



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 07:35 AM UTC

PDB ID : 7KAT / pdb_00007kat
EMDB ID : EMD-22783
Title : Cryo-EM structure of the Sec complex from *S. cerevisiae*, Sec61 pore ring and Sec63 FN3 double mutant, class without Sec62
Authors : Itskanov, S.; Park, E.
Deposited on : 2020-10-01
Resolution : 4.40 Å(reported)

This is a wwPDB EM Validation Summary 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

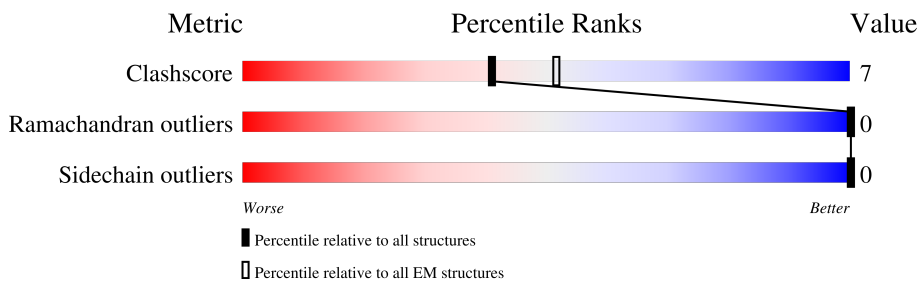
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	480	
2	C	80	
3	B	82	
4	D	676	
5	E	206	
6	F	193	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10431 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	440	3358	2224	541	581	12	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	LEU	MET	variant	UNP P32915
A	185	ILE	THR	variant	UNP P32915
A	294	ILE	MET	variant	UNP P32915
A	450	LEU	MET	variant	UNP P32915

- Molecule 2 is a protein called Protein transport protein SSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	55	435	294	71	69	1	0	0

- Molecule 3 is a protein called Protein transport protein SBH1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	B	32	229	157	38	34	0	0

- Molecule 4 is a protein called Protein translocation protein SEC63.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	485	3809	2482	648	665	14	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-13	GLY	-	expression tag	UNP P14906

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	GLY	-	expression tag	UNP P14906
D	-11	SER	-	expression tag	UNP P14906
D	-10	GLY	-	expression tag	UNP P14906
D	-9	GLY	-	expression tag	UNP P14906
D	-8	SER	-	expression tag	UNP P14906
D	-7	GLY	-	expression tag	UNP P14906
D	-6	GLY	-	expression tag	UNP P14906
D	-5	SER	-	expression tag	UNP P14906
D	-4	GLY	-	expression tag	UNP P14906
D	-3	GLY	-	expression tag	UNP P14906
D	-2	SER	-	expression tag	UNP P14906
D	-1	GLY	-	expression tag	UNP P14906
D	0	GLY	-	expression tag	UNP P14906
D	1	SER	-	expression tag	UNP P14906
D	440	ARG	GLU	engineered mutation	UNP P14906
D	?	-	ASN	deletion	UNP P14906
D	?	-	GLN	deletion	UNP P14906
D	?	-	VAL	deletion	UNP P14906
D	?	-	THR	deletion	UNP P14906
D	?	-	PRO	deletion	UNP P14906
D	?	-	SER	deletion	UNP P14906
D	?	-	SER	deletion	UNP P14906
D	?	-	THR	deletion	UNP P14906
D	481	SER	PHE	engineered mutation	UNP P14906
D	664	GLY	-	expression tag	UNP P14906
D	665	GLU	-	expression tag	UNP P14906
D	666	ASN	-	expression tag	UNP P14906
D	667	LEU	-	expression tag	UNP P14906
D	668	TYR	-	expression tag	UNP P14906
D	669	PHE	-	expression tag	UNP P14906
D	670	GLN	-	expression tag	UNP P14906

- Molecule 5 is a protein called Translocation protein SEC66.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	138	1129	722	200	202	5	0	0

- Molecule 6 is a protein called Translocation protein SEC72.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	190	1471	934	256	274	7	0	0

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	32704	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 ($e^-/\text{\AA}^2$)	48.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	42017	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.11	0/3427	0.30	0/4655
2	C	0.11	0/443	0.27	0/596
3	B	0.11	0/233	0.24	0/318
4	D	0.13	0/3898	0.30	0/5295
5	E	0.13	0/1147	0.31	0/1540
6	F	0.13	0/1491	0.29	0/2018
All	All	0.12	0/10639	0.30	0/14422

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3358	0	3504	61	0
2	C	435	0	481	6	0
3	B	229	0	243	4	0
4	D	3809	0	3852	50	0
5	E	1129	0	1145	10	0
6	F	1471	0	1512	28	0
All	All	10431	0	10737	145	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 145 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:GLY:H	1:A:153:LEU:HD21	1.53	0.72
4:D:470:ILE:HG22	4:D:472:GLU:H	1.57	0.69
4:D:463:PRO:HG3	4:D:549:LYS:HA	1.75	0.68
1:A:44:LEU:HD21	2:C:65:GLY:HA2	1.75	0.68
4:D:6:GLU:H	4:D:207:GLY:HA2	1.58	0.67

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	432/480 (90%)	424 (98%)	8 (2%)	0	100	100
2	C	53/80 (66%)	53 (100%)	0	0	100	100
3	B	30/82 (37%)	30 (100%)	0	0	100	100
4	D	477/676 (71%)	466 (98%)	11 (2%)	0	100	100
5	E	136/206 (66%)	133 (98%)	3 (2%)	0	100	100
6	F	188/193 (97%)	185 (98%)	3 (2%)	0	100	100
All	All	1316/1717 (77%)	1291 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/406 (87%)	353 (100%)	0	100	100
2	C	46/67 (69%)	46 (100%)	0	100	100
3	B	23/69 (33%)	23 (100%)	0	100	100
4	D	414/603 (69%)	414 (100%)	0	100	100
5	E	120/191 (63%)	120 (100%)	0	100	100
6	F	157/165 (95%)	157 (100%)	0	100	100
All	All	1113/1501 (74%)	1113 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	412	GLN
5	E	173	ASN
4	D	416	ASN
6	F	68	ASN
5	E	88	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22783. 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.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

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

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.