wwPDB EM Validation Summary Report (i)

Sep 1, 2026 – 01:51 pm BST

PDB ID	:	9T8S / pdb_00009t8s
EMDB ID	:	EMD-55710
Title	:	E. coli 70S ribosome from delta-10 strain, PTC class 8
Authors	:	Larsson, D.S.D.; Selmer, M.
Deposited on	:	2025-11-13
Resolution	:	2.22 Å(reported)
Based on initial model	:	9T6M

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 (i) 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 (1)) were used in the production of this report:

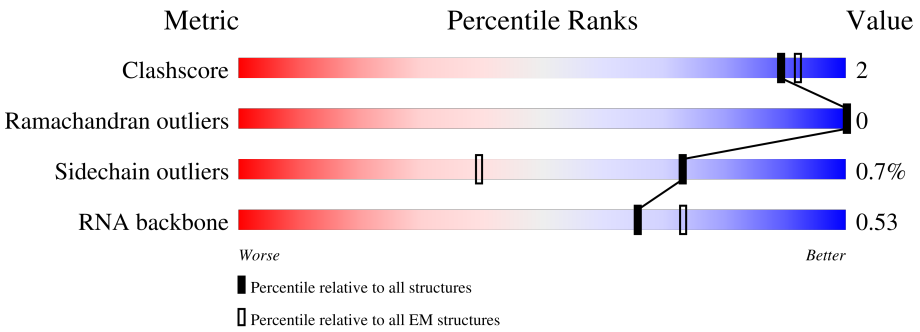
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

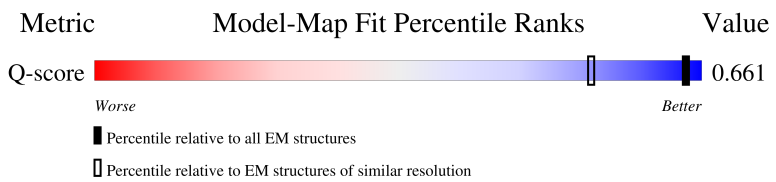
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.22 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	3277 (1.73 - 2.72)

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	Z	77	22% 18% • • 77%
2	a	2904	15% 5% • 80%
3	b	120	• •• 97%

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Mol	Chain	Length	Quality of chain
4	c	273	8% 90%
5	d	209	18% 79%
6	e	201	9% 89%
7	k	144	18% 82%
8	l	136	30% 5% 65%
9	q	103	7% 93%
10	r	110	6% 94%
11	v	85	11% 88%
12	z	57	9% 5% 86%

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 14706 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 tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	Z	18	384	171	72	123	18	0	0

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	a	590	12630	5645	2302	4093	590	0	0

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	b	4	80	36	10	30	4	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	c	26	191	116	41	33	1	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	d	43	333	206	68	58	1	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	e	23	182	115	39	28	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	k	26	182	106	42	33	1	0	0

- Molecule 8 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	l	48	386	242	81	60	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	conflict	UNP A7ZSK2

- Molecule 9 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	q	7	75	48	19	8	0	0

- Molecule 10 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	r	7	53	30	14	9	0	0

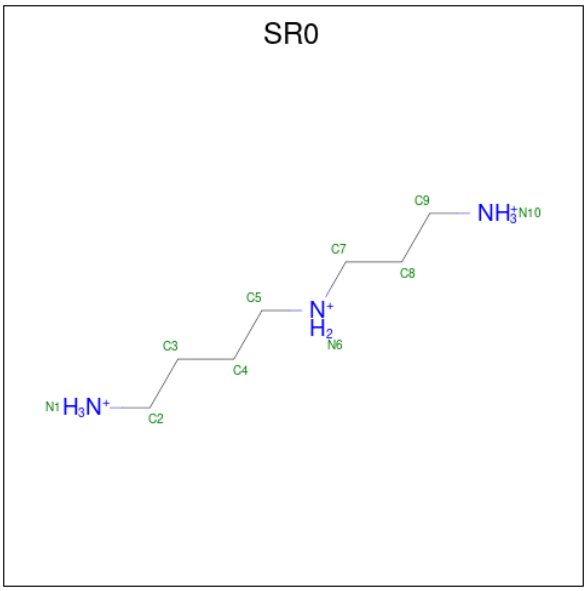
- Molecule 11 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	v	10	74	39	17	18	0	0

- Molecule 12 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	z	8	61	37	12	12	0	0

- Molecule 13 is N 1 -(3-azaniumylpropyl)butane-1,4-diaminium (CCD ID: SR0) (formula: $C_7H_{22}N_3$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
13	a	1	10	7	3	0
			Total	C	N	
13	a	1	10	7	3	0

- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
14	a	33	33	33	0
			Total	Mg	
14	d	1	1	1	0

- Molecule 15 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
15	a	21	21	21	0

3 Residue-property plots (i)

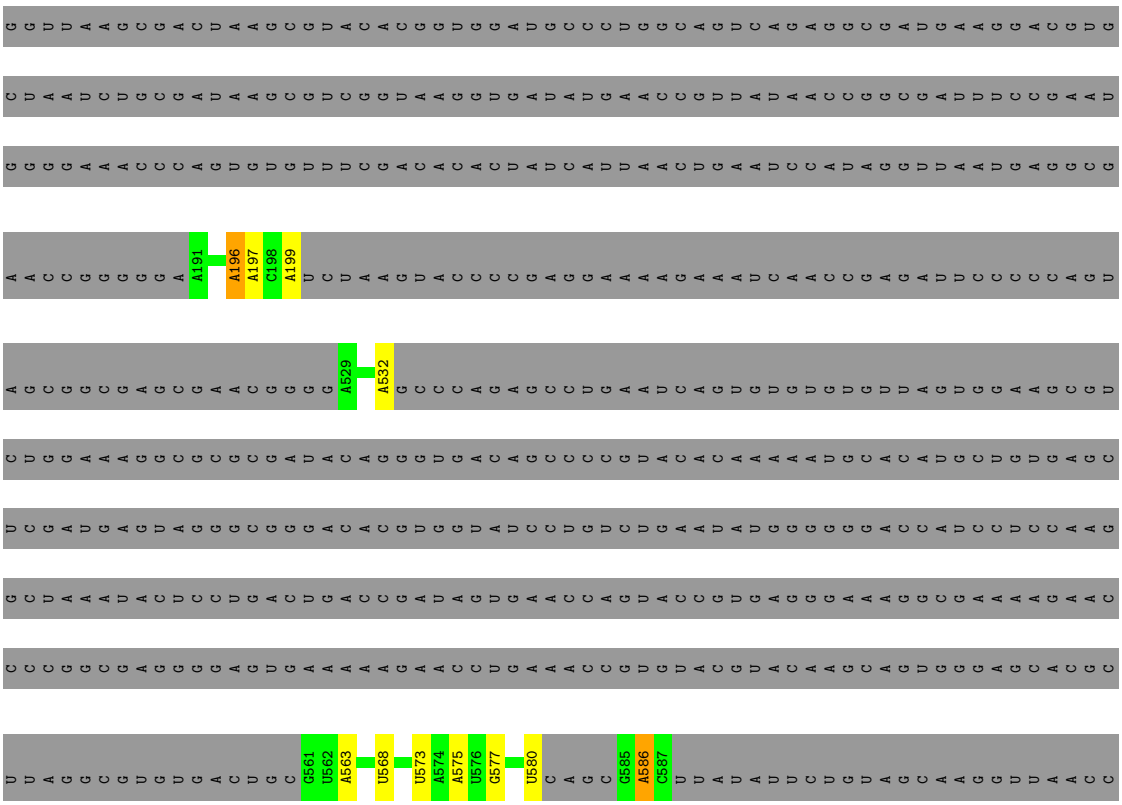
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

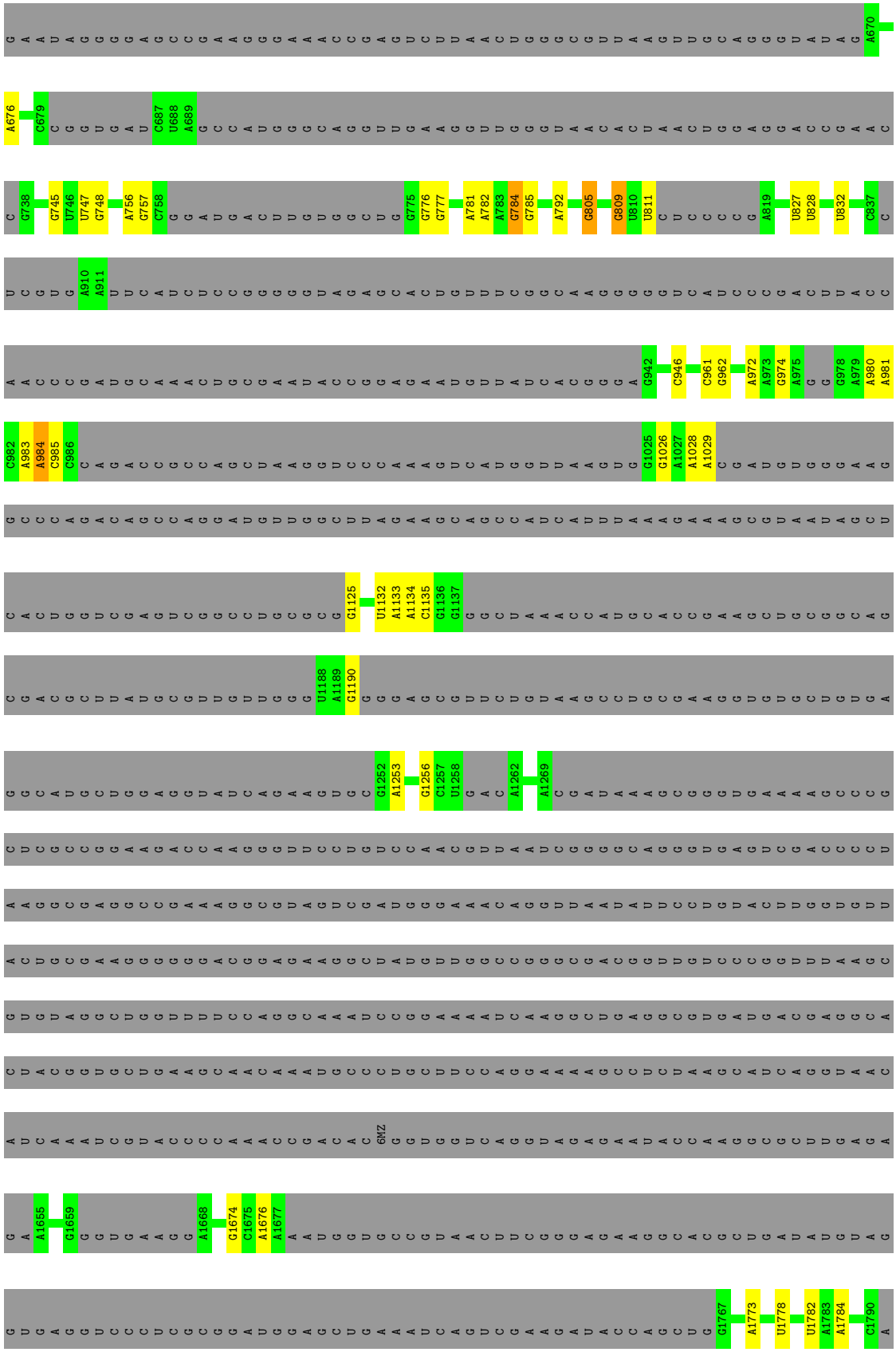
- Molecule 1: tRNA(fMet)

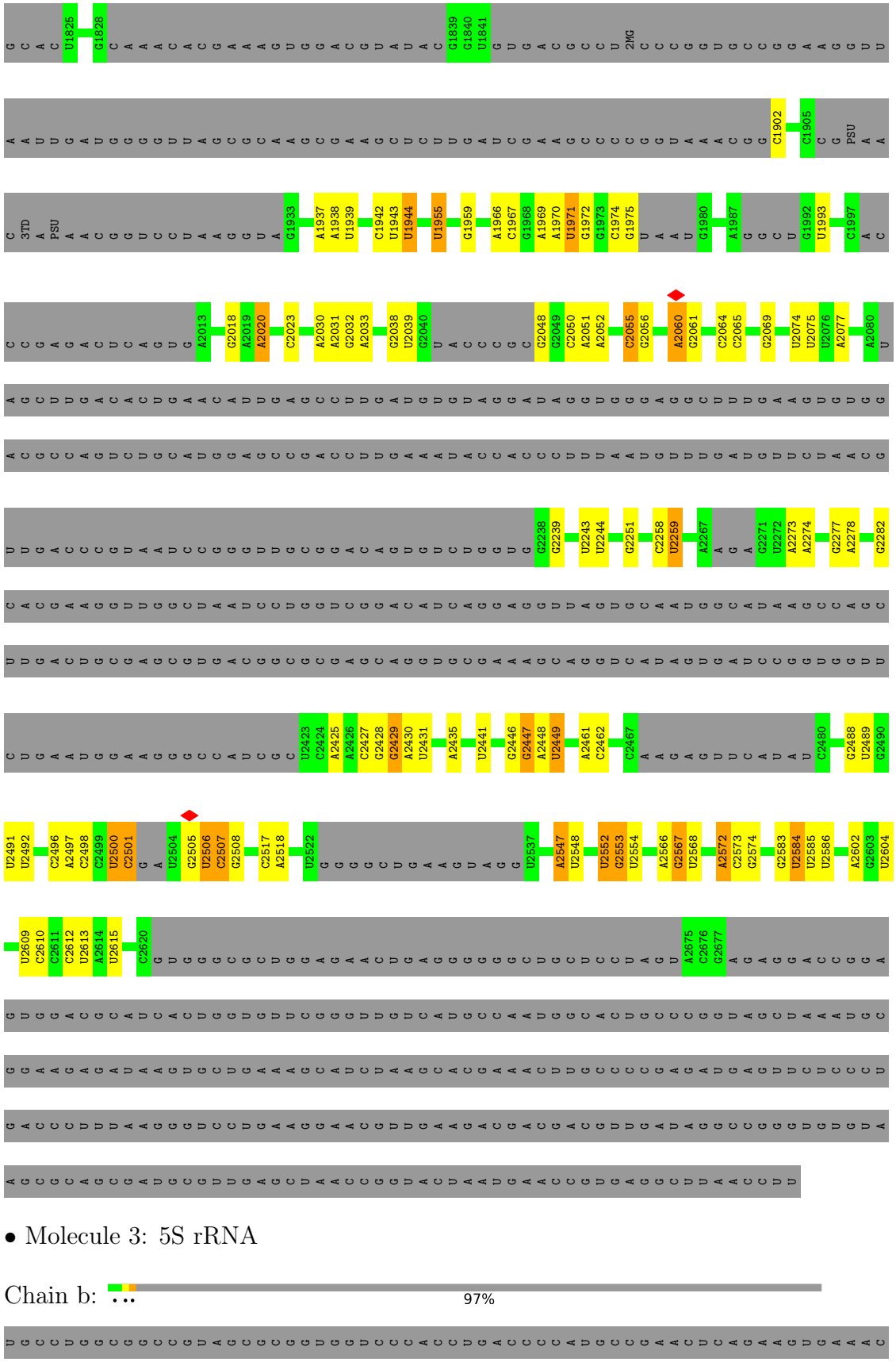
Chain Z:

- Molecule 2: 23S rRNA

Chain a:

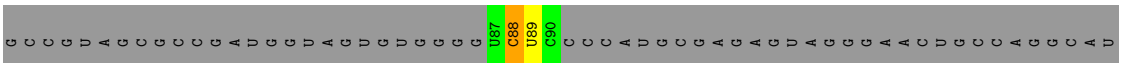



A670
A676 C679 C687 U688 A689
C G738 G745 U746 U747 G748 A756 G757 C758 G775 G776 G777 A781 A782 A783 G784 G785 A792 G805 G809 U810 U811 A819 U827 U828 U832 C837
U C G U G A910 A911 U G942 C946 C961 G962 A972 A973 G974 A975 G G978 A979 A980 A981
C982 A983 A984 C985 C986 G1025 G1026 A1027 A1028 A1029
G1125 U1132 A1133 A1134 C1135 G1136 G1137
U1188 A1189 G1190
G1252 A1253 G1256 C1257 U1258 A1262 A1269
6MZ
A1655 G1659 A1668 G1674 C1675 A1676 A1677
G1767 A1773 U1778 U1782 A1783 A1784 C1790

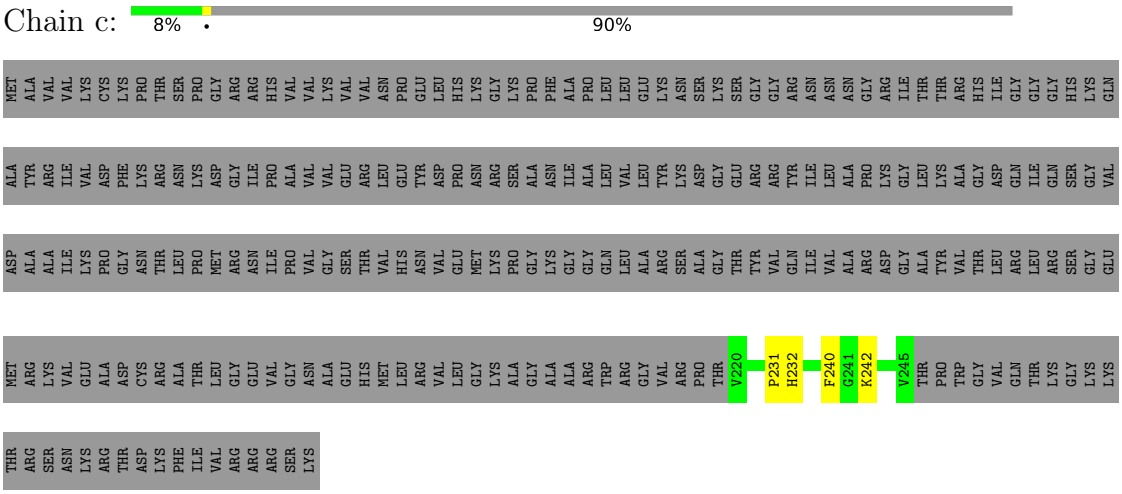


- Molecule 3: 5S rRNA

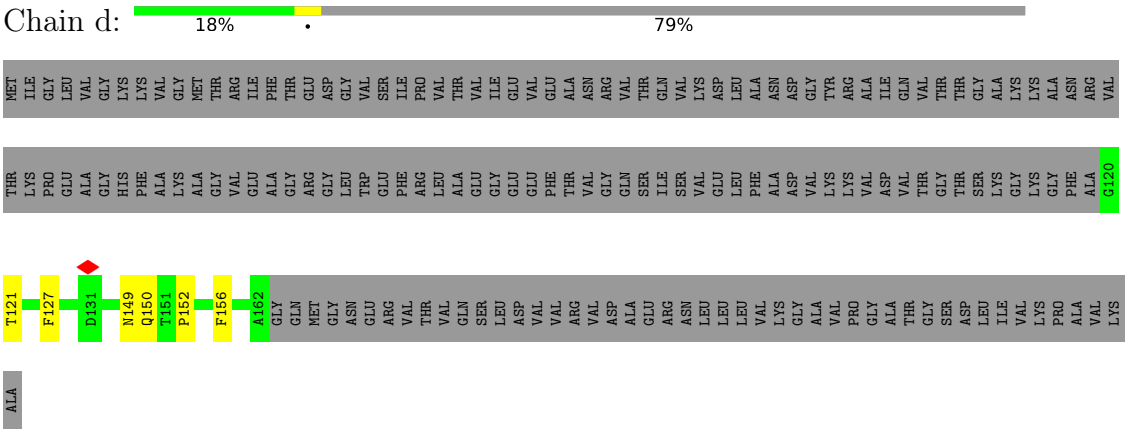
Chain b: 97%



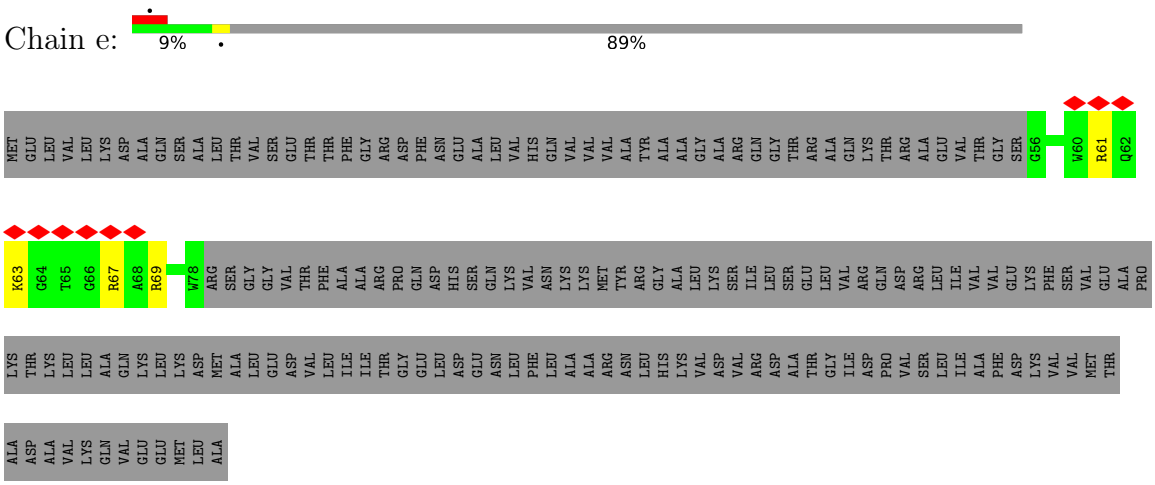
• Molecule 4: Large ribosomal subunit protein uL2



• Molecule 5: Large ribosomal subunit protein uL3



• Molecule 6: Large ribosomal subunit protein uL4



• Molecule 7: Large ribosomal subunit protein uL15

Chain k: 18% 82%

MET ARG LEU ASN THR LEU SER PRO ALA GLU GLY SER LYS LYS ALA GLY LYS ARG LEU GLY ARG GLY ILE GLY SER GLY LEU G28 R47 ARG GLY F50 M55 PRO LEU TYR ARG ARG LEU PRO LYS PHE GLY PHE THR SER ARG LYS ALA ALA ILE THR ALA GLU ILE ARG LEU SER

ASP LEU ALA LYS VAL GLU GLY GLY VAL VAL ASP LEU ASN THR LEU LYS ALA ALA ASN ILE ILE GLY ILE GLN ILE GLU PHE ALA LYS VAL ILE LEU ALA GLY GLU VAL THR THR PRO VAL THR VAL ARG GLY LEU ARG VAL THR LYS GLY ALA ARG ALA ALA ILE GLU ALA ALA GLY GLY

LYS ILE GLU GLU

• Molecule 8: Large ribosomal subunit protein uL16

Chain l: 30% 5% 65%

MET LEU GLN PRO LYS ARG THR LYS F9 R16 N17 R18 A21 GLN GLY THR ASP VAL SER PHE GLY SER PHE GLY LEU LYS ALA VAL GLY R38 T42 A43 R44 Q45 ILE GLU ALA ALA ARG ARG ALA MET THR ARG ALA VAL LYS ARG GLN GLY LYS ILE TRP ILE ARG VAL PHE

P69 T74 4D481 N88 L95 ILE GLN PRO GLY LYS VAL LEU TYR GLU MET ASP GLY VAL PRO GLU GLU LEU ALA ARG GLU ALA PHE LYS LEU ALA ALA ALA LYS LEU PRO ILE LYS THR THR PHE VAL THR LYS THR VAL MET

• Molecule 9: Large ribosomal subunit protein bL21

Chain q: 7% 93%

MET TYR ALA VAL PHE GLN SER GLY GLY LYS GLN HIS ARG VAL SER GLU GLY GLN THR VAL ARG LEU GLU GLU LYS LEU ASP ILE ALA THR GLY GLU THR VAL GLU PHE ALA GLU VAL LEU MET ILE ALA ASN GLY GLU GLU VAL LYS ILE GLY VAL PRO PHE VAL ASP GLY GLY VAL ILE LYS

ALA GLU VAL VAL ALA HIS GLY ARG GLY GLU LYS VAL LYS ILE VAL LYS F77 Y83 ARG LYS GLN GLN GLY HIS ARG GLN TRP PHE THR ASP VAL LYS ILE THR GLY ILE SER ALA

• Molecule 10: Large ribosomal subunit protein uL22

Chain r: 6% 94%

MET GLU THR ILE ALA LYS HIS ARG HIS ALA ARG SER SER ALA GLN LYS VAL ARG LEU VAL ALA ASP LEU ILE ARG GLY LYS LYS VAL SER GLN ALA LEU ASP ILE LEU THR TYR THR ASN LYS LYS ALA ALA VAL LEU VAL LYS LYS VAL LEU GLU SER ALA ILE ALA ASN ALA GLU HIS

ASN ASP GLY ALA ASP ILE ASP ASP LEU LYS VAL THR LYS ILE PHE VAL ASP GLU GLY PRO SER MET LYS ARG ILE MET PRO R88 D94 ARG ILE LEU LYS ARG THR SER HIS ILE THR VAL VAL VAL SER ASP ARG

• Molecule 11: Large ribosomal subunit protein bL27

Chain v: 11% 88%

MET ALA HIS LYS LYS ALA GLY G8 S9 R14 E17 ALA LYS ARG LEU GLY VAL LYS ARG PHE GLY GLY GLU SER VAL LEU ALA GLY SER ILE ILE VAL ARG GLN ARG GLY THR LYS PHE HIS ALA GLY ALA ASN VAL GLY CYS GLY ARG ASP HIS THR LEU PHE ALA LYS ALA ASP

• Molecule 12: Large ribosomal subunit protein bL32

Chain z:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56208	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.107	Depositor
Minimum map value	-0.819	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.099	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	420.608, 420.608, 420.608	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8215, 0.8215, 0.8215	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: 6MZ, MS6, H2U, 5MU, MEQ, 5MC, PSU, 1MG, SR0, K, 4D4, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	Z	0.56	0/427	0.79	0/661
2	a	0.53	0/13916	1.02	38/21612 (0.2%)
3	b	0.60	0/87	0.98	0/132
4	c	0.78	0/197	1.04	0/265
5	d	0.67	0/329	1.04	0/438
6	e	0.64	0/187	1.02	0/248
7	k	0.70	0/182	1.09	0/232
8	l	0.62	0/370	1.13	1/487 (0.2%)
9	q	0.71	0/77	1.03	0/99
10	r	0.76	0/52	0.94	0/66
11	v	0.72	0/73	1.09	0/95
12	z	0.68	0/61	1.10	1/82 (1.2%)
All	All	0.55	0/15958	1.02	40/24417 (0.2%)

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
6	e	0	1
8	l	0	3
11	v	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	a	1971	U	O3'-P-O5'	-11.61	86.59	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	a	1974	C	O3'-P-O5'	-10.47	88.29	104.00
2	a	577	G	O3'-P-O5'	-7.86	92.21	104.00
2	a	2048	G	O3'-P-O5'	-7.65	92.53	104.00
2	a	2050	C	O3'-P-O5'	-6.84	93.73	104.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	e	69	ARG	Sidechain
8	l	16	ARG	Sidechain
8	l	18	ARG	Sidechain
8	l	44	ARG	Sidechain
11	v	14	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z	384	0	200	1	0
2	a	12630	0	6401	33	0
3	b	80	0	43	1	0
4	c	191	0	177	2	0
5	d	333	0	336	3	0
6	e	182	0	193	1	0
7	k	182	0	179	0	0
8	l	386	0	399	1	0
9	q	75	0	76	0	0
10	r	53	0	55	0	0
11	v	74	0	64	0	0
12	z	61	0	62	2	0
13	a	20	0	0	0	0
14	a	33	0	0	0	0
14	d	1	0	0	0	0
15	a	21	0	0	0	0
All	All	14706	0	8185	42	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 2.

The worst 5 of 42 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)
2:a:568:U:H1'	2:a:2030:6MZ:H9C1	1.82	0.60
2:a:2583:G:H3'	2:a:2584:U:H5"	1.86	0.57
2:a:586:A:N1	2:a:809:G:O2'	2.38	0.55
2:a:1028:A:N6	2:a:1125:G:H2'	2.22	0.54
4:c:231:PRO:O	4:c:242:LYS:HE3	2.07	0.53

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	
4	c	24/273 (9%)	23 (96%)	1 (4%)	0	100	100
5	d	40/209 (19%)	36 (90%)	4 (10%)	0	100	100
6	e	21/201 (10%)	19 (90%)	2 (10%)	0	100	100
7	k	22/144 (15%)	20 (91%)	2 (9%)	0	100	100
8	l	40/136 (29%)	39 (98%)	1 (2%)	0	100	100
9	q	5/103 (5%)	5 (100%)	0	0	100	100
10	r	5/110 (4%)	5 (100%)	0	0	100	100
11	v	8/85 (9%)	7 (88%)	1 (12%)	0	100	100
12	z	6/57 (10%)	6 (100%)	0	0	100	100
All	All	171/1318 (13%)	160 (94%)	11 (6%)	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	
4	c	19/218 (9%)	19 (100%)	0	100	100
5	d	34/163 (21%)	34 (100%)	0	100	100
6	e	18/165 (11%)	17 (94%)	1 (6%)	19	22
7	k	16/103 (16%)	16 (100%)	0	100	100
8	l	36/107 (34%)	36 (100%)	0	100	100
9	q	7/84 (8%)	7 (100%)	0	100	100
10	r	4/93 (4%)	4 (100%)	0	100	100
11	v	8/63 (13%)	8 (100%)	0	100	100
12	z	7/48 (15%)	7 (100%)	0	100	100
All	All	149/1044 (14%)	148 (99%)	1 (1%)	73	86

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	e	63	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
11	v	12	ASN
12	z	6	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Z	16/77 (20%)	4 (25%)	1 (6%)
2	a	555/2904 (19%)	95 (17%)	0
3	b	3/120 (2%)	2 (66%)	0
All	All	574/3101 (18%)	101 (17%)	1 (0%)

5 of 101 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Z	7	G
1	Z	74	C
1	Z	75	C
1	Z	76	A
2	a	196	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	Z	74	C

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

11 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	$\#\|Z\| > 2$
2	H2U	a	2449	2	18,21,22	0.34	0	21,30,33	0.57	0
2	1MG	a	745	2	22,26,27	0.57	0	33,39,42	0.58	1 (3%)
8	4D4	l	81	8	9,11,12	0.87	0	8,13,15	1.42	2 (25%)
2	5MC	a	1962	2	18,22,23	0.32	0	26,32,35	0.35	0
2	PSU	a	955	2	18,21,22	0.38	0	22,30,33	0.34	0
2	6MZ	a	2030	2	22,25,26	0.30	0	30,36,39	0.41	0
2	5MU	a	747	2	19,22,23	0.40	0	28,32,35	0.71	0
2	PSU	a	746	2	18,21,22	0.53	0	22,30,33	0.49	0
8	MS6	l	82	8	5,7,8	0.40	0	2,7,9	0.32	0
5	MEQ	d	150	5	8,9,10	0.67	0	5,10,12	0.96	0
2	5MU	a	1939	2	19,22,23	0.38	0	28,32,35	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	H2U	a	2449	2	-	4/7/38/39	0/2/2/2
2	1MG	a	745	2	-	0/7/25/26	0/3/3/3
8	4D4	l	81	8	-	2/11/12/14	-
2	5MC	a	1962	2	-	2/7/25/26	0/2/2/2
2	PSU	a	955	2	-	0/7/25/26	0/2/2/2
2	6MZ	a	2030	2	-	1/9/27/28	0/3/3/3
2	5MU	a	747	2	-	0/7/25/26	0/2/2/2
2	PSU	a	746	2	-	1/7/25/26	0/2/2/2
8	MS6	l	82	8	-	1/4/6/8	-
5	MEQ	d	150	5	-	4/8/9/11	-
2	5MU	a	1939	2	-	0/7/25/26	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	l	81	4D4	O-C-CA	-2.78	117.48	124.78
2	a	745	1MG	C6-C5-C4	-2.32	117.41	119.97
8	l	81	4D4	NE-CZ-NH2	2.31	124.76	120.70

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	d	150	MEQ	C-CA-CB-CG
8	l	81	4D4	N-CA-CB-CG
2	a	2449	H2U	O4'-C1'-N1-C6
2	a	2449	H2U	C2'-C1'-N1-C6
2	a	2449	H2U	C2'-C1'-N1-C2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	a	2449	H2U	1	0
2	a	2030	6MZ	1	0
5	d	150	MEQ	1	0
2	a	1939	5MU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 57 ligands modelled in this entry, 55 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
13	SR0	a	3001	-	9,9,9	0.55	0	8,8,8	0.29	0
13	SR0	a	3002	-	9,9,9	0.56	0	8,8,8	0.34	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SR0	a	3001	-	-	3/7/7/7	-
13	SR0	a	3002	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	a	3002	SR0	N6-C7-C8-C9
13	a	3002	SR0	C8-C7-N6-C5
13	a	3001	SR0	C3-C4-C5-N6
13	a	3002	SR0	C2-C3-C4-C5
13	a	3001	SR0	C2-C3-C4-C5

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.

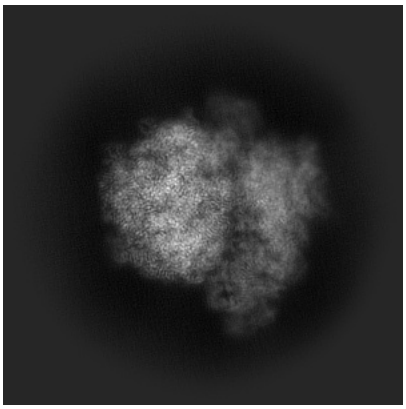
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-55710. These allow visual inspection of the internal detail of the map and identification of artifacts.

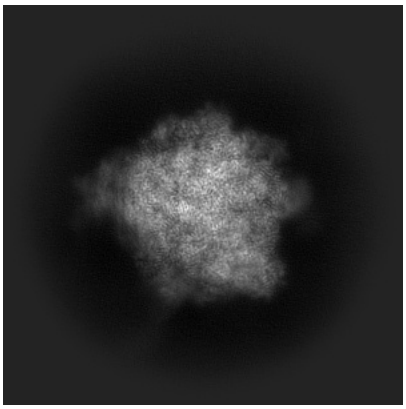
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

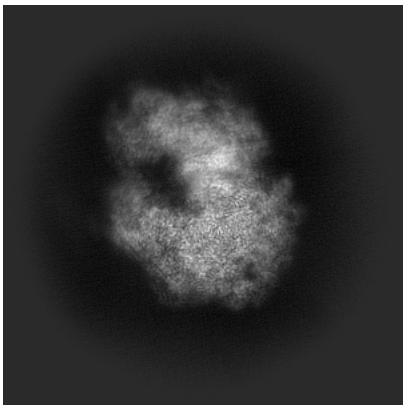
6.1.1 Primary map



X

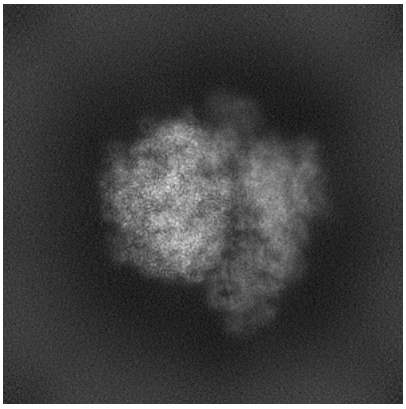


Y

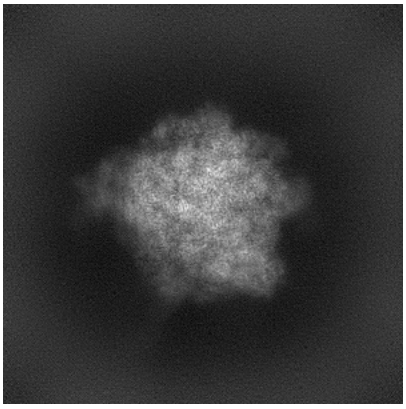


Z

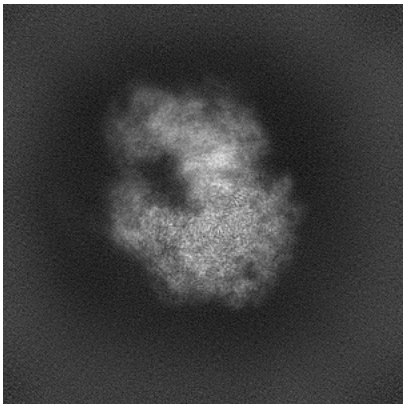
6.1.2 Raw map



X



Y

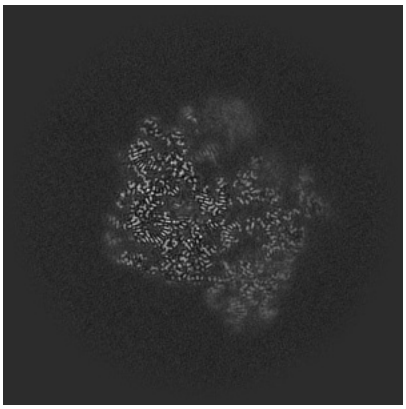


Z

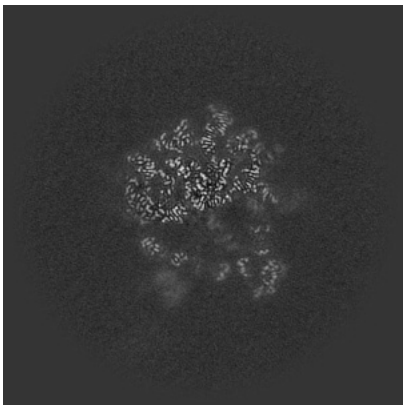
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

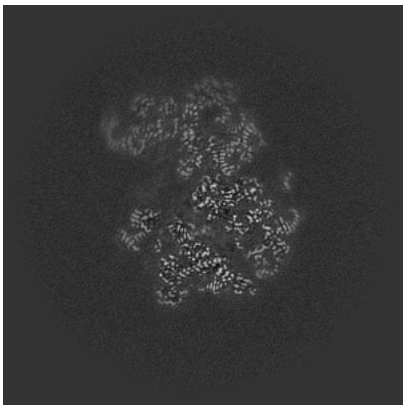
6.2.1 Primary map



X Index: 256

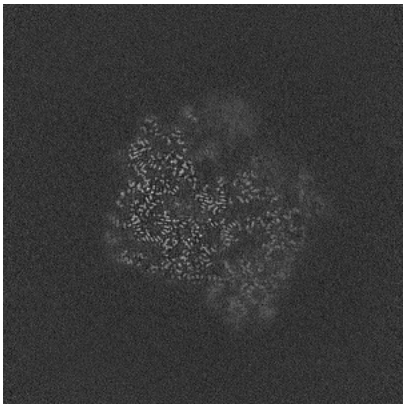


Y Index: 256

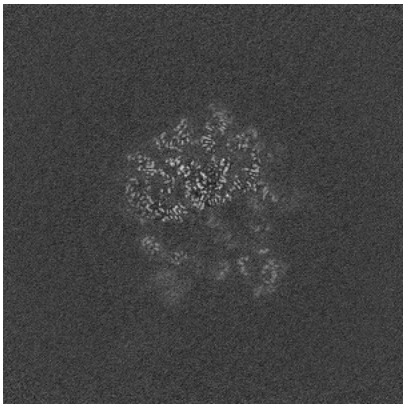


Z Index: 256

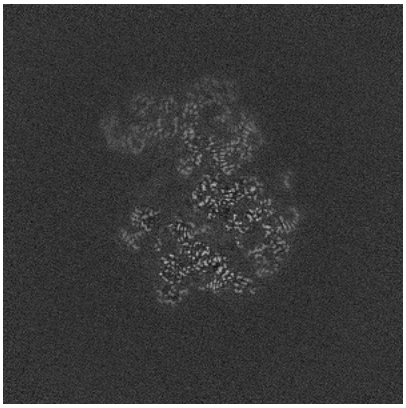
6.2.2 Raw map



X Index: 256



Y Index: 256

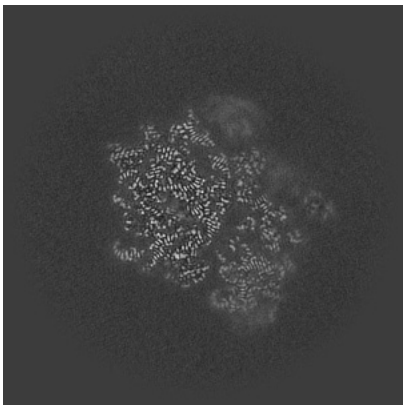


Z Index: 256

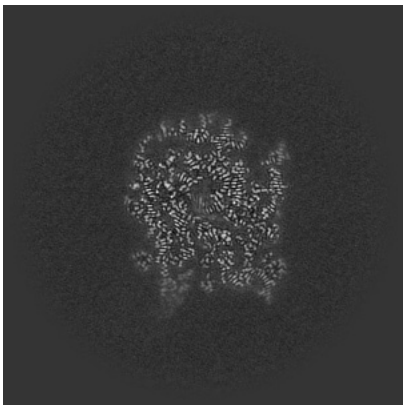
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

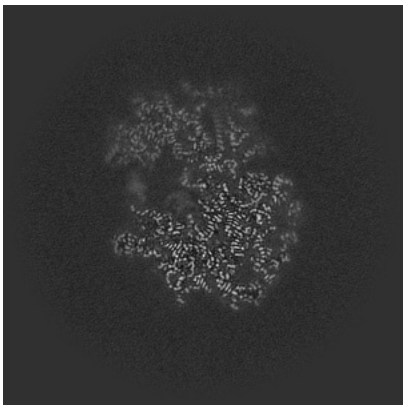
6.3.1 Primary map



X Index: 267

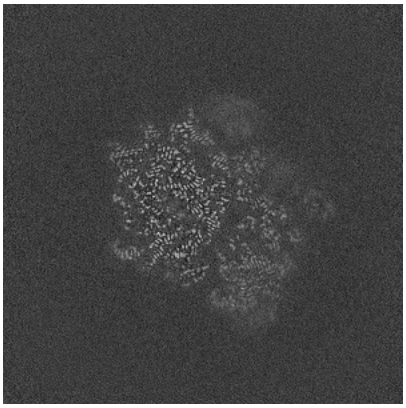


Y Index: 221

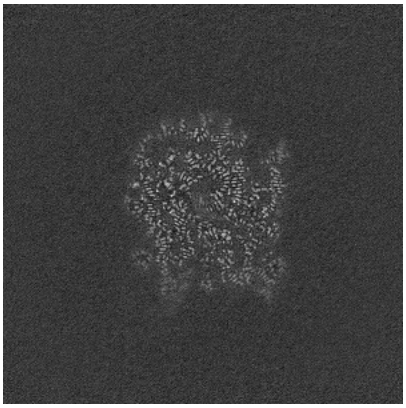


Z Index: 270

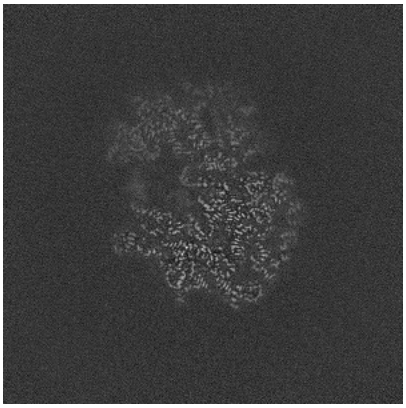
6.3.2 Raw map



X Index: 267



Y Index: 221

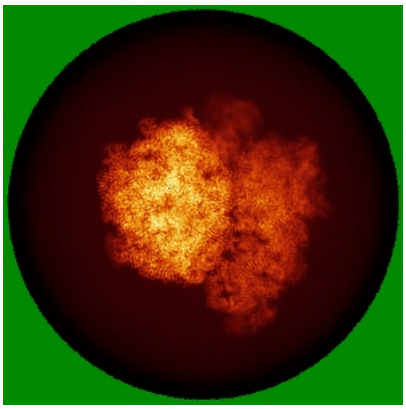


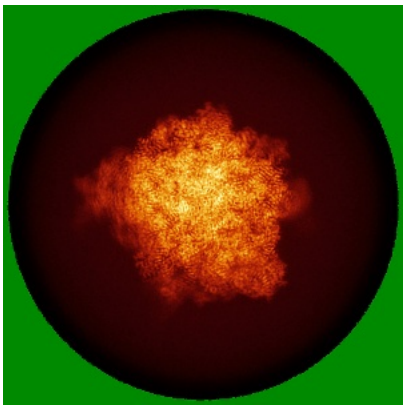
Z Index: 269

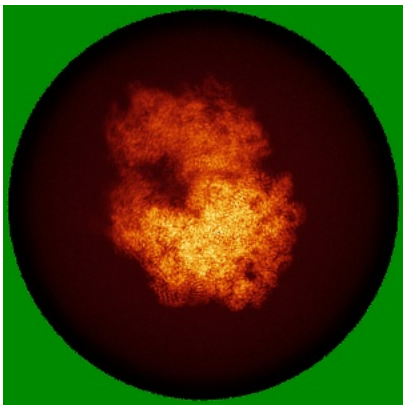
The images above show the largest variance slices of the map in three orthogonal directions.

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

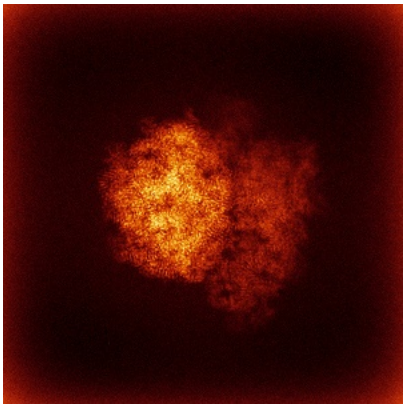
6.4.1 Primary map

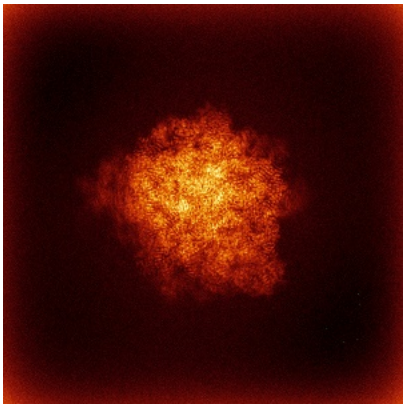

X

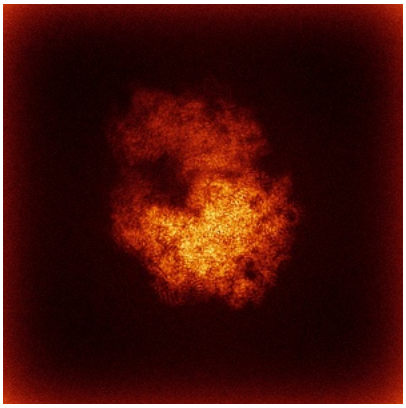

Y


Z

6.4.2 Raw map


X

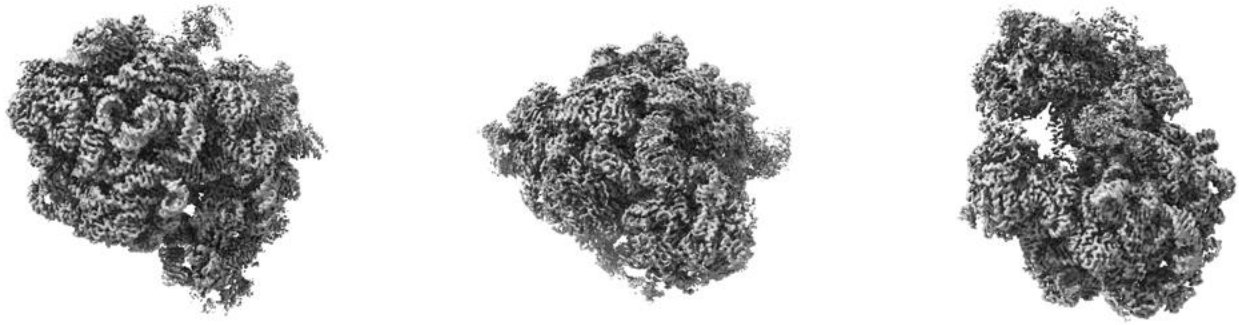

Y


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)

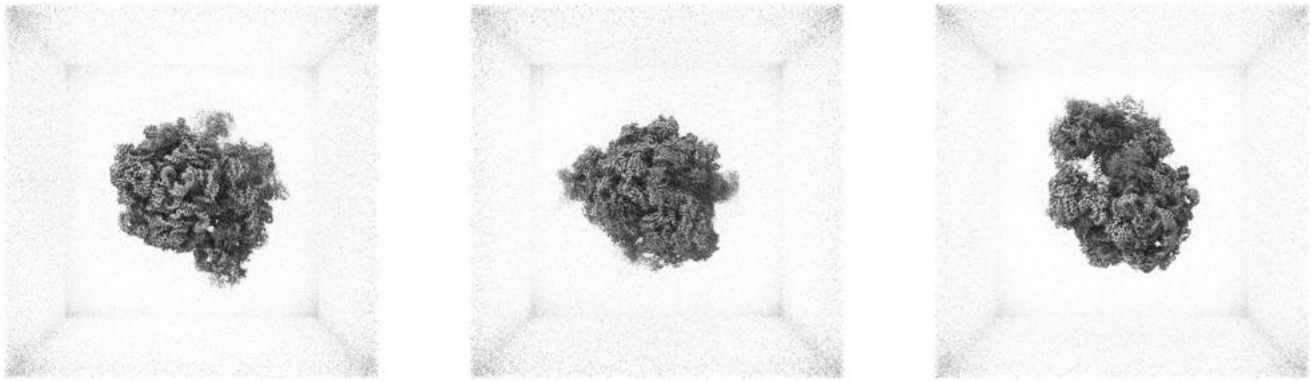
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

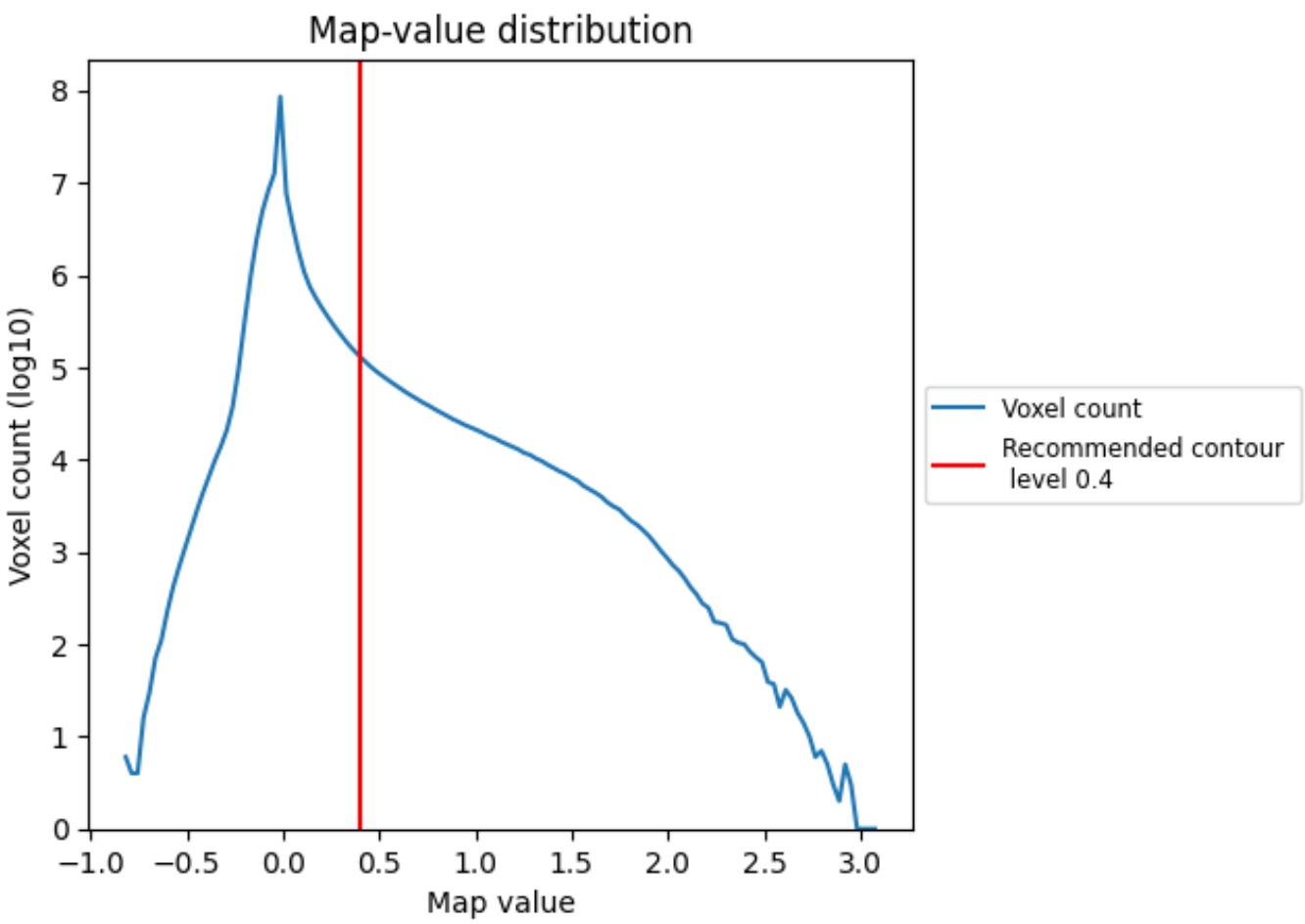
6.6 Mask visualisation (i)

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

7 Map analysis (i)

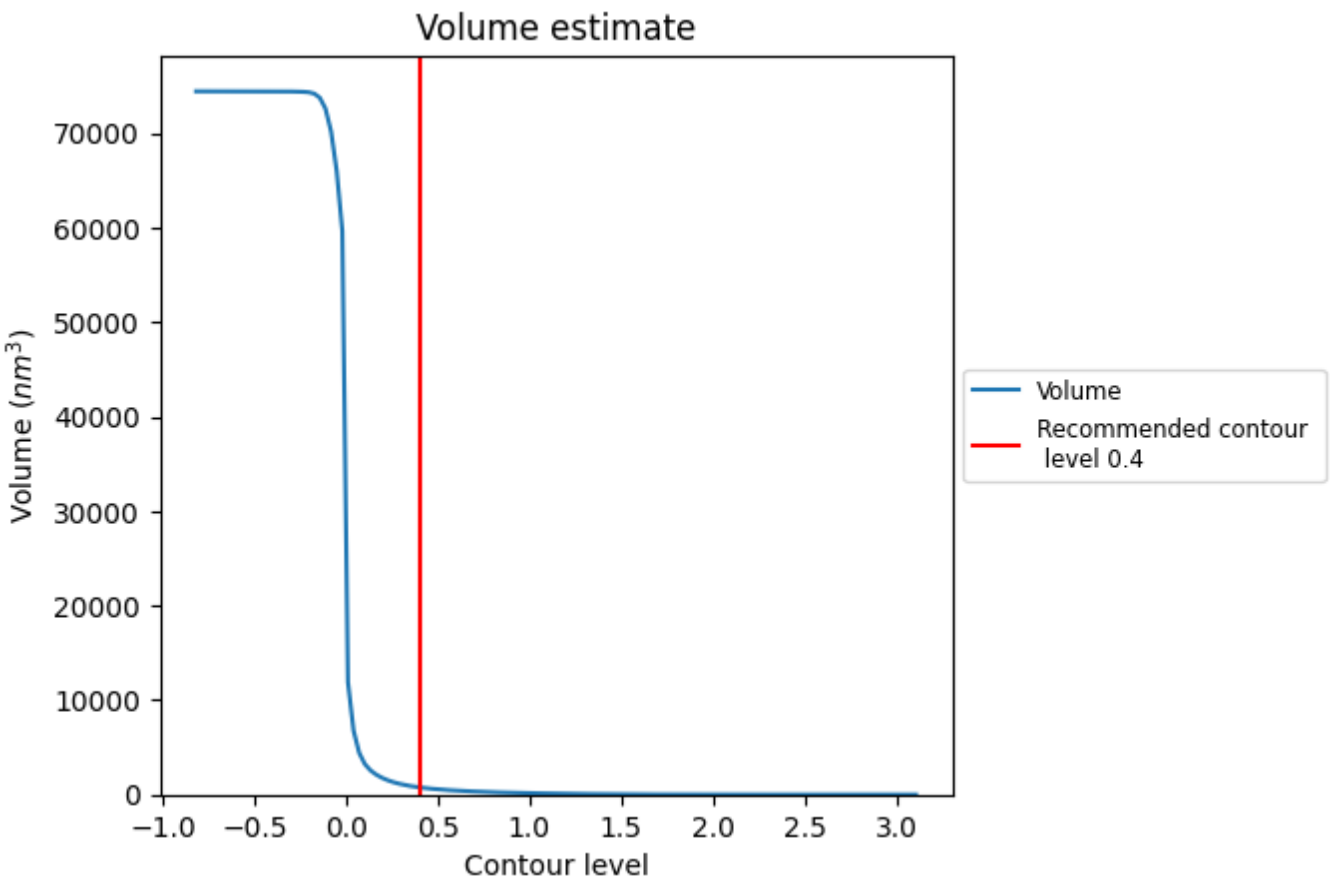
This section contains the results of statistical analysis of the map.

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.

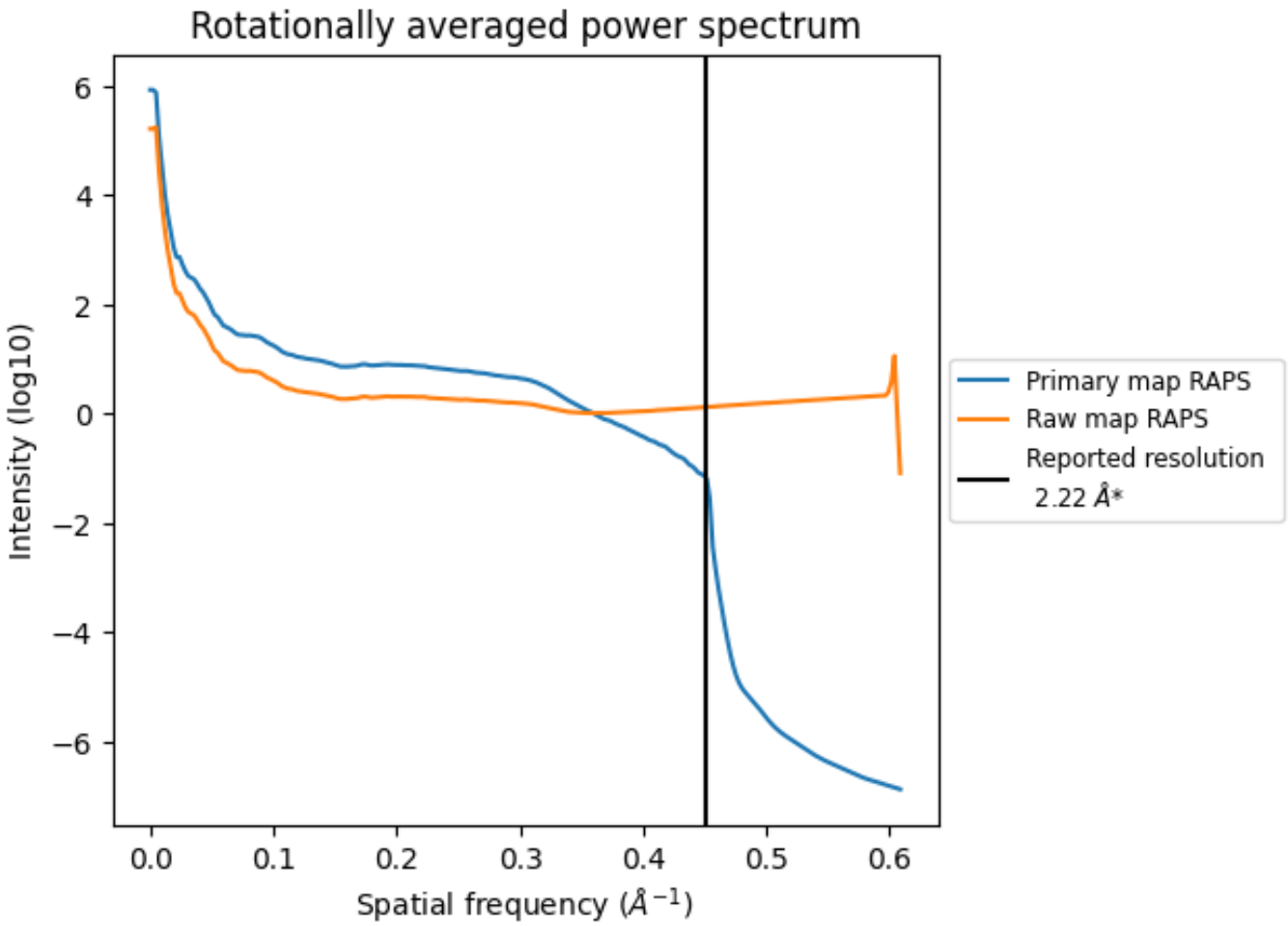
7.2 Volume estimate (i)



The volume at the recommended contour level is 759 nm^3; this corresponds to an approximate mass of 686 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)

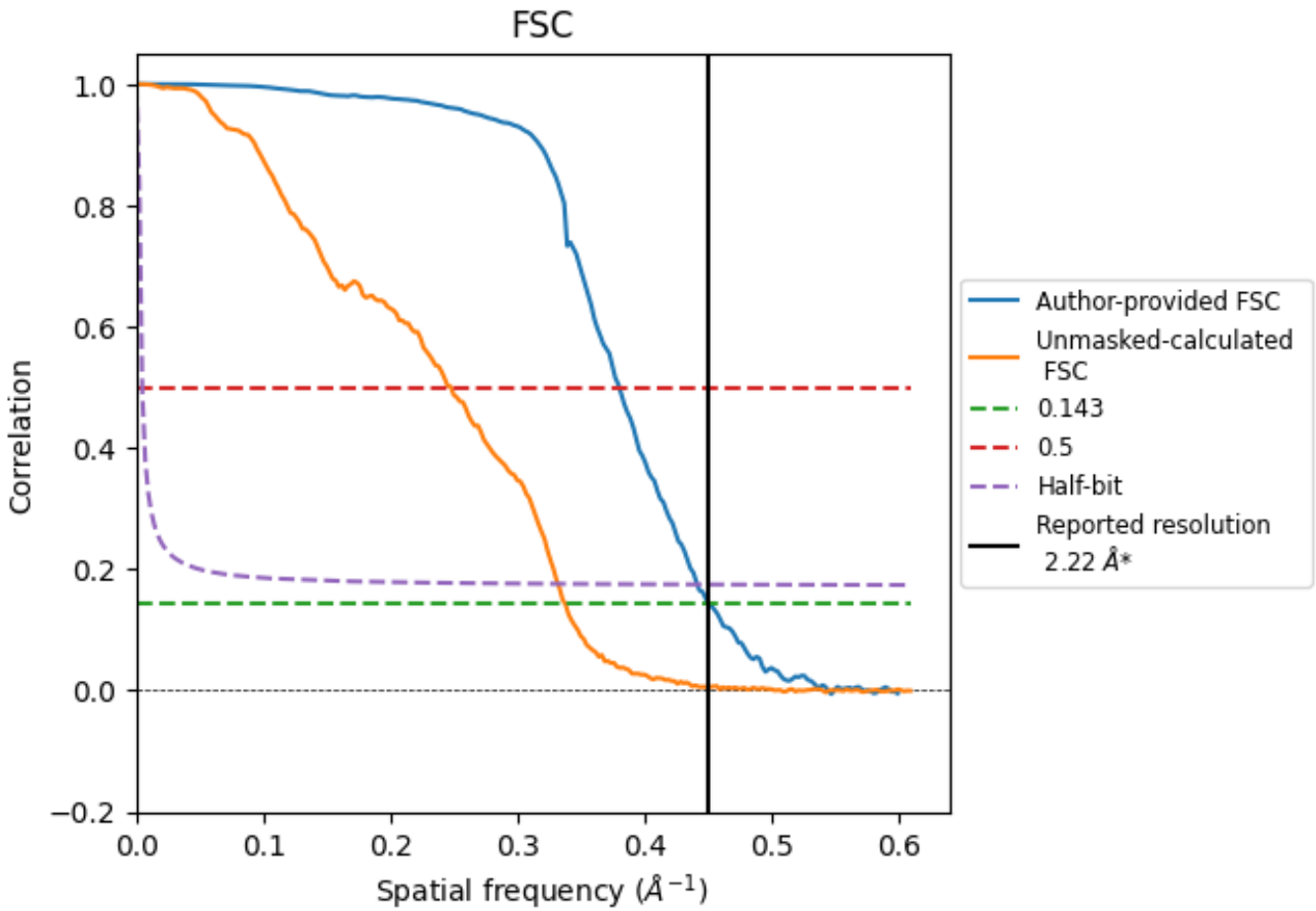


*Reported resolution corresponds to spatial frequency of 0.450 Å^{-1}

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 0.450 Å^{-1}

8.2 Resolution estimates (i)

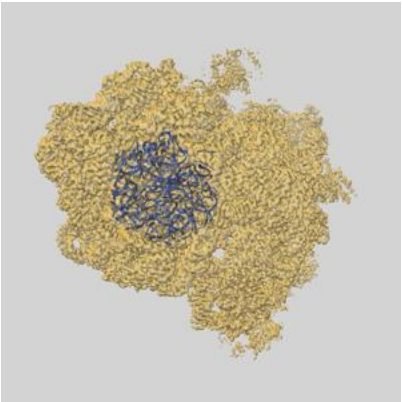
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.22	-	-
Author-provided FSC curve	2.22	2.63	2.27
Unmasked-calculated*	2.97	4.04	3.02

*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 2.97 differs from the reported value 2.22 by more than 10 %

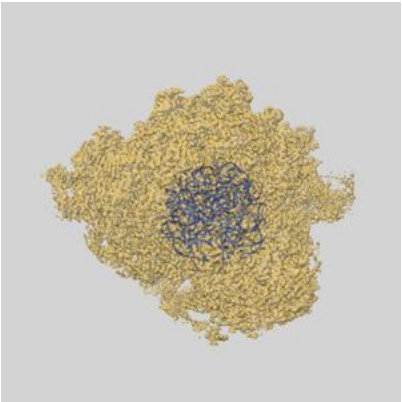
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-55710 and PDB model 9T8S. Per-residue inclusion information can be found in section 3 on page 7.

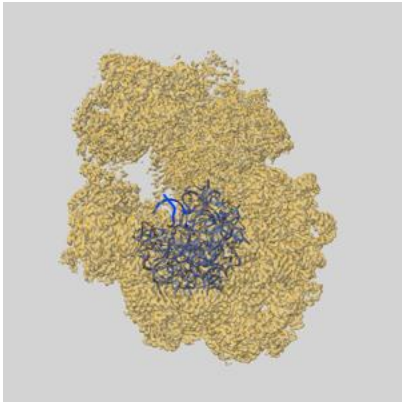
9.1 Map-model overlay (i)



X



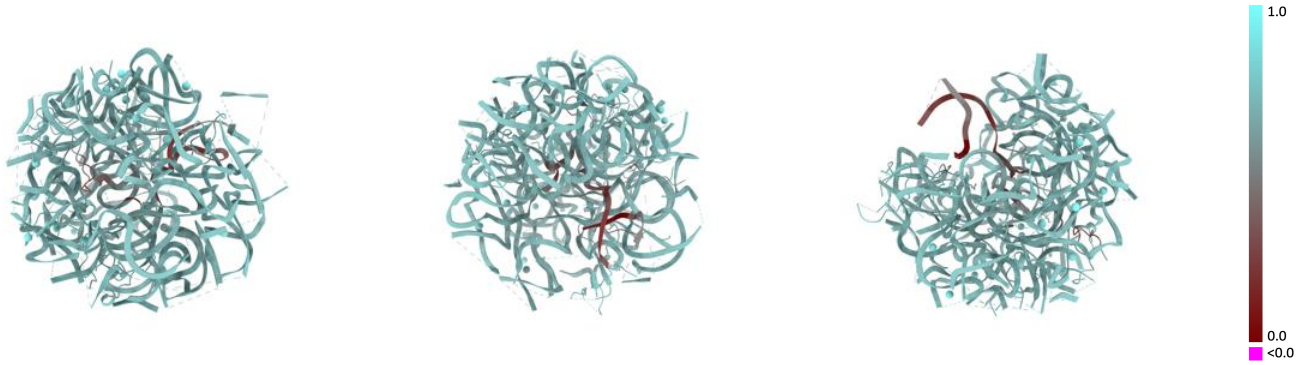
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

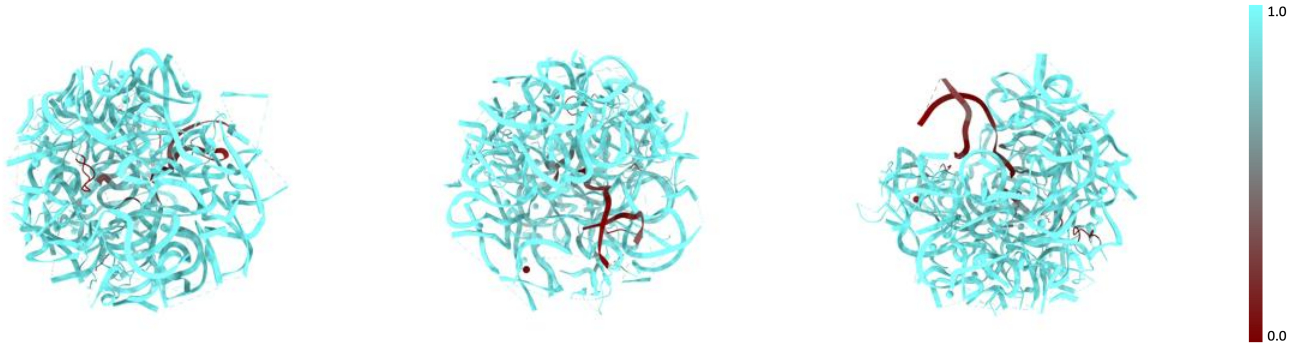
9.2 Q-score mapped to coordinate model (i)



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.

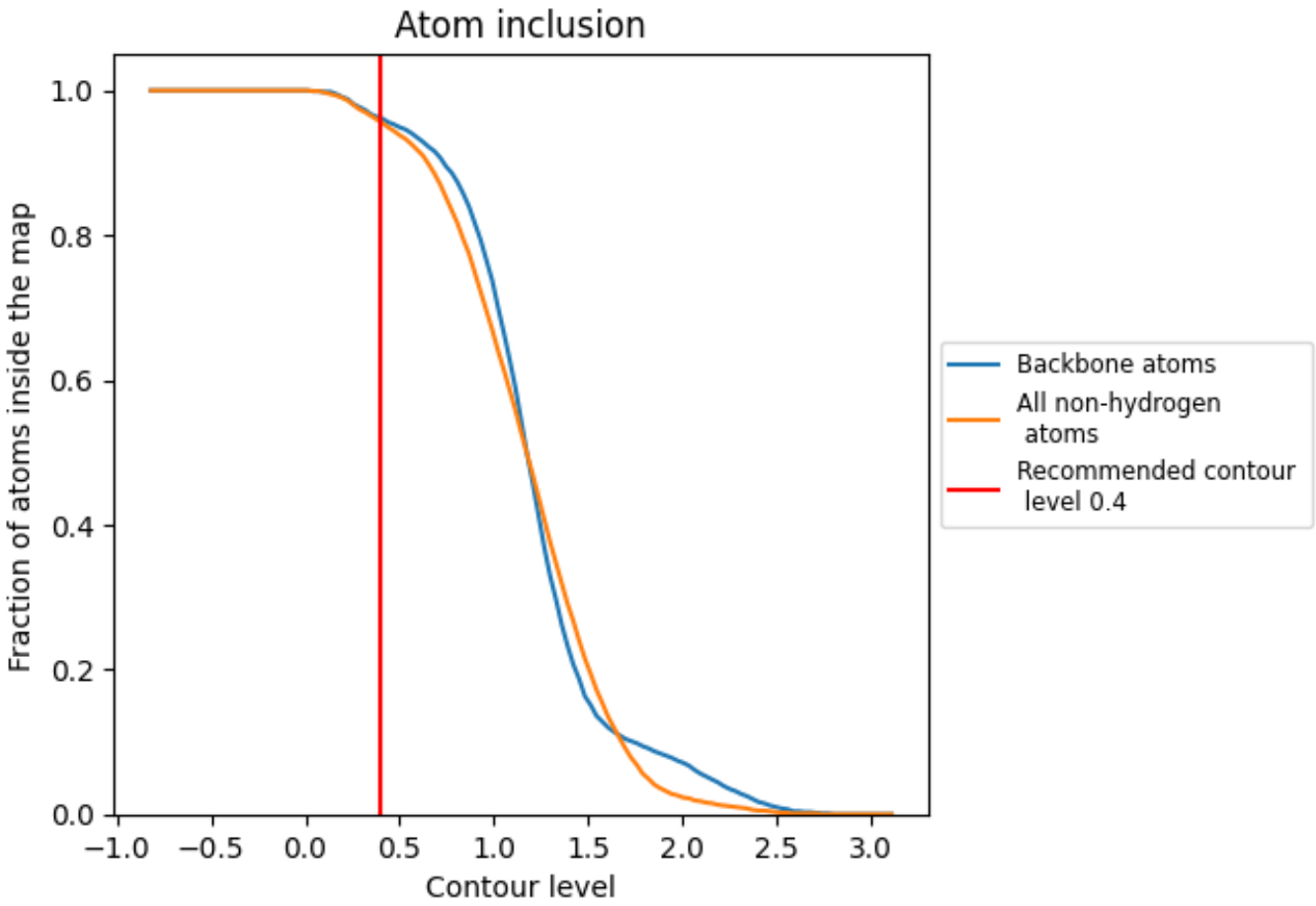
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 96% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9560	0.6610
Z	0.1690	0.2920
a	0.9860	0.6730
b	0.9250	0.6090
c	0.9950	0.6970
d	0.9660	0.6860
e	0.5400	0.4890
k	0.9890	0.7010
l	0.9600	0.6750
q	1.0000	0.6990
r	0.8980	0.6750
v	0.7290	0.5820
z	1.0000	0.7020