wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:50 PM BST

PDB ID	:	3J45
EMDB ID:	:	EMD-5692
Title	:	Structure of a non-translocating SecY protein channel with the 70S ribosome
Authors	:	Menetret, J.F.; Park, E.; Gumbart, J.C.; Ludtke, S.J.; Li, W.; Whynot, A.; Rapoport, T.A.; Akey, C.W.
Deposited on	:	2013-06-18
Resolution	:	9.50 Å(reported)
Based on PDB ID	:	2I2P, 3J01

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

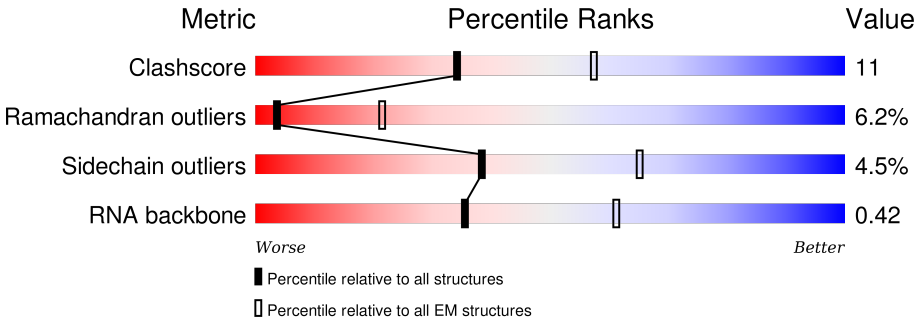
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 9.50 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
RNA backbone	3027	244

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	y	437	74% 21% .
2	E	56	64% 32% .
3	G	65	51% 34% 12% .
4	T	100	67% 26% 7%
5	U	103	68% 22% 9% .
6	Y	63	71% 25% .
7	1	63	46% 38% 16%
8	2	36	50% 36% 14%

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Mol	Chain	Length	Quality of chain
9	3	18	33% 50% 17%
10	4	61	56% 43%
11	5	108	27% 55% 19%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 12465 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	y	437	Total	C	N	O	S	0	1
			3361	2220	554	570	17		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	5	ACE	-	ACETYLATION	UNP P0AGA2
y	441	NH2	-	AMIDATION	UNP P0AGA2

- Molecule 2 is a protein called Preprotein translocase subunit SecE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	56	Total	C	N	O	S	0	1
			433	283	76	73	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	73	ACE	-	ACETYLATION	UNP P0AG96
E	128	NH2	-	AMIDATION	UNP P0AG96

- Molecule 3 is a protein called Protein-export membrane protein SecG.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	65	Total	C	N	O	S	0	0
			457	299	73	81	4		

- Molecule 4 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	100	Total	C	N	O	S	0	0
			787	496	146	143	2		

- Molecule 5 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	U	103	Total	C	N	O	0	0
			789	498	148	143		

- Molecule 6 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 7 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1	63	Total	C	N	O	P	0	0
			1350	603	245	439	63		

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2	36	Total	C	N	O	P	0	0
			775	345	142	252	36		

- Molecule 9 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	3	18	Total	C	N	O	P	0	0
			387	172	71	126	18		

- Molecule 10 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	4	61	Total	C	N	O	P	0	0
			1312	584	240	427	61		

- Molecule 11 is a RNA chain called 23S ribosomal RNA.

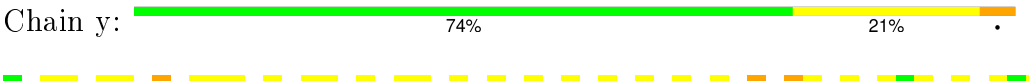
Mol	Chain	Residues	Atoms					AltConf	Trace
11	5	108	Total	C	N	O	P	0	0
			2305	1029	406	762	108		

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 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

Chain y:



- Molecule 2: Preprotein translocase subunit SecE

Chain E:

- Molecule 3: Protein-export membrane protein SecG

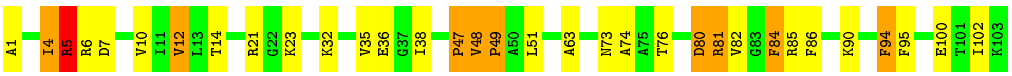
Chain G:

- Molecule 4: 50S ribosomal protein L23

Chain T:

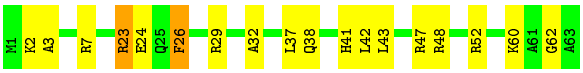
- Molecule 5: 50S ribosomal protein L24

Chain U:



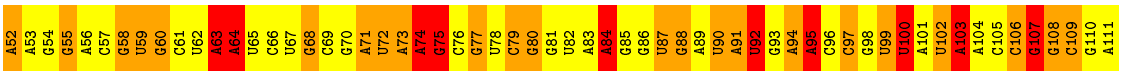
- Molecule 6: 50S ribosomal protein L29

Chain Y:



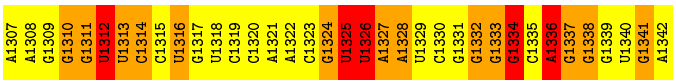
- Molecule 7: 23S ribosomal RNA

Chain 1:



- Molecule 8: 23S ribosomal RNA

Chain 2:

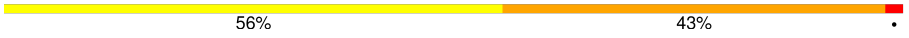


- Molecule 9: 23S ribosomal RNA

Chain 3:

- Molecule 10: 23S ribosomal RNA

Chain 4:



- Molecule 11: 23S ribosomal RNA

Chain 5:


G2152
C2153
A2154
U2155
G2156
G2157
A2158
G2159
C2160
C2161
G2162
A2163
C2164
C2165
U2166
U2167
G2168
A2169
A2170
A2171
U2172
A2173
C2174
C2175
A2176
C2177
C2178
C2179
U2180
U2181
U2182
A2183
A2184
U2185
G2186
U2187
U2188
U2189
G2190
A2191
U2192
G2193
U2194
U2195
C2196
U2197
A2198
A2199

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	39000	Depositor
Resolution determination method	Comparison of 3D map with calculated map of docked ribosomal components, with the second map made with EMAN at 7 Angstrom resolution	Depositor
CTF correction method	per micrograph	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	50000	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, NH2

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	y	1.70	23/3434 (0.7%)	2.02	104/4657 (2.2%)
10	4	3.59	206/1468 (14.0%)	3.69	312/2289 (13.6%)
11	5	3.40	375/2577 (14.6%)	3.71	573/4015 (14.3%)
2	E	1.79	5/437 (1.1%)	2.35	17/596 (2.9%)
3	G	0.27	0/462	1.57	12/620 (1.9%)
4	T	1.64	7/794 (0.9%)	1.92	16/1060 (1.5%)
5	U	1.71	7/797 (0.9%)	1.95	20/1062 (1.9%)
6	Y	1.80	5/510 (1.0%)	1.93	13/677 (1.9%)
7	1	3.51	207/1511 (13.7%)	3.45	299/2354 (12.7%)
8	2	3.40	117/867 (13.5%)	3.56	188/1351 (13.9%)
9	3	3.68	75/432 (17.4%)	3.86	100/672 (14.9%)
All	All	2.75	1027/13289 (7.7%)	3.01	1654/19353 (8.5%)

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	y	0	6
10	4	0	20
11	5	0	54
2	E	0	1
3	G	3	0
4	T	0	1
5	U	0	3
6	Y	0	1
7	1	0	30
8	2	0	15
9	3	0	10
All	All	3	141

The worst 5 of 1027 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	4	1892	C	N1-C6	18.20	1.48	1.37
7	1	114	U	C2-N3	16.37	1.49	1.37
9	3	1532	A	N3-C4	-15.69	1.25	1.34
10	4	1854	A	N9-C4	-15.56	1.28	1.37
10	4	1850	G	N7-C5	-15.20	1.30	1.39

The worst 5 of 1654 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	3	1540	G	N1-C6-O6	26.41	135.75	119.90
11	5	2198	A	N1-C6-N6	26.09	134.26	118.60
10	4	1857	G	N1-C6-O6	24.56	134.64	119.90
10	4	1857	G	C5-C6-O6	-22.03	115.38	128.60
11	5	2171	A	N1-C6-N6	21.65	131.59	118.60

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	45	SER	CA
3	G	48	SER	CA
3	G	51	PHE	CA

5 of 141 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	y	216	HIS	Sidechain
1	y	248	TYR	Sidechain
1	y	25	PHE	Sidechain
1	y	309	TYR	Sidechain
1	y	390	PHE	Sidechain

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	y	3361	0	3514	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	433	0	466	24	0
3	G	457	0	481	63	0
4	T	787	0	846	5	0
5	U	789	0	847	4	0
6	Y	509	0	543	3	0
7	1	1350	0	676	1	0
8	2	775	0	385	0	0
9	3	387	0	196	0	0
10	4	1312	0	659	3	0
11	5	2305	0	1156	4	0
All	All	12465	0	9769	84	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 11.

The worst 5 of 84 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)
2:E:126:ARG:HE	3:G:68:LEU:CD2	1.54	1.20
2:E:126:ARG:CB	3:G:68:LEU:HD21	1.73	1.18
2:E:126:ARG:NH2	3:G:65:ILE:HG12	1.68	1.08
2:E:126:ARG:HE	3:G:68:LEU:HD22	1.02	1.08
2:E:126:ARG:HB3	3:G:68:LEU:CD2	1.87	1.04

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	y	435/437 (100%)	386 (89%)	27 (6%)	22 (5%)	2 30
2	E	54/56 (96%)	49 (91%)	3 (6%)	2 (4%)	4 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	G	63/65 (97%)	50 (79%)	7 (11%)	6 (10%)	1 15
4	T	98/100 (98%)	71 (72%)	18 (18%)	9 (9%)	1 17
5	U	101/103 (98%)	79 (78%)	13 (13%)	9 (9%)	1 17
6	Y	61/63 (97%)	48 (79%)	11 (18%)	2 (3%)	5 40
All	All	812/824 (98%)	683 (84%)	79 (10%)	50 (6%)	4 26

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	y	142	MET
1	y	258	TYR
1	y	266	PRO
1	y	338	ASN
1	y	340	ARG

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	y	353/353 (100%)	336 (95%)	17 (5%)	31 67
2	E	47/47 (100%)	45 (96%)	2 (4%)	35 70
3	G	46/46 (100%)	43 (94%)	3 (6%)	21 58
4	T	84/84 (100%)	80 (95%)	4 (5%)	31 67
5	U	84/84 (100%)	81 (96%)	3 (4%)	42 74
6	Y	55/55 (100%)	54 (98%)	1 (2%)	66 87
All	All	669/669 (100%)	639 (96%)	30 (4%)	38 69

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	y	349	SER
1	y	409	VAL

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Mol	Chain	Res	Type
5	U	23	LYS
1	y	397	VAL
2	E	76	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
4	T	59	ASN
6	Y	41	HIS
4	T	92	ASN
4	T	15	HIS
4	T	70	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	4	60/61 (98%)	2 (3%)	0
11	5	107/108 (99%)	37 (34%)	8 (7%)
7	1	62/63 (98%)	12 (19%)	0
8	2	35/36 (97%)	7 (20%)	2 (5%)
9	3	17/18 (94%)	5 (29%)	0
All	All	281/286 (98%)	63 (22%)	10 (3%)

5 of 63 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	1	63	A
7	1	64	A
7	1	71	A
7	1	74	A
7	1	75	G

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	5	2126	A
11	5	2144	G
11	5	2152	G
11	5	2120	G
11	5	2145	C

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.