



## wwPDB EM Validation Summary Report ⓘ

Nov 3, 2022 – 01:48 AM EDT

PDB ID : 5UYM  
EMDB ID : EMD-8617  
Title : 70S ribosome bound with cognate ternary complex base-paired to A site codon, closed 30S (Structure III)  
Authors : Loveland, A.B.; Demo, G.; Grigorieff, N.; Korostelev, A.A.  
Deposited on : 2017-02-24  
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), 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	:	<b>FAILED</b>
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

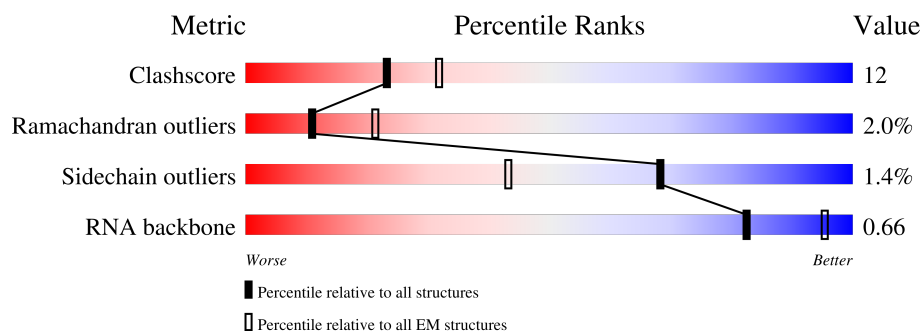
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	04	271	68% 32%
2	05	209	70% 30%
3	06	201	70% 29% .
4	07	177	63% 36% .
5	08	176	73% 26% .
6	09	149	62% 38%
7	10	131	46% 52% ..




















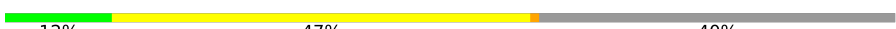





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Mol	Chain	Length	Quality of chain
8	11	141	
9	12	142	
10	13	122	
11	14	143	
12	15	136	
13	16	120	
14	17	116	
15	18	114	
16	19	117	
17	20	103	
18	21	110	
19	22	93	
20	23	102	
21	24	94	
22	25	75	
23	26	77	
24	27	63	
25	28	58	
26	29	66	
27	30	56	
28	31	50	
29	32	46	
30	33	64	
31	34	38	
32	B	218	




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Mol	Chain	Length	Quality of chain
33	C	206	
34	D	205	
35	E	157	
36	F	100	
37	G	151	
38	H	129	
39	I	127	
40	J	98	
41	K	116	
42	L	123	
43	M	114	
44	N	100	
45	O	88	
46	P	82	
47	Q	80	
48	R	65	
49	S	79	
50	T	85	
51	U	65	
52	03	223	
53	A	1539	
54	01	2903	
55	02	120	
56	W	77	
56	X	77	

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Mol	Chain	Length	Quality of chain
57	V	18	 56% 44%
58	Y	76	 61% 36% •
59	Z	392	 37% 57% 5% •

## 2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 154139 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 L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	04	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	05	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	06	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	07	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	08	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	09	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	10	131	Total	C	N	O	S	0	0
			989	625	175	184	5		

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	11	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	12	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	13	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	14	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	15	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	16	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	17	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	18	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	19	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	20	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	21	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	22	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	23	102	Total	C	N	O	0	0
			780	492	146	142		

- Molecule 21 is a protein called 50S ribosomal protein L25.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	24	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	25	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	26	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	27	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	28	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	29	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	30	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	31	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	32	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	33	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	34	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 33 is a protein called 30S ribosomal protein S3.

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

- Molecule 34 is a protein called 30S ribosomal protein S4.

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

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	E	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	F	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 37 is a protein called 30S ribosomal protein S7.

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

- Molecule 38 is a protein called 30S ribosomal protein S8.

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

- Molecule 39 is a protein called 30S ribosomal protein S9.

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

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	J	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	K	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 42 is a protein called 30S ribosomal protein S12.

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

- Molecule 43 is a protein called 30S ribosomal protein S13.

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

- Molecule 44 is a protein called 30S ribosomal protein S14.

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

- Molecule 45 is a protein called 30S ribosomal protein S15.

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

- Molecule 46 is a protein called 30S ribosomal protein S16.

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

- Molecule 47 is a protein called 30S ribosomal protein S17.

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

- Molecule 48 is a protein called 30S ribosomal protein S18.

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

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	S	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	T	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	U	65	Total	C	N	O	S	0	0
			545	335	117	92	1		

- Molecule 52 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	03	134	Total	C	N	O	S	0	0
			1027	645	186	194	2		

- Molecule 53 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	A	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 54 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	01	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
01	747	C	U	conflict	GB 802133627

- Molecule 55 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	02	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

- Molecule 56 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	X	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		
56	W	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 57 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	V	18	Total	C	N	O	P	0	0
			388	175	76	120	17		

- Molecule 58 is a RNA chain called Phe-tRNA<sup>Phe</sup>.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Y	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

- Molecule 59 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Z	392	Total	C	N	O	S	0	0
			3029	1915	521	580	13		

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	12	1	Total	Mg	0
			1	1	
60	25	1	Total	Mg	0
			1	1	
60	N	1	Total	Mg	0
			1	1	
60	A	107	Total	Mg	0
			107	107	
60	01	263	Total	Mg	0
			263	263	

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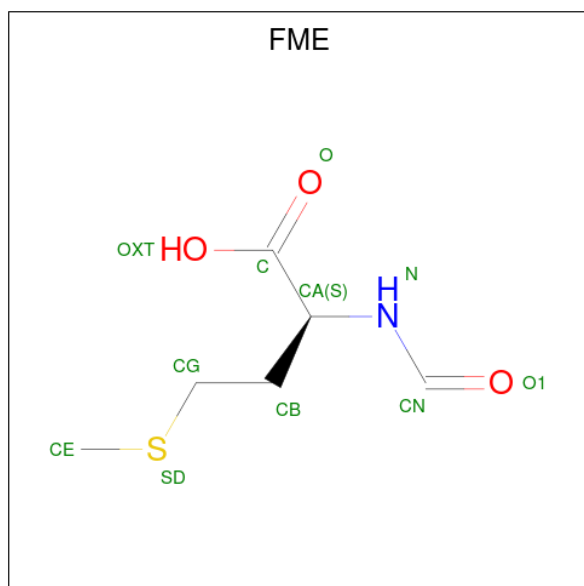
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Mol	Chain	Residues	Atoms		AltConf
60	02	6	Total	Mg	0
			6	6	
60	V	2	Total	Mg	0
			2	2	
60	W	1	Total	Mg	0
			1	1	
60	Z	1	Total	Mg	0
			1	1	

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

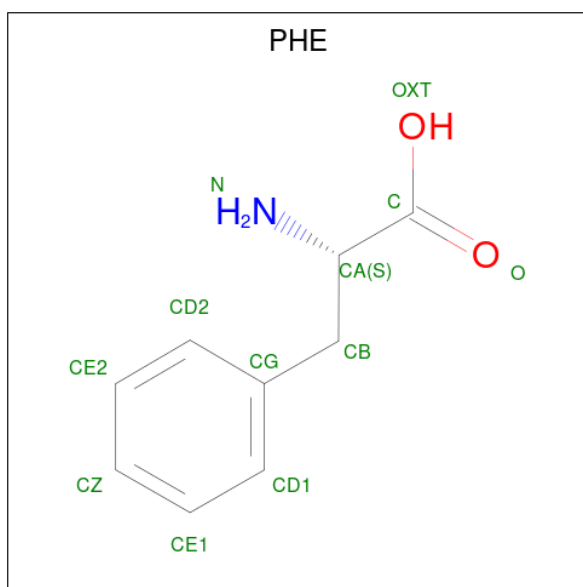
Mol	Chain	Residues	Atoms		AltConf
61	29	1	Total	Zn	0
			1	1	
61	34	1	Total	Zn	0
			1	1	

- Molecule 62 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>3</sub>S).



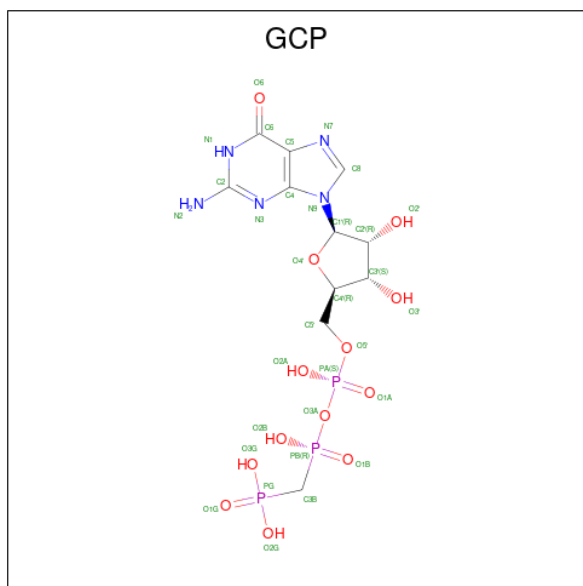
Mol	Chain	Residues	Atoms					AltConf
62	W	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 63 is PHENYLALANINE (three-letter code: PHE) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf
63	Y	1	Total	C	N	O	0
			11	9	1	1	

- Molecule 64 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula:  $C_{11}H_{18}N_5O_{13}P_3$ ).



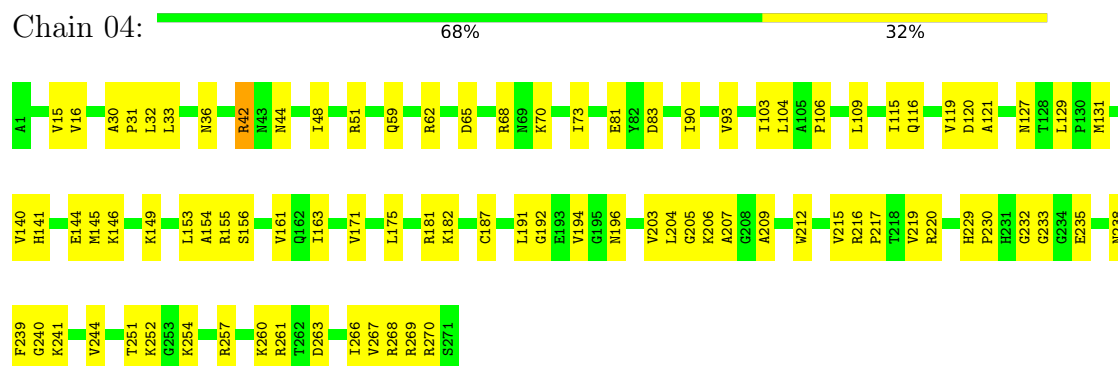
Mol	Chain	Residues	Atoms					AltConf
64	Z	1	Total	C	N	O	P	0
			32	11	5	13	3	



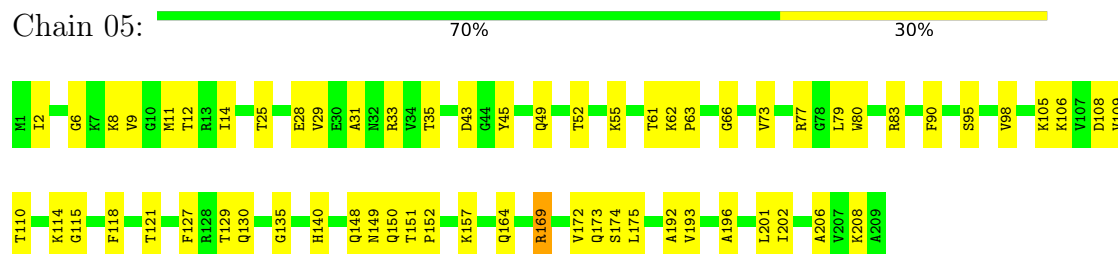
### 3 Residue-property plots

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 L2



- Molecule 2: 50S ribosomal protein L3

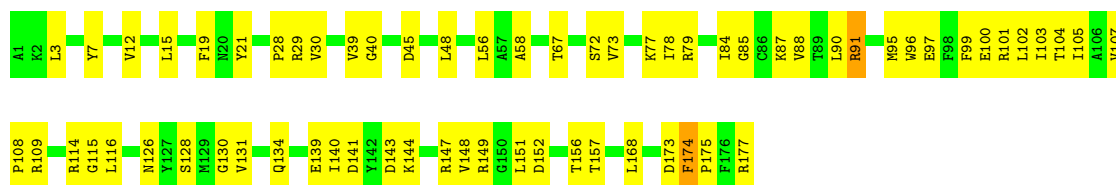


- Molecule 3: 50S ribosomal protein L4



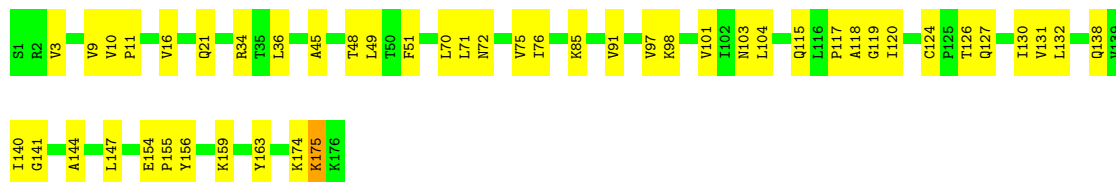
- Molecule 4: 50S ribosomal protein L5





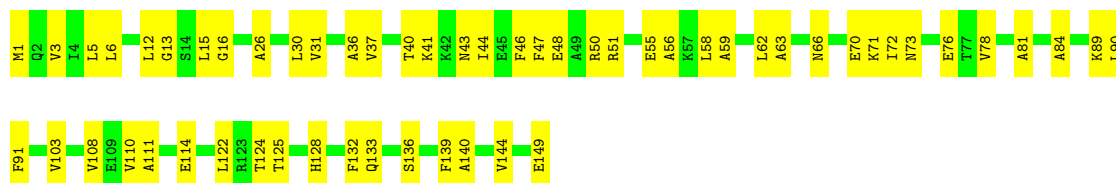
• Molecule 5: 50S ribosomal protein L6

Chain 08: 73% 26% .



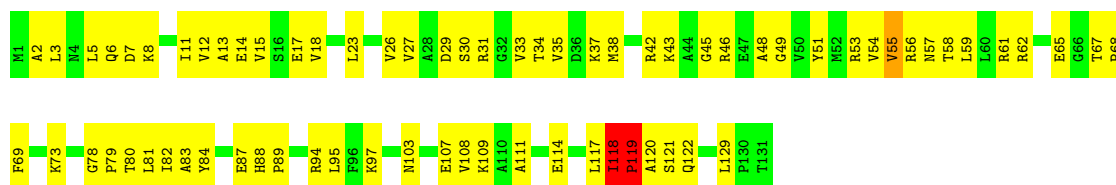
• Molecule 6: 50S ribosomal protein L9

Chain 09: 62% 38%



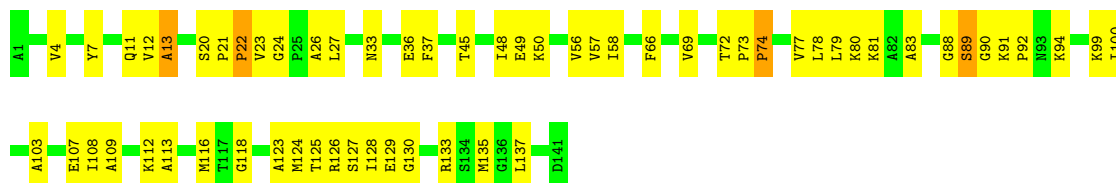
• Molecule 7: 50S ribosomal protein L10

Chain 10: 46% 52% ..



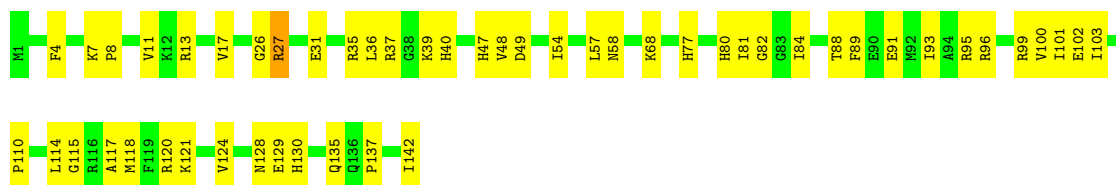
• Molecule 8: 50S ribosomal protein L11

Chain 11: 57% 40% .



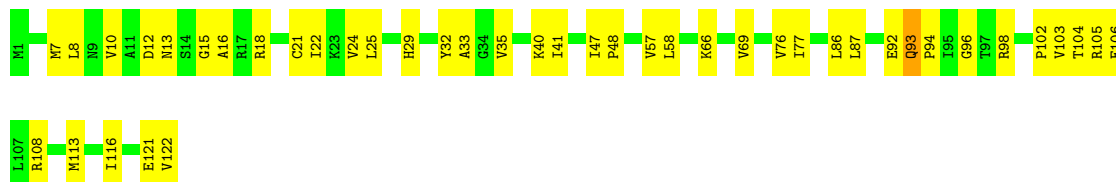
• Molecule 9: 50S ribosomal protein L13

Chain 12: 64% 35% .



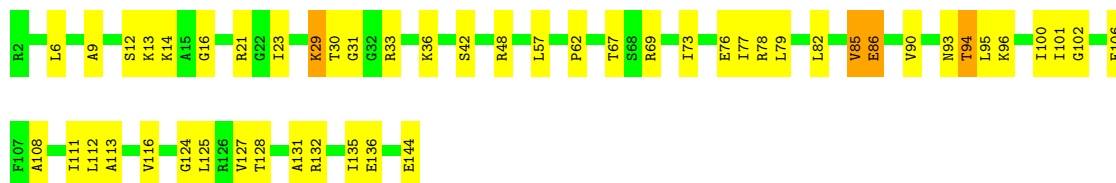
- Molecule 10: 50S ribosomal protein L14

Chain 13: 65% 34% .



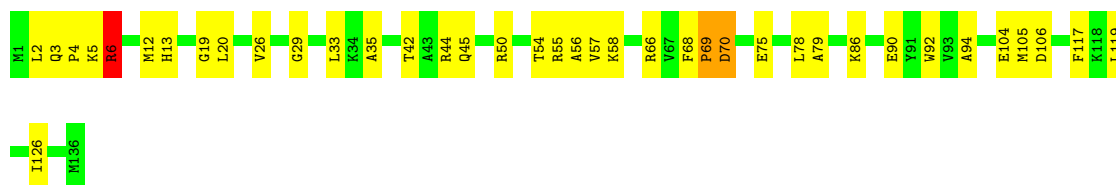
- Molecule 11: 50S ribosomal protein L15

Chain 14: 65% 32% .



- Molecule 12: 50S ribosomal protein L16

Chain 15: 71% 26% ..



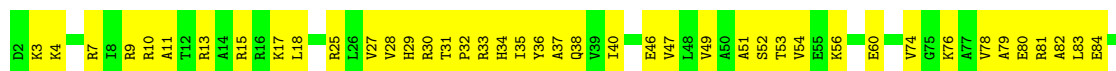
- Molecule 13: 50S ribosomal protein L17

Chain 16: 70% 28% .



- Molecule 14: 50S ribosomal protein L18

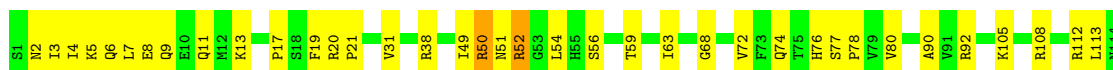
Chain 17: 54% 46%





- Molecule 15: 50S ribosomal protein L19

Chain 18: 68% 31%



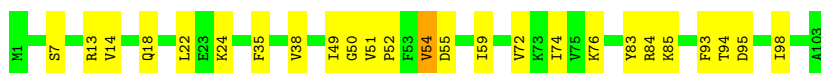
- Molecule 16: 50S ribosomal protein L20

Chain 19: 74% 26%



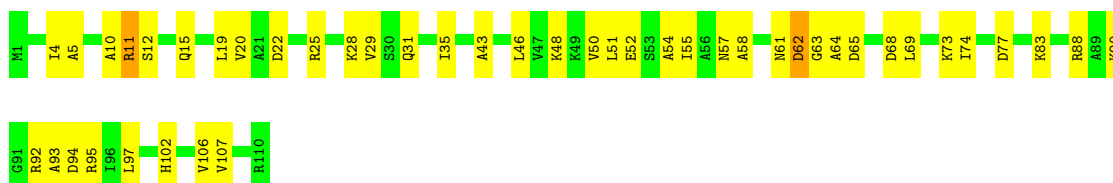
- Molecule 17: 50S ribosomal protein L21

Chain 20: 76% 23%



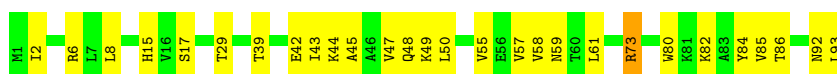
- Molecule 18: 50S ribosomal protein L22

Chain 21: 59% 39%



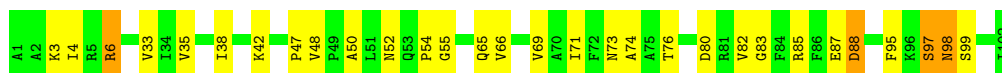
- Molecule 19: 50S ribosomal protein L23

Chain 22: 70% 29%



- Molecule 20: 50S ribosomal protein L24

Chain 23: 71% 25%




- Molecule 21: 50S ribosomal protein L25

Chain 24:  70% 30%




- Molecule 22: 50S ribosomal protein L27

Chain 25:  75% 25%



- Molecule 23: 50S ribosomal protein L28

Chain 26:  78% 22%



- Molecule 24: 50S ribosomal protein L29

Chain 27:  63% 37%



- Molecule 25: 50S ribosomal protein L30

Chain 28:  67% 33%



- Molecule 26: 50S ribosomal protein L31

Chain 29:  71% 27%



- Molecule 27: 50S ribosomal protein L32

Chain 30:  70% 30%



- Molecule 28: 50S ribosomal protein L33

Chain 31:  70% 26% ..



- Molecule 29: 50S ribosomal protein L34

Chain 32:  70% 30%



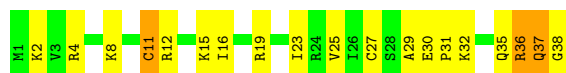
- Molecule 30: 50S ribosomal protein L35

Chain 33:  67% 33%



- Molecule 31: 50S ribosomal protein L36

Chain 34:  50% 42% 8%



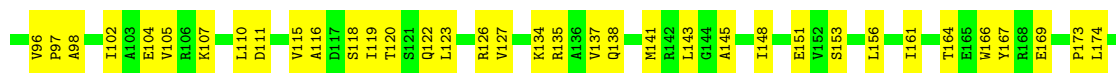
- Molecule 32: 30S ribosomal protein S2

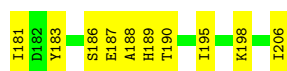
Chain B:  63% 35% .



- Molecule 33: 30S ribosomal protein S3

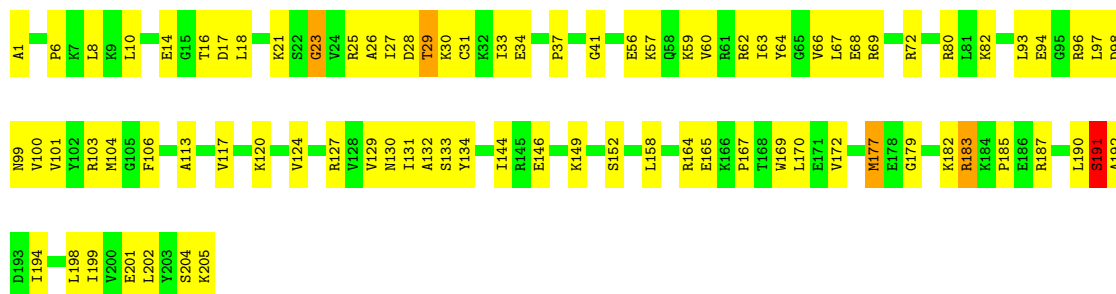
Chain C:  58% 42%





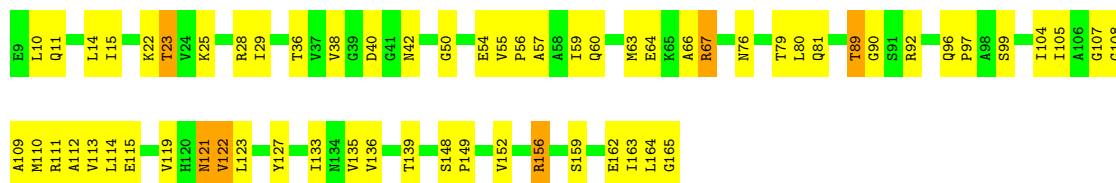
- Molecule 34: 30S ribosomal protein S4

Chain D: 59% 39%



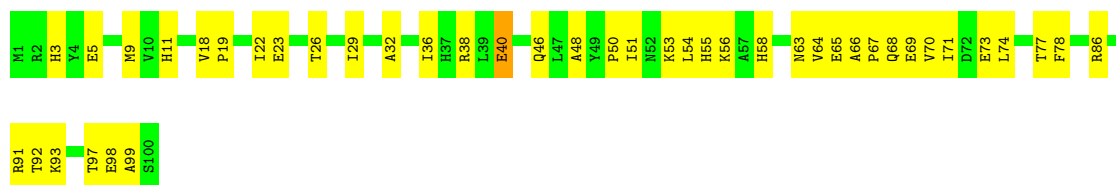
- Molecule 35: 30S ribosomal protein S5

Chain E: 60% 36%



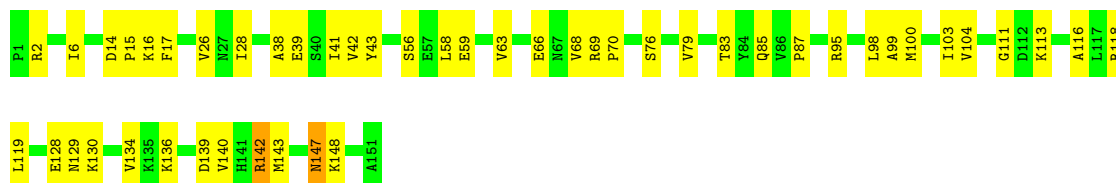
- Molecule 36: 30S ribosomal protein S6

Chain F: 57% 42%



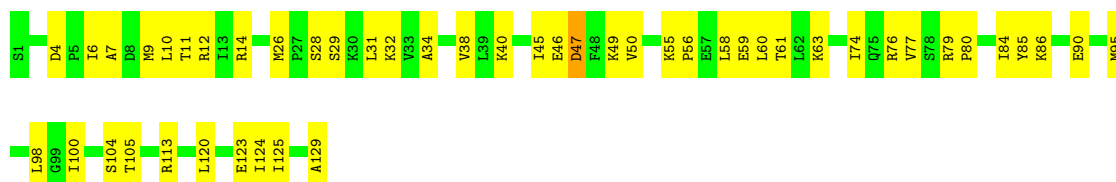
- Molecule 37: 30S ribosomal protein S7

Chain G: 68% 30%



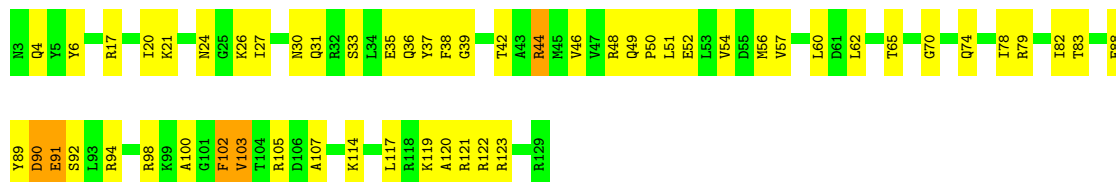
- Molecule 38: 30S ribosomal protein S8

Chain H: 63% 36%



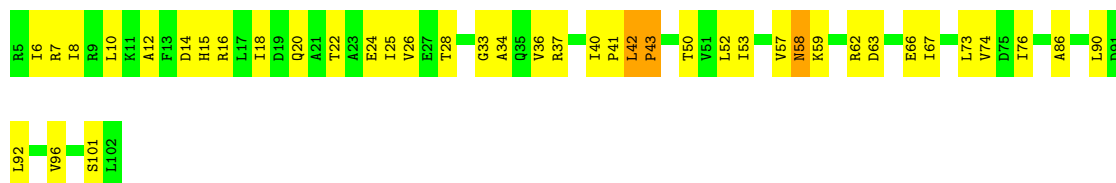
- Molecule 39: 30S ribosomal protein S9

Chain I: 57% 39% .



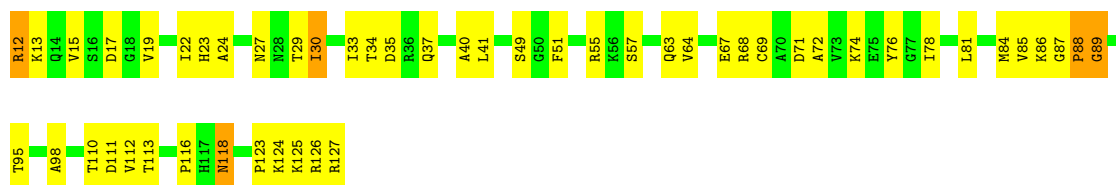
- Molecule 40: 30S ribosomal protein S10

Chain J: 58% 39% .



- Molecule 41: 30S ribosomal protein S11

Chain K: 56% 40% .



- Molecule 42: 30S ribosomal protein S12

Chain L: 68% 30% .



- Molecule 43: 30S ribosomal protein S13

Chain M: 64% 35% .







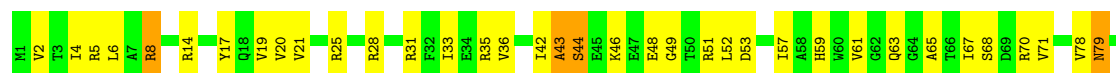
- Molecule 44: 30S ribosomal protein S14



- Molecule 45: 30S ribosomal protein S15



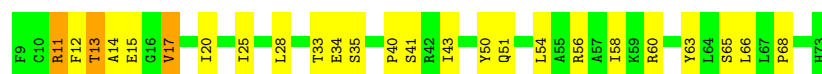
- Molecule 46: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S18

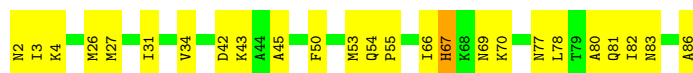


- Molecule 49: 30S ribosomal protein S19



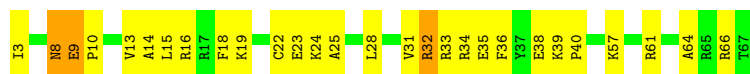
- Molecule 50: 30S ribosomal protein S20

Chain T:  71% 28% .



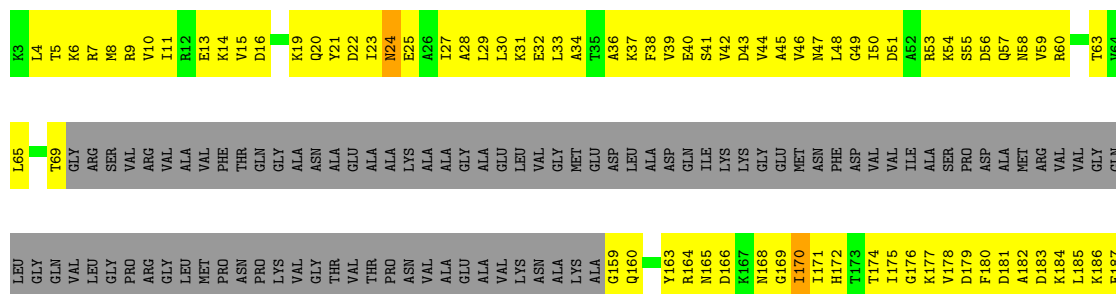
- Molecule 51: 30S ribosomal protein S21

Chain U:  57% 38% 5%



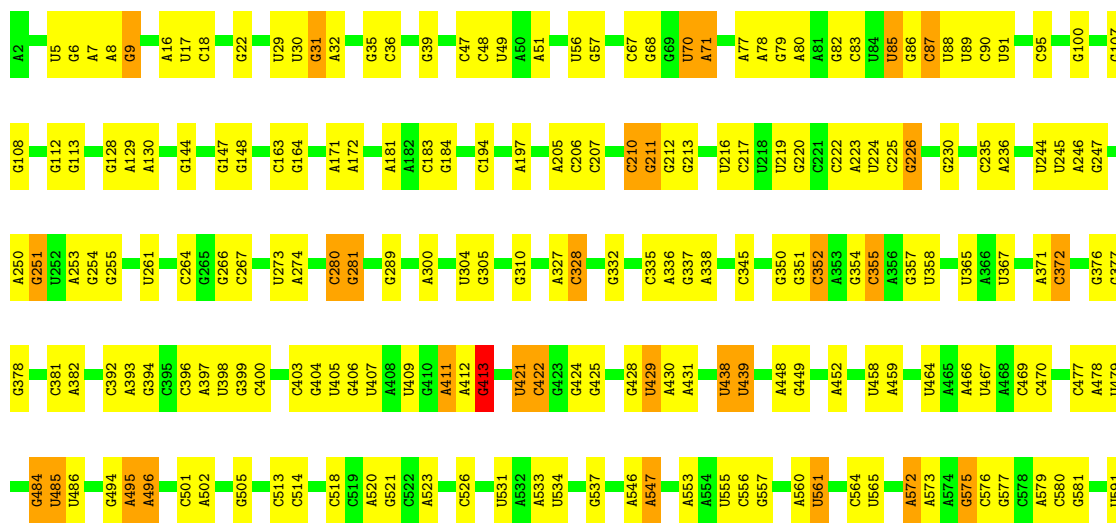
- Molecule 52: 50S ribosomal protein L1

Chain 03:  12% 47% 40%



- Molecule 53: 16S ribosomal RNA

Chain A:  66% 30% .



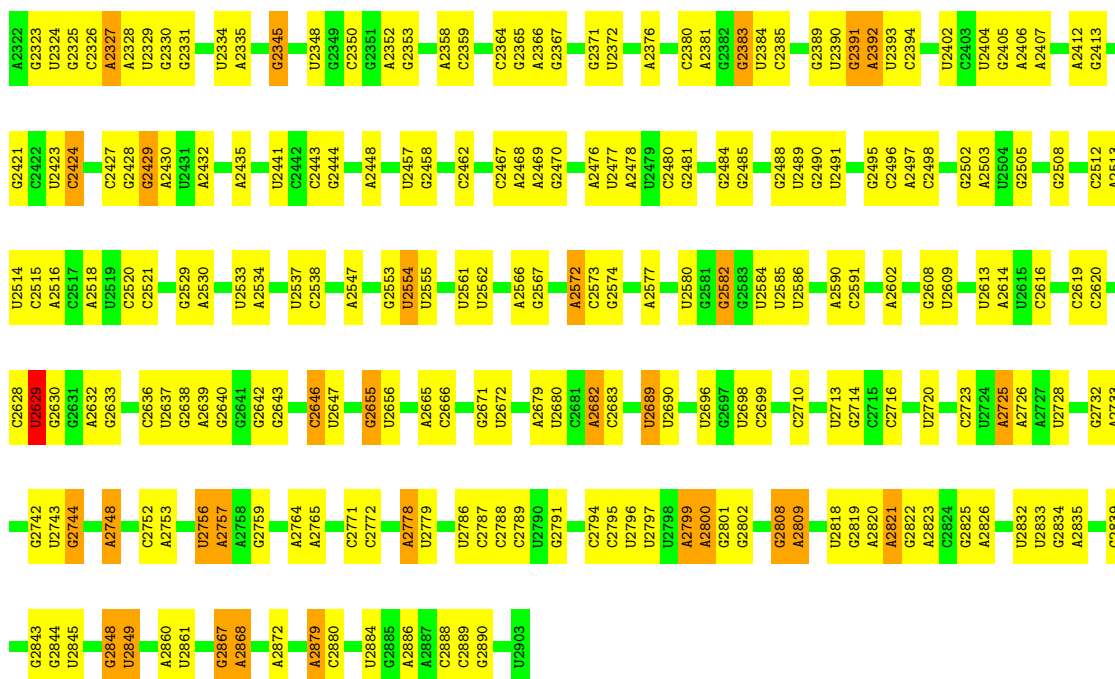
G592	G741	G669	G1003	U1126	C1317	A1447	C1317	C1218	U1126	G1003	G669	G592
G604	G742	G670	A1004	G1127	A1318	C1448	A1318	A1219	G1127	A1004	G670	G604
U605	A743	A872	A1005	C1128	C1319	C1452	C1320	A1220	C1128	A1005	A872	U605
C613	G744	U875	U1007	A1130	C1325	A1456	C1326	G1221	A1130	U1007	U875	C613
C618	U619	A878	U1009	C1136	U1326	G1457	C1327	C1223	C1136	U1009	A878	C618
C620	C620	C982	U1010	C1137	C1328	A1468	C1328	U1224	C1137	U1010	C982	C620
A629	A629	U884	G1015	G1138	G1331	U1471	G1331	A1225	G1138	G1015	U884	A629
A630	A630	G985	A1016	C1140	G1343	U1472	G1343	A1227	C1140	A1016	G985	A630
G633	U757	G886	G1020	C1144	A1346	U1477	A1346	U1235	C1144	G1020	G886	G633
G633	G758	G887	C1027	A1145	G1347	U1478	G1347	A1236	A1145	C1027	G887	G633
U636	U636	G888	U1030	A1146	A1348	U1490	A1348	C1237	A1146	U1030	G888	U636
G761	G761	G890	G1031	C1147	A1349	U1491	A1349	U1240	C1147	G1031	G890	G761
A642	U762	G894	G1032	A1151	A1350	U1492	A1350	G1241	A1151	G1032	G894	A642
C651	G763	G902	G1033	G1157	G1353	U1486	G1353	U1247	G1157	G1033	G902	C651
U653	G764	C902	G1034	A1158	U1354	U1487	U1354	A1248	A1158	G1034	C902	U653
G658	C770	A909	C1038	U1159	A1363	U1498	A1363	G1253	U1159	C1038	A909	G658
G664	A777	C910	G1039	C1162	G1370	A1502	G1370	U1254	C1162	G1039	C910	G664
A665	U780	A915	U1040	A1163	G1371	A1503	G1371	A1256	A1163	U1040	A915	A665
A673	A781	G917	G1041	U1168	U1372	G1496	U1372	A1257	U1168	G1041	G917	A673
G674	A782	A917	U1049	A1169	G1373	U1497	G1373	A1258	A1169	U1049	A917	G674
A676	C783	A923	G1053	A1171	U1379	U1498	U1379	C1259	A1171	G1053	A923	A676
A676	A784	G926	G1058	C1172	U1380	A1507	U1380	G1260	C1172	G1058	G926	A676
G688	G785	G933	U1060	G1175	U1381	A1506	U1381	U1264	G1175	U1060	G933	G688
U692	G786	C934	G1061	G1177	C1382	G1505	C1382	U1264	G1177	G1061	C934	U692
G693	A794	A935	U1062	G1178	C1395	U1506	C1395	U1264	G1178	U1062	A935	G693
A694	A815	A946	C1063	G1182	C1397	A1507	C1397	C1273	A815	C1063	A946	A694
A696	C817	G947	C1069	U1183	C1402	A1513	C1402	A1274	C817	C1069	G947	A696
U697	G818	A955	U1078	G1184	C1403	G1514	C1403	A1275	G818	U1078	A955	U697
G698	A819	U955	G1094	G1190	C1412	G1515	C1412	C1277	A819	G1094	U955	G698
G703	U820	U960	U1099	A1191	U1413	G1517	U1413	G1278	U820	U1099	U960	G703
G711	G830	U961	C1100	C1192	U1414	A1518	U1414	A1280	G830	C1100	U961	G711
A712	A831	G966	A1101	G1193	G1415	G1523	G1415	C1281	A831	A1101	G966	A712
A715	U834	A969	C1102	C1195	G1419	G1529	G1419	U1286	U834	C1102	A969	A715
A716	U835	A975	C1103	A1197	G1422	G1530	G1422	A1287	U835	C1103	A975	A716
G724	U842	G976	G1108	G1198	G1432	C1533	G1432	U1300	U842	G1108	G976	G724
G844	U843	A977	C1109	U1199	A1433	U1540	A1433	U1301	U843	C1109	A977	G844
A845	G844	C990	C1120	A1201	A1441	C1442	A1441	G1304	A845	C1120	C990	A845
G730	A845	U991	U1121	U1202	C1443	U1444	C1443	A1305	G730	U1121	U991	G730
G731	G846	U992	U1122	C1203	U1444	U1445	U1444	A1306	G846	U1122	U992	G731
C736	A865	G993	U1123	U1211	U1445	U1446	U1445	U1315	C736	U1123	G993	C736
C737	C868	G1002	G1124	A1213	A1446		A1446	G1316	C737	G1124	G1002	C737
C738			U1125						C738	U1125		C738

• Molecule 54: 23S ribosomal RNA

Chain 01:  62% 33% 5%

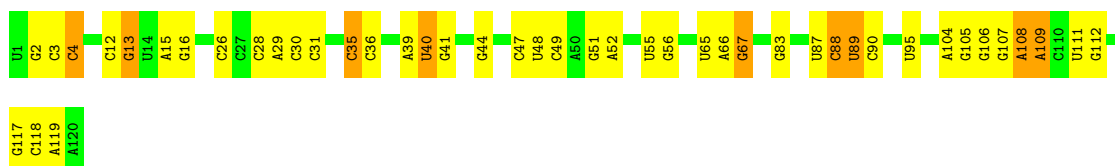
G1	G145	A244	A371	C490	U594	G1	G145	A244	A371	C490	U594
G7	A146	G248	G372	G491	C595	G7	A146	G248	G372	G491	C595
C11	U148	C249	U373	A492	C601	C11	U148	C249	U373	A492	C601
U12	A149	G254	G386	G493	A603	U12	A149	G254	G386	G493	A603
G17	C157	A256	U387	G494	G604	G17	C157	A256	U387	G494	G604
U34	U161	G266	C394	G495	G605	U34	U161	G266	C394	G495	G605
G35	A162	C274	U395	G496	U606	G35	A162	C274	U395	G496	U606
C37	C163	C275	G396	G497	U607	C37	C163	C275	G396	G497	U607
A38	U166	U276	C399	G498	A608	A38	U166	U276	C399	G498	A608
A44	G168	A278	U402	G499	C610	A44	G168	A278	U402	G499	C610
G45	G179	C281	U403	A502	A614	G45	G179	C281	U403	A502	A614
G46	G180	U288	U404	A503	U615	G46	G180	U288	U404	A503	U615
A49	A181	G289	U405	A504	G616	A49	A181	G289	U405	A504	G616
G51	C182	A294	U406	A505	A617	G51	C182	A294	U406	A505	A617
A63	C184	G295	U407	G506	G617	A63	C184	G295	U407	G506	G617
A64	G185	C297	A421	U511	G620	A64	G185	C297	A421	U511	G620
C69	A191	G301	A422	G512	A621	C69	A191	G301	A422	G512	A621
A71	U192	C302	A423	A528	G623	A71	U192	C302	A423	A528	G623
A74	U193	G303	C435	A529	C623	A74	U193	G303	C435	A529	C623
A75	A196	C303	C436	G530	A626	A75	A196	C303	C436	G530	A626
C76	C197	A310	C437	C531	A627	C76	C197	A310	C437	C531	A627
G77	A199	A311	U441	A532	C634	G77	A199	A311	U441	A532	C634
U78	A207	C323	G442	G537	C635	U78	A207	C323	G442	G537	C635
G85	C208	A324	A443	A538	G636	G85	C208	A324	A443	A538	G636
C96	C210	U328	A444	A539	G637	C96	C210	U328	A444	A539	G637
U100	G214	G329	U445	U544	C638	U100	G214	G329	U445	U544	C638
A101	C215	A330	U446	G554	G639	A101	C215	A330	U446	G554	G639
U102	A216	A330	U447	G555	A666	U102	A216	A330	U447	G555	A666
A119	A217	A340	A460	G556	U667	A119	A217	A340	A460	G556	U667
G121	A218	C341	C461	G557	A668	G121	A218	C341	C461	G557	A668
A127	G220	C353	G467	U566	G662	A127	G220	C353	G467	U566	G662
C128	A221	U355	G468	U567	G663	C128	A221	U355	G468	U567	G663
C129	A222	G356	G469	G570	A666	C129	A222	G356	G469	G570	A666
A131	C225	C357	A471	U571	U667	A131	C225	C357	A471	U571	U667
C140	A226	U358	A472	U572	A668	C140	A226	U358	A472	U572	A668
G141	A227	G359	A473	U573	G669	G141	A227	G359	A473	U573	G669
A142	C228	U360	G474	A574	A670	A142	C228	U360	G474	A574	A670
A144	C229	G361	A477	A575	C671	A144	C229	G361	A477	A575	C671
A146	A233	G367	G481	G585	C672	A146	A233	G367	G481	G585	C672
	G242	A368	A482	U588	C673		G242	A368	A482	U588	C673
	U243				G674		U243				G674

G2221	G2222	G2223	G2224	A2225	G2226	U2233	G2234	G2238	G2239	U2240	A2241	G2242	U2243	U2244	G2250	U2257	C2258	U2262	U2265	A2268	C2271	G2277	A2278	A2281	G2282	C2283	A2284	C2285	G2286	A2287	A2288	C2295	U2296	A2297	G2304	U2305	A2309	U2312	C2313	A2317	G2318	G2319	U2320	U2321							
G2140	G2141	A2142	G2143	G2144	G2145	G2146	A2147	G2156	G2157	A2158	G2159	G2160	G2162	A2163	C2164	G2168	A2169	A2170	A2171	U2172	A2173	G2174	G2175	A2176	G2177	A2178	G2179	U2180	A2183	A2184	U2185	G2186	U2189	G2190	C2196	U2197	A2198	G2199	U2195	C2196	U2197	A2201	A2211	A2212	U2213	G2217	G2218	U2219	U2220		
U1943	U1944	U1955	U1956	C1957	C1958	G1959	C1962	U1963	G1964	C1965	A1966	C1967	U1970	A1971	G1972	U1979	G1980	G1989	C1990	U1991	G1992	U1993	C1996	U2005	U2016	G2017	A2018	U2019	G2020	A2021	G2022	A2023	G2024	C2025	U2026	G2038	U2039	A2042	C2043	C2044	G2045	U2130	G2133	A2134	U2139						
C2055	G2056	A2060	G2061	A2062	C2066	C2067	U2068	G2069	A2070	A2071	C2072	C2073	A2074	U2075	C2078	U2079	A2082	G2083	C2096	A2097	U2098	C2104	U2105	U2106	G2107	A2108	U2109	G2110	U2111	G2112	A2114	G2115	G2116	A2117	U2118	U2119	G2120	A2030	A2031	G2032	A2033	G2038	U2039	A2042	C2043	C2044	G2045	U2130	G2133	A2134	U2139
U1816	G1817	U1818	G1824	U1825	G1826	U1827	G1828	A1829	C1833	A1847	A1848	U1856	U1857	A1858	A1866	G1867	A1871	A1872	G1873	A1874	G1875	G1884	A1885	C1893	C1894	A1900	A1901	G1906	G1907	A1913	C1914	U1917	A1918	C1925	U1926	G1929	G1930	U1931	A1932	G1933	A1936	A1937	A1938								
G1715	U1716	G1717	G1718	U1719	U1720	G1721	U1729	G1730	G1731	G1738	A1739	G1740	U1747	U1748	G1753	U1758	G1759	C1760	C1764	U1765	G1766	G1767	A1773	C1774	G1775	G1776	U1779	A1780	A1783	A1784	C1790	A1791	U1794	C1795	U1796	G1797	C1800	A1801	G1807	A1808	A1809	A1810	G1811	U1812							
A1571	A1572	C1577	U1578	G1581	U1584	C1585	C1592	A1593	A1597	A1598	G1601	U1602	A1608	U1609	A1610	C1611	A1614	G1615	A1616	C1625	A1626	A1637	G1645	C1646	U1647	U1648	G1651	A1652	G1653	A1654	G1666	G1667	A1672	G1673	G1674	A1678	A1679	C1685	C1686	A1809	A1810	U1812									
C1349	C1352	A1353	U1354	G1355	G1356	C1357	G1358	A1365	A1366	A1367	G1368	G1369	U1370	G1371	A1372	A1373	A1378	U1379	G1380	A1383	U1386	C1387	U1412	C1413	U1414	U1415	G1416	C1417	G1418	A1419	A1420	G1421	G1424	G1425	G1430	A1431	G1432	G1435	G1436	C1437	U1438	C1447	G1448	C1454							
C1461	A1469	A1470	G1475	U1476	U1481	U1482	A1490	G1491	C1498	C1499	G1500	A1504	A1505	U1506	C1507	A1508	A1509	G1510	A1515	G1524	A1532	C1533	U1534	C1536	C1537	G1538	U1539	G1540	C1541	U1542	G1543	A1548	A1549	G1555	C1558	U1559	G1560	C1564	C1565	A1566	G1567	G1568	A1569	A1570							
G1238	G1245	U1248	G1250	C1251	G1252	A1253	U1255	A1254	G1256	C1257	U1263	A1268	U1269	G1270	G1271	A1272	A1274	A1275	G1280	G1281	U1282	G1283	A1284	A1285	A1286	A1287	C1291	U1292	C1295	G1296	C1297	G1300	A1301	C1306	G1319	C1320	A1321	U1329	C1330	G1331	G1332	U1344	C1345	C1348							
A1103	C1104	U1105	G1106	A1111	G1112	U1113	G1116	C1117	G1122	G1125	U1130	G1131	U1132	A1133	A1134	C1135	G1138	G1139	C1140	U1141	U1142	G1143	G1149	C1150	U1174	A1175	U1176	G1177	C1178	G1179	U1180	U1181	G1182	U1183	G1186	G1187	U1188	G1212	A1213	G1225	U1231	G1232	G1236	A1237							
U1012	C1013	A1020	A1021	G1022	U1023	G1026	A1027	A1028	A1032	U1033	G1038	A1039	C1045	A1046	G1047	C1053	A1054	G1055	G1056	U1057	U1058	G1059	U1060	U1061	G1062	C1063	U1065	U1066	A1069	A1070	G1071	C1076	A1077	U1078	C1079	A1080	U1081	U1082	U1083	A1084	A1085	A1088	C1092	G1093	U1097	A1098					
G879	G880	G881	C885	A886	U887	C888	C890	U894	U895	A896	C897	A899	G903	G904	A910	A917	G923	U927	U928	U932	U933	G940	A941	G942	C946	A947	C948	G949	U955	C961	G962	A973	G974	A975	A983	A984	A988	G989	A990	C995	A996	C1007	A1008	A1009							
A762	A763	G764	G765	C766	C767	G799	A800	G801	A802	U803	G804	A805	C806	C812	U813	C814	G818	A819	A820	A821	G822	U827	U828	G830	A833	G834	U839	C840	A845	U846	U847	C851	C852	C854	G855	G858	G859	U860	A861	G862	A863	G864	C865	U871	U872	A878					
A677	G682	U686	C687	G690	G695	G696	G697	U703	G704	A705	U706	G707	A715	A716	C717	A718	C719	U720	A721	G726	U727	G728	G729	A730	G738	A739	C840	A845	U846	U847	C851	C852	C854	G855	G858	G859	U860	A861	G862	A863	G864	C865	U871	U872	A878						



• Molecule 55: 5S ribosomal RNA

Chain 02: 62% 30% 8%



• Molecule 56: tRNA<sup>fMet</sup>

Chain X: 39% 49% 12%



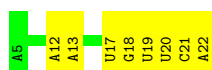
• Molecule 56: tRNA<sup>fMet</sup>

Chain W: 86% 12%



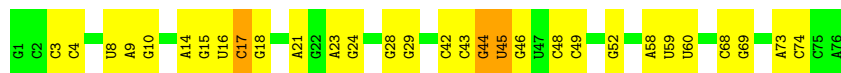
• Molecule 57: mRNA

Chain V: 56% 44%



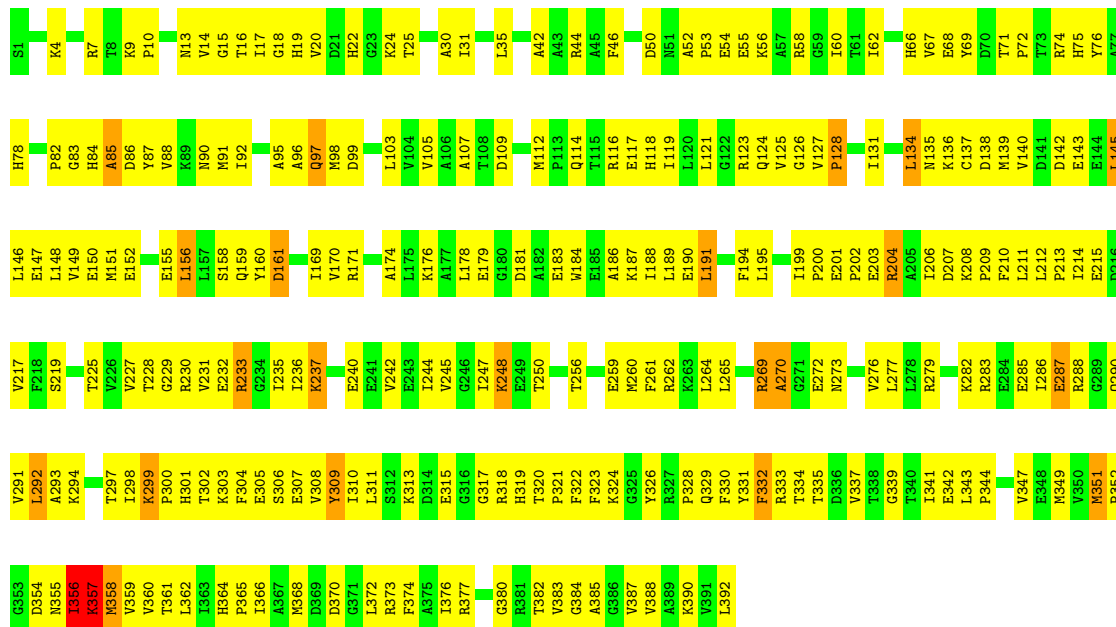
- Molecule 58: Phe-tRNAPhe

Chain Y:  61% 36% •



- Molecule 59: Elongation factor Tu 2

Chain Z:  37% 57% 5% •



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	153597	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND3 was used to determine CTF values. FREALIGN applied CTF correction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	60976	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FME, MG, GCP, ZN

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	04	0.26	0/2122	0.58	0/2852
2	05	0.27	0/1586	0.55	0/2134
3	06	0.26	0/1571	0.55	0/2113
4	07	0.29	0/1435	0.55	0/1926
5	08	0.27	0/1343	0.52	0/1816
6	09	0.29	0/1122	0.63	0/1515
7	10	0.32	0/1002	0.68	0/1350
8	11	0.31	0/1046	0.58	0/1410
9	12	0.27	0/1152	0.54	0/1551
10	13	0.26	0/948	0.59	0/1268
11	14	0.26	0/1054	0.61	0/1403
12	15	0.28	0/1093	0.57	0/1460
13	16	0.26	0/974	0.56	0/1301
14	17	0.25	0/902	0.55	0/1209
15	18	0.27	0/929	0.56	0/1242
16	19	0.28	0/960	0.48	0/1278
17	20	0.28	0/829	0.63	1/1107 (0.1%)
18	21	0.25	0/864	0.58	0/1156
19	22	0.27	0/745	0.54	0/994
20	23	0.28	0/788	0.62	0/1051
21	24	0.29	0/766	0.56	0/1025
22	25	0.28	0/582	0.51	0/769
23	26	0.27	0/635	0.54	0/848
24	27	0.27	0/510	0.51	0/677
25	28	0.25	0/453	0.51	0/605
26	29	0.30	0/532	0.54	0/709
27	30	0.26	0/450	0.56	0/599
28	31	0.30	0/417	0.57	0/554
29	32	0.29	0/380	0.53	0/498
30	33	0.26	0/513	0.60	0/676
31	34	0.26	0/303	0.54	0/397
32	B	0.29	0/1736	0.58	0/2338



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	C	0.28	0/1652	0.52	0/2225
34	D	0.26	0/1665	0.55	0/2227
35	E	0.28	0/1170	0.59	0/1573
36	F	0.29	0/836	0.61	0/1128
37	G	0.25	0/1196	0.53	0/1602
38	H	0.26	0/989	0.57	0/1326
39	I	0.28	0/1034	0.61	0/1375
40	J	0.27	0/797	0.65	0/1077
41	K	0.28	0/886	0.60	0/1195
42	L	0.28	0/969	0.68	1/1300 (0.1%)
43	M	0.25	0/893	0.57	0/1193
44	N	0.26	0/817	0.54	0/1088
45	O	0.26	0/722	0.54	0/964
46	P	0.28	0/659	0.59	0/884
47	Q	0.28	0/658	0.62	0/881
48	R	0.30	0/545	0.55	0/731
49	S	0.28	0/653	0.57	0/877
50	T	0.26	0/671	0.49	0/888
51	U	0.33	0/551	0.61	0/728
52	03	1.37	0/1034	0.73	0/1387
53	A	0.31	0/36963	0.68	1/57662 (0.0%)
54	01	0.32	0/69796	0.67	2/108888 (0.0%)
55	02	0.31	0/2872	0.67	0/4479
56	W	0.31	0/1832	0.67	0/2855
56	X	0.47	0/1832	0.67	0/2855
57	V	0.32	0/436	0.67	0/679
58	Y	0.36	0/1809	0.67	0/2819
59	Z	1.18	0/3085	0.73	1/4173 (0.0%)
All	All	0.36	0/166764	0.65	6/248890 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
54	01	0	3
59	Z	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	20	50	GLY	N-CA-C	-6.04	98.01	113.10
59	Z	71	THR	N-CA-C	-5.68	95.66	111.00
42	L	43	LYS	N-CA-C	5.29	125.29	111.00
54	01	458	G	C1'-O4'-C4'	-5.24	105.71	109.90
53	A	413	G	N9-C1'-C2'	5.11	120.64	114.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
54	01	2629	U	Sidechain
54	01	2725	A	Sidechain
54	01	775	G	Sidechain
59	Z	309	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	04	2083	0	2157	90	0
2	05	1565	0	1616	52	0
3	06	1552	0	1619	50	0
4	07	1411	0	1447	55	0
5	08	1323	0	1374	31	0
6	09	1111	0	1148	45	0
7	10	989	0	1025	75	0
8	11	1032	0	1088	60	0
9	12	1129	0	1162	51	0
10	13	939	0	1012	37	0
11	14	1045	0	1117	46	0
12	15	1074	0	1157	32	0
13	16	961	0	1000	30	0
14	17	892	0	923	45	0
15	18	917	0	965	45	0
16	19	947	0	1022	28	0
17	20	816	0	839	22	0
18	21	857	0	922	28	0
19	22	739	0	807	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	23	780	0	834	26	0
21	24	753	0	780	22	0
22	25	575	0	592	14	0
23	26	625	0	655	9	0
24	27	509	0	543	17	0
25	28	449	0	491	14	0
26	29	523	0	524	13	0
27	30	444	0	461	15	0
28	31	410	0	440	12	0
29	32	377	0	418	15	0
30	33	504	0	574	16	0
31	34	302	0	343	21	0
32	B	1705	0	1732	67	0
33	C	1625	0	1699	64	0
34	D	1643	0	1710	77	0
35	E	1157	0	1199	53	0
36	F	818	0	808	43	0
37	G	1182	0	1240	42	0
38	H	979	0	1034	46	0
39	I	1022	0	1070	47	0
40	J	787	0	828	47	0
41	K	870	0	878	46	0
42	L	955	0	1019	44	0
43	M	884	0	944	41	0
44	N	805	0	847	33	0
45	O	714	0	737	20	0
46	P	649	0	666	42	0
47	Q	649	0	691	34	0
48	R	536	0	552	23	0
49	S	638	0	665	31	0
50	T	665	0	714	16	0
51	U	545	0	579	36	0
52	03	1027	0	1092	155	0
53	A	33012	0	16618	357	0
54	01	62317	0	31346	697	0
55	02	2568	0	1303	38	0
56	W	1640	0	836	4	0
56	X	1640	0	837	33	0
57	V	388	0	196	4	0
58	Y	1619	0	821	12	0
59	Z	3029	0	3043	319	0
60	01	263	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	02	6	0	0	0	0
60	12	1	0	0	0	0
60	25	1	0	0	0	0
60	A	107	0	0	0	0
60	N	1	0	0	0	0
60	V	2	0	0	0	0
60	W	1	0	0	0	0
60	Z	1	0	0	0	0
61	29	1	0	0	0	0
61	34	1	0	0	0	0
62	W	10	0	10	0	0
63	Y	11	0	8	2	0
64	Z	32	0	14	1	0
All	All	154139	0	104791	3196	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 12.

The worst 5 of 3196 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:Z:151:MET:CE	59:Z:151:MET:SD	2.01	1.46
52:03:181:ASP:HB2	52:03:184:LYS:HD3	1.19	1.19
59:Z:212:LEU:HD11	59:Z:229:GLY:HA3	1.32	1.08
35:E:80:LEU:HD13	35:E:122:VAL:HG11	1.31	1.08
59:Z:344:PRO:HG2	59:Z:347:VAL:HG21	1.36	1.06

There are no symmetry-related clashes.

## 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	04	269/271 (99%)	241 (90%)	24 (9%)	4 (2%)	10	44
2	05	207/209 (99%)	191 (92%)	15 (7%)	1 (0%)	29	67
3	06	199/201 (99%)	179 (90%)	19 (10%)	1 (0%)	29	67
4	07	175/177 (99%)	156 (89%)	18 (10%)	1 (1%)	25	64
5	08	174/176 (99%)	155 (89%)	15 (9%)	4 (2%)	6	34
6	09	147/149 (99%)	124 (84%)	21 (14%)	2 (1%)	11	46
7	10	129/131 (98%)	90 (70%)	32 (25%)	7 (5%)	2	14
8	11	139/141 (99%)	113 (81%)	19 (14%)	7 (5%)	2	16
9	12	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
10	13	120/122 (98%)	99 (82%)	19 (16%)	2 (2%)	9	42
11	14	141/143 (99%)	120 (85%)	14 (10%)	7 (5%)	2	16
12	15	134/136 (98%)	118 (88%)	13 (10%)	3 (2%)	6	35
13	16	118/120 (98%)	104 (88%)	12 (10%)	2 (2%)	9	42
14	17	114/116 (98%)	104 (91%)	10 (9%)	0	100	100
15	18	112/114 (98%)	103 (92%)	8 (7%)	1 (1%)	17	56
16	19	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
17	20	101/103 (98%)	87 (86%)	13 (13%)	1 (1%)	15	54
18	21	108/110 (98%)	97 (90%)	8 (7%)	3 (3%)	5	29
19	22	91/93 (98%)	76 (84%)	15 (16%)	0	100	100
20	23	100/102 (98%)	79 (79%)	17 (17%)	4 (4%)	3	21
21	24	92/94 (98%)	84 (91%)	8 (9%)	0	100	100
22	25	73/75 (97%)	62 (85%)	11 (15%)	0	100	100
23	26	75/77 (97%)	68 (91%)	7 (9%)	0	100	100
24	27	61/63 (97%)	57 (93%)	3 (5%)	1 (2%)	9	43
25	28	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
26	29	64/66 (97%)	57 (89%)	7 (11%)	0	100	100
27	30	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
28	31	48/50 (96%)	43 (90%)	3 (6%)	2 (4%)	3	20
29	32	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
30	33	62/64 (97%)	55 (89%)	6 (10%)	1 (2%)	9	43
31	34	36/38 (95%)	30 (83%)	5 (14%)	1 (3%)	5	29
32	B	216/218 (99%)	181 (84%)	30 (14%)	5 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	C	204/206 (99%)	188 (92%)	15 (7%)	1 (0%)	29	67
34	D	203/205 (99%)	172 (85%)	26 (13%)	5 (2%)	5	32
35	E	155/157 (99%)	122 (79%)	26 (17%)	7 (4%)	2	18
36	F	98/100 (98%)	77 (79%)	18 (18%)	3 (3%)	4	26
37	G	149/151 (99%)	131 (88%)	18 (12%)	0	100	100
38	H	127/129 (98%)	118 (93%)	8 (6%)	1 (1%)	19	58
39	I	125/127 (98%)	102 (82%)	17 (14%)	6 (5%)	2	17
40	J	96/98 (98%)	76 (79%)	14 (15%)	6 (6%)	1	10
41	K	114/116 (98%)	94 (82%)	16 (14%)	4 (4%)	3	24
42	L	121/123 (98%)	98 (81%)	18 (15%)	5 (4%)	3	21
43	M	112/114 (98%)	97 (87%)	12 (11%)	3 (3%)	5	30
44	N	98/100 (98%)	78 (80%)	18 (18%)	2 (2%)	7	38
45	O	86/88 (98%)	77 (90%)	8 (9%)	1 (1%)	13	49
46	P	80/82 (98%)	67 (84%)	9 (11%)	4 (5%)	2	16
47	Q	78/80 (98%)	63 (81%)	11 (14%)	4 (5%)	2	15
48	R	63/65 (97%)	54 (86%)	7 (11%)	2 (3%)	4	26
49	S	77/79 (98%)	65 (84%)	10 (13%)	2 (3%)	5	31
50	T	83/85 (98%)	78 (94%)	4 (5%)	1 (1%)	13	49
51	U	63/65 (97%)	43 (68%)	17 (27%)	3 (5%)	2	17
52	03	130/223 (58%)	114 (88%)	14 (11%)	2 (2%)	10	44
59	Z	390/392 (100%)	328 (84%)	54 (14%)	8 (2%)	7	37
All	All	6366/6563 (97%)	5507 (86%)	729 (12%)	130 (2%)	11	38

5 of 130 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	04	232	GLY
3	06	83	VAL
5	08	45	ALA
5	08	119	GLY
7	10	81	LEU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	04	216/216 (100%)	213 (99%)	3 (1%)	67	86
2	05	164/164 (100%)	163 (99%)	1 (1%)	86	94
3	06	165/165 (100%)	163 (99%)	2 (1%)	71	88
4	07	148/148 (100%)	147 (99%)	1 (1%)	84	94
5	08	137/137 (100%)	137 (100%)	0	100	100
6	09	114/114 (100%)	114 (100%)	0	100	100
7	10	100/100 (100%)	98 (98%)	2 (2%)	55	80
8	11	109/109 (100%)	109 (100%)	0	100	100
9	12	116/116 (100%)	115 (99%)	1 (1%)	78	91
10	13	103/103 (100%)	103 (100%)	0	100	100
11	14	102/102 (100%)	102 (100%)	0	100	100
12	15	109/109 (100%)	107 (98%)	2 (2%)	59	82
13	16	100/100 (100%)	99 (99%)	1 (1%)	76	90
14	17	86/86 (100%)	86 (100%)	0	100	100
15	18	99/99 (100%)	97 (98%)	2 (2%)	55	80
16	19	89/89 (100%)	89 (100%)	0	100	100
17	20	84/84 (100%)	84 (100%)	0	100	100
18	21	93/93 (100%)	91 (98%)	2 (2%)	52	79
19	22	80/80 (100%)	78 (98%)	2 (2%)	47	77
20	23	83/83 (100%)	83 (100%)	0	100	100
21	24	78/78 (100%)	78 (100%)	0	100	100
22	25	57/57 (100%)	57 (100%)	0	100	100
23	26	67/67 (100%)	66 (98%)	1 (2%)	65	85
24	27	55/55 (100%)	55 (100%)	0	100	100
25	28	48/48 (100%)	47 (98%)	1 (2%)	53	79
26	29	59/59 (100%)	57 (97%)	2 (3%)	37	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	30	47/47 (100%)	47 (100%)	0	100	100
28	31	45/45 (100%)	44 (98%)	1 (2%)	52	79
29	32	38/38 (100%)	37 (97%)	1 (3%)	46	76
30	33	51/51 (100%)	51 (100%)	0	100	100
31	34	34/34 (100%)	32 (94%)	2 (6%)	19	54
32	B	180/180 (100%)	175 (97%)	5 (3%)	43	74
33	C	170/170 (100%)	170 (100%)	0	100	100
34	D	172/172 (100%)	169 (98%)	3 (2%)	60	83
35	E	119/119 (100%)	117 (98%)	2 (2%)	60	83
36	F	87/87 (100%)	87 (100%)	0	100	100
37	G	124/124 (100%)	122 (98%)	2 (2%)	62	84
38	H	104/104 (100%)	104 (100%)	0	100	100
39	I	105/105 (100%)	102 (97%)	3 (3%)	42	74
40	J	86/86 (100%)	86 (100%)	0	100	100
41	K	89/89 (100%)	86 (97%)	3 (3%)	37	70
42	L	103/103 (100%)	103 (100%)	0	100	100
43	M	92/92 (100%)	91 (99%)	1 (1%)	73	88
44	N	83/83 (100%)	83 (100%)	0	100	100
45	O	76/76 (100%)	76 (100%)	0	100	100
46	P	65/65 (100%)	65 (100%)	0	100	100
47	Q	74/74 (100%)	74 (100%)	0	100	100
48	R	56/56 (100%)	55 (98%)	1 (2%)	59	82
49	S	70/70 (100%)	70 (100%)	0	100	100
50	T	65/65 (100%)	64 (98%)	1 (2%)	65	85
51	U	55/55 (100%)	53 (96%)	2 (4%)	35	69
52	03	110/174 (63%)	108 (98%)	2 (2%)	59	82
59	Z	324/325 (100%)	303 (94%)	21 (6%)	17	51
All	All	5285/5350 (99%)	5212 (99%)	73 (1%)	68	86

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
59	Z	156	LEU

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Mol	Chain	Res	Type
59	Z	357	LYS
59	Z	191	LEU
59	Z	287	GLU
29	32	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
30	33	27	ASN
37	G	129	ASN
59	Z	364	HIS
32	B	176	ASN
34	D	35	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	A	1538/1539 (99%)	147 (9%)	8 (0%)
54	01	2902/2903 (99%)	359 (12%)	22 (0%)
55	02	119/120 (99%)	11 (9%)	1 (0%)
56	W	76/77 (98%)	7 (9%)	0
56	X	76/77 (98%)	18 (23%)	0
57	V	17/18 (94%)	2 (11%)	0
58	Y	75/76 (98%)	12 (16%)	1 (1%)
All	All	4803/4810 (99%)	556 (11%)	32 (0%)

5 of 556 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
53	A	6	G
53	A	9	G
53	A	22	G
53	A	31	G
53	A	32	A

5 of 32 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	01	2808	G
54	01	2848	G

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Mol	Chain	Res	Type
54	01	774	G
54	01	490	C
55	02	88	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 388 ligands modelled in this entry, 385 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	$\# Z  > 2$
64	GCP	Z	402	60	27,34,34	2.53	11 (40%)	34,54,54	3.84	18 (52%)
63	PHE	Y	101	58	10,11,12	0.66	0	10,13,15	0.52	0
62	FME	W	101	-	8,9,10	0.89	0	7,9,11	1.17	1 (14%)

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
64	GCP	Z	402	60	-	9/15/38/38	0/3/3/3
63	PHE	Y	101	58	-	0/5/6/8	0/1/1/1
62	FME	W	101	-	-	3/7/9/11	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	Z	402	GCP	PB-O3A	-5.85	1.51	1.58
64	Z	402	GCP	O4'-C1'	5.16	1.48	1.41
64	Z	402	GCP	C6-N1	4.33	1.40	1.33
64	Z	402	GCP	C5-C6	4.10	1.48	1.41
64	Z	402	GCP	C2'-C1'	4.05	1.59	1.53

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	Z	402	GCP	C1'-N9-C4	12.82	149.17	126.64
64	Z	402	GCP	C5-C6-N1	-8.85	111.32	123.43
64	Z	402	GCP	O1G-PG-C3B	-7.44	95.20	111.24
64	Z	402	GCP	C2-N1-C6	6.89	126.88	115.93
64	Z	402	GCP	O4'-C1'-C2'	-4.88	99.79	106.93

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	W	101	FME	O1-CN-N-CA
62	W	101	FME	O-C-CA-CB
64	Z	402	GCP	PB-C3B-PG-O1G
64	Z	402	GCP	PB-C3B-PG-O2G
64	Z	402	GCP	PG-C3B-PB-O1B

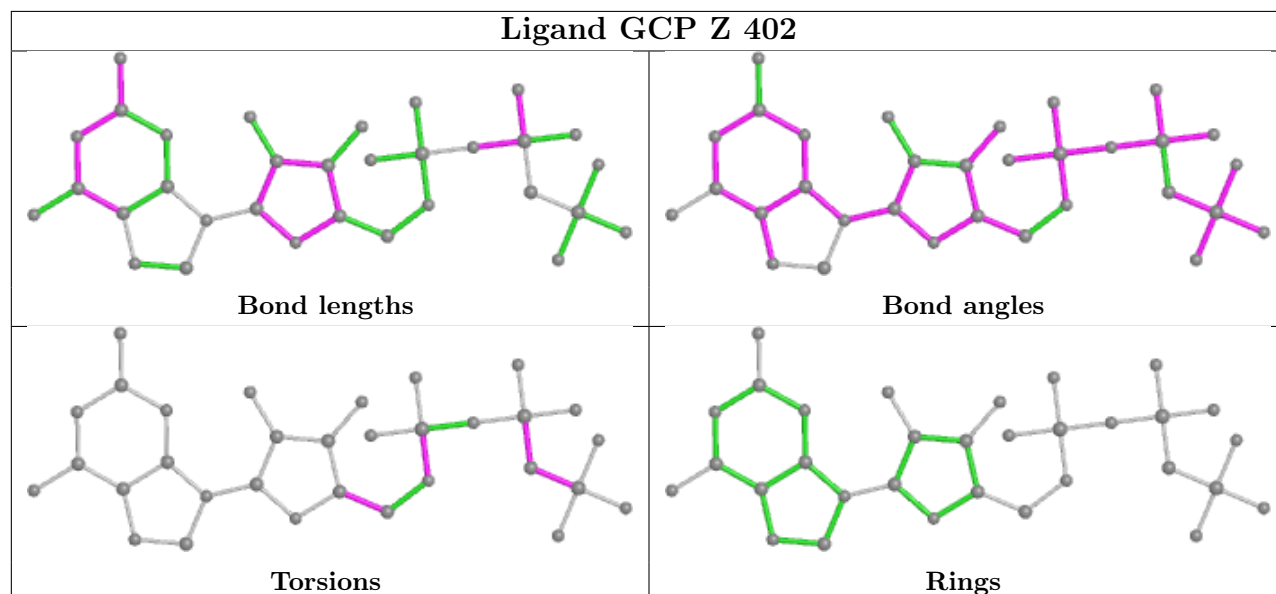
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
64	Z	402	GCP	1	0
63	Y	101	PHE	2	0

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

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8617. 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 surface views

This section was not generated.

### 6.5 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.