



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:39 PM BST

PDB ID : 3DKN  
EMDB ID: : EMD-1528  
Title : Sec61 in the Canine ribosome-channel complex from the endoplasmic reticulum  
Authors : Menetret, J.-F.; Akey, C.  
Deposited on : 2008-06-25  
Resolution : 8.70 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](mailto: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

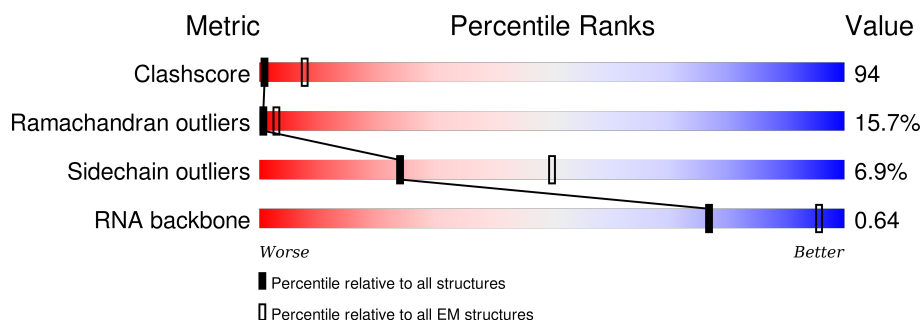
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.70 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  $\geq 3$ , 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	D	20	50% 45% 5%
2	E	17	71% 24% 6%
3	F	32	81% 19%
4	A	430	22% 59% 19% .
5	B	65	22% 63% 14% .
6	C	32	47% 50% .

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5554 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 RNA chain called RNA (5'-R(P\*CP\*GP\*UP\*GP\*CP\*CP\*AP\*AP\*GP\*CP\*UP\*GP\*CP\*GP\*AP\*UP\*AP\*AP\*GP\*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	20	Total	C	N	O	P	0	0
			428	191	79	138	20		

- Molecule 2 is a RNA chain called RNA (5'-R(P\*AP\*GP\*CP\*CP\*GP\*CP\*AP\*CP\*GP\*GP\*AP\*GP\*GP\*CP\*GP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	17	Total	C	N	O	P	0	0
			371	165	75	114	17		

- Molecule 3 is a RNA chain called RNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	32	Total	C	N	O	P	0	0
			683	304	120	227	32		

- Molecule 4 is a protein called Preprotein translocase subunit secY.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	430	Total	C	N	O	S	0	0
			3291	2199	518	555	19		

- Molecule 5 is a protein called Preprotein translocase subunit secE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	65	Total	C	N	O	S	0	0
			524	348	85	90	1		

- Molecule 6 is a protein called Preprotein translocase subunit secG.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	C	32	Total	C	N	O	0	0
			257	172	42	43		

### 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: RNA (5'-R(P\*CP\*GP\*UP\*GP\*CP\*CP\*AP\*AP\*GP\*CP\*UP\*GP\*CP\*GP\*AP\*UP\*AP\*AP\*GP\*C)-3')

Chain D: 




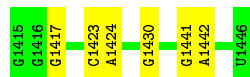
- Molecule 2: RNA (5'-R(P\*AP\*GP\*CP\*CP\*GP\*CP\*AP\*CP\*GP\*GP\*AP\*GP\*GP\*CP\*GP\*A P\*A)-3')

Chain E: 

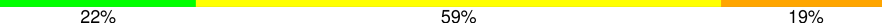


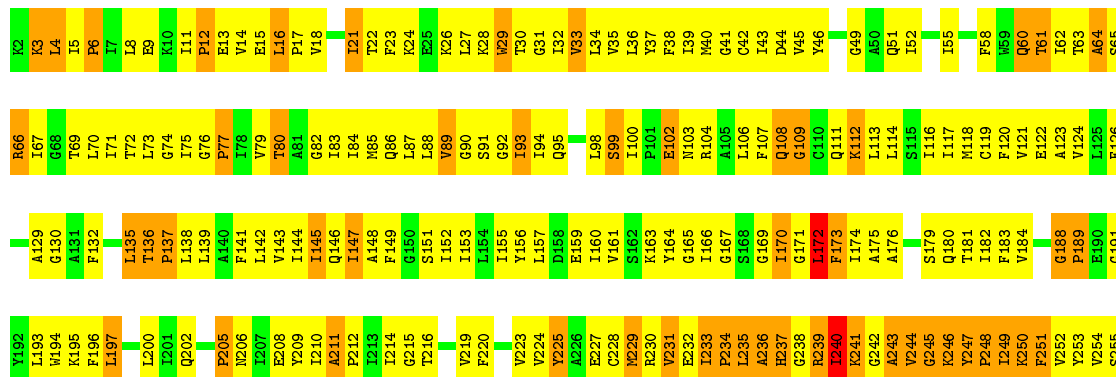
- Molecule 3: RNA (32-MER)

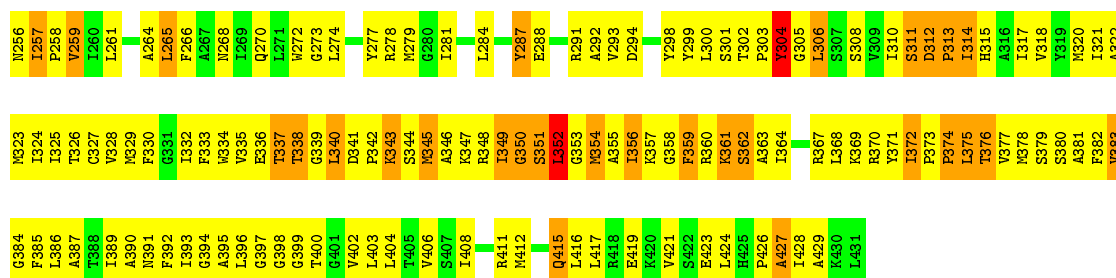
Chain F: 



- Molecule 4: Preprotein translocase subunit secY

Chain A: 





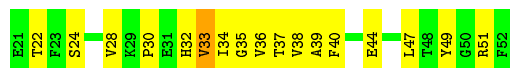
- Molecule 5: Preprotein translocase subunit secE

Chain B: 22% 63% 14% .



- Molecule 6: Preprotein translocase subunit secG

Chain C: 47% 50% .



## 4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	per micrograph	Depositor
Microscope	TF20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1500	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	50000	Depositor
Image detector	film; Kodak SO163	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	D	0.35	0/478	0.70	0/743
2	E	0.30	0/416	0.67	0/648
3	F	0.37	0/762	0.69	0/1186
4	A	0.38	0/3365	0.58	0/4570
5	B	0.33	0/533	0.52	0/719
6	C	0.38	0/262	0.55	0/354
All	All	0.37	0/5816	0.61	0/8220

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
3	F	0	2
4	A	15	0
All	All	15	2

There are no bond length outliers.

There are no bond angle outliers.

5 of 15 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	233	ILE	CB
4	A	234	PRO	CA
4	A	235	LEU	CA
4	A	236	ALA	CA
4	A	237	HIS	CA

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
3	F	1417	G	Sidechain
3	F	1430	G	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	D	428	0	218	14	0
2	E	371	0	188	9	0
3	F	683	0	345	4	0
4	A	3291	0	3504	898	0
5	B	524	0	567	172	0
6	C	257	0	272	30	0
All	All	5554	0	5094	1004	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 94.

The worst 5 of 1004 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)
5:B:22:TRP:CZ3	5:B:23:LEU:HD23	1.41	1.54
4:A:188:GLY:HA2	5:B:52:TYR:CZ	1.55	1.40
4:A:335:VAL:C	4:A:337:THR:HA	1.38	1.40
5:B:35:ALA:HA	5:B:38:LYS:CE	1.52	1.39
4:A:375:LEU:CD1	4:A:379:SER:HB2	1.48	1.39

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	
4	A	428/430 (100%)	244 (57%)	111 (26%)	73 (17%)	0	4
5	B	63/65 (97%)	37 (59%)	17 (27%)	9 (14%)	0	6
6	C	30/32 (94%)	19 (63%)	11 (37%)	0	100	100
All	All	521/527 (99%)	300 (58%)	139 (27%)	82 (16%)	1	5

5 of 82 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	61	THR
4	A	66	ARG
4	A	99	SER
4	A	234	PRO
4	A	236	ALA

### 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	
4	A	349/349 (100%)	323 (93%)	26 (7%)	17	54
5	B	57/57 (100%)	55 (96%)	2 (4%)	43	74
6	C	28/28 (100%)	26 (93%)	2 (7%)	18	55
All	All	434/434 (100%)	404 (93%)	30 (7%)	24	56

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

Mol	Chain	Res	Type
4	A	202	GLN
4	A	239	ARG
5	B	20	ARG
4	A	225	TYR
4	A	240	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
4	A	180	GLN
5	B	6	GLN
4	A	391	ASN
4	A	111	GLN
4	A	268	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	D	19/20 (95%)	5 (26%)	1 (5%)
2	E	16/17 (94%)	2 (12%)	0
3	F	31/32 (96%)	0	0
All	All	66/69 (95%)	7 (10%)	1 (1%)

5 of 7 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	D	60	A
1	D	67	A
1	D	69	A
1	D	70	A
1	D	71	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	D	69	A

## 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 [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.