Full wwPDB EM Validation Report ⓘ

Nov 6, 2023 – 07:42 pm GMT

PDB ID	:	7ZL3
EMDB ID	:	EMD-14776
Title	:	Signal peptide mimicry primes Sec61 for client-selective inhibition
Authors	:	Rehan, S.; Paavilainen O, V.
Deposited on	:	2022-04-13
Resolution	:	3.20 Å(reported)
Based on initial model	:	3JC2

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev70
Mogul	:	NOT EXECUTED
MolProbity	:	FAILED
buster-report	:	NOT EXECUTED
Percentile statistics	:	NOT EXECUTED
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3692 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein transport protein Sec61 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	388	Total	C	N	O	S	0	0
			3020	1992	487	522	19		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PHE	deletion	UNP A0A6P3YN15
A	77	ALA	GLU	conflict	UNP A0A6P3YN15
A	342	HIS	TYR	conflict	UNP A0A6P3YN15
A	362	VAL	ALA	conflict	UNP A0A6P3YN15
A	364	ILE	VAL	conflict	UNP A0A6P3YN15

- Molecule 2 is a protein called Protein transport protein Sec61 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	57	Total	C	N	O	S	0	0
			462	305	81	73	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	29	ASP	VAL	conflict	UNP W5PP18

- Molecule 3 is a protein called Protein transport protein Sec61 subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	28	Total	C	N	O	0	0
			138	82	28	28		

- Molecule 4 is a protein called Cyclic depsipeptide signal peptide mimic.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	6	Total	Br	C	F	N	O	0	0
			72	1	49	6	8	8		

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	47	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

Mogul was not executed - this section is therefore empty.

4.5 Carbohydrates

Mogul was not executed - this section is therefore empty.

4.6 Ligand geometry

Mogul was not executed - this section is therefore empty.

4.7 Other polymers

Mogul was not executed - this section is therefore empty.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Map visualisation

This section contains visualisations of the EMDB entry EMD-14776. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

5.1 Orthogonal projections

This section was not generated.

5.2 Central slices

This section was not generated.

5.3 Largest variance slices

This section was not generated.

5.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

5.5 Orthogonal surface views

This section was not generated.

5.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

6 Map analysis

This section contains the results of statistical analysis of the map.

6.1 Map-value distribution

This section was not generated.

6.2 Volume estimate versus contour level

This section was not generated.

6.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

7 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

8 Map-model fit

This section was not generated.