

# Agenda for EMDataResource Ligand Challenge Wrap Up Meeting

July 26-28 11 AM start, length varies 2-4 hrs per day.

All times noted are US Eastern (New York)

Time Conversion: US PT -3 / US CT -1 / UK +5 / EUR +6

[Ligand Challenge Links](#)

[Possibly Helpful Guides from Previous Challenges](#)

[Zoom Connection Information](#)

[Day 1: presentations by each submitting team \(July 26th; 3.75 hours\)](#)

[Session I](#)

[Session II](#)

[Day 2: presentations by each assessor group \(July 27th; 3 hours\)](#)

[Day 3: Wrap up discussion \(July 28th; 2 hours\)](#)

[Email lists](#)

[Advisors](#)

[EMDR](#)

[Modeling Team Leads](#)

[Assessor Team Leads](#)

[All invitees](#)

## Ligand Challenge Links

Main Challenge Info Page: [2021 Ligand Model Challenge | EM Validation Challenges](#)

Model Compare Analysis: <https://model-compare.emdataresource.org>

## Possibly Helpful Guides from Previous Challenges

[Guidance for Modeler/Assessor Presentations - pdf - \(2017\)](#)

[Guidance for Challenge Discussion - pdf - \(2019\)](#)

## Zoom Connection Information

Topic: Ligand Challenge Wrap Up 3 Day Meeting

Time: Jul 26, 2021 11:00 AM Eastern Time (US and Canada)

Every day, 3 occurrence(s)

Jul 26, 2021 10:30 AM Open for testing, Casual Discussion 11 AM - 3 PM Presentations

Jul 27, 2021 10:30 AM Open for testing, Casual Discussion 11 AM - 2 PM: Presentations

Jul 28, 2021 10:30 AM Open for testing, Casual Discussion 11 AM - 1 PM Discussion

iCalendar (.ics) files to your calendar system:

<https://rutgers.zoom.us/meeting/tJ0sduquqj8qGNbE688-39kN-Ndo0ODFuZ53/ics?icsToken=98tyKuChrzopHNCRsBuFRox5BYj4b-7wiClfjY1fuUm9W20AOwjYe8xGPeJQNP7F>

Join Zoom Meeting

<https://rutgers.zoom.us/j/99113644022?pwd=dGY5LzhGaGIZU2lhb3Z0aWFHNExKUT09>

Join by SIP: 99113644022@zoomcrc.com

Meeting ID: 991 1364 4022

Password: 251406

One tap mobile

+13126266799,,99113644022# US (Chicago)

+16465588656,,99113644022# US (New York)

Join By Phone

+1 312 626 6799 US (Chicago)

+1 646 558 8656 US (New York)

+1 301 715 8592 US (Washington DC)

+1 346 248 7799 US (Houston)

+1 669 900 9128 US (San Jose)

+1 253 215 8782 US (Tacoma)

Meeting ID: 991 1364 4022

Find your local number: <https://rutgers.zoom.us/u/adl8iC4IAx>

Join by Skype for Business: <https://rutgers.zoom.us/skype/99113644022>

If you have any questions, please contact the Office of Information Technology Help Desk:

<https://it.rutgers.edu/help-support/>

**Day 1: presentations by each submitting team (July 26th; 4 hours)**

10:30 - 11:00 (US Eastern) Zoom call opens early for presenter checks, casual discussion

11:00 - 11:10 Welcome, Short Introduction Cathy Lawson/Wah Chiu

11:04 - 15:00 Presentations (10 Minutes per Team plus 4 minutes discussion)

Introduce Team, Summarize methods used, identify any challenges faced, particularly with regards to ligand modeling.

**Session I**

Chair: Cathy Lawson

<b>Team Members/Presenters</b>	<b>Talk Title</b>	<b>Start Time</b>
<u>Colin Palmer</u> , Rob Nicholls, Rangana Warshamanage, Keitaro Yamashita, Garib Murshudov, Paul Bond, Scott Hoh, Mateusz Olek, Kevin Cowtan, Agnel Joseph, Tom Burnley, Martyn Winn	Utilizing Tools in CCP-EM for Model Refinement and Validation	11:10
<u>Dong Si</u> , <u>Sean Lin</u> , Minglei Zhao, Renzhi Cao, Jie Hou	DeepTracer Team 2021 Ligand Model Challenge Summary	11:24
<u>Grzegorz Chojnowski</u>	Modelling the Ligand Challenge targets de novo	11:38
<u>Daisuke Kihara</u> , Genki Terashi, Daipayan Sarkar, Jacob Verburgt	Ligand modeling by Kiharalab	11:52
<u>Abishek Singharoy</u> , Sumit Mittal, Alberto Perez, Daisuke Kihara, <u>Mrinal Shekhar</u> , <u>Daipayan Sarkar</u> , Genki Terashi, Chris Rowley, Reza Esmaeli, Lijun Lang, Arup Mondal, Arthur Campbell	CryoFold Modelling for EMDR Ligand Challenge	12:06
Gunnar Schröder, Luisa Schäfer, <u>Karunakar R. Pothula</u>	Cross-validation approach to fit small molecules into cryo-EM maps	12:20
<u>Andrew Muenks</u> , Frank DiMaio	Density-guided modeling of small molecules and ions with Rosetta	12:34
<b>12 minute break</b>		12:48-13:00

**Session II**

Chair Andriy Kryshtafovych

<b>Team Members/Presenters</b>	<b>Talk Title</b>	<b>Start Time</b>
<u>Wei-Chun Kao</u>	Modeling alternate ligand conformation	13:00
<u>Alberto Perez</u> , Arup Mondal, Reza Esmaeli, Lijun Lang	Extracting Water densities from MD	13:14
Nigel Moriarty, Pavel Afonine, <u>Christopher Schlicksup</u> , Oleg Sobolev	Recent Developments in Phenix for Cryo-EM Model Refinement	13:28
Jianlin Cheng, <u>Nabin Giri</u>	Structure Determination from cryo-EM Density Maps Using a Deep Learning Framework	13:42
Simone Weyand, <u>Sundeep Chaitanya</u> , Tom Blundell, Steven Brohawn	TBD	13:56
<u>Dilip Kumar</u>	Automated or Manual intervention: striking the right balance	14:10
<u>Matthew Baker</u> , Corey Hryc	Beyond Pathwalker: Modeling Ligands in CryoEM Density Maps	14:24
<u>Greg Pintilie</u> , Michael Schmid, Wah Chiu	Modeling ligands, water, ions in CryoEM maps with SegMod and SWIM	14:38
<b>Discussion</b>		14:52-15:00

Modeler group not presenting: Helmut Grubmuller

**Day 2: presentations by each assessor group (July 27th; 3 hours)**

10:30 - 11:00 (US Eastern) Zoom call opens early for presenter checks, casual discussion

11:00 - 11:10 Welcome, Short Introduction Cathy Lawson/Wah Chiu

11:10 - 14:00 Presentations (20 Minutes per Team, including 4 minutes discussion)

Introduce Team, Summarize methods used, identify any challenges faced, particularly with regards to ligand model assessments

Chairs: Helen Berman / Mike Schmid

<b>Assessor Team/Presenter</b>	<b>Talk Title</b>	<b>Start Time</b>
<u>Andriy Kryshfovych</u>	Model Compare Pipeline Trends	11:10
<u>Chenghua Shao</u>	Validation of ligands at the wwPDB	11:30
<u>Paul Emsley</u>	Validating Models using Coot Tools	11:50
Bohdan Schneider, <u>Jiří Černý</u>	Nucleic acid conformations / Protein hydration analysis	12:10
<b>10 Minute Break</b>		12:30
<u>Jane Richardson</u> , Christopher J. Williams, Vincent Chen, David Richardson	Ligands, ions, & waters assessed by contact analysis, partial occupancy, & visual examination	12:40
<u>Chris I. Williams</u> , Chemical Computing Group Support Team	Using Consensus Pharmacophore Fields to Score Placed Fragments	13:00
<u>Ben Sellers</u> , Alberto Gobbi, Alexis Rohou	Assessment of internal strain energy in ligand models	13:20
<u>Greg Pintilie</u> , Michael Schmid, Wah Chiu	Assessment of water, ions and ligands in CryoEM maps with Q-scores	13:40

### **Day 3: Wrap up discussion (July 28th; 2 hours)**

Chair: Cathy Lawson

10:30 - 11:00 (US Eastern) Zoom call opens early for casual discussion

11:00 - 11:10 Short Intro Cathy Lawson

11:10 - 11:40 Discussion: Challenge outcomes: Modellers' perspectives

11:40 - 12:10 Discussion: Challenge outcomes: Assessors' perspectives

Jane Richardson: Ensembles win, occupancy matters, ions need tools, and other stories

12:10 - 12:40 Discussion: Key Outcomes

12:40 - 13:00 Discussion: What's Next

## Participants

### All invitees

Pavel	Afonine	Lawrence Berkeley Laboratory
Matthew L	Baker	University of Texas Houston
Helen	Berman	Rutgers University (Emerita)
Paul	Bond	York University
Stephen	Burley	Rutgers University
Arthur	Campbell	Broad Institute
Renzhi	Cao	Pacific Lutheran University
Jiří	Černý	Czech Academy of Sciences
Sundeeep	Chaitanya	University of Cambridge
Vincent	Chen	Duke University
Jianlin	Cheng	University of Missouri
Chih-Ta	Chien	Stanford University
Wah	Chiu	Stanford University
Grzegorz	Chojnowski	EMBL Hamburg
Frank	DiMaio	University of Washington
Alison	Doerr	Nature Methods (Journal)
Paul	Emsley	MRC-LMB Cambridge
Reza	Esmali	University of Florida
Paula	Flicker	NIH/NIGMS
Michael	Funk	Science (Journal)
Nabin	Giri	University of Missouri
Helmut	Grubmuller	Max Planck Institute Göttingen
Mark	Herzik	University of California San Diego
Scott	Hoh	University of York
Jie	Hou	Saint Louis University
Corey	Hyc	University of Texas Houston
Maxim	Igaev	Max Planck Institute Göttingen
Andrzej	Joachimiak	Argonne National Laboratory
Agnel	Joseph	UKRI Science Technology Facilities Council
Wei-Chun	Kao	University of Freiburg
Daisuke	Kihara	Purdue University
Rachael	Kretsch	Stanford University
Andriy	Kryshchak	University of California Davis
Karin	Kuehnel	Nature Communications (Journal)
Dilip	Kumar	Baylor College of Medicine
Lijun	Lang	University of Florida
Cathy	Lawson	Rutgers University
Sean	Lin	University of Washington
Sumit	Mittal	Arizona State University
Arup	Mondal	University of Florida
Andrew	Muenks	University of Washington
Sigrid	Noreng	Genentech
Nigel	Moriarty	Lawrence Berkeley Laboratory
Mateusz	Olek	Diamond Light Source
Colin	Palmer	UKRI Science Technology Facilities Council
Sushrit	Pasumarthy	Duke University
Alberto	Perez	University of Florida
Grigore	Pintilie	Stanford University

Emmi	Pohjolainen	Max Planck Institute Göttingen
Joann	Polizzi	Stanford University
Karunakar	Pothula	Forschungszentrum Jülich
Michael	Prisant	Duke University
Randy	Read	University of Cambridge
Dave	Richardson	Duke University
Jane	Richardson	Duke University
Alexis	Rohou	Genentech
Chris	Rowley	Arizona State University
Daipayan	Sarkar	Arizona State University
Luisa	Schäfer	Forschungszentrum Jülich
Christopher	Schlicksup	Lawrence Berkeley Laboratory
Michael	Schmid	Stanford University
Bohdan	Schneider	Czech Academy of Sciences
Gunnar	Schröder	Forschungszentrum Jülich
Ben	Sellers	Genentech
Chenghua	Shao	Rutgers University
Mrinal	Shekhar	Broad Institute
Dong	Si	University of Washington
Abhishek	Singharoy	Arizona State University
Oleg	Sobolev	Lawrence Berkeley Laboratory
Elizabeth	Sourial	Chemical Computing Group
Guan Chin	Su	Stanford University
Sai	Subramaniya	Purdue University
Genki	Terashi	Purdue University
Andrea	Vaiana	Max Planck Institute Göttingen
Brinda	Vallat	Rutgers University
Xiao	Wang	Purdue University
Simone	Weyand	University of Cambridge
Chris I	Williams	Chemical Computing Group
Christopher J	Williams	Duke University
Mary Ann	Wu	NIH/NIGMS
Keitaro	Yamashita	MRC-LMB Cambridge
Minglei	Zhao	University of Chicago

### Advisors

Bohdan Schneider, Paul Emsley, Jiří Černý, Alexis Rohou, Andrzej Joachimiak, Randy Read, Jane Richardson

### EMDR

Wah Chiu, Cathy Lawson, Helen Berman, Michael Schmid, Andriy Kryshtafovych, Greg Pintilie

### Modeling Team Leads

Dilip Kumar, Dong Si, Daisuke Kihara, Abhishek Singharoy, Andrew Muenks, Grzegorz Chojnowski, We-Chun Kao, Alberto Perez, Nigel Moriarty, Greg Pintilie, Simon Weyand, Colin Palmer, Matthew Baker, Paul Emsley, Gunnar Schroeder, Helmut Grubmuller, Jianlin Cheng

### Assessor Team Leads

Bohdan Schneider, Jiří Černý, Chenghua Shao, Andriy Kryshtafovych, Elizabeth Sourial, Alexis Rohou, Mark Herzik, Jane Richardson, Ben Sellers, Paul Emsley