WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

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

---

1   Overall quality at a glance ⓘ

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 3020	C 1992	N 487	O 522	S 19	0	0

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 462	C 305	N 81	O 73	S 3	0	0

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 138	C 82	N 28	O 28	0	0

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

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

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

3   Experimental information ⓘ

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 $(e^-/\text{Å}^2)$	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 ⓘ

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

8 Map-model fit (i)

This section was not generated.