wwPDB EM Validation Summary Report

Apr 16, 2024 – 09:52 am BST

PDB ID	:	6YEF
EMDB ID	:	EMD-10791
Title	:	70S initiation complex with assigned rRNA modifications from Staphylococcus aureus
Authors	:	Fatkhullin, B.; Golubev, A.; Khusainov, I.; Yusupova, G.; Yusupov, M.
Deposited on	:	2020-03-24
Resolution	:	3.20 Å(reported)
Based on initial model	:	5LI0

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

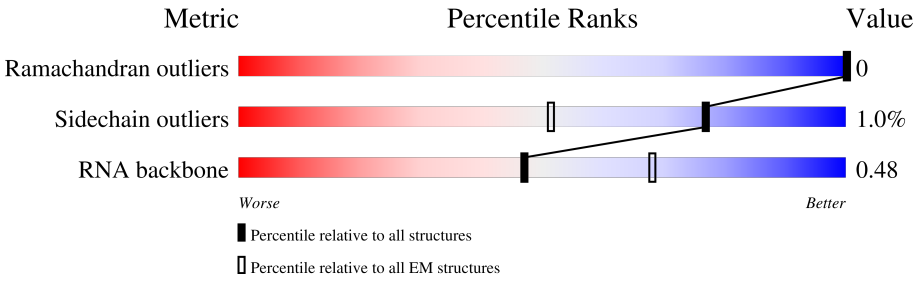
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Mol	Chain	Length	Quality of chain
1	a	1556	77% 21%
2	b	255	85% 14%
3	c	217	92% 8%
4	d	200	98%
5	e	166	93% 5%
6	f	98	96%
7	g	156	94% 6%
8	h	132	99%
9	i	132	95%

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Mol	Chain	Length	Quality of chain
10	j	102	96%
11	k	129	87% 12%
12	l	137	98%
13	m	121	96%
14	n	89	67% 33%
15	o	89	99%
16	p	91	99%
17	q	87	97%
18	r	80	80% 20%
19	s	92	85% 11%
20	t	83	96%
21	v	29	45% 24% 28%
22	A	2923	75% 22%
23	B	115	81% 17%
24	D	277	96%
25	E	220	98%
26	F	207	96%
27	G	179	85% 14%
28	H	178	88% 10%
29	M	145	100%
30	N	122	99%
31	O	146	96%
32	P	144	93% 5%
33	Q	122	97%
34	R	119	99%

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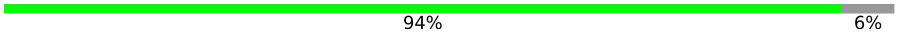
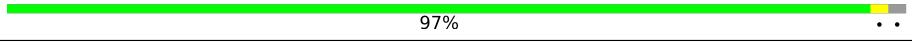
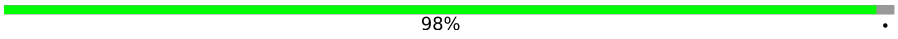
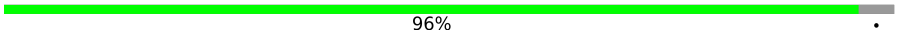
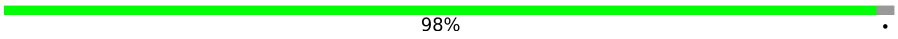
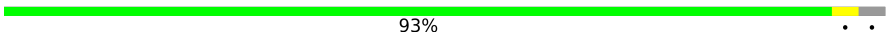
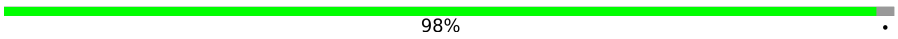
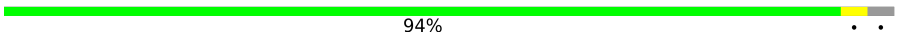
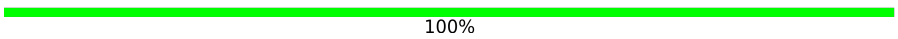
Mol	Chain	Length	Quality of chain
35	S	116	
36	T	118	
37	U	102	
38	V	117	
39	W	91	
40	X	105	
41	Y	217	
42	Z	94	
43	0	62	
44	1	69	
45	2	59	
46	3	84	
47	4	58	
48	5	49	
49	6	45	
50	7	66	
51	8	37	
52	x	77	

2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 141837 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
			Total	C	N	O	P		
1	a	1545	33097	14781	6034	10737	1545	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	219	1762	1123	307	325	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	200	1578	993	296	287	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	197	1600	1009	300	289	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	157	1169	735	214	218	2	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	96	798	503	139	153	3	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	146	Total	C	N	O	S	0	0
			1176	733	225	214	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	131	Total	C	N	O	S	0	0
			1032	652	183	193	4		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	127	Total	C	N	O	S	0	0
			1008	623	201	183	1		

- Molecule 10 is a protein called ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	98	Total	C	N	O	S	0	0
			783	494	143	145	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	113	Total	C	N	O	S	0	0
			833	514	156	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	117	Total	C	N	O	S	0	0
			927	569	184	173	1		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	60	Total 481	C 296	N 103	O 80	S 2	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total 738	C 454	N 153	O 130	S 1	0	0

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	90	Total 712	C 448	N 132	O 131	S 1	0	0

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	85	Total 698	C 441	N 125	O 131	S 1	0	0

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	64	Total 527	C 335	N 97	O 92	S 3	0	0

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	82	Total 661	C 426	N 118	O 115	S 2	0	0

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	80	Total 606	C 367	N 119	O 118	S 2	0	0

- Molecule 21 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	v	21	Total	C	N	O	P	0	0
			462	207	96	138	21		

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	A	2881	Total	C	N	O	P	0	0
			61802	27593	11324	20004	2881		

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B	115	Total	C	N	O	P	0	0
			2445	1094	436	801	114		

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	D	274	Total	C	N	O	S	0	0
			2094	1303	415	371	5		

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	E	216	Total	C	N	O	S	0	0
			1635	1023	301	306	5		

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	F	203	Total	C	N	O	S	0	0
			1540	966	284	288	2		

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	G	154	Total	C	N	O	S	0	0
			1191	751	206	228	6		

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	H	160	Total	C	N	O	S	0	0
			1250	781	222	244	3		

- Molecule 29 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	M	145	Total	C	N	O	S	0	0
			1151	717	211	220	3		

- Molecule 30 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	N	122	Total	C	N	O	S	0	0
			920	572	174	170	4		

- Molecule 31 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	O	146	Total	C	N	O	S	0	0
			1098	680	215	202	1		

- Molecule 32 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	P	137	Total	C	N	O	S	0	0
			1097	704	207	182	4		

- Molecule 33 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Q	119	Total	C	N	O	S	0	0
			940	575	181	183	1		

- Molecule 34 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	R	118	Total	C	N	O	0	0
			911	568	173	170		

- Molecule 35 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	S	109	Total 877	C 552	N 176	O 149	0	0

- Molecule 36 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	T	116	Total 943	C 593	N 189	O 157	S 4	0	0

- Molecule 37 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	U	100	Total 784	C 497	N 140	O 146	S 1	0	0

- Molecule 38 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	V	112	Total 862	C 537	N 164	O 158	S 3	0	0

- Molecule 39 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	W	89	Total 725	C 457	N 130	O 134	S 4	0	0

- Molecule 40 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	X	87	Total 662	C 420	N 119	O 122	S 1	0	0

- Molecule 41 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Y	94	Total 731	C 465	N 131	O 133	S 2	0	0

- Molecule 42 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	Z	82	Total 626	C 386	N 122	O 118	0	0

- Molecule 43 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	0	45	Total 358	C 222	N 78	O 58	0	0

- Molecule 44 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	1	65	Total 536	C 330	N 101	O 105	0	0

- Molecule 45 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	2	57	Total 441	C 274	N 83	O 84	0	0

- Molecule 46 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3	75	Total 593	C 371	N 106	O 113	S 3	0	0

- Molecule 47 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	4	52	Total 411	C 249	N 85	O 72	S 5	0	0

- Molecule 48 is a protein called 50S ribosomal protein L33 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5	44	Total 371	C 223	N 76	O 68	S 4	0	0

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	6	44	Total	C	N	O	S	0	0
			373	228	90	54	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	7	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	8	37	Total	C	N	O	S	0	0
			296	186	60	46	4		

- Molecule 52 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	x	77	Total	C	N	O	P	S	0	0
			1659	741	299	541	76	2		

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	a	54	Total	Mg	0
			54	54	
53	v	1	Total	Mg	0
			1	1	
53	A	207	Total	Mg	0
			207	207	
53	B	2	Total	Mg	0
			2	2	
53	D	1	Total	Mg	0
			1	1	
53	O	1	Total	Mg	0
			1	1	
53	X	1	Total	Mg	0
			1	1	
53	x	1	Total	Mg	0
			1	1	

- Molecule 54 is POTASSIUM ION (three-letter code: K) (formula: K).

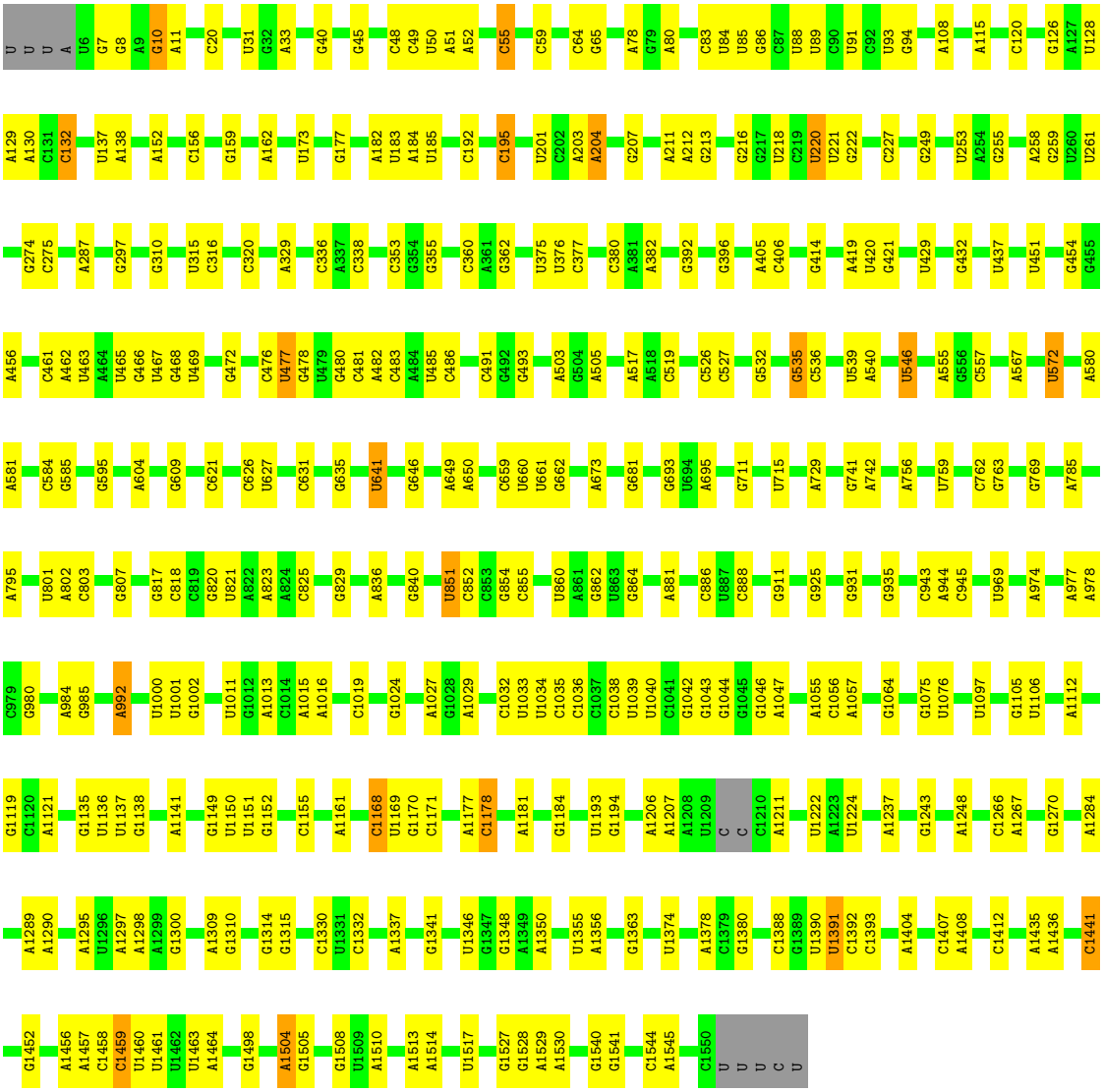
Mol	Chain	Residues	Atoms	AltConf
54	a	2	Total K 2 2	0
54	A	18	Total K 18 18	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 rRNA

Chain a:



- Molecule 2: 30S ribosomal protein S2

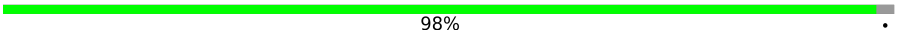
Chain b:

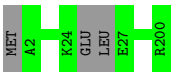
• Molecule 3: 30S ribosomal protein S3

Chain c:

• Molecule 4: 30S ribosomal protein S4

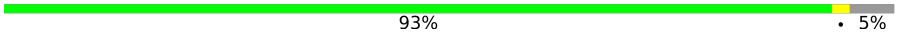
Chain d:

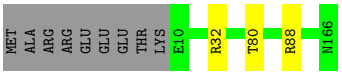




• Molecule 5: 30S ribosomal protein S5

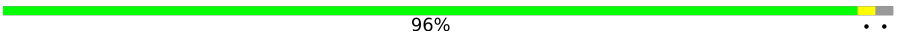
Chain e:

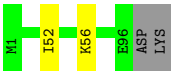




• Molecule 6: 30S ribosomal protein S6

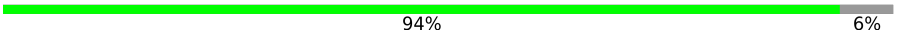
Chain f:

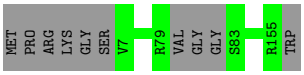




• Molecule 7: 30S ribosomal protein S7

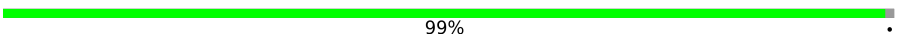
Chain g:





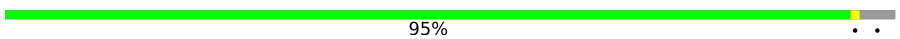
• Molecule 8: 30S ribosomal protein S8

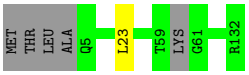
Chain h:



• Molecule 9: 30S ribosomal protein S9

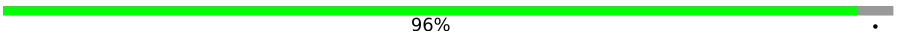
Chain i:

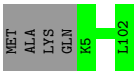




• Molecule 10: ribosomal protein uS10

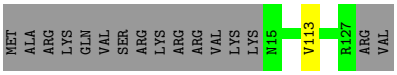
Chain j:





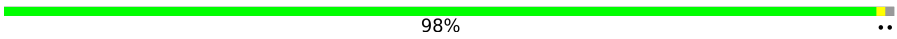
• Molecule 11: 30S ribosomal protein S11

Chain k:



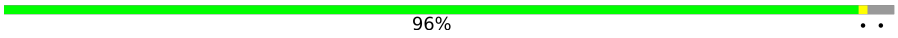
• Molecule 12: 30S ribosomal protein S12

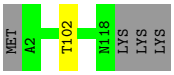
Chain l:



• Molecule 13: 30S ribosomal protein S13

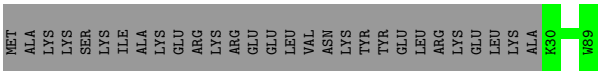
Chain m:





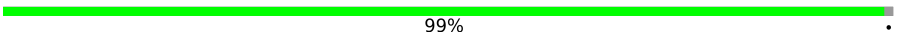
• Molecule 14: 30S ribosomal protein S14

Chain n:



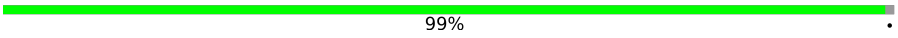
• Molecule 15: 30S ribosomal protein S15

Chain o:



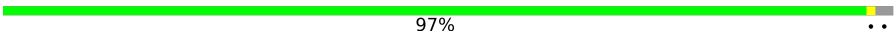
• Molecule 16: 30S ribosomal protein S16

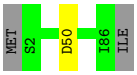
Chain p:



• Molecule 17: 30S ribosomal protein S17

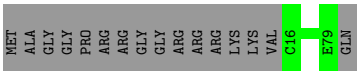
Chain q:





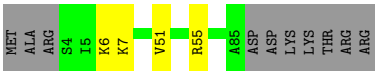
• Molecule 18: 30S ribosomal protein S18

Chain r:



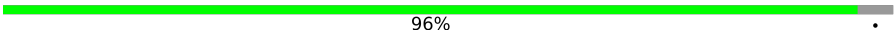
• Molecule 19: 30S ribosomal protein S19

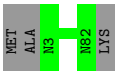
Chain s:



• Molecule 20: 30S ribosomal protein S20

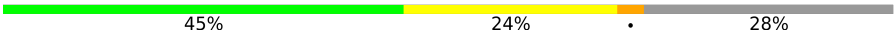
Chain t:

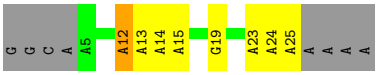




• Molecule 21: mRNA

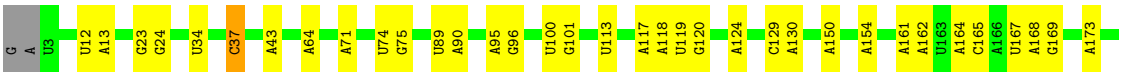
Chain v:

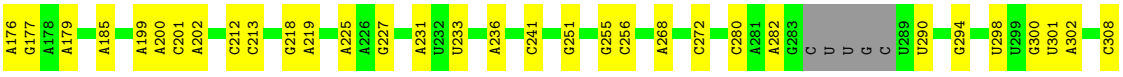


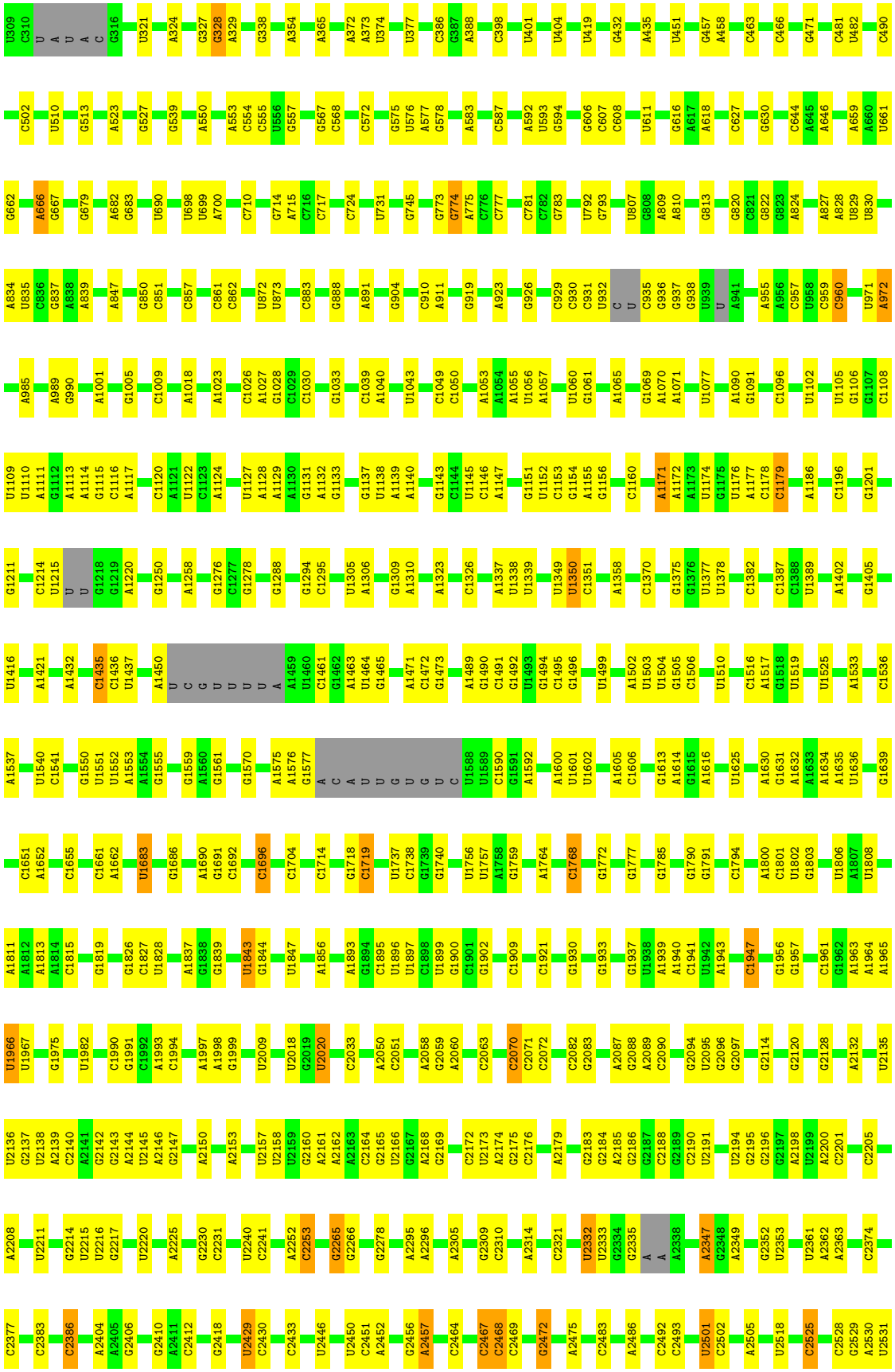


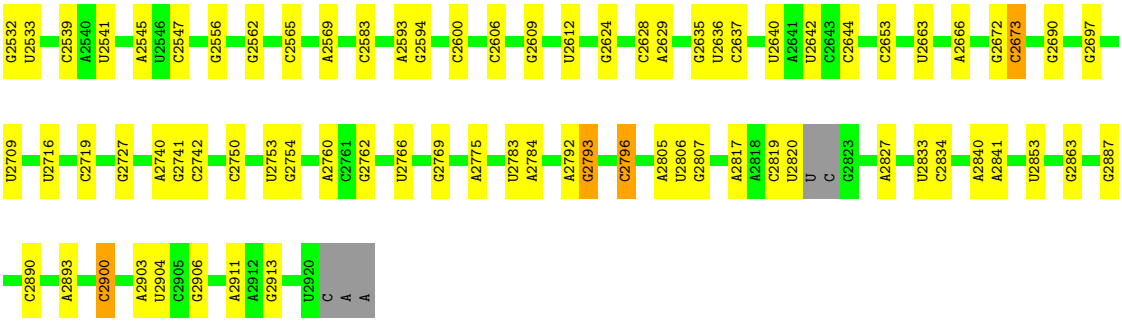
• Molecule 22: 23S rRNA

Chain A:



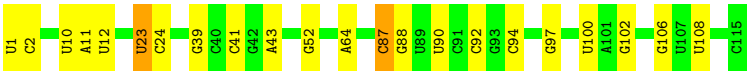






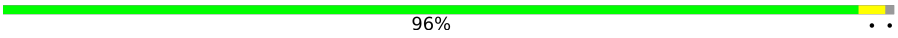
• Molecule 23: 5S rRNA

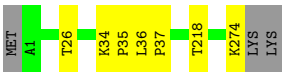
Chain B:



• Molecule 24: 50S ribosomal protein L2

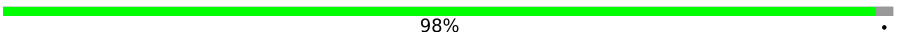
Chain D:

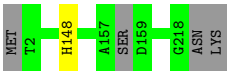




• Molecule 25: 50S ribosomal protein L3

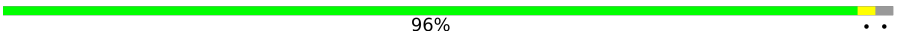
Chain E:





• Molecule 26: 50S ribosomal protein L4

Chain F:



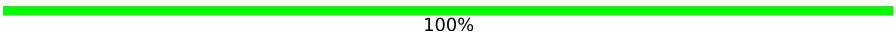
• Molecule 27: 50S ribosomal protein L5

Chain G:

• Molecule 28: 50S ribosomal protein L6

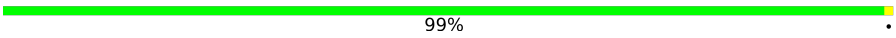
Chain H:

• Molecule 29: 50S ribosomal protein L13

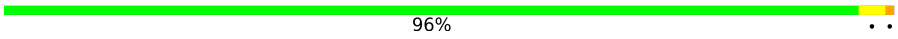
Chain M: 

There are no outlier residues recorded for this chain.

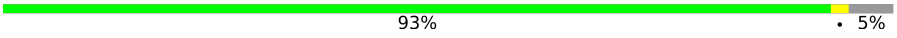
• Molecule 30: 50S ribosomal protein L14

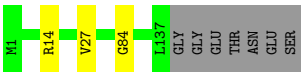
Chain N: 

• Molecule 31: 50S ribosomal protein L15

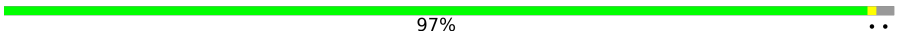
Chain O: 

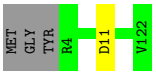
• Molecule 32: 50S ribosomal protein L16

Chain P: 

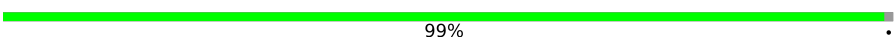


• Molecule 33: 50S ribosomal protein L17

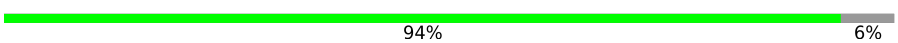
Chain Q: 

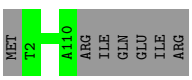


• Molecule 34: 50S ribosomal protein L18

Chain R: 

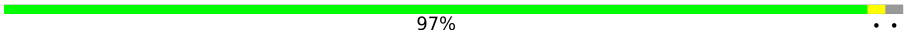
• Molecule 35: 50S ribosomal protein L19

Chain S: 



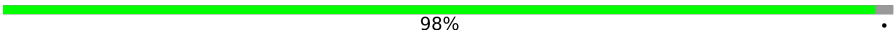
• Molecule 36: 50S ribosomal protein L20

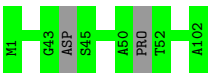
Chain T:



• Molecule 37: 50S ribosomal protein L21

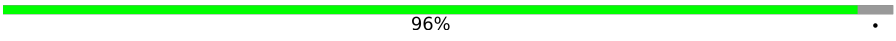
Chain U:





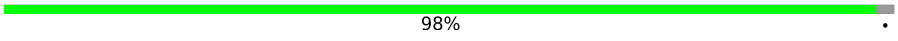
• Molecule 38: 50S ribosomal protein L22

Chain V:



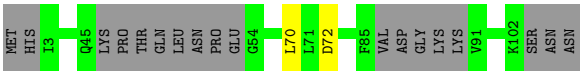
• Molecule 39: 50S ribosomal protein L23

Chain W:



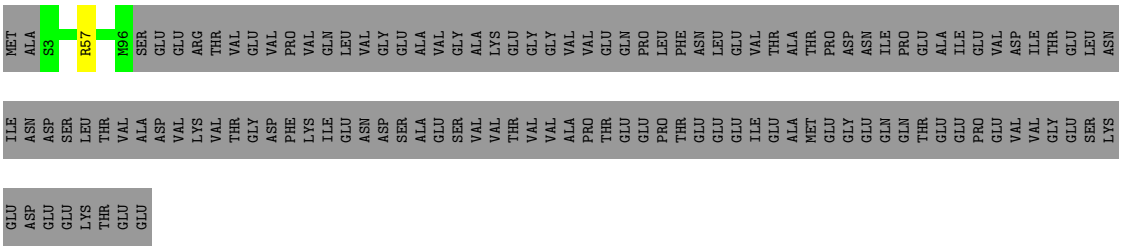
• Molecule 40: 50S ribosomal protein L24

Chain X:



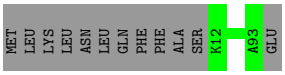
• Molecule 41: 50S ribosomal protein L25

Chain Y:



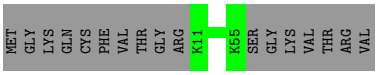
• Molecule 42: 50S ribosomal protein L27

Chain Z:



• Molecule 43: 50S ribosomal protein L28

Chain 0:

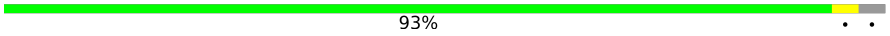


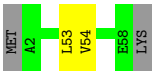
• Molecule 44: 50S ribosomal protein L29

Chain 1:

• Molecule 45: 50S ribosomal protein L30

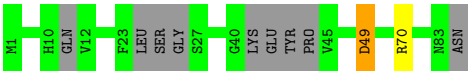
Chain 2:





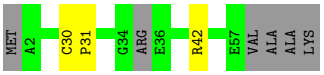
• Molecule 46: 50S ribosomal protein L31 type B

Chain 3:



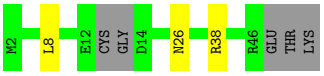
• Molecule 47: 50S ribosomal protein L32

Chain 4:



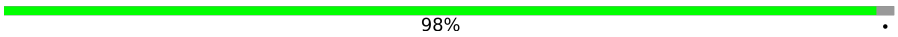
• Molecule 48: 50S ribosomal protein L33 2

Chain 5:



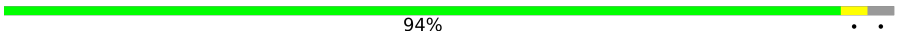
• Molecule 49: 50S ribosomal protein L34

Chain 6:



• Molecule 50: 50S ribosomal protein L35

Chain 7:



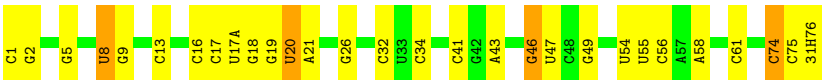
• Molecule 51: 50S ribosomal protein L36

Chain 8:

There are no outlier residues recorded for this chain.

• Molecule 52: P-site tRNA

Chain x:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	83000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	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: PSU, 2MA, 4OC, MG, H2U, OMC, K, 31H, 4SU, 7MG, MA6, 2MG, OMG, 5MU

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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	a	0.47	1/36920 (0.0%)	0.98	103/57570 (0.2%)
2	b	0.29	0/1788	0.53	0/2397
3	c	0.27	0/1598	0.52	0/2145
4	d	0.30	0/1629	0.54	0/2185
5	e	0.30	0/1183	0.57	1/1595 (0.1%)
6	f	0.30	0/809	0.51	0/1085
7	g	0.29	0/1192	0.50	0/1603
8	h	0.29	0/1044	0.56	0/1401
9	i	0.30	0/1023	0.58	1/1372 (0.1%)
10	j	0.28	0/795	0.55	0/1071
11	k	0.28	0/848	0.50	0/1147
12	l	0.30	0/1075	0.58	0/1439
13	m	0.28	0/934	0.56	0/1253
14	n	0.26	0/490	0.49	0/650
15	o	0.25	0/747	0.45	0/996
16	p	0.30	0/723	0.56	0/971
17	q	0.28	0/706	0.56	0/944
18	r	0.28	0/536	0.51	0/718
19	s	0.27	0/679	0.50	0/912
20	t	0.23	0/606	0.47	0/810
21	v	0.43	0/521	1.02	1/812 (0.1%)
22	A	0.78	4/69062 (0.0%)	1.06	202/107697 (0.2%)
23	B	0.49	0/2733	1.06	21/4257 (0.5%)
24	D	0.45	2/2129 (0.1%)	0.64	2/2858 (0.1%)
25	E	0.40	0/1659	0.59	1/2224 (0.0%)
26	F	0.39	0/1563	0.56	0/2113
27	G	0.29	0/1201	0.53	0/1610
28	H	0.29	0/1267	0.53	0/1710
29	M	0.35	0/1173	0.52	0/1578
30	N	0.39	0/927	0.58	0/1243
31	O	0.42	1/1112 (0.1%)	0.63	1/1482 (0.1%)
32	P	0.39	0/1121	0.58	1/1504 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Q	0.34	0/943	0.57	0/1259
34	R	0.29	0/920	0.53	0/1230
35	S	0.37	0/889	0.61	0/1189
36	T	0.40	0/955	0.52	0/1265
37	U	0.37	0/791	0.55	0/1051
38	V	0.36	0/870	0.58	0/1171
39	W	0.36	0/733	0.57	0/978
40	X	0.32	0/666	0.66	1/886 (0.1%)
41	Y	0.29	0/738	0.54	0/989
42	Z	0.43	0/632	0.55	0/838
43	0	0.39	0/363	0.66	0/486
44	1	0.29	0/537	0.49	0/714
45	2	0.34	0/443	0.61	1/597 (0.2%)
46	3	0.31	0/602	0.61	1/802 (0.1%)
47	4	0.52	1/416 (0.2%)	0.63	1/550 (0.2%)
48	5	0.31	0/373	0.69	1/495 (0.2%)
49	6	0.41	0/377	0.56	0/491
50	7	0.37	0/526	0.56	0/690
51	8	0.36	0/299	0.53	0/392
52	x	0.46	0/1671	1.08	10/2605 (0.4%)
All	All	0.61	9/153537 (0.0%)	0.94	349/230030 (0.2%)

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
3	c	0	1
5	e	0	1
26	F	0	1
30	N	0	1
36	T	0	1
44	1	0	2
48	5	0	1
All	All	0	8

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	774	G	N9-C4	-6.94	1.32	1.38
22	A	774	G	C2-N3	-6.62	1.27	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	774	G	N3-C4	-5.88	1.31	1.35
1	a	204	A	N9-C4	5.49	1.41	1.37
31	O	8	PRO	N-CD	5.43	1.55	1.47

The worst 5 of 349 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	774	G	N3-C4-N9	-13.61	117.83	126.00
22	A	12	U	N1-C2-O2	12.05	131.24	122.80
22	A	12	U	N3-C2-O2	-11.78	113.95	122.20
22	A	12	U	C2-N1-C1'	11.58	131.59	117.70
23	B	87	C	N1-C2-O2	10.47	125.19	118.90

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	F	188	ASN	Peptide
30	N	17	ARG	Sidechain
36	T	25	PHE	Peptide
3	c	155	ARG	Sidechain
5	e	32	ARG	Sidechain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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
2	b	215/255 (84%)	202 (94%)	13 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	194/217 (89%)	186 (96%)	8 (4%)	0	100	100
4	d	193/200 (96%)	187 (97%)	6 (3%)	0	100	100
5	e	155/166 (93%)	151 (97%)	4 (3%)	0	100	100
6	f	94/98 (96%)	92 (98%)	2 (2%)	0	100	100
7	g	142/156 (91%)	137 (96%)	5 (4%)	0	100	100
8	h	129/132 (98%)	125 (97%)	4 (3%)	0	100	100
9	i	123/132 (93%)	117 (95%)	6 (5%)	0	100	100
10	j	96/102 (94%)	90 (94%)	6 (6%)	0	100	100
11	k	111/129 (86%)	105 (95%)	6 (5%)	0	100	100
12	l	133/137 (97%)	126 (95%)	7 (5%)	0	100	100
13	m	115/121 (95%)	113 (98%)	2 (2%)	0	100	100
14	n	58/89 (65%)	58 (100%)	0	0	100	100
15	o	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	p	88/91 (97%)	83 (94%)	5 (6%)	0	100	100
17	q	83/87 (95%)	75 (90%)	8 (10%)	0	100	100
18	r	62/80 (78%)	60 (97%)	2 (3%)	0	100	100
19	s	80/92 (87%)	78 (98%)	2 (2%)	0	100	100
20	t	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
24	D	272/277 (98%)	265 (97%)	7 (3%)	0	100	100
25	E	214/220 (97%)	205 (96%)	9 (4%)	0	100	100
26	F	201/207 (97%)	192 (96%)	9 (4%)	0	100	100
27	G	148/179 (83%)	139 (94%)	9 (6%)	0	100	100
28	H	156/178 (88%)	145 (93%)	11 (7%)	0	100	100
29	M	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
30	N	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
31	O	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
32	P	135/144 (94%)	134 (99%)	1 (1%)	0	100	100
33	Q	117/122 (96%)	114 (97%)	3 (3%)	0	100	100
34	R	116/119 (98%)	114 (98%)	2 (2%)	0	100	100
35	S	107/116 (92%)	101 (94%)	6 (6%)	0	100	100
36	T	114/118 (97%)	110 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	U	94/102 (92%)	90 (96%)	4 (4%)	0	100	100
38	V	110/117 (94%)	106 (96%)	4 (4%)	0	100	100
39	W	87/91 (96%)	84 (97%)	3 (3%)	0	100	100
40	X	81/105 (77%)	75 (93%)	6 (7%)	0	100	100
41	Y	92/217 (42%)	90 (98%)	2 (2%)	0	100	100
42	Z	80/94 (85%)	76 (95%)	4 (5%)	0	100	100
43	0	43/62 (69%)	38 (88%)	5 (12%)	0	100	100
44	1	63/69 (91%)	62 (98%)	1 (2%)	0	100	100
45	2	55/59 (93%)	51 (93%)	4 (7%)	0	100	100
46	3	67/84 (80%)	62 (92%)	5 (8%)	0	100	100
47	4	47/58 (81%)	45 (96%)	2 (4%)	0	100	100
48	5	40/49 (82%)	36 (90%)	4 (10%)	0	100	100
49	6	42/45 (93%)	40 (95%)	2 (5%)	0	100	100
50	7	62/66 (94%)	56 (90%)	6 (10%)	0	100	100
51	8	35/37 (95%)	35 (100%)	0	0	100	100
All	All	5220/5804 (90%)	5003 (96%)	217 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	
2	b	189/221 (86%)	187 (99%)	2 (1%)	73	88
3	c	162/175 (93%)	162 (100%)	0	100	100
4	d	172/175 (98%)	172 (100%)	0	100	100
5	e	123/131 (94%)	122 (99%)	1 (1%)	81	93
6	f	84/86 (98%)	82 (98%)	2 (2%)	49	77
7	g	125/132 (95%)	125 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	h	112/113 (99%)	112 (100%)	0	100	100
9	i	105/109 (96%)	105 (100%)	0	100	100
10	j	88/91 (97%)	88 (100%)	0	100	100
11	k	89/104 (86%)	88 (99%)	1 (1%)	73	88
12	l	117/119 (98%)	116 (99%)	1 (1%)	78	91
13	m	100/104 (96%)	99 (99%)	1 (1%)	76	90
14	n	50/78 (64%)	50 (100%)	0	100	100
15	o	80/81 (99%)	80 (100%)	0	100	100
16	p	76/77 (99%)	76 (100%)	0	100	100
17	q	80/82 (98%)	79 (99%)	1 (1%)	69	87
18	r	57/68 (84%)	57 (100%)	0	100	100
19	s	71/80 (89%)	67 (94%)	4 (6%)	21	57
20	t	67/69 (97%)	67 (100%)	0	100	100
24	D	221/224 (99%)	218 (99%)	3 (1%)	67	86
25	E	173/177 (98%)	173 (100%)	0	100	100
26	F	163/169 (96%)	158 (97%)	5 (3%)	40	72
27	G	131/158 (83%)	130 (99%)	1 (1%)	81	93
28	H	141/155 (91%)	137 (97%)	4 (3%)	43	74
29	M	123/123 (100%)	123 (100%)	0	100	100
30	N	100/100 (100%)	100 (100%)	0	100	100
31	O	112/112 (100%)	107 (96%)	5 (4%)	27	63
32	P	114/119 (96%)	112 (98%)	2 (2%)	59	82
33	Q	100/102 (98%)	99 (99%)	1 (1%)	76	90
34	R	93/95 (98%)	93 (100%)	0	100	100
35	S	95/102 (93%)	95 (100%)	0	100	100
36	T	96/98 (98%)	95 (99%)	1 (1%)	76	90
37	U	84/86 (98%)	84 (100%)	0	100	100
38	V	91/94 (97%)	91 (100%)	0	100	100
39	W	80/82 (98%)	80 (100%)	0	100	100
40	X	72/90 (80%)	71 (99%)	1 (1%)	67	86
41	Y	82/190 (43%)	81 (99%)	1 (1%)	71	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
42	Z	64/75 (85%)	64 (100%)	0	100 100
43	0	37/52 (71%)	37 (100%)	0	100 100
44	1	59/62 (95%)	59 (100%)	0	100 100
45	2	51/53 (96%)	50 (98%)	1 (2%)	55 80
46	3	63/75 (84%)	61 (97%)	2 (3%)	39 71
47	4	46/51 (90%)	45 (98%)	1 (2%)	52 79
48	5	43/47 (92%)	42 (98%)	1 (2%)	50 78
49	6	39/40 (98%)	39 (100%)	0	100 100
50	7	55/57 (96%)	53 (96%)	2 (4%)	35 69
51	8	34/35 (97%)	34 (100%)	0	100 100
All	All	4509/4918 (92%)	4465 (99%)	44 (1%)	77 90

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
31	O	129	SER
40	X	72	ASP
31	O	134	GLU
32	P	27	VAL
45	2	54	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
46	3	55	HIS
46	3	83	ASN
50	7	31	HIS
17	q	49	HIS
15	o	68	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1541/1556 (99%)	310 (20%)	0
21	v	20/29 (68%)	8 (40%)	0
22	A	2870/2923 (98%)	584 (20%)	8 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	B	114/115 (99%)	17 (14%)	1 (0%)
52	x	75/77 (97%)	21 (28%)	0
All	All	4620/4700 (98%)	940 (20%)	9 (0%)

5 of 940 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	7	G
1	a	8	G
1	a	10	G
1	a	11	A
1	a	31	U

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	A	2783	U
23	B	23	U
22	A	971	U
22	A	1503	U
22	A	1550	G

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

18 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	$\#\|Z\| > 2$
52	H2U	x	20	52	22,22,22	0.94	2 (9%)	28,33,33	2.84	6 (21%)
22	OMG	A	2278	22,52	18,26,27	2.31	7 (38%)	19,38,41	1.51	4 (21%)
1	2MG	a	1527	1	18,26,27	2.37	7 (38%)	16,38,41	1.43	3 (18%)
52	4SU	x	8	52	22,22,22	1.71	4 (18%)	33,33,33	2.82	13 (39%)
1	MA6	a	1530	1	18,26,27	1.03	2 (11%)	19,38,41	3.52	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
52	31H	x	76	52,53	28,34,35	4.57	13 (46%)	23,47,50	2.80	6 (26%)
22	5MU	A	1966	22,54	19,22,23	4.82	7 (36%)	28,32,35	3.83	9 (32%)
22	2MA	A	2530	22,54,53	17,25,26	2.41	5 (29%)	17,37,40	1.55	4 (23%)
52	5MU	x	54	52	23,23,23	4.53	7 (30%)	35,35,35	3.83	15 (42%)
1	7MG	a	535	1	22,26,27	3.80	10 (45%)	29,39,42	2.07	9 (31%)
52	7MG	x	46	52	26,27,27	3.49	10 (38%)	36,42,42	2.74	15 (41%)
22	2MG	A	2472	22	18,26,27	2.25	7 (38%)	16,38,41	1.66	4 (25%)
52	OMC	x	32	52	23,23,23	2.73	8 (34%)	33,34,34	2.28	8 (24%)
22	OMC	A	1947	22	19,22,23	2.84	8 (42%)	26,31,34	0.88	1 (3%)
22	OMC	A	2525	22	19,22,23	2.75	7 (36%)	26,31,34	0.99	1 (3%)
1	MA6	a	1529	1	18,26,27	1.04	2 (11%)	19,38,41	3.12	2 (10%)
1	4OC	a	1412	1	20,23,24	3.07	8 (40%)	26,32,35	1.04	2 (7%)
52	PSU	x	55	52	22,22,22	1.25	3 (13%)	29,33,33	2.75	11 (37%)

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
52	H2U	x	20	52	-	4/10/39/39	0/2/2/2
22	OMG	A	2278	22,52	-	0/5/27/28	0/3/3/3
1	2MG	a	1527	1	-	0/5/27/28	0/3/3/3
52	4SU	x	8	52	-	1/10/26/26	0/2/2/2
1	MA6	a	1530	1	-	2/7/29/30	0/3/3/3
52	31H	x	76	52,53	-	14/18/40/41	0/3/3/3
22	5MU	A	1966	22,54	-	2/7/25/26	0/2/2/2
22	2MA	A	2530	22,54,53	-	2/3/25/26	0/3/3/3
52	5MU	x	54	52	-	2/10/26/26	0/2/2/2
1	7MG	a	535	1	-	2/7/37/38	0/3/3/3
52	7MG	x	46	52	-	5/10/38/38	0/3/3/3
22	2MG	A	2472	22	-	2/5/27/28	0/3/3/3
52	OMC	x	32	52	-	4/12/28/28	0/2/2/2
22	OMC	A	1947	22	-	2/9/27/28	0/2/2/2
22	OMC	A	2525	22	-	2/9/27/28	0/2/2/2
1	MA6	a	1529	1	-	1/7/29/30	0/3/3/3
1	4OC	a	1412	1	-	2/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	PSU	x	55	52	-	4/10/26/26	0/2/2/2

The worst 5 of 117 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	x	76	31H	C4'-C3'	-13.83	1.28	1.52
52	x	54	5MU	C2-N1	11.56	1.57	1.38
52	x	54	5MU	C6-N1	11.11	1.57	1.38
22	A	1966	5MU	C6-N1	10.80	1.56	1.38
22	A	1966	5MU	C2-N1	10.59	1.55	1.38

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	1530	MA6	N1-C6-N6	-13.63	102.72	117.06
22	A	1966	5MU	C5-C4-N3	12.76	126.20	115.31
52	x	54	5MU	C5-C4-N3	12.34	125.84	115.31
1	a	1529	MA6	N1-C6-N6	-12.04	104.38	117.06
22	A	1966	5MU	C5-C6-N1	-11.02	112.00	123.34

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	1530	MA6	O4'-C4'-C5'-O5'
22	A	1947	OMC	O4'-C4'-C5'-O5'
52	x	20	H2U	O4'-C4'-C5'-O5'
52	x	32	OMC	C5'-O5'-P-OP1
52	x	46	7MG	C5'-O5'-P-OP3

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 288 ligands modelled in this entry, 288 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
47	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	53:GLU	C	57:GLU	N	9.89

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10791. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.