



wwPDB EM Validation Summary Report ⓘ

Jul 13, 2026 – 05:01 pm BST

PDB ID : 9RVC / pdb_00009rvc
EMDB ID : EMD-54286
Title : staphylococcus aureus 70S initiation complex with natural mRNA
Authors : Bahena, R.; Klaholz, B.; Marzi, S.
Deposited on : 2025-07-07
Resolution : 2.90 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.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

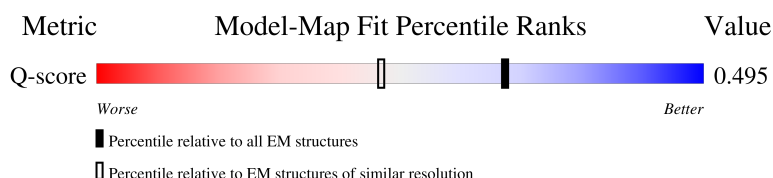
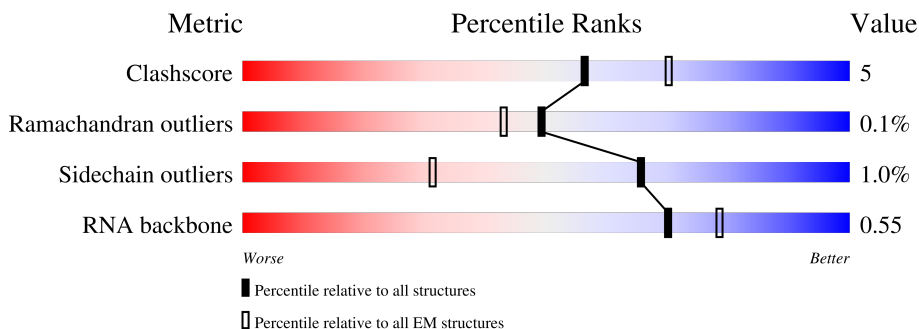
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	0	49	 90% 10%
2	1	45	 96%
3	2	66	 82% 17%

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Mol	Chain	Length	Quality of chain
4	3	37	
5	4	84	
6	A	1553	
7	B	255	
8	C	217	
9	D	200	
10	E	166	
11	F	98	
12	G	156	
13	H	132	
14	I	132	
15	J	145	
16	K	129	
17	L	137	
18	M	121	
19	N	61	
20	O	89	
21	P	91	
22	Q	87	
23	R	80	
24	S	92	
25	T	83	
26	U	122	
27	X	23	
28	Y	76	

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Mol	Chain	Length	Quality of chain
29	Z	76	
30	a	2914	
31	b	114	
32	c	277	
33	d	220	
34	e	207	
35	f	179	
36	g	178	
37	j	102	
38	k	146	
39	l	144	
40	m	122	
41	n	119	
42	o	116	
43	p	118	
44	q	102	
45	r	117	
46	s	91	
47	t	105	
48	u	217	
49	v	94	
50	w	62	
51	x	69	
52	y	59	
53	z	58	

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 240710 atoms, of which 96041 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 Large ribosomal subunit protein bL33B.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	49	Total	C	H	N	O	S	0	0
			822	243	416	82	76	5		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1	44	Total	C	H	N	O	S	0	0
			793	228	420	90	54	1		

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	2	65	Total	C	H	N	O	S	0	0
			1130	330	600	115	83	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	3	37	Total	C	H	N	O	S	0	0
			638	186	342	60	45	5		

- Molecule 5 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	4	80	Total	C	H	N	O	S	0	0
			1282	417	630	109	123	3		

- Molecule 6 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	A	1547	Total	C	H	N	O	P	0	0
			49804	14790	16678	6036	10753	1547		

- Molecule 7 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	B	226	Total	C	H	N	O	S	0	0
			3698	1158	1881	317	335	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	206	ILE	ALA	conflict	UNP Q2FZ25
B	207	ALA	ILE	conflict	UNP Q2FZ25

- Molecule 8 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	C	203	Total	C	H	N	O	S	0	0
			3262	1007	1662	301	290	2		

- Molecule 9 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	D	198	Total	C	H	N	O	S	0	0
			3244	1014	1636	301	291	2		

- Molecule 10 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	E	157	Total	C	H	N	O	S	0	0
			2397	735	1229	214	217	2		

- Molecule 11 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	F	95	Total	C	H	N	O	S	0	0
			1577	498	788	138	150	3		

- Molecule 12 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	G	153	Total	C	H	N	O	S	0	0
			2478	759	1257	236	222	4		

- Molecule 13 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	H	131	Total	C	H	N	O	S	0	0
			2114	652	1083	183	192	4		

- Molecule 14 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	I	127	Total	C	H	N	O	S	0	0
			2034	623	1026	201	183	1		

- Molecule 15 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	J	145	Total	C	H	N	O	S	0	0
			2295	717	1145	211	219	3		

- Molecule 16 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	K	117	Total	C	H	N	O	S	0	0
			1753	537	886	163	164	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	117	LYS	ARG	conflict	UNP Q2FW31

- Molecule 17 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	L	135	Total	C	H	N	O	S	0	0
			2192	658	1130	218	184	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	55	ARG	LYS	conflict	UNP P0A0H0
L	100	ARG	LYS	conflict	UNP P0A0H0

- Molecule 18 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	M	118	Total	C	H	N	O	S	0	0
			1925	575	989	186	174	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS14B.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	N	60	Total	C	H	N	O	S	0	0
			1029	317	528	100	79	5		

- Molecule 20 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	O	88	Total	C	H	N	O	S	0	0
			1507	454	770	153	129	1		

- Molecule 21 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	P	87	Total	C	H	N	O	S	0	0
			1402	433	714	127	127	1		

- Molecule 22 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	Q	83	Total	C	H	N	O	S	0	0
			1406	432	722	123	128	1		

- Molecule 23 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	R	66	Total	C	H	N	O	S	0	0
			1123	347	580	101	92	3		

- Molecule 24 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	S	84	Total	C	H	N	O	S	0	0
			1360	435	683	123	117	2		

- Molecule 25 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	T	82	Total	C	H	N	O	S	0	0
			1286	375	668	121	120	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	80	SER	ASN	conflict	UNP Q2FXY6

- Molecule 26 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	U	122	Total	C	H	N	O	S	0	0
			1900	572	981	174	169	4		

- Molecule 27 is a RNA chain called spa mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	X	23	Total	C	H	N	O	P	0	0
			742	221	246	89	163	23		

- Molecule 28 is a RNA chain called A-site tRNA-Lys.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	Y	76	Total	C	H	N	O	P	0	0
			2431	721	817	282	535	76		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
29	Z	76	Total	C	H	N	O	P	0	0
			2448	723	825	294	530	76		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
30	a	2914	Total	C	H	N	O	P	0	0
			93870	27893	31391	11427	20245	2914		

- Molecule 31 is a RNA chain called 5S.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	b	114	Total	C	H	N	O	P	0	0
			3659	1086	1229	436	794	114		

- Molecule 32 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	c	273	Total	C	H	N	O	S	0	0
			4278	1297	2193	413	370	5		

- Molecule 33 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	d	215	Total	C	H	N	O	S	0	0
			3298	1018	1670	299	306	5		

- Molecule 34 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	e	206	Total	C	H	N	O	S	0	0
			3193	986	1620	288	297	2		

- Molecule 35 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	f	179	Total	C	H	N	O	S	0	0
			2902	902	1482	245	265	8		

- Molecule 36 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	g	175	Total	C	H	N	O	S	0	0
			2768	850	1400	250	265	3		

- Molecule 37 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	j	98	Total	C	H	N	O	S	0	0
			1608	494	825	143	145	1		

- Molecule 38 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	k	146	Total	C	H	N	O	S	0	0
			2240	680	1142	215	202	1		

- Molecule 39 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	l	138	Total	C	H	N	O	S	0	0
			2270	706	1169	208	183	4		

- Molecule 40 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	m	119	Total	C	H	N	O	S	0	0
			1930	575	991	181	182	1		

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	n	118	Total	C	H	N	O	S	0	0
			1867	564	960	173	169	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	62	ILE	ASP	conflict	UNP Q2FW22
n	63	ALA	ILE	conflict	UNP Q2FW22

- Molecule 42 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	o	109	Total	C	H	N	O		0	0
			1822	552	945	176	149			

- Molecule 43 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	p	115	Total	C	H	N	O	S	0	0
			1942	588	1006	188	156	4		

- Molecule 44 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	q	102	Total	C	H	N	O	S	0	0
			1634	506	836	142	149	1		

- Molecule 45 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	r	112	Total	C	H	N	O	S	0	0
			1782	537	920	164	158	3		

- Molecule 46 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	s	89	Total	C	H	N	O	S	0	0
			1486	457	761	130	134	4		

- Molecule 47 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	t	90	Total	C	H	N	O	S	0	0
			1439	434	750	129	125	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
t	53	ALA	GLU	conflict	UNP Q2FW17
t	54	GLN	GLY	conflict	UNP Q2FW17

- Molecule 48 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	u	93	Total	C	H	N	O	S	0	0
			1509	466	779	130	133	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	161	SER	GLY	conflict	UNP Q2G0S0

- Molecule 49 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	v	81	Total	C	H	N	O	0	0
			1262	383	641	121	117		

- Molecule 50 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	w	61	Total	C	H	N	O	S	0	0
			1005	298	524	104	78	1		

- Molecule 51 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	65	Total	C	H	N	O	0	0
			1104	330	568	101	105		

- Molecule 52 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	y	56	Total	C	H	N	O	0	0
			909	271	473	82	83		

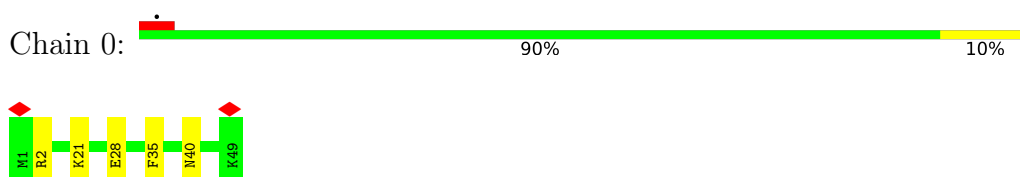
- Molecule 53 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace	
53	z	54	Total	C	H	N	O	S	0	0
			861	259	434	87	76	5		

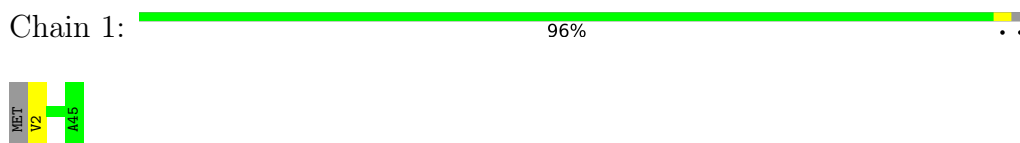
3 Residue-property plots [i](#)

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.

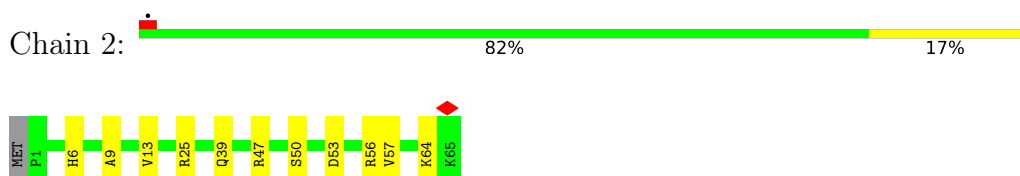
- Molecule 1: Large ribosomal subunit protein bL33B



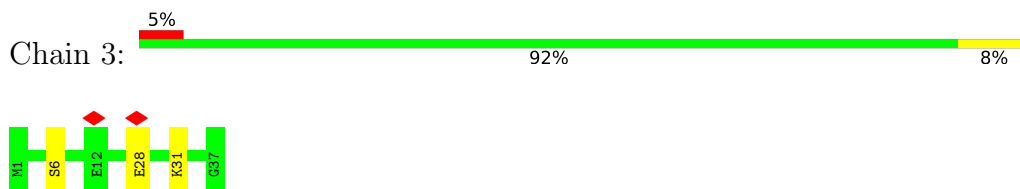
- Molecule 2: Large ribosomal subunit protein bL34



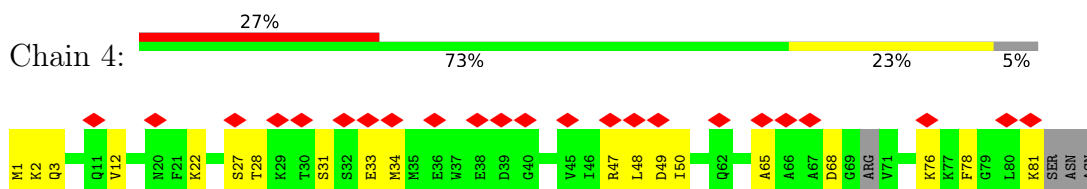
- Molecule 3: Large ribosomal subunit protein bL35



- Molecule 4: Large ribosomal subunit protein bL36

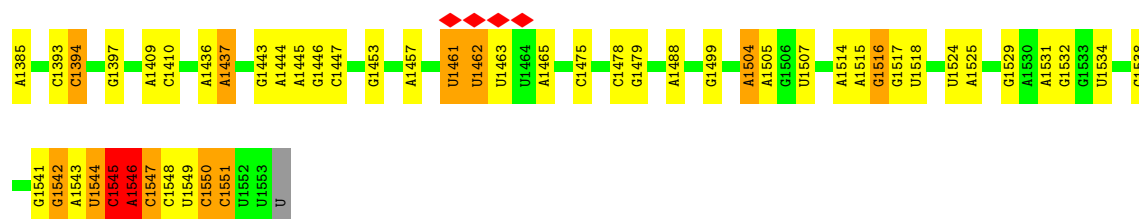


- Molecule 5: Large ribosomal subunit protein bL31B

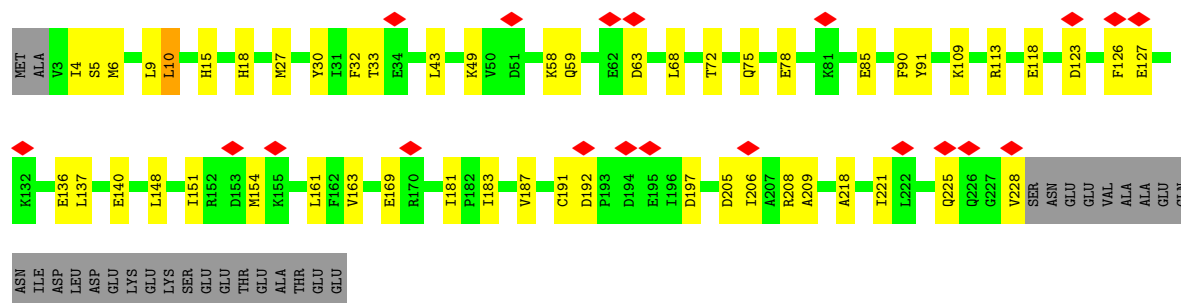


Chain A:

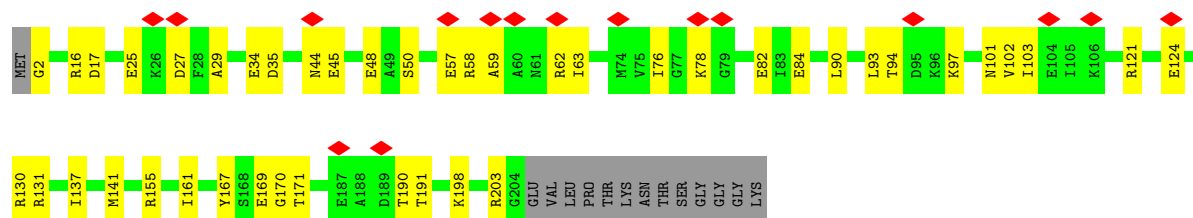
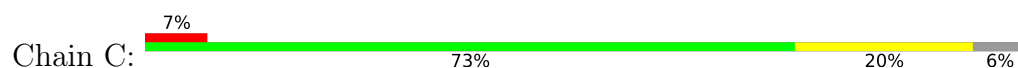




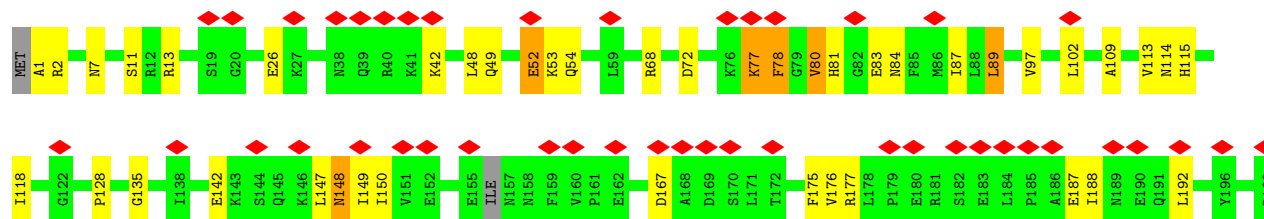
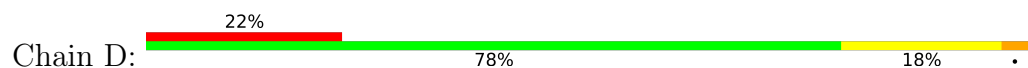
• Molecule 7: Small ribosomal subunit protein uS2



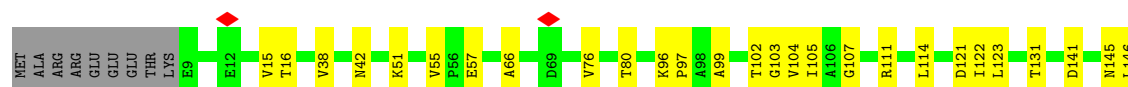
• Molecule 8: Small ribosomal subunit protein uS3



• Molecule 9: Small ribosomal subunit protein uS4

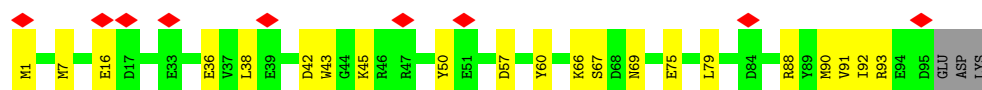
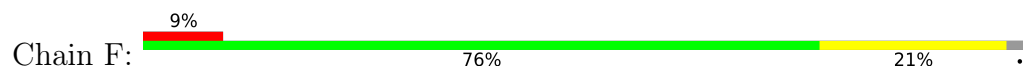


• Molecule 10: Small ribosomal subunit protein uS5

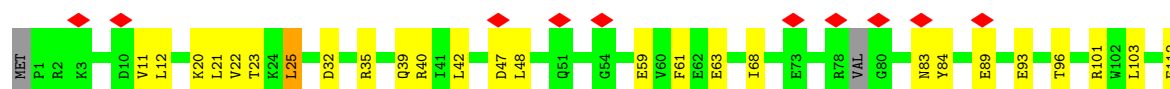
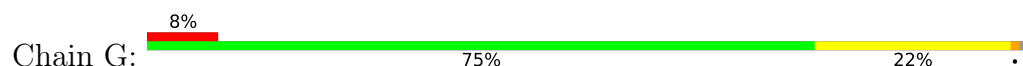




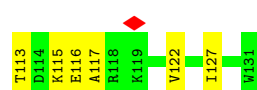
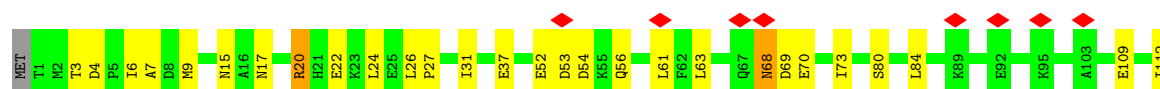
- Molecule 11: Small ribosomal subunit protein bS6



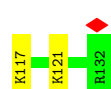
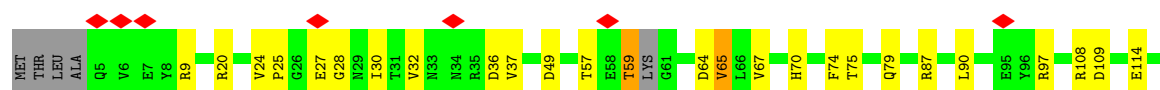
- Molecule 12: Small ribosomal subunit protein uS7



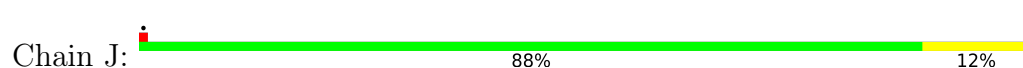
- Molecule 13: Small ribosomal subunit protein uS8



- Molecule 14: Small ribosomal subunit protein uS9

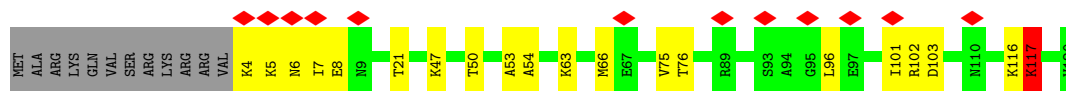
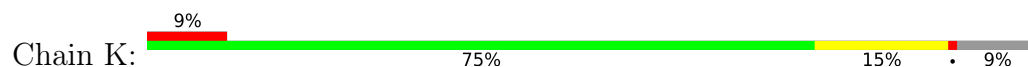


- Molecule 15: Large ribosomal subunit protein uL13

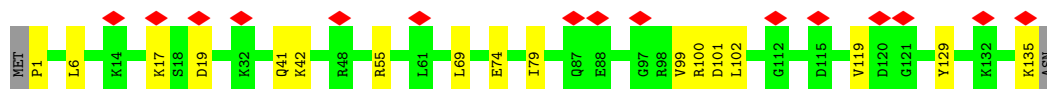
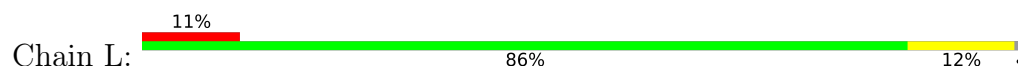




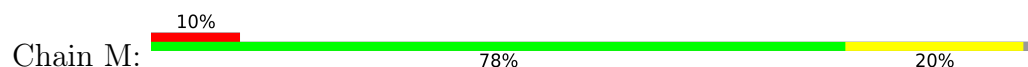
- Molecule 16: Small ribosomal subunit protein uS11



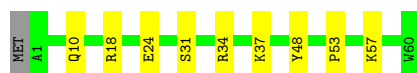
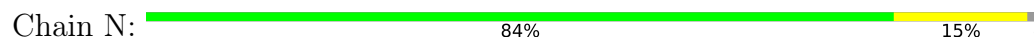
- Molecule 17: Small ribosomal subunit protein uS12



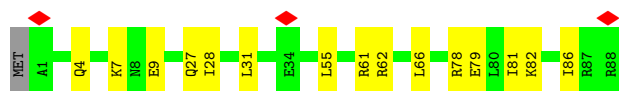
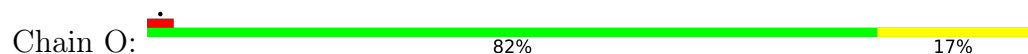
- Molecule 18: Small ribosomal subunit protein uS13



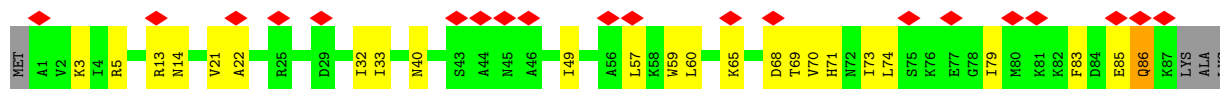
- Molecule 19: Small ribosomal subunit protein uS14B



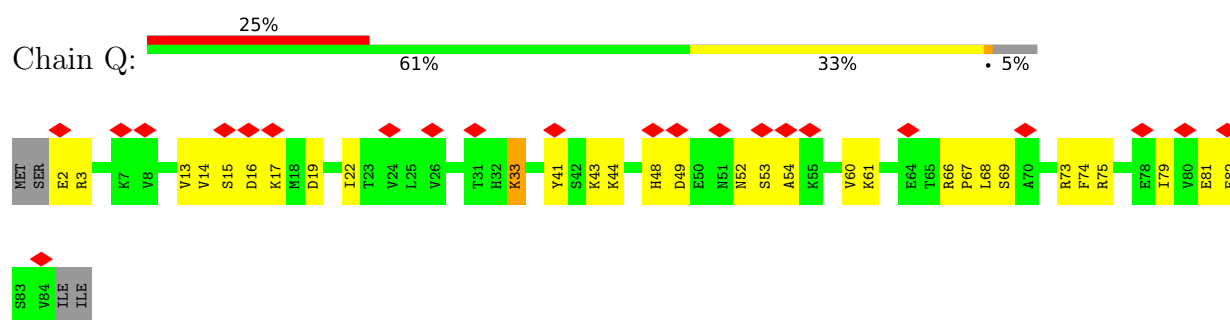
- Molecule 20: Small ribosomal subunit protein uS15



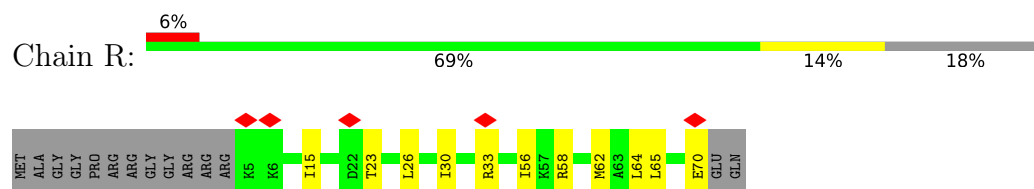
- Molecule 21: Small ribosomal subunit protein bS16



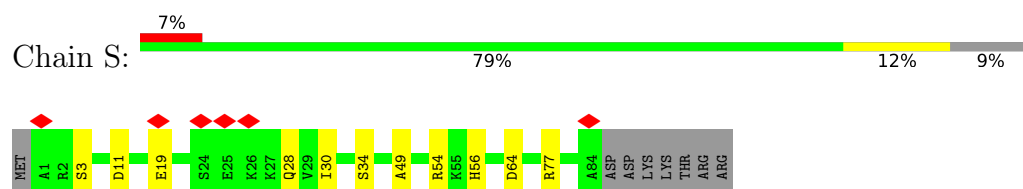
- Molecule 22: Small ribosomal subunit protein uS17



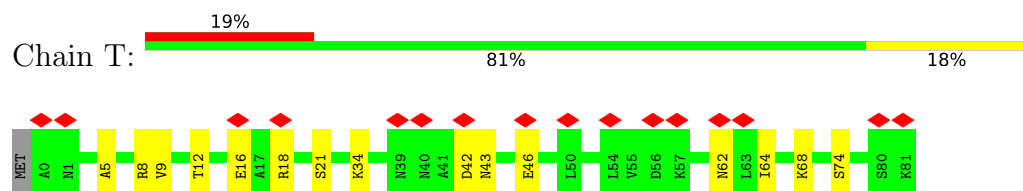
- Molecule 23: Small ribosomal subunit protein bS18



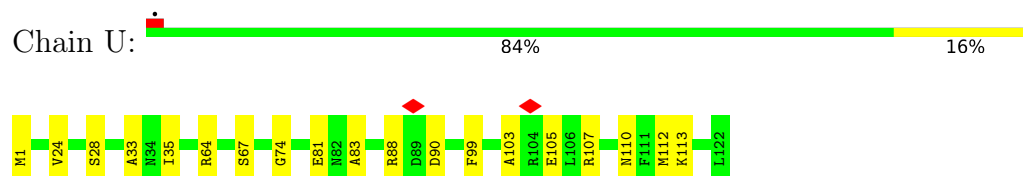
- Molecule 24: Small ribosomal subunit protein uS19



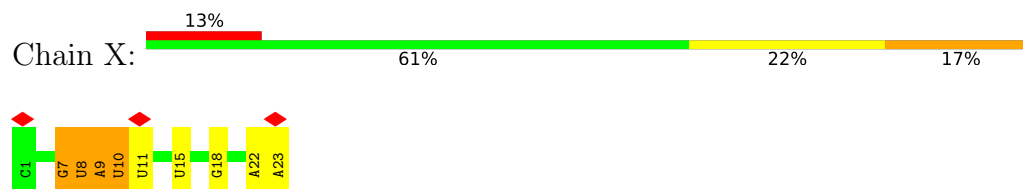
- Molecule 25: Small ribosomal subunit protein bS20



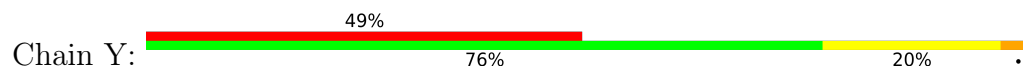
- Molecule 26: Large ribosomal subunit protein uL14

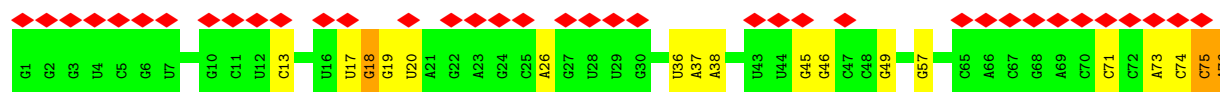


- Molecule 27: spa mRNA

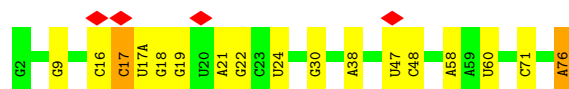
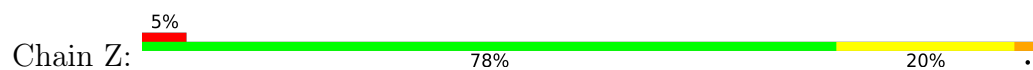


- Molecule 28: A-site tRNA-Lys

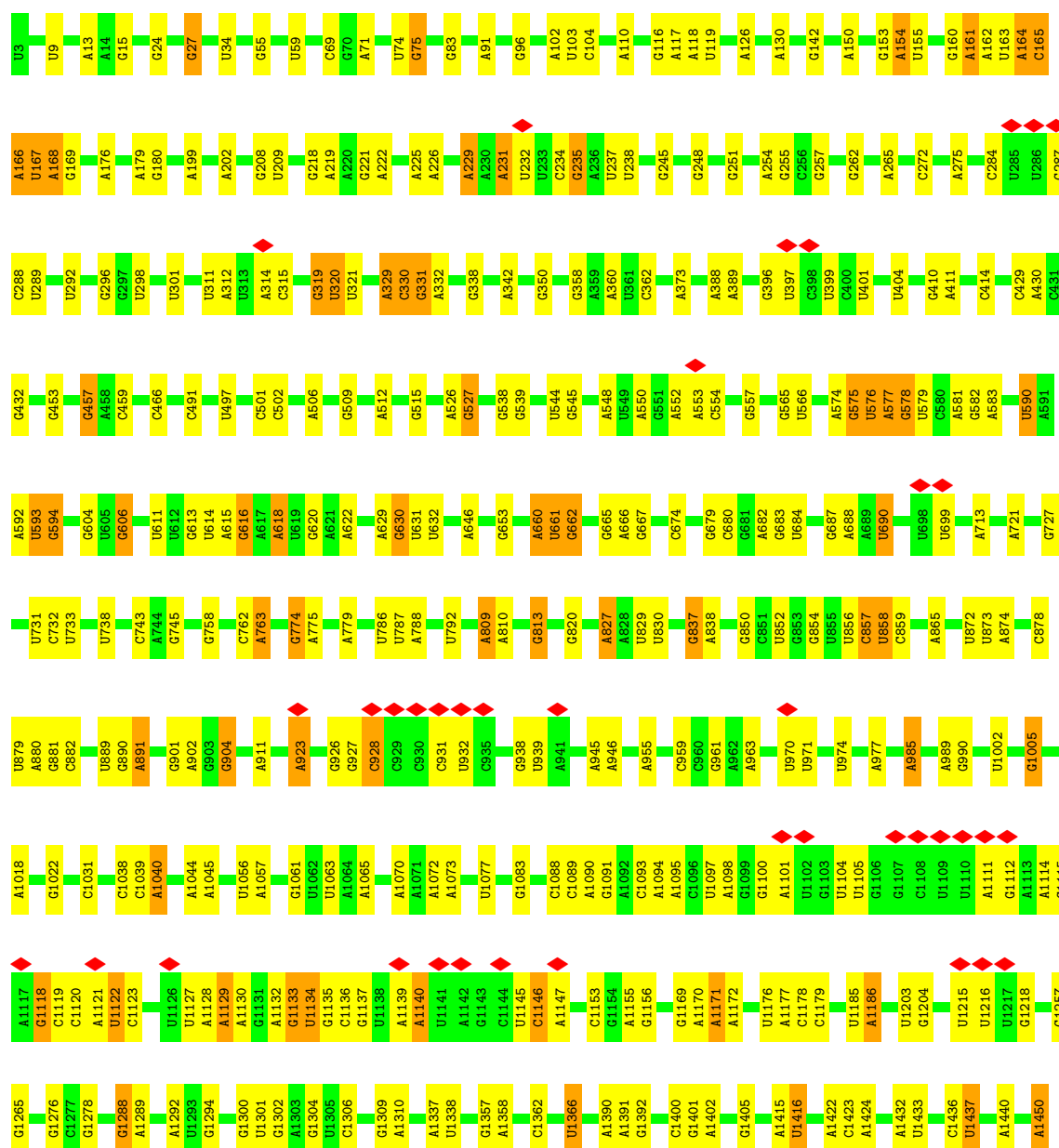


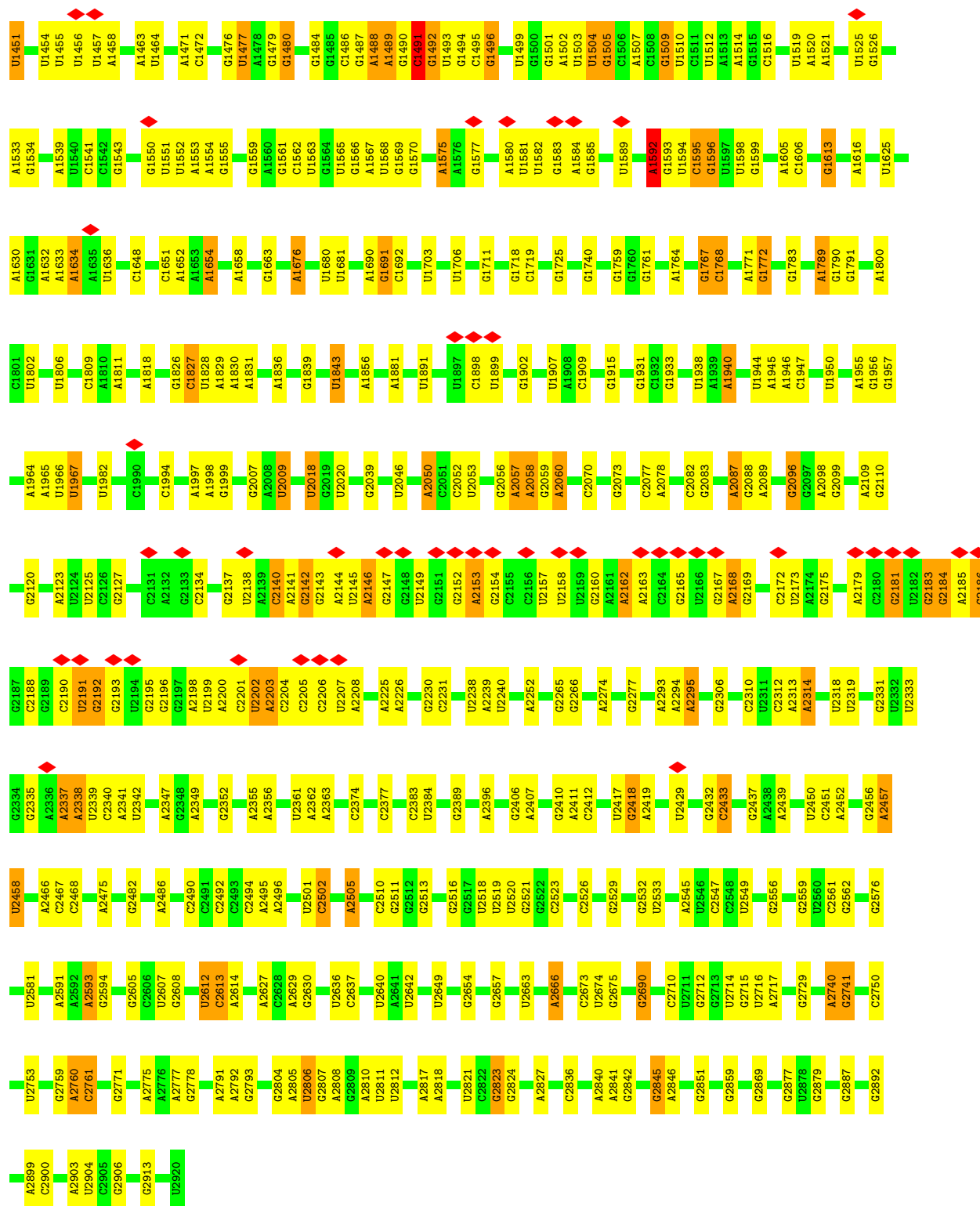


• Molecule 29: P-site tRNA-Met



• Molecule 30: 23S rRNA





• Molecule 31: 5S

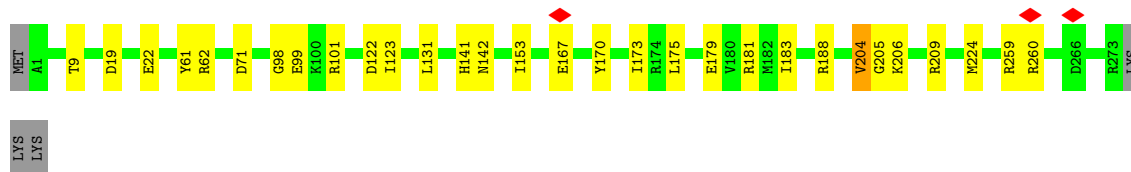
Chain b:





- Molecule 32: Large ribosomal subunit protein uL2

Chain c: 88% 10%



- Molecule 33: Large ribosomal subunit protein uL3

Chain d: 90% 8%



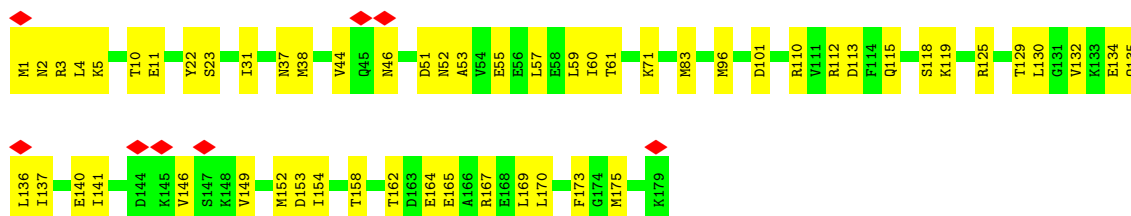
- Molecule 34: Large ribosomal subunit protein uL4

Chain e: 93% 7%



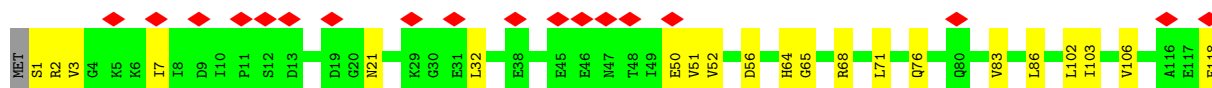
- Molecule 35: Large ribosomal subunit protein uL5

Chain f: 69% 31%



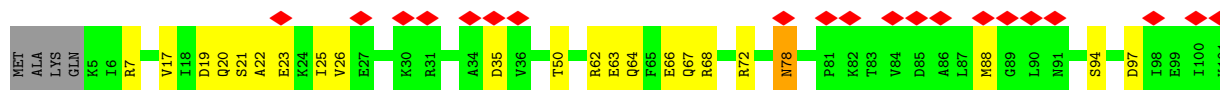
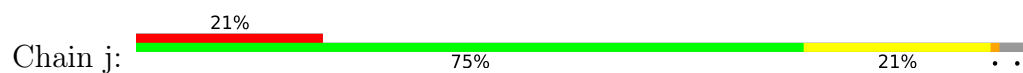
- Molecule 36: Large ribosomal subunit protein uL6

Chain g: 13% 83% 16%

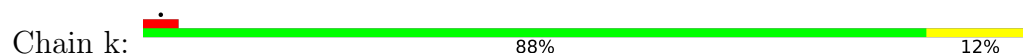




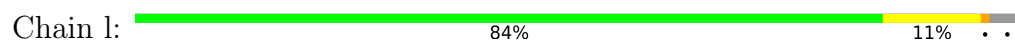
- Molecule 37: Small ribosomal subunit protein uS10



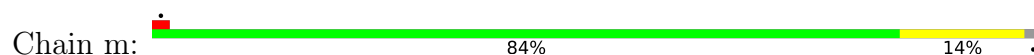
- Molecule 38: Large ribosomal subunit protein uL15



- Molecule 39: Large ribosomal subunit protein uL16



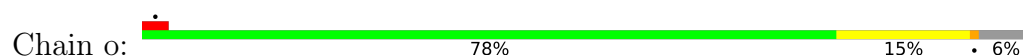
- Molecule 40: Large ribosomal subunit protein bL17



- Molecule 41: Large ribosomal subunit protein uL18



- Molecule 42: Large ribosomal subunit protein bL19



ASN
LEU
GLU
GLU
VAL
THR
ALA
THR
PRO
ASP
ASN
ILE
PRO
GLU
ALA
ILE
GLU
PRO
VAL
ASP
ILE
THR
GLU
LEU
ASN
ILE
ASN
ASP
SER
LEU
THR
VAL
ALA
ASP
VAL
LYS
THR
SER
ASP
PHE
LYS
ILE
GLU
ASN
ASP
SER
ALA
GLU
SER
VAL
VAL
THR
VAL
ALA
PRO
THR
GLU
PRO
THR

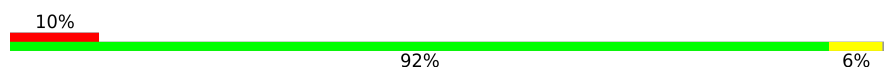
GLU
GLU
ILE
GLU
ALA
MET
GLY
ASN
GLN
THR
GLU
GLU
PRO
VAL
VAL
GLY
GLU
SER
LYS
ASN
ILE
ASN
ASP
GLU
GLU
LYS
THR
GLU
GLU

- Molecule 49: Large ribosomal subunit protein bL27

Chain v:  73% 13% 14%

MET
LEU
LYS
LEU
ASN
LEU
GLN
PHE
SER
ALA
K1
K2
G3
V4
S5
G30
I42
E46
D53
D54
T55
L56
D61
R71
V81
ALA
GLU

- Molecule 50: Large ribosomal subunit protein bL28

Chain w:  10% 92% 6%

MET
G1
V6
T7
L38
V39
D40
G41
K42
K54
S55
G56
K57
V61

- Molecule 51: Large ribosomal subunit protein uL29

Chain x:  81% 12% 6%

MET
K1
A2
K3
R6
T9
E12
E37
R41
R59
E62
Q63
S64
R65
ALA
ASN
GLN

- Molecule 52: Large ribosomal subunit protein uL30

Chain y:  85% 10% 5%

MET
ALA
K2
R9
T17
A24
Q45
K48
V49
E57
LYS

- Molecule 53: Large ribosomal subunit protein bL32

Chain z:  79% 14% 7%

MET
A1
R5
K12
R15
E28
N31
C32
G33
ARG
E34
C42
C45
C46
E51
A54
ALA
LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21621	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	1.257	Depositor
Minimum map value	-0.466	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	450.0, 450.0, 450.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9, 0.9, 0.9	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	0	0.17	0/409	0.35	0/544
2	1	0.20	0/377	0.36	0/491
3	2	0.18	0/535	0.35	0/701
4	3	0.20	0/299	0.50	0/393
5	4	0.24	0/669	0.56	0/897
6	A	0.39	27/37086 (0.1%)	0.47	49/57833 (0.1%)
7	B	0.22	0/1844	0.50	0/2475
8	C	0.23	0/1622	0.51	0/2178
9	D	0.20	0/1638	0.47	0/2200
10	E	0.41	1/1182 (0.1%)	0.45	0/1595
11	F	0.22	0/800	0.59	0/1073
12	G	0.22	0/1239	0.52	0/1665
13	H	0.26	0/1043	0.49	0/1401
14	I	0.20	0/1024	0.53	0/1375
15	J	0.20	0/1172	0.37	0/1578
16	K	0.70	4/882 (0.5%)	0.63	3/1190 (0.3%)
17	L	0.18	0/1079	0.42	0/1445
18	M	0.24	0/943	0.48	0/1264
19	N	0.21	0/511	0.45	0/678
20	O	0.22	0/746	0.50	0/996
21	P	0.24	0/699	0.60	0/942
22	Q	0.26	0/692	0.58	0/925
23	R	0.19	0/552	0.43	0/738
24	S	0.21	0/695	0.44	0/933
25	T	0.28	0/618	0.55	0/825
26	U	0.20	0/926	0.39	0/1243
27	X	1.03	7/555 (1.3%)	1.25	13/862 (1.5%)
28	Y	0.11	0/1802	0.26	0/2805
29	Z	0.17	0/1813	0.31	1/2825 (0.0%)
30	a	0.22	0/69970	0.34	4/109124 (0.0%)
31	b	0.16	0/2717	0.28	0/4232
32	c	0.19	0/2120	0.42	0/2847
33	d	0.20	0/1652	0.36	0/2216
34	e	0.20	0/1596	0.37	0/2155

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	f	0.26	0/1438	0.53	0/1928
36	g	0.21	0/1386	0.50	0/1865
37	j	0.23	0/795	0.56	1/1071 (0.1%)
38	k	0.18	0/1112	0.34	0/1482
39	l	0.31	0/1125	0.55	0/1509
40	m	0.19	0/942	0.42	0/1259
41	n	0.24	0/915	0.38	0/1224
42	o	0.20	0/889	0.39	0/1189
43	p	0.22	0/947	0.44	0/1254
44	q	0.20	0/808	0.36	0/1080
45	r	0.19	0/870	0.43	0/1171
46	s	0.18	0/733	0.37	0/978
47	t	0.20	0/694	0.49	0/923
48	u	0.19	0/738	0.38	0/990
49	v	0.29	0/627	0.48	0/831
50	w	0.19	0/487	0.31	0/649
51	x	0.23	0/537	0.48	0/714
52	y	0.18	0/438	0.34	0/590
53	z	0.21	0/434	0.37	0/578
All	All	0.28	39/157422 (0.0%)	0.41	71/235929 (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
4	3	0	1
9	D	0	3
13	H	0	1
16	K	0	1
22	Q	0	3
32	c	0	2
34	e	0	1
39	l	0	1
51	x	0	1
All	All	0	14

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	939	A	P-OP1	-20.88	1.07	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	938	G	P-OP2	-18.76	1.11	1.49
6	A	938	G	P-OP1	-18.71	1.11	1.49
6	A	1544	U	P-O5'	-15.14	1.37	1.59
6	A	1548	C	P-O5'	-13.32	1.39	1.59

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1546	A	O3'-P-O5'	-39.83	44.26	104.00
6	A	1550	C	C2'-C3'-O3'	-16.38	89.13	113.70
6	A	1546	A	C2'-C3'-O3'	-15.96	89.76	113.70
6	A	1550	C	C1'-C2'-O2'	-15.44	85.24	108.40
6	A	1542	G	O3'-P-O5'	13.64	124.46	104.00

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	3	28	GLU	Peptide
9	D	77	LYS	Peptide
9	D	78	PHE	Peptide
9	D	80	VAL	Peptide
13	H	20	ARG	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	0	406	416	416	3	0
2	1	373	420	420	1	0
3	2	530	600	601	8	0
4	3	296	342	342	2	0
5	4	652	630	631	14	0
6	A	33126	16678	16670	241	0
7	B	1817	1881	1881	37	0
8	C	1600	1662	1662	40	0
9	D	1608	1636	1638	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	E	1168	1229	1229	24	0
11	F	789	788	788	17	0
12	G	1221	1257	1259	26	0
13	H	1031	1083	1085	29	0
14	I	1008	1026	1026	23	0
15	J	1150	1145	1145	16	0
16	K	867	886	886	15	0
17	L	1062	1130	1132	12	0
18	M	936	989	991	24	0
19	N	501	528	530	9	0
20	O	737	770	772	13	0
21	P	688	714	716	20	0
22	Q	684	722	722	24	0
23	R	543	580	580	11	0
24	S	677	683	685	8	0
25	T	618	668	670	12	0
26	U	919	981	981	15	0
27	X	496	246	245	4	0
28	Y	1614	817	817	4	0
29	Z	1623	825	825	5	0
30	a	62479	31391	31404	315	0
31	b	2430	1229	1229	17	0
32	c	2085	2193	2195	25	0
33	d	1628	1670	1670	15	0
34	e	1573	1620	1622	12	0
35	f	1420	1482	1482	51	0
36	g	1368	1400	1402	22	0
37	j	783	825	825	19	0
38	k	1098	1142	1142	12	0
39	l	1101	1169	1169	11	0
40	m	939	991	993	12	0
41	n	907	960	960	7	0
42	o	877	945	945	17	0
43	p	936	1006	1006	10	0
44	q	798	836	836	10	0
45	r	862	920	920	14	0
46	s	725	761	761	3	0
47	t	689	750	750	13	0
48	u	730	779	781	9	0
49	v	621	641	643	5	0
50	w	481	524	526	2	0
51	x	536	568	570	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	y	436	473	473	5	0
53	z	427	434	436	7	0
All	All	144669	96041	96085	1138	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 5.

The worst 5 of 1138 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)
6:A:938:G:OP1	6:A:938:G:P	1.11	1.50
6:A:938:G:P	6:A:938:G:OP2	1.11	1.49
6:A:939:A:OP1	6:A:939:A:P	1.07	1.44
6:A:938:G:OP1	6:A:938:G:OP2	1.79	0.98
6:A:938:G:O3'	6:A:939:A:OP1	1.83	0.93

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
2	1	42/45 (93%)	42 (100%)	0	0	100	100
3	2	63/66 (96%)	62 (98%)	1 (2%)	0	100	100
4	3	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
5	4	78/84 (93%)	67 (86%)	10 (13%)	1 (1%)	9	32
7	B	224/255 (88%)	215 (96%)	9 (4%)	0	100	100
8	C	201/217 (93%)	195 (97%)	6 (3%)	0	100	100
9	D	196/200 (98%)	185 (94%)	9 (5%)	2 (1%)	12	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	E	155/166 (93%)	154 (99%)	1 (1%)	0	100	100
11	F	93/98 (95%)	91 (98%)	2 (2%)	0	100	100
12	G	151/156 (97%)	144 (95%)	7 (5%)	0	100	100
13	H	129/132 (98%)	121 (94%)	8 (6%)	0	100	100
14	I	125/132 (95%)	116 (93%)	9 (7%)	0	100	100
15	J	143/145 (99%)	143 (100%)	0	0	100	100
16	K	115/129 (89%)	110 (96%)	5 (4%)	0	100	100
17	L	133/137 (97%)	129 (97%)	4 (3%)	0	100	100
18	M	116/121 (96%)	114 (98%)	2 (2%)	0	100	100
19	N	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
20	O	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
21	P	85/91 (93%)	75 (88%)	10 (12%)	0	100	100
22	Q	81/87 (93%)	74 (91%)	7 (9%)	0	100	100
23	R	64/80 (80%)	64 (100%)	0	0	100	100
24	S	82/92 (89%)	82 (100%)	0	0	100	100
25	T	80/83 (96%)	77 (96%)	3 (4%)	0	100	100
26	U	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
32	c	271/277 (98%)	258 (95%)	12 (4%)	1 (0%)	30	59
33	d	213/220 (97%)	203 (95%)	10 (5%)	0	100	100
34	e	204/207 (99%)	197 (97%)	7 (3%)	0	100	100
35	f	177/179 (99%)	172 (97%)	5 (3%)	0	100	100
36	g	173/178 (97%)	157 (91%)	16 (9%)	0	100	100
37	j	96/102 (94%)	92 (96%)	4 (4%)	0	100	100
38	k	144/146 (99%)	138 (96%)	6 (4%)	0	100	100
39	l	136/144 (94%)	131 (96%)	4 (3%)	1 (1%)	18	48
40	m	117/122 (96%)	110 (94%)	7 (6%)	0	100	100
41	n	116/119 (98%)	113 (97%)	3 (3%)	0	100	100
42	o	107/116 (92%)	106 (99%)	1 (1%)	0	100	100
43	p	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
44	q	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
45	r	110/117 (94%)	109 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	s	87/91 (96%)	87 (100%)	0	0	100	100
47	t	86/105 (82%)	77 (90%)	9 (10%)	0	100	100
48	u	91/217 (42%)	88 (97%)	3 (3%)	0	100	100
49	v	79/94 (84%)	76 (96%)	3 (4%)	0	100	100
50	w	59/62 (95%)	56 (95%)	3 (5%)	0	100	100
51	x	63/69 (91%)	63 (100%)	0	0	100	100
52	y	54/59 (92%)	52 (96%)	2 (4%)	0	100	100
53	z	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
All	All	5350/5776 (93%)	5138 (96%)	207 (4%)	5 (0%)	49	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	4	65	ALA
39	l	85	ALA
9	D	77	LYS
9	D	78	PHE
32	c	205	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/47 (100%)	47 (100%)	0	100	100
2	1	39/40 (98%)	39 (100%)	0	100	100
3	2	56/57 (98%)	56 (100%)	0	100	100
4	3	35/35 (100%)	35 (100%)	0	100	100
5	4	71/75 (95%)	68 (96%)	3 (4%)	26	60
7	B	196/221 (89%)	194 (99%)	2 (1%)	68	89
8	C	164/175 (94%)	162 (99%)	2 (1%)	63	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	D	173/175 (99%)	168 (97%)	5 (3%)	37	71
10	E	123/131 (94%)	123 (100%)	0	100	100
11	F	83/86 (96%)	82 (99%)	1 (1%)	63	86
12	G	129/132 (98%)	126 (98%)	3 (2%)	44	76
13	H	112/113 (99%)	111 (99%)	1 (1%)	70	90
14	I	105/109 (96%)	103 (98%)	2 (2%)	50	79
15	J	123/123 (100%)	122 (99%)	1 (1%)	73	90
16	K	93/104 (89%)	92 (99%)	1 (1%)	65	88
17	L	117/119 (98%)	115 (98%)	2 (2%)	53	82
18	M	101/104 (97%)	100 (99%)	1 (1%)	68	89
19	N	52/53 (98%)	51 (98%)	1 (2%)	50	79
20	O	80/81 (99%)	80 (100%)	0	100	100
21	P	74/77 (96%)	71 (96%)	3 (4%)	27	61
22	Q	78/82 (95%)	77 (99%)	1 (1%)	61	86
23	R	59/68 (87%)	59 (100%)	0	100	100
24	S	72/80 (90%)	71 (99%)	1 (1%)	59	85
25	T	68/69 (99%)	68 (100%)	0	100	100
26	U	100/100 (100%)	99 (99%)	1 (1%)	68	89
32	c	220/224 (98%)	220 (100%)	0	100	100
33	d	173/177 (98%)	172 (99%)	1 (1%)	78	93
34	e	168/169 (99%)	168 (100%)	0	100	100
35	f	158/158 (100%)	155 (98%)	3 (2%)	50	79
36	g	153/155 (99%)	153 (100%)	0	100	100
37	j	88/91 (97%)	88 (100%)	0	100	100
38	k	112/112 (100%)	111 (99%)	1 (1%)	70	90
39	l	114/119 (96%)	113 (99%)	1 (1%)	70	90
40	m	100/102 (98%)	99 (99%)	1 (1%)	68	89
41	n	93/94 (99%)	92 (99%)	1 (1%)	65	88
42	o	95/102 (93%)	93 (98%)	2 (2%)	47	77
43	p	95/98 (97%)	95 (100%)	0	100	100
44	q	86/86 (100%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	r	91/94 (97%)	91 (100%)	0	100	100
46	s	80/82 (98%)	80 (100%)	0	100	100
47	t	75/90 (83%)	74 (99%)	1 (1%)	61	86
48	u	82/191 (43%)	82 (100%)	0	100	100
49	v	64/75 (85%)	60 (94%)	4 (6%)	16	45
50	w	51/52 (98%)	51 (100%)	0	100	100
51	x	59/62 (95%)	59 (100%)	0	100	100
52	y	51/53 (96%)	51 (100%)	0	100	100
53	z	48/51 (94%)	48 (100%)	0	100	100
All	All	4606/4893 (94%)	4560 (99%)	46 (1%)	65	89

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	Q	33	LYS
38	k	122	THR
24	S	28	GLN
35	f	23	SER
40	m	37	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
33	d	199	ASN
48	u	11	GLN
35	f	63	GLN
40	m	9	GLN
50	w	29	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	22/23 (95%)	4 (18%)	0
28	Y	75/76 (98%)	15 (20%)	0
29	Z	75/76 (98%)	11 (14%)	0
30	a	2908/2914 (99%)	482 (16%)	0
31	b	113/114 (99%)	16 (14%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	A	1546/1553 (99%)	314 (20%)	13 (0%)
All	All	4739/4756 (99%)	842 (17%)	13 (0%)

5 of 842 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	10	G
6	A	23	G
6	A	33	A
6	A	40	G
6	A	44	C

5 of 13 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	492	G
6	A	524	U
6	A	1550	C
6	A	627	U
6	A	1488	A

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 oligosaccharides 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
30	a	3
16	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	939:U	O3'	941:A	P	12.05
1	a	932:U	O3'	935:C	P	11.38
1	a	2149:U	O3'	2151:G	P	11.11
1	K	116:LYS	C	117:LYS	N	1.17

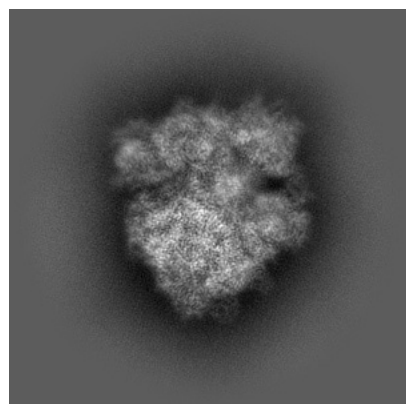
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54286. These allow visual inspection of the internal detail of the map and identification of artifacts.

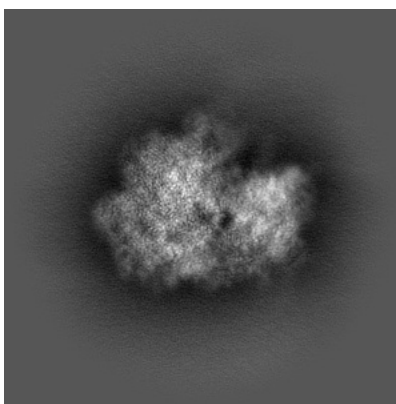
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

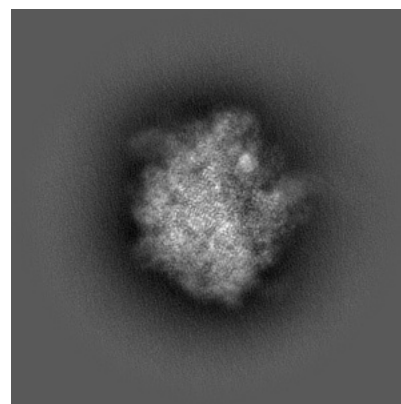
6.1.1 Primary map



X

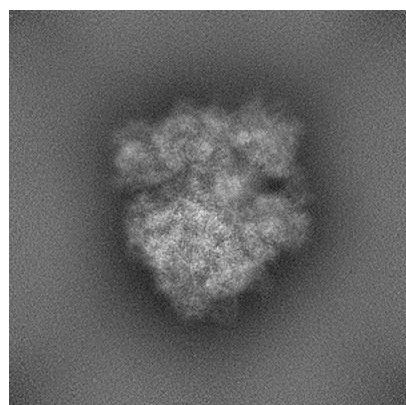


Y

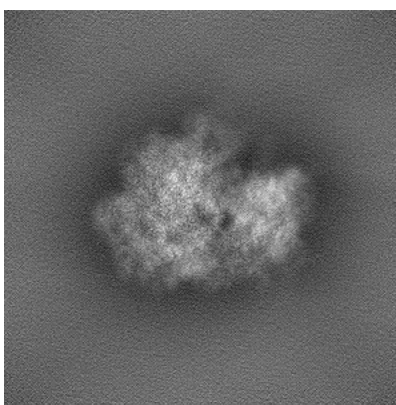


Z

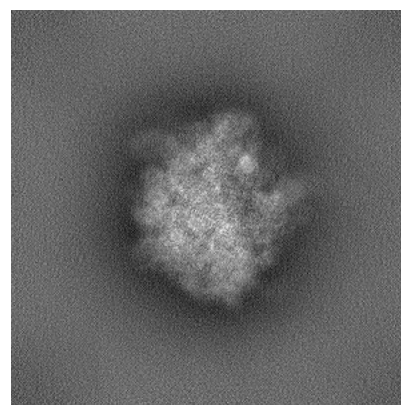
6.1.2 Raw map



X



Y

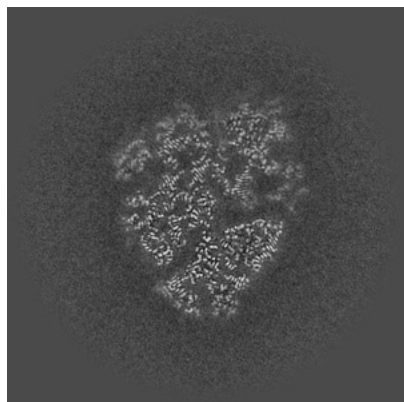


Z

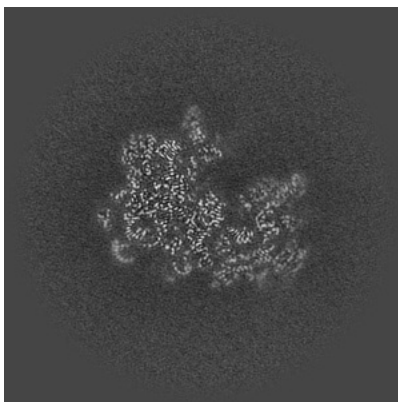
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

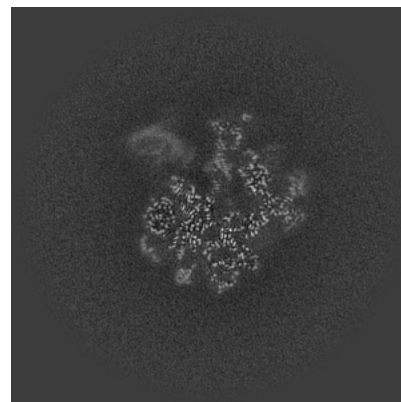
6.2.1 Primary map



X Index: 250

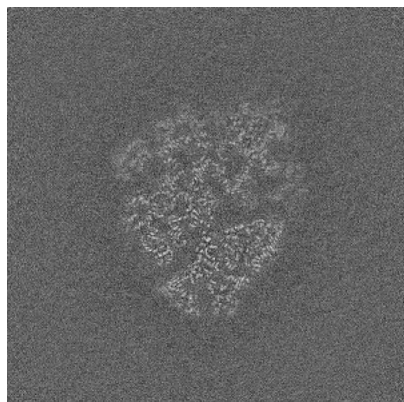


Y Index: 250

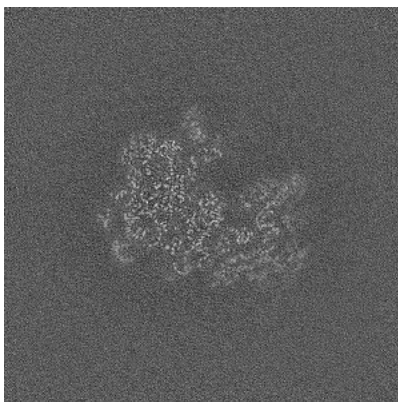


Z Index: 250

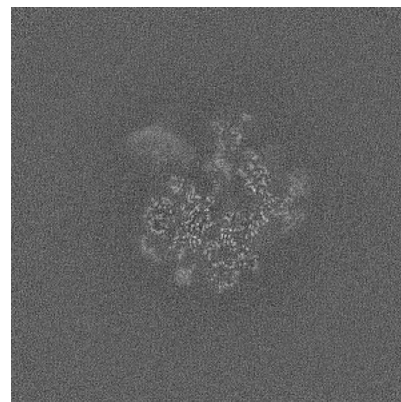
6.2.2 Raw map



X Index: 250



Y Index: 250

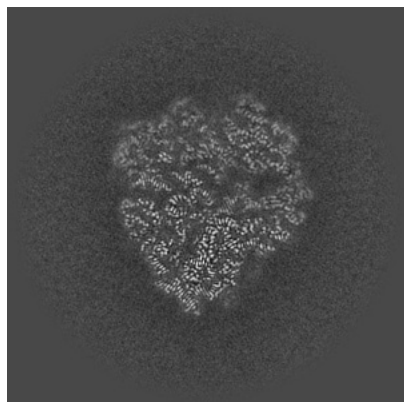


Z Index: 250

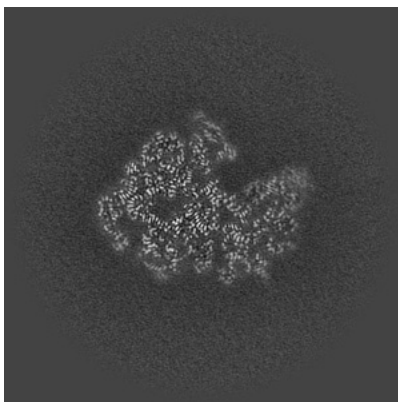
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

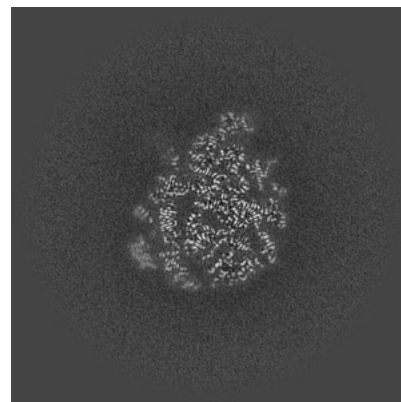
6.3.1 Primary map



X Index: 260

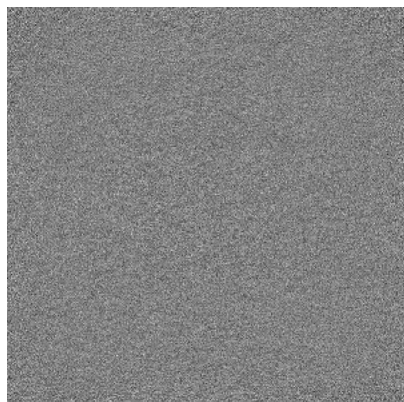


Y Index: 232

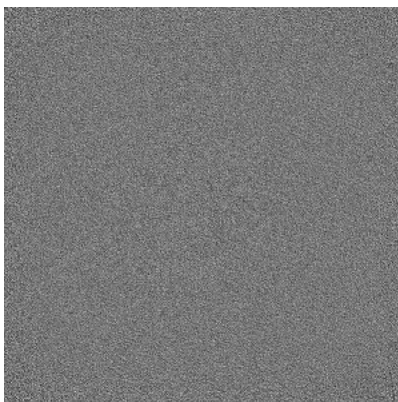


Z Index: 208

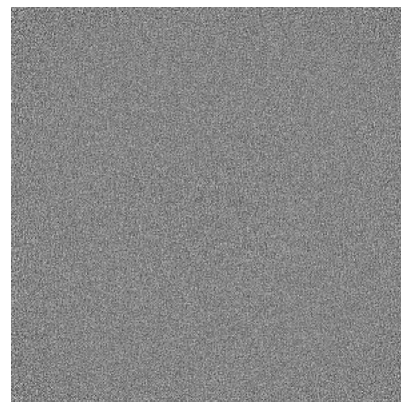
6.3.2 Raw map



X Index: 0



Y Index: 0

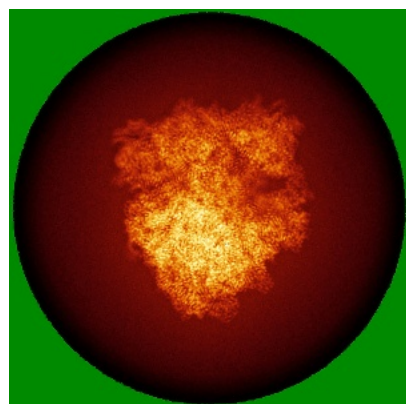


Z Index: 0

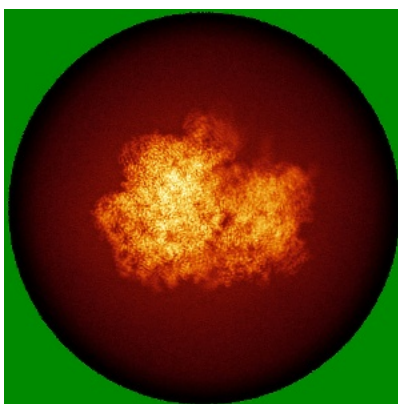
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

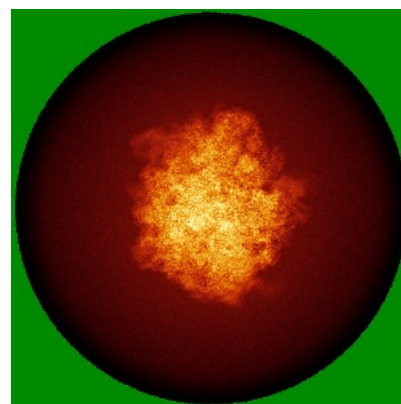
6.4.1 Primary map



X

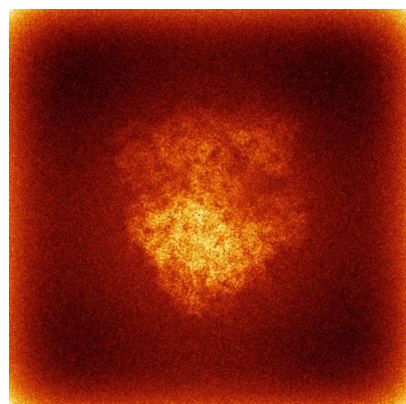


Y

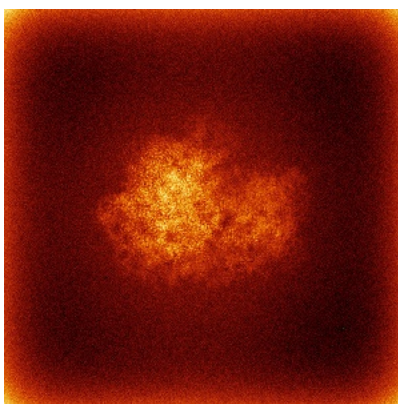


Z

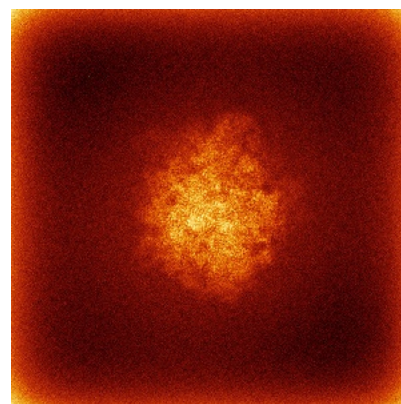
6.4.2 Raw map



X



Y

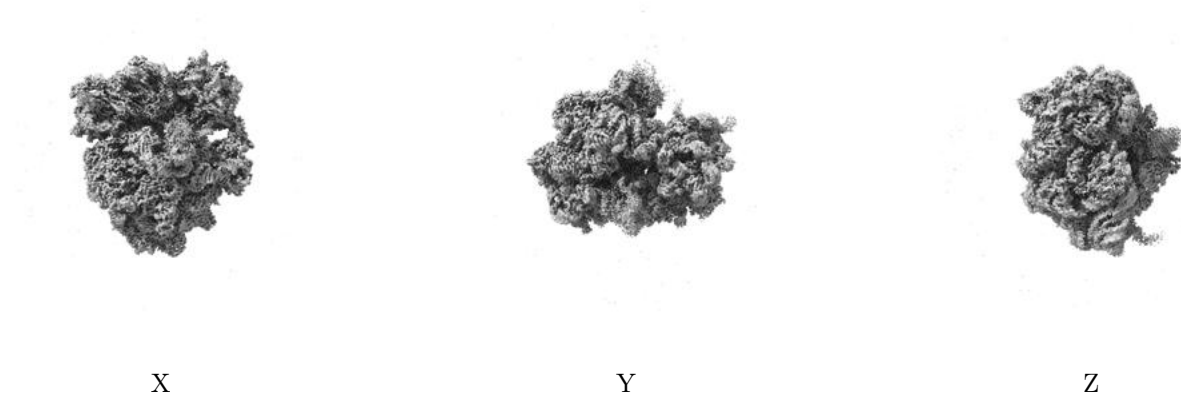


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

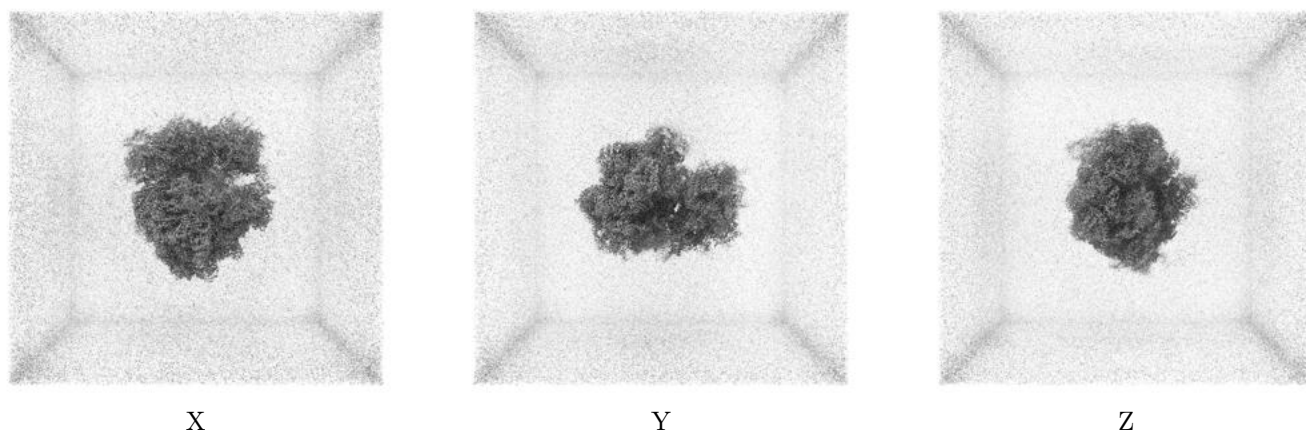
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

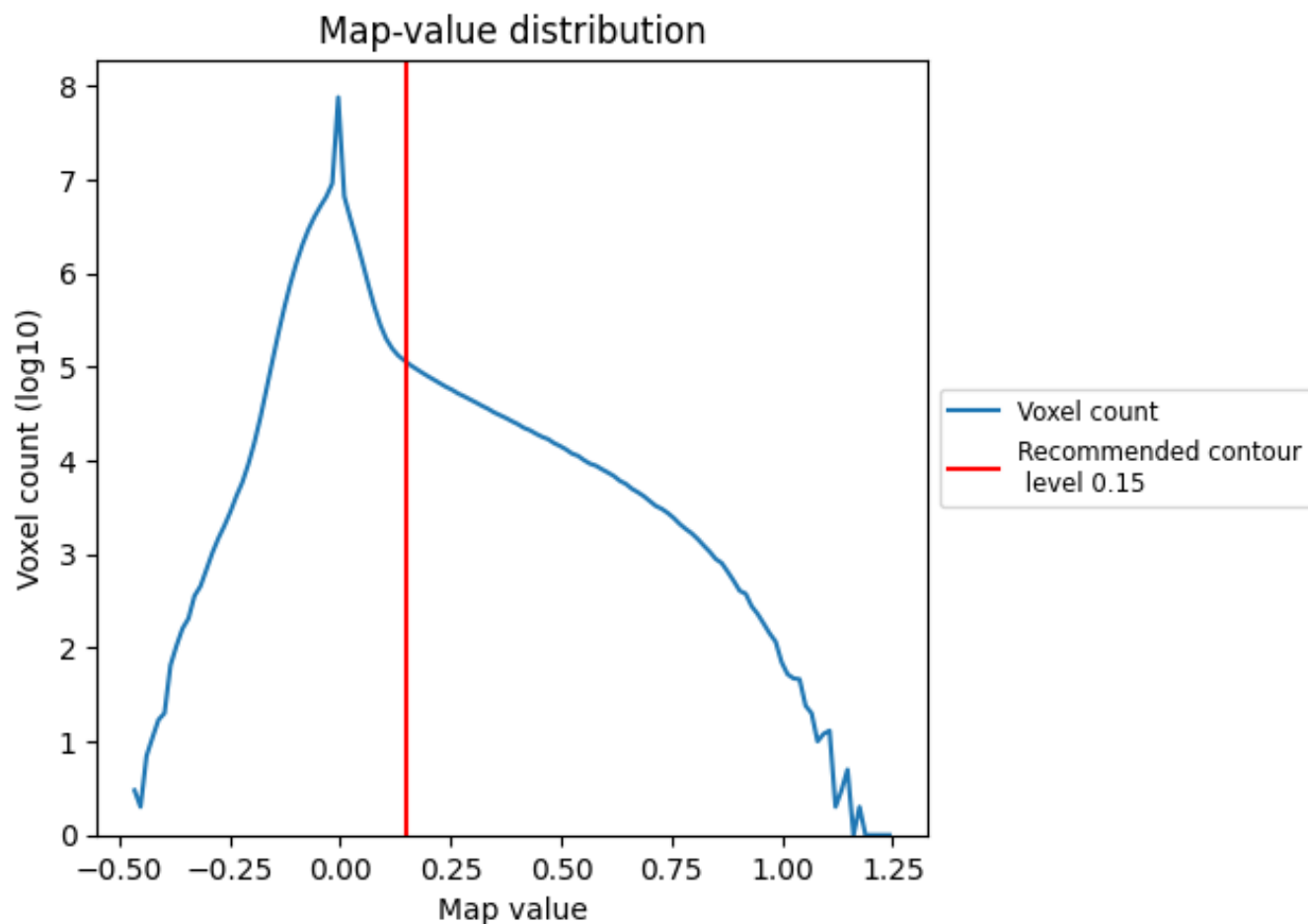
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

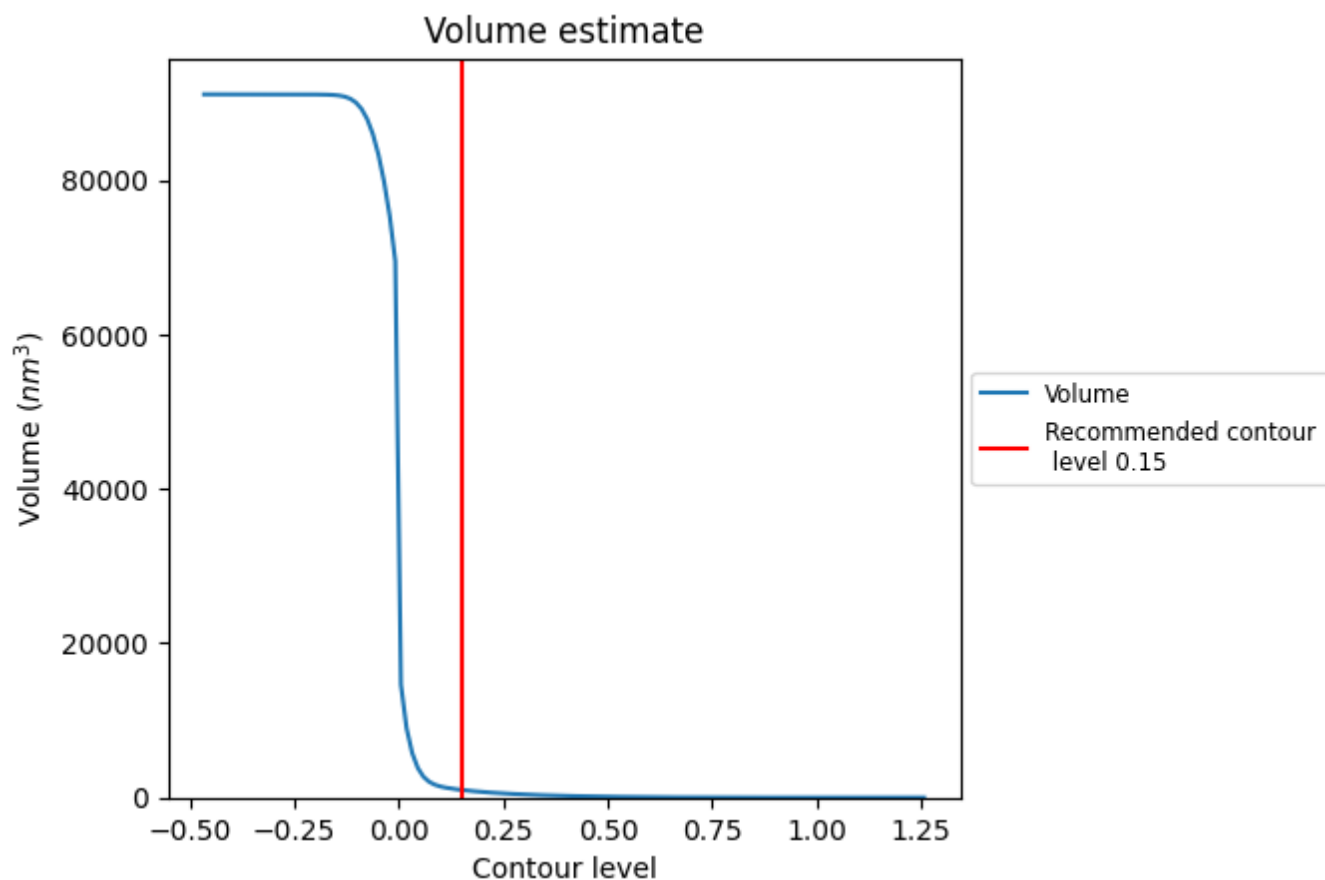
This section contains the results of statistical analysis of the map.

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.

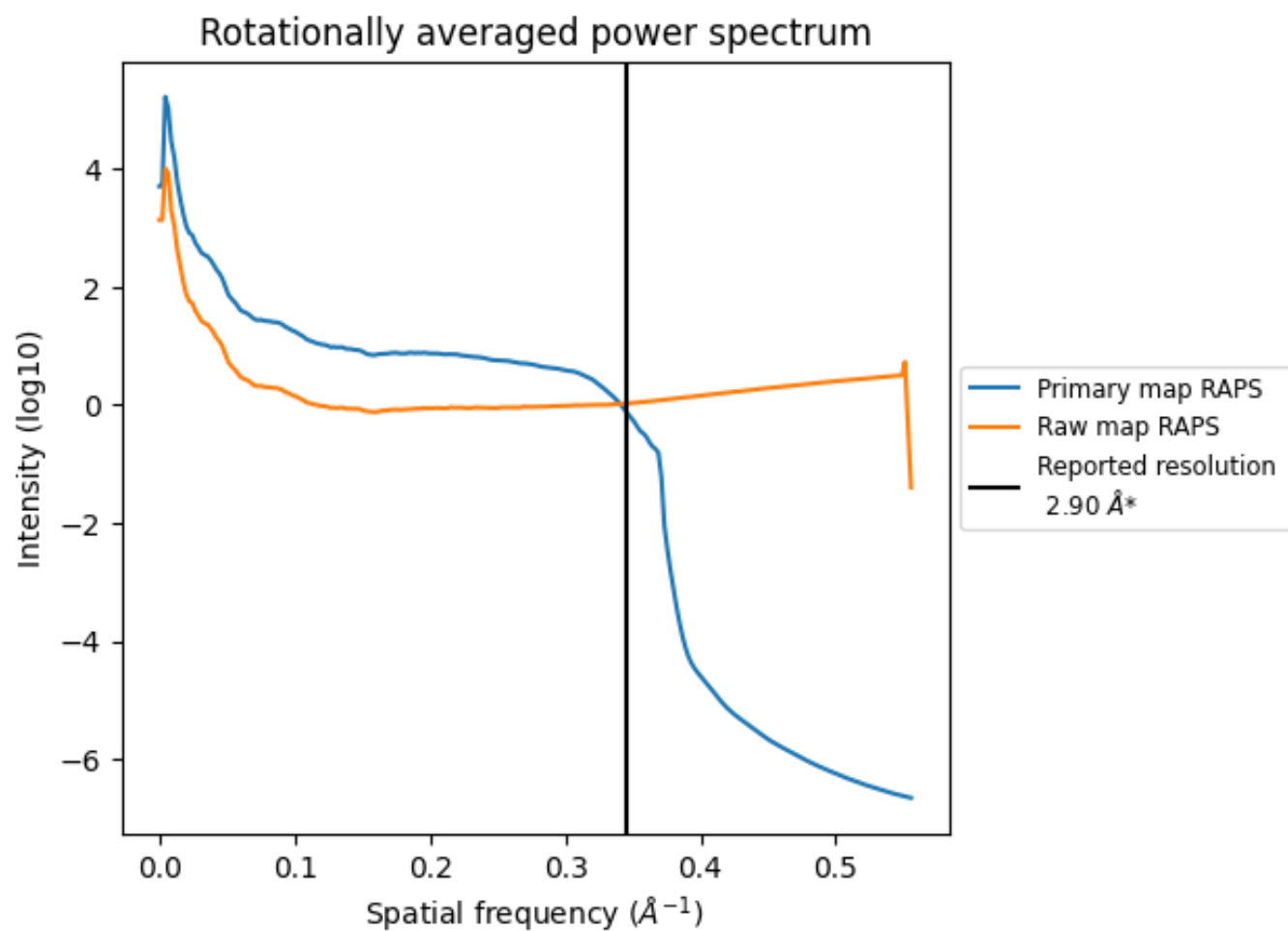
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 991 nm³; this corresponds to an approximate mass of 895 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 ⓘ

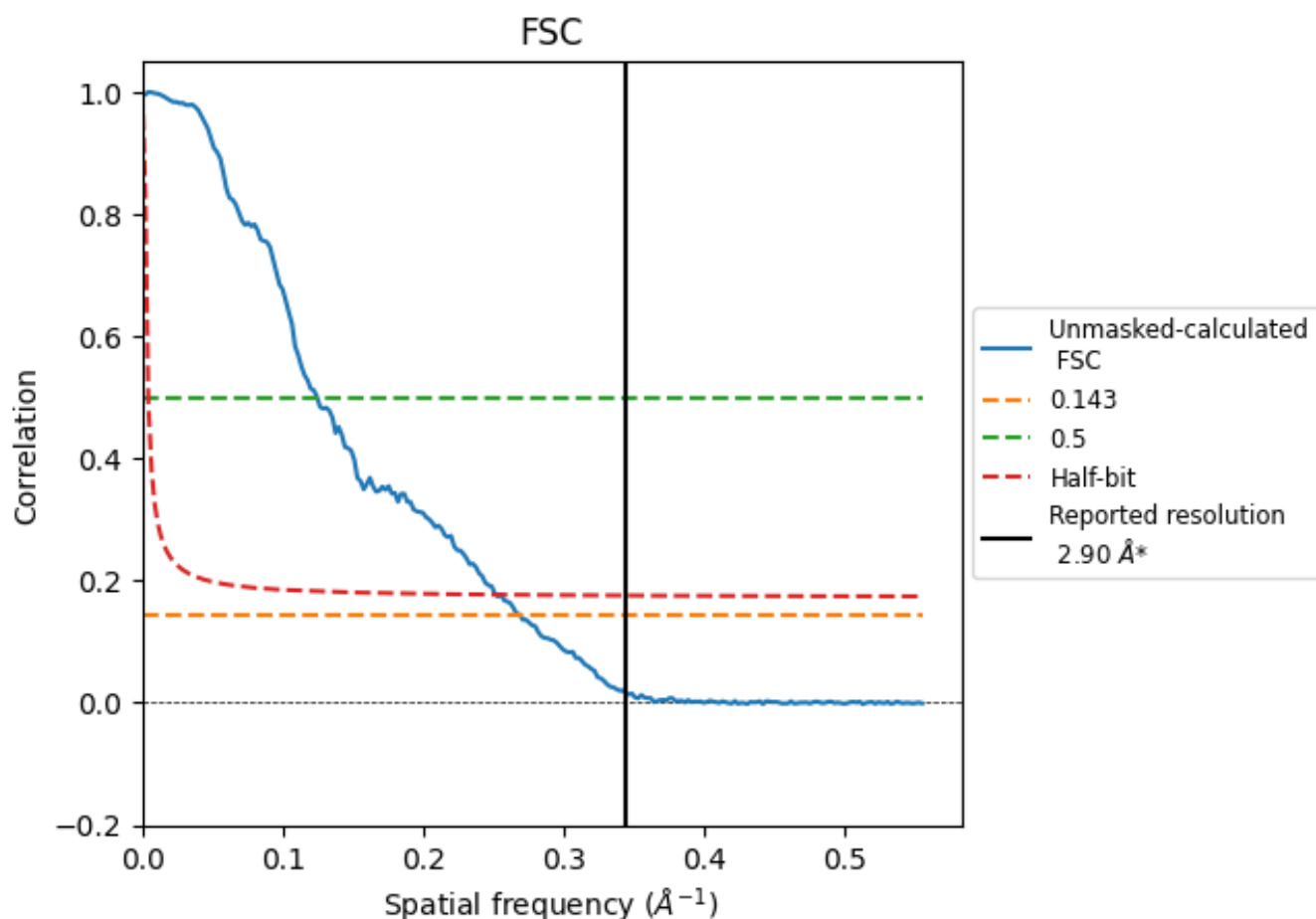


*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

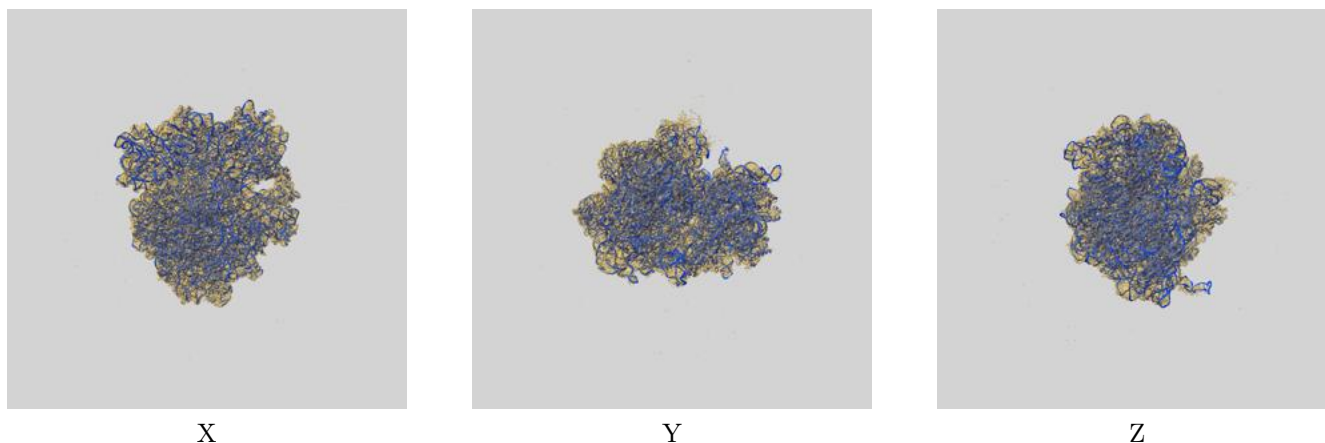
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.71	8.03	3.97

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.71 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

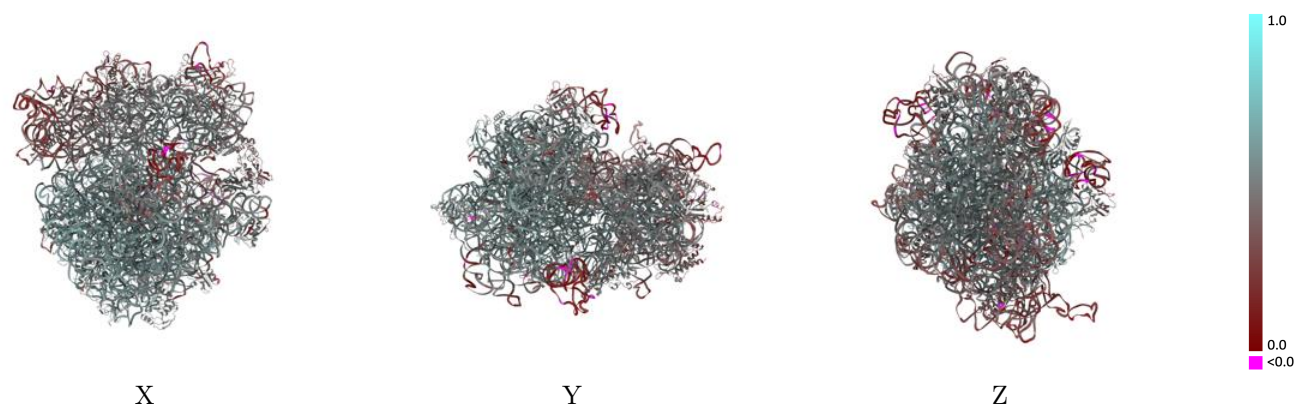
This section contains information regarding the fit between EMDB map EMD-54286 and PDB model 9RVC. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



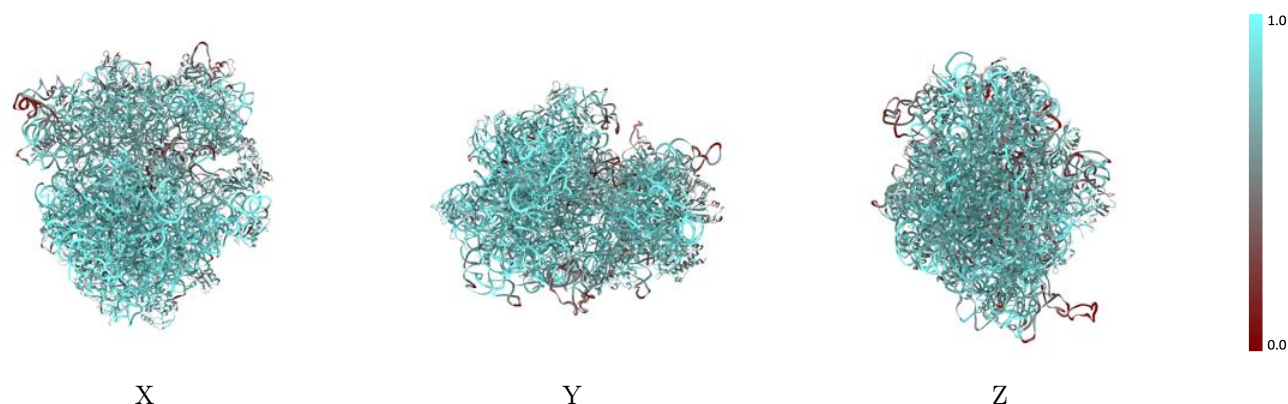
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



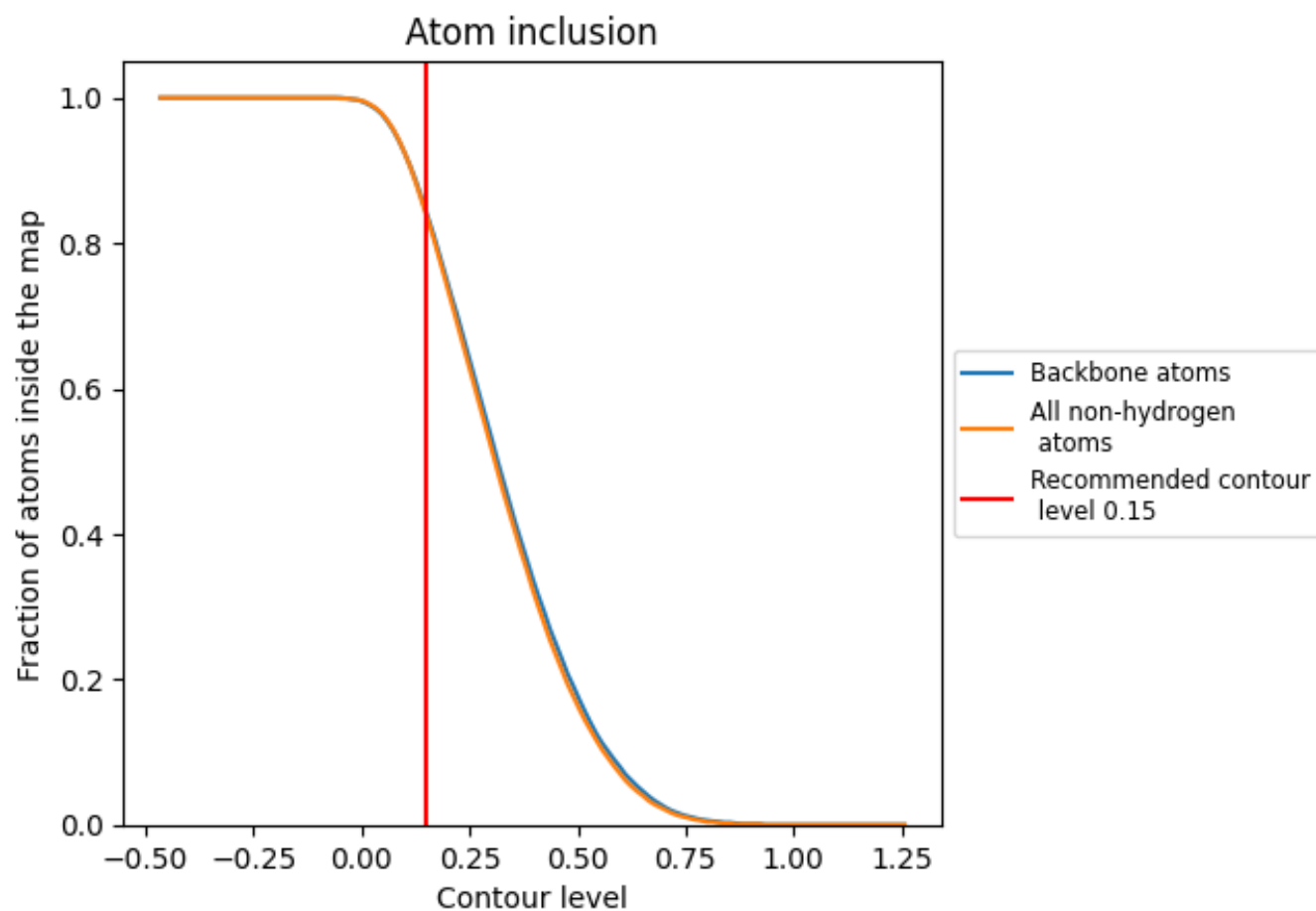
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8380	 0.4950
0	 0.8240	 0.5320
1	 0.9150	 0.6000
2	 0.8610	 0.5650
3	 0.8280	 0.5190
4	 0.5580	 0.3500
A	 0.8490	 0.4470
B	 0.6440	 0.4250
C	 0.6830	 0.4560
D	 0.5980	 0.3550
E	 0.7400	 0.4750
F	 0.7100	 0.4710
G	 0.6730	 0.4480
H	 0.6960	 0.4380
I	 0.7320	 0.4400
J	 0.8710	 0.5680
K	 0.6830	 0.4810
L	 0.6780	 0.4630
M	 0.6720	 0.4420
N	 0.8480	 0.5130
O	 0.7290	 0.4540
P	 0.5870	 0.3430
Q	 0.5470	 0.3460
R	 0.7140	 0.4610
S	 0.6880	 0.4570
T	 0.5890	 0.3470
U	 0.8150	 0.5630
X	 0.7120	 0.4610
Y	 0.4420	 0.4000
Z	 0.8150	 0.4930
a	 0.9190	 0.5280
b	 0.9070	 0.4920
c	 0.8620	 0.5780
d	 0.8660	 0.5760
e	 0.8090	 0.5370



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Chain	Atom inclusion	Q-score
f	 0.6950	 0.4520
g	 0.6700	 0.4170
j	 0.6150	 0.4030
k	 0.8000	 0.5290
l	 0.8490	 0.5470
m	 0.8390	 0.5680
n	 0.7780	 0.4980
o	 0.8380	 0.5670
p	 0.8530	 0.5600
q	 0.7980	 0.5520
r	 0.8240	 0.5620
s	 0.8270	 0.5520
t	 0.7670	 0.5050
u	 0.7240	 0.4770
v	 0.8470	 0.5480
w	 0.7900	 0.5110
x	 0.7880	 0.5170
y	 0.8110	 0.5470
z	 0.8570	 0.5710