



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:47 PM BST

PDB ID : 3J5Y
EMDB ID: : EMD-5801
Title : Structure of the mammalian ribosomal pre-termination complex associated with eRF1-eRF3-GDPNP
Authors : des Georges, A.; Hashem, Y.; Unbehaun, A.; Grassucci, R.A.; Taylor, D.; Hellen, C.U.T.; Pestova, T.V.; Frank, J.
Deposited on : 2013-11-21
Resolution : 9.70 Å(reported)
Based on PDB ID : 2KTU, 1R5O, 3E1Y, 1R5B, 3VMF

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

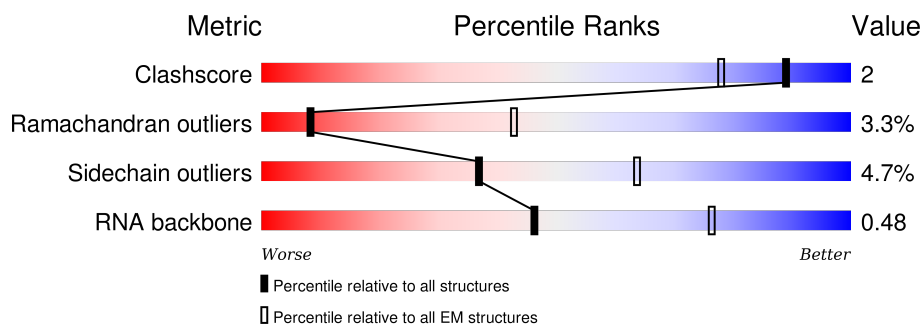
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.70 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 ≥ 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	414	70% 25% 5%
2	B	428	70% 25% .
3	C	10	60% 40%
4	D	88	38% 34% 28%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8724 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 Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	414	Total	C	N	O	S	0	0
			3269	2080	557	621	11		

- Molecule 2 is a protein called Eukaryotic peptide chain release factor GTP-binding subunit ERF3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	428	Total	C	N	O	S	0	0
			3367	2144	578	624	21		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	369	ILE	ASN	CONFLICT	UNP P15170
B	389	SER	ASN	CONFLICT	UNP P15170
B	407	ILE	LEU	CONFLICT	UNP P15170
B	418	THR	ILE	CONFLICT	UNP P15170
B	436	ILE	VAL	CONFLICT	UNP P15170

- Molecule 3 is a RNA chain called 5'-R(*AP*UP*UP*GP*UP*AP*AP*AP*AP*A)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	10	Total	C	N	O	P	0	0
			212	97	41	65	9		

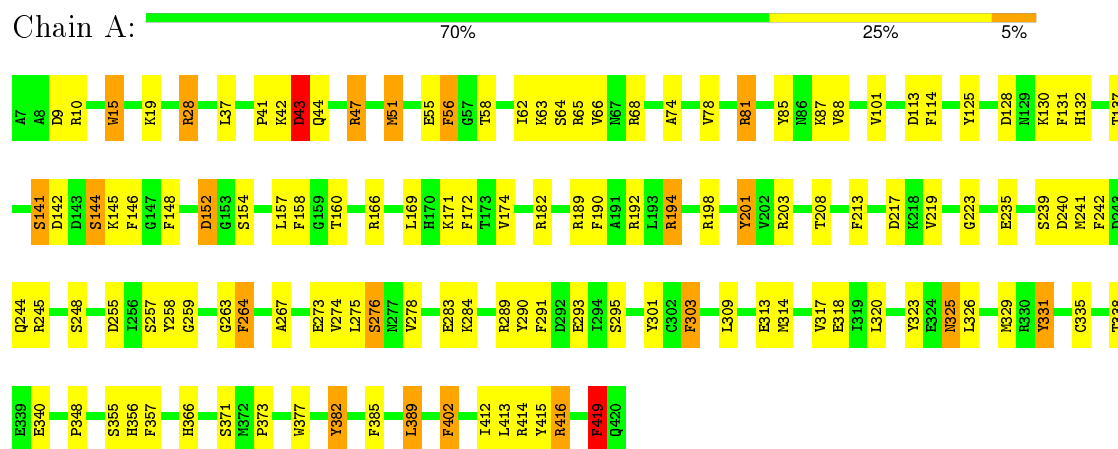
- Molecule 4 is a RNA chain called tRNA-Leu.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	88	Total	C	N	O	P	0	0
			1876	836	339	614	87		

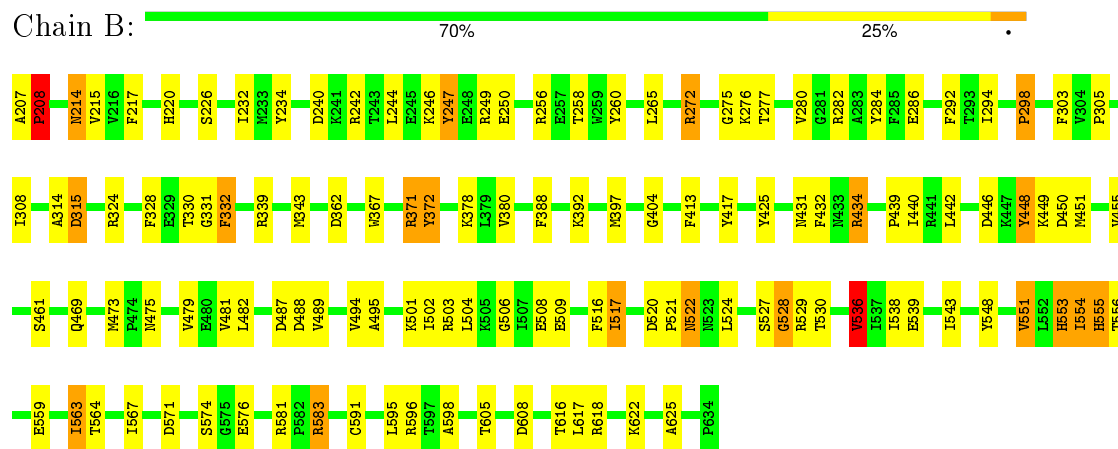
3 Residue-property plots

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: Eukaryotic peptide chain release factor subunit 1



- Molecule 2: Eukaryotic peptide chain release factor GTP-binding subunit ERF3A



- Molecule 3: 5'-R(*AP*UP*UP*GP*UP*AP*AP*AP*AP*A)-3'



- Molecule 4: tRNA-Leu

Chain D:



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	48973	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each Particle	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	TVIPS TEMCAM-F415 (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	A	1.62	28/3322 (0.8%)	2.00	87/4466 (1.9%)
2	B	1.57	14/3434 (0.4%)	1.98	91/4630 (2.0%)
3	C	3.46	38/238 (16.0%)	3.23	39/369 (10.6%)
4	D	3.24	252/2095 (12.0%)	3.32	394/3266 (12.1%)
All	All	2.15	332/9089 (3.7%)	2.44	611/12731 (4.8%)

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	17
2	B	0	23
3	C	0	7
4	D	0	42
All	All	0	89

The worst 5 of 332 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	14	A	P-O5'	-13.49	1.46	1.59
4	D	77	G	N3-C4	-12.40	1.26	1.35
4	D	17	C	N1-C6	12.07	1.44	1.37
4	D	6	G	C6-N1	11.74	1.47	1.39
4	D	22	C	P-O5'	-11.66	1.48	1.59

The worst 5 of 611 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	91	U	P-O3'-C3'	20.04	143.75	119.70
4	D	23	A	P-O3'-C3'	19.36	142.93	119.70
1	A	203	ARG	NE-CZ-NH2	-17.01	111.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	13	G	N1-C6-O6	16.61	129.87	119.90
4	D	80	C	N3-C4-C5	-15.23	115.81	121.90

There are no chirality outliers.

5 of 89 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	HIS	Sidechain
1	A	141	SER	Peptide
1	A	142	ASP	Peptide
1	A	28	ARG	Sidechain
1	A	81	ARG	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	3269	0	3314	10	0
2	B	3367	0	3424	11	0
3	C	212	0	106	8	0
4	D	1876	0	938	15	0
All	All	8724	0	7782	37	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 2.

The worst 5 of 37 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:C:91:U:N3	4:D:39:A:N1	2.19	0.90
3:C:92:U:C2	4:D:38:A:C2	2.81	0.69
4:D:39:A:H3'	4:D:40:G:C8	2.30	0.67
2:B:308:ILE:HG21	2:B:553:HIS:CE1	2.34	0.63
2:B:617:LEU:HD23	2:B:625:ALA:HB3	1.84	0.57

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	
1	A	412/414 (100%)	365 (89%)	34 (8%)	13 (3%)	5	41
2	B	426/428 (100%)	374 (88%)	37 (9%)	15 (4%)	4	39
All	All	838/842 (100%)	739 (88%)	71 (8%)	28 (3%)	8	40

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ARG
1	A	145	LYS
1	A	326	LEU
2	B	298	PRO
2	B	315	ASP

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	
1	A	357/357 (100%)	342 (96%)	15 (4%)	36	70
2	B	372/372 (100%)	353 (95%)	19 (5%)	29	66
All	All	729/729 (100%)	695 (95%)	34 (5%)	37	68

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	214	ASN

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Mol	Chain	Res	Type
2	B	305	PRO
2	B	551	VAL
2	B	276	LYS
1	A	201	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	214	ASN
2	B	540	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	9/10 (90%)	6 (66%)	1 (11%)
4	D	87/88 (98%)	23 (26%)	6 (6%)
All	All	96/98 (97%)	29 (30%)	7 (7%)

5 of 29 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	91	U
3	C	92	U
3	C	94	U
3	C	96	A
3	C	97	A

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	D	23	A
4	D	72	U
4	D	60	C
4	D	9	U
4	D	70	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 [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.