



wwPDB EM Validation Summary Report ⓘ

May 26, 2024 – 06:58 AM EDT

PDB ID : 7S0S
EMDB ID : EMD-24792
Title : M. tuberculosis ribosomal RNA methyltransferase TlyA bound to M. smegmatis 50S ribosomal subunit
Authors : Laughlin, Z.T.; Dunham, C.M.; Conn, G.L.
Deposited on : 2021-08-31
Resolution : 3.05 Å (reported)
Based on initial models : 5O60, 5KYG, 3HP7

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.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

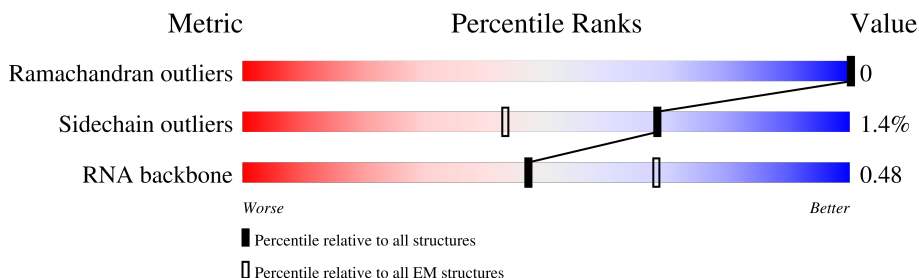
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.05 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	3	23	
2	B	284	
3	C	3120	
4	D	275	
5	E	214	
6	F	210	
7	G	182	
8	H	176	

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Mol	Chain	Length	Quality of chain
9	I	151	84% 99% 99%
10	J	126	100% 98%
11	K	133	100%
12	L	146	8% 99%
13	M	122	8% 100%
14	N	145	7% 100%
15	O	136	16% 99%
16	P	118	100%
17	Q	126	32% 100%
18	R	113	26% 100%
19	S	124	6% 100%
20	T	100	7% 100%
21	U	114	98% .
22	V	97	18% 100%
23	W	105	9% 92% 8%
24	X	192	63% 100%
25	Y	79	9% 100%
26	Z	63	10% 100%
27	a	64	12% 97% .
28	b	59	15% 100%
29	c	54	96% .
30	d	49	98% .
31	e	46	100%
32	f	63	100%
33	g	37	16% 100%

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Mol	Chain	Length	Quality of chain
34	h	48	<div><div></div><div>85%</div><div></div><div>100%</div></div>
35	i	118	<div><div></div><div>8%</div><div></div><div>82%</div><div>17%</div><div></div></div>

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 100057 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ribosomal protein bL37.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	3	23	Total	C	N	O	0	0
			189	111	50	28		

- Molecule 2 is a protein called 16S/23S rRNA (Cytidine-2'-O)-methyltransferase TlyA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	265	Total	C	N	O	S	0	0
			1954	1221	372	359	2		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	initiating methionine	UNP A0A045KH60
B	-14	HIS	-	expression tag	UNP A0A045KH60
B	-13	HIS	-	expression tag	UNP A0A045KH60
B	-12	HIS	-	expression tag	UNP A0A045KH60
B	-11	HIS	-	expression tag	UNP A0A045KH60
B	-10	HIS	-	expression tag	UNP A0A045KH60
B	-9	HIS	-	expression tag	UNP A0A045KH60
B	-8	ALA	-	expression tag	UNP A0A045KH60
B	-7	SER	-	expression tag	UNP A0A045KH60
B	-6	GLY	-	expression tag	UNP A0A045KH60
B	-5	LEU	-	expression tag	UNP A0A045KH60
B	-4	VAL	-	expression tag	UNP A0A045KH60
B	-3	PRO	-	expression tag	UNP A0A045KH60
B	-2	ARG	-	expression tag	UNP A0A045KH60
B	-1	GLY	-	expression tag	UNP A0A045KH60
B	0	SER	-	expression tag	UNP A0A045KH60

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	3119	Total	C	N	O	P	0	0
			67010	29871	12320	21700	3119		

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	275	Total	C	N	O	S	0	0
			2110	1298	438	370	4		

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1587	982	310	290	5		

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	209	Total	C	N	O	S	0	0
			1569	969	295	303	2		

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	182	Total	C	N	O	S	0	0
			1445	907	271	261	6		

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	176	Total	C	N	O	S	0	0
			1348	845	249	253	1		

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	151	Total	C	N	O	S	0	0
			1018	635	188	194	1		

- Molecule 10 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	126	Total	C	N	O	S	0	0
			918	580	156	180	2		

- Molecule 11 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	133	Total	C	N	O	S	0	0
			990	625	175	187	3		

- Molecule 12 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	146	Total	C	N	O	S	0	0
			1130	722	207	200	1		

- Molecule 13 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	122	Total	C	N	O	S	0	0
			938	586	179	170	3		

- Molecule 14 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	145	Total	C	N	O	S	0	0
			1078	676	205	194	3		

- Molecule 15 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	136	Total	C	N	O	S	0	0
			1092	690	213	187	2		

- Molecule 16 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	118	Total	C	N	O	S	0	0
			928	583	180	163	2		

- Molecule 17 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	126	Total	C	N	O	0	0
			956	586	199	171		

- Molecule 18 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	113	Total	C	N	O	S	0
			907	570	171	165	1	0

- Molecule 19 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	S	124	Total	C	N	O		0
			988	613	203	172		0

- Molecule 20 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	T	100	Total	C	N	O	0	0
			754	478	137	139		

- Molecule 21 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	114	Total	C	N	O	0	0
			873	543	171	159		

- Molecule 22 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	97	Total	C	N	O	0	0
			756	479	138	139		

- Molecule 23 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	W	97	Total	C	N	O	S	0
			732	456	137	137	2	0

- Molecule 24 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	192	Total	C	N	O	0	0
			1428	881	255	292		

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	79	Total	C	N	O	0	0
			586	361	123	102		

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	63	Total	C	N	O	S	0	0
			470	283	103	80	4		

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	64	Total	C	N	O	S	0	0
			531	324	103	103	1		

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	b	59	Total	C	N	O	0	0
			474	292	95	87		

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	54	Total	C	N	O	S	0	0
			423	260	93	69	1		

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	49	Total	C	N	O	S	0	0
			405	248	82	71	4		

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	46	Total	C	N	O	S	0	0
			377	225	97	54	1		

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	63	Total	C	N	O		0	0
			502	302	115	85			

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	37	Total	C	N	O	S	0	0
			299	181	66	47	5		

- Molecule 34 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	48	Total	C	N	O	S	0	0
			364	225	63	71	5		

- Molecule 35 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	118	Total	C	N	O	P	0	0
			2522	1126	468	810	118		

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	C	380	Total	Mg	0
			380	380	
36	D	5	Total	Mg	0
			5	5	
36	E	2	Total	Mg	0
			2	2	
36	N	1	Total	Mg	0
			1	1	
36	O	4	Total	Mg	0
			4	4	
36	U	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
36	i	9	Total 9	Mg 9	0

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
37	Z	1	Total 1	Zn 1	0
37	d	1	Total 1	Zn 1	0
37	g	1	Total 1	Zn 1	0
37	h	1	Total 1	Zn 1	0

3 Residue-property plots [i](#)


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

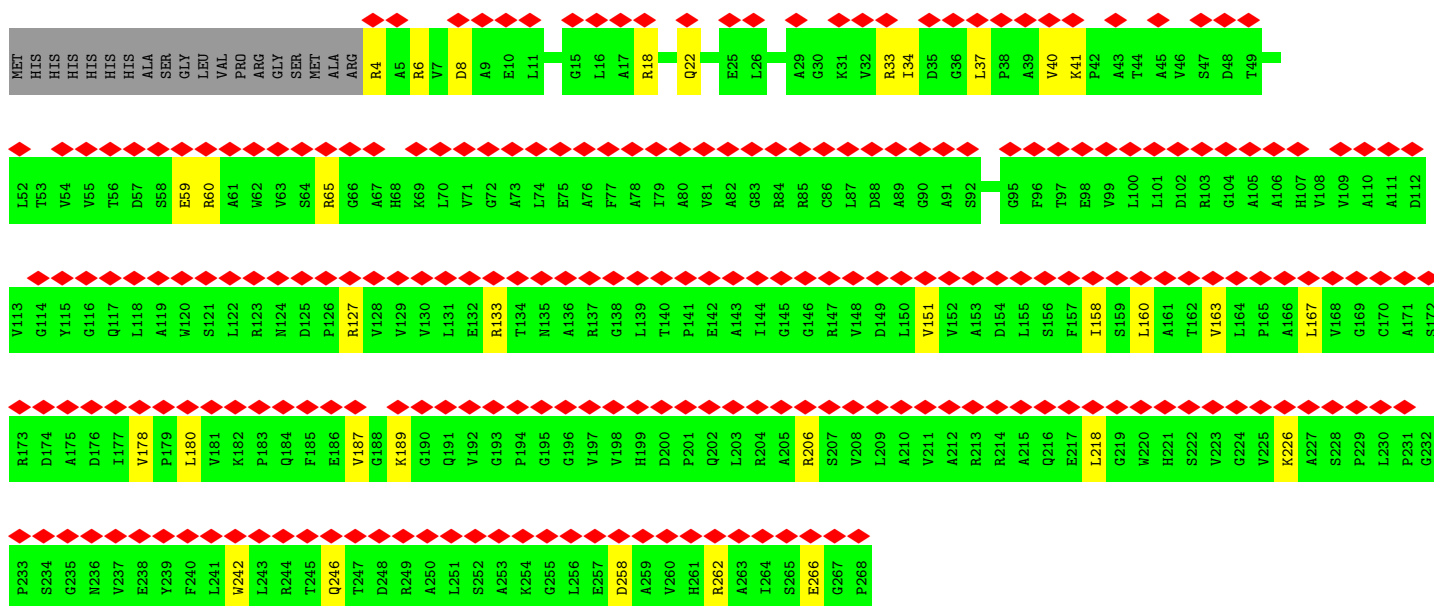
- Molecule 1: ribosomal protein bL37

Chain 3:  100%




- Molecule 2: 16S/23S rRNA (Cytidine-2'-O)-methyltransferase TlyA

Chain B:  84% 82% 11% 7%

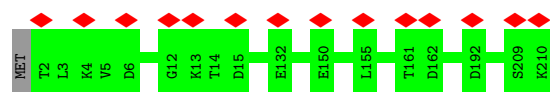


- Molecule 3: 23S rRNA

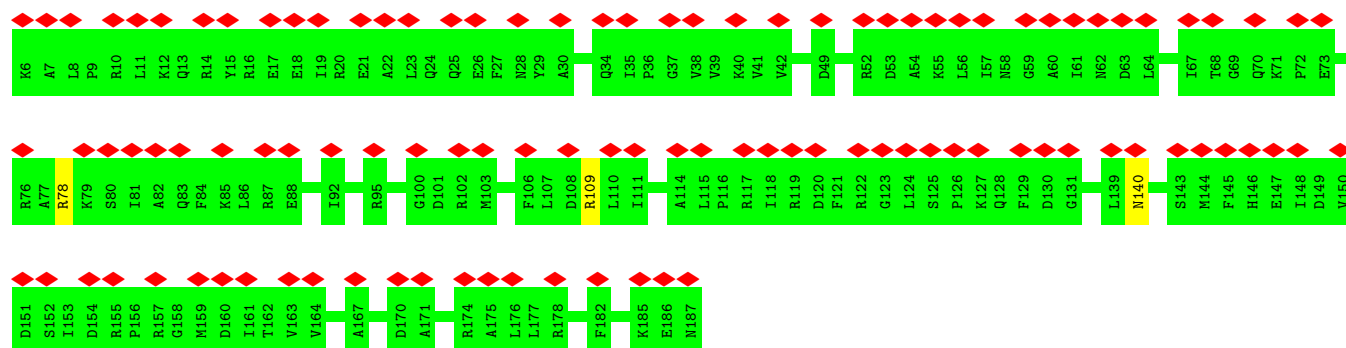
Chain C:  12% 77% 22%



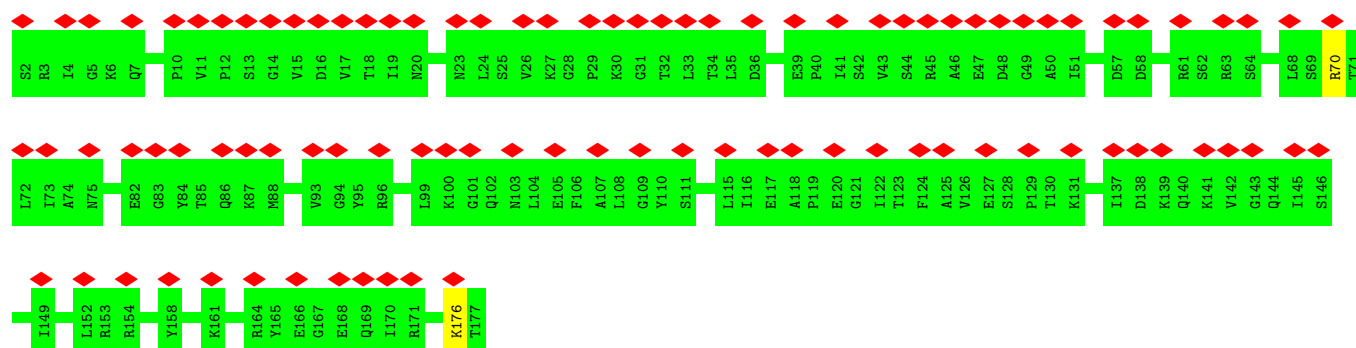




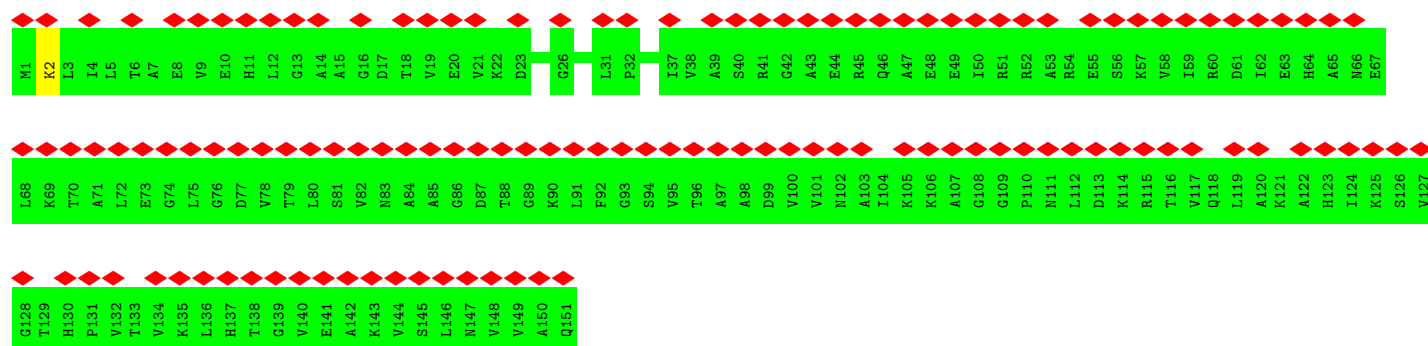
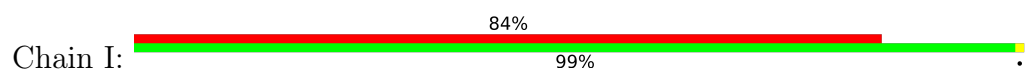
- Molecule 7: 50S ribosomal protein L5



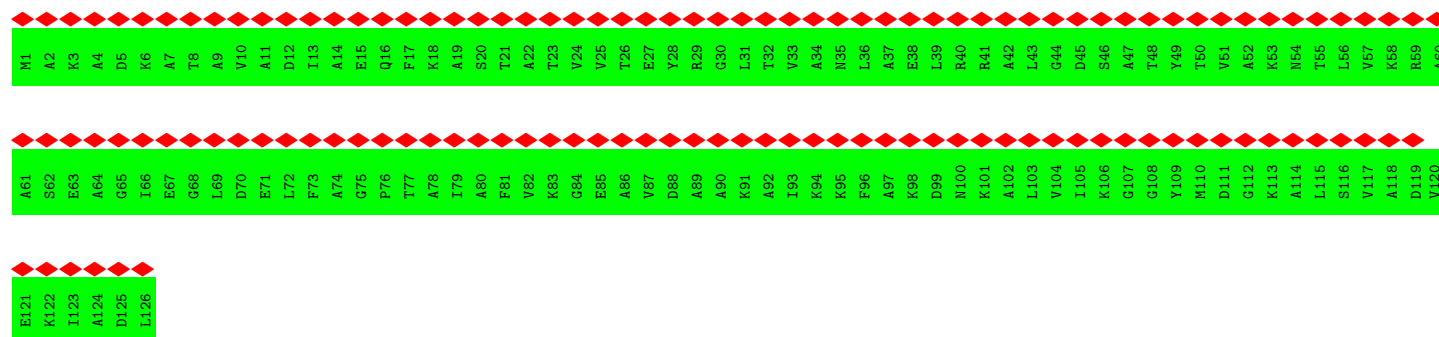
- Molecule 8: 50S ribosomal protein L6



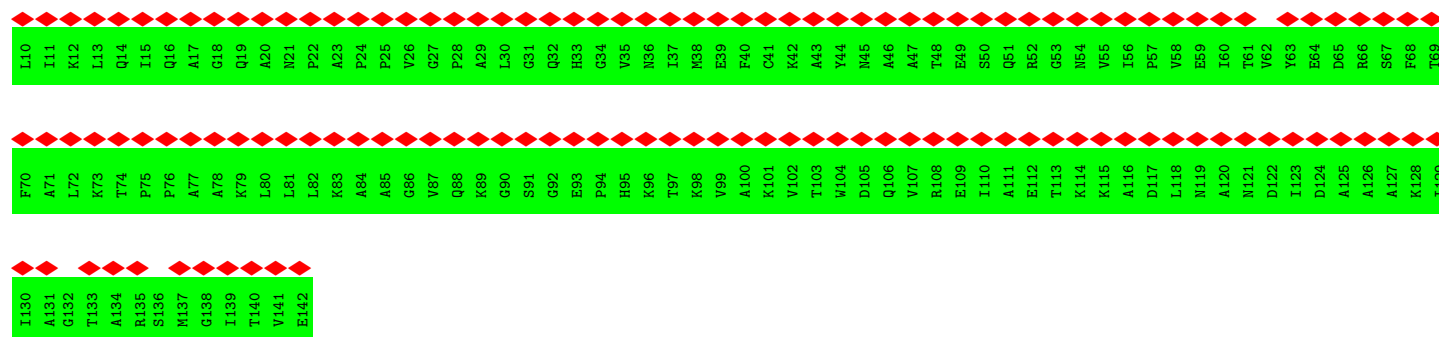
- Molecule 9: 50S ribosomal protein L9



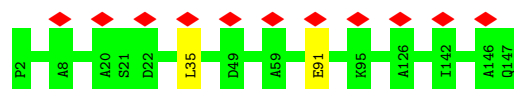
- Molecule 10: 50S ribosomal protein L10



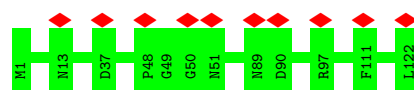
- Molecule 11: 50S ribosomal protein L11



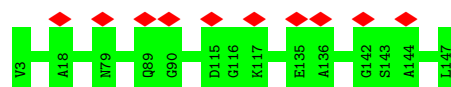
- Molecule 12: 50S ribosomal protein L13



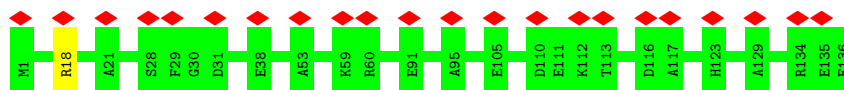
- Molecule 13: 50S ribosomal protein L14



- Molecule 14: 50S ribosomal protein L15



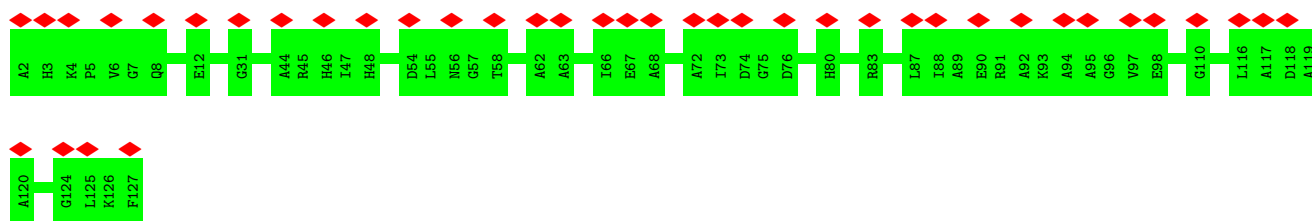
- Molecule 15: 50S ribosomal protein L16



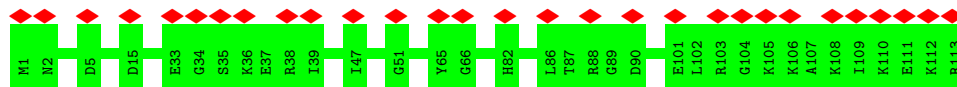
- Molecule 16: 50S ribosomal protein L17



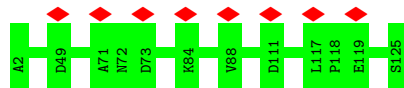
- Molecule 17: 50S ribosomal protein L18



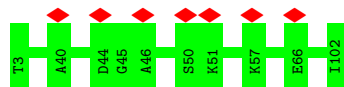
- Molecule 18: 50S ribosomal protein L19



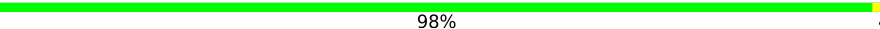
- Molecule 19: 50S ribosomal protein L20



- Molecule 20: 50S ribosomal protein L21



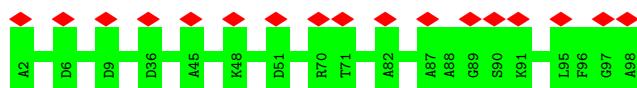
- Molecule 21: 50S ribosomal protein L22

Chain U:  98%




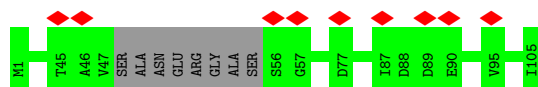
- Molecule 22: 50S ribosomal protein L23

Chain V:  18% 100%



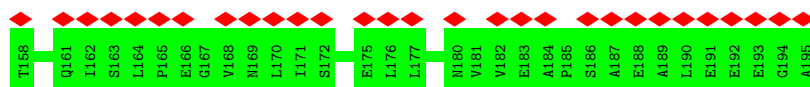
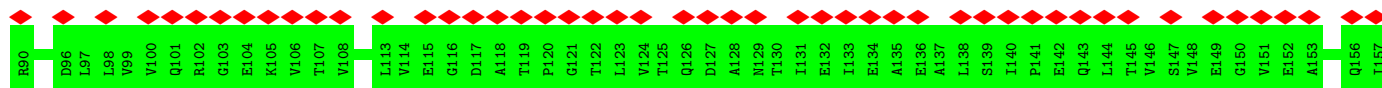
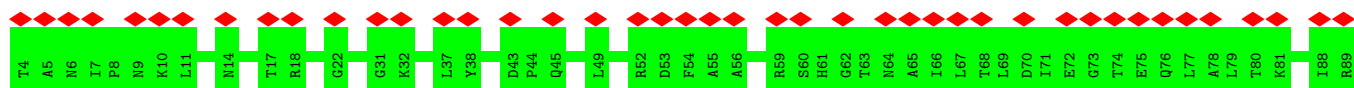
- Molecule 23: 50S ribosomal protein L24

Chain W:  9% 92% 8%



- Molecule 24: 50S ribosomal protein L25

Chain X:  63% 100%



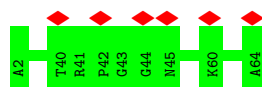
- Molecule 25: 50S ribosomal protein L27

Chain Y:  9% 100%

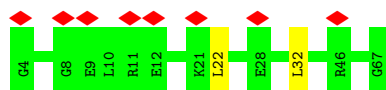


- Molecule 26: 50S ribosomal protein L28

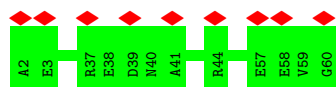
Chain Z:  10% 100%



- Molecule 27: 50S ribosomal protein L29



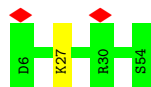
- Molecule 28: 50S ribosomal protein L30



- Molecule 29: 50S ribosomal protein L32



- Molecule 30: 50S ribosomal protein L33



- Molecule 31: 50S ribosomal protein L34



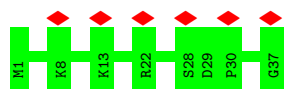
There are no outlier residues recorded for this chain.

- Molecule 32: 50S ribosomal protein L35

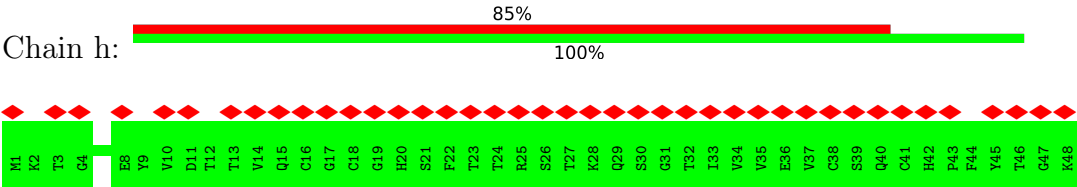


There are no outlier residues recorded for this chain.

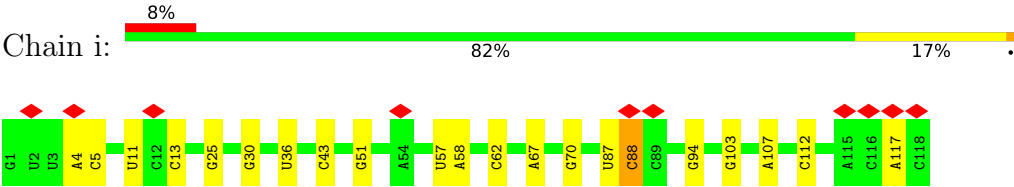
- Molecule 33: 50S ribosomal protein L36



- Molecule 34: 50S ribosomal protein L31



● Molecule 35: 5S rRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	129011	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.79	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.163	Depositor
Minimum map value	-0.097	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0179	Depositor
Map size (\AA)	299.32, 299.32, 299.32	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.069, 1.069, 1.069	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AI5, ZN, MG

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	3	0.38	0/191	0.73	0/247
2	B	0.50	0/1986	0.64	0/2702
3	C	0.82	0/74978	0.91	73/116989 (0.1%)
4	D	0.45	0/2153	0.65	0/2895
5	E	0.46	0/1609	0.66	1/2165 (0.0%)
6	F	0.45	0/1592	0.61	0/2153
7	G	0.33	0/1467	0.64	0/1973
8	H	0.34	0/1369	0.61	0/1848
9	I	0.31	0/1027	0.58	0/1398
10	J	0.28	0/925	0.53	0/1246
11	K	0.28	0/1006	0.53	0/1364
12	L	0.48	0/1157	0.60	1/1567 (0.1%)
13	M	0.44	0/946	0.64	0/1268
14	N	0.43	0/1091	0.63	0/1457
15	O	0.42	0/1118	0.63	0/1506
16	P	0.45	0/945	0.63	0/1267
17	Q	0.33	0/966	0.61	0/1298
18	R	0.43	0/921	0.62	0/1236
19	S	0.44	0/1000	0.65	0/1341
20	T	0.46	0/764	0.54	0/1030
21	U	0.46	0/887	0.65	1/1204 (0.1%)
22	V	0.44	0/766	0.57	0/1030
23	W	0.44	0/738	0.61	0/987
24	X	0.33	0/1443	0.61	0/1970
25	Y	0.46	0/595	0.66	0/798
26	Z	0.47	0/478	0.65	0/641
27	a	0.41	0/534	0.75	2/713 (0.3%)
28	b	0.46	0/477	0.66	0/640
29	c	0.46	0/427	0.74	1/572 (0.2%)
30	d	0.42	0/413	0.60	0/553
31	e	0.42	0/380	0.78	0/500
32	f	0.41	0/507	0.67	0/672

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
33	g	0.44	0/303	0.69	0/401
34	h	0.29	0/372	0.50	0/503
35	i	0.61	0/2821	0.92	5/4396 (0.1%)
All	All	0.73	0/108352	0.85	84/162530 (0.1%)

There are no bond length outliers.

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2088	C	N3-C2-O2	-10.92	114.26	121.90
3	C	2088	C	N1-C2-O2	9.64	124.68	118.90
3	C	2089	C	N3-C2-O2	-8.77	115.76	121.90
3	C	2154	G	C2'-C3'-O3'	8.12	127.36	109.50
3	C	1001	C	N3-C2-O2	-7.86	116.40	121.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	21/23 (91%)	19 (90%)	2 (10%)	0	100	100
2	B	263/284 (93%)	229 (87%)	34 (13%)	0	100	100
4	D	273/275 (99%)	255 (93%)	18 (7%)	0	100	100
5	E	212/214 (99%)	200 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
7	G	180/182 (99%)	159 (88%)	21 (12%)	0	100	100
8	H	174/176 (99%)	168 (97%)	6 (3%)	0	100	100
9	I	149/151 (99%)	134 (90%)	15 (10%)	0	100	100
10	J	124/126 (98%)	113 (91%)	11 (9%)	0	100	100
11	K	131/133 (98%)	119 (91%)	12 (9%)	0	100	100
12	L	144/146 (99%)	137 (95%)	7 (5%)	0	100	100
13	M	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
14	N	143/145 (99%)	129 (90%)	14 (10%)	0	100	100
15	O	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
16	P	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
17	Q	124/126 (98%)	118 (95%)	6 (5%)	0	100	100
18	R	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
19	S	122/124 (98%)	116 (95%)	6 (5%)	0	100	100
20	T	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
21	U	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
22	V	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
23	W	93/105 (89%)	88 (95%)	5 (5%)	0	100	100
24	X	190/192 (99%)	181 (95%)	9 (5%)	0	100	100
25	Y	77/79 (98%)	73 (95%)	4 (5%)	0	100	100
26	Z	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
27	a	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
28	b	57/59 (97%)	53 (93%)	4 (7%)	0	100	100
29	c	52/54 (96%)	52 (100%)	0	0	100	100
30	d	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
31	e	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
32	f	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
33	g	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
34	h	46/48 (96%)	43 (94%)	3 (6%)	0	100	100
All	All	3878/3974 (98%)	3637 (94%)	241 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	3	18/18 (100%)	18 (100%)	0	100	100
2	B	197/212 (93%)	165 (84%)	32 (16%)	2	9
4	D	215/215 (100%)	214 (100%)	1 (0%)	88	94
5	E	160/160 (100%)	160 (100%)	0	100	100
6	F	169/170 (99%)	169 (100%)	0	100	100
7	G	151/151 (100%)	148 (98%)	3 (2%)	55	78
8	H	148/148 (100%)	146 (99%)	2 (1%)	67	84
9	I	90/116 (78%)	89 (99%)	1 (1%)	73	88
10	J	89/89 (100%)	89 (100%)	0	100	100
11	K	102/102 (100%)	102 (100%)	0	100	100
12	L	119/119 (100%)	118 (99%)	1 (1%)	81	91
13	M	100/100 (100%)	100 (100%)	0	100	100
14	N	112/112 (100%)	112 (100%)	0	100	100
15	O	114/114 (100%)	113 (99%)	1 (1%)	78	90
16	P	97/97 (100%)	97 (100%)	0	100	100
17	Q	93/93 (100%)	93 (100%)	0	100	100
18	R	100/100 (100%)	100 (100%)	0	100	100
19	S	97/97 (100%)	97 (100%)	0	100	100
20	T	81/81 (100%)	81 (100%)	0	100	100
21	U	90/90 (100%)	89 (99%)	1 (1%)	73	88
22	V	83/83 (100%)	83 (100%)	0	100	100
23	W	81/86 (94%)	81 (100%)	0	100	100
24	X	155/155 (100%)	155 (100%)	0	100	100
25	Y	58/58 (100%)	58 (100%)	0	100	100
26	Z	50/50 (100%)	50 (100%)	0	100	100
27	a	58/58 (100%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	b	52/52 (100%)	52 (100%)	0	100	100
29	c	43/43 (100%)	42 (98%)	1 (2%)	50	75
30	d	47/47 (100%)	46 (98%)	1 (2%)	53	77
31	e	35/35 (100%)	35 (100%)	0	100	100
32	f	53/53 (100%)	53 (100%)	0	100	100
33	g	35/35 (100%)	35 (100%)	0	100	100
34	h	43/43 (100%)	43 (100%)	0	100	100
All	All	3135/3182 (98%)	3091 (99%)	44 (1%)	68	84

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	246	GLN
7	G	140	ASN
2	B	258	ASP
4	D	157	ARG
8	H	176	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
34	h	6	HIS
34	h	40	GLN
7	G	70	GLN
9	I	118	GLN
11	K	19	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	3117/3120 (99%)	671 (21%)	28 (0%)
35	i	117/118 (99%)	20 (17%)	0
All	All	3234/3238 (99%)	691 (21%)	28 (0%)

5 of 691 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	6	G
3	C	10	A
3	C	11	A
3	C	12	G
3	C	20	G

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	C	1213	A
3	C	3002	A
3	C	1510	A
3	C	2398	C
3	C	1234	U

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
3	AI5	C	2144	3	47,53,53	3.67	22 (46%)	55,76,76	1.81	13 (23%)

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
3	AI5	C	2144	3	-	9/27/65/65	0/5/5/5

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2144	AI5	O25-C26	14.22	1.60	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2144	AI5	C48-C17	-10.61	1.29	1.52
3	C	2144	AI5	O25-C24	-7.36	1.28	1.45
3	C	2144	AI5	C39-C37	-6.54	1.35	1.53
3	C	2144	AI5	C39-C24	4.89	1.65	1.53

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2144	AI5	N29-C30-N31	-4.84	121.12	128.68
3	C	2144	AI5	N13-C12-N11	4.41	125.71	117.97
3	C	2144	AI5	C08-N09-C10	4.38	128.20	118.42
3	C	2144	AI5	C08-N09-C15	-4.00	112.11	120.84
3	C	2144	AI5	O16-C10-N11	-4.00	115.83	122.33

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2144	AI5	C48-C17-O18-C19
3	C	2144	AI5	C41-C42-C43-N44
3	C	2144	AI5	C17-C08-N09-C15
3	C	2144	AI5	C17-C08-N09-C10
3	C	2144	AI5	O18-C19-C20-N21

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 406 ligands modelled in this entry, 406 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

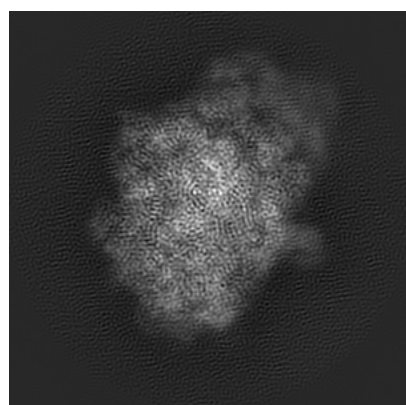
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24792. These allow visual inspection of the internal detail of the map and identification of artifacts.

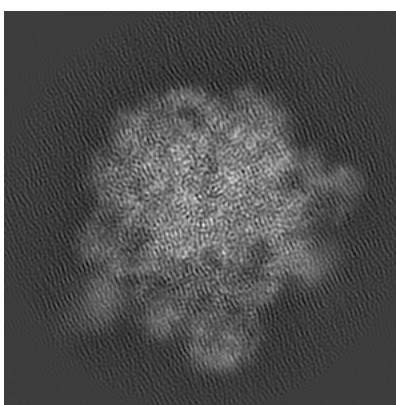
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

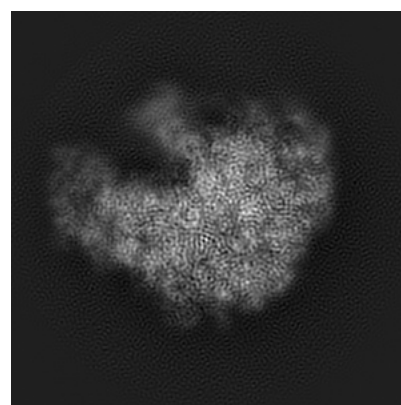
6.1.1 Primary map



X



Y

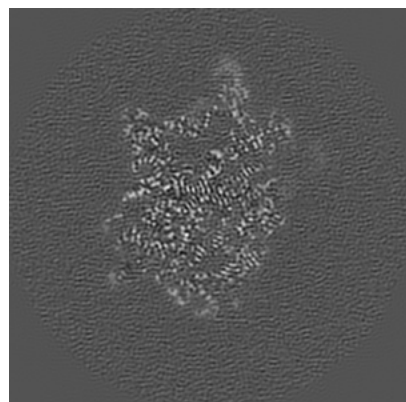


Z

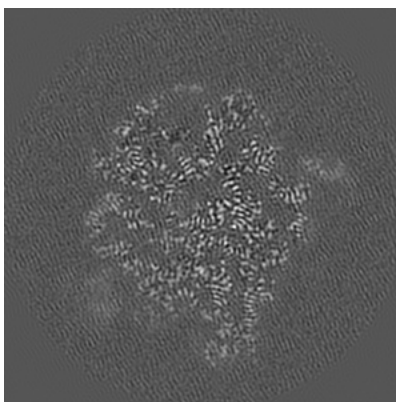
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

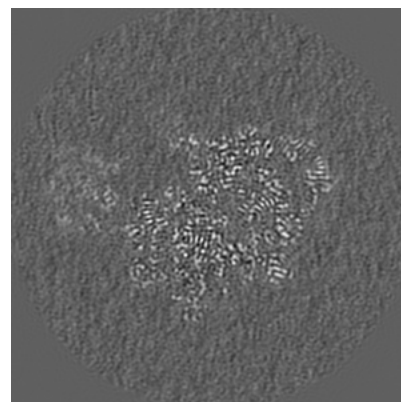
6.2.1 Primary map



X Index: 140



Y Index: 140

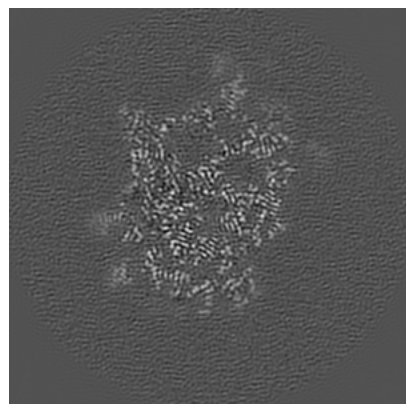


Z Index: 140

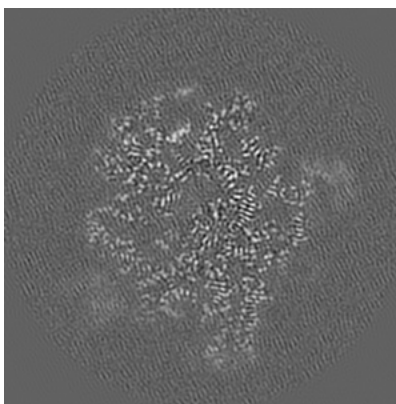
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

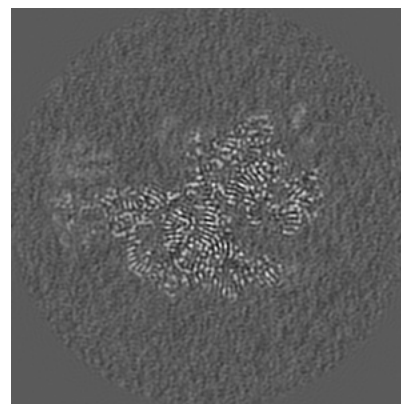
6.3.1 Primary map



X Index: 145



Y Index: 142

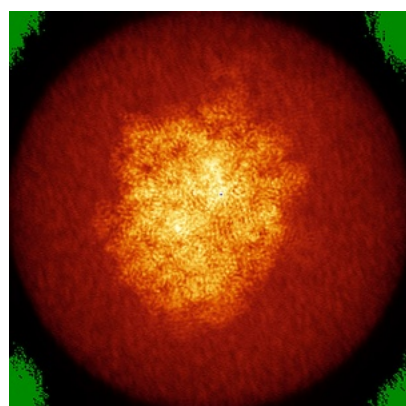


Z Index: 152

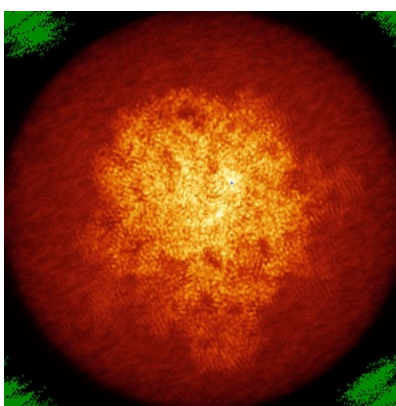
The images above show the largest variance slices of the map in three orthogonal directions.

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

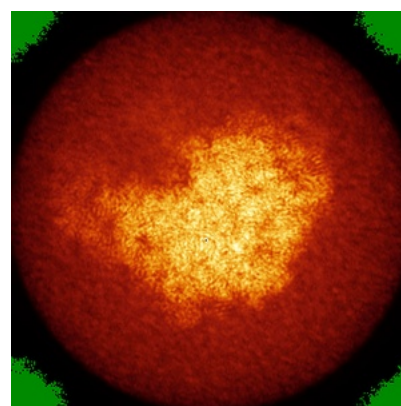
6.4.1 Primary map



X



Y

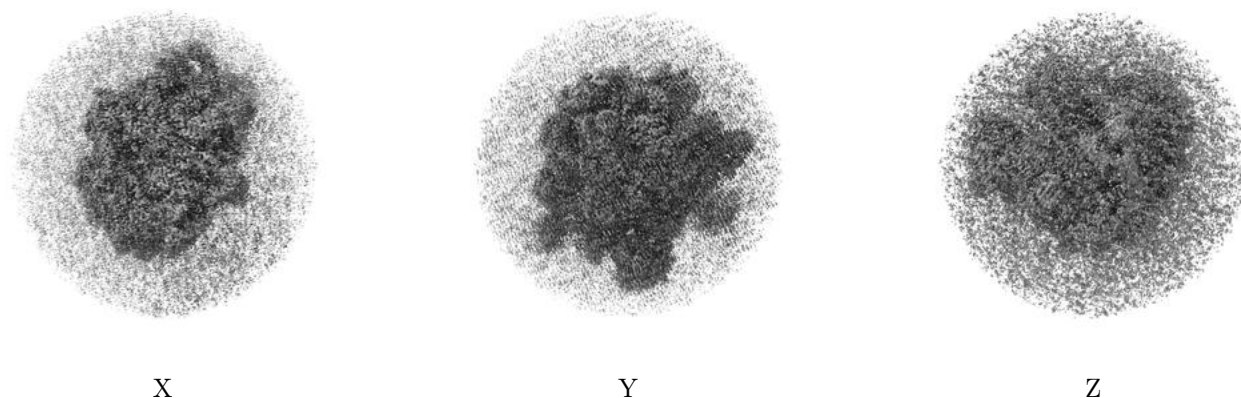


Z

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 0.0179. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

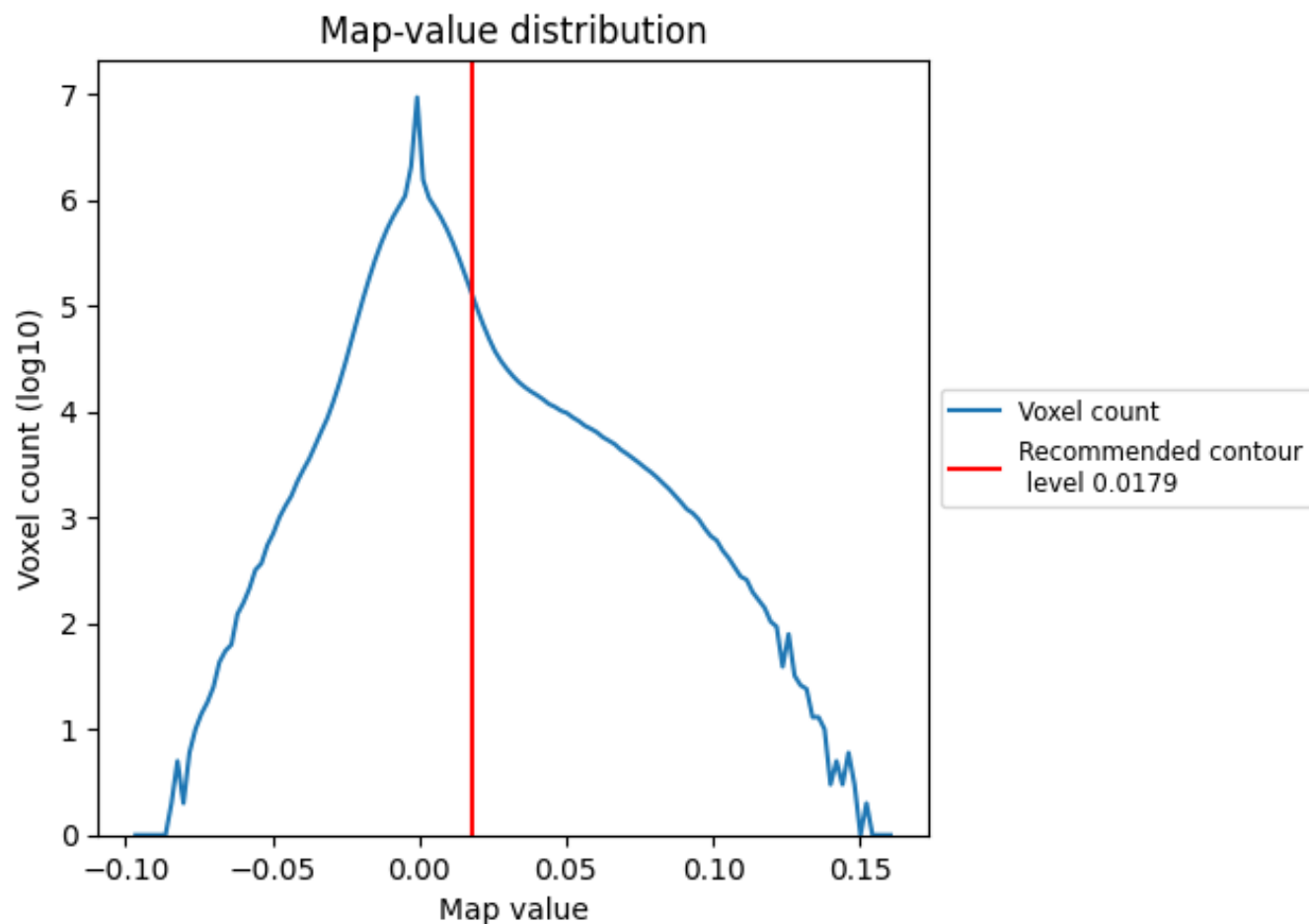
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

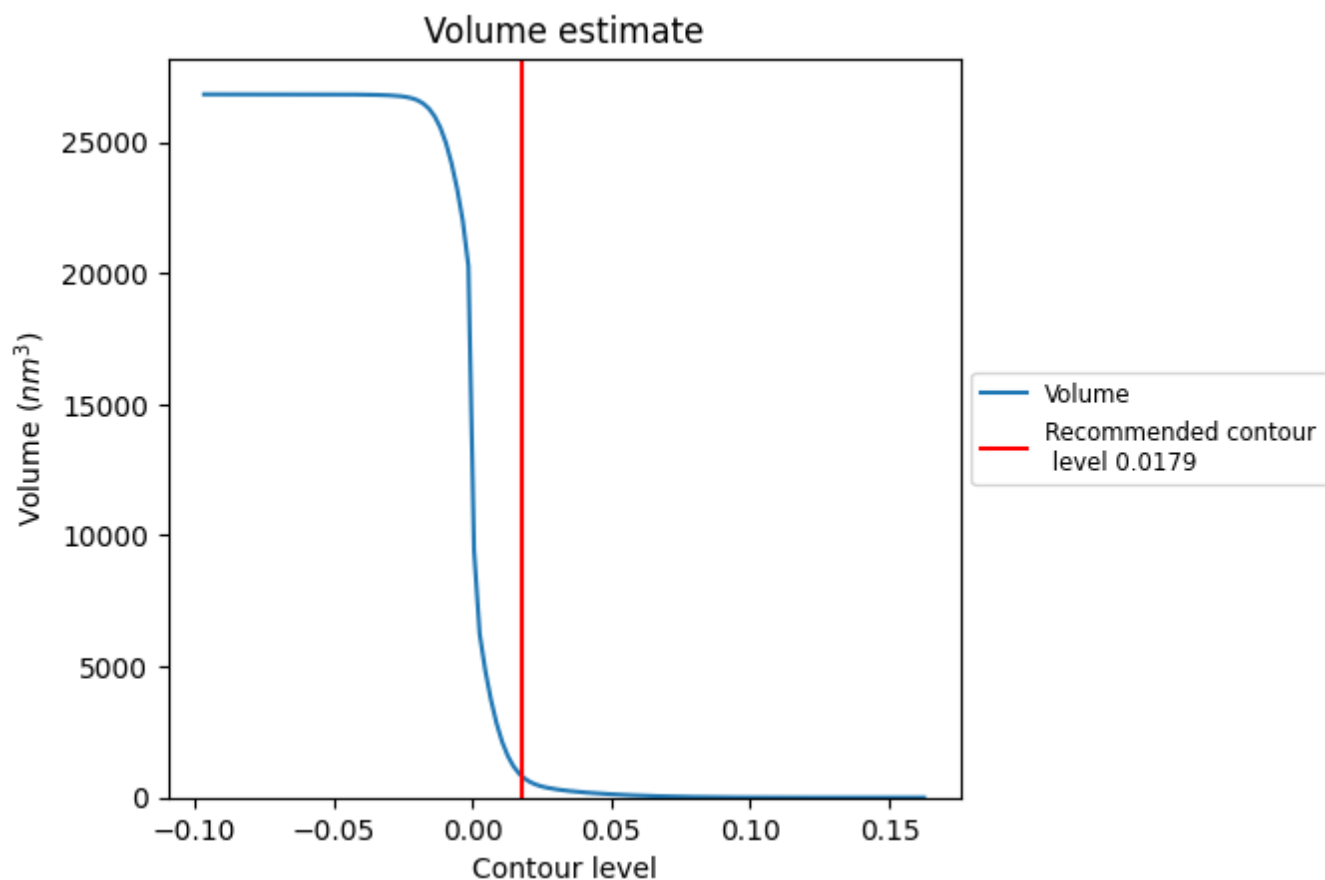
This section contains the results of statistical analysis of the map.

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.

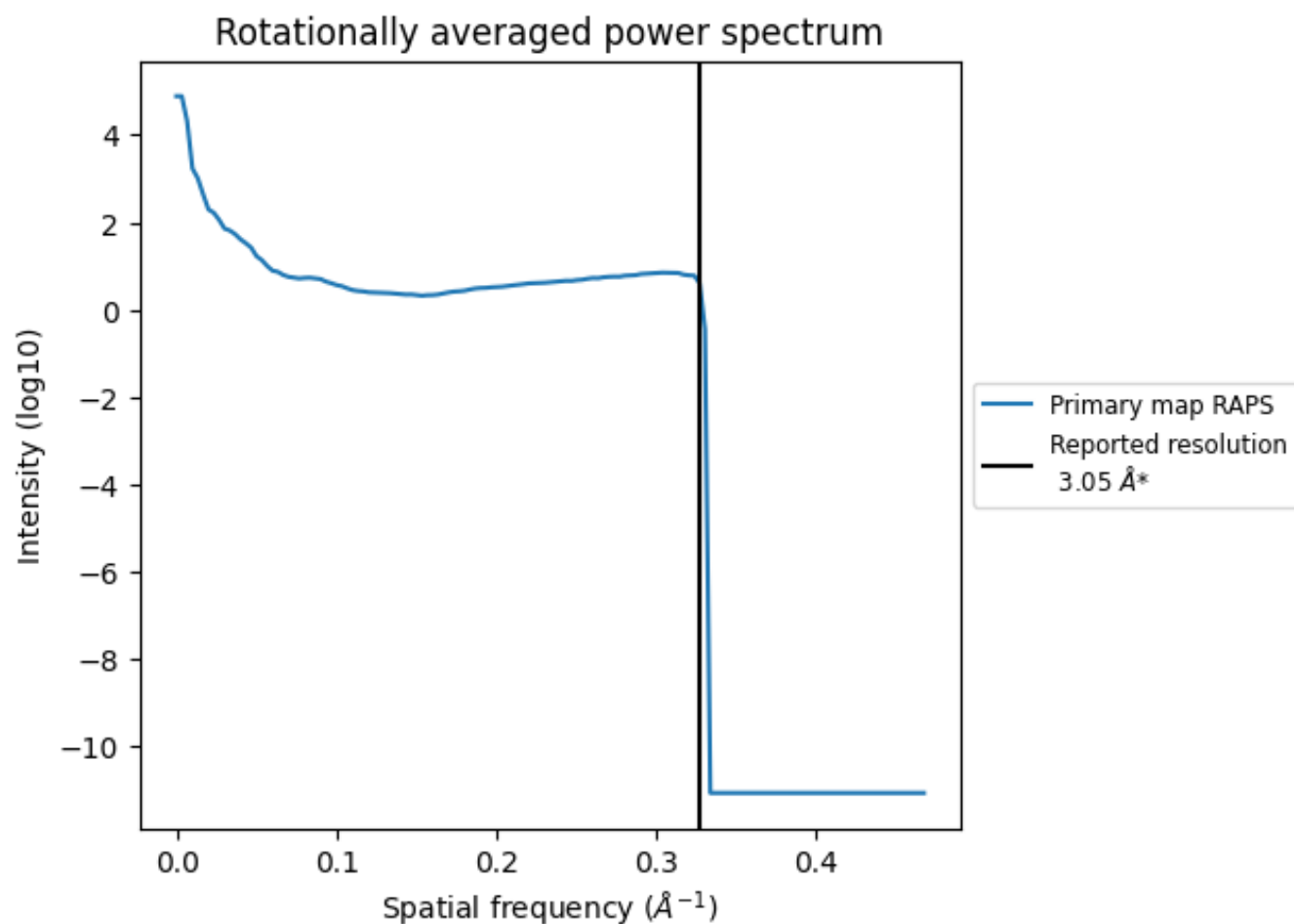
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 809 nm³; this corresponds to an approximate mass of 731 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 ⓘ

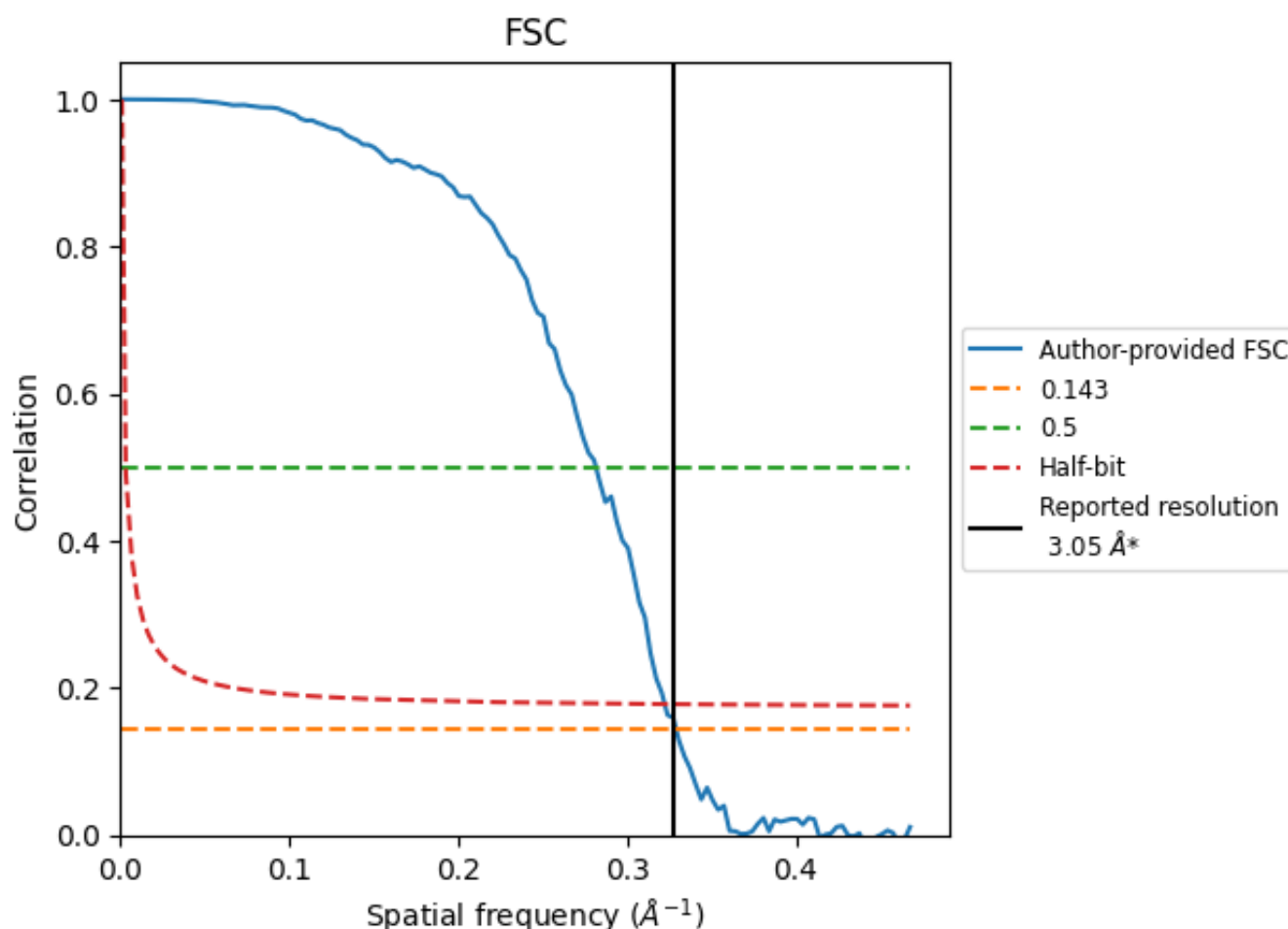


*Reported resolution corresponds to spatial frequency of 0.328 Å⁻¹

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 0.328 Å⁻¹

8.2 Resolution estimates [i](#)

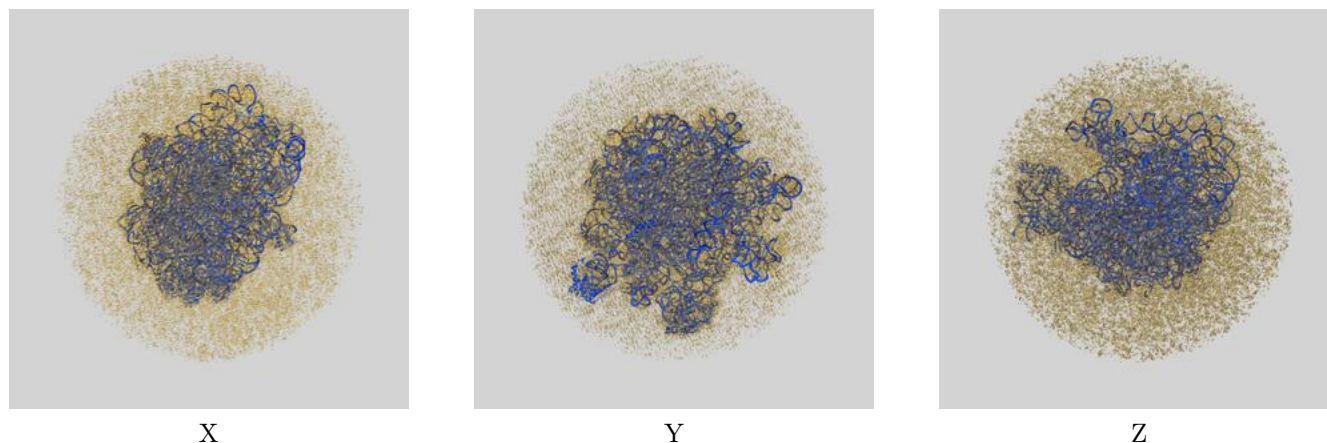
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.05	-	-
Author-provided FSC curve	3.04	3.55	3.10
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

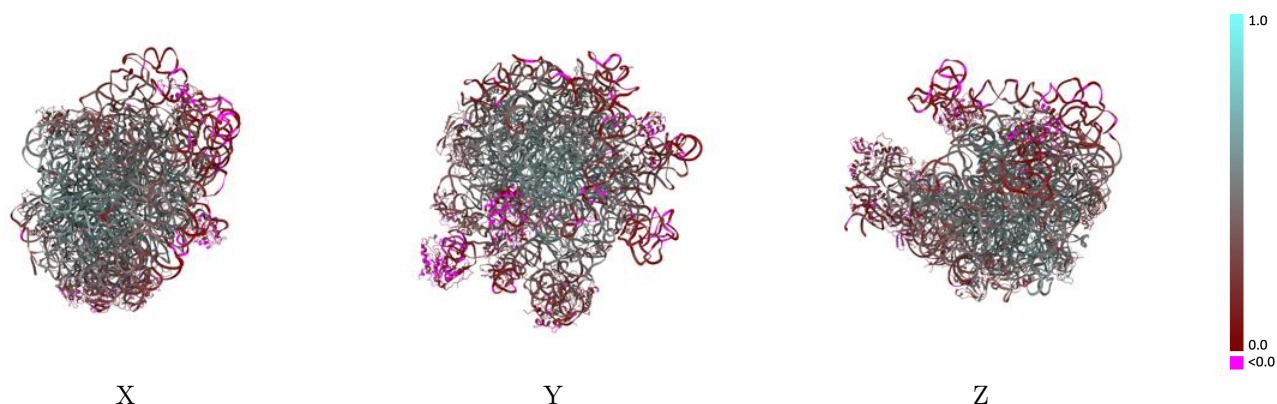
This section contains information regarding the fit between EMDB map EMD-24792 and PDB model 7S0S. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



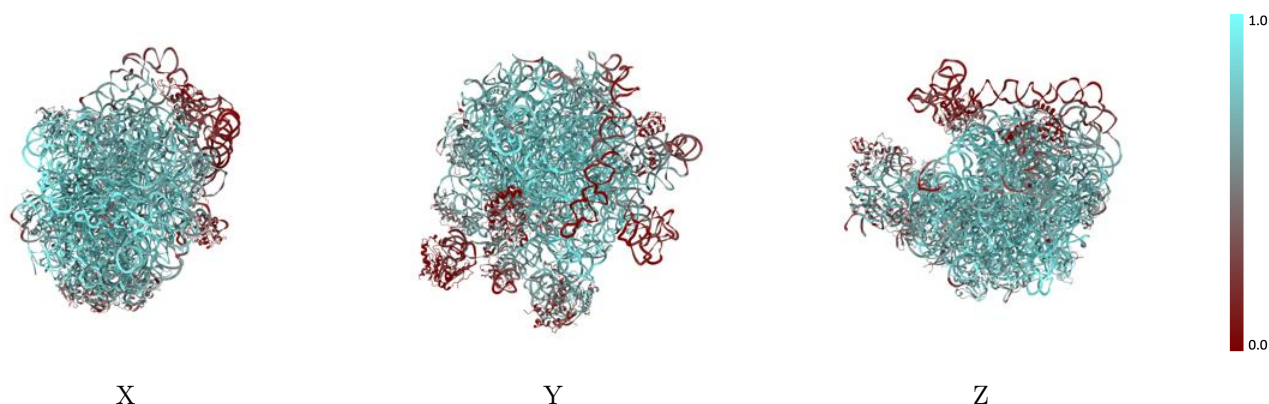
The images above show the 3D surface view of the map at the recommended contour level 0.0179 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



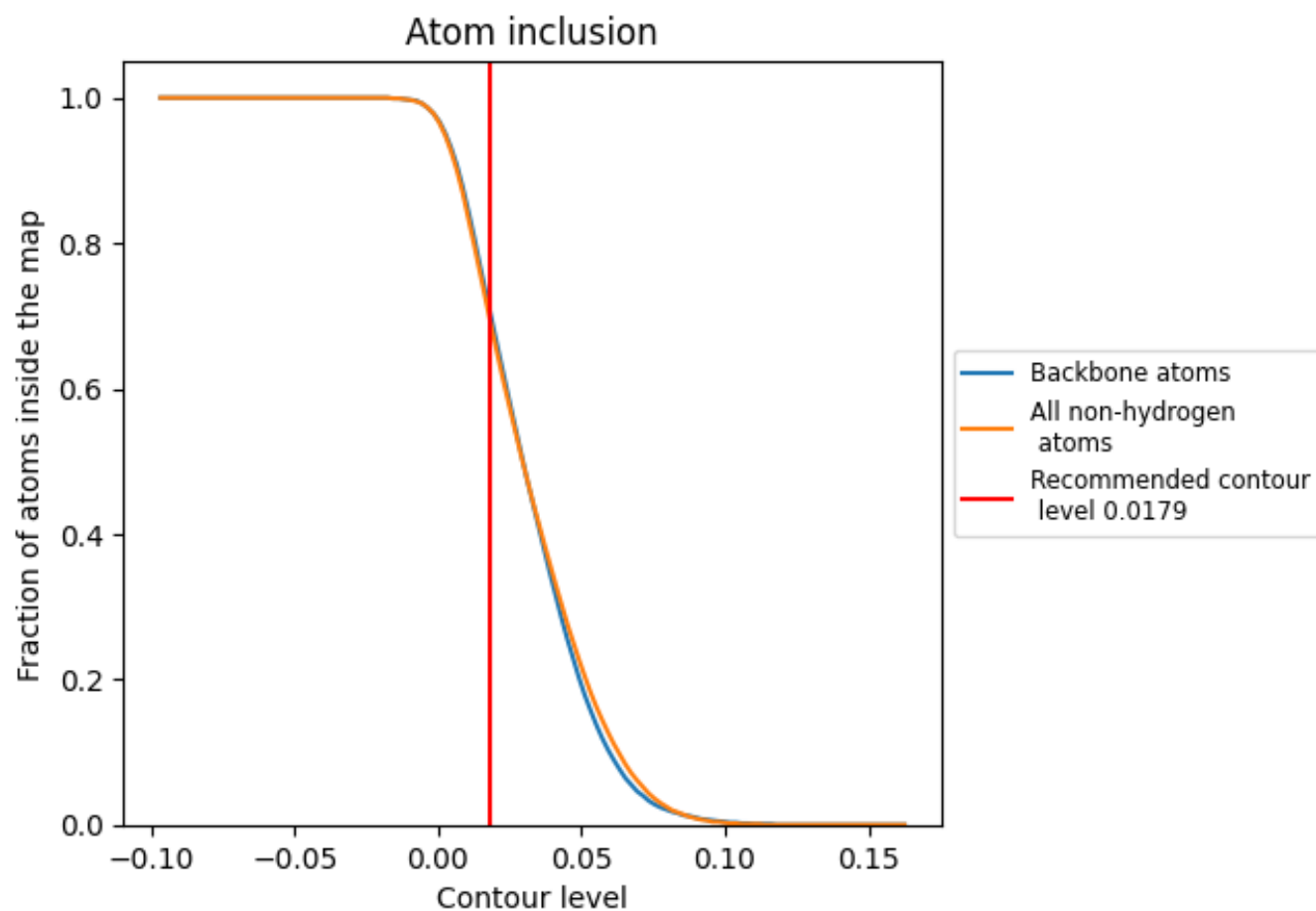
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0179).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 70% 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 (0.0179) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6990	 0.3830
3	 0.7320	 0.4390
B	 0.1620	 0.0740
C	 0.7590	 0.4130
D	 0.7740	 0.4540
E	 0.7320	 0.4120
F	 0.7290	 0.4170
G	 0.3590	 0.2190
H	 0.3810	 0.1650
I	 0.1990	 0.1710
J	 0.0430	 0.0460
K	 0.0420	 0.0630
L	 0.7120	 0.3830
M	 0.6540	 0.3610
N	 0.7480	 0.4230
O	 0.6490	 0.3660
P	 0.8130	 0.4790
Q	 0.5350	 0.2300
R	 0.5610	 0.2960
S	 0.7520	 0.4290
T	 0.7140	 0.3920
U	 0.8670	 0.5750
V	 0.6680	 0.3910
W	 0.7070	 0.4300
X	 0.3210	 0.1470
Y	 0.7240	 0.3960
Z	 0.7340	 0.4330
a	 0.6470	 0.3290
b	 0.6780	 0.3390
c	 0.8380	 0.5420
d	 0.7850	 0.4530
e	 0.8570	 0.5370
f	 0.8420	 0.4900
g	 0.5970	 0.2840
h	 0.2100	 0.1460
i	 0.6500	 0.3020

