



## wwPDB EM Validation Summary Report ⓘ

Mar 6, 2025 – 02:25 pm GMT

PDB ID : 8AYE  
EMDB ID : EMD-15712  
Title : E. coli 70S ribosome bound to thermorubin and fMet-tRNA  
Authors : Sanyal, S.; Parajuli, N.P.; Emmerich, A.G.  
Deposited on : 2022-09-02  
Resolution : 1.96 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](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:

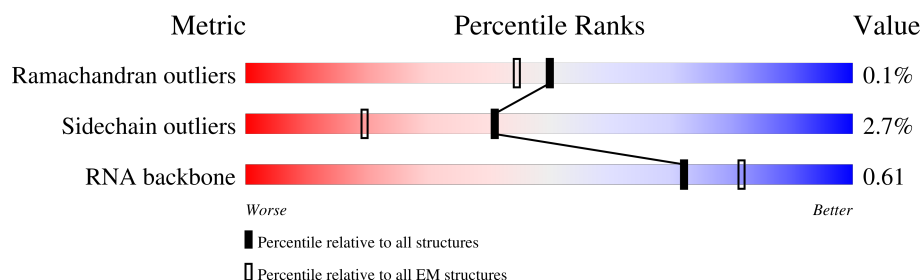
EMDB validation analysis	: <b>FAILED</b>
Mogul	: 1.8.4, CSD as541be (2020)
MolProbity	: 4.02b-467
buster-report	: 1.1.7 (2018)
Percentile statistics	: 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	: <b>FAILED</b>
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (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 1.96 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.



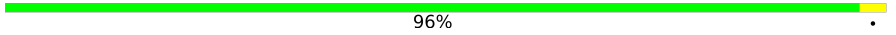
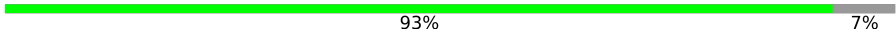


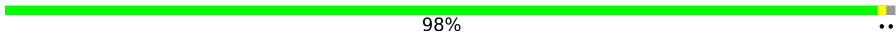
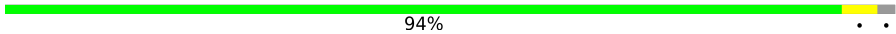


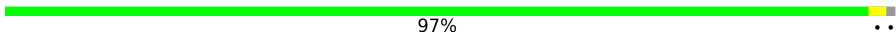
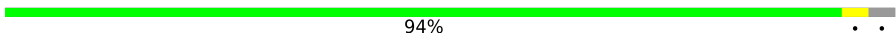
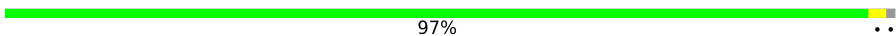
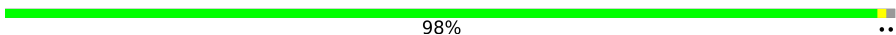
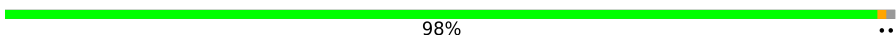



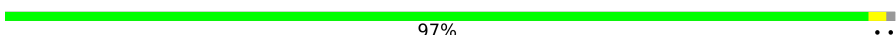
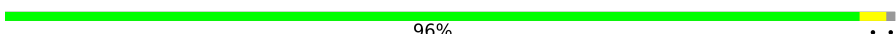
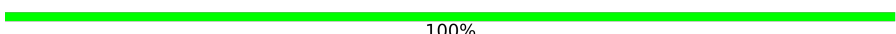



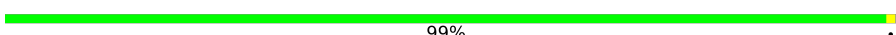
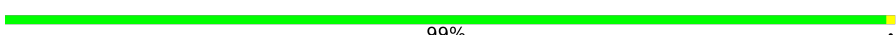
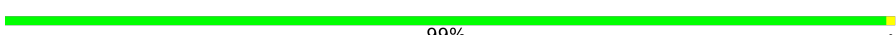
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	5	2	
7	A	1542	
8	B	241	
9	C	233	

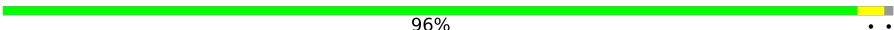
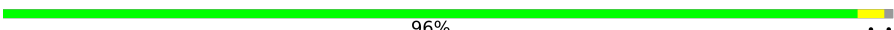

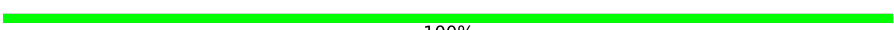
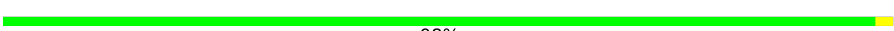







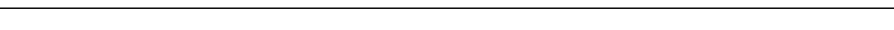
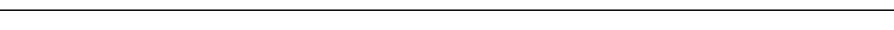
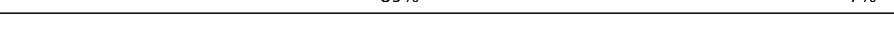
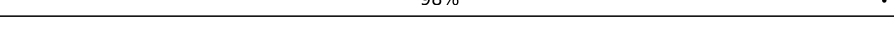
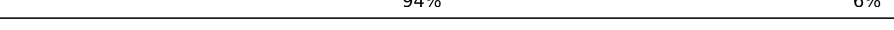
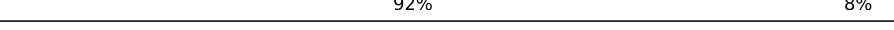
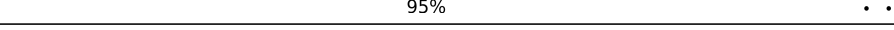
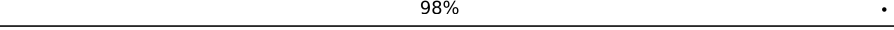
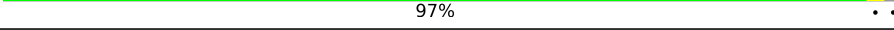
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Mol	Chain	Length	Quality of chain
10	D	206	 96% .
11	E	167	 93% 7%
12	F	135	 73% . 24%
13	G	179	 82% . 15%
14	H	130	 98% ..
15	I	130	 94% . .
16	J	103	 92% . 5%
17	K	129	 88% . . 9%
18	L	124	 97% ..
19	M	118	 94% . .
20	N	101	 97% ..
21	O	89	 98% ..
22	P	82	 98% ..
23	Q	84	 88% 6% 6%
24	R	75	 83% . . 12%
25	S	92	 90% . 9%
26	T	87	 97% ..
27	U	71	 96% . .
28	X	6	 100%
29	Z	76	 74% 26%
30	a	2903	 82% 13% 5%
31	b	120	 89% 10% .
32	c	273	 99% ..
33	d	209	 99% .
34	e	201	 99% .

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Mol	Chain	Length	Quality of chain
35	f	179	 96% . .
36	g	177	 96% . .
37	h	149	 26% . 72%
38	i	142	 100%
39	j	123	 98% .
40	k	144	 99% .
41	l	136	 99% .
42	m	127	 92% . 7%
43	n	117	 98% . .
44	o	115	 97% . .
45	p	118	 98% . .
46	q	103	 94% 6%
47	r	110	 98% .
48	s	100	 89% . 7%
49	t	104	 98% .
50	u	94	 94% 6%
51	v	85	 92% 8%
52	w	78	 95% . .
53	x	63	 98% .
54	y	59	 97% . .
55	z	57	 96% . .

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 140205 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	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	1519	Total	C	N	O	P	0	0
			32612	14552	5986	10555	1519		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	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	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 12 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	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	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 17 is a protein called 30S ribosomal protein S11.

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	ASP	ASN	conflict	UNP P0A7R9

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

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

- 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 30S ribosomal protein S15.

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	81	Total	C	N	O	S	0	0
			643	403	127	112	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	66	Total	C	N	O	S	0	0
			544	345	102	96	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	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 28 is a RNA chain called mRNA.

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

- Molecule 29 is a RNA chain called P-site tRNA-fMet.

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

- Molecule 30 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	2753	Total	C	N	O	P	0	0
			59129	26383	10897	19096	2753		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	2163	G	A	conflict	GB 937521852

- Molecule 31 is a RNA chain called 5S rRNA.

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

- Molecule 32 is a protein called 50S ribosomal protein L2.

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

- Molecule 33 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 34 is a protein called 50S ribosomal protein L4.

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

- Molecule 35 is a protein called 50S ribosomal protein L5.

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

- Molecule 36 is a protein called 50S ribosomal protein L6.

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

- Molecule 37 is a protein called 50S ribosomal protein L9.

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

- Molecule 38 is a protein called 50S ribosomal protein L13.

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

- Molecule 39 is a protein called 50S ribosomal protein L14.

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

- Molecule 40 is a protein called 50S ribosomal protein L15.

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

- Molecule 41 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 42 is a protein called 50S ribosomal protein L17.

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

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

- Molecule 44 is a protein called 50S ribosomal protein L19.

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

- Molecule 45 is a protein called 50S ribosomal protein L20.

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

- Molecule 46 is a protein called 50S ribosomal protein L21.

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

- Molecule 47 is a protein called 50S ribosomal protein L22.

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

- Molecule 48 is a protein called 50S ribosomal protein L23.

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

- Molecule 49 is a protein called 50S ribosomal protein L24.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

- Molecule 52 is a protein called 50S ribosomal protein L28.

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

- Molecule 53 is a protein called 50S ribosomal protein L29.

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

- Molecule 54 is a protein called 50S ribosomal protein L30.

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

- Molecule 55 is a protein called 50S ribosomal protein L32.

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

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	3	1	Total	Zn	0
			1	1	
56	4	1	Total	Zn	0
			1	1	

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	A	89	Total	Mg	0
			89	89	
57	E	1	Total	Mg	0
			1	1	
57	N	1	Total	Mg	0
			1	1	
57	Q	1	Total	Mg	0
			1	1	
57	a	207	Total	Mg	0
			207	207	
57	b	5	Total	Mg	0
			5	5	
57	d	1	Total	Mg	0
			1	1	
57	k	1	Total	Mg	0
			1	1	
57	p	1	Total	Mg	0
			1	1	
57	z	1	Total	Mg	0
			1	1	

- Molecule 58 is Thermorubin (three-letter code: T8B) (formula: C<sub>32</sub>H<sub>24</sub>O<sub>12</sub>) (labeled as "Ligand of Interest" by depositor).



### 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.

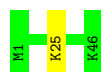
- Molecule 1: 50S ribosomal protein L33

Chain 0:  91% 7%



- Molecule 2: 50S ribosomal protein L34

Chain 1:  98%



- Molecule 3: 50S ribosomal protein L35

Chain 2:  97%




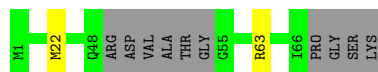
- Molecule 4: 50S ribosomal protein L36

Chain 3:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: 50S ribosomal protein L31

Chain 4:  83% 14%

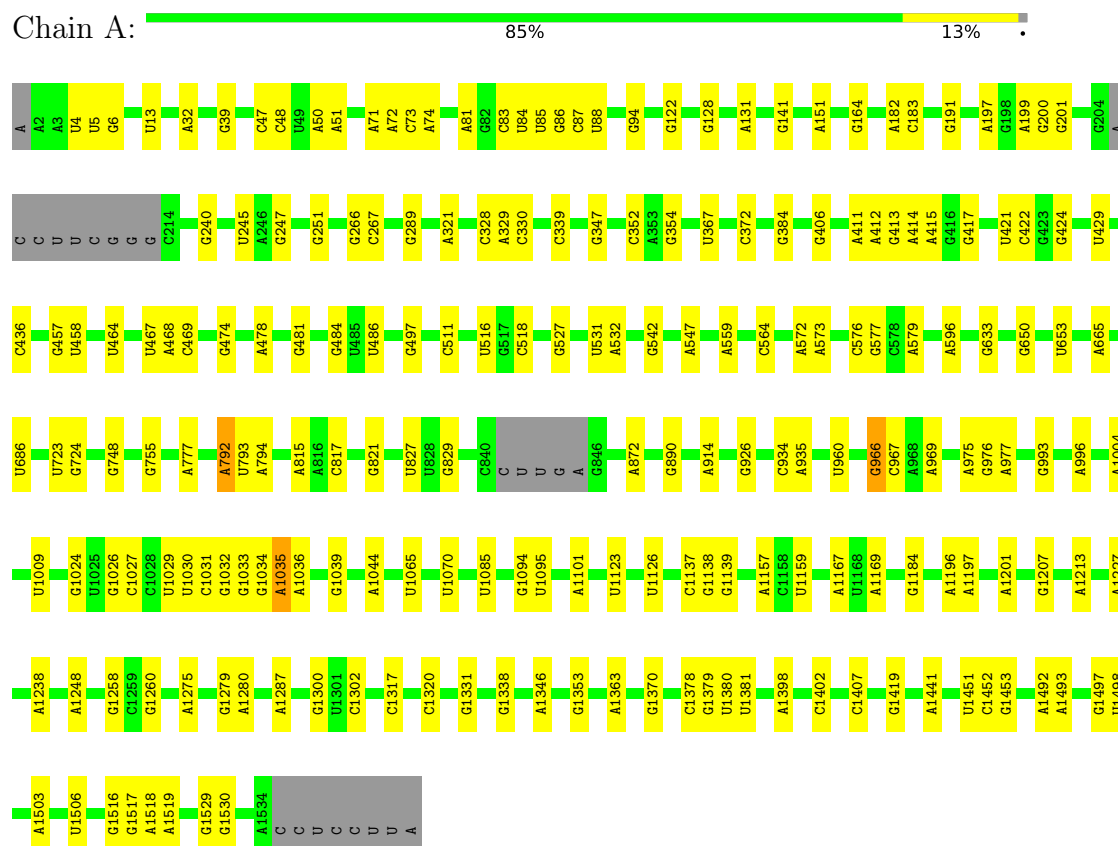


- Molecule 6: E-site tRNA

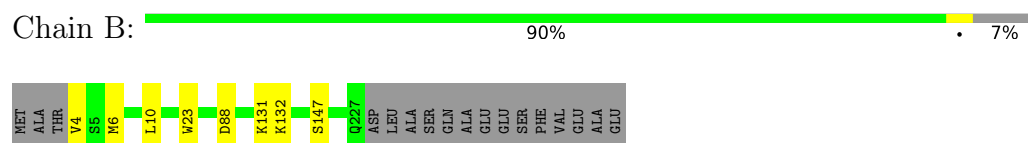
Chain 5:  50% 50%



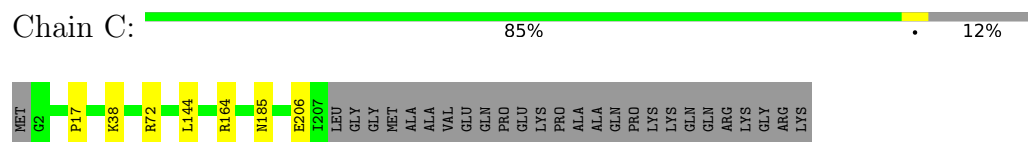
- Molecule 7: 16S rRNA



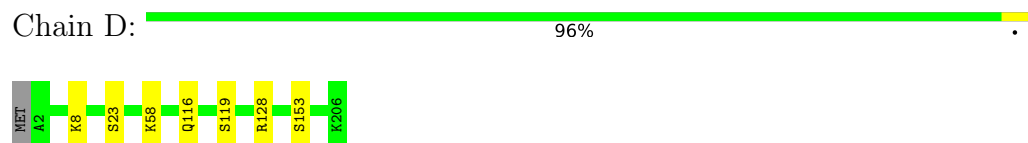
- Molecule 8: 30S ribosomal protein S2



- Molecule 9: 30S ribosomal protein S3



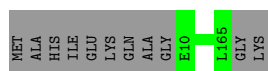
- Molecule 10: 30S ribosomal protein S4



- Molecule 11: 30S ribosomal protein S5

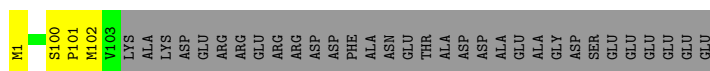


Chain E:  93% 7%




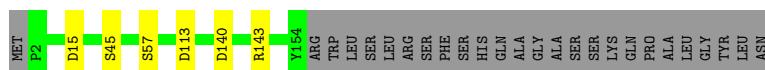
- Molecule 12: 30S ribosomal protein S6, fully modified isoform

Chain F:  73% 24%



- Molecule 13: 30S ribosomal protein S7

Chain G:  82% 15%



- Molecule 14: 30S ribosomal protein S8

Chain H:  98% ..



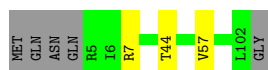
- Molecule 15: 30S ribosomal protein S9

Chain I:  94% ..




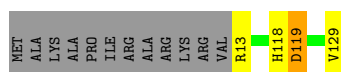
- Molecule 16: 30S ribosomal protein S10

Chain J:  92% 5%



- Molecule 17: 30S ribosomal protein S11

Chain K:  88% .. 9%



- Molecule 18: 30S ribosomal protein S12

Chain L:  97% ..



- Molecule 19: 30S ribosomal protein S13

Chain M:  94% ..



- Molecule 20: 30S ribosomal protein S14

Chain N:  97% ..



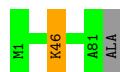
- Molecule 21: 30S ribosomal protein S15

Chain O:  98% ..




- Molecule 22: 30S ribosomal protein S16

Chain P:  98% ..




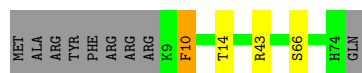
- Molecule 23: 30S ribosomal protein S17

Chain Q:  88% 6% 6%




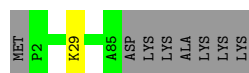
- Molecule 24: 30S ribosomal protein S18

Chain R:  83% .. 12%



- Molecule 25: 30S ribosomal protein S19

Chain S:  90% 9%



- Molecule 26: 30S ribosomal protein S20

Chain T:  97%



- Molecule 27: 30S ribosomal protein S21

Chain U:  96%



- Molecule 28: mRNA

Chain X:  100%


There are no outlier residues recorded for this chain.

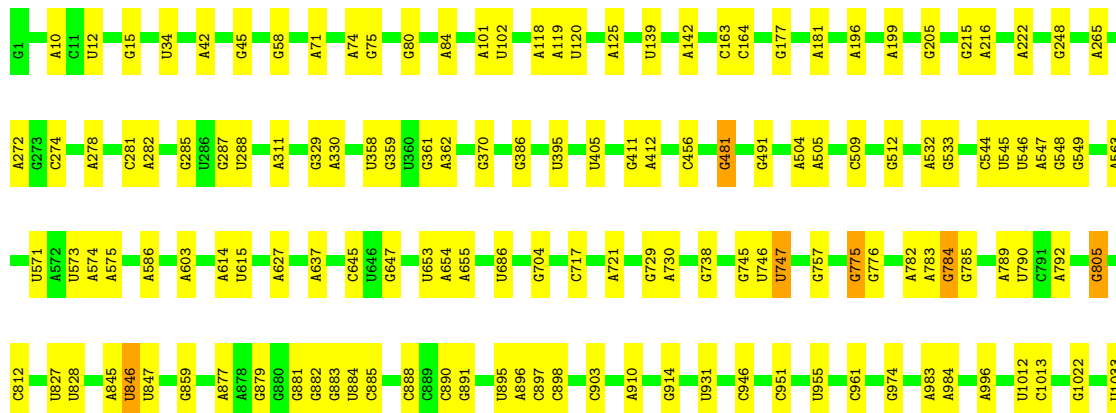
- Molecule 29: P-site tRNA-fMet

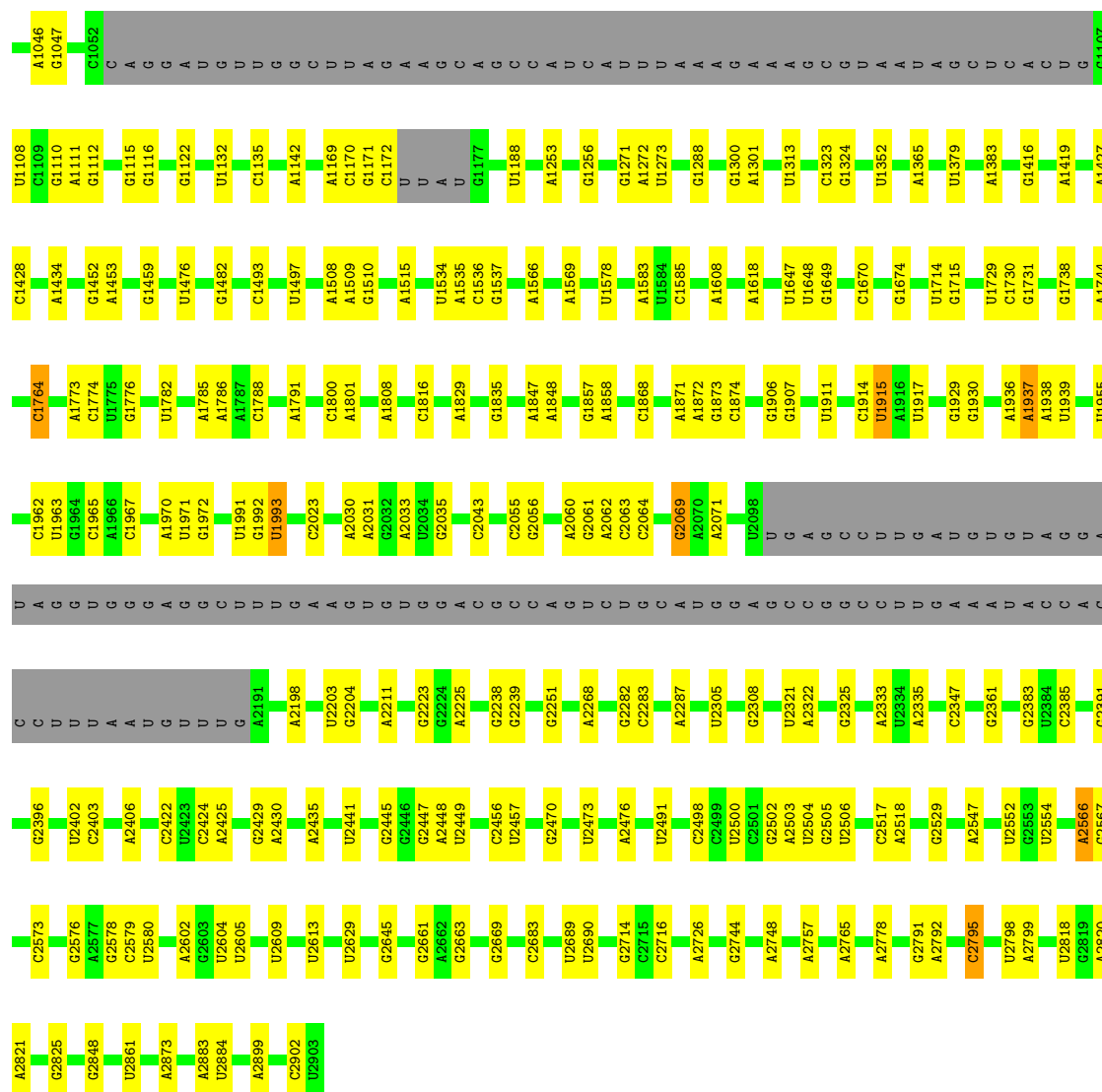
Chain Z:  74% 26%



- Molecule 30: 23S rRNA

Chain a:  82% 13% 5%





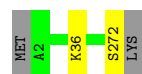
### ● Molecule 31: 5S rRNA

Chain b: 89% 10%



### ● Molecule 32: 50S ribosomal protein L2

Chain c: 99%



### ● Molecule 33: 50S ribosomal protein L3

Chain d: 99%



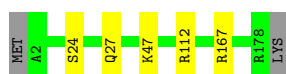
- Molecule 34: 50S ribosomal protein L4

Chain e: 99%



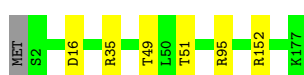
- Molecule 35: 50S ribosomal protein L5

Chain f: 96%



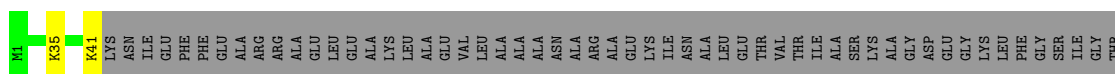
- Molecule 36: 50S ribosomal protein L6

Chain g: 96%



- Molecule 37: 50S ribosomal protein L9

Chain h: 26%



- Molecule 38: 50S ribosomal protein L13

Chain i: 100%

There are no outlier residues recorded for this chain.

- Molecule 39: 50S ribosomal protein L14

Chain j: 98%



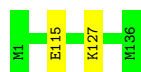
- Molecule 40: 50S ribosomal protein L15

Chain k: 99%



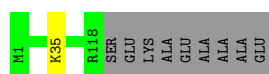
- Molecule 41: 50S ribosomal protein L16

Chain l: 99%



- Molecule 42: 50S ribosomal protein L17

Chain m: 92% 7%



- Molecule 43: 50S ribosomal protein L18

Chain n: 98%



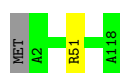
- Molecule 44: 50S ribosomal protein L19

Chain o: 97%



- Molecule 45: 50S ribosomal protein L20

Chain p: 98%



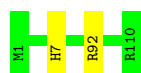
- Molecule 46: 50S ribosomal protein L21

Chain q: 94% 6%



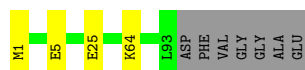
- Molecule 47: 50S ribosomal protein L22

Chain r: 98%



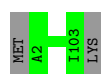
- Molecule 48: 50S ribosomal protein L23

Chain s: 89% 7%



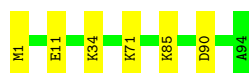
- Molecule 49: 50S ribosomal protein L24

Chain t: 98%



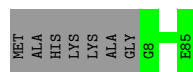
- Molecule 50: 50S ribosomal protein L25

Chain u: 94% 6%



- Molecule 51: 50S ribosomal protein L27

Chain v: 92% 8%



- Molecule 52: 50S ribosomal protein L28

Chain w: 95% 2%



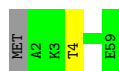
- Molecule 53: 50S ribosomal protein L29

Chain x: 98%



- Molecule 54: 50S ribosomal protein L30

Chain y: 97% 2%



- Molecule 55: 50S ribosomal protein L32

Chain z:  96% ..





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1088035	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 ( $e^-/\text{\AA}^2$ )	30.745	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (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: 1MG, ZN, MA6, 6MZ, T8B, MG, G7M, UR3, OMC, 2MA, MEQ, 5MU, OMU, 4OC, 2MG, 5MC, OMG, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	0	0.38	0/424	0.57	0/565
2	1	0.33	0/380	0.73	0/498
3	2	0.35	0/513	0.60	0/676
4	3	0.38	0/303	0.60	0/397
5	4	0.29	0/488	0.53	0/649
6	5	0.62	0/46	0.87	0/69
7	A	0.77	0/36236	0.93	8/56520 (0.0%)
8	B	0.35	0/1784	0.55	0/2403
9	C	0.34	0/1651	0.58	0/2225
10	D	0.32	0/1665	0.58	0/2227
11	E	0.37	0/1165	0.58	0/1568
12	F	0.42	1/858 (0.1%)	0.70	3/1160 (0.3%)
13	G	0.33	0/1219	0.59	0/1635
14	H	0.37	0/989	0.58	0/1326
15	I	0.37	0/1034	0.62	0/1375
16	J	0.38	0/796	0.62	0/1077
17	K	0.33	0/893	0.64	1/1205 (0.1%)
18	L	0.36	0/969	0.63	0/1300
19	M	0.32	0/900	0.59	0/1204
20	N	0.34	0/817	0.60	0/1088
21	O	0.33	0/722	0.57	0/964
22	P	0.34	0/653	0.61	0/877
23	Q	0.39	0/650	0.60	0/871
24	R	0.36	0/553	0.63	0/742
25	S	0.31	0/685	0.54	0/922
26	T	0.32	0/676	0.54	0/895
27	U	0.36	0/597	0.61	0/792
28	X	0.71	0/147	0.91	0/227
29	Z	0.66	0/1813	0.94	0/2825
30	a	0.91	8/65696 (0.0%)	1.03	78/102485 (0.1%)
31	b	0.74	0/2850	0.87	0/4444

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	c	0.40	0/2121	0.64	0/2852
33	d	0.36	0/1576	0.58	0/2119
34	e	0.34	0/1571	0.55	0/2113
35	f	0.35	0/1434	0.55	0/1926
36	g	0.35	0/1343	0.56	0/1816
37	h	0.31	0/306	0.57	0/413
38	i	0.38	0/1152	0.57	0/1551
39	j	0.39	0/955	0.66	0/1279
40	k	0.34	0/1062	0.62	0/1413
41	l	0.37	0/1092	0.64	0/1457
42	m	0.38	0/958	0.66	0/1281
43	n	0.35	0/902	0.61	0/1209
44	o	0.38	0/929	0.61	0/1242
45	p	0.37	0/960	0.61	0/1278
46	q	0.37	0/829	0.60	0/1107
47	r	0.36	0/864	0.58	0/1156
48	s	0.34	0/744	0.56	0/994
49	t	0.33	0/787	0.56	0/1051
50	u	0.38	0/766	0.56	0/1025
51	v	0.37	0/593	0.58	0/785
52	w	0.37	0/635	0.61	0/848
53	x	0.31	0/502	0.55	0/667
54	y	0.34	0/453	0.63	0/605
55	z	0.37	0/450	0.64	0/599
All	All	0.74	9/151156 (0.0%)	0.91	90/225997 (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
52	w	0	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2449	U	C5-C6	17.63	1.50	1.34
30	a	2449	U	C2-N3	13.90	1.47	1.37
30	a	2449	U	N1-C2	10.25	1.47	1.38
30	a	2449	U	C4-O4	-8.77	1.16	1.23
30	a	2449	U	N1-C6	8.54	1.45	1.38

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	2449	U	C2-N3-C4	-11.12	120.33	127.00
12	F	101	PRO	N-CD-CG	-10.47	87.50	103.20
30	a	2449	U	N1-C2-N3	10.27	121.06	114.90
30	a	512	G	O4'-C1'-N9	9.19	115.55	108.20
30	a	2449	U	N3-C4-C5	8.38	119.63	114.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
52	w	16	ASN	Peptide

## 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	49/55 (89%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (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%)	52 (93%)	4 (7%)	0	100	100
8	B	222/241 (92%)	216 (97%)	5 (2%)	1 (0%)	25	16
9	C	204/233 (88%)	195 (96%)	9 (4%)	0	100	100
10	D	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
11	E	154/167 (92%)	152 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	F	101/135 (75%)	100 (99%)	1 (1%)	0	100	100
13	G	151/179 (84%)	143 (95%)	8 (5%)	0	100	100
14	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
15	I	125/130 (96%)	121 (97%)	4 (3%)	0	100	100
16	J	96/103 (93%)	92 (96%)	3 (3%)	1 (1%)	13	5
17	K	115/129 (89%)	109 (95%)	5 (4%)	1 (1%)	14	7
18	L	121/124 (98%)	116 (96%)	5 (4%)	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%)	85 (99%)	1 (1%)	0	100	100
22	P	79/82 (96%)	71 (90%)	7 (9%)	1 (1%)	10	3
23	Q	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
24	R	64/75 (85%)	61 (95%)	2 (3%)	1 (2%)	8	2
25	S	82/92 (89%)	82 (100%)	0	0	100	100
26	T	84/87 (97%)	84 (100%)	0	0	100	100
27	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
32	c	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
33	d	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
34	e	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
35	f	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
36	g	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
37	h	39/149 (26%)	36 (92%)	3 (8%)	0	100	100
38	i	140/142 (99%)	140 (100%)	0	0	100	100
39	j	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
40	k	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
41	l	132/136 (97%)	126 (96%)	6 (4%)	0	100	100
42	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
43	n	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
44	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
45	p	115/118 (98%)	115 (100%)	0	0	100	100
46	q	101/103 (98%)	99 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
48	s	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
49	t	100/104 (96%)	90 (90%)	10 (10%)	0	100	100
50	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
51	v	76/85 (89%)	74 (97%)	2 (3%)	0	100	100
52	w	75/78 (96%)	75 (100%)	0	0	100	100
53	x	60/63 (95%)	60 (100%)	0	0	100	100
54	y	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	7	2
55	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
All	All	5484/5913 (93%)	5333 (97%)	145 (3%)	6 (0%)	50	42

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	R	10	PHE
16	J	57	VAL
17	K	119	ASP
22	P	46	LYS
54	y	4	THR

### 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	41
2	1	38/38 (100%)	37 (97%)	1 (3%)	41	33
3	2	51/52 (98%)	50 (98%)	1 (2%)	50	44
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	55/62 (89%)	53 (96%)	2 (4%)	30	20
8	B	186/199 (94%)	179 (96%)	7 (4%)	28	18
9	C	170/190 (90%)	163 (96%)	7 (4%)	26	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	D	172/173 (99%)	165 (96%)	7 (4%)	26	15
11	E	119/126 (94%)	119 (100%)	0	100	100
12	F	90/116 (78%)	87 (97%)	3 (3%)	33	23
13	G	126/147 (86%)	120 (95%)	6 (5%)	21	10
14	H	104/105 (99%)	103 (99%)	1 (1%)	73	72
15	I	105/107 (98%)	100 (95%)	5 (5%)	21	10
16	J	86/90 (96%)	84 (98%)	2 (2%)	45	39
17	K	90/99 (91%)	87 (97%)	3 (3%)	33	23
18	L	103/104 (99%)	100 (97%)	3 (3%)	37	28
19	M	93/96 (97%)	89 (96%)	4 (4%)	25	14
20	N	83/84 (99%)	81 (98%)	2 (2%)	44	37
21	O	76/77 (99%)	75 (99%)	1 (1%)	65	62
22	P	65/65 (100%)	64 (98%)	1 (2%)	60	57
23	Q	73/78 (94%)	68 (93%)	5 (7%)	13	4
24	R	57/65 (88%)	53 (93%)	4 (7%)	12	4
25	S	72/79 (91%)	71 (99%)	1 (1%)	62	59
26	T	65/66 (98%)	63 (97%)	2 (3%)	35	25
27	U	60/61 (98%)	58 (97%)	2 (3%)	33	23
32	c	216/218 (99%)	214 (99%)	2 (1%)	75	75
33	d	163/163 (100%)	161 (99%)	2 (1%)	67	65
34	e	165/165 (100%)	162 (98%)	3 (2%)	54	49
35	f	148/150 (99%)	143 (97%)	5 (3%)	32	22
36	g	137/138 (99%)	131 (96%)	6 (4%)	24	13
37	h	32/114 (28%)	30 (94%)	2 (6%)	15	6
38	i	116/116 (100%)	116 (100%)	0	100	100
39	j	104/104 (100%)	102 (98%)	2 (2%)	52	47
40	k	103/103 (100%)	102 (99%)	1 (1%)	73	72
41	l	109/109 (100%)	107 (98%)	2 (2%)	54	49
42	m	98/103 (95%)	97 (99%)	1 (1%)	73	72
43	n	86/87 (99%)	85 (99%)	1 (1%)	67	65
44	o	99/100 (99%)	97 (98%)	2 (2%)	50	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	p	89/90 (99%)	88 (99%)	1 (1%)	70	68
46	q	84/84 (100%)	78 (93%)	6 (7%)	12	4
47	r	93/93 (100%)	91 (98%)	2 (2%)	47	41
48	s	80/84 (95%)	76 (95%)	4 (5%)	20	10
49	t	83/85 (98%)	83 (100%)	0	100	100
50	u	78/78 (100%)	72 (92%)	6 (8%)	10	3
51	v	58/63 (92%)	58 (100%)	0	100	100
52	w	67/68 (98%)	65 (97%)	2 (3%)	36	27
53	x	54/55 (98%)	54 (100%)	0	100	100
54	y	48/49 (98%)	48 (100%)	0	100	100
55	z	47/48 (98%)	46 (98%)	1 (2%)	48	43
All	All	4576/4829 (95%)	4454 (97%)	122 (3%)	41	31

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	Q	9	GLN
48	s	5	GLU
32	c	36	LYS
48	s	1	MET
50	u	90	ASP

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

Mol	Chain	Res	Type
8	B	122	GLN
13	G	68	ASN
13	G	130	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	X	5/6 (83%)	0	0
29	Z	75/76 (98%)	20 (26%)	0
30	a	2746/2903 (94%)	308 (11%)	0
31	b	118/120 (98%)	12 (10%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	5	1/2 (50%)	1 (100%)	0
7	A	1513/1542 (98%)	186 (12%)	6 (0%)
All	All	4458/4649 (95%)	527 (11%)	6 (0%)

5 of 527 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	5	76	A
7	A	4	U
7	A	5	U
7	A	6	G
7	A	13	U

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	1026	G
7	A	1035	A
7	A	1492	A
7	A	199	A
7	A	5	U

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

34 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	2MG	A	1516	7	18,26,27	2.58	7 (38%)	16,38,41	1.40	2 (12%)
30	1MG	a	745	30	18,26,27	2.56	6 (33%)	19,39,42	1.51	3 (15%)
30	5MU	a	1939	30	19,22,23	7.11	8 (42%)	28,32,35	3.45	8 (28%)
30	OMC	a	2498	57,30	19,22,23	2.89	8 (42%)	26,31,34	0.96	1 (3%)
7	G7M	A	527	7	20,26,27	2.31	7 (35%)	17,39,42	1.17	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	PSU	a	955	30	18,21,22	1.20	1 (5%)	22,30,33	2.04	3 (13%)
7	4OC	A	1402	7	20,23,24	2.92	8 (40%)	26,32,35	1.19	2 (7%)
30	2MA	a	2503	57,30	19,25,26	2.99	7 (36%)	21,37,40	2.50	4 (19%)
30	6MZ	a	1618	30	18,25,26	2.11	3 (16%)	16,36,39	2.59	4 (25%)
7	5MC	A	967	7	18,22,23	3.61	7 (38%)	26,32,35	1.05	2 (7%)
30	6MZ	a	2030	30	18,25,26	1.95	2 (11%)	16,36,39	2.85	3 (18%)
30	2MG	a	2445	30	18,26,27	2.79	7 (38%)	16,38,41	1.57	3 (18%)
30	PSU	a	2457	30	18,21,22	1.15	1 (5%)	22,30,33	1.90	4 (18%)
33	MEQ	d	150	33	8,9,10	0.83	0	5,10,12	0.98	0
30	5MU	a	747	30	19,22,23	7.18	8 (42%)	28,32,35	3.41	8 (28%)
7	2MG	A	966	7	18,26,27	2.58	6 (33%)	16,38,41	1.51	4 (25%)
30	OMG	a	2251	29,30	18,26,27	2.38	8 (44%)	19,38,41	1.67	5 (26%)
7	UR3	A	1498	7,57	19,22,23	2.76	8 (42%)	26,32,35	1.47	1 (3%)
7	5MC	A	1407	7	18,22,23	3.48	7 (38%)	26,32,35	1.18	3 (11%)
30	PSU	a	1911	30	18,21,22	1.14	1 (5%)	22,30,33	1.88	4 (18%)
7	2MG	A	1207	7	18,26,27	2.66	6 (33%)	16,38,41	1.45	3 (18%)
30	G7M	a	2069	30	20,26,27	2.14	7 (35%)	17,39,42	1.05	1 (5%)
30	PSU	a	2504	30	18,21,22	1.14	1 (5%)	22,30,33	1.89	2 (9%)
7	MA6	A	1519	7	18,26,27	1.48	4 (22%)	19,38,41	3.68	3 (15%)
30	2MG	a	1835	30	18,26,27	2.53	7 (38%)	16,38,41	1.55	3 (18%)
7	PSU	A	516	7	18,21,22	1.20	1 (5%)	22,30,33	1.79	5 (22%)
30	PSU	a	2605	30	18,21,22	1.14	1 (5%)	22,30,33	1.74	4 (18%)
30	PSU	a	2604	30	18,21,22	1.10	1 (5%)	22,30,33	1.80	4 (18%)
30	PSU	a	1917	30	18,21,22	1.06	1 (5%)	22,30,33	1.70	3 (13%)
7	MA6	A	1518	7	18,26,27	1.49	3 (16%)	19,38,41	3.36	3 (15%)
30	PSU	a	2580	30	18,21,22	1.14	2 (11%)	22,30,33	1.80	5 (22%)
30	PSU	a	746	57,30	18,21,22	1.23	1 (5%)	22,30,33	1.67	4 (18%)
30	5MC	a	1962	30	18,22,23	3.47	7 (38%)	26,32,35	1.05	1 (3%)
30	OMU	a	2552	30	19,22,23	2.94	8 (42%)	26,31,34	1.72	4 (15%)

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	2MG	A	1516	7	-	0/5/27/28	0/3/3/3
30	1MG	a	745	30	-	0/3/25/26	0/3/3/3
30	5MU	a	1939	30	-	0/7/25/26	0/2/2/2
30	OMC	a	2498	57,30	-	0/9/27/28	0/2/2/2
7	G7M	A	527	7	-	0/3/25/26	0/3/3/3
30	PSU	a	955	30	-	0/7/25/26	0/2/2/2
7	4OC	A	1402	7	-	0/9/29/30	0/2/2/2
30	2MA	a	2503	57,30	-	2/3/25/26	0/3/3/3
30	6MZ	a	1618	30	-	0/5/27/28	0/3/3/3
7	5MC	A	967	7	-	0/7/25/26	0/2/2/2
30	6MZ	a	2030	30	-	2/5/27/28	0/3/3/3
30	2MG	a	2445	30	-	0/5/27/28	0/3/3/3
30	PSU	a	2457	30	-	0/7/25/26	0/2/2/2
33	MEQ	d	150	33	-	2/8/9/11	-
30	5MU	a	747	30	-	1/7/25/26	0/2/2/2
7	2MG	A	966	7	-	0/5/27/28	0/3/3/3
30	OMG	a	2251	29,30	-	1/5/27/28	0/3/3/3
7	UR3	A	1498	7,57	-	0/7/25/26	0/2/2/2
7	5MC	A	1407	7	-	0/7/25/26	0/2/2/2
30	PSU	a	1911	30	-	1/7/25/26	0/2/2/2
7	2MG	A	1207	7	-	0/5/27/28	0/3/3/3
30	G7M	a	2069	30	-	2/3/25/26	0/3/3/3
30	PSU	a	2504	30	-	0/7/25/26	0/2/2/2
7	MA6	A	1519	7	-	2/7/29/30	0/3/3/3
30	2MG	a	1835	30	-	0/5/27/28	0/3/3/3
7	PSU	A	516	7	-	0/7/25/26	0/2/2/2
30	PSU	a	2605	30	-	0/7/25/26	0/2/2/2
30	PSU	a	2604	30	-	0/7/25/26	0/2/2/2
30	PSU	a	1917	30	-	0/7/25/26	0/2/2/2
7	MA6	A	1518	7	-	0/7/29/30	0/3/3/3
30	PSU	a	2580	30	-	0/7/25/26	0/2/2/2
30	PSU	a	746	57,30	-	3/7/25/26	0/2/2/2
30	5MC	a	1962	30	-	0/7/25/26	0/2/2/2
30	OMU	a	2552	30	-	1/9/27/28	0/2/2/2

The worst 5 of 160 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	747	5MU	C4-C5	20.47	1.78	1.44
30	a	1939	5MU	C4-C5	20.34	1.78	1.44
30	a	747	5MU	C6-N1	15.03	1.63	1.38
30	a	1939	5MU	C6-N1	14.78	1.63	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	747	5MU	C6-C5	-12.22	1.14	1.34

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1519	MA6	N1-C6-N6	-14.26	102.05	117.06
7	A	1518	MA6	N1-C6-N6	-12.36	104.05	117.06
30	a	1939	5MU	C5-C4-N3	10.68	124.43	115.31
30	a	747	5MU	C5-C4-N3	9.36	123.30	115.31
30	a	1939	5MU	C5-C6-N1	-9.07	114.01	123.34

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	a	746	PSU	C2'-C1'-C5-C4
30	a	746	PSU	O4'-C1'-C5-C6
30	a	2030	6MZ	O4'-C4'-C5'-O5'
30	a	2030	6MZ	C3'-C4'-C5'-O5'
33	d	150	MEQ	NE2-CD-CG-CB

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](#)

Of 311 ligands modelled in this entry, 310 are monoatomic - leaving 1 for Mogul analysis.

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
58	T8B	A	1689	57	48,48,48	0.80	2 (4%)	63,71,71	1.07	2 (3%)

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
58	T8B	A	1689	57	-	2/26/26/26	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	A	1689	T8B	C10-C11	3.91	1.38	1.34
58	A	1689	T8B	O1-C1	-2.19	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	A	1689	T8B	C21-C23-C24	-5.27	118.89	125.03
58	A	1689	T8B	O7-C16-C15	-2.61	116.08	121.29

There are no chirality outliers.

All (2) torsion outliers are listed below:

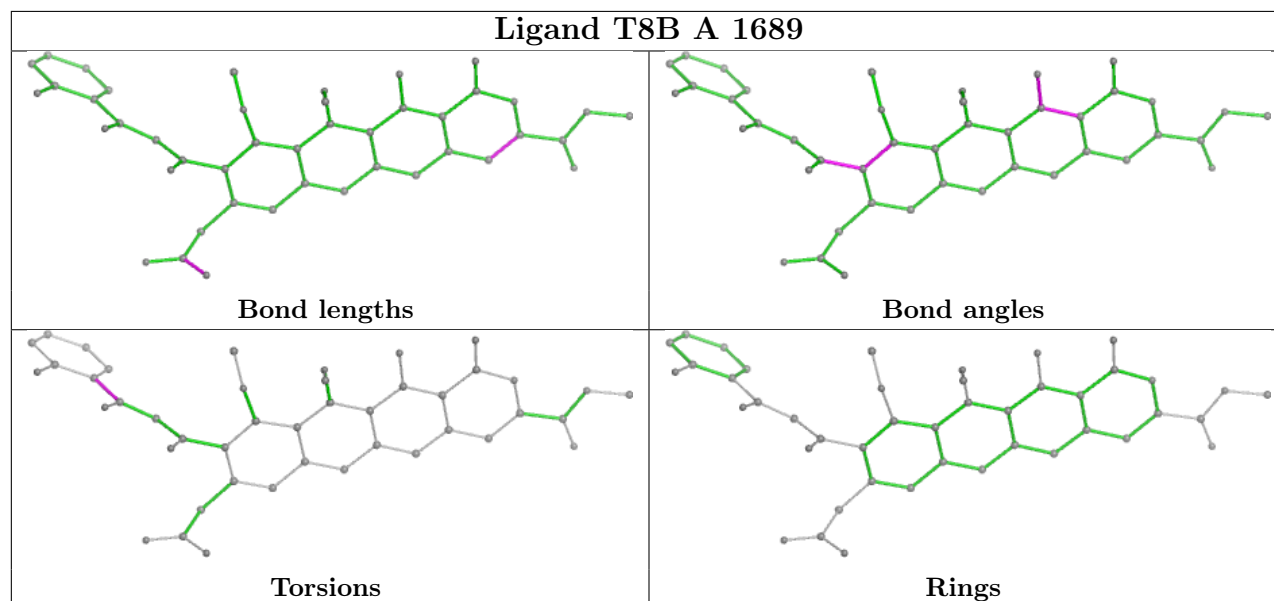
Mol	Chain	Res	Type	Atoms
58	A	1689	T8B	O11-C26-C27-C32
58	A	1689	T8B	C25-C26-C27-C28

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
41	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	81:ARG	C	82:MET	N	2.56