



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:07 PM BST

PDB ID : 5A6U
EMDB ID: : EMD-3068
Title : Native mammalian ribosome-bound Sec61 protein-conducting channel in the
'non-inserting' state
Authors : Pfeffer, S.; Burbaum, L.; Unverdorben, P.; Pech, M.; Chen, Y.; Zimmermann,
R.; Beckmann, R.; Foerster, F.
Deposited on : 2015-07-01
Resolution : 9.00 Å(reported)
Based on PDB ID : 3J7Q

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

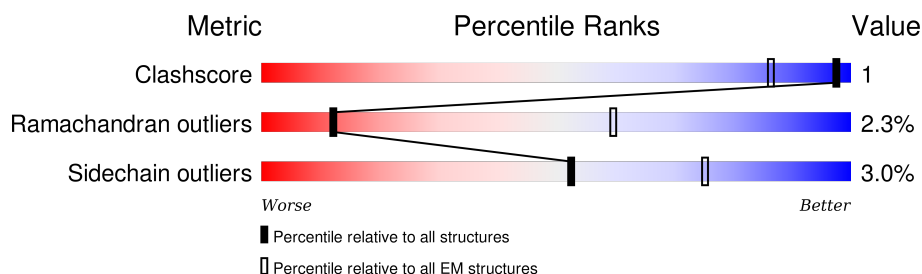
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.00 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	451	 70% 14% • 12%
2	B	36	 78% 17% • •
3	G	62	 73% 26% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7775 atoms, of which 3997 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 SEC61A.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	396	Total	C	H	N	O	S	0	4
			6185	1967	3170	497	532	19		

- Molecule 2 is a protein called SEC61B.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	36	Total	C	H	N	O	S	0	0
			576	186	297	44	47	2		

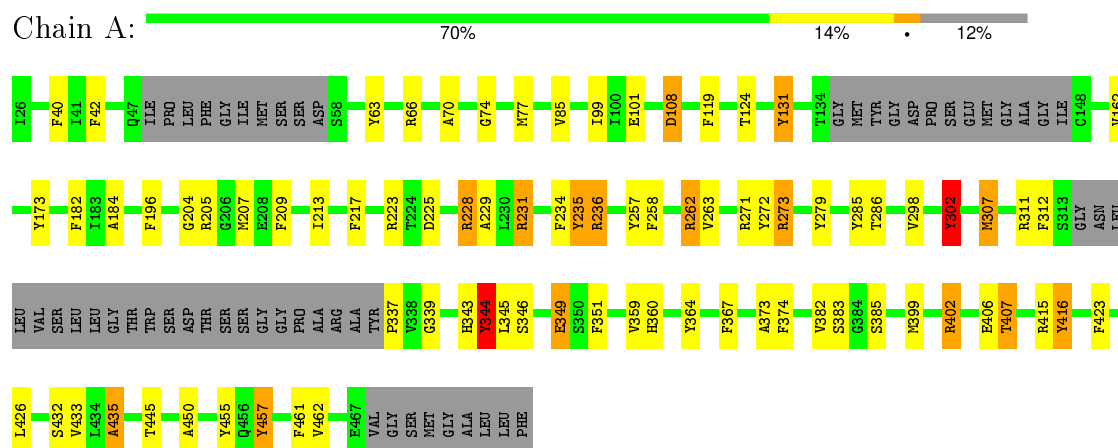
- Molecule 3 is a protein called SEC61G.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	62	Total	C	H	N	O	S	0	0
			1014	316	530	86	79	3		

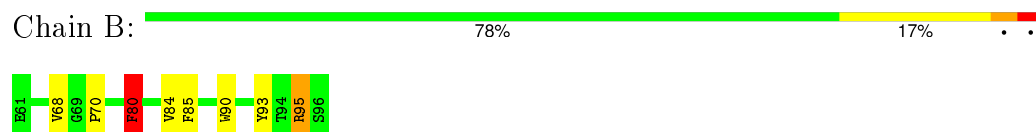
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

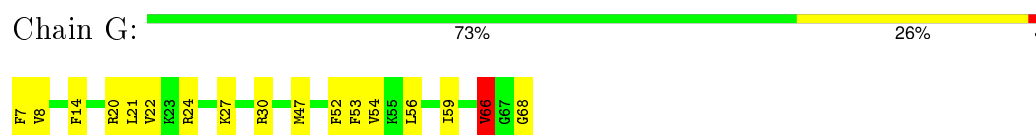
• Molecule 1: SEC61A



• Molecule 2: SEC61B



• Molecule 3: SEC61G



4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH TILT IMAGE	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 (4K 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 >2	RMSZ	# Z >2
1	A	1.73	25/3078 (0.8%)	1.94	72/4186 (1.7%)
2	B	1.61	1/287 (0.3%)	1.90	7/389 (1.8%)
3	G	1.74	2/494 (0.4%)	2.01	15/663 (2.3%)
All	All	1.72	28/3859 (0.7%)	1.95	94/5238 (1.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	11
2	B	0	2
3	G	0	1
All	All	2	14

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	ARG	CZ-NH2	8.32	1.43	1.33
1	A	337	PRO	N-CA	6.93	1.59	1.47
1	A	432	SER	CA-CB	6.80	1.63	1.52
1	A	311	ARG	CZ-NH2	6.23	1.41	1.33
1	A	63	TYR	CG-CD2	6.04	1.47	1.39

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	ARG	NE-CZ-NH2	-13.97	113.32	120.30
1	A	235	TYR	CB-CG-CD2	-12.74	113.36	121.00
1	A	257	TYR	CB-CG-CD1	-12.55	113.47	121.00
1	A	131	TYR	CB-CG-CD2	-11.61	114.04	121.00
1	A	344	TYR	CB-CG-CD1	11.57	127.94	121.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	188	CYS	CA
1	A	447	ILE	CB

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	TYR	Sidechain
1	A	228	ARG	Sidechain
1	A	231	ARG	Sidechain
1	A	235	TYR	Sidechain
1	A	40	PHE	Sidechain

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	A	3015	3170	2959	4	0
2	B	279	297	284	1	0
3	G	484	530	477	1	0
All	All	3778	3997	3720	6	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 1.

The worst 5 of 6 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:74:GLY:H	1:A:77:MET:HB3	1.73	0.54
2:B:80:PHE:O	2:B:84:VAL:HG23	2.12	0.49
1:A:302:TYR:CZ	1:A:345:LEU:HD13	2.49	0.48
1:A:339:GLY:O	1:A:343:HIS:CD2	2.69	0.45
1:A:184:ALA:HB2	1:A:450:ALA:CB	2.46	0.45

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	388/451 (86%)	338 (87%)	41 (11%)	9 (2%)	8	48
2	B	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
3	G	60/62 (97%)	57 (95%)	1 (2%)	2 (3%)	5	40
All	All	482/549 (88%)	428 (89%)	43 (9%)	11 (2%)	12	48

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	ILE
1	A	406	GLU
1	A	407	THR
1	A	445	THR
1	A	349	GLU

5.3.2 Protein sidechains

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	290/374 (78%)	280 (97%)	10 (3%)	44	75
2	B	30/32 (94%)	30 (100%)	0	100	100
3	G	43/53 (81%)	42 (98%)	1 (2%)	58	83
All	All	363/459 (79%)	352 (97%)	11 (3%)	52	77

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	307	MET
1	A	344	TYR
1	A	402	ARG
1	A	286	THR
1	A	359	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	154	GLN
1	A	259	GLN
1	A	343	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 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](#)

There are no chain breaks in this entry.