



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:33 am GMT

PDB ID : 3J5S
EMDB ID: : EMD-5784
Title : EttA binds to ribosome exit site and regulates translation by restricting ribosome and tRNA dynamics
Authors : Hashem, Y.
Deposited on : 2013-11-15
Resolution : 7.50 Å(reported)
Based on PDB ID : 3R8O, 3R8T, 2WDG, 4FIN

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) : recalc29047

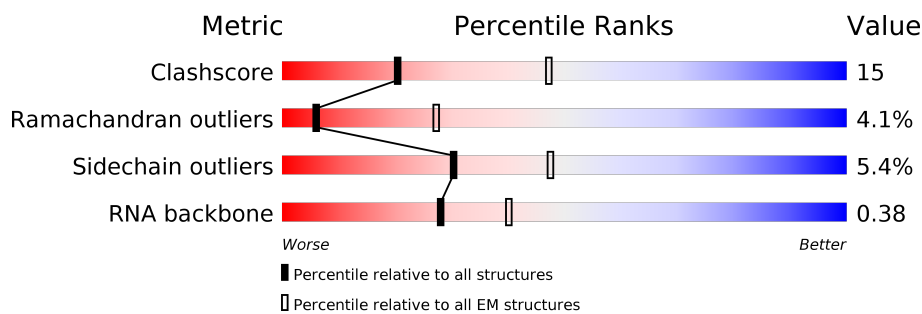
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.50 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
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	B	101	12% 14% 6% 68%
2	A	360	16% 19% 13% 52%
3	E	77	40% 43% 17%
4	D	561	65% 25% 8% .
5	F	234	64% 29% 6% .
6	G	178	71% 22% 7%
7	H	50	74% 18% 8%
8	I	151	61% 30% 7% .

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15196 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	32	Total	C	N	O	P	0	0
			687	306	126	223	32		

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	174	Total	C	N	O	P	0	0
			3731	1663	674	1220	174		

- Molecule 3 is a RNA chain called P-site tRNA FMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 4 is a protein called Energy-dependent translational throttle A (EttA).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	554	Total	C	N	O	S	0	0
			4393	2764	781	837	11		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	EXPRESSION TAG	UNP P0A9W3
D	-4	HIS	-	EXPRESSION TAG	UNP P0A9W3
D	-3	HIS	-	EXPRESSION TAG	UNP P0A9W3
D	-2	HIS	-	EXPRESSION TAG	UNP P0A9W3
D	-1	HIS	-	EXPRESSION TAG	UNP P0A9W3
D	0	HIS	-	EXPRESSION TAG	UNP P0A9W3

- Molecule 5 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 7 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 8 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

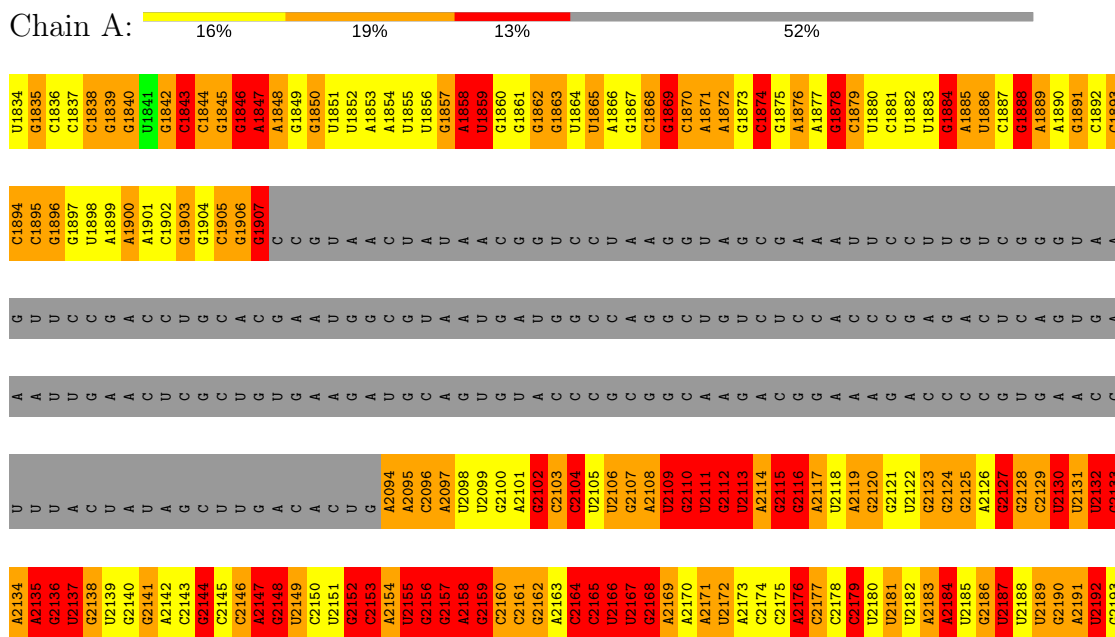
3 Residue-property plots

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.

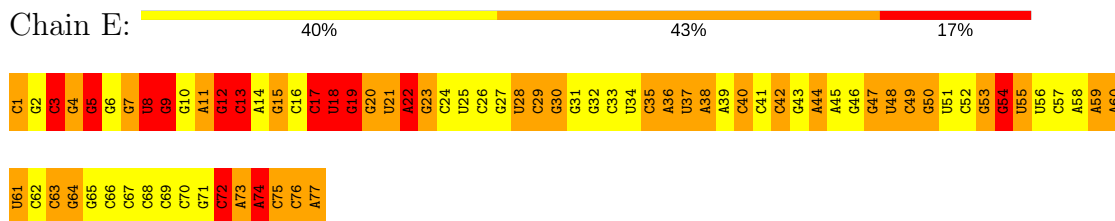
• Molecule 1: 16S ribosomal RNA



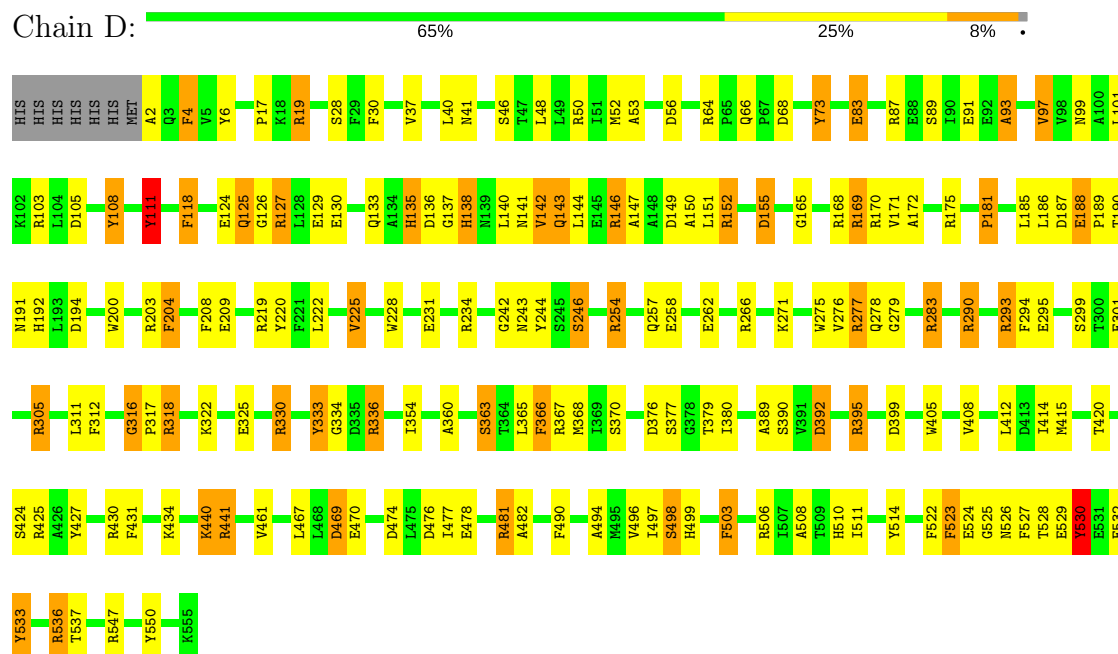
• Molecule 2: 23S ribosomal RNA



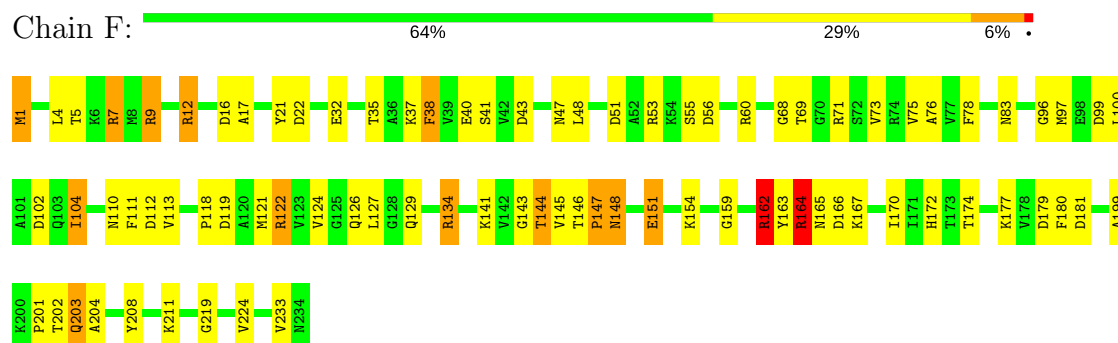
• Molecule 3: P-site tRNA FMet



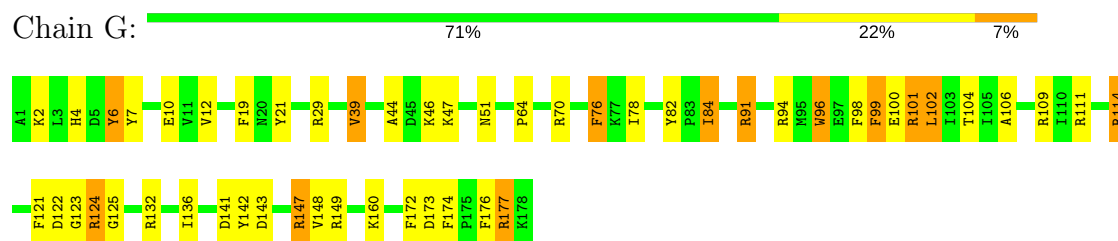
• Molecule 4: Energy-dependent translational throttle A (EttA)



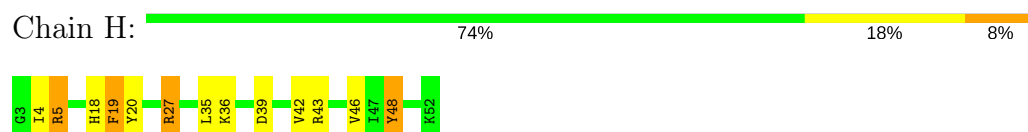
• Molecule 5: 50S ribosomal protein L1



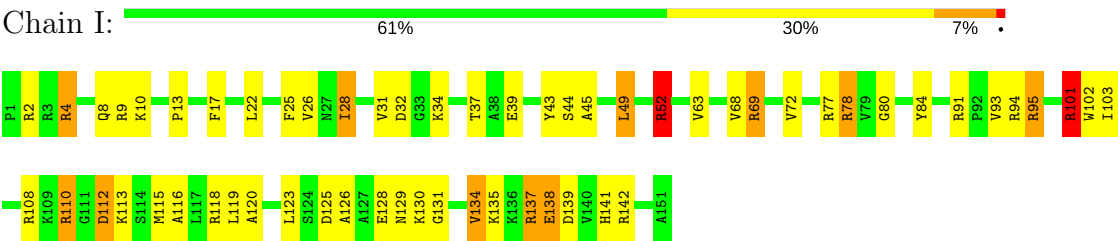
• Molecule 6: 50S ribosomal protein L5



• Molecule 7: 50S ribosomal protein L33



● Molecule 8: 30S ribosomal protein S7



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	39316	Depositor
Resolution determination method	gold standard FSC 0.143	Depositor
CTF correction method	Each micrograph	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	17	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	110637	Depositor
Image detector	GATAN UltraScan 4000 (4k x 4k)	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	B	3.33	96/766 (12.5%)	3.35	147/1188 (12.4%)
2	A	3.17	486/4174 (11.6%)	3.15	702/6507 (10.8%)
3	E	3.23	213/1832 (11.6%)	3.28	351/2855 (12.3%)
4	D	1.58	22/4474 (0.5%)	2.04	130/6034 (2.2%)
5	F	1.52	5/1748 (0.3%)	1.97	49/2355 (2.1%)
6	G	1.65	8/1444 (0.6%)	2.08	40/1937 (2.1%)
7	H	1.63	2/417 (0.5%)	2.02	11/554 (2.0%)
8	I	1.61	6/1196 (0.5%)	2.31	50/1602 (3.1%)
All	All	2.41	838/16051 (5.2%)	2.65	1480/23032 (6.4%)

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	B	0	12
2	A	0	84
3	E	0	34
4	D	0	23
5	F	0	9
6	G	0	6
7	H	0	4
8	I	0	6
All	All	0	178

The worst 5 of 838 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	36	A	N9-C4	-18.05	1.27	1.37
1	B	1297	G	N9-C8	15.82	1.49	1.37
2	A	1879	C	N1-C6	14.46	1.45	1.37
1	B	1242	G	C8-N7	-13.58	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1236	A	C5-C4	13.00	1.47	1.38

The worst 5 of 1480 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	91	ARG	NE-CZ-NH2	-25.82	107.39	120.30
4	D	430	ARG	NE-CZ-NH1	23.11	131.85	120.30
1	B	1236	A	N1-C6-N6	19.82	130.49	118.60
1	B	1334	G	C5-C6-O6	-18.89	117.27	128.60
1	B	1334	G	N1-C6-O6	17.55	130.43	119.90

There are no chirality outliers.

5 of 178 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1239	A	Sidechain
1	B	1242	G	Sidechain
1	B	1243	C	Sidechain
1	B	1290	G	Sidechain
1	B	1295	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	B	687	0	342	24	0
2	A	3731	0	1828	67	0
3	E	1640	0	827	29	0
4	D	4393	0	4377	333	0
5	F	1733	0	1824	152	0
6	G	1420	0	1460	10	0
7	H	410	0	440	1	0
8	I	1182	0	1240	124	0
All	All	15196	0	12338	421	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 15.

The worst 5 of 421 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)
1:B:1240:U:C4	8:I:31:VAL:HG12	1.20	1.68
4:D:108:TYR:HA	5:F:118:PRO:CB	1.17	1.59
4:D:108:TYR:CA	5:F:118:PRO:HB2	1.27	1.57
4:D:108:TYR:CE2	5:F:121:MET:HB3	1.34	1.57
4:D:523:PHE:CD1	8:I:130:LYS:HB2	1.37	1.57

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	
4	D	552/561 (98%)	508 (92%)	27 (5%)	17 (3%)	5	36
5	F	232/234 (99%)	199 (86%)	23 (10%)	10 (4%)	3	29
6	G	176/178 (99%)	138 (78%)	26 (15%)	12 (7%)	1	20
7	H	48/50 (96%)	38 (79%)	9 (19%)	1 (2%)	8	45
8	I	149/151 (99%)	119 (80%)	23 (15%)	7 (5%)	3	28
All	All	1157/1174 (99%)	1002 (87%)	108 (9%)	47 (4%)	6	30

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	83	GLU
4	D	91	GLU
4	D	143	GLN
4	D	317	PRO
6	G	102	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	
4	D	465/472 (98%)	436 (94%)	29 (6%)	21	54
5	F	181/181 (100%)	170 (94%)	11 (6%)	22	55
6	G	149/149 (100%)	143 (96%)	6 (4%)	36	65
7	H	45/45 (100%)	44 (98%)	1 (2%)	57	79
8	I	124/124 (100%)	119 (96%)	5 (4%)	36	65
All	All	964/971 (99%)	912 (95%)	52 (5%)	30	58

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	474	ASP
5	F	1	MET
8	I	39	GLU
4	D	477	ILE
4	D	498	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	278	GLN
5	F	126	GLN
5	F	172	HIS
4	D	257	GLN
5	F	129	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	29/101 (28%)	12 (41%)	0
2	A	172/360 (47%)	53 (30%)	0
3	E	76/77 (98%)	19 (25%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	277/538 (51%)	84 (30%)	0

5 of 84 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	1238	A
1	B	1240	U
1	B	1243	C
1	B	1292	G
1	B	1293	C

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](#)

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.