2021 Ligand Model Challenge Summary Statistics

Challenge Target

beta-galactosidase 1.9 Å (EMD-7770)	23
SARS-CoV-2 RNA polymerase 2.5 Å (EMD-30210)	17
SARS-Cov-2 ORF3a ion channel 2.1 Å (EMD-22898)	21

Polymer Modelling Category

ab initio+optimized	22
optimized	32
not optimized	7

Ligand Modelling Category

independently refit	49
optimized	12

Effort type

fully automated	9
partially automated, some manual steps	49
manual	3

Ligand initial source

PDB Chemical Component Dictionary (CCD)	10
Crystallography Online Database (COD)	3
coordinates from PDB entry	36
Other	12

Ligand restraints software

BUSTER/Grade	1
phenix elbow	26
ccp4 acedrg	6
other/MD Force Field	13
other/PyRosetta	7
other/Multiple Sources	7
other/COOT mon_lib	3
other/CGENFF	1
other/Schrodinger LigPrep	1
other/Antechamber	1
other/OpenBabel	1

Modelling software (indicate all used)

AMBER	1
ARP/wARP	3
CCP-EM	3
Chimera	31
ChimeraX	7
COOT	15
CDMD	1
DeepTracer	8
EMDA	3
ISOLDE	4
LAFTER	2
mainmast	2
MDFF	10
modeller	3
pathwalker	3
phenix	7
ProSMART	3
pymol	7
refmac	6
rosetta	15
Schrodinger	7
servalcat	3
VMD	11

Restraints/Methods (indicate all used)

bond lengths, angles	30
dihedrals angles	27
planarity	27
chirality	33
secondary structure-protein	21
secondary structure-nucleic acid	14
nonbonded (vdW)	18
riding hydrogen atoms	5
explicit hydrogen atoms	23
charge assignments	18
molecular dynamics force field	28
other	31

Atomic Displacement (B) and Occupancy

single overall B value applied to entire model	2
grouped B (per residue)	6
individual B for each atom	23
neigbor restraints	11
occupancy refinement or occupancy reduced for specific atoms/residues	6
other	3
none	29

Final model optimization software

Chimera	7
COOT	3
CDMD	4
MDFF	10
phenix	20
refmac	3
rosetta	10
Schrodinger	1
VMD	3

Did you modify the map?

yes	4
no	57

EMDR information release

yes	61

Below are screenshots of the ligand submission form with example values entered.

2021 Ligand Challenge Submission Form

Instructions:

1. Carefully check the coordinate file: make sure it follows all **Challenge instructions**. **Remove any remarks that identify users and/or software**.
2. Next go to **PDBextract**. Select "EM" method and upload your coordinates. Don't fill any info on second page, just submit.
3. Copy **THE FULL LINK for** the PDBextract-generated output cif file. Paste this link in the form below**.**
4. Fill out the remainder of the submission form as completely as possible.

Use "next page" "previous page" buttons to navigate (browser navigation may reset your submission). You will have an opportunity to review all of your answers prior to submission. Questions/issues/comments? Contact **challenges@emdataresource.org**.

You must be logged in to fill out this form.

Note: PDBextract is used for file upload because it automates file conversion to mmCIF.

Page 1: Submission info

Entry Info — Categories — Ligand — Modeling Method — Validation — Additional Info — Preview — Submission

PDBextract full URL *

https://pdb-extract.wwpdb.org//users_data/em_dir_2019_5_28_15_2

Submission Title *

Unique title for this submission (will not be shared during blinded assessment).

RNAP optimized using ModelX (example submission)

Challenge Target *

- ○ beta-galactosidase 1.9 Å (EMD-7770)
- ◉ SARS-CoV-2 RNA polymerase 2.5 Å (EMD-30210)
- ○ SARS-Cov-2 ORF3a ion channel 2.1 Å (EMD-22898)

Page 2: Categories

Polymer Modelling Category *

Indicate modeling category for polymer chains (protein,RNA)

- (•) ab initio+optimized
- ( ) optimized
- ( ) not optimized

Ligand Modelling Category *

For the submitted model, please indicate modeling category for ligand(s)

- (•) independently refit
- ( ) optimized

Effort type *

Indicate to what extent your process involved interactive (manual) modeling steps

- (•) fully automated
- ( ) partially automated, some manual steps
- ( ) manual

Estimated human effort *

10 person-hours

Estimated computing time *

2 CPU-hours

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Conditional: PDB info is also requested if polymer modelling category is “optimized”:

Polymer model resources *

List all PDB ids (comma separated)

Page 3: Ligand

Entry Info | Categories | Ligand | Modeling Method | Validation | Additional Info | Preview | Submission

Ligand initial source *

resource(s) used for initial ligand chemistry/valence geometry definition (email us to suggest additional options).

- [x] PDB Chemical Component Dictionary (CCD)
- [ ] Crystallography Online Database (COD)
- [ ] coordinates from PDB entry
- [ ] Other

Ligand restraints software *

Indicate all software used to create modeling restraints for the ligand (email us to suggest additional options)

- [x] phenix elbow
- [ ] phenix reel
- [ ] ccp4 acedrg
- [ ] other

Ligand restraints description *

Describe how you obtained and any software used to encode the ligand chemistry / geometry / restraint information for model refinement. List all resources including database names/dictionary ids.

```
Ligand restraints were build using phenix elbow gui. Input was F86 from the PDB Chemical Component dictionary.
Optimized using eLBOW AM1 QM method.
```

Ligand restraints file *

F86.cif Remove

Upload the file describing the ligand geometry /chemistry that was used for fitting, dynamics and minimization (non-CIF files can be added to the allowed list--please email us).

Files must be less than **2 MB**.

Allowed file types: **cif**.

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Page 4: Modeling Method

Entry Info — Categories — Ligand — Modeling Method — Validation — Additional Info — Preview — Submission

Modelling software (indicate all used) *

Additional software can be added to his list--send requests to challenges@emdataresource.org. Software descriptions/links can be found **here**.

- [ ] ARP/wARP
- [ ] Buccaneer
- [ ] CCP-EM
- [ ] Chimera
- [ ] ChimeraX
- [ ] COOT
- [ ] CDMD
- [ ] direX
- [ ] EMfit
- [ ] flex-EM
- [ ] GemSpot
- [ ] gorgon
- [ ] hermitefit
- [ ] iMDFF
- [ ] ISOLDE
- [ ] mainmast
- [ ] MDFF
- [ ] modeller
- [ ] MOE
- [ ] pathwalker
- [ ] phenix
- [ ] pymol
- [ ] refmac
- [ ] rosetta
- [ ] Schrodinger
- [ ] situs
- [ ] TEMPy
- [ ] VMD

Restraints/Methods (indicate all used) *

Indicate restraints used during any modeling step.

- [ ] bond lengths, angles
- [ ] dihedrals angles
- [ ] planarity
- [ ] chirality
- [ ] secondary structure-protein
- [ ] secondary structure-nucleic acid
- [ ] bfactor neighbor
- [ ] nonbonded (vdW)
- [ ] riding hydrogen atoms
- [ ] explicit hydrogen atoms
- [ ] charge assignments
- [ ] molecular dynamics force field
- [ ] other

Atomic Displacement (B) and Occupancy *

Indicate all types used (or none).

- [ ] single overall B value applied to entire model
- [ ] grouped B (segments)
- [ ] grouped B (per residue)
- [ ] individual B for each atom
- [ ] neigbor restraints
- [ ] occupancy refinement for specific atoms/residues
- [ ] other
- [ ] none

Final model optimization software *

Additional software can be added to his list--send requests to challenges@emdataresource.org. Software descriptions/links can be found **here**.

(same answer list as “Modelling software” above, but only one can be selected)

Modelling details *

step-by-step text description of the modelling process used. For each software package used, indicate version, package module(s), relevant parameters and settings.

Page 5: Validation

Entry Info — Categories — Ligand — Modeling Method — Validation — Additional Info — Preview — Submission

Validation details *

Indicate types of validation performed, including software package(s)/parameters/settings used.

```
checked final model using wwPDB validation service
```

Page 6: Additional info (including modified map upload)

Entry Info — Categories — Ligand — Modeling Method — Validation — Additional Info — Preview — Submission

Did you modify the map? *

- ○ yes
- ◉ no

Additional Details

If you have any further details relevant to your modelling process that were not captured by the previous questions, please provide here!

EMDR information release *

EMDataResource is permitted to publicly release the model and all information provided in this submission (software and author info will be temporarily withheld until blinded analysis is completed).

- ◉ yes

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Extra form elements if answer to map modification is “yes”:

Did you modify the map? *

- ◉ yes
- ○ no

Map preparation details *

Step-by-step description of all map modification steps, including software/parameters used.

Map Upload

Choose File | No file chosen | Upload

Upload the modified map used for model/ligand optimization. Upload may take a few minutes

Files must be less than **300 MB**.

Allowed file types: **mrc map**.