



Full wwPDB EM Validation Report ⓘ

Jun 21, 2026 – 01:01 pm BST

PDB ID : 9Q87 / pdb_00009q87
EMDB ID : EMD-15793
Title : Principles of ion binding to RNA inferred from the analysis of a 1.55 Angstrom resolution bacterial ribosome structure - Part I: Mg²⁺
Authors : Leonarski, F.; Henning-Knechtel, A.; Kirmizialtin, S.; Ennifar, E.; Auffinger, P.
Deposited on : 2025-02-23
Resolution : 1.55 Å (reported)
Based on initial model : 8B0X

This is a Full wwPDB EM Validation 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:

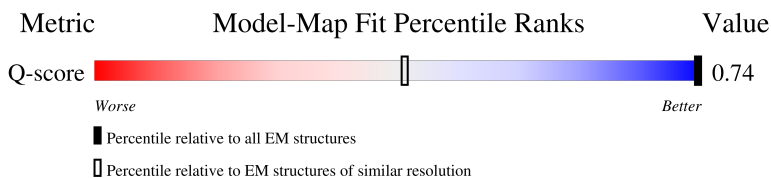
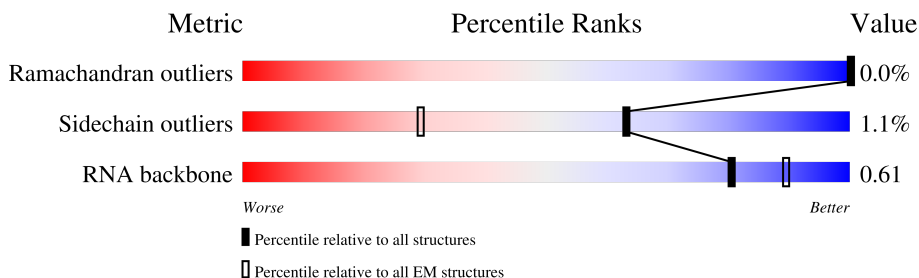
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 1.55 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.



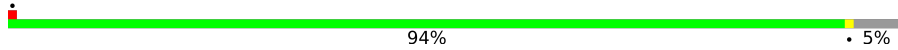
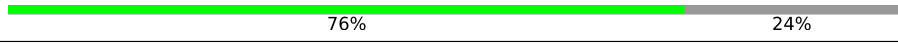
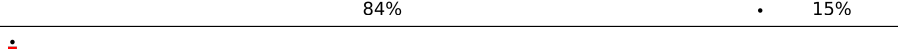
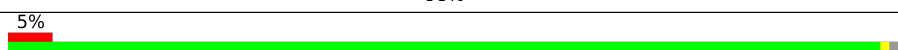
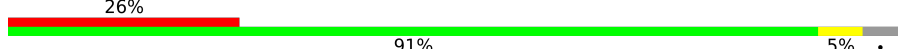
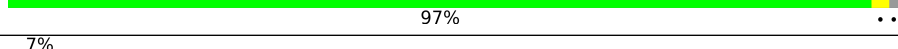
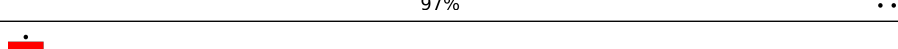
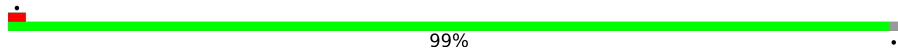
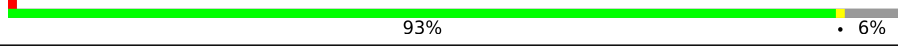
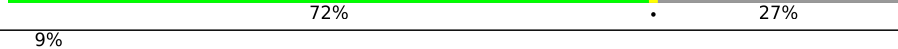
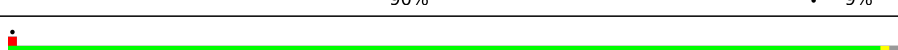
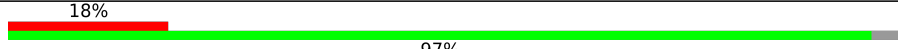
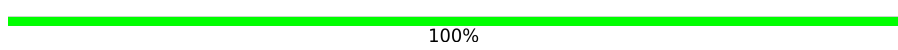
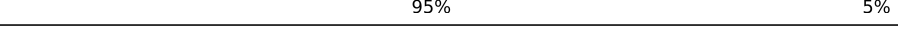
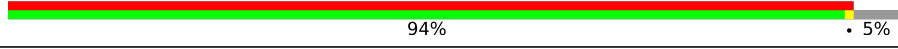
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	289 (1.05 - 2.05)

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	A	1554	
2	B	233	
3	C	233	
4	D	206	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	167	
6	F	135	
7	G	179	
8	H	130	
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	X	6	
23	Z	77	
24	0	55	
25	1	46	
26	2	65	
27	3	38	
28	5	141	
29	6	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	a	2908	
31	b	120	
32	c	273	
33	d	209	
34	e	201	
35	f	179	
36	g	177	
37	h	149	
38	i	142	
39	j	123	
40	k	144	
41	l	135	
42	m	127	
43	n	117	
44	o	115	
45	p	118	
46	q	103	
47	r	110	
48	s	100	
49	t	104	
50	u	94	
51	v	85	
52	w	78	
53	x	63	
54	y	59	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
55	z	57	 98%

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 166869 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 30S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1533	Total	C	N	O	P	0	0
			32912	14685	6040	10654	1533		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	233	Total	C	N	O	S	0	0
			1817	1146	325	338	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	deletion	UNP P0A7V0

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	158	Total	C	N	O	S	0	0
			1166	725	220	215	6		

- Molecule 6 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

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

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	129	Total	C	N	O	S	0	0
			1036	642	208	183	3		

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	99	Total	C	N	O	S	0	0
			791	495	151	144	1		

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP P0A7R9

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	69	Total	C	N	O	S	0	0
			577	357	124	95	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	6	Total	C	N	O	P	0	0
			132	59	27	40	6		

- Molecule 23 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	Z	77	Total	C	N	O	P	S	0	0
			1646	734	297	537	77	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	34	U	C	conflict	GB 1173003849

- Molecule 24 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	0	52	Total	C	N	O	0	0
			427	275	78	74		

- Molecule 25 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 26 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 27 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 28 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 29 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	6	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	2907	Total	C	N	O	P	0	0
			62424	27854	11483	20180	2907		

- Molecule 31 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

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

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

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

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

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

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

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

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

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

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

- Molecule 37 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 38 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 40 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 41 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	135	Total	C	N	O	S	0	0
			1067	681	204	177	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	?	-	ARG	deletion	UNP C3SQX7
l	81	4D4	MET	conflict	UNP C3SQX7

- Molecule 42 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 43 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 44 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 45 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 46 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 47 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 48 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 49 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	t	103	Total	C	N	O	0	0
			789	498	148	143		

- Molecule 50 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 51 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	78	Total	C	N	O	S	0	0
			592	365	119	107	1		

- Molecule 52 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 53 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 54 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 55 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 56 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
56	A	66	Total	K	0
			66	66	
56	D	1	Total	K	0
			1	1	
56	F	1	Total	K	0
			1	1	
56	a	159	Total	K	0
			159	159	
56	b	1	Total	K	0
			1	1	
56	c	4	Total	K	0
			4	4	
56	d	1	Total	K	0
			1	1	
56	e	1	Total	K	0
			1	1	
56	f	1	Total	K	0
			1	1	

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	A	89	Total 89	Mg 89	0
57	B	1	Total 1	Mg 1	0
57	M	1	Total 1	Mg 1	0
57	Z	1	Total 1	Mg 1	0
57	a	311	Total 311	Mg 311	0
57	b	6	Total 6	Mg 6	0
57	c	2	Total 2	Mg 2	0
57	d	1	Total 1	Mg 1	0
57	k	1	Total 1	Mg 1	0
57	p	1	Total 1	Mg 1	0
57	z	1	Total 1	Mg 1	0

- Molecule 58 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
58	A	1	Total 1	Cu 1	0
58	a	3	Total 3	Cu 3	0
58	w	1	Total 1	Cu 1	0

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	3	1	Total 1	Zn 1	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		AltConf
60	A	3993	Total 3993	O 3993	0
60	B	25	Total 25	O 25	0
60	C	36	Total 36	O 36	0
60	D	35	Total 35	O 35	0
60	E	63	Total 63	O 63	0
60	F	12	Total 12	O 12	0
60	G	9	Total 9	O 9	0
60	H	64	Total 64	O 64	0
60	I	18	Total 18	O 18	0
60	J	20	Total 20	O 20	0
60	K	33	Total 33	O 33	0
60	L	58	Total 58	O 58	0
60	M	7	Total 7	O 7	0
60	N	14	Total 14	O 14	0
60	O	41	Total 41	O 41	0
60	P	32	Total 32	O 32	0
60	Q	18	Total 18	O 18	0
60	R	16	Total 16	O 16	0
60	S	4	Total 4	O 4	0
60	T	30	Total 30	O 30	0
60	U	29	Total 29	O 29	0
60	X	27	Total 27	O 27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
60	Z	46	Total 46	O 46	0
60	0	44	Total 44	O 44	0
60	1	94	Total 94	O 94	0
60	2	80	Total 80	O 80	0
60	3	34	Total 34	O 34	0
60	6	12	Total 12	O 12	0
60	a	13616	Total 13616	O 13616	0
60	b	364	Total 364	O 364	0
60	c	330	Total 330	O 330	0
60	d	225	Total 225	O 225	0
60	e	180	Total 180	O 180	0
60	f	6	Total 6	O 6	0
60	g	26	Total 26	O 26	0
60	h	10	Total 10	O 10	0
60	i	185	Total 185	O 185	0
60	j	91	Total 91	O 91	0
60	k	172	Total 172	O 172	0
60	l	150	Total 150	O 150	0
60	m	123	Total 123	O 123	0
60	n	55	Total 55	O 55	0
60	o	119	Total 119	O 119	0

Continued on next page...

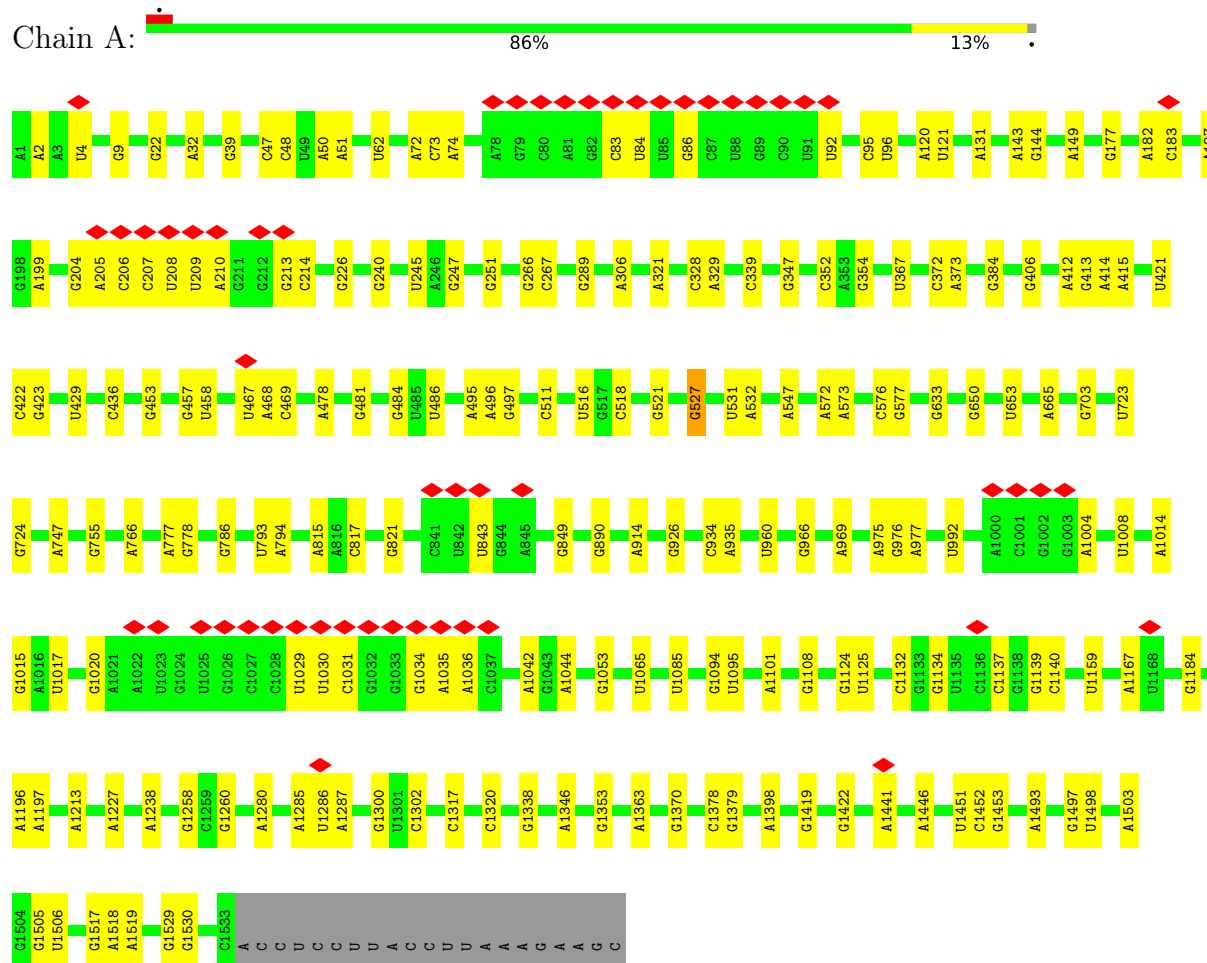
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
60	p	126	Total 126	O 126	0
60	q	93	Total 93	O 93	0
60	r	122	Total 122	O 122	0
60	s	51	Total 51	O 51	0
60	t	65	Total 65	O 65	0
60	u	51	Total 51	O 51	0
60	v	90	Total 90	O 90	0
60	w	80	Total 80	O 80	0
60	x	19	Total 19	O 19	0
60	y	63	Total 63	O 63	0
60	z	82	Total 82	O 82	0

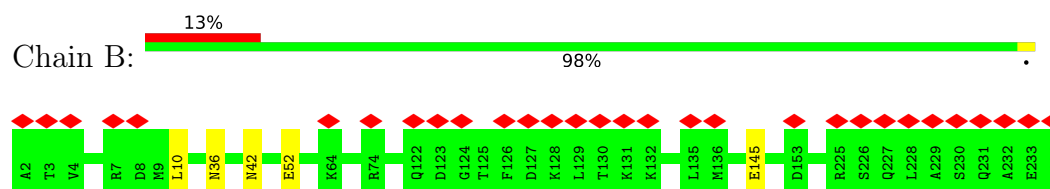
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: 30S

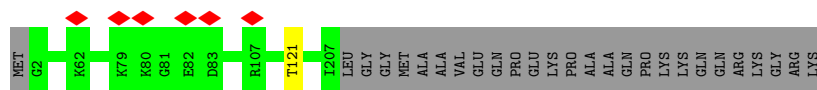


• Molecule 2: Small ribosomal subunit protein uS2

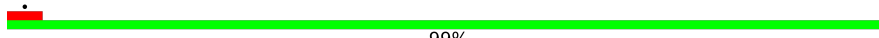


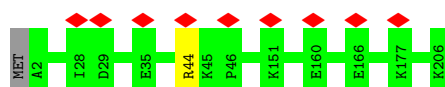
- Molecule 3: Small ribosomal subunit protein uS3

Chain C:  88% 12%

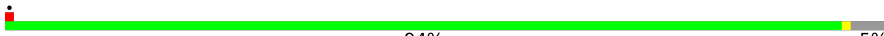


- Molecule 4: Small ribosomal subunit protein uS4

Chain D:  99%



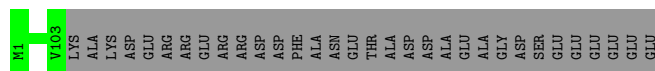
- Molecule 5: Small ribosomal subunit protein uS5

Chain E:  94% 5%



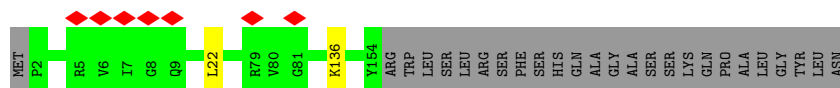
- Molecule 6: Small ribosomal subunit protein bS6, fully modified isoform

Chain F:  76% 24%

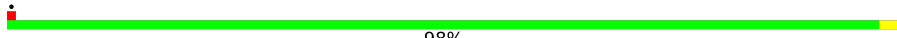


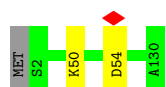
- Molecule 7: Small ribosomal subunit protein uS7

Chain G:  84% 15%



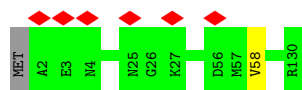
- Molecule 8: Small ribosomal subunit protein uS8

Chain H:  98%

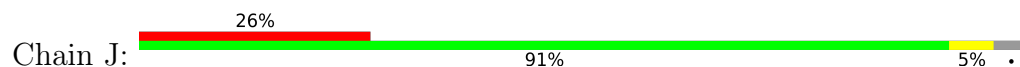


- Molecule 9: Small ribosomal subunit protein uS9

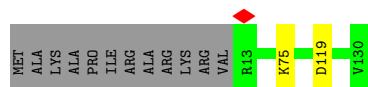
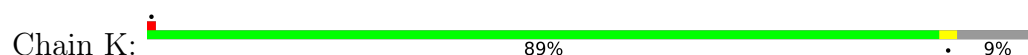
Chain I:  5% 98%



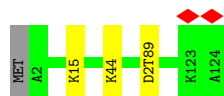
- Molecule 10: Small ribosomal subunit protein uS10



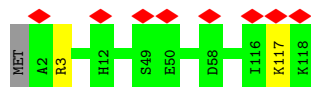
- Molecule 11: Small ribosomal subunit protein uS11



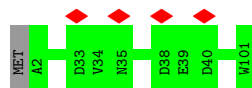
- Molecule 12: Small ribosomal subunit protein uS12



- Molecule 13: Small ribosomal subunit protein uS13



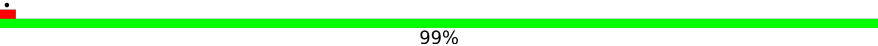
- Molecule 14: Small ribosomal subunit protein uS14

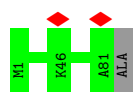


- Molecule 15: Small ribosomal subunit protein uS15

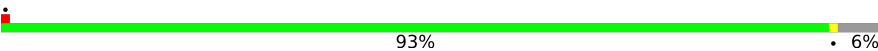


- Molecule 16: Small ribosomal subunit protein bS16

Chain P:  99%



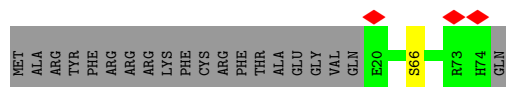
- Molecule 17: Small ribosomal subunit protein uS17

Chain Q:  93% 6%



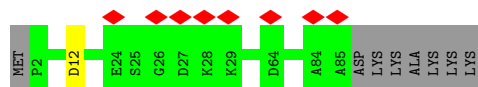
- Molecule 18: Small ribosomal subunit protein bS18

Chain R:  72% 27%

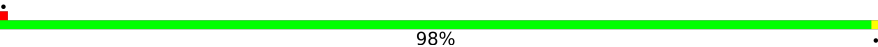


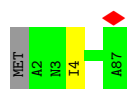
- Molecule 19: Small ribosomal subunit protein uS19

Chain S:  9% 90% 9%

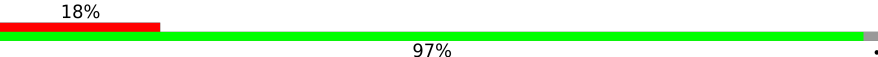


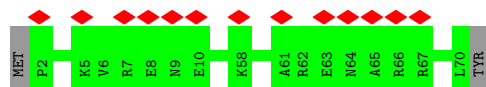
- Molecule 20: Small ribosomal subunit protein bS20

Chain T:  98%

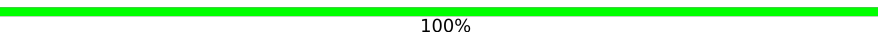


- Molecule 21: Small ribosomal subunit protein bS21

Chain U:  18% 97%

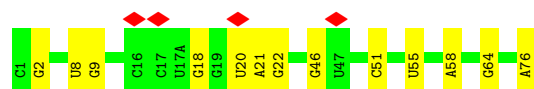
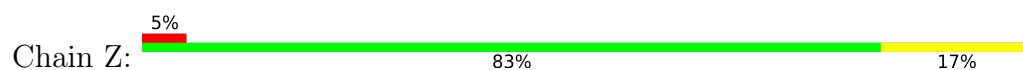


- Molecule 22: mRNA

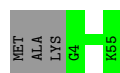
Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 23: P-site tRNA



- Molecule 24: Large ribosomal subunit protein bL33



- Molecule 25: Large ribosomal subunit protein bL34



There are no outlier residues recorded for this chain.

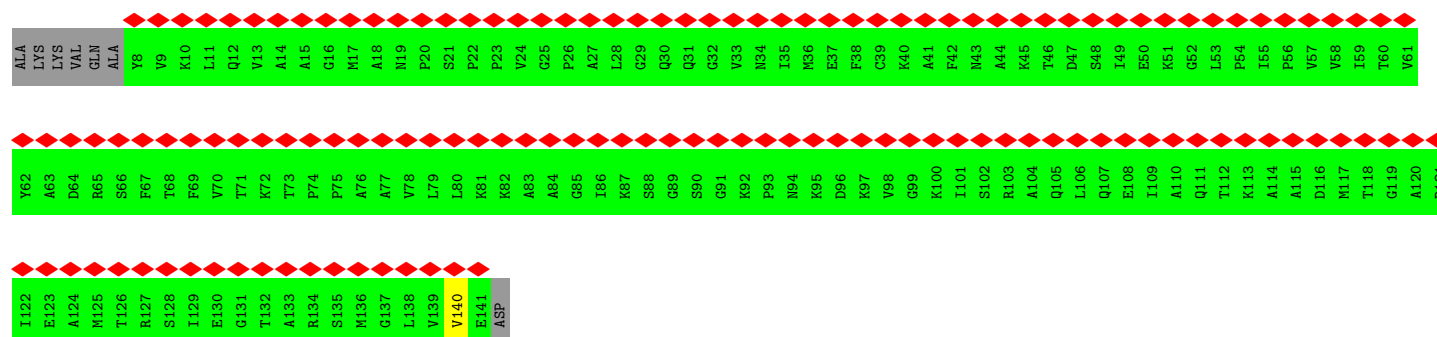
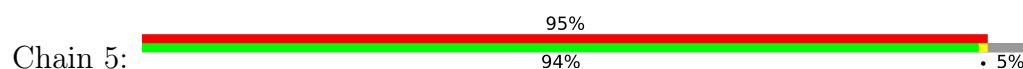
- Molecule 26: Large ribosomal subunit protein bL35



- Molecule 27: Large ribosomal subunit protein bL36A



- Molecule 28: Large ribosomal subunit protein uL11



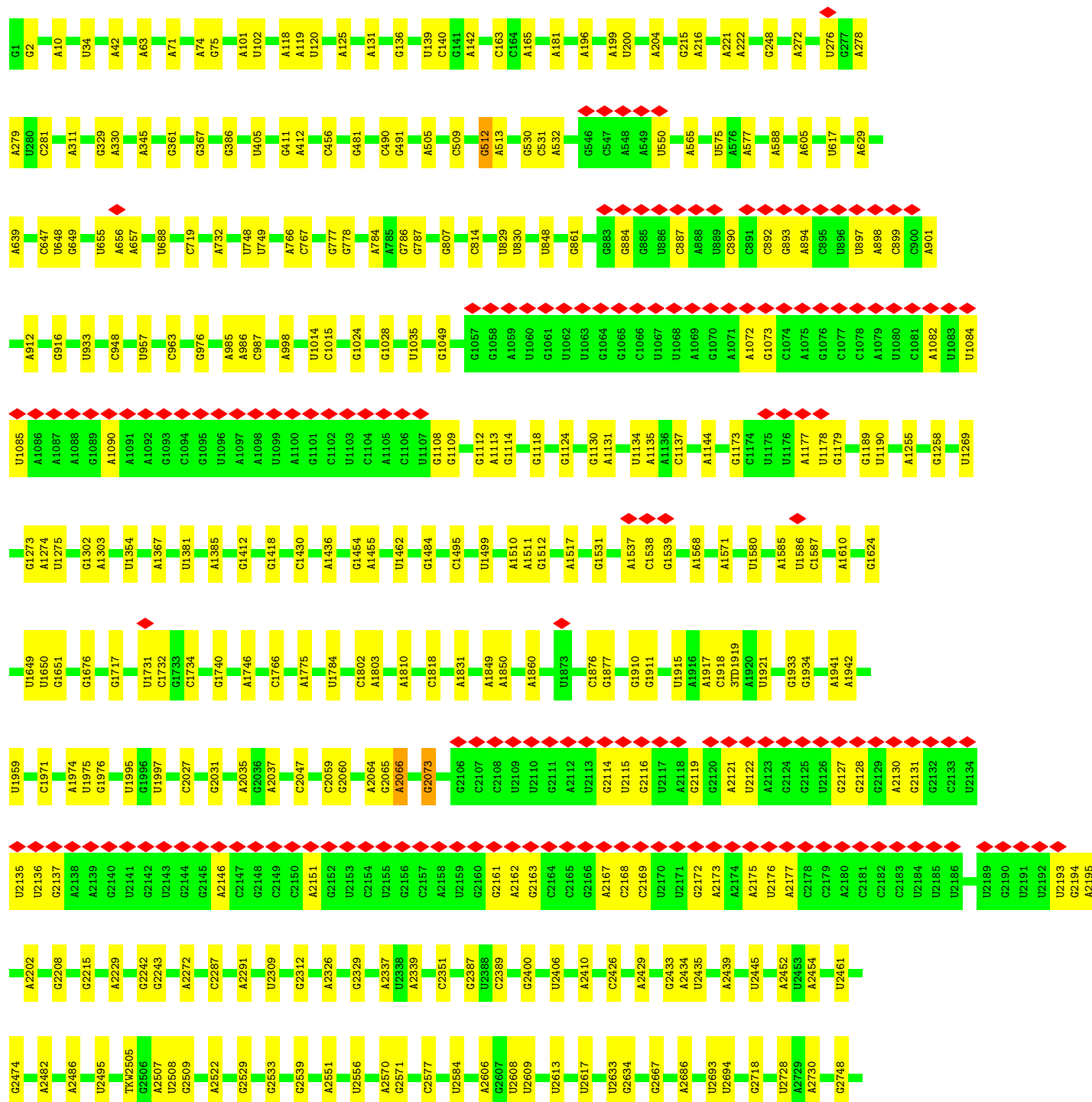
- Molecule 29: A-site tRNA



C75
A76

• Molecule 30: 23S rRNA

Chain a:  6% 88% 11%

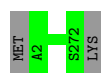




- Molecule 31: 5S rRNA



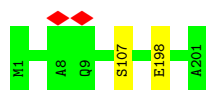
- Molecule 32: Large ribosomal subunit protein uL2



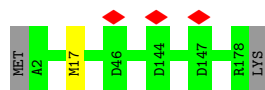
- Molecule 33: Large ribosomal subunit protein uL3



- Molecule 34: Large ribosomal subunit protein uL4



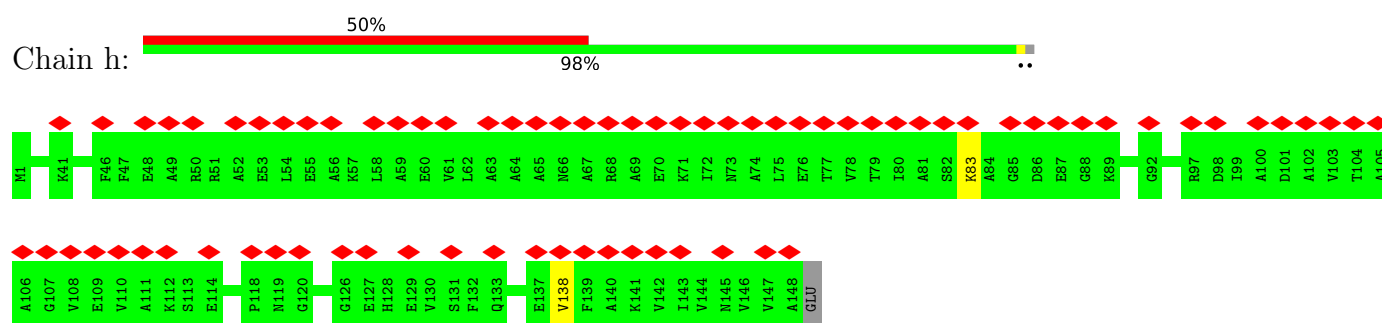
- Molecule 35: Large ribosomal subunit protein uL5



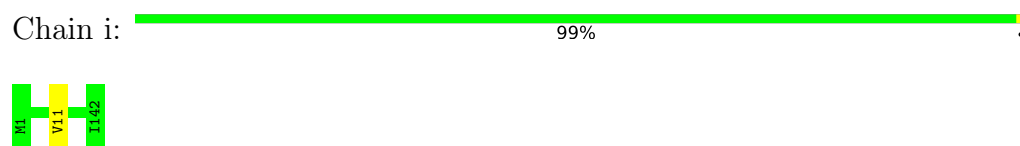
- Molecule 36: Large ribosomal subunit protein uL6



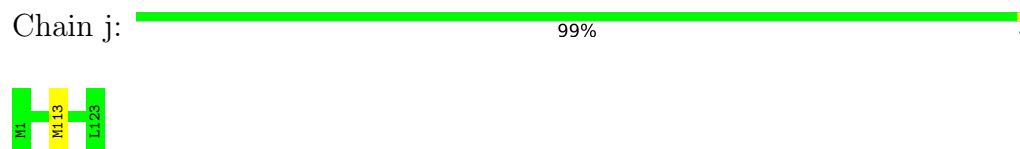
- Molecule 37: Large ribosomal subunit protein bL9



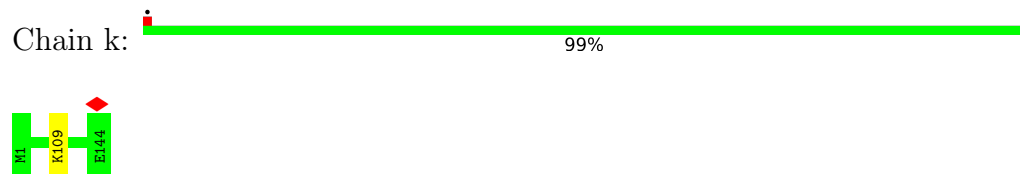
- Molecule 38: Large ribosomal subunit protein uL13



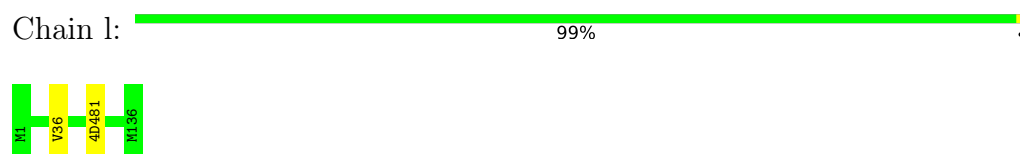
- Molecule 39: Large ribosomal subunit protein uL14



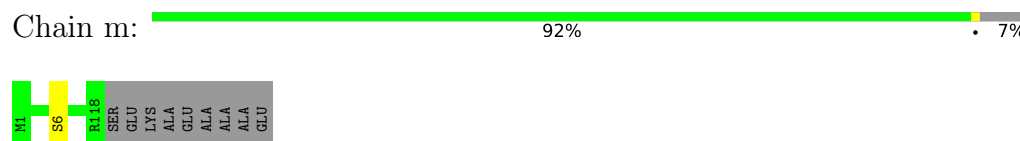
- Molecule 40: Large ribosomal subunit protein uL15



- Molecule 41: Large ribosomal subunit protein uL16



- Molecule 42: Large ribosomal subunit protein bL17



- Molecule 43: Large ribosomal subunit protein uL18





- Molecule 44: Large ribosomal subunit protein bL19

Chain o: 99%



- Molecule 45: Large ribosomal subunit protein bL20

Chain p: 99%



- Molecule 46: Large ribosomal subunit protein bL21

Chain q: 100%

There are no outlier residues recorded for this chain.

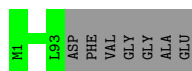
- Molecule 47: Large ribosomal subunit protein uL22

Chain r: 99%



- Molecule 48: Large ribosomal subunit protein uL23

Chain s: 93% 7%



- Molecule 49: Large ribosomal subunit protein uL24

Chain t: 5% 97%

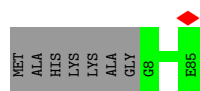
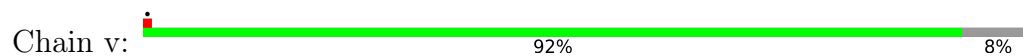


- Molecule 50: Large ribosomal subunit protein bL25

Chain u: 97%



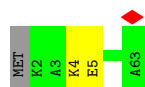
- Molecule 51: Large ribosomal subunit protein bL27



- Molecule 52: Large ribosomal subunit protein bL28



- Molecule 53: Large ribosomal subunit protein uL29



- Molecule 54: Large ribosomal subunit protein uL30



- Molecule 55: Large ribosomal subunit protein bL32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	506020	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	7.947	Depositor
Minimum map value	-2.498	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.093	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	409.36002, 409.36002, 409.36002	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.731, 0.731, 0.731	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, D2T, MEQ, ZN, UR3, 1MG, 4OC, 6MZ, MG, MA6, IAS, 5MC, 4D4, OMU, 3TD, TKW, AP7, 2MG, OMG, PSU, 2MA, K, OMC, CU1, G7M, 5MU, H2U

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.26	0/36573	0.38	0/57049
2	B	0.15	0/1848	0.32	0/2489
3	C	0.15	0/1651	0.28	0/2225
4	D	0.15	0/1665	0.29	0/2227
5	E	0.19	0/1179	0.33	0/1584
6	F	0.16	0/858	0.29	0/1160
7	G	0.15	0/1219	0.30	0/1635
8	H	0.18	0/989	0.32	0/1326
9	I	0.14	0/1048	0.27	0/1394
10	J	0.29	0/801	0.47	0/1082
11	K	0.16	0/884	0.31	0/1191
12	L	0.29	0/960	0.45	0/1286
13	M	0.12	0/919	0.28	0/1226
14	N	0.14	0/817	0.26	0/1088
15	O	0.31	0/722	0.45	0/964
16	P	0.17	0/653	0.34	0/877
17	Q	0.17	0/650	0.32	0/871
18	R	0.18	0/462	0.27	0/621
19	S	0.12	0/685	0.25	0/922
20	T	0.22	0/676	0.35	0/895
21	U	0.13	0/584	0.24	0/774
22	X	0.47	0/148	0.54	0/227
23	Z	0.29	0/1726	0.38	0/2689
24	0	0.23	0/434	0.42	0/576
25	1	0.63	0/380	0.88	0/498
26	2	0.36	0/513	0.60	0/676
27	3	0.29	0/303	0.41	0/397
28	5	0.13	0/993	0.35	0/1341
29	6	0.21	0/46	0.32	0/69
30	a	0.38	1/69290 (0.0%)	0.56	6/108088 (0.0%)
31	b	0.26	0/2873	0.34	0/4478

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.43	0/2121	0.58	0/2852
33	d	0.42	0/1576	0.56	0/2119
34	e	0.31	0/1571	0.50	0/2113
35	f	0.15	0/1434	0.32	0/1926
36	g	0.17	0/1343	0.33	1/1816 (0.1%)
37	h	0.17	0/1112	0.38	0/1503
38	i	0.31	0/1152	0.50	0/1551
39	j	0.30	0/956	0.47	0/1279
40	k	0.45	0/1062	0.63	0/1413
41	l	0.28	0/1073	0.47	1/1433 (0.1%)
42	m	0.59	0/958	0.78	0/1281
43	n	0.17	0/902	0.34	0/1209
44	o	0.29	0/929	0.48	0/1242
45	p	0.39	0/960	0.55	0/1278
46	q	0.39	0/829	0.61	0/1107
47	r	0.48	0/864	0.66	0/1156
48	s	0.33	0/744	0.50	0/994
49	t	0.22	0/797	0.38	0/1062
50	u	0.21	0/766	0.37	0/1025
51	v	0.32	0/599	0.47	0/792
52	w	0.40	0/635	0.73	2/848 (0.2%)
53	x	0.19	0/502	0.27	0/667
54	y	0.28	0/453	0.44	0/605
55	z	0.32	0/450	0.51	0/599
All	All	0.33	1/156337 (0.0%)	0.48	10/233795 (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
10	J	0	1
30	a	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2556	OMU	O3'-P	5.21	1.61	1.56

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	513	A	P-O3'-C3'	7.20	131.00	120.20
30	a	204	A	O3'-P-O5'	-7.05	93.42	104.00
30	a	2824	A	O3'-P-O5'	6.75	114.12	104.00
30	a	512	G	O4'-C1'-N9	6.24	117.56	108.20
52	w	17	ASN	CB-CA-C	-5.66	100.19	109.53
41	l	36	VAL	N-CA-C	-5.35	107.61	112.96
36	g	46	ALA	CB-CA-C	-5.22	110.13	117.23
30	a	1269	U	O3'-P-O5'	5.18	111.77	104.00
30	a	2066	A	C2'-C3'-O3'	5.13	117.20	109.50
52	w	17	ASN	N-CA-C	-5.12	101.36	109.96

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	37	ARG	Sidechain
30	a	512	G	Sidechain

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	
2	B	231/233 (99%)	225 (97%)	6 (3%)	0	100	100
3	C	204/233 (88%)	196 (96%)	8 (4%)	0	100	100
4	D	203/206 (98%)	202 (100%)	1 (0%)	0	100	100
5	E	156/167 (93%)	152 (97%)	4 (3%)	0	100	100
6	F	101/135 (75%)	99 (98%)	2 (2%)	0	100	100
7	G	151/179 (84%)	141 (93%)	10 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
9	I	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
10	J	97/103 (94%)	94 (97%)	2 (2%)	1 (1%)	12	3
11	K	113/129 (88%)	108 (96%)	5 (4%)	0	100	100
12	L	120/124 (97%)	118 (98%)	2 (2%)	0	100	100
13	M	115/118 (98%)	112 (97%)	3 (3%)	0	100	100
14	N	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
15	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	P	79/82 (96%)	77 (98%)	2 (2%)	0	100	100
17	Q	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
18	R	53/75 (71%)	53 (100%)	0	0	100	100
19	S	82/92 (89%)	81 (99%)	1 (1%)	0	100	100
20	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	U	67/71 (94%)	66 (98%)	1 (2%)	0	100	100
24	0	50/55 (91%)	49 (98%)	1 (2%)	0	100	100
25	1	44/46 (96%)	44 (100%)	0	0	100	100
26	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
27	3	36/38 (95%)	36 (100%)	0	0	100	100
28	5	132/141 (94%)	121 (92%)	11 (8%)	0	100	100
32	c	269/273 (98%)	260 (97%)	9 (3%)	0	100	100
33	d	206/209 (99%)	202 (98%)	4 (2%)	0	100	100
34	e	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
35	f	175/179 (98%)	170 (97%)	5 (3%)	0	100	100
36	g	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
37	h	146/149 (98%)	141 (97%)	5 (3%)	0	100	100
38	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
39	j	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
40	k	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
41	l	131/135 (97%)	126 (96%)	5 (4%)	0	100	100
42	m	116/127 (91%)	114 (98%)	2 (2%)	0	100	100
43	n	114/117 (97%)	112 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
45	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
46	q	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
47	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
48	s	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
49	t	101/104 (97%)	95 (94%)	6 (6%)	0	100	100
50	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
51	v	76/85 (89%)	74 (97%)	2 (3%)	0	100	100
52	w	75/78 (96%)	75 (100%)	0	0	100	100
53	x	60/63 (95%)	60 (100%)	0	0	100	100
54	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
55	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
All	All	5669/5975 (95%)	5527 (98%)	141 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	57	VAL

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	
2	B	192/192 (100%)	187 (97%)	5 (3%)	40	13
3	C	170/190 (90%)	169 (99%)	1 (1%)	78	64
4	D	172/173 (99%)	171 (99%)	1 (1%)	78	64
5	E	120/126 (95%)	119 (99%)	1 (1%)	73	56
6	F	90/116 (78%)	90 (100%)	0	100	100
7	G	126/147 (86%)	124 (98%)	2 (2%)	55	28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	104/105 (99%)	102 (98%)	2 (2%)	50	22
9	I	106/107 (99%)	105 (99%)	1 (1%)	70	51
10	J	86/90 (96%)	83 (96%)	3 (4%)	32	7
11	K	89/98 (91%)	88 (99%)	1 (1%)	65	43
12	L	102/103 (99%)	100 (98%)	2 (2%)	48	20
13	M	95/96 (99%)	93 (98%)	2 (2%)	47	19
14	N	83/84 (99%)	83 (100%)	0	100	100
15	O	76/77 (99%)	75 (99%)	1 (1%)	61	36
16	P	65/65 (100%)	65 (100%)	0	100	100
17	Q	73/78 (94%)	72 (99%)	1 (1%)	59	33
18	R	48/65 (74%)	47 (98%)	1 (2%)	47	19
19	S	72/79 (91%)	71 (99%)	1 (1%)	59	33
20	T	65/66 (98%)	64 (98%)	1 (2%)	57	31
21	U	59/61 (97%)	59 (100%)	0	100	100
24	0	47/49 (96%)	47 (100%)	0	100	100
25	1	38/38 (100%)	38 (100%)	0	100	100
26	2	51/52 (98%)	51 (100%)	0	100	100
27	3	34/34 (100%)	33 (97%)	1 (3%)	37	10
28	5	104/109 (95%)	103 (99%)	1 (1%)	68	47
32	c	216/218 (99%)	216 (100%)	0	100	100
33	d	163/163 (100%)	162 (99%)	1 (1%)	78	64
34	e	165/165 (100%)	163 (99%)	2 (1%)	63	40
35	f	148/150 (99%)	147 (99%)	1 (1%)	76	59
36	g	137/138 (99%)	133 (97%)	4 (3%)	37	10
37	h	113/114 (99%)	111 (98%)	2 (2%)	51	24
38	i	116/116 (100%)	115 (99%)	1 (1%)	70	51
39	j	104/104 (100%)	103 (99%)	1 (1%)	68	47
40	k	103/103 (100%)	102 (99%)	1 (1%)	68	47
41	l	107/107 (100%)	107 (100%)	0	100	100
42	m	98/103 (95%)	97 (99%)	1 (1%)	68	47
43	n	86/87 (99%)	85 (99%)	1 (1%)	63	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	o	99/100 (99%)	99 (100%)	0	100	100
45	p	89/90 (99%)	89 (100%)	0	100	100
46	q	84/84 (100%)	84 (100%)	0	100	100
47	r	93/93 (100%)	92 (99%)	1 (1%)	65	43
48	s	80/84 (95%)	80 (100%)	0	100	100
49	t	84/85 (99%)	82 (98%)	2 (2%)	43	15
50	u	78/78 (100%)	75 (96%)	3 (4%)	29	5
51	v	59/63 (94%)	59 (100%)	0	100	100
52	w	67/68 (98%)	67 (100%)	0	100	100
53	x	54/55 (98%)	52 (96%)	2 (4%)	30	6
54	y	48/49 (98%)	48 (100%)	0	100	100
55	z	47/48 (98%)	47 (100%)	0	100	100
All	All	4705/4865 (97%)	4654 (99%)	51 (1%)	63	43

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	10	LEU
2	B	36	ASN
2	B	42	ASN
2	B	52	GLU
2	B	145	GLU
3	C	121	THR
4	D	44	ARG
5	E	142	ASP
7	G	22	LEU
7	G	136	LYS
8	H	50	LYS
8	H	54	ASP
9	I	58	VAL
10	J	31	ARG
10	J	36	VAL
10	J	40	ILE
11	K	75	LYS
12	L	15	LYS
12	L	44	LYS
13	M	3	ARG
13	M	117	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	O	80	GLN
17	Q	42	THR
18	R	66	SER
19	S	12	ASP
20	T	4	ILE
27	3	36	ARG
28	5	140	VAL
33	d	1	MET
34	e	107	SER
34	e	198	GLU
35	f	17	MET
36	g	6	LYS
36	g	17	VAL
36	g	51	THR
36	g	81	GLU
37	h	83	LYS
37	h	138	VAL
38	i	11	VAL
39	j	113	MET
40	k	109	LYS
42	m	6	SER
43	n	20	GLU
47	r	66	ILE
49	t	27	ASN
49	t	52	LEU
50	u	41	GLU
50	u	61	LEU
50	u	65	VAL
53	x	4	LYS
53	x	5	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	42	ASN
2	B	58	ASN
2	B	227	GLN
4	D	74	ASN
4	D	116	GLN
4	D	198	HIS
5	E	121	HIS
6	F	55	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	4	GLN
9	I	32	GLN
10	J	58	ASN
11	K	22	HIS
11	K	38	GLN
11	K	118	HIS
14	N	4	GLN
14	N	60	GLN
15	O	38	HIS
15	O	40	GLN
18	R	52	GLN
18	R	54	GLN
20	T	13	GLN
20	T	70	ASN
25	1	26	ASN
27	3	13	ASN
28	5	30	GLN
32	c	86	ASN
32	c	117	GLN
32	c	134	ASN
32	c	153	GLN
34	e	94	GLN
34	e	115	GLN
34	e	156	ASN
35	f	5	HIS
36	g	30	ASN
36	g	73	ASN
37	h	18	GLN
37	h	66	ASN
38	i	131	ASN
38	i	138	GLN
41	l	3	GLN
42	m	107	ASN
43	n	98	GLN
43	n	116	GLN
44	o	3	ASN
44	o	10	GLN
44	o	52	ASN
46	q	6	GLN
47	r	31	GLN
48	s	92	ASN
49	t	46	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	t	74	ASN
50	u	5	ASN
50	u	49	ASN
50	u	75	GLN
53	x	15	ASN
53	x	20	ASN
53	x	31	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1532/1554 (98%)	189 (12%)	11 (0%)
22	X	5/6 (83%)	0	0
23	Z	76/77 (98%)	11 (14%)	0
29	6	1/2 (50%)	1 (100%)	0
30	a	2904/2908 (99%)	319 (10%)	0
31	b	119/120 (99%)	8 (6%)	0
All	All	4637/4667 (99%)	528 (11%)	11 (0%)

All (528) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	A
1	A	4	U
1	A	9	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	72	A
1	A	73	C
1	A	74	A
1	A	83	C
1	A	84	U
1	A	86	G
1	A	92	U
1	A	95	C
1	A	96	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	120	A
1	A	121	U
1	A	131	A
1	A	143	A
1	A	144	G
1	A	149	A
1	A	177	G
1	A	182	A
1	A	183	C
1	A	197	A
1	A	204	G
1	A	205	A
1	A	206	C
1	A	207	C
1	A	208	U
1	A	209	U
1	A	210	A
1	A	213	G
1	A	214	C
1	A	226	G
1	A	240	G
1	A	245	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	306	A
1	A	321	A
1	A	328	C
1	A	329	A
1	A	339	C
1	A	347	G
1	A	352	C
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	384	G
1	A	406	G
1	A	412	A
1	A	413	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	414	A
1	A	415	A
1	A	421	U
1	A	422	C
1	A	423	G
1	A	429	U
1	A	436	C
1	A	453	G
1	A	457	G
1	A	458	U
1	A	467	U
1	A	468	A
1	A	469	C
1	A	478	A
1	A	481	G
1	A	484	G
1	A	486	U
1	A	495	A
1	A	496	A
1	A	497	G
1	A	511	C
1	A	518	C
1	A	521	G
1	A	527	G7M
1	A	531	U
1	A	532	A
1	A	547	A
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	633	G
1	A	650	G
1	A	653	U
1	A	665	A
1	A	703	G
1	A	723	U
1	A	724	G
1	A	747	A
1	A	755	G
1	A	777	A
1	A	793	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	794	A
1	A	815	A
1	A	817	C
1	A	821	G
1	A	843	U
1	A	849	G
1	A	890	G
1	A	914	A
1	A	926	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	966	2MG
1	A	969	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	992	U
1	A	1004	A
1	A	1008	U
1	A	1014	A
1	A	1015	G
1	A	1017	U
1	A	1020	G
1	A	1029	U
1	A	1030	U
1	A	1031	C
1	A	1034	G
1	A	1035	A
1	A	1036	A
1	A	1042	A
1	A	1044	A
1	A	1053	G
1	A	1065	U
1	A	1085	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1124	G
1	A	1125	U
1	A	1132	C
1	A	1134	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1137	C
1	A	1139	G
1	A	1140	C
1	A	1159	U
1	A	1167	A
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1227	A
1	A	1238	A
1	A	1258	G
1	A	1260	G
1	A	1280	A
1	A	1285	A
1	A	1286	U
1	A	1287	A
1	A	1300	G
1	A	1302	C
1	A	1317	C
1	A	1320	C
1	A	1338	G
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1370	G
1	A	1378	C
1	A	1379	G
1	A	1398	A
1	A	1419	G
1	A	1422	G
1	A	1441	A
1	A	1446	A
1	A	1451	U
1	A	1452	C
1	A	1453	G
1	A	1493	A
1	A	1497	G
1	A	1503	A
1	A	1505	G
1	A	1506	U
1	A	1517	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1529	G
1	A	1530	G
23	Z	2	G
23	Z	9	G
23	Z	18	G
23	Z	20	H2U
23	Z	21	A
23	Z	22	G
23	Z	46	G
23	Z	51	C
23	Z	58	A
23	Z	64	G
23	Z	76	A
29	6	76	A
30	a	2	G
30	a	10	A
30	a	34	U
30	a	42	A
30	a	63	A
30	a	71	A
30	a	74	A
30	a	75	G
30	a	101	A
30	a	102	U
30	a	118	A
30	a	119	A
30	a	120	U
30	a	125	A
30	a	131	A
30	a	136	G
30	a	139	U
30	a	140	C
30	a	142	A
30	a	163	C
30	a	165	A
30	a	181	A
30	a	196	A
30	a	199	A
30	a	200	U
30	a	215	G
30	a	216	A
30	a	221	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	222	A
30	a	248	G
30	a	272	A
30	a	276	U
30	a	278	A
30	a	279	A
30	a	281	C
30	a	311	A
30	a	329	G
30	a	330	A
30	a	345	A
30	a	361	G
30	a	367	G
30	a	386	G
30	a	405	U
30	a	411	G
30	a	412	A
30	a	456	C
30	a	481	G
30	a	490	C
30	a	491	G
30	a	505	A
30	a	509	C
30	a	530	G
30	a	531	C
30	a	532	A
30	a	550	U
30	a	565	A
30	a	575	U
30	a	577	A
30	a	588	A
30	a	605	A
30	a	617	U
30	a	629	A
30	a	639	A
30	a	647	C
30	a	648	U
30	a	649	G
30	a	655	U
30	a	656	A
30	a	657	A
30	a	688	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	719	C
30	a	732	A
30	a	749	5MU
30	a	766	A
30	a	767	C
30	a	777	G
30	a	778	G
30	a	784	A
30	a	786	G
30	a	787	G
30	a	807	G
30	a	814	C
30	a	829	U
30	a	830	U
30	a	848	U
30	a	861	G
30	a	884	G
30	a	887	C
30	a	890	C
30	a	892	C
30	a	893	G
30	a	894	A
30	a	897	U
30	a	898	A
30	a	899	C
30	a	901	A
30	a	912	A
30	a	916	G
30	a	933	U
30	a	948	C
30	a	963	C
30	a	976	G
30	a	985	A
30	a	986	A
30	a	987	C
30	a	998	A
30	a	1014	U
30	a	1015	C
30	a	1024	G
30	a	1028	G
30	a	1035	U
30	a	1049	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	1072	A
30	a	1073	G
30	a	1082	A
30	a	1084	U
30	a	1085	U
30	a	1090	A
30	a	1108	G
30	a	1109	G
30	a	1112	G
30	a	1113	A
30	a	1114	G
30	a	1118	G
30	a	1124	G
30	a	1130	G
30	a	1131	A
30	a	1134	U
30	a	1135	A
30	a	1137	C
30	a	1144	A
30	a	1173	G
30	a	1177	A
30	a	1178	U
30	a	1179	G
30	a	1189	G
30	a	1190	U
30	a	1255	A
30	a	1258	G
30	a	1273	G
30	a	1274	A
30	a	1275	U
30	a	1302	G
30	a	1303	A
30	a	1354	U
30	a	1367	A
30	a	1381	U
30	a	1385	A
30	a	1412	G
30	a	1418	G
30	a	1430	C
30	a	1436	A
30	a	1454	G
30	a	1455	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	1462	U
30	a	1484	G
30	a	1495	C
30	a	1499	U
30	a	1510	A
30	a	1511	A
30	a	1512	G
30	a	1517	A
30	a	1531	G
30	a	1537	A
30	a	1538	C
30	a	1539	G
30	a	1568	A
30	a	1571	A
30	a	1580	U
30	a	1585	A
30	a	1586	U
30	a	1587	C
30	a	1610	A
30	a	1624	G
30	a	1649	U
30	a	1650	U
30	a	1651	G
30	a	1676	G
30	a	1717	G
30	a	1731	U
30	a	1732	C
30	a	1734	C
30	a	1740	G
30	a	1746	A
30	a	1766	C
30	a	1775	A
30	a	1784	U
30	a	1802	C
30	a	1803	A
30	a	1810	A
30	a	1818	C
30	a	1831	A
30	a	1849	A
30	a	1850	A
30	a	1860	A
30	a	1876	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	1877	G
30	a	1910	G
30	a	1911	G
30	a	1917	A
30	a	1918	C
30	a	1933	G
30	a	1934	G
30	a	1941	A
30	a	1942	A
30	a	1959	U
30	a	1971	C
30	a	1974	A
30	a	1975	U
30	a	1976	G
30	a	1995	U
30	a	1997	U
30	a	2027	C
30	a	2031	G
30	a	2035	A
30	a	2037	A
30	a	2047	C
30	a	2059	C
30	a	2060	G
30	a	2064	A
30	a	2065	G
30	a	2066	A
30	a	2073	G7M
30	a	2114	G
30	a	2115	U
30	a	2116	G
30	a	2119	G
30	a	2121	A
30	a	2122	U
30	a	2127	G
30	a	2128	G
30	a	2130	A
30	a	2131	G
30	a	2135	U
30	a	2136	U
30	a	2137	G
30	a	2146	A
30	a	2151	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	2161	G
30	a	2162	A
30	a	2163	G
30	a	2167	A
30	a	2168	C
30	a	2169	C
30	a	2172	G
30	a	2173	A
30	a	2175	A
30	a	2176	U
30	a	2177	A
30	a	2193	U
30	a	2194	G
30	a	2195	A
30	a	2202	A
30	a	2208	G
30	a	2215	G
30	a	2229	A
30	a	2242	G
30	a	2243	G
30	a	2272	A
30	a	2287	C
30	a	2291	A
30	a	2309	U
30	a	2312	G
30	a	2326	A
30	a	2329	G
30	a	2337	A
30	a	2339	A
30	a	2351	C
30	a	2387	G
30	a	2389	C
30	a	2400	G
30	a	2406	U
30	a	2410	A
30	a	2426	C
30	a	2429	A
30	a	2433	G
30	a	2434	A
30	a	2435	U
30	a	2439	A
30	a	2445	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	a	2452	A
30	a	2474	G
30	a	2482	A
30	a	2486	A
30	a	2495	U
30	a	2509	G
30	a	2522	A
30	a	2529	G
30	a	2533	G
30	a	2539	G
30	a	2551	A
30	a	2570	A
30	a	2571	G
30	a	2577	C
30	a	2606	A
30	a	2613	U
30	a	2617	U
30	a	2633	U
30	a	2634	G
30	a	2667	G
30	a	2686	A
30	a	2693	U
30	a	2694	U
30	a	2718	G
30	a	2728	U
30	a	2730	A
30	a	2748	G
30	a	2752	A
30	a	2769	A
30	a	2782	A
30	a	2802	U
30	a	2824	A
30	a	2825	A
30	a	2839	A
30	a	2865	U
30	a	2887	A
30	a	2888	U
30	a	2906	C
30	a	2907	U
31	b	35	C
31	b	45	A
31	b	56	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	b	67	G
31	b	89	U
31	b	90	C
31	b	99	A
31	b	109	A

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	62	U
1	A	182	A
1	A	199	A
1	A	213	G
1	A	766	A
1	A	778	G
1	A	786	G
1	A	793	U
1	A	1035	A
1	A	1108	G
1	A	1124	G

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

46 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	MA6	A	1519	1	23,26,27	0.47	0	34,38,41	0.94	1 (2%)
30	2MG	a	1837	30	23,26,27	0.39	0	32,38,41	0.46	0
1	PSU	A	516	1,57	18,21,22	1.01	1 (5%)	22,30,33	0.77	1 (4%)
30	OMG	a	2255	30,56,23	23,26,27	0.27	0	33,38,41	0.42	0
30	PSU	a	2508	30,56	18,21,22	0.95	1 (5%)	22,30,33	0.86	0
30	PSU	a	2584	30	18,21,22	1.05	2 (11%)	22,30,33	0.79	1 (4%)
1	5MC	A	1407	1	18,22,23	0.41	0	26,32,35	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	5MU	a	749	30	19,22,23	0.40	0	28,32,35	0.49	0
41	4D4	l	81	41	9,11,12	0.45	0	8,13,15	1.10	1 (12%)
30	G7M	a	2073	30,56	23,26,27	0.75	1 (4%)	35,39,42	0.70	1 (2%)
1	4OC	A	1402	1	20,23,24	0.47	0	26,32,35	0.63	0
30	PSU	a	1921	30	18,21,22	1.02	1 (5%)	22,30,33	0.74	0
30	6MZ	a	2034	30	22,25,26	0.40	0	30,36,39	0.70	0
30	OMC	a	2502	57,30	19,22,23	0.35	0	26,31,34	0.60	0
23	4SU	Z	8	23	18,21,22	0.43	0	26,30,33	1.11	2 (7%)
30	5MC	a	1966	30,56	18,22,23	0.43	0	26,32,35	0.56	0
30	TKW	a	2505	30,56	18,22,23	0.55	0	28,32,35	1.08	1 (3%)
30	2MA	a	2507	57,30,56	22,25,26	0.82	1 (4%)	33,37,40	1.13	4 (12%)
1	2MG	A	1207	1,56	23,26,27	0.39	0	32,38,41	0.42	0
30	PSU	a	748	57,30	18,21,22	1.04	1 (5%)	22,30,33	0.52	0
30	3TD	a	1919	30	18,22,23	2.89	1 (5%)	22,32,35	0.93	1 (4%)
30	PSU	a	2609	30	18,21,22	0.99	1 (5%)	22,30,33	0.89	0
30	OMU	a	2556	57,30	19,22,23	0.27	0	26,31,34	0.46	0
30	PSU	a	957	30	18,21,22	1.02	1 (5%)	22,30,33	0.77	0
1	MA6	A	1518	1	23,26,27	0.30	0	34,38,41	0.74	1 (2%)
33	MEQ	d	150	33	8,9,10	0.41	0	5,10,12	0.51	0
23	PSU	Z	55	23	18,21,22	0.99	1 (5%)	22,30,33	0.78	0
30	H2U	a	2453	30	18,21,22	0.58	0	21,30,33	0.73	0
1	5MC	A	967	1	18,22,23	0.37	0	26,32,35	0.54	0
1	UR3	A	1498	1	19,22,23	0.37	0	26,32,35	0.83	1 (3%)
23	H2U	Z	20	23	18,21,22	0.50	0	21,30,33	0.67	0
30	6MZ	a	1620	30	22,25,26	0.37	0	30,36,39	0.63	0
23	OMC	Z	32	23	19,22,23	0.40	0	26,31,34	0.58	0
30	2MG	a	2449	30	23,26,27	0.41	0	32,38,41	0.53	0
30	PSU	a	2461	30	18,21,22	1.02	1 (5%)	22,30,33	0.71	0
11	IAS	K	119	11	6,7,8	0.96	0	6,8,10	1.28	1 (16%)
30	PSU	a	2608	30	18,21,22	1.02	1 (5%)	22,30,33	0.94	0
12	D2T	L	89	12	7,9,10	1.00	0	6,11,13	1.84	3 (50%)
30	PSU	a	1915	30	18,21,22	0.97	1 (5%)	22,30,33	0.74	0
1	G7M	A	527	1,56	23,26,27	0.67	1 (4%)	35,39,42	0.63	0
30	5MU	a	1943	30,56	19,22,23	0.42	0	28,32,35	0.49	0
1	2MG	A	966	1	23,26,27	0.38	0	32,38,41	0.47	0
30	AP7	a	2454	30	21,24,25	0.39	0	31,35,38	0.91	2 (6%)
30	1MG	a	747	30	22,26,27	0.48	0	33,39,42	0.74	0
1	2MG	A	1516	1	23,26,27	0.44	0	32,38,41	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	5MU	Z	54	23	19,22,23	0.38	0	28,32,35	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	A	1519	1	-	1/11/29/30	0/3/3/3
30	2MG	a	1837	30	-	0/9/27/28	0/3/3/3
1	PSU	A	516	1,57	-	0/7/25/26	0/2/2/2
30	OMG	a	2255	30,56,23	-	1/9/27/28	0/3/3/3
30	PSU	a	2508	30,56	-	0/7/25/26	0/2/2/2
30	PSU	a	2584	30	-	0/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
30	5MU	a	749	30	-	0/7/25/26	0/2/2/2
41	4D4	l	81	41	-	0/11/12/14	-
30	G7M	a	2073	30,56	-	2/7/25/26	0/3/3/3
1	4OC	A	1402	1	-	0/9/29/30	0/2/2/2
30	PSU	a	1921	30	-	0/7/25/26	0/2/2/2
30	6MZ	a	2034	30	-	2/9/27/28	0/3/3/3
30	OMC	a	2502	57,30	-	0/9/27/28	0/2/2/2
23	4SU	Z	8	23	-	1/7/25/26	0/2/2/2
30	5MC	a	1966	30,56	-	0/7/25/26	0/2/2/2
30	TKW	a	2505	30,56	-	3/7/25/26	0/2/2/2
30	2MA	a	2507	57,30,56	-	2/7/25/26	0/3/3/3
1	2MG	A	1207	1,56	-	0/9/27/28	0/3/3/3
30	PSU	a	748	57,30	-	1/7/25/26	0/2/2/2
30	3TD	a	1919	30	-	0/7/25/26	0/2/2/2
30	PSU	a	2609	30	-	0/7/25/26	0/2/2/2
30	OMU	a	2556	57,30	-	0/9/27/28	0/2/2/2
30	PSU	a	957	30	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/11/29/30	0/3/3/3
33	MEQ	d	150	33	-	3/8/9/11	-
23	PSU	Z	55	23	-	0/7/25/26	0/2/2/2
30	H2U	a	2453	30	-	0/7/38/39	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
23	H2U	Z	20	23	-	3/7/38/39	0/2/2/2
30	6MZ	a	1620	30	-	0/9/27/28	0/3/3/3
23	OMC	Z	32	23	-	2/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	2MG	a	2449	30	-	0/9/27/28	0/3/3/3
30	PSU	a	2461	30	-	0/7/25/26	0/2/2/2
11	IAS	K	119	11	-	1/7/7/8	-
30	PSU	a	2608	30	-	0/7/25/26	0/2/2/2
12	D2T	L	89	12	-	3/7/12/14	-
30	PSU	a	1915	30	-	0/7/25/26	0/2/2/2
1	G7M	A	527	1,56	-	3/7/25/26	0/3/3/3
30	5MU	a	1943	30,56	-	0/7/25/26	0/2/2/2
1	2MG	A	966	1	-	0/9/27/28	0/3/3/3
30	AP7	a	2454	30	-	0/7/25/26	0/3/3/3
30	1MG	a	747	30	-	0/7/25/26	0/3/3/3
1	2MG	A	1516	1	-	0/9/27/28	0/3/3/3
23	5MU	Z	54	23	-	0/7/25/26	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	1919	3TD	C6-C5	11.98	1.49	1.35
23	Z	55	PSU	C6-C5	3.47	1.39	1.35
30	a	957	PSU	C6-C5	3.47	1.39	1.35
30	a	1921	PSU	C6-C5	3.44	1.39	1.35
1	A	516	PSU	C6-C5	3.41	1.39	1.35
30	a	1915	PSU	C6-C5	3.39	1.39	1.35
30	a	2461	PSU	C6-C5	3.38	1.39	1.35
30	a	748	PSU	C6-C5	3.37	1.39	1.35
30	a	2584	PSU	C6-C5	3.22	1.39	1.35
30	a	2608	PSU	C6-C5	3.21	1.39	1.35
30	a	2508	PSU	C6-C5	3.15	1.39	1.35
30	a	2609	PSU	C6-C5	3.07	1.38	1.35
30	a	2073	G7M	C8-N7	2.43	1.37	1.33
30	a	2507	2MA	C6-N6	-2.39	1.28	1.34
1	A	527	G7M	C8-N7	2.32	1.37	1.33
30	a	2584	PSU	O4'-C1'	-2.09	1.40	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	2505	TKW	OAC-C5-C4	4.05	120.54	114.43
23	Z	8	4SU	C4-N3-C2	-3.75	123.69	127.34
1	A	1518	MA6	C2-N1-C6	3.24	119.41	111.75
30	a	2507	2MA	C2-N1-C6	3.00	122.76	118.08
1	A	1519	MA6	C2-N1-C6	2.95	118.73	111.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	2454	AP7	N6-C6-N1	2.88	122.78	118.70
41	l	81	4D4	O-C-CA	-2.85	117.30	124.78
12	L	89	D2T	OD1-CG-CB	-2.65	116.88	122.44
12	L	89	D2T	O-C-CA	-2.63	117.89	124.78
30	a	2507	2MA	N3-C2-N1	-2.59	120.96	125.72
30	a	2507	2MA	C5-C4-N3	-2.55	124.33	127.19
23	Z	8	4SU	C5-C4-N3	2.55	117.05	114.69
30	a	1919	3TD	C5-C6-N1	-2.48	118.39	122.11
11	K	119	IAS	OD1-CG-CB	-2.46	118.26	125.43
30	a	2584	PSU	O4'-C1'-C2'	2.38	108.50	105.14
30	a	2454	AP7	C2-N1-C6	2.33	121.96	118.61
30	a	2507	2MA	CM2-C2-N1	2.32	120.77	117.15
1	A	1498	UR3	C6-N1-C2	-2.28	119.75	121.79
1	A	516	PSU	O4'-C1'-C2'	2.27	108.35	105.14
12	L	89	D2T	OD2-CG-CB	2.21	117.92	113.15
30	a	2073	G7M	N9-C8-N7	-2.12	106.97	112.21

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	G7M	C3'-C4'-C5'-O5'
23	Z	20	H2U	O4'-C1'-N1-C6
30	a	748	PSU	O4'-C1'-C5-C6
30	a	2034	6MZ	O4'-C4'-C5'-O5'
23	Z	20	H2U	O4'-C1'-N1-C2
30	a	2034	6MZ	C3'-C4'-C5'-O5'
33	d	150	MEQ	NE2-CD-CG-CB
33	d	150	MEQ	OE1-CD-CG-CB
1	A	527	G7M	O4'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C10
30	a	2505	TKW	O4'-C1'-N1-C6
33	d	150	MEQ	CA-CB-CG-CD
30	a	2505	TKW	C2'-C1'-N1-C6
1	A	527	G7M	C4'-C5'-O5'-P
30	a	2073	G7M	C4'-C5'-O5'-P
30	a	2505	TKW	O4'-C1'-N1-C2
11	K	119	IAS	N-CA-CB-CG
12	L	89	D2T	CA-CB-SB-CB1
12	L	89	D2T	SB-CB-CG-OD2
23	Z	32	OMC	C1'-C2'-O2'-CM2
30	a	2255	OMG	C1'-C2'-O2'-CM2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	Z	8	4SU	C2'-C1'-N1-C2
23	Z	20	H2U	O4'-C4'-C5'-O5'
12	L	89	D2T	CG-CB-SB-CB1
23	Z	32	OMC	C2'-C1'-N1-C2
30	a	2073	G7M	O4'-C4'-C5'-O5'
30	a	2507	2MA	C4'-C5'-O5'-P
30	a	2507	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 656 ligands modelled in this entry, 656 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
41	l	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	81:4D4	C	83:GLY	N	3.91

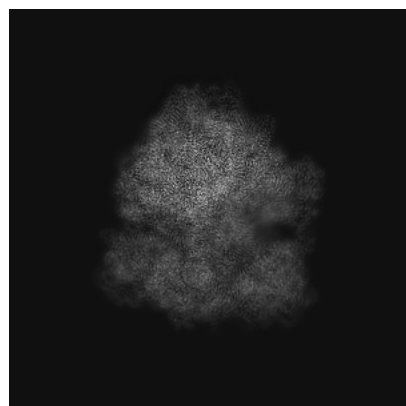
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15793. These allow visual inspection of the internal detail of the map and identification of artifacts.

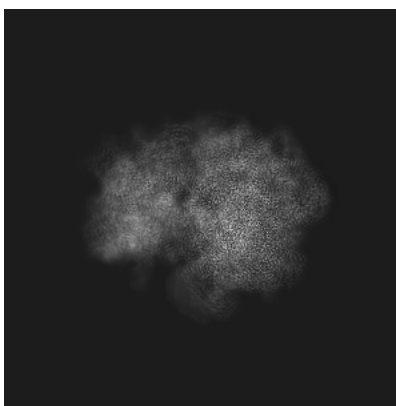
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

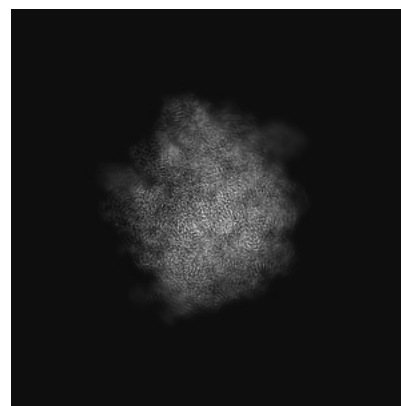
6.1.1 Primary map



X

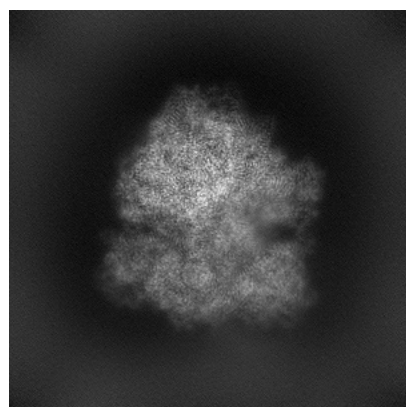


Y

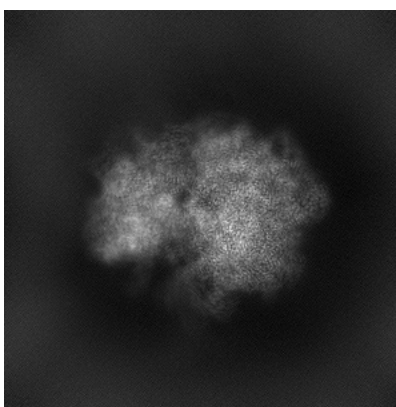


Z

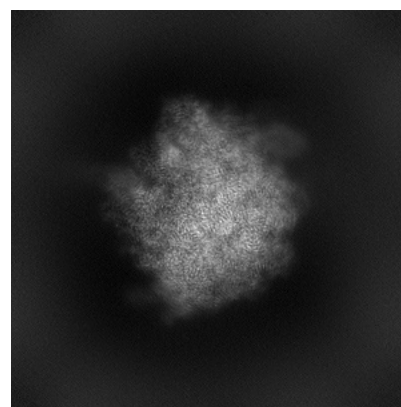
6.1.2 Raw map



X



Y

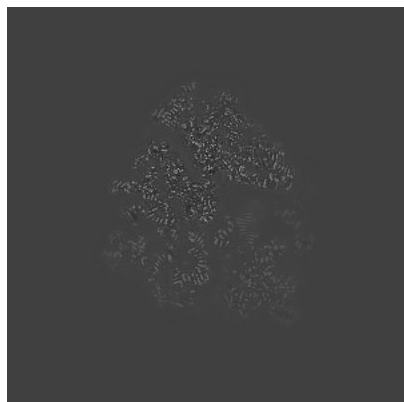


Z

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

6.2 Central slices [i](#)

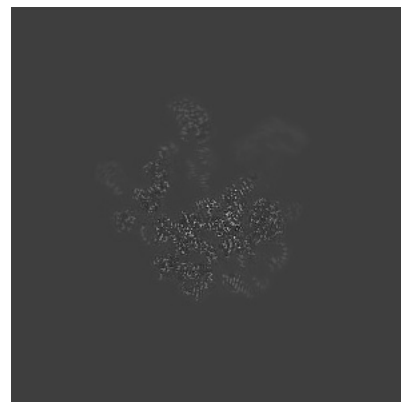
6.2.1 Primary map



X Index: 280

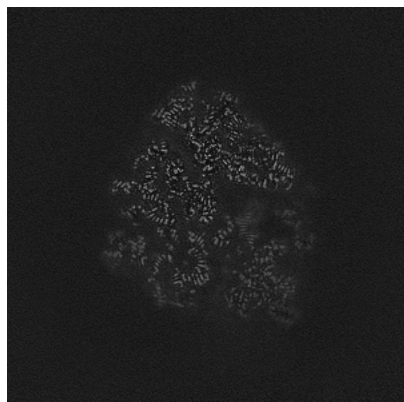


Y Index: 280

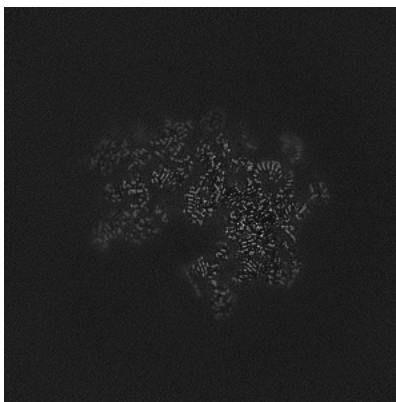


Z Index: 280

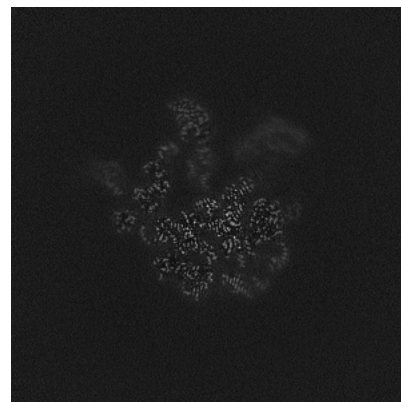
6.2.2 Raw map



X Index: 280



Y Index: 280

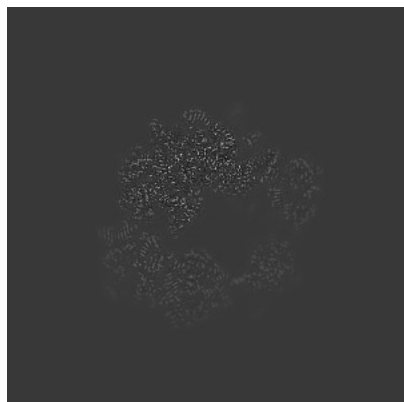


Z Index: 280

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

6.3 Largest variance slices [i](#)

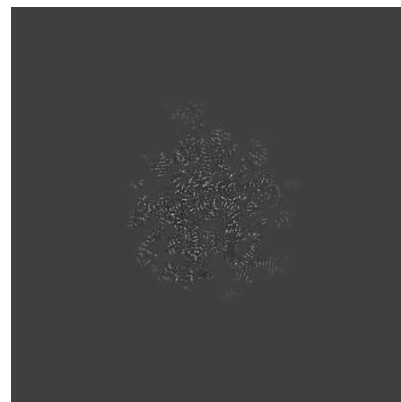
6.3.1 Primary map



X Index: 246

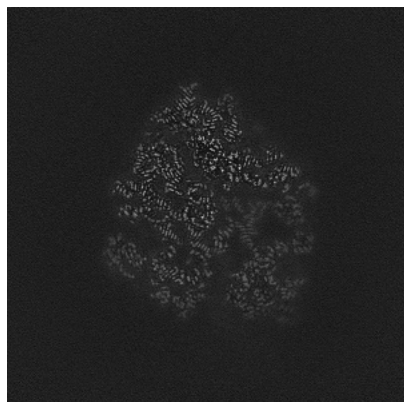


Y Index: 260

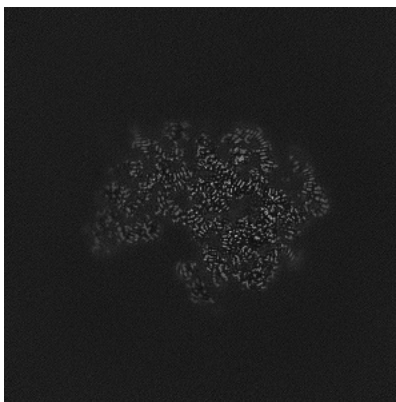


Z Index: 342

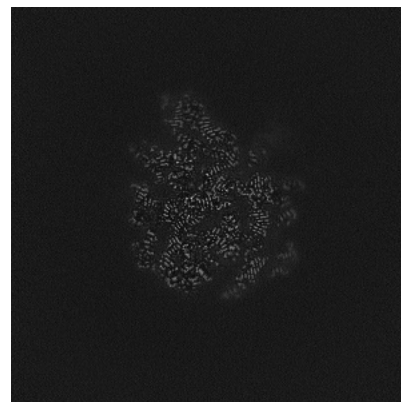
6.3.2 Raw map



X Index: 274



Y Index: 260

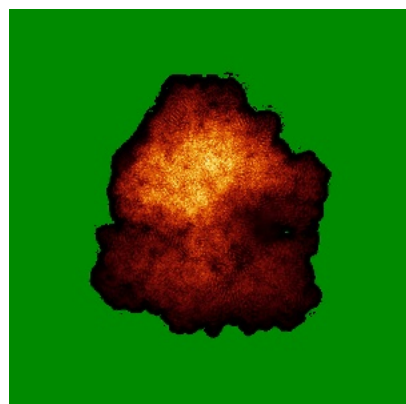


Z Index: 334

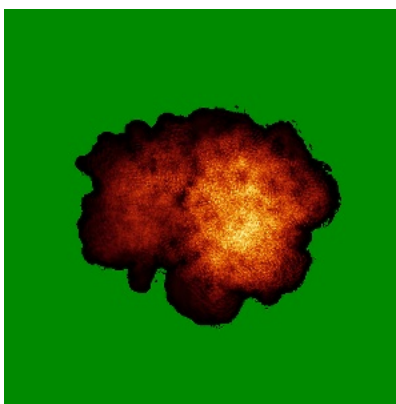
The images above show the largest variance slices of the map in three orthogonal directions.

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

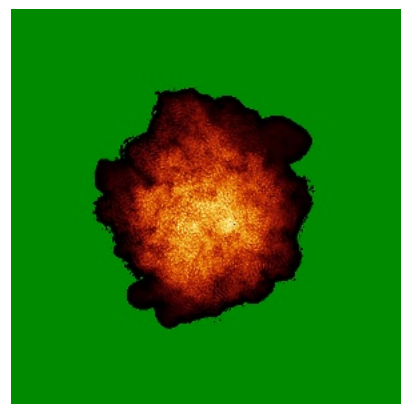
6.4.1 Primary map



X

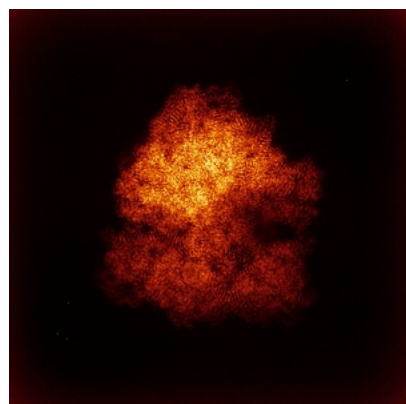


Y

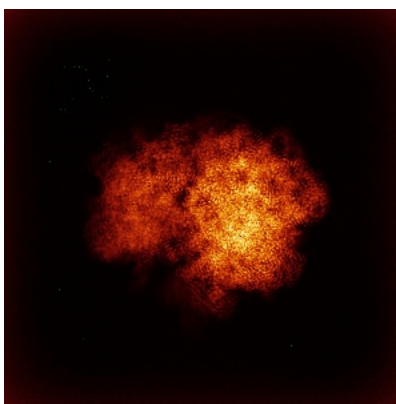


Z

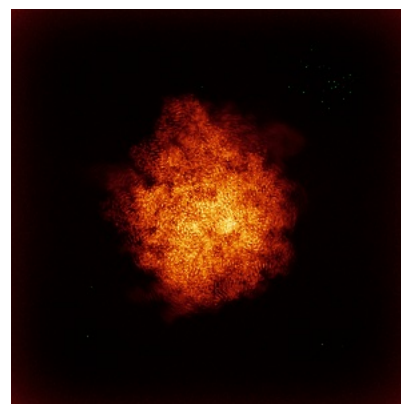
6.4.2 Raw map



X



Y

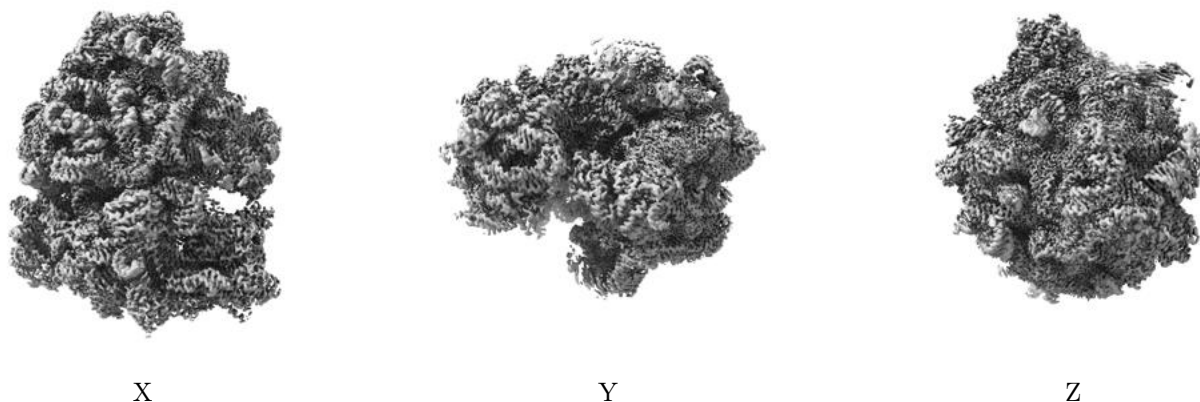


Z

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.

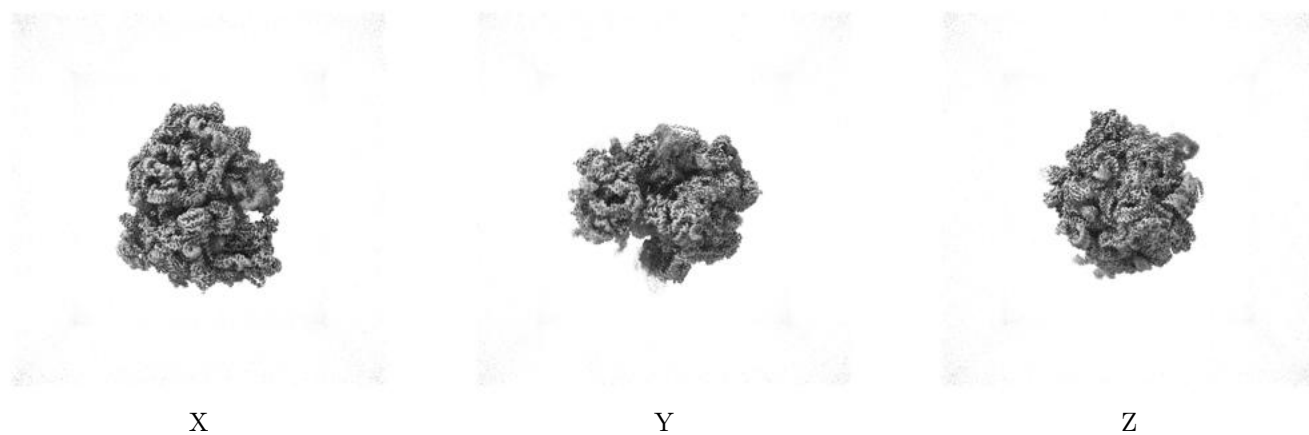
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

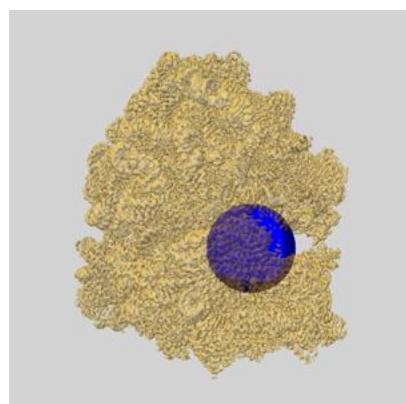
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

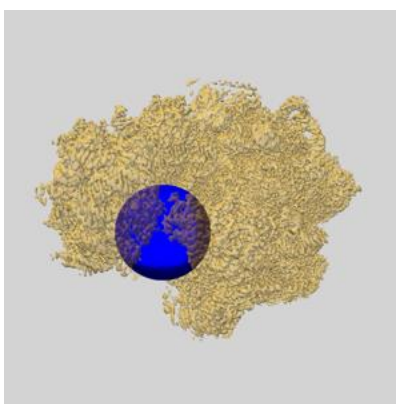
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

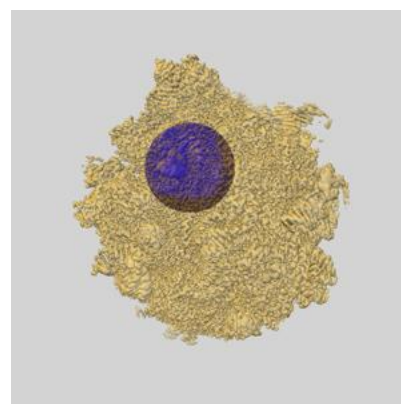
6.6.1 emd_15793_msk_1.map [i](#)



X

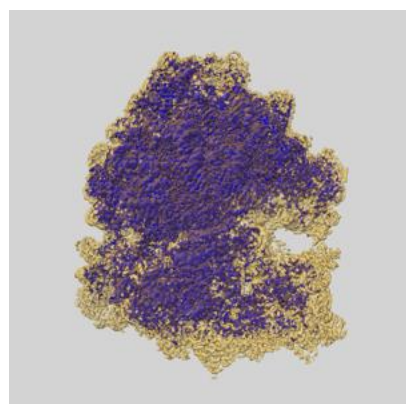


Y

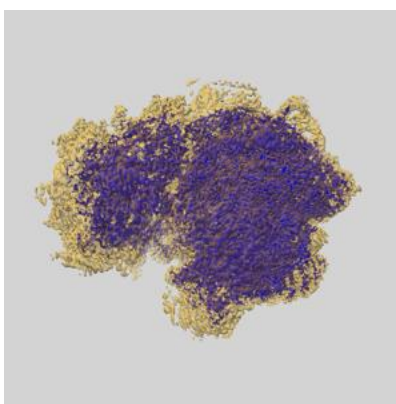


Z

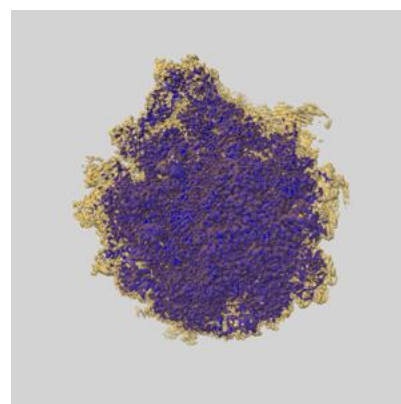
6.6.2 emd_15793_msk_2.map [i](#)



X



Y

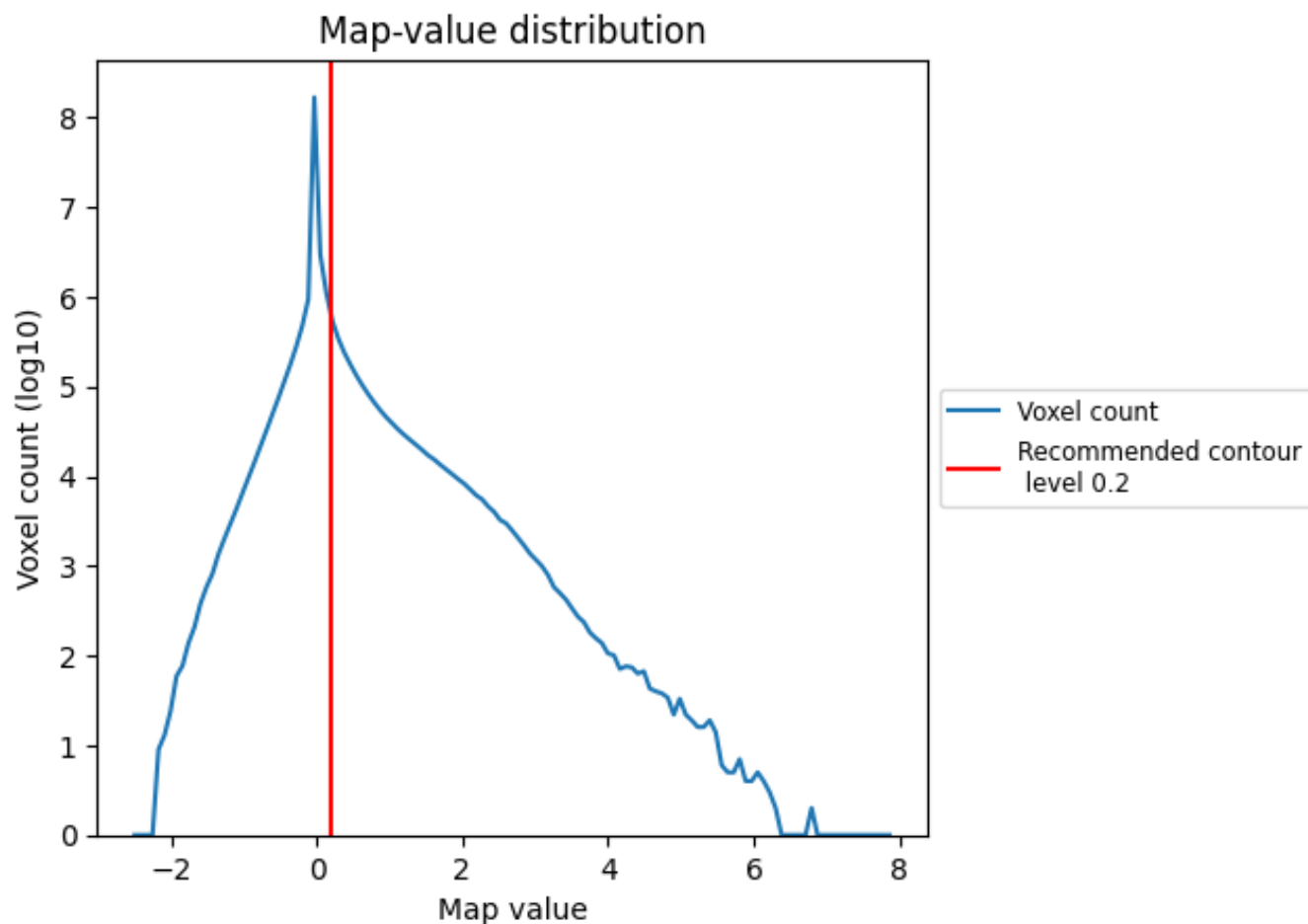


Z

7 Map analysis [i](#)

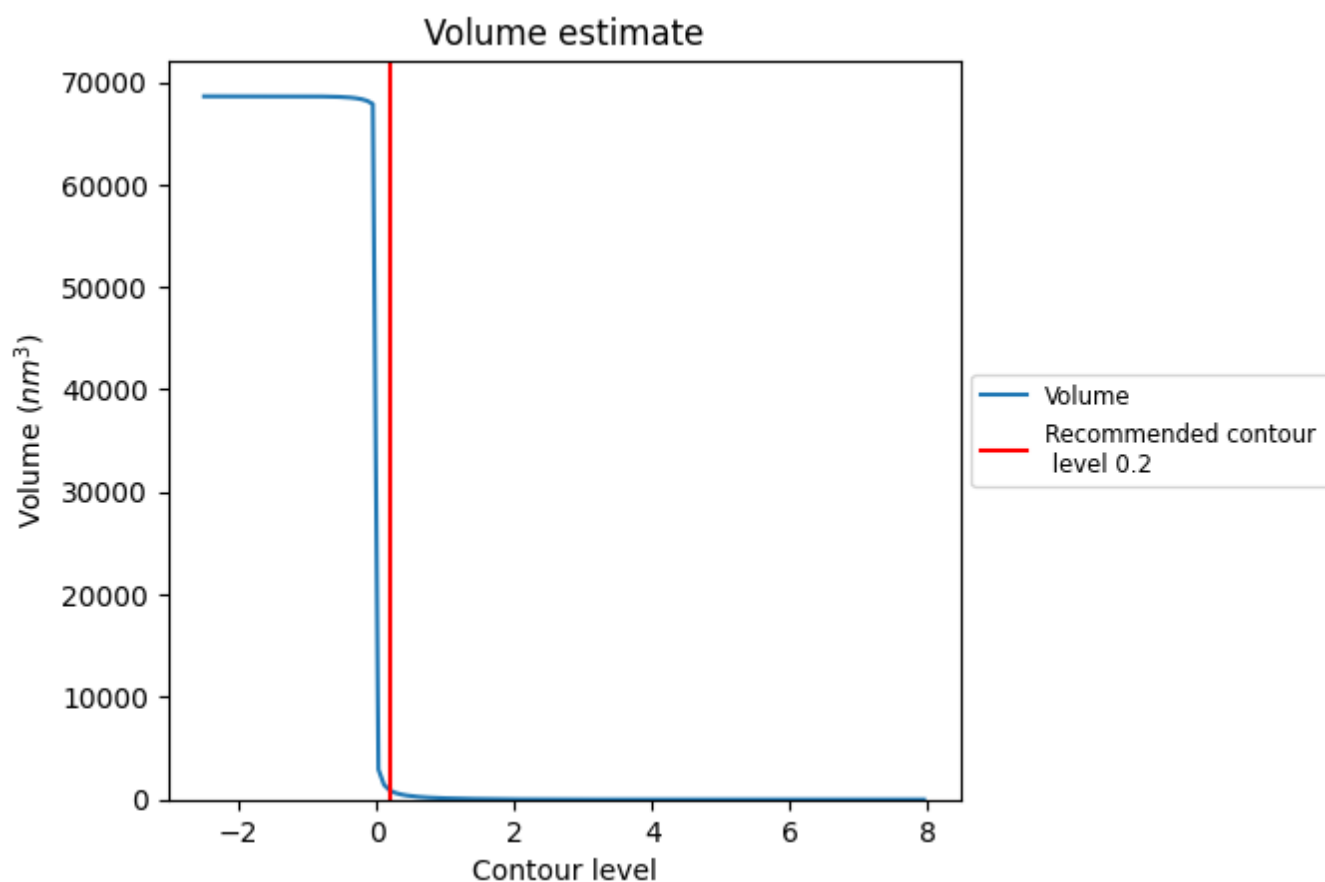
This section contains the results of statistical analysis of the map.

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.

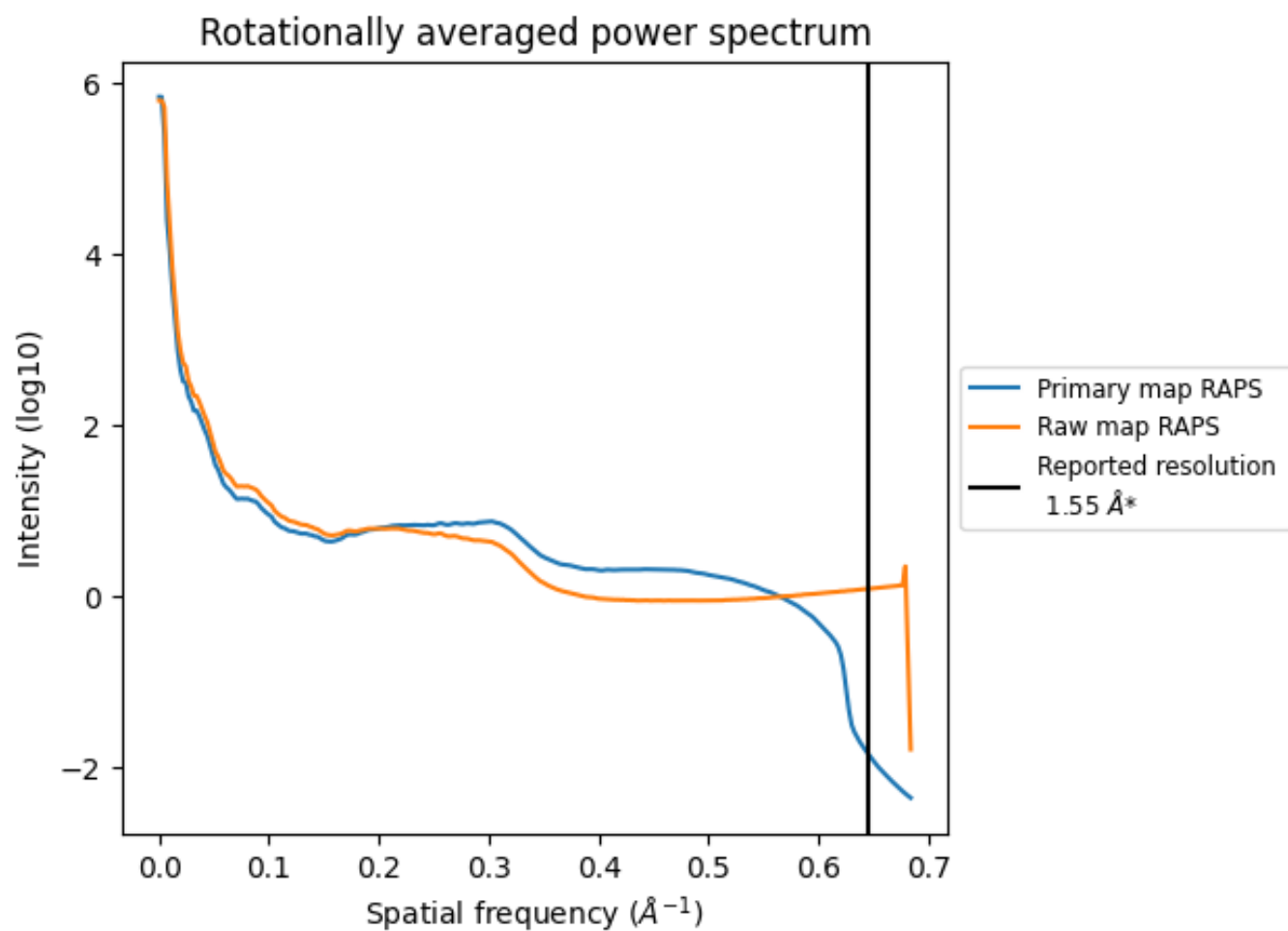
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 882 nm³; this corresponds to an approximate mass of 797 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 ⓘ

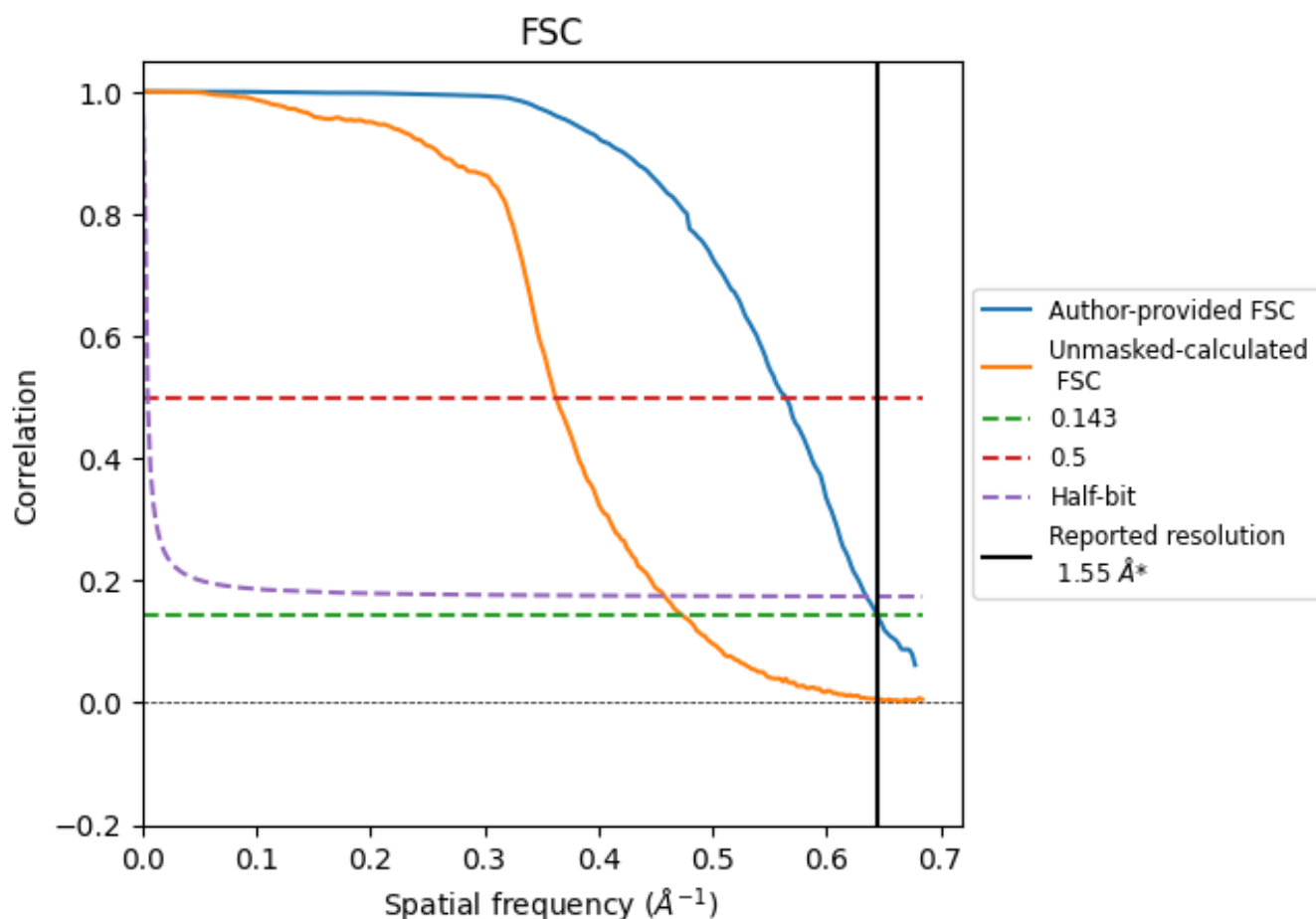


*Reported resolution corresponds to spatial frequency of 0.645 Å⁻¹

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 0.645 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

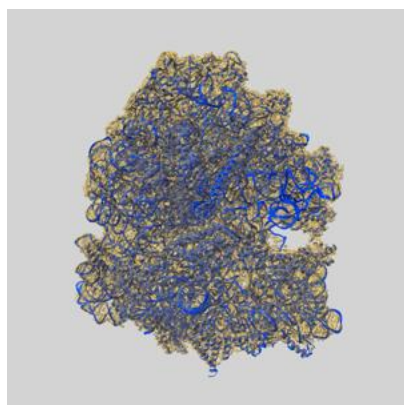
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.55	-	-
Author-provided FSC curve	1.55	1.77	1.57
Unmasked-calculated*	2.11	2.76	2.18

*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 2.11 differs from the reported value 1.55 by more than 10 %

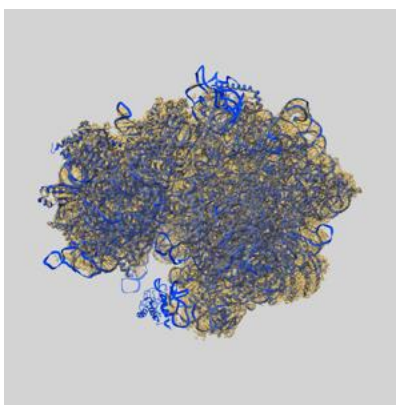
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15793 and PDB model 9Q87. Per-residue inclusion information can be found in section [3](#) on page [19](#).

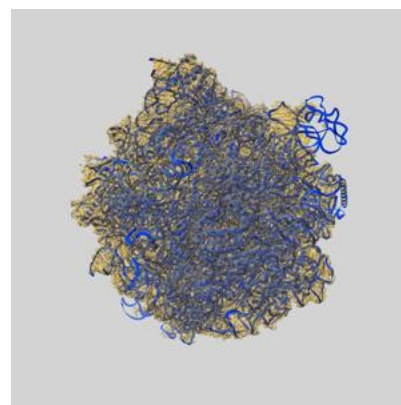
9.1 Map-model overlay [i](#)



X



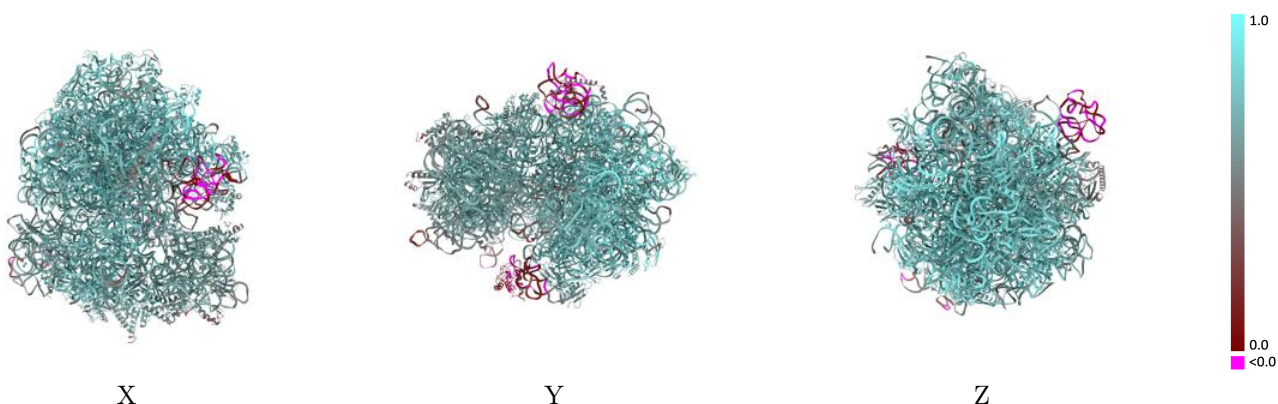
Y



Z

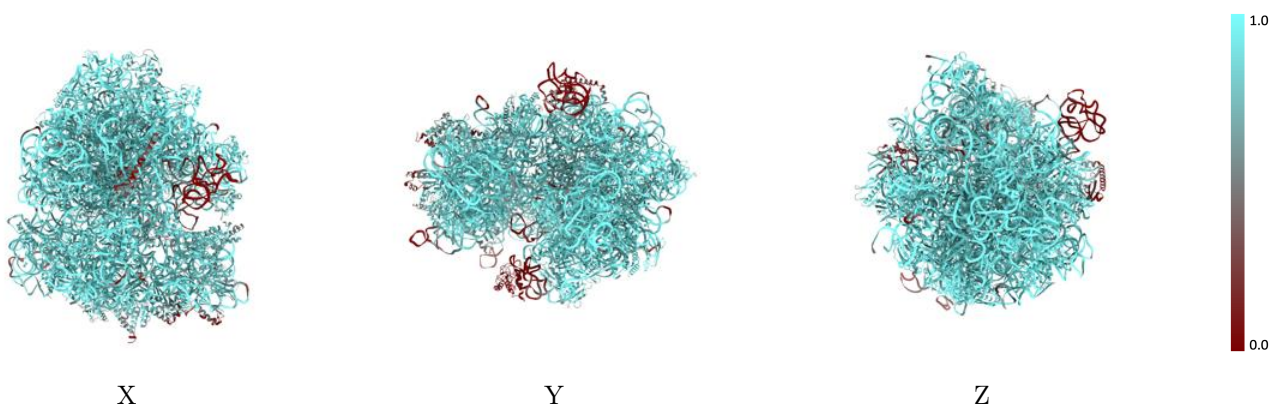
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



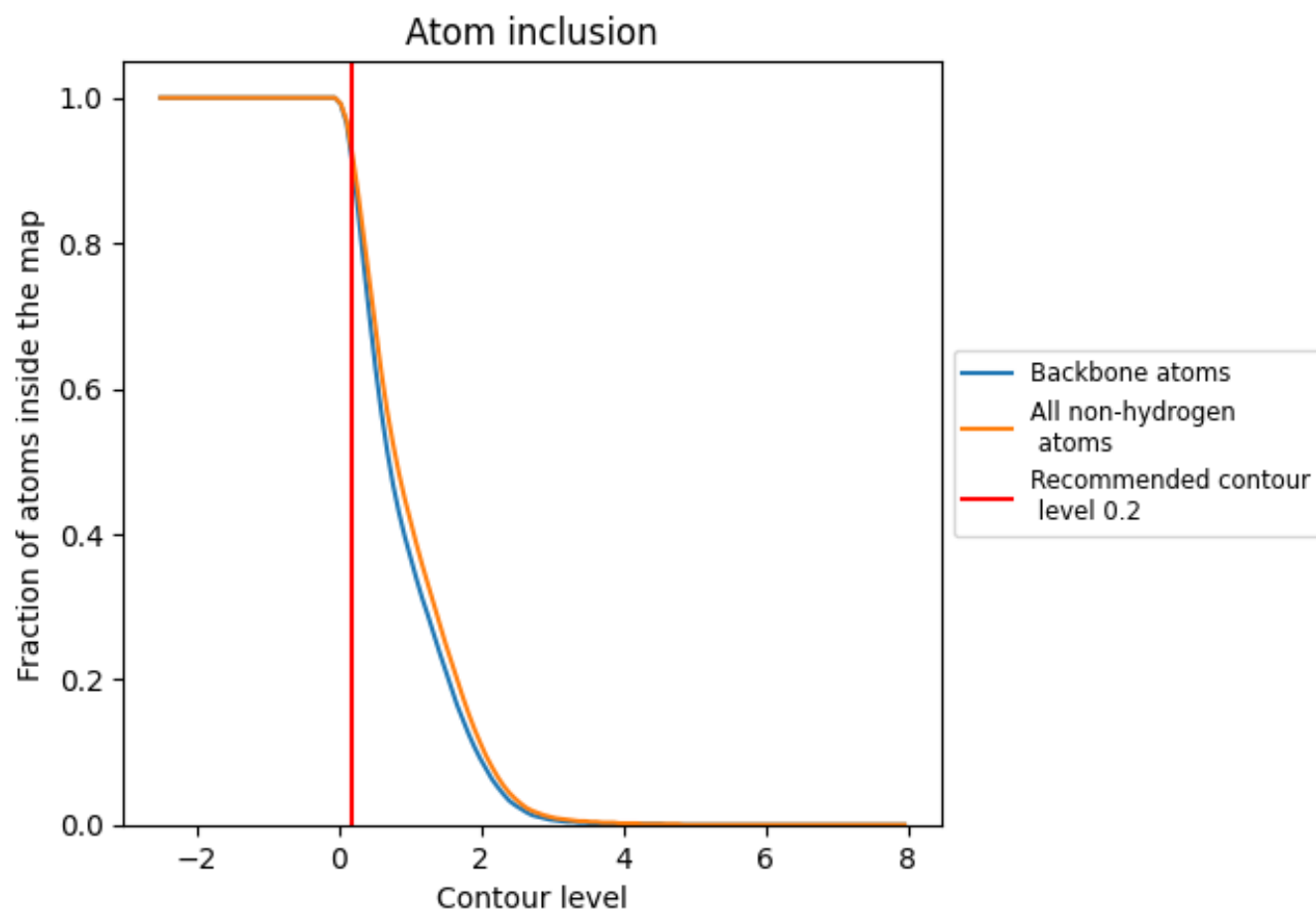
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 92% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9190	 0.7400
0	 0.9450	 0.7930
1	 0.9920	 0.8740
2	 0.9960	 0.8710
3	 0.9760	 0.8190
5	 0.0000	 0.0200
6	 0.9520	 0.7380
A	 0.9460	 0.7020
B	 0.7200	 0.6150
C	 0.8770	 0.6730
D	 0.8510	 0.6660
E	 0.9400	 0.7500
F	 0.8930	 0.6690
G	 0.7970	 0.6220
H	 0.9470	 0.7560
I	 0.8300	 0.6290
J	 0.6550	 0.5810
K	 0.9280	 0.6990
L	 0.9430	 0.7410
M	 0.7910	 0.6170
N	 0.8760	 0.6530
O	 0.9410	 0.7400
P	 0.9320	 0.7060
Q	 0.8980	 0.6730
R	 0.9110	 0.7070
S	 0.7530	 0.5870
T	 0.9270	 0.7100
U	 0.6880	 0.6190
X	 0.9470	 0.7110
Z	 0.8570	 0.6080
a	 0.9340	 0.7760
b	 0.9740	 0.7260
c	 0.9900	 0.8540
d	 0.9750	 0.8450
e	 0.9400	 0.7970



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	 0.8600	 0.6480
g	 0.8870	 0.6670
h	 0.4810	 0.5560
i	 0.9860	 0.8460
j	 0.9790	 0.8410
k	 0.9790	 0.8340
l	 0.9840	 0.8260
m	 0.9980	 0.8690
n	 0.9430	 0.7360
o	 0.9690	 0.8320
p	 0.9970	 0.8660
q	 0.9590	 0.8120
r	 0.9800	 0.8470
s	 0.9420	 0.7840
t	 0.9160	 0.7510
u	 0.9290	 0.7510
v	 0.9720	 0.8260
w	 0.9780	 0.8290
x	 0.9260	 0.7420
y	 0.9610	 0.8310
z	 0.9670	 0.8270