wwPDB EM Validation Summary Report (i)

Aug 17, 2026 – 06:15 pm BST

PDB ID	:	9T1I / pdb_00009t1i
EMDB ID	:	EMD-55436
Title	:	E. coli 70S ribosome from delta-RlmE strain, PTC class 8
Authors	:	Larsson, D.S.D.; Selmer, M.
Deposited on	:	2025-10-21
Resolution	:	2.30 Å(reported)
Based on initial model	:	9SYH

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:

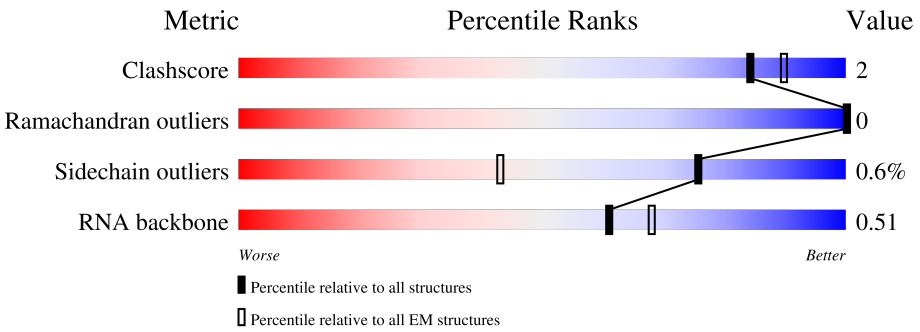
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal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

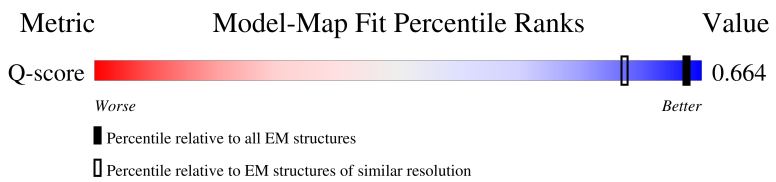
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	4254 (1.80 - 2.80)

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	16% 9% 13% • 77%
2	a	2904	14% 5% • 79%
3	b	120	• • • 97%

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Mol	Chain	Length	Quality of chain
4	c	273	9% 90%
5	d	209	16% 79%
6	e	201	9% 89%
7	i	142	5% 94%
8	k	144	18% 82%
9	l	136	30% 5% 65%
10	q	103	7% 93%
11	r	110	6% 94%
12	v	85	11% 16% 81%
13	z	57	9% 5% 86%

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 15041 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	596	12772	5710	2332	4134	596	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 uL13.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	i	8	55	34	12	9	0	0

- Molecule 8 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	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 10 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 11 is a protein called Large ribosomal subunit protein uL22.

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

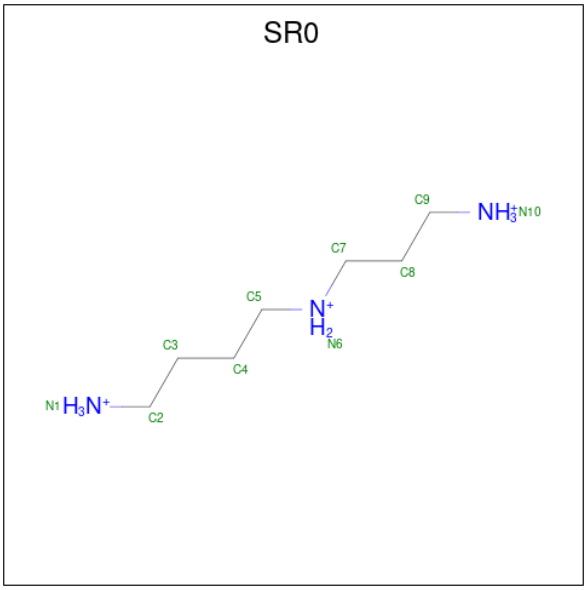
- Molecule 12 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	v	16	116	65	27	24	0	0

- Molecule 13 is a protein called Large ribosomal subunit protein bL32.

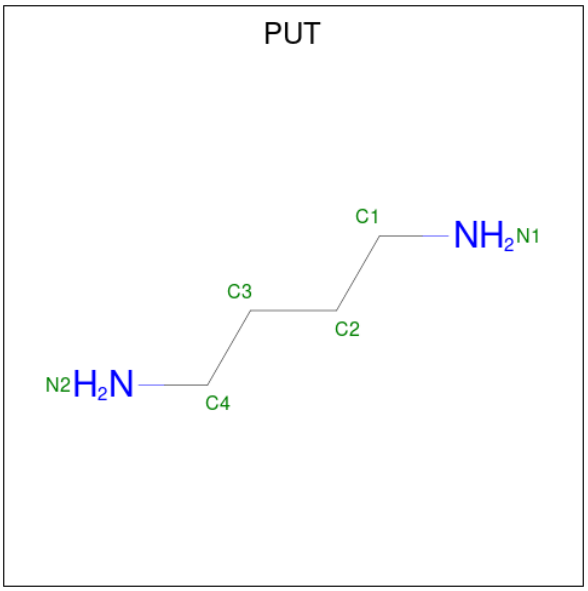
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	z	8	61	37	12	12	0	0

- Molecule 14 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	
14	a	1	10	7	3	0
			Total	C	N	
14	a	1	10	7	3	0

- Molecule 15 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
15	a	1	6	4	2	0

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
16	a	101	101	101	0
16	d	1	1	1	0

- Molecule 17 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
17	a	42	42	42	0
17	e	1	1	1	0

3 Residue-property plots (i)

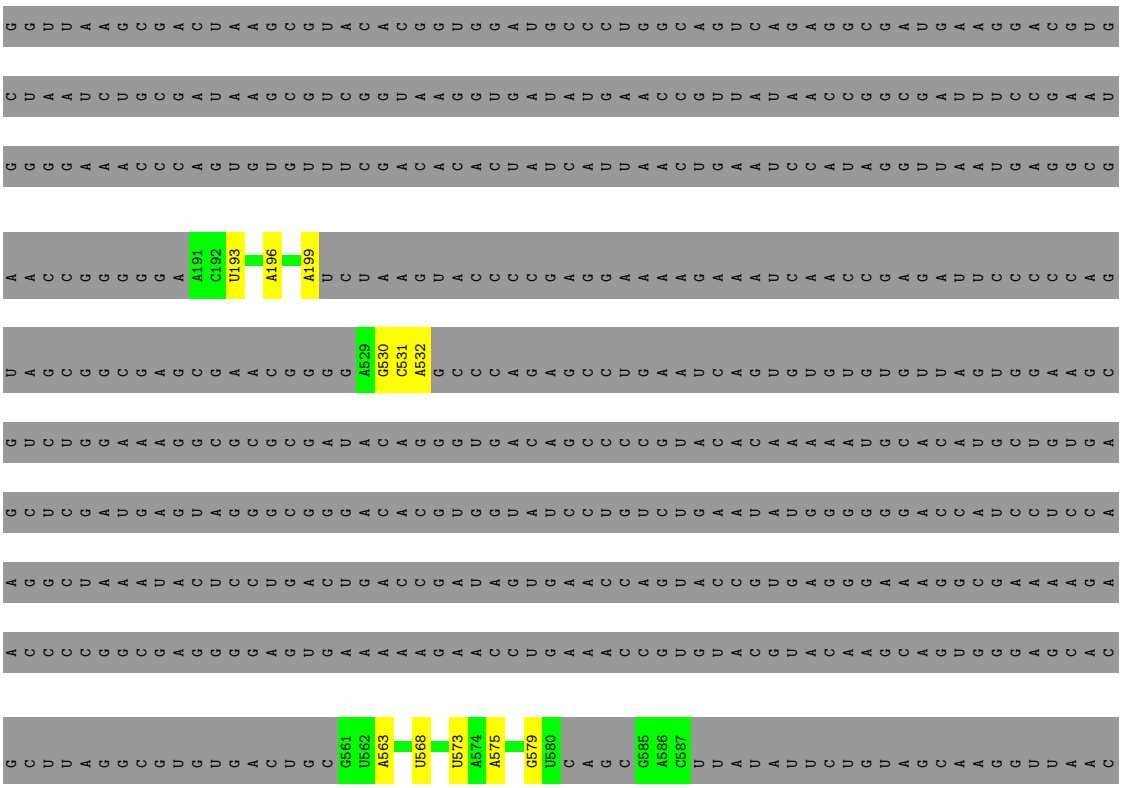
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

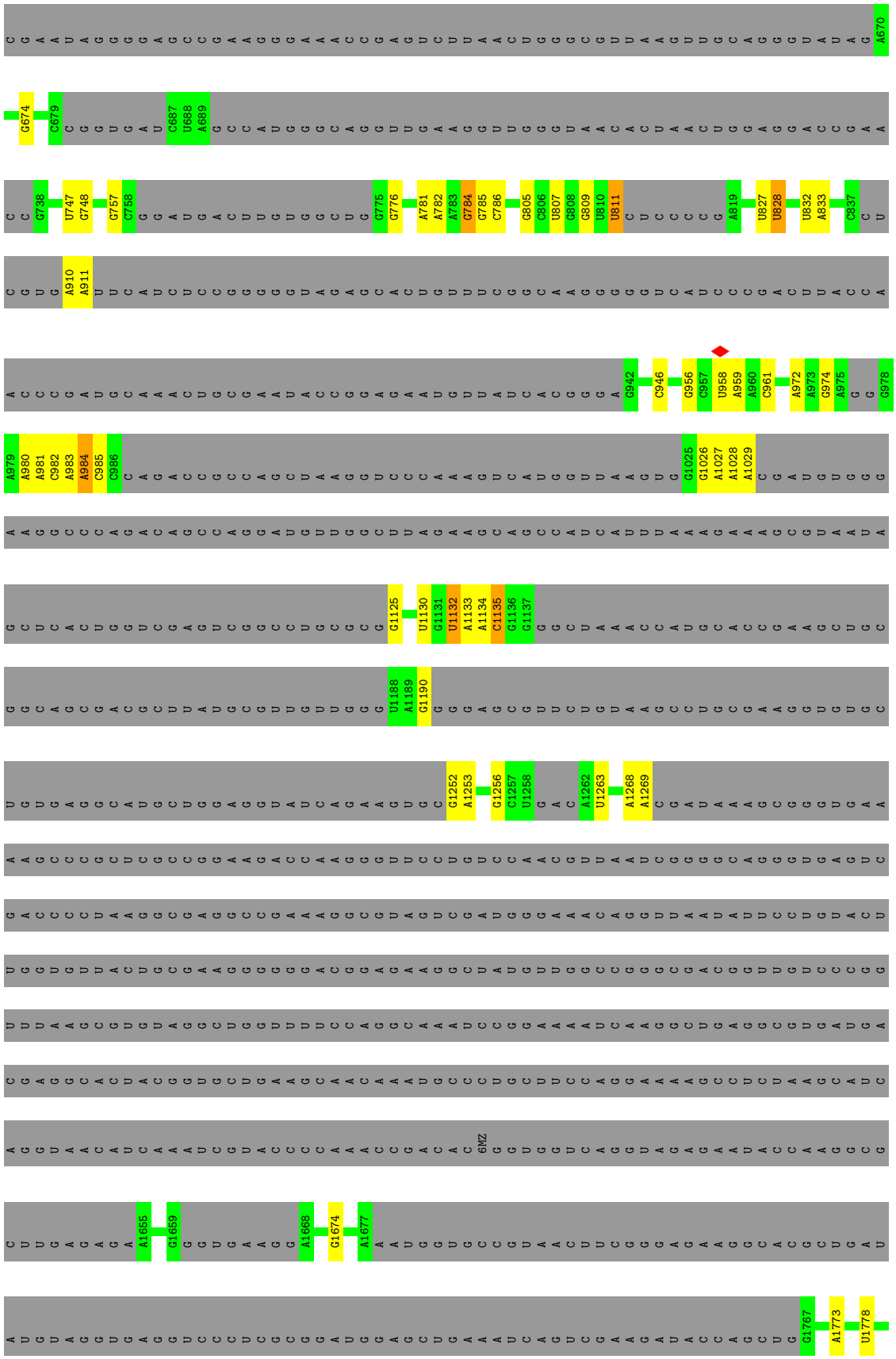
- Molecule 1: tRNA(fMet)

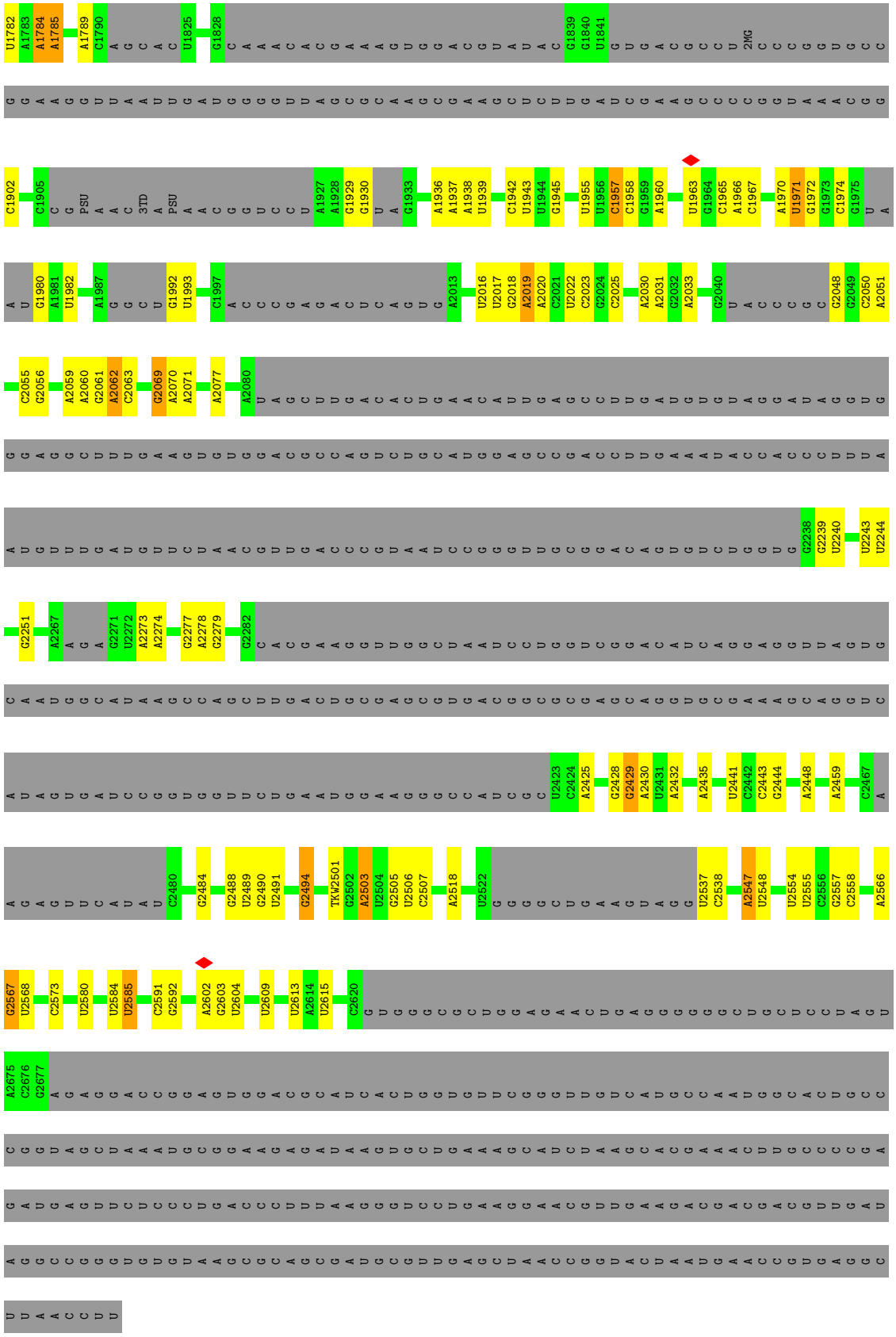
Chain Z:

- Molecule 2: 23S rRNA

Chain a:




A670
G674
C679
C687
U688
A689
G738
U747
G748
G757
C758
G775
G776
A781
A782
A783
G784
G785
C786
G805
C806
U807
G808
G809
U810
U811
A819
U827
U828
U832
A833
C837
A910
A911
G942
C946
G956
C957
U958
A959
A960
C961
A972
A973
G974
A975
G978
A979
A980
A981
C982
A983
A984
C985
C986
G1025
G1026
A1027
A1028
A1029
G1125
U1130
G1131
U1132
A1133
A1134
C1135
G1136
G1137
U1188
A1189
G1190
G1252
A1253
G1256
C1257
U1258
A1262
U1263
A1268
A1269
6MZ
A1655
G1659
A1668
G1674
A1677
G1767
A1773
U1778



- Molecule 3: 5S rRNA

Chain b: 97%

U G C C U G G C G G C C G U A G C G C G G U G G U C C C A C C U G A C C C C A U G C C G A A C U C A G A A A C

G C C G U A G C G C C C G A U G G U A G U G U G G G G U87 C88 U89 C90 C C C A U G C G A G A G U A G G G G A A C U G C C A G G C A U

- Molecule 4: Large ribosomal subunit protein uL2

Chain c: 9% 90%

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

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

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

MET ARG LYS VAL GLU ALA ASP CYS ARG ALA THR LEU GLY GLU VAL GLY ASN ALA GLU HIS MET LEU ARG VAL LEU GLY LYS ALA GLY ALA ALA ARG TRP ARG GLY VAL ARG PRO THR V220 F240 G241 K242 V245 THR PRO TRP GLY VAL GLN THR LYS GLY LYS LYS THR ARG SER

ASN LYS ARG THR ASP LYS PHE ILE VAL ARG ARG ARG SER LYS

- Molecule 5: Large ribosomal subunit protein uL3

Chain d: 16% 79%

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

THR LYS PRO GLU ALA GLY HIS PHE ALA LYS ALA GLY VAL GLU ALA GLY ARG GLY LEU TRP GLU PHE ARG LEU ALA GLU GLY GLU GLU PHE THR VAL GLY GLN SER ILE SER VAL VAL GLU LEU PHE ALA ASP VAL LYS LYS VAL ASP VAL THR GLY THR SER LYS GLY LYS GLY PHE ALA G120

T121 F127 R128 T129 N149 Q150 T151 P152 F156 K157 G158 K159 A162 GLY GLN MET GLY ASN GLU ARG VAL THR VAL GLN SER LEU ASP VAL VAL ARG VAL ASP ALA GLU ARG ASN LEU LEU LEU VAL LYS GLY ALA VAL PRO GLY ALA THR GLY SER ASP LEU ILE VAL LYS PRO

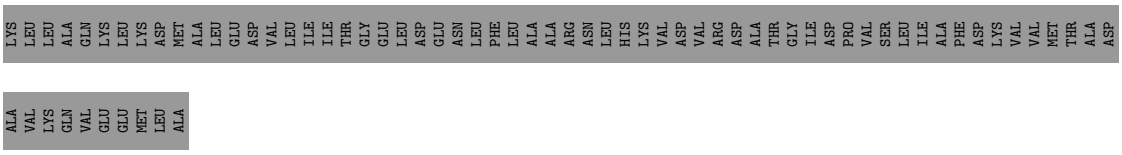
ALA VAL LYS ALA

- Molecule 6: Large ribosomal subunit protein uL4

Chain e: 9% 89%

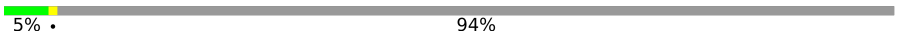
MET GLU LEU VAL LEU LYS ASP ALA GLN SER ALA LEU THR VAL SER GLU THR THR PHE GLY ARG ASP PHE ASN GLU ALA LEU VAL HIS GLN VAL VAL VAL ALA TYR ALA ALA GLY ALA ARG GLN GLY THR ARG ALA GLN LYS THR ARG ALA GLU VAL THR GLY SER G56 K57 R61

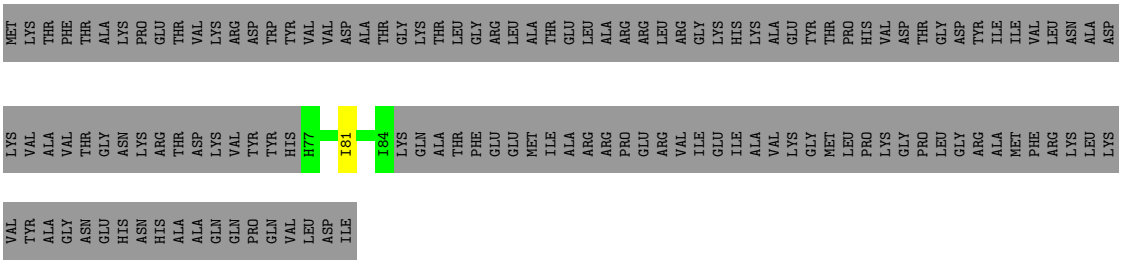
R67 A68 R69 S70 G71 W78 ARG SER GLY GLY VAL THR PHE ALA ALA ARG PRO GLN ASP HIS SER GLN LYS VAL ASN LYS LYS MET TYR ARG GLY ALA LEU LYS SER ILE LEU SER GLU LEU VAL ARG GLN ASP ARG LEU ILE VAL ARG GLU LYS PHE SER VAL GLU ALA PRO LYS THR



• Molecule 7: Large ribosomal subunit protein uL13

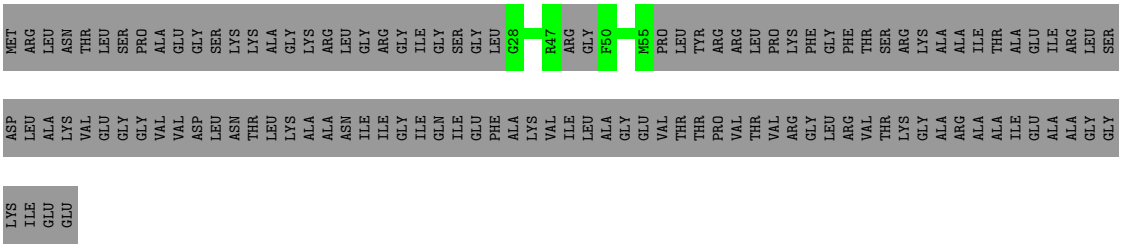
Chain i:





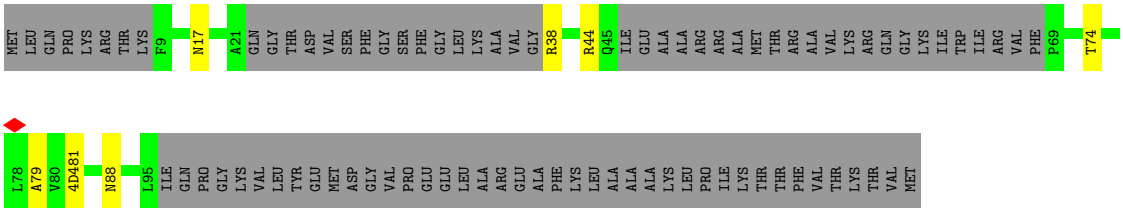
• Molecule 8: Large ribosomal subunit protein uL15

Chain k:



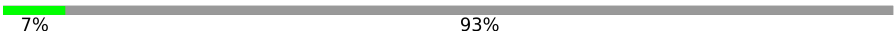
• Molecule 9: Large ribosomal subunit protein uL16

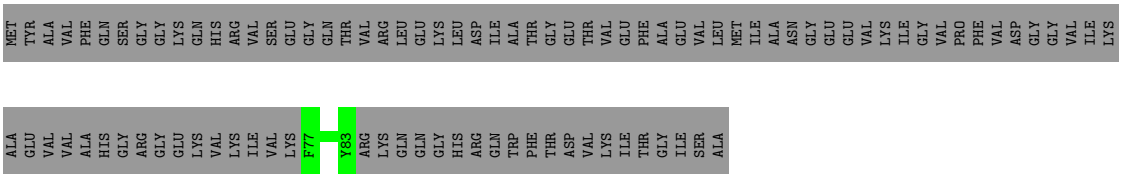
Chain l:



• Molecule 10: Large ribosomal subunit protein bL21

Chain q:





• Molecule 11: 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 12: Large ribosomal subunit protein bL27

Chain v: 11% 16% 81%

MET A2 H3 K4 K5 A6 G7 G8 S9 T10 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 GLY LYS VAL LYS PHE GLU VAL LYS GLY PRO LYS ASN ARG LYS PHE ILE SER ILE GLU ALA GLU

- Molecule 13: Large ribosomal subunit protein bL32

Chain z: 9% 5% 86%

MET A2 V3 Q4 P8 T9 ARG SER LYS ARG GLY MET ARG ARG SER HIS ASP ALA LEU THR ALA VAL THR SER LEU SER VAL ASP LYS THR SER GLY GLU LYS HIS LEU ARG HIS HIS ILE THR ALA ASP GLY TYR TYR ARG GLY ARG LYS VAL ILE ALA LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53129	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 ($e^-/Å^2$)	42.1	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.517	Depositor
Minimum map value	-0.133	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	421.2736, 421.2736, 421.2736	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8228, 0.8228, 0.8228	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, G7M, 1MG, 2MG, 5MC, SR0, MG, PSU, K, 4D4, 2MA, TKW, MS6, PUT, OMG, 5MU, H2U, 6MZ, MEQ

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	0.55	0/427	0.87	0/661
2	a	0.55	1/13812 (0.0%)	1.05	49/21450 (0.2%)
3	b	0.58	0/87	1.08	0/132
4	c	0.76	0/197	0.96	0/265
5	d	0.72	0/329	1.12	1/438 (0.2%)
6	e	0.71	0/187	0.95	0/248
7	i	0.71	0/56	1.15	0/74
8	k	0.74	0/182	1.19	0/232
9	l	0.65	0/370	1.02	0/487
10	q	0.67	0/77	1.15	0/99
11	r	0.74	0/52	0.87	0/66
12	v	0.66	0/116	0.91	0/151
13	z	0.71	0/61	1.00	0/82
All	All	0.56	1/15953 (0.0%)	1.05	50/24385 (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	2
9	l	0	1
12	v	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	a	2069	G7M	O3'-P	5.16	1.61	1.56

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	a	1132	U	O3'-P-O5'	-21.52	71.72	104.00
2	a	980	A	O3'-P-O5'	-12.13	85.80	104.00
2	a	1971	U	O3'-P-O5'	-10.42	88.37	104.00
2	a	980	A	C4'-C3'-O3'	8.77	126.16	113.00
2	a	1957	C	O3'-P-O5'	-8.25	91.62	104.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	e	61	ARG	Sidechain
6	e	67	ARG	Sidechain
9	l	44	ARG	Sidechain
12	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	5	0
2	a	12772	0	6467	40	0
3	b	80	0	43	0	0
4	c	191	0	177	1	0
5	d	333	0	336	5	0
6	e	182	0	193	4	0
7	i	55	0	51	1	0
8	k	182	0	179	0	0
9	l	386	0	399	3	0
10	q	75	0	76	0	0
11	r	53	0	55	0	0
12	v	116	0	110	1	0
13	z	61	0	62	4	0
14	a	20	0	0	1	0
15	a	6	0	12	0	0
16	a	101	0	0	0	0
16	d	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	a	42	0	0	0	0
17	e	1	0	0	0	0
All	All	15041	0	8360	53	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 53 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:674:G:H5"	6:e:71:GLY:H	1.39	0.86
2:a:568:U:H1'	2:a:2030:6MZ:H9C1	1.66	0.78
9:l:17:ASN:O	9:l:38:ARG:HD3	1.93	0.66
2:a:674:G:H5"	6:e:71:GLY:N	2.11	0.64
2:a:1778:U:H2'	2:a:1784:A:N6	2.13	0.64

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%)	21 (100%)	0	0	100	100
7	i	6/142 (4%)	6 (100%)	0	0	100	100
8	k	22/144 (15%)	19 (86%)	3 (14%)	0	100	100
9	l	40/136 (29%)	39 (98%)	1 (2%)	0	100	100
10	q	5/103 (5%)	5 (100%)	0	0	100	100
11	r	5/110 (4%)	5 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	v	14/85 (16%)	12 (86%)	2 (14%)	0	100	100
13	z	6/57 (10%)	6 (100%)	0	0	100	100
All	All	183/1460 (12%)	172 (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	28
7	i	5/116 (4%)	5 (100%)	0	100	100
8	k	16/103 (16%)	16 (100%)	0	100	100
9	l	36/107 (34%)	36 (100%)	0	100	100
10	q	7/84 (8%)	7 (100%)	0	100	100
11	r	4/93 (4%)	4 (100%)	0	100	100
12	v	11/63 (18%)	11 (100%)	0	100	100
13	z	7/48 (15%)	7 (100%)	0	100	100
All	All	157/1160 (14%)	156 (99%)	1 (1%)	76	89

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

Mol	Chain	Res	Type
6	e	57	LYS

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

Mol	Chain	Res	Type
8	k	54	GLN
13	z	6	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Z	16/77 (20%)	6 (37%)	0
2	a	559/2904 (19%)	85 (15%)	0
3	b	3/120 (2%)	3 (100%)	0
All	All	578/3101 (18%)	94 (16%)	0

5 of 94 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Z	4	G
1	Z	6	G
1	Z	7	G
1	Z	71	C
1	Z	74	C

There are no RNA pucker outliers to report.

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

22 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	5MU	a	1939	2,17	19,22,23	0.51	0	28,32,35	0.62	0
2	PSU	a	2504	2,17	18,21,22	0.26	0	22,30,33	0.38	0
2	OMG	a	2251	2,1,17	23,26,27	0.38	0	33,38,41	0.28	0
2	5MC	a	1962	2,17	18,22,23	0.31	0	26,32,35	0.32	0
9	MS6	l	82	9	5,7,8	0.24	0	2,7,9	0.15	0
2	6MZ	a	2030	2	22,25,26	0.26	0	30,36,39	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	2MA	a	2503	16,2,17	22,25,26	0.99	2 (9%)	33,37,40	1.30	3 (9%)
2	OMC	a	2498	16,2	19,22,23	0.22	0	26,31,34	0.36	0
2	1MG	a	745	2	22,26,27	0.64	0	33,39,42	0.49	0
2	H2U	a	2449	2	18,21,22	0.46	0	21,30,33	0.36	0
2	PSU	a	2457	2	18,21,22	0.36	0	22,30,33	0.37	0
2	PSU	a	2604	2	18,21,22	0.36	0	22,30,33	0.49	0
2	PSU	a	2605	2	18,21,22	0.27	0	22,30,33	0.49	0
2	PSU	a	2580	2	18,21,22	0.42	0	22,30,33	0.62	1 (4%)
2	PSU	a	955	2	18,21,22	0.37	0	22,30,33	0.33	0
5	MEQ	d	150	5	8,9,10	0.75	0	5,10,12	1.30	1 (20%)
2	TKW	a	2501	2,17	18,22,23	0.37	0	28,32,35	0.89	1 (3%)
2	G7M	a	2069	2,17	23,26,27	0.40	0	35,39,42	0.52	0
2	5MU	a	747	2	19,22,23	0.33	0	28,32,35	0.44	0
2	PSU	a	746	16,2	18,21,22	0.38	0	22,30,33	0.40	0
2	2MG	a	2445	2	23,26,27	0.49	0	32,38,41	0.31	0
9	4D4	l	81	9	9,11,12	0.70	0	8,13,15	0.97	1 (12%)

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	5MU	a	1939	2,17	-	0/7/25/26	0/2/2/2
2	PSU	a	2504	2,17	-	0/7/25/26	0/2/2/2
2	OMG	a	2251	2,1,17	-	1/9/27/28	0/3/3/3
2	5MC	a	1962	2,17	-	0/7/25/26	0/2/2/2
9	MS6	l	82	9	-	1/4/6/8	-
2	6MZ	a	2030	2	-	2/9/27/28	0/3/3/3
2	2MA	a	2503	16,2,17	-	3/7/25/26	0/3/3/3
2	OMC	a	2498	16,2	-	0/9/27/28	0/2/2/2
2	1MG	a	745	2	-	0/7/25/26	0/3/3/3
2	H2U	a	2449	2	-	0/7/38/39	0/2/2/2
2	PSU	a	2457	2	-	0/7/25/26	0/2/2/2
2	PSU	a	2604	2	-	0/7/25/26	0/2/2/2
2	PSU	a	2605	2	-	0/7/25/26	0/2/2/2
2	PSU	a	2580	2	-	0/7/25/26	0/2/2/2
2	PSU	a	955	2	-	0/7/25/26	0/2/2/2
5	MEQ	d	150	5	-	3/8/9/11	-
2	TKW	a	2501	2,17	-	4/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G7M	a	2069	2,17	-	2/7/25/26	0/3/3/3
2	5MU	a	747	2	-	0/7/25/26	0/2/2/2
2	PSU	a	746	16,2	-	1/7/25/26	0/2/2/2
2	2MG	a	2445	2	-	0/9/27/28	0/3/3/3
9	4D4	l	81	9	-	0/11/12/14	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	a	2503	2MA	C6-N6	-3.41	1.25	1.34
2	a	2503	2MA	C6-N1	2.03	1.37	1.35

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	a	2503	2MA	N6-C6-N1	5.19	124.37	117.03
2	a	2501	TKW	OAC-C5-C4	3.98	120.43	114.43
2	a	2503	2MA	C2-N1-C6	3.21	123.08	118.08
2	a	2503	2MA	C5-C6-N1	-3.12	113.63	119.01
9	l	81	4D4	O-C-CA	-2.41	118.45	124.78

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	d	150	MEQ	C-CA-CB-CG
2	a	2251	OMG	C1'-C2'-O2'-CM2
2	a	2030	6MZ	O4'-C4'-C5'-O5'
5	d	150	MEQ	NE2-CD-CG-CB
5	d	150	MEQ	OE1-CD-CG-CB

There are no ring outliers.

6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	a	1939	5MU	1	0
2	a	2251	OMG	1	0
2	a	2030	6MZ	1	0
2	a	2503	2MA	1	0
2	a	2604	PSU	1	0
5	d	150	MEQ	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 148 ligands modelled in this entry, 145 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
15	PUT	a	3003	-	5,5,5	0.28	0	4,4,4	0.30	0
14	SR0	a	3002	-	9,9,9	0.54	0	8,8,8	0.54	0
14	SR0	a	3001	-	9,9,9	0.51	0	8,8,8	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PUT	a	3003	-	-	0/3/3/3	-
14	SR0	a	3002	-	-	3/7/7/7	-
14	SR0	a	3001	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	a	3002	SR0	N6-C7-C8-C9
14	a	3002	SR0	C8-C7-N6-C5
14	a	3002	SR0	C2-C3-C4-C5
14	a	3001	SR0	N1-C2-C3-C4
14	a	3001	SR0	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	a	3001	SR0	1	0

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.

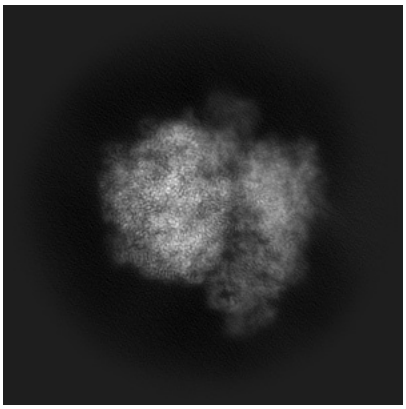
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-55436. 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



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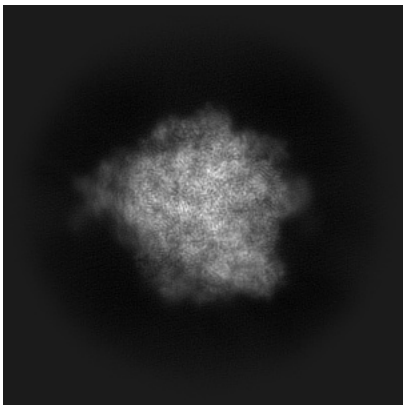

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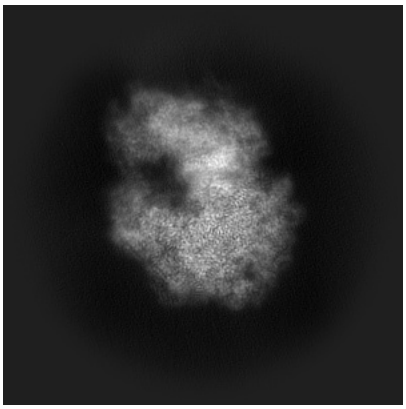

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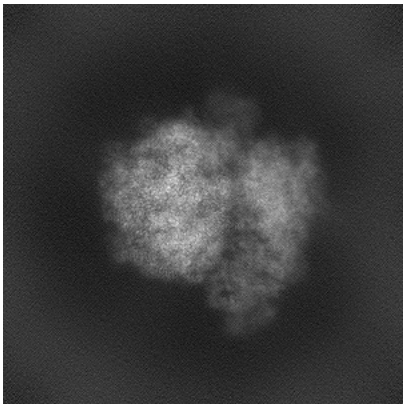
6.1.2 Raw map



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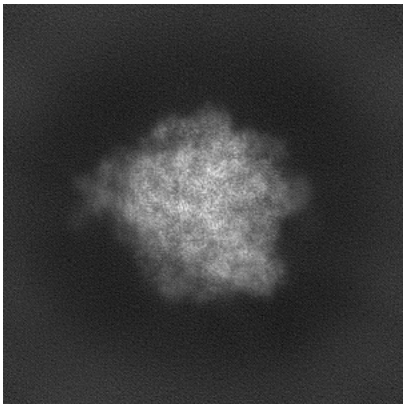

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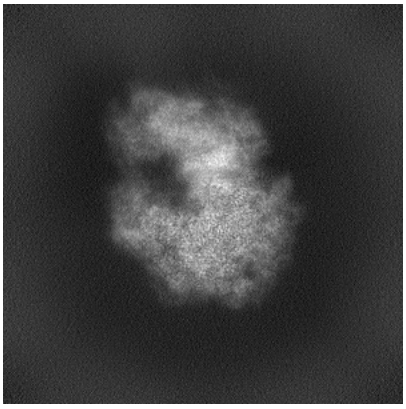
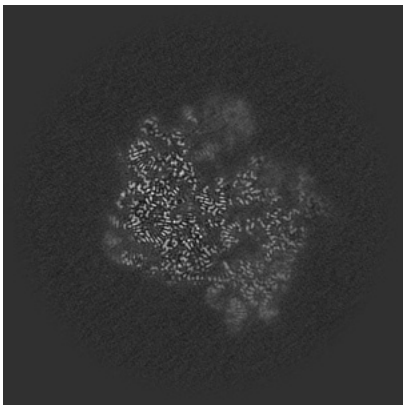


Z

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

6.2 Central slices (i)

6.2.1 Primary map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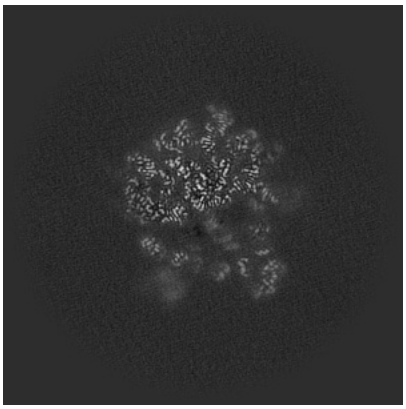
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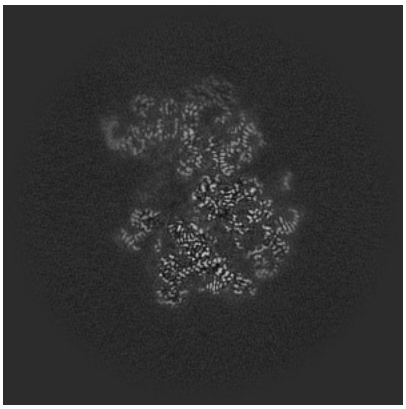
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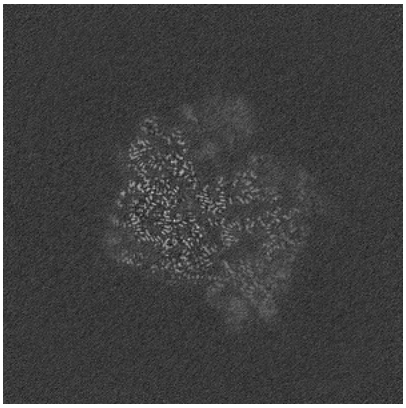
6.2.2 Raw map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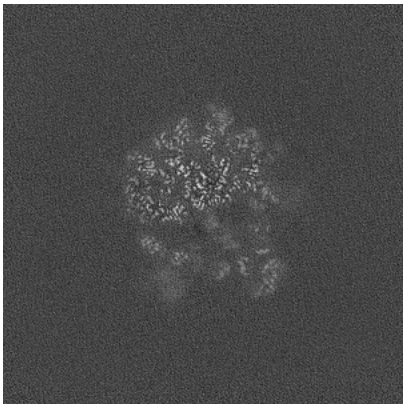
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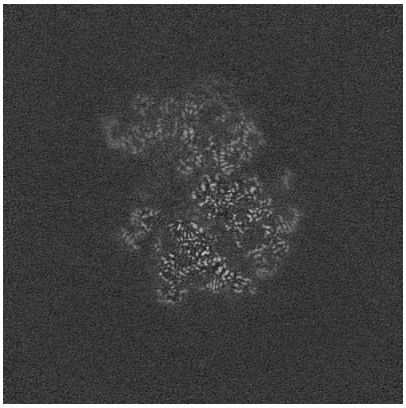
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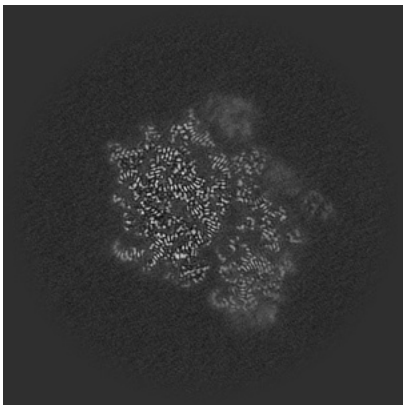
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



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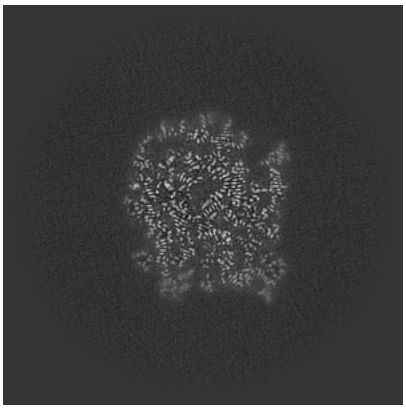

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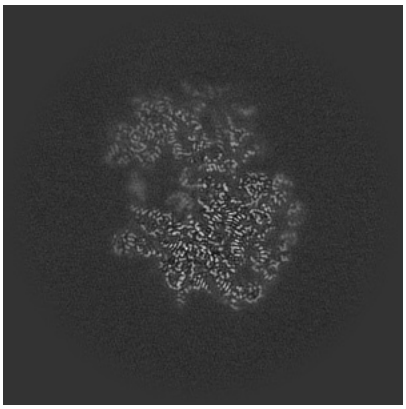
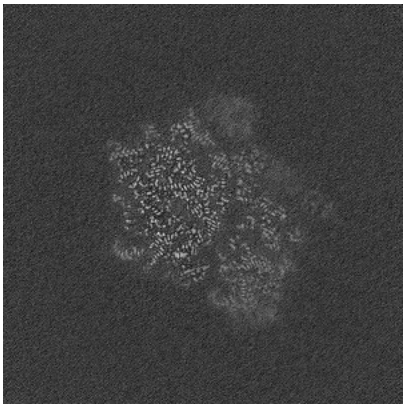


Z Index: 269

6.3.2 Raw map



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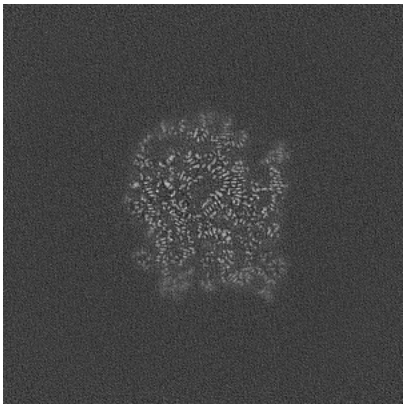

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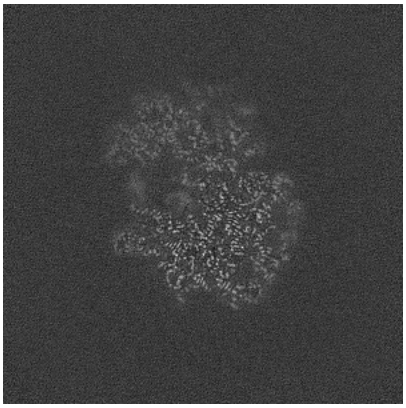
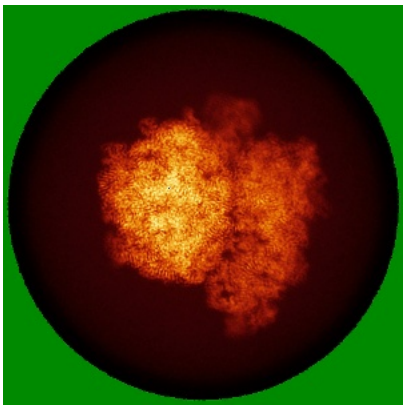


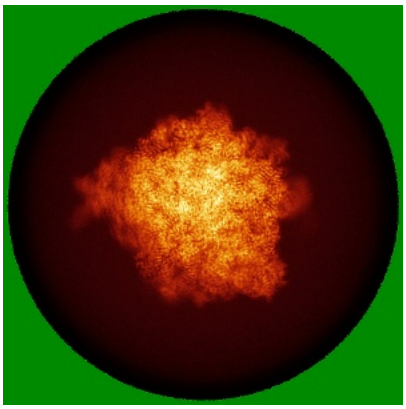
Z Index: 270

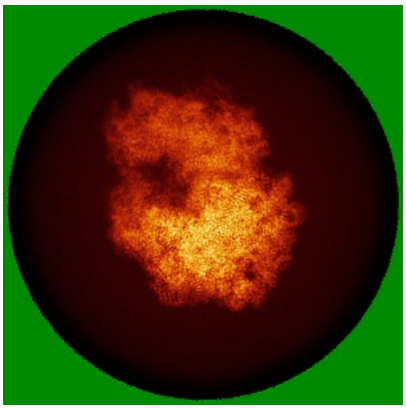
The images above show the largest variance slices of the map in three orthogonal directions.

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

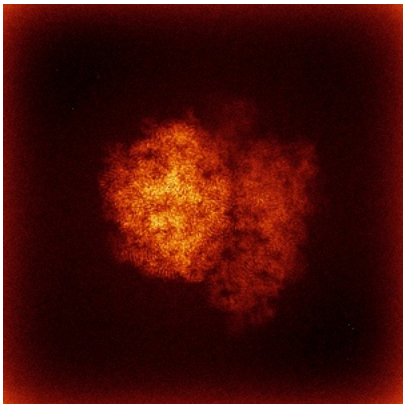
6.4.1 Primary map

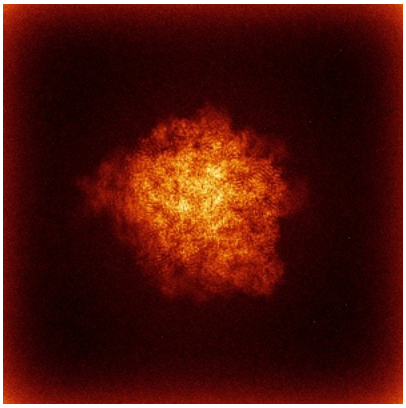

X

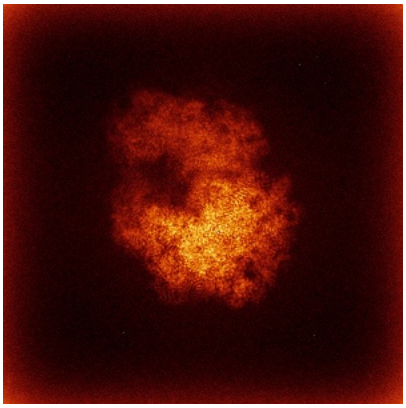

Y


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 0.1. 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.

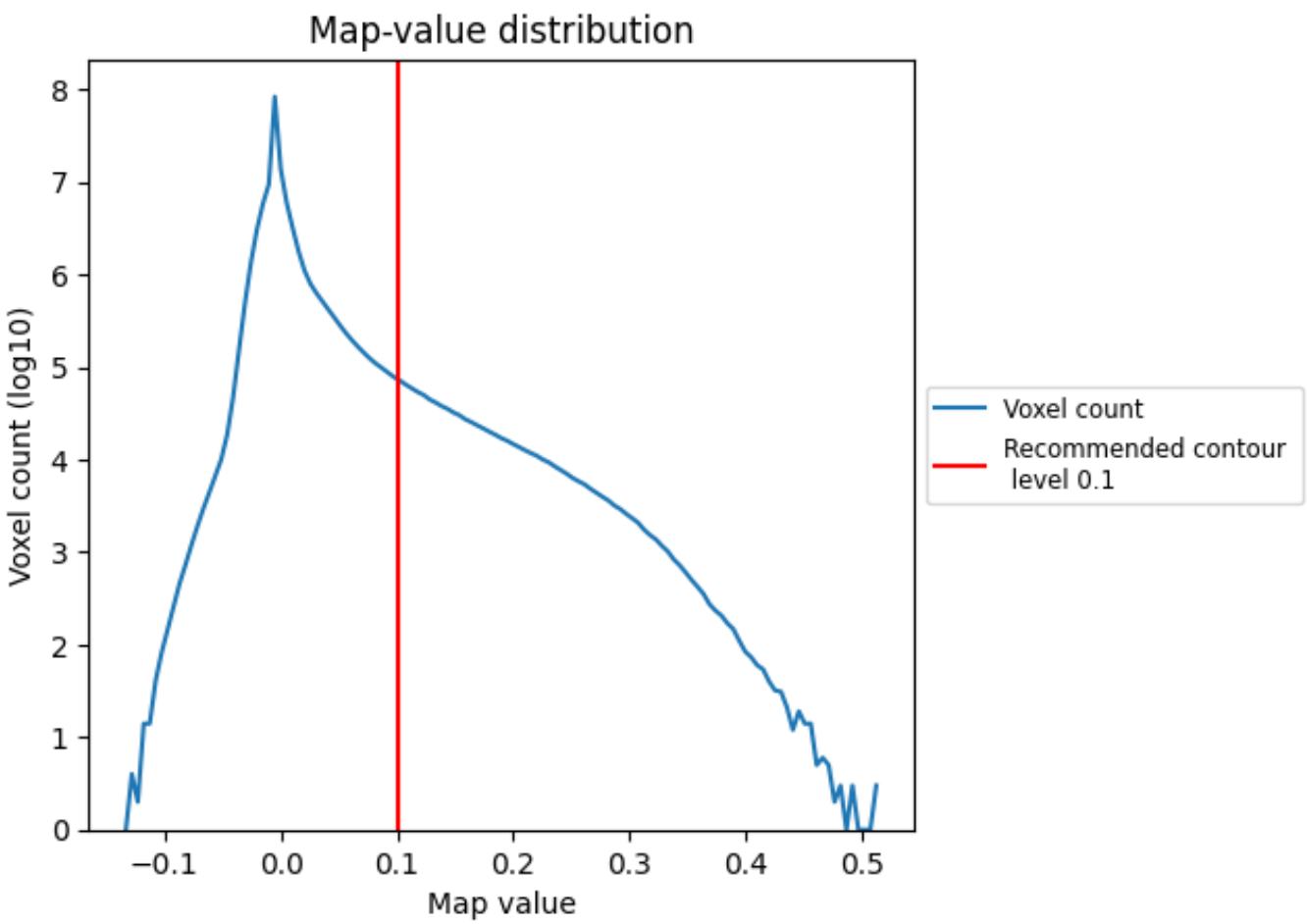
6.6 Mask visualisation (i)

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

7 Map analysis (i)

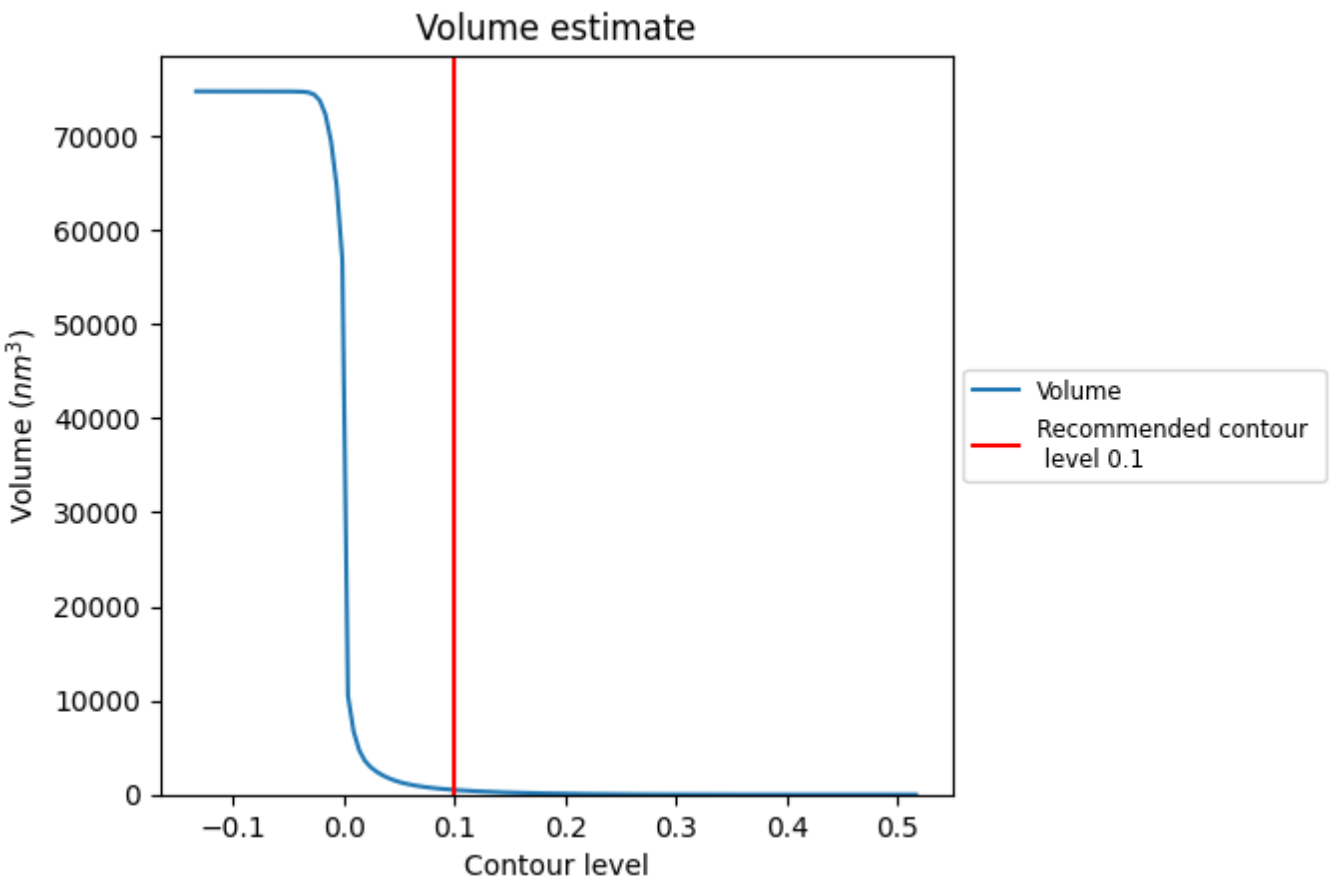
This section contains the results of statistical analysis of the map.

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.

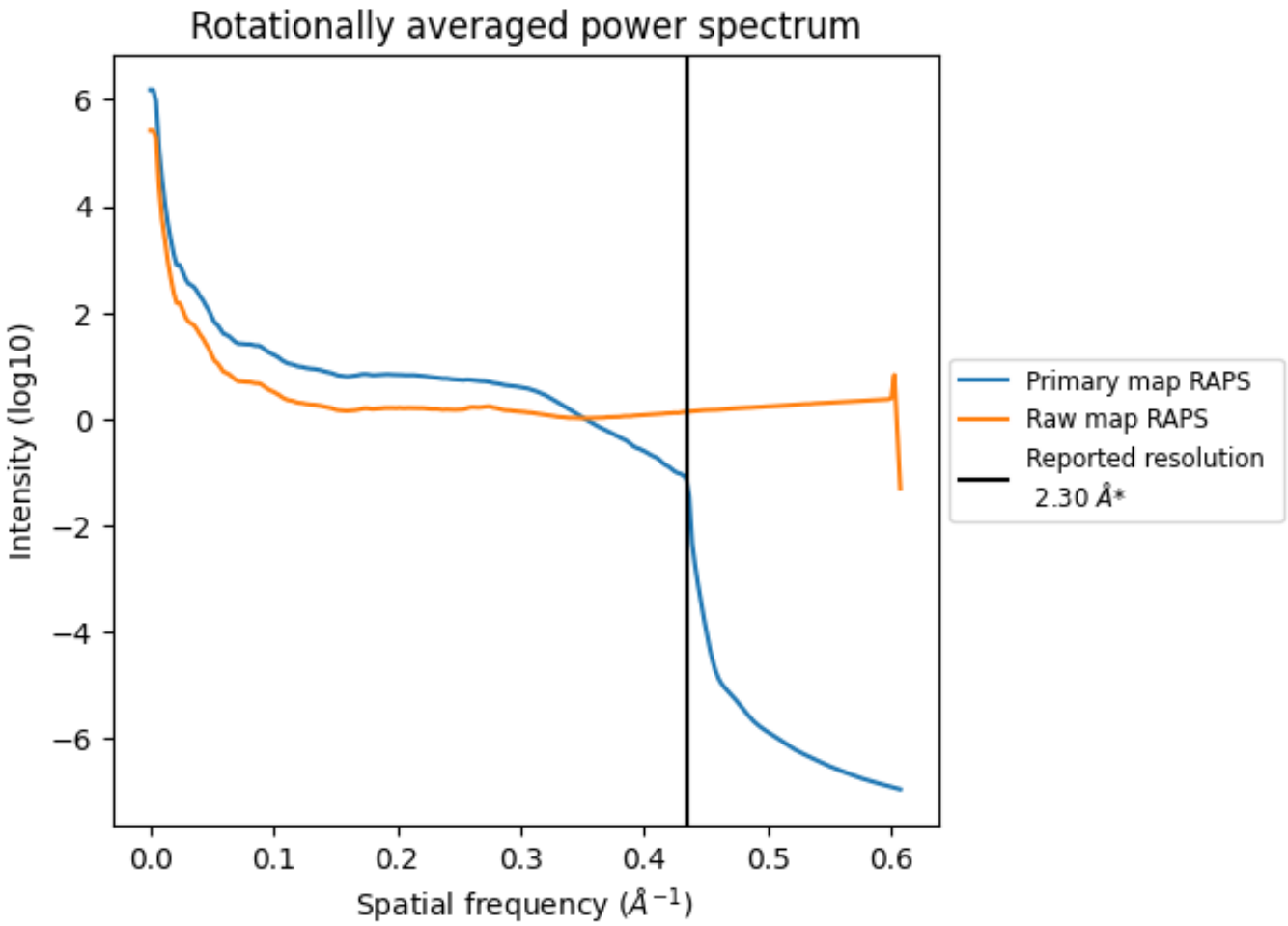
7.2 Volume estimate (i)



The volume at the recommended contour level is 496 nm^3; this corresponds to an approximate mass of 448 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)

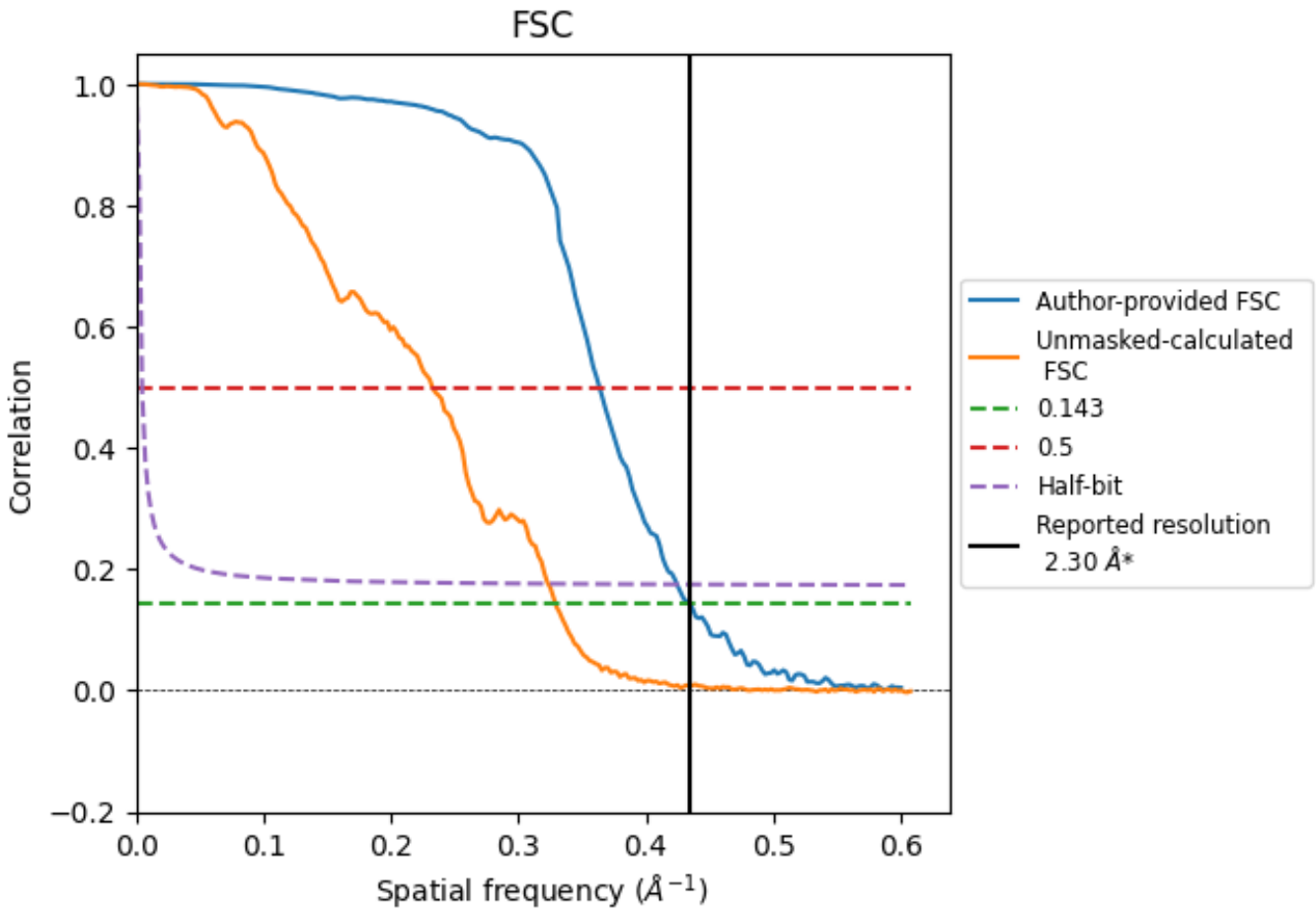


*Reported resolution corresponds to spatial frequency of 0.435 Å^{-1}

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 0.435 Å^{-1}

8.2 Resolution estimates (i)

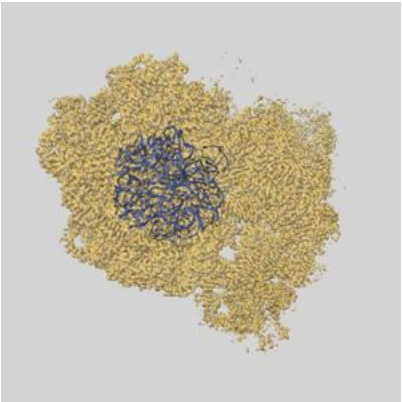
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.30	2.75	2.36
Unmasked-calculated*	3.04	4.30	3.09

*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 3.04 differs from the reported value 2.3 by more than 10 %

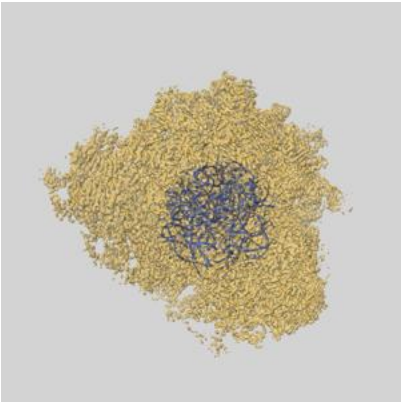
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-55436 and PDB model 9T1I. Per-residue inclusion information can be found in section 3 on page 8.

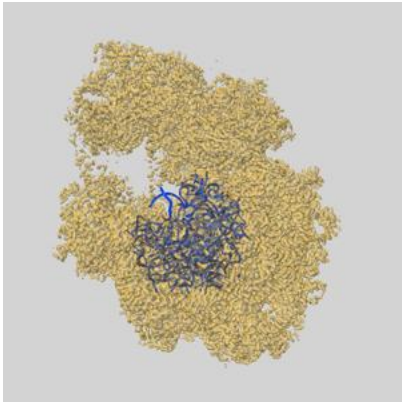
9.1 Map-model overlay (i)



X



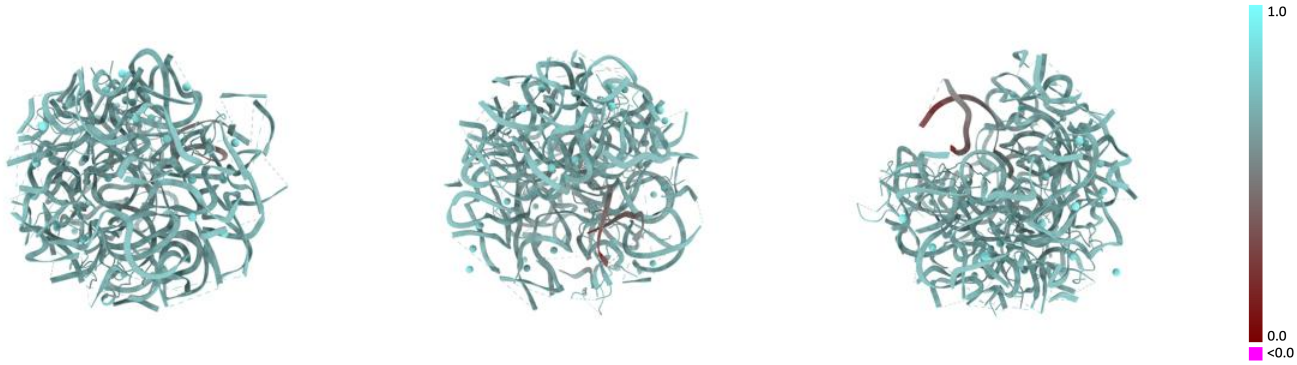
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

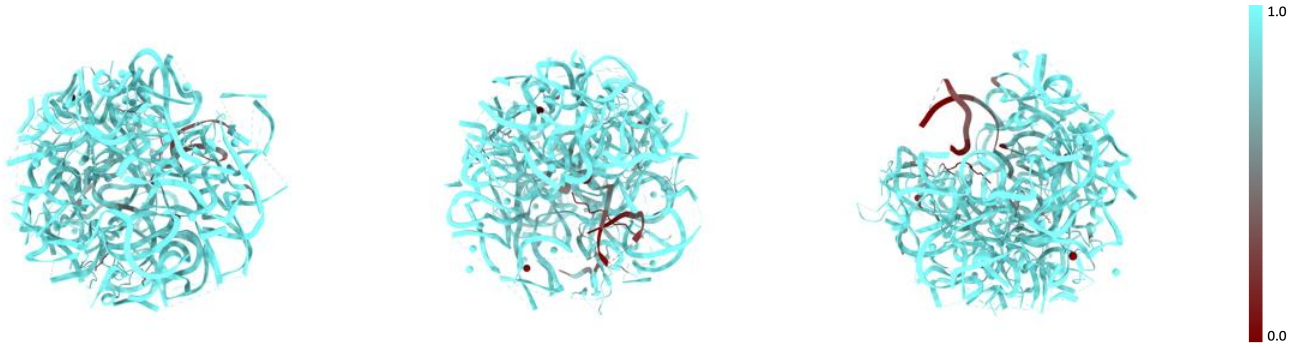
9.2 Q-score mapped to coordinate model (i)



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.

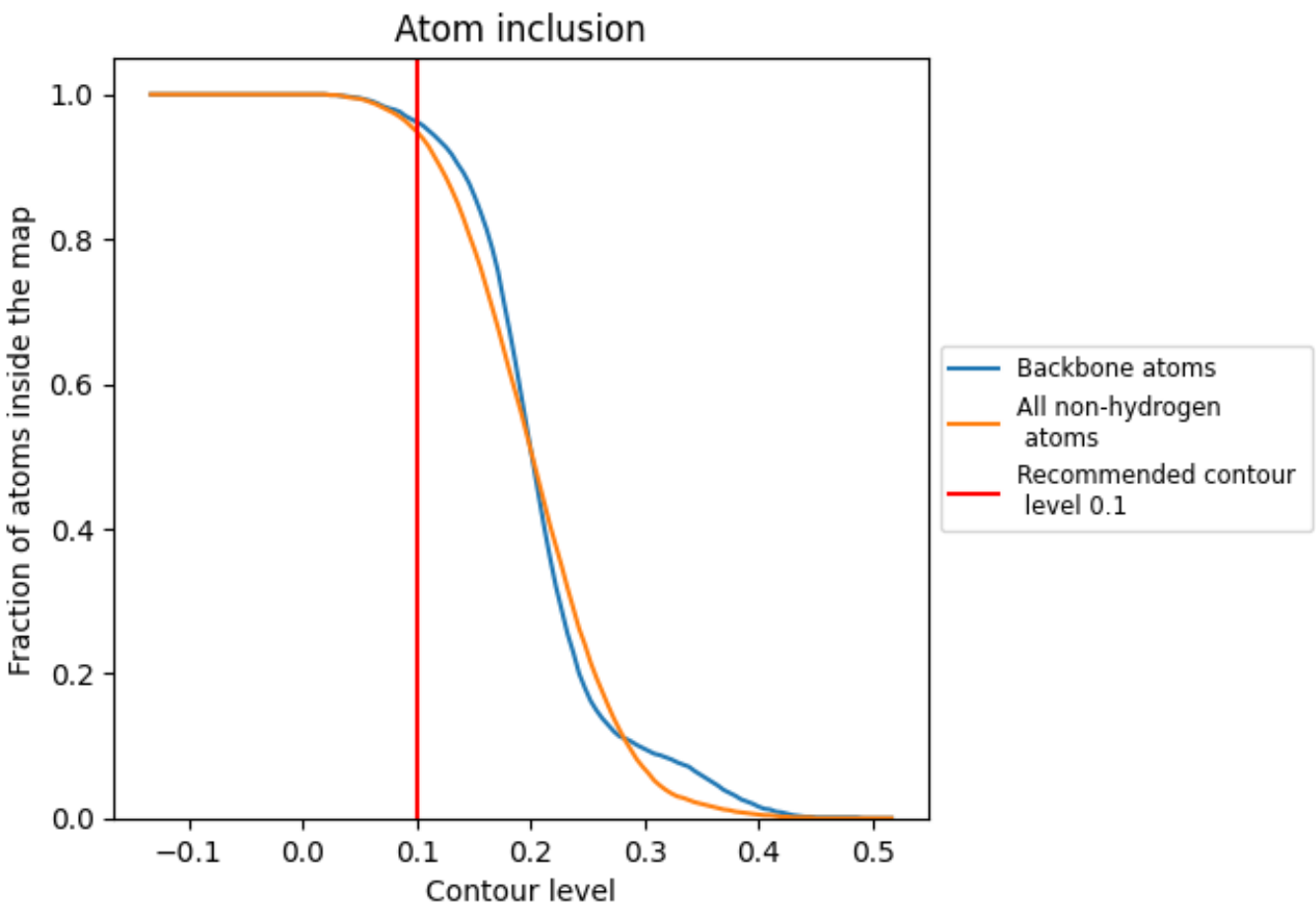
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9490	0.6640
Z	0.3180	0.4280
a	0.9780	0.6700
b	0.6500	0.5840
c	0.9570	0.6840
d	0.9360	0.6860
e	0.9200	0.6750
i	0.9270	0.6830
k	0.9430	0.6840
l	0.8730	0.6660
q	1.0000	0.6860
r	0.7960	0.6610
v	0.3840	0.5770
z	0.9670	0.6890