wwPDB EM Validation Summary Report

Mar 6, 2025 – 03:02 pm GMT

PDB ID	:	8AP4
EMDB ID	:	EMD-15558
Title	:	Structure of Escherischia coli heat shock protein Hsp15 in complex with ribosomal 50S subunits bearing peptidyl-tRNA
Authors	:	Safdari, H.A.; Wilson, D.N.
Deposited on	:	2022-08-09
Resolution	:	3.00 Å(reported)

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 ⓘ 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 ⓘ) were used in the production of this report:

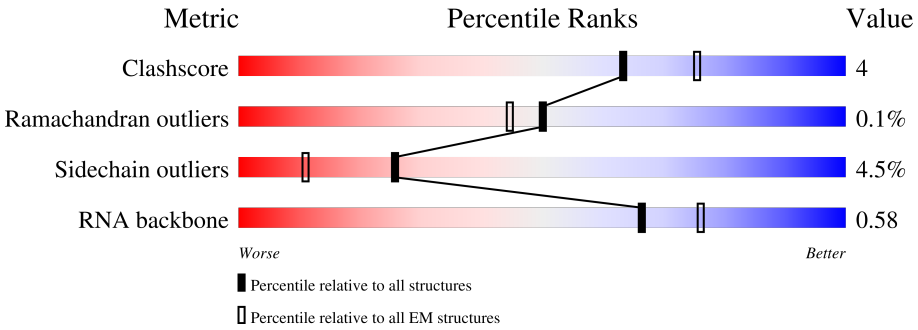
EMDB validation analysis	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	0	55	85% 7% 7%
2	1	46	91% 9%
3	2	65	89% 6%
4	3	38	89% 11%
5	4	70	54% 14% 31%
6	A	133	65% 11% 23%
7	Z	76	64% 13% 9% 7% 7%

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Mol	Chain	Length	Quality of chain
8	a	2904	83% 11% 5%
9	b	120	88% 12%
10	c	273	94% 5%
11	d	209	98%
12	e	201	96%
13	f	179	87% 12%
14	g	177	95%
15	h	149	27% 72%
16	i	142	96%
17	j	123	96%
18	k	144	97%
19	l	136	98%
20	m	127	91% 7%
21	n	117	91% 8%
22	o	115	93% 6%
23	p	118	97%
24	q	103	93% 7%
25	r	110	95% 5%
26	s	100	89% 7%
27	t	104	97%
28	u	94	98%
29	v	85	86% 5% 8%
30	w	78	97%
31	x	63	94% 5%
32	y	59	98%

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Mol	Chain	Length	Quality of chain
33	z	57	96%

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 88614 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 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	48	Total	C	N	O	S	0	0
			373	232	66	69	6		

- Molecule 6 is a protein called Heat shock protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	102	Total	C	N	O	S	0	0
			820	513	155	150	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Z	71	Total	C	N	O	P	0	0
			1521	677	280	493	71		

- Molecule 8 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	2750	Total	C	N	O	P	0	0
			59067	26355	10887	19075	2750		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1915	N	U	conflict	GB 939732440

- Molecule 9 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 10 is a protein called 50S ribosomal protein L2.

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

- Molecule 11 is a protein called 50S ribosomal protein L3.

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

- Molecule 12 is a protein called 50S ribosomal protein L4.

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

- Molecule 13 is a protein called 50S ribosomal protein L5.

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

- Molecule 14 is a protein called 50S ribosomal protein L6.

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

- Molecule 15 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 16 is a protein called 50S ribosomal protein L13.

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

- Molecule 17 is a protein called 50S ribosomal protein L14.

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

- Molecule 18 is a protein called 50S ribosomal protein L15.

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

- Molecule 19 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	l	135	Total	C	N	O	S	0	0
			1066	681	204	176	5		

- Molecule 20 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	m	118	Total 945	C 585	N 194	O 161	S 5	0	0

- Molecule 21 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	n	116	Total 892	C 552	N 178	O 162	0	0

- Molecule 22 is a protein called 50S ribosomal protein L19.

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

- Molecule 23 is a protein called 50S ribosomal protein L20.

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

- Molecule 24 is a protein called 50S ribosomal protein L21.

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

- Molecule 25 is a protein called 50S ribosomal protein L22.

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

- Molecule 26 is a protein called 50S ribosomal protein L23.

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

- Molecule 27 is a protein called 50S ribosomal protein L24.

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

- Molecule 28 is a protein called 50S ribosomal protein L25.

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

- Molecule 29 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	v	78	Total 592	C 365	N 119	O 107	S 1	0	0

- Molecule 30 is a protein called 50S ribosomal protein L28.

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

- Molecule 31 is a protein called 50S ribosomal protein L29.

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

- Molecule 32 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	y	58	Total 449	C 281	N 87	O 79	S 2	0	0

- Molecule 33 is a protein called 50S ribosomal protein L32.

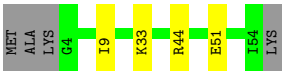
Mol	Chain	Residues	Atoms					AltConf	Trace
33	z	56	Total 444	C 269	N 94	O 80	S 1	0	0

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.

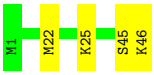
- Molecule 1: 50S ribosomal protein L33

Chain 0:



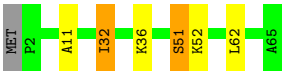
- Molecule 2: 50S ribosomal protein L34

Chain 1:



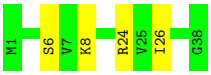
- Molecule 3: 50S ribosomal protein L35

Chain 2:



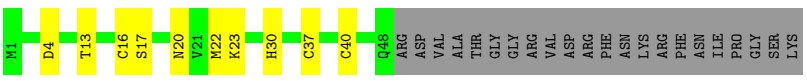
- Molecule 4: 50S ribosomal protein L36

Chain 3:



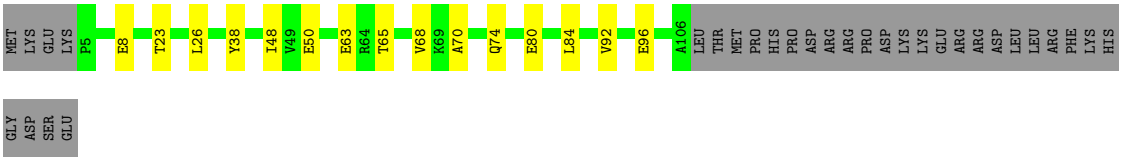
- Molecule 5: 50S ribosomal protein L31

Chain 4:



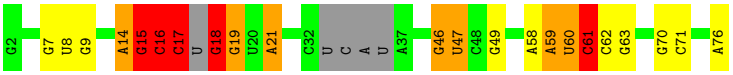
- Molecule 6: Heat shock protein 15

Chain A:



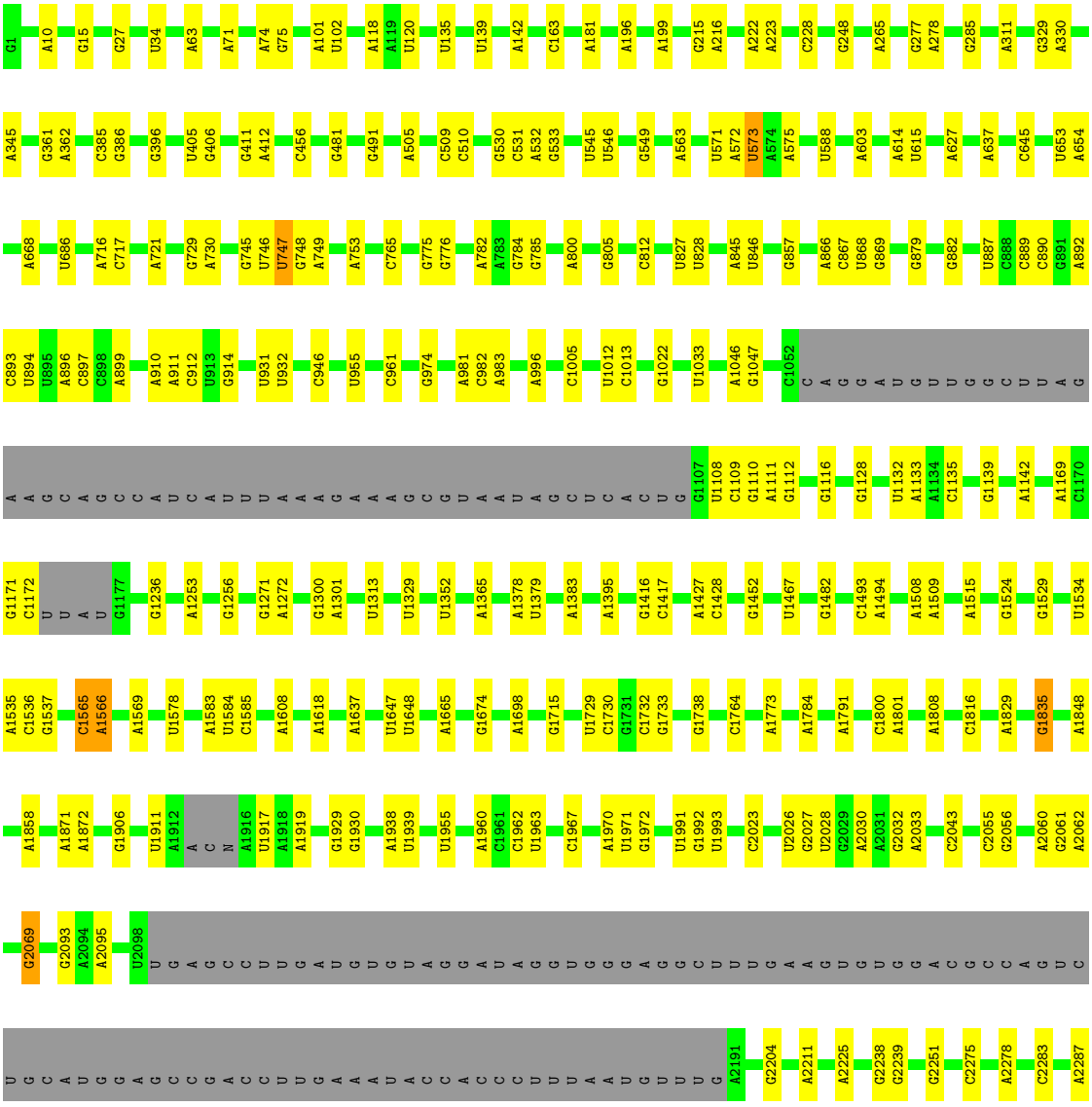
• Molecule 7: P-tRNA

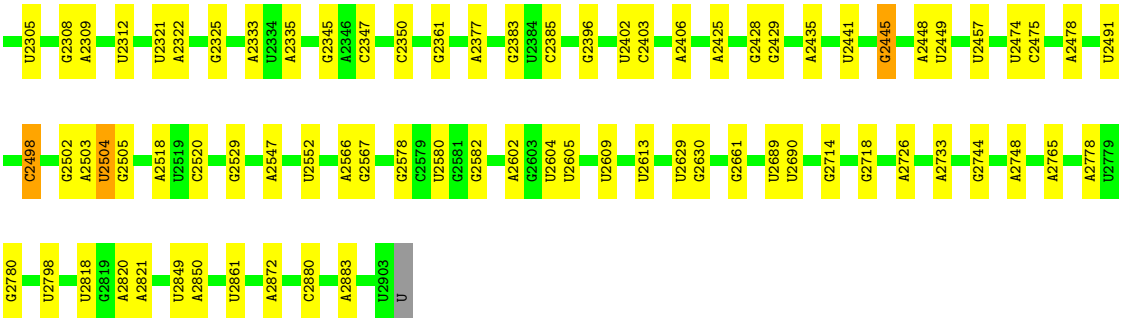
Chain Z:



• Molecule 8: 23S rRNA

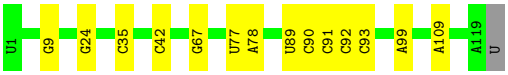
Chain a:





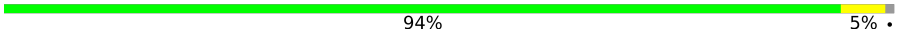
• Molecule 9: 5S rRNA

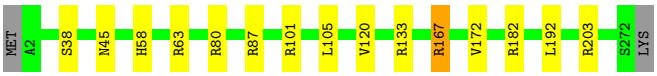
Chain b:



• Molecule 10: 50S ribosomal protein L2

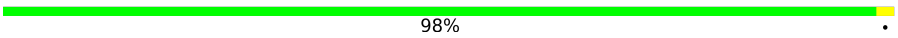
Chain c:

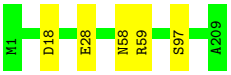




• Molecule 11: 50S ribosomal protein L3

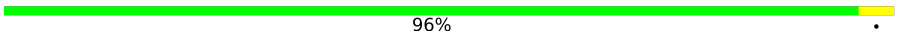
Chain d:





• Molecule 12: 50S ribosomal protein L4

Chain e:

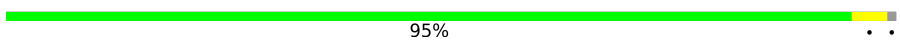


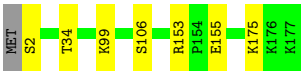
• Molecule 13: 50S ribosomal protein L5

Chain f:

• Molecule 14: 50S ribosomal protein L6

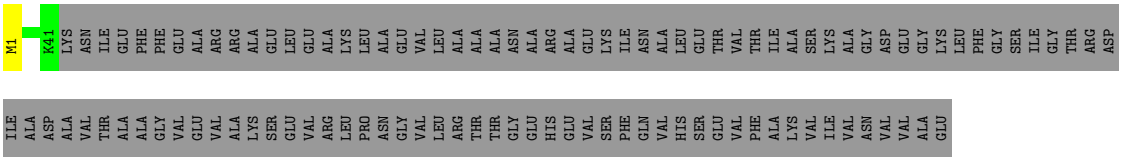
Chain g:





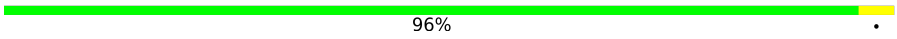
• Molecule 15: 50S ribosomal protein L9

Chain h:



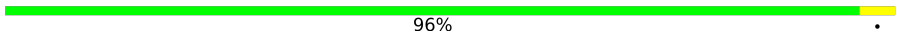
• Molecule 16: 50S ribosomal protein L13

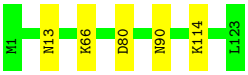
Chain i:



• Molecule 17: 50S ribosomal protein L14

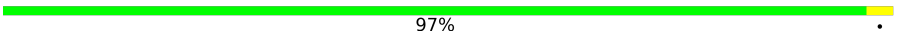
Chain j:

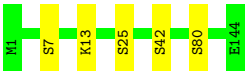




• Molecule 18: 50S ribosomal protein L15

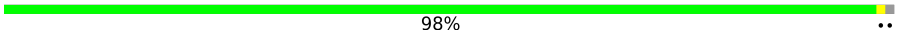
Chain k:





• Molecule 19: 50S ribosomal protein L16

Chain l:

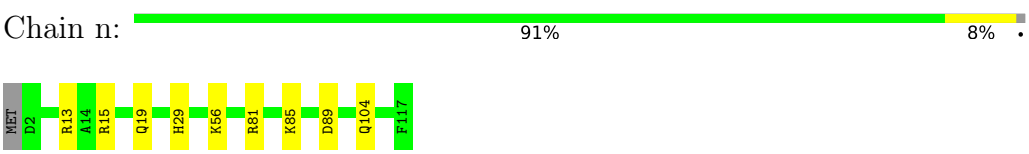


• Molecule 20: 50S ribosomal protein L17

Chain m:

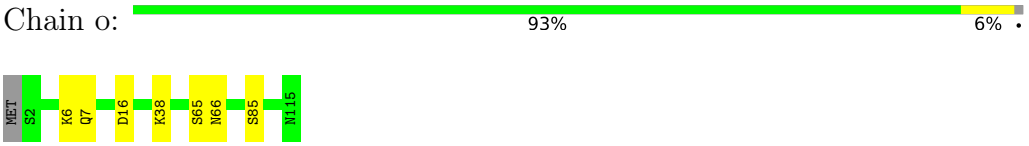
• Molecule 21: 50S ribosomal protein L18

Chain n:



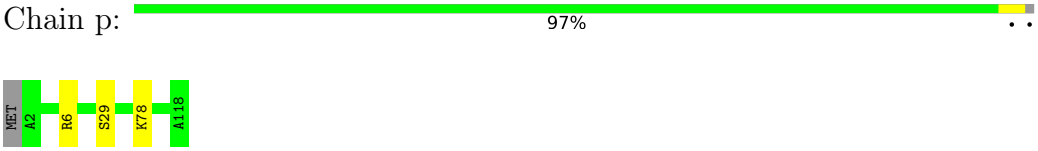
• Molecule 22: 50S ribosomal protein L19

Chain o:



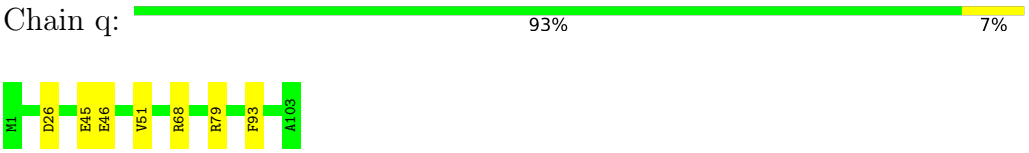
• Molecule 23: 50S ribosomal protein L20

Chain p:



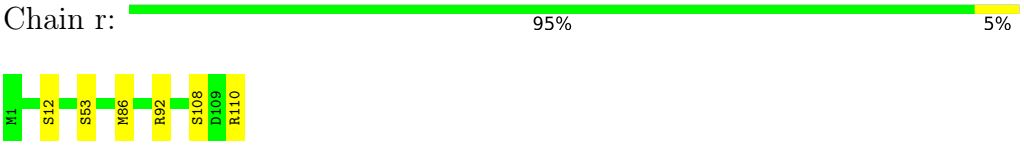
• Molecule 24: 50S ribosomal protein L21

Chain q:



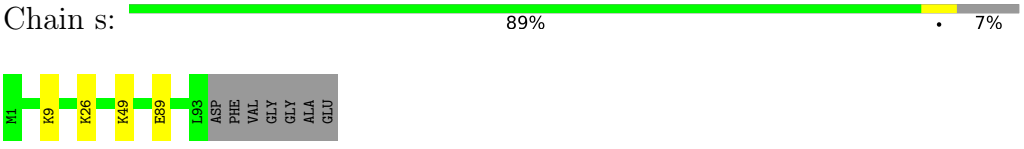
• Molecule 25: 50S ribosomal protein L22

Chain r:



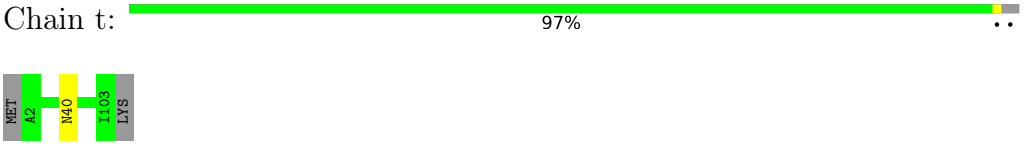
• Molecule 26: 50S ribosomal protein L23

Chain s:



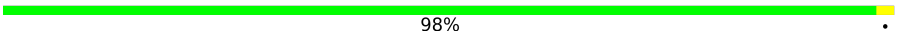
• Molecule 27: 50S ribosomal protein L24

Chain t:



• Molecule 28: 50S ribosomal protein L25

Chain u:

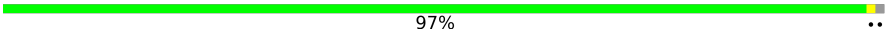


• Molecule 29: 50S ribosomal protein L27

Chain v:

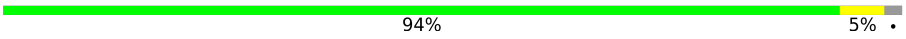
• Molecule 30: 50S ribosomal protein L28

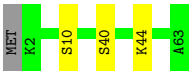
Chain w:



• Molecule 31: 50S ribosomal protein L29

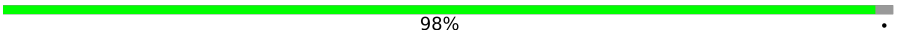
Chain x:





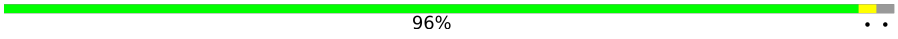
• Molecule 32: 50S ribosomal protein L30

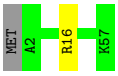
Chain y:



• Molecule 33: 50S ribosomal protein L32

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	247060	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 ($e^-/Å^2$)	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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: 6MZ, OMU, 5MC, 5MU, 2MA, G7M, OMC, PSU, 2MG, OMG, 1MG

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	0	0.44	0/424	0.64	0/565
2	1	0.35	0/380	0.77	0/498
3	2	0.36	0/513	0.65	0/676
4	3	0.36	0/303	0.69	0/397
5	4	0.36	0/380	0.68	1/508 (0.2%)
6	A	0.29	0/831	0.59	0/1116
7	Z	0.40	0/1699	1.00	8/2646 (0.3%)
8	a	0.77	7/65626 (0.0%)	0.83	26/102374 (0.0%)
9	b	0.64	0/2850	0.84	5/4444 (0.1%)
10	c	0.51	0/2121	0.69	0/2852
11	d	0.40	0/1586	0.62	1/2134 (0.0%)
12	e	0.38	0/1571	0.68	2/2113 (0.1%)
13	f	0.40	0/1434	0.78	2/1926 (0.1%)
14	g	0.38	0/1343	0.65	0/1816
15	h	0.42	0/306	0.70	0/413
16	i	0.43	0/1152	0.63	0/1551
17	j	0.38	0/955	0.70	0/1279
18	k	0.36	0/1062	0.68	0/1413
19	l	0.41	0/1085	0.66	0/1450
20	m	0.37	0/958	0.71	0/1281
21	n	0.36	0/902	0.73	1/1209 (0.1%)
22	o	0.38	0/929	0.70	0/1242
23	p	0.46	0/960	0.64	0/1278
24	q	0.43	0/829	0.73	0/1107
25	r	0.36	0/864	0.68	0/1156
26	s	0.39	0/744	0.66	0/994
27	t	0.33	0/787	0.64	0/1051
28	u	0.42	0/766	0.66	0/1025
29	v	0.41	0/599	0.71	1/792 (0.1%)
30	w	0.40	0/635	0.70	0/848
31	x	0.34	0/502	0.69	0/667
32	y	0.33	0/453	0.67	0/605

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	z	0.37	0/450	0.68	0/599
All	All	0.68	7/95999 (0.0%)	0.80	47/144025 (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
10	c	0	8

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	2449	U	C5-C6	15.97	1.48	1.34
8	a	2449	U	C2-N3	15.62	1.48	1.37
8	a	2449	U	N1-C2	10.02	1.47	1.38
8	a	2449	U	N3-C4	7.29	1.45	1.38
8	a	2449	U	N1-C6	7.11	1.44	1.38

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	a	2449	U	C2-N3-C4	-12.33	119.60	127.00
7	Z	15	G	P-O3'-C3'	-11.49	105.92	119.70
8	a	2449	U	C5-C4-O4	-10.53	119.58	125.90
7	Z	60	U	P-O3'-C3'	-10.40	107.22	119.70
9	b	93	C	P-O3'-C3'	-10.07	107.62	119.70

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	c	101	ARG	Sidechain
10	c	133	ARG	Sidechain
10	c	63	ARG	Sidechain
10	c	80	ARG	Sidechain
10	c	87	ARG	Sidechain

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	0	417	0	451	2	0
2	1	377	0	418	1	0
3	2	504	0	572	3	0
4	3	302	0	343	2	0
5	4	373	0	371	4	0
6	A	820	0	851	8	0
7	Z	1521	0	774	23	0
8	a	59067	0	29732	0	0
9	b	2549	0	1291	0	0
10	c	2082	0	2154	0	0
11	d	1565	0	1616	0	0
12	e	1552	0	1619	0	0
13	f	1410	0	1444	0	0
14	g	1323	0	1371	0	0
15	h	303	0	327	0	0
16	i	1129	0	1162	0	0
17	j	946	0	1023	0	0
18	k	1053	0	1129	0	0
19	l	1066	0	1148	0	0
20	m	945	0	989	0	0
21	n	892	0	923	0	0
22	o	917	0	962	0	0
23	p	947	0	1019	0	0
24	q	816	0	839	0	0
25	r	857	0	922	0	0
26	s	738	0	807	0	0
27	t	779	0	831	0	0
28	u	753	0	780	0	0
29	v	592	0	607	0	0
30	w	625	0	652	0	0
31	x	501	0	531	0	0
32	y	449	0	488	0	0
33	z	444	0	458	0	0
All	All	88614	0	58604	43	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 4.

The worst 5 of 43 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)
6:A:38:TYR:OH	6:A:50:GLU:OE1	2.02	0.76
6:A:74:GLN:N	6:A:74:GLN:OE1	2.25	0.69
5:4:37:CYS:N	5:4:40:CYS:SG	2.69	0.65
2:1:45:SER:OG	2:1:46:LYS:N	2.31	0.64
6:A:63:GLU:OE2	6:A:65:THR:OG1	2.18	0.62

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	0	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
2	1	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
3	2	62/65 (95%)	61 (98%)	0	1 (2%)	8	34
4	3	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
5	4	46/70 (66%)	45 (98%)	1 (2%)	0	100	100
6	A	100/133 (75%)	96 (96%)	4 (4%)	0	100	100
10	c	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
11	d	207/209 (99%)	195 (94%)	12 (6%)	0	100	100
12	e	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
13	f	175/179 (98%)	169 (97%)	5 (3%)	1 (1%)	22	57
14	g	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
15	h	39/149 (26%)	36 (92%)	3 (8%)	0	100	100
16	i	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
17	j	121/123 (98%)	118 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	k	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
19	l	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
20	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
21	n	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
22	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
23	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
24	q	101/103 (98%)	96 (95%)	4 (4%)	1 (1%)	13	46
25	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
26	s	91/100 (91%)	84 (92%)	6 (7%)	1 (1%)	12	44
27	t	100/104 (96%)	92 (92%)	8 (8%)	0	100	100
28	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
29	v	76/85 (89%)	73 (96%)	3 (4%)	0	100	100
30	w	75/78 (96%)	75 (100%)	0	0	100	100
31	x	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
32	y	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
33	z	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
All	All	3206/3470 (92%)	3086 (96%)	116 (4%)	4 (0%)	50	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	f	159	THR
24	q	51	VAL
26	s	89	GLU
3	2	32	ILE

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
1	0	46/49 (94%)	45 (98%)	1 (2%)	47 76
2	1	38/38 (100%)	36 (95%)	2 (5%)	19 51
3	2	51/52 (98%)	50 (98%)	1 (2%)	50 78
4	3	34/34 (100%)	32 (94%)	2 (6%)	16 47
5	4	44/62 (71%)	42 (96%)	2 (4%)	23 57
6	A	84/114 (74%)	83 (99%)	1 (1%)	67 86
10	c	216/218 (99%)	208 (96%)	8 (4%)	29 63
11	d	164/164 (100%)	160 (98%)	4 (2%)	44 74
12	e	165/165 (100%)	158 (96%)	7 (4%)	25 59
13	f	148/150 (99%)	130 (88%)	18 (12%)	4 18
14	g	137/138 (99%)	130 (95%)	7 (5%)	20 53
15	h	32/114 (28%)	31 (97%)	1 (3%)	35 68
16	i	116/116 (100%)	111 (96%)	5 (4%)	25 58
17	j	104/104 (100%)	99 (95%)	5 (5%)	21 55
18	k	103/103 (100%)	98 (95%)	5 (5%)	21 54
19	l	108/109 (99%)	106 (98%)	2 (2%)	52 79
20	m	98/103 (95%)	95 (97%)	3 (3%)	35 68
21	n	86/87 (99%)	78 (91%)	8 (9%)	7 29
22	o	99/100 (99%)	92 (93%)	7 (7%)	12 40
23	p	89/90 (99%)	86 (97%)	3 (3%)	32 66
24	q	84/84 (100%)	78 (93%)	6 (7%)	12 40
25	r	93/93 (100%)	87 (94%)	6 (6%)	14 43
26	s	80/84 (95%)	77 (96%)	3 (4%)	28 62
27	t	83/85 (98%)	82 (99%)	1 (1%)	67 86
28	u	78/78 (100%)	76 (97%)	2 (3%)	41 72
29	v	59/63 (94%)	54 (92%)	5 (8%)	8 33
30	w	67/68 (98%)	66 (98%)	1 (2%)	60 83
31	x	54/55 (98%)	51 (94%)	3 (6%)	17 49
32	y	48/49 (98%)	48 (100%)	0	100 100
33	z	47/48 (98%)	46 (98%)	1 (2%)	48 77
All	All	2655/2817 (94%)	2535 (96%)	120 (4%)	26 57

5 of 120 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	i	118	MET
29	v	25	ARG
20	m	6	SER
28	u	51	GLN
31	x	44	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
10	c	53	HIS
10	c	86	ASN
10	c	117	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	Z	69/76 (90%)	15 (21%)	1 (1%)
8	a	2742/2904 (94%)	302 (11%)	0
9	b	118/120 (98%)	9 (7%)	0
All	All	2929/3100 (94%)	326 (11%)	1 (0%)

5 of 326 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	Z	8	U
7	Z	9	G
7	Z	14	A
7	Z	15	G
7	Z	16	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	Z	16	C

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

22 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	$\#\|Z\| > 2$
8	OMU	a	2552	8	19,22,23	3.00	7 (36%)	26,31,34	1.67	5 (19%)
8	PSU	a	746	8	18,21,22	4.47	9 (50%)	22,30,33	1.59	4 (18%)
8	1MG	a	745	8	18,26,27	2.74	6 (33%)	19,39,42	1.73	5 (26%)
8	G7M	a	2069	8	20,26,27	2.69	7 (35%)	17,39,42	1.15	3 (17%)
8	2MG	a	1835	8	18,26,27	2.79	7 (38%)	16,38,41	1.33	3 (18%)
8	5MC	a	1962	8	18,22,23	3.80	7 (38%)	26,32,35	1.06	2 (7%)
8	PSU	a	2504	8	18,21,22	4.46	8 (44%)	22,30,33	1.92	5 (22%)
8	6MZ	a	2030	8	18,25,26	0.70	0	16,36,39	0.96	2 (12%)
8	PSU	a	2604	8	18,21,22	4.43	8 (44%)	22,30,33	1.87	5 (22%)
8	PSU	a	1911	8	18,21,22	4.64	8 (44%)	22,30,33	1.81	5 (22%)
8	PSU	a	1917	8	18,21,22	4.72	8 (44%)	22,30,33	1.78	6 (27%)
8	PSU	a	2457	8	18,21,22	4.32	9 (50%)	22,30,33	2.01	6 (27%)
8	OMC	a	2498	8	19,22,23	3.04	8 (42%)	26,31,34	0.69	0
8	5MU	a	747	8	19,22,23	7.09	7 (36%)	28,32,35	3.50	10 (35%)
8	PSU	a	2605	8	18,21,22	4.39	8 (44%)	22,30,33	1.82	5 (22%)
8	OMG	a	2251	8,7	18,26,27	2.69	8 (44%)	19,38,41	1.50	4 (21%)
8	2MG	a	2445	8	18,26,27	2.62	7 (38%)	16,38,41	1.36	4 (25%)
8	PSU	a	955	8	18,21,22	4.39	9 (50%)	22,30,33	1.80	5 (22%)
8	PSU	a	2580	8	18,21,22	4.45	9 (50%)	22,30,33	1.96	6 (27%)
8	2MA	a	2503	8	19,25,26	3.38	7 (36%)	21,37,40	3.26	4 (19%)
8	6MZ	a	1618	8	18,25,26	2.01	3 (16%)	16,36,39	2.24	4 (25%)
8	5MU	a	1939	8	19,22,23	7.06	7 (36%)	28,32,35	3.24	10 (35%)

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
8	OMU	a	2552	8	-	0/9/27/28	0/2/2/2
8	PSU	a	746	8	-	1/7/25/26	0/2/2/2
8	1MG	a	745	8	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	G7M	a	2069	8	-	1/3/25/26	0/3/3/3
8	2MG	a	1835	8	-	2/5/27/28	0/3/3/3
8	5MC	a	1962	8	-	0/7/25/26	0/2/2/2
8	PSU	a	2504	8	-	2/7/25/26	0/2/2/2
8	6MZ	a	2030	8	-	1/5/27/28	0/3/3/3
8	PSU	a	2604	8	-	0/7/25/26	0/2/2/2
8	PSU	a	1911	8	-	0/7/25/26	0/2/2/2
8	PSU	a	1917	8	-	2/7/25/26	0/2/2/2
8	PSU	a	2457	8	-	0/7/25/26	0/2/2/2
8	OMC	a	2498	8	-	0/9/27/28	0/2/2/2
8	5MU	a	747	8	-	0/7/25/26	0/2/2/2
8	PSU	a	2605	8	-	0/7/25/26	0/2/2/2
8	OMG	a	2251	8,7	-	0/5/27/28	0/3/3/3
8	2MG	a	2445	8	-	2/5/27/28	0/3/3/3
8	PSU	a	955	8	-	1/7/25/26	0/2/2/2
8	PSU	a	2580	8	-	2/7/25/26	0/2/2/2
8	2MA	a	2503	8	-	1/3/25/26	0/3/3/3
8	6MZ	a	1618	8	-	2/5/27/28	0/3/3/3
8	5MU	a	1939	8	-	0/7/25/26	0/2/2/2

The worst 5 of 157 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	a	747	5MU	C4-C5	20.98	1.79	1.44
8	a	1939	5MU	C4-C5	20.61	1.79	1.44
8	a	1939	5MU	C6-N1	15.31	1.64	1.38
8	a	747	5MU	C6-N1	14.96	1.63	1.38
8	a	1917	PSU	C6-C5	12.38	1.49	1.35

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	a	2503	2MA	C1'-N9-C4	12.93	149.35	126.64
8	a	747	5MU	C5-C4-N3	10.82	124.55	115.31
8	a	1939	5MU	C5-C4-N3	10.23	124.04	115.31
8	a	747	5MU	C5-C6-N1	-8.16	114.95	123.34
8	a	1939	5MU	C5-C6-N1	-7.41	115.72	123.34

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	a	1618	6MZ	C5-C6-N6-C9
8	a	1618	6MZ	N1-C6-N6-C9
8	a	2445	2MG	C3'-C4'-C5'-O5'
8	a	2504	PSU	O4'-C4'-C5'-O5'
8	a	1835	2MG	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.