wwPDB EM Validation Summary Report (i)

Nov 7, 2023 – 07:25 am GMT

PDB ID	:	7ZTA
EMDB ID	:	EMD-14956
Title	:	Structure of an Escherichia coli 70S ribosome stalled by Tetracenomycin X during translation of an MAAAPQK(C) peptide
Authors	:	Leroy, E.C.; Perry, T.N.; Renault, T.T.; Innis, C.A.
Deposited on	:	2022-05-09
Resolution	:	2.70 Å(reported)
Based on initial model	:	6TC3

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 (1)) were used in the production of this report:

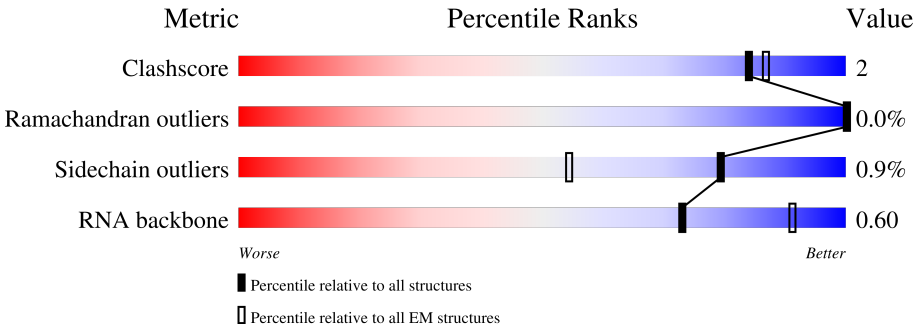
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	16S1	1534	87% 13%
2	S021	224	99% .
3	S031	206	99% .
4	S041	205	100%
5	S051	155	99% .
6	S061	106	100%
7	S071	151	100%

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Mol	Chain	Length	Quality of chain
8	S081	129	100%
9	S091	127	98%
10	S101	99	99%
11	S111	117	99%
12	S121	123	99%
13	S131	114	97%
14	S141	101	100%
15	S151	88	100%
16	S161	82	100%
17	S171	80	99%
18	S181	65	100%
19	S191	83	99%
20	S201	86	99%
21	S211	56	100%
22	23S1	2903	90% 9%
23	05S1	120	92% 8%
24	L021	271	100%
25	L031	209	98%
26	L041	201	99%
27	L051	177	100%
28	L061	176	99%
29	L091	149	97%
30	L131	142	100%
31	L141	123	100%
32	L151	144	99%

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Mol	Chain	Length	Quality of chain
33	L161	136	99%
34	L171	118	99%
35	L181	117	100%
36	L191	114	100%
37	L201	117	98%
38	L211	103	100%
39	L221	110	99%
40	L231	93	99%
41	L241	102	100%
42	L251	94	100%
43	L271	84	100%
44	L281	77	97%
45	L291	62	100%
46	L301	58	98%
47	L311	66	98%
48	L321	56	100%
49	L331	51	100%
50	L341	46	98%
51	L351	64	98%
52	L361	38	97%
53	ATR1	74	64% 34%
54	PTR1	76	80% 11% 5%
55	PQK1	7	71% 29%
56	ETR1	75	72% 21%
57	MRN1	14	86% 14%

2 Entry composition (i)

There are 64 unique types of molecules in this entry. The entry contains 148592 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	16S1	1534	32930	14694	6041	10661	1534	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	S021	224	1753	1109	315	321	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	S031	206	1625	1028	305	289	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	S041	205	1643	1026	315	298	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	S051	155	1144	711	216	211	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	S061	106	862	545	156	154	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S071	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S081	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S091	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S101	99	Total	C	N	O	S	0	0
			796	498	152	145	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S111	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S121	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S131	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S141	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S141	35	ALA	-	insertion	UNP P0AG59

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S151	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S161	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S171	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S181	65	Total	C	N	O	S	0	0
			536	339	100	96	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S191	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S201	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S211	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	23S1	2903	Total	C	N	O	P	0	0
			62334	27815	11467	20149	2903		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	05S1	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	L021	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L031	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	L041	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	L051	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	L061	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	L091	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 30 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	L131	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 31 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L141	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 32 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	L151	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 33 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L161	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 34 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	L171	118	Total 945	C 585	N 194	O 161	S 5	0	0

- Molecule 35 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L181	117	Total 900	C 557	N 179	O 163	S 1	0	0

- Molecule 36 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	L191	114	Total 917	C 574	N 179	O 163	S 1	0	0

- Molecule 37 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	L201	117	Total 947	C 604	N 192	O 151	0	0

- Molecule 38 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	L211	103	Total 816	C 516	N 153	O 145	S 2	0	0

- Molecule 39 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	L221	110	Total 857	C 532	N 166	O 156	S 3	0	0

- Molecule 40 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	L231	93	Total 739	C 466	N 139	O 132	S 2	0	0

- Molecule 41 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	L241	102	Total 780	C 492	N 146	O 142	0	0

- Molecule 42 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	L251	94	Total 753	C 479	N 137	O 134	S 3	0	0

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	L271	84	Total 634	C 391	N 129	O 113	S 1	0	0

- Molecule 44 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	L281	77	Total 625	C 388	N 129	O 106	S 2	0	0

- Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	L291	62	Total 501	C 308	N 98	O 94	S 1	0	0

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	L301	58	Total 449	C 281	N 87	O 79	S 2	0	0

- Molecule 47 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	L311	66	Total 522	C 323	N 99	O 94	S 6	0	0

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	L321	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	L331	51	Total	C	N	O	0	0
			414	266	76	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	L341	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	L351	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	L361	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 53 is a RNA chain called tRNA-Cys.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	ATR1	72	Total	C	N	O	P	S	0	0
			1540	692	276	499	71	2		

- Molecule 54 is a RNA chain called tRNA-Lys.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	PTR1	73	Total	C	N	O	P	S	0	0
			1569	703	277	515	73	1		

- Molecule 55 is a protein called MAAAPQK nascent peptide.

Mol	Chain	Residues	Atoms	AltConf	Trace
55	PQK1	5	Total C N O 35 22 7 6	0	0

- Molecule 56 is a RNA chain called tRNA-Gln.

Mol	Chain	Residues	Atoms	AltConf	Trace
56	ETR1	72	Total C N O P S 1537 688 274 502 72 1	0	0

- Molecule 57 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms	AltConf	Trace
57	MRN1	14	Total C N O P 303 135 58 96 14	0	0

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

Mol	Chain	Residues	Atoms	AltConf
58	16S1	76	Total Mg 76 76	0
58	23S1	209	Total Mg 209 209	0
58	05S1	1	Total Mg 1 1	0
58	L021	1	Total Mg 1 1	0
58	L031	1	Total Mg 1 1	0
58	L041	1	Total Mg 1 1	0

- Molecule 59 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
59	16S1	31	Total K 31 31	0
59	S131	1	Total K 1 1	0
59	23S1	81	Total K 81 81	0
59	05S1	1	Total K 1 1	0

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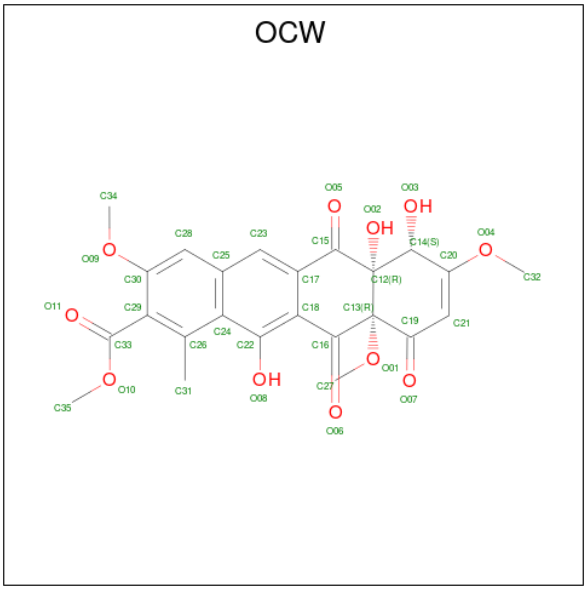
Mol	Chain	Residues	Atoms	AltConf
59	L021	1	Total K 1 1	0

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

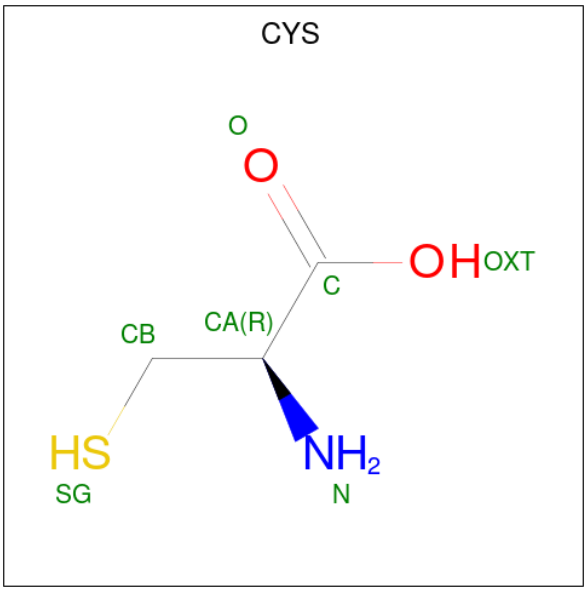
Mol	Chain	Residues	Atoms	AltConf
60	S021	1	Total Zn 1 1	0
60	L311	1	Total Zn 1 1	0
60	L361	1	Total Zn 1 1	0

- Molecule 61 is Tetracenomycin X (three-letter code: OCW) (formula: $C_{24}H_{22}O_{11}$) (labeled as "Ligand of Interest" by depositor).



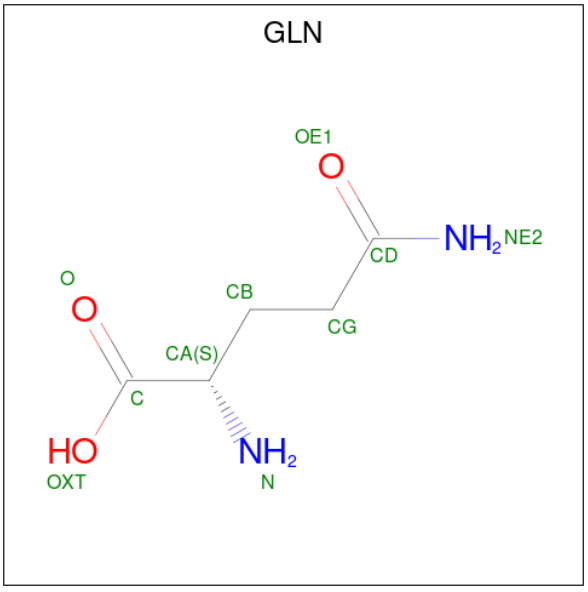
Mol	Chain	Residues	Atoms	AltConf
61	23S1	1	Total C O 35 24 11	0

- Molecule 62 is CYSTEINE (three-letter code: CYS) (formula: $C_3H_7NO_2S$).



Mol	Chain	Residues	Atoms					AltConf
62	ATR1	1	Total	C	N	O	S	0
			6	3	1	1	1	

- Molecule 63 is GLUTAMINE (three-letter code: GLN) (formula: $C_5H_{10}N_2O_3$).



Mol	Chain	Residues	Atoms				AltConf
63	ETR1	1	Total	C	N	O	0
			9	5	2	2	

- Molecule 64 is water.

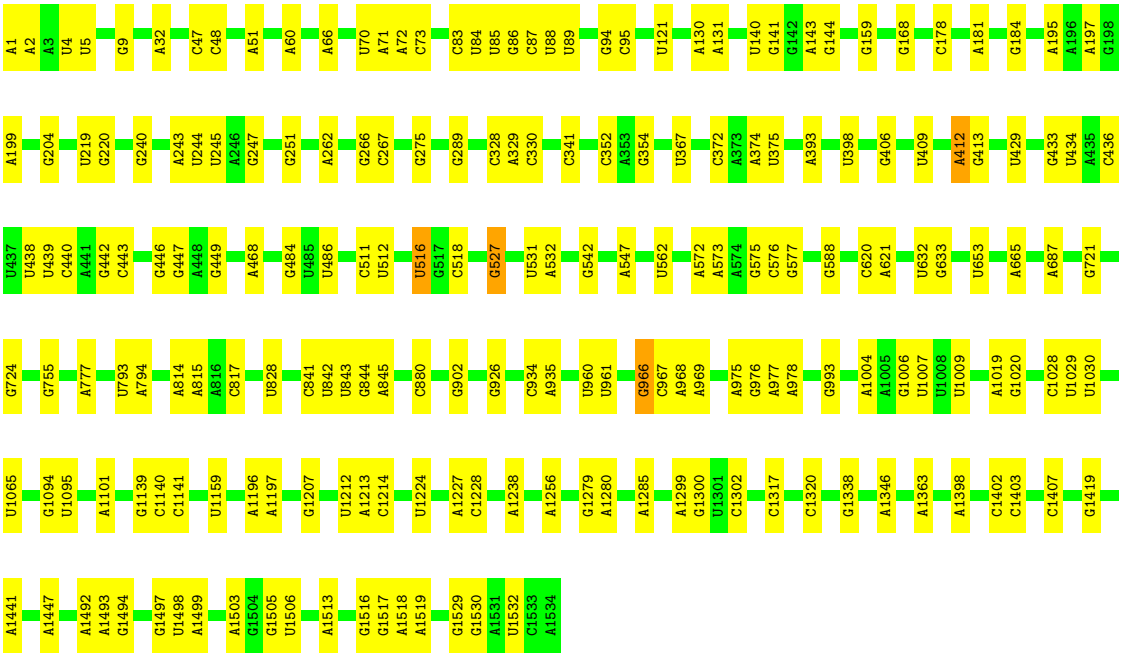
Mol	Chain	Residues	Atoms	AltConf
64	16S1	147	Total O 147 147	0
64	S111	1	Total O 1 1	0
64	S141	2	Total O 2 2	0
64	23S1	604	Total O 604 604	0
64	05S1	5	Total O 5 5	0
64	L021	7	Total O 7 7	0
64	L031	4	Total O 4 4	0
64	L131	1	Total O 1 1	0
64	L171	4	Total O 4 4	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

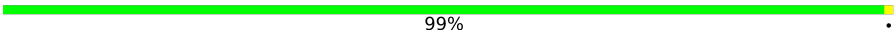
• Molecule 1: 16S ribosomal RNA

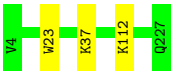
Chain 16S1:



• Molecule 2: 30S ribosomal protein S2

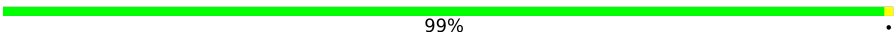
Chain S021:





• Molecule 3: 30S ribosomal protein S3

Chain S031:



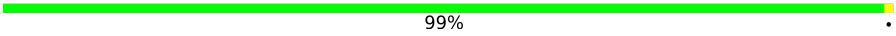
• Molecule 4: 30S ribosomal protein S4

Chain S041:

There are no outlier residues recorded for this chain.

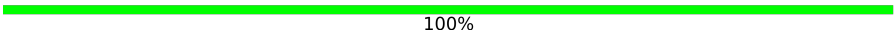
• Molecule 5: 30S ribosomal protein S5

Chain S051:



• Molecule 6: 30S ribosomal protein S6, fully modified isoform

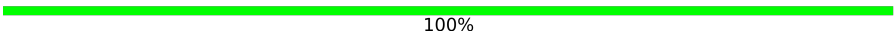
Chain S061:



There are no outlier residues recorded for this chain.

• Molecule 7: 30S ribosomal protein S7

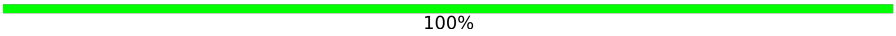
Chain S071:



There are no outlier residues recorded for this chain.

• Molecule 8: 30S ribosomal protein S8

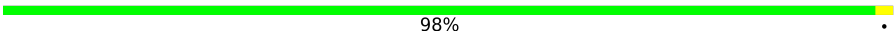
Chain S081:

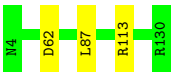


There are no outlier residues recorded for this chain.

• Molecule 9: 30S ribosomal protein S9

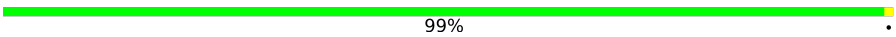
Chain S091:





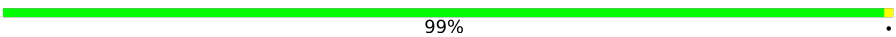
• Molecule 10: 30S ribosomal protein S10

Chain S101:

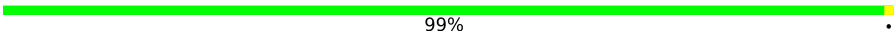


• Molecule 11: 30S ribosomal protein S11

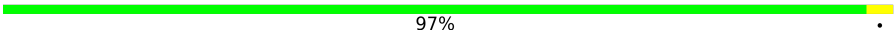
Chain S111:

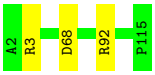


• Molecule 12: 30S ribosomal protein S12

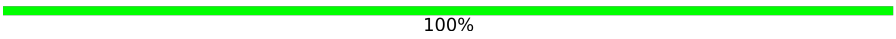
Chain S121: 

• Molecule 13: 30S ribosomal protein S13

Chain S131: 

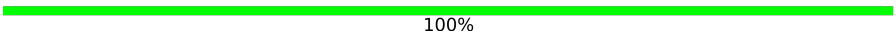


• Molecule 14: 30S ribosomal protein S14

Chain S141: 

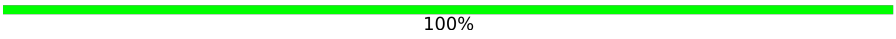
There are no outlier residues recorded for this chain.

• Molecule 15: 30S ribosomal protein S15

Chain S151: 

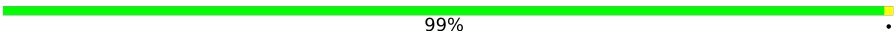
There are no outlier residues recorded for this chain.

• Molecule 16: 30S ribosomal protein S16

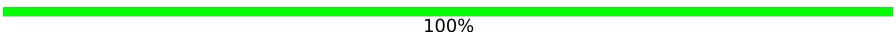
Chain S161: 

There are no outlier residues recorded for this chain.

• Molecule 17: 30S ribosomal protein S17

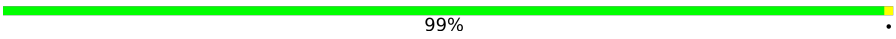
Chain S171: 

• Molecule 18: 30S ribosomal protein S18

Chain S181: 

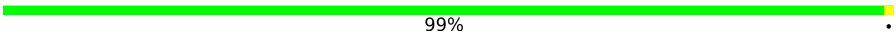
There are no outlier residues recorded for this chain.

• Molecule 19: 30S ribosomal protein S19

Chain S191: 

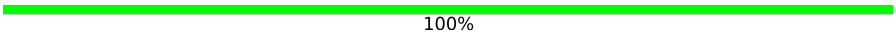
• Molecule 20: 30S ribosomal protein S20

Chain S201:



• Molecule 21: 30S ribosomal protein S21

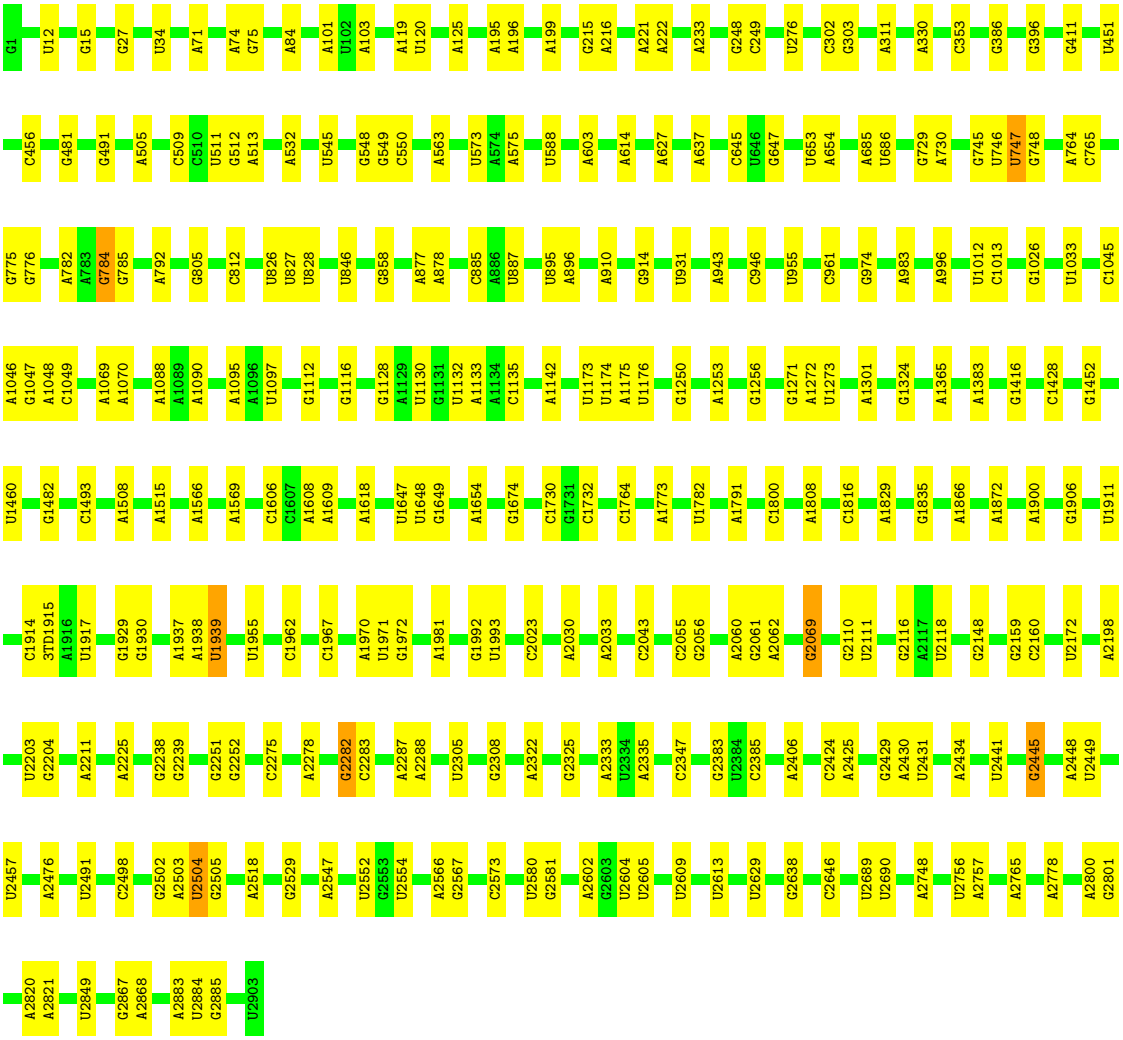
Chain S211:



There are no outlier residues recorded for this chain.

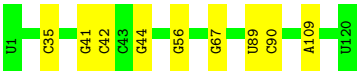
• Molecule 22: 23S ribosomal RNA

Chain 23S1:

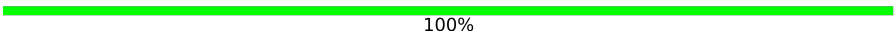


• Molecule 23: 5S ribosomal RNA

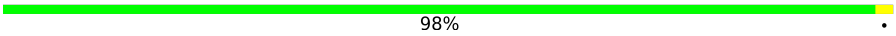
Chain 05S1:



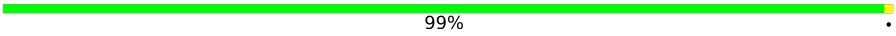
• Molecule 24: 50S ribosomal protein L2

Chain L021: 

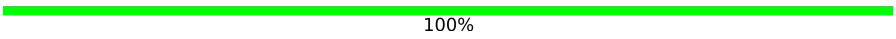
• Molecule 25: 50S ribosomal protein L3

Chain L031: 

• Molecule 26: 50S ribosomal protein L4

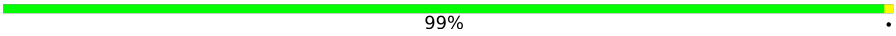
Chain L041: 

• Molecule 27: 50S ribosomal protein L5

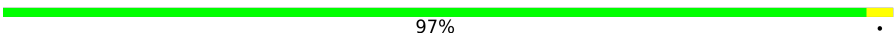
Chain L051: 

There are no outlier residues recorded for this chain.

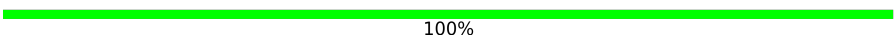
• Molecule 28: 50S ribosomal protein L6

Chain L061: 

• Molecule 29: 50S ribosomal protein L9

Chain L091: 

• Molecule 30: 50S ribosomal protein L13

Chain L131: 

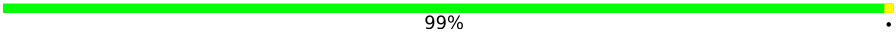
There are no outlier residues recorded for this chain.

• Molecule 31: 50S ribosomal protein L14

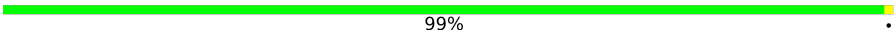
Chain L141: 

There are no outlier residues recorded for this chain.

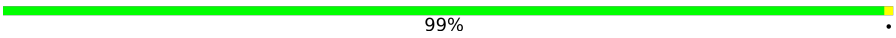
• Molecule 32: 50S ribosomal protein L15

Chain L151: 

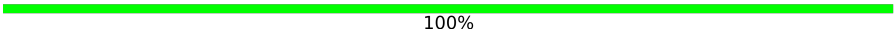
• Molecule 33: 50S ribosomal protein L16

Chain L161: 

• Molecule 34: 50S ribosomal protein L17

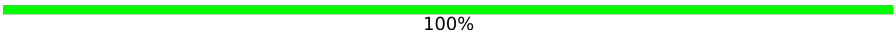
Chain L171: 

• Molecule 35: 50S ribosomal protein L18

Chain L181: 

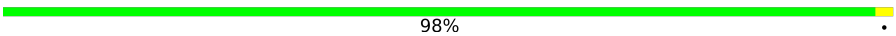
There are no outlier residues recorded for this chain.

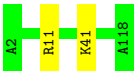
• Molecule 36: 50S ribosomal protein L19

Chain L191: 

There are no outlier residues recorded for this chain.

• Molecule 37: 50S ribosomal protein L20

Chain L201: 

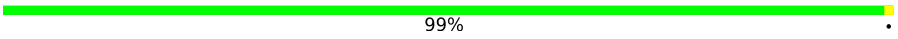


• Molecule 38: 50S ribosomal protein L21

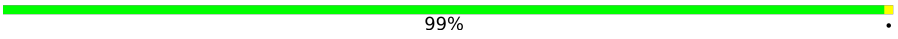
Chain L211: 

There are no outlier residues recorded for this chain.

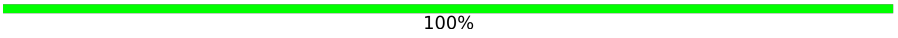
• Molecule 39: 50S ribosomal protein L22

Chain L221: 

• Molecule 40: 50S ribosomal protein L23

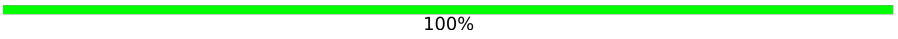
Chain L231: 

• Molecule 41: 50S ribosomal protein L24

Chain L241: 

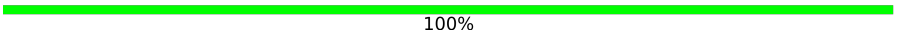
There are no outlier residues recorded for this chain.

• Molecule 42: 50S ribosomal protein L25

Chain L251: 

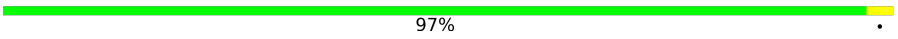
There are no outlier residues recorded for this chain.

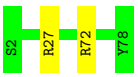
• Molecule 43: 50S ribosomal protein L27

Chain L271: 

There are no outlier residues recorded for this chain.

• Molecule 44: 50S ribosomal protein L28

Chain L281: 

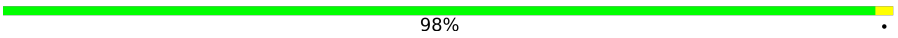


• Molecule 45: 50S ribosomal protein L29

Chain L291: 

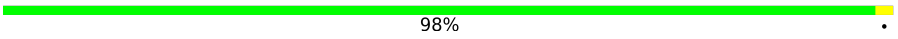
There are no outlier residues recorded for this chain.

• Molecule 46: 50S ribosomal protein L30

Chain L301: 

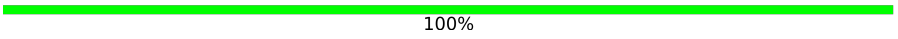
• Molecule 47: 50S ribosomal protein L31

Chain L311:



• Molecule 48: 50S ribosomal protein L32

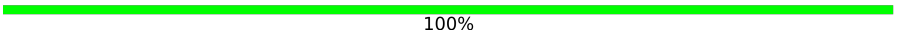
Chain L321:



There are no outlier residues recorded for this chain.

• Molecule 49: 50S ribosomal protein L33

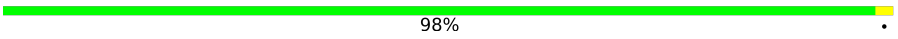
Chain L331:



There are no outlier residues recorded for this chain.

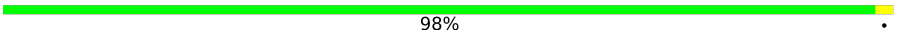
• Molecule 50: 50S ribosomal protein L34

Chain L341:



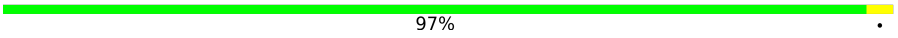
• Molecule 51: 50S ribosomal protein L35

Chain L351:



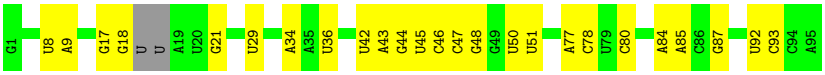
• Molecule 52: 50S ribosomal protein L36

Chain L361:



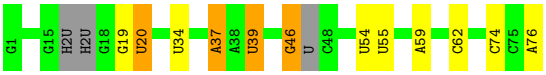
• Molecule 53: tRNA-Cys

Chain ATR1:



• Molecule 54: tRNA-Lys

Chain PTR1:

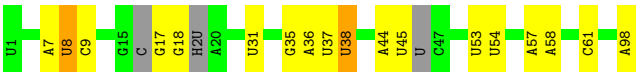


• Molecule 55: MAAAPQK nascent peptide

Chain PQK1:

• Molecule 56: tRNA-Gln

Chain ETR1:



• Molecule 57: mRNA

Chain MRN1:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	86672	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	35.71	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	1800	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: 6MZ, 4OC, 4SU, 2MG, D2T, OMG, ZN, PSU, 4D4, OMC, 1MG, UR3, MG, 5MC, MIA, OMU, 3TD, 2MA, MEQ, U8U, MA6, OCW, G7M, K, T6A, 5MU, H2U

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	16S1	0.70	0/36593	0.89	3/57081 (0.0%)
2	S021	0.28	0/1784	0.52	0/2403
3	S031	0.31	0/1652	0.55	0/2225
4	S041	0.29	0/1665	0.57	0/2227
5	S051	0.34	0/1157	0.58	0/1557
6	S061	0.33	0/881	0.54	0/1189
7	S071	0.28	0/1196	0.58	0/1602
8	S081	0.32	0/989	0.55	0/1326
9	S091	0.31	0/1034	0.62	0/1375
10	S101	0.29	0/806	0.60	0/1089
11	S111	0.33	0/893	0.60	0/1205
12	S121	0.33	0/960	0.62	0/1286
13	S131	0.29	0/893	0.61	0/1193
14	S141	0.29	0/811	0.60	0/1081
15	S151	0.32	0/722	0.59	0/964
16	S161	0.30	0/659	0.58	0/884
17	S171	0.31	0/658	0.54	0/881
18	S181	0.35	0/545	0.58	0/731
19	S191	0.29	0/680	0.55	0/915
20	S201	0.28	0/676	0.51	0/895
21	S211	0.32	0/472	0.61	0/627
22	23S1	0.96	0/69239	0.91	6/108014 (0.0%)
23	05S1	0.75	0/2872	0.82	0/4478
24	L021	0.42	0/2122	0.62	0/2852
25	L031	0.40	0/1576	0.56	0/2119
26	L041	0.37	0/1571	0.53	0/2113
27	L051	0.32	0/1435	0.54	0/1926
28	L061	0.31	0/1343	0.53	0/1816
29	L091	0.27	0/1121	0.49	0/1515
30	L131	0.41	0/1152	0.54	0/1551
31	L141	0.38	0/955	0.60	0/1279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	L151	0.37	0/1062	0.62	0/1413
33	L161	0.40	0/1081	0.58	0/1443
34	L171	0.41	0/958	0.62	0/1281
35	L181	0.34	0/910	0.58	0/1219
36	L191	0.40	0/929	0.59	0/1242
37	L201	0.48	0/960	0.61	0/1278
38	L211	0.41	0/829	0.56	0/1107
39	L221	0.35	0/864	0.56	0/1156
40	L231	0.36	0/745	0.53	0/994
41	L241	0.33	0/788	0.52	0/1051
42	L251	0.35	0/766	0.51	0/1025
43	L271	0.40	0/642	0.58	0/848
44	L281	0.38	0/635	0.62	0/848
45	L291	0.29	0/502	0.53	0/667
46	L301	0.35	0/453	0.60	0/605
47	L311	0.29	0/531	0.54	0/709
48	L321	0.41	0/450	0.62	0/599
49	L331	0.37	0/421	0.55	0/561
50	L341	0.40	0/380	0.76	0/498
51	L351	0.38	0/513	0.60	0/676
52	L361	0.40	0/303	0.60	0/397
53	ATR1	0.62	0/1575	0.99	0/2450
54	PTR1	0.63	0/1572	0.91	0/2441
55	PQK1	0.32	0/35	0.43	0/46
56	ETR1	0.48	0/1527	1.01	0/2374
57	MRN1	0.64	0/339	0.83	0/527
All	All	0.75	0/158882	0.83	9/237854 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	23S1	784	G	O5'-P-OP2	8.06	120.37	110.70
1	16S1	412	A	O4'-C1'-N9	6.83	113.66	108.20
22	23S1	195	A	N9-C4-C5	6.21	108.28	105.80
22	23S1	2638	G	O4'-C1'-N9	5.36	112.48	108.20
1	16S1	60	A	C8-N9-C4	-5.27	103.69	105.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	16S1	32930	0	0	0	0
2	S021	1753	0	0	0	0
3	S031	1625	0	0	0	0
4	S041	1643	0	0	0	0
5	S051	1144	0	0	0	0
6	S061	862	0	0	0	0
7	S071	1182	0	0	0	0
8	S081	979	0	0	0	0
9	S091	1022	0	0	0	0
10	S101	796	0	0	0	0
11	S111	877	0	0	0	0
12	S121	957	0	0	0	0
13	S131	884	0	0	0	0
14	S141	799	0	0	0	0
15	S151	714	0	0	0	0
16	S161	649	0	0	0	0
17	S171	649	0	0	0	0
18	S181	536	0	0	0	0
19	S191	663	0	0	0	0
20	S201	670	0	0	0	0
21	S211	465	0	0	0	0
22	23S1	62334	0	0	0	0
23	05S1	2569	0	0	0	0
24	L021	2083	0	0	0	0
25	L031	1566	0	0	0	0
26	L041	1552	0	0	0	0
27	L051	1411	0	0	0	0
28	L061	1323	0	0	0	0
29	L091	1110	0	0	0	0
30	L131	1129	0	0	0	0
31	L141	946	0	0	0	0
32	L151	1053	0	0	0	0
33	L161	1075	0	0	0	0
34	L171	945	0	0	0	0
35	L181	900	0	0	0	0
36	L191	917	0	0	0	0
37	L201	947	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	L211	816	0	0	0	0
39	L221	857	0	0	0	0
40	L231	739	0	0	0	0
41	L241	780	0	0	0	0
42	L251	753	0	0	0	0
43	L271	634	0	0	0	0
44	L281	625	0	0	0	0
45	L291	501	0	0	0	0
46	L301	449	0	0	0	0
47	L311	522	0	0	0	0
48	L321	444	0	0	0	0
49	L331	414	0	0	0	0
50	L341	377	0	0	0	0
51	L351	504	0	0	0	0
52	L361	302	0	0	0	0
53	ATR1	1540	0	0	0	0
54	PTR1	1569	0	0	0	0
55	PQK1	35	0	0	0	0
56	ETR1	1537	0	0	0	0
57	MRN1	303	0	0	0	0
58	05S1	1	0	0	0	0
58	16S1	76	0	0	0	0
58	23S1	209	0	0	0	0
58	L021	1	0	0	0	0
58	L031	1	0	0	0	0
58	L041	1	0	0	0	0
59	05S1	1	0	0	0	0
59	16S1	31	0	0	0	0
59	23S1	81	0	0	0	0
59	L021	1	0	0	0	0
59	S131	1	0	0	0	0
60	L311	1	0	0	0	0
60	L361	1	0	0	0	0
60	S021	1	0	0	0	0
61	23S1	35	0	0	0	0
62	ATR1	6	0	0	0	0
63	ETR1	9	0	0	0	0
64	05S1	5	0	0	0	0
64	16S1	147	0	0	0	0
64	23S1	604	0	0	0	0
64	L021	7	0	0	0	0
64	L031	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	L131	1	0	0	0	0
64	L171	4	0	0	0	0
64	S111	1	0	0	0	0
64	S141	2	0	0	0	0
All	All	148592	0	0	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S021	222/224 (99%)	217 (98%)	5 (2%)	0	100	100
3	S031	204/206 (99%)	202 (99%)	2 (1%)	0	100	100
4	S041	203/205 (99%)	201 (99%)	2 (1%)	0	100	100
5	S051	153/155 (99%)	150 (98%)	3 (2%)	0	100	100
6	S061	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
7	S071	149/151 (99%)	146 (98%)	3 (2%)	0	100	100
8	S081	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
9	S091	125/127 (98%)	119 (95%)	6 (5%)	0	100	100
10	S101	97/99 (98%)	96 (99%)	0	1 (1%)	15	37
11	S111	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
12	S121	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
13	S131	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
14	S141	99/101 (98%)	95 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	S151	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
16	S161	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
17	S171	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
18	S181	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
19	S191	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
20	S201	84/86 (98%)	84 (100%)	0	0	100	100
21	S211	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
24	L021	269/271 (99%)	259 (96%)	10 (4%)	0	100	100
25	L031	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	29	54
26	L041	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
27	L051	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
28	L061	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
29	L091	147/149 (99%)	141 (96%)	6 (4%)	0	100	100
30	L131	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
31	L141	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
32	L151	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
33	L161	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
34	L171	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
35	L181	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
36	L191	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
37	L201	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
38	L211	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
39	L221	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
40	L231	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
41	L241	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
42	L251	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
43	L271	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
44	L281	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
45	L291	60/62 (97%)	60 (100%)	0	0	100	100
46	L301	56/58 (97%)	56 (100%)	0	0	100	100
47	L311	64/66 (97%)	62 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	L321	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
49	L331	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
50	L341	44/46 (96%)	44 (100%)	0	0	100	100
51	L351	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
52	L361	36/38 (95%)	36 (100%)	0	0	100	100
55	PQK1	3/7 (43%)	3 (100%)	0	0	100	100
All	All	5597/5702 (98%)	5466 (98%)	129 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	L031	149	ASN
10	S101	57	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S021	186/186 (100%)	183 (98%)	3 (2%)	62	85
3	S031	170/170 (100%)	168 (99%)	2 (1%)	71	88
4	S041	172/172 (100%)	172 (100%)	0	100	100
5	S051	118/118 (100%)	116 (98%)	2 (2%)	60	84
6	S061	92/92 (100%)	92 (100%)	0	100	100
7	S071	124/124 (100%)	124 (100%)	0	100	100
8	S081	104/104 (100%)	104 (100%)	0	100	100
9	S091	105/105 (100%)	102 (97%)	3 (3%)	42	71
10	S101	87/87 (100%)	87 (100%)	0	100	100
11	S111	90/90 (100%)	89 (99%)	1 (1%)	73	90
12	S121	102/102 (100%)	102 (100%)	0	100	100
13	S131	92/92 (100%)	89 (97%)	3 (3%)	38	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	S141	79/83 (95%)	79 (100%)	0	100	100
15	S151	76/76 (100%)	76 (100%)	0	100	100
16	S161	65/65 (100%)	65 (100%)	0	100	100
17	S171	74/74 (100%)	73 (99%)	1 (1%)	67	86
18	S181	56/56 (100%)	56 (100%)	0	100	100
19	S191	72/72 (100%)	71 (99%)	1 (1%)	67	86
20	S201	65/65 (100%)	64 (98%)	1 (2%)	65	86
21	S211	48/48 (100%)	48 (100%)	0	100	100
24	L021	216/216 (100%)	215 (100%)	1 (0%)	88	96
25	L031	163/163 (100%)	160 (98%)	3 (2%)	59	83
26	L041	165/165 (100%)	163 (99%)	2 (1%)	71	88
27	L051	148/148 (100%)	148 (100%)	0	100	100
28	L061	137/137 (100%)	136 (99%)	1 (1%)	84	94
29	L091	114/114 (100%)	110 (96%)	4 (4%)	36	65
30	L131	116/116 (100%)	116 (100%)	0	100	100
31	L141	104/104 (100%)	104 (100%)	0	100	100
32	L151	103/103 (100%)	102 (99%)	1 (1%)	76	91
33	L161	108/108 (100%)	107 (99%)	1 (1%)	78	92
34	L171	98/98 (100%)	97 (99%)	1 (1%)	76	91
35	L181	87/87 (100%)	87 (100%)	0	100	100
36	L191	99/99 (100%)	99 (100%)	0	100	100
37	L201	89/89 (100%)	87 (98%)	2 (2%)	52	79
38	L211	84/84 (100%)	84 (100%)	0	100	100
39	L221	93/93 (100%)	92 (99%)	1 (1%)	73	90
40	L231	80/80 (100%)	79 (99%)	1 (1%)	69	87
41	L241	83/83 (100%)	83 (100%)	0	100	100
42	L251	78/78 (100%)	78 (100%)	0	100	100
43	L271	62/62 (100%)	62 (100%)	0	100	100
44	L281	67/67 (100%)	65 (97%)	2 (3%)	41	70
45	L291	54/54 (100%)	54 (100%)	0	100	100
46	L301	48/48 (100%)	47 (98%)	1 (2%)	53	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
47	L311	59/59 (100%)	58 (98%)	1 (2%)	60 84
48	L321	47/47 (100%)	47 (100%)	0	100 100
49	L331	45/46 (98%)	45 (100%)	0	100 100
50	L341	38/38 (100%)	37 (97%)	1 (3%)	46 75
51	L351	51/51 (100%)	50 (98%)	1 (2%)	55 81
52	L361	34/34 (100%)	33 (97%)	1 (3%)	42 71
55	PQK1	3/4 (75%)	3 (100%)	0	100 100
All	All	4650/4656 (100%)	4608 (99%)	42 (1%)	79 92

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	L151	2	ARG
44	L281	27	ARG
33	L161	111	GLU
37	L201	41	LYS
46	L301	58	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16S1	1531/1534 (99%)	184 (12%)	15 (0%)
22	23S1	2898/2903 (99%)	250 (8%)	24 (0%)
23	05S1	119/120 (99%)	9 (7%)	1 (0%)
53	ATR1	69/74 (93%)	19 (27%)	3 (4%)
54	PTR1	69/76 (90%)	9 (13%)	2 (2%)
56	ETR1	67/75 (89%)	11 (16%)	2 (2%)
57	MRN1	13/14 (92%)	2 (15%)	0
All	All	4766/4796 (99%)	484 (10%)	47 (0%)

5 of 484 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16S1	2	A
1	16S1	4	U

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Mol	Chain	Res	Type
1	16S1	5	U
1	16S1	9	G
1	16S1	32	A

5 of 47 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	23S1	1175	A
22	23S1	2430	A
22	23S1	1608	A
22	23S1	2110	G
22	23S1	2756	U

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

59 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	$\#\|Z\| > 2$
22	6MZ	23S1	1618	22	18,25,26	1.43	3 (16%)	16,36,39	2.08	4 (25%)
1	2MG	16S1	966	1	18,26,27	2.14	6 (33%)	16,38,41	1.41	3 (18%)
1	2MG	16S1	1207	59,1	18,26,27	2.06	6 (33%)	16,38,41	1.45	3 (18%)
22	PSU	23S1	1917	22	18,21,22	4.11	6 (33%)	22,30,33	2.71	5 (22%)
54	PSU	PTR1	39	54	18,21,22	4.13	7 (38%)	22,30,33	2.62	5 (22%)
1	G7M	16S1	527	1	20,26,27	2.15	7 (35%)	17,39,42	1.17	2 (11%)
22	PSU	23S1	1911	22	18,21,22	4.09	6 (33%)	22,30,33	2.71	5 (22%)
54	PSU	PTR1	55	54	18,21,22	4.21	6 (33%)	22,30,33	2.59	5 (22%)
1	5MC	16S1	1407	1	18,22,23	3.30	7 (38%)	26,32,35	0.95	1 (3%)
1	UR3	16S1	1498	1	19,22,23	2.93	8 (42%)	26,32,35	1.32	2 (7%)
1	5MC	16S1	967	1	18,22,23	3.45	7 (38%)	26,32,35	1.03	1 (3%)
1	2MG	16S1	1516	1	18,26,27	2.06	6 (33%)	16,38,41	1.46	4 (25%)
22	PSU	23S1	2580	22,59	18,21,22	3.90	7 (38%)	22,30,33	2.77	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
53	5MU	ATR1	50	53	19,22,23	3.65	7 (36%)	28,32,35	4.56	10 (35%)
1	MA6	16S1	1518	1	19,26,27	1.28	2 (10%)	18,38,41	2.06	2 (11%)
22	5MU	23S1	747	22	19,22,23	4.52	7 (36%)	28,32,35	3.92	10 (35%)
22	PSU	23S1	2504	22,59	18,21,22	3.90	6 (33%)	22,30,33	2.64	5 (22%)
56	4SU	ETR1	8	56	18,21,22	3.64	8 (44%)	26,30,33	2.29	4 (15%)
12	D2T	S121	89	12	7,9,10	1.01	0	6,11,13	2.83	3 (50%)
56	OMG	ETR1	17	56	18,26,27	2.36	7 (38%)	19,38,41	1.79	5 (26%)
22	PSU	23S1	2605	22	18,21,22	3.94	6 (33%)	22,30,33	2.77	6 (27%)
56	PSU	ETR1	37	56	18,21,22	4.23	7 (38%)	22,30,33	2.66	5 (22%)
22	PSU	23S1	746	22,58	18,21,22	4.00	8 (44%)	22,30,33	2.53	5 (22%)
22	6MZ	23S1	2030	22	18,25,26	1.46	3 (16%)	16,36,39	2.16	4 (25%)
54	G7M	PTR1	46	54	20,26,27	2.25	7 (35%)	17,39,42	1.08	1 (5%)
56	OMU	ETR1	31	56	19,22,23	3.00	8 (42%)	26,31,34	1.72	4 (15%)
22	1MG	23S1	745	22	18,26,27	2.41	5 (27%)	19,39,42	1.41	3 (15%)
54	T6A	PTR1	37	54	27,34,35	2.23	6 (22%)	29,49,52	2.09	5 (17%)
22	2MG	23S1	1835	22	18,26,27	1.98	6 (33%)	16,38,41	1.49	4 (25%)
22	PSU	23S1	955	22	18,21,22	3.96	6 (33%)	22,30,33	2.83	6 (27%)
22	OMC	23S1	2498	22,58	19,22,23	2.74	7 (36%)	26,31,34	0.84	0
22	G7M	23S1	2069	22,59	20,26,27	2.11	7 (35%)	17,39,42	1.19	1 (5%)
25	MEQ	L031	150	25	8,9,10	0.92	0	5,10,12	0.74	0
33	4D4	L161	81	33	9,11,12	2.48	3 (33%)	8,13,15	0.86	0
22	PSU	23S1	2457	22	18,21,22	3.87	7 (38%)	22,30,33	2.89	5 (22%)
22	5MC	23S1	1962	22,59	18,22,23	3.21	7 (38%)	26,32,35	0.99	2 (7%)
54	U8U	PTR1	34	54,57	19,24,25	2.46	6 (31%)	23,34,37	1.27	4 (17%)
56	2MA	ETR1	36	56	17,25,26	2.47	4 (23%)	17,37,40	1.14	2 (11%)
53	4SU	ATR1	8	53	18,21,22	3.51	8 (44%)	26,30,33	2.20	5 (19%)
53	PSU	ATR1	29	53	18,21,22	4.19	6 (33%)	22,30,33	2.74	6 (27%)
22	H2U	23S1	2449	22	18,21,22	0.78	0	21,30,33	0.95	2 (9%)
54	5MU	PTR1	54	54	19,22,23	4.70	7 (36%)	28,32,35	3.63	9 (32%)
22	3TD	23S1	1915	22	19,22,23	3.82	6 (31%)	21,32,35	1.80	3 (14%)
53	PSU	ATR1	51	53	18,21,22	4.19	7 (38%)	22,30,33	2.72	5 (22%)
1	MA6	16S1	1519	1	19,26,27	1.29	2 (10%)	18,38,41	2.31	2 (11%)
54	H2U	PTR1	20	54	18,21,22	1.16	2 (11%)	21,30,33	0.98	2 (9%)
22	2MG	23S1	2445	22	18,26,27	1.97	6 (33%)	16,38,41	1.51	4 (25%)
22	OMG	23S1	2251	22,54,59	18,26,27	2.34	8 (44%)	19,38,41	1.53	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	16S1	516	58,1	18,21,22	4.16	8 (44%)	22,30,33	2.43	5 (22%)
22	OMU	23S1	2552	22	19,22,23	2.69	7 (36%)	26,31,34	1.86	6 (23%)
22	2MA	23S1	2503	22,58,59	17,25,26	2.35	5 (29%)	17,37,40	1.39	4 (23%)
22	PSU	23S1	2604	22	18,21,22	3.89	6 (33%)	22,30,33	2.81	5 (22%)
56	PSU	ETR1	54	56	18,21,22	4.40	7 (38%)	22,30,33	2.65	5 (22%)
53	MIA	ATR1	34	53	24,31,32	2.53	4 (16%)	26,44,47	2.54	8 (30%)
1	4OC	16S1	1402	58,1	20,23,24	2.95	8 (40%)	26,32,35	0.88	1 (3%)
56	PSU	ETR1	38	56	18,21,22	4.28	7 (38%)	22,30,33	2.56	5 (22%)
53	PSU	ATR1	36	53	18,21,22	4.15	6 (33%)	22,30,33	2.70	5 (22%)
56	5MU	ETR1	53	56	19,22,23	3.72	6 (31%)	28,32,35	4.39	10 (35%)
22	5MU	23S1	1939	22,59	19,22,23	4.64	7 (36%)	28,32,35	3.65	10 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	6MZ	23S1	1618	22	-	0/5/27/28	0/3/3/3
1	2MG	16S1	966	1	-	2/5/27/28	0/3/3/3
1	2MG	16S1	1207	59,1	-	0/5/27/28	0/3/3/3
22	PSU	23S1	1917	22	-	0/7/25/26	0/2/2/2
54	PSU	PTR1	39	54	-	2/7/25/26	0/2/2/2
1	G7M	16S1	527	1	-	2/3/25/26	0/3/3/3
22	PSU	23S1	1911	22	-	0/7/25/26	0/2/2/2
54	PSU	PTR1	55	54	-	0/7/25/26	0/2/2/2
1	5MC	16S1	1407	1	-	0/7/25/26	0/2/2/2
1	UR3	16S1	1498	1	-	1/7/25/26	0/2/2/2
1	5MC	16S1	967	1	-	0/7/25/26	0/2/2/2
1	2MG	16S1	1516	1	-	0/5/27/28	0/3/3/3
22	PSU	23S1	2580	22,59	-	1/7/25/26	0/2/2/2
53	5MU	ATR1	50	53	-	0/7/25/26	0/2/2/2
1	MA6	16S1	1518	1	-	1/7/29/30	0/3/3/3
22	5MU	23S1	747	22	-	0/7/25/26	0/2/2/2
22	PSU	23S1	2504	22,59	-	2/7/25/26	0/2/2/2
56	4SU	ETR1	8	56	-	0/7/25/26	0/2/2/2
12	D2T	S121	89	12	-	2/7/12/14	-
56	OMG	ETR1	17	56	-	2/5/27/28	0/3/3/3
22	PSU	23S1	2605	22	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	PSU	ETR1	37	56	-	0/7/25/26	0/2/2/2
22	PSU	23S1	746	22,58	-	1/7/25/26	0/2/2/2
22	6MZ	23S1	2030	22	-	2/5/27/28	0/3/3/3
54	G7M	PTR1	46	54	-	1/3/25/26	0/3/3/3
56	OMU	ETR1	31	56	-	2/9/27/28	0/2/2/2
22	1MG	23S1	745	22	-	0/3/25/26	0/3/3/3
54	T6A	PTR1	37	54	-	4/19/41/42	0/3/3/3
22	2MG	23S1	1835	22	-	0/5/27/28	0/3/3/3
22	PSU	23S1	955	22	-	0/7/25/26	0/2/2/2
22	OMC	23S1	2498	22,58	-	0/9/27/28	0/2/2/2
22	G7M	23S1	2069	22,59	-	3/3/25/26	0/3/3/3
25	MEQ	L031	150	25	-	2/8/9/11	-
33	4D4	L161	81	33	-	2/11/12/14	-
22	PSU	23S1	2457	22	-	1/7/25/26	0/2/2/2
22	5MC	23S1	1962	22,59	-	2/7/25/26	0/2/2/2
54	U8U	PTR1	34	54,57	-	0/9/28/29	0/2/2/2
56	2MA	ETR1	36	56	-	0/3/25/26	0/3/3/3
53	4SU	ATR1	8	53	-	0/7/25/26	0/2/2/2
53	PSU	ATR1	29	53	-	0/7/25/26	0/2/2/2
22	H2U	23S1	2449	22	-	0/7/38/39	0/2/2/2
54	5MU	PTR1	54	54	-	0/7/25/26	0/2/2/2
22	3TD	23S1	1915	22	-	2/7/25/26	0/2/2/2
53	PSU	ATR1	51	53	-	0/7/25/26	0/2/2/2
1	MA6	16S1	1519	1	-	2/7/29/30	0/3/3/3
54	H2U	PTR1	20	54	-	7/7/38/39	0/2/2/2
22	2MG	23S1	2445	22	-	2/5/27/28	0/3/3/3
22	OMG	23S1	2251	22,54,59	-	0/5/27/28	0/3/3/3
1	PSU	16S1	516	58,1	-	0/7/25/26	0/2/2/2
22	OMU	23S1	2552	22	-	0/9/27/28	0/2/2/2
22	2MA	23S1	2503	22,58,59	-	2/3/25/26	0/3/3/3
22	PSU	23S1	2604	22	-	0/7/25/26	0/2/2/2
56	PSU	ETR1	54	56	-	0/7/25/26	0/2/2/2
53	MIA	ATR1	34	53	-	2/11/33/34	0/3/3/3
1	4OC	16S1	1402	58,1	-	2/9/29/30	0/2/2/2
56	PSU	ETR1	38	56	-	2/7/25/26	0/2/2/2
53	PSU	ATR1	36	53	-	0/7/25/26	0/2/2/2
56	5MU	ETR1	53	56	-	0/7/25/26	0/2/2/2
22	5MU	23S1	1939	22,59	-	2/7/25/26	0/2/2/2

The worst 5 of 345 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	ETR1	54	PSU	C6-C5	12.15	1.49	1.35
56	ETR1	38	PSU	C6-C5	11.73	1.49	1.35
22	23S1	1915	3TD	C6-C5	11.73	1.49	1.35
56	ETR1	37	PSU	C6-C5	11.43	1.48	1.35
53	ATR1	36	PSU	C6-C5	11.43	1.48	1.35

The worst 5 of 248 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	PTR1	54	5MU	C5-C4-N3	12.90	126.32	115.31
22	23S1	747	5MU	C5-C4-N3	12.62	126.08	115.31
22	23S1	1939	5MU	C5-C4-N3	12.51	125.98	115.31
53	ATR1	50	5MU	C4-N3-C2	-11.84	112.02	127.35
53	ATR1	50	5MU	C5-C4-N3	11.54	125.17	115.31

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16S1	527	G7M	O4'-C4'-C5'-O5'
1	16S1	527	G7M	C3'-C4'-C5'-O5'
1	16S1	966	2MG	O4'-C4'-C5'-O5'
1	16S1	966	2MG	C3'-C4'-C5'-O5'
12	S121	89	D2T	CG-CB-SB-CB1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 410 ligands modelled in this entry, 407 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
61	OCW	23S1	3001	58	34,38,38	0.50	0	41,61,61	0.95	2 (4%)
63	GLN	ETR1	101	56	7,8,9	0.45	0	4,9,11	0.04	0
62	CYS	ATR1	101	53	4,5,6	0.55	0	1,5,7	0.12	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
61	OCW	23S1	3001	58	-	2/13/62/62	0/4/4/4
63	GLN	ETR1	101	56	-	3/6/7/9	-
62	CYS	ATR1	101	53	-	0/1/4/6	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
61	23S1	3001	OCW	O04-C20-C14	3.45	112.99	110.06
61	23S1	3001	OCW	C12-C14-C20	2.85	114.87	110.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	23S1	3001	OCW	C12-C13-O01-C27
63	ETR1	101	GLN	CA-CB-CG-CD
63	ETR1	101	GLN	OE1-CD-CG-CB
63	ETR1	101	GLN	NE2-CD-CG-CB
61	23S1	3001	OCW	C16-C13-O01-C27

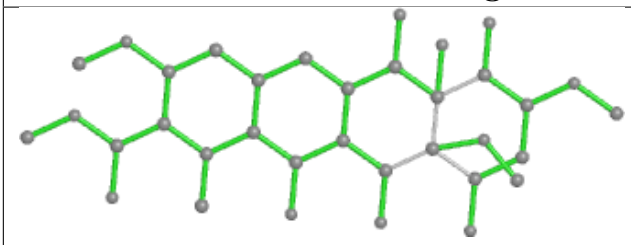
There are no ring outliers.

No monomer is involved in short contacts.

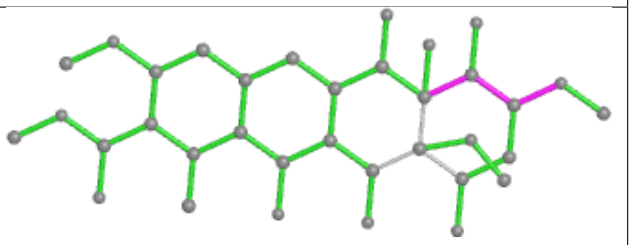
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

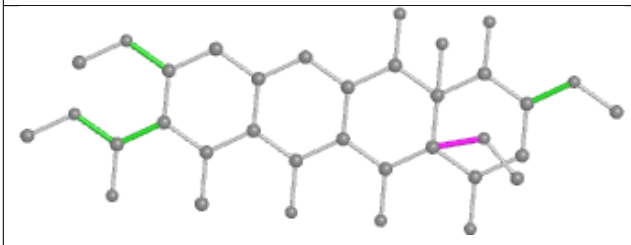
Ligand OCW 23S1 3001



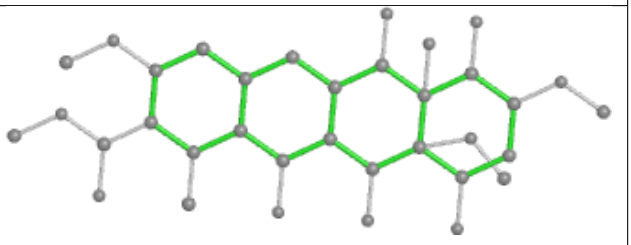
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14956. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

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

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.