



wwPDB/EMDatabank EM Map/Model Validation Summary Report

Aug 21, 2017 – 08:21 AM EDT

PDB ID : 4UE5
EMDB ID: : EMD-2844
Title : Structural basis for targeting and elongation arrest of Bacillus signal recognition particle
Authors : Beckert, B.; Kedrov, A.; Sohmen, D.; Kempf, G.; Wild, K.; Sinning, I.; Stahlberg, H.; Wilson, D.N.; Beckmann, R.
Deposited on : unknown
Resolution : 9.00 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
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the  symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

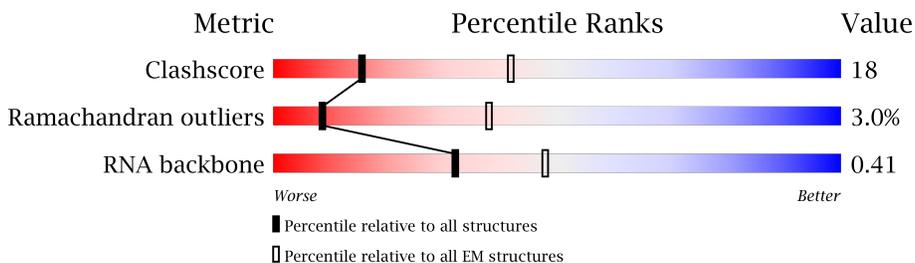
1 Overall quality at a glance

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	125131	1336
Ramachandran outliers	121729	1120
RNA backbone	3398	335

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	299	 45% 37% 15%
2	B	75	 87% 12%
3	C	195	 88% 8%
4	D	433	 70% 28%
5	E	74	 81% 18%
6	F	107	 81% 19%
7	S	18	 100%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9948 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 7S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	299	6403	2852	1167	2086	298	0	0

- Molecule 2 is a protein called SRP14.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	75	300	150	75	75	0	0

- Molecule 3 is a protein called SIGNAL RECOGNITION PARTICLE SUBUNIT SRP68.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	179	716	358	179	179	0	0

- Molecule 4 is a protein called SIGNAL RECOGNITION PARTICLE 54 KDA PROTEIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	433	1732	866	433	433	0	0

- Molecule 5 is a protein called SRP9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	74	296	148	74	74	0	0

- Molecule 6 is a protein called SIGNAL RECOGNITION PARTICLE 9 KDA PROTEIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	F	107	429	214	107	108	0	0

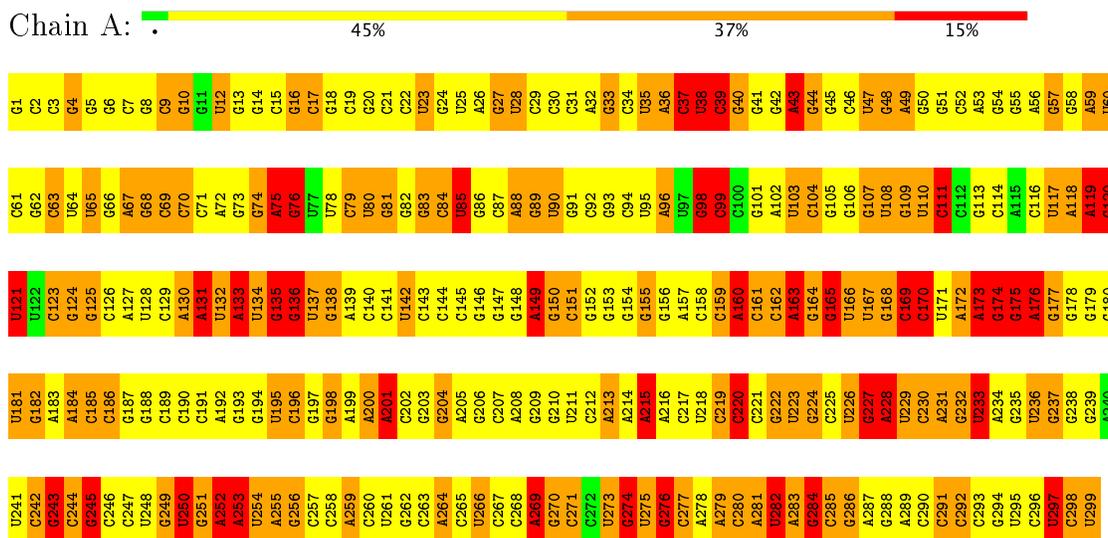
- Molecule 7 is a protein called SIGNAL SEQUENCE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	S	18	72	36	18	18	0	0

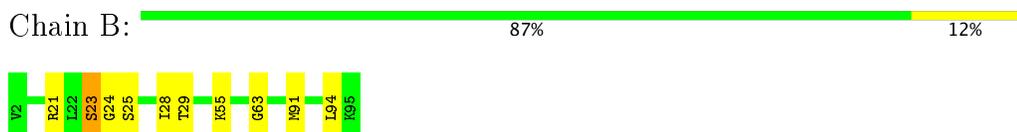
3 Residue-property plots

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

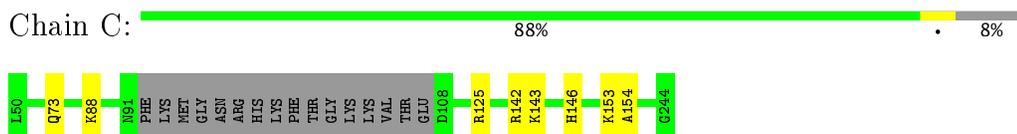
- Molecule 1: 7S RNA



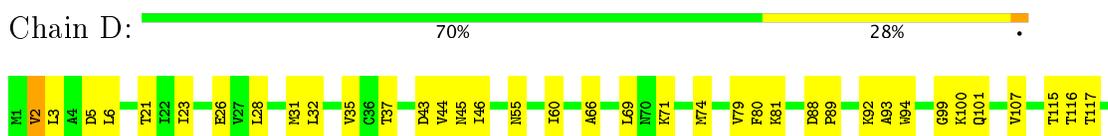
- Molecule 2: SRP14

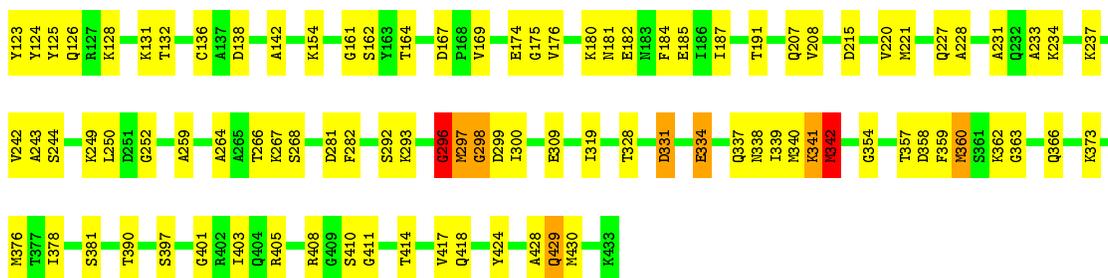


- Molecule 3: SIGNAL RECOGNITION PARTICLE SUBUNIT SRP68



- Molecule 4: SIGNAL RECOGNITION PARTICLE 54 KDA PROTEIN





- Molecule 5: SRP9

Chain E: 81% 18%



- Molecule 6: SIGNAL RECOGNITION PARTICLE 9 KDA PROTEIN

Chain F: 81% 19%



- Molecule 7: SIGNAL SEQUENCE

Chain S: 100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	19096	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	MICROGRAPH	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	Depositor
Image detector	TVIPS TEMCAM-F816 (8k x 8k)	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	1.55	31/7161 (0.4%)	2.59	812/11171 (7.3%)
2	B	0.40	0/298	0.74	0/369
3	C	0.25	0/714	0.48	0/889
4	D	0.73	0/1731	0.94	0/2162
5	E	0.37	0/295	0.73	0/367
6	F	0.40	0/428	0.68	0/532
7	S	0.44	0/71	0.72	0/87
All	All	1.31	31/10698 (0.3%)	2.23	812/15577 (5.2%)

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	38
2	B	4	0
3	C	4	0
4	D	0	108
5	E	4	0
All	All	12	146

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	C	O3'-P	-8.07	1.51	1.61
1	A	229	U	O3'-P	-7.93	1.51	1.61
1	A	198	G	C2-N3	7.58	1.38	1.32
1	A	131	A	C6-N6	6.36	1.39	1.33
1	A	201	A	N7-C5	-6.30	1.35	1.39

The worst 5 of 812 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	G	O5'-P-OP2	-25.39	80.23	110.70
1	A	59	A	C4'-C3'-O3'	20.59	154.17	113.00
1	A	59	A	P-O3'-C3'	-18.37	97.66	119.70
1	A	201	A	N1-C6-N6	17.49	129.09	118.60
1	A	47	U	P-O3'-C3'	17.26	140.41	119.70

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	21	ARG	CA
2	B	23	SER	CA
2	B	26	VAL	CA
2	B	27	PHE	CA
3	C	143	LYS	CA

5 of 146 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39	C	Sidechain
1	A	43	A	Sidechain
1	A	75	A	Sidechain
1	A	83	G	Sidechain
1	A	85	U	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	6403	0	3239	206	0
2	B	300	0	74	22	0
3	C	716	0	184	27	0
4	D	1732	0	488	27	0
5	E	296	0	71	26	0
6	F	429	0	109	11	0
7	S	72	0	18	0	0
All	All	9948	0	4183	255	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 18.

The worst 5 of 255 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:B:94:LEU:CA	5:E:55:GLN:CA	1.96	1.43
2:B:94:LEU:N	5:E:56:ALA:H	1.26	1.31
2:B:94:LEU:H	5:E:56:ALA:N	1.30	1.28
1:A:196:C:H4'	6:F:69:SER:CA	1.65	1.26
2:B:94:LEU:CA	5:E:56:ALA:H	1.49	1.25

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	B	71/75 (95%)	61 (86%)	9 (13%)	1 (1%)	13	54
3	C	175/195 (90%)	168 (96%)	7 (4%)	0	100	100
4	D	431/433 (100%)	360 (84%)	55 (13%)	16 (4%)	4	33
5	E	72/74 (97%)	61 (85%)	9 (12%)	2 (3%)	6	39
6	F	105/107 (98%)	87 (83%)	11 (10%)	7 (7%)	1	21
7	S	16/18 (89%)	14 (88%)	2 (12%)	0	100	100
All	All	870/902 (96%)	751 (86%)	93 (11%)	26 (3%)	9	37

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	342	MET
6	F	42	GLU
6	F	75	ASP
4	D	296	GLY
4	D	297	MET

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](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	298/299 (99%)	69 (23%)	10 (3%)

5 of 69 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	G
1	A	10	G
1	A	27	G
1	A	28	U
1	A	33	G

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	110	U
1	A	172	A
1	A	185	C
1	A	98	G
1	A	176	A

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	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	34:ASP	C	54:ASN	N	9.50