



wwPDB EM Validation Summary Report ⓘ

Feb 8, 2025 – 02:01 PM EST

PDB ID : 9DUK
EMDB ID : EMD-47168
Title : Structure of mutant 30S subunit with extended helix 26, version 3
Authors : Boyko, K.; Cate, J.
Deposited on : 2024-10-03
Resolution : 2.56 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

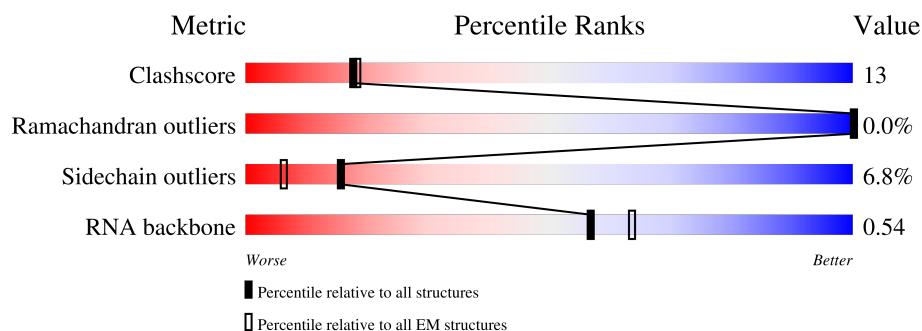
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.56 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	234	<div> <div>96%</div> <div>68% 25% . .</div> </div>
2	C	233	<div> <div>88%</div> <div>54% 34% . 12%</div> </div>
3	D	206	<div> <div>51%</div> <div>58% 34% 7%</div> </div>
4	E	167	<div> <div>17%</div> <div>68% 25% . 7%</div> </div>
5	F	135	<div> <div>67%</div> <div>53% 23% 24%</div> </div>
6	G	179	<div> <div>85%</div> <div>57% 25% . 15%</div> </div>
7	H	130	<div> <div>36%</div> <div>67% 30% . .</div> </div>

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Mol	Chain	Length	Quality of chain
8	I	130	
9	J	103	
10	K	129	
11	L	124	
12	M	118	
13	N	101	
14	O	89	
15	P	82	
16	Q	84	
17	R	75	
18	S	92	
19	T	87	
20	U	71	
21	A	1533	

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 51578 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 protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 2 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 7 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 8 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 9 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 10 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	116	Total	C	N	O	S	0	0
			869	536	172	158	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP A0A0H3PWX2

- Molecule 11 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 13 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 16 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 18 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

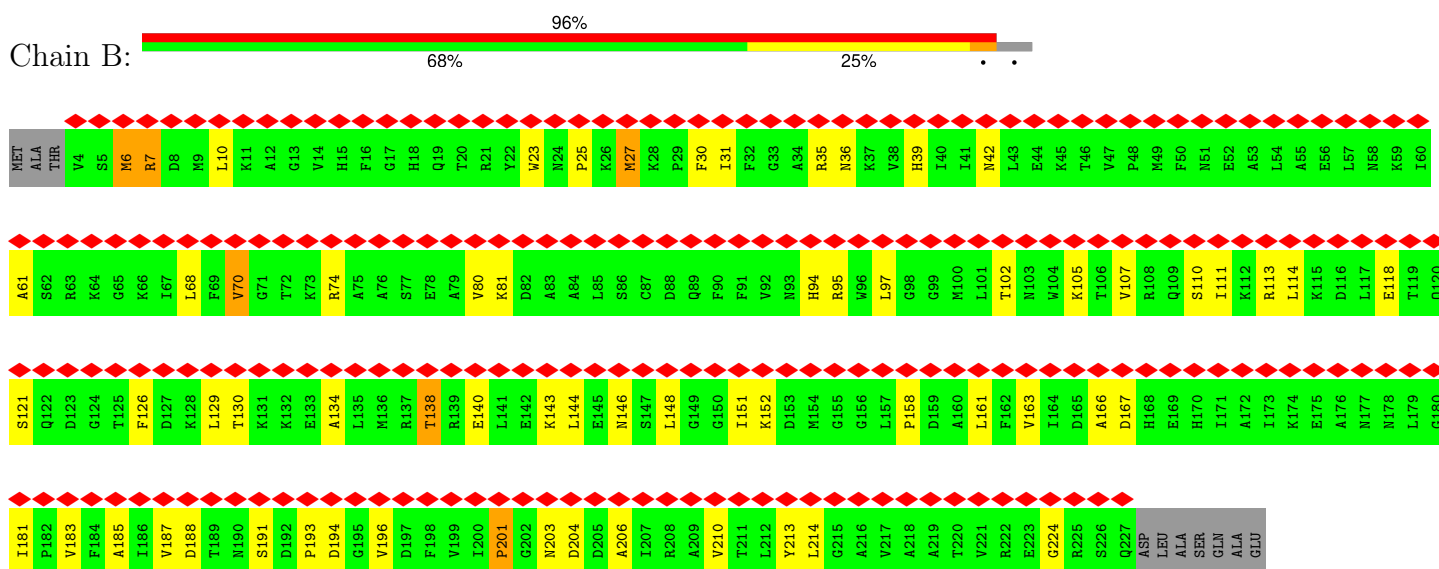
- Molecule 21 is a RNA chain called 16S rRNA.

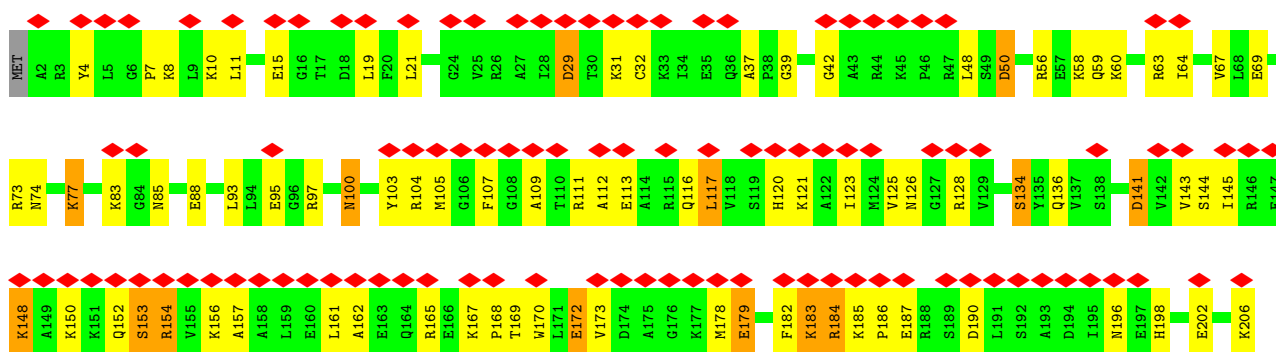
Mol	Chain	Residues	Atoms					AltConf	Trace
21	A	1518	Total	C	N	O	P	0	0
			32586	14539	5981	10548	1518		

3 Residue-property plots

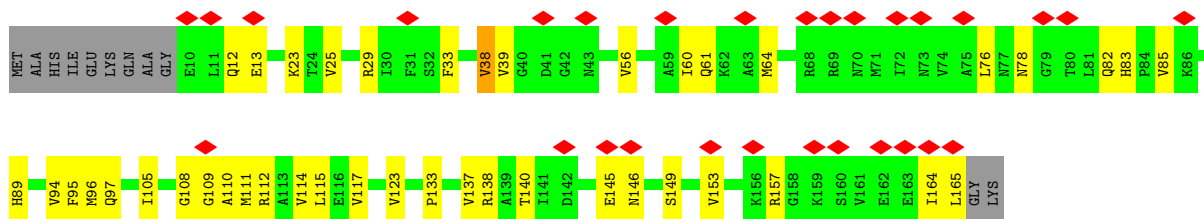
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Small ribosomal subunit protein uS2

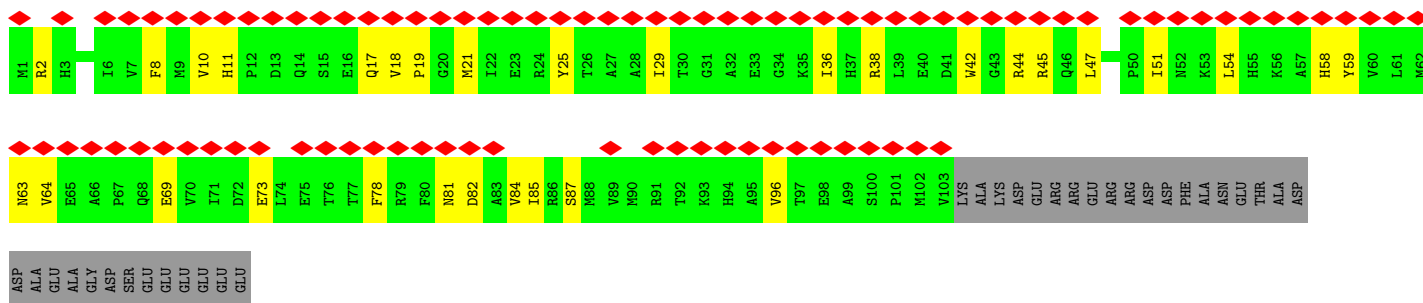




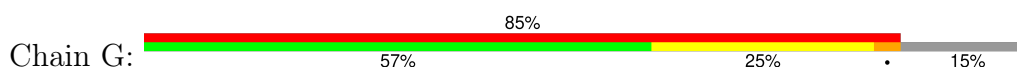
• Molecule 4: 30S ribosomal protein S5

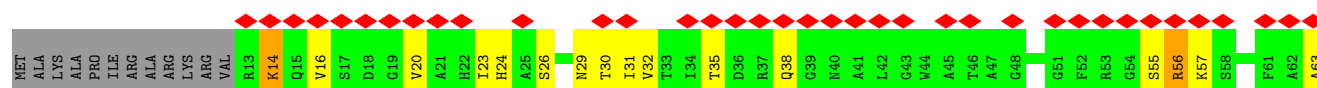


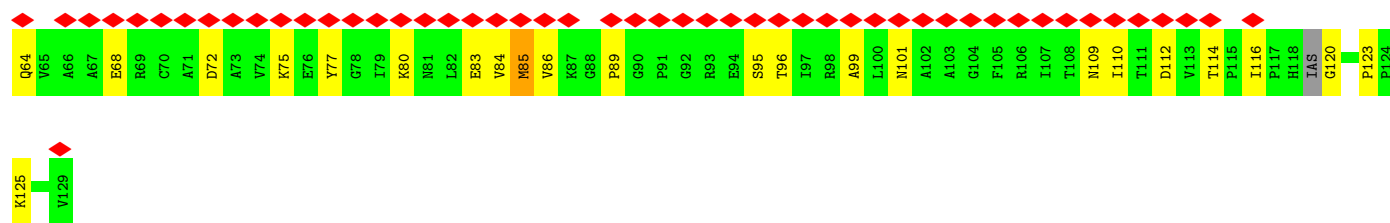
• Molecule 5: 30S ribosomal protein S6



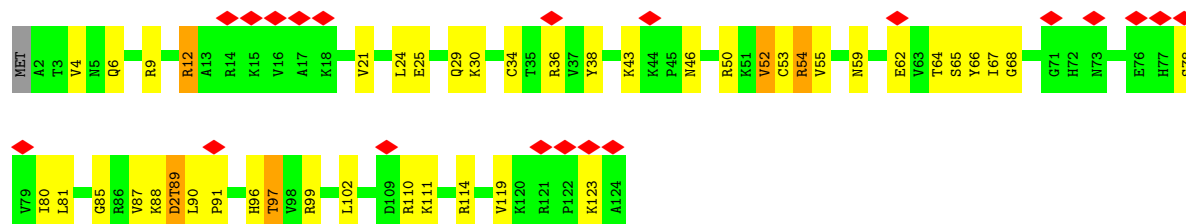
• Molecule 6: 30S ribosomal protein S7







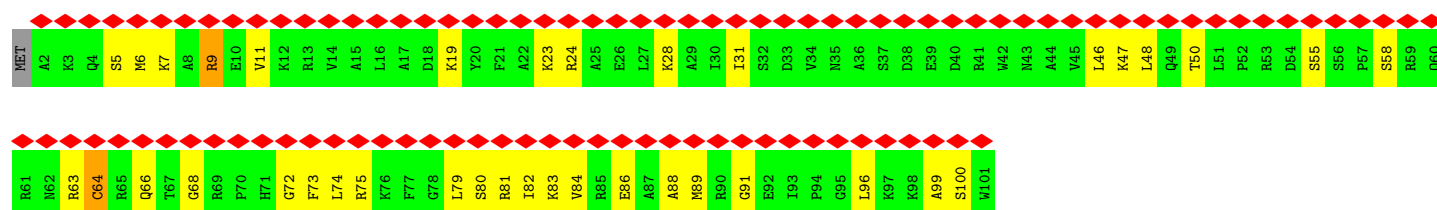
- Molecule 11: Small ribosomal subunit protein uS12



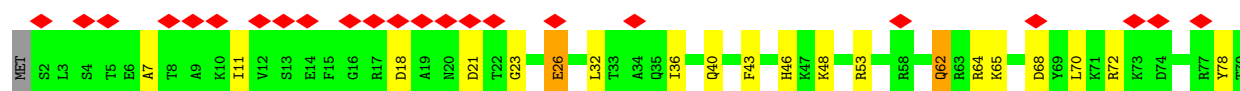
- Molecule 12: 30S ribosomal protein S13

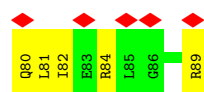


- Molecule 13: Small ribosomal subunit protein uS14

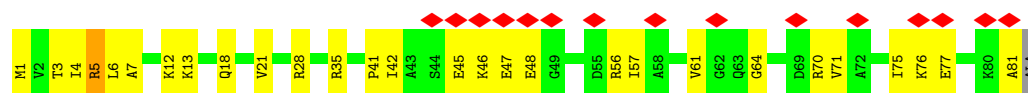


- Molecule 14: Small ribosomal subunit protein uS15

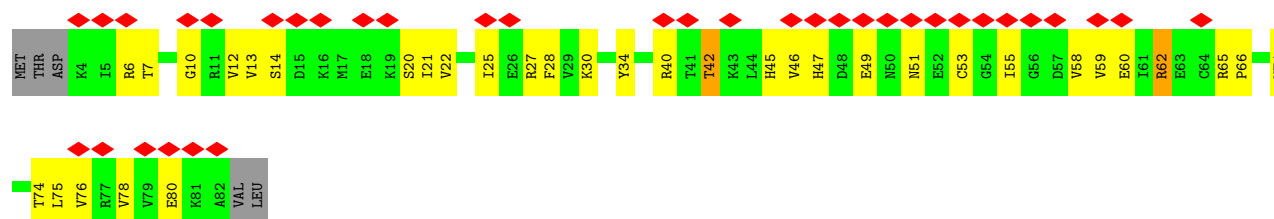
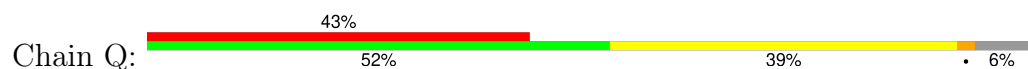




- Molecule 15: 30S ribosomal protein S16



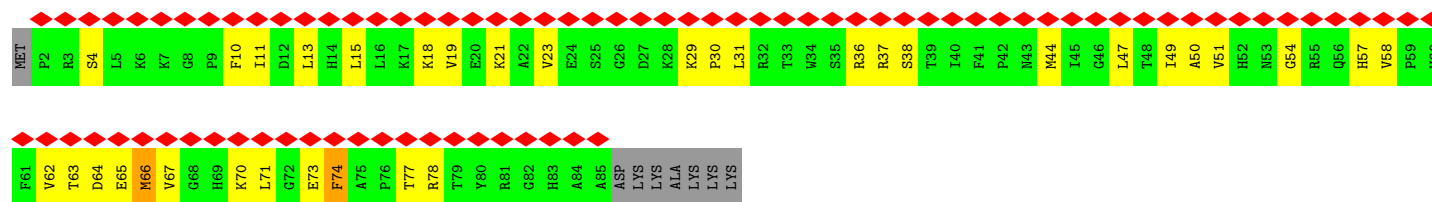
- Molecule 16: Small ribosomal subunit protein uS17



- Molecule 17: 30S ribosomal protein S18

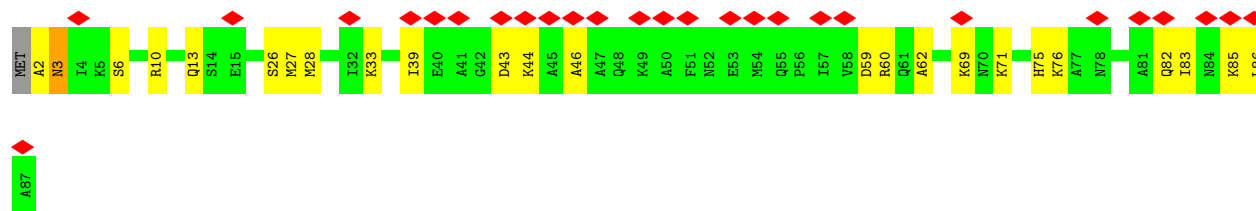


- Molecule 18: Small ribosomal subunit protein uS19

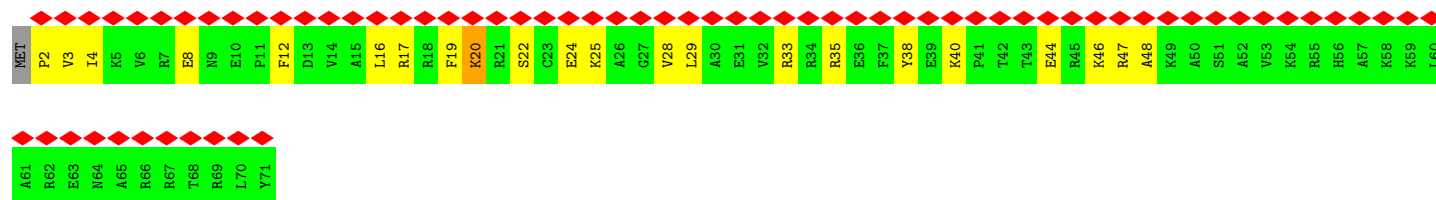


- Molecule 19: 30S ribosomal protein S20

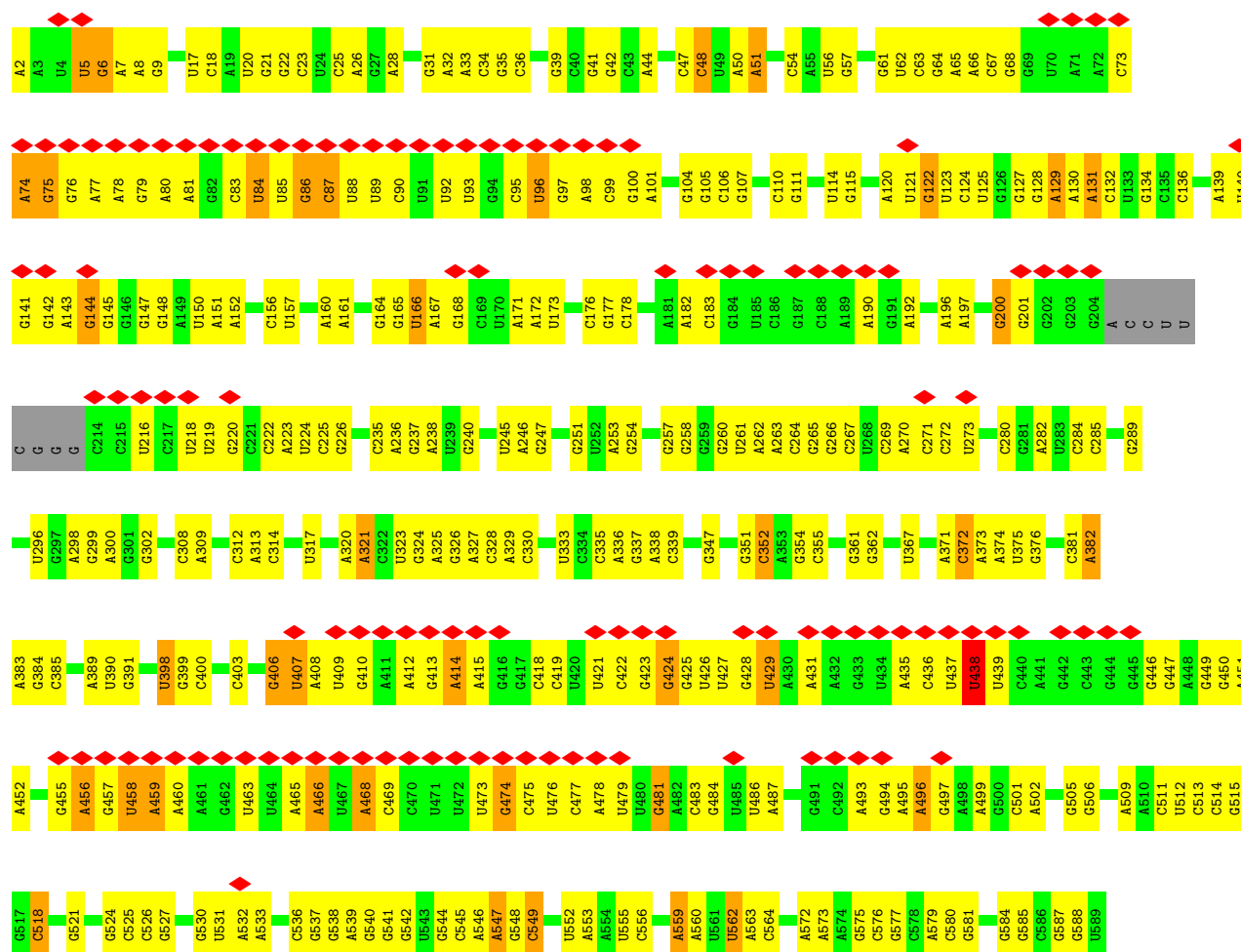
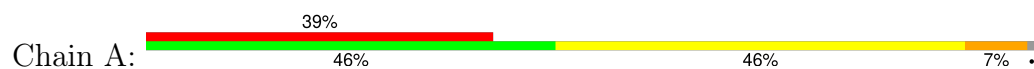


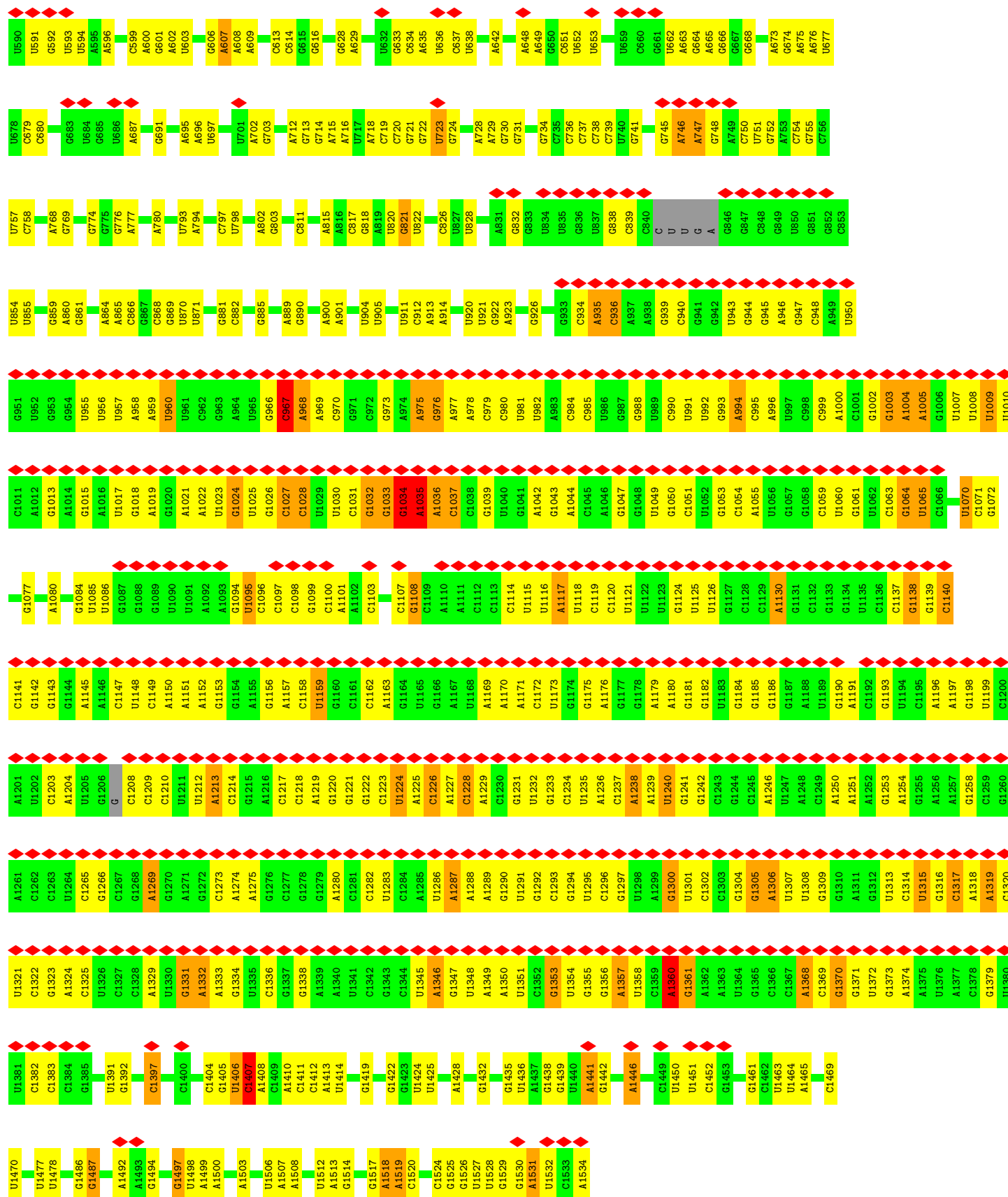


• Molecule 20: 30S ribosomal protein S21



• Molecule 21: 16S rRNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51527	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.594	Depositor
Minimum map value	-1.801	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.256	Depositor
Map size (Å)	369.6, 369.6, 369.6	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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: 4OC, PSU, G7M, UR3, MA6, D2T, 5MC

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	B	0.26	0/1784	0.51	0/2403
2	C	0.26	0/1651	0.53	0/2225
3	D	0.72	1/1665 (0.1%)	0.64	1/2227 (0.0%)
4	E	0.27	0/1165	0.53	0/1568
5	F	0.28	0/858	0.54	0/1160
6	G	0.25	0/1219	0.56	0/1635
7	H	0.26	0/989	0.52	0/1326
8	I	0.27	0/1034	0.62	0/1375
9	J	0.87	2/796 (0.3%)	0.97	3/1077 (0.3%)
10	K	0.27	0/884	0.56	0/1191
11	L	0.30	0/960	0.62	0/1286
12	M	0.25	0/900	0.58	0/1204
13	N	0.24	0/817	0.58	0/1088
14	O	0.26	0/722	0.56	0/964
15	P	0.28	0/653	0.61	0/877
16	Q	0.27	0/650	0.55	0/871
17	R	0.28	0/553	0.55	0/742
18	S	0.25	0/685	0.53	0/922
19	T	0.26	0/676	0.52	0/895
20	U	0.26	0/597	0.60	0/792
21	A	0.63	2/36287 (0.0%)	0.96	12/56598 (0.0%)
All	All	0.55	5/55545 (0.0%)	0.86	16/82426 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
3	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	7	PRO	N-CD	-27.13	1.09	1.47
9	J	55	PRO	N-CD	20.81	1.76	1.47
9	J	55	PRO	CG-CD	-10.87	1.14	1.50
21	A	1406	U	C4'-C3'	-6.81	1.45	1.53
21	A	1406	U	C2'-O2'	6.56	1.50	1.41

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	55	PRO	N-CD-CG	-21.59	70.82	103.20
3	D	7	PRO	N-CD-CG	11.90	121.06	103.20
9	J	55	PRO	CA-CB-CG	-9.60	85.76	104.00
21	A	1406	U	C1'-O4'-C4'	-7.86	103.61	109.90
9	J	55	PRO	CA-N-CD	-6.98	101.73	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	59	ARG	Sidechain
3	D	154	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	B	1753	0	1780	40	0
2	C	1624	0	1696	67	0
3	D	1643	0	1707	74	0
4	E	1152	0	1196	30	0
5	F	839	0	833	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	1203	0	1254	35	0
7	H	979	0	1031	31	0
8	I	1022	0	1070	70	0
9	J	786	0	828	25	0
10	K	869	0	880	29	0
11	L	957	0	1017	33	0
12	M	891	0	952	43	0
13	N	805	0	844	48	0
14	O	714	0	734	14	0
15	P	643	0	661	22	0
16	Q	641	0	682	24	0
17	R	544	0	565	17	0
18	S	668	0	693	35	0
19	T	670	0	719	19	0
20	U	589	0	629	20	0
21	A	32586	0	16416	588	0
All	All	51578	0	36187	1128	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 13.

The worst 5 of 1128 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)
9:J:55:PRO:CD	9:J:55:PRO:N	1.77	1.23
8:I:88:MET:HE1	8:I:104:VAL:HG13	1.40	1.03
8:I:42:GLU:HG2	8:I:45:ARG:NH2	1.80	0.96
9:J:53:ILE:HD12	21:A:1060:U:H5''	1.47	0.96
8:I:45:ARG:HG2	8:I:46:MET:HE3	1.48	0.94

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	
1	B	222/234 (95%)	206 (93%)	16 (7%)	0	100	100
2	C	204/233 (88%)	192 (94%)	12 (6%)	0	100	100
3	D	203/206 (98%)	196 (97%)	7 (3%)	0	100	100
4	E	154/167 (92%)	147 (96%)	7 (4%)	0	100	100
5	F	101/135 (75%)	95 (94%)	6 (6%)	0	100	100
6	G	151/179 (84%)	137 (91%)	14 (9%)	0	100	100
7	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
8	I	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
9	J	96/103 (93%)	94 (98%)	1 (1%)	1 (1%)	13	17
10	K	112/129 (87%)	104 (93%)	8 (7%)	0	100	100
11	L	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
12	M	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
13	N	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
14	O	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	P	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
16	Q	77/84 (92%)	73 (95%)	4 (5%)	0	100	100
17	R	64/75 (85%)	58 (91%)	6 (9%)	0	100	100
18	S	82/92 (89%)	79 (96%)	3 (4%)	0	100	100
19	T	84/87 (97%)	84 (100%)	0	0	100	100
20	U	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
All	All	2366/2569 (92%)	2245 (95%)	120 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	57	VAL

5.3.2 Protein sidechains ⓘ

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	
1	B	186/193 (96%)	169 (91%)	17 (9%)	7	9
2	C	170/190 (90%)	163 (96%)	7 (4%)	26	37
3	D	172/173 (99%)	152 (88%)	20 (12%)	4	4
4	E	119/126 (94%)	114 (96%)	5 (4%)	25	36
5	F	90/116 (78%)	86 (96%)	4 (4%)	24	34
6	G	126/147 (86%)	117 (93%)	9 (7%)	12	16
7	H	104/105 (99%)	97 (93%)	7 (7%)	13	18
8	I	105/107 (98%)	100 (95%)	5 (5%)	21	30
9	J	86/90 (96%)	76 (88%)	10 (12%)	4	4
10	K	89/98 (91%)	81 (91%)	8 (9%)	8	9
11	L	102/103 (99%)	94 (92%)	8 (8%)	10	13
12	M	93/96 (97%)	89 (96%)	4 (4%)	25	36
13	N	83/84 (99%)	80 (96%)	3 (4%)	30	43
14	O	76/77 (99%)	72 (95%)	4 (5%)	19	26
15	P	65/65 (100%)	63 (97%)	2 (3%)	35	49
16	Q	73/78 (94%)	66 (90%)	7 (10%)	7	8
17	R	57/65 (88%)	53 (93%)	4 (7%)	12	17
18	S	72/79 (91%)	70 (97%)	2 (3%)	38	53
19	T	65/66 (98%)	60 (92%)	5 (8%)	10	14
20	U	60/61 (98%)	56 (93%)	4 (7%)	13	18
All	All	1993/2119 (94%)	1858 (93%)	135 (7%)	16	17

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	Q	28	PHE
16	Q	65	ARG
19	T	85	LYS
4	E	146	ASN
4	E	145	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	39	HIS
2	C	102	ASN
5	F	11	HIS
6	G	86	GLN
17	R	52	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	A	1511/1533 (98%)	256 (16%)	7 (0%)

5 of 256 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	A	5	U
21	A	6	G
21	A	9	G
21	A	32	A
21	A	39	G

5 of 7 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	A	1026	G
21	A	1035	A
21	A	1530	G
21	A	1319	A
21	A	966	G

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

9 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
21	5MC	A	967	21	19,22,23	0.83	1 (5%)	26,32,35	0.67	0
21	UR3	A	1498	21	19,22,23	0.30	0	26,32,35	0.72	0
21	PSU	A	516	21	18,21,22	1.10	1 (5%)	21,30,33	1.99	6 (28%)
21	G7M	A	527	21	20,26,27	1.17	2 (10%)	16,39,42	0.59	0
21	4OC	A	1402	21	20,23,24	0.39	0	25,32,35	0.45	0
21	MA6	A	1518	21	19,26,27	0.97	2 (10%)	18,38,41	0.64	0
11	D2T	L	89	11	8,9,10	1.26	2 (25%)	6,11,13	1.67	3 (50%)
21	MA6	A	1519	21	19,26,27	0.98	2 (10%)	18,38,41	0.69	0
21	5MC	A	1407	21	19,22,23	0.91	2 (10%)	26,32,35	0.78	1 (3%)

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
21	5MC	A	967	21	-	2/7/25/26	0/2/2/2
21	UR3	A	1498	21	-	0/7/25/26	0/2/2/2
21	PSU	A	516	21	-	0/7/25/26	0/2/2/2
21	G7M	A	527	21	-	1/3/25/26	0/3/3/3
21	4OC	A	1402	21	-	0/9/29/30	0/2/2/2
21	MA6	A	1518	21	-	2/7/29/30	0/3/3/3
11	D2T	L	89	11	-	4/7/12/14	-
21	MA6	A	1519	21	-	2/7/29/30	0/3/3/3
21	5MC	A	1407	21	-	0/7/25/26	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	516	PSU	C6-C5	3.43	1.39	1.35
21	A	527	G7M	C5-C4	3.42	1.45	1.39
21	A	967	5MC	C5-C4	-3.31	1.41	1.44
21	A	1407	5MC	C5-C4	-2.99	1.41	1.44
21	A	527	G7M	C6-N1	-2.61	1.33	1.37

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	516	PSU	N1-C2-N3	4.90	120.34	115.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	516	PSU	C4-N3-C2	-4.88	119.65	126.37
21	A	516	PSU	O2-C2-N1	-3.07	119.63	122.79
11	L	89	D2T	O-C-CA	-2.52	118.29	124.77
21	A	516	PSU	C6-N1-C2	-2.41	120.46	122.69

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	L	89	D2T	CA-CB-CG-OD1
11	L	89	D2T	CA-CB-CG-OD2
21	A	967	5MC	O4'-C1'-N1-C2
21	A	1518	MA6	N1-C6-N6-C9
21	A	967	5MC	O4'-C1'-N1-C6

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	967	5MC	2	0
21	A	1498	UR3	1	0
21	A	1518	MA6	3	0
11	L	89	D2T	1	0
21	A	1519	MA6	1	0
21	A	1407	5MC	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 ⓘ

There are no chain breaks in this entry.

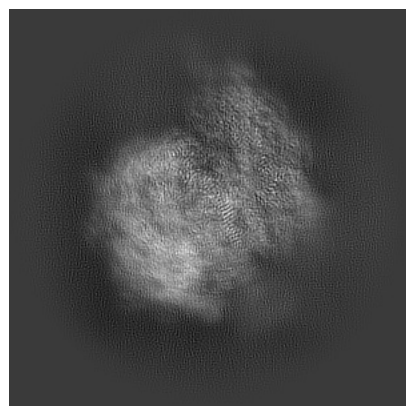
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47168. These allow visual inspection of the internal detail of the map and identification of artifacts.

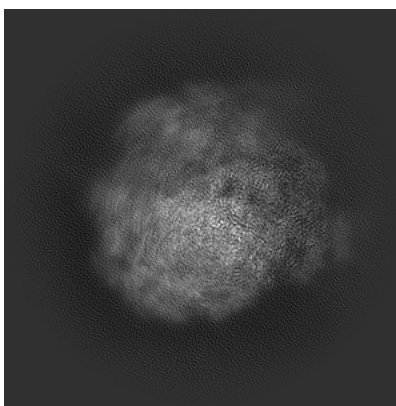
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

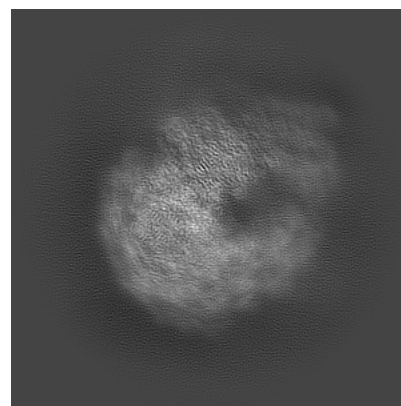
6.1.1 Primary map



X

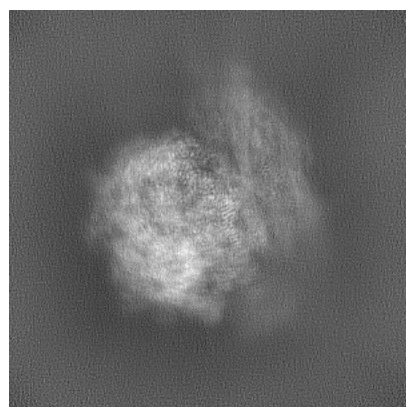


Y

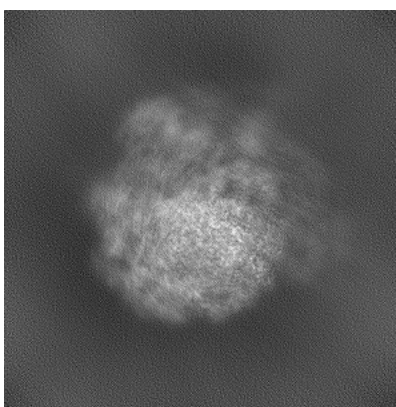


Z

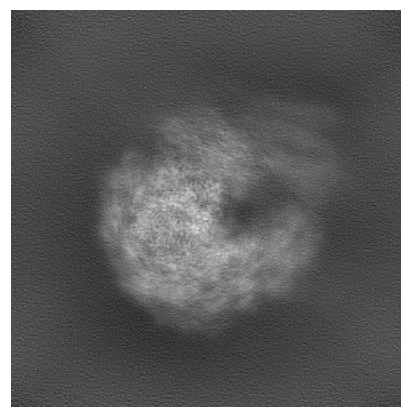
6.1.2 Raw map



X



Y

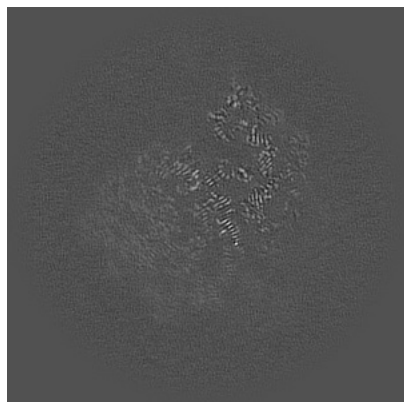


Z

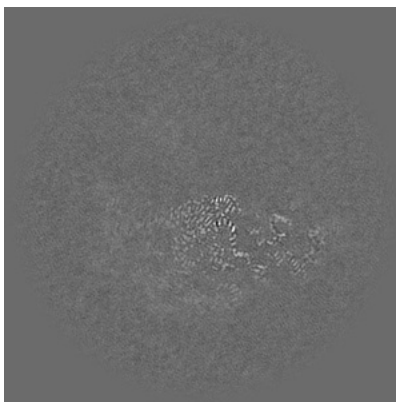
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

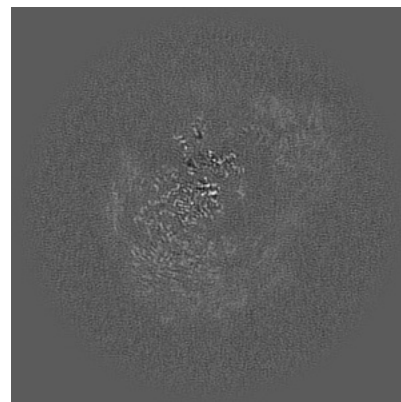
6.2.1 Primary map



X Index: 224

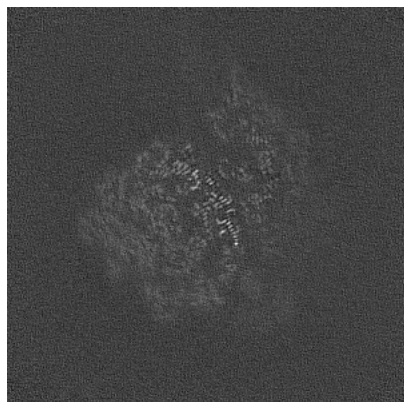


Y Index: 224

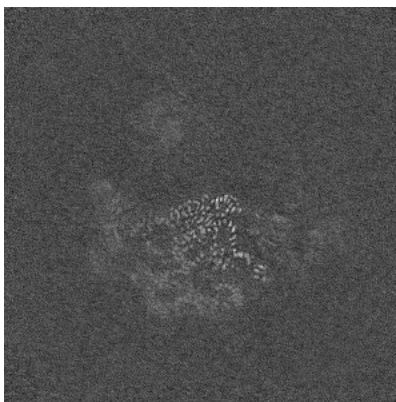


Z Index: 224

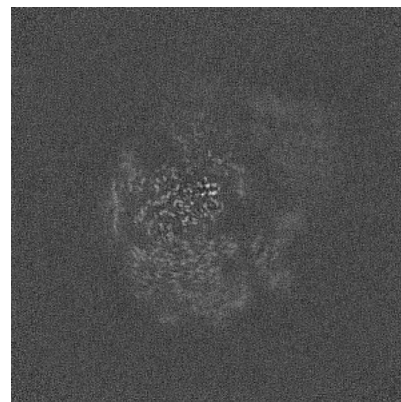
6.2.2 Raw map



X Index: 224



Y Index: 224

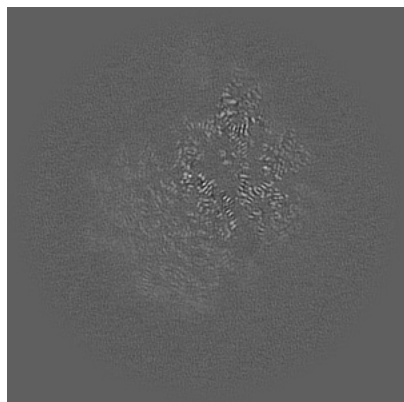


Z Index: 224

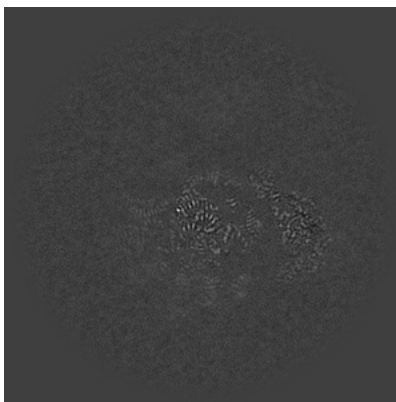
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

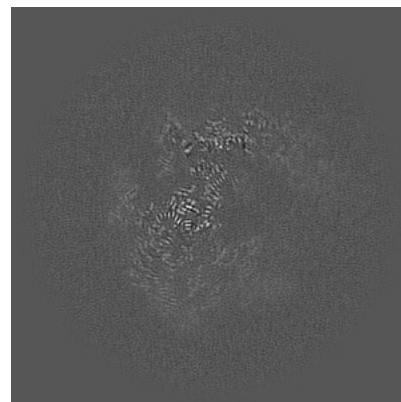
6.3.1 Primary map



X Index: 208

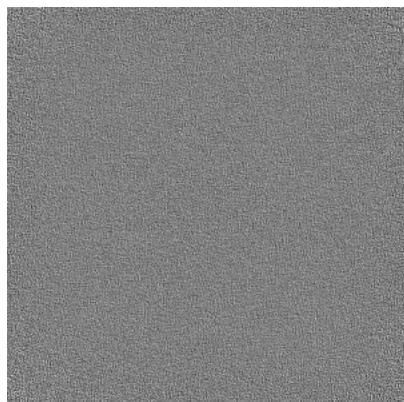


Y Index: 244

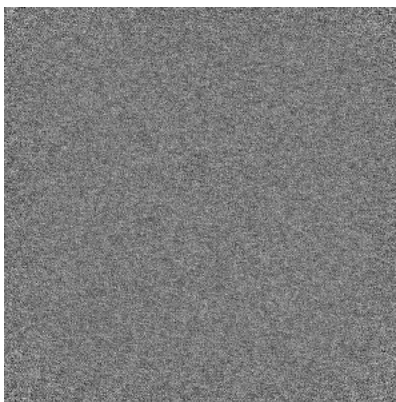


Z Index: 256

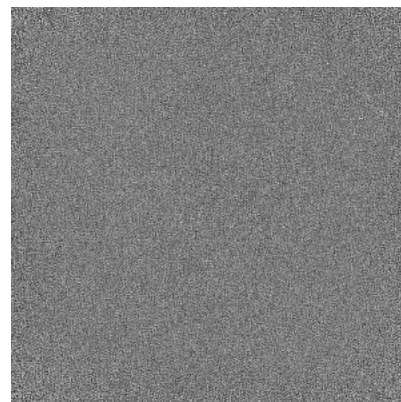
6.3.2 Raw map



X Index: 0



Y Index: 0

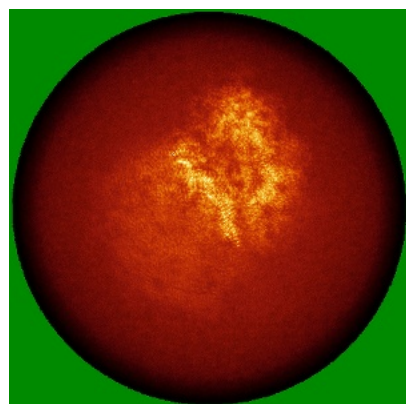


Z Index: 0

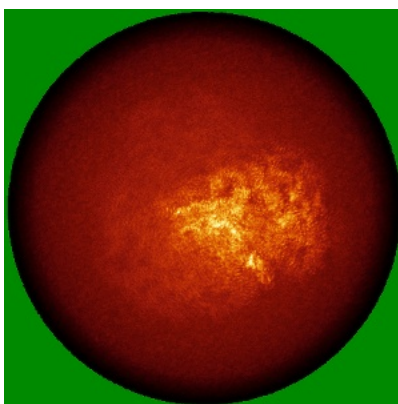
The images above show the largest variance slices of the map in three orthogonal directions.

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

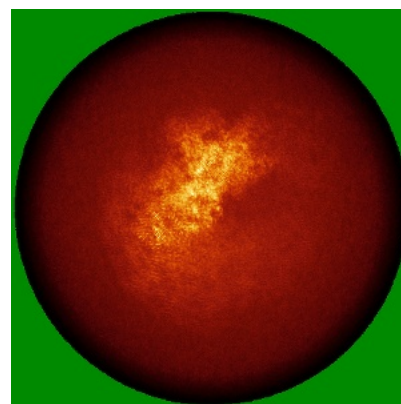
6.4.1 Primary map



X

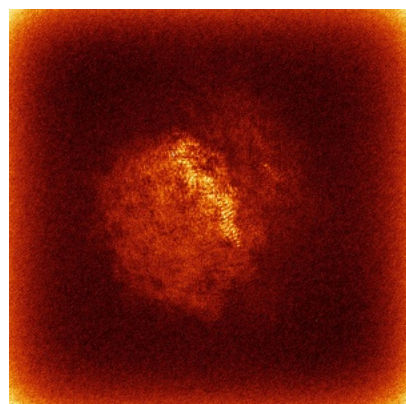


Y

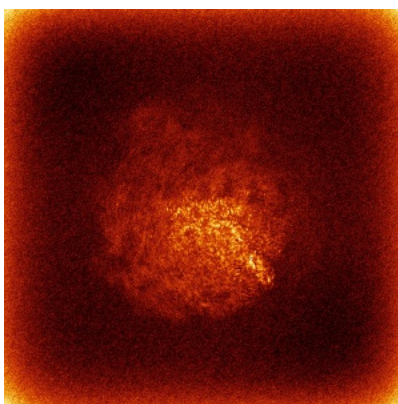


Z

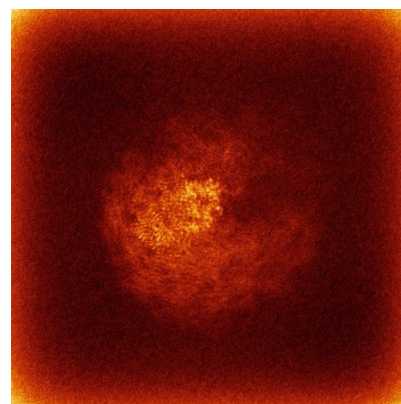
6.4.2 Raw map



X



Y

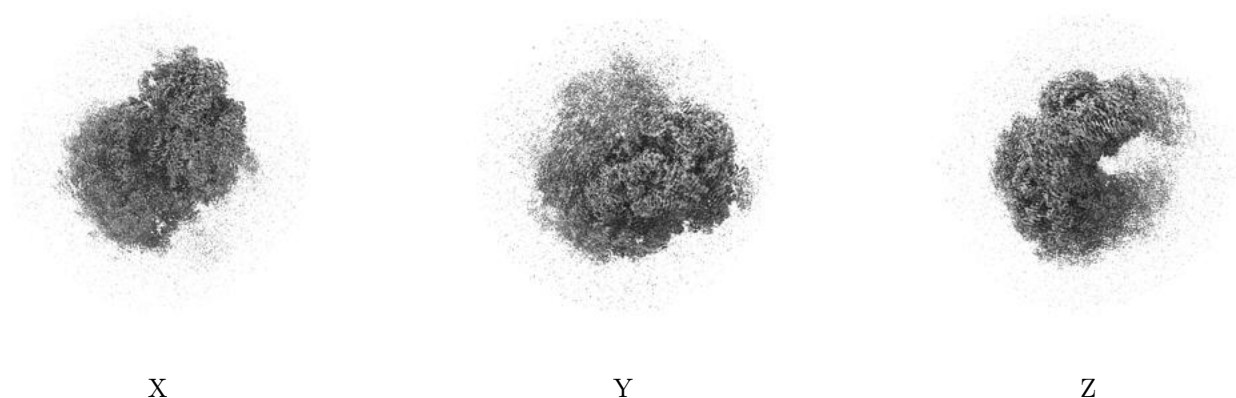


Z

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

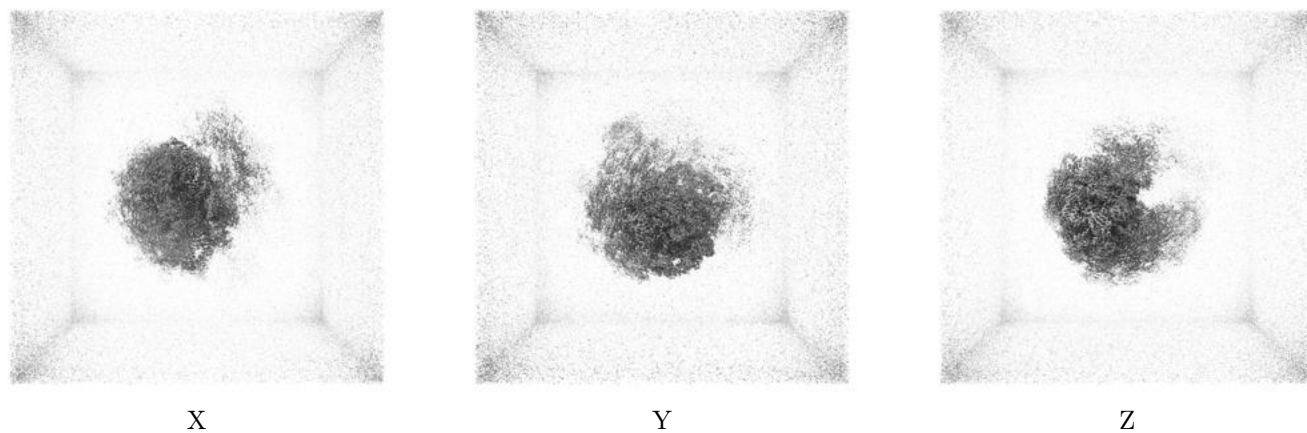
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.256. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

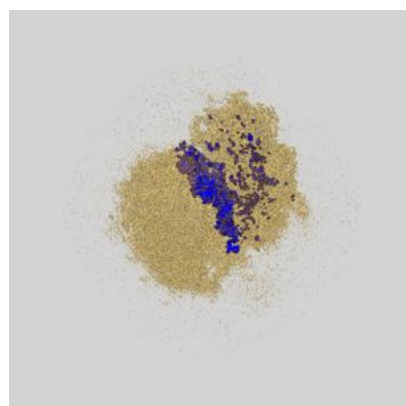
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

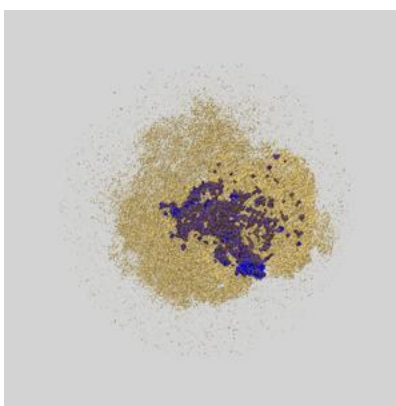
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

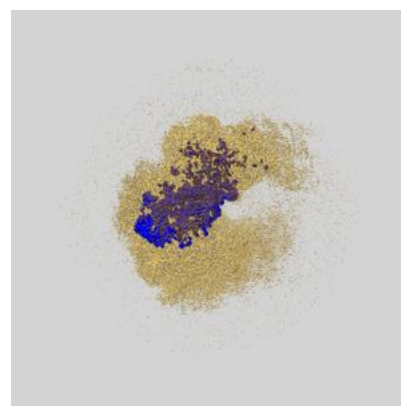
6.6.1 emd_47168_msk_1.map [i](#)



X



Y

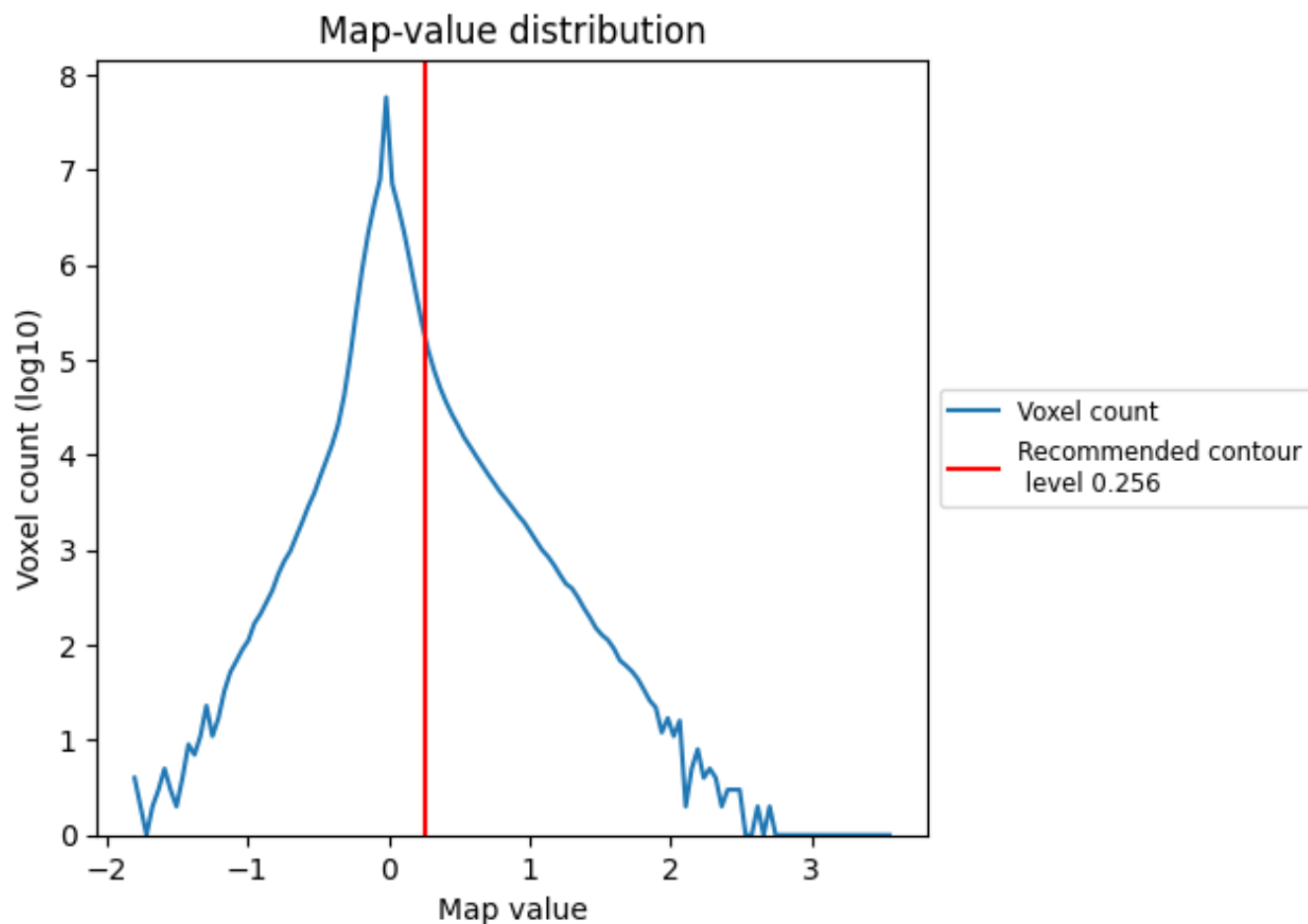


Z

7 Map analysis [i](#)

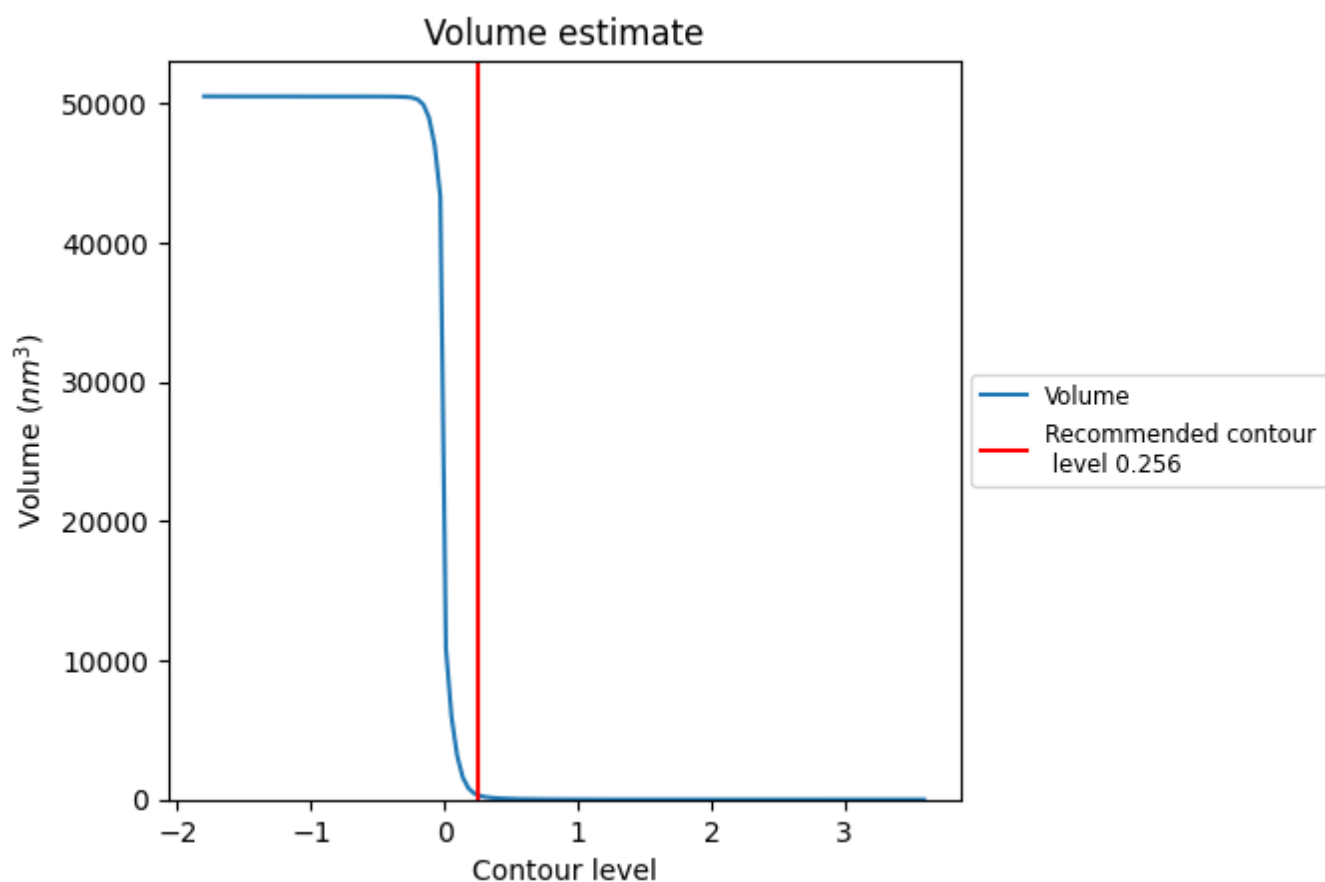
This section contains the results of statistical analysis of the map.

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.

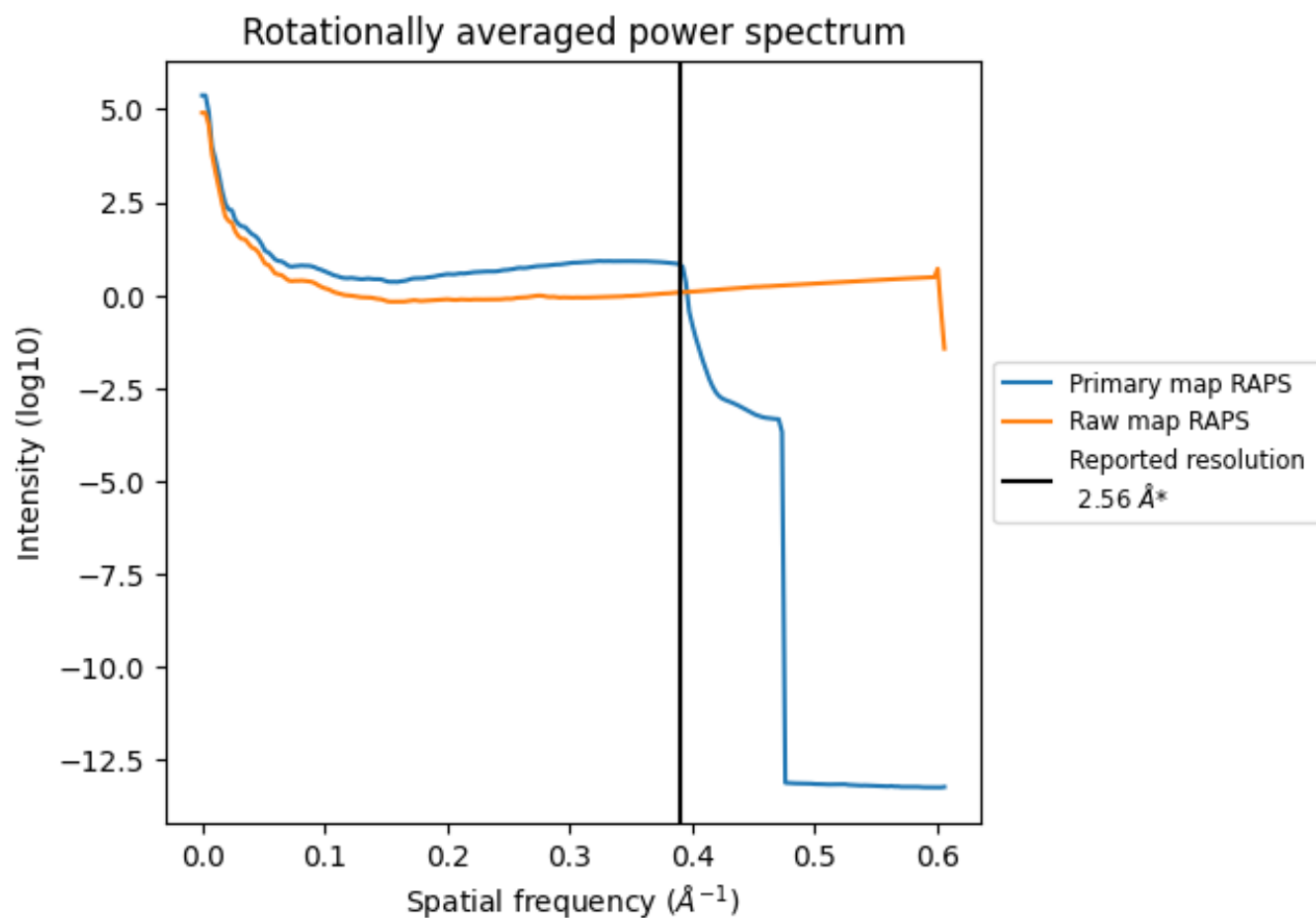
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 310 nm³; this corresponds to an approximate mass of 280 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

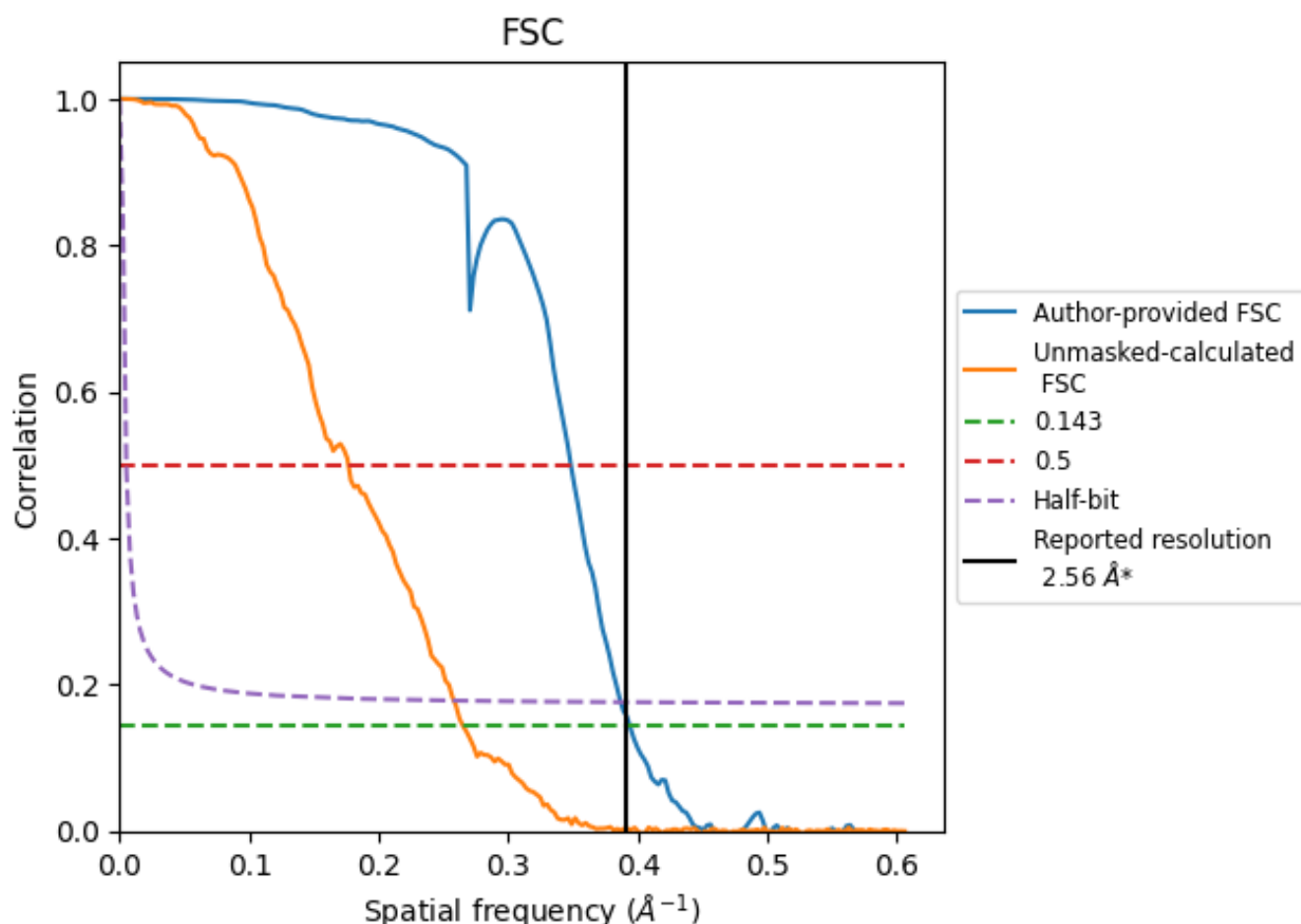


*Reported resolution corresponds to spatial frequency of 0.391 \AA^{-1}

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 0.391 \AA^{-1}

8.2 Resolution estimates [i](#)

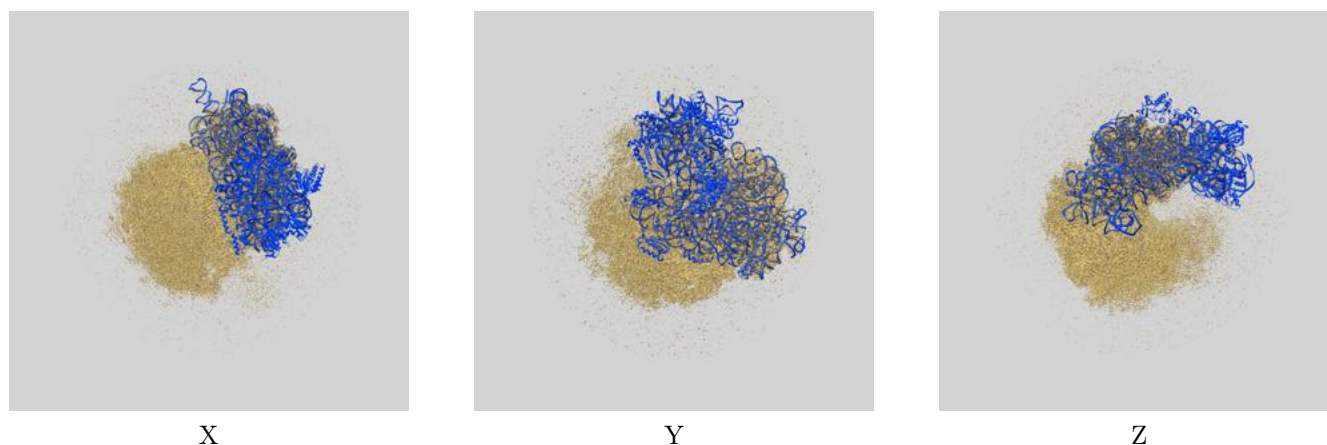
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.56	-	-
Author-provided FSC curve	2.54	2.87	2.58
Unmasked-calculated*	3.77	5.66	3.87

*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 3.77 differs from the reported value 2.56 by more than 10 %

9 Map-model fit [i](#)

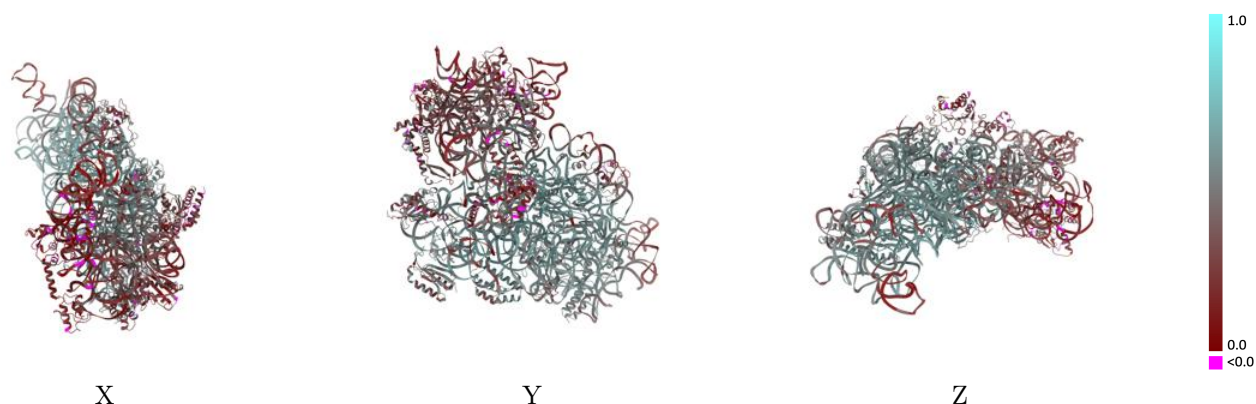
This section contains information regarding the fit between EMDB map EMD-47168 and PDB model 9DUK. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



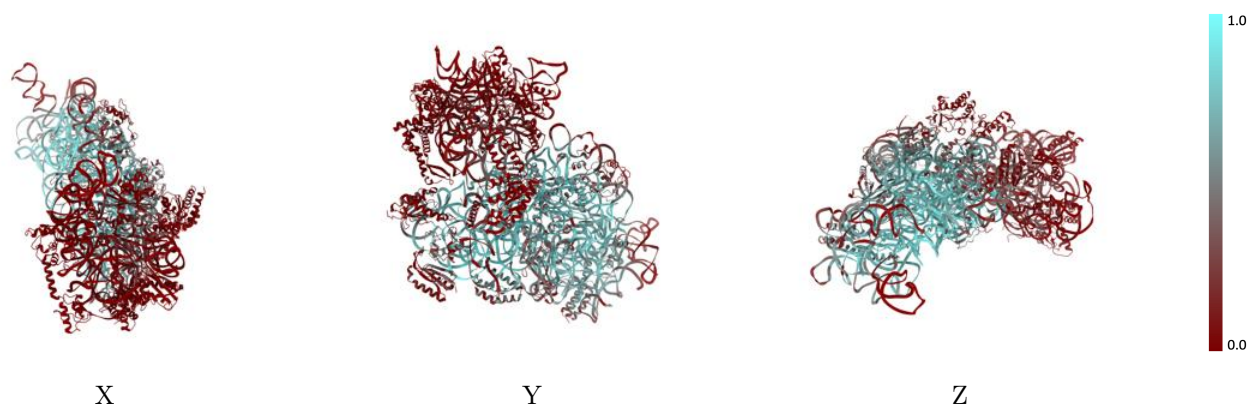
The images above show the 3D surface view of the map at the recommended contour level 0.256 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



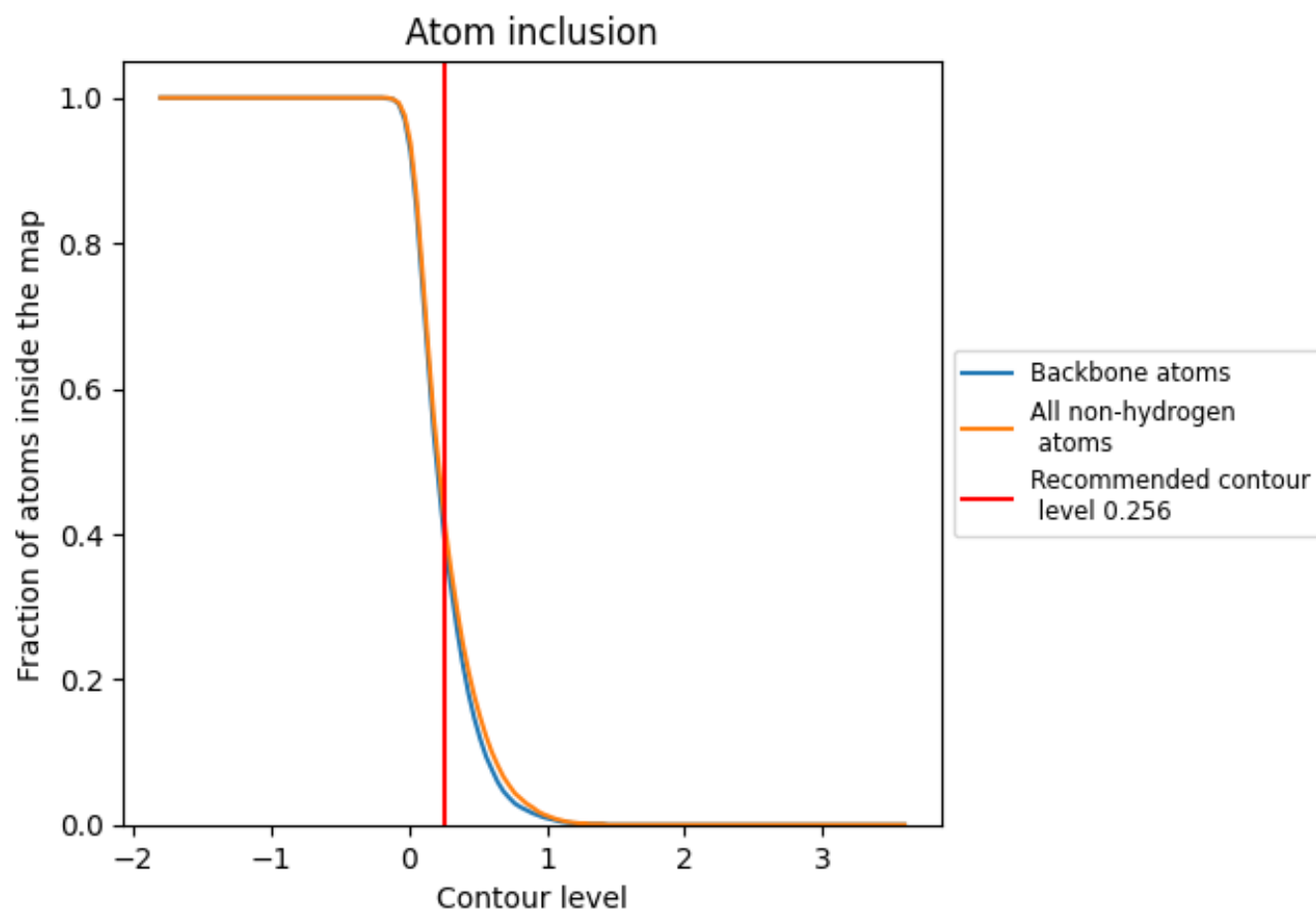
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.256).













































9.4 Atom inclusion ⓘ



At the recommended contour level, 40% of all backbone atoms, 42% 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 (0.256) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4200	 0.4460
A	 0.5170	 0.4680
B	 0.0030	 0.2580
C	 0.0610	 0.3890
D	 0.4120	 0.4480
E	 0.5980	 0.5930
F	 0.1980	 0.4540
G	 0.0140	 0.3150
H	 0.5010	 0.5580
I	 0.0310	 0.3120
J	 0.0340	 0.3450
K	 0.2620	 0.4840
L	 0.6480	 0.5750
M	 0.0050	 0.2180
N	 0.0280	 0.2670
O	 0.5460	 0.5580
P	 0.6420	 0.5730
Q	 0.4370	 0.5200
R	 0.3160	 0.4900
S	 0.0020	 0.1870
T	 0.5650	 0.5600
U	 0.0070	 0.1950

