wwPDB EM Validation Summary Report

Apr 15, 2024 – 12:36 PM JST

PDB ID	:	8J1Z
EMDB ID	:	EMD-35939
Title	:	The global structure of pre50S related to DbpA in state3
Authors	:	Yu, T.; Zeng, F.
Deposited on	:	2023-04-13
Resolution	:	2.60 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:

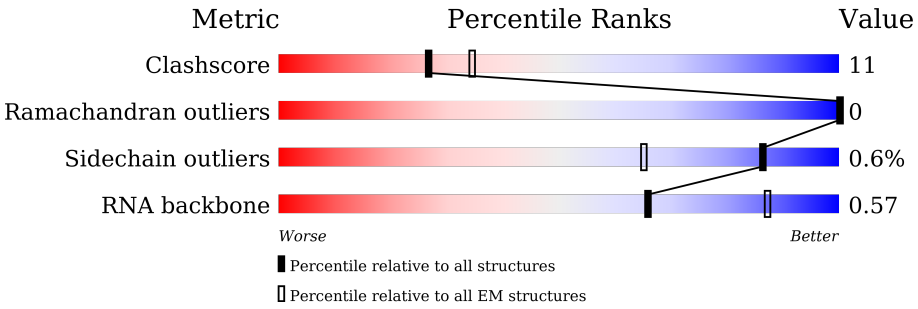
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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)
Clashscore	158937	4297
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 <=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	75% 12% 13%
2	b	120	88% 11%
3	c	273	96%
4	d	209	89% 11%
5	e	201	96%
6	f	179	29% 97%
7	i	142	100%

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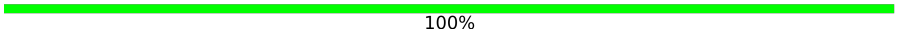
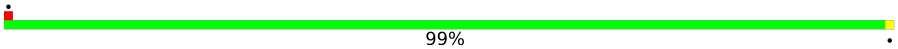
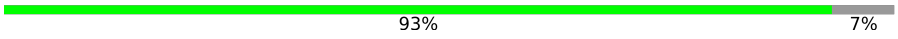
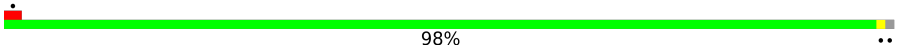
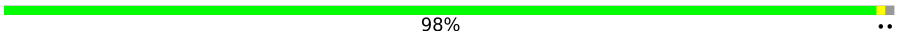
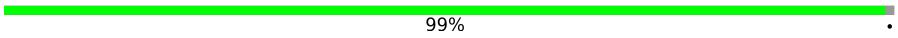
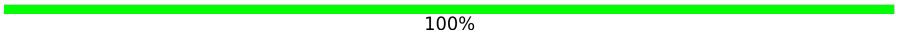
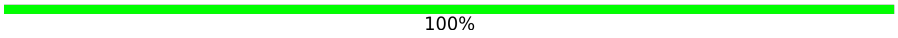
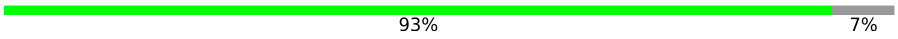
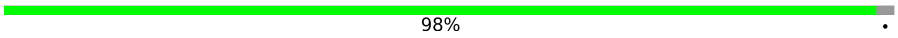
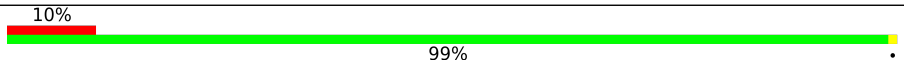
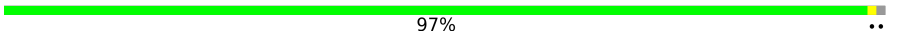
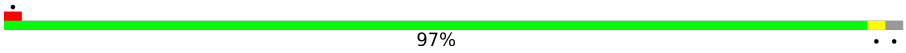
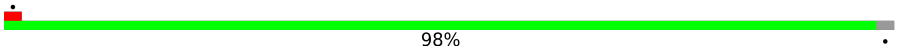
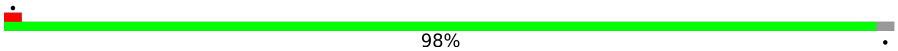
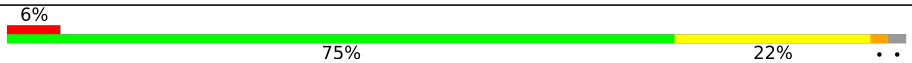
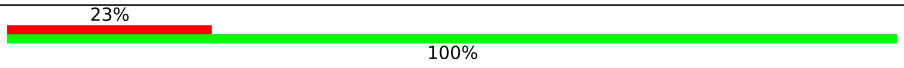
Mol	Chain	Length	Quality of chain
8	j	123	
9	k	144	
10	m	127	
11	n	117	
12	o	115	
13	p	118	
14	q	103	
15	r	110	
16	s	100	
17	t	104	
18	u	94	
19	v	85	
20	w	78	
21	x	63	
22	y	59	
23	z	57	
24	0	55	
25	1	46	
26	2	65	
27	h	149	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	G7M	a	2069	X	-	-	-

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 79520 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
			Total	C	N	O	P		
1	a	2513	54003	24093	9979	17418	2513	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	b	119	2549	1135	466	829	119	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	265	2035	1260	413	355	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	186	1397	882	253	258	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	193	1483	932	266	280	5	0	0

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

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

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

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

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

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

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

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

- Molecule 10 is a protein called 50S ribosomal protein L17.

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

- Molecule 11 is a protein called 50S ribosomal protein L18.

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

- Molecule 12 is a protein called 50S ribosomal protein L19.

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

- Molecule 13 is a protein called 50S ribosomal protein L20.

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

- Molecule 14 is a protein called 50S ribosomal protein L21.

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

- Molecule 15 is a protein called 50S ribosomal protein L22.

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

- Molecule 16 is a protein called 50S ribosomal protein L23.

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

- Molecule 17 is a protein called 50S ribosomal protein L24.

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

- Molecule 18 is a protein called 50S ribosomal protein L25.

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

- Molecule 19 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	v	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

- Molecule 20 is a protein called 50S ribosomal protein L28.

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

- Molecule 21 is a protein called 50S ribosomal protein L29.

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

- Molecule 22 is a protein called 50S ribosomal protein L30.

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

- Molecule 23 is a protein called 50S ribosomal protein L32.

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

- Molecule 24 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 25 is a protein called 50S ribosomal protein L34.

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 50S ribosomal protein L35.

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 50S ribosomal protein L9.

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

- Molecule 28 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
28	a	202	Total Mg 202 202	0
28	b	5	Total Mg 5 5	0
28	c	1	Total Mg 1 1	0
28	p	1	Total Mg 1 1	0
28	z	1	Total Mg 1 1	0

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	AltConf
29	a	137	Total O 137 137	0
29	b	117	Total O 117 117	0
29	c	63	Total O 63 63	0
29	d	17	Total O 17 17	0
29	e	22	Total O 22 22	0
29	f	22	Total O 22 22	0
29	i	13	Total O 13 13	0
29	j	14	Total O 14 14	0
29	k	28	Total O 28 28	0
29	m	28	Total O 28 28	0
29	n	34	Total O 34 34	0
29	o	9	Total O 9 9	0
29	p	22	Total O 22 22	0
29	q	17	Total O 17 17	0
29	r	15	Total O 15 15	0

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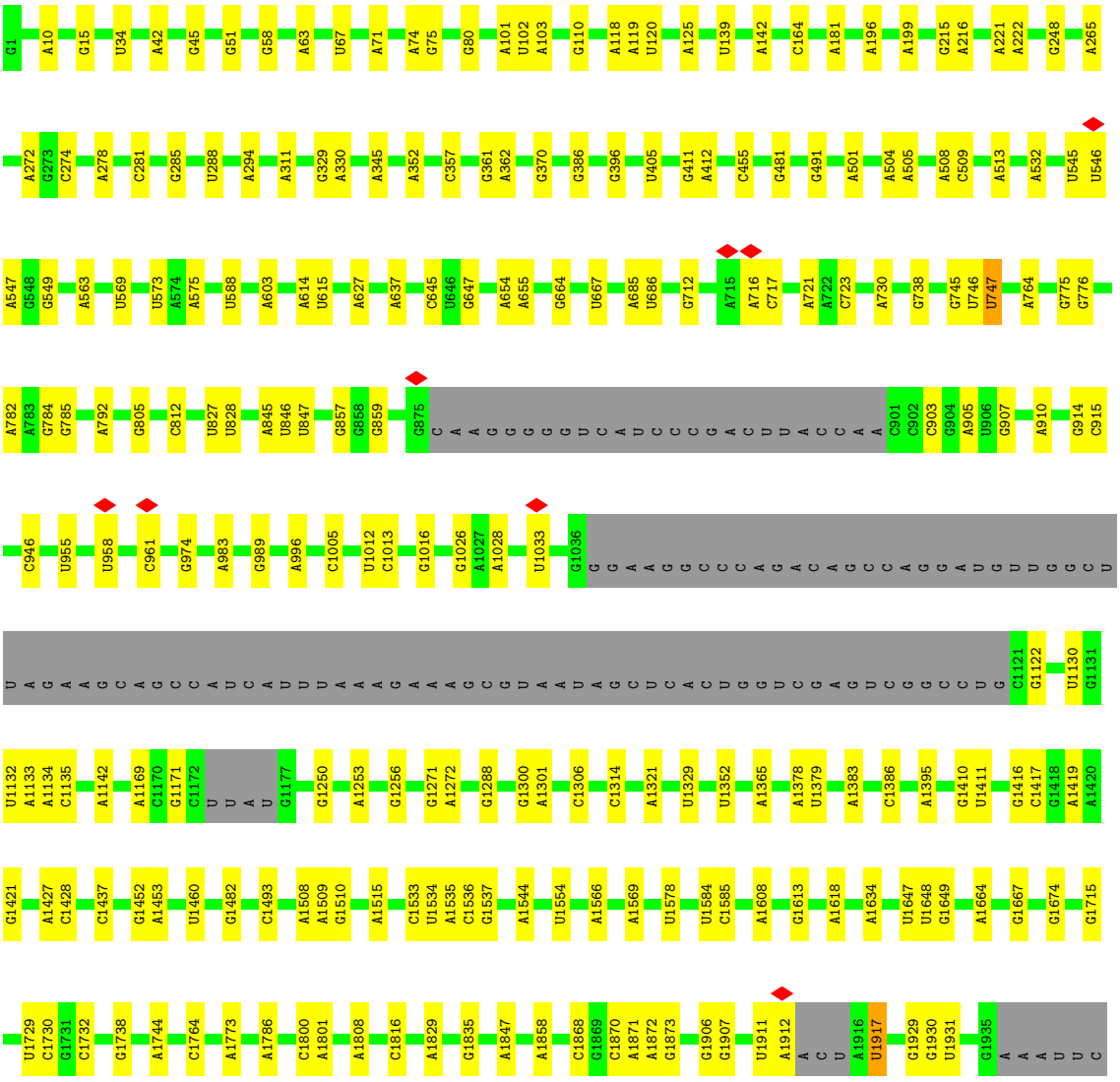
Mol	Chain	Residues	Atoms	AltConf
29	s	6	Total O 6 6	0
29	t	2	Total O 2 2	0
29	u	2	Total O 2 2	0
29	v	12	Total O 12 12	0
29	w	15	Total O 15 15	0
29	y	6	Total O 6 6	0
29	z	17	Total O 17 17	0
29	0	6	Total O 6 6	0
29	1	25	Total O 25 25	0
29	2	15	Total O 15 15	0

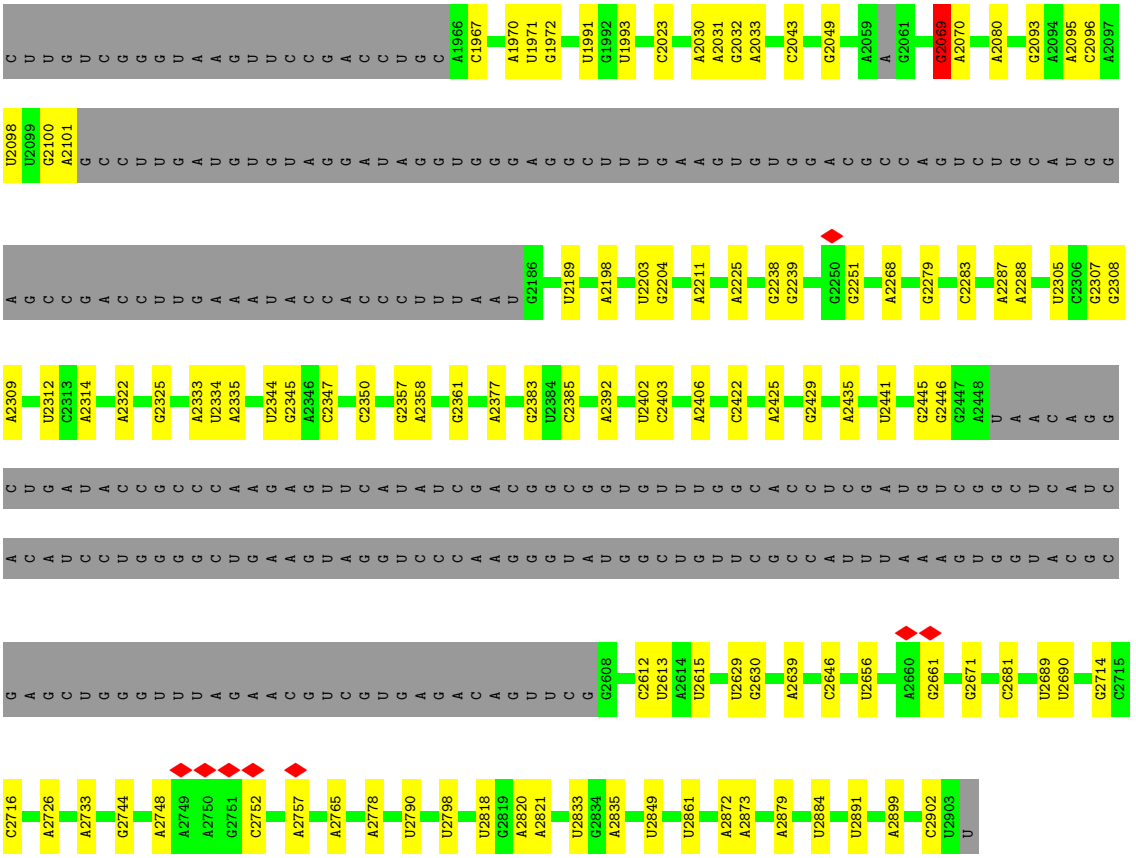
3 Residue-property plots (i)

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: 23S rRNA

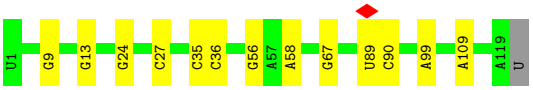
Chain a:





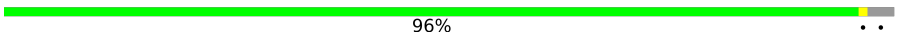
• Molecule 2: 5S rRNA

Chain b:



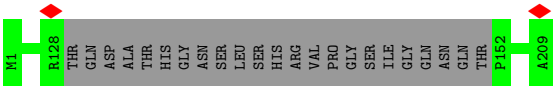
• Molecule 3: 50S ribosomal protein L2

Chain c:



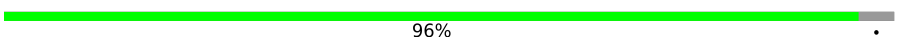
• Molecule 4: 50S ribosomal protein L3

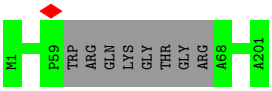
Chain d:



• Molecule 5: 50S ribosomal protein L4

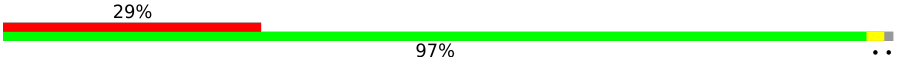
Chain e:

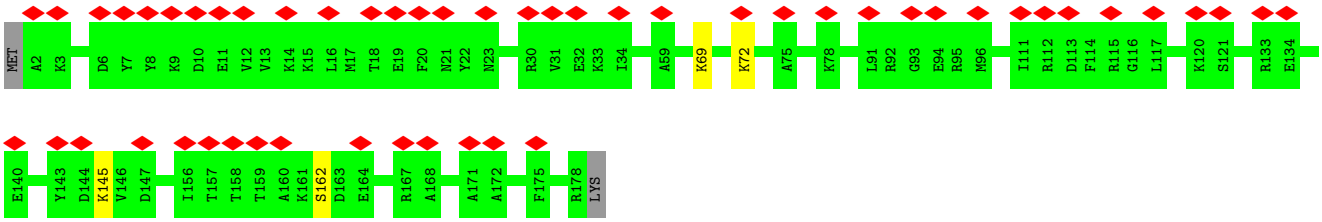




• Molecule 6: 50S ribosomal protein L5

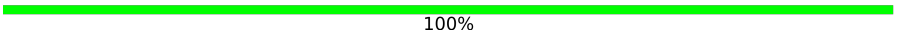
Chain f:





• Molecule 7: 50S ribosomal protein L13

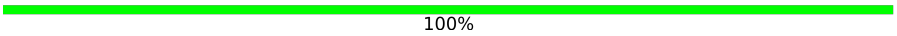
Chain i:



There are no outlier residues recorded for this chain.

• Molecule 8: 50S ribosomal protein L14

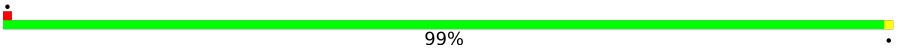
Chain j:

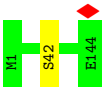


There are no outlier residues recorded for this chain.

• Molecule 9: 50S ribosomal protein L15

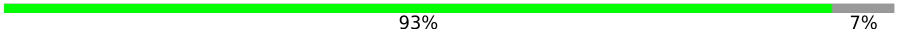
Chain k:





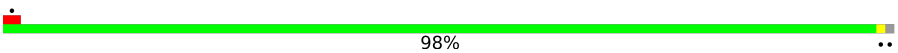
• Molecule 10: 50S ribosomal protein L17

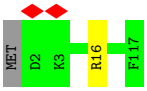
Chain m:



• Molecule 11: 50S ribosomal protein L18

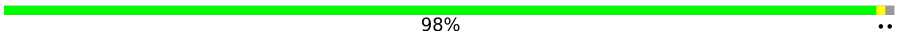
Chain n:

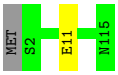




• Molecule 12: 50S ribosomal protein L19

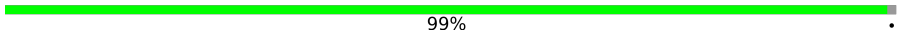
Chain o:





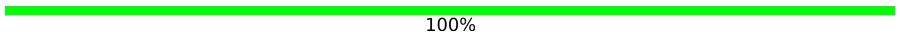
• Molecule 13: 50S ribosomal protein L20

Chain p:



• Molecule 14: 50S ribosomal protein L21

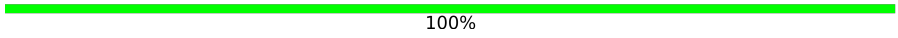
Chain q:



There are no outlier residues recorded for this chain.

• Molecule 15: 50S ribosomal protein L22

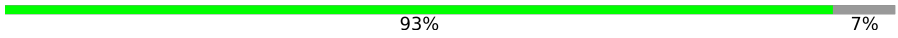
Chain r:



There are no outlier residues recorded for this chain.

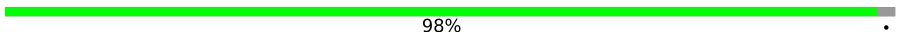
• Molecule 16: 50S ribosomal protein L23

Chain s:



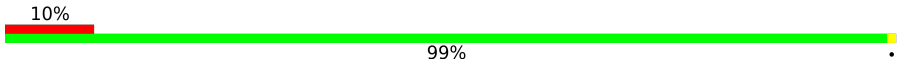
• Molecule 17: 50S ribosomal protein L24

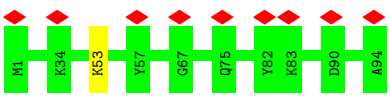
Chain t:



• Molecule 18: 50S ribosomal protein L25

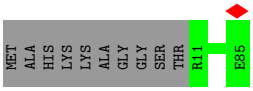
Chain u:





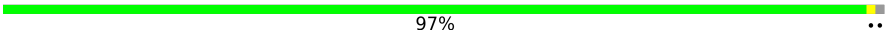
• Molecule 19: 50S ribosomal protein L27

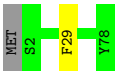
Chain v:



• Molecule 20: 50S ribosomal protein L28

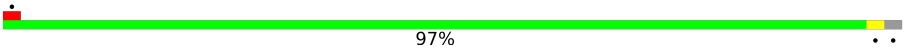
Chain w:

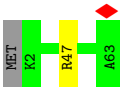




• Molecule 21: 50S ribosomal protein L29

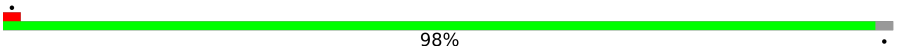
Chain x:





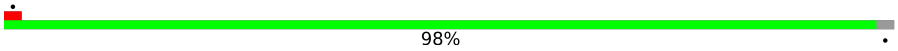
• Molecule 22: 50S ribosomal protein L30

Chain y:



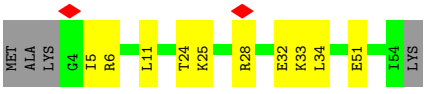
• Molecule 23: 50S ribosomal protein L32

Chain z:



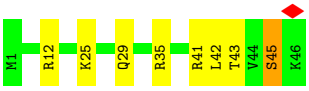
• Molecule 24: 50S ribosomal protein L33

Chain 0:



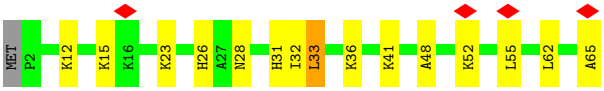
• Molecule 25: 50S ribosomal protein L34

Chain 1:



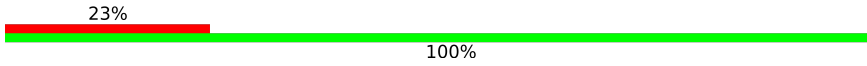
• Molecule 26: 50S ribosomal protein L35

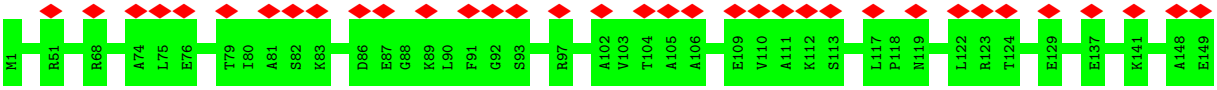
Chain 2:



• Molecule 27: 50S ribosomal protein L9

Chain h:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55280	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 ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	403.19998, 403.19998, 403.19998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: G7M, PSU, MG, 2MG, 1MG, OMG, 6MZ, 5MU

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	1.31	0/60188	0.87	3/93883 (0.0%)
2	b	0.66	0/2850	0.81	0/4444
3	c	0.57	0/2072	0.57	0/2786
4	d	0.61	0/1414	0.55	0/1897
5	e	0.56	0/1499	0.58	0/2016
6	f	0.31	0/1434	0.56	0/1926
7	i	0.61	0/1152	0.52	0/1551
8	j	0.51	0/955	0.57	0/1279
9	k	0.51	0/1062	0.57	0/1413
10	m	0.63	0/958	0.55	0/1281
11	n	0.38	0/902	0.52	0/1209
12	o	0.58	0/929	0.53	0/1242
13	p	0.72	0/960	0.50	0/1278
14	q	0.60	0/829	0.54	0/1107
15	r	0.59	0/864	0.56	0/1156
16	s	0.56	0/744	0.55	0/994
17	t	0.57	0/787	0.61	0/1051
18	u	0.31	0/766	0.47	0/1025
19	v	0.48	0/576	0.48	0/762
20	w	0.63	1/635 (0.2%)	0.59	0/848
21	x	0.45	0/502	0.55	0/667
22	y	0.47	0/453	0.56	0/605
23	z	0.62	0/450	0.58	0/599
24	0	0.37	0/424	0.51	0/565
25	1	0.63	0/380	0.58	0/498
26	2	0.38	0/513	0.47	0/676
27	h	0.38	0/1122	0.52	0/1515
All	All	1.14	1/85420 (0.0%)	0.81	3/128273 (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
1	a	3	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	w	29	PHE	C-N	-5.39	1.21	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	67	U	C5-C4-O4	-5.65	122.51	125.90
1	a	1314	C	C2-N1-C1'	5.50	124.85	118.80
1	a	370	G	O4'-C1'-N9	-5.19	104.05	108.20

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	2069	G7M	C4',C2',C3'

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	54003	0	27172	0	0
2	b	2549	0	1291	0	0
3	c	2035	0	2113	0	0
4	d	1397	0	1461	0	0
5	e	1483	0	1548	0	0
6	f	1410	0	1444	0	0
7	i	1129	0	1162	0	0
8	j	946	0	1023	0	0
9	k	1053	0	1129	0	0
10	m	945	0	989	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	n	892	0	923	0	0
12	o	917	0	962	0	0
13	p	947	0	1019	0	0
14	q	816	0	839	0	0
15	r	857	0	922	0	0
16	s	738	0	807	0	0
17	t	779	0	831	0	0
18	u	753	0	780	0	0
19	v	569	0	581	0	0
20	w	625	0	652	0	0
21	x	501	0	531	0	0
22	y	449	0	488	0	0
23	z	444	0	458	0	0
24	0	417	0	451	6	0
25	1	377	0	418	7	0
26	2	504	0	572	10	0
27	h	1111	0	1148	0	0
28	a	202	0	0	0	0
28	b	5	0	0	0	0
28	c	1	0	0	0	0
28	p	1	0	0	0	0
28	z	1	0	0	0	0
29	0	6	0	0	0	0
29	1	25	0	0	2	0
29	2	15	0	0	1	0
29	a	137	0	0	0	0
29	b	117	0	0	0	0
29	c	63	0	0	0	0
29	d	17	0	0	0	0
29	e	22	0	0	0	0
29	f	22	0	0	0	0
29	i	13	0	0	0	0
29	j	14	0	0	0	0
29	k	28	0	0	0	0
29	m	28	0	0	0	0
29	n	34	0	0	0	0
29	o	9	0	0	0	0
29	p	22	0	0	0	0
29	q	17	0	0	0	0
29	r	15	0	0	0	0
29	s	6	0	0	0	0
29	t	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	u	2	0	0	0	0
29	v	12	0	0	0	0
29	w	15	0	0	0	0
29	y	6	0	0	0	0
29	z	17	0	0	0	0
All	All	79520	0	51714	23	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 11.

The worst 5 of 23 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)
24:0:25:LYS:NZ	24:0:51:GLU:OE1	2.25	0.70
26:2:62:LEU:HB3	26:2:65:ALA:HB2	1.75	0.69
26:2:28:ASN:O	26:2:36:LYS:NZ	2.21	0.68
24:0:6:ARG:HG2	24:0:24:THR:HB	1.81	0.62
26:2:15:LYS:HB2	26:2:23:LYS:HE3	1.85	0.58

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	261/273 (96%)	256 (98%)	5 (2%)	0	100	100
4	d	182/209 (87%)	181 (100%)	1 (0%)	0	100	100
5	e	189/201 (94%)	184 (97%)	5 (3%)	0	100	100
6	f	175/179 (98%)	163 (93%)	12 (7%)	0	100	100
7	i	140/142 (99%)	140 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	j	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
9	k	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
10	m	116/127 (91%)	109 (94%)	7 (6%)	0	100	100
11	n	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
12	o	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
13	p	115/118 (98%)	115 (100%)	0	0	100	100
14	q	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
15	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
16	s	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
17	t	100/104 (96%)	93 (93%)	7 (7%)	0	100	100
18	u	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
19	v	73/85 (86%)	70 (96%)	3 (4%)	0	100	100
20	w	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
21	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
22	y	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
23	z	54/57 (95%)	54 (100%)	0	0	100	100
24	0	49/55 (89%)	49 (100%)	0	0	100	100
25	1	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
26	2	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
27	h	147/149 (99%)	126 (86%)	21 (14%)	0	100	100
All	All	2779/2916 (95%)	2676 (96%)	103 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	212/218 (97%)	210 (99%)	2 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	d	145/164 (88%)	145 (100%)	0	100 100
5	e	159/165 (96%)	159 (100%)	0	100 100
6	f	148/150 (99%)	144 (97%)	4 (3%)	44 71
7	i	116/116 (100%)	116 (100%)	0	100 100
8	j	104/104 (100%)	104 (100%)	0	100 100
9	k	103/103 (100%)	102 (99%)	1 (1%)	76 90
10	m	98/103 (95%)	98 (100%)	0	100 100
11	n	86/87 (99%)	85 (99%)	1 (1%)	71 87
12	o	99/100 (99%)	98 (99%)	1 (1%)	76 90
13	p	89/90 (99%)	89 (100%)	0	100 100
14	q	84/84 (100%)	84 (100%)	0	100 100
15	r	93/93 (100%)	93 (100%)	0	100 100
16	s	80/84 (95%)	80 (100%)	0	100 100
17	t	83/85 (98%)	83 (100%)	0	100 100
18	u	78/78 (100%)	77 (99%)	1 (1%)	69 86
19	v	56/63 (89%)	56 (100%)	0	100 100
20	w	67/68 (98%)	67 (100%)	0	100 100
21	x	54/55 (98%)	53 (98%)	1 (2%)	57 79
22	y	48/49 (98%)	48 (100%)	0	100 100
23	z	47/48 (98%)	47 (100%)	0	100 100
24	0	46/49 (94%)	46 (100%)	0	100 100
25	1	38/38 (100%)	36 (95%)	2 (5%)	22 45
26	2	51/52 (98%)	50 (98%)	1 (2%)	55 78
27	h	114/114 (100%)	114 (100%)	0	100 100
All	All	2298/2360 (97%)	2284 (99%)	14 (1%)	86 95

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	n	16	ARG
12	o	11	GLU
26	2	33	LEU
25	1	41	ARG
25	1	45	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
12	o	75	GLN
14	q	86	GLN
23	z	6	ASN
23	z	5	GLN
5	e	94	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	2502/2904 (86%)	326 (13%)	0
2	b	118/120 (98%)	13 (11%)	0
All	All	2620/3024 (86%)	339 (12%)	0

5 of 339 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	10	A
1	a	15	G
1	a	34	U
1	a	42	A
1	a	45	G

There are no RNA pucker outliers to report.

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

12 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	2MG	a	2445	1	18,26,27	1.08	1 (5%)	16,38,41	1.15	2 (12%)
1	1MG	a	745	1	18,26,27	0.64	0	19,39,42	1.16	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	a	1917	1	18,21,22	1.11	1 (5%)	22,30,33	1.71	5 (22%)
1	PSU	a	1911	1	18,21,22	1.09	1 (5%)	22,30,33	1.91	5 (22%)
1	6MZ	a	2030	1	18,25,26	0.79	0	16,36,39	2.45	5 (31%)
1	PSU	a	955	1	18,21,22	1.03	1 (5%)	22,30,33	2.03	5 (22%)
1	2MG	a	1835	1	18,26,27	0.98	1 (5%)	16,38,41	1.25	3 (18%)
1	OMG	a	2251	1	18,26,27	0.96	1 (5%)	19,38,41	1.10	2 (10%)
1	G7M	a	2069	1	20,26,27	1.12	2 (10%)	17,39,42	0.99	0
1	6MZ	a	1618	1	18,25,26	0.81	0	16,36,39	2.31	4 (25%)
1	PSU	a	746	1	18,21,22	1.00	2 (11%)	22,30,33	2.13	5 (22%)
1	5MU	a	747	1	19,22,23	1.42	4 (21%)	28,32,35	2.16	6 (21%)

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	2MG	a	2445	1	-	0/5/27/28	0/3/3/3
1	1MG	a	745	1	-	0/3/25/26	0/3/3/3
1	PSU	a	1917	1	-	2/7/25/26	0/2/2/2
1	PSU	a	1911	1	-	2/7/25/26	0/2/2/2
1	6MZ	a	2030	1	-	2/5/27/28	0/3/3/3
1	PSU	a	955	1	-	0/7/25/26	0/2/2/2
1	2MG	a	1835	1	-	2/5/27/28	0/3/3/3
1	OMG	a	2251	1	-	0/5/27/28	0/3/3/3
1	G7M	a	2069	1	3/3/5/5	1/3/25/26	0/3/3/3
1	6MZ	a	1618	1	-	0/5/27/28	0/3/3/3
1	PSU	a	746	1	-	0/7/25/26	0/2/2/2
1	5MU	a	747	1	-	2/7/25/26	0/2/2/2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1911	PSU	C6-C5	3.53	1.39	1.35
1	a	1917	PSU	C6-C5	3.53	1.39	1.35
1	a	747	5MU	C4-N3	-3.38	1.32	1.38
1	a	2445	2MG	C6-N1	-3.26	1.33	1.37
1	a	1835	2MG	C6-N1	-3.05	1.33	1.37

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	2030	6MZ	C2-N1-C6	6.43	122.11	116.59
1	a	1618	6MZ	C2-N1-C6	5.83	121.59	116.59
1	a	1618	6MZ	C9-N6-C6	-5.42	118.20	122.87
1	a	955	PSU	N1-C2-N3	5.36	121.20	115.13
1	a	747	5MU	C4-N3-C2	-5.32	120.46	127.35

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	2069	G7M	C4'
1	a	2069	G7M	C2'
1	a	2069	G7M	C3'

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	1917	PSU	C3'-C4'-C5'-O5'
1	a	1917	PSU	O4'-C4'-C5'-O5'
1	a	747	5MU	C3'-C4'-C5'-O5'
1	a	747	5MU	O4'-C4'-C5'-O5'
1	a	2030	6MZ	O4'-C4'-C5'-O5'

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 210 ligands modelled in this entry, 210 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.

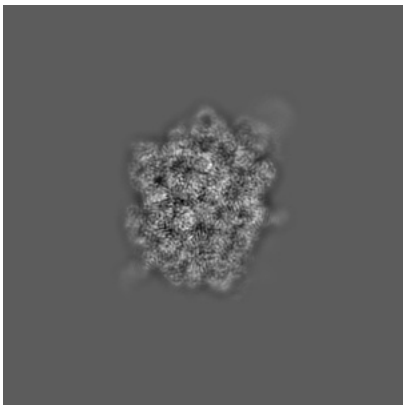
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35939. These allow visual inspection of the internal detail of the map and identification of artifacts.

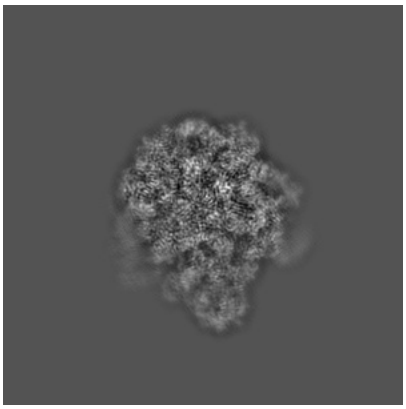
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

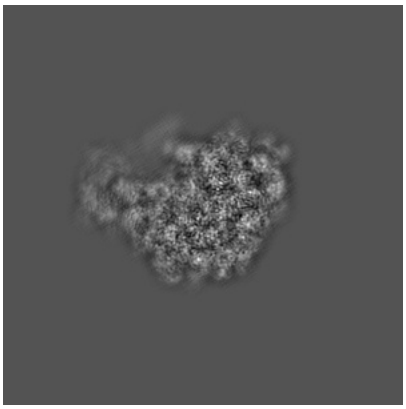
6.1.1 Primary map



X

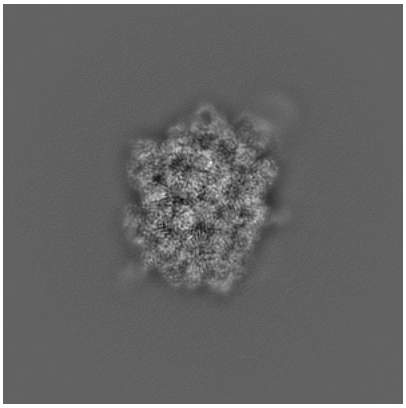


Y

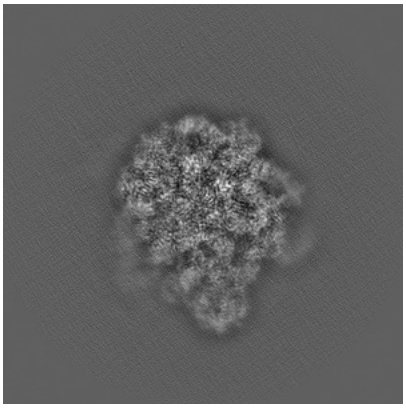


Z

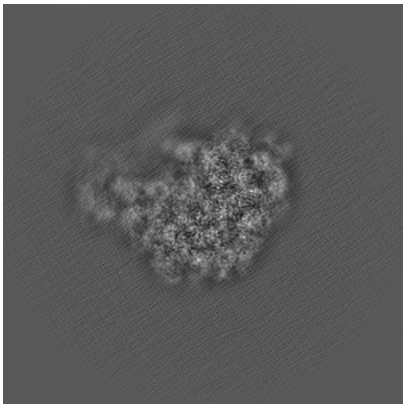
6.1.2 Raw map



X



Y

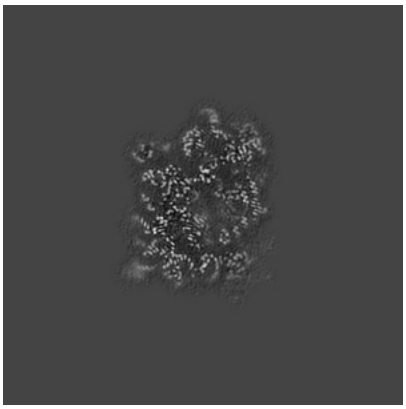


Z

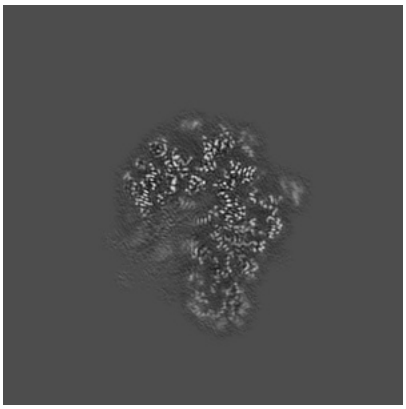
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

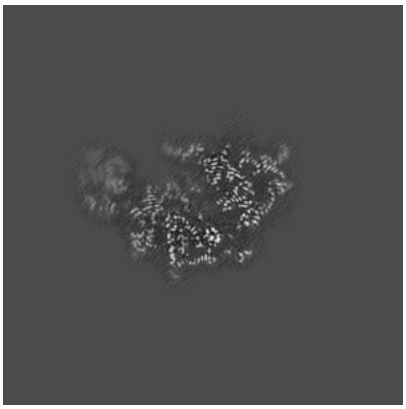
6.2.1 Primary map



X Index: 192

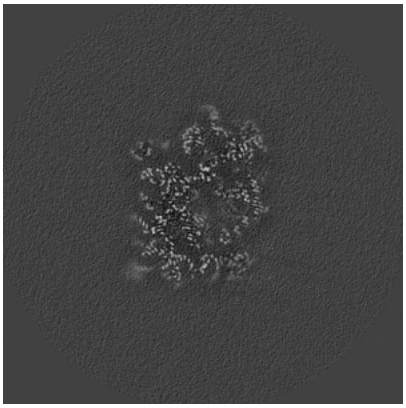


Y Index: 192

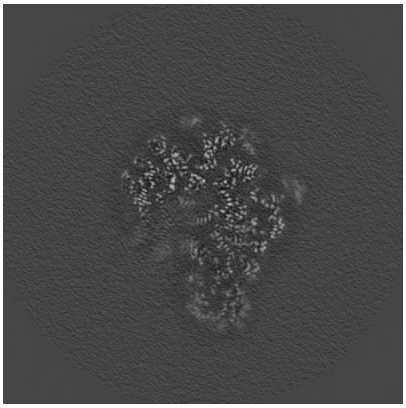


Z Index: 192

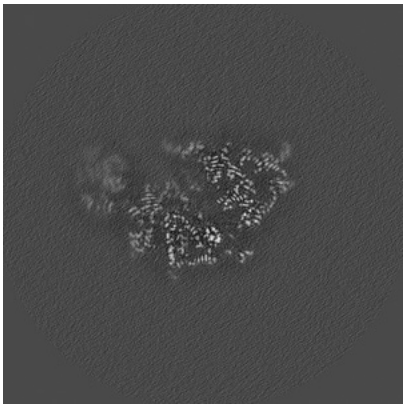
6.2.2 Raw map



X Index: 192



Y Index: 192

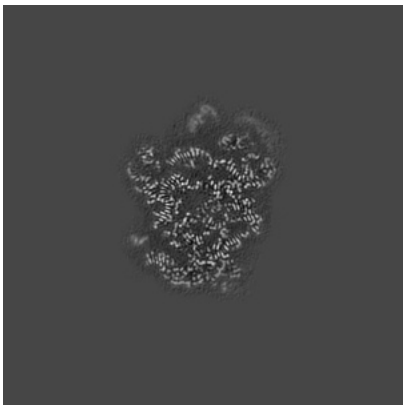


Z Index: 192

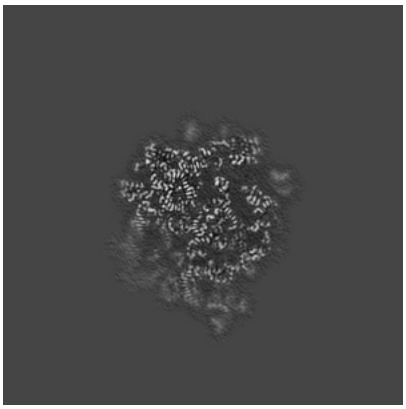
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

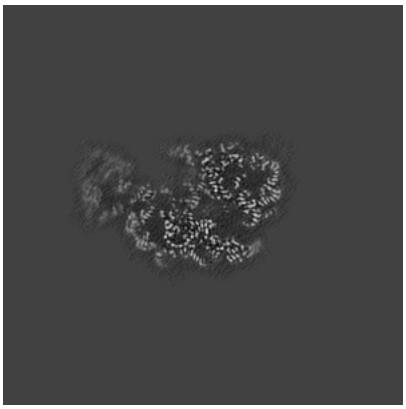
6.3.1 Primary map



X Index: 205

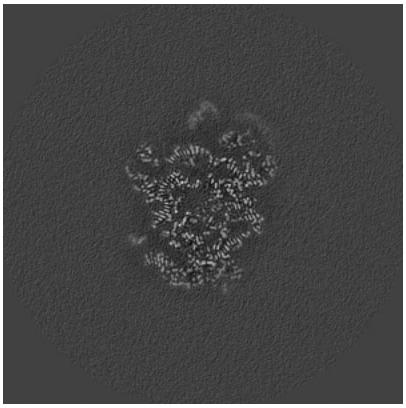


Y Index: 179

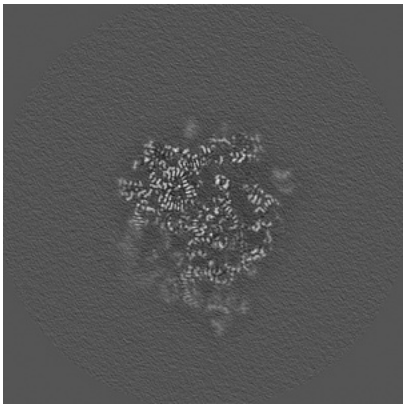


Z Index: 199

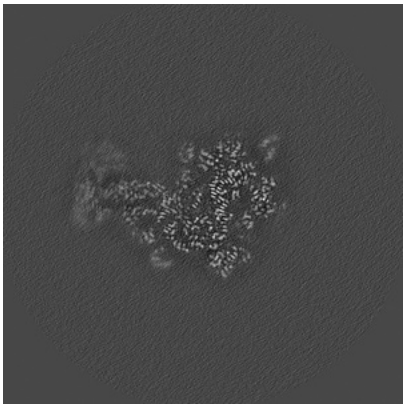
6.3.2 Raw map



X Index: 205



Y Index: 179

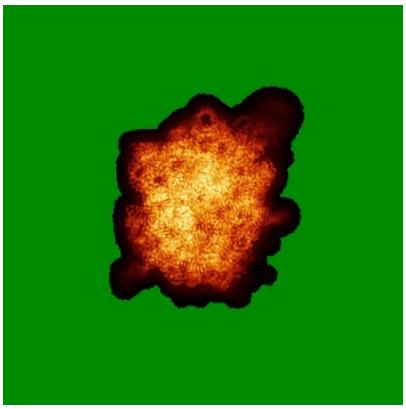


Z Index: 209

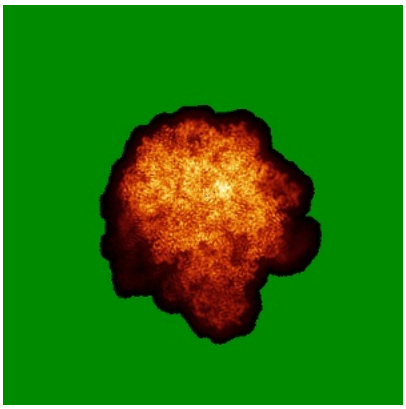
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

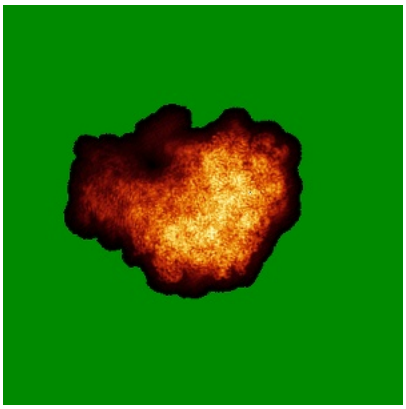
6.4.1 Primary map



X

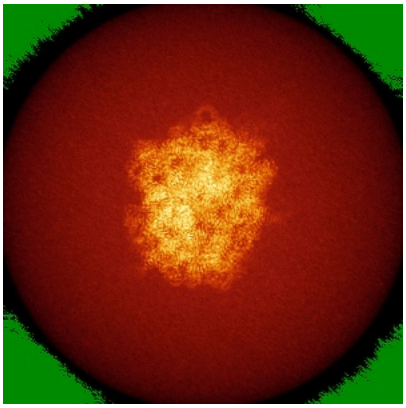


Y

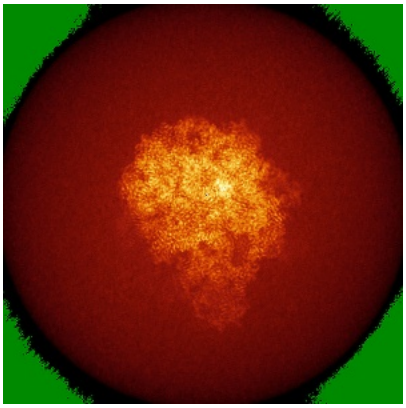


Z

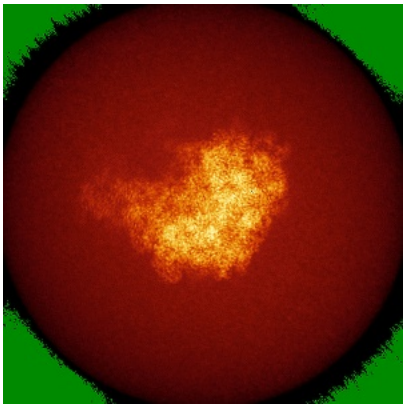
6.4.2 Raw map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.005. 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

X Y Z

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.

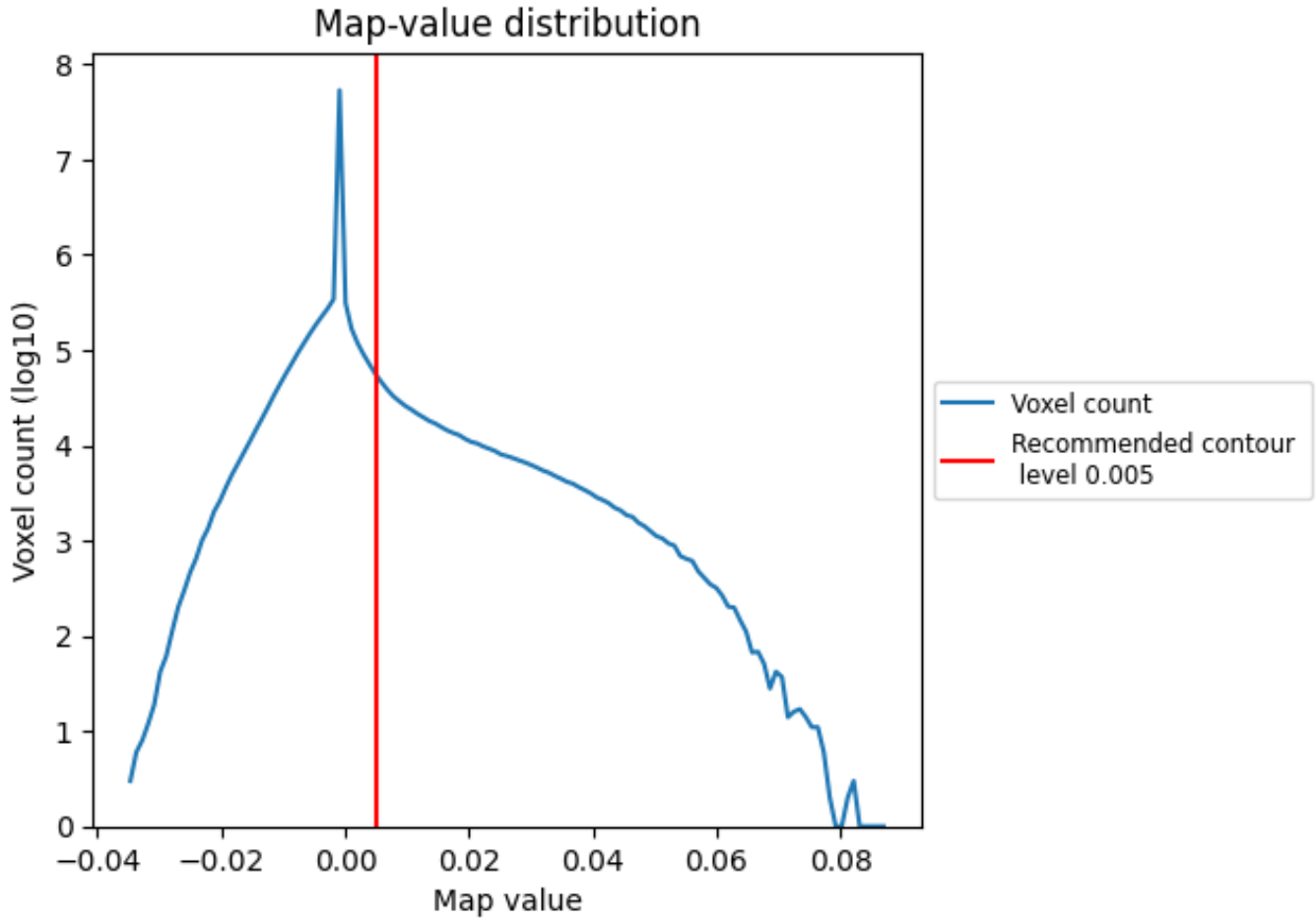
6.6 Mask visualisation (i)

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

7 Map analysis

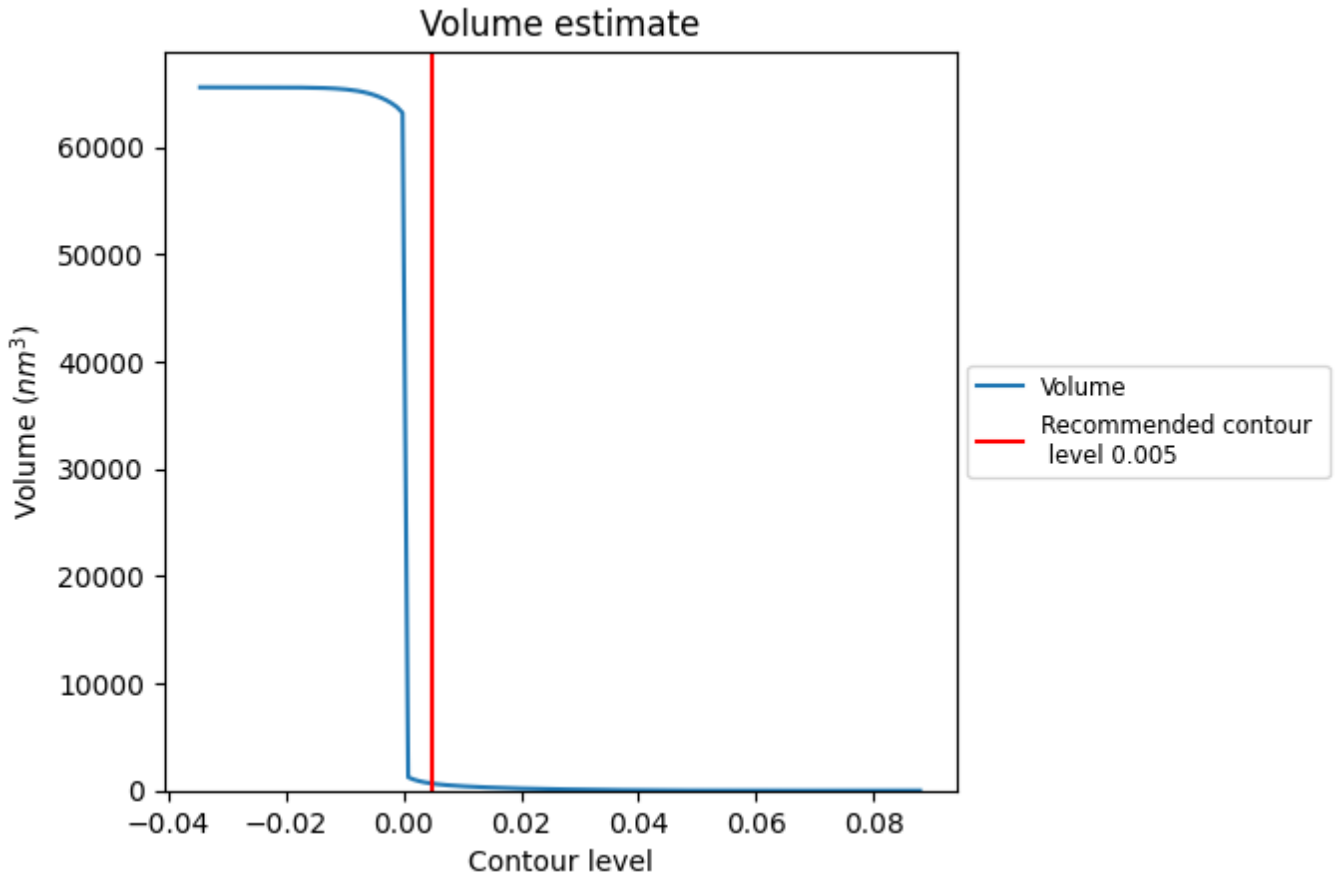
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

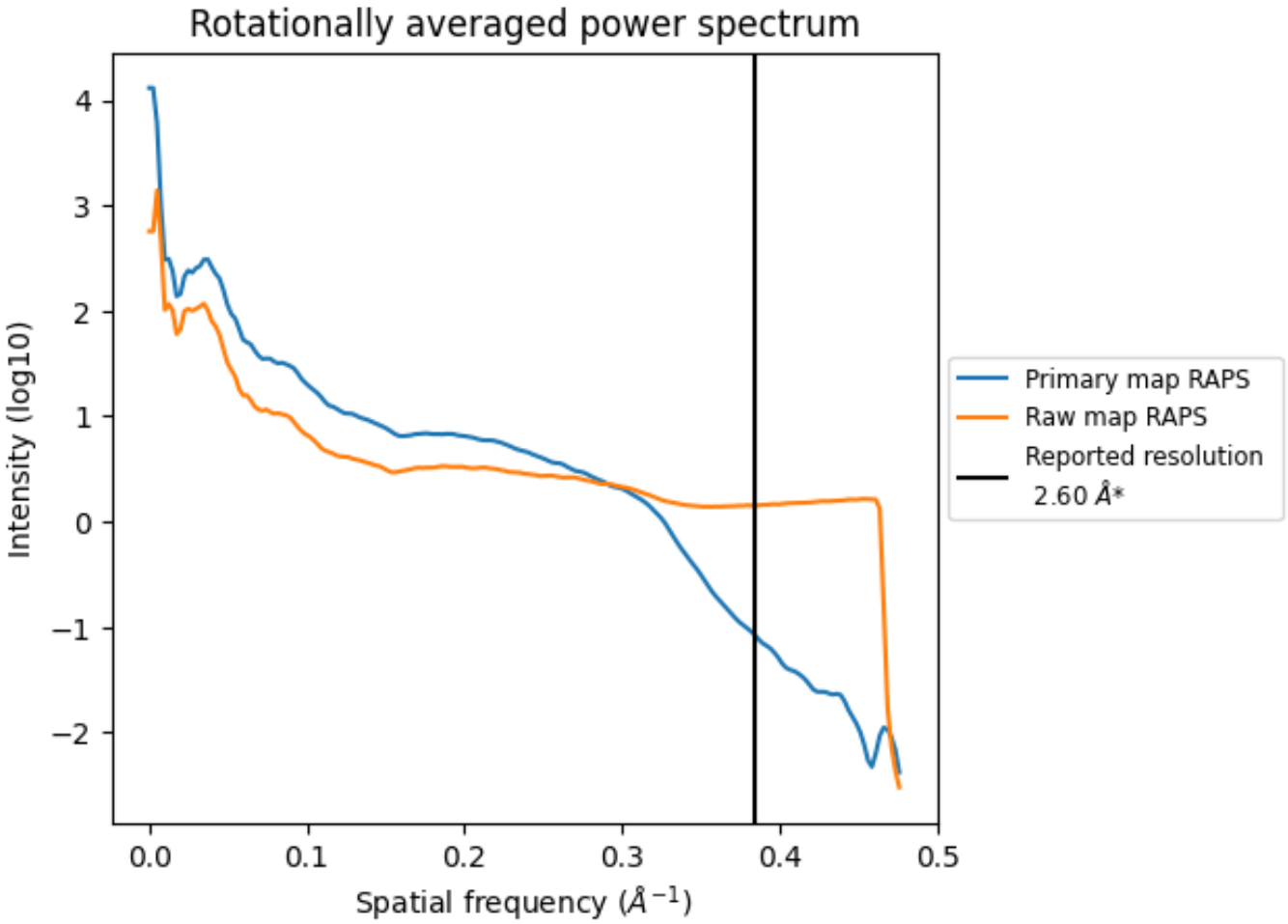
7.2 Volume estimate (i)



The volume at the recommended contour level is 647 nm^3; this corresponds to an approximate mass of 584 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 (i)

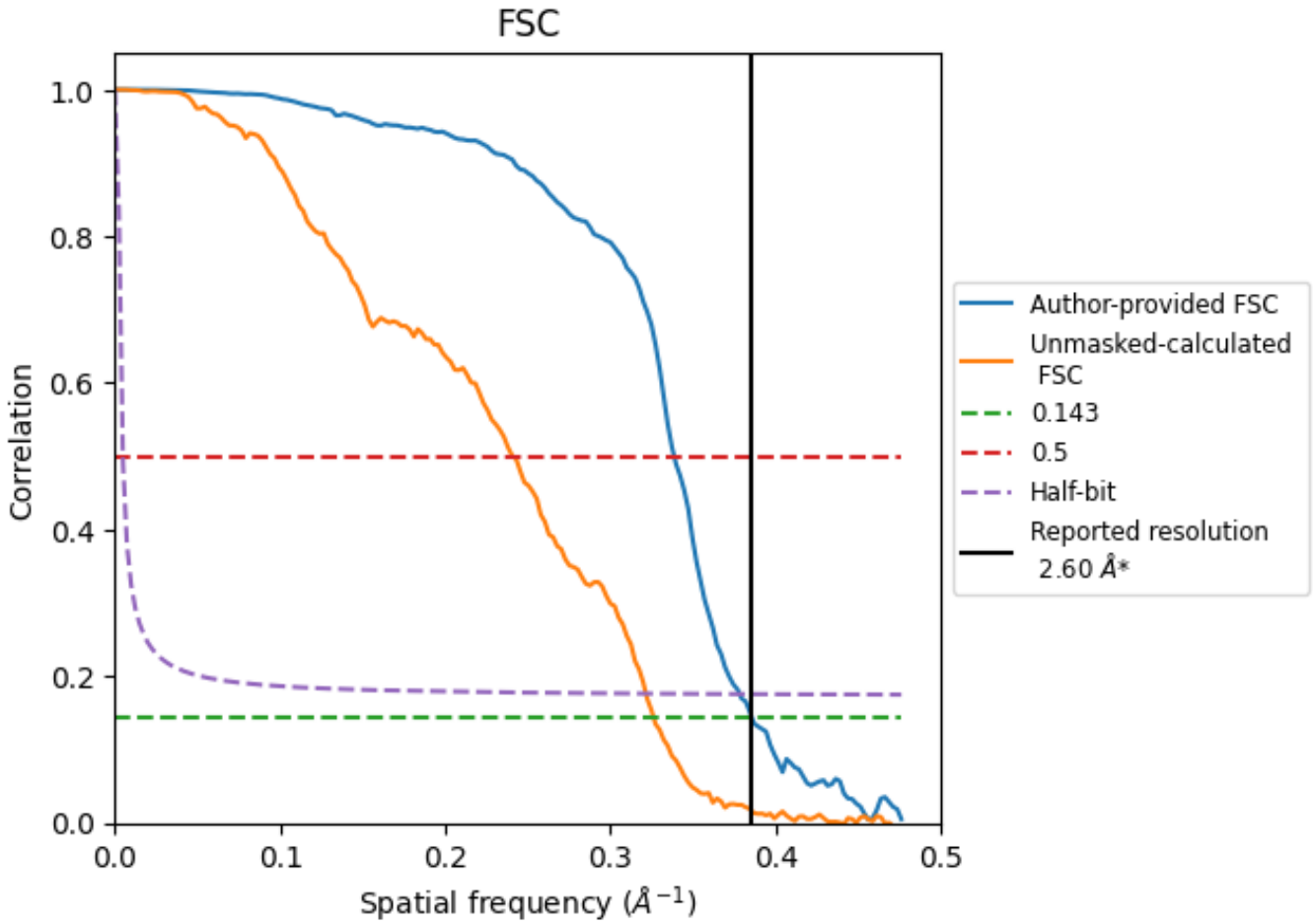


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8.2 Resolution estimates (i)

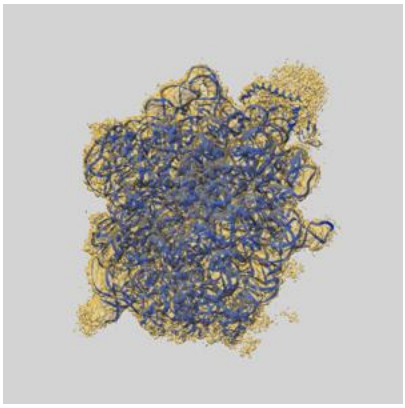
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.59	2.95	2.64
Unmasked-calculated*	3.06	4.15	3.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.06 differs from the reported value 2.6 by more than 10 %

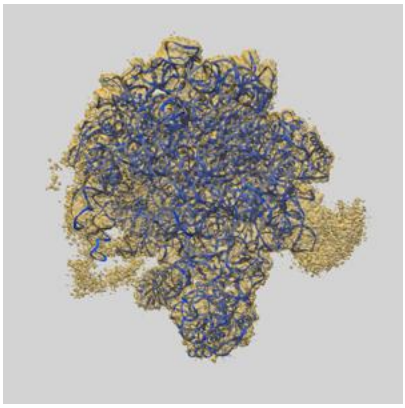
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35939 and PDB model 8J1Z. Per-residue inclusion information can be found in section 3 on page 10.

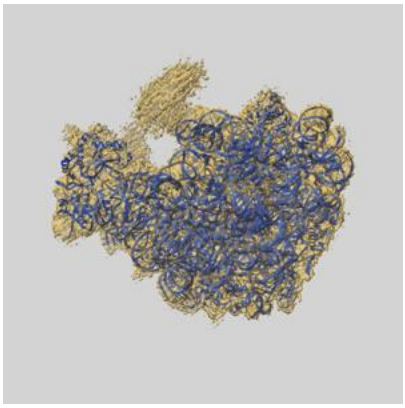
9.1 Map-model overlay



X



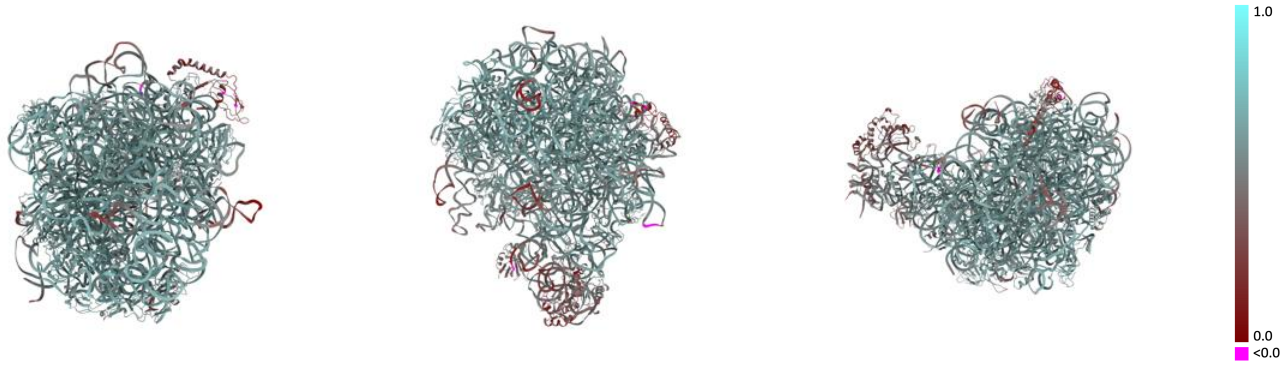
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.005 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.

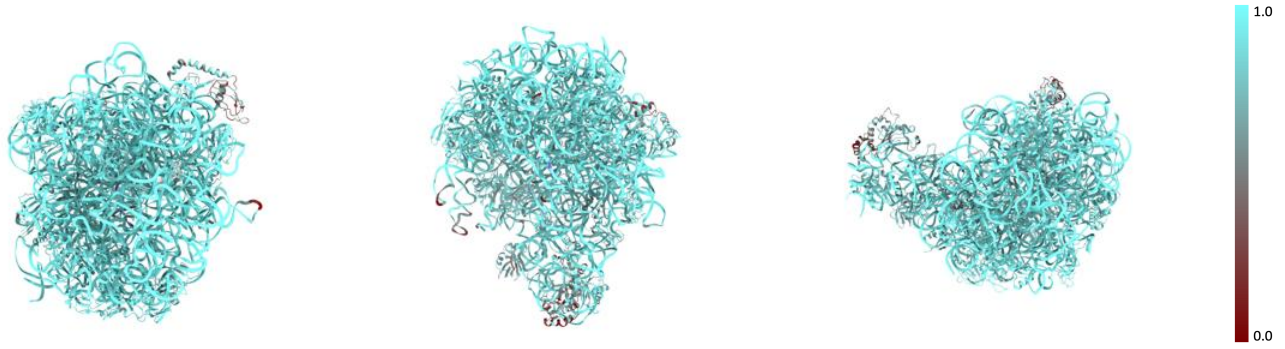
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

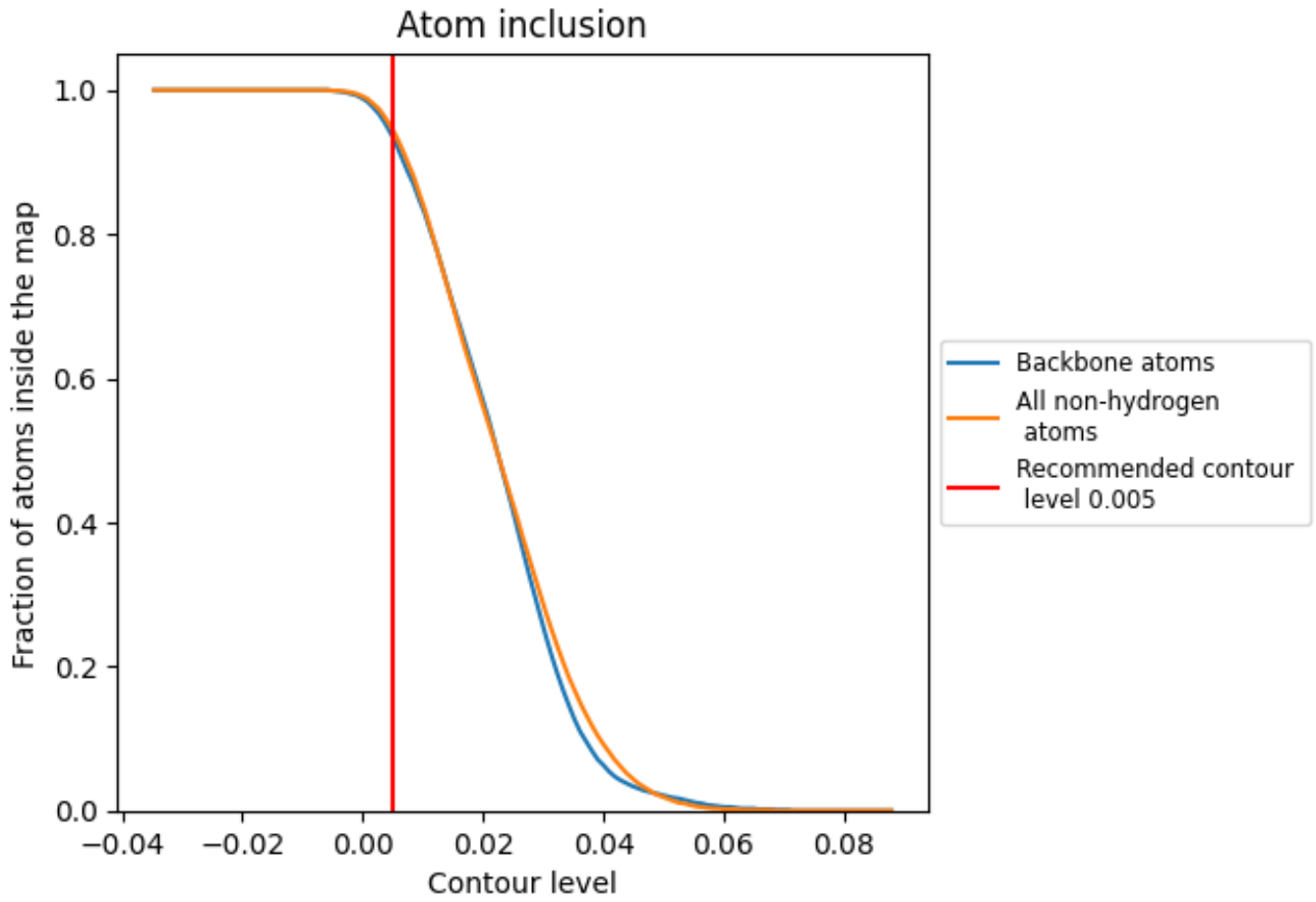
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.005).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9450	0.5820
0	0.7510	0.5440
1	0.9490	0.6370
2	0.7350	0.6080
a	0.9750	0.5950
b	0.9390	0.4940
c	0.9420	0.6210
d	0.9480	0.6120
e	0.9370	0.5910
f	0.5340	0.3220
h	0.6290	0.3420
i	0.9370	0.6090
j	0.9020	0.5730
k	0.9160	0.5950
m	0.9700	0.6350
n	0.8510	0.4790
o	0.9230	0.5860
p	0.9640	0.6350
q	0.9560	0.6090
r	0.9410	0.6230
s	0.9240	0.5990
t	0.9560	0.5880
u	0.7210	0.3970
v	0.8830	0.5820
w	0.9300	0.6100
x	0.9300	0.5640
y	0.9200	0.5810
z	0.9370	0.6130