wwPDB/EMDataBank EM Map/Model Validation Summary Report (i)

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PDB ID	:	6R7L
EMDB ID:	:	EMD-4743
Title	:	Ribosome-bound SecYEG translocon in a nanodisc
Authors	:	Kater, L.; Beckmann, R.; Kedrov, A.
Deposited on	:	2019-03-29
Resolution	:	6.00 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB 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 (i) symbol.

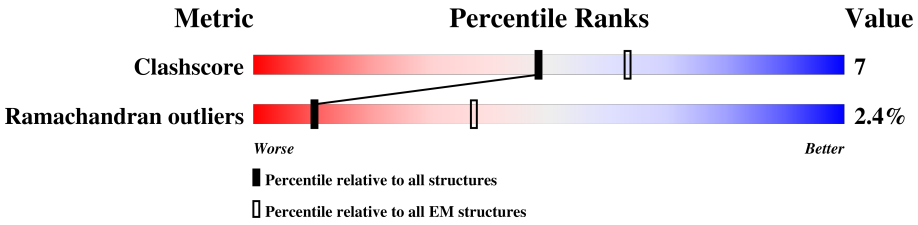
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

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 6.00 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	136327	1886
Ramachandran outliers	132723	1663

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=5%

Mol	Chain	Length	Quality of chain
1	G	22	100%
2	E	107	91% · 8%
3	Y	443	82% 8% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2567 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 SecG.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	G	22	110	66	22	22	0	0

- Molecule 2 is a protein called SecE,Protein translocase subunit SecE,Protein translocase subunit SecE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	E	98	487	291	98	98	0	0

- Molecule 3 is a protein called Protein translocase subunit SecY.

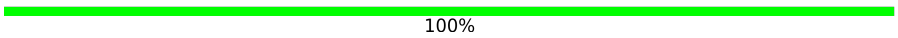
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	Y	401	1970	1168	401	401	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: SecG

Chain G:



There are no outlier residues recorded for this chain.

- Molecule 2: SecE,Protein translocase subunit SecE,Protein translocase subunit SecE

Chain E:

- Molecule 3: Protein translocase subunit SecY

Chain Y:

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	112366	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2.5	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
2	E	0.34	0/291	0.54	0/404
3	Y	0.48	0/1967	0.89	0/2728
All	All	0.47	0/2258	0.86	0/3132

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

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	G	110	0	24	0	0
2	E	487	0	183	1	0
3	Y	1970	0	928	25	0
All	All	2567	0	1135	25	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 25 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)
3:Y:62:GLU:C	3:Y:399:PHE:CB	2.02	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:63:MET:N	3:Y:399:PHE:CB	2.11	1.12
3:Y:62:GLU:O	3:Y:399:PHE:CB	2.33	0.76
3:Y:99:HIS:O	3:Y:102:LEU:N	2.18	0.76
3:Y:63:MET:CA	3:Y:399:PHE:CB	2.66	0.73

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
2	E	57/107 (53%)	56 (98%)	1 (2%)	0	100 100
3	Y	395/443 (89%)	356 (90%)	28 (7%)	11 (3%)	5 37
All	All	452/550 (82%)	412 (91%)	29 (6%)	11 (2%)	10 40

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Y	140	PRO
3	Y	269	VAL
3	Y	272	ALA
3	Y	310	LEU
3	Y	396	LYS

5.3.2 Protein sidechains (i)

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

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 carbohydrates 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	18:UNK	C	21:UNK	N	8.57
1	E	41:UNK	C	60:LEU	N	8.13