



## wwPDB EM Validation Summary Report ⓘ

Mar 15, 2025 – 06:20 pm GMT

PDB ID : 9GHD  
EMDB ID : EMD-51353  
Title : Escherichia coli 70S ribosome in complex with Staphylococcus aureus FusB-EF-G (FusB-EF-G-70S\*)  
Authors : Gonzalez-Lopez, A.; Selmer, M.  
Deposited on : 2024-08-15  
Resolution : 2.41 Å (reported)  
Based on initial models : 8P2H, 9GHE

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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

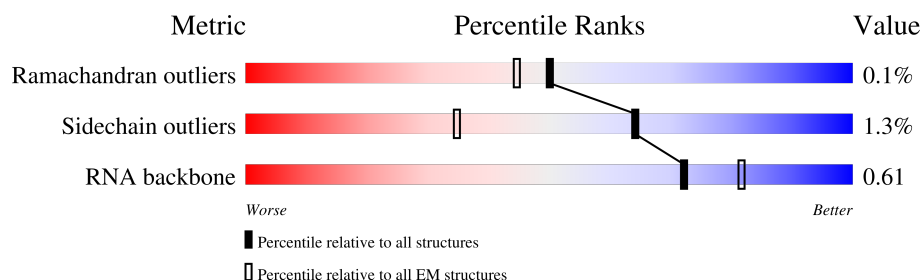
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.41 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.



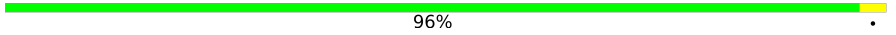



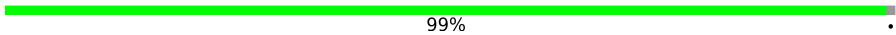
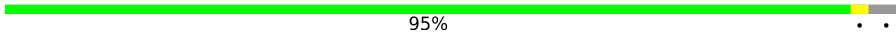


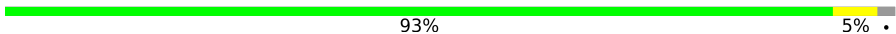
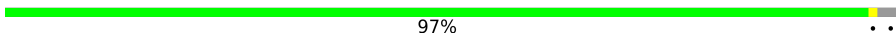
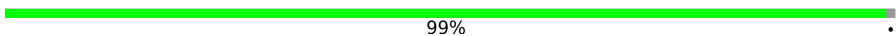

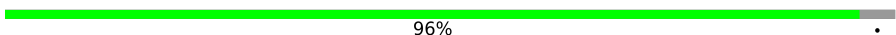
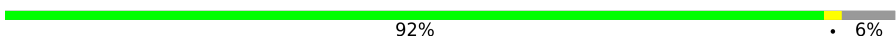


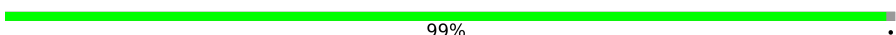

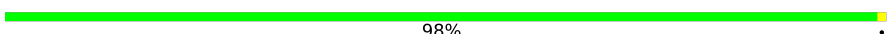



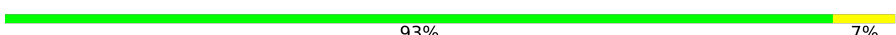
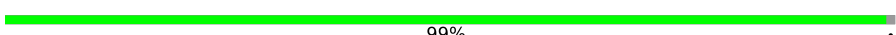
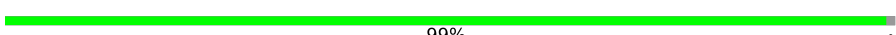
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	0	55	
2	1	46	
3	2	65	
4	3	38	
5	4	70	
6	9	24	
7	A	1554	
8	B	241	
9	C	233	


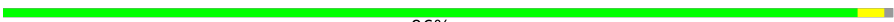












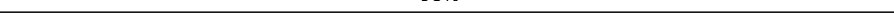
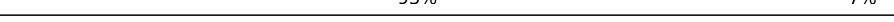

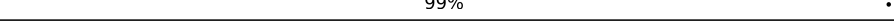

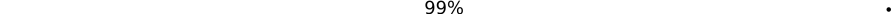
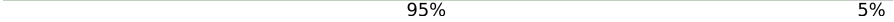
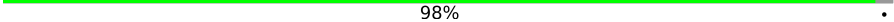
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Mol	Chain	Length	Quality of chain
10	D	206	 96% .
11	E	167	 90% . 8%
12	F	135	 75% 25%
13	G	179	 80% . 16%
14	H	130	 99% .
15	I	130	 95% . .
16	J	103	 89% . 7%
17	K	129	 89% . 9%
18	L	124	 93% 5% .
19	M	118	 97% . .
20	N	101	 99% .
21	O	89	 99% .
22	P	82	 96% .
23	Q	84	 92% . 6%
24	R	75	 85% 15%
25	S	92	 91% 9%
26	T	87	 99% .
27	U	71	 76% . 23%
28	V	213	 98% .
29	W	693	 30% 69%
30	Z	77	 75% 23% .
31	a	2930	 84% 11% 5%
32	b	119	 93% 7%
33	c	273	 99% .
34	d	209	 99% .

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Mol	Chain	Length	Quality of chain
35	e	201	 100%
36	f	179	 96% ..
37	g	177	 94% • 5%
38	h	149	 26% • 72%
39	i	142	 99% •
40	j	123	 99% •
41	k	144	 99% •
42	l	136	 99% •
43	m	127	 93% 7%
44	n	117	 97% • •
45	o	115	 98% • •
46	p	118	 99% •
47	q	103	 99% •
48	r	110	 98% • •
49	s	100	 93% 7%
50	t	104	 89% 11%
51	u	94	 99% •
52	v	85	 88% 12%
53	w	78	 99% •
54	x	63	 95% 5%
55	y	59	 98% •
56	z	57	 95% 5%

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 143666 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 Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	50	Total	C	N	O	0	0
			413	267	75	71		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	45	Total	C	N	O	S	0	0
			367	222	88	55	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	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	9	7	Total	C	N	O	P	0	0
			154	69	32	46	7		

- Molecule 7 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	1514	Total	C	N	O	P	0	0
			32500	14503	5963	10520	1514		

- Molecule 8 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	222	Total	C	N	O	S	0	0
			1737	1099	312	318	8		

- Molecule 9 is a protein called 30S ribosomal protein S3.

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

- Molecule 10 is a protein called 30S ribosomal protein S4.

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

- Molecule 11 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	154	Total	C	N	O	S	0	0
			1135	706	215	208	6		

- Molecule 12 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	101	Total	C	N	O	S	0	0
			824	520	149	149	6		

- Molecule 13 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	150	Total	C	N	O	S	0	0
			1176	732	226	214	4		

- Molecule 14 is a protein called 30S ribosomal protein S8.

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

- Molecule 15 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	125	Total	C	N	O	S	0	0
			1001	622	200	176	3		

- Molecule 16 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	96	Total	C	N	O	S	0	0
			775	487	148	139	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	modified residue	UNP P0A7R9

- Molecule 18 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	121	Total	C	N	O	S	0	0
			942	582	193	162	5		

- Molecule 19 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 20 is a protein called 30S ribosomal protein S14.

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

- Molecule 21 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 22 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	79	Total	C	N	O	S	0	0
			629	394	124	110	1		

- Molecule 23 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 24 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	64	Total	C	N	O	S	0	0
			524	330	99	94	1		

- Molecule 25 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 26 is a protein called 30S ribosomal protein S20.

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

- Molecule 27 is a protein called 30S ribosomal protein S21.



Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	55	Total	C	N	O	S	0	0
			460	287	95	77	1		

- Molecule 28 is a protein called Far1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	212	Total	C	N	O	S	0	0
			1765	1139	290	328	8		

- Molecule 29 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	214	Total	C	N	O	S	0	0
			1647	1035	277	323	12		

- Molecule 30 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

- Molecule 31 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	2782	Total	C	N	O	P	0	0
			59756	26665	11017	19292	2782		

- Molecule 32 is a RNA chain called 5S rRNA.

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

- Molecule 33 is a protein called 50S ribosomal protein L2.

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

- Molecule 34 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	207	Total	C	N	O	S	0	0
			1552	972	286	291	3		

- Molecule 35 is a protein called 50S ribosomal protein L4.

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

- Molecule 36 is a protein called 50S ribosomal protein L5.

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

- Molecule 37 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	168	Total	C	N	O	S	0	0
			1255	791	228	234	2		

- Molecule 38 is a protein called 50S ribosomal protein L9.

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

- Molecule 39 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	141	Total	C	N	O	S	0	0
			1121	709	211	198	3		

- Molecule 40 is a protein called 50S ribosomal protein L14.

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

- Molecule 41 is a protein called 50S ribosomal protein L15.

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

- Molecule 42 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	modified residue	UNP P0ADY7

- Molecule 43 is a protein called 50S ribosomal protein L17.

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

- Molecule 44 is a protein called 50S ribosomal protein L18.

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

- Molecule 45 is a protein called 50S ribosomal protein L19.

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

- Molecule 46 is a protein called 50S ribosomal protein L20.

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

- Molecule 47 is a protein called 50S ribosomal protein L21.

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

- Molecule 48 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 49 is a protein called 50S ribosomal protein L23.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	93	Total	C	N	O	S	0	0
			717	452	135	130			

- Molecule 51 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	93	Total	C	N	O	S	0	0
			745	474	136	133	2		

- Molecule 52 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	v	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

- Molecule 53 is a protein called 50S ribosomal protein L28.

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

- Molecule 54 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	x	60	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 55 is a protein called 50S ribosomal protein L30.

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

- Molecule 56 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	z	54	Total	C	N	O	S	0	0
			429	260	91	77	1		

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	3	1	Total	Zn	0
			1	1	
57	4	1	Total	Zn	0
			1	1	

- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
58	A	31	Total	K	0
			31	31	
58	F	1	Total	K	0
			1	1	
58	M	1	Total	K	0
			1	1	
58	a	76	Total	K	0
			76	76	
58	c	2	Total	K	0
			2	2	
58	e	1	Total	K	0
			1	1	

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	A	55	Total 55	Mg 55	0
59	a	240	Total 240	Mg 240	0
59	b	3	Total 3	Mg 3	0
59	c	2	Total 2	Mg 2	0
59	d	1	Total 1	Mg 1	0
59	p	1	Total 1	Mg 1	0
59	z	1	Total 1	Mg 1	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: Large ribosomal subunit protein bL33

Chain 0:  89% 9%



- Molecule 2: Large ribosomal subunit protein bL34

Chain 1:  98%



- Molecule 3: 50S ribosomal protein L35

Chain 2:  97%




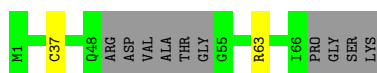
- Molecule 4: 50S ribosomal protein L36

Chain 3:  97%



- Molecule 5: 50S ribosomal protein L31

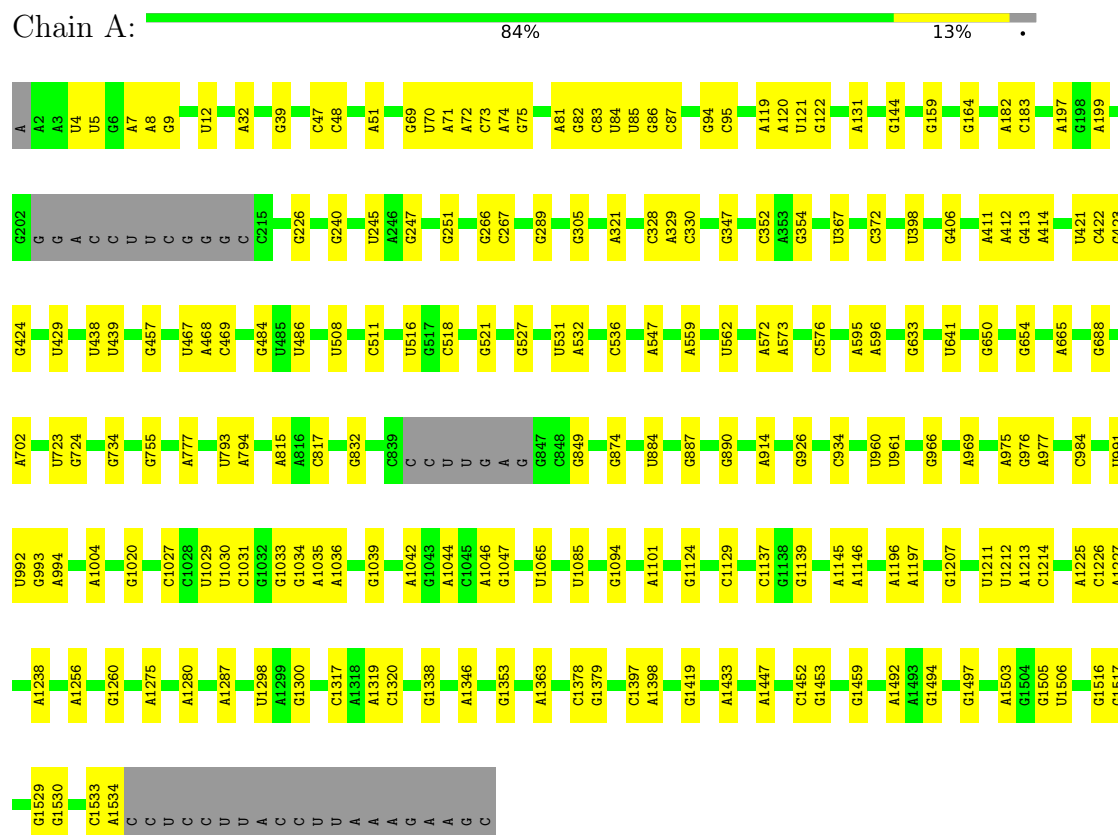
Chain 4:  83% 14%



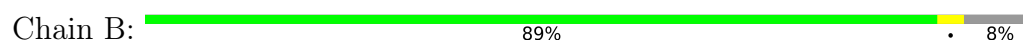
- Molecule 6: mRNA

Chain 9:  25% 71%

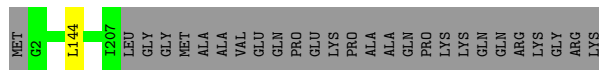
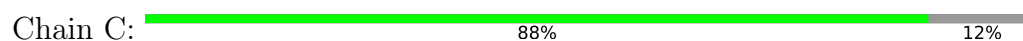
- Molecule 7: 16S rRNA



- Molecule 8: 30S ribosomal protein S2



- Molecule 9: 30S ribosomal protein S3




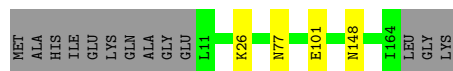
- Molecule 10: 30S ribosomal protein S4





- Molecule 11: 30S ribosomal protein S5

Chain E:  90% 8%




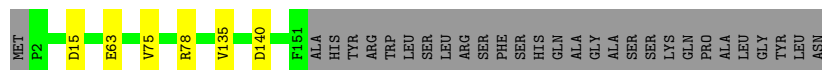
- Molecule 12: 30S ribosomal protein S6

Chain F:  75% 25%



- Molecule 13: 30S ribosomal protein S7

Chain G:  80% 16%



- Molecule 14: 30S ribosomal protein S8

Chain H:  99%




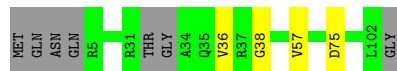
- Molecule 15: 30S ribosomal protein S9

Chain I:  95%




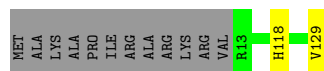
- Molecule 16: 30S ribosomal protein S10

Chain J:  89% 7%



- Molecule 17: Small ribosomal subunit protein uS11

Chain K:  89% 9%



- Molecule 18: 30S ribosomal protein S12

Chain L:  93% 5% .



- Molecule 19: 30S ribosomal protein S13

Chain M:  97% . .



- Molecule 20: 30S ribosomal protein S14

Chain N:  99% .



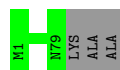
- Molecule 21: Small ribosomal subunit protein uS15

Chain O:  99% .



- Molecule 22: 30S ribosomal protein S16

Chain P:  96% .




- Molecule 23: 30S ribosomal protein S17

Chain Q:  92% . 6%



- Molecule 24: 30S ribosomal protein S18

Chain R:  85% 15%



- Molecule 25: 30S ribosomal protein S19

MET
P2
A85
ASP
LYS
LYS
ALA
LYS
LYS
LYS

- |     |    |     |
|-----|----|-----|
| MET | A2 | A87 |
|-----|----|-----|

- |     |
|-----|
| MET |
| P2  |
| R34 |
| H56 |
| ALA |
| LYS |
| LYS |
| LEU |
| ALA |
| ARG |
| GLU |
| ASN |
| ALA |
| ARG |
| ARG |
| THR |
| ARG |
| LEU |
| TYR |

- 

- MET ALA ARG GLU PHE SER LEU LEU GLN THR LYS THR ARG ASN ILE ILE GLY ILE MET MET ALA ALA GLY LYS THR THR THR THR ARG GLU ILE ILE LEU TYR TYR TYR TYR GLY ARG ARG ILE ILE HIS HIS LYS ILE ILE GLU THR HIS HIS GLU GLY ALA SER GLN MET MET ASP TRP MET GLU GLN GLU GLN ASP ARG

ILE	THR	ILE	THR	SER	ALA	THR	THR	ALA	ALA	ALA	TRP	GLU	GLY	HIS	ARG	ASN	ILE	ILE	ASP	THR	THR	PRO	GLY	HIS	VAL	VAL	ASP	PHE	THR	THR	VAL	GLU	VAL	VAL	GLU	ARG	SER	LEU	LEU	VAL	ASP	GLY	ALA	VAL	THR	THR	VAL	LEU	LEU	ASP	GLN	GLN	SER	GLY	VAL	GLU	PRO	THR	THR	THR	VAL
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ARG	GLN	ALA	THR	THR	TYR	GLY	VAL	PRO	ARG	ARG	ILE	LEU	PHE	VAL	ASN	LYS	MET	ASP	LYS	LEU	GLY	ALA	ASN	PHE	GLU	TYR	SER	SER	THR	LEU	HIS	ASP	ARG	LEU	GLN	LEU	ALA	ASN	ALA	ALA	ALA	PRO	ILE	GLN	LEU	PRO	ILE	GLY	ALA	GLU	ASP	PHE	GLU	ALA	ILE	ILE	ASP	LEU	VAL
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MET	LYS	CYS	PHE	LYS	TYR	THR	ASN	ASP	LEU	GLY	THR	GLU	ILE	GLU	GLY	ILE	GLU	ILE	PRO	ARG	ALA	GLU	GLY	HIS	ASP	LEU	ASP	ALA	ARG	ALA	GLY	GLU	ALA	GLY	THR	SER	ASP	GLU	GLY	LEU	MET	LYS	TYR	LEU	GLY	ASP	GLU	VAL	SER	SER	VAL	SER	GLY
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LYS GLU ALA ALA ILE ARG GLN ALA THR THR ASN ASN VAL VAL VAL PHE TYR VAL GLU PHE TYR PRO PRO VAL LEU LEU CYS GLY THR THR ALA ALA PHE PHE LYS LYS ASN LYS LYS GLY GLY VAL VAL GLN GLN LEU LEU MET LEU LEU ASP ASP PRO PRO PRO PRO PRO LEU LEU ASP VAL VAL LYS LYS PRO PRO ILE ILE ILE GLY HIS ARG HIS ALA ALA SER ASN ASN GLU GLU GLU VAL

ALA	LYS	ALA	ASP	SER	ALA	ALA	ALA	LEU	ALA	PHE	LYS	MET	THR	ASP	PRO	TYR	VAL	GLY	LYS	LEU	THR	PHE	PHE	ARG	VAL	TYR	SER	SER	THR	MET	THR	SER	GLY	THR	LYS	VAL	VAL	LYS	ASN	SER	SER	THR	GLY	ARG	GLY	LEU	LEU	GLN	MET	HIS
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ASN SER ARG GLN GLU ILE ASP THR VAL TYR SER SER GLY ASP ILE ALA ALA VAL GLY LEU LYS ASP THR THR GLY ASP THR GLU GLU LYS ASN ASP ILE ILE LEU GLU MET SER GLU PHE PRO GLU PRO VAL ILE HIS LEU SER VAL PRO LYS SER LYS ALA ASP

	ASP	GYS	MET	THR	GLN	ALA	LEU	VAL	VAL	GLY	ASN	PHE	GLU	LYS	CYS	ASN	VAL	VAL	GLY	GLY	ALA	PRO	ARG
--	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



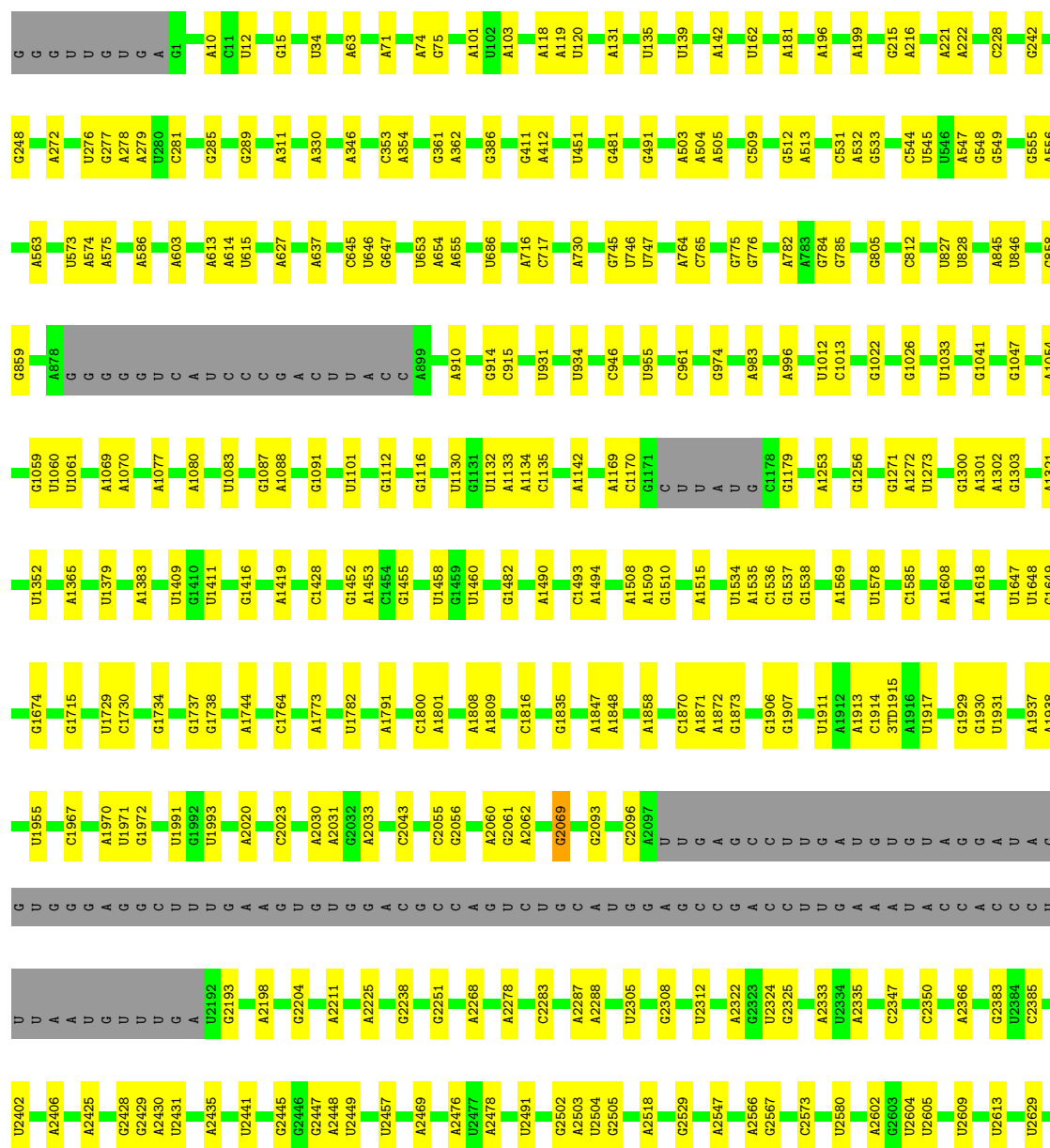
- Molecule 30: tRNA

Chain Z: 75% 23%



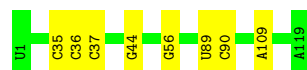
- Molecule 31: 23S rRNA

Chain a: 84% 11% 5%





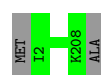
• Molecule 32: 5S rRNA



• Molecule 33: 50S ribosomal protein L2



• Molecule 34: 50S ribosomal protein L3



• Molecule 35: 50S ribosomal protein L4

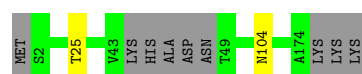


There are no outlier residues recorded for this chain.

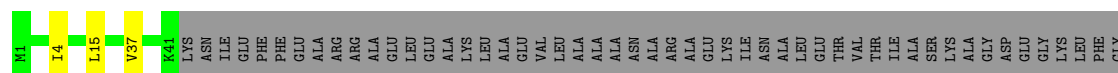
• Molecule 36: 50S ribosomal protein L5



• Molecule 37: 50S ribosomal protein L6



• Molecule 38: 50S ribosomal protein L9



SER  
ILE  
GLY  
THR  
ARG  
ASP  
TLE  
ALA  
ASP  
ALA  
VAL  
THR  
ALA  
ALA  
GLY  
VAL  
VAL  
GLU  
VAL  
ALA  
LYS  
SER  
GLU  
VAL  
VAL  
ARG  
LEU  
PRO  
ASN  
GLY  
VAL  
LEU  
ARG  
THR  
THR  
GLY  
GLU  
HIS  
GLU  
VAL  
SER  
PHE  
GLN  
VAL  
HIS  
SER  
GLU  
VAL  
PHE  
ALA  
LYS  
VAL  
TLE  
VAL  
ASN  
VAL  
VAL  
ALA  
GLU

- Molecule 39: 50S ribosomal protein L13

Chain i:  99% .

MET  
K2  
I142

- Molecule 40: 50S ribosomal protein L14

Chain j:  99% .

M1  
L58  
L123

- Molecule 41: 50S ribosomal protein L15

Chain k:  99% .

M1  
K29  
E144

- Molecule 42: Large ribosomal subunit protein uL16

Chain l:  99% .

M1  
R6  
M136

- Molecule 43: 50S ribosomal protein L17

Chain m:  93% 7%

M1  
R118  
SER  
GLU  
LYS  
ALA  
GLU  
ALA  
ALA  
ALA  
GLU

- Molecule 44: 50S ribosomal protein L18

Chain n:  97% ..

MET  
D2  
V49  
K56  
F117

- Molecule 45: 50S ribosomal protein L19

Chain o:  98% ..



- Molecule 46: 50S ribosomal protein L20

Chain p: 99%



- Molecule 47: 50S ribosomal protein L21

Chain q: 99%



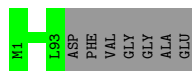
- Molecule 48: 50S ribosomal protein L22

Chain r: 98%



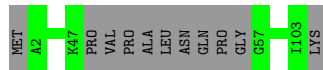
- Molecule 49: 50S ribosomal protein L23

Chain s: 93% 7%



- Molecule 50: 50S ribosomal protein L24

Chain t: 89% 11%



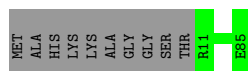
- Molecule 51: 50S ribosomal protein L25

Chain u: 99%



- Molecule 52: Large ribosomal subunit protein bL27

Chain v: 88% 12%



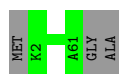
- Molecule 53: 50S ribosomal protein L28

Chain w:  99% .



- Molecule 54: 50S ribosomal protein L29

Chain x:  95% 5% .



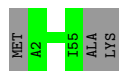
- Molecule 55: 50S ribosomal protein L30

Chain y:  98% .



- Molecule 56: 50S ribosomal protein L32

Chain z:  95% 5% .





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30847	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45.47	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 1MG, OMG, MEQ, ZN, MS6, MG, UR3, IAS, H2U, K, G7M, PSU, D2T, 2MG, 5MU, 4OC, 2MA, 3TD, MA6, OMU, 4D4, 5MC, 6MZ

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	0.31	0/420	0.54	0/560
2	1	0.30	0/370	0.58	0/487
3	2	0.33	0/513	0.54	0/676
4	3	0.30	0/303	0.58	0/397
5	4	0.32	0/488	0.56	0/649
6	9	0.47	0/173	0.83	0/268
7	A	0.42	0/36110	0.89	0/56322
8	B	0.29	0/1768	0.54	0/2381
9	C	0.28	0/1651	0.53	0/2225
10	D	0.29	0/1665	0.54	0/2227
11	E	0.29	0/1148	0.54	0/1545
12	F	0.28	0/843	0.50	0/1140
13	G	0.29	0/1190	0.52	0/1595
14	H	0.29	0/989	0.55	0/1326
15	I	0.29	0/1013	0.56	0/1350
16	J	0.28	0/784	0.60	0/1059
17	K	0.30	0/884	0.53	0/1191
18	L	0.29	0/945	0.61	0/1268
19	M	0.29	0/900	0.54	0/1204
20	N	0.30	0/817	0.53	0/1088
21	O	0.29	0/722	0.50	0/964
22	P	0.28	0/639	0.56	0/859
23	Q	0.28	0/650	0.56	0/871
24	R	0.28	0/532	0.55	0/715
25	S	0.32	0/685	0.54	0/922
26	T	0.28	0/676	0.48	0/895
27	U	0.32	0/467	0.60	0/620
28	V	0.29	0/1798	0.49	0/2415
29	W	0.30	0/1679	0.51	0/2261
30	Z	0.45	0/1813	0.89	0/2825
31	a	0.41	0/66355	0.89	4/103511 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	b	0.43	0/2850	0.90	0/4444
33	c	0.29	0/2121	0.57	0/2852
34	d	0.29	0/1562	0.52	0/2102
35	e	0.28	0/1571	0.51	0/2113
36	f	0.29	0/1434	0.54	0/1926
37	g	0.29	0/1273	0.54	0/1725
38	h	0.30	0/306	0.55	0/413
39	i	0.28	0/1144	0.52	0/1541
40	j	0.28	0/955	0.55	0/1279
41	k	0.31	0/1062	0.52	0/1413
42	l	0.29	0/1073	0.55	0/1433
43	m	0.28	0/958	0.53	0/1281
44	n	0.29	0/902	0.54	0/1209
45	o	0.29	0/929	0.54	0/1242
46	p	0.28	0/960	0.52	0/1278
47	q	0.30	0/829	0.54	0/1107
48	r	0.28	0/852	0.55	0/1142
49	s	0.27	0/744	0.54	0/994
50	t	0.30	0/721	0.56	0/956
51	u	0.29	0/758	0.54	0/1015
52	v	0.32	0/576	0.54	0/762
53	w	0.30	0/635	0.54	0/848
54	x	0.26	0/492	0.48	0/655
55	y	0.29	0/453	0.51	0/605
56	z	0.30	0/435	0.56	0/581
All	All	0.38	0/154585	0.81	4/230732 (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
4	3	0	1
10	D	0	1
16	J	0	1
17	K	0	1
27	U	0	1
All	All	0	5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	512	G	O4'-C1'-N9	6.25	113.20	108.20
31	a	2447	G	C3'-C2'-C1'	-5.36	97.21	101.50
31	a	242	G	C3'-C2'-C1'	-5.03	97.47	101.50
31	a	512	G	C1'-O4'-C4'	-5.01	105.89	109.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	3	36	ARG	Sidechain
10	D	184	ARG	Sidechain
16	J	38	GLY	Peptide
17	K	118	HIS	Peptide
27	U	34	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	
1	0	48/55 (87%)	48 (100%)	0	0	100	100
2	1	43/46 (94%)	43 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	55 (98%)	1 (2%)	0	100	100
8	B	220/241 (91%)	214 (97%)	5 (2%)	1 (0%)	25	36
9	C	204/233 (88%)	198 (97%)	6 (3%)	0	100	100
10	D	203/206 (98%)	202 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	E	152/167 (91%)	150 (99%)	2 (1%)	0	100	100
12	F	99/135 (73%)	98 (99%)	1 (1%)	0	100	100
13	G	148/179 (83%)	147 (99%)	1 (1%)	0	100	100
14	H	127/130 (98%)	127 (100%)	0	0	100	100
15	I	123/130 (95%)	120 (98%)	3 (2%)	0	100	100
16	J	92/103 (89%)	87 (95%)	4 (4%)	1 (1%)	12	17
17	K	113/129 (88%)	111 (98%)	2 (2%)	0	100	100
18	L	118/124 (95%)	114 (97%)	4 (3%)	0	100	100
19	M	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
20	N	98/101 (97%)	98 (100%)	0	0	100	100
21	O	86/89 (97%)	86 (100%)	0	0	100	100
22	P	77/82 (94%)	75 (97%)	2 (3%)	0	100	100
23	Q	77/84 (92%)	77 (100%)	0	0	100	100
24	R	62/75 (83%)	62 (100%)	0	0	100	100
25	S	82/92 (89%)	81 (99%)	1 (1%)	0	100	100
26	T	84/87 (97%)	84 (100%)	0	0	100	100
27	U	53/71 (75%)	53 (100%)	0	0	100	100
28	V	210/213 (99%)	208 (99%)	2 (1%)	0	100	100
29	W	212/693 (31%)	209 (99%)	3 (1%)	0	100	100
33	c	269/273 (98%)	265 (98%)	4 (2%)	0	100	100
34	d	204/209 (98%)	200 (98%)	4 (2%)	0	100	100
35	e	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
36	f	175/179 (98%)	174 (99%)	1 (1%)	0	100	100
37	g	164/177 (93%)	162 (99%)	2 (1%)	0	100	100
38	h	39/149 (26%)	38 (97%)	1 (3%)	0	100	100
39	i	139/142 (98%)	138 (99%)	1 (1%)	0	100	100
40	j	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
41	k	142/144 (99%)	139 (98%)	2 (1%)	1 (1%)	19	27
42	l	132/136 (97%)	131 (99%)	1 (1%)	0	100	100
43	m	116/127 (91%)	113 (97%)	3 (3%)	0	100	100
44	n	114/117 (97%)	112 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
46	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
47	q	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
48	r	107/110 (97%)	106 (99%)	1 (1%)	0	100	100
49	s	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
50	t	89/104 (86%)	89 (100%)	0	0	100	100
51	u	91/94 (97%)	90 (99%)	1 (1%)	0	100	100
52	v	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
53	w	75/78 (96%)	75 (100%)	0	0	100	100
54	x	58/63 (92%)	58 (100%)	0	0	100	100
55	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
56	z	52/57 (91%)	52 (100%)	0	0	100	100
All	All	5832/6819 (86%)	5752 (99%)	77 (1%)	3 (0%)	50	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	J	57	VAL
41	k	29	LYS
8	B	165	ASP

### 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	0	46/49 (94%)	45 (98%)	1 (2%)	47	65
2	1	37/38 (97%)	37 (100%)	0	100	100
3	2	51/52 (98%)	50 (98%)	1 (2%)	50	68
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	55/62 (89%)	53 (96%)	2 (4%)	30	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	B	184/199 (92%)	178 (97%)	6 (3%)	33	51
9	C	170/190 (90%)	169 (99%)	1 (1%)	84	92
10	D	172/173 (99%)	166 (96%)	6 (4%)	31	49
11	E	117/126 (93%)	113 (97%)	4 (3%)	32	50
12	F	88/116 (76%)	88 (100%)	0	100	100
13	G	124/147 (84%)	118 (95%)	6 (5%)	21	35
14	H	104/105 (99%)	104 (100%)	0	100	100
15	I	103/107 (96%)	101 (98%)	2 (2%)	52	70
16	J	85/90 (94%)	83 (98%)	2 (2%)	44	63
17	K	89/98 (91%)	88 (99%)	1 (1%)	70	84
18	L	101/103 (98%)	96 (95%)	5 (5%)	20	34
19	M	93/96 (97%)	92 (99%)	1 (1%)	70	84
20	N	83/84 (99%)	83 (100%)	0	100	100
21	O	76/77 (99%)	76 (100%)	0	100	100
22	P	64/65 (98%)	64 (100%)	0	100	100
23	Q	73/78 (94%)	71 (97%)	2 (3%)	40	58
24	R	55/65 (85%)	55 (100%)	0	100	100
25	S	72/79 (91%)	72 (100%)	0	100	100
26	T	65/66 (98%)	65 (100%)	0	100	100
27	U	48/61 (79%)	48 (100%)	0	100	100
28	V	203/204 (100%)	200 (98%)	3 (2%)	60	77
29	W	174/579 (30%)	171 (98%)	3 (2%)	56	73
33	c	216/218 (99%)	215 (100%)	1 (0%)	86	94
34	d	162/163 (99%)	162 (100%)	0	100	100
35	e	165/165 (100%)	165 (100%)	0	100	100
36	f	148/150 (99%)	143 (97%)	5 (3%)	32	50
37	g	130/138 (94%)	128 (98%)	2 (2%)	60	77
38	h	32/114 (28%)	29 (91%)	3 (9%)	7	10
39	i	115/116 (99%)	115 (100%)	0	100	100
40	j	104/104 (100%)	103 (99%)	1 (1%)	73	85
41	k	103/103 (100%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	l	107/107 (100%)	106 (99%)	1 (1%)	75	87
43	m	98/103 (95%)	98 (100%)	0	100	100
44	n	86/87 (99%)	83 (96%)	3 (4%)	31	49
45	o	99/100 (99%)	98 (99%)	1 (1%)	73	85
46	p	89/90 (99%)	89 (100%)	0	100	100
47	q	84/84 (100%)	83 (99%)	1 (1%)	67	82
48	r	92/93 (99%)	91 (99%)	1 (1%)	70	84
49	s	80/84 (95%)	80 (100%)	0	100	100
50	t	76/85 (89%)	76 (100%)	0	100	100
51	u	77/78 (99%)	77 (100%)	0	100	100
52	v	56/63 (89%)	56 (100%)	0	100	100
53	w	67/68 (98%)	67 (100%)	0	100	100
54	x	54/55 (98%)	54 (100%)	0	100	100
55	y	48/49 (98%)	48 (100%)	0	100	100
56	z	46/48 (96%)	46 (100%)	0	100	100
All	All	4900/5608 (87%)	4835 (99%)	65 (1%)	64	80

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	j	58	LEU
44	n	2	ASP
13	G	78	ARG
13	G	75	VAL
44	n	49	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
29	W	551	ASN
47	q	43	ASN
33	c	37	ASN
46	p	44	GLN
51	u	49	ASN



### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	Z	75/77 (97%)	17 (22%)	3 (4%)
31	a	2774/2930 (94%)	310 (11%)	0
32	b	118/119 (99%)	8 (6%)	0
6	9	6/24 (25%)	1 (16%)	0
7	A	1508/1554 (97%)	177 (11%)	37 (2%)
All	All	4481/4704 (95%)	513 (11%)	40 (0%)

5 of 513 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	9	19	G
7	A	4	U
7	A	5	U
7	A	8	A
7	A	9	G

5 of 40 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	1225	A
7	A	1459	G
7	A	1298	U
7	A	1397	C
30	Z	7	G

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

39 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
7	PSU	A	516	59,7	18,21,22	0.90	1 (5%)	22,30,33	0.64	0
31	5MC	a	1962	31	18,22,23	0.33	0	26,32,35	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	5MC	A	1407	7	18,22,23	0.33	0	26,32,35	0.58	0
31	OMC	a	2498	31,59	19,22,23	0.27	0	26,31,34	0.48	0
31	G7M	a	2069	31	20,26,27	1.15	3 (15%)	17,39,42	0.48	0
7	5MC	A	967	7	18,22,23	0.32	0	26,32,35	0.49	0
7	4OC	A	1402	7	20,23,24	0.37	0	26,32,35	0.49	0
7	2MG	A	1207	58,7	18,26,27	1.02	2 (11%)	16,38,41	0.75	0
7	MA6	A	1519	7	18,26,27	0.74	0	19,38,41	0.56	0
34	MEQ	d	150	34	8,9,10	0.42	0	5,10,12	0.54	0
31	2MG	a	2445	31	18,26,27	1.03	2 (11%)	16,38,41	0.69	0
7	G7M	A	527	7	20,26,27	1.14	2 (10%)	17,39,42	0.50	0
7	UR3	A	1498	7	19,22,23	0.28	0	26,32,35	0.68	0
31	5MU	a	1939	31,58	19,22,23	0.28	0	28,32,35	0.35	0
31	OMU	a	2552	31	19,22,23	0.20	0	26,31,34	0.46	0
18	D2T	L	89	18	7,9,10	0.95	0	6,11,13	2.24	4 (66%)
42	4D4	l	81	42	9,11,12	0.50	0	8,13,15	0.60	0
31	2MG	a	1835	31	18,26,27	1.04	2 (11%)	16,38,41	0.67	0
17	IAS	K	119	17	6,7,8	0.92	0	6,8,10	1.01	0
31	PSU	a	2605	31	18,21,22	0.93	1 (5%)	22,30,33	0.74	0
31	3TD	a	1915	31	18,22,23	0.96	1 (5%)	22,32,35	0.63	0
31	PSU	a	2604	31	18,21,22	0.91	1 (5%)	22,30,33	0.69	0
31	6MZ	a	1618	31	18,25,26	0.67	0	16,36,39	0.70	1 (6%)
31	PSU	a	2504	31,58	18,21,22	0.89	1 (5%)	22,30,33	0.69	0
31	PSU	a	1917	31	18,21,22	0.90	1 (5%)	22,30,33	0.54	0
31	H2U	a	2449	31	18,21,22	0.61	0	21,30,33	0.85	2 (9%)
31	6MZ	a	2030	31	18,25,26	0.68	0	16,36,39	0.77	1 (6%)
31	OMG	a	2251	31,58,30	18,26,27	1.00	2 (11%)	19,38,41	0.69	0
31	2MA	a	2503	31,59,58	19,25,26	1.03	1 (5%)	21,37,40	1.81	5 (23%)
31	PSU	a	2580	31,58	18,21,22	0.94	1 (5%)	22,30,33	0.78	1 (4%)
31	5MU	a	747	31	19,22,23	0.27	0	28,32,35	0.37	0
31	PSU	a	955	31	18,21,22	0.92	1 (5%)	22,30,33	0.58	0
7	2MG	A	966	7	18,26,27	1.01	2 (11%)	16,38,41	0.81	0
31	PSU	a	2457	31	18,21,22	0.91	1 (5%)	22,30,33	0.60	0
7	MA6	A	1518	7	18,26,27	0.75	0	19,38,41	0.46	0
31	PSU	a	1911	31	18,21,22	0.89	1 (5%)	22,30,33	0.65	0
7	2MG	A	1516	7	18,26,27	1.01	2 (11%)	16,38,41	0.79	0
31	PSU	a	746	31,59	18,21,22	0.91	1 (5%)	22,30,33	0.62	0
31	1MG	a	745	31	18,26,27	0.97	1 (5%)	19,39,42	0.53	0

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
7	PSU	A	516	59,7	-	0/7/25/26	0/2/2/2
31	5MC	a	1962	31	-	4/7/25/26	0/2/2/2
7	5MC	A	1407	7	-	0/7/25/26	0/2/2/2
31	OMC	a	2498	31,59	-	0/9/27/28	0/2/2/2
31	G7M	a	2069	31	-	2/3/25/26	0/3/3/3
7	5MC	A	967	7	-	0/7/25/26	0/2/2/2
7	4OC	A	1402	7	-	0/9/29/30	0/2/2/2
7	2MG	A	1207	58,7	-	0/5/27/28	0/3/3/3
7	MA6	A	1519	7	-	0/7/29/30	0/3/3/3
34	MEQ	d	150	34	-	2/8/9/11	-
31	2MG	a	2445	31	-	0/5/27/28	0/3/3/3
7	G7M	A	527	7	-	1/3/25/26	0/3/3/3
7	UR3	A	1498	7	-	0/7/25/26	0/2/2/2
31	5MU	a	1939	31,58	-	0/7/25/26	0/2/2/2
31	OMU	a	2552	31	-	0/9/27/28	0/2/2/2
18	D2T	L	89	18	-	2/7/12/14	-
42	4D4	l	81	42	-	1/11/12/14	-
31	2MG	a	1835	31	-	0/5/27/28	0/3/3/3
17	IAS	K	119	17	-	2/7/7/8	-
31	PSU	a	2605	31	-	0/7/25/26	0/2/2/2
31	3TD	a	1915	31	-	2/7/25/26	0/2/2/2
31	PSU	a	2604	31	-	0/7/25/26	0/2/2/2
31	6MZ	a	1618	31	-	0/5/27/28	0/3/3/3
31	PSU	a	2504	31,58	-	0/7/25/26	0/2/2/2
31	PSU	a	1917	31	-	0/7/25/26	0/2/2/2
31	H2U	a	2449	31	-	0/7/38/39	0/2/2/2
31	6MZ	a	2030	31	-	2/5/27/28	0/3/3/3
31	OMG	a	2251	31,58,30	-	1/5/27/28	0/3/3/3
31	2MA	a	2503	31,59,58	-	2/3/25/26	0/3/3/3
31	PSU	a	2580	31,58	-	0/7/25/26	0/2/2/2
31	5MU	a	747	31	-	0/7/25/26	0/2/2/2
31	PSU	a	955	31	-	0/7/25/26	0/2/2/2
7	2MG	A	966	7	-	0/5/27/28	0/3/3/3
31	PSU	a	2457	31	-	0/7/25/26	0/2/2/2
7	MA6	A	1518	7	-	0/7/29/30	0/3/3/3
31	PSU	a	1911	31	-	2/7/25/26	0/2/2/2
7	2MG	A	1516	7	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PSU	a	746	31,59	-	3/7/25/26	0/2/2/2
31	1MG	a	745	31	-	0/3/25/26	0/3/3/3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	2580	PSU	C6-C5	3.74	1.39	1.35
31	a	2605	PSU	C6-C5	3.66	1.39	1.35
31	a	1915	3TD	C6-C5	3.64	1.39	1.35
31	a	746	PSU	C6-C5	3.62	1.39	1.35
31	a	2457	PSU	C6-C5	3.59	1.39	1.35

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	2503	2MA	C5-C6-N1	-5.49	117.40	121.01
31	a	2503	2MA	C5-C6-N6	4.23	126.79	120.35
18	L	89	D2T	CB-CA-N	3.81	117.23	109.10
31	a	2503	2MA	CM2-C2-N1	2.85	121.61	117.15
18	L	89	D2T	OD1-CG-CB	-2.53	117.15	122.44

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	a	746	PSU	C2'-C1'-C5-C4
31	a	1911	PSU	O4'-C1'-C5-C4
31	a	1911	PSU	O4'-C1'-C5-C6
31	a	1915	3TD	C3'-C4'-C5'-O5'
31	a	1915	3TD	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 417 ligands modelled in this entry, 417 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

There are no chain breaks in this entry.