



Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 01:50 PM EST

PDB ID : 6V3E
EMDB ID : EMD-21034
Title : Cryo-EM structure of the Acinetobacter baumannii Ribosome: 30S subunit
Authors : Morgan, C.E.; Yu, E.W.
Deposited on : 2019-11-25
Resolution : 4.40 Å (reported)
Based on initial model : 5AFI

This is a Full wwPDB EM Validation 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:

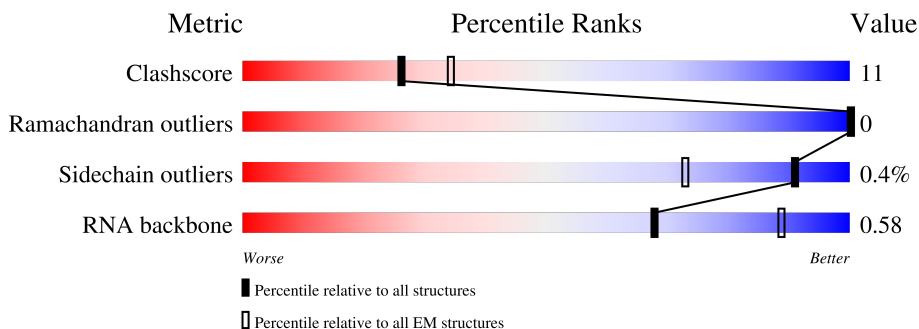
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 4.40 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.



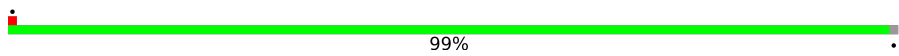
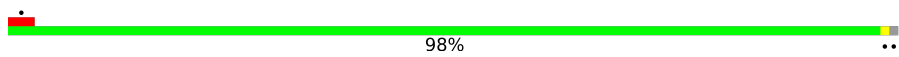
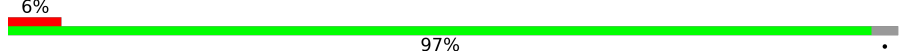

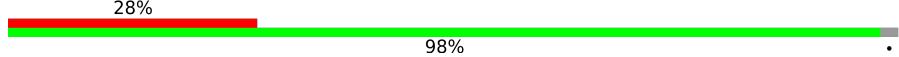
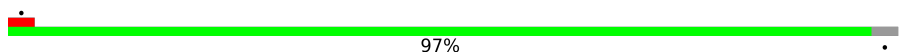
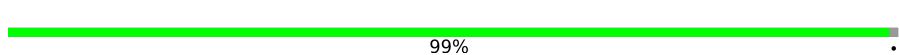
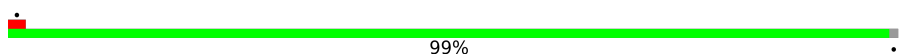

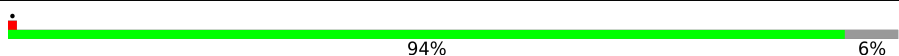
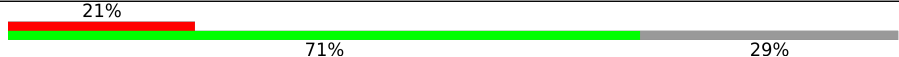
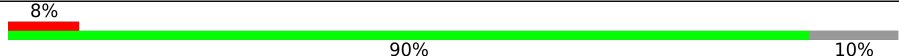
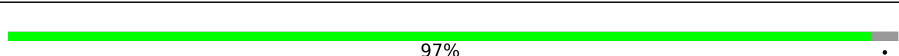
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. 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	sN1	1544	
2	b	250	
3	c	250	
4	d	208	
5	e	165	
6	f	127	
7	g	156	

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Mol	Chain	Length	Quality of chain
8	h	131	 99%
9	i	128	 98%
10	j	103	 97%
11	k	128	 89%
12	l	124	 98%
13	m	118	 97%
14	n	101	 99%
15	o	89	 99%
16	p	101	 81%
17	q	85	 94%
18	r	75	 71%
19	s	91	 90%
20	t	88	 97%

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 50850 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
			Total	C	N	O	P		
1	sN1	1528	32782	14631	5994	10630	1527	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	225	1769	1110	328	325	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	215	1690	1065	318	299	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	207	1631	1017	313	299	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	155	1129	700	217	207	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	94	793	499	147	143	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	g	133	1047	657	193	191	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	h	130	985	615	177	187	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	i	127	995	621	198	175	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	j	100	801	500	150	148	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	k	117	862	535	167	159	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	l	122	945	580	193	167	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	m	115	903	558	184	158	3	0	0

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			792	493	158	137	4		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			705	434	144	126	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	83	Total	C	N	O	S	0	0
			649	406	129	113	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			630	396	118	115	1		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	53	Total	C	N	O	0	0
			438	282	75	81		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	82	Total	C	N	O	S	0	0
			646	412	125	107	2		

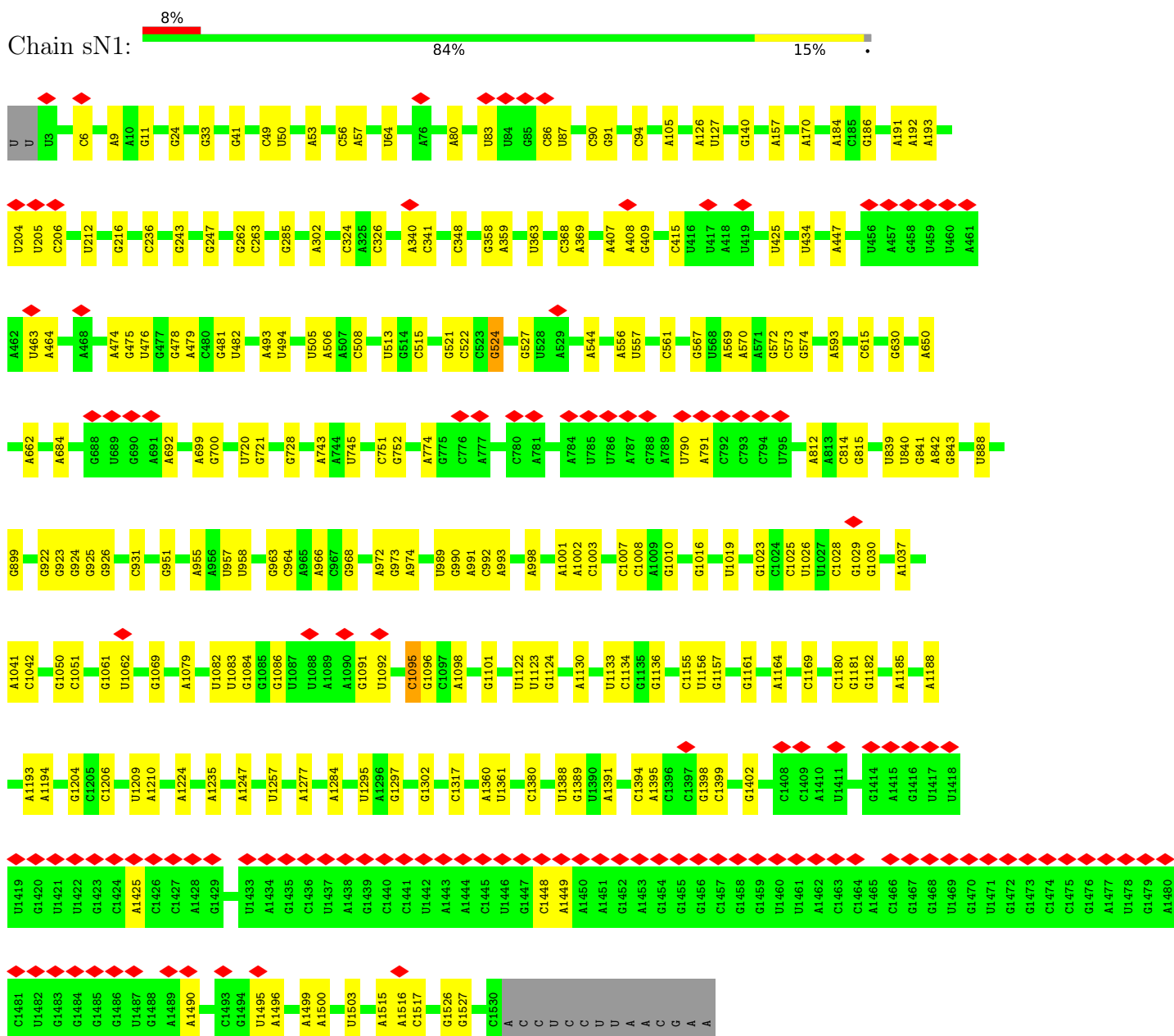
- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	85	Total	C	N	O	S	0	0
			658	406	138	112	2		

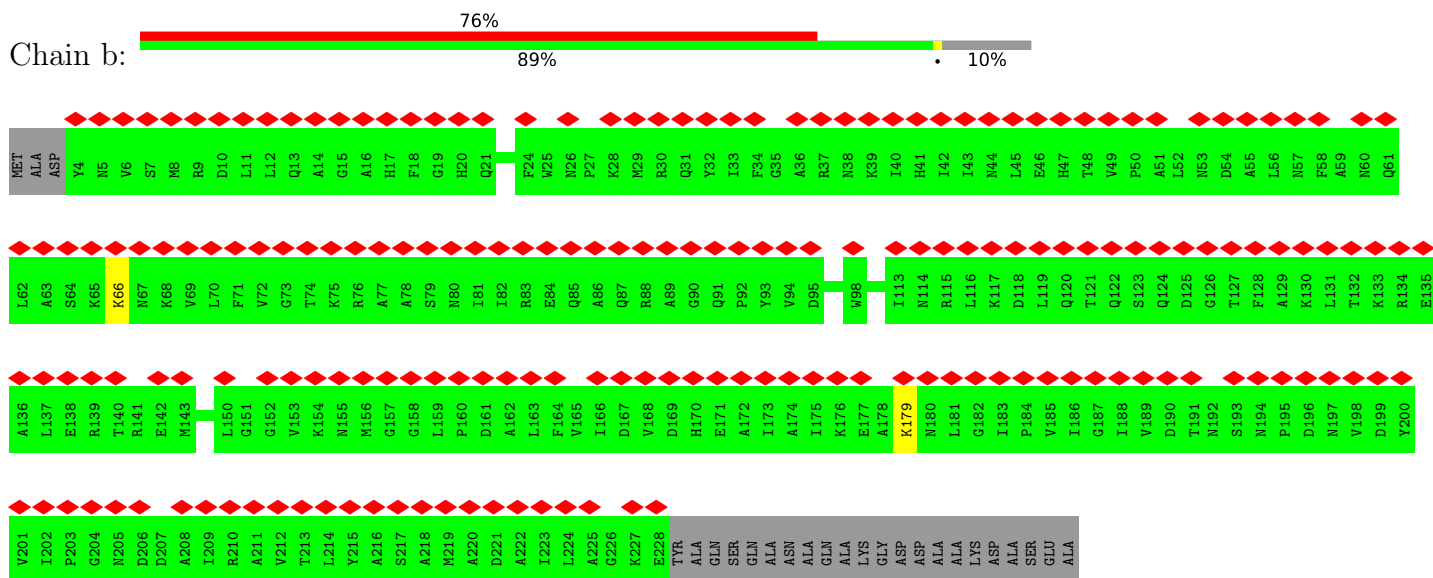
3 Residue-property plots

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.

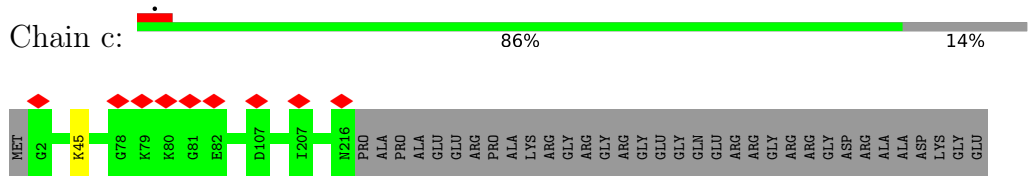
- Molecule 1: 16s Ribosomal RNA



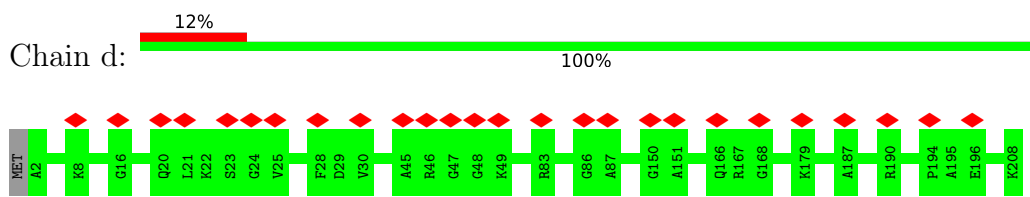
• Molecule 2: 30S ribosomal protein S2



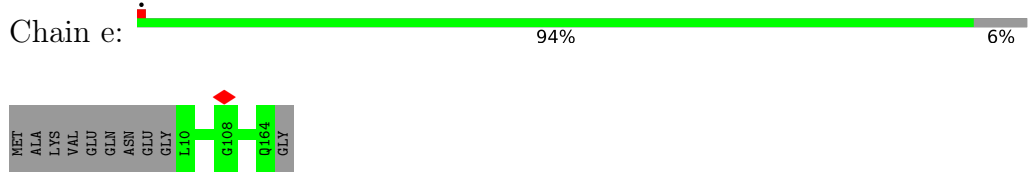
• Molecule 3: 30S ribosomal protein S3



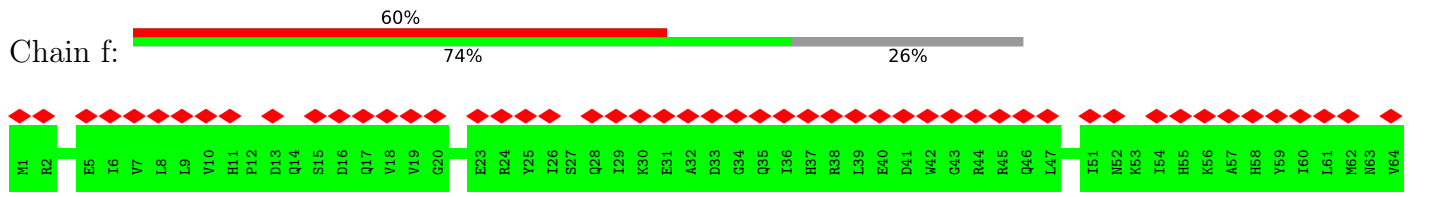
• Molecule 4: 30S ribosomal protein S4

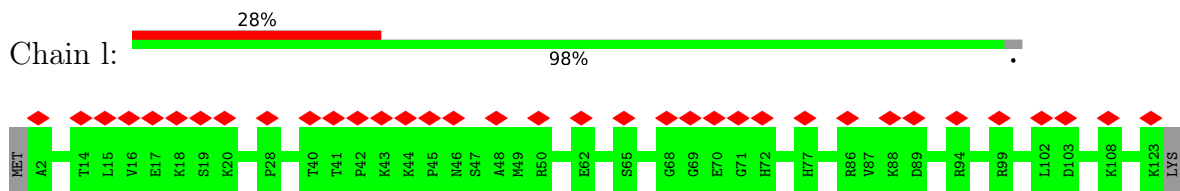


• Molecule 5: 30S ribosomal protein S5

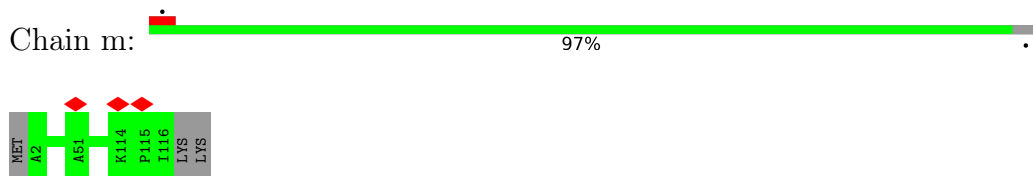


• Molecule 6: 30S ribosomal protein S6

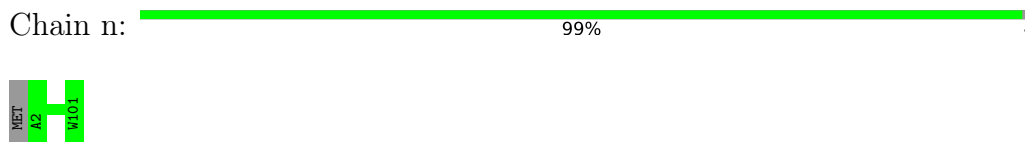




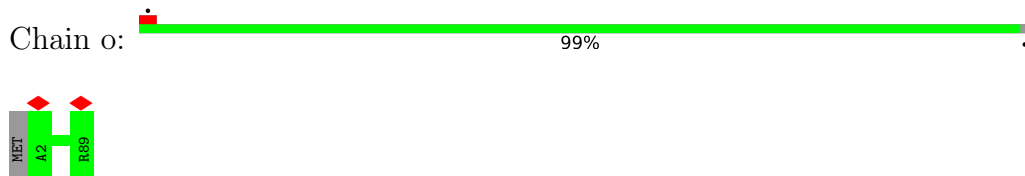
• Molecule 13: 30S ribosomal protein S13



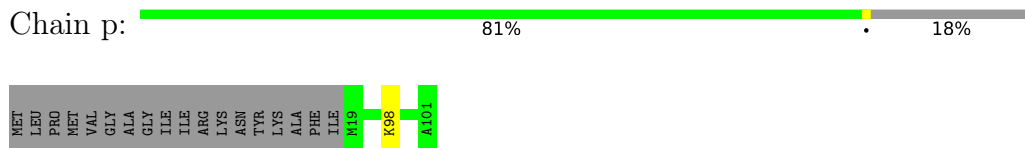
• Molecule 14: 30S ribosomal protein S14



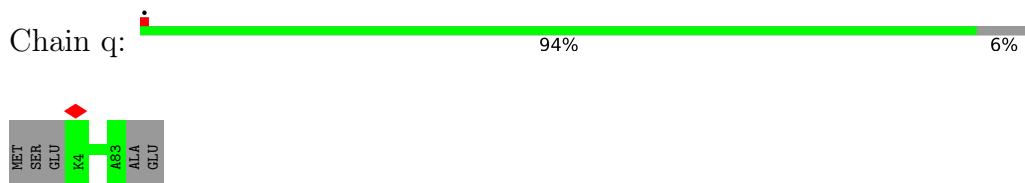
• Molecule 15: 30S ribosomal protein S15



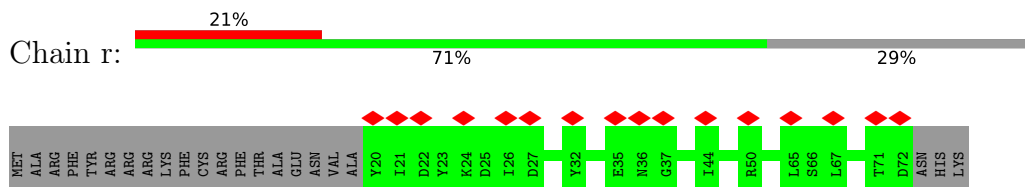
• Molecule 16: 30S ribosomal protein S16



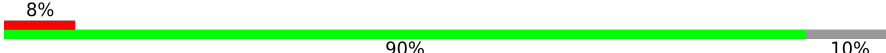
• Molecule 17: 30S ribosomal protein S17

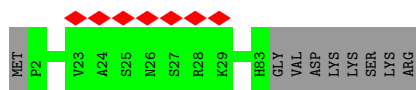


• Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19

Chain s:  8% 90% 10%



- Molecule 20: 30S ribosomal protein S20

Chain t:  97%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10555	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 ($e^-/\text{\AA}^2$)	40	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	1.777	Depositor
Minimum map value	-0.324	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	544.768, 544.768, 544.768	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	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, 2MG, 5MC, PSU, 7MG, MA6, UR3

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	sN1	0.18	0/36476	0.75	6/56895 (0.0%)
2	b	0.25	0/1799	0.46	0/2429
3	c	0.23	0/1714	0.41	0/2304
4	d	0.24	0/1653	0.41	0/2213
5	e	0.25	0/1141	0.44	0/1537
6	f	0.22	0/808	0.43	0/1089
7	g	0.23	0/1062	0.39	0/1424
8	h	0.24	0/993	0.41	0/1331
9	i	0.24	0/1006	0.42	0/1346
10	j	0.23	0/811	0.44	0/1096
11	k	0.24	0/878	0.43	0/1189
12	l	0.25	0/958	0.45	0/1284
13	m	0.22	0/913	0.41	0/1226
14	n	0.23	0/803	0.39	0/1071
15	o	0.22	0/715	0.35	0/958
16	p	0.24	0/660	0.41	0/886
17	q	0.23	0/637	0.44	0/858
18	r	0.22	0/445	0.38	0/601
19	s	0.24	0/664	0.42	0/897
20	t	0.23	0/664	0.33	0/885
All	All	0.20	0/54800	0.67	6/81519 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	sN1	415	C	N3-C2-O2	-7.27	116.81	121.90
1	sN1	1095	C	N1-C2-O2	6.23	122.64	118.90
1	sN1	1095	C	N3-C2-O2	-6.23	117.54	121.90
1	sN1	751	C	C2-N1-C1'	5.25	124.58	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	sN1	1155	C	C2-N1-C1'	5.25	124.57	118.80
1	sN1	1155	C	N1-C2-O2	5.19	122.02	118.90

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	sN1	32782	0	16508	0	0
2	b	1769	0	1787	0	0
3	c	1690	0	1774	0	0
4	d	1631	0	1691	0	0
5	e	1129	0	1174	0	0
6	f	793	0	788	0	0
7	g	1047	0	1088	0	0
8	h	985	0	1047	0	0
9	i	995	0	1053	0	0
10	j	801	0	832	0	0
11	k	862	0	877	0	0
12	l	945	0	996	0	0
13	m	903	0	962	0	0
14	n	792	0	833	0	0
15	o	705	0	712	0	0
16	p	649	0	660	0	0
17	q	630	0	678	0	0
18	r	438	0	456	0	0
19	s	646	0	663	0	0
20	t	658	0	710	0	0
All	All	50850	0	35289	0	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 11.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	223/250 (89%)	212 (95%)	11 (5%)	0	100	100
3	c	213/250 (85%)	210 (99%)	3 (1%)	0	100	100
4	d	205/208 (99%)	203 (99%)	2 (1%)	0	100	100
5	e	153/165 (93%)	149 (97%)	4 (3%)	0	100	100
6	f	92/127 (72%)	87 (95%)	5 (5%)	0	100	100
7	g	131/156 (84%)	130 (99%)	1 (1%)	0	100	100
8	h	128/131 (98%)	124 (97%)	4 (3%)	0	100	100
9	i	125/128 (98%)	122 (98%)	3 (2%)	0	100	100
10	j	98/103 (95%)	93 (95%)	5 (5%)	0	100	100
11	k	115/128 (90%)	112 (97%)	3 (3%)	0	100	100
12	l	120/124 (97%)	116 (97%)	4 (3%)	0	100	100
13	m	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
14	n	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
15	o	86/89 (97%)	86 (100%)	0	0	100	100
16	p	81/101 (80%)	81 (100%)	0	0	100	100
17	q	78/85 (92%)	76 (97%)	2 (3%)	0	100	100
18	r	51/75 (68%)	51 (100%)	0	0	100	100
19	s	80/91 (88%)	79 (99%)	1 (1%)	0	100	100
20	t	83/88 (94%)	83 (100%)	0	0	100	100
All	All	2273/2518 (90%)	2219 (98%)	54 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	185/200 (92%)	183 (99%)	2 (1%)	73	85
3	c	175/198 (88%)	174 (99%)	1 (1%)	86	92
4	d	170/171 (99%)	170 (100%)	0	100	100
5	e	113/120 (94%)	113 (100%)	0	100	100
6	f	86/111 (78%)	86 (100%)	0	100	100
7	g	110/128 (86%)	110 (100%)	0	100	100
8	h	108/109 (99%)	108 (100%)	0	100	100
9	i	99/100 (99%)	98 (99%)	1 (1%)	76	86
10	j	89/91 (98%)	89 (100%)	0	100	100
11	k	88/98 (90%)	85 (97%)	3 (3%)	37	61
12	l	104/106 (98%)	104 (100%)	0	100	100
13	m	95/98 (97%)	95 (100%)	0	100	100
14	n	81/82 (99%)	81 (100%)	0	100	100
15	o	71/72 (99%)	71 (100%)	0	100	100
16	p	63/77 (82%)	62 (98%)	1 (2%)	62	79
17	q	72/76 (95%)	72 (100%)	0	100	100
18	r	47/66 (71%)	47 (100%)	0	100	100
19	s	70/78 (90%)	70 (100%)	0	100	100
20	t	65/67 (97%)	65 (100%)	0	100	100
All	All	1891/2048 (92%)	1883 (100%)	8 (0%)	91	94

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	66	LYS
2	b	179	LYS
3	c	45	LYS
9	i	104	ARG

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Mol	Chain	Res	Type
11	k	55	ARG
11	k	71	LYS
11	k	79	LYS
16	p	98	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	5	ASN
2	b	41	HIS
2	b	57	ASN
2	b	120	GLN
2	b	122	GLN
2	b	180	ASN
3	c	18	HIS
3	c	28	GLN
4	d	73	GLN
4	d	102	ASN
4	d	118	GLN
4	d	138	GLN
4	d	154	GLN
5	e	121	ASN
6	f	11	HIS
6	f	35	GLN
6	f	52	ASN
6	f	55	HIS
6	f	94	HIS
7	g	21	GLN
7	g	29	HIS
7	g	32	GLN
8	h	53	GLN
9	i	4	ASN
10	j	56	HIS
10	j	58	ASN
11	k	118	ASN
13	m	52	GLN
14	n	8	ASN
14	n	82	ASN
15	o	42	HIS
17	q	32	HIS
18	r	54	GLN
19	s	83	HIS

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Mol	Chain	Res	Type
20	t	13	GLN
20	t	21	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	sN1	1524/1544 (98%)	222 (14%)	0

All (222) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	sN1	6	C
1	sN1	9	A
1	sN1	11	G
1	sN1	24	G
1	sN1	33	G
1	sN1	41	G
1	sN1	49	C
1	sN1	50	U
1	sN1	53	A
1	sN1	56	C
1	sN1	57	A
1	sN1	64	U
1	sN1	80	A
1	sN1	83	U
1	sN1	86	C
1	sN1	87	U
1	sN1	90	C
1	sN1	91	G
1	sN1	94	C
1	sN1	105	A
1	sN1	126	A
1	sN1	127	U
1	sN1	140	G
1	sN1	157	A
1	sN1	170	A
1	sN1	184	A
1	sN1	186	G
1	sN1	191	A
1	sN1	192	A
1	sN1	193	A

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Mol	Chain	Res	Type
1	sN1	204	U
1	sN1	205	U
1	sN1	206	C
1	sN1	212	U
1	sN1	216	G
1	sN1	236	C
1	sN1	243	G
1	sN1	247	G
1	sN1	262	G
1	sN1	263	C
1	sN1	285	G
1	sN1	302	A
1	sN1	324	C
1	sN1	326	C
1	sN1	340	A
1	sN1	341	C
1	sN1	348	C
1	sN1	358	G
1	sN1	359	A
1	sN1	363	U
1	sN1	368	C
1	sN1	369	A
1	sN1	407	A
1	sN1	408	A
1	sN1	409	G
1	sN1	425	U
1	sN1	434	U
1	sN1	447	A
1	sN1	463	U
1	sN1	464	A
1	sN1	474	A
1	sN1	475	G
1	sN1	476	U
1	sN1	478	G
1	sN1	479	A
1	sN1	481	G
1	sN1	482	U
1	sN1	493	A
1	sN1	494	U
1	sN1	505	U
1	sN1	506	A
1	sN1	508	C

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Mol	Chain	Res	Type
1	sN1	515	C
1	sN1	521	G
1	sN1	522	C
1	sN1	524	7MG
1	sN1	527	G
1	sN1	544	A
1	sN1	556	A
1	sN1	557	U
1	sN1	561	C
1	sN1	567	G
1	sN1	569	A
1	sN1	570	A
1	sN1	572	G
1	sN1	573	C
1	sN1	574	G
1	sN1	593	A
1	sN1	615	C
1	sN1	630	G
1	sN1	650	A
1	sN1	662	A
1	sN1	684	A
1	sN1	692	A
1	sN1	699	A
1	sN1	700	G
1	sN1	720	U
1	sN1	721	G
1	sN1	728	G
1	sN1	743	A
1	sN1	745	U
1	sN1	752	G
1	sN1	774	A
1	sN1	790	U
1	sN1	791	A
1	sN1	812	A
1	sN1	814	C
1	sN1	815	G
1	sN1	839	U
1	sN1	840	U
1	sN1	841	G
1	sN1	842	A
1	sN1	843	G
1	sN1	888	U

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Mol	Chain	Res	Type
1	sN1	899	G
1	sN1	922	G
1	sN1	923	G
1	sN1	924	G
1	sN1	925	G
1	sN1	926	G
1	sN1	931	C
1	sN1	951	G
1	sN1	955	A
1	sN1	957	U
1	sN1	958	U
1	sN1	966	A
1	sN1	968	G
1	sN1	972	A
1	sN1	973	G
1	sN1	974	A
1	sN1	989	U
1	sN1	990	G
1	sN1	991	A
1	sN1	992	C
1	sN1	993	A
1	sN1	998	A
1	sN1	1001	A
1	sN1	1002	A
1	sN1	1003	C
1	sN1	1007	C
1	sN1	1008	C
1	sN1	1010	G
1	sN1	1016	G
1	sN1	1019	U
1	sN1	1023	G
1	sN1	1025	C
1	sN1	1026	U
1	sN1	1028	C
1	sN1	1029	G
1	sN1	1030	G
1	sN1	1037	A
1	sN1	1041	A
1	sN1	1042	C
1	sN1	1050	G
1	sN1	1051	C
1	sN1	1061	G

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Mol	Chain	Res	Type
1	sN1	1062	U
1	sN1	1069	G
1	sN1	1079	A
1	sN1	1082	U
1	sN1	1083	U
1	sN1	1084	G
1	sN1	1086	G
1	sN1	1091	G
1	sN1	1092	U
1	sN1	1095	C
1	sN1	1096	G
1	sN1	1098	A
1	sN1	1101	G
1	sN1	1122	U
1	sN1	1123	U
1	sN1	1124	G
1	sN1	1130	A
1	sN1	1133	U
1	sN1	1134	C
1	sN1	1136	G
1	sN1	1156	U
1	sN1	1157	G
1	sN1	1161	G
1	sN1	1164	A
1	sN1	1169	C
1	sN1	1180	C
1	sN1	1181	G
1	sN1	1182	G
1	sN1	1185	A
1	sN1	1188	A
1	sN1	1193	A
1	sN1	1194	A
1	sN1	1206	C
1	sN1	1209	U
1	sN1	1210	A
1	sN1	1224	A
1	sN1	1235	A
1	sN1	1247	A
1	sN1	1257	U
1	sN1	1277	A
1	sN1	1284	A
1	sN1	1295	U

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Mol	Chain	Res	Type
1	sN1	1297	G
1	sN1	1302	G
1	sN1	1317	C
1	sN1	1360	A
1	sN1	1361	U
1	sN1	1380	C
1	sN1	1388	U
1	sN1	1389	G
1	sN1	1391	A
1	sN1	1394	C
1	sN1	1395	A
1	sN1	1398	G
1	sN1	1402	G
1	sN1	1425	A
1	sN1	1448	C
1	sN1	1449	A
1	sN1	1490	A
1	sN1	1496	A
1	sN1	1499	A
1	sN1	1500	A
1	sN1	1503	U
1	sN1	1517	C
1	sN1	1526	G
1	sN1	1527	G

There are no RNA pucker outliers to report.

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

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	$\# Z > 2$
1	4OC	sN1	1399	1	20,23,24	3.21	8 (40%)	26,32,35	0.90	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MA6	sN1	1516	1	19,26,27	1.03	2 (10%)	18,38,41	3.67	2 (11%)
1	2MG	sN1	963	1	18,26,27	2.55	7 (38%)	16,38,41	1.37	3 (18%)
1	UR3	sN1	1495	1	19,22,23	2.93	6 (31%)	26,32,35	1.29	1 (3%)
1	MA6	sN1	1515	1	19,26,27	1.02	2 (10%)	18,38,41	3.64	2 (11%)
1	PSU	sN1	513	1	18,21,22	1.12	1 (5%)	22,30,33	1.58	3 (13%)
1	5MC	sN1	964	1	18,22,23	3.61	7 (38%)	26,32,35	1.01	2 (7%)
1	7MG	sN1	524	1	22,26,27	3.90	10 (45%)	29,39,42	2.03	9 (31%)
1	2MG	sN1	1204	1	18,26,27	2.53	7 (38%)	16,38,41	1.36	3 (18%)

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	4OC	sN1	1399	1	-	0/9/29/30	0/2/2/2
1	MA6	sN1	1516	1	-	3/7/29/30	0/3/3/3
1	2MG	sN1	963	1	-	0/5/27/28	0/3/3/3
1	UR3	sN1	1495	1	-	2/7/25/26	0/2/2/2
1	MA6	sN1	1515	1	-	0/7/29/30	0/3/3/3
1	PSU	sN1	513	1	-	0/7/25/26	0/2/2/2
1	5MC	sN1	964	1	-	0/7/25/26	0/2/2/2
1	7MG	sN1	524	1	-	3/7/37/38	0/3/3/3
1	2MG	sN1	1204	1	-	0/5/27/28	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	sN1	524	7MG	C8-N9	9.94	1.51	1.46
1	sN1	964	5MC	C6-C5	9.20	1.49	1.34
1	sN1	524	7MG	C5-N7	7.80	1.44	1.35
1	sN1	1495	UR3	C2-N1	7.14	1.48	1.38
1	sN1	1399	4OC	C4-N3	7.00	1.45	1.32
1	sN1	1495	UR3	C6-C5	6.84	1.51	1.35
1	sN1	964	5MC	C4-N3	6.58	1.45	1.34
1	sN1	1399	4OC	C6-C5	6.34	1.49	1.35
1	sN1	1399	4OC	C2-N3	6.22	1.49	1.36
1	sN1	964	5MC	C2-N3	6.21	1.49	1.36
1	sN1	524	7MG	C2-N3	5.98	1.47	1.33
1	sN1	1495	UR3	C2-N3	5.87	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	sN1	524	7MG	C4-N9	5.65	1.44	1.37
1	sN1	524	7MG	C4-N3	5.64	1.47	1.34
1	sN1	963	2MG	C2-N2	5.54	1.45	1.33
1	sN1	1204	2MG	C2-N2	5.48	1.45	1.33
1	sN1	963	2MG	C4-N3	5.03	1.49	1.37
1	sN1	1204	2MG	C4-N3	4.99	1.49	1.37
1	sN1	1399	4OC	C4-N4	4.94	1.46	1.35
1	sN1	524	7MG	C2-N2	4.94	1.45	1.34
1	sN1	963	2MG	C2-N1	4.92	1.44	1.36
1	sN1	1204	2MG	C2-N1	4.90	1.44	1.36
1	sN1	964	5MC	C6-N1	4.58	1.45	1.38
1	sN1	964	5MC	C4-N4	4.39	1.45	1.34
1	sN1	1399	4OC	C2-N1	4.35	1.49	1.40
1	sN1	964	5MC	C2-N1	4.32	1.49	1.40
1	sN1	1399	4OC	C5-C4	3.90	1.49	1.40
1	sN1	524	7MG	C2-N1	3.87	1.47	1.37
1	sN1	963	2MG	C6-N1	3.82	1.43	1.37
1	sN1	1204	2MG	C6-N1	3.76	1.43	1.37
1	sN1	513	PSU	C6-C5	3.71	1.39	1.35
1	sN1	524	7MG	C5-C6	3.57	1.52	1.43
1	sN1	1495	UR3	C6-N1	3.44	1.46	1.38
1	sN1	1399	4OC	C6-N1	3.41	1.46	1.38
1	sN1	524	7MG	C6-N1	3.33	1.45	1.38
1	sN1	1204	2MG	C5-C6	3.14	1.53	1.47
1	sN1	963	2MG	C5-C6	3.14	1.53	1.47
1	sN1	964	5MC	O2-C2	-2.74	1.18	1.23
1	sN1	1516	MA6	C2-N3	2.62	1.36	1.32
1	sN1	1515	MA6	C2-N3	2.61	1.36	1.32
1	sN1	1399	4OC	O2-C2	-2.59	1.18	1.23
1	sN1	1515	MA6	C5-C4	-2.57	1.34	1.40
1	sN1	524	7MG	O6-C6	-2.56	1.18	1.23
1	sN1	1516	MA6	C5-C4	-2.54	1.34	1.40
1	sN1	1204	2MG	C5-C4	-2.48	1.36	1.43
1	sN1	963	2MG	C5-C4	-2.45	1.36	1.43
1	sN1	1495	UR3	C4-N3	2.41	1.46	1.40
1	sN1	1495	UR3	C5-C4	2.31	1.49	1.43
1	sN1	1204	2MG	O6-C6	-2.17	1.18	1.23
1	sN1	963	2MG	O6-C6	-2.17	1.18	1.23

All (26) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	sN1	1516	MA6	N1-C6-N6	-14.34	101.96	117.06
1	sN1	1515	MA6	N1-C6-N6	-14.15	102.16	117.06
1	sN1	1515	MA6	N3-C2-N1	-5.56	119.99	128.68
1	sN1	1516	MA6	N3-C2-N1	-5.48	120.11	128.68
1	sN1	524	7MG	C5-C6-N1	4.96	119.74	110.99
1	sN1	1495	UR3	C4-N3-C2	-4.69	120.15	124.56
1	sN1	524	7MG	C2-N3-C4	4.42	120.18	112.30
1	sN1	524	7MG	C5-C4-N3	-4.16	120.20	128.13
1	sN1	513	PSU	C4-N3-C2	-4.14	120.37	126.34
1	sN1	513	PSU	N1-C2-N3	3.93	119.58	115.13
1	sN1	1204	2MG	C5-C6-N1	3.45	120.04	113.95
1	sN1	963	2MG	C5-C6-N1	3.43	120.01	113.95
1	sN1	964	5MC	C5-C6-N1	-3.28	119.97	123.34
1	sN1	524	7MG	C4-C5-N7	3.15	109.91	105.53
1	sN1	524	7MG	C5-C4-N9	3.03	110.28	106.35
1	sN1	524	7MG	C2-N1-C6	-2.82	119.96	125.10
1	sN1	524	7MG	O6-C6-C5	-2.76	120.78	127.54
1	sN1	524	7MG	N9-C4-N3	2.72	129.53	125.47
1	sN1	963	2MG	C8-N7-C5	2.69	108.11	102.99
1	sN1	1204	2MG	C8-N7-C5	2.65	108.05	102.99
1	sN1	524	7MG	N9-C8-N7	2.34	106.72	103.38
1	sN1	1399	4OC	C6-C5-C4	2.28	119.75	116.96
1	sN1	963	2MG	O6-C6-C5	-2.23	120.03	124.37
1	sN1	1204	2MG	O6-C6-C5	-2.21	120.06	124.37
1	sN1	513	PSU	O4'-C1'-C2'	2.12	108.14	105.14
1	sN1	964	5MC	CM5-C5-C6	-2.09	120.06	122.85

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	sN1	524	7MG	C3'-C4'-C5'-O5'
1	sN1	1516	MA6	C5-C6-N6-C9
1	sN1	1516	MA6	C5-C6-N6-C10
1	sN1	524	7MG	O4'-C4'-C5'-O5'
1	sN1	1495	UR3	O4'-C4'-C5'-O5'
1	sN1	1495	UR3	C3'-C4'-C5'-O5'
1	sN1	1516	MA6	N1-C6-N6-C9
1	sN1	524	7MG	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

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.

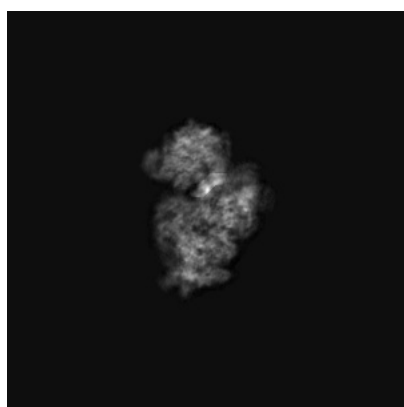
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21034. These allow visual inspection of the internal detail of the map and identification of artifacts.

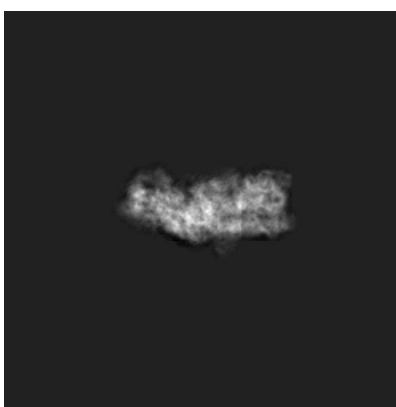
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

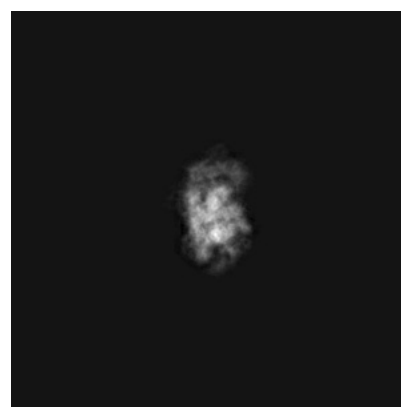
6.1.1 Primary map



X



Y

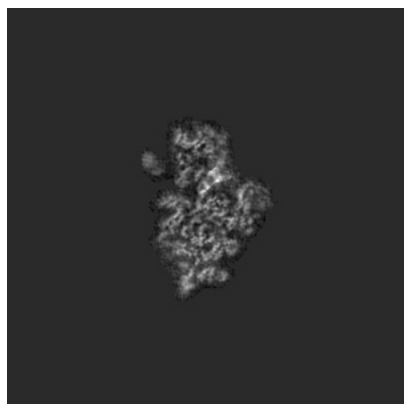


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 256



Y Index: 256

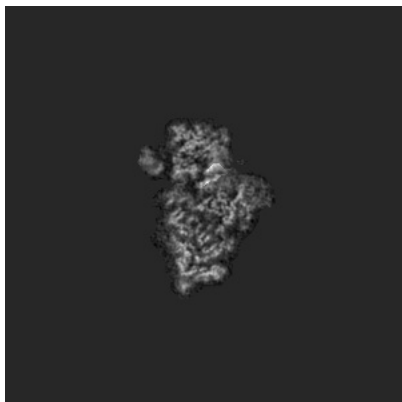


Z Index: 256

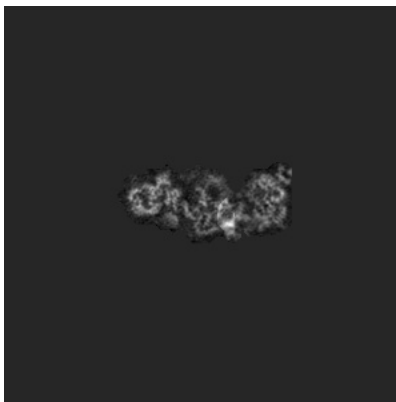
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

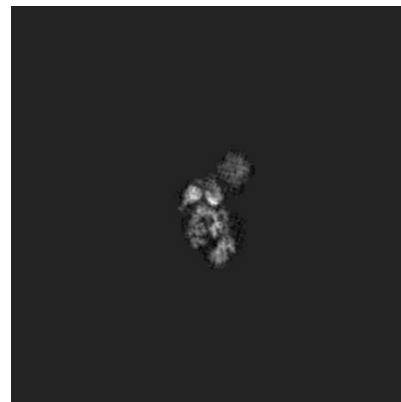
6.3.1 Primary map



X Index: 261



Y Index: 251



Z Index: 301

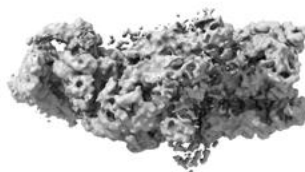
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

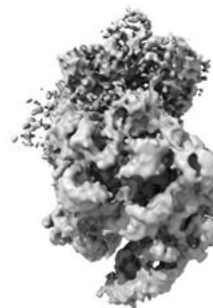
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

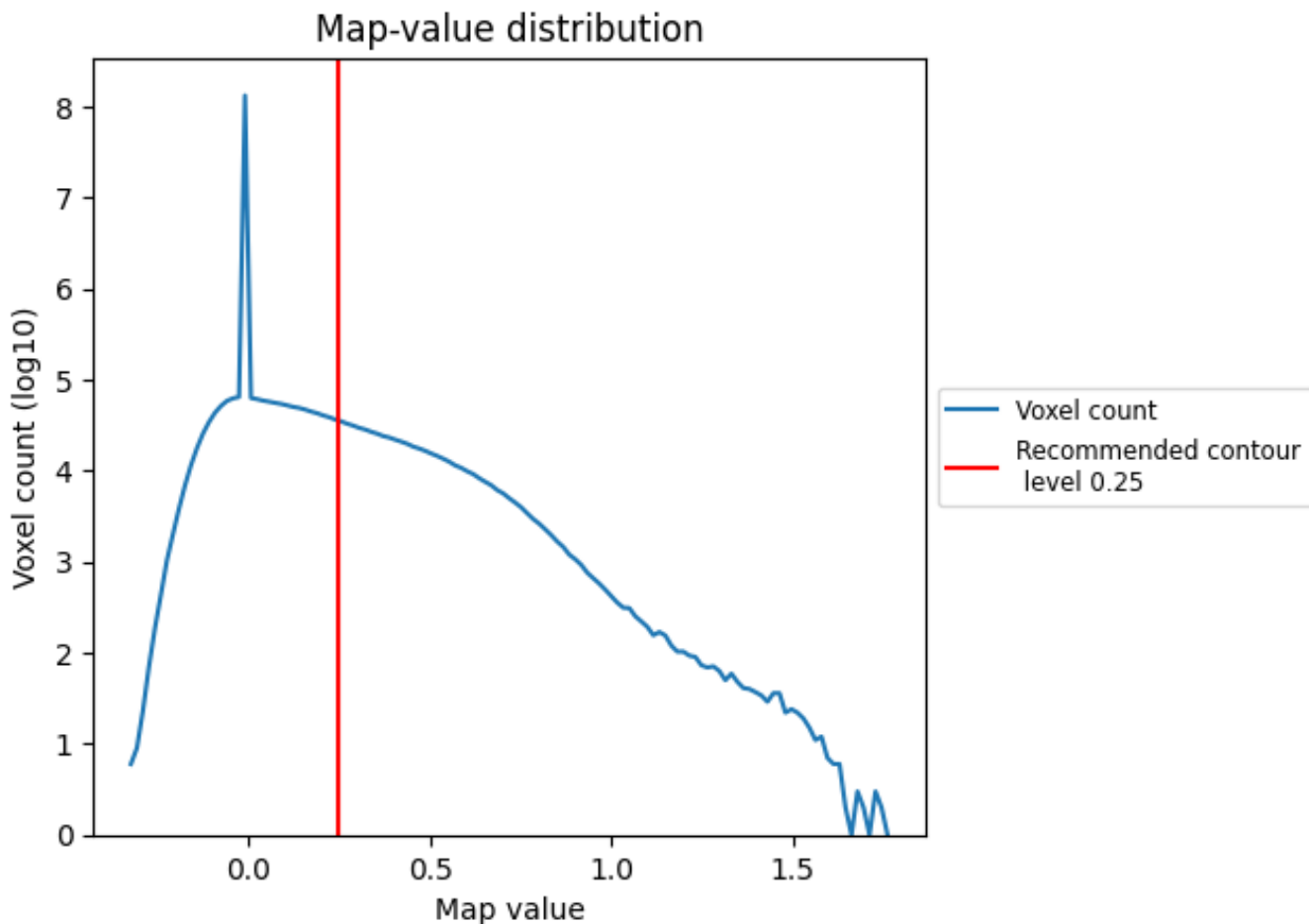
6.5 Mask visualisation

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

7 Map analysis [i](#)

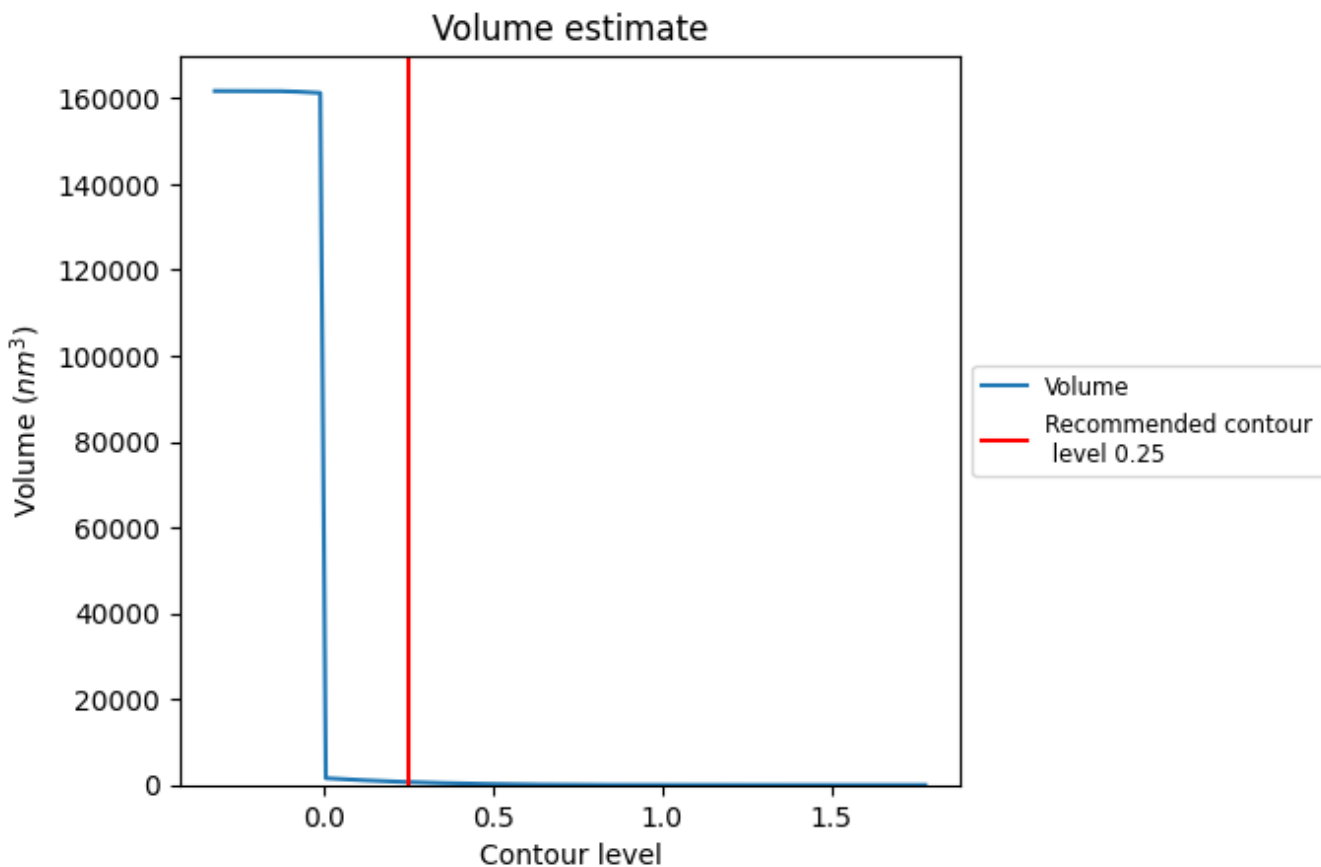
This section contains the results of statistical analysis of the map.

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.

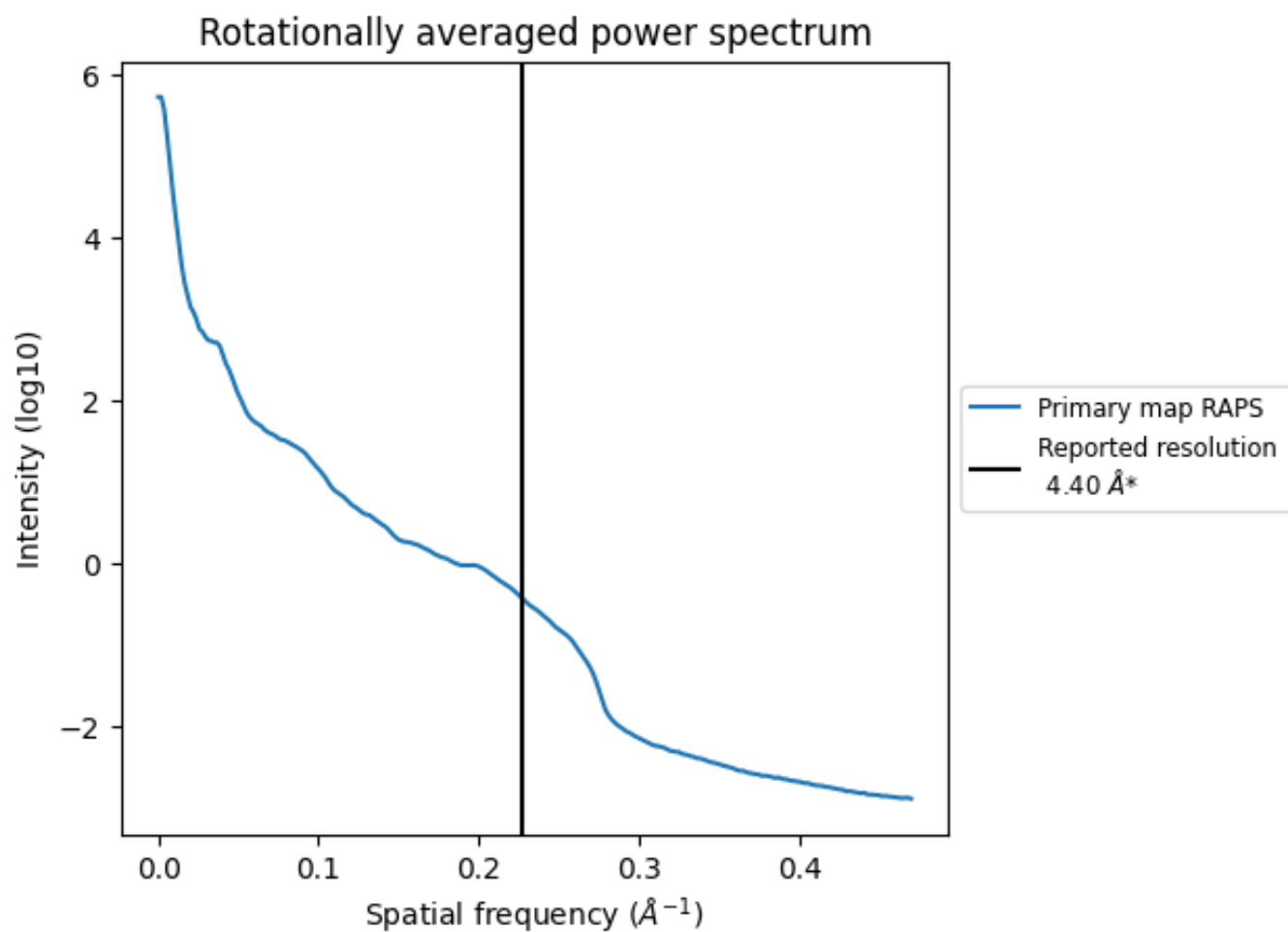
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 668 nm³; this corresponds to an approximate mass of 603 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 0.227\AA^{-1}

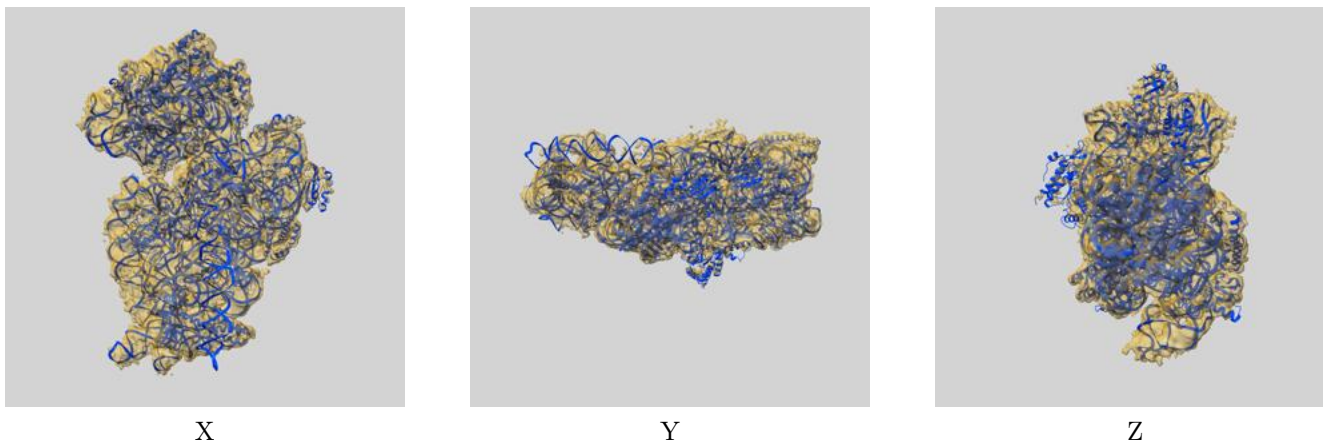
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

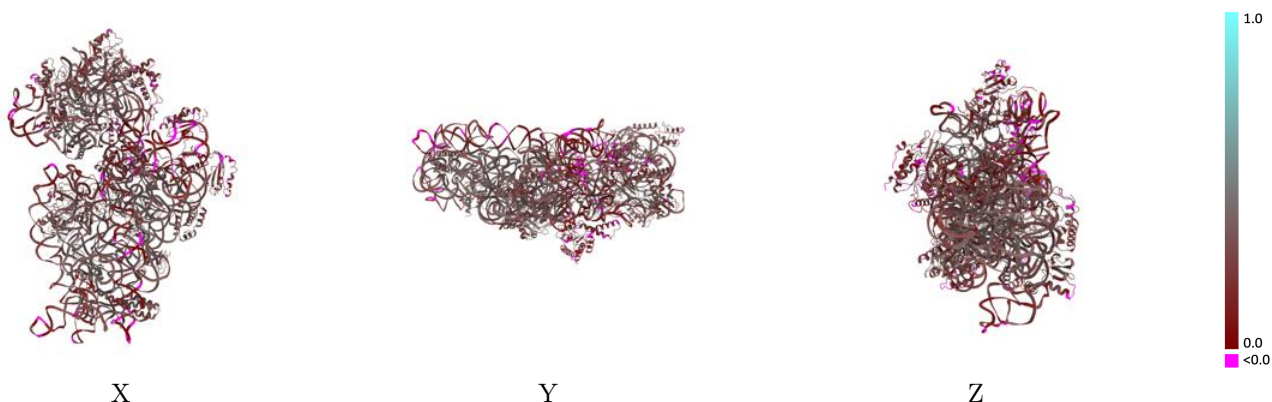
This section contains information regarding the fit between EMDB map EMD-21034 and PDB model 6V3E. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



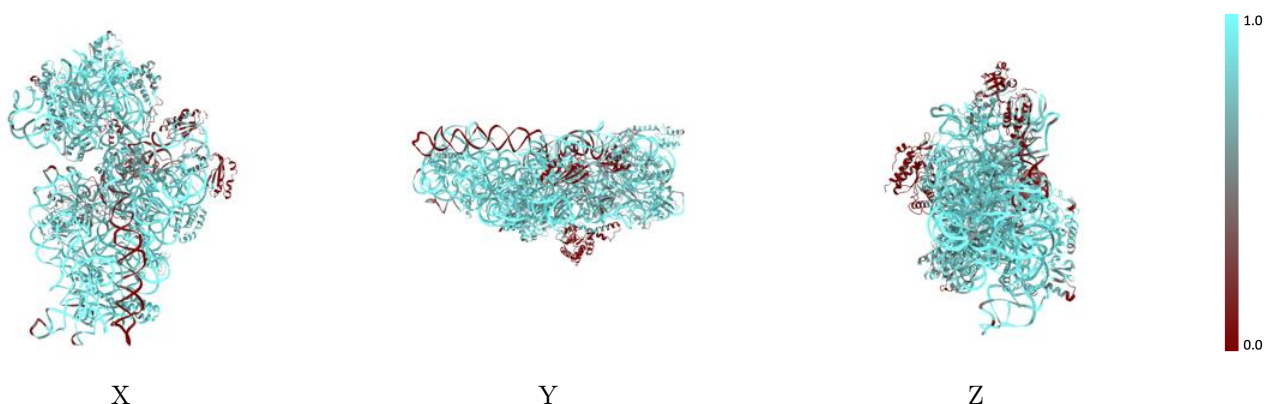
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



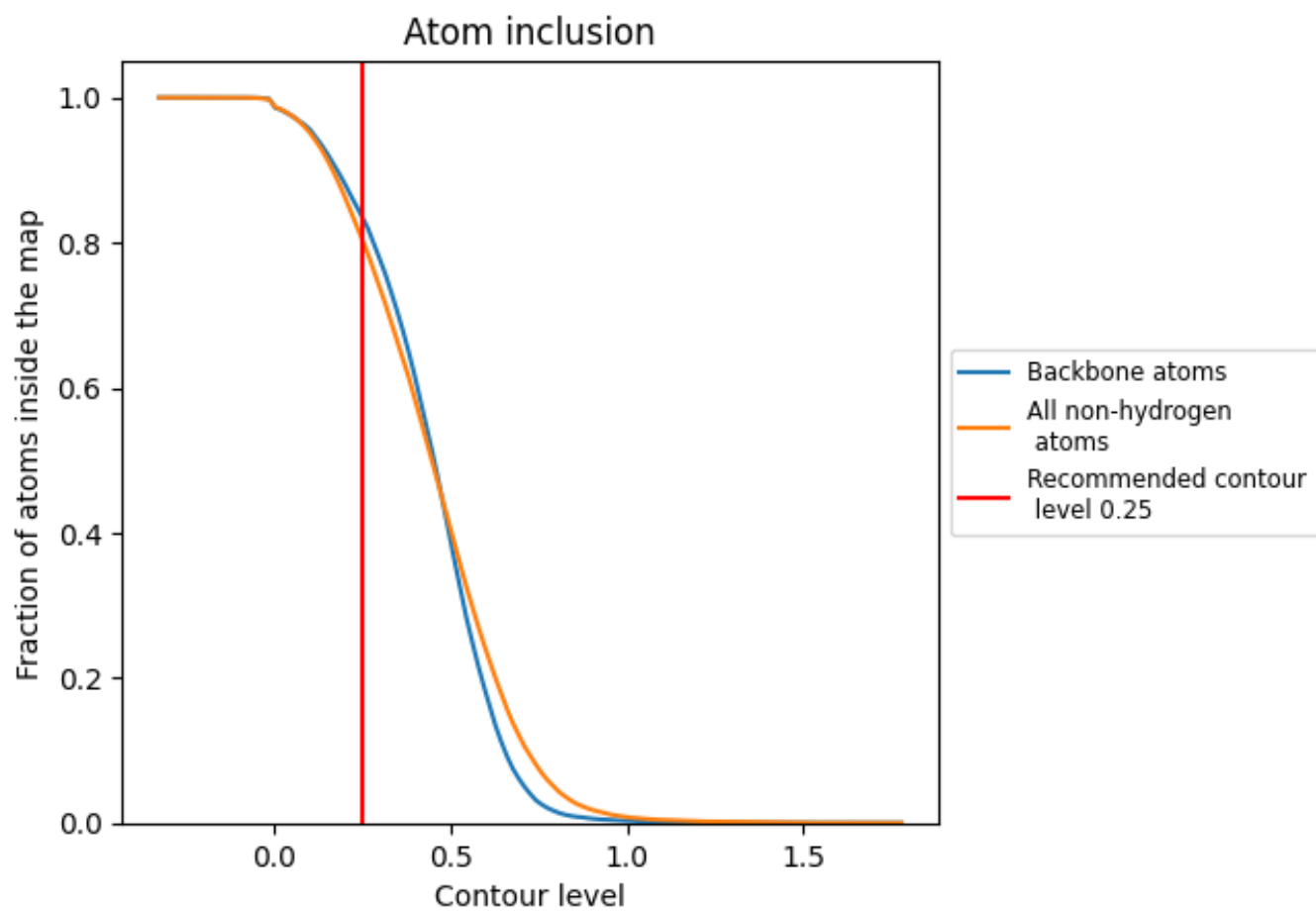
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.25).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 81% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8056	 0.2800
b	 0.1849	 0.1510
c	 0.7824	 0.2980
d	 0.6909	 0.2580
e	 0.8432	 0.3070
f	 0.2055	 0.1800
g	 0.6922	 0.2130
h	 0.8520	 0.3580
i	 0.8036	 0.3100
j	 0.7805	 0.3270
k	 0.2152	 0.1300
l	 0.5510	 0.3120
m	 0.7871	 0.2850
n	 0.8052	 0.3280
o	 0.8404	 0.3050
p	 0.9203	 0.3740
q	 0.8880	 0.3500
r	 0.5967	 0.1980
s	 0.7714	 0.2830
sN1	 0.8806	 0.2850
t	 0.8932	 0.3290

