



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 04:34 PM UTC

PDB ID : 9GUQ / pdb_00009guq
EMDB ID : EMD-51616
Title : 30S PIC (Pre-Initiation complex)
Authors : Rahil, H.; Weixlbaumer, A.; Webster, M.W.
Deposited on : 2024-09-20
Resolution : 3.10 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:

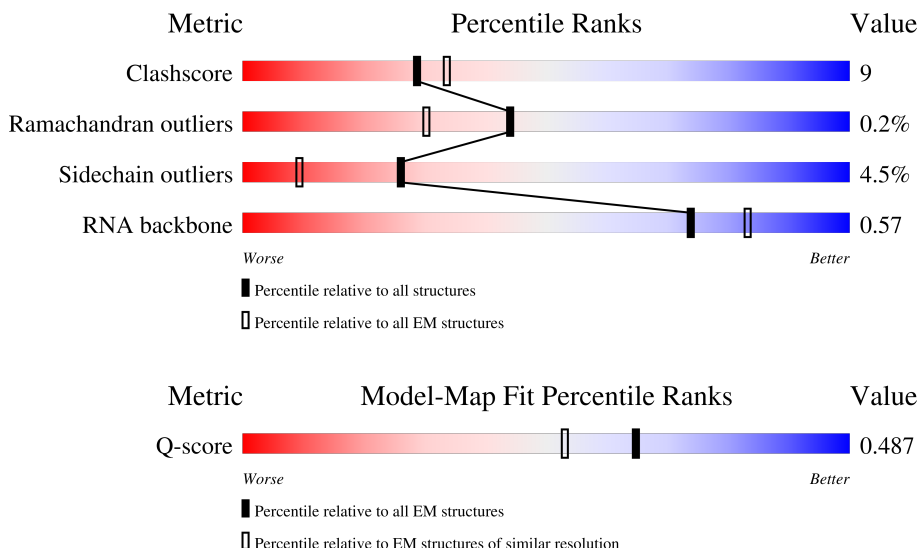
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.10 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.



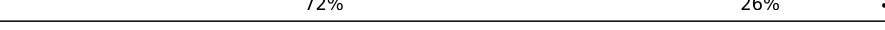
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	A	1541	
2	B	557	
3	C	241	

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Mol	Chain	Length	Quality of chain
4	D	233	
5	E	206	
6	F	156	
7	G	131	
8	H	156	
9	I	130	
10	J	130	
11	K	103	
12	L	129	
13	M	124	
14	N	118	
15	O	101	
16	P	89	
17	Q	82	
18	R	84	
19	S	75	
20	T	92	
21	U	87	
22	V	71	
23	W	77	
24	X	53	

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 55411 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1539	Total	C	N	O	P	0	0
			33023	14736	6046	10702	1539		

- Molecule 2 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	172	Total	C	N	O	0	0
			1094	674	196	224		

- Molecule 3 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	226	Total	C	N	O	S	0	0
			1765	1116	317	324	8		

- Molecule 4 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	211	Total	C	N	O	S	0	0
			1653	1046	310	293	4		

- Molecule 5 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 6 is a protein called 30S ribosomal protein S5.

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

- Molecule 7 is a protein called Small ribosomal subunit protein bS6, non-modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	125	ASP	GLU	conflict	UNP P02358

- Molecule 8 is a protein called 30S ribosomal protein S7.

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

- Molecule 9 is a protein called 30S ribosomal protein S8.

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

- Molecule 10 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	128	Total	C	N	O	S	0	0
			1031	639	207	182	3		

- Molecule 11 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			808	504	155	148	1		

- Molecule 12 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 13 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	122	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 14 is a protein called 30S ribosomal protein S13.

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

- Molecule 15 is a protein called 30S ribosomal protein S14.

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 17 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 18 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 19 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	67	Total	C	N	O	S	0	0
			554	350	104	99	1		

- Molecule 20 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 21 is a protein called 30S ribosomal protein S20.

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

- Molecule 22 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 23 is a RNA chain called tRNA(fmet) P-site.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	77	Total	C	N	O	P	S	
			1645	734	297	536	77	1	0

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	20	Total	C	N	O	P		
			427	191	77	139	20	0	0

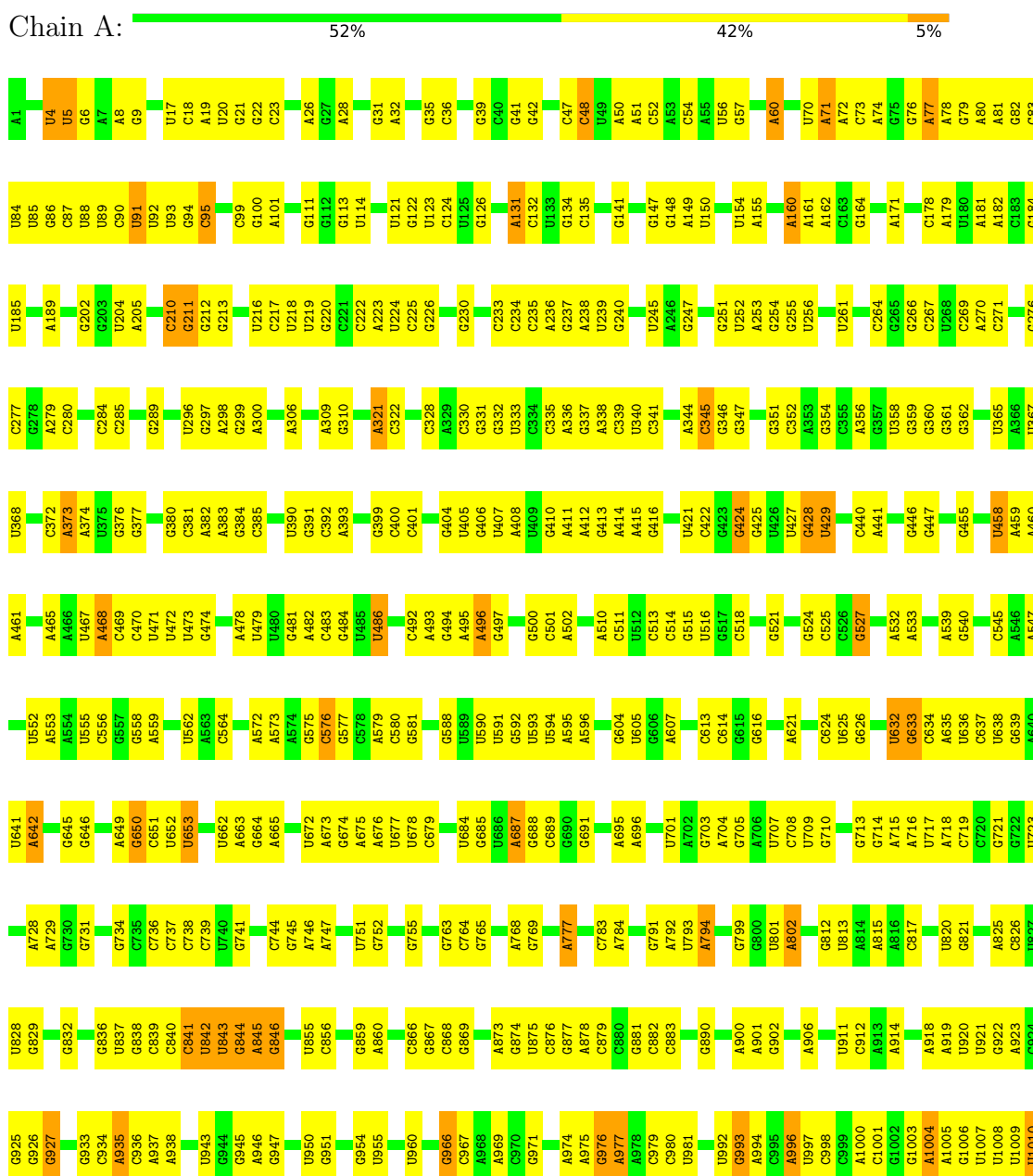
- Molecule 25 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

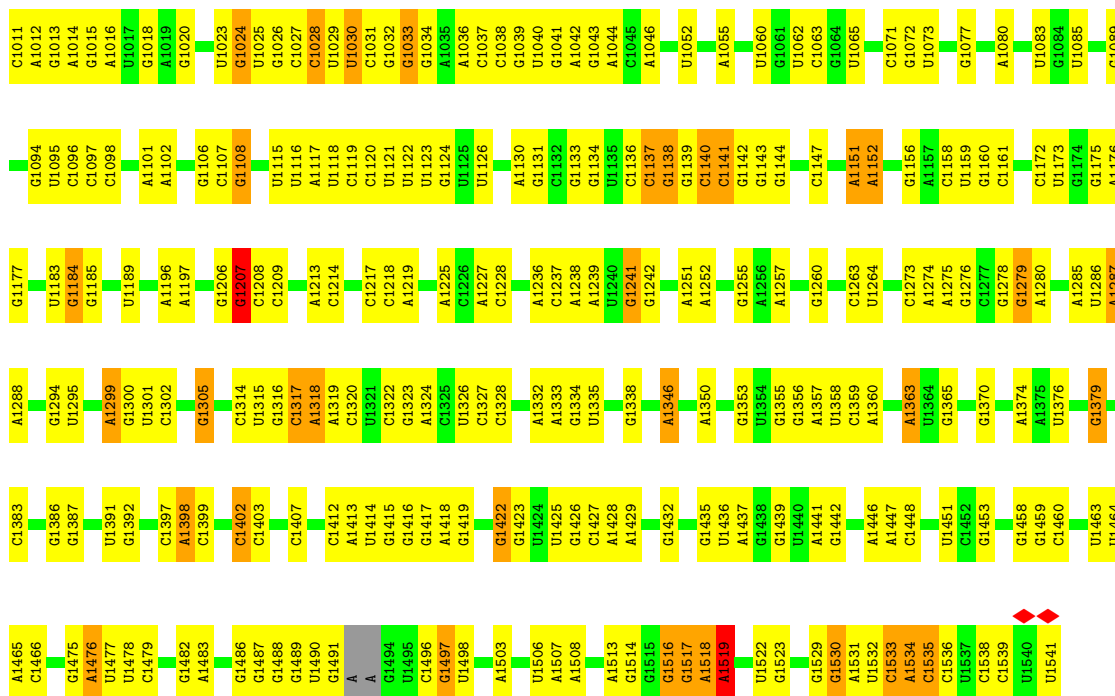
Mol	Chain	Residues	Atoms		AltConf
25	A	127	Total	Mg	0
			127	127	
25	X	1	Total	Mg	0
			1	1	

3 Residue-property plots

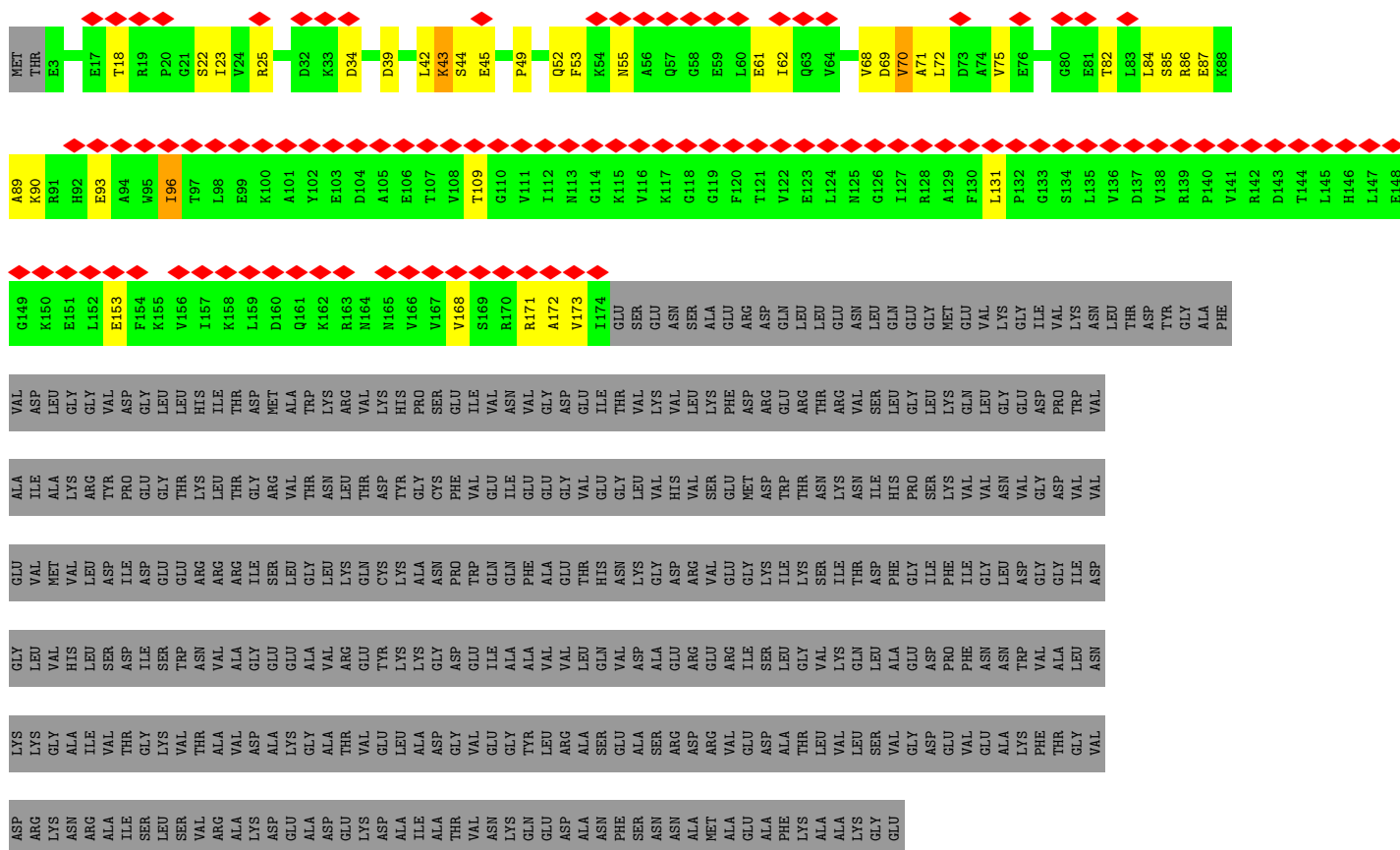
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S ribosomal RNA

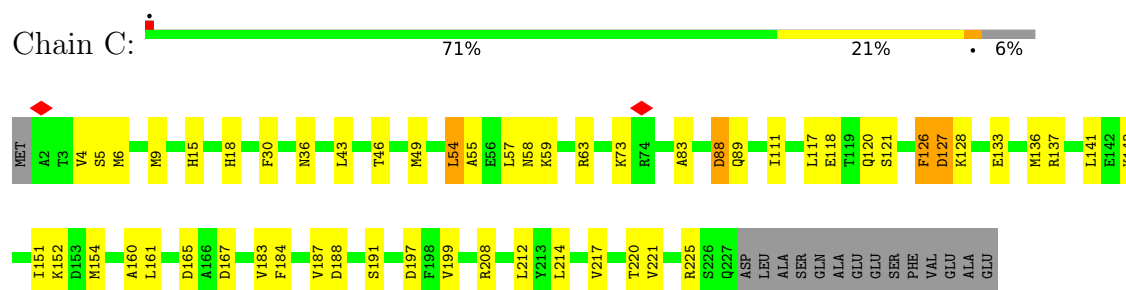




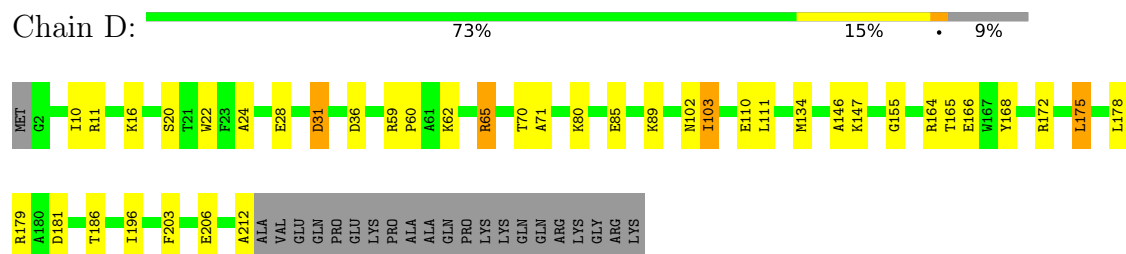
• Molecule 2: 30S ribosomal protein S1



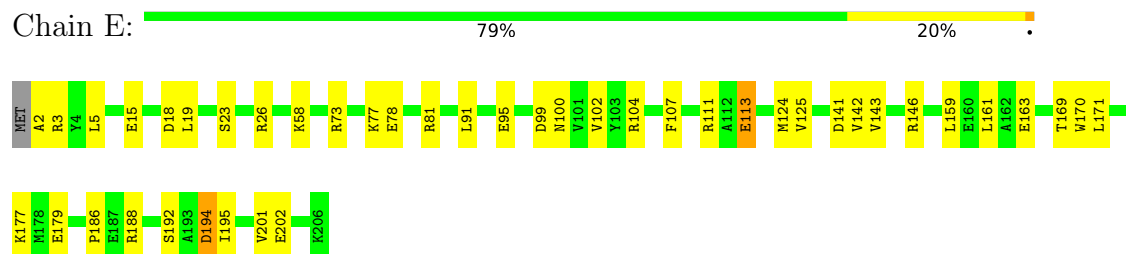
- Molecule 3: 30S ribosomal protein S2



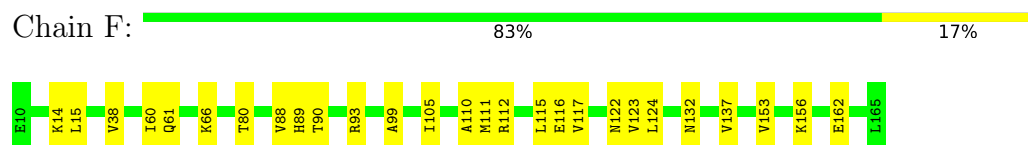
- Molecule 4: Small ribosomal subunit protein uS3



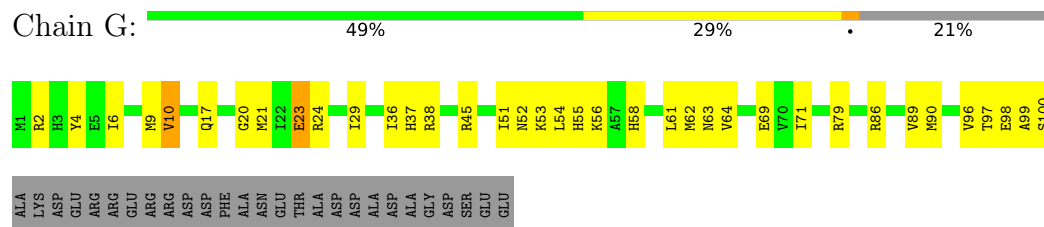
- Molecule 5: Small ribosomal subunit protein uS4



- Molecule 6: 30S ribosomal protein S5

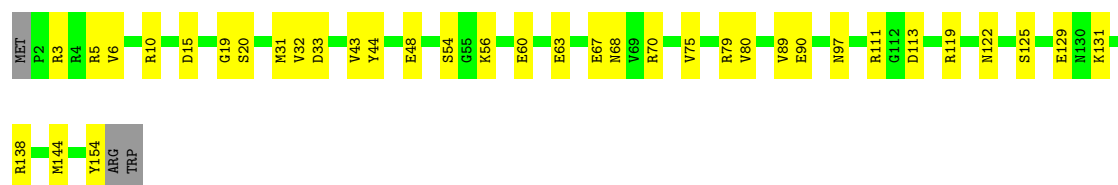


- Molecule 7: Small ribosomal subunit protein bS6, non-modified isoform



- Molecule 8: 30S ribosomal protein S7

Chain H:  75% 23%



- Molecule 9: 30S ribosomal protein S8

Chain I:  78% 20%



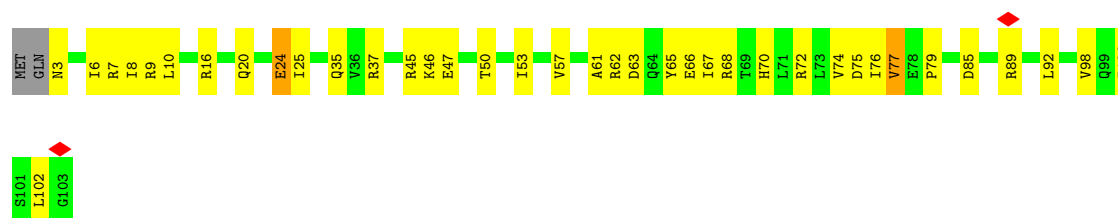
- Molecule 10: 30S ribosomal protein S9

Chain J:  78% 20%



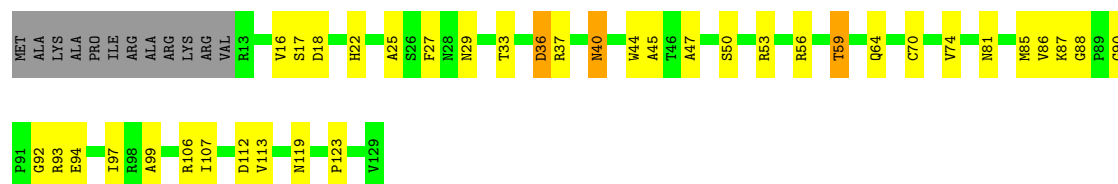
- Molecule 11: 30S ribosomal protein S10

Chain K:  61% 35%



- Molecule 12: 30S ribosomal protein S11

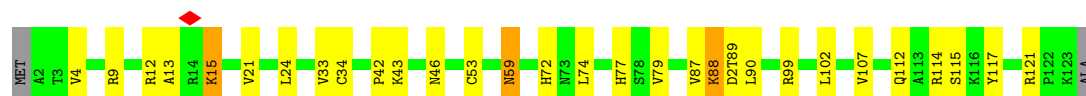
Chain L:  61% 27% 9%



- Molecule 13: 30S ribosomal protein S12

Chain M:  74% 22%





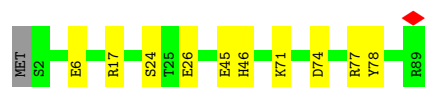
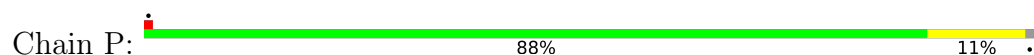
- Molecule 14: 30S ribosomal protein S13



- Molecule 15: 30S ribosomal protein S14



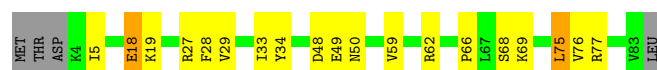
- Molecule 16: Small ribosomal subunit protein uS15



- Molecule 17: 30S ribosomal protein S16



- Molecule 18: 30S ribosomal protein S17



- Molecule 19: 30S ribosomal protein S18



- Molecule 20: 30S ribosomal protein S19

Chain T:  72% 17% 10%



- Molecule 21: 30S ribosomal protein S20

Chain U:  77% 22%



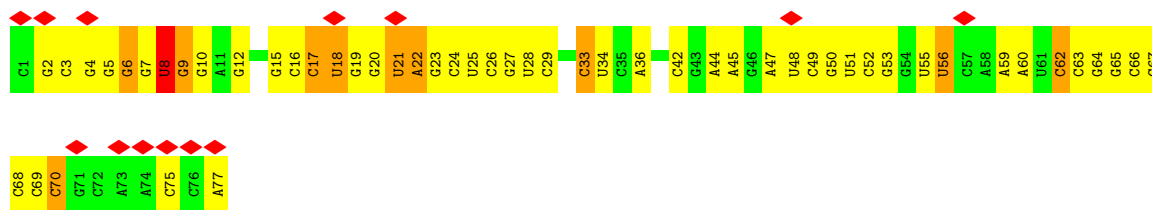
- Molecule 22: 30S ribosomal protein S21

Chain V:  76% 21%



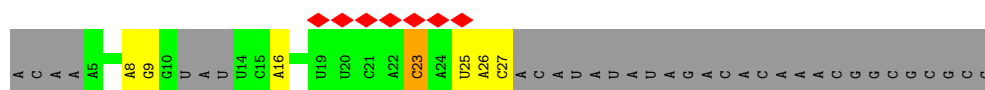
- Molecule 23: tRNA(fmet) P-site

Chain W:  17% 31% 55% 13%



- Molecule 24: mRNA

Chain X:  13% 25% 11% 62%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20551	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 ($e^-/\text{\AA}^2$)	49.95	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	1.745	Depositor
Minimum map value	-0.554	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.253	Depositor
Map size (Å)	420.0, 420.0, 420.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4OC, PSU, MA6, UR3, 2MG, H2U, 5MU, D2T, 5MC, OMC, MG, G7M, 4SU

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	0.28	0/36692	0.29	0/57230
2	B	0.10	0/1102	0.26	0/1504
3	C	0.21	0/1796	0.32	0/2420
4	D	0.25	0/1680	0.30	0/2263
5	E	0.23	0/1665	0.31	0/2227
6	F	0.25	0/1165	0.34	0/1568
7	G	0.23	0/867	0.34	0/1171
8	H	0.20	0/1219	0.31	0/1635
9	I	0.25	0/989	0.31	0/1326
10	J	0.26	0/1043	0.35	0/1387
11	K	0.24	0/818	0.34	0/1105
12	L	0.23	0/893	0.30	0/1205
13	M	0.26	0/954	0.34	0/1279
14	N	0.22	0/900	0.34	0/1204
15	O	0.26	0/817	0.27	0/1088
16	P	0.22	0/722	0.27	0/964
17	Q	0.27	0/659	0.29	0/884
18	R	0.21	0/657	0.29	0/881
19	S	0.24	0/563	0.33	0/754
20	T	0.25	0/680	0.27	0/915
21	U	0.22	0/676	0.28	0/895
22	V	0.17	0/598	0.27	0/792
23	W	0.21	0/1725	0.32	0/2687
24	X	0.15	0/476	0.23	0/737
All	All	0.26	0/59356	0.30	0/88121

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	33023	0	16643	512	0
2	B	1094	0	866	28	0
3	C	1765	0	1792	37	0
4	D	1653	0	1727	22	0
5	E	1643	0	1707	32	0
6	F	1152	0	1196	19	0
7	G	848	0	846	29	0
8	H	1203	0	1254	20	0
9	I	979	0	1031	17	0
10	J	1031	0	1076	16	0
11	K	808	0	845	26	0
12	L	877	0	887	23	0
13	M	951	0	1010	20	0
14	N	891	0	952	19	0
15	O	805	0	844	24	0
16	P	714	0	734	5	0
17	Q	649	0	666	18	0
18	R	648	0	691	10	0
19	S	554	0	573	9	0
20	T	663	0	688	16	0
21	U	670	0	719	11	0
22	V	590	0	629	10	0
23	W	1645	0	842	45	0
24	X	427	0	217	4	0
25	A	127	0	0	0	0
25	X	1	0	0	0	0
All	All	55411	0	38435	867	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 9.

The worst 5 of 867 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:1425:U:H3	1:A:1475:G:H1	1.05	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1006:G:H1	1:A:1023:U:H3	1.21	0.88
23:W:8:4SU:H5'	23:W:50:G:H5'	1.55	0.85
1:A:1418:A:N6	1:A:1482:G:O2'	2.08	0.85
1:A:1423:G:H1	1:A:1477:U:H3	1.24	0.85

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	170/557 (30%)	161 (95%)	8 (5%)	1 (1%)	21	52
3	C	224/241 (93%)	208 (93%)	16 (7%)	0	100	100
4	D	209/233 (90%)	201 (96%)	8 (4%)	0	100	100
5	E	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
6	F	154/156 (99%)	140 (91%)	14 (9%)	0	100	100
7	G	102/131 (78%)	97 (95%)	5 (5%)	0	100	100
8	H	151/156 (97%)	140 (93%)	11 (7%)	0	100	100
9	I	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
10	J	126/130 (97%)	114 (90%)	12 (10%)	0	100	100
11	K	99/103 (96%)	95 (96%)	3 (3%)	1 (1%)	12	41
12	L	115/129 (89%)	106 (92%)	9 (8%)	0	100	100
13	M	119/124 (96%)	107 (90%)	11 (9%)	1 (1%)	16	47
14	N	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
15	O	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
16	P	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
17	Q	80/82 (98%)	80 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	78/84 (93%)	73 (94%)	5 (6%)	0	100	100
19	S	65/75 (87%)	59 (91%)	5 (8%)	1 (2%)	8	32
20	T	81/92 (88%)	81 (100%)	0	0	100	100
21	U	84/87 (97%)	84 (100%)	0	0	100	100
22	V	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
All	All	2552/3095 (82%)	2421 (95%)	127 (5%)	4 (0%)	44	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	172	ALA
19	S	23	TYR
13	M	88	LYS
11	K	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	
2	B	74/461 (16%)	70 (95%)	4 (5%)	20	50
3	C	187/199 (94%)	177 (95%)	10 (5%)	20	51
4	D	172/190 (90%)	164 (95%)	8 (5%)	23	55
5	E	172/173 (99%)	164 (95%)	8 (5%)	23	55
6	F	119/119 (100%)	118 (99%)	1 (1%)	73	81
7	G	91/112 (81%)	86 (94%)	5 (6%)	19	50
8	H	126/129 (98%)	121 (96%)	5 (4%)	28	60
9	I	104/105 (99%)	100 (96%)	4 (4%)	29	60
10	J	106/107 (99%)	99 (93%)	7 (7%)	15	43
11	K	88/90 (98%)	85 (97%)	3 (3%)	32	63
12	L	90/99 (91%)	84 (93%)	6 (7%)	15	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	102/103 (99%)	97 (95%)	5 (5%)	22	53
14	N	93/96 (97%)	89 (96%)	4 (4%)	26	57
15	O	83/84 (99%)	80 (96%)	3 (4%)	31	62
16	P	76/77 (99%)	75 (99%)	1 (1%)	61	77
17	Q	65/65 (100%)	63 (97%)	2 (3%)	35	64
18	R	74/78 (95%)	67 (90%)	7 (10%)	8	30
19	S	58/65 (89%)	56 (97%)	2 (3%)	32	63
20	T	72/79 (91%)	70 (97%)	2 (3%)	38	66
21	U	65/66 (98%)	62 (95%)	3 (5%)	24	55
22	V	60/61 (98%)	56 (93%)	4 (7%)	15	43
All	All	2077/2558 (81%)	1983 (96%)	94 (4%)	26	56

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	40	ASN
15	O	61	ARG
12	L	74	VAL
13	M	112	GLN
17	Q	55	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
11	K	4	GLN
16	P	35	GLN
21	U	70	ASN
15	O	49	GLN
17	Q	18	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1537/1541 (99%)	229 (14%)	2 (0%)
23	W	76/77 (98%)	16 (21%)	1 (1%)
24	X	18/53 (33%)	4 (22%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	1631/1671 (97%)	249 (15%)	3 (0%)

5 of 249 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	U
1	A	9	G
1	A	32	A
1	A	39	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	641	U
1	A	1533	C
23	W	20	G

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

17 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	UR3	A	1498	1,25	19,22,23	2.65	8 (42%)	26,32,35	1.57	2 (7%)
1	2MG	A	1516	1	23,26,27	2.84	9 (39%)	33,38,41	2.99	11 (33%)
1	MA6	A	1518	1	23,26,27	1.61	6 (26%)	33,38,41	3.59	11 (33%)
23	OMC	W	33	23	19,22,23	2.77	8 (42%)	25,31,34	0.65	0
23	PSU	W	56	23	18,21,22	1.00	1 (5%)	21,30,33	1.94	5 (23%)
13	D2T	M	89	13	8,9,10	1.61	1 (12%)	6,11,13	2.22	2 (33%)
1	PSU	A	516	1,25	18,21,22	1.10	3 (16%)	21,30,33	1.93	5 (23%)
23	5MU	W	55	23	19,22,23	1.42	6 (31%)	27,32,35	2.04	6 (22%)
1	2MG	A	966	1	23,26,27	2.84	9 (39%)	33,38,41	3.06	12 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4OC	A	1402	1	20,23,24	3.42	9 (45%)	25,32,35	0.89	1 (4%)
23	H2U	W	21	23	18,21,22	2.83	5 (27%)	19,30,33	1.58	4 (21%)
1	G7M	A	527	1	23,26,27	2.52	10 (43%)	34,39,42	2.98	11 (32%)
1	2MG	A	1207	1	23,26,27	2.88	9 (39%)	33,38,41	3.01	11 (33%)
1	5MC	A	967	1	19,22,23	4.21	8 (42%)	26,32,35	1.05	2 (7%)
1	MA6	A	1519	1	23,26,27	1.62	6 (26%)	33,38,41	3.70	11 (33%)
23	4SU	W	8	23	18,21,22	4.09	8 (44%)	25,30,33	2.44	6 (24%)
1	5MC	A	1407	1	19,22,23	4.21	8 (42%)	26,32,35	0.94	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
1	UR3	A	1498	1,25	-	0/7/25/26	0/2/2/2
1	2MG	A	1516	1	-	2/9/27/28	0/3/3/3
1	MA6	A	1518	1	-	0/11/29/30	0/3/3/3
23	OMC	W	33	23	-	1/9/27/28	0/2/2/2
23	PSU	W	56	23	-	0/7/25/26	0/2/2/2
13	D2T	M	89	13	-	1/7/12/14	-
1	PSU	A	516	1,25	-	0/7/25/26	0/2/2/2
23	5MU	W	55	23	-	0/7/25/26	0/2/2/2
1	2MG	A	966	1	-	2/9/27/28	0/3/3/3
1	4OC	A	1402	1	-	1/9/29/30	0/2/2/2
23	H2U	W	21	23	-	7/7/38/39	0/2/2/2
1	G7M	A	527	1	-	3/7/25/26	0/3/3/3
1	2MG	A	1207	1	-	2/9/27/28	0/3/3/3
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	3/11/29/30	0/3/3/3
23	4SU	W	8	23	-	2/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	2/7/25/26	0/2/2/2

The worst 5 of 114 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	967	5MC	C6-C5	9.97	1.50	1.34
1	A	1407	5MC	C6-C5	9.94	1.50	1.34
23	W	8	4SU	C4-N3	9.07	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C2-N3	8.44	1.48	1.32
23	W	21	H2U	C2-N1	8.40	1.47	1.35

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1519	MA6	N1-C6-N6	-14.24	99.50	116.86
1	A	1518	MA6	N1-C6-N6	-13.76	100.09	116.86
1	A	1519	MA6	C5-C6-N6	9.65	140.60	125.33
1	A	1518	MA6	C5-C6-N6	9.43	140.25	125.33
1	A	966	2MG	C1'-N9-C8	-9.15	100.73	126.73

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1207	2MG	O4'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
23	W	21	H2U	O4'-C1'-N1-C6
23	W	33	OMC	C1'-C2'-O2'-CM2
1	A	527	G7M	C3'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1516	2MG	1	0
1	A	1518	MA6	2	0
23	W	33	OMC	3	0
23	W	56	PSU	1	0
1	A	1402	4OC	2	0
1	A	1207	2MG	1	0
1	A	1519	MA6	2	0
23	W	8	4SU	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 128 ligands modelled in this entry, 128 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

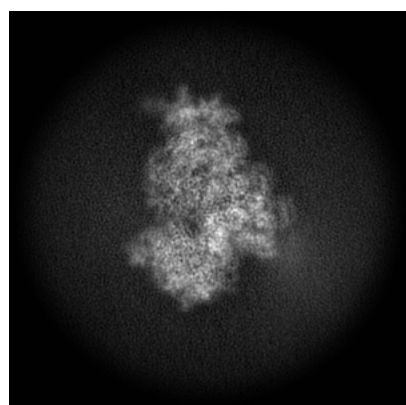
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51616. These allow visual inspection of the internal detail of the map and identification of artifacts.

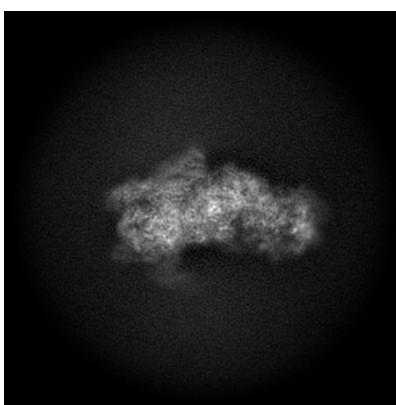
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

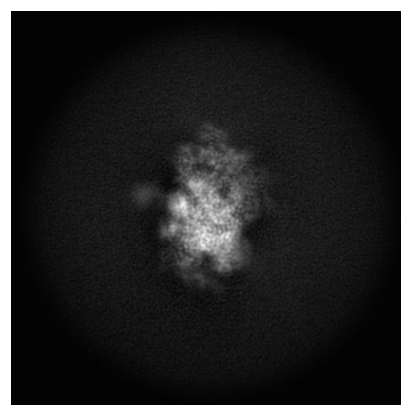
6.1.1 Primary map



X



Y

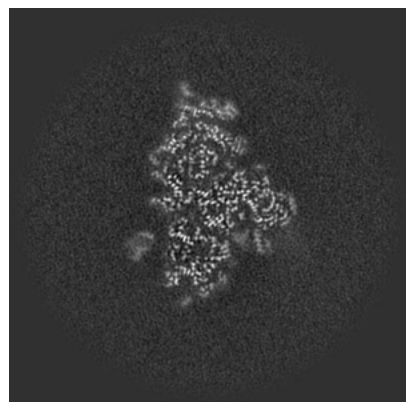


Z

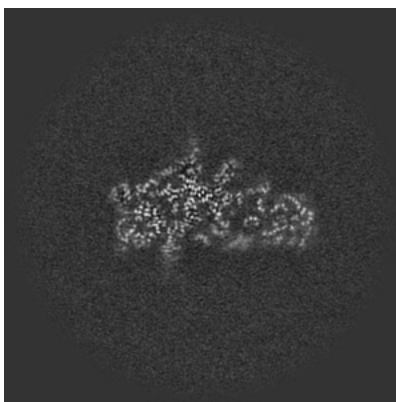
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

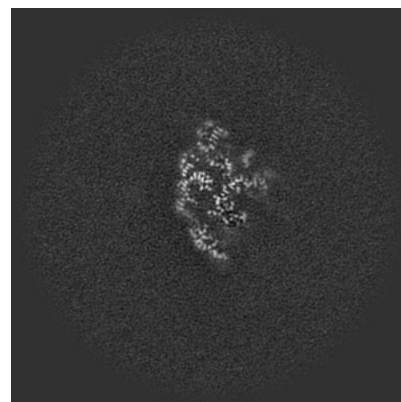
6.2.1 Primary map



X Index: 250



Y Index: 250

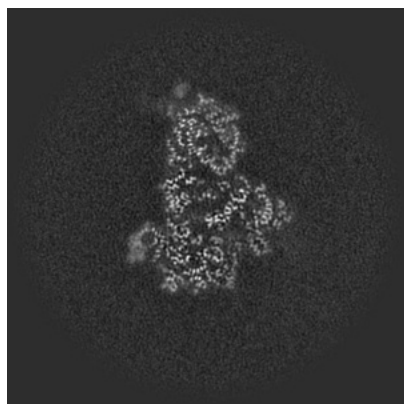


Z Index: 250

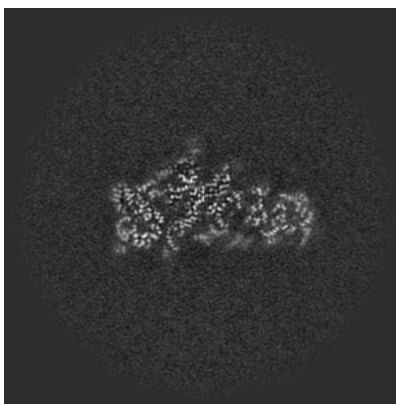
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

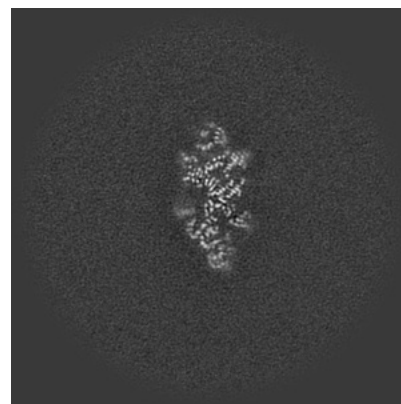
6.3.1 Primary map



X Index: 238



Y Index: 248

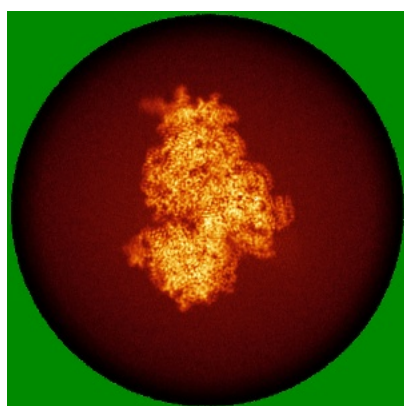


Z Index: 257

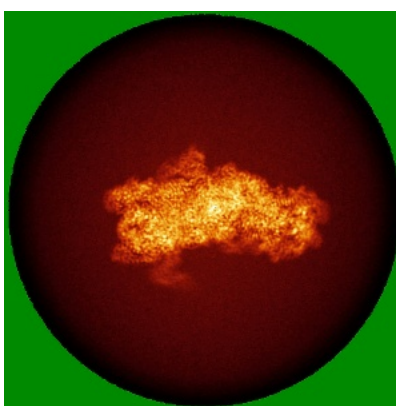
The images above show the largest variance slices of the map in three orthogonal directions.

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

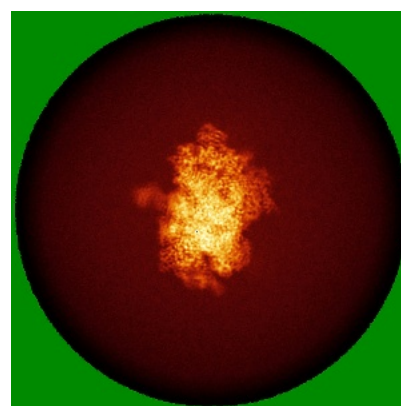
6.4.1 Primary map



X



Y

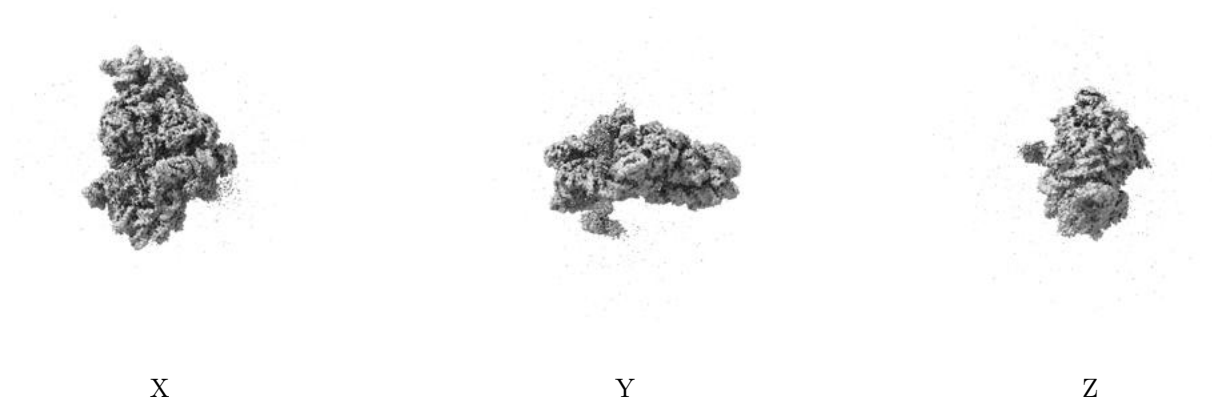


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.253. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

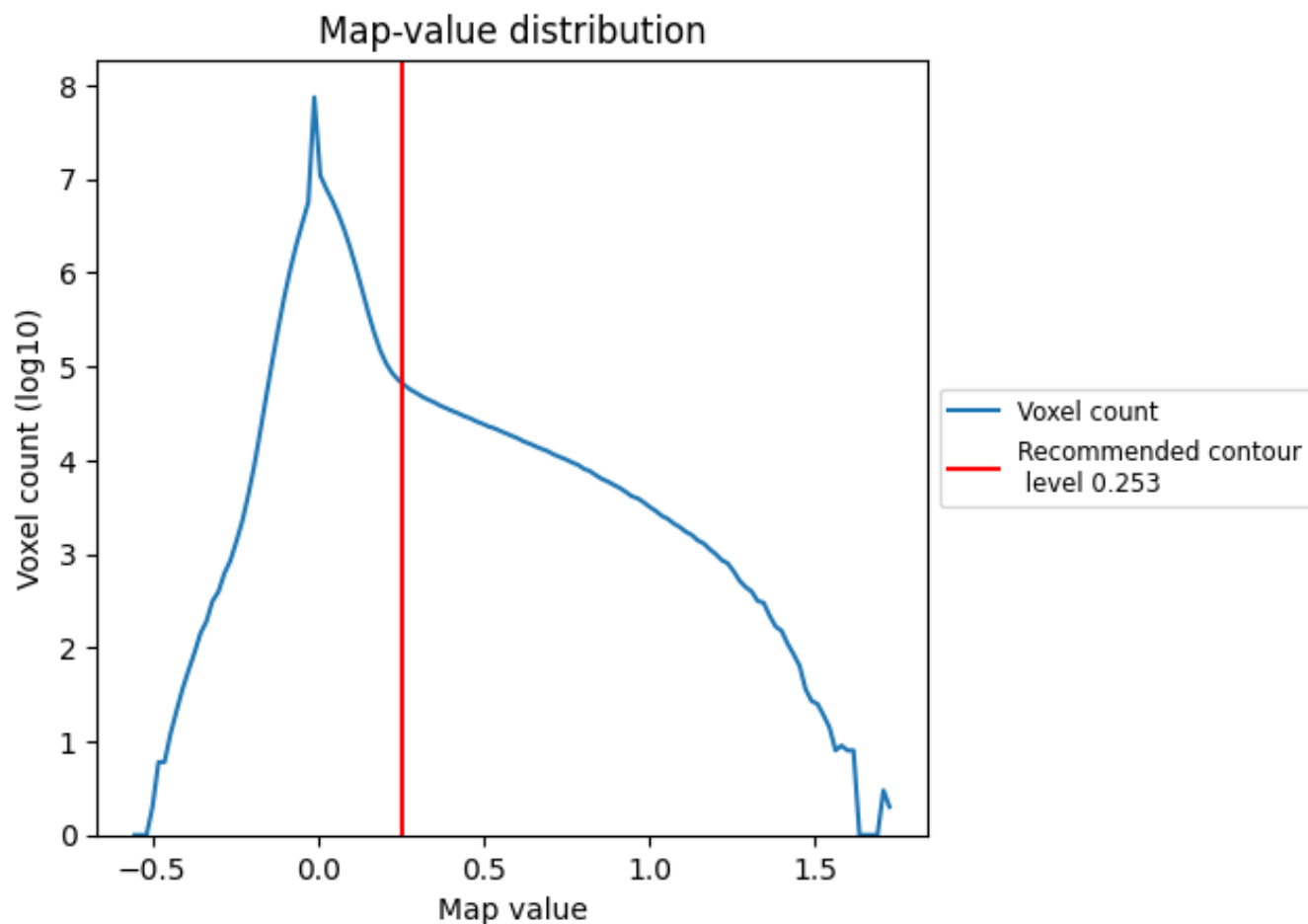
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

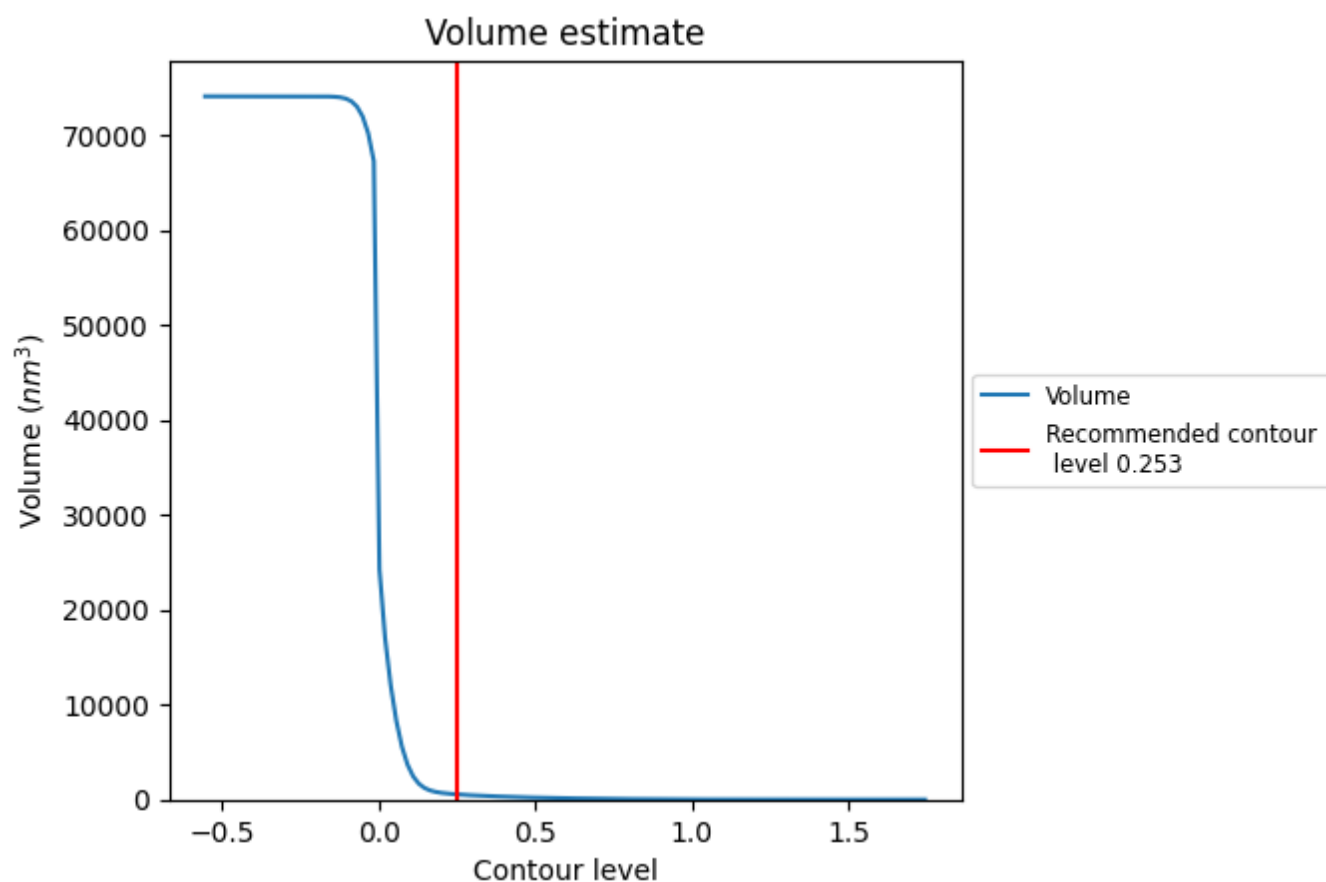
This section contains the results of statistical analysis of the map.

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.

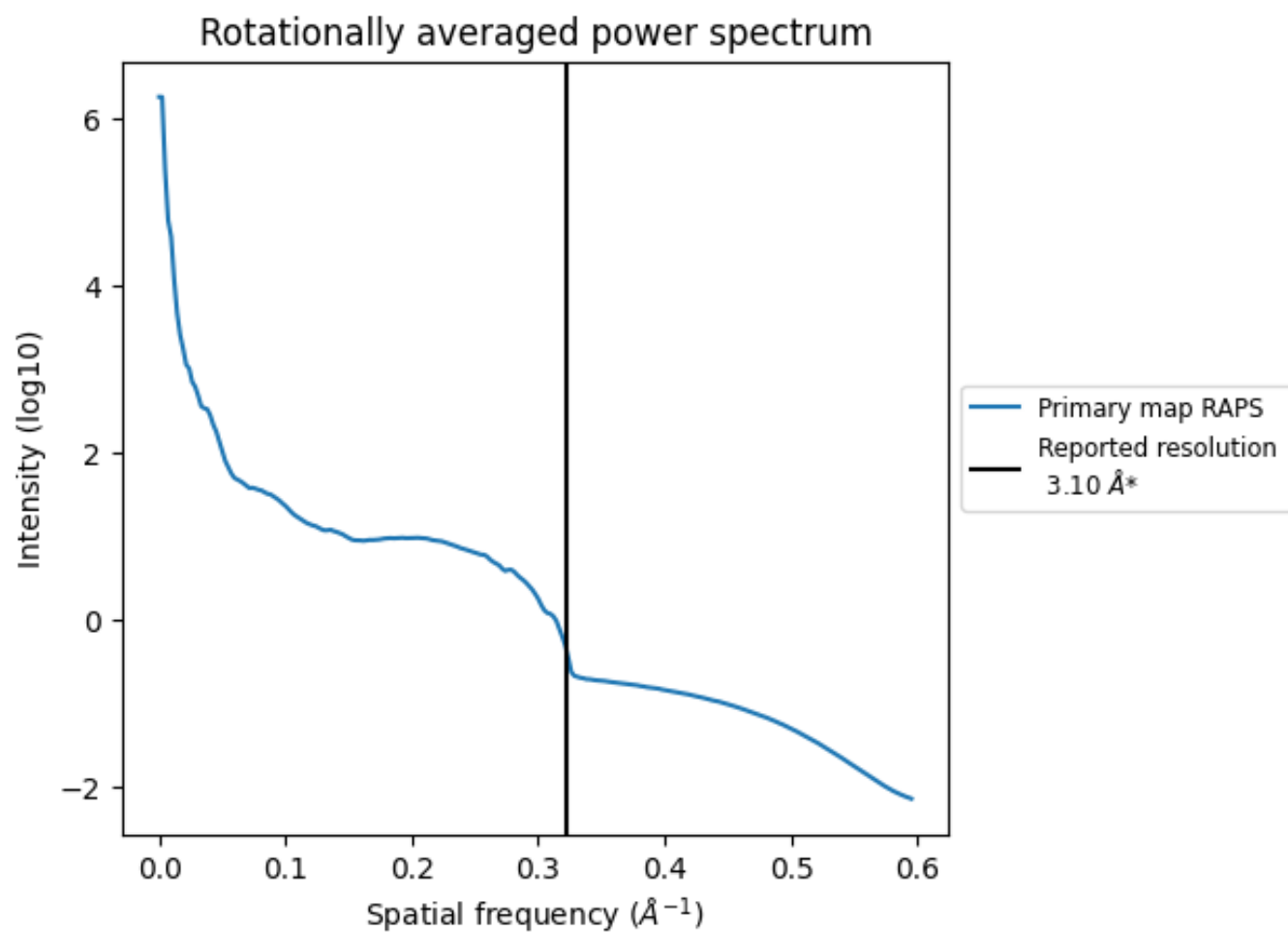
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 541 nm³; this corresponds to an approximate mass of 489 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 0.323 Å⁻¹

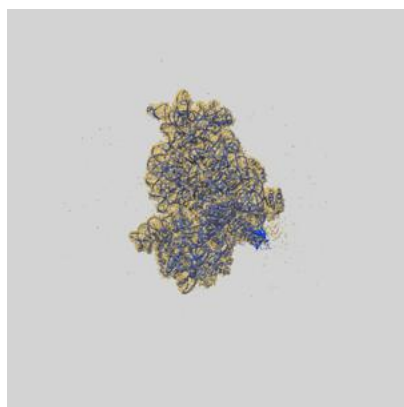
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

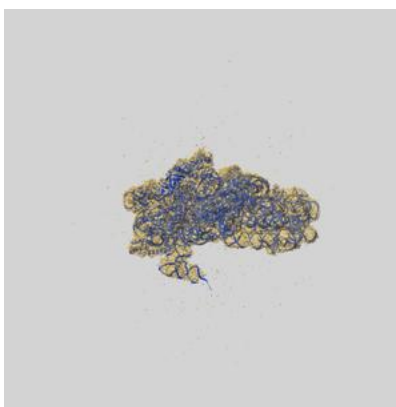
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51616 and PDB model 9GUQ. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

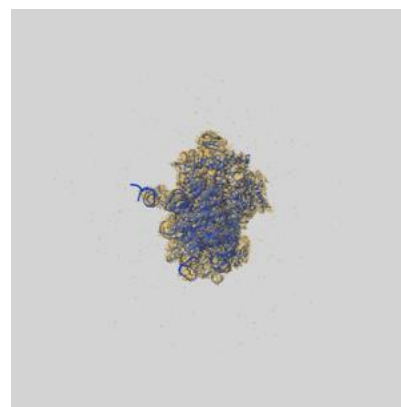
9.1 Map-model overlay [i](#)



X



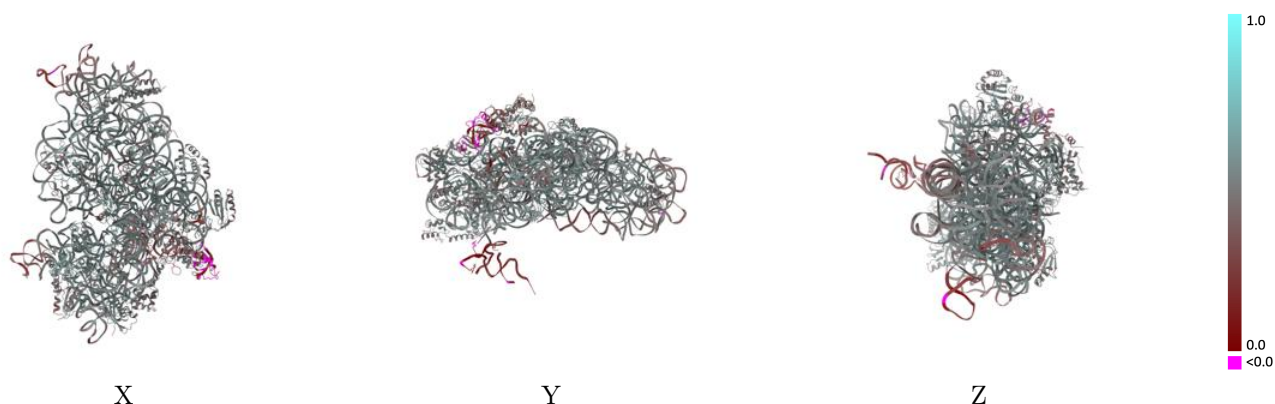
Y



Z

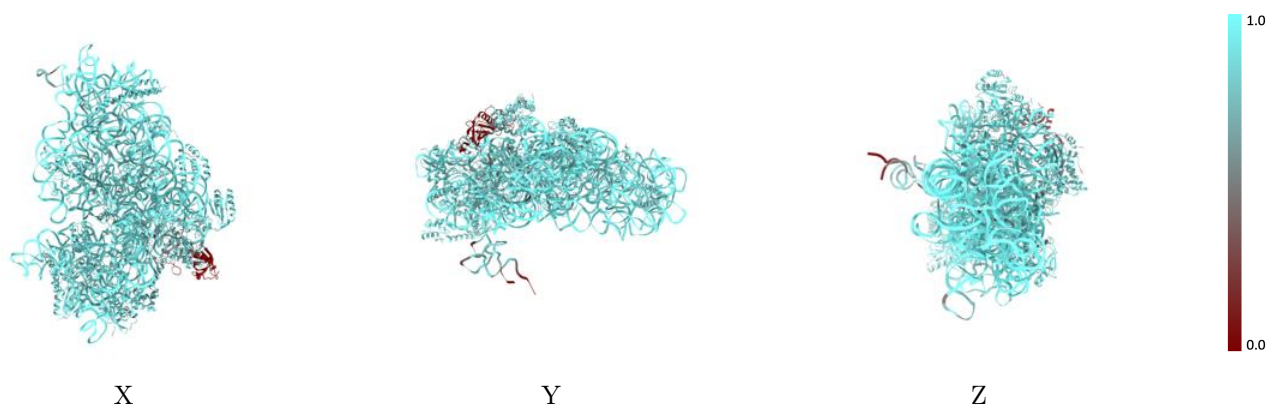
The images above show the 3D surface view of the map at the recommended contour level 0.253 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



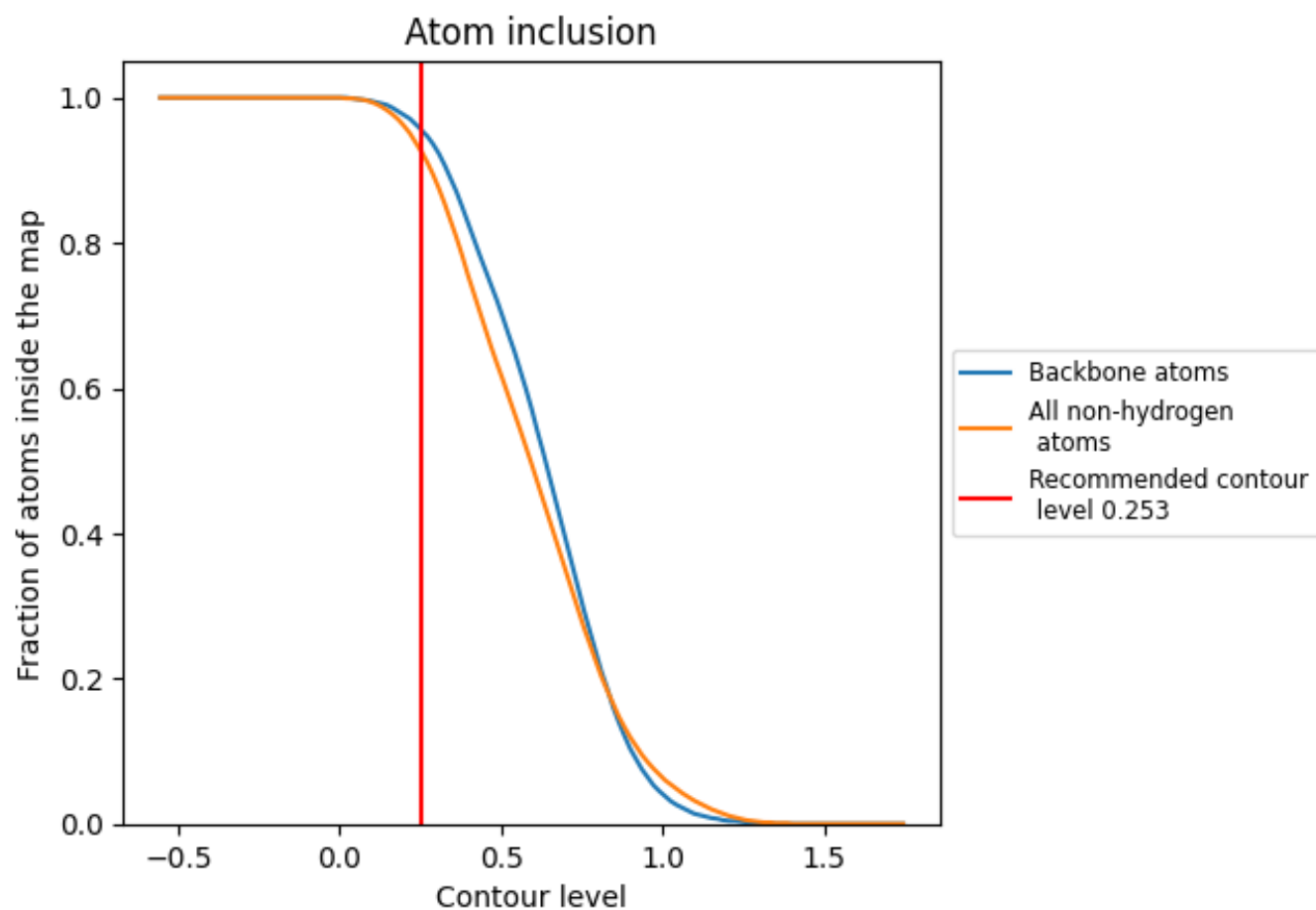
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.253).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% 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 (0.253) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9260	 0.4870
A	 0.9840	 0.5000
B	 0.3630	 0.2480
C	 0.8600	 0.4740
D	 0.8890	 0.5220
E	 0.8880	 0.5010
F	 0.8880	 0.5240
G	 0.8830	 0.4770
H	 0.8550	 0.4700
I	 0.8930	 0.5350
J	 0.9010	 0.5150
K	 0.8570	 0.4880
L	 0.8860	 0.5000
M	 0.9030	 0.5300
N	 0.8910	 0.4820
O	 0.9160	 0.5300
P	 0.8990	 0.4980
Q	 0.9110	 0.5150
R	 0.8700	 0.4990
S	 0.8710	 0.5010
T	 0.9230	 0.5100
U	 0.8990	 0.4790
V	 0.7700	 0.4510
W	 0.7240	 0.2640
X	 0.5940	 0.3110

