EMDataBank 2015/2016 Model Challenge Website Archive

This document collates the information provided at the website challenges.emdatabank.org for the 2015/2016 Model Challenge. Some information/links may be outdated.

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News Archive

EMDataBank Challenges
published Tue, 07/14/2015

EMDataBank is hosting community-wide challenges to critically evaluate 3DEM methods that are coming into use, with the ultimate goal of developing recommendations for validation criteria associated with every 3DEM map deposited to the EM Data Bank (EMDB) and map-derived model deposited to Protein Data Bank (PDB).

Committees comprised of respected 3DEM community members are charged to formulate the details for each challenge, including:

- choosing challenge reference data
- deciding what information participants will need to submit
- deciding on criteria for validation and comparison of results
- deciding on the timeline for challenge events
- promoting worldwide participation
- emphasizing the challenge as a collaborative and constructive activity
- evaluating the results and producing a report

In 2015/2016 we are hosting two challenges that focus, respectively, on reconstruction and modelling at moderate to high resolution, with the goals of establishing benchmarks, comparing current practices, and evolving criteria for evaluation of results. Click here to view a mini-poster about the challenges that we have presented at recent meetings. In the future we plan to host additional challenges for reconstruction and interpretation at lower resolution.

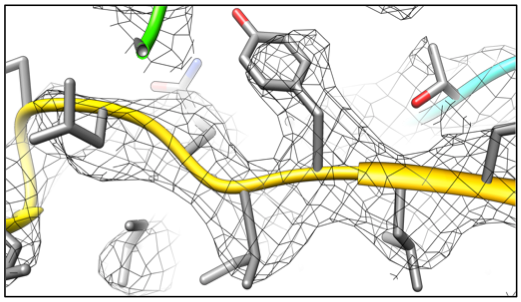
Model Challenge Workshop
published Mon, 07/20/2015

The model challenge committee held a weekend workshop on June 20/21 with a selected group of cryoEM specialists and model software developers to share results and develop plans for the model challenge. The outcome of this meeting is the recommendation by this group to launch a community wide challenge to model 5-7 selected cryoEM density maps that have been reported to be determined at 3.0-4.5 Å gold-standard resolution.

This resolution range was selected for two reasons: (1) envisioned growth in the number of maps in the next few years at this resolution range; and (2) the various technical challenges that exist for interpreting maps as atomic models in this resolution range. The chosen map targets will cover different symmetry, size, and multiple resolution structures by previous cryoEM and X-ray studies. We anticipate engaging the committee, as well as the community, to assess the submitted models and develop tools for assessment.

Announcing the 2nd EMDataBank Model Challenge

published Wed, 10/14/2015



EMDataBank is pleased to announce the 2015/2016 **Model Challenge**.

All members of the Scientific Community--at all levels of experience--are invited to participate as **Challengers**, and/or as **Assessors**.

Benchmark targets of varying size and complexity have been selected from recently deposited 3DEM structures based on current state-of-the-art detectors and processing methods, in the resolution range 2.2-4.5 Å.

Challengers are sought to create and validate models from challenge target maps in four different categories (1. optimize current cryoEM model, 2. fit known related cryoEM, crystallographic, or comparative models, 3. ab initio model building, 4. any other method of map interpretation), and upload their results with associated details.

Assessors are sought to participate in evaluating submitted models.

Registration is now open for all interested participants. Challengers may submit their models between November and April. Before submissions open, all are encouraged to provide feedback on submission requirements. An open assessment period will commence in late 2016.

To learn more about this challenge and to register, please visit http://challenges.emdatabank.org and click on "MODEL CHALLENGE" in the menu bar.

The model challenge is the second of two community-wide challenges being sponsored by EMDataBank this year to critically evaluate 3DEM methods that are coming into use, with the ultimate goal of developing validation criteria associated with every 3DEM map and map-derived model. The first challenge is focused on creating reconstructions from raw 2D image data and is currently in progress (click on "MAP CHALLENGE" in the menu bar).

New Publications
published Mon, 11/23/2015

New open access articles about EMDataBank and EMDB access are now available online, in advance of publication in the upcoming January 2016 Nucleic Acids Research Database Issue.

- EMDataBank unified data resource for 3DEM provides an overview of the rapidly growing 3DEM structural data archives, which include maps in EM Data Bank and map-derived models in the Protein Data Bank. Also, discussion of progress and approaches toward development of validation protocols and methods, working with the scientific community, in order to create a validation pipeline for 3DEM data.
- PDBe: improved accessibility of macromolecular structure data from PDB and EMDB describes PDBe's website redesign, API access to the PDB and EMDB archives, and value-added annotations.

Challenge Submissions Update
published Thu, 01/28/2016

The following updates have been made to the challenges site this week:

1. Model challenge submissions are now open.
2. Challenge submissions (both map and model) now require login to the challenges site. Emails have been sent out to all challenger registrants with their login information.
3. Challenge news is now available via rss feed.

Model Challenge Submission Deadline Extended
published Tue, 04/26/2016

The deadline for model challenge submissions is now changed to Friday June 17 (21:00 UTC).

We hope that this extension will be helpful to all of our challengers.

In addition, please be aware that indicated symmetry centers in the model challenge guide may not be exact.

This issue was just raised by one participant—we are investigating and will send a further update about this soon.

Model Challenge: Symmetry Info Updated
published Thu, 04/28/2016 - 12:11

The model challenge guide now holds corrected symmetry center info and BIOMT matrices for the proteasome, GroEL, and β-galactosidase targets. The changes are highlighted with red text and update date.

The previously posted symmetry info had used rounded values for the voxel sizes, yielding imprecise center coordinate and matrix element values. We apologize for the errors.

Model Challenge Submission Deadline is Friday June 17
published Wed, 06/15/2016

EMDataBank Challenge Modellers, Please complete your model submissions this week--the deadline is this coming Friday at 21:00 UTC. Any questions/issues please let us know (challenges@emdatabank.org). Thanks for participating!

Assessment Phases are Coming Soon
published Fri, 10/28/2016 - 11:20

Following two amazing challenge submission finishes in April (66 maps!) and in June (106 models!), we have been working with our respective committees to prepare and organize the data for blinded assessments and to perform preliminary analyses. This process has taken more time than originally anticipated, so we have been making adjustments to assessment phase timelines. For the map challenge, we plan to announce the beginning of the assessment phase in early November. Watch this space for more details!

Model Challenge Comparison Site
published Thu, 02/23/2017

The model challenge assessment period is still in progress. Interested to see how we the results are being assessed? Please visit the model-compare pages at http://model-compare.emdatabank.org. There you can view and compare the submitted models via more than a dozen different whole-model and residue level metrics, as summarized here.

Model Challenge Face-to-Face Meeting
published Fri, 06/09/2017

Update for the Model Challenge: A face-to-face meeting was held Monday May 29, 2017 to discuss model assessments and how to move forward with completing the challenge. The challenge has been designed to enable assessment of current approaches to interpretation of higher resolution (3-5Å) cryoEM maps with atomic models, to critically evaluate the map interpretation, model fitting, model refinement, and validation methods that are now coming into use. Initial assessments of the 106 submissions from 16 modellers have been prepared and can be viewed at the model comparison site. Notes from the May 29 meeting are available in the provided attachment.

Joint Challenges Wrap-Up Meeting Oct 6-8
published Wed, 08/16/2017

In 2016 EMDataBank ran two community challenges in parallel to create awareness of the need for cryoEM structure validation as a routine process in research studies and publications, and to expedite development of quantitative tools for assessment. The Map and Model Challenges were developed by cryoEM and modeling community experts, respectively, who have been charged with developing challenge tasks, promoting worldwide participation, evaluating the results, and producing a report. In each case, benchmark datasets (i.e. raw single particle

images and 3D density maps) have been assembled for molecular machines of varying size and complexity, based on current state-of-the-art detectors and processing methods, in the resolution range 2-5 Å. Challenge tasks are designed to be suitable for all levels of expertise.

The cryoEM and modelling scientific communities have responded enthusiastically : a grand total of 83 scientists have participated as committee members, challengers, and/or assessors. There were 66 submissions to the Map Challenge, and 107 submissions to the Model Challenge, each with supporting details about workflow from benchmark data to final result. Analyses of all of these depositions is now nearing completion, making use of both currently available as well as novel procedures, conducted by volunteers and experts.

In order to share and fully explore the results and analyses of both challenges with the community, we plan to hold a joint Challenges Wrap-Up Workshop October 6-8, 2017 at the Conference Center of SLAC National Accelerator Laboratory, Stanford University, Menlo Park, California. We are inviting all of the participants from both challenges to present and discuss their findings, providing a unique opportunity for two somewhat separate communities (3DEM reconstruction and molecular modelling) to come together to review the challenge results, to address the need for robust validation procedures for maps and models, and to make recommendations for future challenge events for increasingly complex data with high compositional and/or conformational heterogeneity.

The format of the meeting is to have the first day devoted to density map generation from raw single particle images and the second day devoted to modeling from 3D density maps. Each of these two sessions will have presentations from assessors and challengers on their chosen computational approaches and their rationales of adoptions. The session discussion leaders will be drawn from our Committee experts. The third day will be devoted to the necessary metrics of cryoEM structure validation report for structures archived in EMDB and PDB, discucssion on integration of map and model validation, and possible topics and formats for future challenge events. After the workshop, we plan to organize a journal special issue that will be contributed by the assessors and challengers so that the outcomes will be disseminated freely to the entire scientific community.

If you are interested, please join us! The workshop registration site is here: http://ncmi.bcm.edu/ncmi/events/workshops/workshops_163

Joint Challenges Wrap Up Workshop: Thanks to Our Participants!

published Thu, 10/12/2017

The Oct 6-8, 2017 Joint Challenges Wrap-Up workshop at Stanford/SLAC was a tremendous success.

With more than 60 scientists attending, participants of the 2016 Map and Model Challenges, including challengers, assessors, committee members presented and discussed their findings, and to help to develop recommendations for future challenge events. More outcome details will be posted soon.

JSB Special Issue on Outcomes of the Map and Model Challenges

published Mon, 11/13/2017

We are pleased to announce that the *Journal of Structural Biology* has agreed to produce a special issue on the 2016 Map and Model Challenges.

For those planning to submit a manuscript, here are the particulars:

Submission Format and Guidelines

All submitted papers must be clearly written in excellent English and contain only original work which has not been published by or is currently under review for any other journal or conference. A detailed submission guideline is available as "Guide to Authors" at: https://www.elsevier.com/journals/journal-of-structural-biology/1047-8477/guide-for-authors

All manuscripts and any supplementary material should be submitted through Elsevier Editorial System (EES). Select **VSI:2016 CryoEM Challenges** when you reach the **Article Type** step in the submission process. This will ensure that all manuscripts are correctly identified for inclusion into the special issue.

We have been advised that there will be no publication charges to authors, and use of color figures will be free. In addition, Elsevier has agreed to give the entire issue promotional free access during the 1st 6 months following publication.

The earliest submission date will be **February 1, 2018**. The final submission deadline is **March 1, 2018.**

The EES submission site is located at: https://ees.elsevier.com/jsb/default.asp

Please refer to the journal's Guide for Authors for specific advice on how to prepare your paper.

All papers will be peer-reviewed by three independent reviewers.

Requests for additional information should be addressed to the guest editors, Wah Chiu and Cathy Lawson.

Goals

- Establish a benchmark set of 3DEM maps in the 3.0-4.5 Å resolution range, where significant growth in the number of maps is anticipated over the next few years and where a number of technical challenges exist to map interpretation and fitting
- Encourage developers of modelling software packages and biological end users to analyze these maps and present modelling results with the best practice
- Evolve criteria for evaluation and validation of 3DEM map-derived models
- Compare and contrast the various modelling and analysis approaches in a positive spirit

Model Committee

Paul Adams (Chair), Axel Brunger, Randy Read, Torsten Schwede, Maya Topf, Gerard Kleywegt, Cathy Lawson, Wah Chiu, Ardan Patwardhan

How to Participate

All members of the Scientific Community--at all levels of experience--are invited to participate as **Challengers**, and/or as **Assessors**.

Challengers will create and submit their own atomic coordinate models of one or more challenge targets using the supplied target maps.

There are four modelling categories:

1. **Optimize the current cryoEM model** for the target, improving fit to the cryo-EM map density and/or model stereochemistry
2. **Fit known related cryoEM, crystallographic, or comparative models** to the cryo-EM map, optionally followed by model optimization
3. **Ab initio model building**, without reference to any existing cryo-EM or crystallographic models related to the cryo-EM map
4. **Any other method** that seeks to interpret, or create a model based on, the cryo-EM map

For each submission, challengers will provide their final model, target map (if modified from original), and basic information about their modelling process. **Researchers are expected to disclose all of the prior information used in their method.** For full challenge rules and additional information see the model challenge guide.

Assessors will contribute to the challenge assessment phase. Following a short initial review period by the model committee, challenge data and files will be made publicly available (entry

authorship suppressed) for anyone to assess. The intention is to enable comparisons of the various modelling methodologies available and their options in a positive spirit. Assessors will be able to share their results via a planned workshop (~Fall 2016) as well as manuscript submissions to a Journal special issue.

****All participants--challengers and assessors--are required to register****

Timeline

2015	**DEVELOPMENT PHASE**
February-June	Model Committee meets monthly to discuss possible scope of challenge
June 20/21	Face-to-face meeting to define challenge targets, goals, and parameters
July-September	Finalization of challenge formulation. Requests to map contributors to provide any missing data (e.g., half-maps, unfiltered, unsharpened, unmasked maps)
2015/2016	**CHALLENGE PHASE**
October 14	Pre-Challenge Announcement, Challenger and Assessor Registration Opens
January-**June 17**	Challenge Site Open for Model Entry Submissions
June 17 21:00 UTC	Model entry submission window closes
2016/2017	**ASSESSMENT PHASE**
June-November	Challenge Data review by the Model Committee
December-May	Challenge Data review opened to volunteer assessors (blind analysis--entry authorship suppressed)
May 29	Face-to-Face Meeting to discuss preliminary outcomes of assessments
mid July	Assessors provide written reports on their results
mid July	Reports on Models sent to Challengers; Full workflow info provided to all challengers and assessors
Aug 15	Feedback from Challengers on their reports
Sept 1	Deadline for Assessors to update their reports
Oct 5-8	Challenges Meeting (Maps and Models)
Post-workshop	Challenge Writeups (multiple articles) for a Journal Special Issue

Model Challenge Targets

The eight targets chosen by the model challenge committee are shown below. All are based on recently reported 3DEM structures. The target order is according to unique molecular weight, from 19 kDa (TMV) at left to 2500 kDa (ribosome) at right. For challenge rules and additional information about each target see the model challenge guide.

April 28: Corrected symmetry center info and BIOMT matrix files for the proteasome and beta-galactosidase targets, see the model challenge guide.

May 3: Corrected BIOMT matrix file containing Icosahedral transformations for Brome Mosaic Virus, see the model challenge guide.

Target Map Download: You can use this rsync script to download target maps from one of three wwPDB ftp sites. Alternately, you can download individual maps from EMDB atlas pages (click on EMDB entry link in the table below, select "download" tab).

	1. Tobacco Mosaic Virus	2. T20S Proteasome	3. GroEL	4. TRPV1 Channel	5. Brome Mosaic Virus	6. β-Galactosidase	7. γ-Secretase	8. 70S Ribosome
target								
Map "A" EMDB entry; Primary Citation; Reported Resolution (Å)	EMD-2842 Fromm et al 3.3	EMD-5623 Li et al 3.3	EMD-6422 -- 4.1	EMD-5778 Liao et al 3.3	EMD-6000 Wang et al 3.8	EMD-5995 Bartesaghi et al 3.2	EMD-2677 Lu et al 4.5	EMD-2847 Fischer et al 2.9
Reference Model(s) Map "A"	4udv (EM) 1ei7 (Xray)	1yar (Xray) 3j9i (EM)	3cau (EM) 1ss8 (Xray) 1svt (Xray)	3j5p (EM)	3j7l (EM) 1js9 (Xray)	3j7h (EM) 1jz7 (Xray)	4upc/superceded by 5a63 (EM)	5afi (EM)
Map "B" EMDB entry; Primary Citation; Reported Resolution (Å)		EMD-6287 Campbell et al 2.8				EMD-2984 Bartesaghi et al 2.2	EMD-3061 Bai et al 3.4	EMD-6316 Li et al 3.6
Reference Model(s) Map "B"		1yar (Xray)				5a1a (EM) 1jz7 (Xray)	5a63 (EM)	3ja1 (EM)
Imposed Map Symmetry	Helical	Dihedral (D7)	Dihedral (D7)	Cyclic (C4)	Icosahedral (I)	Dihedral (D2)	None (C1)	None (C1)
Sample MW (MDa)	--	0.7	0.8	0.3	4.6	0.47	0.17	2.5
Unique MW (kDa)	19	50	56	80	80	120	170	2500
Map Contributors (Thank You!)	***Simon Fromm, Carsten Sachse***	***Jean-Paul Armache, Yifan Cheng Melody Campbell, Bridget Carragher***	***Soung-Hun Roh, Corey Hryc, Wah Chiu***	***Jean-Paul Armache, Maofu Liao, Yifan Cheng***	***Zhao Wang, Wah Chiu***	***Alberto Bartesaghi, Sriram Subramaniam***	***Xiaochen Bai, Sjors Scheres***	***Niels Fischer, Holger Stark Wen Li, Zheng Liu, Joachim Frank***

Download maps via rsync script

```
################################################################################
# template for downloading map files associated with the 2015 EMDataBank Model
Challenge #
################################################################################
# Before running, uncomment the rsync command of your preferred download site.
# If you do not want to download files for every target, adjust "foreach" to your
# desired download list.
#
# Individual target EMDB entry ids are:
# 1. Tobacco Mosaic Virus EMD-2842
# 2. T20S Proteasome      EMD-5623 EMD-6287
# 3. GroEL                EMD-6422
# 4. TrpV1 Channel        EMD-5778
# 5. Brome Mosaic Virus   EMD-6000
# 6. Beta Galactosidase   EMD-5995 EMD-2984
# 7. Gamma Secretase      EMD-2677 EMD-3061
# 8. Ribosome             EMD-2847 EMD-6316
#
# Following download, each target map will have its own directory with EMDB entry id.
# subdirectory "map" contains the depositor's original map, which may have been
masked/filtered.
# subdirectory "other" contains additional maps specifically requested for the
challenge.
# filenames in most cases are: full reconstruction (no masking/filtering):
EMD-####-full.map.gz
#                  half-maps : EMD-####-half-1.map.gz; EMD-####-half-2.map.gz
#                  mask (if used to calculate FSC) : EMD-####-FSC-mask.map.gz
# Full guidelines for the maps that may be used either for modelling or validation in
the challenge
# for each target are provided in the 2015 Model Challenge Guide http://bit.ly/1Gcexvi
################################################################################
#/bin/csh -f

foreach entry(2842 5623 6287 6422 5778 6000 5995 2984 2677 3061 2847 6316)

# download from EUROPE (PDBe)
#rsync -rlpt -v -z --delete
rsync.ebi.ac.uk::pub/databases/emdb/structures/EMD-${entry}/ ./EMD-${entry}

# download from USA (RCSB)
#rsync -rlpt -v -z --delete --port=33444
rsync.wwpdb.org::emdb/structures/EMD-${entry}/ ./EMD-${entry}

# download from ASIA (PDBj)
#rsync -rlpt -v -z --delete ftp.pdbj.org::emdb/structures/EMD-${entry}/ ./EMD-${entry}

end
```

Model Challenge Guide

2015-2016 Model Challenge Guide

Last Update: June 2, 2016

Overview

Welcome to the 2015/2016 EMDataBank Model Challenge! Please see the Main Model Challenge Website for overview information including goals, participation info, timeline, and target table. Refer to this guide for the challenge rules and additional target information.

Updates to this guide are being made as required; look for red text with update date.
April 28: corrected symmetry center info and BIOMT matrices for the proteasome and β-galactosidase targets.
May 3: corrected BIOMT matrices for Brome Mosaic Virus.
Questions/Comments/Suggestions? Please email challenges@emdatabank.org

Challenge Rules

- Challengers must use one or more of the map files included in the target EMDB entries as their starting point(s) for modelling. Use of the original, unmodified map from the reconstruction software, and/or independent maps generated for Fourier Shell Correlation calculation is STRONGLY encouraged (see individual target sections for filenames).
- Starting maps may be modified, e.g., filtered, sharpened, and/or segmented. If a map is modified for fitting, you will be asked to upload it along with the final model.
- The committee strongly recommends that models be validated before they are submitted, using tools of the challenger's choosing. Tools can include, but are not limited to, those listed in the section below.
- Challengers are encouraged to explore ab initio modelling approaches, but are also permitted to utilize publicly available coordinates as starting points for fitting.
- Researchers are expected to disclose all of the prior information used in their modelling method.
- Uploaded models must:
- be positioned within the target map
- have the same symmetry as the map
- use the UNIPROT or PDB sequence/residue numbering indicated below

Validation Tools

Challengers are encouraged to validate their final model using procedures of their choosing, checking (i) internal model consistency and (ii) fit of map to the model. The software packages listed here are suggestions and are meant to serve as a starting point. Suggestions for additions to this list are welcome (challenges@emdatabank.org).

Software packages with model geometry and/or map-model fit assessment tools	Model Quality Estimation (QE) tools developed for CASP
• Molprobity • WHAT_CHECK	• QE comparison/overview • ProQ

• CCP4 package • Phenix package • UCSF Chimera • COOT • EMRinger • TEMPy	• VERIFY3D • Dfire • ModFold • QMEAN • DOPE • PROSA

Planned Submission Questions & Uploads

The following information will be collected for each model challenge submission.

1. Name, institution address, email, list of collaborators
2. Challenge target (select from list)
3. Submission Title
4. Target map(s) used for fitting (checklist)
5. Modelling category (choices are: 1. optimize current cryoEM model, 2. fit known related cryoEM, crystallographic, or comparative models, 3. ab initio model building, 4. any other method of map interpretation)
6. Description of the modelling process
    a. Map preparation: description of any modifications (combination of yes/no questions and free text description)
        i. filtering/sharpening
        ii. segmentation
    b. Source coordinates(s) used for fitting (PDB ids, free-text description of any modifications to model before use)
    c. Process/effort type (select from list): manual, automated, manual+automated
    d. Space of refinement/model optimization (select from list): real, reciprocal
    e. Modelling software package(s) used, with text description of parameters and settings
    f. Text description of the modelling process
    g. Was map scale adjusted as part of model optimization? (yes/no; if yes, final A/pixel).
    h. Estimated time/effort to create the model (cpu hours, person/days)
7. Target map(s) used for validation (checklist).
8. Description of validation(s) performed.
    a. Internal Model Consistency
    b. Fit of Model to the Map
9. Upload: Final model file from refinement program
10. Upload: Final Model in PDBx/mmCIF format, produced using PDBextract
11. Upload: Map used for fitting (if modified from original)

Target 1. Tobacco Mosaic Virus

TMV Capsid Sequence: Uniprot P69687

```
>sp|P69687|CAPSD_TMV Capsid protein OS=Tobacco mosaic virus (strain vulgare) GN=CP PE=1 SV=2
MSYSITTPSQFVFLSSAWADPIELINLCTNALGNQFQTQQARTVVQRQFSEVWKPSPQVT
VRFPDSDFKVYRYNAVLDPLVTALLGAFDTRNRIIEVENQANPTTAETLDATRRVDDATV
AIRSAINNLIVELIRGTGSYNRSSFESSSGLVWTSGPAT
```

Map A:

EMDB entry: EMD-2842 primary map: emd_2842.map

Dimensions (voxels):	210	210	190	
Voxel spacing:	1.06 Å	1.06 Å	1.06 Å	
Map extent:	223.0 Å	223.0 Å	201.8 Å	
Origin (voxels):	-105	-105	-95	
Map statistics:	**Minimum**	**Maximum**	**Average**	**Standard deviation**
	-3.43	5.53	0.02	0.74
Recommended contour level:	1.2 (source: author)			

Helical symmetry: rise 1.41, angle 22.03
Symmetry Matrices

original, unmodified map from reconstruction software: EMD-2842-full.map
maps and mask for FSC calculation: EMD-2842-half-1.map, EMD-2842-half-2.map, EMD-2842-FSC-mask.map

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Target 2. T20S Proteasome

Sequences:
Proteasome Subunit alpha: Uniprot P25156
Proteasome Subunit beta: Uniprot P28061

```
>sp|P25156|PSA_THEAC Proteasome subunit alpha OS=Thermoplasma acidophilum (strain ATCC 25905 /
DSM 1728 / JCM 9062 / NBRC 15155 / AMRC-C165) GN=psmA PE=1 SV=2
MQQGQMAYDRAITVFSPDGRLFQVEYAREAVKKGSTALGMKFANGVLLISDKKVRSRLIE
QNSIEKIQLIDDYVAAVTSGLVADARVLVDFARISAQQEKVTYGSLVNIENLVKRVADQM
QQYTQYGGVRPYGVSLIFAGIDQIGPRLFDCDPAGTINEYKATAIGSGKDAVVSFLEREY
KENLPEKEAVTLGIKALKSSLEEGEELKAPEIASITVGNKYRIYDQEEVKKFL
>sp|P28061|PSB_THEAC Proteasome subunit beta OS=Thermoplasma acidophilum (strain ATCC 25905 /
DSM 1728 / JCM 9062 / NBRC 15155 / AMRC-C165) GN=psmB PE=1 SV=1
MNQTLETGTTTVGITLKDAVIMATERRVTMENFIMHKNGKKLFQIDTYTGMTIAGLVGDA
QVLVRYMKAELELYRLQRRVNMPIEAVATLLSNMLNQVKYMPYMVQLLVGGIDTAPHVFS
IDAAGGSVEDIYASTGSGSPFVYGVLESQYSEKMTVDEGVDLVIRAISAAKQRDSASGGM
IDVAVITRKDGYVQLPTDQIESRIRKLGLIL
```

Map A:
EMDB entry: EMD-5623

Dimensions (voxels):	256	256	256	
Voxel spacing:	1.22 Å	1.22 Å	1.22 Å	
Map extent:	311.2 Å	311.2 Å	311.2 Å	
Origin (voxels):	0	0	0	
Map statistics:	**Minimum**	**Maximum**	**Average**	**Standard deviation**
	-0.55	1.20	-0.01	0.05
Recommended contour level:	0.25 (source: author)			

~~D7 symmetry center position is at 128,128,128 voxels; 156.16,156.16,156.16 Å~~
Correction 4/28: true voxel edge is 1.2156 Å (value shown in box above is rounded)
D7 symmetry center position at 128, 128, 128 voxels; 155.5968, 155.5968, 155.5968 Å

Symmetry Matrices **<==updated**

primary map: emd_5623.map
original, unmodified map from reconstruction software: EMD-5623-full.map
maps for FSC calculation: EMD-5623-half-1.map, EMD-5623-half-2.map

Map B:
EMDB entry: EMD-6287

Dimensions (voxels):	300	300	300	
Voxel spacing:	0.98 Å	0.98 Å	0.98 Å	
Map extent:	294.6 Å	294.6 Å	294.6 Å	
Origin (voxels):	0	0	0	
Map statistics:	**Minimum**	**Maximum**	**Average**	**Standard deviation**
	-0.13	0.20	0.00	0.01
Recommended contour level:	0.025 (source: emdb)			

~~D7 symmetry center position is at 150,150,150 voxels; 147.0,147.0,147.0 Å~~
Correction 4/28: true voxel edge is 0.982 Å (value shown in box above is rounded)
D7 symmetry center position at 150, 150, 150 voxels: 147.3, 147.3, 147.3 Å

Symmetry Matrices **<==updated**

primary map: emd_6287.map
original, unmodified map from reconstruction software: EMD-6287-full.map

maps for FSC calculation: EMD-6287-half-1.map, EMD-6287-half-2.map

---

Target 3. Escherichia coli GroEL

GroEL Sequence: Uniprot P0A6F5

```
>sp|P0A6F5|CH60_ECOLI 60 kDa chaperonin OS=Escherichia coli (strain K12) GN=groL PE=1 SV=2
MAAKDVKFGNDARVKMLRGVNVLADAVKVTLGPKGRNVVLDKSFGAPTITKDGVSVAREI
ELEDKFENMGAQMVKEVASKANDAAGDGTTTATVLAQAIITEGLKAVAAGMNPMDLKRGI
DKAVTAAVEELKALSVPCSDSKAIAQVGTISANSDETVGKLIAEAMDKVGKEGVITVEDG
TGLQDELDVVEGMQFDRGYLSPYFINKPETGAVELESPFILLADKKISNIREMLPVLEAV
AKAGKPLLIIAEDVEGEALATLVVNTMRGIVKVAAVKAPGFGDRRKAMLQDIATLTGGTV
ISEEIGMELEKATLEDLGQAKRVVINKDTTTIIDGVGEEAAIQGRVAQIRQQIEEATSDY
DREKLQERVAKLAGGVAVIKVGAATEVEMKEKKARVEDALHATRAAVEEGVVAGGGVALI
RVASKLADLRGQNEDQNVGIKVALRAMEAPLRQIVLNCGEEPSVVANTVKGGDGNYGYNA
ATEEYGNMIDMGILDPTKVTRSALQYAASVAGLMITTECMVTDLPKNDAADLGAAGGMGG
MGGMGGMM
```

Map A:

EMDB entry: EMD-6422

Dimensions (voxels):	240	240	240	
Voxel spacing:	1.07 Å	1.07 Å	1.07 Å	
Map extent:	256.8 Å	256.8 Å	256.8 Å	
Origin (voxels):	0	0	0	
Map statistics:	**Minimum**	**Maximum**	**Average**	**Standard deviation**
	-8.84	16.47	0.0000	1.00
Recommended contour level:	3.5 (source: author)			

D7 symmetry center position is at 120, 120, 120 voxels; 128.4, 128.4, 128.4 Å
(symmetry center is ok -- rechecked 4/28)
Symmetry Matrices

primary map: emd_6422.map
original, unmodified map from reconstruction software: EMD-6422-full.map
maps for FSC calculation: EMD-6422-half-1.map, EMD-6422-half-2.map

---

Target 4. TrpV1 Channel

TrpV1 Sequence: Uniprot O35433

```
>sp|O35433|TRPV1_RAT Transient receptor potential cation channel subfamily V member 1
OS=Rattus norvegicus GN=Trpv1 PE=1 SV=1
MEQRASLDSEESESPPQENSCLDPPDRDPNCKPPPVKPHIFTTRSRTRLFGKGDSEEASP
LDCPYEEGGLASCPIITVSSVLTIQRPGDGPASVRPSSQDSVSAGEKPPRLYDRRSIFDA
VAQSNCQELESLLPFLQRSKKRLTDSEFKDPETGKTCLLKAMLNLHNGQNDTIALLLDVA
RKTDSLKQFVNASYTDSYYKGQTALHIAIERRNMTLVTLLVENGADVQAAANGDFFKKTK
GRPGFYFGELPLSLAACTNQLAIVKFLLQNSWQPADISARDSVGNTVLHALVEVADNTVD
NTKFVTSMYNEILILGAKLHPTLKLEEITNRKGLTPLALAASSGKIGVLAYILQREIHEP
ECRHLSRKFTEWAYGPVHSSLYDLSCIDTCEKNSVLEVIAYSSSETPNRHDMLLVEPLNR
```

```
LLQDKWDRFVKRIFYFNFFVYCLYMIIFTAAAYYRPVEGLPPYKLKNTVGDYFRVTGEIL
SVSGGVYFFFRGIQYFLQRRPSLKSLFVDSYSEILFFVQSLFMLVSVVLYFSQRKEYVAS
MVFSLAMGWTNMLYYTRGFQQMGIYAVMIEKMILRDLCRFMFVYLVFLFGFSTAVVTLIE
DGKNNSLPMESTPHKCRGSACKPGNSYNSLYSTCLELFKFTIGMGDLEFTENYDFKAVFI
ILLLAYVILTYILLLNMLIALMGETVNKIAQESKNIWKLQRAITILDTEKSFLKCMRKAF
RSGKLLQVGFTPDGKDDYRWCFRVDEVNWTTWNTNVGIINEDPGNCEGVKRTLSFSLRSG
RVSGRNWKNFALVPLLRDASTRDRHATQQEEVQLKHYTGSLKPEDAEVFKDSMVPGEK
```

[note added Nov 11: quote from the primary citation: "The rat TRPV1 construct used for this study consists of residues 110 to 764 (indicated by red arrows), excluding the highly divergent region (604–626, highlighted by cyan box)"]

Map A:
EMDB entry EMD-5778

Dimensions (voxels):	256	256	256	
Voxel spacing:	1.22 Å	1.22 Å	1.22 Å	
Map extent:	311.2 Å	311.2 Å	311.2 Å	
Origin (voxels):	-128	-128	-128	
Map statistics:	**Minimum**	**Maximum**	**Average**	**Standard deviation**
	-13.65	26.52	0.0000	1.00
Recommended contour level:	7 (source: author)			

Note: true voxel edge is 1.2156 Å (value shown in box above is rounded)
C4 symmetry center position is at 128, 128, (125) voxels; 0, 0, (0) Å
(symmetry center is ok -- rechecked 4/28)
Symmetry Matrices

primary map: emd_5778.map
original, unmodified map from reconstruction software: EMD-5778-full.map
maps for FSC calculation: EMD-5778-half-1.map, EMD-5778-half-2.map

additional maps available for this entry:
EMD-5778-full-sharpened.map
TRPV1_sharpened_-100_3.4A.map

Target 5. Brome Mosaic Virus

Symmetry: I (T=3)
BMV Capsid Sequence: Uniprot P03602

```
>sp|P03602|CAPSD_BMV Capsid protein OS=Brome mosaic virus GN=ORF3b PE=1 SV=1
MSTSGTGKMTRAQRRAAARRNRWTARVQPVIVEPLAAGQGKAIKAIAGYSISKWEASSDA
```

```
ITAKATNAMSITLPHELSSEKNKELKVGRVLLWLGLLPSVAGRIKACVAEKQAQAEAAFQ
VALAVADSSKEVVAAMYTDAFRGATLGDLLNLQIYLYASEAVPAKAVVVHLEVEHVRPTF
DDFFTPVYR
```

EMDB entry: EMD-6000

Dimensions (voxels):	420		420	420
Voxel spacing:	0.99 Å		0.99 Å	0.99 Å
Map extent:	415.8 Å		415.8 Å	415.8 Å
Origin (voxels):	0		0	0
Map statistics:	**Minimum**	**Maximum**	**Average**	**Standard deviation**
	-10.34	17.47	0.0000	1.11
Recommended contour level:	5 (source: emdb)			

Icosahedral symmetry center position is at 210, 210, 210 voxels; 207.9, 207.9, 207.9 Å
Icosahedral orientation is n25r with 2-fold symmetry axis along y, 5-fold symmetry axis along z.
(symmetry is center ok -- rechecked 4/28)
Symmetry Matrices **<==updated May 3**

primary map: emd_6000.map
original, unmodified map from reconstruction software: emd_6000.map
maps for FSC calculation: BMV-set1.map, BMV-set2.map

additional segmented maps are available for this entry:
subunitA.map, subunitB.map, subunitC.map

Target 6. ß-Galactosidase

Beta-galactosidase sequence: Uniprot P00722

```
>sp|P00722|BGAL_ECOLI Beta-galactosidase OS=Escherichia coli (strain K12) GN=lacZ PE=1 SV=2
MTMITDSLAVVLQRRDWENPGVTQLNRLAAHPPFASWRNSEEARTDRPSQQLRSLNGEWR
FAWFPAPEAVPESWLECDLPEADTVVVPSNWQMHGYDAPIYTNVTYPITVNPPFVPTENP
TGCYSLTFNVDESWLQEGQTRIIFDGVNSAFHLWCNGRWVGYGQDSRLPSEFDLSAFLRA
GENRLAVMVLRWSDGSYLEDQDMWRMSGIFRDVSLLHKPTTQISDFHVATRFNDDFSRAV
LEAEVQMCGELRDYLRVTVSLWQGETQVASGTAPFGGEIIDERGGYADRVTLRLNVENPK
LWSAEIPNLYRAVVELHTADGTLIEAEACDVGFREVRIENGLLLLNGKPLLIRGVNRHEH
HPLHGQVMDEQTMVQDILLMKQNNFNAVRCSHYPNHPLWYTLCDRYGLYVVDEANIETHG
MVPMNRLTDDPRWLPAMSERVTRMVQRDRNHPSVIIWSLGNESGHGANHDALYRWIKSVD
PSRPVQYEGGGADTTATDIICPMYARVDEDQPFPAVPKWSIKKWLSLPGETRPLILCEYA
HAMGNSLGGFAKYWQAFRQYPRLQGGFVWDWVDQSLIKYDENGNPWSAYGGDFGDTPNDR
QFCMNGLVFADRTPHPALTEAKHQQQFFQFRLSGQTIEVTSEYLFRHSDNELLHWMVALD
GKPLASGEVPLDVAPQGKQLIELPELPQPESAGQLWLTVRVVQPNATAWSEAGHISAWQQ
WRLAENLSVTLPAASHAIPHLTTSEMDFCIELGNKRWQFNRQSGFLSQMWIGDKKQLLTP
LRDQFTRAPLDNDIGVSEATRIDPNAWVERWKAAGHYQAEAALLQCTADTLADAVLITTA
HAWQHQGKTLFISRKTYRIDGSGQMAITVDVEVASDTPHPARIGLNCQLAQVAERVNWLG
LGPQENYPDRLTAACFDRWDLPLSDMYTPYVFPSENGLRCGTRELNYGPHQWRGDFQFNI
SRYSQQQLMETSHRHLLHAEEGTWLNIDGFHMGIGGDDSWSPSVSAEFQLSAGRYHYQLV
WCQK
```

Map A:
EMDB entry EMD-5995

Dimensions (voxels):	340	340	340	
Voxel spacing:	0.64 Å	0.64 Å	0.64 Å	
Map extent:	216.8 Å	216.8 Å	216.8 Å	
Origin (voxels):	0	0	0	
Map statistics:	**Minimum**	**Maximum**	**Average**	**Standard deviation**
	-0.05	0.09	0.00	0.01
Recommended contour level:	0.0224 (source: author)			

~~D2 symmetry center position at 170,170,170 voxels; 108.8, 108.8, 108.8 Å~~
Correction 4/28: true voxel edge is 0.6375 Å (value shown in box above is rounded)
D2 symmetry center position at 170,170,170 voxels; 108.375, 108.375, 108.375 Å

Symmetry Matrices **<==updated**

primary map: emd_5995.map
original, unmodified map from reconstruction software: EMD-5995-full.map
maps for FSC calculation: EMD-5995-half-1.map, EMD-5995-half-2.map

Map B:
EMDB entry EMD-2984

Dimensions (voxels):	292	292	292	
Voxel spacing:	0.64 Å	0.64 Å	0.64 Å	
Map extent:	186.0 Å	186.0 Å	186.0 Å	
Origin (voxels):	0	0	0	
Map statistics:	**Minimum**	**Maximum**	**Average**	**Standard deviation**
	-0.12	0.17	-0.00	0.02
Recommended contour level:	0.05 (source: author)			

~~D2 symmetry center position at 146,146,146 voxels; 93.44, 93.44, 93.44 Å~~
Correction 4/27: true voxel edge is 0.637 Å (value shown in box above is rounded)
D2 symmetry center position at 146,146,146 voxels; 93.002, 93.002, 93.002 Å

Symmetry Matrices **<==updated**

primary map: emd_2984.map
original, unmodified map from reconstruction software: EMD-2984-full.map
maps for FSC calculation: EMD-2984-half-1.map, EMD-2984-half-2.map

Target 7. Recombinant γ-Secretase

Sequences:

Presenilin (PS1, 1-467) Uniprot P49768

PEN-2 (1-101) Uniprot Q9NZ42

APH-1 (APH-1aL, 1-265) Uniprot Q96BI3

Nicastrin (1-709) Uniprot Q92542

[note added Nov 12: For each of these sequences, the original study authors always used the 1st isoform.]

```
>sp|P49768|PSN1_HUMAN Presenilin-1 OS=Homo sapiens GN=PSEN1 PE=1 SV=1
MTELPAPLSYFQNAQMSEDNHLSNTVRSQNDNRERQEHNDRRSLGHPEPLSNGRPQGNSR
QVVEQDEEEDEELTLKYGAKHVIMLFVPVTLCMVVVVATIKSVSFYTRKDGQLIYTPFTE
DTETVGQRALHSILNAAIMISVIVVMTILLVVLYKYRCYKVIHAWLIISSLLLLFFFSFI
YLGEVFKTYNVAVDYITVALLIWNFGVVGMISIHWKGPLRLQQAYLIMISALMALVFIKY
LPEWTAWLILAVISVYDLVAVLCPKGPLRMLVETAQERNETLFPALIYSSTMVWLVNMAE
GDPEAQRRVSKNSKYNAESTERESQDTVAENDDGGFSEEWEAQRDSHLGPHRSTPESRAA
VQELSSSILAGEDPEERGVKLGLGDFIFYSVLVGKASATASGDWNTTIACFVAILIGLCL
TLLLLAIFKKALPALPISITFGLVFYFATDYLVQPFMDQLAFHQFYI
>sp|Q9NZ42|PEN2_HUMAN Gamma-secretase subunit PEN-2 OS=Homo sapiens GN=PSENEN PE=1 SV=1
MNLERVSNEEKLNLCRKYYLGGFAFLPFLWLVNIFWFFREAFLVPAYTEQSQIKGYVWRS
AVGFLFWVIVLTSWITIFQIYRPRWGALGDYLSFTIPLGTP
>sp|Q96BI3|APH1A_HUMAN Gamma-secretase subunit APH-1A OS=Homo sapiens GN=APH1A PE=1 SV=1
MGAAVFFGCTFVAFGPAFALFLITVAGDPLRVIILVAGAFFWLVSLLLASVVWFILVHVT
DRSDARLQYGLLIFGAAVSVLLQEVFRFAYYKLLKKADEGLASLSEDGRSPISIRQMAYV
SGLSFGIISGVFSVINILADALGPGVVGIHGDSPYYFLTSAFLTAAIILLHTFWGVVFFD
ACERRRYWALGLVVGSHLLTSGLTFLNPWYEASLLPIYAVTVSMGLWAFITAGGSLRSIQ
RSLLCRRQEDSRVMVYSALRIPPED
>sp|Q92542|NICA_HUMAN Nicastrin OS=Homo sapiens GN=NCSTN PE=1 SV=2
MATAGGGSGADPGSRGLLRLLSFCVLLAGLCRGNSVERKIYIPLNKTAPCVRLLNATHQI
GCQSSISGDTGVIHVVEKEEDLQWVLTDGPNPPYMVLLESKHFTRDLMEKLKGRTSRIAG
LAVSLTKPSPASGFSPSVQCPNDGFGVYSNSYGPEFAHCREIQWNSLGNGLAYEDFSFPI
FLLEDENETKVIKQCYQDHNLSQNGSAPTFPLCAMQLFSHMHAVISTATCMRRSSIQSTF
SINPEIVCDPLSDYNVWSMLKPINTTGTLKPDDRVVVAATRLDSRSFFWNVAPGAESAVA
SFVTQLAAAEALQKAPDVTTLPRNVMFVFFQGETFDYIGSSRMVYDMEKGKFPVQLENVD
SFVELGQVALRTSLELWMHTDPVSQKNESVRNQVEDLLATLEKSGAGVPAVILRRPNQSQ
PLPPSSLQRFLRARNISGVVLADHSGAFHNKYYQSIYDTAENINVSYPEWLSPEEDLNFV
TDTAKALADVATVLGRALYELAGGTNFSDTVQADPQTVTRLLYGFLIKANNSWFQSILRQ
DLRSYLGDGPLQHYIAVSSPTNTTYVVQYALANLTGTVVNLTREQCQDPSKVPSENKDLY
EYSWVQGPLHSNETDRLPRCVRSTARLARALSPAFELSQWSSTEYSTWTESRWKDIRARI
FLIASKELELITLTVGFGILIFSLIVTYCINAKADVLFIAPREPGAVSY
```

Map A:

EMDB entry: EMD-2677

Dimensions (voxels):	140	140	140	
Voxel spacing:	1.76 Å	1.76 Å	1.76 Å	
Map extent:	246.4 Å	246.4 Å	246.4 Å	
Origin (voxels):	0	0	0	
Map statistics:	**Minimum**	**Maximum**	**Average**	**Standard deviation**
	-0.25	0.41	0.00	0.02
Recommended contour level:	0.12 (source: author)			

primary map: emd_2677.map
original, unmodified map from reconstruction software: EMD-2677-full.map
maps for FSC calculation: EMD-2677-half-1.map, EMD-2677-half-2.map

Map B:
EMDB entry: EMD-3061

Dimensions (voxels):	180	180	180	
Voxel spacing:	1.40 Å	1.40 Å	1.40 Å	
Map extent:	252.0 Å	252.0 Å	252.0 Å	
Origin (voxels):	0	0	0	
Map statistics:	**Minimum**	**Maximum**	**Average**	**Standard deviation**
	-0.27	0.45	0.00	0.02
Recommended contour level:	0.08 (source: author)			

primary map: emd_3061.map
original, unmodified map from reconstruction software: EMD-3061-full.map
maps for FSC calculation: EMD-3061-half-1.map, EMD-3061-half-2.map

---

Target 8. 70S Ribosome

Map A (70S with EF-Tu-GDP, kirromycin, tRNAs):
EMDB entry: EMD-2847
Sequence reference: PDB entry 5afi at RCSB-PDB, PDBe, PDBj

Dimensions (voxels):	420		420	420
Voxel spacing:	0.76 Å		0.76 Å	0.76 Å
Map extent:	317.2 Å		317.2 Å	317.2 Å
Origin (voxels):	0		0	0
Map statistics:	**Minimum**	**Maximum**	**Average**	**Standard deviation**
	-2.43	4.71	0.00	0.21
Recommended contour level:	0.43 (source: emdb)			

primary map: emd_2847.map
original, unmodified map from reconstruction software: EMD-2847-full.map
maps and mask for FSC calculation: EMD-2847-half-1.map, EMD-2847-half-2.map, EMD-2847-FSC-mask.map

Map B (70S with Elongation factor G):
EMDB entry: EMD-6316
Sequence reference: PDB entry 3ja1 at RCSB-PDB, PDBe, PDBj

Dimensions (voxels):	360		360	360
Voxel spacing:	1.05 Å		1.05 Å	1.05 Å
Map extent:	378.0 Å		378.0 Å	378.0 Å
Origin (voxels):	0		0	0
Map statistics:	**Minimum**	**Maximum**	**Average**	**Standard deviation**
	-0.08	0.21	0.00	0.01
Recommended contour level:	0.03 (source: author)			

primary map: emd_6316.map
original, unmodified map from reconstruction software: EMD-6316-full.map
maps and mask for FSC calculation: EMD-6316-half-1.map, EMD-6316-half-2.map, EMD-6316-FSC-mask.map

Model Submissions Summary

Model Challenge Analysis Website
http://model-compare.emdatabank.org

Download All of the Submissions Metadata
http://model-compare.emdatabank.org/data/models/model-challenge-workflow...

Statistics
- 16 modellers submitted 106 entries total

Modelling Category

Optimized a current cryoEM model	47
Fitted/Optimized another known model	16
Created an ab initio model	44

Challenge Target

1. Tobacco Mosaic Virus	11
2. T20S Proteasome	18
3. GroEL	8
4. TRPVI Channel	13
5. Brome Mosaic Virus	12
6. β-Galactosidase	16
7. γ-Secretase	22
8. Ribosome	6

Was the model fitted to the "map A" or "map B" target?

Map A	80
Map B	27

Which target map was used for fitting?

primary map of the EMDB entry (emd_####.map)	83
original, unmodified map from reconstruction software (EMD-####-full.map)	15
half-map 1 for the FSC calculation (EMD-####-half-1.map)	9

Did you modify the provided map?

yes	60
no	47

Map preparation procedures used

	yes	no
low pass filter	18	41
high pass filter	1	58
segmentation	41	19
applied a mask	27	33

Effort type

fully automated	66
partially automated, some manual steps	37
manual	4

Refinement space

real	96
reciprocal	11

Modelling software used

Chimera	35
COOT	25
direX	8
flex-EM	3
MDFF	6
phenix	63
pymol	1
rosetta	19
situs	1
TEMPy	3
VMD	6
other breakdown of "other" based on detailed description: amber (1), gmfit (1), gromacs (1), HermiteFit (10), iMDFF (4), MainMast (4), Modeller (12), Pathwalker (13), PULCHRA (4), Remo (4), scwrl (1)	36

Which target criteria were used to identify model improvements?

map vs. model correlation coefficient	102
map vs. model FSC curve	12
energy function	35
cross-validation procedure	23
other	13

Was the map scale (voxel size) adjusted during the modelling process?

yes	9
no	98

Validation Checks

	yes	**no**
internal model consistency	90	17
fit of model to the target map	105	2
fit of model to map other than target (cross-validation)	18	85

Website Footer

EMDataBank Validation Challenges are supported by NIH National Institute of General Medical Sciences

Please send your challenge questions, comments and feedback to challenges@emdatabank.org