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)	
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	
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:

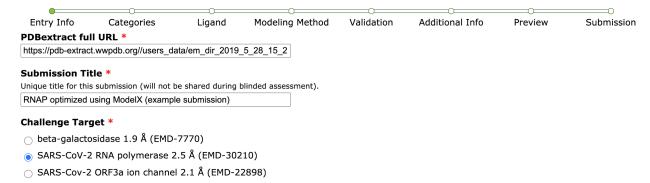
- Carefully check the coordinate file: make sure it follows all Challenge instructions. Remove any remarks that identify users and/or software.
- 2. Next go to PDBextract. Select "EM" method and upload your coordinates. Don't fill any info on second page, just submit.
- 3. Copy THE FULL LINK for the 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



Page 2: Categories

•							
Entry Info	Categories	Ligand	Modeling Method	Validation	Additional Info	Preview	Submission
Polymer Mode	lling Category *						
Indicate modeling	category for polymer c	hains (protein,Ri	NA)				
ab initio+op	timized						
\bigcirc optimized							
o not optimize	ed						
_	ing Category * model, please indicate	modeling catego	ory for ligand(s)				
independent	tly refit						
$\bigcirc \ optimized$							
Effort type *							
Indicate to what e	xtent your process invo	lved interactive	(manual) modeling steps				
fully automa	ated						
partially aut	omated, some man	ual steps					
○ manual							
Estimated hun	nan effort *						
10	person-hours	5					
Estimated con	nputing time *						
2	CPU-hours						
Save Draft < P	revious Page Next F	Page >					

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



Page 3: Ligand

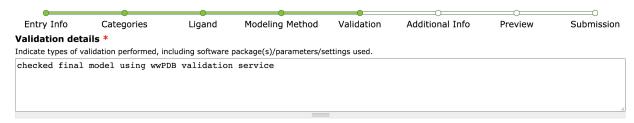
0							
Entry Info	Categories	Ligand	Modeling Method	Validation	Additional Info	Preview	Submissio
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esource(s) used fo	r initial ligand chemis	try/valence geom	etry definition (email us t	o suggest addition	al options).		
PDB Chemica	al Component Dicti	onary (CCD)					
Crystallograp	hy Online Databas	se (COD)					
coordinates f	rom PDB entry						
Other							
ndicate all softwar		eling restraints for	the ligand (email us to s	uggest additional o	options)		
phenix elbow	I						
phenix reel							
ccp4 acedrg							
other							
igand restrair	nts description *						
-	•	ware used to enco	de the ligand chemistry /	geometry / restra	int information for mode	l refinement. List a	Il resources
cluding database	names/dictionary ids.						
	ints were build and eLBOW AM1 QM		elbow gui. Input w	as F86 from t	he PDB Chemical Co	omponent dicti	onary.
F86.cif Rem pload the file desc lease email us). illes must be less tillowed file types:	nove cribing the ligand geor	metry /chemistry (that was used for fitting,	dynamics and mini	imization (non-CIF files o	an be added to the	e allowed list
Save Draft < Pr	revious Page Next F	Page >					

Page 4: Modeling Method

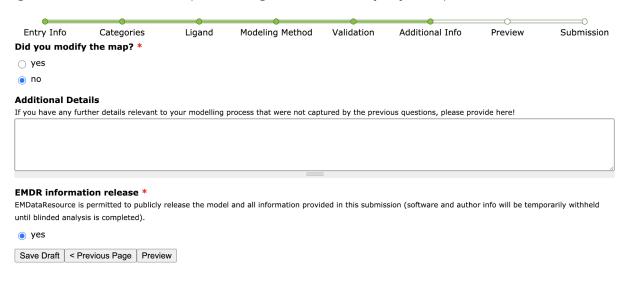
Atomic Displacement (B) and Occupancy * ABP/WARP	0							
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Page 5: Validation

Allowed file types: mrc map.



Page 6: Additional info (including modified map upload)



Extra form elements if answer to map modification is "yes":

