



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

Jan 30, 2017 – 01:18 PM EST

PDB ID : 5H5U  
EMDB ID: : EMD-6667  
Title : Mechanistic insights into the alternative translation termination by ArfA and RF2  
Authors : Ma, C.; Kurita, D.; Li, N.; Chen, Y.; Himeno, H.; Gao, N.  
Deposited on : 2016-11-09  
Resolution : 3.00 Å(reported)

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  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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) : rb-20028442

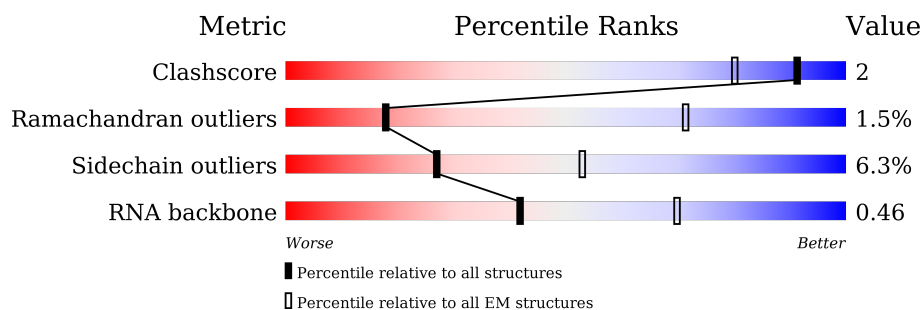
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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.





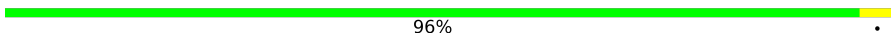












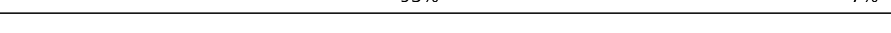
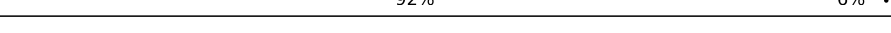







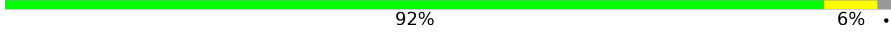
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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  $\geq 3$ , 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	1	86	95% ..
2	2	70	71% 9% 20%
3	3	72	43% 15% . 38%
4	4	365	82% 14% ..
5	5	76	71% 29%
6	7	6	50% 50%
7	A	2903	78% 20% .
8	B	120	84% 16%




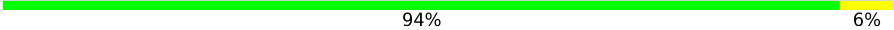
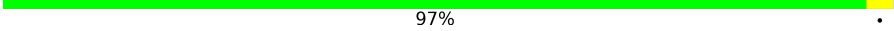



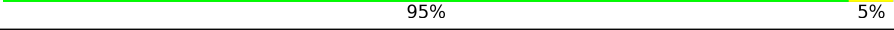



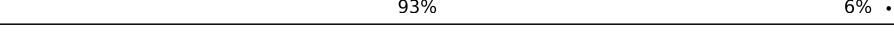
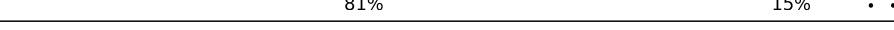







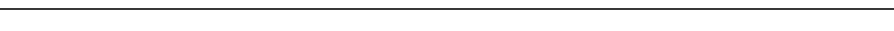


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Mol	Chain	Length	Quality of chain
9	C	272	 84% 14% .
10	D	209	 87% 11% .
11	E	201	 96% .
12	F	178	 87% 11% ..
13	G	176	 91% 9%
14	H	149	 91% 7% ..
15	I	164	 76% 5% . 18%
16	J	141	 45% . . 50%
17	K	142	 96% . .
18	L	123	 92% 7% .
19	M	144	 85% 14% .
20	N	136	 92% 7% ..
21	O	127	 89% 9% .
22	P	117	 92% 7% .
23	Q	114	 93% 7%
24	R	117	 92% 6% .
25	S	103	 77% 20% .
26	T	110	 86% 12% .
27	U	100	 80% 12% . 7%
28	V	103	 78% 18% . .
29	W	94	 87% 12% .
30	X	84	 83% 6% . 10%
31	Y	77	 81% 16% .
32	Z	63	 92% 6% .
33	a	58	 97% .

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Mol	Chain	Length	Quality of chain
34	b	56	 89% 11%
35	c	54	 85% 9% 6%
36	d	46	 91% 9%
37	e	64	 94% 6%
38	f	38	 97% .
39	h	1534	 81% 19%
40	i	240	 84% 9% . 7%
41	j	232	 82% 6% 11%
42	k	205	 95% 5%
43	l	166	 84% 10% 7%
44	m	135	 70% 7% . 21%
45	n	178	 75% 9% . 15%
46	o	129	 93% 6% .
47	p	129	 81% 15% . .
48	q	103	 85% 10% . .
49	r	128	 77% 13% . 9%
50	s	123	 89% 10% .
51	t	117	 87% 9% . .
52	u	100	 90% 9% .
53	v	88	 94% 6%
54	w	82	 89% 10% .
55	x	83	 87% 10% .
56	y	74	 70% . 26%
57	z	91	 79% 7% . 13%

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 148128 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 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 2 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 3 is a protein called Alternative ribosome-rescue factor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	45	Total	C	N	O	S	0	0
			369	229	76	63	1		

- Molecule 4 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	357	Total	C	N	O	S	0	0
			2829	1740	499	580	10		

- Molecule 5 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	76	Total	C	N	O	P	0	0
			1620	723	294	528	75		

- Molecule 6 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	6	Total	C	N	O	P	0	0
			127	57	22	42	6		

- Molecule 7 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	2897	Total	C	N	O	P	3	0
			62240	27765	11457	20119	2899		

- Molecule 8 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 9 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 10 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 11 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 12 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 13 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 14 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	148	Total	C	N	O	S	0	0
			1101	694	196	210	1		

- Molecule 15 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	135	Total	C	N	O	S	0	0
			1023	649	179	192	3		

- Molecule 16 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	71	Total	C	N	O	S	0	0
			509	313	93	100	3		

- Molecule 17 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 18 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 20 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	136	Total	C	N	O	S	1	0
			1082	691	208	177	6		

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

- Molecule 22 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 23 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 24 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 25 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 26 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 27 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 28 is a protein called 50S ribosomal protein L24.



Mol	Chain	Residues	Atoms				AltConf	Trace
28	V	102	Total	C	N	O		
			779	492	146	141	0	0

- Molecule 29 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	94	Total	C	N	O	S		
			753	479	137	134	3	0	0

- Molecule 30 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	76	Total	C	N	O	S		
			591	365	121	104	1	1	0

- Molecule 31 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	77	Total	C	N	O	S		
			625	388	129	106	2	0	0

- Molecule 32 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	62	Total	C	N	O	S		
			501	308	98	94	1	0	0

- Molecule 33 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	58	Total	C	N	O	S		
			463	290	90	81	2	2	0

- Molecule 34 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	56	Total	C	N	O	S		
			444	269	94	80	1	0	0

- Molecule 35 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	c	51	Total	C	N	O	0	0
			414	266	76	72		

- Molecule 36 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 37 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 38 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 39 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	1534	Total	C	N	O	P	0	0
			32917	14681	6041	10661	1534		

- Molecule 40 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 41 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 42 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 43 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

- Molecule 44 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 45 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 46 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 47 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 48 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

- Molecule 49 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 50 is a protein called 30S ribosomal protein S12.

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

- Molecule 51 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 52 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 53 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	v	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 54 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	w	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 55 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	x	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 56 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	y	55	Total	C	N	O	0	0
			455	288	86	81		

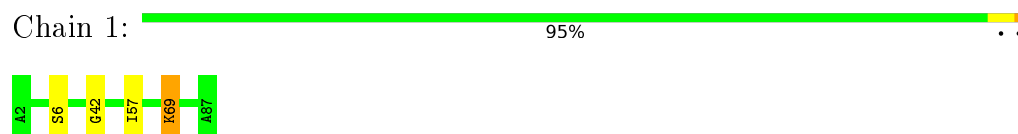
- Molecule 57 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	z	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

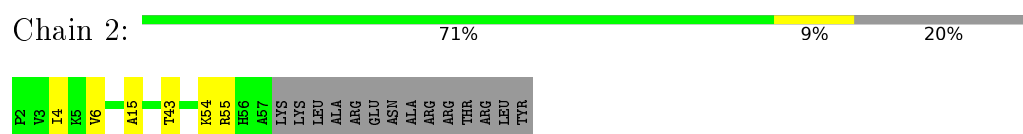
### 3 Residue-property plots

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.

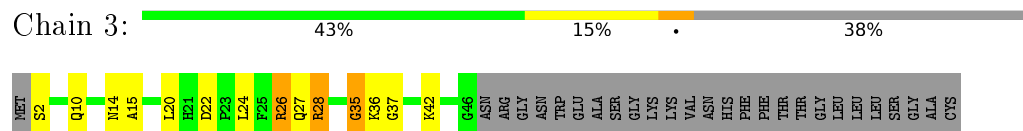
- Molecule 1: 30S ribosomal protein S20



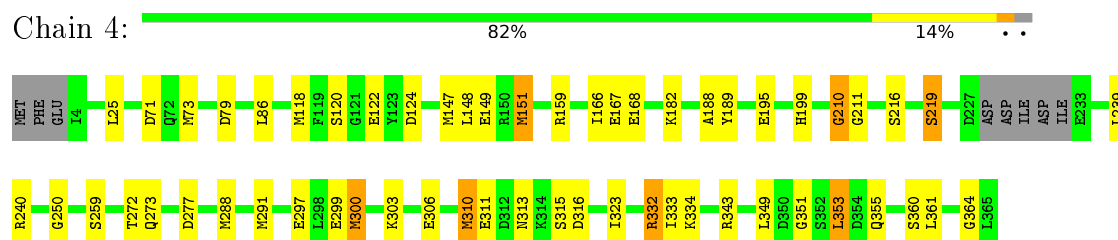
- Molecule 2: 30S ribosomal protein S21



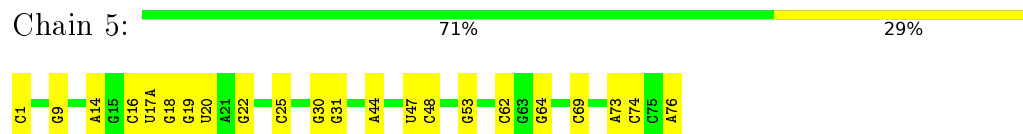
- Molecule 3: Alternative ribosome-rescue factor A



- Molecule 4: Peptide chain release factor 2



- Molecule 5: P-site tRNA

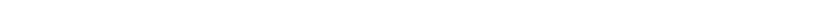


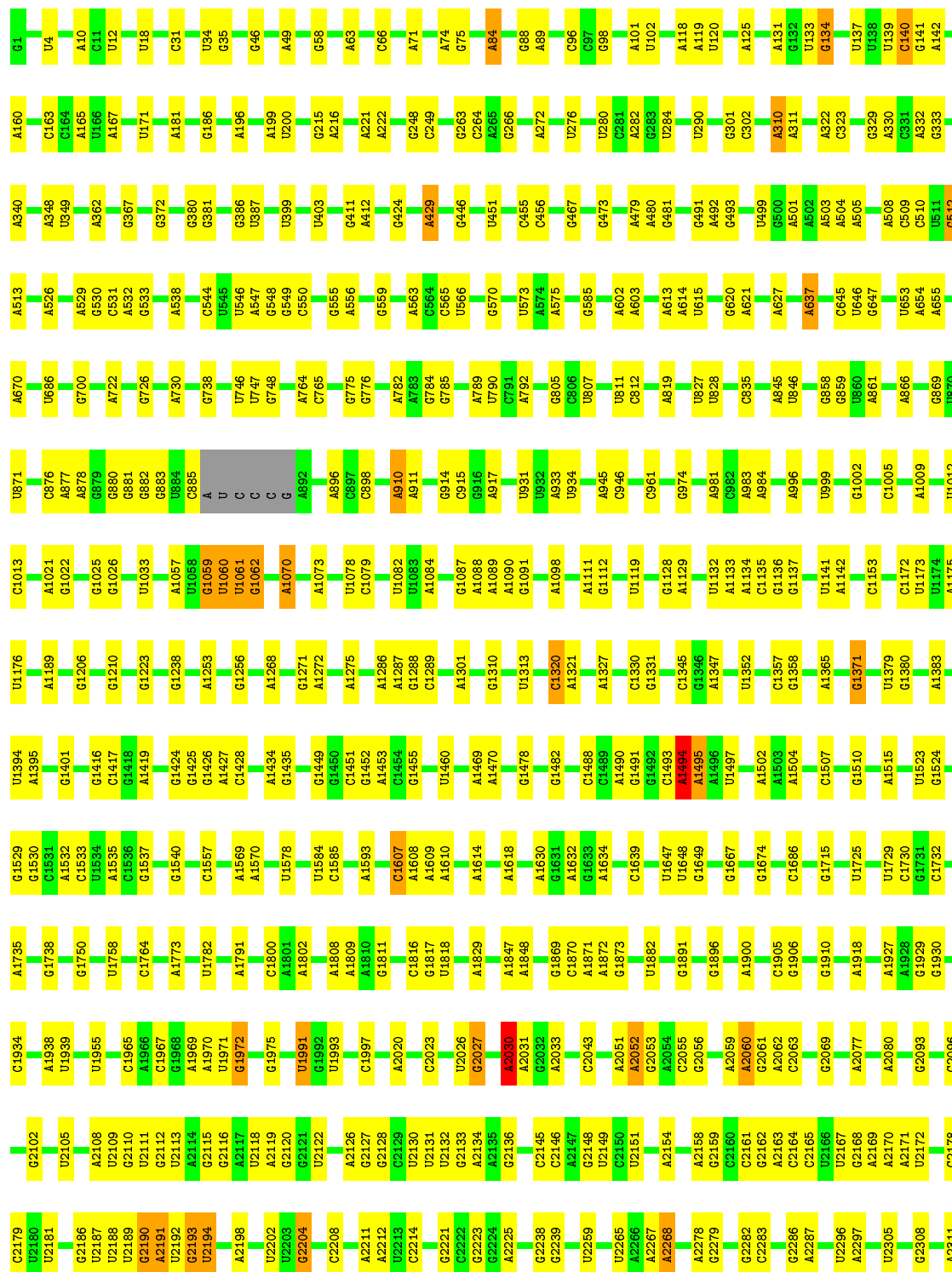
- Molecule 6: mRNA

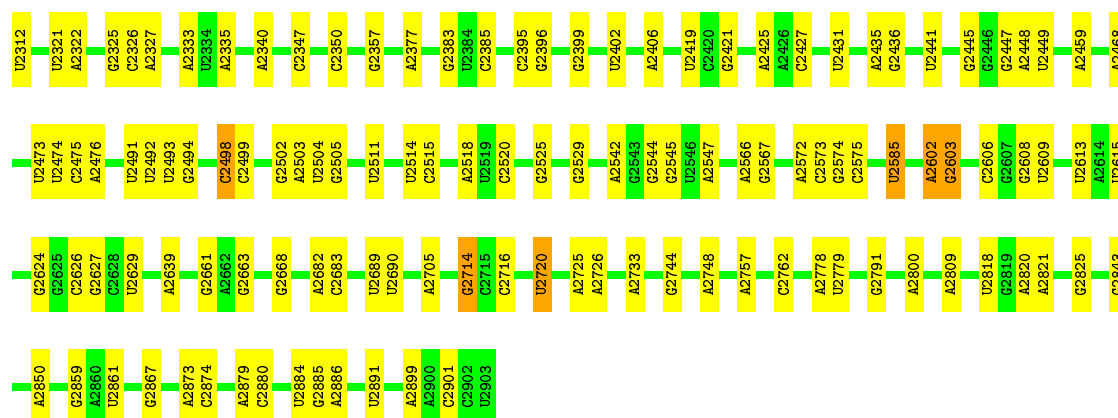




- Molecule 7: 23S rRNA

Chain A:  78% 20%





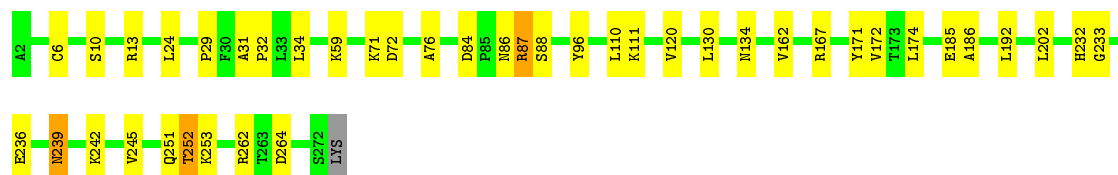
- Molecule 8: 5S Ribosomal RNA

Chain B: 84% 16%



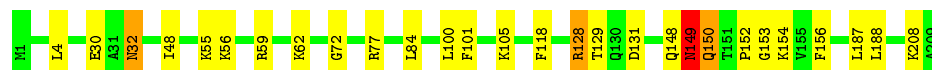
- Molecule 9: 50S ribosomal protein L2

Chain C: 84% 14%



- Molecule 10: 50S ribosomal protein L3

Chain D: 87% 11%



- Molecule 11: 50S ribosomal protein L4

Chain E: 96%



- Molecule 12: 50S ribosomal protein L5

Chain F: 87% 11%



- Molecule 13: 50S ribosomal protein L6



Chain G:  91% 9%



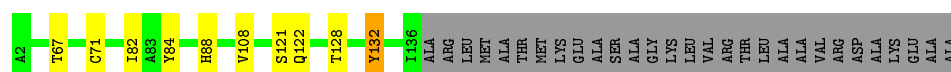
- Molecule 14: 50S ribosomal protein L9

Chain H:  91% 7% ..



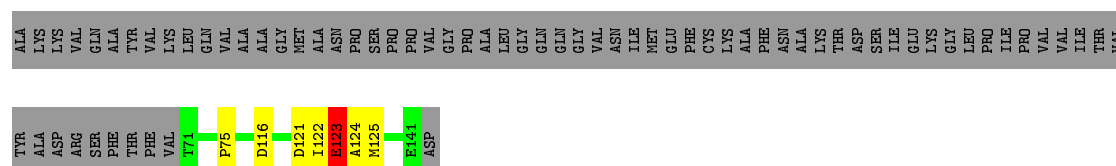
- Molecule 15: 50S ribosomal protein L10

Chain I:  76% 5% • 18%



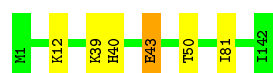
- Molecule 16: 50S ribosomal protein L11

Chain J:  45% • • 50%



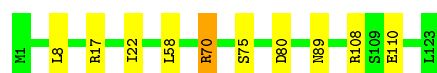
- Molecule 17: 50S ribosomal protein L13

Chain K:  96% • •




- Molecule 18: 50S ribosomal protein L14

Chain L:  92% 7% •



- Molecule 19: 50S ribosomal protein L15

Chain M:  85% 14% •



- Molecule 20: 50S ribosomal protein L16

Chain N:  92% 7% ..



- Molecule 21: 50S ribosomal protein L17

Chain O:  89% 9% .



- Molecule 22: 50S ribosomal protein L18

Chain P:  92% 7% .



- Molecule 23: 50S ribosomal protein L19

Chain Q:  93% 7%




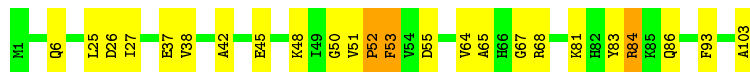
- Molecule 24: 50S ribosomal protein L20

Chain R:  92% 6% .



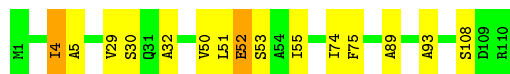
- Molecule 25: 50S ribosomal protein L21

Chain S:  77% 20% .




- Molecule 26: 50S ribosomal protein L22

Chain T:  86% 12% .

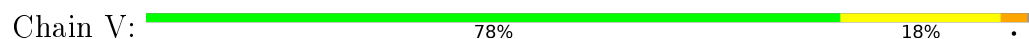


- Molecule 27: 50S ribosomal protein L23

Chain U:  80% 12% . 7%



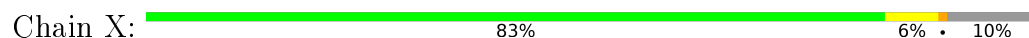
- Molecule 28: 50S ribosomal protein L24



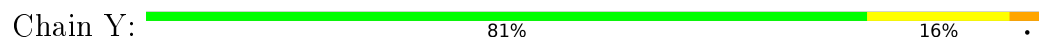
- Molecule 29: 50S ribosomal protein L25



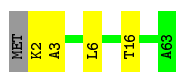
- Molecule 30: 50S ribosomal protein L27



- Molecule 31: 50S ribosomal protein L28



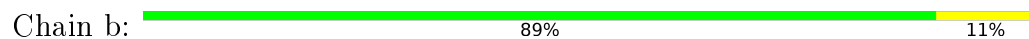
- Molecule 32: 50S ribosomal protein L29




- Molecule 33: 50S ribosomal protein L30



- Molecule 34: 50S ribosomal protein L32



- Molecule 35: 50S ribosomal protein L33

Chain c:  85% 9% 6%



- Molecule 36: 50S ribosomal protein L34

Chain d:  91% 9%



- Molecule 37: 50S ribosomal protein L35

Chain e:  94% 6%




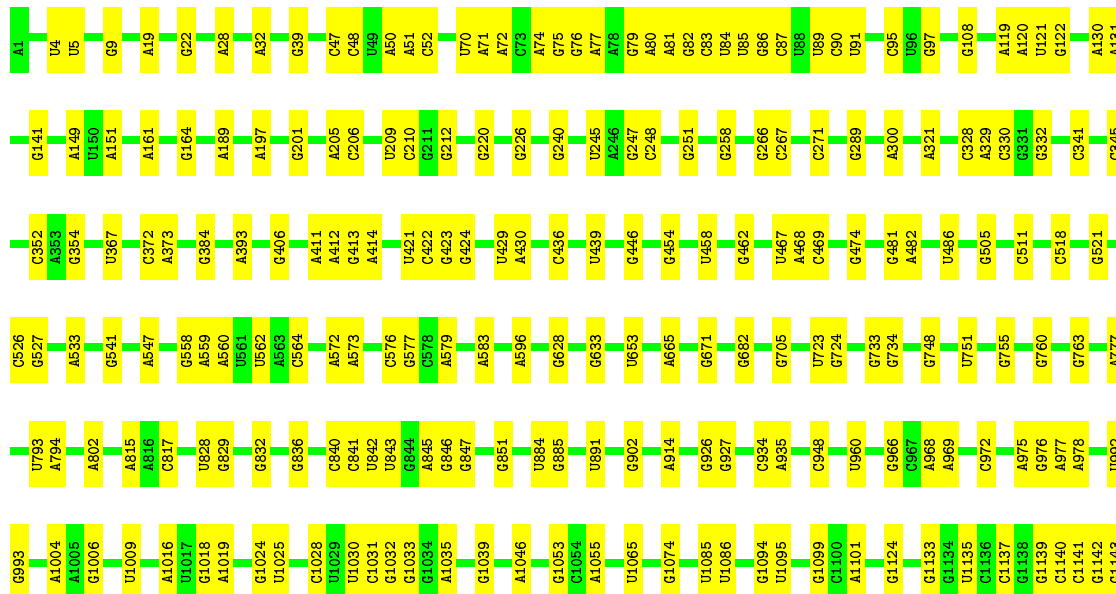
- Molecule 38: 50S ribosomal protein L36

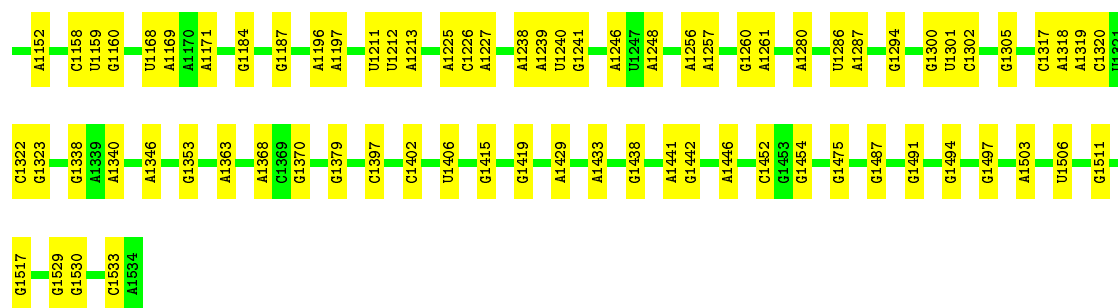
Chain f:  97%



- Molecule 39: 16S rRNA

Chain h:  81% 19%





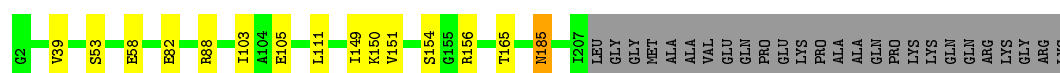
- Molecule 40: 30S ribosomal protein S2

Chain i: 84% 9% 7%



- Molecule 41: 30S ribosomal protein S3

Chain j: 82% 6% 11%



- Molecule 42: 30S ribosomal protein S4

Chain k: 95% 5%



- Molecule 43: 30S ribosomal protein S5

Chain l: 84% 10% 7%



- Molecule 44: 30S ribosomal protein S6

Chain m: 70% 7% 21%



- Molecule 45: 30S ribosomal protein S7

Chain n: 75% 9% 15%




ASN

- Molecule 46: 30S ribosomal protein S8

Chain o:  93% 6%




- Molecule 47: 30S ribosomal protein S9

Chain p:  81% 15%




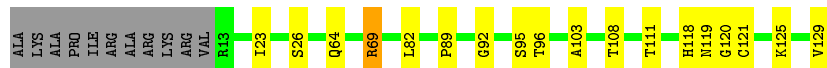
- Molecule 48: 30S ribosomal protein S10

Chain q:  85% 10%




- Molecule 49: 30S ribosomal protein S11

Chain r:  77% 13% 9%




- Molecule 50: 30S ribosomal protein S12

Chain s:  89% 10%




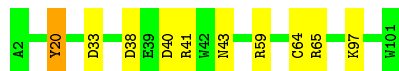
- Molecule 51: 30S ribosomal protein S13

Chain t:  87% 9%

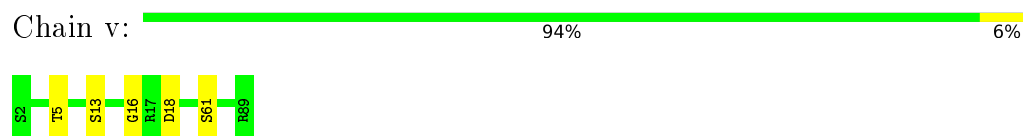


- Molecule 52: 30S ribosomal protein S14

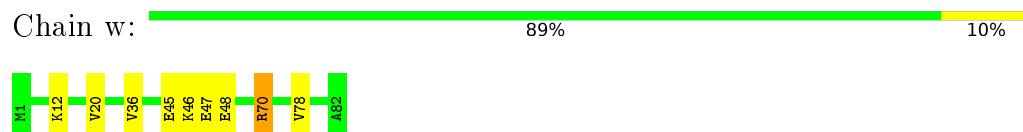
Chain u:  90% 9%



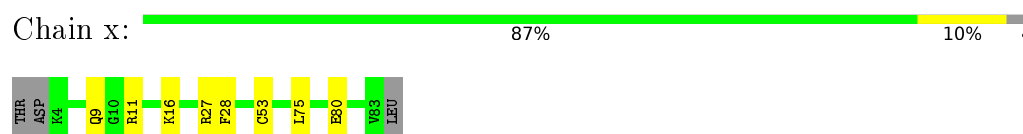
- Molecule 53: 30S ribosomal protein S15



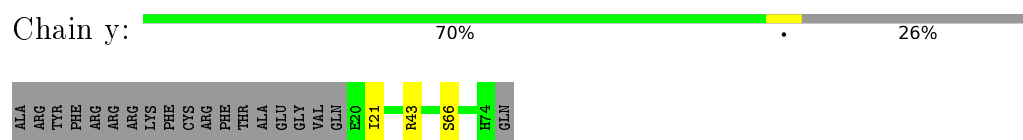
- Molecule 54: 30S ribosomal protein S16



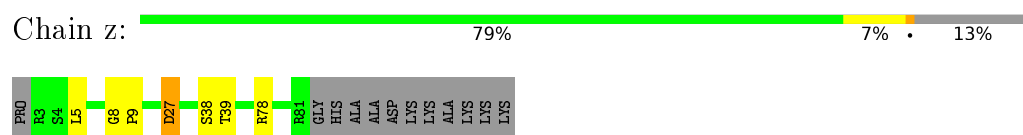
- Molecule 55: 30S ribosomal protein S17



- Molecule 56: 30S ribosomal protein S18



- Molecule 57: 30S ribosomal protein S19



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	13693	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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	1	0.38	0/676	0.62	0/895
10	D	0.42	0/1586	0.68	0/2134
11	E	0.38	0/1571	0.60	0/2113
12	F	0.40	0/1434	0.58	0/1926
13	G	0.38	0/1343	0.58	0/1816
14	H	0.42	0/1112	0.52	0/1503
15	I	0.44	0/1037	0.53	0/1402
16	J	0.41	0/511	0.49	0/683
17	K	0.40	0/1152	0.64	0/1551
18	L	0.40	0/955	0.71	0/1279
19	M	0.41	0/1062	0.68	0/1413
2	2	0.49	0/472	0.73	0/627
20	N	0.44	0/1104	0.69	0/1474
21	O	0.43	0/1006	0.75	0/1345
22	P	0.37	0/910	0.64	0/1219
23	Q	0.42	0/929	0.70	0/1242
24	R	0.42	0/960	0.72	0/1278
25	S	0.42	0/829	0.61	0/1107
26	T	0.41	0/864	0.67	0/1156
27	U	0.41	0/744	0.65	0/994
28	V	0.39	0/787	0.56	0/1051
29	W	0.39	0/766	0.61	0/1025
3	3	0.43	0/375	0.81	0/494
30	X	0.46	0/598	0.75	0/790
31	Y	0.42	0/635	0.66	0/848
32	Z	0.37	0/502	0.68	0/667
33	a	0.35	0/467	0.65	0/623
34	b	0.40	0/450	0.74	0/599
35	c	0.42	0/421	0.72	0/561
36	d	0.49	0/380	0.91	0/498
37	e	0.38	0/513	0.65	0/676
38	f	0.36	0/303	0.72	0/397
39	h	0.31	0/36859	0.72	3/57501 (0.0%)
4	4	0.43	0/2868	0.61	0/3861

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
40	i	0.41	0/1784	0.60	0/2403
41	j	0.42	0/1651	0.68	0/2225
42	k	0.41	0/1665	0.61	0/2227
43	l	0.44	0/1157	0.70	0/1557
44	m	0.42	0/881	0.66	0/1189
45	n	0.42	0/1195	0.70	0/1602
46	o	0.41	0/989	0.67	0/1326
47	p	0.42	0/1034	0.76	1/1375 (0.1%)
48	q	0.40	0/805	0.69	0/1089
49	r	0.42	0/893	0.70	0/1205
5	5	0.27	0/1810	0.72	2/2821 (0.1%)
50	s	0.44	0/969	0.77	2/1300 (0.2%)
51	t	0.41	0/892	0.68	0/1193
52	u	0.44	0/817	0.71	0/1088
53	v	0.39	0/722	0.64	0/964
54	w	0.47	0/659	0.75	1/884 (0.1%)
55	x	0.39	0/657	0.64	0/881
56	y	0.46	0/462	0.71	0/621
57	z	0.45	0/652	0.64	1/877 (0.1%)
6	7	0.49	0/141	0.90	0/217
7	A	0.33	2/69735 (0.0%)	0.71	11/108791 (0.0%)
8	B	0.26	0/2872	0.69	0/4478
9	C	0.41	0/2121	0.76	1/2852 (0.0%)
All	All	0.35	2/160744 (0.0%)	0.70	22/239913 (0.0%)

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	1	0	1
10	D	0	3
11	E	0	3
12	F	0	4
13	G	0	6
14	H	0	1
15	I	0	3
18	L	0	1
19	M	0	2
2	2	0	1
20	N	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
21	O	0	1
22	P	0	1
23	Q	0	2
25	S	0	3
26	T	0	1
27	U	0	3
28	V	0	1
29	W	0	1
3	3	0	4
31	Y	0	2
32	Z	0	1
35	c	0	2
36	d	0	1
4	4	0	6
40	i	0	4
41	j	0	4
42	k	0	4
43	l	0	1
44	m	0	2
45	n	0	3
46	o	0	4
47	p	0	5
48	q	0	3
49	r	0	4
50	s	0	1
51	t	0	4
52	u	0	3
53	v	0	1
54	w	0	2
55	x	0	1
56	y	0	1
57	z	0	2
9	C	0	6
All	All	0	111

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1607	C	O3'-P	5.24	1.67	1.61
7	A	2498	C	O3'-P	-5.23	1.54	1.61

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	h	560	A	O5'-P-OP1	-8.87	97.72	105.70
7	A	1607	C	C2'-C3'-O3'	7.92	126.92	109.50
54	w	70	ARG	NE-CZ-NH1	7.05	123.83	120.30
7	A	2498	C	C2'-C3'-O3'	6.74	124.48	113.70
7	A	1494	A	C2'-C3'-O3'	6.68	124.38	113.70

There are no chirality outliers.

5 of 111 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	42	GLY	Peptide
2	2	55	ARG	Peptide
3	3	2	SER	Peptide
3	3	35	GLY	Peptide
3	3	36	LYS	Peptide

## 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	1	670	0	719	0	0
2	2	465	0	491	1	0
3	3	369	0	381	3	0
4	4	2829	0	2734	42	0
5	5	1620	0	826	0	0
6	7	127	0	65	0	0
7	A	62240	0	31297	86	0
8	B	2569	0	1301	1	0
9	C	2082	0	2154	13	0
10	D	1565	0	1616	26	0
11	E	1552	0	1619	0	0
12	F	1410	0	1444	7	0
13	G	1323	0	1371	9	0
14	H	1101	0	1142	3	0
15	I	1023	0	1052	3	0
16	J	509	0	547	4	0
17	K	1129	0	1162	3	0
18	L	946	0	1023	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	M	1053	0	1129	23	0
20	N	1082	0	1170	6	0
21	O	993	0	1034	3	0
22	P	900	0	935	5	0
23	Q	917	0	962	2	0
24	R	947	0	1019	4	0
25	S	816	0	839	35	0
26	T	857	0	922	12	0
27	U	738	0	807	4	0
28	V	779	0	831	12	0
29	W	753	0	780	4	0
30	X	591	0	606	4	0
31	Y	625	0	652	8	0
32	Z	501	0	531	1	0
33	a	463	0	504	0	0
34	b	444	0	458	0	0
35	c	414	0	442	0	0
36	d	377	0	418	0	0
37	e	504	0	572	0	0
38	f	302	0	343	0	0
39	h	32917	0	16564	0	0
40	i	1753	0	1780	0	0
41	j	1624	0	1696	0	0
42	k	1643	0	1707	0	0
43	l	1144	0	1185	0	0
44	m	862	0	864	0	0
45	n	1181	0	1238	0	0
46	o	979	0	1031	0	0
47	p	1022	0	1070	0	0
48	q	795	0	836	0	0
49	r	877	0	885	0	0
50	s	955	0	1016	0	0
51	t	883	0	941	0	0
52	u	805	0	844	0	0
53	v	714	0	734	0	0
54	w	649	0	666	0	0
55	x	648	0	691	0	0
56	y	455	0	478	0	0
57	z	637	0	665	0	0
All	All	148128	0	100789	297	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 297 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)
25:S:37:GLU:CB	25:S:53:PHE:HE1	1.04	1.67
25:S:37:GLU:HB3	25:S:53:PHE:CE1	1.25	1.64
25:S:37:GLU:CB	25:S:53:PHE:CE1	1.88	1.39
7:A:1061:U:H1'	7:A:1070:A:C1'	1.54	1.34
25:S:37:GLU:CG	25:S:53:PHE:CE1	2.13	1.31

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	1	84/86 (98%)	79 (94%)	4 (5%)	1 (1%)	16	56
2	2	54/70 (77%)	51 (94%)	3 (6%)	0	100	100
3	3	43/72 (60%)	32 (74%)	8 (19%)	3 (7%)	1	7
4	4	353/365 (97%)	316 (90%)	31 (9%)	6 (2%)	11	46
9	C	269/272 (99%)	245 (91%)	24 (9%)	0	100	100
10	D	207/209 (99%)	189 (91%)	16 (8%)	2 (1%)	19	61
11	E	199/201 (99%)	188 (94%)	10 (5%)	1 (0%)	34	76
12	F	175/178 (98%)	157 (90%)	15 (9%)	3 (2%)	11	46
13	G	174/176 (99%)	156 (90%)	18 (10%)	0	100	100
14	H	146/149 (98%)	131 (90%)	13 (9%)	2 (1%)	14	51
15	I	133/164 (81%)	116 (87%)	14 (10%)	3 (2%)	8	36
16	J	69/141 (49%)	61 (88%)	7 (10%)	1 (1%)	14	51
17	K	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
18	L	121/123 (98%)	108 (89%)	11 (9%)	2 (2%)	11	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	M	142/144 (99%)	127 (89%)	14 (10%)	1 (1%)	26	70
20	N	135/136 (99%)	125 (93%)	6 (4%)	4 (3%)	5	29
21	O	123/127 (97%)	110 (89%)	12 (10%)	1 (1%)	24	66
22	P	115/117 (98%)	112 (97%)	2 (2%)	1 (1%)	21	64
23	Q	112/114 (98%)	99 (88%)	13 (12%)	0	100	100
24	R	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
25	S	101/103 (98%)	93 (92%)	6 (6%)	2 (2%)	9	41
26	T	108/110 (98%)	101 (94%)	7 (6%)	0	100	100
27	U	91/100 (91%)	83 (91%)	4 (4%)	4 (4%)	3	18
28	V	100/103 (97%)	88 (88%)	8 (8%)	4 (4%)	4	21
29	W	92/94 (98%)	83 (90%)	8 (9%)	1 (1%)	17	58
30	X	75/84 (89%)	66 (88%)	9 (12%)	0	100	100
31	Y	75/77 (97%)	66 (88%)	6 (8%)	3 (4%)	4	21
32	Z	60/63 (95%)	56 (93%)	4 (7%)	0	100	100
33	a	57/58 (98%)	52 (91%)	5 (9%)	0	100	100
34	b	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
35	c	49/54 (91%)	45 (92%)	4 (8%)	0	100	100
36	d	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
37	e	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
38	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
40	i	222/240 (92%)	196 (88%)	17 (8%)	9 (4%)	3	20
41	j	204/232 (88%)	176 (86%)	25 (12%)	3 (2%)	13	50
42	k	203/205 (99%)	193 (95%)	10 (5%)	0	100	100
43	l	153/166 (92%)	130 (85%)	20 (13%)	3 (2%)	9	41
44	m	104/135 (77%)	91 (88%)	11 (11%)	2 (2%)	10	43
45	n	149/178 (84%)	130 (87%)	16 (11%)	3 (2%)	9	41
46	o	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
47	p	125/129 (97%)	106 (85%)	14 (11%)	5 (4%)	4	21
48	q	97/103 (94%)	87 (90%)	8 (8%)	2 (2%)	9	40
49	r	115/128 (90%)	94 (82%)	17 (15%)	4 (4%)	4	24
50	s	121/123 (98%)	106 (88%)	13 (11%)	2 (2%)	11	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	t	112/117 (96%)	94 (84%)	12 (11%)	6 (5%)	2	14
52	u	98/100 (98%)	83 (85%)	10 (10%)	5 (5%)	2	15
53	v	86/88 (98%)	78 (91%)	8 (9%)	0	100	100
54	w	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	15	53
55	x	78/83 (94%)	73 (94%)	5 (6%)	0	100	100
56	y	53/74 (72%)	49 (92%)	3 (6%)	1 (2%)	10	43
57	z	77/91 (85%)	69 (90%)	7 (9%)	1 (1%)	15	53
All	All	6117/6556 (93%)	5506 (90%)	519 (8%)	92 (2%)	18	50

5 of 92 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	E	73	ILE
14	H	50	ARG
19	M	132	ARG
20	N	81	ARG
27	U	2	ILE

### 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	1	65/65 (100%)	62 (95%)	3 (5%)	33	73
2	2	48/60 (80%)	45 (94%)	3 (6%)	22	60
3	3	38/59 (64%)	31 (82%)	7 (18%)	2	10
4	4	303/311 (97%)	277 (91%)	26 (9%)	13	44
9	C	216/217 (100%)	198 (92%)	18 (8%)	14	46
10	D	164/164 (100%)	150 (92%)	14 (8%)	13	45
11	E	165/165 (100%)	161 (98%)	4 (2%)	57	87
12	F	148/149 (99%)	138 (93%)	10 (7%)	20	56
13	G	137/137 (100%)	135 (98%)	2 (2%)	72	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	H	113/114 (99%)	106 (94%)	7 (6%)	23	60
15	I	103/122 (84%)	102 (99%)	1 (1%)	82	95
16	J	53/109 (49%)	50 (94%)	3 (6%)	25	64
17	K	116/116 (100%)	111 (96%)	5 (4%)	35	75
18	L	104/104 (100%)	97 (93%)	7 (7%)	20	57
19	M	103/103 (100%)	98 (95%)	5 (5%)	31	71
20	N	110/109 (101%)	108 (98%)	2 (2%)	66	91
21	O	102/103 (99%)	98 (96%)	4 (4%)	39	77
22	P	87/87 (100%)	87 (100%)	0	100	100
23	Q	99/99 (100%)	96 (97%)	3 (3%)	48	83
24	R	89/89 (100%)	83 (93%)	6 (7%)	20	57
25	S	84/84 (100%)	77 (92%)	7 (8%)	14	46
26	T	93/93 (100%)	91 (98%)	2 (2%)	60	88
27	U	80/84 (95%)	77 (96%)	3 (4%)	40	78
28	V	83/84 (99%)	74 (89%)	9 (11%)	8	30
29	W	78/78 (100%)	75 (96%)	3 (4%)	40	78
30	X	58/62 (94%)	55 (95%)	3 (5%)	29	68
31	Y	67/67 (100%)	61 (91%)	6 (9%)	12	41
32	Z	54/55 (98%)	53 (98%)	1 (2%)	65	90
33	a	49/48 (102%)	47 (96%)	2 (4%)	37	76
34	b	47/47 (100%)	41 (87%)	6 (13%)	5	23
35	c	45/48 (94%)	42 (93%)	3 (7%)	20	57
36	d	38/38 (100%)	35 (92%)	3 (8%)	15	48
37	e	51/51 (100%)	47 (92%)	4 (8%)	16	49
38	f	34/34 (100%)	33 (97%)	1 (3%)	50	84
40	i	186/198 (94%)	174 (94%)	12 (6%)	21	58
41	j	170/189 (90%)	161 (95%)	9 (5%)	28	67
42	k	172/172 (100%)	165 (96%)	7 (4%)	37	76
43	l	118/125 (94%)	106 (90%)	12 (10%)	9	33
44	m	92/116 (79%)	84 (91%)	8 (9%)	13	43
45	n	124/146 (85%)	112 (90%)	12 (10%)	10	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
46	o	104/104 (100%)	98 (94%)	6 (6%)	25 63
47	p	105/106 (99%)	89 (85%)	16 (15%)	3 16
48	q	87/90 (97%)	80 (92%)	7 (8%)	15 47
49	r	90/98 (92%)	79 (88%)	11 (12%)	6 25
50	s	103/103 (100%)	93 (90%)	10 (10%)	10 37
51	t	92/95 (97%)	89 (97%)	3 (3%)	45 82
52	u	83/83 (100%)	80 (96%)	3 (4%)	42 79
53	v	76/76 (100%)	72 (95%)	4 (5%)	28 67
54	w	65/65 (100%)	59 (91%)	6 (9%)	11 40
55	x	74/77 (96%)	67 (90%)	7 (10%)	11 38
56	y	48/64 (75%)	47 (98%)	1 (2%)	61 89
57	z	70/78 (90%)	66 (94%)	4 (6%)	25 64
All	All	5083/5340 (95%)	4762 (94%)	321 (6%)	27 60

5 of 321 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	V	68	SER
37	e	38	THR
52	u	59	ARG
28	V	86	ARG
32	Z	16	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
22	P	98	GLN
24	R	72	ASN
46	o	67	GLN
23	Q	12	GLN
23	Q	115	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
39	h	1533/1534 (99%)	287 (18%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	5	75/76 (98%)	20 (26%)	2 (2%)
6	7	5/6 (83%)	3 (60%)	1 (20%)
7	A	2892/2903 (99%)	533 (18%)	62 (2%)
8	B	119/120 (99%)	17 (14%)	0
All	All	4624/4639 (99%)	860 (18%)	65 (1%)

5 of 860 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	5	9	G
5	5	14	A
5	5	17(A)	U
5	5	18	G
5	5	19	G

5 of 65 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	1089	A
7	A	1451	C
7	A	2529	G
7	A	1128	G
7	A	1286	A

## 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 ⓘ

There are no chain breaks in this entry.