wwPDB EM Validation Summary Report (i)

Mar 4, 2024 – 04:41 PM EST

PDB ID	:	6DZK
EMDB ID	:	EMD-8934
Title	:	Cryo-EM Structure of Mycobacterium smegmatis C(minus) 30S ribosomal subunit with MPY
Authors	:	Sharma, M.R.; Li, Y.; Korripella, R.; Yang, Y.; Kaushal, P.S.; Lin, Q.; Wade, J.T.; Gray, A.G.; Derbyshire, K.M.; Agrawal, R.K.; Ojha, A.
Deposited on	:	2018-07-05
Resolution	:	3.60 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 (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 (i)) were used in the production of this report:

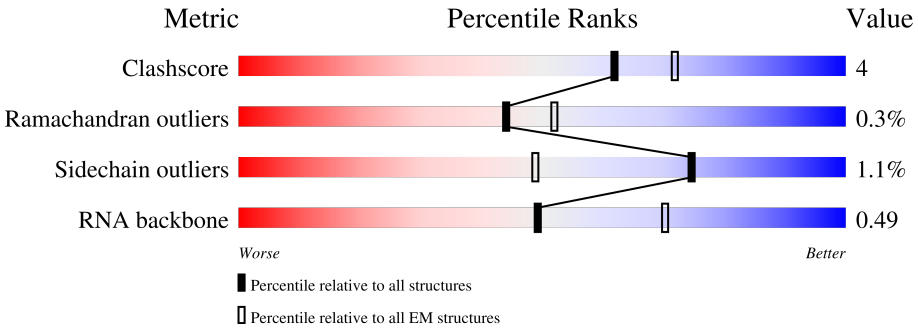
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.60 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	1511	62% 31% 7%
2	B	32	88% 12%
3	C	275	59% 15% 24%
4	D	201	85% 13%
5	E	213	79% 5% 15%
6	F	96	82% 17%
7	G	156	82% 17%

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Mol	Chain	Length	Quality of chain
8	H	131	
9	I	150	
10	J	101	
11	K	138	
12	L	124	
13	M	124	
14	O	88	
15	P	156	
16	Q	98	
17	S	93	
18	T	86	
19	V	277	
20	r	85	
21	Y	230	
22	N	100	
23	g	82	

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 90307 atoms, of which 37538 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 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	1511	48753	14448	16314	5930	10550	1511	0	0

- Molecule 2 is a protein called Conserved domain protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	32	622	172	342	71	36	1	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	208	3367	1036	1707	322	298	4	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	200	3309	1028	1668	316	295	2	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	180	2656	812	1360	245	235	4	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	96	1568	486	797	138	145	2	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	155	Total	C	H	N	O	S	0	0
			2514	768	1282	241	221	2		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	131	Total	C	H	N	O	S	0	0
			2056	633	1046	189	187	1		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	126	Total	C	H	N	O	0	0
			2044	630	1050	194	170		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	99	Total	C	H	N	O	S	0	0
			1607	495	819	146	144	3		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	115	Total	C	H	N	O	S	0	0
			1718	528	863	170	156	1		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	122	Total	C	H	N	O	S	0	0
			2003	594	1045	197	165	2		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	116	Total	C	H	N	O	S	0	0
			1921	572	986	191	169	3		

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	88	Total	C	H	N	O	0	0
			1480	449	760	147	124		

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	113	Total	C	H	N	O	0	0
			1826	570	935	162	159		

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	Q	94	Total	C	H	N	O	S	0	0
			1543	469	795	142	135	2		

- Molecule 17 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	S	82	Total	C	H	N	O	S	0	0
			1339	425	677	124	112	1		

- Molecule 18 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	85	Total	C	H	N	O	0	0
			1372	402	712	139	119		

- Molecule 19 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	V	228	Total	C	H	N	O	S	0	0
			3632	1132	1839	322	330	9		

- Molecule 20 is a protein called 30S ribosomal protein S18 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	r	84	Total	C	H	N	O	S	0	0
			1375	408	717	131	115	4		

- Molecule 21 is a protein called Ribosome hibernation promoting factor.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	Y	103	Total	C	H	N	O	S	0	0
			1720	529	860	175	154	2		

- Molecule 22 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	N	100	Total	C	H	N	O	S	0	0
			1685	497	866	183	138	1		

- Molecule 23 is a protein called 50S ribosomal protein L31.

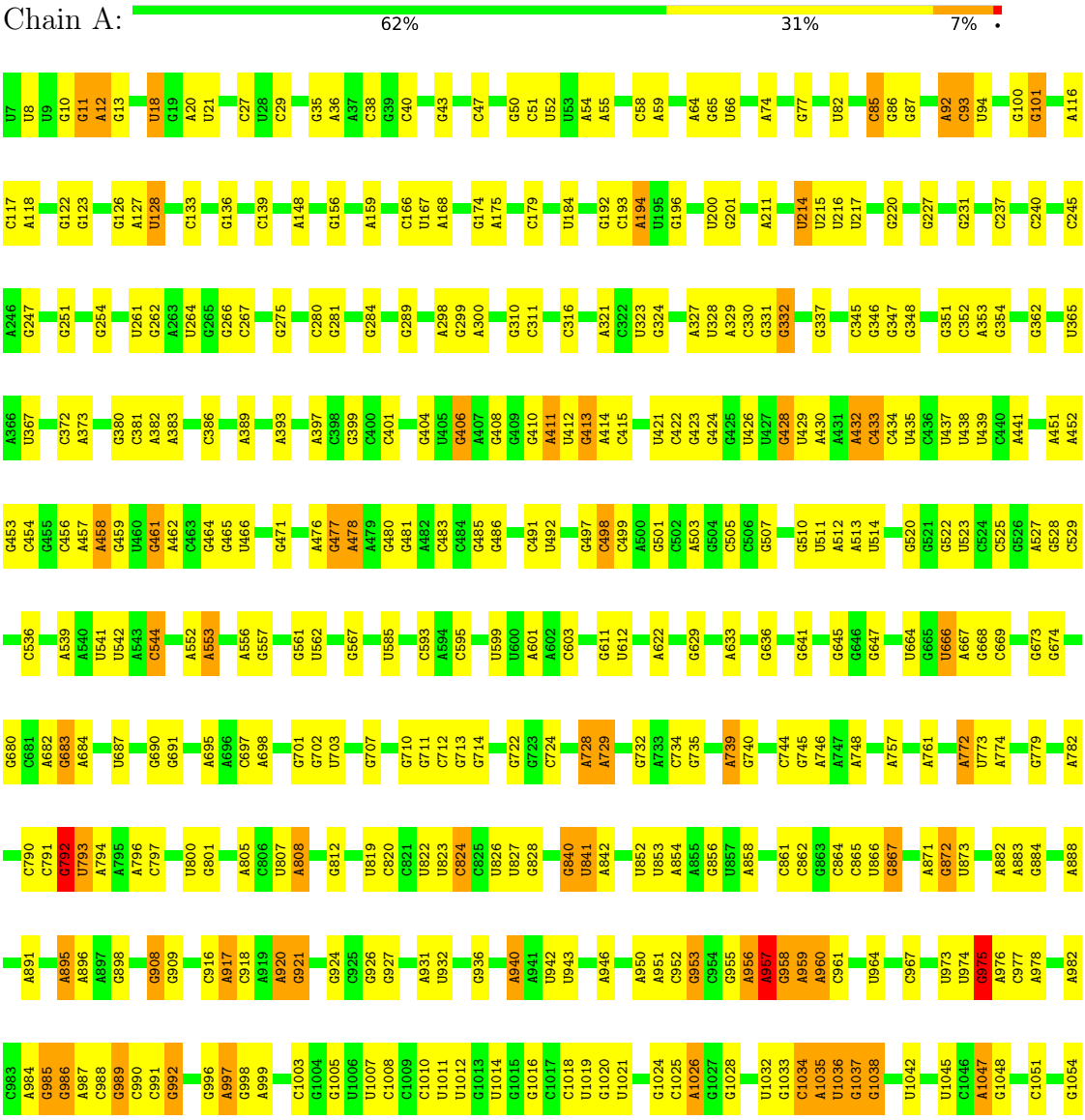
Mol	Chain	Residues	Atoms					AltConf	Trace
23	g	11	Total	C	H	N	O	0	0
			197	61	98	22	16		

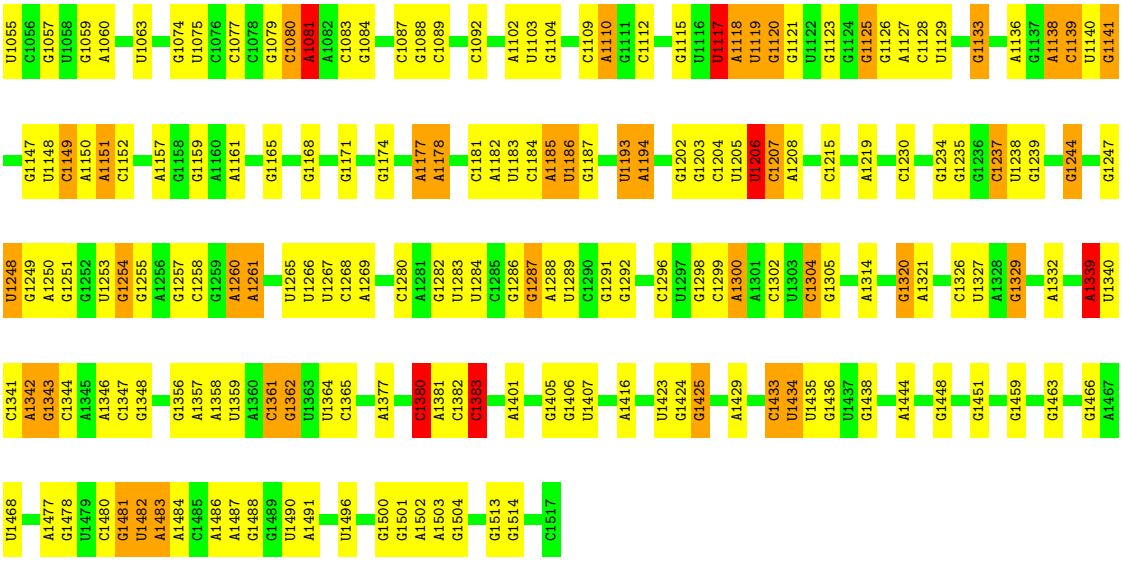
3 Residue-property plots (i)

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: 16S rRNA

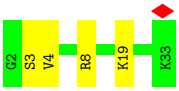
Chain A:





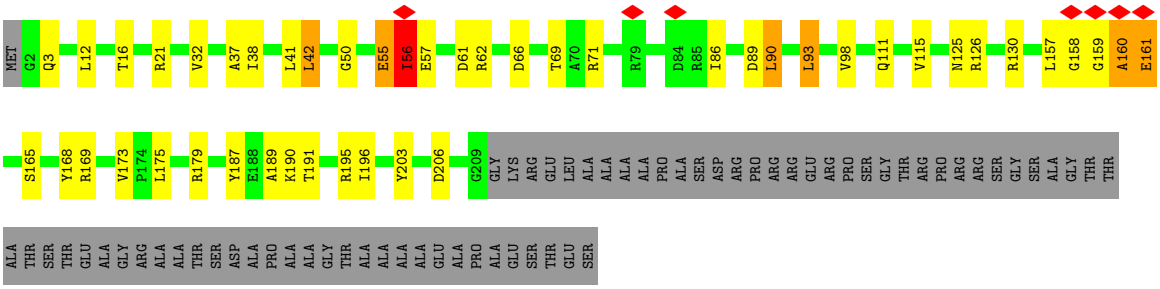
• Molecule 2: Conserved domain protein

Chain B:



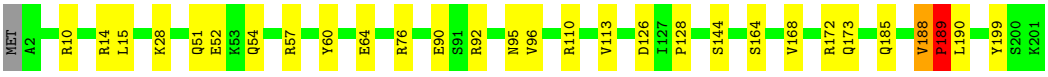
• Molecule 3: 30S ribosomal protein S3

Chain C:



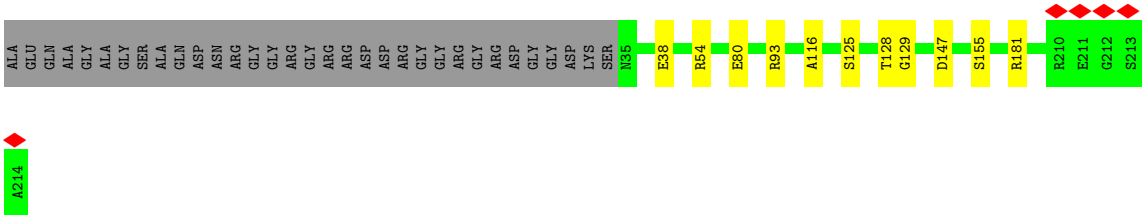
• Molecule 4: 30S ribosomal protein S4

Chain D:



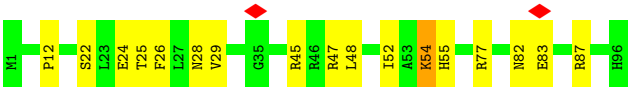
• Molecule 5: 30S ribosomal protein S5

Chain E:



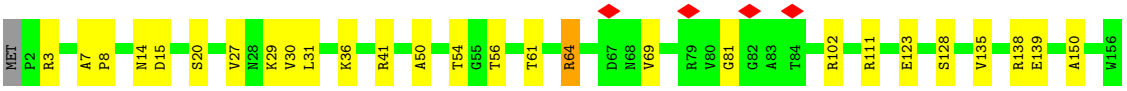
• Molecule 6: 30S ribosomal protein S6

Chain F:



• Molecule 7: 30S ribosomal protein S7

Chain G:

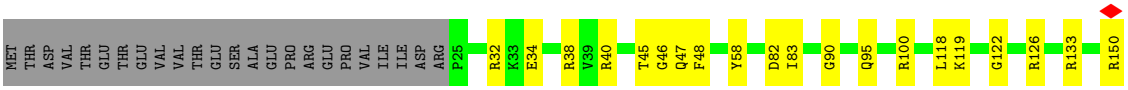


• Molecule 8: 30S ribosomal protein S8

Chain H:

• Molecule 9: 30S ribosomal protein S9

Chain I:

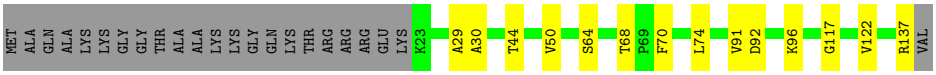


• Molecule 10: 30S ribosomal protein S10

Chain J:

• Molecule 11: 30S ribosomal protein S11

Chain K:

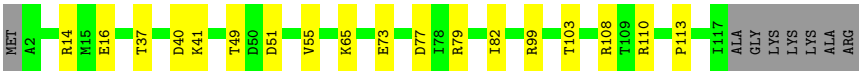


• Molecule 12: 30S ribosomal protein S12

Chain L:

• Molecule 13: 30S ribosomal protein S13

Chain M:

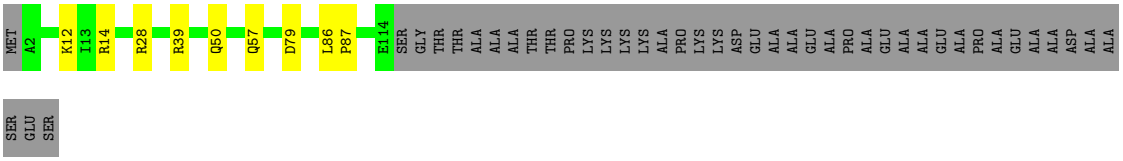


• Molecule 14: 30S ribosomal protein S15

Chain O:

• Molecule 15: 30S ribosomal protein S16

Chain P:

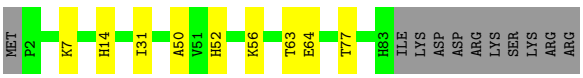


• Molecule 16: 30S ribosomal protein S17

Chain Q:

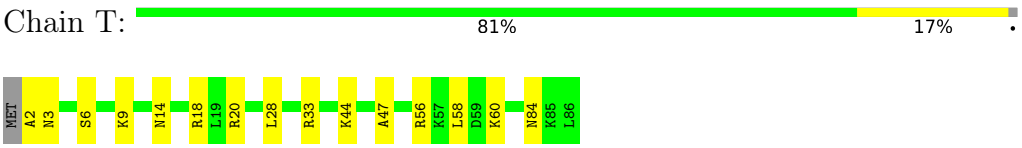
• Molecule 17: 30S ribosomal protein S19

Chain S:



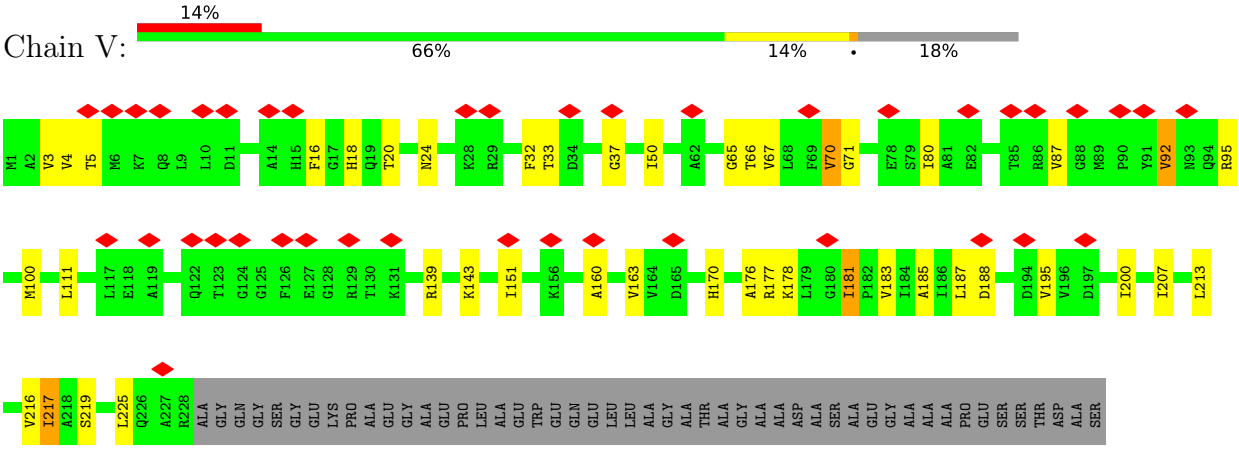
• Molecule 18: 30S ribosomal protein S20

Chain T:



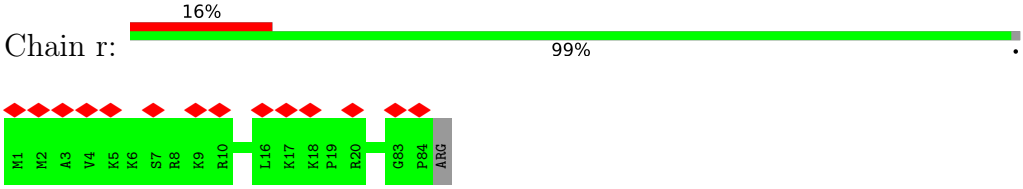
• Molecule 19: 30S ribosomal protein S2

Chain V:



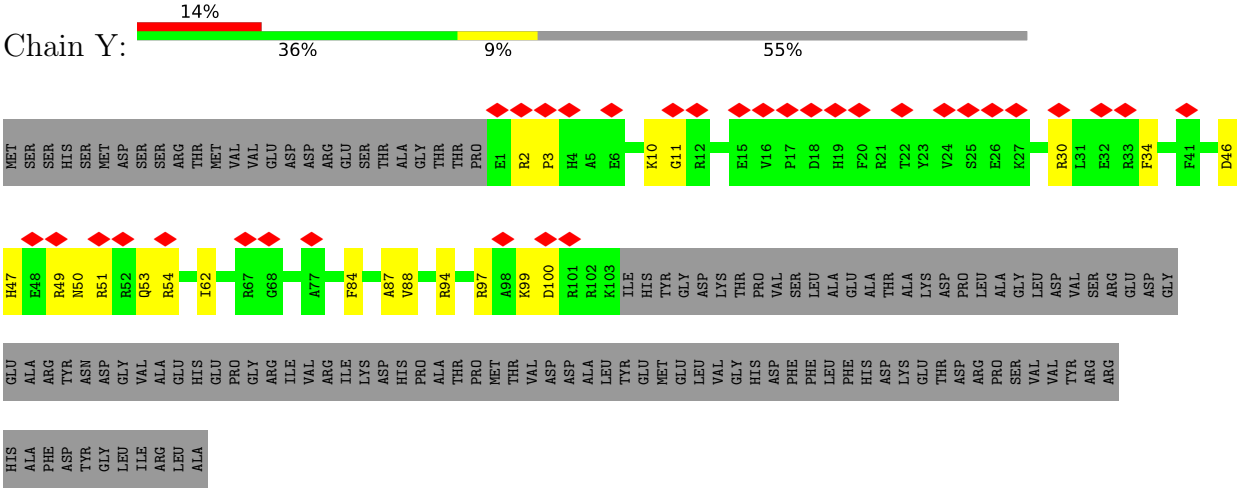
• Molecule 20: 30S ribosomal protein S18 1

Chain r:



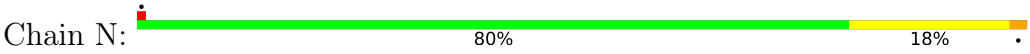
• Molecule 21: Ribosome hibernation promoting factor

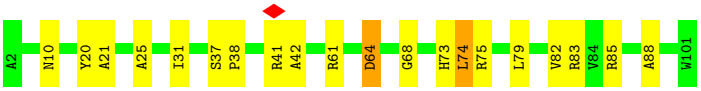
Chain Y:



• Molecule 22: 30S ribosomal protein S14

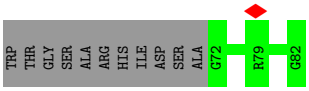
Chain N:





• Molecule 23: 50S ribosomal protein L31

Chain g:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	66840	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 ($e^-/Å^2$)	67	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.211	Depositor
Minimum map value	-0.099	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	485.78003, 485.78003, 485.78003	wwPDB
Map dimensions	454, 454, 454	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.82	0/36309	1.09	63/56657 (0.1%)
2	B	0.42	0/280	0.85	0/359
3	C	0.44	0/1684	0.88	11/2261 (0.5%)
4	D	0.46	0/1672	0.64	0/2251
5	E	0.49	0/1312	0.61	0/1772
6	F	0.38	0/782	0.59	0/1059
7	G	0.34	0/1252	0.62	0/1690
8	H	0.53	0/1025	0.67	1/1385 (0.1%)
9	I	0.35	0/1012	0.63	0/1362
10	J	0.41	0/802	0.60	0/1086
11	K	0.39	0/873	0.58	0/1180
12	L	0.48	0/969	0.79	3/1294 (0.2%)
13	M	0.31	0/942	0.66	0/1260
14	O	0.43	0/729	0.68	0/977
15	P	0.53	0/908	0.62	0/1226
16	Q	0.46	0/759	0.71	0/1016
17	S	0.36	0/680	0.63	0/915
18	T	0.44	0/663	0.66	0/882
19	V	0.36	0/1822	1.05	23/2457 (0.9%)
20	r	0.38	0/664	0.67	0/889
21	Y	0.34	0/874	0.69	0/1169
22	N	0.38	0/830	0.81	4/1106 (0.4%)
23	g	0.36	0/100	0.83	0/128
All	All	0.70	0/56943	0.98	105/84381 (0.1%)

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
3	C	0	7
4	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
15	P	0	2
16	Q	0	1
19	V	0	2
All	All	0	13

There are no bond length outliers.

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1339	A	O4'-C1'-N9	10.57	116.65	108.20
1	A	1037	G	O4'-C1'-N9	10.36	116.49	108.20
1	A	1081	A	O4'-C1'-N9	10.04	116.23	108.20
1	A	1038	G	O4'-C1'-N9	9.00	115.40	108.20
19	V	18	HIS	C-N-CA	8.49	142.93	121.70

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	126	ARG	Peptide
3	C	157	LEU	Peptide
3	C	158	GLY	Peptide
3	C	55	GLU	Peptide
3	C	56	ILE	Peptide

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	32439	16314	16321	218	0
2	B	280	342	342	3	0
3	C	1660	1707	1707	23	0
4	D	1641	1668	1668	21	0
5	E	1296	1360	1360	7	0
6	F	771	797	797	8	0
7	G	1232	1282	1282	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1010	1046	1046	11	0
9	I	994	1050	1050	11	0
10	J	788	819	819	9	0
11	K	855	863	863	9	0
12	L	958	1045	1045	16	0
13	M	935	986	986	11	0
14	O	720	760	760	7	0
15	P	891	935	935	4	0
16	Q	748	795	795	8	0
17	S	662	677	677	6	0
18	T	660	712	712	10	0
19	V	1793	1839	1839	16	0
20	r	658	717	717	0	0
21	Y	860	860	862	19	0
22	N	819	866	866	12	0
23	g	99	98	98	0	0
All	All	52769	37538	37547	354	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 4.

The worst 5 of 354 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:C:O3'	16:Q:44:LYS:NZ	2.13	0.82
1:A:985:G:N2	1:A:1018:C:O2	2.12	0.81
1:A:1110:A:O2'	9:I:40:ARG:NH2	2.14	0.81
1:A:1118:A:O2'	1:A:1119:U:O4'	2.00	0.80
1:A:987:A:OP2	1:A:1007:U:O2'	2.00	0.79

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	
2	B	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
3	C	206/275 (75%)	164 (80%)	37 (18%)	5 (2%)	6	37
4	D	198/201 (98%)	179 (90%)	18 (9%)	1 (0%)	29	68
5	E	178/213 (84%)	155 (87%)	23 (13%)	0	100	100
6	F	94/96 (98%)	84 (89%)	10 (11%)	0	100	100
7	G	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
8	H	129/131 (98%)	119 (92%)	10 (8%)	0	100	100
9	I	124/150 (83%)	113 (91%)	11 (9%)	0	100	100
10	J	97/101 (96%)	91 (94%)	6 (6%)	0	100	100
11	K	113/138 (82%)	104 (92%)	9 (8%)	0	100	100
12	L	120/124 (97%)	102 (85%)	18 (15%)	0	100	100
13	M	114/124 (92%)	102 (90%)	12 (10%)	0	100	100
14	O	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
15	P	111/156 (71%)	98 (88%)	12 (11%)	1 (1%)	17	57
16	Q	92/98 (94%)	86 (94%)	6 (6%)	0	100	100
17	S	80/93 (86%)	78 (98%)	2 (2%)	0	100	100
18	T	83/86 (96%)	82 (99%)	1 (1%)	0	100	100
19	V	226/277 (82%)	196 (87%)	30 (13%)	0	100	100
20	r	82/85 (96%)	71 (87%)	11 (13%)	0	100	100
21	Y	101/230 (44%)	88 (87%)	13 (13%)	0	100	100
22	N	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
23	g	9/82 (11%)	9 (100%)	0	0	100	100
All	All	2524/3036 (83%)	2270 (90%)	247 (10%)	7 (0%)	44	75

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	160	ALA
3	C	56	ILE
3	C	161	GLU
3	C	125	ASN
15	P	87	PRO

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	
2	B	30/30 (100%)	30 (100%)	0	100	100
3	C	170/212 (80%)	168 (99%)	2 (1%)	71	87
4	D	175/176 (99%)	174 (99%)	1 (1%)	86	94
5	E	127/146 (87%)	127 (100%)	0	100	100
6	F	85/85 (100%)	82 (96%)	3 (4%)	36	68
7	G	131/132 (99%)	129 (98%)	2 (2%)	65	84
8	H	107/107 (100%)	106 (99%)	1 (1%)	78	90
9	I	102/125 (82%)	99 (97%)	3 (3%)	42	72
10	J	89/90 (99%)	89 (100%)	0	100	100
11	K	89/105 (85%)	88 (99%)	1 (1%)	73	88
12	L	103/105 (98%)	102 (99%)	1 (1%)	76	88
13	M	99/104 (95%)	99 (100%)	0	100	100
14	O	76/76 (100%)	75 (99%)	1 (1%)	69	86
15	P	92/118 (78%)	92 (100%)	0	100	100
16	Q	80/83 (96%)	77 (96%)	3 (4%)	33	66
17	S	73/84 (87%)	73 (100%)	0	100	100
18	T	69/70 (99%)	65 (94%)	4 (6%)	20	55
19	V	191/218 (88%)	190 (100%)	1 (0%)	88	95
20	r	70/71 (99%)	70 (100%)	0	100	100
21	Y	91/199 (46%)	91 (100%)	0	100	100
22	N	85/85 (100%)	85 (100%)	0	100	100
23	g	9/70 (13%)	9 (100%)	0	100	100
All	All	2143/2491 (86%)	2120 (99%)	23 (1%)	74	88

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	O	88	ARG
16	Q	89	ARG
16	Q	54	ARG
18	T	18	ARG
7	G	41	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
20	r	72	ASN
18	T	14	ASN
14	O	46	HIS
7	G	129	ASN
14	O	48	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1511 (99%)	379 (25%)	25 (1%)

5 of 379 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	U
1	A	10	G
1	A	11	G
1	A	12	A
1	A	13	G

5 of 25 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1038	G
1	A	1119	U
1	A	1482	U
1	A	1117	U
1	A	1149	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

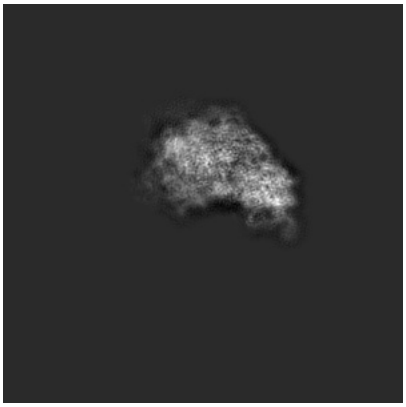
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8934. These allow visual inspection of the internal detail of the map and identification of artifacts.

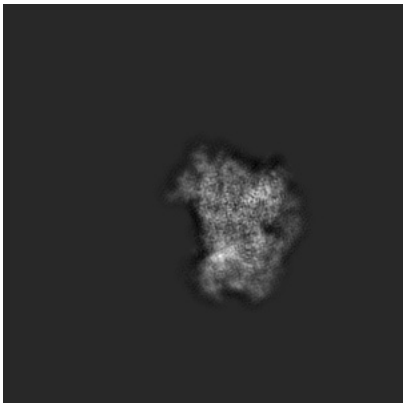
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

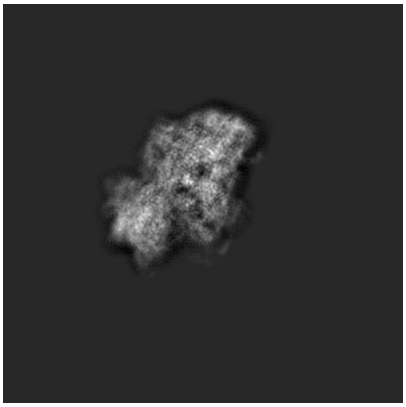
6.1.1 Primary map



X



Y

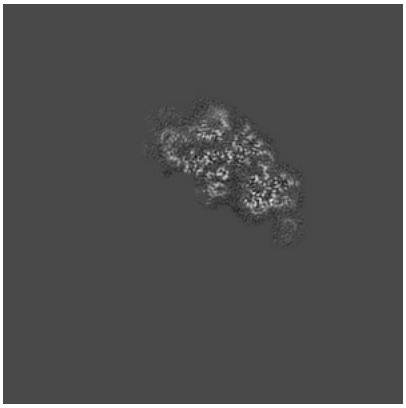


Z

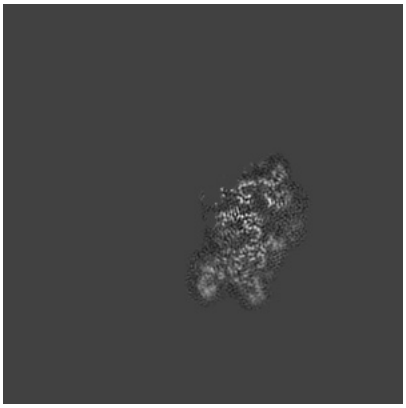
The images above show the map projected in three orthogonal directions.

6.2 Central slices

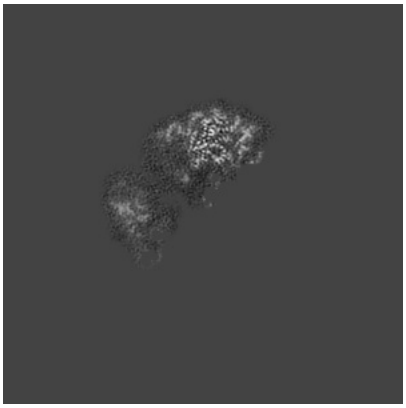
6.2.1 Primary map



X Index: 227



Y Index: 227

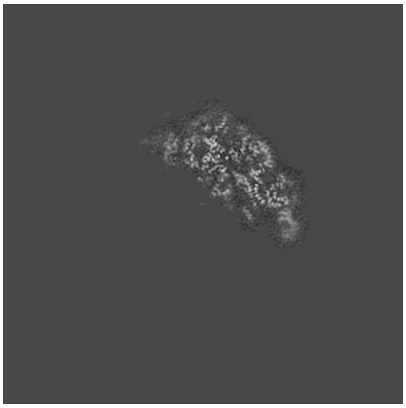


Z Index: 227

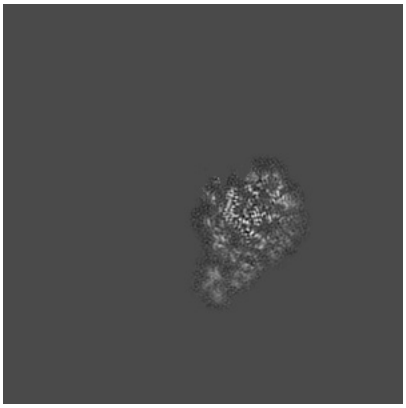
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

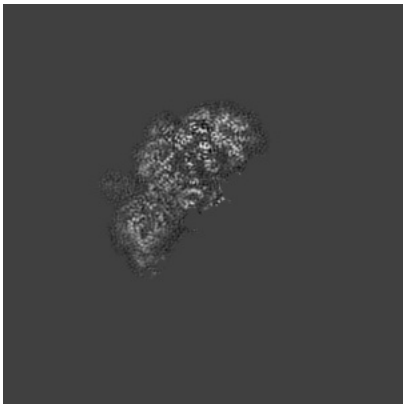
6.3.1 Primary map



X Index: 234



Y Index: 250

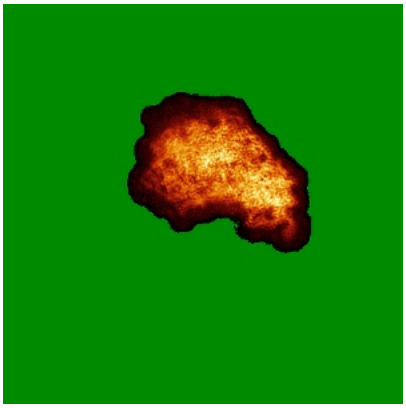


Z Index: 251

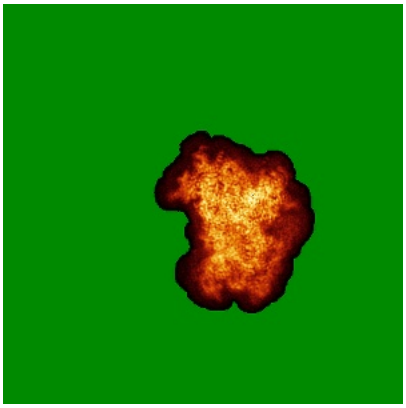
The images above show the largest variance slices of the map in three orthogonal directions.

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

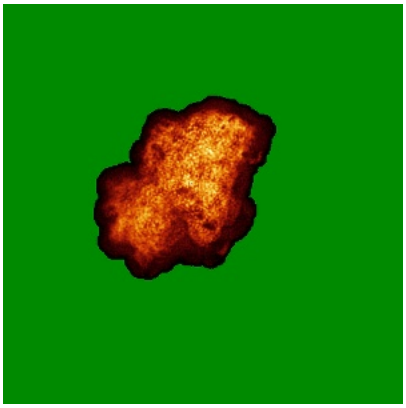
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

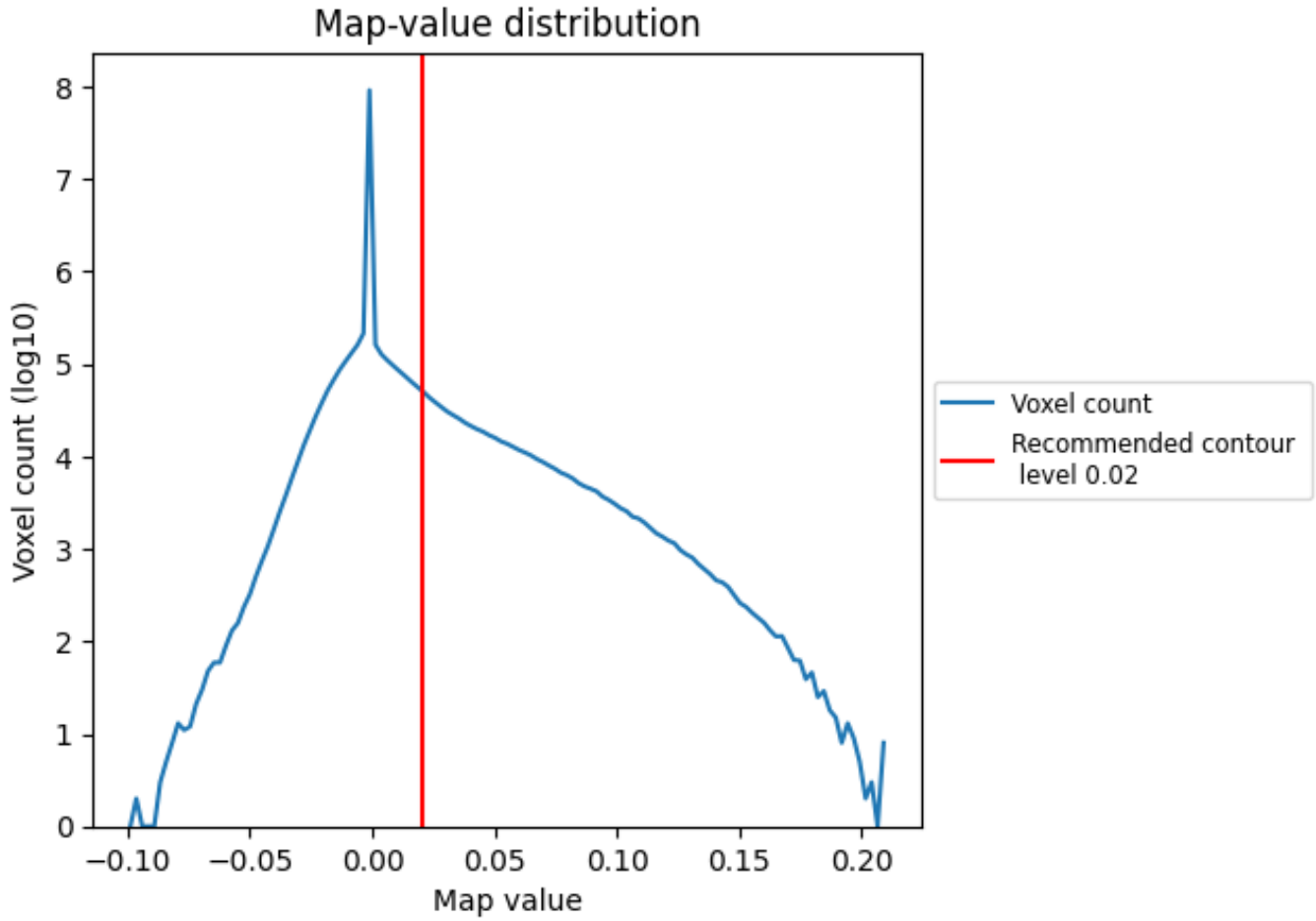
6.6 Mask visualisation (i)

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

7 Map analysis

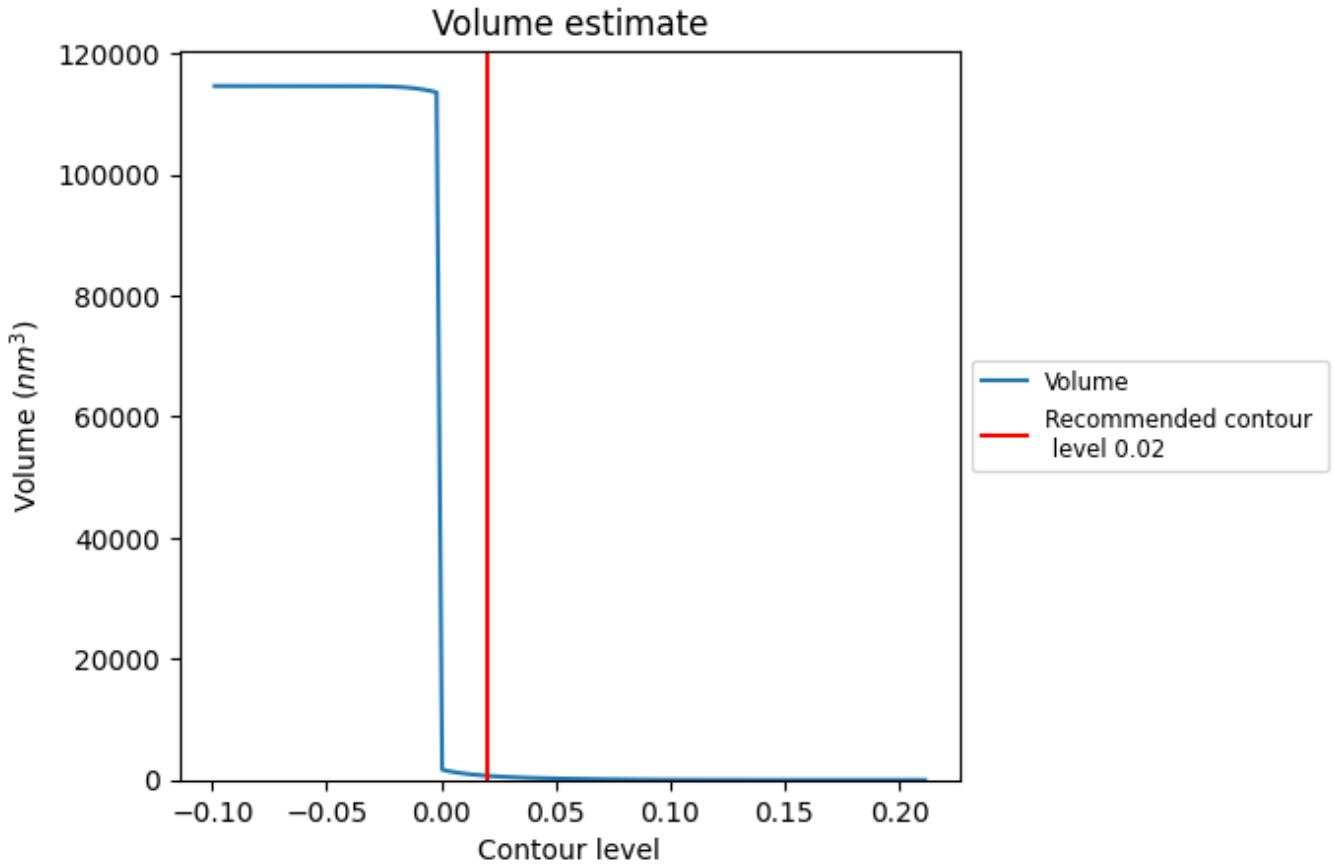
This section contains the results of statistical analysis of the map.

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.

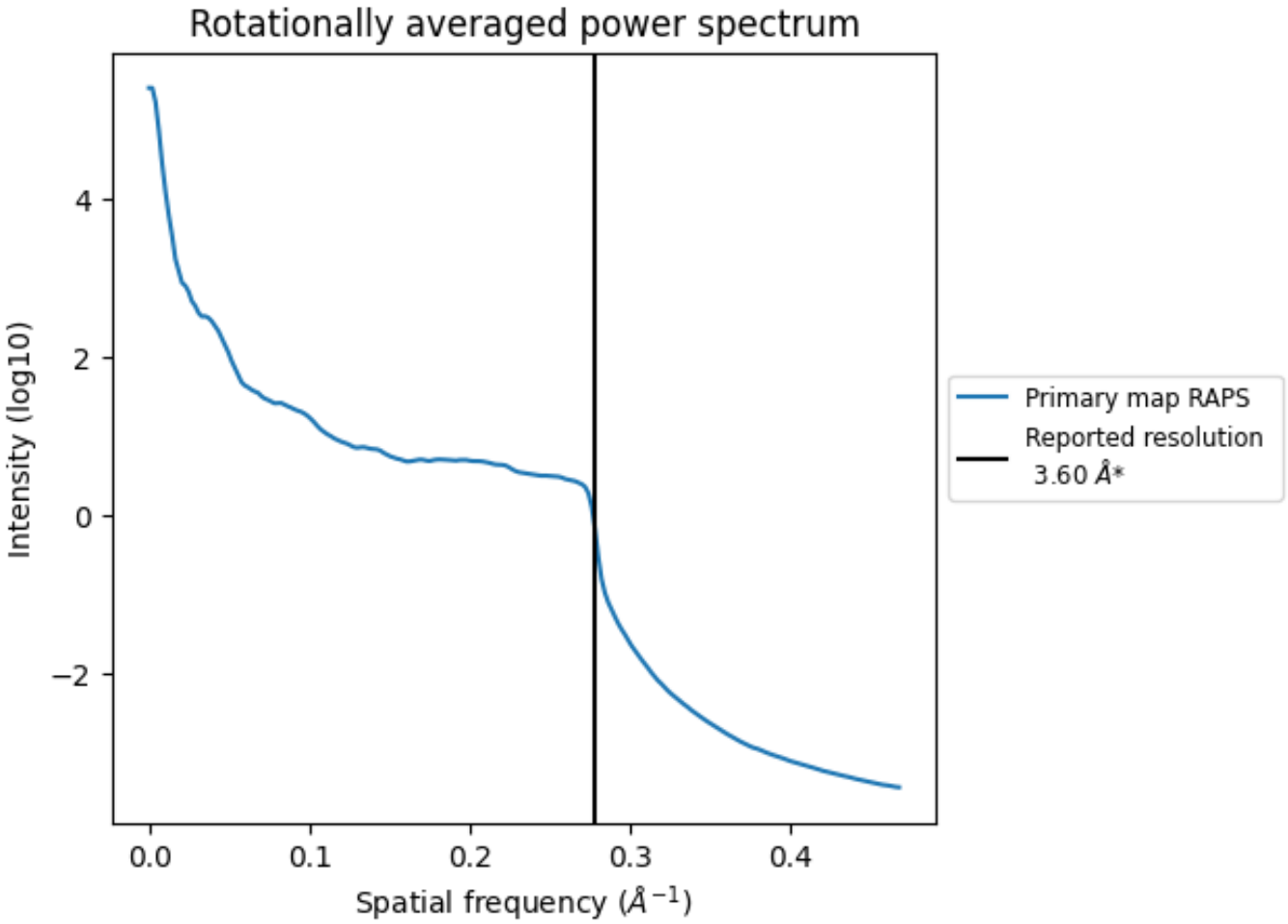
7.2 Volume estimate



The volume at the recommended contour level is 693 nm^3; this corresponds to an approximate mass of 626 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)

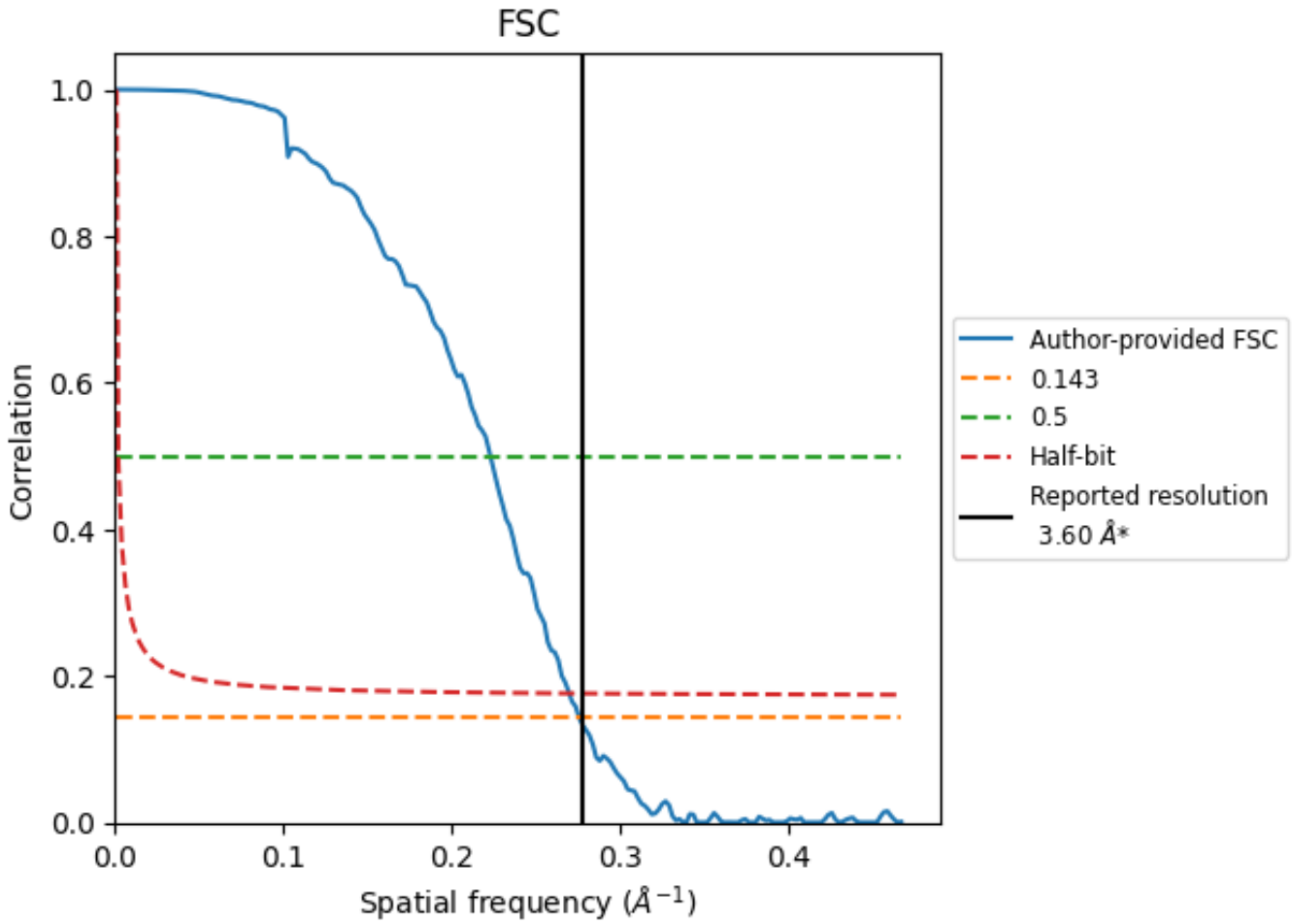


*Reported resolution corresponds to spatial frequency of 0.278 $Å^{-1}$

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

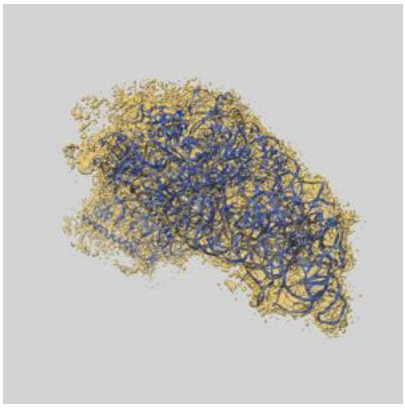
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.62	4.48	3.70
Unmasked-calculated*	-	-	-

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

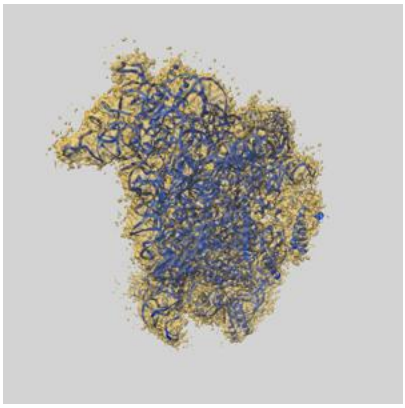
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8934 and PDB model 6DZK. Per-residue inclusion information can be found in section 3 on page 8.

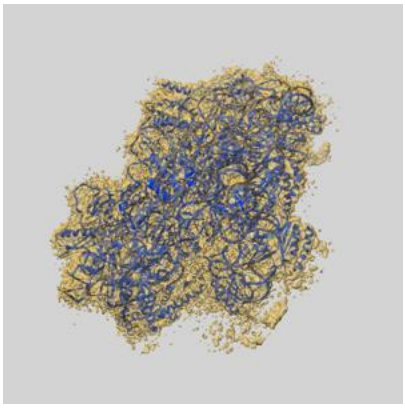
9.1 Map-model overlay



X



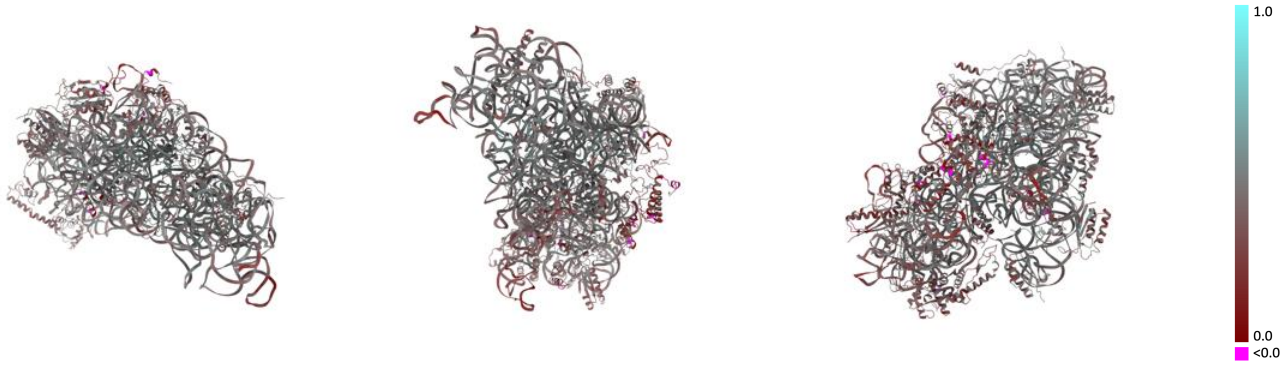
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

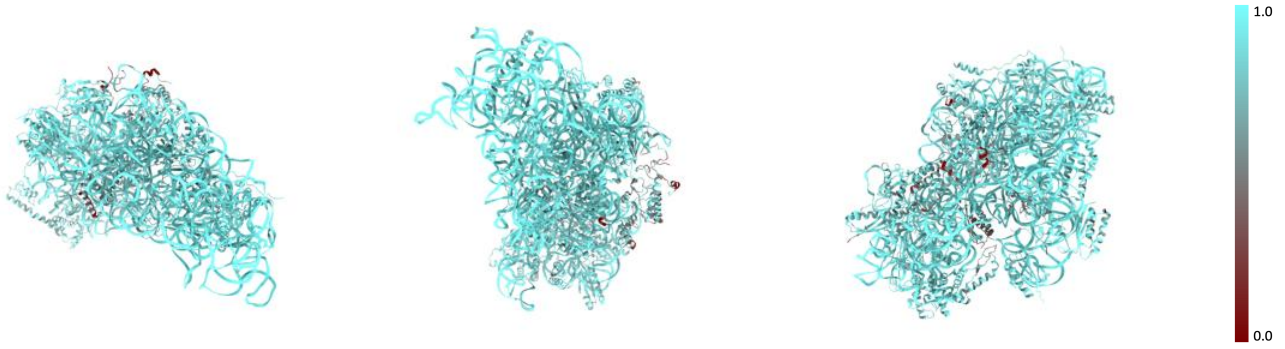
9.2 Q-score mapped to coordinate model (i)



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.

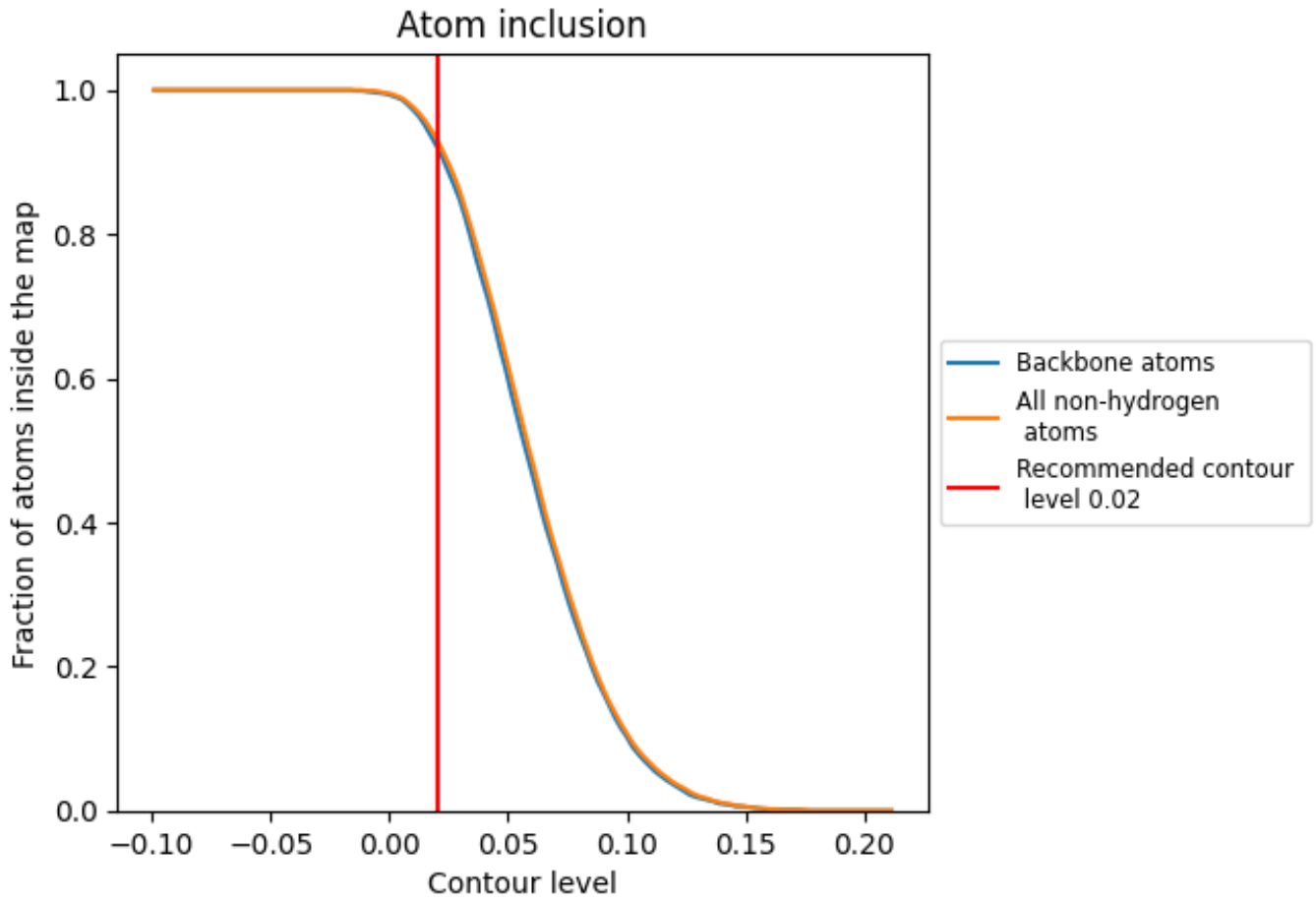
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9320	0.4190
A	0.9810	0.4420
B	0.7860	0.4250
C	0.8500	0.3640
D	0.8930	0.3830
E	0.8780	0.4350
F	0.8570	0.3840
G	0.8520	0.3710
H	0.9280	0.4600
I	0.9070	0.3910
J	0.8640	0.3800
K	0.9080	0.4430
L	0.8830	0.4570
M	0.8860	0.3490
N	0.8890	0.3630
O	0.9220	0.4240
P	0.9040	0.4420
Q	0.9060	0.4490
S	0.9020	0.3820
T	0.9000	0.4170
V	0.6440	0.2540
Y	0.5320	0.3040
g	0.8480	0.2470
r	0.7380	0.3370