



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:56 PM BST

PDB ID : 3ZN8
EMDB ID: : EMD-2316
Title : Structural Basis of Signal Sequence Surveillance and Selection by the SRP-SR Complex
Authors : von Loeffelholz, O.; Knoop, K.; Ariosa, A.; Zhang, X.; Karuppasamy, M.; Huard, K.; Schoehn, G.; Berger, I.; Shan, S.O.; Schaffitzel, C.
Deposited on : 2013-02-13
Resolution : 12.00 Å (reported)
Based on PDB ID : 1FFH,1FTS,3KL4,2XXA

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

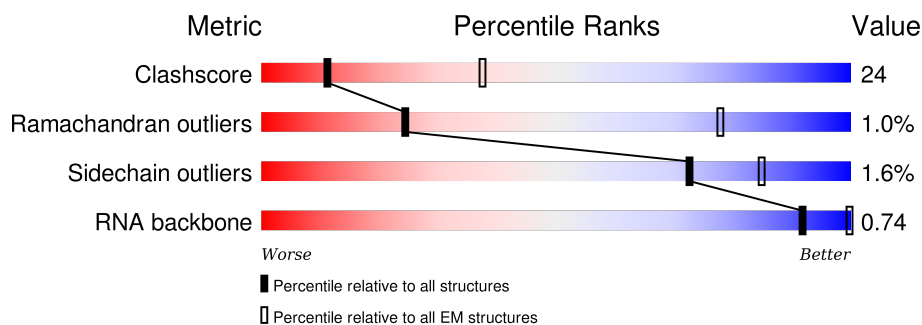
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 12.00 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
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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	294	60% 37% .
2	D	295	55% 44% .
3	G	88	42% 55% .
4	M	125	33% 47% . . 15%
5	S	14	64% 29% 7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7453 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 SIGNAL RECOGNITION PARTICLE PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	288	Total	C	N	O	S	0	1
			2215	1391	406	413	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	THR	ALA	CONFLICT	UNP O07347

- Molecule 2 is a protein called SIGNAL RECOGNITION PARTICLE RECEPTOR FTSY.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	295	Total	C	N	O	S	0	0
			2261	1430	394	431	6		

- Molecule 3 is a RNA chain called 4.5 S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	88	Total	C	N	O	P	0	0
			1886	840	346	613	87		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	106	Total	C	N	O	S	0	0
			861	547	153	155	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	307	LEU	-	EXPRESSION TAG	UNP Q97ZE7

- Molecule 5 is a protein called DIPEPTIDYL AMINOPEPTIDASE B.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	S	14	Total	C	N	O	0	0
			108	77	15	16		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Mg	0
			1	1	

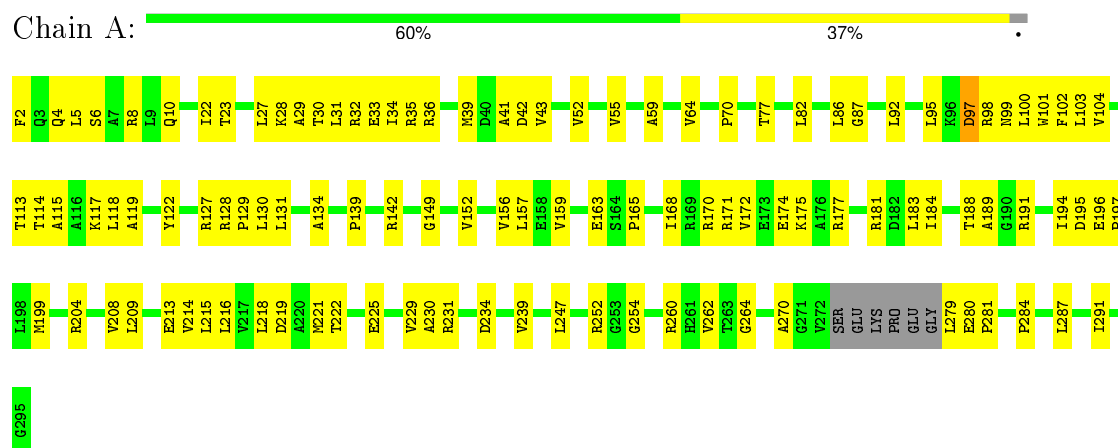
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	121	Total	O	0
			121	121	

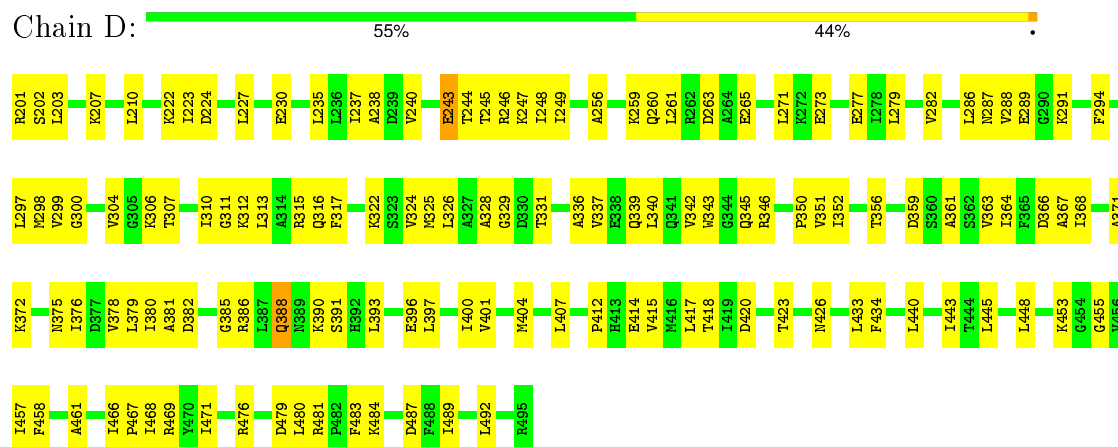
3 Residue-property plots

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.

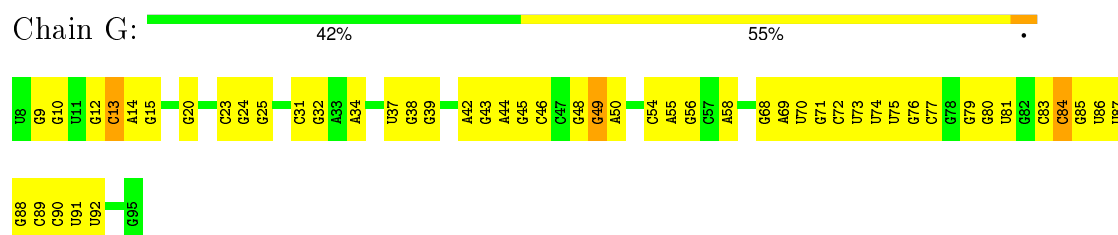
• Molecule 1: SIGNAL RECOGNITION PARTICLE PROTEIN



• Molecule 2: SIGNAL RECOGNITION PARTICLE RECEPTOR FTSY



• Molecule 3: 4.5 S RNA



Chain M: 33% 47% •• 15%



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	MICROGRAPH	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	5700	Depositor
Magnification	59000	Depositor
Image detector	GATAN 4K X 4K CCD	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.23	0/2238	0.39	0/3013
2	D	0.24	0/2287	0.40	0/3078
3	G	0.13	0/2109	0.63	0/3290
4	M	0.23	0/872	0.42	0/1170
5	S	0.34	0/109	0.49	0/148
All	All	0.21	0/7615	0.48	0/10699

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	2215	0	2313	91	0
2	D	2261	0	2333	121	0
3	G	1886	0	956	40	0
4	M	861	0	907	88	0
5	S	108	0	128	7	0
6	A	1	0	0	0	0
7	A	121	0	0	0	0
All	All	7453	0	6637	329	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 24.

The worst 5 of 329 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)
3:G:45:G:H1	3:G:54:C:H42	1.09	0.94
2:D:388:GLN:H	2:D:388:GLN:NE2	1.68	0.92
1:A:28:LYS:HB3	1:A:32:ARG:HH12	1.38	0.88
1:A:189:ALA:HB1	1:A:191:ARG:HH12	1.41	0.84
4:M:343:GLY:HA3	4:M:344:PRO:C	1.99	0.83

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	284/294 (97%)	264 (93%)	18 (6%)	2 (1%)	26	71
2	D	293/295 (99%)	256 (87%)	36 (12%)	1 (0%)	46	83
4	M	103/125 (82%)	78 (76%)	21 (20%)	4 (4%)	4	36
5	S	12/14 (86%)	10 (83%)	2 (17%)	0	100	100
All	All	692/728 (95%)	608 (88%)	77 (11%)	7 (1%)	24	65

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	M	344	PRO
1	A	262	VAL
4	M	342	MET
1	A	97	ASP
4	M	345	LEU

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	A	227/233 (97%)	227 (100%)	0	100	100
2	D	238/238 (100%)	235 (99%)	3 (1%)	76	89
4	M	95/112 (85%)	90 (95%)	5 (5%)	28	64
5	S	12/12 (100%)	11 (92%)	1 (8%)	14	49
All	All	572/595 (96%)	563 (98%)	9 (2%)	72	88

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	M	337	ILE
5	S	457	TRP
4	M	345	LEU
2	D	388	GLN
4	M	344	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	316	GLN
2	D	319	GLN
2	D	388	GLN
2	D	251	ASN
2	D	355	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	G	87/88 (98%)	8 (9%)	0

5 of 8 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	G	13	C
3	G	37	U
3	G	49	G
3	G	72	C
3	G	73	U

There are no RNA pucker outliers to report.

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.