



wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 11:58 PM EST

PDB ID : 6OGG
EMDB ID : EMD-20057
Title : 70S termination complex with RF2 bound to the UGA codon. Rotated ribosome with RF2 bound (Structure IV).
Authors : Svidritskiy, E.; Demo, G.; Loveland, A.B.; Xu, C.; Korostelev, A.A.
Deposited on : 2019-04-02
Resolution : 4.20 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

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>.

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

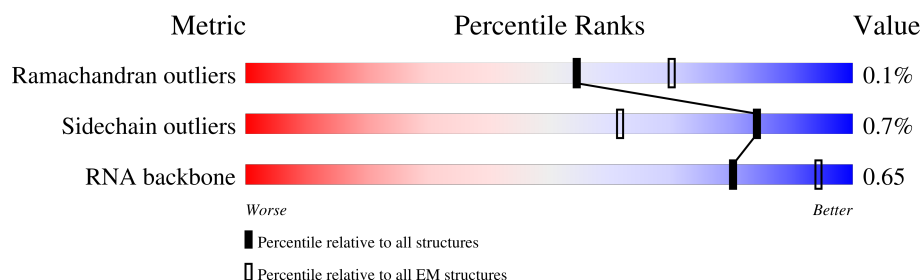
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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.



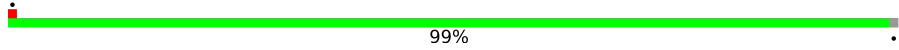
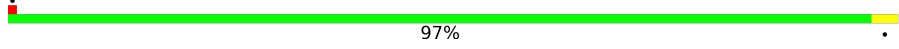
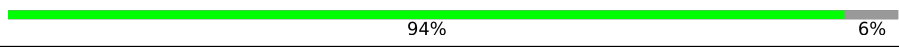
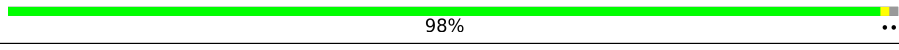
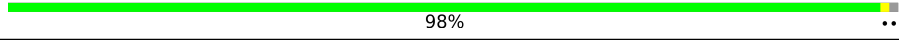
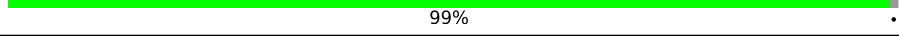
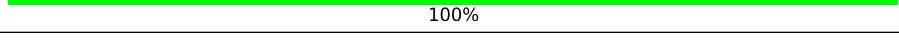
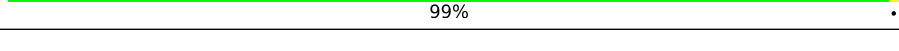
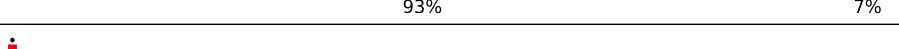
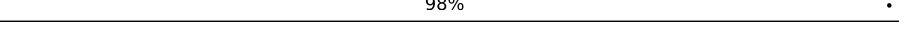
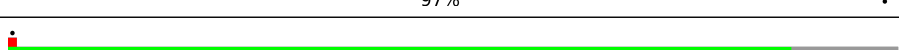

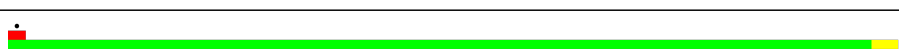
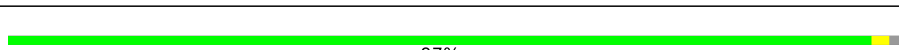
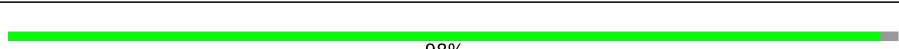

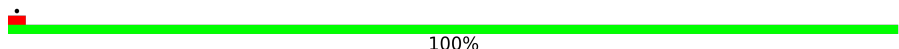
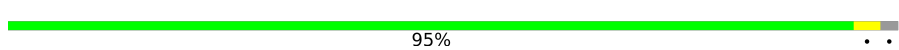
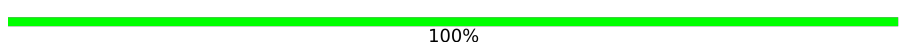
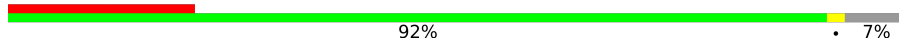
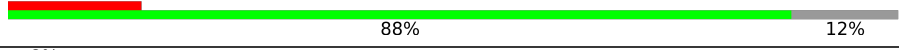
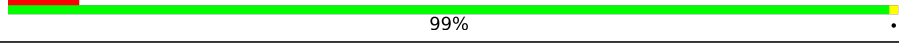
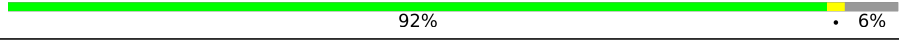


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	b	273	
2	c	209	
3	d	201	
4	e	179	
5	f	177	
6	g	149	
7	j	142	
8	k	123	

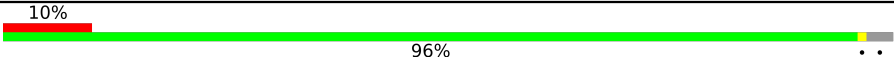
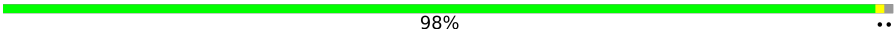
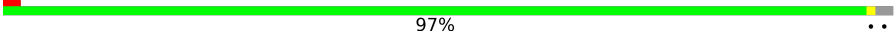
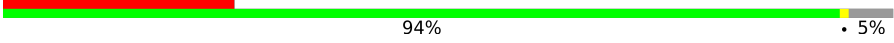

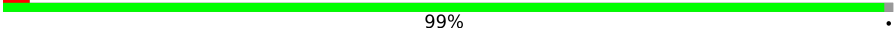
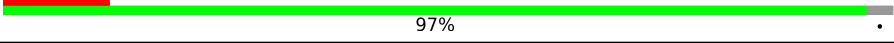
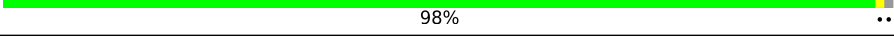
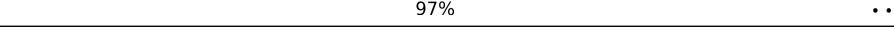
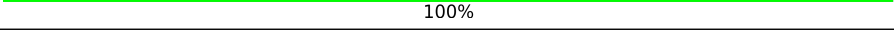
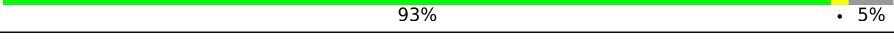
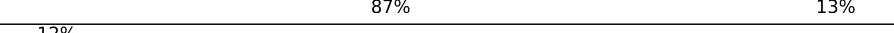
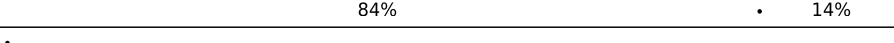
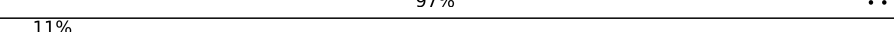
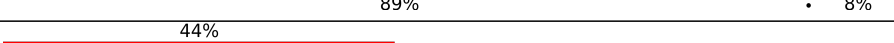





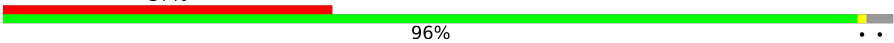

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Mol	Chain	Length	Quality of chain
9	l	144	
10	m	136	
11	n	127	
12	o	117	
13	p	115	
14	q	118	
15	r	103	
16	s	110	
17	t	100	
18	u	104	
19	v	94	
20	w	85	
21	x	78	
22	y	63	
23	z	59	
24	B	57	
25	C	55	
26	D	46	
27	E	65	
28	F	38	
29	G	241	
30	H	233	
31	I	206	
32	J	167	
33	K	131	

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Mol	Chain	Length	Quality of chain
34	L	156	
35	M	130	
36	N	130	
37	O	103	
38	P	129	
39	Q	124	
40	R	118	
41	S	101	
42	T	89	
43	U	82	
44	V	84	
45	W	75	
46	X	92	
47	Y	87	
48	Z	71	
49	a	234	
50	3	1539	
51	1	2903	
52	2	120	
53	5	77	
54	4	27	
55	8	371	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 147733 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	b	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	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	d	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	e	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	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	g	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 7 is a protein called 50S ribosomal protein L13.

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

- Molecule 8 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	k	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 9 is a protein called 50S ribosomal protein L15.

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

- Molecule 10 is a protein called 50S ribosomal protein L16.

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

- Molecule 11 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	n	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 12 is a protein called 50S ribosomal protein L18.

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

- Molecule 13 is a protein called 50S ribosomal protein L19.

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

- Molecule 14 is a protein called 50S ribosomal protein L20.

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

- Molecule 15 is a protein called 50S ribosomal protein L21.

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

- Molecule 16 is a protein called 50S ribosomal protein L22.

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

- Molecule 17 is a protein called 50S ribosomal protein L23.

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

- Molecule 18 is a protein called 50S ribosomal protein L24.

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

- Molecule 19 is a protein called 50S ribosomal protein L25.

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

- Molecule 20 is a protein called 50S ribosomal protein L27.

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

- Molecule 21 is a protein called 50S ribosomal protein L28.

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

- Molecule 22 is a protein called 50S ribosomal protein L29.

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

- Molecule 23 is a protein called 50S ribosomal protein L30.

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

- Molecule 24 is a protein called 50S ribosomal protein L32.

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

- Molecule 25 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	C	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 26 is a protein called 50S ribosomal protein L34.

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

- Molecule 27 is a protein called 50S ribosomal protein L35.

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

- Molecule 28 is a protein called 50S ribosomal protein L36.

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

- Molecule 29 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	G	225	Total	C	N	O	S	0	0
			1756	1111	315	322	8		

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

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

- Molecule 31 is a protein called 30S ribosomal protein S4.

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

- Molecule 32 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	J	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 33 is a protein called 30S ribosomal protein S6.

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

- Molecule 34 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	L	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 35 is a protein called 30S ribosomal protein S8.

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

- Molecule 36 is a protein called 30S ribosomal protein S9.

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

- Molecule 37 is a protein called 30S ribosomal protein S10.

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

- Molecule 38 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	P	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 39 is a protein called 30S ribosomal protein S12.

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

- Molecule 40 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	R	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 41 is a protein called 30S ribosomal protein S14.

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

- Molecule 42 is a protein called 30S ribosomal protein S15.

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

- Molecule 43 is a protein called 30S ribosomal protein S16.

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

- Molecule 44 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	V	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 45 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	W	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 46 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	X	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 47 is a protein called 30S ribosomal protein S20.

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

- Molecule 48 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Z	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 49 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	a	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 50 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 51 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1	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
1	747	C	U	conflict	GB 1036415628

- Molecule 52 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	2	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	120	A	-	expression tag	GB 1370526515

- Molecule 53 is a RNA chain called tRNA^{fMet}.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	5	73	Total	C	N	O	P	0	0
			1556	694	281	509	72		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	20	Total	C	N	O	P	0	0
			437	197	91	130	19		

- Molecule 55 is a protein called Peptide chain release factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	8	361	Total	C	N	O	S	0	0
			2860	1758	503	589	10		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	-5	MET	-	initiating methionine	UNP A0A2S5ZJX2
8	-4	HIS	-	expression tag	UNP A0A2S5ZJX2
8	-3	HIS	-	expression tag	UNP A0A2S5ZJX2
8	-2	HIS	-	expression tag	UNP A0A2S5ZJX2
8	-1	HIS	-	expression tag	UNP A0A2S5ZJX2
8	0	HIS	-	expression tag	UNP A0A2S5ZJX2
8	1	HIS	-	expression tag	UNP A0A2S5ZJX2

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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

Chain b:  98% ..



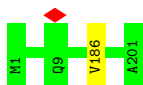
- Molecule 2: 50S ribosomal protein L3

Chain c:  98% .



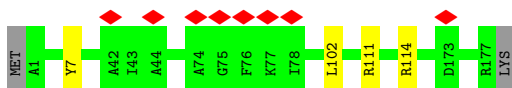
- Molecule 3: 50S ribosomal protein L4

Chain d:  100%



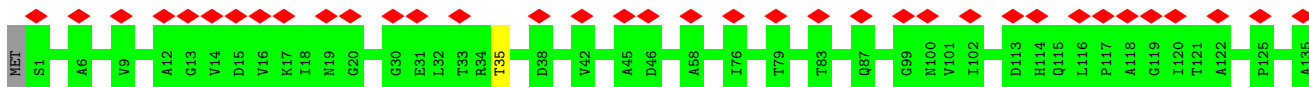
- Molecule 4: 50S ribosomal protein L5

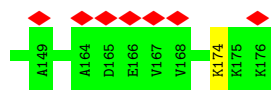
Chain e:  97% ..



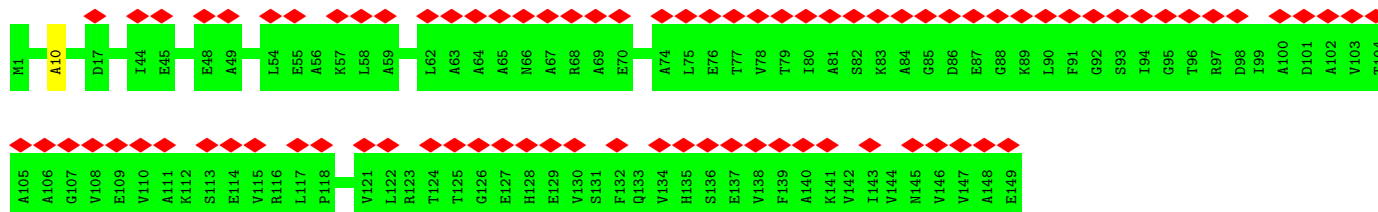
- Molecule 5: 50S ribosomal protein L6

Chain f:  24% 98% ..





- Molecule 6: 50S ribosomal protein L9



- Molecule 7: 50S ribosomal protein L13



There are no outlier residues recorded for this chain.

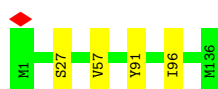
- Molecule 8: 50S ribosomal protein L14



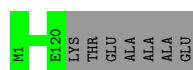
- Molecule 9: 50S ribosomal protein L15



- Molecule 10: 50S ribosomal protein L16



- Molecule 11: 50S ribosomal protein L17



- Molecule 12: 50S ribosomal protein L18

Chain o:  98% ..



- Molecule 13: 50S ribosomal protein L19

Chain p:  98% ..



- Molecule 14: 50S ribosomal protein L20

Chain q:  99% .



- Molecule 15: 50S ribosomal protein L21

Chain r:  100%

There are no outlier residues recorded for this chain.

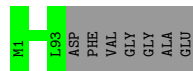
- Molecule 16: 50S ribosomal protein L22

Chain s:  99% .



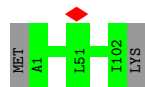
- Molecule 17: 50S ribosomal protein L23

Chain t:  93% 7%



- Molecule 18: 50S ribosomal protein L24

Chain u:  98% .




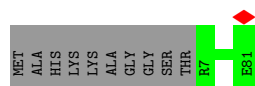
- Molecule 19: 50S ribosomal protein L25

Chain v:  97% .



- Molecule 20: 50S ribosomal protein L27

Chain w:  88% 12%



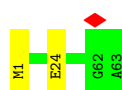
- Molecule 21: 50S ribosomal protein L28

Chain x:  97% ..



- Molecule 22: 50S ribosomal protein L29

Chain y:  97% .



- Molecule 23: 50S ribosomal protein L30

Chain z:  97% ..




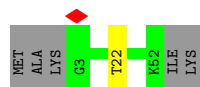
- Molecule 24: 50S ribosomal protein L32

Chain B:  98% .



- Molecule 25: 50S ribosomal protein L33

Chain C:  89% . 9%



- Molecule 26: 50S ribosomal protein L34

Chain D:  100%



- Molecule 27: 50S ribosomal protein L35

Chain E:  95%

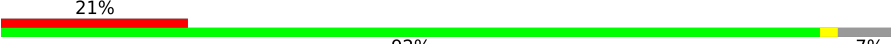


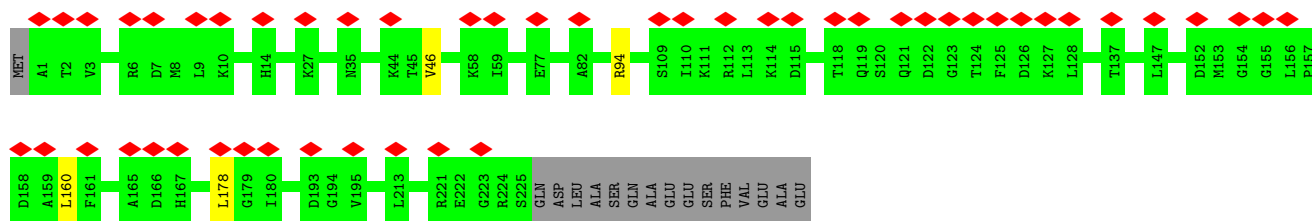
- Molecule 28: 50S ribosomal protein L36

Chain F:  100%


There are no outlier residues recorded for this chain.

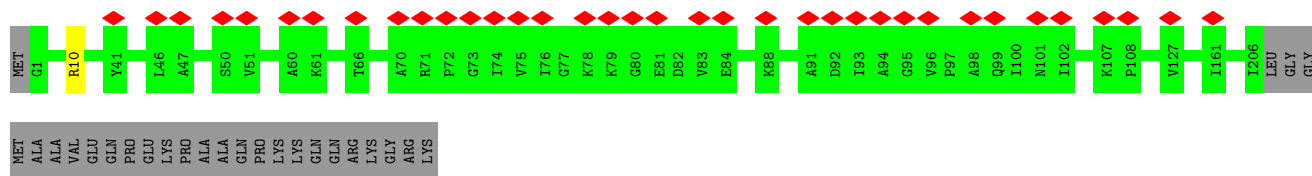
- Molecule 29: 30S ribosomal protein S2

Chain G:  21% 92% 7%



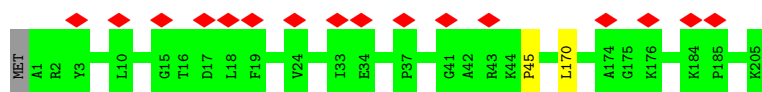
- Molecule 30: 30S ribosomal protein S3

Chain H:  15% 88% 12%




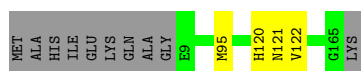
- Molecule 31: 30S ribosomal protein S4

Chain I:  8% 99%

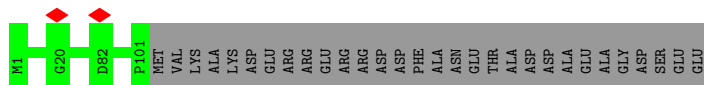
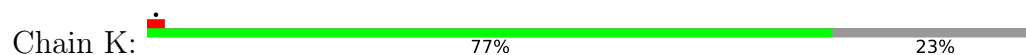


- Molecule 32: 30S ribosomal protein S5

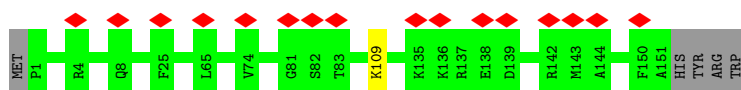
Chain J:  92% 6%



- Molecule 33: 30S ribosomal protein S6



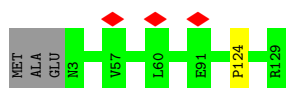
- Molecule 34: 30S ribosomal protein S7



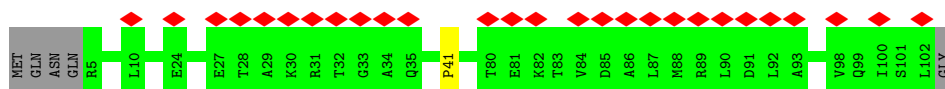
- Molecule 35: 30S ribosomal protein S8



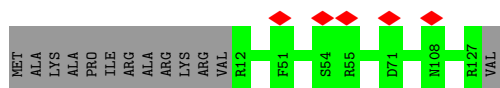
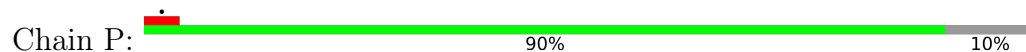
- Molecule 36: 30S ribosomal protein S9



- Molecule 37: 30S ribosomal protein S10

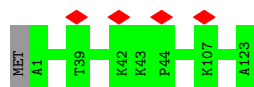


- Molecule 38: 30S ribosomal protein S11



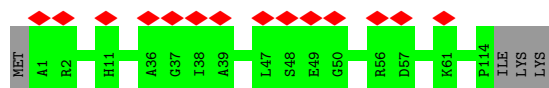
- Molecule 39: 30S ribosomal protein S12

Chain Q:  99%



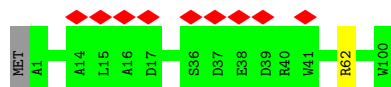
- Molecule 40: 30S ribosomal protein S13

Chain R:  12% 97%



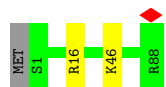
- Molecule 41: 30S ribosomal protein S14

Chain S:  9% 98%



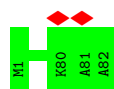
- Molecule 42: 30S ribosomal protein S15

Chain T:  97%



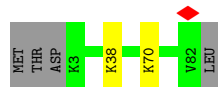
- Molecule 43: 30S ribosomal protein S16

Chain U:  100%




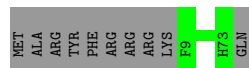
- Molecule 44: 30S ribosomal protein S17

Chain V:  93% 5%

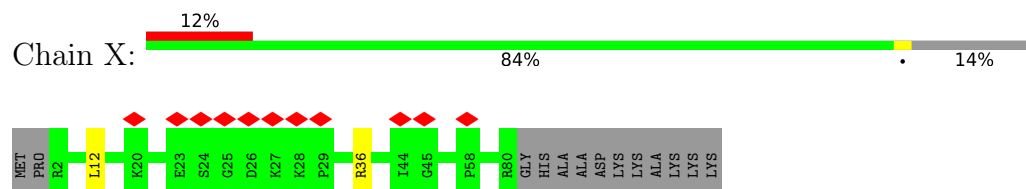


- Molecule 45: 30S ribosomal protein S18

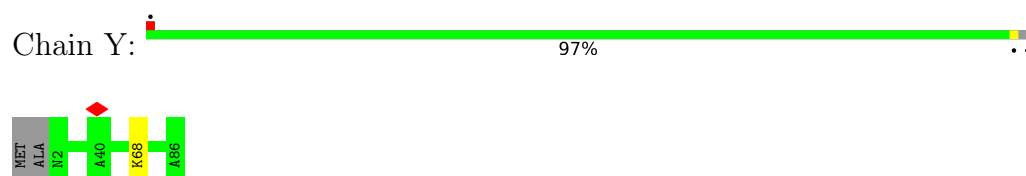
Chain W:  87% 13%



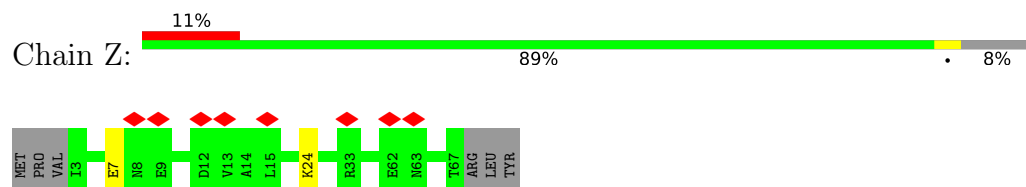
- Molecule 46: 30S ribosomal protein S19



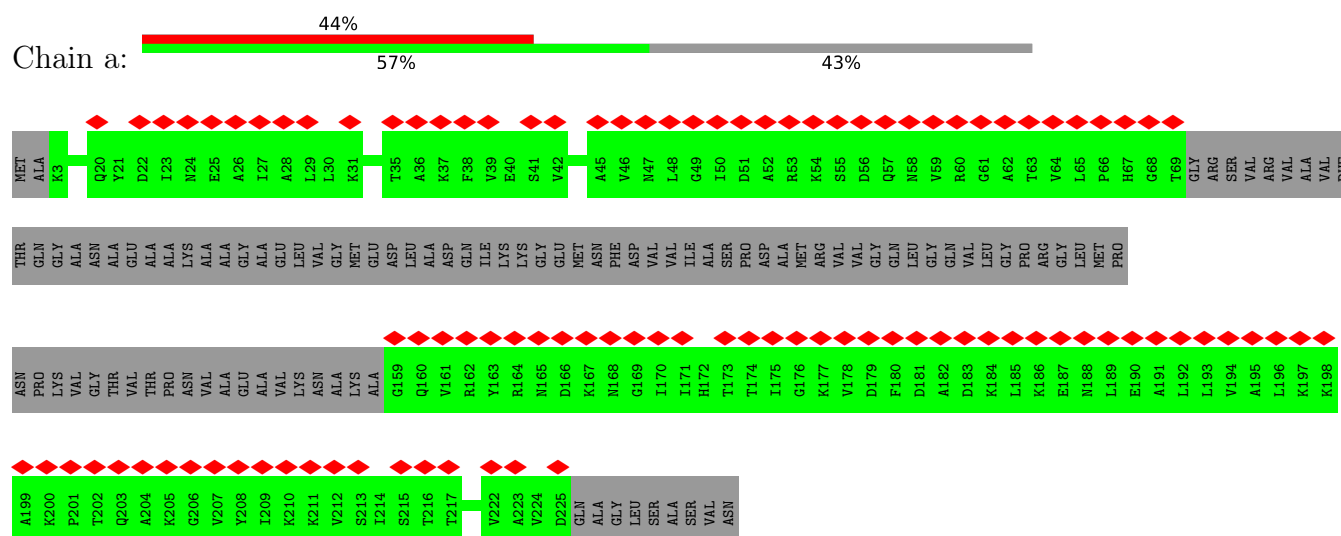
- Molecule 47: 30S ribosomal protein S20



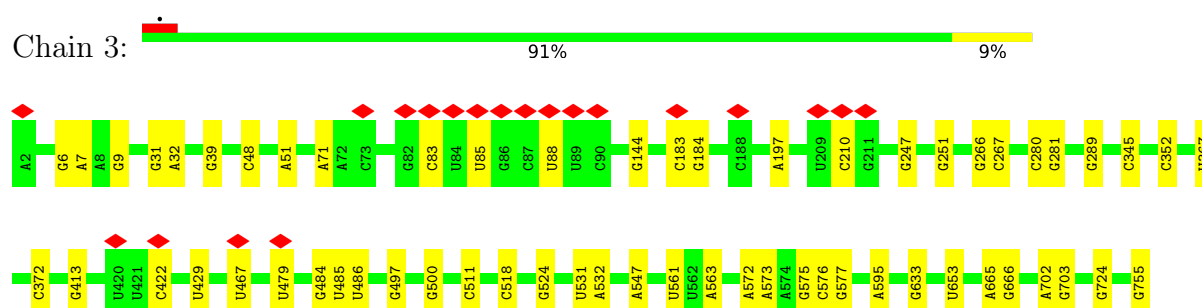
- Molecule 48: 30S ribosomal protein S21

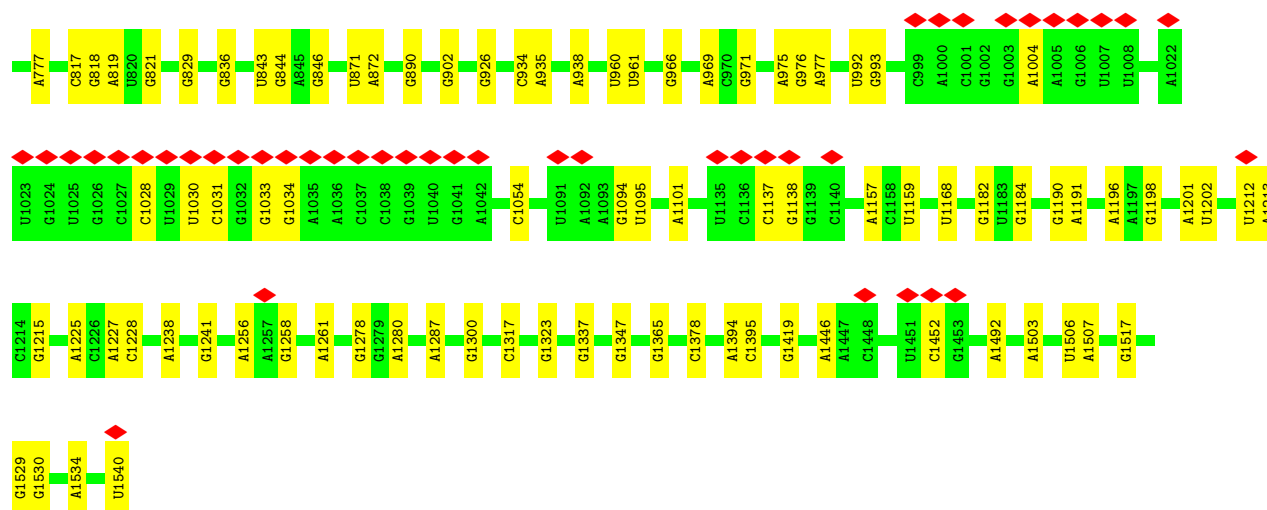


- Molecule 49: 50S ribosomal protein L1

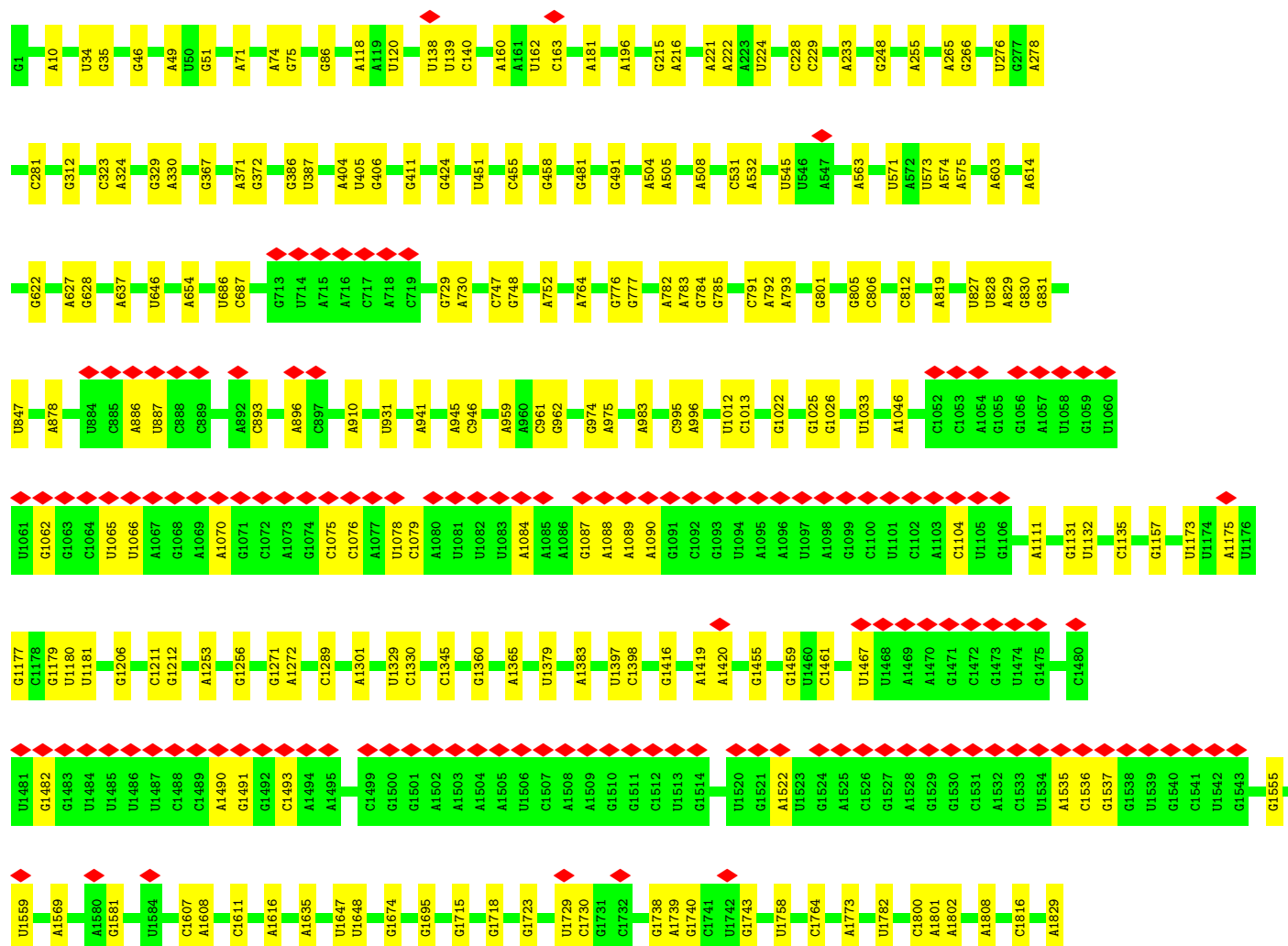
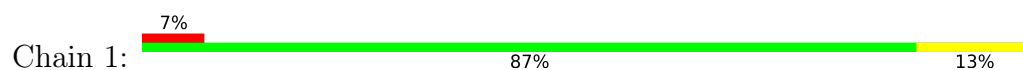


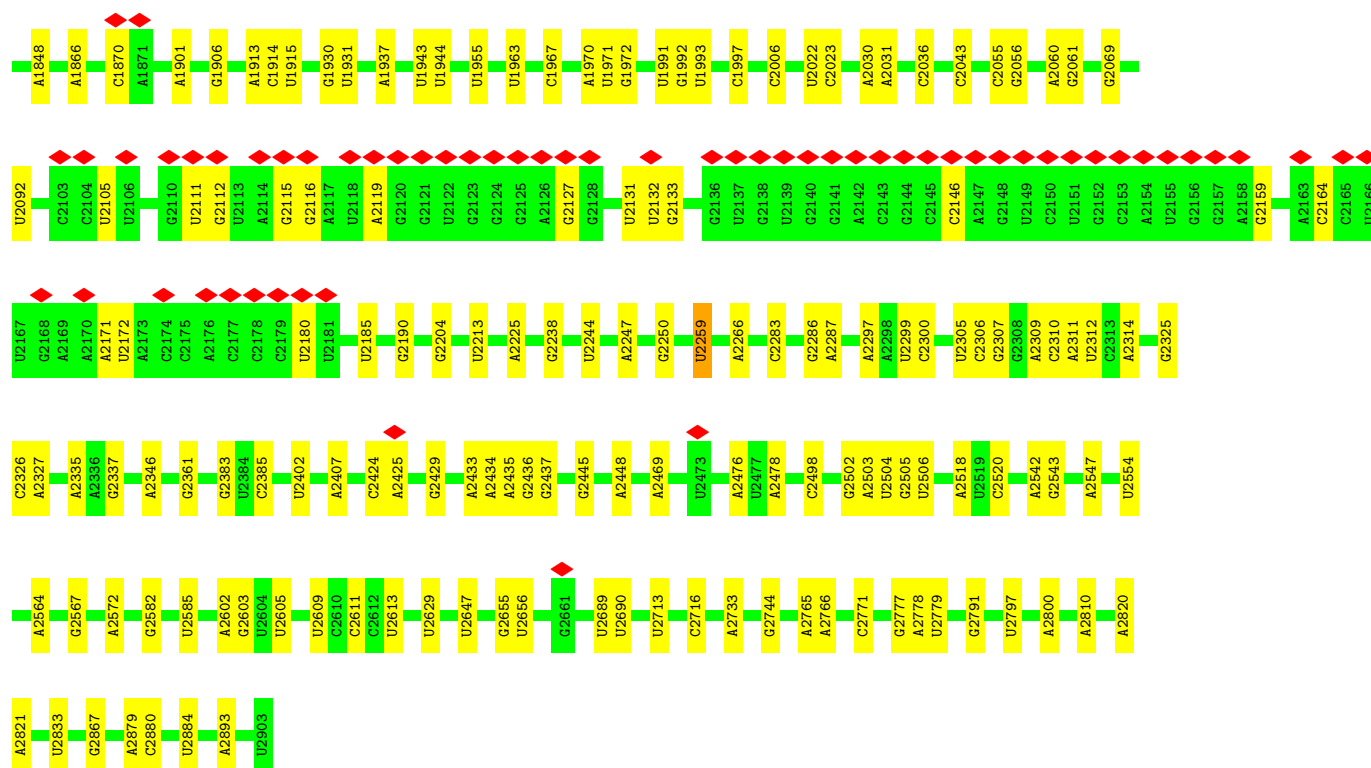
- Molecule 50: 16S ribosomal RNA





• Molecule 51: 23S ribosomal RNA





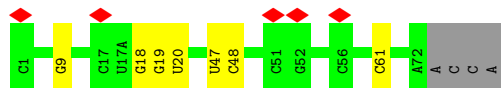
- Molecule 52: 5S ribosomal RNA

Chain 2: 91% 9%



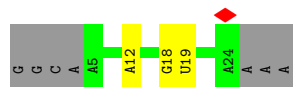
- Molecule 53: tRNAfMet

Chain 5: 6% 86% 9% 5%



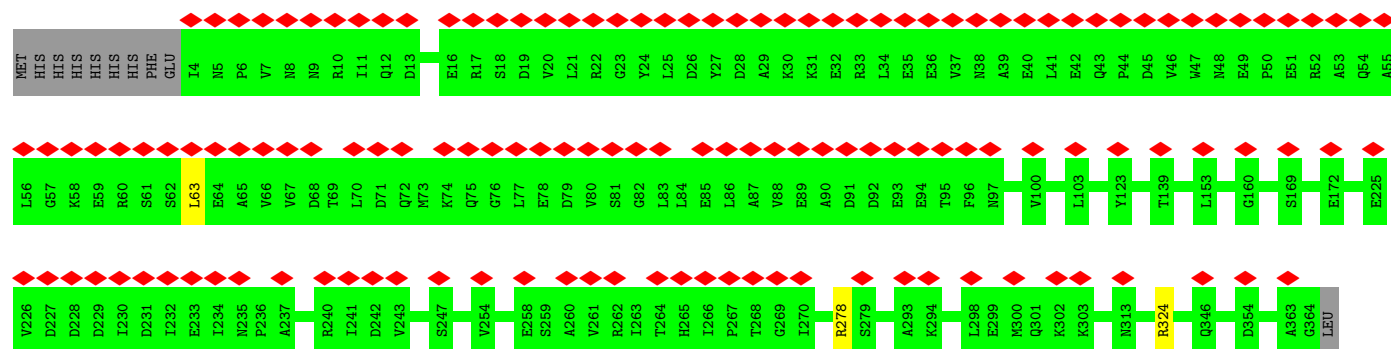
- Molecule 54: mRNA

Chain 4: 63% 11% 26%



- Molecule 55: Peptide chain release factor 2

Chain 8: 37% 96% 2%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	5881	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	29.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.429	Depositor
Minimum map value	-2.704	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.455	Depositor
Recommended contour level	0.9	Depositor
Map size (Å)	416.208, 416.208, 416.208	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.334, 1.334, 1.334	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	b	0.40	0/2121	0.62	0/2852
2	c	0.40	0/1586	0.61	1/2134 (0.0%)
3	d	0.39	0/1571	0.55	0/2113
4	e	0.34	0/1434	0.60	0/1926
5	f	0.34	0/1343	0.61	0/1816
6	g	0.33	0/1122	0.65	0/1515
7	j	0.40	0/1152	0.54	0/1551
8	k	0.42	0/947	0.61	0/1268
9	l	0.37	0/1054	0.60	0/1403
10	m	0.42	1/1093 (0.1%)	0.61	0/1460
11	n	0.37	0/973	0.58	0/1301
12	o	0.33	0/902	0.55	0/1209
13	p	0.41	0/929	0.56	0/1242
14	q	0.39	0/960	0.47	0/1278
15	r	0.40	0/829	0.61	0/1107
16	s	0.35	0/864	0.60	0/1156
17	t	0.39	0/744	0.55	0/994
18	u	0.40	0/787	0.57	0/1051
19	v	0.43	1/766 (0.1%)	0.56	0/1025
20	w	0.37	0/582	0.61	0/769
21	x	0.37	0/635	0.59	1/848 (0.1%)
22	y	0.33	0/510	0.56	0/677
23	z	0.38	0/453	0.56	0/605
24	B	0.38	0/450	0.65	0/599
25	C	0.39	0/416	0.64	0/554
26	D	0.39	0/380	0.54	0/498
27	E	0.38	0/513	0.66	0/676
28	F	0.35	0/303	0.58	0/397
29	G	0.30	0/1787	0.62	1/2408 (0.0%)
30	H	0.31	0/1651	0.56	0/2225
31	I	0.33	0/1665	0.57	1/2227 (0.0%)
32	J	0.31	0/1169	0.60	0/1573
33	K	0.35	0/843	0.59	0/1140
34	L	0.29	0/1195	0.55	0/1602

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	M	0.33	0/989	0.55	0/1326
36	N	0.31	0/1034	0.60	0/1375
37	O	0.32	0/796	0.64	0/1077
38	P	0.30	0/885	0.63	0/1195
39	Q	0.41	0/969	0.69	0/1300
40	R	0.27	0/892	0.57	0/1193
41	S	0.30	0/817	0.55	0/1088
42	T	0.28	0/722	0.59	0/964
43	U	0.32	0/659	0.53	0/884
44	V	0.38	0/657	0.60	0/881
45	W	0.31	0/544	0.56	0/731
46	X	0.33	0/652	0.62	1/877 (0.1%)
47	Y	0.32	0/671	0.52	0/888
48	Z	0.31	0/550	0.67	0/728
49	a	0.29	0/1033	0.55	0/1387
50	3	0.25	0/36963	0.63	0/57662
51	1	0.24	0/69796	0.63	1/108888 (0.0%)
52	2	0.25	0/2872	0.63	0/4479
53	5	0.25	0/1738	0.64	0/2709
54	4	0.22	0/493	0.61	0/769
55	8	0.35	0/2900	0.64	1/3908 (0.0%)
All	All	0.28	2/160361 (0.0%)	0.62	7/239508 (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
5	f	0	1
6	g	0	1
10	m	0	2
13	p	0	1
27	E	0	1
32	J	0	1
44	V	0	1
48	Z	0	1
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	m	96	ILE	C-N	-6.28	1.19	1.34
19	v	25	LYS	C-N	-5.12	1.22	1.34

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	8	63	LEU	CA-CB-CG	6.76	130.85	115.30
46	X	12	LEU	CA-CB-CG	6.33	129.85	115.30
29	G	178	LEU	CA-CB-CG	6.20	129.56	115.30
21	x	21	LEU	CA-CB-CG	6.10	129.33	115.30
31	I	170	LEU	CA-CB-CG	5.30	127.48	115.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	f	174	LYS	Peptide
6	g	10	ALA	Peptide
10	m	27	SER	Peptide
10	m	57	VAL	Peptide
13	p	15	ASP	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	269/273 (98%)	239 (89%)	30 (11%)	0	100	100
2	c	207/209 (99%)	187 (90%)	20 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	d	199/201 (99%)	183 (92%)	16 (8%)	0	100	100
4	e	175/179 (98%)	152 (87%)	22 (13%)	1 (1%)	25	64
5	f	174/177 (98%)	154 (88%)	20 (12%)	0	100	100
6	g	147/149 (99%)	123 (84%)	24 (16%)	0	100	100
7	j	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
8	k	120/123 (98%)	108 (90%)	12 (10%)	0	100	100
9	l	141/144 (98%)	131 (93%)	10 (7%)	0	100	100
10	m	134/136 (98%)	116 (87%)	18 (13%)	0	100	100
11	n	118/127 (93%)	104 (88%)	14 (12%)	0	100	100
12	o	114/117 (97%)	104 (91%)	10 (9%)	0	100	100
13	p	112/115 (97%)	99 (88%)	13 (12%)	0	100	100
14	q	115/118 (98%)	112 (97%)	3 (3%)	0	100	100
15	r	101/103 (98%)	90 (89%)	11 (11%)	0	100	100
16	s	108/110 (98%)	98 (91%)	10 (9%)	0	100	100
17	t	91/100 (91%)	85 (93%)	6 (7%)	0	100	100
18	u	100/104 (96%)	89 (89%)	11 (11%)	0	100	100
19	v	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
20	w	73/85 (86%)	63 (86%)	10 (14%)	0	100	100
21	x	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
22	y	61/63 (97%)	59 (97%)	1 (2%)	1 (2%)	9	45
23	z	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
24	B	54/57 (95%)	46 (85%)	8 (15%)	0	100	100
25	C	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
26	D	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
27	E	62/65 (95%)	52 (84%)	9 (14%)	1 (2%)	9	45
28	F	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
29	G	223/241 (92%)	210 (94%)	13 (6%)	0	100	100
30	H	204/233 (88%)	186 (91%)	18 (9%)	0	100	100
31	I	203/206 (98%)	181 (89%)	21 (10%)	1 (0%)	29	68
32	J	155/167 (93%)	137 (88%)	16 (10%)	2 (1%)	12	48
33	K	99/131 (76%)	83 (84%)	16 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	L	149/156 (96%)	135 (91%)	14 (9%)	0	100	100
35	M	127/130 (98%)	117 (92%)	10 (8%)	0	100	100
36	N	125/130 (96%)	102 (82%)	22 (18%)	1 (1%)	19	60
37	O	96/103 (93%)	83 (86%)	12 (12%)	1 (1%)	15	54
38	P	114/129 (88%)	93 (82%)	21 (18%)	0	100	100
39	Q	121/124 (98%)	93 (77%)	28 (23%)	0	100	100
40	R	112/118 (95%)	99 (88%)	13 (12%)	0	100	100
41	S	98/101 (97%)	84 (86%)	14 (14%)	0	100	100
42	T	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	13	50
43	U	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
44	V	78/84 (93%)	64 (82%)	14 (18%)	0	100	100
45	W	63/75 (84%)	55 (87%)	8 (13%)	0	100	100
46	X	77/92 (84%)	71 (92%)	6 (8%)	0	100	100
47	Y	83/87 (95%)	80 (96%)	3 (4%)	0	100	100
48	Z	63/71 (89%)	43 (68%)	20 (32%)	0	100	100
49	a	130/234 (56%)	114 (88%)	16 (12%)	0	100	100
55	8	359/371 (97%)	328 (91%)	31 (9%)	0	100	100
All	All	6011/6421 (94%)	5366 (89%)	636 (11%)	9 (0%)	54	85

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	y	24	GLU
32	J	121	ASN
32	J	122	VAL
42	T	46	LYS
4	e	111	ARG

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	b	216/218 (99%)	212 (98%)	4 (2%)	57	74
2	c	164/164 (100%)	161 (98%)	3 (2%)	59	76
3	d	165/165 (100%)	164 (99%)	1 (1%)	86	92
4	e	148/150 (99%)	145 (98%)	3 (2%)	55	73
5	f	137/138 (99%)	136 (99%)	1 (1%)	84	90
6	g	114/114 (100%)	114 (100%)	0	100	100
7	j	116/116 (100%)	116 (100%)	0	100	100
8	k	103/104 (99%)	102 (99%)	1 (1%)	76	86
9	l	102/103 (99%)	102 (100%)	0	100	100
10	m	109/109 (100%)	108 (99%)	1 (1%)	78	87
11	n	100/104 (96%)	100 (100%)	0	100	100
12	o	86/87 (99%)	85 (99%)	1 (1%)	71	83
13	p	99/100 (99%)	99 (100%)	0	100	100
14	q	89/90 (99%)	89 (100%)	0	100	100
15	r	84/84 (100%)	84 (100%)	0	100	100
16	s	93/93 (100%)	92 (99%)	1 (1%)	73	84
17	t	80/84 (95%)	80 (100%)	0	100	100
18	u	83/85 (98%)	83 (100%)	0	100	100
19	v	78/78 (100%)	76 (97%)	2 (3%)	46	67
20	w	57/63 (90%)	57 (100%)	0	100	100
21	x	67/68 (98%)	67 (100%)	0	100	100
22	y	55/55 (100%)	54 (98%)	1 (2%)	59	76
23	z	48/49 (98%)	47 (98%)	1 (2%)	53	71
24	B	47/48 (98%)	47 (100%)	0	100	100
25	C	45/49 (92%)	44 (98%)	1 (2%)	52	70
26	D	38/38 (100%)	38 (100%)	0	100	100
27	E	51/52 (98%)	51 (100%)	0	100	100
28	F	34/34 (100%)	34 (100%)	0	100	100
29	G	186/199 (94%)	183 (98%)	3 (2%)	62	79
30	H	170/190 (90%)	169 (99%)	1 (1%)	86	92
31	I	172/173 (99%)	172 (100%)	0	100	100
32	J	119/126 (94%)	118 (99%)	1 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	K	88/112 (79%)	88 (100%)	0	100	100
34	L	124/129 (96%)	123 (99%)	1 (1%)	81	89
35	M	104/105 (99%)	103 (99%)	1 (1%)	76	86
36	N	105/107 (98%)	105 (100%)	0	100	100
37	O	86/90 (96%)	86 (100%)	0	100	100
38	P	89/99 (90%)	89 (100%)	0	100	100
39	Q	103/104 (99%)	103 (100%)	0	100	100
40	R	92/96 (96%)	92 (100%)	0	100	100
41	S	83/84 (99%)	82 (99%)	1 (1%)	71	83
42	T	76/77 (99%)	75 (99%)	1 (1%)	69	82
43	U	65/65 (100%)	65 (100%)	0	100	100
44	V	74/78 (95%)	73 (99%)	1 (1%)	67	80
45	W	56/65 (86%)	56 (100%)	0	100	100
46	X	70/79 (89%)	69 (99%)	1 (1%)	67	80
47	Y	65/66 (98%)	64 (98%)	1 (2%)	65	80
48	Z	55/61 (90%)	54 (98%)	1 (2%)	59	76
49	a	110/181 (61%)	110 (100%)	0	100	100
55	8	307/317 (97%)	305 (99%)	2 (1%)	84	90
All	All	5007/5245 (96%)	4971 (99%)	36 (1%)	84	90

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	S	62	ARG
55	8	324	ARG
42	T	16	ARG
47	Y	68	LYS
8	k	31	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
32	J	145	ASN
39	Q	95	HIS
33	K	46	GLN

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Mol	Chain	Res	Type
36	N	74	GLN
42	T	41	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
50	3	1538/1539 (99%)	145 (9%)	2 (0%)
51	1	2902/2903 (99%)	365 (12%)	6 (0%)
52	2	119/120 (99%)	11 (9%)	1 (0%)
53	5	72/77 (93%)	7 (9%)	0
54	4	19/27 (70%)	3 (15%)	0
All	All	4650/4666 (99%)	531 (11%)	9 (0%)

5 of 531 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
50	3	6	G
50	3	7	A
50	3	9	G
50	3	31	G
50	3	32	A

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
51	1	2436	G
52	2	88	C
51	1	1738	G
51	1	2286	G
51	1	2299	U

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	m	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	m	96:ILE	C	97:GLN	N	1.19

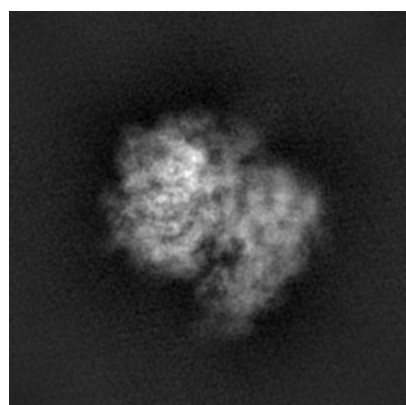
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20057. These allow visual inspection of the internal detail of the map and identification of artifacts.

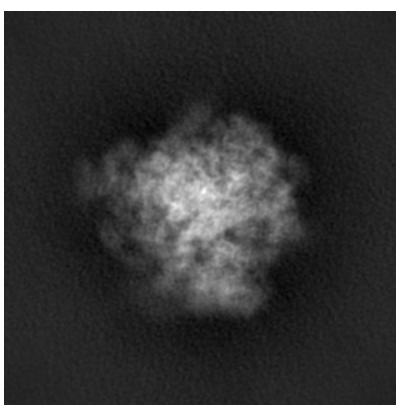
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

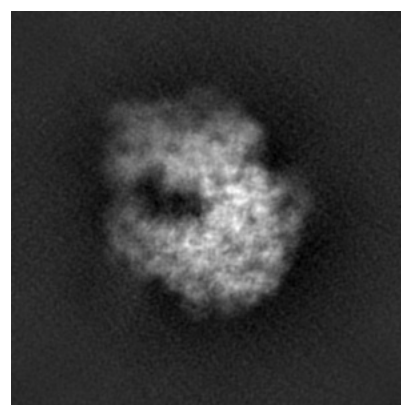
6.1.1 Primary map



X



Y

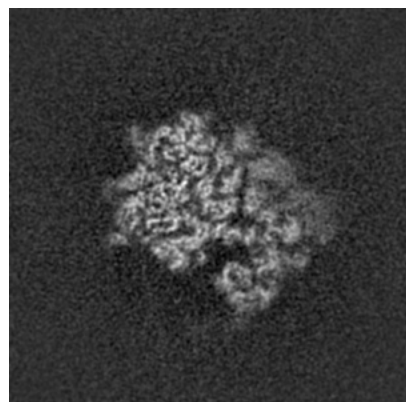


Z

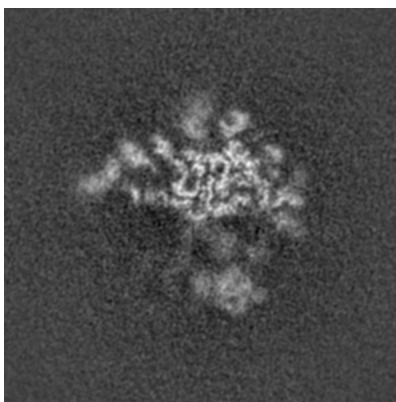
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

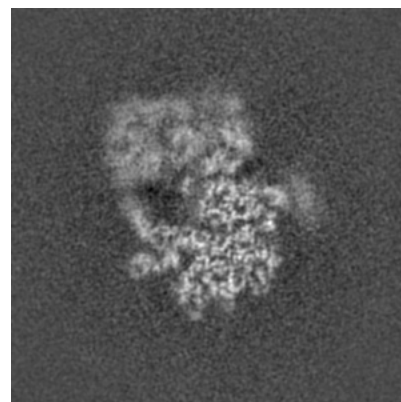
6.2.1 Primary map



X Index: 156



Y Index: 156

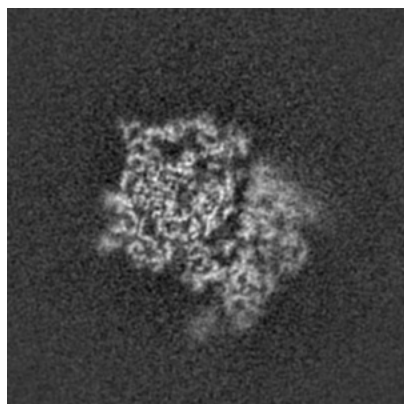


Z Index: 156

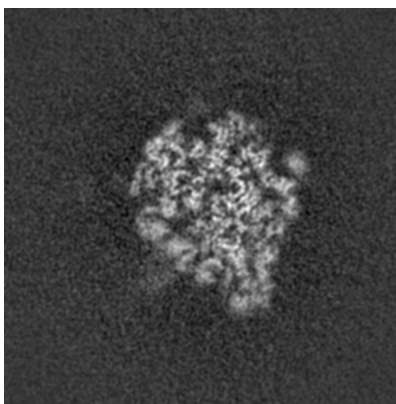
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

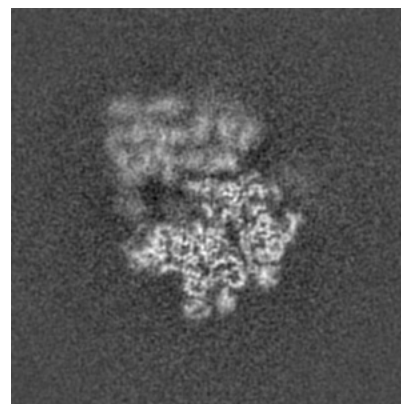
6.3.1 Primary map



X Index: 167



Y Index: 138



Z Index: 164

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

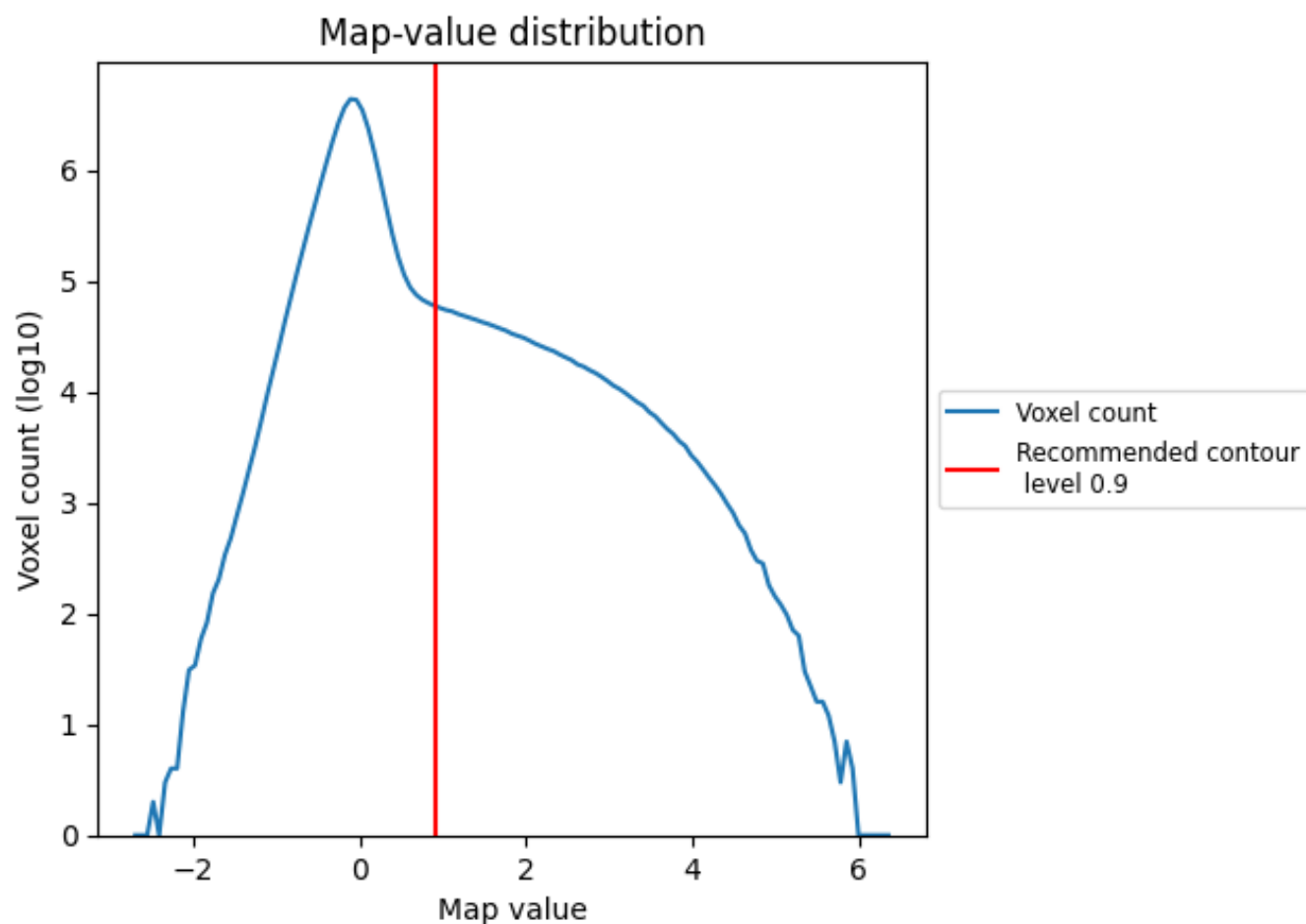
6.5 Mask visualisation

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

7 Map analysis [i](#)

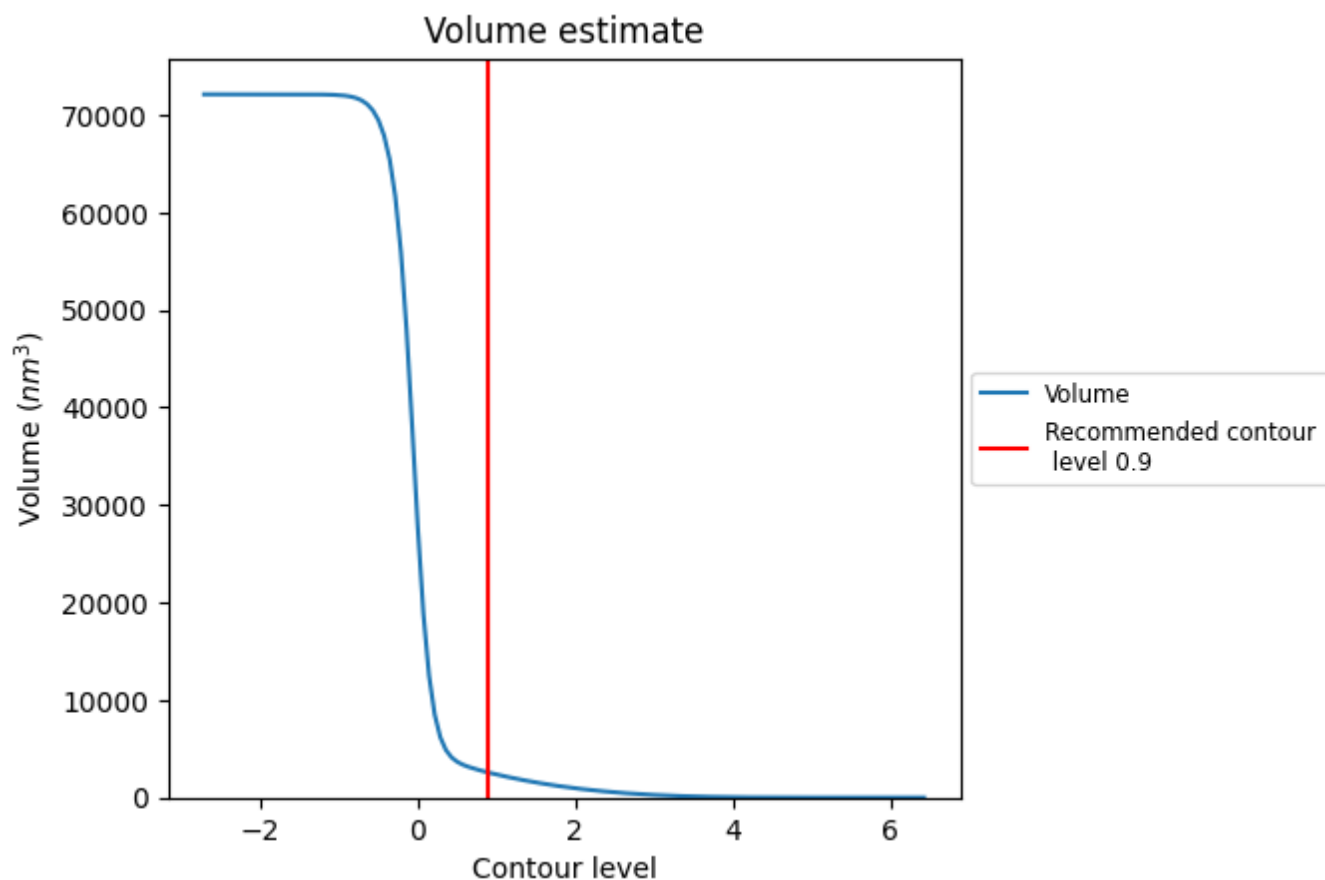
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

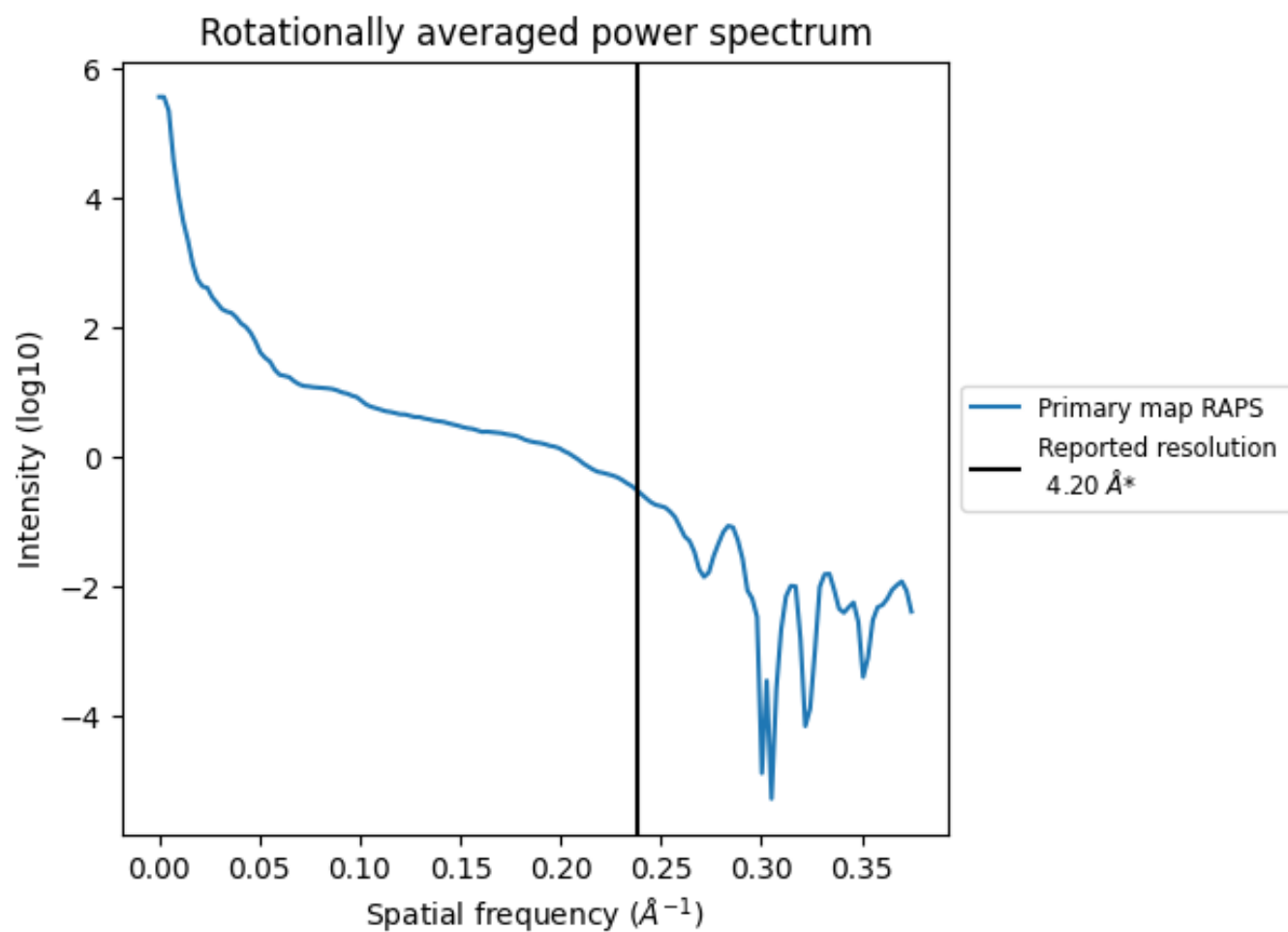
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2573 nm³; this corresponds to an approximate mass of 2324 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

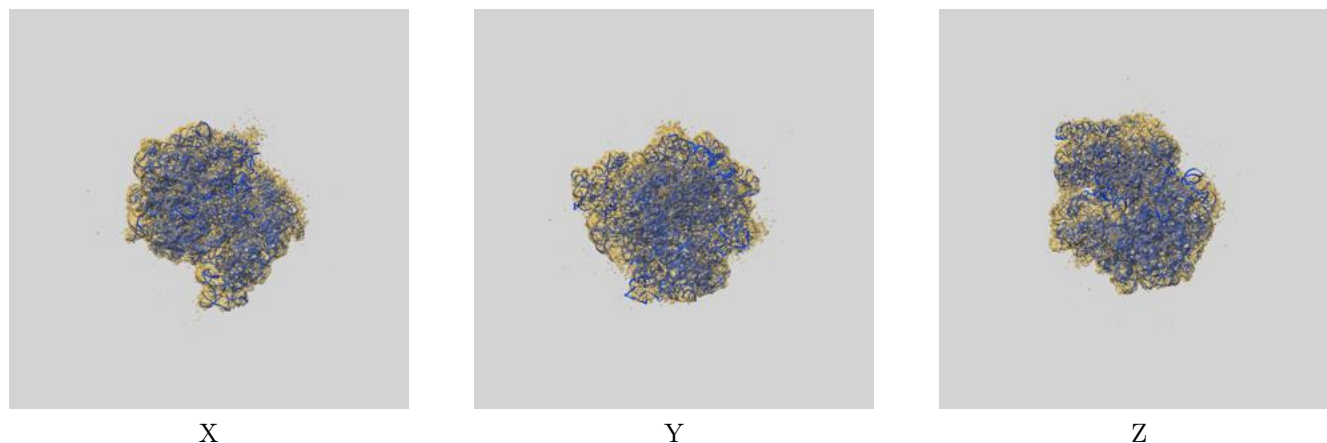
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

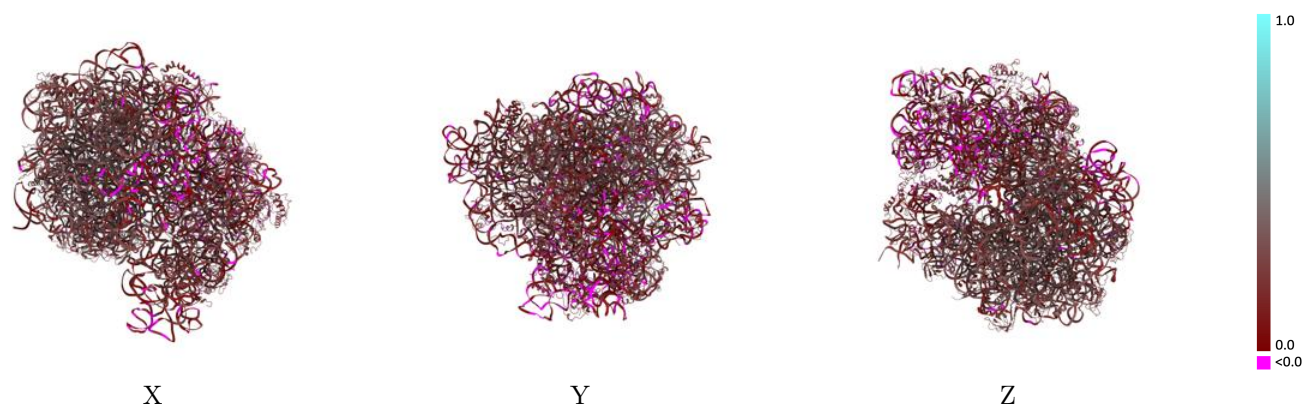
This section contains information regarding the fit between EMDB map EMD-20057 and PDB model 6OGG. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



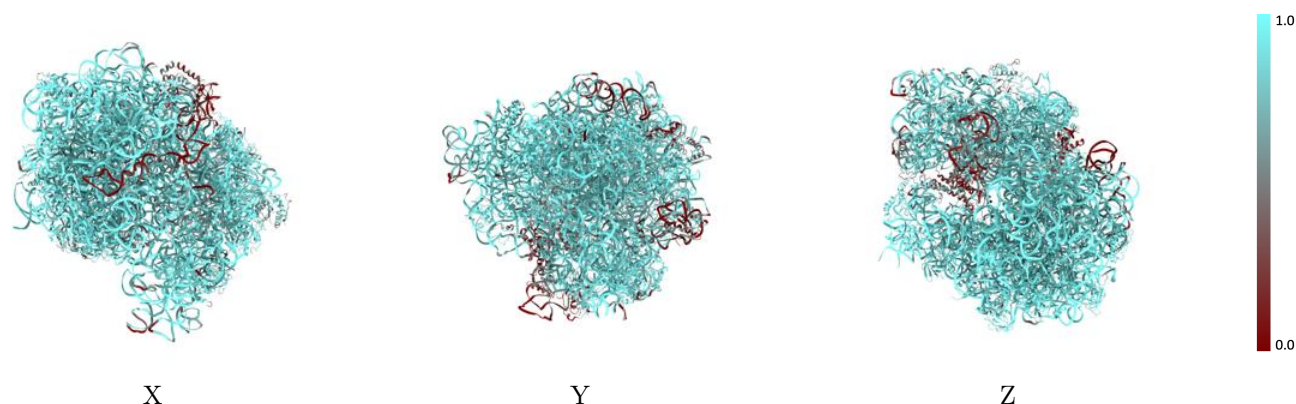
The images above show the 3D surface view of the map at the recommended contour level 0.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



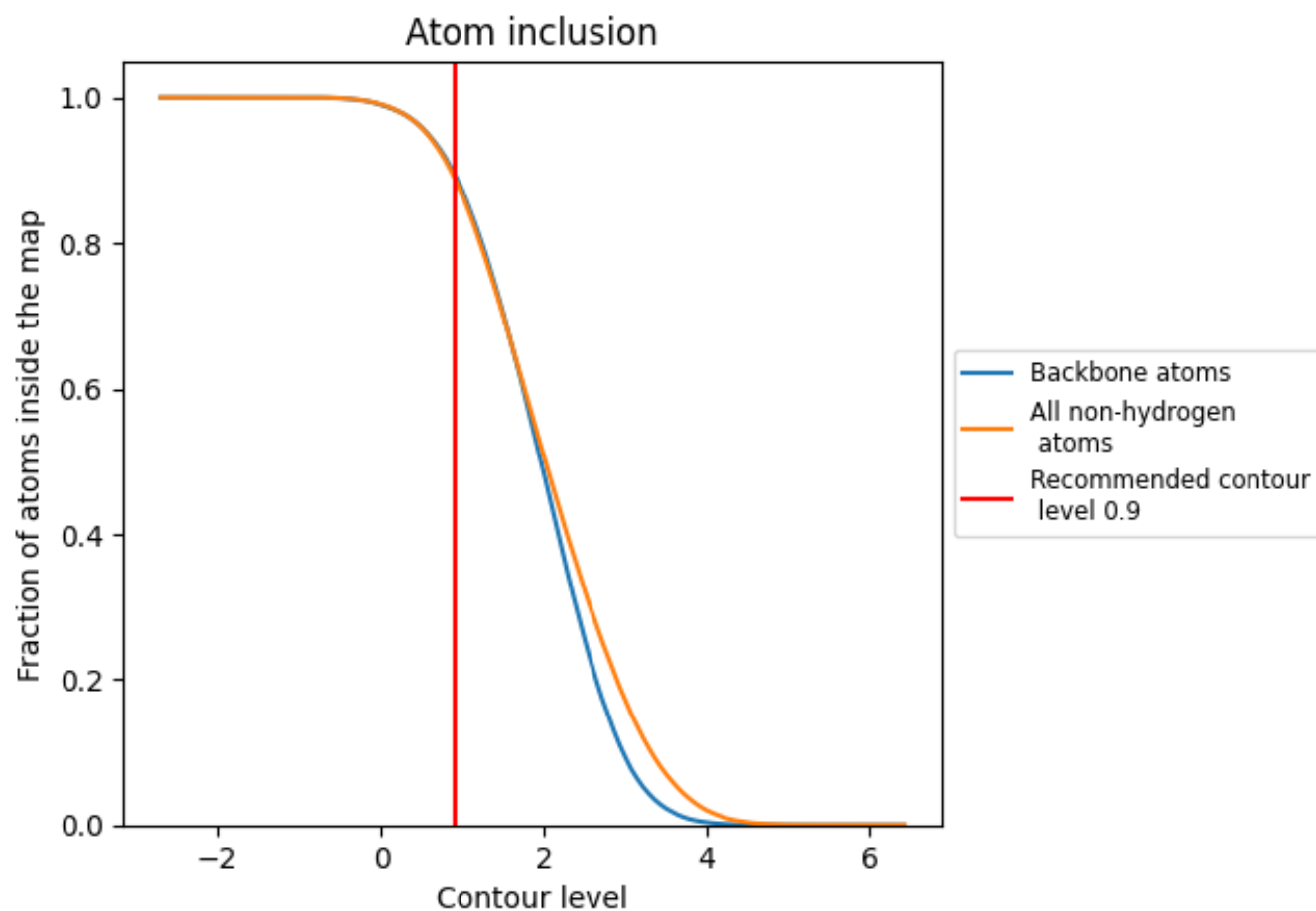
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.9).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ











































The table lists the average atom inclusion at the recommended contour level (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8906	 0.2240
1	 0.9075	 0.2460
2	 0.9724	 0.2100
3	 0.9148	 0.1580
4	 0.8924	 0.0830
5	 0.7783	 0.0890
8	 0.5659	 0.1900
B	 0.9696	 0.3210
C	 0.8603	 0.2750
D	 0.9465	 0.3110
E	 0.9633	 0.3070
F	 0.9384	 0.1780
G	 0.6852	 0.2020
H	 0.7364	 0.1980
I	 0.8403	 0.2070
J	 0.9480	 0.2500
K	 0.9502	 0.1840
L	 0.7762	 0.1760
M	 0.9490	 0.2290
N	 0.9009	 0.1530
O	 0.6478	 0.1950
P	 0.9053	 0.1660
Q	 0.8893	 0.2380
R	 0.8143	 0.1920
S	 0.8501	 0.1540
T	 0.9420	 0.2000
U	 0.9506	 0.2700
V	 0.9794	 0.2460
W	 0.9747	 0.1860
X	 0.8277	 0.1600
Y	 0.9292	 0.2280
Z	 0.7621	 0.2340
a	 0.2299	 0.2050
b	 0.9688	 0.2920
c	 0.9720	 0.3200



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Chain	Atom inclusion	Q-score
d	 0.9257	 0.3050
e	 0.8922	 0.2010
f	 0.6369	 0.2340
g	 0.4015	 0.2340
j	 0.9709	 0.3010
k	 0.9518	 0.3240
l	 0.9636	 0.3080
m	 0.9549	 0.3070
n	 0.9707	 0.3070
o	 0.9745	 0.2480
p	 0.9662	 0.3250
q	 0.9548	 0.2920
r	 0.9511	 0.3100
s	 0.9581	 0.3230
t	 0.9363	 0.2830
u	 0.9426	 0.2850
v	 0.9661	 0.2750
w	 0.9696	 0.3240
x	 0.9434	 0.2910
y	 0.9477	 0.2760
z	 0.9703	 0.3110