wwPDB EM Validation Summary Report (i)

Mar 6, 2025 – 05:56 pm GMT

PDB ID	:	9GR1
EMDB ID	:	EMD-51517
Title	:	E. coli 70S-TEC complex in delivery state
Authors	:	Webster, M.W.; Weixlbaumer, A.
Deposited on	:	2024-09-10
Resolution	:	3.17 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

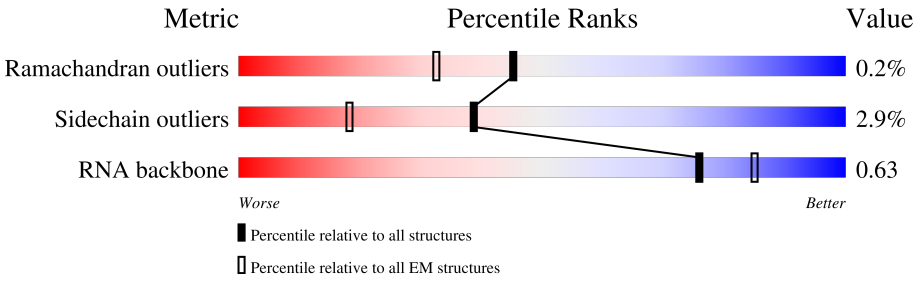
EMDB validation analysis	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.17 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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	0	55	89% · 7%
2	1	46	98% ·
3	2	65	97% · ·
4	3	38	97% ·
5	A	1542	85% 13% ·
6	B	241	88% 5% 7%
7	C	233	85% · 12%
8	D	206	99%
9	E	167	92% · 7%

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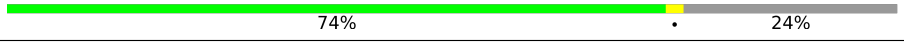
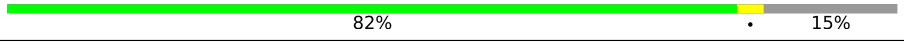
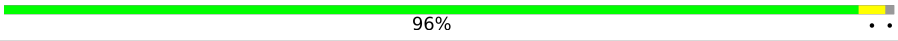
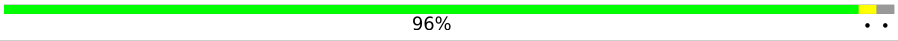
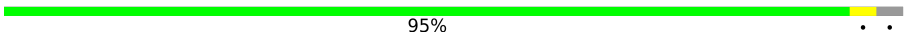
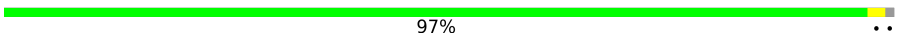
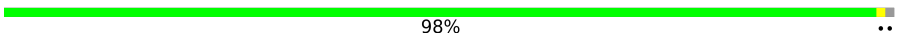
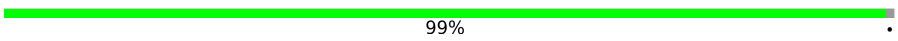
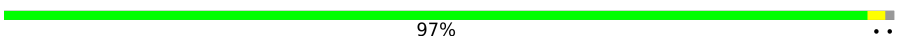
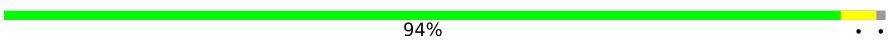
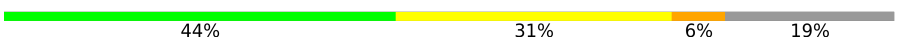
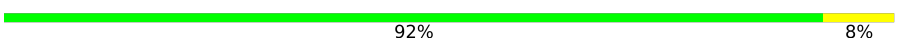
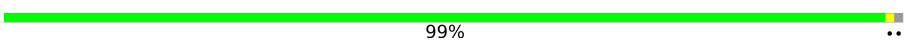
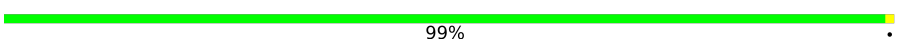
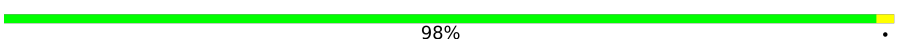
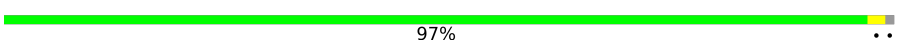
Mol	Chain	Length	Quality of chain
10	F	135	
11	G	179	
12	H	130	
13	I	130	
14	J	103	
15	K	129	
16	L	124	
17	M	118	
18	N	101	
19	O	89	
20	P	82	
21	Q	84	
22	R	75	
23	S	92	
24	T	87	
25	U	71	
26	X	16	
27	Z	76	
28	a	2925	
29	b	119	
30	c	273	
31	d	209	
32	e	201	
33	f	179	
34	g	177	

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Mol	Chain	Length	Quality of chain
35	h	149	94% 5%
36	i	142	99%
37	j	123	98%
38	k	144	100%
39	l	136	99%
40	m	127	92% 7%
41	n	117	97%
42	o	115	98%
43	p	118	99%
44	q	103	99%
45	r	110	99%
46	s	100	89% 7%
47	t	104	94%
48	u	94	99%
49	v	85	91% 8%
50	w	78	96%
51	x	63	98%
52	y	59	98%
53	z	57	96%
54	4	10	50% 50%
55	Y	77	79% 18%

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 142297 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 RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	1513	Total	C	N	O	P	0	0
			32478	14493	5961	10511	1513		

- Molecule 6 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 7 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 8 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 10 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 12 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	116	Total	C	N	O	S	0	0
			902	558	183	156	5		

- Molecule 17 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 20 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 21 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 22 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 23 is a protein called 30S ribosomal protein S19.

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

- Molecule 24 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 25 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 26 is a RNA chain called mRNA in ribosome channel.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	13	Total	C	N	O	P	0	0
			271	122	44	92	13		

- Molecule 27 is a RNA chain called Phe-NH-tRNA(Phe) A-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	Z	76	Total	C	N	O	P	S	0	0
			1624	724	290	533	76	1		

- Molecule 28 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	2748	Total	C	N	O	P	0	0
			59025	26336	10876	19065	2748		

- Molecule 29 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 30 is a protein called 50S ribosomal protein L2.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 32 is a protein called 50S ribosomal protein L4.

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

- Molecule 33 is a protein called 50S ribosomal protein L5.

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

- Molecule 34 is a protein called 50S ribosomal protein L6.

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

- Molecule 35 is a protein called 50S ribosomal protein L9.

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

- Molecule 36 is a protein called 50S ribosomal protein L13.

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

- Molecule 37 is a protein called 50S ribosomal protein L14.

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

- Molecule 38 is a protein called 50S ribosomal protein L15.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	77	ILE	VAL	conflict	UNP A0A140N711

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	l	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 40 is a protein called 50S ribosomal protein L17.

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

- Molecule 41 is a protein called 50S ribosomal protein L18.

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

- Molecule 42 is a protein called 50S ribosomal protein L19.

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

- Molecule 43 is a protein called 50S ribosomal protein L20.

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

- Molecule 44 is a protein called 50S ribosomal protein L21.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L23.

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

- Molecule 47 is a protein called 50S ribosomal protein L24.

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

- Molecule 48 is a protein called 50S ribosomal protein L25.

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

- Molecule 49 is a protein called 50S ribosomal protein L27.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L29.

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

- Molecule 52 is a protein called 50S ribosomal protein L30.

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

- Molecule 53 is a protein called 50S ribosomal protein L32.

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

- Molecule 54 is a RNA chain called mRNA in SD-aSD duplex.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	10	Total	C	N	O	P	0	0
			223	99	48	66	10		

- Molecule 55 is a RNA chain called tRNA(fmet) P-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	Y	77	Total	C	N	O	P	S	0	0
			1645	734	297	536	77	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	

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
57	A	48	Total	K	0
			48	48	
57	a	112	Total	K	0
			112	112	
57	b	1	Total	K	0
			1	1	
57	c	4	Total	K	0
			4	4	
57	d	1	Total	K	0
			1	1	
57	e	1	Total	K	0
			1	1	
57	f	1	Total	K	0
			1	1	

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	A	95	Total	Mg	0
			95	95	
58	N	1	Total	Mg	0
			1	1	
58	a	254	Total	Mg	0
			254	254	
58	b	5	Total	Mg	0
			5	5	
58	c	1	Total	Mg	0
			1	1	
58	d	1	Total	Mg	0
			1	1	

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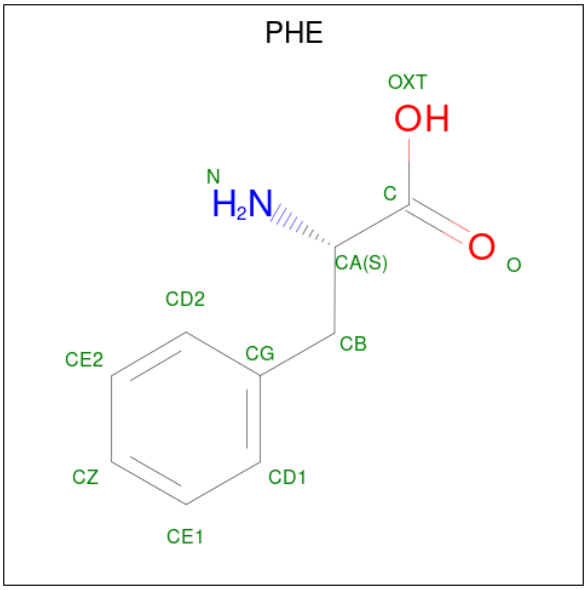
Mol	Chain	Residues	Atoms	AltConf
58	k	1	Total Mg 1 1	0
58	z	1	Total Mg 1 1	0
58	Y	1	Total Mg 1 1	0

- Molecule 59 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms	AltConf
59	a	1	Total C N O 11 9 1 1	0

3 Residue-property plots (i)

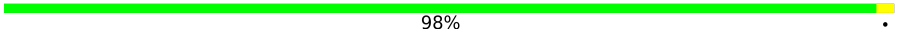
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: 50S ribosomal protein L33

Chain 0:

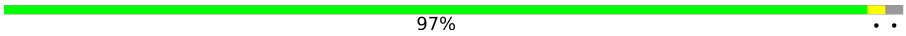
- Molecule 2: 50S ribosomal protein L34

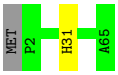
Chain 1:



- Molecule 3: 50S ribosomal protein L35

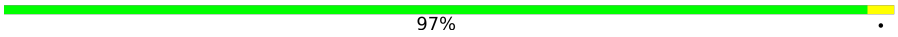
Chain 2:





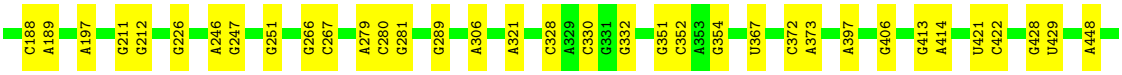
- Molecule 4: 50S ribosomal protein L36

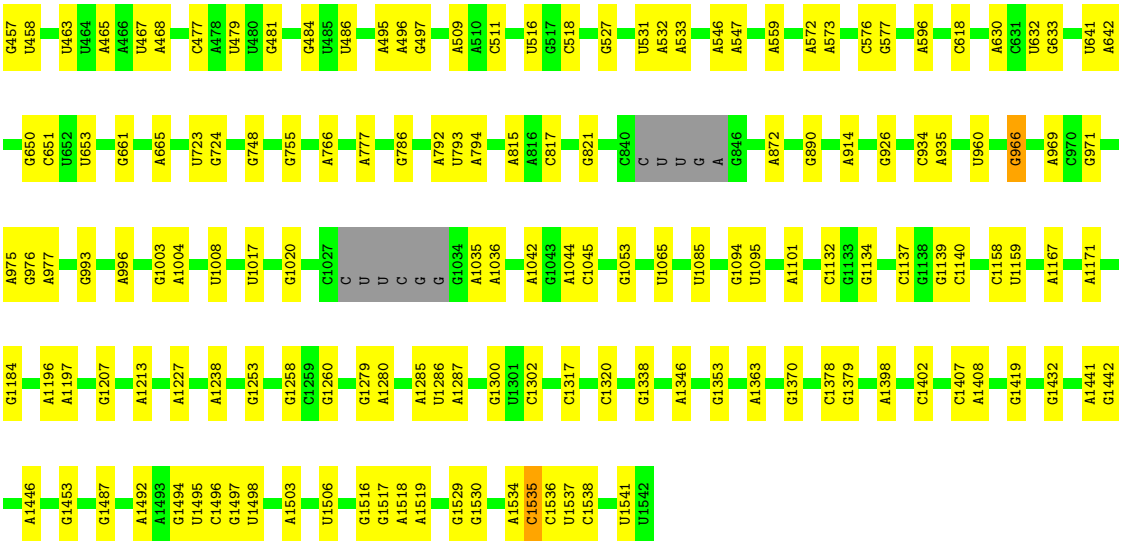
Chain 3:



- Molecule 5: 16S ribosomal RNA

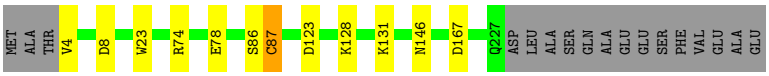
Chain A:





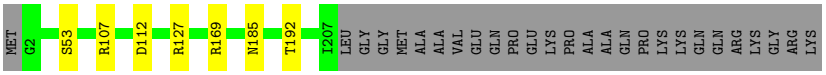
• Molecule 6: Small ribosomal subunit protein uS2

Chain B:



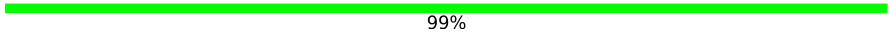
• Molecule 7: Small ribosomal subunit protein uS3

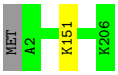
Chain C:



• Molecule 8: Small ribosomal subunit protein uS4

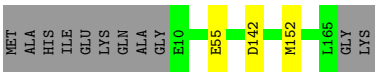
Chain D:





• Molecule 9: Small ribosomal subunit protein uS5

Chain E:

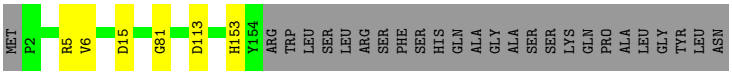


• Molecule 10: Small ribosomal subunit protein bS6, fully modified isoform

Chain F:

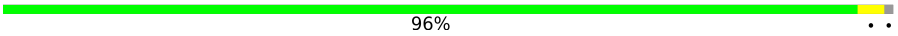
• Molecule 11: Small ribosomal subunit protein uS7

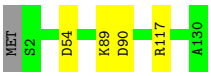
Chain G:



• Molecule 12: Small ribosomal subunit protein uS8

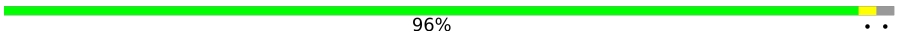
Chain H:

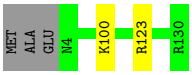




• Molecule 13: Small ribosomal subunit protein uS9

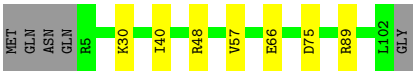
Chain I:





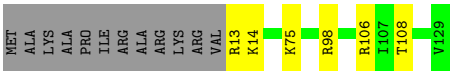
• Molecule 14: Small ribosomal subunit protein uS10

Chain J:



• Molecule 15: Small ribosomal subunit protein uS11

Chain K:

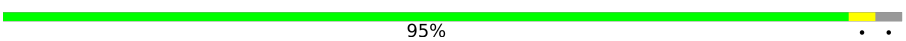


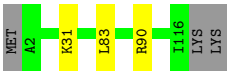
• Molecule 16: Small ribosomal subunit protein uS12

Chain L:

• Molecule 17: Small ribosomal subunit protein uS13

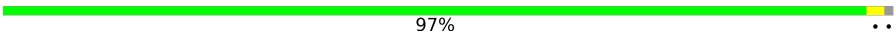
Chain M:

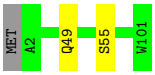




• Molecule 18: Small ribosomal subunit protein uS14

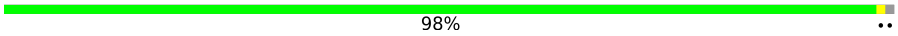
Chain N:





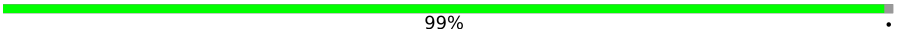
• Molecule 19: Small ribosomal subunit protein uS15

Chain O:



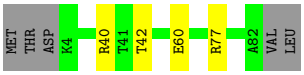
• Molecule 20: 30S ribosomal protein S16

Chain P:



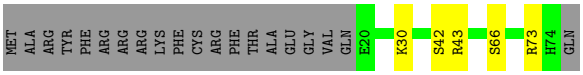
• Molecule 21: Small ribosomal subunit protein uS17

Chain Q:



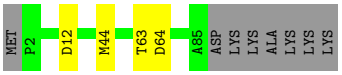
• Molecule 22: Small ribosomal subunit protein bS18

Chain R:



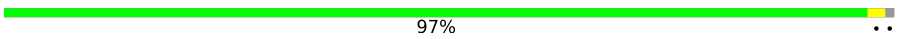
• Molecule 23: 30S ribosomal protein S19

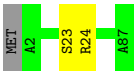
Chain S:



• Molecule 24: Small ribosomal subunit protein bS20

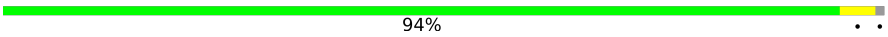
Chain T:





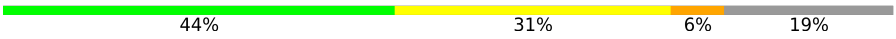
• Molecule 25: Small ribosomal subunit protein bS21

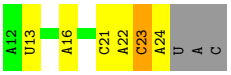
Chain U:



• Molecule 26: mRNA in ribosome channel

Chain X:



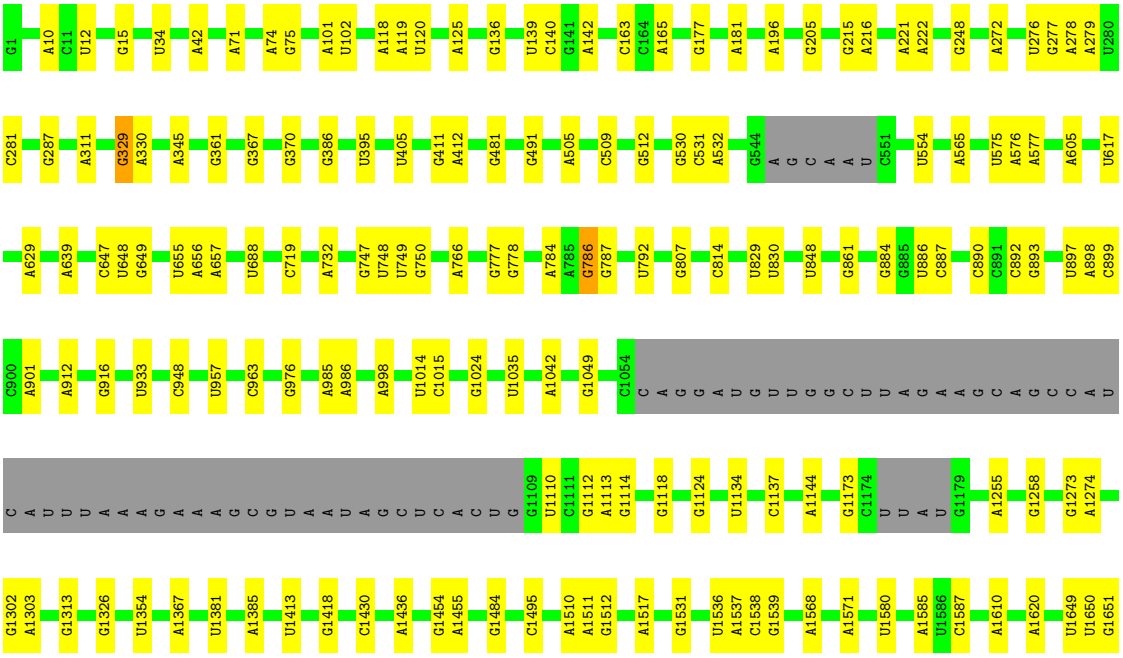


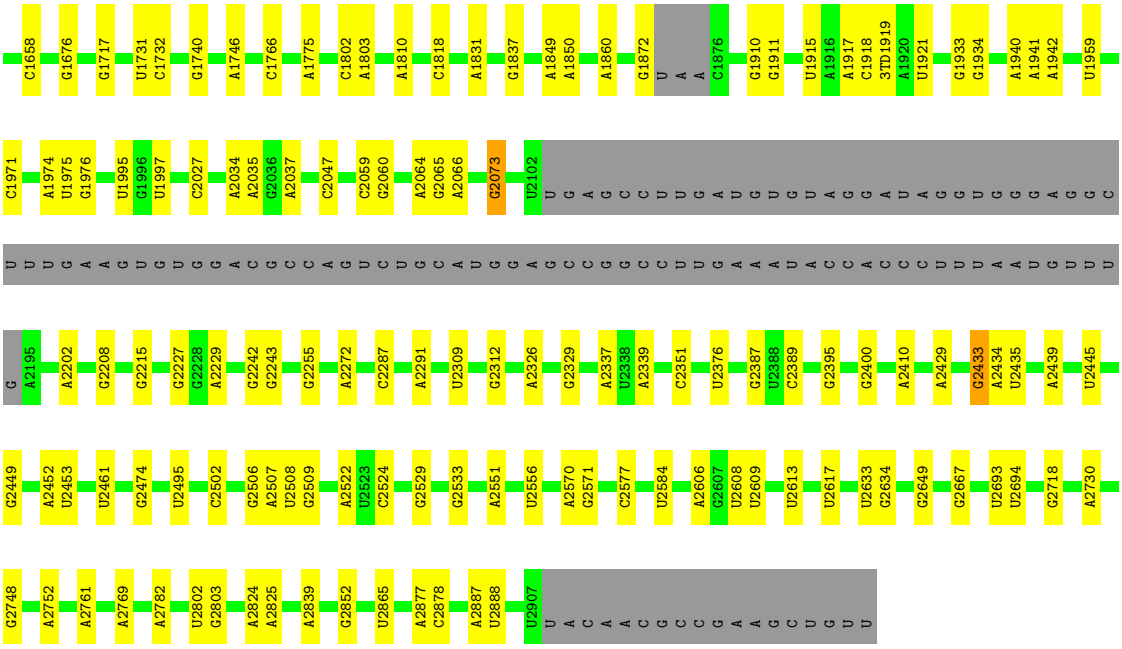
• Molecule 27: Phe-NH-tRNA(Phe) A-site

Chain Z:

• Molecule 28: 23S ribosomal RNA

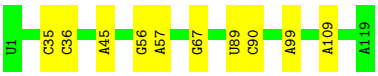
Chain a:





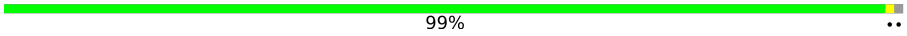
• Molecule 29: 5S ribosomal RNA

Chain b:



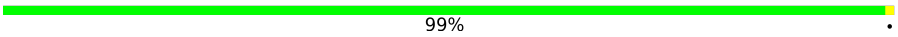
• Molecule 30: 50S ribosomal protein L2

Chain c:



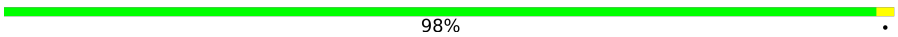
• Molecule 31: Large ribosomal subunit protein uL3

Chain d:



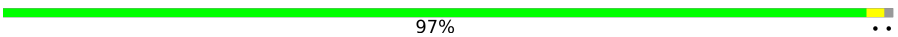
• Molecule 32: 50S ribosomal protein L4

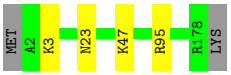
Chain e:



• Molecule 33: 50S ribosomal protein L5

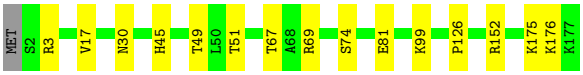
Chain f:





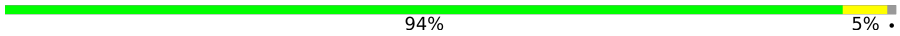
• Molecule 34: 50S ribosomal protein L6

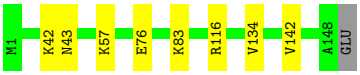
Chain g:



• Molecule 35: 50S ribosomal protein L9

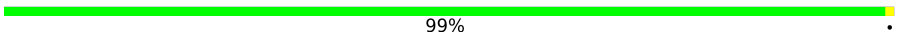
Chain h:





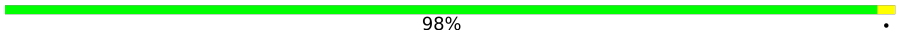
• Molecule 36: 50S ribosomal protein L13

Chain i:



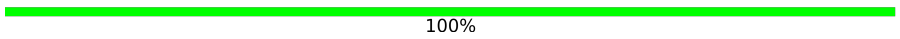
• Molecule 37: 50S ribosomal protein L14

Chain j:



• Molecule 38: 50S ribosomal protein L15

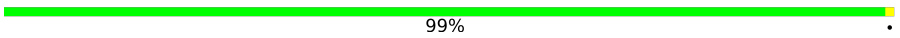
Chain k:



There are no outlier residues recorded for this chain.

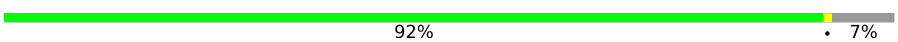
• Molecule 39: 50S ribosomal protein L16

Chain l:



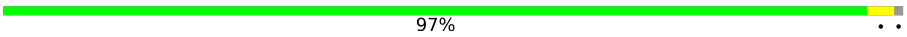
• Molecule 40: 50S ribosomal protein L17

Chain m:



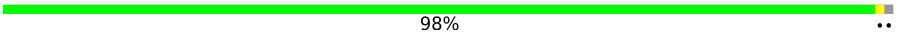
• Molecule 41: 50S ribosomal protein L18

Chain n:



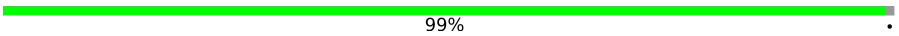
• Molecule 42: 50S ribosomal protein L19

Chain o:



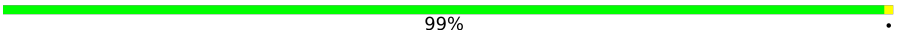
• Molecule 43: 50S ribosomal protein L20

Chain p:



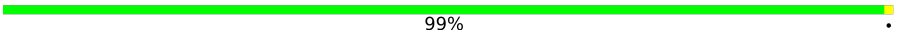
• Molecule 44: 50S ribosomal protein L21

Chain q:



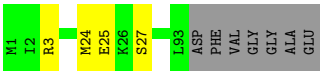
• Molecule 45: 50S ribosomal protein L22

Chain r:



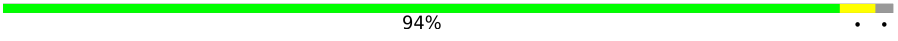
• Molecule 46: 50S ribosomal protein L23

Chain s:



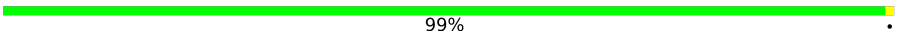
• Molecule 47: 50S ribosomal protein L24

Chain t:



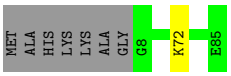
• Molecule 48: 50S ribosomal protein L25

Chain u:



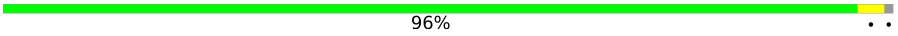
• Molecule 49: 50S ribosomal protein L27

Chain v:



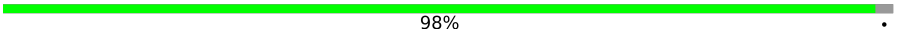
• Molecule 50: 50S ribosomal protein L28

Chain w:



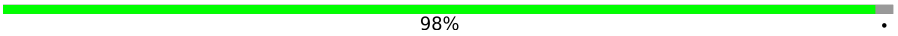
• Molecule 51: 50S ribosomal protein L29

Chain x:



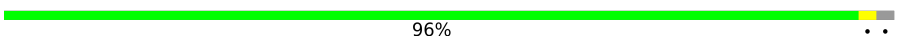
• Molecule 52: 50S ribosomal protein L30

Chain y:



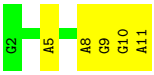
• Molecule 53: 50S ribosomal protein L32

Chain z:



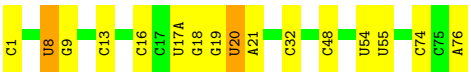
• Molecule 54: mRNA in SD-aSD duplex

Chain 4:



• Molecule 55: tRNA(fmet) P-site

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39139	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, 4SU, MA6, 1MG, 7MG, 3TD, 3AU, MG, 5MU, 4D4, G7M, OMC, 5MC, OMU, 4OC, MIA, UR3, PSU, ZN, K, 2MA, MEQ, D2T, H2U, 2MG, 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	0.37	0/424	0.55	0/565
2	1	0.37	0/380	0.70	0/498
3	2	0.37	0/513	0.57	0/676
4	3	0.37	0/303	0.60	0/397
5	A	0.58	1/36083 (0.0%)	0.80	16/56274 (0.0%)
6	B	0.30	0/1784	0.51	0/2403
7	C	0.32	0/1651	0.53	0/2225
8	D	0.28	0/1665	0.55	0/2227
9	E	0.35	0/1165	0.54	0/1568
10	F	0.35	0/858	0.54	0/1160
11	G	0.29	0/1219	0.53	0/1635
12	H	0.34	0/989	0.50	0/1326
13	I	0.31	0/1034	0.59	0/1375
14	J	0.31	0/796	0.57	0/1077
15	K	0.34	0/893	0.58	0/1205
16	L	0.36	0/904	0.62	0/1211
17	M	0.28	0/900	0.56	0/1204
18	N	0.30	0/817	0.57	0/1088
19	O	0.30	0/722	0.53	0/964
20	P	0.29	0/653	0.64	0/877
21	Q	0.36	0/650	0.55	0/871
22	R	0.37	0/462	0.60	0/621
23	S	0.30	0/685	0.53	0/922
24	T	0.28	0/676	0.50	0/895
25	U	0.30	0/597	0.58	0/792
26	X	0.39	0/301	1.22	5/465 (1.1%)
27	Z	0.35	1/1584 (0.1%)	0.72	0/2463
28	a	0.98	0/65531	0.91	26/102222 (0.0%)
29	b	0.80	0/2850	0.77	0/4444
30	c	0.41	0/2121	0.61	0/2852
31	d	0.39	0/1576	0.56	0/2119

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	e	0.37	0/1571	0.54	0/2113
33	f	0.33	0/1434	0.52	0/1926
34	g	0.36	0/1343	0.53	0/1816
35	h	0.33	0/1112	0.53	0/1503
36	i	0.40	0/1152	0.54	0/1551
37	j	0.39	0/955	0.62	0/1279
38	k	0.36	0/1062	0.62	0/1413
39	l	0.38	0/1081	0.58	0/1443
40	m	0.37	0/958	0.60	0/1281
41	n	0.36	0/902	0.57	0/1209
42	o	0.40	0/929	0.56	0/1242
43	p	0.39	0/960	0.57	0/1278
44	q	0.41	0/829	0.57	0/1107
45	r	0.35	0/864	0.55	0/1156
46	s	0.38	0/744	0.54	0/994
47	t	0.36	0/787	0.54	0/1051
48	u	0.39	0/766	0.52	0/1025
49	v	0.38	0/593	0.55	0/785
50	w	0.37	0/635	0.60	0/848
51	x	0.30	0/502	0.50	0/667
52	y	0.33	0/453	0.59	0/605
53	z	0.40	0/450	0.65	0/599
54	4	0.29	0/251	0.85	0/391
55	Y	0.38	1/1725 (0.1%)	0.80	0/2687
All	All	0.73	3/152844 (0.0%)	0.80	47/228590 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1407	5MC	O3'-P	20.37	1.85	1.61
55	Y	1	C	OP3-P	-10.62	1.48	1.61
27	Z	1	G	OP3-P	-10.60	1.48	1.61

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1495	U	P-O3'-C3'	15.04	137.74	119.70
5	A	1495	U	OP2-P-O3'	-14.46	73.40	105.20
5	A	1495	U	OP1-P-O3'	9.75	126.66	105.20
5	A	1407	5MC	O3'-P-O5'	8.46	120.08	104.00
28	a	2433	G	P-O3'-C3'	-8.18	109.88	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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
6	B	222/241 (92%)	210 (95%)	9 (4%)	3 (1%)	9	38
7	C	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
8	D	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
9	E	154/167 (92%)	150 (97%)	4 (3%)	0	100	100
10	F	101/135 (75%)	99 (98%)	2 (2%)	0	100	100
11	G	151/179 (84%)	136 (90%)	13 (9%)	2 (1%)	10	39
12	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
13	I	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
14	J	96/103 (93%)	88 (92%)	7 (7%)	1 (1%)	13	45
15	K	115/129 (89%)	109 (95%)	6 (5%)	0	100	100
16	L	111/124 (90%)	107 (96%)	3 (3%)	1 (1%)	14	47
17	M	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
18	N	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
19	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	P	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
21	Q	77/84 (92%)	70 (91%)	7 (9%)	0	100	100
22	R	53/75 (71%)	51 (96%)	1 (2%)	1 (2%)	6	31
23	S	82/92 (89%)	74 (90%)	8 (10%)	0	100	100
24	T	84/87 (97%)	84 (100%)	0	0	100	100
25	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
30	c	269/273 (98%)	259 (96%)	10 (4%)	0	100	100
31	d	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
32	e	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
33	f	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
34	g	174/177 (98%)	160 (92%)	13 (8%)	1 (1%)	22	55
35	h	146/149 (98%)	134 (92%)	10 (7%)	2 (1%)	9	38
36	i	140/142 (99%)	140 (100%)	0	0	100	100
37	j	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
38	k	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
39	l	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
40	m	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
41	n	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
42	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
43	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
44	q	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
45	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
46	s	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
47	t	100/104 (96%)	96 (96%)	3 (3%)	1 (1%)	13	45
48	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
49	v	76/85 (89%)	75 (99%)	1 (1%)	0	100	100
50	w	75/78 (96%)	75 (100%)	0	0	100	100
51	x	60/63 (95%)	60 (100%)	0	0	100	100
52	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
53	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
All	All	5515/5843 (94%)	5313 (96%)	190 (3%)	12 (0%)	45	73

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	87	CYS
6	B	131	LYS
11	G	81	GLY
14	J	57	VAL
34	g	126	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	44 (96%)	2 (4%)	25	54
2	1	38/38 (100%)	37 (97%)	1 (3%)	41	68
3	2	51/52 (98%)	50 (98%)	1 (2%)	50	73
4	3	34/34 (100%)	33 (97%)	1 (3%)	37	65
6	B	186/199 (94%)	176 (95%)	10 (5%)	18	48
7	C	170/190 (90%)	163 (96%)	7 (4%)	26	56
8	D	172/173 (99%)	171 (99%)	1 (1%)	84	92
9	E	119/126 (94%)	116 (98%)	3 (2%)	42	68
10	F	90/116 (78%)	87 (97%)	3 (3%)	33	62
11	G	126/147 (86%)	122 (97%)	4 (3%)	34	63
12	H	104/105 (99%)	100 (96%)	4 (4%)	28	58
13	I	105/107 (98%)	103 (98%)	2 (2%)	52	74
14	J	86/90 (96%)	80 (93%)	6 (7%)	12	39
15	K	90/99 (91%)	84 (93%)	6 (7%)	13	41
16	L	96/103 (93%)	95 (99%)	1 (1%)	73	86
17	M	93/96 (97%)	90 (97%)	3 (3%)	34	63
18	N	83/84 (99%)	81 (98%)	2 (2%)	44	69
19	O	76/77 (99%)	75 (99%)	1 (1%)	65	82
20	P	65/65 (100%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	Q	73/78 (94%)	69 (94%)	4 (6%)	18 47
22	R	48/65 (74%)	44 (92%)	4 (8%)	9 32
23	S	72/79 (91%)	68 (94%)	4 (6%)	17 47
24	T	65/66 (98%)	63 (97%)	2 (3%)	35 63
25	U	60/61 (98%)	57 (95%)	3 (5%)	20 50
30	c	216/218 (99%)	214 (99%)	2 (1%)	75 88
31	d	163/163 (100%)	160 (98%)	3 (2%)	54 75
32	e	165/165 (100%)	160 (97%)	5 (3%)	36 64
33	f	148/150 (99%)	144 (97%)	4 (3%)	40 67
34	g	137/138 (99%)	123 (90%)	14 (10%)	6 23
35	h	113/114 (99%)	107 (95%)	6 (5%)	19 48
36	i	116/116 (100%)	114 (98%)	2 (2%)	56 77
37	j	104/104 (100%)	102 (98%)	2 (2%)	52 74
38	k	103/103 (100%)	103 (100%)	0	100 100
39	l	108/108 (100%)	107 (99%)	1 (1%)	75 88
40	m	98/103 (95%)	97 (99%)	1 (1%)	73 86
41	n	86/87 (99%)	83 (96%)	3 (4%)	31 60
42	o	99/100 (99%)	98 (99%)	1 (1%)	73 86
43	p	89/90 (99%)	89 (100%)	0	100 100
44	q	84/84 (100%)	83 (99%)	1 (1%)	67 83
45	r	93/93 (100%)	92 (99%)	1 (1%)	70 84
46	s	80/84 (95%)	76 (95%)	4 (5%)	20 50
47	t	83/85 (98%)	80 (96%)	3 (4%)	30 59
48	u	78/78 (100%)	77 (99%)	1 (1%)	65 82
49	v	58/63 (92%)	57 (98%)	1 (2%)	56 77
50	w	67/68 (98%)	65 (97%)	2 (3%)	36 64
51	x	54/55 (98%)	54 (100%)	0	100 100
52	y	48/49 (98%)	48 (100%)	0	100 100
53	z	47/48 (98%)	46 (98%)	1 (2%)	48 72
All	All	4585/4765 (96%)	4452 (97%)	133 (3%)	39 65

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	n	13	ARG
44	q	60	LYS
50	w	42	SER
15	K	98	ARG
15	K	75	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
46	s	59	ASN
50	w	36	HIS
52	y	20	HIS
47	t	54	GLN
30	c	226	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	X	12/16 (75%)	5 (41%)	0
27	Z	73/76 (96%)	12 (16%)	1 (1%)
28	a	2738/2925 (93%)	257 (9%)	0
29	b	118/119 (99%)	10 (8%)	0
5	A	1505/1542 (97%)	191 (12%)	5 (0%)
54	4	9/10 (90%)	5 (55%)	0
55	Y	76/77 (98%)	12 (15%)	0
All	All	4531/4765 (95%)	492 (10%)	6 (0%)

5 of 492 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	2	A
5	A	3	A
5	A	4	U
5	A	5	U
5	A	9	G

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	1035	A
5	A	1535	C

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Mol	Chain	Res	Type
27	Z	19	G
5	A	766	A
5	A	641	U

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

53 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	$\#\|Z\| > 2$
28	PSU	a	957	28	18,21,22	1.07	1 (5%)	22,30,33	1.79	2 (9%)
27	3AU	Z	47	27	18,21,29	3.38	8 (44%)	26,30,43	1.64	5 (19%)
27	PSU	Z	55	27	18,21,22	1.10	1 (5%)	22,30,33	1.81	5 (22%)
55	H2U	Y	20	55	18,21,22	3.11	5 (27%)	21,30,33	1.96	5 (23%)
5	UR3	A	1498	5	19,22,23	2.57	6 (31%)	26,32,35	1.38	3 (11%)
28	1MG	a	747	28	18,26,27	2.52	5 (27%)	19,39,42	1.16	2 (10%)
55	PSU	Y	55	55	18,21,22	1.12	1 (5%)	22,30,33	1.76	4 (18%)
28	PSU	a	2461	28	18,21,22	1.09	1 (5%)	22,30,33	1.84	4 (18%)
28	6MZ	a	1620	28	18,25,26	2.12	3 (16%)	16,36,39	2.21	4 (25%)
28	PSU	a	1915	28	18,21,22	1.01	1 (5%)	22,30,33	1.78	3 (13%)
28	5MC	a	1966	28,57	18,22,23	0.81	0	26,32,35	0.53	0
28	6MZ	a	2034	28	18,25,26	2.08	5 (27%)	16,36,39	2.18	4 (25%)
28	OMC	a	2502	28,58	19,22,23	0.81	1 (5%)	26,31,34	0.66	0
28	2MA	a	2507	28,58,57	19,25,26	3.17	8 (42%)	21,37,40	2.64	4 (19%)
5	MA6	A	1518	5	18,26,27	1.01	1 (5%)	19,38,41	2.66	3 (15%)
55	5MU	Y	54	55	19,22,23	1.39	5 (26%)	28,32,35	2.07	6 (21%)
28	H2U	a	2453	28	18,21,22	0.64	0	21,30,33	1.07	3 (14%)
16	D2T	L	89	16	7,9,10	1.36	1 (14%)	6,11,13	1.79	2 (33%)
28	2MG	a	1837	28	18,26,27	1.36	3 (16%)	16,38,41	0.81	1 (6%)
28	PSU	a	2508	28,57	18,21,22	1.03	1 (5%)	22,30,33	1.87	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	2MG	A	1207	5,57	18,26,27	1.20	3 (16%)	16,38,41	0.92	1 (6%)
5	PSU	A	516	5	18,21,22	0.99	1 (5%)	22,30,33	1.71	5 (22%)
27	MIA	Z	37	27	18,24,32	1.53	3 (16%)	18,35,47	1.54	3 (16%)
27	4SU	Z	8	27	18,21,22	4.19	8 (44%)	26,30,33	2.25	4 (15%)
28	OMG	a	2255	28,55,57	18,26,27	1.31	3 (16%)	19,38,41	0.80	1 (5%)
5	2MG	A	1516	5	18,26,27	1.33	3 (16%)	16,38,41	0.90	1 (6%)
5	5MC	A	1407	5	18,22,23	0.83	1 (5%)	26,32,35	0.58	0
5	G7M	A	527	5	20,26,27	2.42	7 (35%)	17,39,42	1.14	1 (5%)
5	2MG	A	966	5	18,26,27	1.26	3 (16%)	16,38,41	0.84	0
28	PSU	a	748	28,58	18,21,22	1.10	2 (11%)	22,30,33	1.60	3 (13%)
28	PSU	a	2584	28	18,21,22	1.07	2 (11%)	22,30,33	1.77	3 (13%)
27	H2U	Z	16	27	18,21,22	3.06	5 (27%)	21,30,33	2.09	5 (23%)
28	3TD	a	1919	28	18,22,23	4.02	7 (38%)	22,32,35	1.79	3 (13%)
27	PSU	Z	32	27	18,21,22	1.06	1 (5%)	22,30,33	1.77	5 (22%)
28	PSU	a	2608	28	18,21,22	1.06	1 (5%)	22,30,33	1.85	3 (13%)
28	PSU	a	2609	28	18,21,22	1.08	1 (5%)	22,30,33	1.89	4 (18%)
39	4D4	l	81	39	9,11,12	0.54	0	8,13,15	1.03	1 (12%)
27	PSU	Z	39	27	18,21,22	1.05	1 (5%)	22,30,33	1.80	5 (22%)
55	4SU	Y	8	55	18,21,22	4.19	8 (44%)	26,30,33	2.26	5 (19%)
5	MA6	A	1519	5	18,26,27	1.04	1 (5%)	19,38,41	2.77	3 (15%)
28	OMU	a	2556	28,58,57	19,22,23	3.07	7 (36%)	26,31,34	1.66	4 (15%)
28	PSU	a	1921	28	18,21,22	1.04	1 (5%)	22,30,33	1.84	4 (18%)
5	4OC	A	1402	5	20,23,24	2.98	8 (40%)	26,32,35	0.94	1 (3%)
28	G7M	a	2073	28,57	20,26,27	2.45	7 (35%)	17,39,42	1.12	2 (11%)
27	7MG	Z	46	27	20,25,27	3.36	10 (50%)	27,37,42	2.11	8 (29%)
27	5MU	Z	54	27	19,22,23	1.38	5 (26%)	28,32,35	2.09	6 (21%)
28	2MG	a	2449	28	18,26,27	1.46	3 (16%)	16,38,41	0.66	0
28	5MU	a	749	28	19,22,23	0.72	0	28,32,35	0.56	0
28	5MU	a	1943	28,57	19,22,23	0.81	0	28,32,35	0.46	0
27	H2U	Z	20	27	18,21,22	3.13	5 (27%)	21,30,33	1.99	5 (23%)
5	5MC	A	967	5	18,22,23	0.76	0	26,32,35	0.61	0
55	OMC	Y	32	55	19,22,23	3.01	8 (42%)	26,31,34	0.90	2 (7%)
31	MEQ	d	150	31	8,9,10	0.82	0	5,10,12	0.76	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
28	PSU	a	957	28	-	0/7/25/26	0/2/2/2
27	3AU	Z	47	27	-	2/7/25/35	0/2/2/2
27	PSU	Z	55	27	-	0/7/25/26	0/2/2/2
55	H2U	Y	20	55	-	7/7/38/39	0/2/2/2
5	UR3	A	1498	5	-	0/7/25/26	0/2/2/2
28	1MG	a	747	28	-	0/3/25/26	0/3/3/3
55	PSU	Y	55	55	-	0/7/25/26	0/2/2/2
28	PSU	a	2461	28	-	0/7/25/26	0/2/2/2
28	6MZ	a	1620	28	-	0/5/27/28	0/3/3/3
28	PSU	a	1915	28	-	0/7/25/26	0/2/2/2
28	5MC	a	1966	28,57	-	0/7/25/26	0/2/2/2
28	6MZ	a	2034	28	-	2/5/27/28	0/3/3/3
28	OMC	a	2502	28,58	-	0/9/27/28	0/2/2/2
28	2MA	a	2507	28,58,57	-	2/3/25/26	0/3/3/3
5	MA6	A	1518	5	-	0/7/29/30	0/3/3/3
55	5MU	Y	54	55	-	0/7/25/26	0/2/2/2
28	H2U	a	2453	28	-	0/7/38/39	0/2/2/2
16	D2T	L	89	16	-	3/7/12/14	-
28	2MG	a	1837	28	-	0/5/27/28	0/3/3/3
28	PSU	a	2508	28,57	-	0/7/25/26	0/2/2/2
5	2MG	A	1207	5,57	-	0/5/27/28	0/3/3/3
5	PSU	A	516	5	-	0/7/25/26	0/2/2/2
27	MIA	Z	37	27	-	0/3/25/34	0/3/3/3
27	4SU	Z	8	27	-	2/7/25/26	0/2/2/2
28	OMG	a	2255	28,55,57	-	1/5/27/28	0/3/3/3
5	2MG	A	1516	5	-	0/5/27/28	0/3/3/3
5	5MC	A	1407	5	-	0/7/25/26	0/2/2/2
5	G7M	A	527	5	-	0/3/25/26	0/3/3/3
5	2MG	A	966	5	-	0/5/27/28	0/3/3/3
28	PSU	a	748	28,58	-	1/7/25/26	0/2/2/2
28	PSU	a	2584	28	-	0/7/25/26	0/2/2/2
27	H2U	Z	16	27	-	0/7/38/39	0/2/2/2
28	3TD	a	1919	28	-	2/7/25/26	0/2/2/2
27	PSU	Z	32	27	-	0/7/25/26	0/2/2/2
28	PSU	a	2608	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2609	28	-	0/7/25/26	0/2/2/2
39	4D4	l	81	39	-	6/11/12/14	-
27	PSU	Z	39	27	-	0/7/25/26	0/2/2/2
55	4SU	Y	8	55	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MA6	A	1519	5	-	3/7/29/30	0/3/3/3
28	OMU	a	2556	28,58,57	-	0/9/27/28	0/2/2/2
28	PSU	a	1921	28	-	0/7/25/26	0/2/2/2
5	4OC	A	1402	5	-	0/9/29/30	0/2/2/2
28	G7M	a	2073	28,57	-	2/3/25/26	0/3/3/3
27	7MG	Z	46	27	-	2/7/34/38	0/3/3/3
27	5MU	Z	54	27	-	0/7/25/26	0/2/2/2
28	2MG	a	2449	28	-	0/5/27/28	0/3/3/3
28	5MU	a	749	28	-	0/7/25/26	0/2/2/2
28	5MU	a	1943	28,57	-	0/7/25/26	0/2/2/2
27	H2U	Z	20	27	-	2/7/38/39	0/2/2/2
5	5MC	A	967	5	-	0/7/25/26	0/2/2/2
55	OMC	Y	32	55	-	3/9/27/28	0/2/2/2
31	MEQ	d	150	31	-	2/8/9/11	-

The worst 5 of 172 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	1919	3TD	C6-C5	12.08	1.49	1.35
27	Z	20	H2U	C2-N1	9.70	1.49	1.35
55	Y	20	H2U	C2-N1	9.65	1.49	1.35
55	Y	8	4SU	C4-N3	9.58	1.47	1.37
27	Z	8	4SU	C4-N3	9.41	1.47	1.37

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1519	MA6	N1-C6-N6	-9.71	106.84	117.06
28	a	2507	2MA	C1'-N9-C4	9.39	143.13	126.64
5	A	1518	MA6	N1-C6-N6	-9.21	107.36	117.06
55	Y	8	4SU	C4-N3-C2	-7.98	119.59	127.34
27	Z	8	4SU	C4-N3-C2	-7.85	119.72	127.34

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	Z	46	7MG	O4'-C4'-C5'-O5'
39	l	81	4D4	NH1-CZ-NE-CD
55	Y	20	H2U	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
55	Y	32	OMC	C1'-C2'-O2'-CM2
28	a	2034	6MZ	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 530 ligands modelled in this entry, 529 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	$\#\|Z\| > 2$
59	PHE	a	3001	-	10,11,12	0.43	0	10,13,15	0.30	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
59	PHE	a	3001	-	-	0/5/6/8	0/1/1/1

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 (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
5	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1532:U	O3'	1533:C	P	3.52
1	A	1407:5MC	O3'	1408:A	P	1.85