



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 10:34 PM UTC

PDB ID : 8W51 / pdb_00008w51
EMDB ID : EMD-37271
Title : Structure of YchF(H114A) on E.coli 50S ribosomal subunit
Authors : Yu, T.; Li, X.; Zeng, F.
Deposited on : 2023-08-25
Resolution : 2.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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

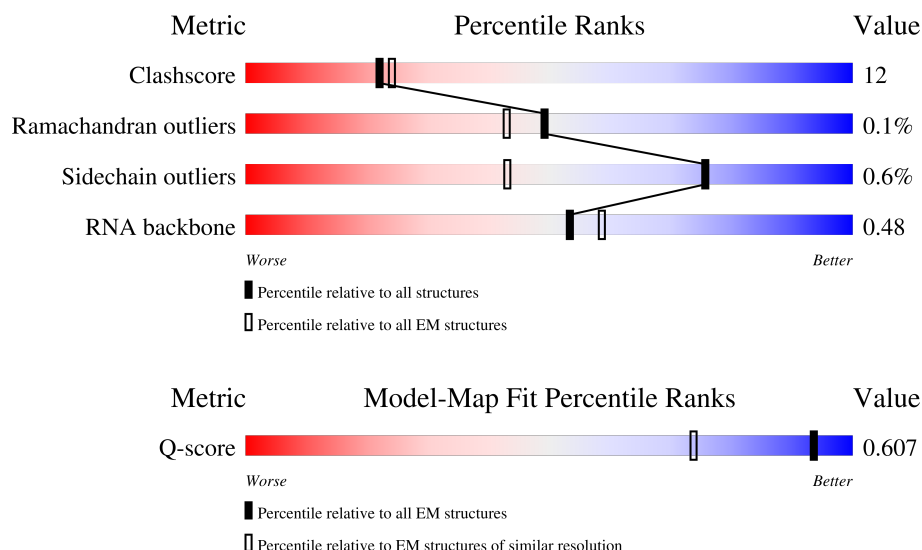
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	2904	
2	B	118	
3	C	273	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	209	
5	E	201	
6	F	179	
7	G	177	
8	H	149	
9	J	142	
10	K	142	
11	L	123	
12	M	144	
13	N	136	
14	O	127	
15	P	117	
16	Q	115	
17	R	118	
18	S	103	
19	T	110	
20	U	100	
21	V	104	
22	W	94	
23	X	85	
24	Y	78	
25	Z	63	
26	0	59	
27	1	57	
28	2	55	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	3	46	78% 22%
30	4	65	74% 22% ...
31	5	38	76% 24%
32	y	379	80% 59% 37% .

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 93901 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 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2904	Total	C	N	O	P	0	0
			62351	27820	11472	20155	2904		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L9.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL11.

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

- Molecule 10 is a protein called 50S ribosomal protein L13.

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

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 12 is a protein called 50S ribosomal protein L15.

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

- Molecule 13 is a protein called 50S ribosomal protein L16.

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

- Molecule 14 is a protein called 50S ribosomal protein L17.

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

- Molecule 15 is a protein called 50S ribosomal protein L18.

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

- Molecule 16 is a protein called 50S ribosomal protein L19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	117	Total	C	N	O	S	0	0
			947	604	192	151			

- Molecule 18 is a protein called 50S ribosomal protein L21.

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

- Molecule 19 is a protein called 50S ribosomal protein L22.

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

- Molecule 20 is a protein called 50S ribosomal protein L23.

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

- Molecule 21 is a protein called 50S ribosomal protein L24.

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

- Molecule 22 is a protein called 50S ribosomal protein L25.

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

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	X	77	Total	C	N	O	S	
			588	363	118	106	1	0

- Molecule 24 is a protein called 50S ribosomal protein L28.

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

- Molecule 25 is a protein called 50S ribosomal protein L29.

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

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	0	58	Total	C	N	O	S	
			449	281	87	79	2	0

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	2	50	Total	C	N	O	0	0
			409	263	75	71		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	5	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called Ribosome-binding ATPase YchF.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	y	363	Total	C	N	O	S	0	0
			2781	1757	470	540	14		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	-15	MET	-	initiating methionine	UNP P0ABU2
y	-14	GLY	-	expression tag	UNP P0ABU2
y	-13	HIS	-	expression tag	UNP P0ABU2
y	-12	HIS	-	expression tag	UNP P0ABU2
y	-11	HIS	-	expression tag	UNP P0ABU2
y	-10	HIS	-	expression tag	UNP P0ABU2
y	-9	HIS	-	expression tag	UNP P0ABU2
y	-8	HIS	-	expression tag	UNP P0ABU2
y	-7	GLU	-	expression tag	UNP P0ABU2
y	-6	ASN	-	expression tag	UNP P0ABU2
y	-5	LEU	-	expression tag	UNP P0ABU2
y	-4	TYR	-	expression tag	UNP P0ABU2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
y	-3	PHE	-	expression tag	UNP P0ABU2
y	-2	GLN	-	expression tag	UNP P0ABU2
y	-1	GLY	-	expression tag	UNP P0ABU2
y	0	HIS	-	expression tag	UNP P0ABU2
y	114	ALA	HIS	engineered mutation	UNP P0ABU2

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	A	99	Total	Mg	0
			99	99	
33	B	4	Total	Mg	0
			4	4	
33	D	1	Total	Mg	0
			1	1	

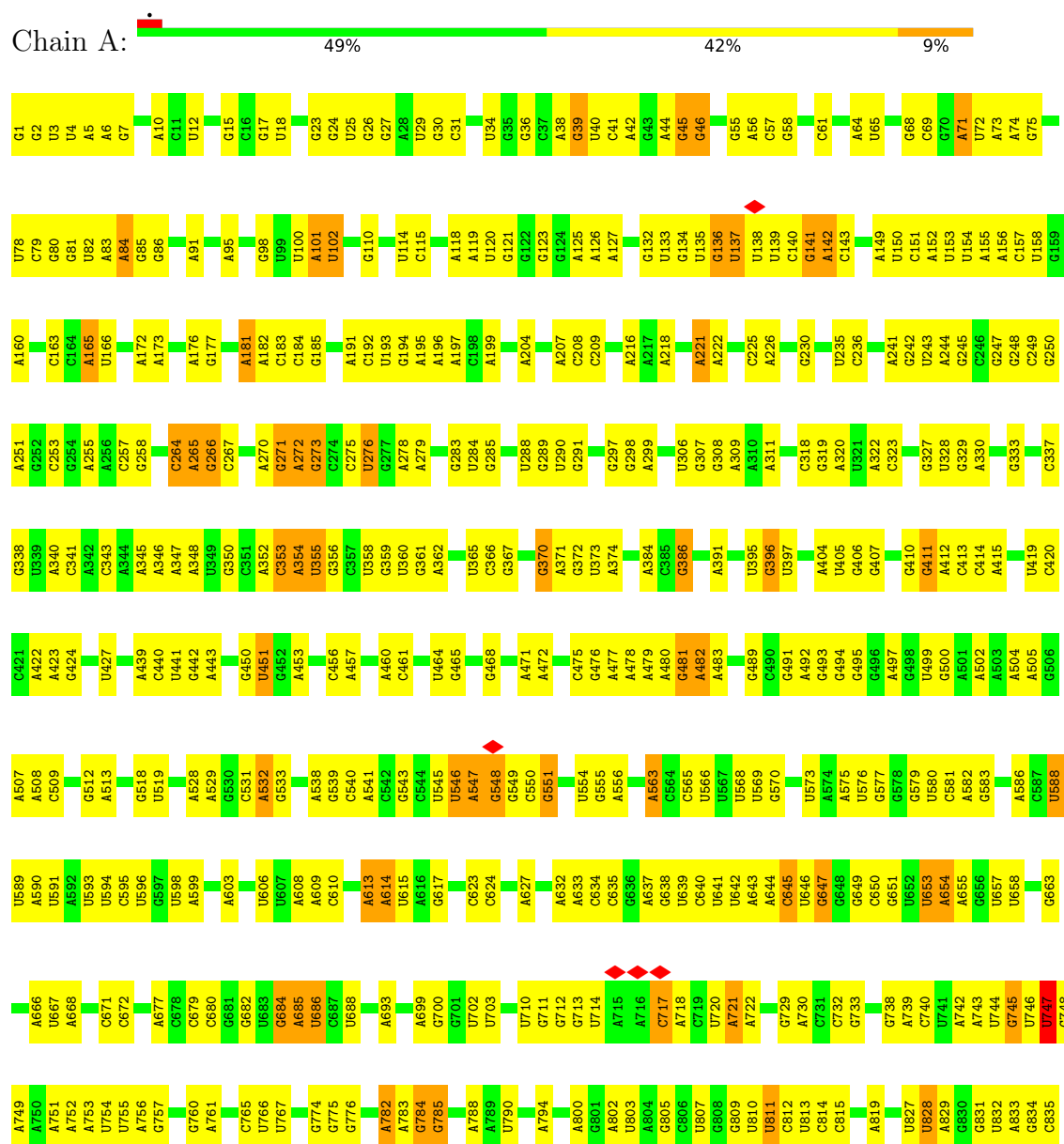
- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

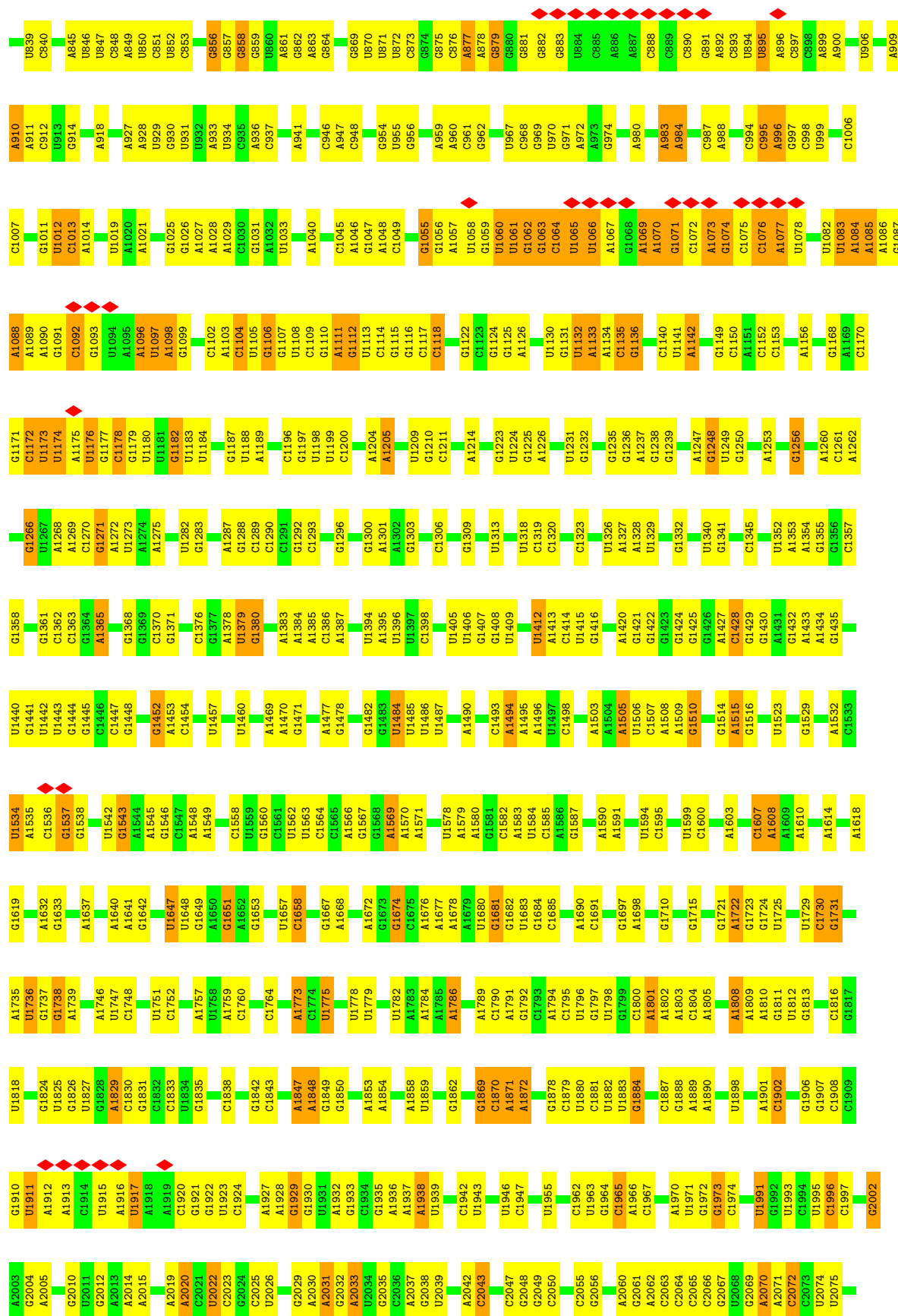
Mol	Chain	Residues	Atoms		AltConf
34	5	1	Total	Zn	0
			1	1	

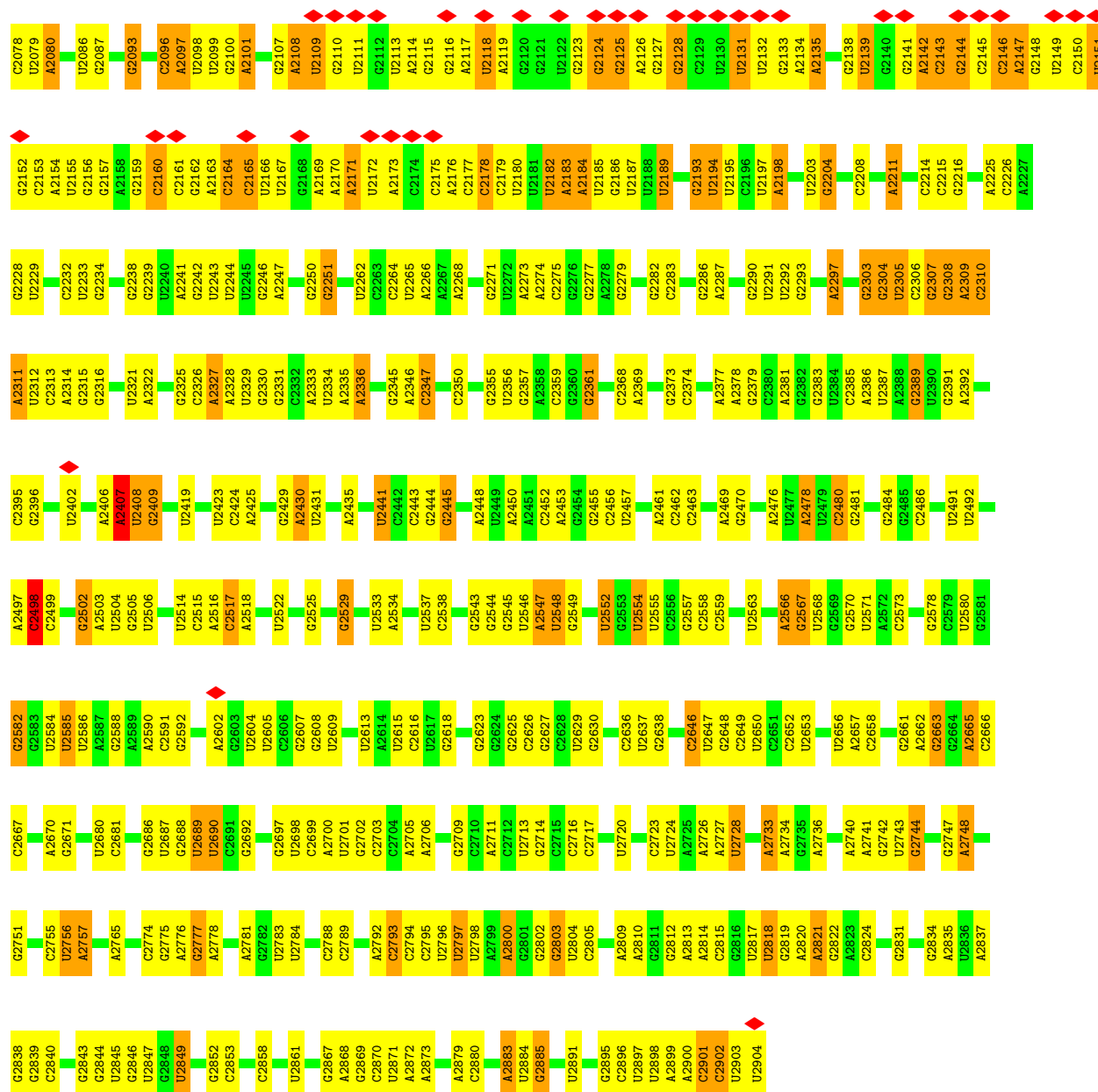
3 Residue-property plots

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: 23S rRNA

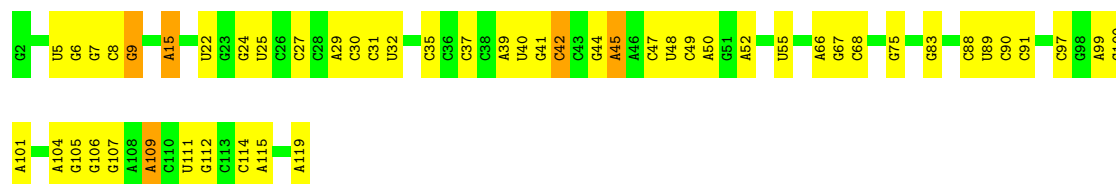






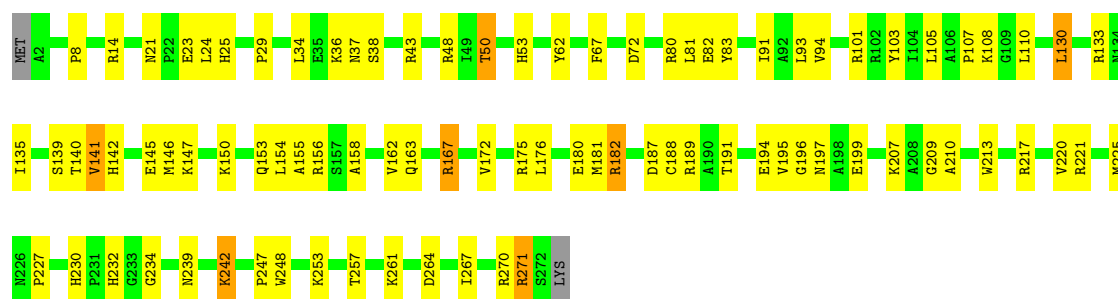
• Molecule 2: 5S rRNA

Chain B: 57% 39%



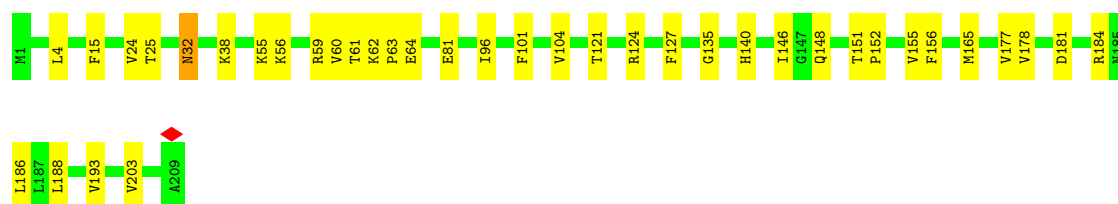
• Molecule 3: 50S ribosomal protein L2

Chain C: 67% 30%



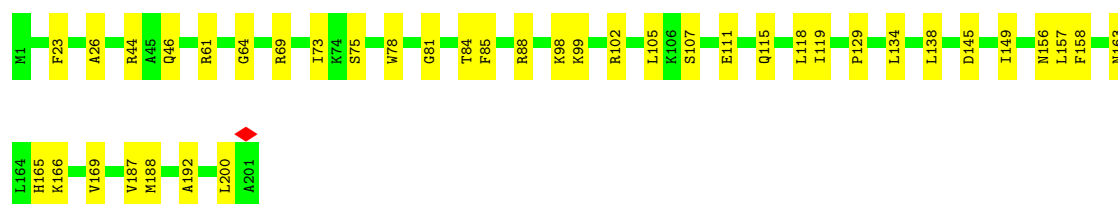
• Molecule 4: 50S ribosomal protein L3

Chain D: 82% 18%



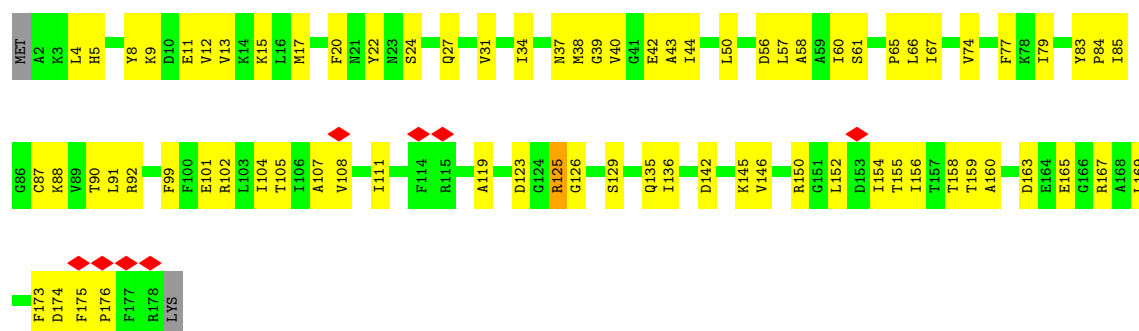
• Molecule 5: 50S ribosomal protein L4

Chain E: 81% 19%



• Molecule 6: 50S ribosomal protein L5

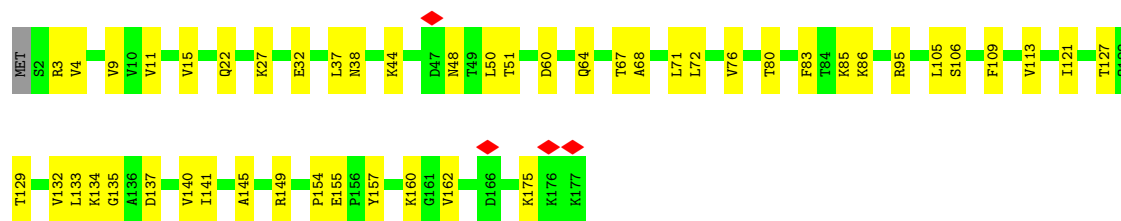
Chain F: 56% 42% ..



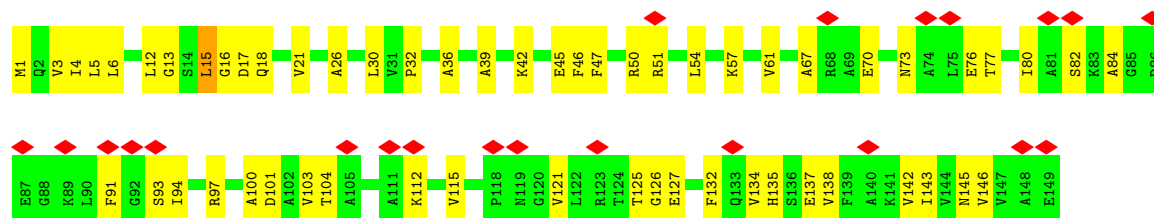
• Molecule 7: 50S ribosomal protein L6

Chain G: 72% 27%

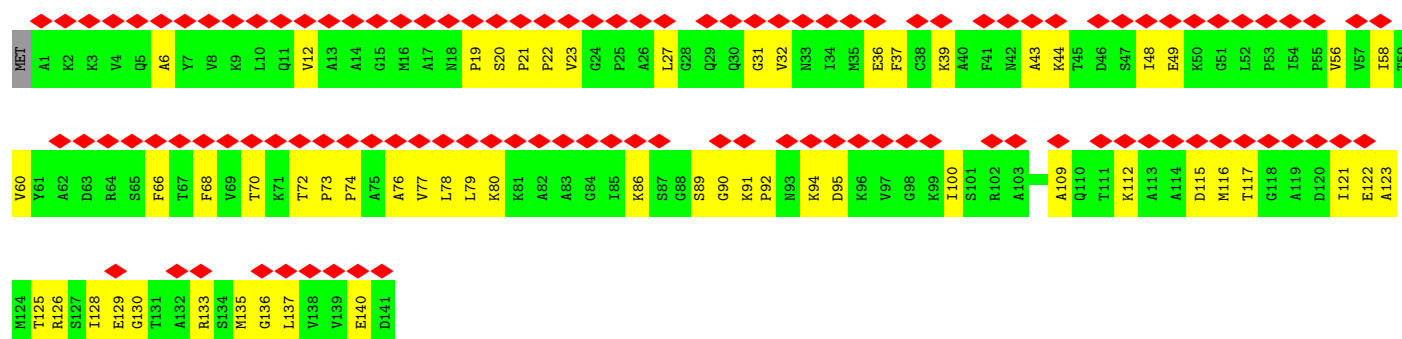
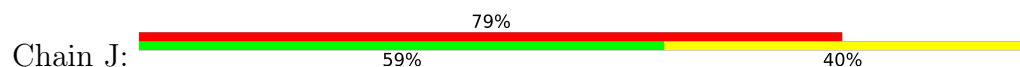




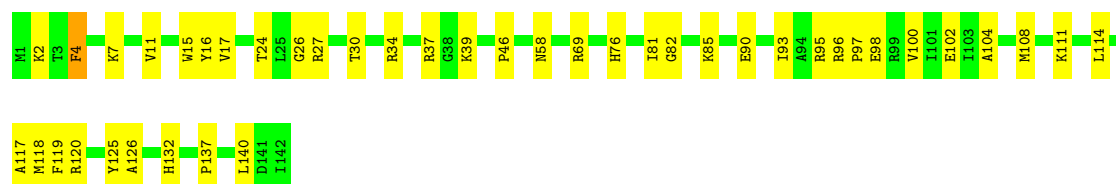
• Molecule 8: 50S ribosomal protein L9



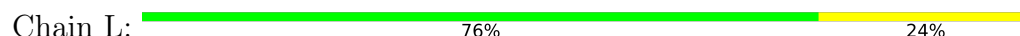
• Molecule 9: Large ribosomal subunit protein uL11



• Molecule 10: 50S ribosomal protein L13



• Molecule 11: 50S ribosomal protein L14



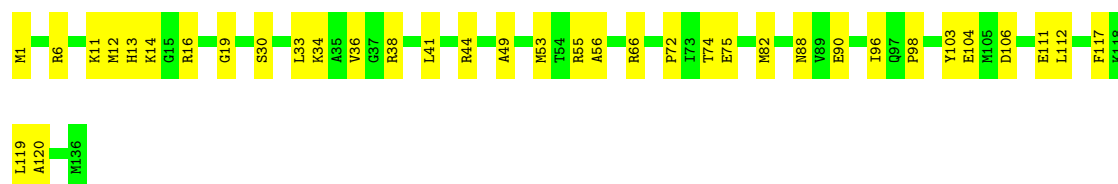
- Molecule 12: 50S ribosomal protein L15

Chain M:  78% 22%



- Molecule 13: 50S ribosomal protein L16

Chain N:  74% 26%



- Molecule 14: 50S ribosomal protein L17

Chain O:  72% 23% 6%



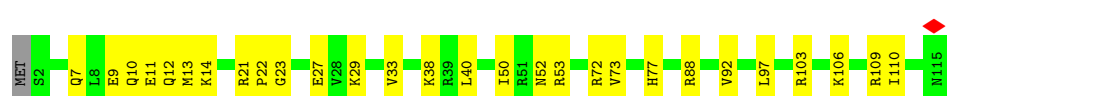
- Molecule 15: 50S ribosomal protein L18

Chain P:  63% 35% 2%



- Molecule 16: 50S ribosomal protein L19

Chain Q:  75% 24%



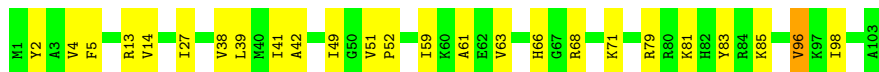
- Molecule 17: 50S ribosomal protein L20

Chain R:  70% 28%

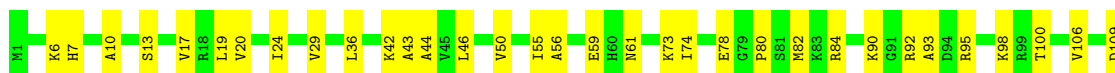


A118

- Molecule 18: 50S ribosomal protein L21

Chain S:  76% 23%


- Molecule 19: 50S ribosomal protein L22

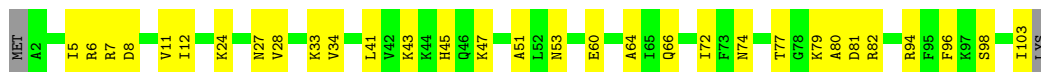
Chain T:  70% 30%


R110

- Molecule 20: 50S ribosomal protein L23

Chain U:  78% 15% 7%

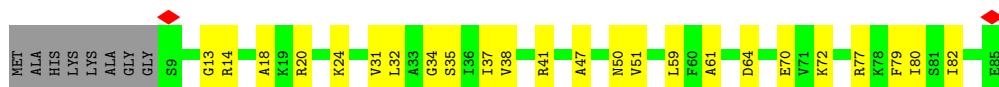

- Molecule 21: 50S ribosomal protein L24

Chain V:  68% 30%


- Molecule 22: 50S ribosomal protein L25

Chain W:  81% 19%


- Molecule 23: 50S ribosomal protein L27

Chain X:  62% 28% 9%


- Molecule 24: 50S ribosomal protein L28

Chain Y:  65% 33%



- Molecule 25: 50S ribosomal protein L29

Chain Z:  78% 21%



- Molecule 26: 50S ribosomal protein L30

Chain 0:  69% 29%



- Molecule 27: 50S ribosomal protein L32

Chain 1:  68% 30%



- Molecule 28: 50S ribosomal protein L33

Chain 2:  62% 29% 9%



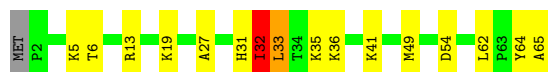
- Molecule 29: 50S ribosomal protein L34

Chain 3:  78% 22%



- Molecule 30: 50S ribosomal protein L35

Chain 4:  74% 22%



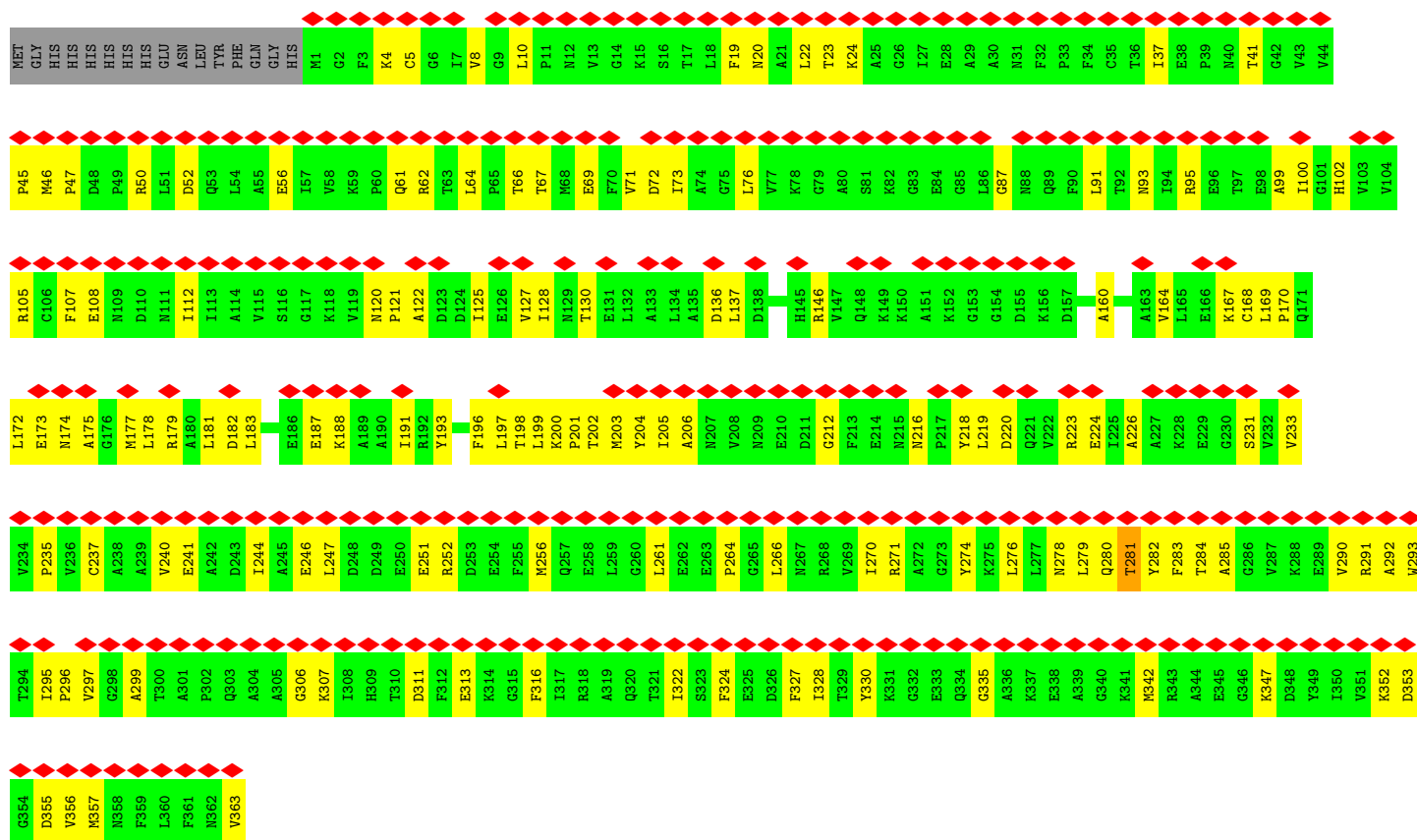
- Molecule 31: 50S ribosomal protein L36

Chain 5:  76% 24%



● Molecule 32: Ribosome-binding ATPase YchF

Chain y:  80% 59% 37% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	137631	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.103	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.006	Depositor
Map size ($\text{\AA}$)	403.19998, 403.19998, 403.19998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.05, 1.05, 1.05	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: OMC, 2MG, 5MC, PSU, MG, 1MG, ZN, 5MU, OMU, OMG

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	0.69	0/69434	0.47	5/108325 (0.0%)
2	B	0.55	0/2828	0.40	0/4410
3	C	0.63	0/2121	0.60	0/2852
4	D	0.63	0/1586	0.60	0/2134
5	E	0.59	0/1571	0.55	0/2113
6	F	0.35	0/1434	0.64	0/1926
7	G	0.44	0/1343	0.54	0/1816
8	H	0.29	0/1122	0.51	0/1515
9	J	0.20	0/1046	0.53	0/1410
10	K	0.61	0/1152	0.55	0/1551
11	L	0.61	0/955	0.59	0/1279
12	M	0.58	0/1062	0.64	0/1413
13	N	0.61	0/1093	0.56	0/1460
14	O	0.62	0/973	0.60	0/1301
15	P	0.54	1/902 (0.1%)	0.60	0/1209
16	Q	0.58	0/929	0.59	0/1242
17	R	0.65	0/960	0.66	1/1278 (0.1%)
18	S	0.61	0/829	0.65	0/1107
19	T	0.63	0/864	0.59	0/1156
20	U	0.56	0/744	0.61	0/994
21	V	0.52	0/787	0.60	0/1051
22	W	0.51	0/766	0.48	0/1025
23	X	0.63	0/595	0.63	0/787
24	Y	0.61	0/635	0.62	0/848
25	Z	0.45	0/502	0.50	0/667
26	0	0.57	0/453	0.60	0/605
27	1	0.65	0/450	0.59	0/599
28	2	0.57	0/416	0.57	0/554
29	3	0.66	0/380	0.56	0/498
30	4	0.60	0/513	0.67	1/676 (0.1%)
31	5	0.65	0/303	0.58	0/397
32	y	0.21	0/2825	0.46	1/3819 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.65	1/101573 (0.0%)	0.50	8/152017 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	P	11	ALA	CA-CB	-6.11	1.44	1.53

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	R	50	ARG	N-CA-C	-10.32	100.11	111.36
30	4	33	LEU	N-CA-C	8.05	121.06	111.33
32	y	281	THR	N-CA-C	5.97	118.85	108.76
1	A	355	U	C2'-C3'-O3'	-5.49	105.47	113.70
1	A	1256	G	C4'-C3'-O3'	-5.39	104.92	113.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62351	0	31373	1067	0
2	B	2529	0	1281	35	0
3	C	2082	0	2154	80	0
4	D	1565	0	1616	31	0
5	E	1552	0	1619	30	0
6	F	1410	0	1444	68	0
7	G	1323	0	1371	31	0
8	H	1111	0	1148	42	0
9	J	1032	0	1088	51	0
10	K	1129	0	1162	36	0
11	L	946	0	1023	21	0
12	M	1053	0	1129	35	0
13	N	1074	0	1157	34	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	O	960	0	1000	23	0
15	P	892	0	923	34	0
16	Q	917	0	962	21	0
17	R	947	0	1019	32	0
18	S	816	0	839	20	0
19	T	857	0	922	28	0
20	U	738	0	807	12	0
21	V	779	0	831	27	0
22	W	753	0	780	13	0
23	X	588	0	604	16	0
24	Y	625	0	652	21	0
25	Z	501	0	531	11	0
26	0	449	0	488	11	0
27	1	444	0	458	25	0
28	2	409	0	440	11	0
29	3	377	0	418	10	0
30	4	504	0	572	18	0
31	5	302	0	340	8	0
32	y	2781	0	2788	109	0
33	A	99	0	0	0	0
33	B	4	0	0	0	0
33	D	1	0	0	0	0
34	5	1	0	0	0	0
All	All	93901	0	62939	1772	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 1772 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2885:G:H22	27:1:40:ARG:NH1	1.37	1.20
32:y:280:GLN:NE2	32:y:295:ILE:HD11	1.64	1.10
1:A:2885:G:N2	27:1:40:ARG:HH12	1.52	1.05
1:A:1779:U:H5	1:A:1784:A:N7	1.59	0.99
1:A:1813:G:N3	3:C:50:THR:HG21	1.77	0.98

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	269/273 (98%)	257 (96%)	12 (4%)	0	100	100
4	D	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
5	E	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
6	F	175/179 (98%)	158 (90%)	16 (9%)	1 (1%)	21	32
7	G	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
8	H	147/149 (99%)	131 (89%)	16 (11%)	0	100	100
9	J	139/142 (98%)	119 (86%)	20 (14%)	0	100	100
10	K	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
11	L	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
12	M	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
13	N	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
14	O	118/127 (93%)	115 (98%)	3 (2%)	0	100	100
15	P	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
16	Q	112/115 (97%)	104 (93%)	8 (7%)	0	100	100
17	R	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
18	S	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
19	T	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
20	U	91/100 (91%)	85 (93%)	6 (7%)	0	100	100
21	V	100/104 (96%)	89 (89%)	11 (11%)	0	100	100
22	W	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
23	X	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
24	Y	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
25	Z	60/63 (95%)	56 (93%)	4 (7%)	0	100	100
26	0	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	2	48/55 (87%)	41 (85%)	7 (15%)	0	100	100
29	3	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
30	4	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	7	11
31	5	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
32	y	361/379 (95%)	345 (96%)	16 (4%)	0	100	100
All	All	3669/3788 (97%)	3484 (95%)	183 (5%)	2 (0%)	49	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	174	ASP
30	4	32	ILE

5.3.2 Protein sidechains [i](#)

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	
3	C	216/218 (99%)	209 (97%)	7 (3%)	34	56
4	D	164/164 (100%)	163 (99%)	1 (1%)	78	89
5	E	165/165 (100%)	165 (100%)	0	100	100
6	F	148/150 (99%)	147 (99%)	1 (1%)	76	88
7	G	137/138 (99%)	137 (100%)	0	100	100
8	H	114/114 (100%)	112 (98%)	2 (2%)	51	73
9	J	109/110 (99%)	109 (100%)	0	100	100
10	K	116/116 (100%)	115 (99%)	1 (1%)	70	85
11	L	104/104 (100%)	104 (100%)	0	100	100
12	M	103/103 (100%)	103 (100%)	0	100	100
13	N	109/109 (100%)	109 (100%)	0	100	100
14	O	100/103 (97%)	100 (100%)	0	100	100
15	P	86/87 (99%)	86 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	Q	99/100 (99%)	98 (99%)	1 (1%)	68	84
17	R	89/90 (99%)	88 (99%)	1 (1%)	65	82
18	S	84/84 (100%)	83 (99%)	1 (1%)	63	81
19	T	93/93 (100%)	93 (100%)	0	100	100
20	U	80/84 (95%)	80 (100%)	0	100	100
21	V	83/85 (98%)	83 (100%)	0	100	100
22	W	78/78 (100%)	78 (100%)	0	100	100
23	X	59/63 (94%)	59 (100%)	0	100	100
24	Y	67/68 (98%)	66 (98%)	1 (2%)	57	77
25	Z	54/55 (98%)	54 (100%)	0	100	100
26	0	48/49 (98%)	48 (100%)	0	100	100
27	1	47/48 (98%)	47 (100%)	0	100	100
28	2	45/49 (92%)	45 (100%)	0	100	100
29	3	38/38 (100%)	38 (100%)	0	100	100
30	4	51/52 (98%)	50 (98%)	1 (2%)	48	70
31	5	34/34 (100%)	34 (100%)	0	100	100
32	y	293/307 (95%)	292 (100%)	1 (0%)	86	93
All	All	3013/3058 (98%)	2995 (99%)	18 (1%)	76	89

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	S	96	VAL
32	y	281	THR
30	4	32	ILE
6	F	125	ARG
17	R	92	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
8	H	18	GLN
25	Z	36	GLN
9	J	104	GLN
32	y	267	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	T	7	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2903/2904 (99%)	519 (17%)	19 (0%)
2	B	117/118 (99%)	18 (15%)	0
All	All	3020/3022 (99%)	537 (17%)	19 (0%)

5 of 537 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	15	G
1	A	23	G
1	A	34	U
1	A	39	G

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2308	G
1	A	2756	U
1	A	2873	A
1	A	2518	A
1	A	1379	U

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

17 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	5MU	A	1939	1	19,22,23	1.49	3 (15%)	27,32,35	2.50	8 (29%)
1	5MC	A	1962	1	19,22,23	1.39	3 (15%)	26,32,35	1.05	2 (7%)
1	OMC	A	2498	33,1	19,22,23	0.92	2 (10%)	25,31,34	0.93	1 (4%)
1	1MG	A	745	1	23,26,27	1.18	3 (13%)	33,39,42	1.71	5 (15%)
1	5MU	A	747	1	19,22,23	1.54	3 (15%)	27,32,35	2.16	7 (25%)
1	PSU	A	2580	1	18,21,22	1.24	3 (16%)	21,30,33	1.98	5 (23%)
1	PSU	A	2504	1	18,21,22	1.29	1 (5%)	21,30,33	2.04	6 (28%)
1	PSU	A	2457	1	18,21,22	1.23	2 (11%)	21,30,33	2.22	5 (23%)
1	2MG	A	1835	1	23,26,27	1.34	4 (17%)	33,38,41	2.16	10 (30%)
1	PSU	A	746	33,1	18,21,22	1.18	2 (11%)	21,30,33	2.14	6 (28%)
1	OMU	A	2552	1	19,22,23	1.50	4 (21%)	25,31,34	1.95	4 (16%)
1	PSU	A	1917	1	18,21,22	1.08	1 (5%)	21,30,33	1.84	4 (19%)
1	2MG	A	2445	1	23,26,27	1.47	6 (26%)	33,38,41	2.30	11 (33%)
1	PSU	A	2605	1	18,21,22	1.22	2 (11%)	21,30,33	2.34	7 (33%)
1	OMG	A	2251	1	23,26,27	1.20	3 (13%)	32,38,41	2.09	7 (21%)
1	PSU	A	955	1	18,21,22	1.12	2 (11%)	21,30,33	1.86	4 (19%)
1	PSU	A	1911	1	18,21,22	1.20	1 (5%)	21,30,33	2.00	6 (28%)

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	5MU	A	1939	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1962	1	-	0/7/25/26	0/2/2/2
1	OMC	A	2498	33,1	-	0/9/27/28	0/2/2/2
1	1MG	A	745	1	-	0/7/25/26	0/3/3/3
1	5MU	A	747	1	-	1/7/25/26	0/2/2/2
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	A	2504	1	-	1/7/25/26	0/2/2/2
1	PSU	A	2457	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1835	1	-	0/9/27/28	0/3/3/3
1	PSU	A	746	33,1	-	2/7/25/26	0/2/2/2
1	OMU	A	2552	1	-	0/9/27/28	0/2/2/2
1	PSU	A	1917	1	-	1/7/25/26	0/2/2/2
1	2MG	A	2445	1	-	1/9/27/28	0/3/3/3
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	A	2251	1	-	1/9/27/28	0/3/3/3
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1911	1	-	3/7/25/26	0/2/2/2

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1962	5MC	C5-C4	4.49	1.47	1.44
1	A	1911	PSU	C6-C5	4.02	1.39	1.35
1	A	2504	PSU	C6-C5	3.93	1.39	1.35
1	A	1917	PSU	C6-C5	3.76	1.39	1.35
1	A	2552	OMU	C4-N3	-3.72	1.32	1.38

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2445	2MG	C2-N3-C4	7.21	121.02	112.00
1	A	1835	2MG	C2-N3-C4	6.73	120.42	112.00
1	A	1939	5MU	C4-N3-C2	-6.21	119.20	127.34
1	A	2605	PSU	C4-N3-C2	-6.08	118.00	126.37
1	A	2605	PSU	N1-C2-N3	6.05	121.55	115.17

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	2251	OMG	C1'-C2'-O2'-CM2
1	A	747	5MU	C3'-C4'-C5'-O5'
1	A	2445	2MG	C3'-C4'-C5'-O5'
1	A	1911	PSU	O4'-C4'-C5'-O5'
1	A	2504	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	2498	OMC	3	0
1	A	745	1MG	1	0
1	A	747	5MU	2	0
1	A	2552	OMU	1	0
1	A	1917	PSU	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	2445	2MG	1	0
1	A	2251	OMG	1	0
1	A	1911	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 105 ligands modelled in this entry, 105 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](#)

There are no chain breaks in this entry.

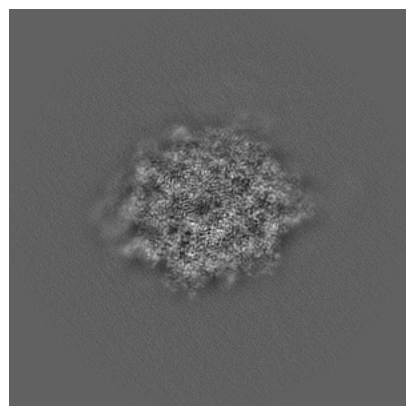
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37271. These allow visual inspection of the internal detail of the map and identification of artifacts.

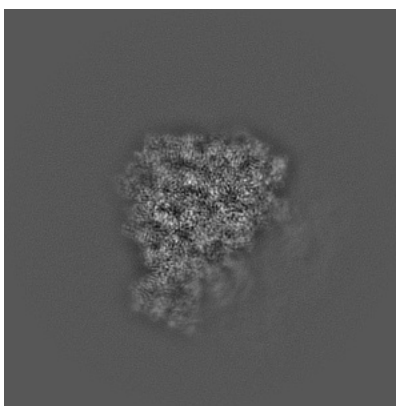
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

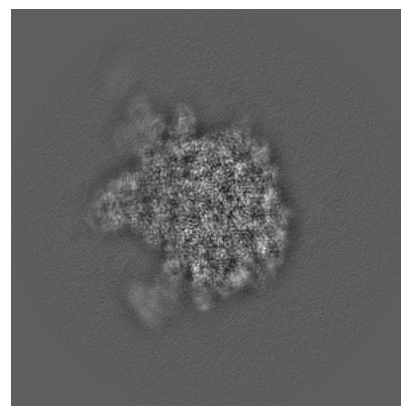
6.1.1 Primary map



X

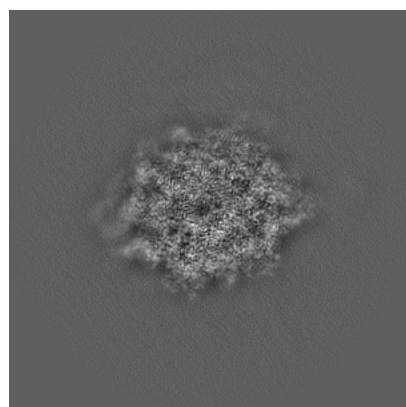


Y

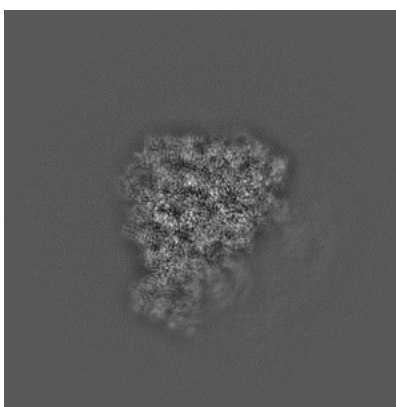


Z

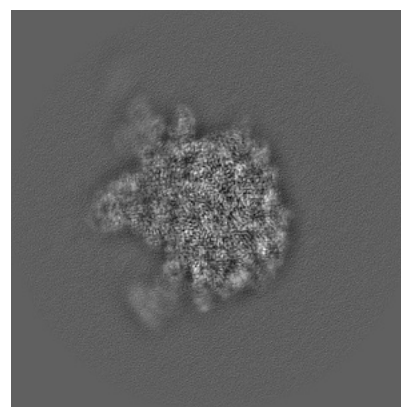
6.1.2 Raw map



X



Y

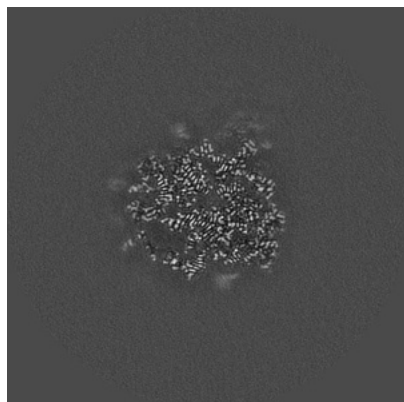


Z

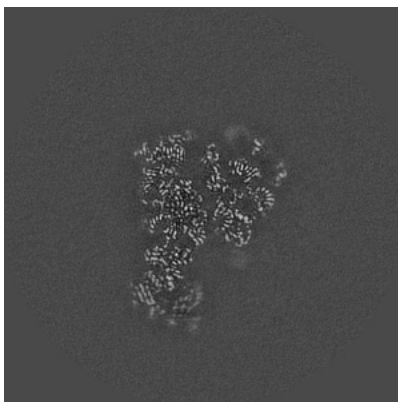
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

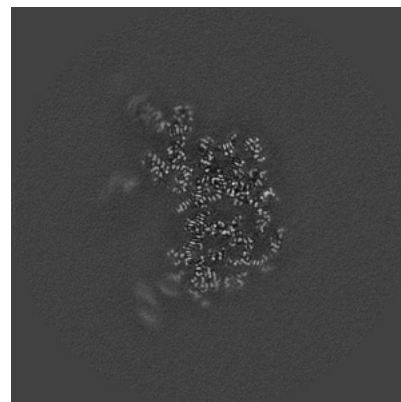
6.2.1 Primary map



X Index: 192

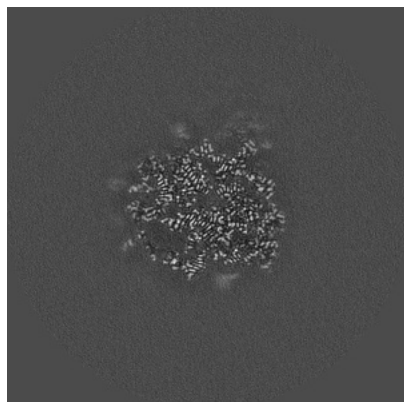


Y Index: 192

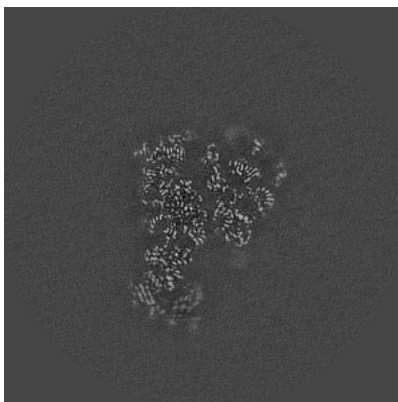


Z Index: 192

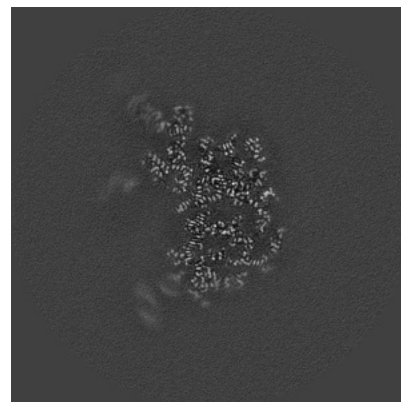
6.2.2 Raw map



X Index: 192



Y Index: 192

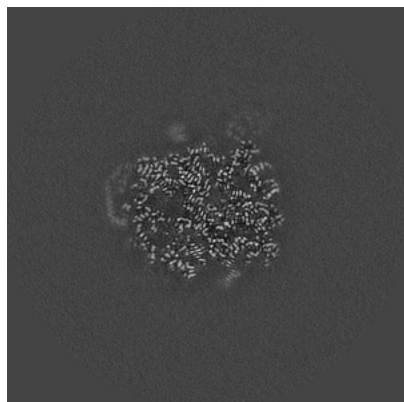


Z Index: 192

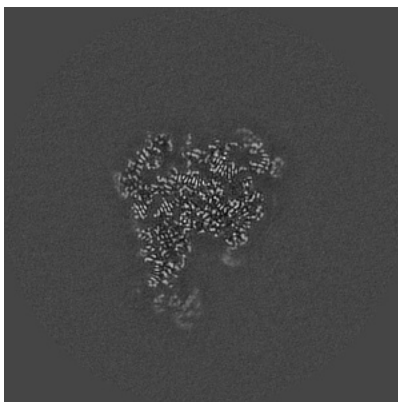
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

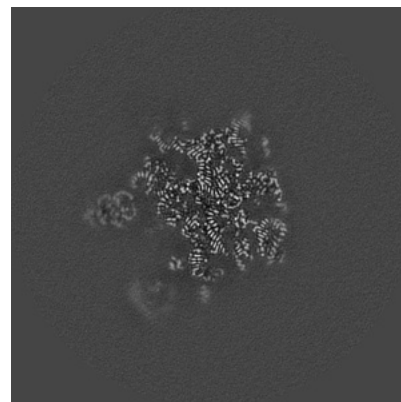
6.3.1 Primary map



X Index: 187

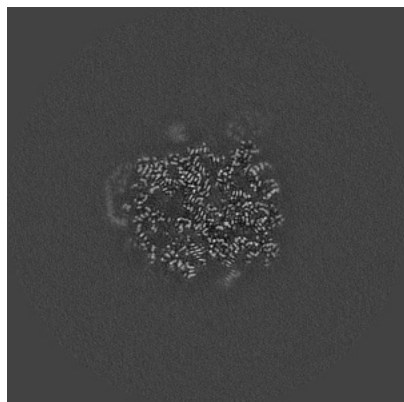


Y Index: 176

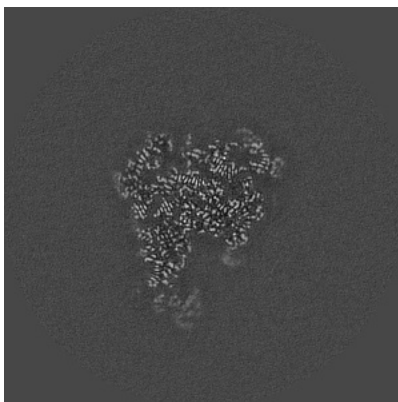


Z Index: 177

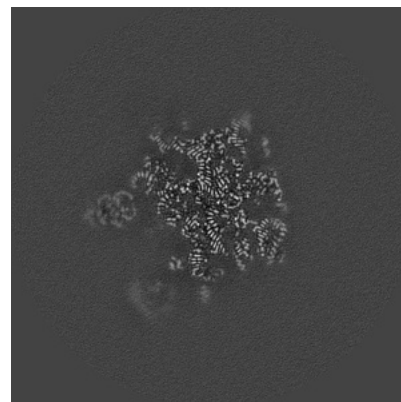
6.3.2 Raw map



X Index: 187



Y Index: 176

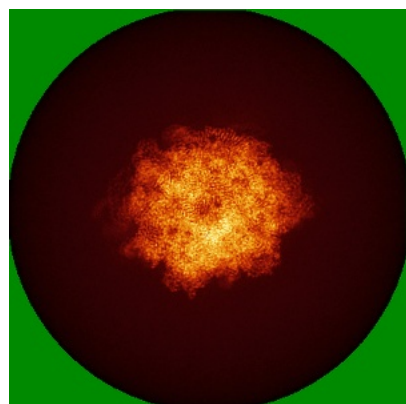


Z Index: 177

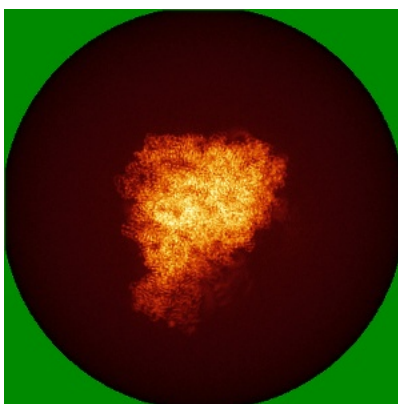
The images above show the largest variance slices of the map in three orthogonal directions.

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

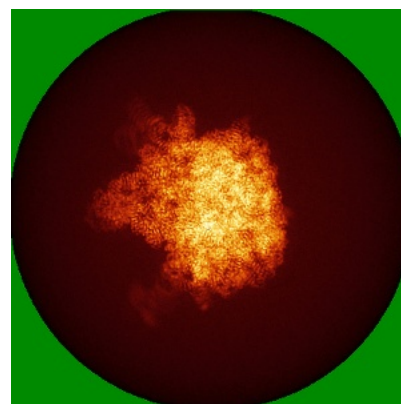
6.4.1 Primary map



X

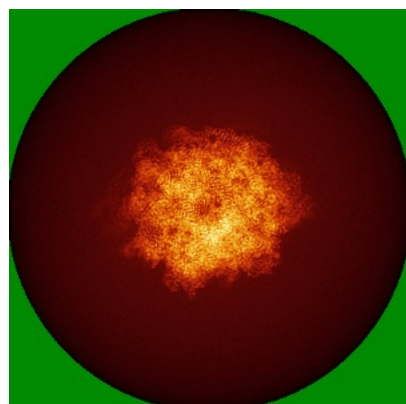


Y

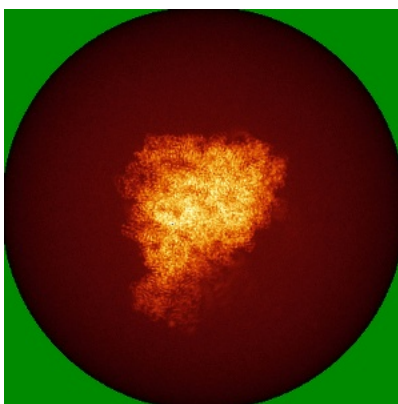


Z

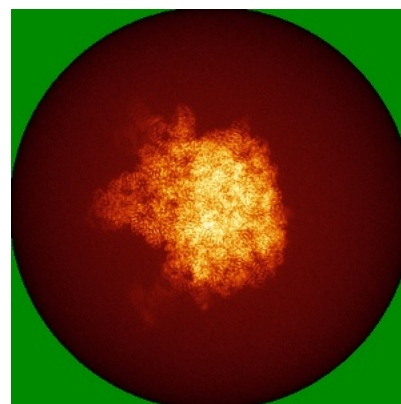
6.4.2 Raw map



X



Y

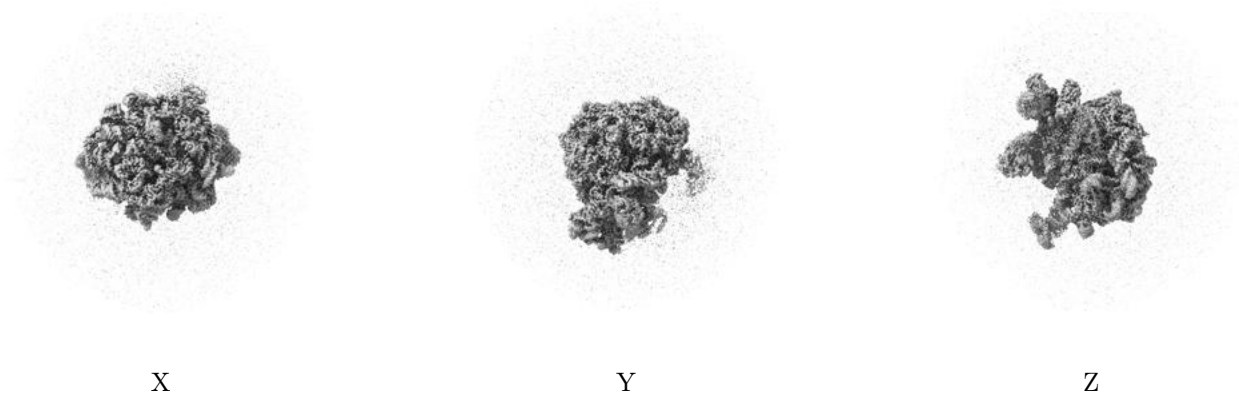


Z

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.

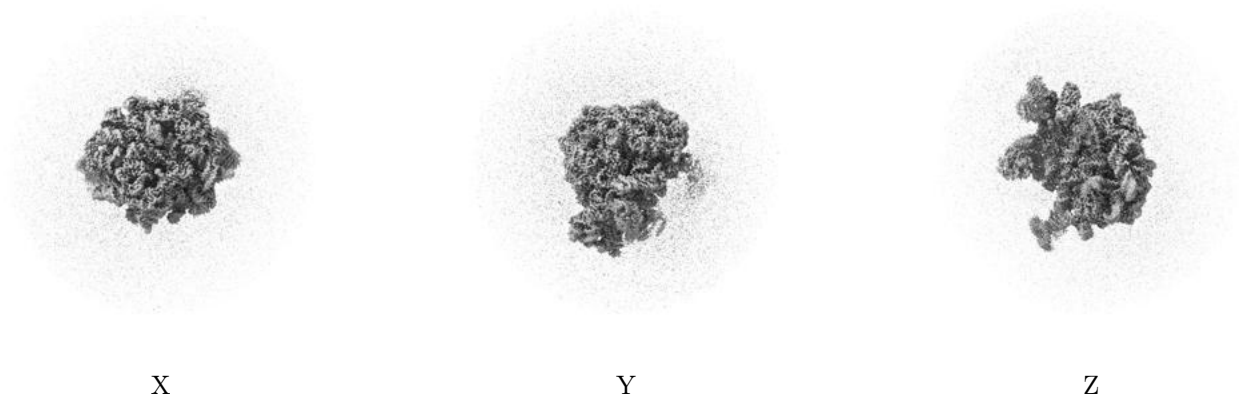
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

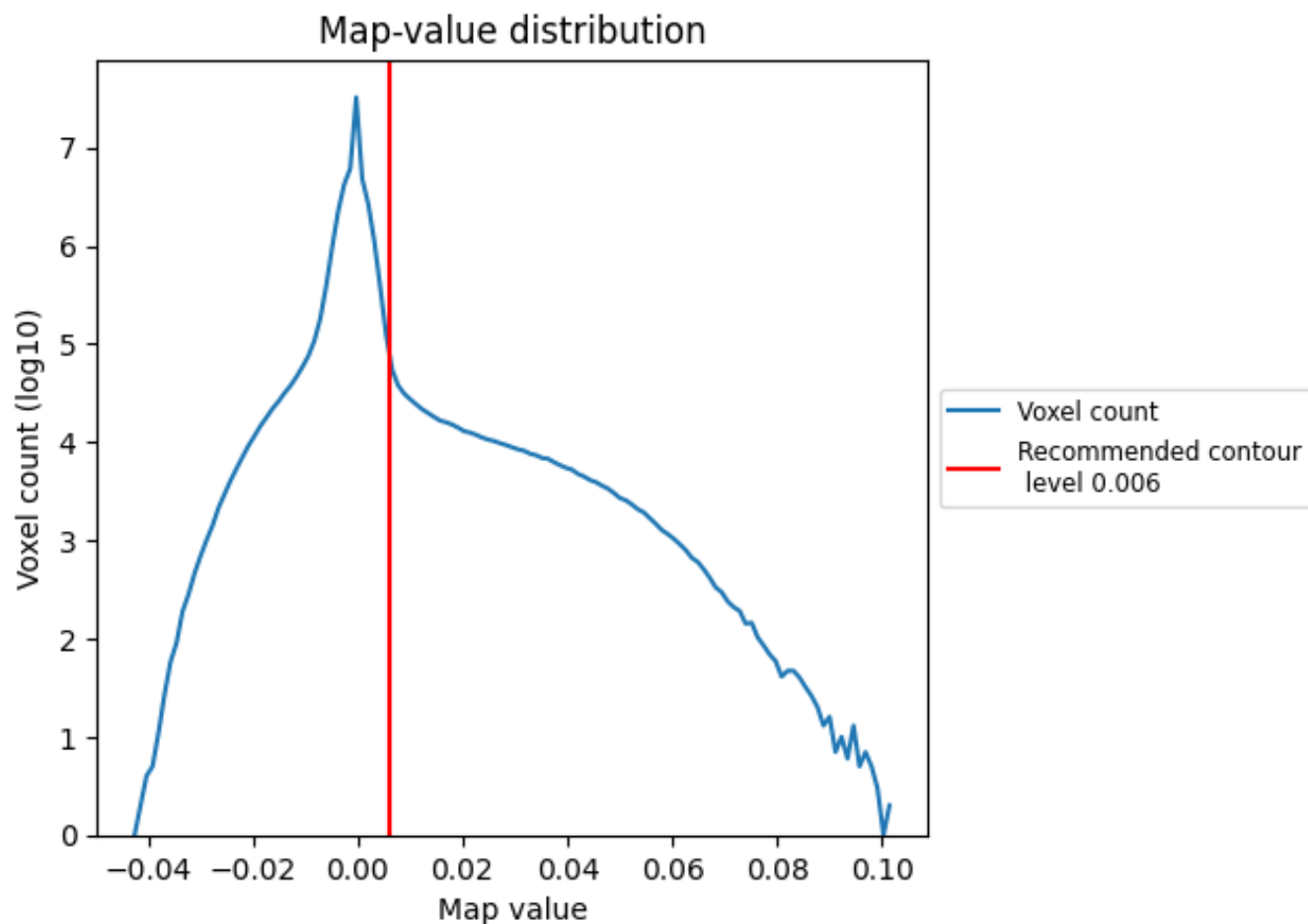
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

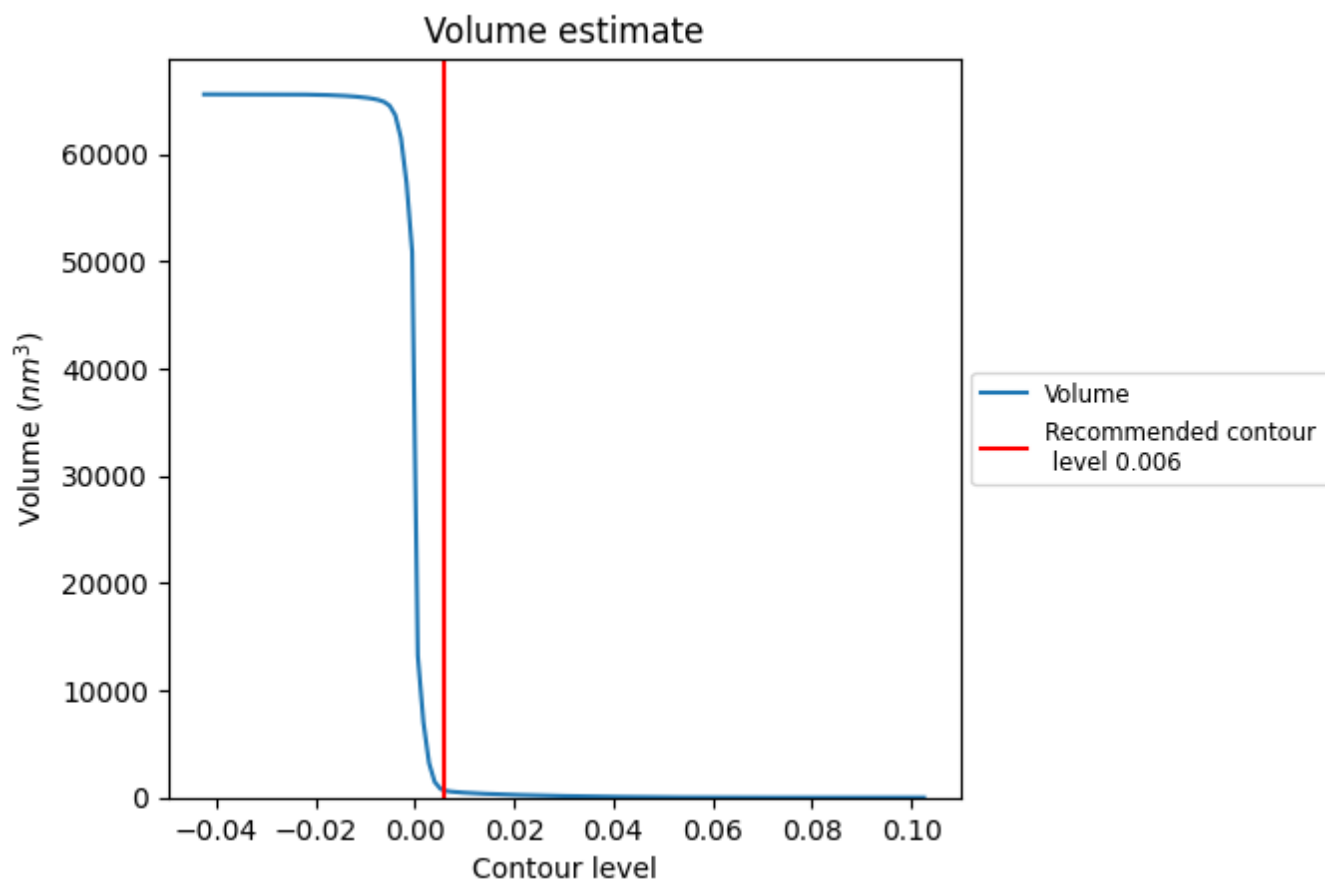
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

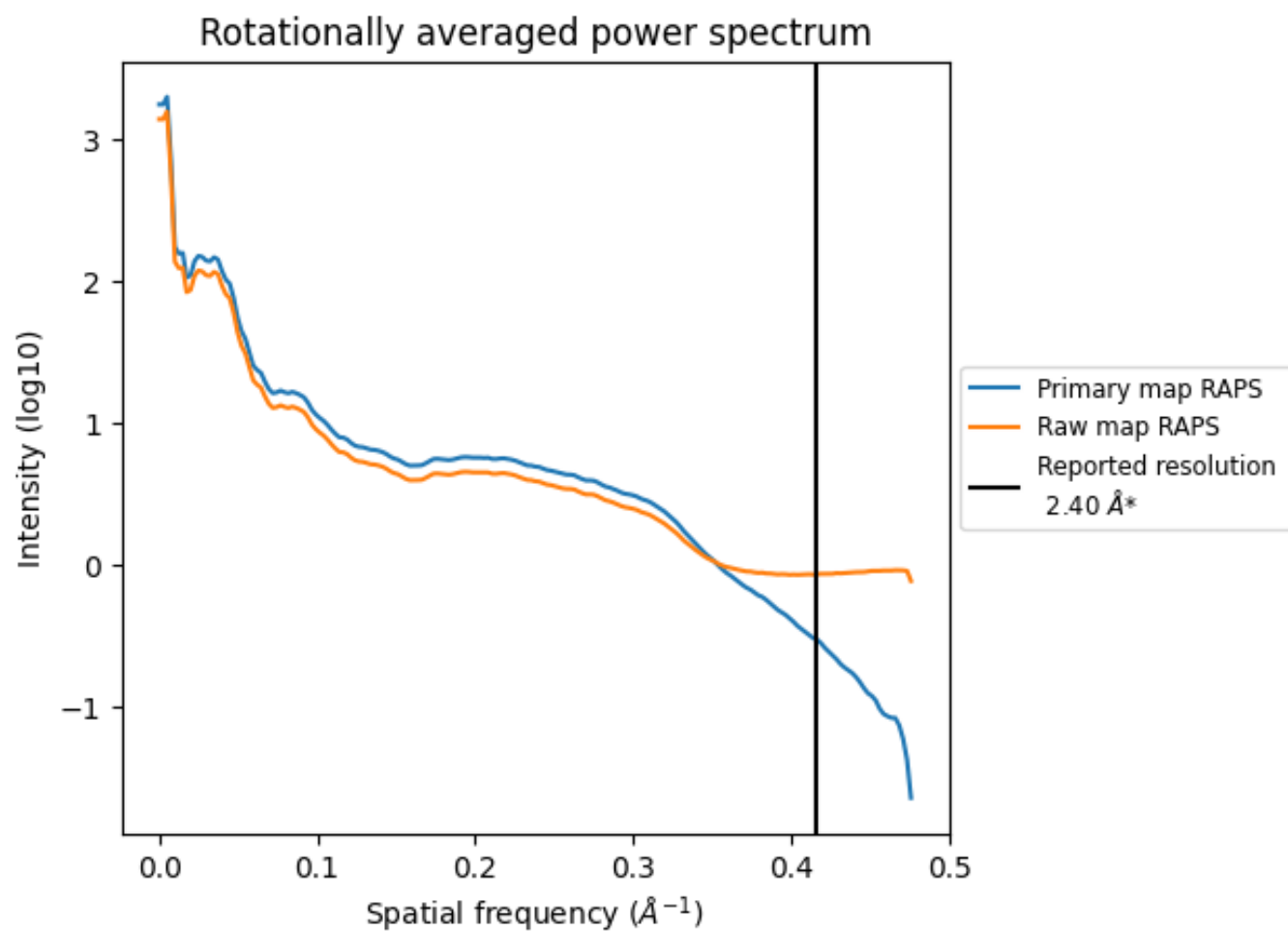
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 667 nm^3 ; this corresponds to an approximate mass of 603 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 ⓘ

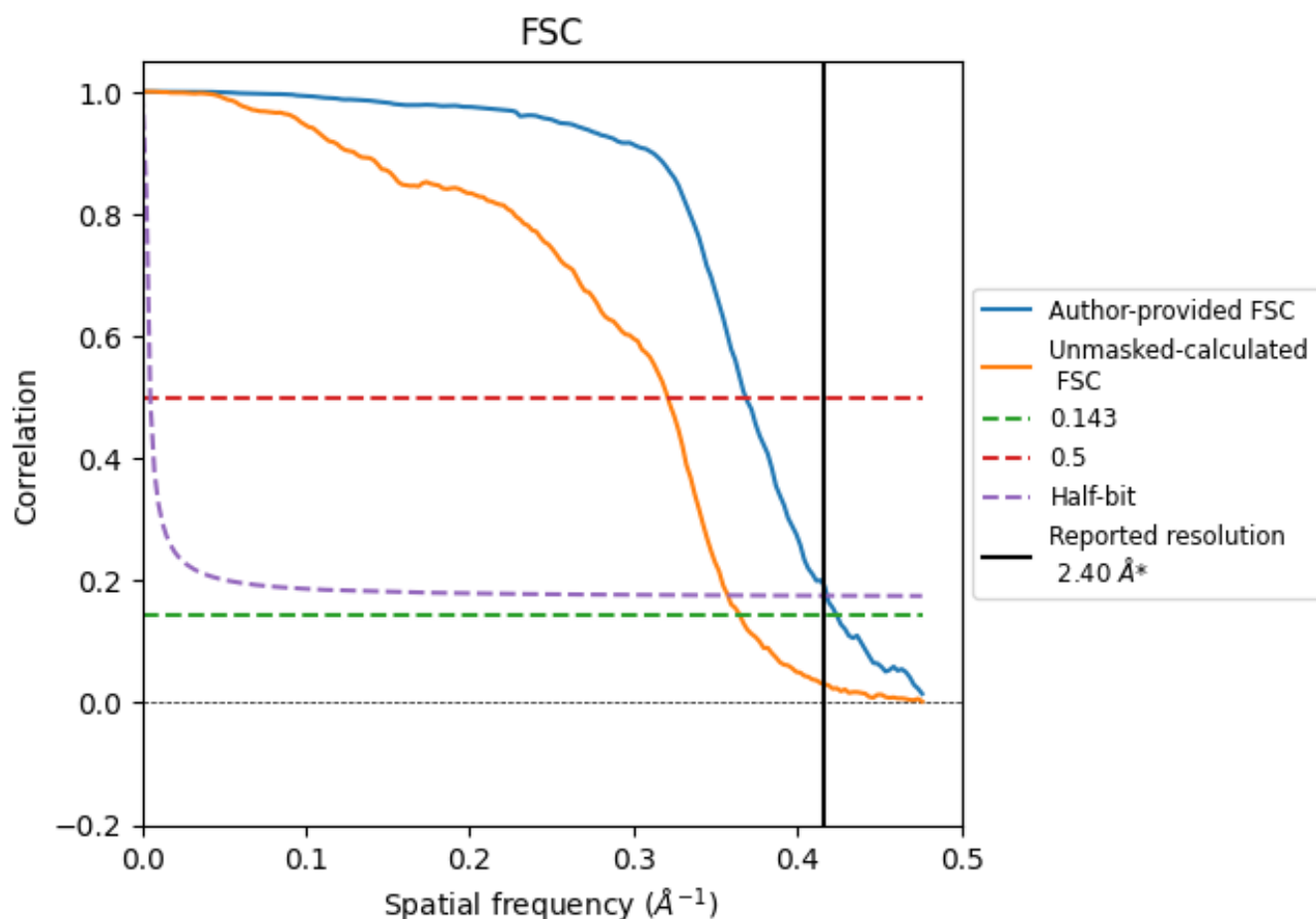


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

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 0.417 Å⁻¹

8.2 Resolution estimates [i](#)

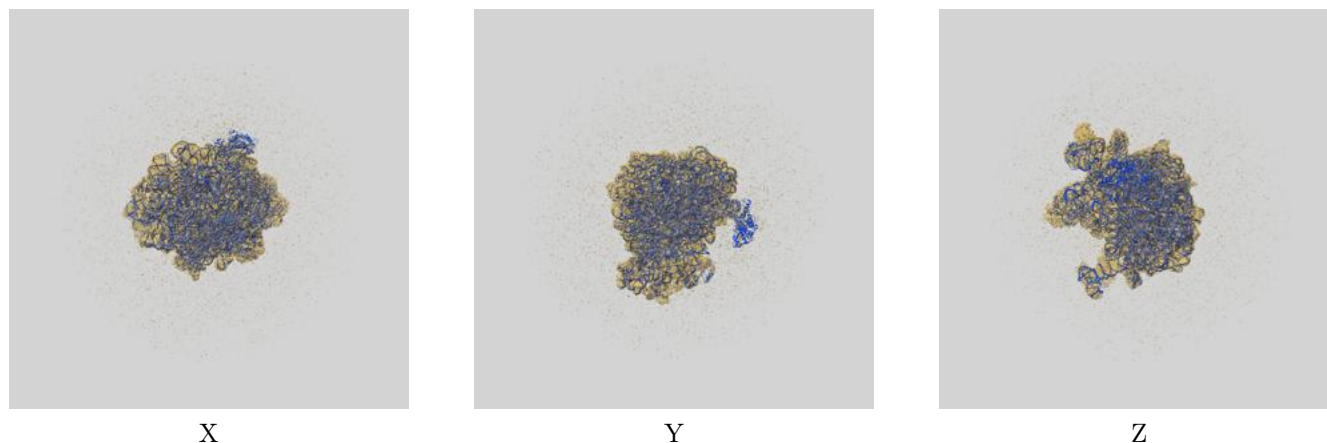
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.36	2.71	2.39
Unmasked-calculated*	2.74	3.12	2.80

*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 2.74 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

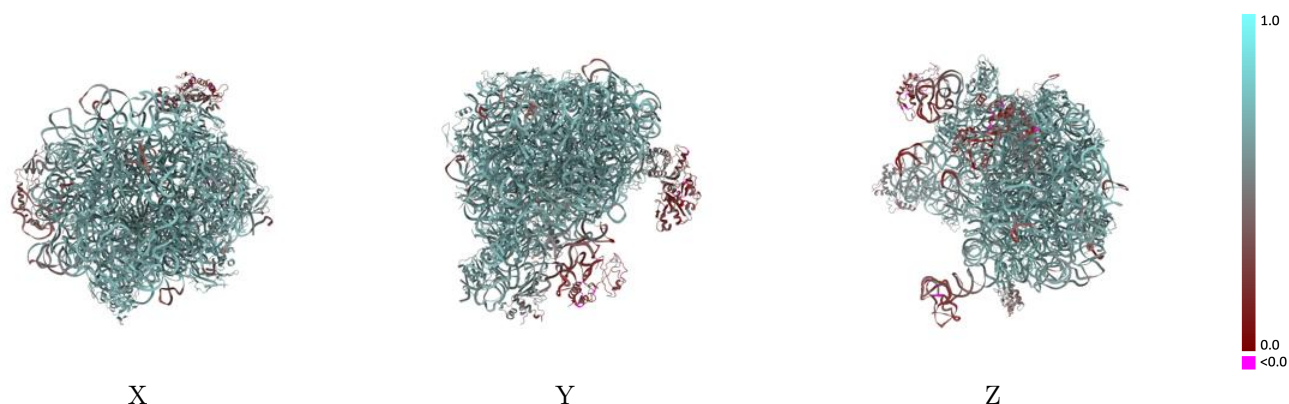
This section contains information regarding the fit between EMDB map EMD-37271 and PDB model 8W51. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



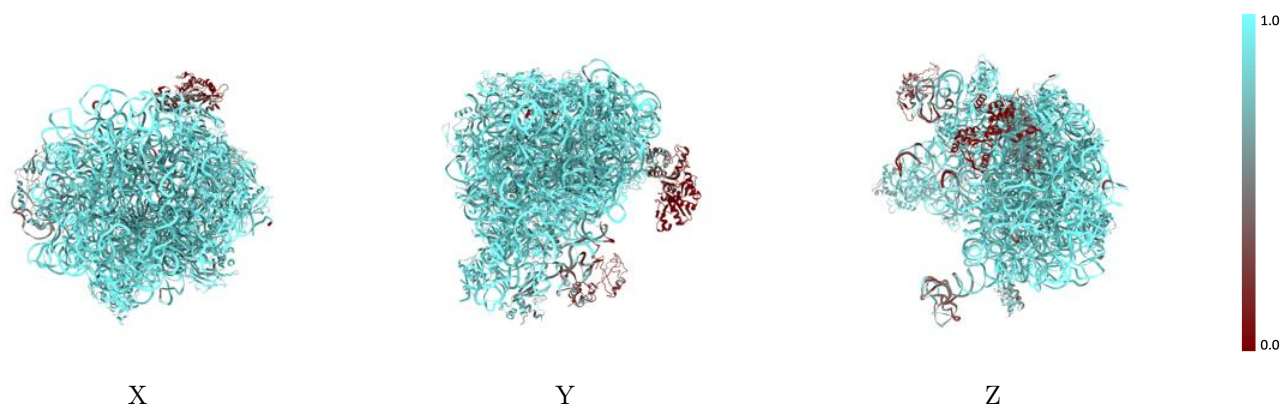
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



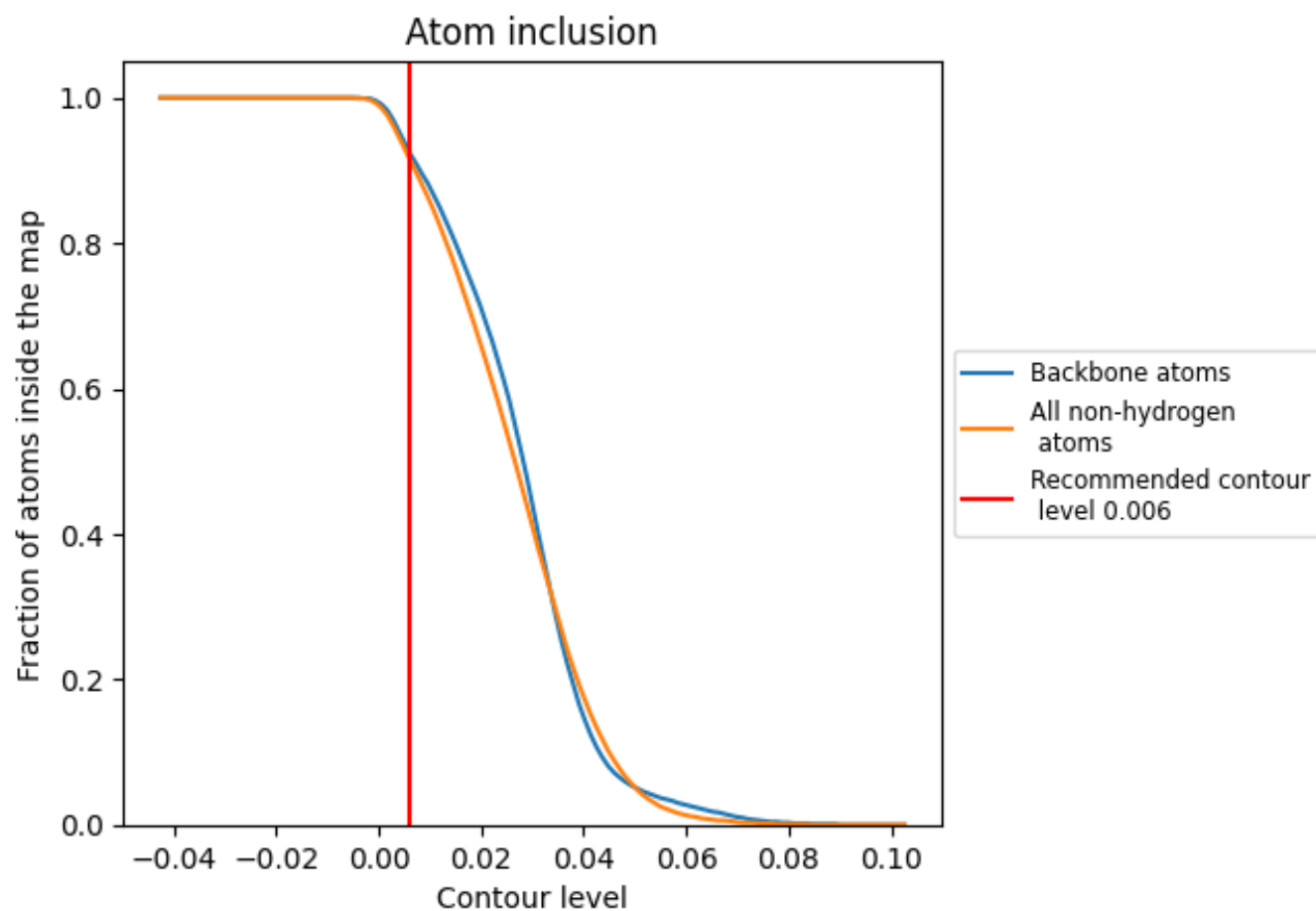
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9160	 0.6070
0	 0.9450	 0.6410
1	 0.9350	 0.6560
2	 0.9350	 0.6110
3	 0.9630	 0.6840
4	 0.9610	 0.6710
5	 0.9490	 0.6540
A	 0.9580	 0.6200
B	 0.9800	 0.6140
C	 0.9590	 0.6630
D	 0.9530	 0.6580
E	 0.9350	 0.6350
F	 0.7570	 0.4720
G	 0.8890	 0.5750
H	 0.6740	 0.4440
J	 0.2260	 0.2220
K	 0.9460	 0.6490
L	 0.9450	 0.6430
M	 0.9420	 0.6430
N	 0.9520	 0.6560
O	 0.9700	 0.6660
P	 0.8960	 0.5970
Q	 0.9270	 0.6350
R	 0.9640	 0.6690
S	 0.9310	 0.6350
T	 0.9390	 0.6540
U	 0.8930	 0.6100
V	 0.9100	 0.6080
W	 0.9160	 0.6200
X	 0.9270	 0.6530
Y	 0.9400	 0.6450
Z	 0.8920	 0.6040
y	 0.1760	 0.3150

