



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:09 PM BST

PDB ID : 5ABB
EMDB ID: : EMD-2446
Title : Visualization of a polytopic membrane protein during SecY-mediated membrane insertion
Authors : Bischoff, L.; Wickles, S.; Berninghausen, O.; vanderSluis, E.; Beckmann, R.
Deposited on : 2015-08-05
Resolution : 8.00 Å(reported)

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

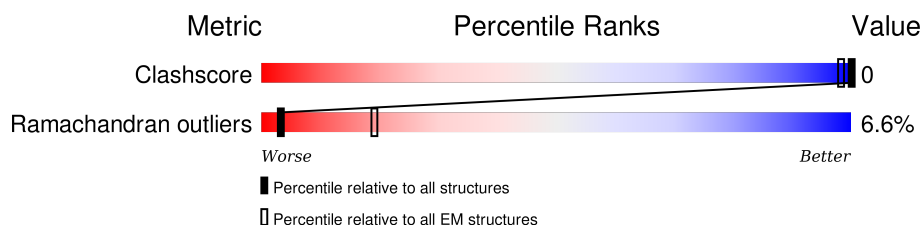
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 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

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	443	
2	B	116	
3	Z	69	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2512 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 TRANSLOCASE SUBUNIT SECY.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	443	Total	C	N	O	0	0
			1772	886	443	443		

- Molecule 2 is a protein called PROTEIN TRANSLOCASE SUBUNIT SECE.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	116	Total	C	N	O	0	0
			464	232	116	116		

- Molecule 3 is a protein called GREEN-LIGHT ABSORBING PROTEORHODOPSIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	Z	69	Total	C	N	O	0	0
			276	138	69	69		

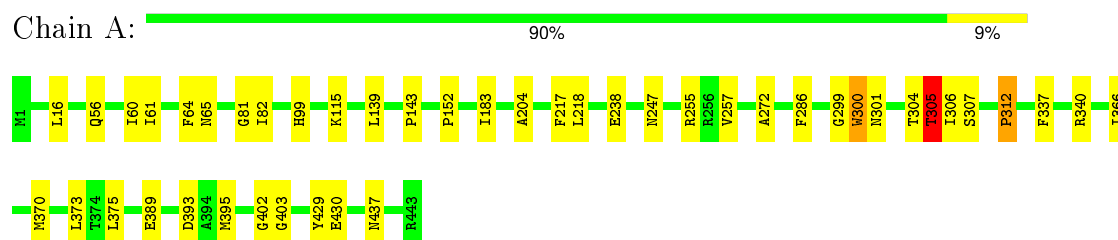
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	84	THR	-	EXPRESSION TAG	UNP Q9F7P4
Z	85	ALA	-	EXPRESSION TAG	UNP Q9F7P4
Z	86	GLY	-	EXPRESSION TAG	UNP Q9F7P4
Z	87	ARG	-	EXPRESSION TAG	UNP Q9F7P4

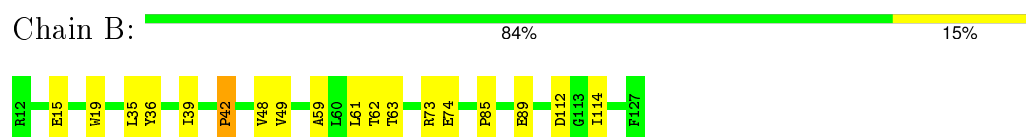
3 Residue-property plots

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.

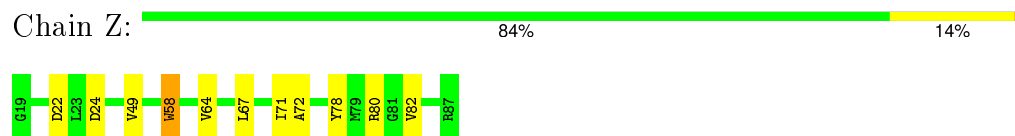
- Molecule 1: PROTEIN TRANSLOCASE SUBUNIT SECY



- Molecule 2: PROTEIN TRANSLOCASE SUBUNIT SECE



- Molecule 3: GREEN-LIGHT ABSORBING PROTEORHODOPSIN



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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
1	A	0.57	0/1771	1.03	2/2212 (0.1%)
2	B	0.57	0/463	1.02	0/577
3	Z	0.56	0/275	1.15	0/342
All	All	0.57	0/2509	1.04	2/3131 (0.1%)

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	0	23
2	B	0	10
3	Z	0	9
All	All	0	42

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	TRP	C-N-CA	7.20	139.70	121.70
1	A	305	THR	N-CA-C	5.27	125.23	111.00

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	LYS	Mainchain
1	A	16	LEU	Mainchain
1	A	183	ILE	Mainchain,Peptide
1	A	204	ALA	Mainchain
1	A	218	LEU	Mainchain

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Mol	Chain	Res	Type	Group
1	A	238	GLU	Peptide
1	A	272	ALA	Peptide
1	A	286	PHE	Mainchain
1	A	299	GLY	Peptide
1	A	300	TRP	Mainchain
1	A	305	THR	Mainchain
1	A	312	PRO	Mainchain
1	A	340	ARG	Mainchain
1	A	366	ILE	Mainchain
1	A	370	MET	Mainchain
1	A	373	LEU	Mainchain
1	A	375	LEU	Mainchain
1	A	389	GLU	Mainchain
1	A	393	ASP	Mainchain
1	A	403	GLY	Mainchain
1	A	65	ASN	Mainchain
1	A	99	HIS	Peptide
2	B	112	ASP	Mainchain,Peptide
2	B	15	GLU	Peptide
2	B	19	TRP	Mainchain
2	B	42	PRO	Mainchain
2	B	59	ALA	Mainchain
2	B	61	LEU	Mainchain,Peptide
2	B	62	THR	Mainchain,Peptide
3	Z	58	TRP	Mainchain
3	Z	64	VAL	Peptide
3	Z	67	LEU	Mainchain
3	Z	71	ILE	Mainchain
3	Z	72	ALA	Mainchain
3	Z	78	TYR	Mainchain
3	Z	80	ARG	Mainchain
3	Z	82	VAL	Mainchain,Peptide

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	1772	0	511	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	464	0	129	0	0
3	Z	276	0	84	0	0
All	All	2512	0	724	0	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 0.

There are no clashes within the asymmetric unit.

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	441/443 (100%)	367 (83%)	49 (11%)	25 (6%)	2	28
2	B	114/116 (98%)	88 (77%)	14 (12%)	12 (10%)	1	12
3	Z	67/69 (97%)	52 (78%)	11 (16%)	4 (6%)	2	26
All	All	622/628 (99%)	507 (82%)	74 (12%)	41 (7%)	3	24

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ILE
1	A	82	ILE
1	A	257	VAL
1	A	305	THR
1	A	312	PRO
2	B	35	LEU
2	B	48	VAL
2	B	63	THR
1	A	81	GLY
1	A	217	PHE
1	A	307	SER

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Mol	Chain	Res	Type
1	A	337	PHE
1	A	402	GLY
1	A	429	TYR
2	B	42	PRO
2	B	89	GLU
2	B	114	ILE
3	Z	22	ASP
3	Z	24	ASP
1	A	143	PRO
1	A	247	ASN
1	A	304	THR
2	B	36	TYR
2	B	39	ILE
1	A	56	GLN
1	A	64	PHE
1	A	139	LEU
1	A	430	GLU
1	A	437	ASN
2	B	73	ARG
2	B	74	GLU
1	A	301	ASN
1	A	306	ILE
1	A	395	MET
2	B	85	PRO
1	A	255	ARG
3	Z	58	TRP
1	A	61	ILE
1	A	152	PRO
2	B	49	VAL
3	Z	49	VAL

5.3.2 Protein sidechains ⓘ

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

5.3.3 RNA ⓘ

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.