



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 15, 2018 – 11:54 pm GMT

PDB ID : 5A8L  
EMDB ID: : EMD-3099  
Title : Human eRF1 and the hCMV nascent peptide in the translation termination complex  
Authors : Matheisl, S.; Berninghausen, O.; Becker, T.; Beckmann, R.  
Deposited on : 2015-07-16  
Resolution : 3.80 Å(reported)  
Based on PDB ID : 3E1Y

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

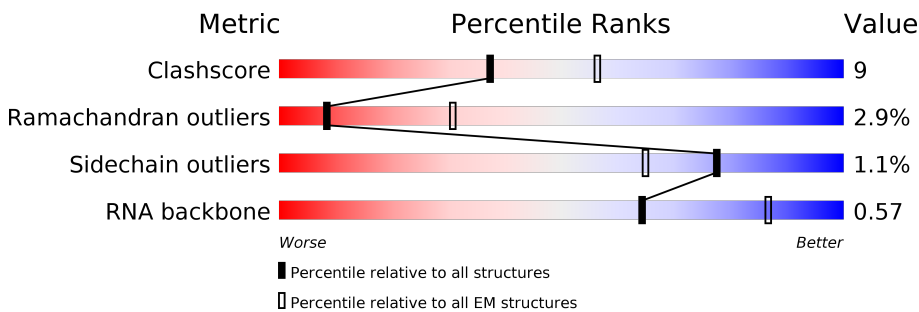
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MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

**i**

ELECTRON MICROSCOPY

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	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531
RNA backbone	3744	458

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	A	5025	95%
2	B	1869	96%
3	D	184	9%      89%
4	G	165	62%      21%      16%
5	H	427	97%
6	P	18	72%      22%      6%
7	Q	431	73%      26%
8	R	9	56%      33%      11%

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Mol	Chain	Length	Quality of chain
9	Z	22	 A horizontal bar chart showing the quality of chain 9. The bar is divided into three segments: green (14%), yellow (55%), and orange (32%).

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12264 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 28S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	253	Total	C	N	O	P	0	0
			5401	2413	971	1764	253		

- Molecule 2 is a RNA chain called HUMAN 18S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	67	Total	C	N	O	P	0	0
			1423	636	252	468	67		

- Molecule 3 is a protein called 60S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	21	Total	C	N	O	S	0	0
			179	110	40	27	2		

- Molecule 4 is a protein called 60S RIBOSOMAL PROTEIN L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	138	Total	C	N	O	S	0	0
			1046	654	196	193	3		

- Molecule 5 is a protein called 60S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	H	12	Total	C	N	O	0	0
			88	49	24	15		

- Molecule 6 is a RNA chain called P-SITE TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	18	Total	C	N	O	P	0	0
			382	172	71	122	17		

- Molecule 7 is a protein called EUKARYOTIC RELEASE FACTOR ERF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	431	Total	C	N	O	S	0	0
			3410	2168	575	655	12		

- Molecule 8 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	R	9	Total	C	N	O	P	0	0
			190	86	35	60	9		

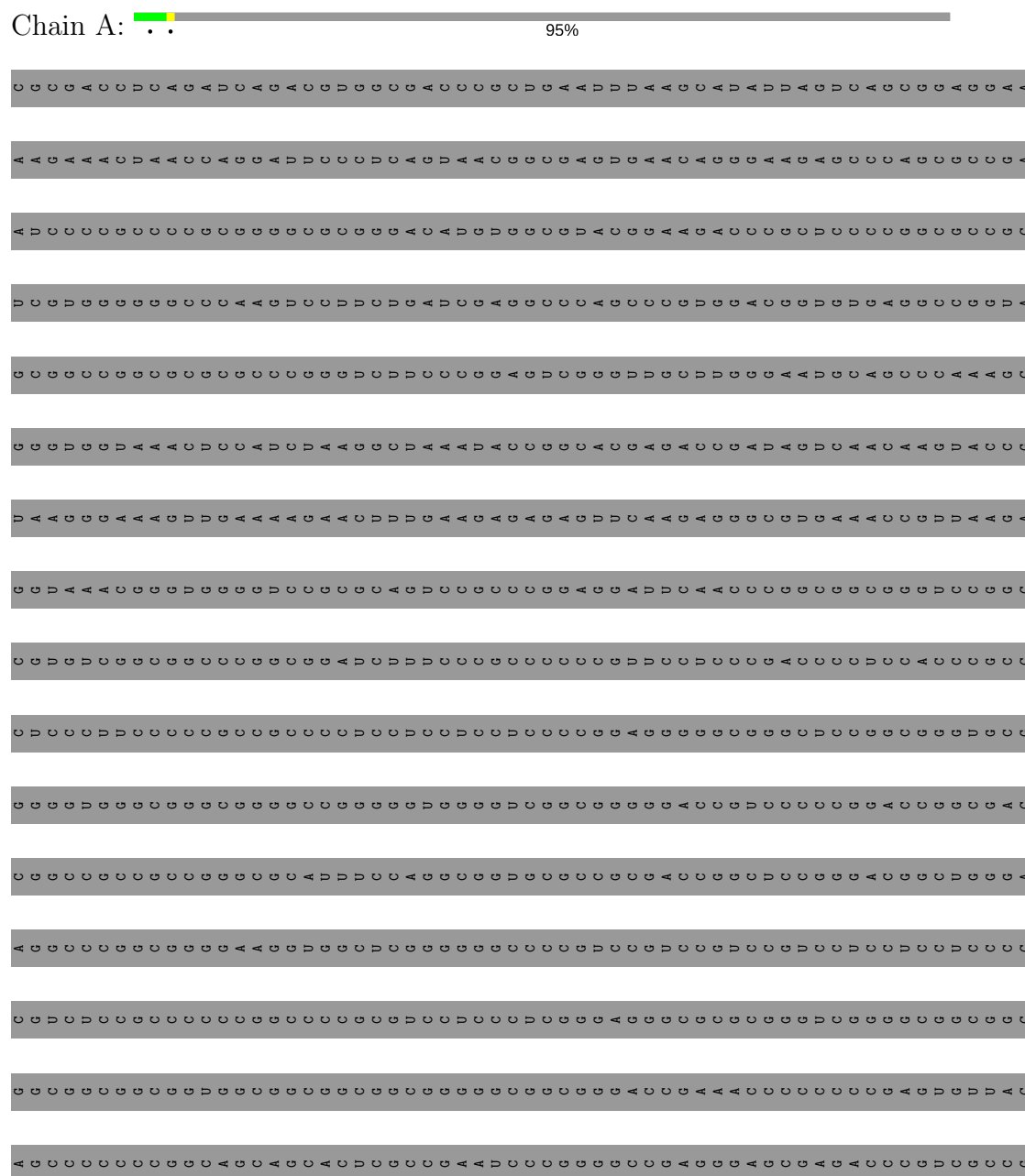
- Molecule 9 is a protein called NASCENT CHAIN.

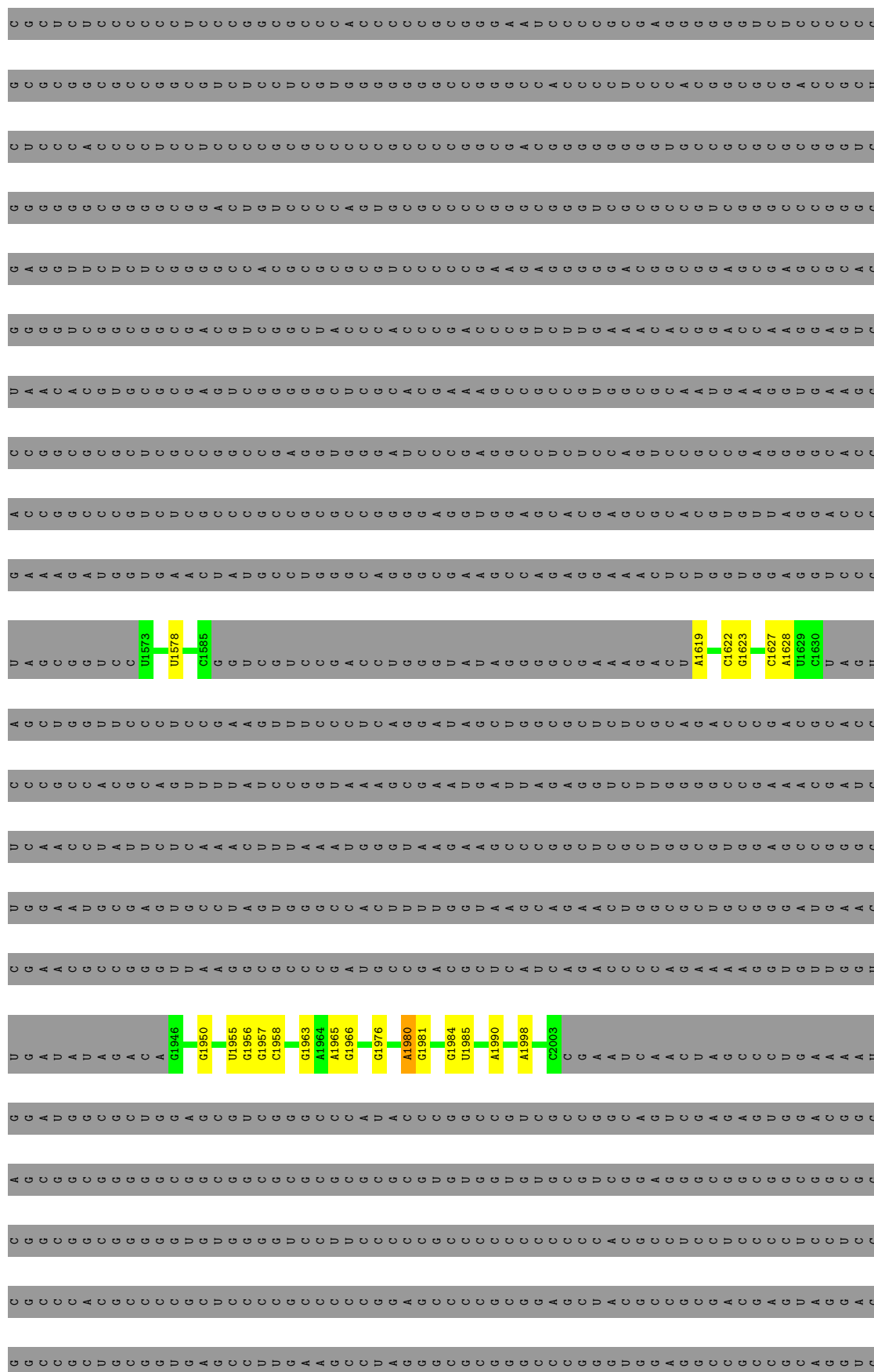
Mol	Chain	Residues	Atoms					AltConf	Trace
9	Z	22	Total	C	N	O	S	0	0
			145	92	25	27	1		

### 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: 28S RIBOSOMAL RNA





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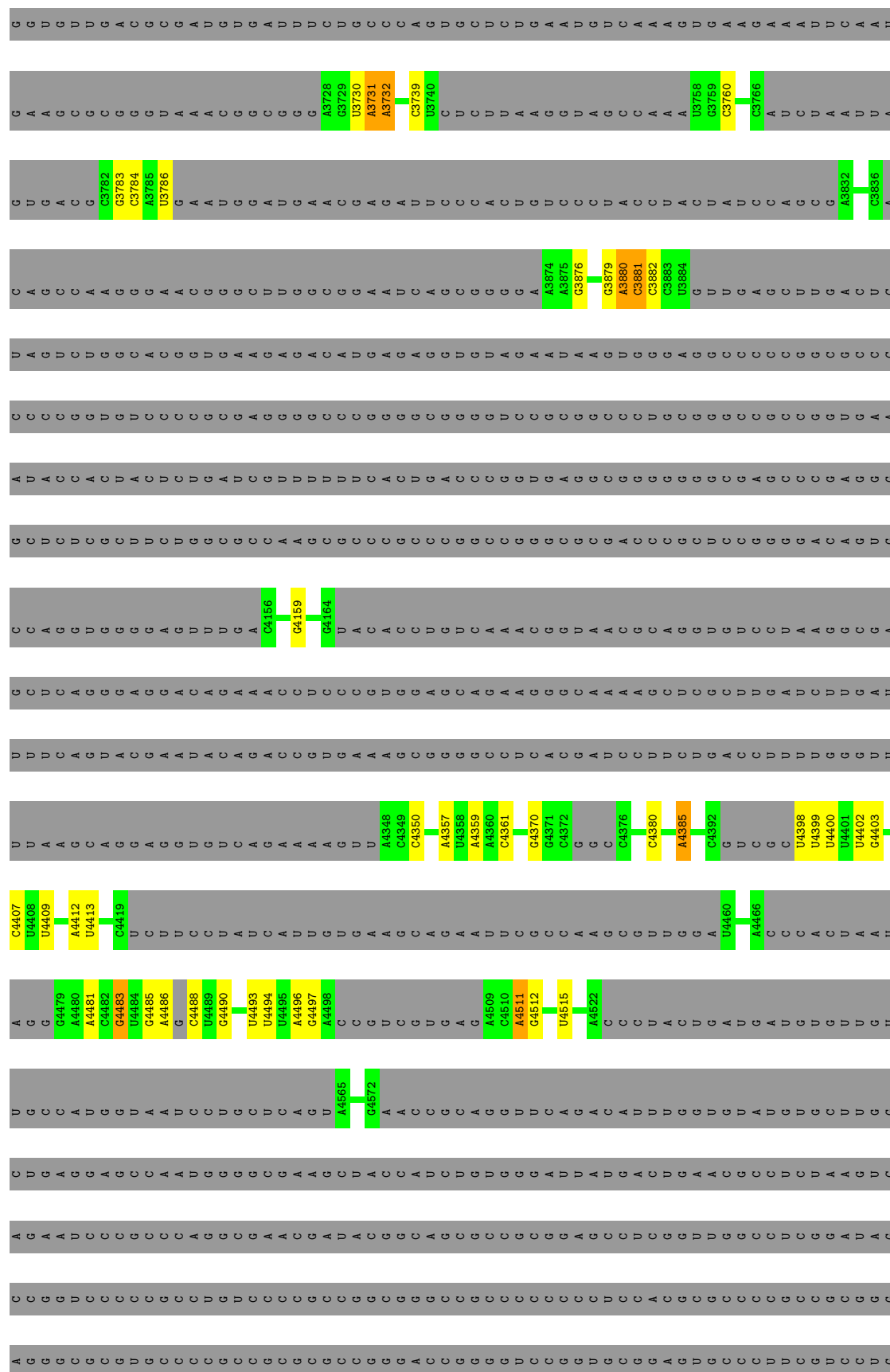
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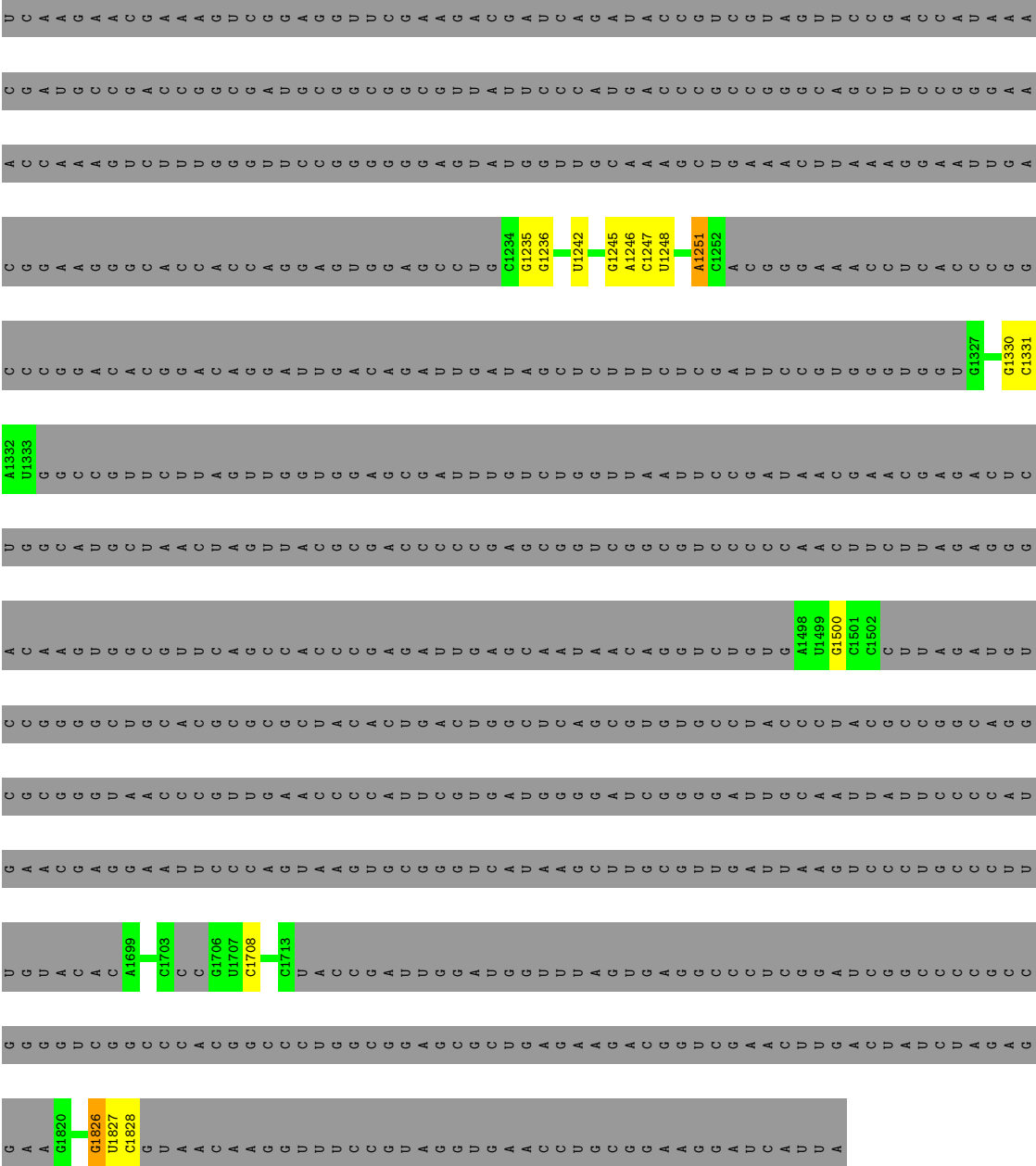


[illegible]

- Molecule 2: HUMAN 18S RIBOSOMAL RNA

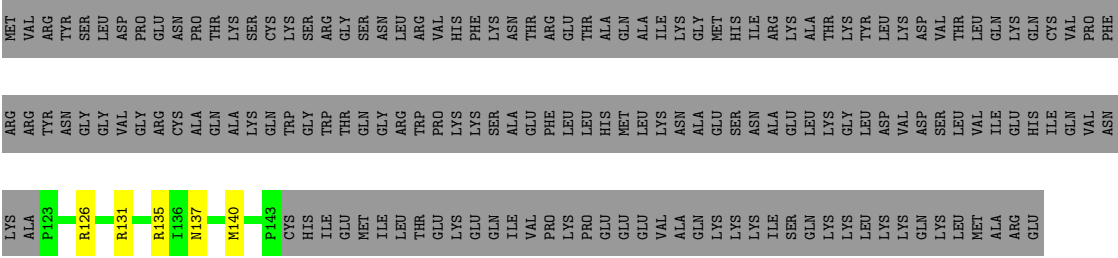
Chain B:  96%

[illegible]



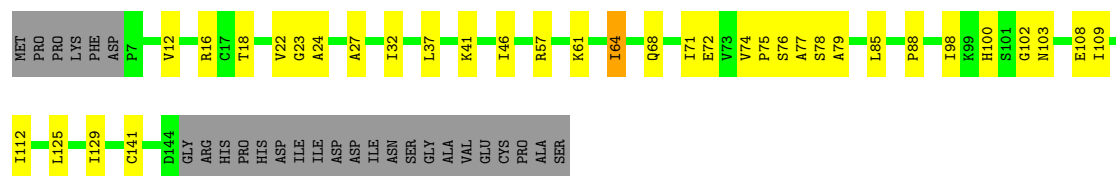
● Molecule 3: 60S RIBOSOMAL PROTEIN L17

Chain D: 9% 89%



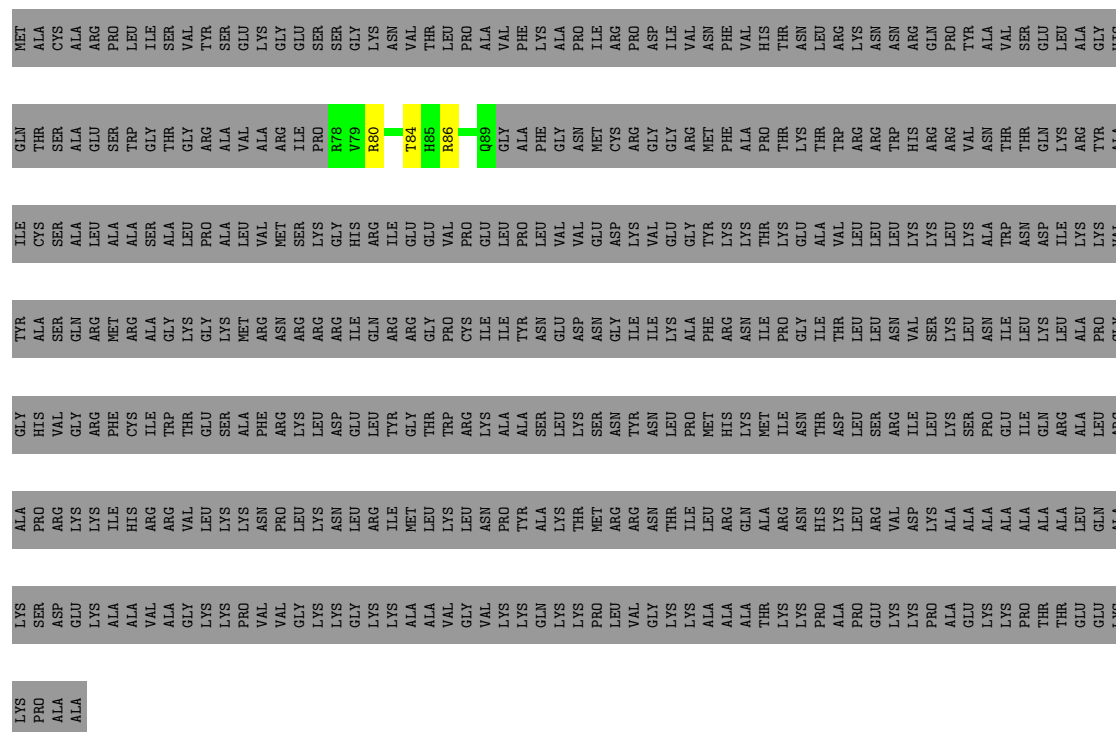
● Molecule 4: 60S RIBOSOMAL PROTEIN L12

Chain G:  62% 21% • 16%



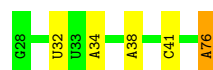
- Molecule 5: 60S RIBOSOMAL PROTEIN L4

Chain H:  97%



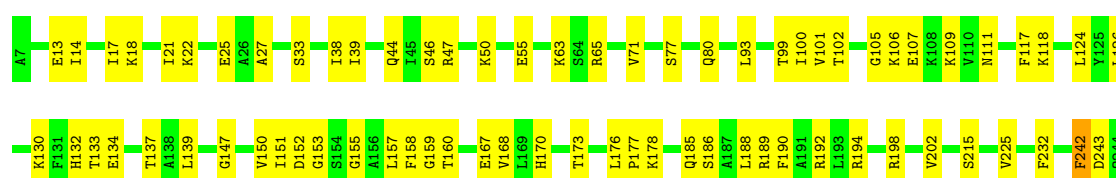
- Molecule 6: P-SITE TRNA

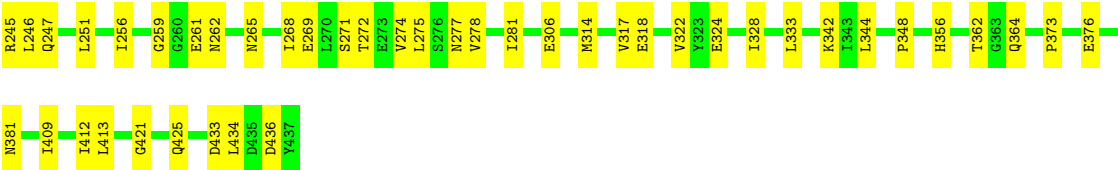
Chain P: 



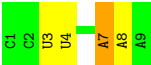
- Molecule 7: EUKARYOTIC RELEASE FACTOR ERF1

Chain Q:  73% 26%

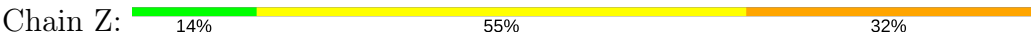




● Molecule 8: MRNA



● Molecule 9: NASCENT CHAIN



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	33165	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	DEFOCUS GROUPS	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	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	0.11	0/6024	0.66	0/9344
2	B	0.11	0/1582	0.65	0/2445
3	D	0.48	0/184	0.53	0/244
4	G	0.36	0/1058	0.50	0/1424
5	H	0.18	0/88	0.30	0/114
6	P	0.10	0/426	0.63	0/660
7	Q	0.27	0/3467	0.42	0/4661
8	R	0.17	0/212	0.69	0/327
9	Z	0.52	0/147	0.78	0/195
All	All	0.21	0/13188	0.60	0/19414

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	5401	0	2742	46	0
2	B	1423	0	730	9	0
3	D	179	0	184	4	0
4	G	1046	0	1116	18	0
5	H	88	0	86	3	0
6	P	382	0	197	3	0
7	Q	3410	0	3419	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	R	190	0	98	3	0
9	Z	145	0	145	49	0
All	All	12264	0	8717	179	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 9.

The worst 5 of 179 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)
9:Z:15:LEU:CA	9:Z:18:LYS:HE3	1.62	1.29
9:Z:8:ALA:O	9:Z:12:SER:HB3	1.22	1.26
9:Z:15:LEU:O	9:Z:18:LYS:HD2	1.23	1.26
1:A:3880:A:H2'	9:Z:19:TYR:CE2	1.82	1.14
9:Z:9:LYS:HD2	9:Z:11:LEU:HB2	1.15	1.14

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	
3	D	19/184 (10%)	18 (95%)	1 (5%)	0	100	100
4	G	136/165 (82%)	103 (76%)	27 (20%)	6 (4%)	3	30
5	H	10/427 (2%)	10 (100%)	0	0	100	100
7	Q	429/431 (100%)	390 (91%)	33 (8%)	6 (1%)	12	52
9	Z	20/22 (91%)	12 (60%)	2 (10%)	6 (30%)	0	0
All	All	614/1229 (50%)	533 (87%)	63 (10%)	18 (3%)	8	40

5 of 18 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
4	G	98	ILE
4	G	109	ILE
7	Q	242	PHE
9	Z	3	PRO
9	Z	4	LEU

### 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	
3	D	19/163 (12%)	19 (100%)	0	100	100
4	G	114/137 (83%)	114 (100%)	0	100	100
5	H	8/348 (2%)	8 (100%)	0	100	100
7	Q	371/371 (100%)	371 (100%)	0	100	100
9	Z	15/21 (71%)	9 (60%)	6 (40%)	0	0
All	All	527/1040 (51%)	521 (99%)	6 (1%)	77	88

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	Z	13	SER
9	Z	19	TYR
9	Z	15	LEU
9	Z	10	LYS
9	Z	18	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
7	Q	132	HIS
7	Q	366	HIS
7	Q	265	ASN
7	Q	44	GLN
7	Q	356	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	234/5025 (4%)	33 (14%)	1 (0%)
2	B	59/1869 (3%)	11 (18%)	0
6	P	16/18 (88%)	2 (12%)	0
8	R	8/9 (88%)	3 (37%)	0
All	All	317/6921 (4%)	49 (15%)	1 (0%)

5 of 49 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1623	G
1	A	1955	U
1	A	1956	G
1	A	1957	G
1	A	1965	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	3730	U

## 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 ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.