



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 30, 2017 – 02:31 PM EST

PDB ID : 5U4J
EMDB ID: : EMD-8506
Title : Structural Basis of Co-translational Quality Control by ArfA and RF2 Bound to Ribosome
Authors : Zeng, F.; Chen, Y.; Remis, J.; Shekhar, M.; Phillips, J.C.; Tajkhorshid, E.; Jin, H.
Deposited on : 2016-12-04
Resolution : 3.70 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation 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
Mogul : 1.7.1 (RC1), CSD as537be (2016)
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) : rb-20028442

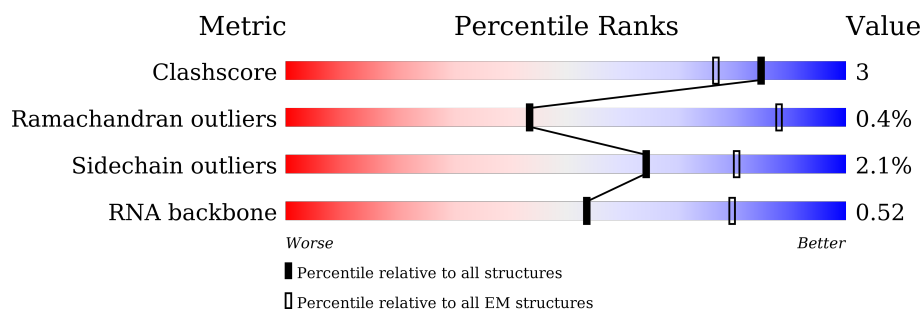
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	1533	15% 5% 80%
2	A	2904	100%
3	c	233	9% 91%
4	d	206	32% 68%
5	e	167	80% 19%
6	z	18	28% 6% 67%
7	x	77	19% 81%
8	l	124	98% ..

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Mol	Chain	Length	Quality of chain
9	v	383	<div><div></div><div>34%</div><div></div><div>66%</div></div>
10	w	57	<div><div></div><div>72%</div><div>11%</div><div>18%</div></div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11360 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	307	Total	C	N	O	P	0	0
			6591	2944	1198	2142	307		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	11	Total	C	N	O	P	0	0
			233	105	42	75	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	887	A	U	conflict	GB 42756

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	c	21	Total	C	N	O	0	0
			169	105	32	32		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	65	Total	C	N	O	S	0	0
			523	327	106	89	1		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	136	Total	C	N	O	S	0	0
			1001	625	190	182	4		

- Molecule 6 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	z	6	Total	C	N	O	P	0	0
			131	59	27	39	6		

- Molecule 7 is a RNA chain called P-site tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	x	15	Total	C	N	O	P	0	0
			315	141	54	105	15		

- Molecule 8 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 9 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	v	132	Total	C	N	O	S	0	0
			1054	659	182	208	5		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	-17	HIS	-	expression tag	UNP P07012
v	-16	HIS	-	expression tag	UNP P07012
v	-15	HIS	-	expression tag	UNP P07012
v	-14	HIS	-	expression tag	UNP P07012
v	-13	HIS	-	expression tag	UNP P07012
v	-12	HIS	-	expression tag	UNP P07012
v	-11	SER	-	expression tag	UNP P07012
v	-10	ALA	-	expression tag	UNP P07012
v	-9	ALA	-	expression tag	UNP P07012
v	-8	LEU	-	expression tag	UNP P07012
v	-7	GLU	-	expression tag	UNP P07012
v	-6	VAL	-	expression tag	UNP P07012
v	-5	LEU	-	expression tag	UNP P07012
v	-4	PHE	-	expression tag	UNP P07012
v	-3	GLN	-	expression tag	UNP P07012
v	-2	GLY	-	expression tag	UNP P07012
v	-1	PRO	-	expression tag	UNP P07012
v	0	GLY	-	expression tag	UNP P07012

- Molecule 10 is a protein called Alternative ribosome-rescue factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	w	47	Total	C	N	O	S	0	0
			388	239	82	66	1		

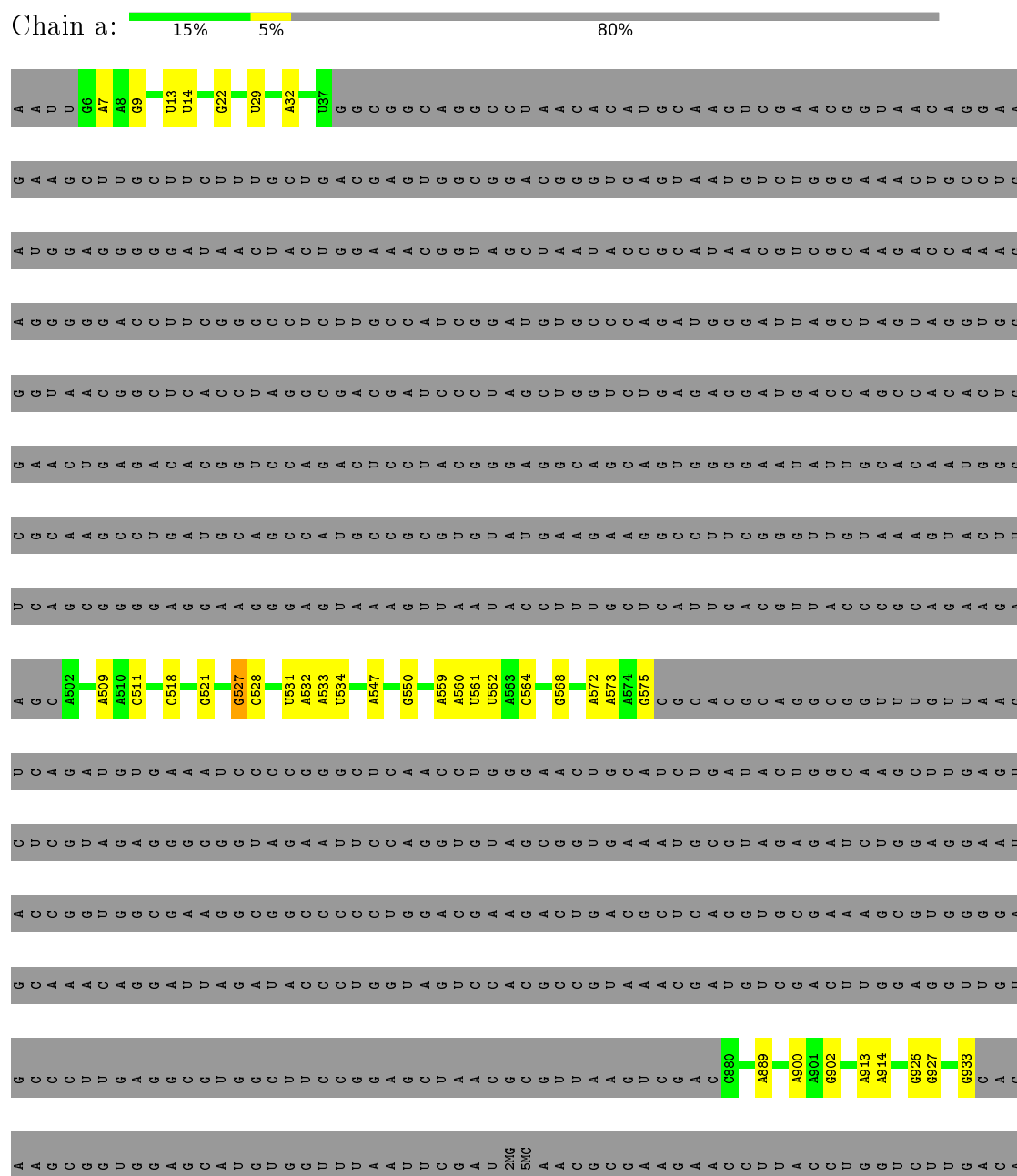
There are 2 discrepancies between the modelled and reference sequences:

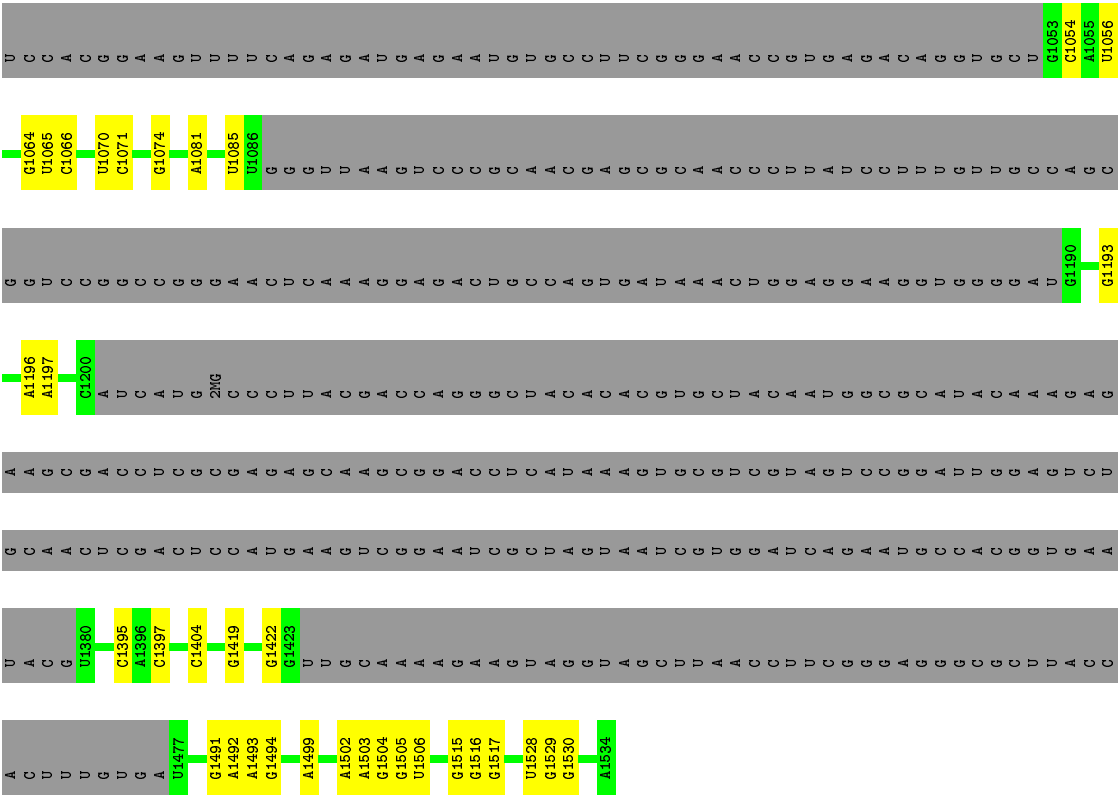
Chain	Residue	Modelled	Actual	Comment	Reference
w	-1	GLY	-	expression tag	UNP P36675
w	0	SER	-	expression tag	UNP P36675

3 Residue-property plots [i](#)

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: 16S rRNA





● Molecule 2: 23S rRNA

Chain A:  100%



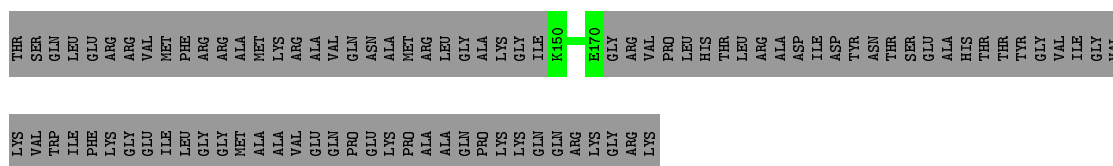



[illegible]

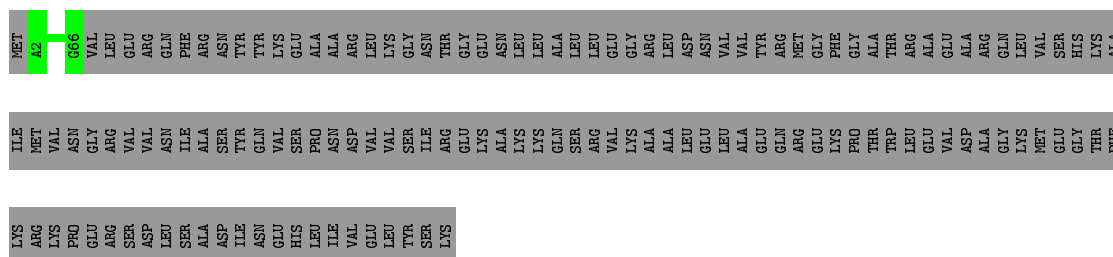
- Molecule 3: 30S ribosomal protein S3

Chain c: 9% 91%

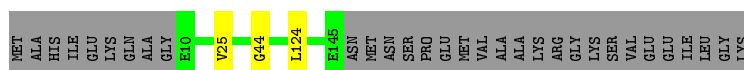
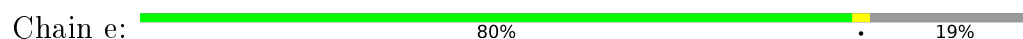
[illegible]



- Molecule 4: 30S ribosomal protein S4



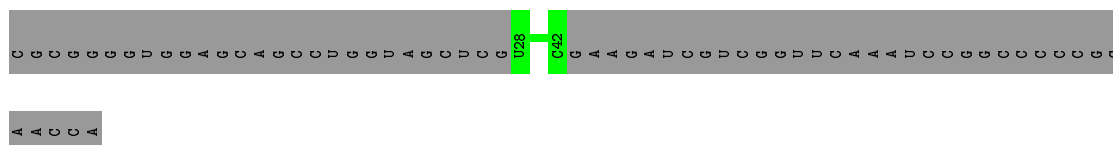
- Molecule 5: 30S ribosomal protein S5



- Molecule 6: mRNA



- Molecule 7: P-site tRNA fMet

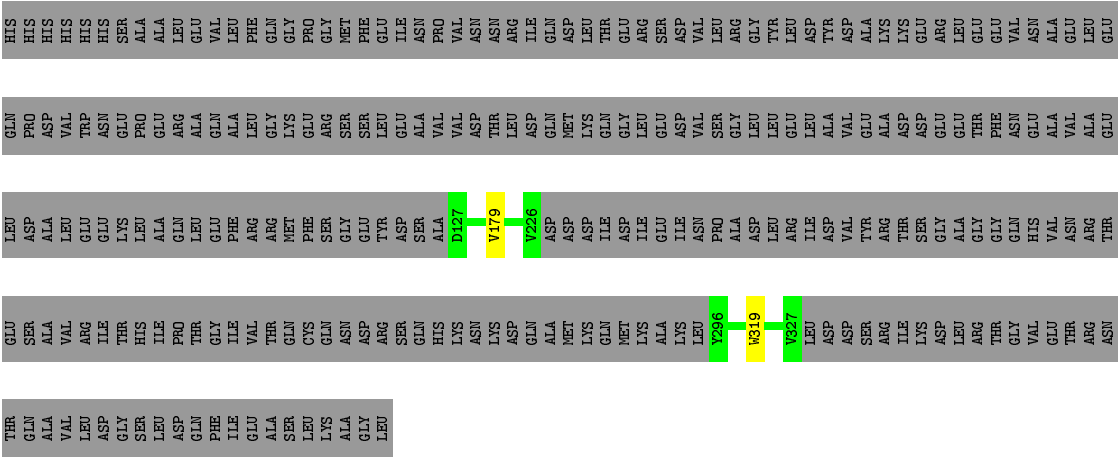


- Molecule 8: 30S ribosomal protein S12

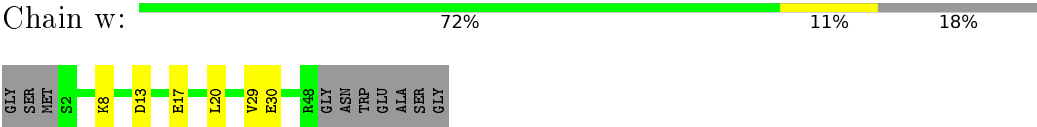


- Molecule 9: Peptide chain release factor 2





● Molecule 10: Alternative ribosome-rescue factor A



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	155440	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	83822	Depositor
Image detector	Not provided	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: MA6, G7M, 2MG, 5MC, UR3, 4OC, PSU

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	0/7167	0.64	3/11159 (0.0%)
10	w	0.34	0/394	0.69	2/519 (0.4%)
2	A	0.18	0/216	0.63	0/334
3	c	0.37	0/171	0.51	0/228
4	d	0.37	0/530	0.55	0/704
5	e	0.36	0/1013	0.56	0/1365
6	z	0.19	0/147	0.59	0/227
7	x	0.20	0/350	0.63	0/542
8	l	0.35	0/969	0.59	0/1300
9	v	0.39	0/1075	0.52	0/1443
All	All	0.28	0/12032	0.62	5/17821 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	527	G7M	O3'-P-O5'	9.93	122.87	104.00
10	w	8	LYS	CB-CA-C	5.74	121.87	110.40
1	a	528	C	OP1-P-OP2	-5.62	111.17	119.60
10	w	20	LEU	CA-CB-CG	5.23	127.33	115.30
1	a	1070	U	C2'-C3'-O3'	5.02	121.73	113.70

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	6591	0	3340	0	0
2	A	233	0	119	0	0
3	c	169	0	165	0	0
4	d	523	0	558	0	0
5	e	1001	0	1039	0	0
6	z	131	0	66	0	0
7	x	315	0	163	0	0
8	l	955	0	1016	0	0
9	v	1054	0	1004	0	0
10	w	388	0	400	0	0
All	All	11360	0	7870	0	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 3.

There are no clashes within the asymmetric unit.

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	c	19/233 (8%)	18 (95%)	1 (5%)	0	100	100
4	d	63/206 (31%)	62 (98%)	1 (2%)	0	100	100
5	e	134/167 (80%)	123 (92%)	10 (8%)	1 (1%)	26	72
8	l	121/124 (98%)	114 (94%)	6 (5%)	1 (1%)	24	70
9	v	128/383 (33%)	121 (94%)	7 (6%)	0	100	100
10	w	45/57 (79%)	41 (91%)	4 (9%)	0	100	100
All	All	510/1170 (44%)	479 (94%)	29 (6%)	2 (0%)	43	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	l	44	LYS
5	e	44	GLY

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	c	16/190 (8%)	16 (100%)	0	100	100
4	d	54/173 (31%)	54 (100%)	0	100	100
5	e	102/126 (81%)	100 (98%)	2 (2%)	63	87
8	l	103/104 (99%)	102 (99%)	1 (1%)	82	92
9	v	110/325 (34%)	108 (98%)	2 (2%)	66	89
10	w	40/46 (87%)	36 (90%)	4 (10%)	9	44
All	All	425/964 (44%)	416 (98%)	9 (2%)	64	86

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	e	25	VAL
5	e	124	LEU
8	l	52	VAL
9	v	179	VAL
9	v	319	TRP
10	w	13	ASP
10	w	17	GLU
10	w	29	VAL
10	w	30	GLU

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

Mol	Chain	Res	Type
5	e	132	ASN

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Mol	Chain	Res	Type
9	v	214	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	297/1533 (19%)	68 (22%)	0
2	A	10/2904 (0%)	2 (20%)	1 (10%)
6	z	5/18 (27%)	1 (20%)	0
7	x	14/77 (18%)	0	0
All	All	326/4532 (7%)	71 (21%)	1 (0%)

All (71) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	7	A
1	a	9	G
1	a	13	U
1	a	14	U
1	a	22	G
1	a	29	U
1	a	32	A
1	a	509	A
1	a	511	C
1	a	518	C
1	a	521	G
1	a	527	G7M
1	a	531	U
1	a	532	A
1	a	533	A
1	a	534	U
1	a	547	A
1	a	550	G
1	a	559	A
1	a	560	A
1	a	561	U
1	a	562	U
1	a	564	C
1	a	568	G
1	a	572	A
1	a	573	A
1	a	575	G

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Mol	Chain	Res	Type
1	a	889	A
1	a	900	A
1	a	902	G
1	a	913	A
1	a	914	A
1	a	926	G
1	a	927	G
1	a	933	G
1	a	1054	C
1	a	1056	U
1	a	1064	G
1	a	1065	U
1	a	1066	C
1	a	1071	C
1	a	1074	G
1	a	1081	A
1	a	1085	U
1	a	1193	G
1	a	1196	A
1	a	1197	A
1	a	1395	C
1	a	1397	C
1	a	1404	C
1	a	1419	G
1	a	1422	G
1	a	1491	G
1	a	1492	A
1	a	1493	A
1	a	1494	G
1	a	1499	A
1	a	1502	A
1	a	1503	A
1	a	1504	G
1	a	1505	G
1	a	1506	U
1	a	1515	G
1	a	1516	2MG
1	a	1517	G
1	a	1528	U
1	a	1529	G
1	a	1530	G
2	A	1913	A

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Mol	Chain	Res	Type
2	A	1914	C
6	z	46	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	1913	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	A	1911	2	15,21,22	1.09	1 (6%)	16,30,33	2.31	5 (31%)
2	PSU	A	1917	2	15,21,22	1.11	1 (6%)	16,30,33	2.38	5 (31%)
1	4OC	a	1402	1	15,23,24	0.70	0	21,32,35	2.03	5 (23%)
1	5MC	a	1407	1	14,22,23	1.58	2 (14%)	17,32,35	1.10	1 (5%)
1	UR3	a	1498	1	13,22,23	1.07	1 (7%)	18,32,35	1.07	1 (5%)
1	2MG	a	1516	1	18,26,27	1.39	2 (11%)	21,38,41	2.44	8 (38%)
1	MA6	a	1518	1	18,26,27	1.26	1 (5%)	15,38,41	2.34	4 (26%)
1	MA6	a	1519	1	18,26,27	1.23	1 (5%)	15,38,41	2.51	3 (20%)
1	PSU	a	516	1	15,21,22	1.10	1 (6%)	16,30,33	2.39	5 (31%)
1	G7M	a	527	1	18,26,27	1.04	1 (5%)	21,39,42	2.27	5 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	A	1911	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PSU	A	1917	2	-	0/7/25/26	0/2/2/2
1	4OC	a	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	a	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	a	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	a	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	a	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
1	G7M	a	527	1	-	0/3/25/26	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	516	PSU	C5-C1'	-3.04	1.49	1.52
2	A	1917	PSU	C5-C1'	-2.98	1.49	1.52
2	A	1911	PSU	C5-C1'	-2.95	1.49	1.52
1	a	1407	5MC	O4'-C1'	2.06	1.44	1.41
1	a	1498	UR3	C4-N3	3.07	1.42	1.38
1	a	1516	2MG	C5-C4	3.25	1.47	1.40
1	a	1518	MA6	C5-C4	3.35	1.48	1.40
1	a	1519	MA6	C5-C4	3.40	1.48	1.40
1	a	527	G7M	C6-C5	3.67	1.48	1.41
1	a	1516	2MG	C6-C5	3.70	1.48	1.41
1	a	1407	5MC	C5-C4	5.23	1.49	1.41

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1519	MA6	N3-C2-N1	-7.04	123.34	128.87
1	a	1518	MA6	N3-C2-N1	-6.72	123.59	128.87
1	a	527	G7M	C5-C6-N1	-4.88	117.14	123.52
1	a	527	G7M	C1'-N9-C4	-4.84	121.41	126.81
1	a	1516	2MG	C5-C6-N1	-4.03	118.26	123.52
2	A	1917	PSU	C5-C1'-C2'	-3.59	109.34	115.44
1	a	527	G7M	N3-C2-N1	-3.31	123.05	127.56
1	a	1516	2MG	C6-C5-C4	-3.29	117.10	120.86
1	a	516	PSU	C5-C6-N1	-3.27	119.81	124.38
2	A	1911	PSU	C5-C6-N1	-3.26	119.84	124.38
2	A	1917	PSU	C5-C6-N1	-3.15	119.99	124.38
1	a	516	PSU	C5-C1'-C2'	-3.15	110.09	115.44
2	A	1911	PSU	C5-C1'-C2'	-3.15	110.09	115.44
1	a	1516	2MG	N3-C2-N1	-2.85	121.93	126.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1519	MA6	C10-N6-C9	-2.43	108.02	115.96
1	a	1518	MA6	C2'-C1'-N9	-2.34	107.21	113.47
1	a	527	G7M	C6-C5-C4	-2.32	118.21	120.86
1	a	1516	2MG	C2'-C1'-N9	-2.25	107.45	113.47
1	a	1402	4OC	C5-C4-N3	-2.16	119.32	123.22
2	A	1917	PSU	C4'-O4'-C1'	2.02	111.62	109.54
1	a	1518	MA6	O4'-C1'-N9	2.04	111.96	108.11
1	a	1402	4OC	C4'-O4'-C1'	2.23	112.01	109.64
2	A	1911	PSU	C3'-C2'-C1'	2.25	104.37	101.71
2	A	1911	PSU	O4'-C1'-C2'	2.35	107.23	104.69
1	a	1516	2MG	O4'-C1'-N9	2.43	112.70	108.11
1	a	516	PSU	O4'-C1'-C2'	2.55	107.45	104.69
1	a	1498	UR3	O4'-C1'-N1	2.60	113.04	108.10
1	a	1402	4OC	O4'-C1'-N1	2.73	113.29	108.10
1	a	1407	5MC	O4'-C1'-N1	2.81	113.44	108.10
2	A	1917	PSU	C3'-C2'-C1'	2.96	105.22	101.71
1	a	516	PSU	C3'-C2'-C1'	3.19	105.49	101.71
1	a	1516	2MG	N2-C2-N3	3.45	120.94	116.94
1	a	1518	MA6	C2-N1-C6	4.47	122.17	111.64
1	a	1402	4OC	C2-N3-C4	4.59	121.28	115.43
1	a	1519	MA6	C2-N1-C6	4.65	122.61	111.64
1	a	527	G7M	C6-N1-C2	5.09	121.84	115.88
1	a	1516	2MG	C6-N1-C2	5.18	122.66	115.24
1	a	1402	4OC	C6-C5-C4	5.97	119.77	117.42
1	a	1516	2MG	C2-N3-C4	5.99	121.56	114.99
1	a	516	PSU	C4-N3-C2	6.86	120.88	115.16
2	A	1917	PSU	C4-N3-C2	6.97	120.97	115.16
2	A	1911	PSU	C4-N3-C2	6.99	120.99	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.