



Full wwPDB EM Validation Report ⓘ

Mar 12, 2025 – 11:02 AM EDT

PDB ID : 9D89
EMDB ID : EMD-46632
Title : E. coli 50S ribosomal subunit in complex with PrAMP rumicidin-2 (focused refinement)
Authors : Pichkur, E.B.; Panteleev, P.V.; Konevega, A.L.
Deposited on : 2024-08-19
Resolution : 1.95 Å(reported)
Based on initial model : 8B0X

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.dev117
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) : 2.41.4

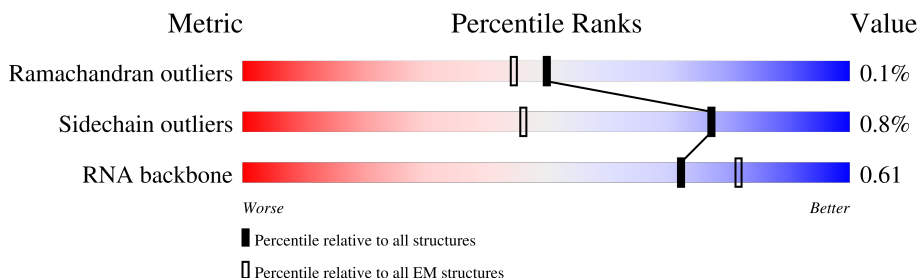
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.95 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.




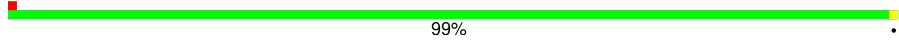
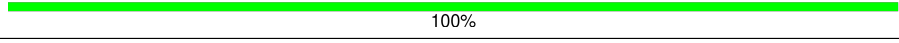
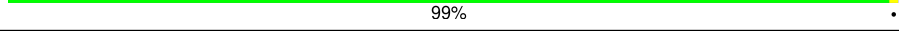
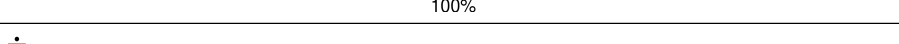
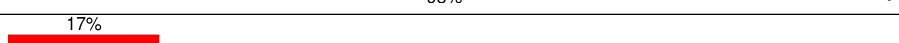


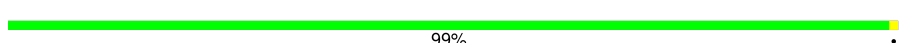
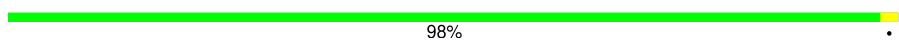
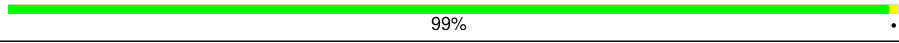
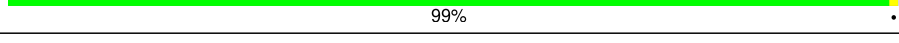
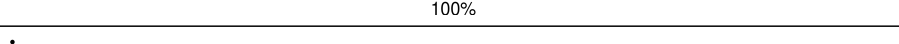
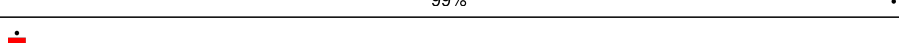


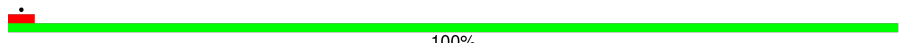
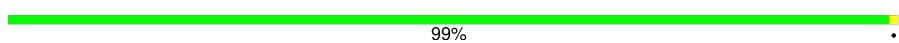

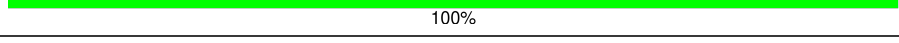
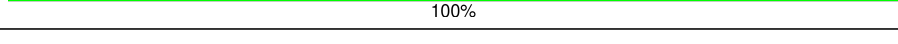


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	0	55	
2	1	46	
3	B	65	
4	C	38	
5	D	2728	
6	E	119	
7	F	273	
8	G	209	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	H	201	 100%
10	I	144	 99%
11	J	118	 100%
12	K	93	 99%
13	L	78	 100%
14	M	56	 98%
15	f	177	 99%
16	g	176	 100%
17	h	38	 100%
18	i	142	 99%
19	j	123	 98%
20	l	135	 99%
21	n	116	 99%
22	o	114	 100%
23	p	117	 99%
24	q	103	 100%
25	r	110	 97%
26	t	102	 97%
27	u	94	 100%
28	w	77	 99%
29	x	62	 100%
30	y	58	 100%
31	T	16	 100%

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 90166 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 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	2728	Total	C	N	O	P	0	0
			58601	26147	10802	18924	2728		

- Molecule 6 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 11 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 12 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 13 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

- Molecule 14 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 15 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 16 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 17 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	h	38	Total	C	N	O	S	0	0
			282	181	50	50	1		

- Molecule 18 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	i	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 19 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 20 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	135	Total	C	N	O	S	0	0
			1067	681	204	177	5		

- Molecule 21 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	n	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 22 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	o	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 23 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	p	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 24 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	q	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 25 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	r	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 26 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	t	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 27 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	u	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 28 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	w	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 29 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 30 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	y	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 31 is a protein called Rumicidin-2 (12-27).

Mol	Chain	Residues	Atoms				AltConf	Trace
31	T	16	Total	C	N	O	0	0
			143	96	31	16		

- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
32	C	1	Total	Zn	0
			1	1	

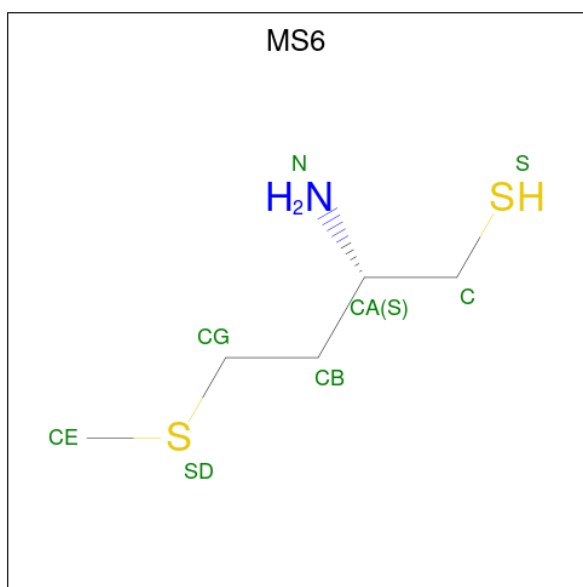
- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	D	198	Total	Mg	0
			198	198	
33	E	3	Total	Mg	0
			3	3	
33	F	1	Total	Mg	0
			1	1	
33	G	1	Total	Mg	0
			1	1	
33	M	1	Total	Mg	0
			1	1	

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
34	D	88	Total	K	0
			88	88	
34	F	4	Total	K	0
			4	4	
34	H	1	Total	K	0
			1	1	

- Molecule 35 is (2S)-2-amino-4-(methylsulfanyl)butane-1-thiol (three-letter code: MS6) (formula: $C_5H_{13}NS_2$).



Mol	Chain	Residues	Atoms				AltConf
35	1	1	Total	C	N	S	0
			8	5	1	2	

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
36	1	15	Total	O	0
			15	15	
36	B	19	Total	O	0
			19	19	
36	C	3	Total	O	0
			3	3	
36	D	3780	Total	O	0
			3780	3780	
36	E	48	Total	O	0
			48	48	

Continued on next page...

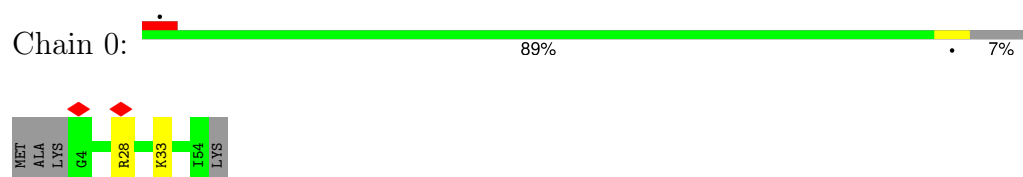
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
36	F	79	Total 79	O 79	0
36	G	38	Total 38	O 38	0
36	H	36	Total 36	O 36	0
36	I	38	Total 38	O 38	0
36	J	22	Total 22	O 22	0
36	K	12	Total 12	O 12	0
36	L	14	Total 14	O 14	0
36	M	25	Total 25	O 25	0
36	h	1	Total 1	O 1	0
36	i	22	Total 22	O 22	0
36	j	12	Total 12	O 12	0
36	l	26	Total 26	O 26	0
36	o	13	Total 13	O 13	0
36	p	32	Total 32	O 32	0
36	q	19	Total 19	O 19	0
36	r	30	Total 30	O 30	0
36	t	6	Total 6	O 6	0
36	u	3	Total 3	O 3	0
36	w	9	Total 9	O 9	0
36	x	1	Total 1	O 1	0
36	y	5	Total 5	O 5	0

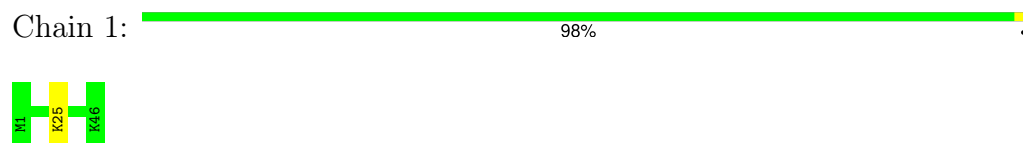
3 Residue-property plots [i](#)

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

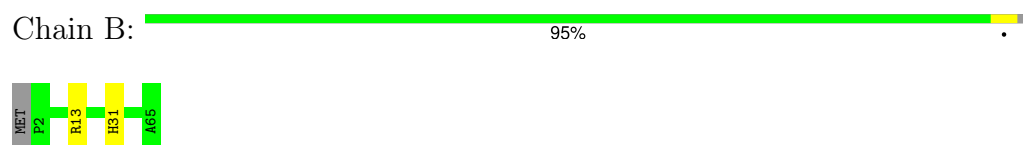
- Molecule 1: 50S ribosomal protein L33



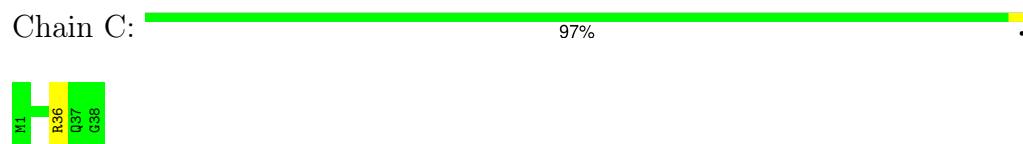
- Molecule 2: 50S ribosomal protein L34



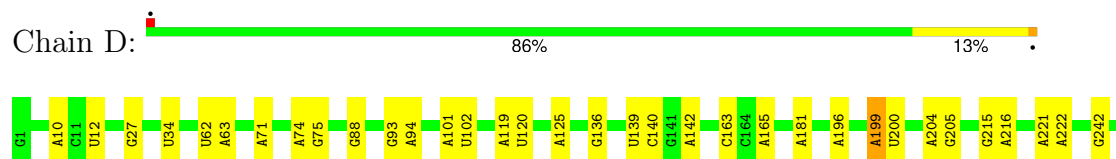
- Molecule 3: 50S ribosomal protein L35



- Molecule 4: 50S ribosomal protein L36

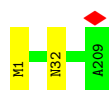


- Molecule 5: 23S rRNA



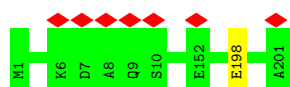
- Molecule 8: 50S ribosomal protein L3

Chain G:  99%



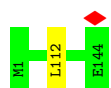
- Molecule 9: 50S ribosomal protein L4

Chain H:  100%



- Molecule 10: 50S ribosomal protein L15

Chain I:  99%



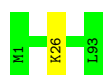
- Molecule 11: 50S ribosomal protein L17

Chain J:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: Large ribosomal subunit protein uL23

Chain K:  99%



- Molecule 13: 50S ribosomal protein L27

Chain L:  100%

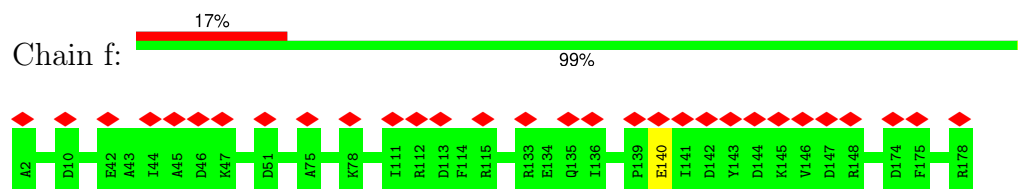


- Molecule 14: 50S ribosomal protein L32

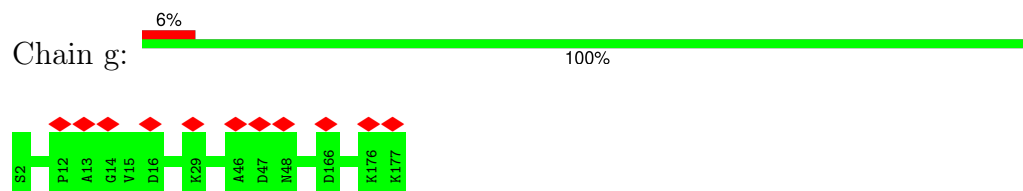
Chain M:  98%



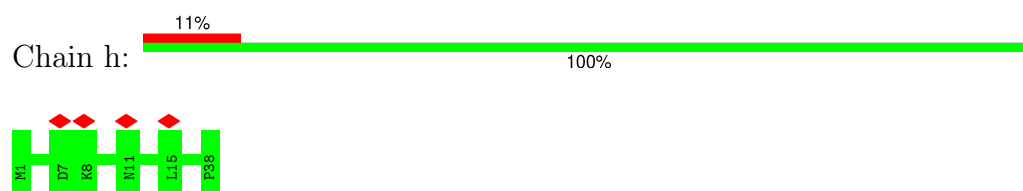
• Molecule 15: 50S ribosomal protein L5



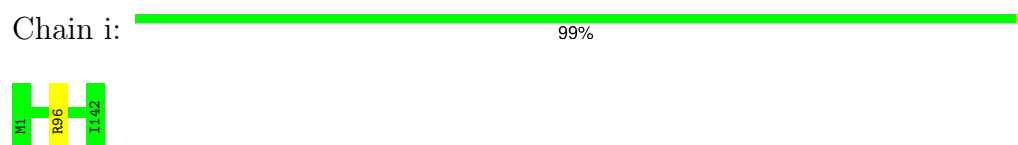
• Molecule 16: Large ribosomal subunit protein uL6



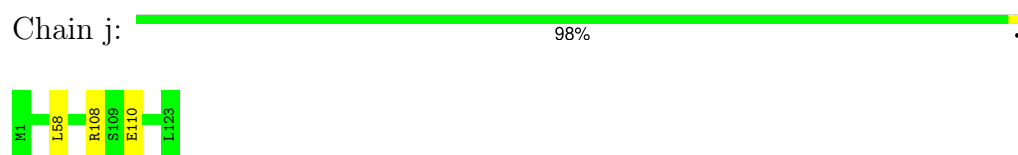
• Molecule 17: 50S ribosomal protein L9



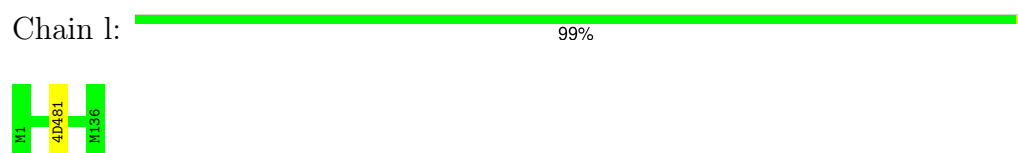
• Molecule 18: Large ribosomal subunit protein uL13



• Molecule 19: 50S ribosomal protein L14

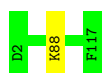


• Molecule 20: 50S ribosomal protein L16



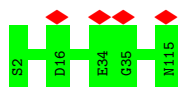
• Molecule 21: 50S ribosomal protein L18





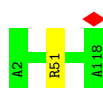
- Molecule 22: 50S ribosomal protein L19

Chain o: 100%



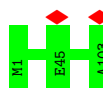
- Molecule 23: Large ribosomal subunit protein bL20

Chain p: 99%



- Molecule 24: 50S ribosomal protein L21

Chain q: 100%



- Molecule 25: 50S ribosomal protein L22

Chain r: 97%



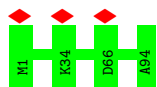
- Molecule 26: Large ribosomal subunit protein uL24

Chain t: 6%



- Molecule 27: Large ribosomal subunit protein bL25

Chain u: 100%



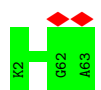
- Molecule 28: 50S ribosomal protein L28

Chain w:  99% .



- Molecule 29: Large ribosomal subunit protein uL29

Chain x:  100%



- Molecule 30: 50S ribosomal protein L30

Chain y:  100%



- Molecule 31: Rumicidin-2 (12-27)

Chain T:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	371000	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 ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	20000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	6.240	Depositor
Minimum map value	-0.674	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	0.274	Depositor
Recommended contour level	1.1	Depositor
Map size (Å)	441.856, 441.856, 441.856	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.863, 0.863, 0.863	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 5MC, OMU, H2U, K, 5MU, MS6, PSU, MG, ZN, G7M, 1MG, MEQ, 6MZ, 2MG, OMG, 3TD, 4D4, 2MA

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	0	0.31	0/424	0.57	0/565
2	1	0.33	0/380	0.76	0/498
3	B	0.36	0/513	0.61	0/676
4	C	0.32	0/303	0.71	0/397
5	D	0.44	0/65057	0.98	58/101481 (0.1%)
6	E	0.44	0/2850	0.93	0/4444
7	F	0.31	0/2121	0.66	0/2852
8	G	0.32	0/1576	0.60	0/2119
9	H	0.30	0/1571	0.58	0/2113
10	I	0.33	0/1062	0.58	0/1413
11	J	0.31	0/958	0.63	0/1281
12	K	0.29	0/744	0.58	0/994
13	L	0.33	0/593	0.64	0/785
14	M	0.33	0/450	0.65	0/599
15	f	0.29	0/1434	0.53	0/1926
16	g	0.29	0/1343	0.55	0/1816
17	h	0.30	0/285	0.55	0/385
18	i	0.30	0/1152	0.59	0/1551
19	j	0.30	0/955	0.61	0/1279
20	l	0.30	0/1073	0.61	0/1433
21	n	0.28	0/902	0.55	0/1209
22	o	0.31	0/929	0.60	0/1242
23	p	0.31	0/960	0.66	0/1278
24	q	0.31	0/829	0.62	0/1107
25	r	0.32	0/864	0.63	0/1156
26	t	0.30	0/787	0.57	0/1051
27	u	0.30	0/766	0.55	0/1025
28	w	0.31	0/635	0.62	0/848
29	x	0.27	0/502	0.53	0/667
30	y	0.29	0/453	0.59	0/605
31	T	0.41	0/154	0.68	0/213

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.41	0/92625	0.90	58/139008 (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
3	B	0	1
5	D	0	1
7	F	0	1
28	w	0	1
All	All	0	4

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	512	G	O4'-C1'-N9	11.65	117.52	108.20
5	D	576	A	O5'-P-OP1	-11.52	95.33	105.70
5	D	576	A	O5'-P-OP2	9.79	122.45	110.70
5	D	739	C	O5'-P-OP2	-8.59	97.97	105.70
5	D	739	C	O5'-P-OP1	8.55	120.97	110.70
5	D	2054	C	O3'-P-O5'	-8.10	88.60	104.00
5	D	2728	U	O5'-P-OP2	-7.44	99.00	105.70
5	D	204	A	O3'-P-O5'	-7.41	89.93	104.00
5	D	1975	U	O3'-P-O5'	-7.11	90.50	104.00
5	D	1940	A	O4'-C1'-N9	7.10	113.88	108.20
5	D	2057	G	O5'-P-OP2	-7.09	99.31	105.70
5	D	2852	G	O4'-C1'-N9	7.04	113.83	108.20
5	D	750	G	C1'-O4'-C4'	-6.82	104.44	109.90
5	D	2226	C	O3'-P-O5'	-6.61	91.43	104.00
5	D	2649	G	O4'-C1'-N9	6.60	113.48	108.20
5	D	1640	C	O3'-P-O5'	-6.51	91.63	104.00
5	D	395	U	O4'-C1'-N1	6.49	113.39	108.20
5	D	1641	C	O5'-P-OP2	6.39	118.36	110.70
5	D	242	G	C3'-C2'-C1'	-6.36	96.42	101.50
5	D	329	G	O3'-P-O5'	-6.29	92.06	104.00
5	D	1313	G	O4'-C1'-N9	6.28	113.22	108.20
5	D	2072	U	O5'-P-OP2	-6.25	100.08	105.70
5	D	783	A	O3'-P-O5'	-6.24	92.14	104.00
5	D	2521	C	O4'-C1'-N1	6.22	113.18	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	974	A	O5'-P-OP2	-6.21	100.11	105.70
5	D	1978	C	O3'-P-O5'	-6.19	92.24	104.00
5	D	1775	A	O5'-P-OP2	-6.07	100.24	105.70
5	D	2451	G	C3'-C2'-C1'	-6.06	96.65	101.50
5	D	786	G	OP1-P-O3'	6.00	118.41	105.20
5	D	786	G	P-O3'-C3'	5.97	126.86	119.70
5	D	27	G	O4'-C1'-N9	5.90	112.92	108.20
5	D	512	G	C1'-O4'-C4'	-5.83	105.24	109.90
5	D	1188	G	O3'-P-O5'	-5.83	92.93	104.00
5	D	1934	G	C3'-C2'-C1'	-5.79	96.87	101.50
5	D	986	A	O4'-C1'-N9	5.71	112.77	108.20
5	D	954	G	O3'-P-O5'	-5.71	93.16	104.00
5	D	777	G	O4'-C1'-N9	5.70	112.76	108.20
5	D	1940	A	C1'-O4'-C4'	-5.66	105.37	109.90
5	D	2286	G	O4'-C1'-N9	5.65	112.72	108.20
5	D	1375	A	O3'-P-O5'	-5.65	93.27	104.00
5	D	2065	G	OP2-P-O3'	5.64	117.61	105.20
5	D	2585	G	O4'-C1'-N9	5.56	112.64	108.20
5	D	1326	G	O4'-C1'-N9	5.52	112.62	108.20
5	D	2877	A	C1'-O4'-C4'	-5.43	105.56	109.90
5	D	706	G	O4'-C1'-N9	5.39	112.52	108.20
5	D	739	C	O3'-P-O5'	-5.38	93.77	104.00
5	D	1130	G	C1'-O4'-C4'	-5.29	105.67	109.90
5	D	1773	C	O5'-P-OP2	-5.29	100.94	105.70
5	D	1214	G	O4'-C1'-N9	5.22	112.37	108.20
5	D	1623	U	OP1-P-O3'	5.21	116.66	105.20
5	D	863	A	O5'-P-OP2	-5.17	101.05	105.70
5	D	776	G	O4'-C1'-N9	5.16	112.33	108.20
5	D	1933	G	O3'-P-O5'	-5.15	94.22	104.00
5	D	199	A	C1'-O4'-C4'	-5.13	105.80	109.90
5	D	2031	G	O5'-P-OP2	-5.12	101.09	105.70
5	D	1941	A	O4'-C1'-N9	5.10	112.28	108.20
5	D	205	G	C3'-C2'-C1'	-5.05	97.46	101.50
5	D	2438	A	C1'-O4'-C4'	-5.04	105.87	109.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	13	ARG	Sidechain
5	D	512	G	Sidechain
7	F	43	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
28	w	16	ASN	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	0	49/55 (89%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	B	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	C	36/38 (95%)	36 (100%)	0	0	100	100
7	F	269/273 (98%)	260 (97%)	9 (3%)	0	100	100
8	G	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
9	H	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
10	I	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
11	J	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
12	K	91/93 (98%)	89 (98%)	2 (2%)	0	100	100
13	L	76/78 (97%)	74 (97%)	2 (3%)	0	100	100
14	M	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
15	f	175/177 (99%)	165 (94%)	10 (6%)	0	100	100
16	g	174/176 (99%)	160 (92%)	14 (8%)	0	100	100
17	h	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
18	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
19	j	121/123 (98%)	116 (96%)	4 (3%)	1 (1%)	16	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	l	131/135 (97%)	128 (98%)	3 (2%)	0	100	100
21	n	114/116 (98%)	108 (95%)	5 (4%)	1 (1%)	14	7
22	o	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
23	p	115/117 (98%)	115 (100%)	0	0	100	100
24	q	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
25	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
26	t	100/102 (98%)	96 (96%)	3 (3%)	1 (1%)	13	5
27	u	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
28	w	75/77 (97%)	75 (100%)	0	0	100	100
29	x	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
30	y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
31	T	14/16 (88%)	12 (86%)	2 (14%)	0	100	100
All	All	3068/3136 (98%)	2977 (97%)	88 (3%)	3 (0%)	50	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	j	108	ARG
21	n	88	LYS
26	t	39	ILE

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	0	46/49 (94%)	44 (96%)	2 (4%)	25	14
2	1	38/38 (100%)	37 (97%)	1 (3%)	41	33
3	B	51/52 (98%)	50 (98%)	1 (2%)	50	44
4	C	34/34 (100%)	33 (97%)	1 (3%)	37	28
7	F	216/218 (99%)	216 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	G	163/163 (100%)	161 (99%)	2 (1%)	67	65
9	H	165/165 (100%)	164 (99%)	1 (1%)	84	83
10	I	103/103 (100%)	102 (99%)	1 (1%)	73	72
11	J	98/98 (100%)	98 (100%)	0	100	100
12	K	80/80 (100%)	79 (99%)	1 (1%)	65	62
13	L	58/59 (98%)	58 (100%)	0	100	100
14	M	47/47 (100%)	46 (98%)	1 (2%)	48	43
15	f	148/148 (100%)	147 (99%)	1 (1%)	81	81
16	g	137/137 (100%)	137 (100%)	0	100	100
17	h	30/30 (100%)	30 (100%)	0	100	100
18	i	116/116 (100%)	115 (99%)	1 (1%)	75	75
19	j	104/104 (100%)	102 (98%)	2 (2%)	52	47
20	l	107/107 (100%)	107 (100%)	0	100	100
21	n	86/86 (100%)	86 (100%)	0	100	100
22	o	99/99 (100%)	99 (100%)	0	100	100
23	p	89/89 (100%)	88 (99%)	1 (1%)	70	68
24	q	84/84 (100%)	84 (100%)	0	100	100
25	r	93/93 (100%)	90 (97%)	3 (3%)	34	24
26	t	83/83 (100%)	81 (98%)	2 (2%)	44	37
27	u	78/78 (100%)	78 (100%)	0	100	100
28	w	67/67 (100%)	67 (100%)	0	100	100
29	x	54/54 (100%)	54 (100%)	0	100	100
30	y	48/48 (100%)	48 (100%)	0	100	100
31	T	16/16 (100%)	16 (100%)	0	100	100
All	All	2538/2545 (100%)	2517 (99%)	21 (1%)	77	78

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	28	ARG
1	0	33	LYS
2	1	25	LYS
3	B	31	HIS
4	C	36	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	G	1	MET
8	G	32	ASN
9	H	198	GLU
10	I	112	LEU
12	K	26	LYS
14	M	57	LYS
15	f	140	GLU
18	i	96	ARG
19	j	58	LEU
19	j	110	GLU
23	p	51	ARG
25	r	82	MET
25	r	83	LYS
25	r	92	ARG
26	t	15	THR
26	t	52	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
9	H	9	GLN
10	I	104	GLN
14	M	42	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	D	2717/2728 (99%)	302 (11%)	47 (1%)
6	E	118/119 (99%)	14 (11%)	1 (0%)
All	All	2835/2847 (99%)	316 (11%)	48 (1%)

All (316) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	D	10	A
5	D	12	U
5	D	34	U
5	D	63	A
5	D	71	A
5	D	74	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	D	75	G
5	D	88	G
5	D	93	G
5	D	94	A
5	D	101	A
5	D	102	U
5	D	119	A
5	D	120	U
5	D	125	A
5	D	136	G
5	D	139	U
5	D	140	C
5	D	142	A
5	D	163	C
5	D	165	A
5	D	181	A
5	D	196	A
5	D	199	A
5	D	200	U
5	D	215	G
5	D	216	A
5	D	221	A
5	D	222	A
5	D	248	G
5	D	272	A
5	D	276	U
5	D	280	U
5	D	281	C
5	D	285	G
5	D	287	G
5	D	291	G
5	D	311	A
5	D	330	A
5	D	345	A
5	D	361	G
5	D	386	G
5	D	404	A
5	D	405	U
5	D	411	G
5	D	412	A
5	D	420	C
5	D	451	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	D	456	C
5	D	480	A
5	D	481	G
5	D	491	G
5	D	503	A
5	D	504	A
5	D	505	A
5	D	509	C
5	D	530	G
5	D	531	C
5	D	532	A
5	D	533	G
5	D	538	A
5	D	565	A
5	D	575	U
5	D	577	A
5	D	605	A
5	D	617	U
5	D	620	G
5	D	629	A
5	D	639	A
5	D	647	C
5	D	648	U
5	D	649	G
5	D	656	A
5	D	687	A
5	D	688	U
5	D	719	C
5	D	732	A
5	D	749	5MU
5	D	766	A
5	D	767	C
5	D	777	G
5	D	778	G
5	D	784	A
5	D	786	G
5	D	787	G
5	D	791	A
5	D	794	A
5	D	807	G
5	D	814	C
5	D	829	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	D	830	U
5	D	848	U
5	D	860	G
5	D	861	G
5	D	876	G
5	D	878	C
5	D	879	A
5	D	903	C
5	D	912	A
5	D	916	G
5	D	917	C
5	D	929	A
5	D	933	U
5	D	934	U
5	D	936	U
5	D	948	C
5	D	963	C
5	D	976	G
5	D	985	A
5	D	998	A
5	D	1007	C
5	D	1014	U
5	D	1015	C
5	D	1024	G
5	D	1035	U
5	D	1049	G
5	D	1113	A
5	D	1114	G
5	D	1118	G
5	D	1124	G
5	D	1130	G
5	D	1131	A
5	D	1134	U
5	D	1135	A
5	D	1137	C
5	D	1144	A
5	D	1173	G
5	D	1212	G
5	D	1213	U
5	D	1255	A
5	D	1258	G
5	D	1273	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	D	1274	A
5	D	1302	G
5	D	1303	A
5	D	1307	C
5	D	1323	A
5	D	1354	U
5	D	1367	A
5	D	1381	U
5	D	1385	A
5	D	1413	U
5	D	1418	G
5	D	1422	A
5	D	1430	C
5	D	1436	A
5	D	1453	C
5	D	1454	G
5	D	1457	G
5	D	1460	U
5	D	1462	U
5	D	1484	G
5	D	1492	A
5	D	1495	C
5	D	1510	A
5	D	1511	A
5	D	1512	G
5	D	1517	A
5	D	1531	G
5	D	1537	A
5	D	1538	C
5	D	1539	G
5	D	1571	A
5	D	1580	U
5	D	1585	A
5	D	1586	U
5	D	1587	C
5	D	1588	A
5	D	1609	C
5	D	1610	A
5	D	1628	A
5	D	1629	G
5	D	1649	U
5	D	1650	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	D	1676	G
5	D	1717	G
5	D	1731	U
5	D	1732	C
5	D	1734	C
5	D	1740	G
5	D	1752	G
5	D	1766	C
5	D	1775	A
5	D	1784	U
5	D	1802	C
5	D	1803	A
5	D	1810	A
5	D	1818	C
5	D	1831	A
5	D	1841	G
5	D	1850	A
5	D	1860	A
5	D	1871	G
5	D	1910	G
5	D	1911	G
5	D	1917	A
5	D	1918	C
5	D	1933	G
5	D	1934	G
5	D	1935	U
5	D	1941	A
5	D	1942	A
5	D	1959	U
5	D	1969	C
5	D	1971	C
5	D	1974	A
5	D	1975	U
5	D	1976	G
5	D	1979	G
5	D	1995	U
5	D	1997	U
5	D	2027	C
5	D	2035	A
5	D	2037	A
5	D	2047	C
5	D	2059	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	D	2060	G
5	D	2064	A
5	D	2065	G
5	D	2066	A
5	D	2073	G7M
5	D	2197	G
5	D	2202	A
5	D	2208	G
5	D	2215	G
5	D	2229	A
5	D	2242	G
5	D	2243	G
5	D	2272	A
5	D	2287	C
5	D	2291	A
5	D	2309	U
5	D	2312	G
5	D	2316	U
5	D	2325	U
5	D	2326	A
5	D	2329	G
5	D	2330	C
5	D	2337	A
5	D	2339	A
5	D	2351	C
5	D	2354	C
5	D	2376	U
5	D	2387	G
5	D	2389	C
5	D	2406	U
5	D	2407	C
5	D	2410	A
5	D	2426	C
5	D	2429	A
5	D	2433	G
5	D	2434	A
5	D	2435	U
5	D	2436	A
5	D	2437	A
5	D	2438	A
5	D	2439	A
5	D	2445	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	D	2452	A
5	D	2474	G
5	D	2478	U
5	D	2480	A
5	D	2484	C
5	D	2495	U
5	D	2506	G
5	D	2509	G
5	D	2522	A
5	D	2529	G
5	D	2533	G
5	D	2551	A
5	D	2558	U
5	D	2570	A
5	D	2571	G
5	D	2577	C
5	D	2589	U
5	D	2606	A
5	D	2607	G
5	D	2613	U
5	D	2617	U
5	D	2633	U
5	D	2667	G
5	D	2686	A
5	D	2693	U
5	D	2694	U
5	D	2718	G
5	D	2730	A
5	D	2748	G
5	D	2752	A
5	D	2761	A
5	D	2762	A
5	D	2769	A
5	D	2782	A
5	D	2794	U
5	D	2795	G
5	D	2802	U
5	D	2803	G
5	D	2824	A
5	D	2825	A
5	D	2865	U
5	D	2888	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	D	2889	G
5	D	2903	A
6	E	11	C
6	E	13	G
6	E	25	U
6	E	35	C
6	E	36	C
6	E	56	G
6	E	64	G
6	E	67	G
6	E	89	U
6	E	90	C
6	E	99	A
6	E	108	A
6	E	109	A
6	E	112	G

All (48) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	D	62	U
5	D	199	A
5	D	221	A
5	D	249	C
5	D	310	A
5	D	404	A
5	D	503	A
5	D	512	G
5	D	655	U
5	D	766	A
5	D	778	G
5	D	786	G
5	D	829	U
5	D	860	G
5	D	963	C
5	D	986	A
5	D	1027	G
5	D	1130	G
5	D	1135	A
5	D	1143	U
5	D	1144	A
5	D	1255	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	D	1288	A
5	D	1303	A
5	D	1453	C
5	D	1492	A
5	D	1499	U
5	D	1537	A
5	D	1585	A
5	D	1628	A
5	D	1649	U
5	D	1849	A
5	D	1917	A
5	D	2229	A
5	D	2286	G
5	D	2315	A
5	D	2328	U
5	D	2406	U
5	D	2434	A
5	D	2436	A
5	D	2437	A
5	D	2438	A
5	D	2760	U
5	D	2802	U
5	D	2824	A
5	D	2871	G
5	D	2877	A
6	E	108	A

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

26 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	$\# Z > 2$
8	MEQ	G	150	8	8,9,10	0.49	0	5,10,12	0.65	0
5	G7M	D	2073	5,34	20,26,27	1.20	3 (15%)	16,39,42	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PSU	D	2584	5	18,21,22	0.94	1 (5%)	21,30,33	0.81	0
5	1MG	D	747	5	19,26,27	1.16	2 (10%)	18,39,42	0.68	0
5	PSU	D	2609	5	18,21,22	0.96	1 (5%)	21,30,33	0.90	1 (4%)
5	5MU	D	749	5	19,22,23	0.28	0	27,32,35	0.51	0
5	PSU	D	1915	5	18,21,22	0.96	1 (5%)	21,30,33	0.62	0
5	6MZ	D	2034	5	17,25,26	1.12	2 (11%)	15,36,39	0.95	1 (6%)
5	PSU	D	748	33,5	18,21,22	0.97	1 (5%)	21,30,33	0.66	0
5	2MG	D	2449	5	18,26,27	1.11	3 (16%)	16,38,41	0.85	1 (6%)
5	2MA	D	2507	33,5,34	18,25,26	1.04	1 (5%)	20,37,40	1.58	5 (25%)
5	PSU	D	2608	5	18,21,22	0.99	1 (5%)	21,30,33	0.87	1 (4%)
5	H2U	D	2453	5	18,21,22	0.62	0	19,30,33	0.97	2 (10%)
5	5MC	D	1966	5,34	19,22,23	0.64	1 (5%)	26,32,35	0.47	0
5	PSU	D	2508	5,34	18,21,22	0.94	1 (5%)	21,30,33	0.93	0
5	PSU	D	1921	5	18,21,22	0.97	1 (5%)	21,30,33	0.63	0
5	5MU	D	1943	5,34	19,22,23	0.33	0	27,32,35	0.53	0
5	OMG	D	2255	5,34	19,26,27	1.05	1 (5%)	21,38,41	0.73	1 (4%)
5	OMU	D	2556	5	19,22,23	0.26	0	25,31,34	0.58	1 (4%)
5	3TD	D	1919	5	19,22,23	1.26	2 (10%)	23,32,35	0.76	0
5	6MZ	D	1620	5	17,25,26	1.04	2 (11%)	15,36,39	0.82	1 (6%)
5	2MG	D	1837	5	18,26,27	1.09	1 (5%)	16,38,41	0.83	1 (6%)
5	PSU	D	957	5	18,21,22	0.91	1 (5%)	21,30,33	0.74	0
20	4D4	l	81	20	9,11,12	0.53	0	7,13,15	1.06	1 (14%)
5	OMC	D	2502	33,5	19,22,23	0.29	0	25,31,34	0.59	0
5	PSU	D	2461	5	18,21,22	0.96	1 (5%)	21,30,33	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MEQ	G	150	8	-	3/8/9/11	-
5	G7M	D	2073	5,34	-	1/3/25/26	0/3/3/3
5	PSU	D	2584	5	-	0/7/25/26	0/2/2/2
5	1MG	D	747	5	-	0/3/25/26	0/3/3/3
5	PSU	D	2609	5	-	0/7/25/26	0/2/2/2
5	5MU	D	749	5	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PSU	D	1915	5	-	0/7/25/26	0/2/2/2
5	6MZ	D	2034	5	-	2/5/27/28	0/3/3/3
5	PSU	D	748	33,5	-	2/7/25/26	0/2/2/2
5	2MG	D	2449	5	-	0/5/27/28	0/3/3/3
5	2MA	D	2507	33,5,34	-	1/3/25/26	0/3/3/3
5	PSU	D	2608	5	-	0/7/25/26	0/2/2/2
5	H2U	D	2453	5	-	0/7/38/39	0/2/2/2
5	5MC	D	1966	5,34	-	0/7/25/26	0/2/2/2
5	PSU	D	2508	5,34	-	0/7/25/26	0/2/2/2
5	PSU	D	1921	5	-	0/7/25/26	0/2/2/2
5	5MU	D	1943	5,34	-	0/7/25/26	0/2/2/2
5	OMG	D	2255	5,34	-	0/5/27/28	0/3/3/3
5	OMU	D	2556	5	-	0/9/27/28	0/2/2/2
5	3TD	D	1919	5	-	2/7/25/26	0/2/2/2
5	6MZ	D	1620	5	-	0/5/27/28	0/3/3/3
5	2MG	D	1837	5	-	0/5/27/28	0/3/3/3
5	PSU	D	957	5	-	0/7/25/26	0/2/2/2
20	4D4	I	81	20	-	1/11/12/14	-
5	OMC	D	2502	33,5	-	0/9/27/28	0/2/2/2
5	PSU	D	2461	5	-	0/7/25/26	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1919	3TD	C6-C5	3.89	1.39	1.35
5	D	1921	PSU	C6-C5	3.81	1.39	1.35
5	D	1915	PSU	C6-C5	3.81	1.39	1.35
5	D	2608	PSU	C6-C5	3.80	1.39	1.35
5	D	748	PSU	C6-C5	3.79	1.39	1.35
5	D	2461	PSU	C6-C5	3.78	1.39	1.35
5	D	2508	PSU	C6-C5	3.71	1.39	1.35
5	D	2584	PSU	C6-C5	3.57	1.39	1.35
5	D	2609	PSU	C6-C5	3.56	1.39	1.35
5	D	1919	3TD	C4-C5	-3.32	1.40	1.47
5	D	957	PSU	C6-C5	3.32	1.39	1.35
5	D	2073	G7M	C8-N9	3.30	1.39	1.33
5	D	2255	OMG	C5-C6	-2.89	1.41	1.47
5	D	2034	6MZ	C6-C5	-2.80	1.40	1.44
5	D	1837	2MG	C5-C6	-2.71	1.42	1.47
5	D	2034	6MZ	C1'-N9	-2.68	1.43	1.49
5	D	2449	2MG	C5-C6	-2.67	1.42	1.47
5	D	2073	G7M	C8-N7	2.61	1.37	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1620	6MZ	C6-C5	-2.48	1.41	1.44
5	D	1966	5MC	C5-C4	-2.37	1.42	1.44
5	D	2073	G7M	C5-C6	-2.29	1.39	1.45
5	D	2449	2MG	C8-N7	-2.28	1.31	1.34
5	D	747	1MG	C5-C4	-2.27	1.37	1.43
5	D	747	1MG	C5-C6	-2.11	1.41	1.47
5	D	1620	6MZ	C1'-N9	-2.06	1.44	1.49
5	D	2449	2MG	C5-C4	-2.06	1.38	1.43
5	D	2507	2MA	C6-N1	2.06	1.37	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	2507	2MA	C5-C6-N6	3.75	126.03	120.31
5	D	2507	2MA	CM2-C2-N1	3.46	122.31	117.13
5	D	2453	H2U	O2-C2-N1	-2.99	119.51	123.10
5	D	2507	2MA	C5-C6-N1	-2.82	117.50	120.84
20	l	81	4D4	O-C-CA	-2.62	118.04	124.77
5	D	2453	H2U	N3-C2-N1	2.57	119.23	116.65
5	D	2034	6MZ	C2-N1-C6	2.52	118.55	116.60
5	D	2507	2MA	N3-C2-N1	-2.43	121.52	125.77
5	D	2507	2MA	C2-N1-C6	2.41	121.81	118.10
5	D	2608	PSU	C2'-C3'-C4'	-2.41	97.95	102.61
5	D	2449	2MG	O6-C6-C5	2.30	128.89	124.32
5	D	1620	6MZ	C2-N1-C6	2.11	118.24	116.60
5	D	1837	2MG	O6-C6-C5	2.11	128.51	124.32
5	D	2609	PSU	C2'-C3'-C4'	-2.08	98.60	102.61
5	D	2255	OMG	O6-C6-C5	2.05	128.38	124.32
5	D	2556	OMU	O2'-C2'-C1'	2.05	112.87	108.99

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1919	3TD	O4'-C4'-C5'-O5'
8	G	150	MEQ	NE2-CD-CG-CB
8	G	150	MEQ	OE1-CD-CG-CB
5	D	1919	3TD	C3'-C4'-C5'-O5'
5	D	2034	6MZ	O4'-C4'-C5'-O5'
5	D	2034	6MZ	C3'-C4'-C5'-O5'
20	l	81	4D4	NE-CD-CG-CB
5	D	2073	G7M	C4'-C5'-O5'-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	D	748	PSU	O4'-C1'-C5-C6
8	G	150	MEQ	C-CA-CB-CG
5	D	748	PSU	C2'-C1'-C5-C6
5	D	2507	2MA	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 299 ligands modelled in this entry, 298 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
35	MS6	1	201	-	7,7,7	0.57	0	7,7,7	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	MS6	1	201	-	-	1/4/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	1	201	MS6	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	D	6
20	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	880:A	O3'	901:A	P	17.61
1	D	544:G	O3'	551:C	P	17.04
1	D	1054:C	O3'	1109:G	P	17.03
1	D	2102:U	O3'	2195:A	P	16.99
1	D	1174:C	O3'	1179:G	P	15.94
1	D	1872:G	O3'	1876:C	P	12.48
1	1	81:4D4	C	83:GLY	N	5.21

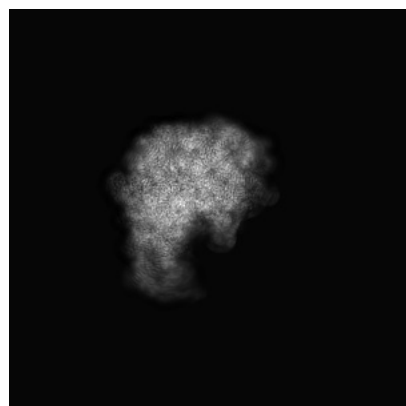
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46632. These allow visual inspection of the internal detail of the map and identification of artifacts.

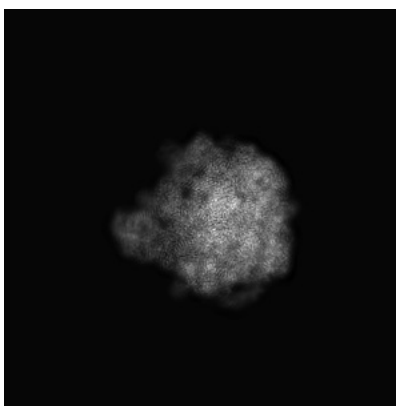
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

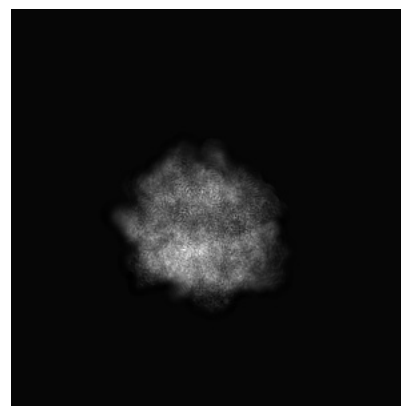
6.1.1 Primary map



X

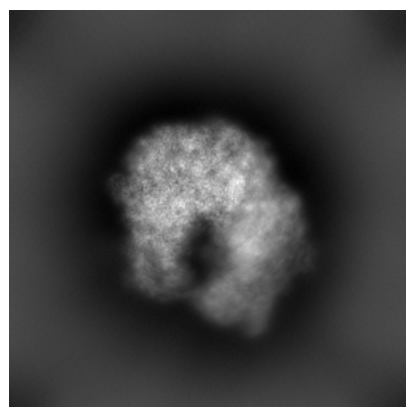


Y

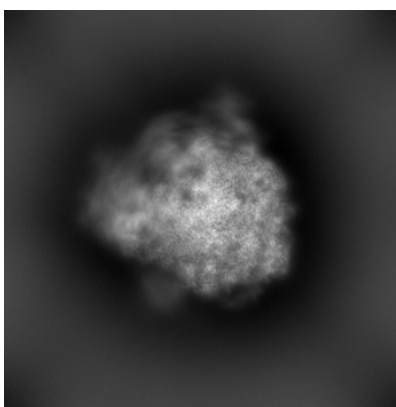


Z

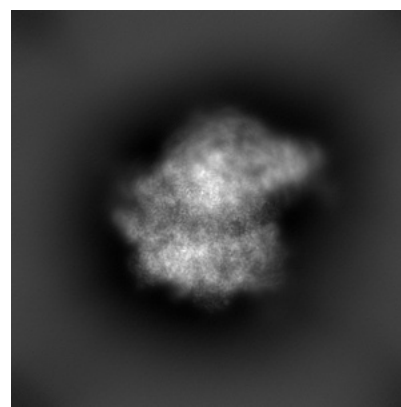
6.1.2 Raw map



X



Y

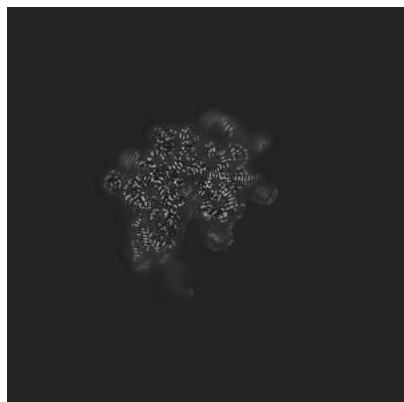


Z

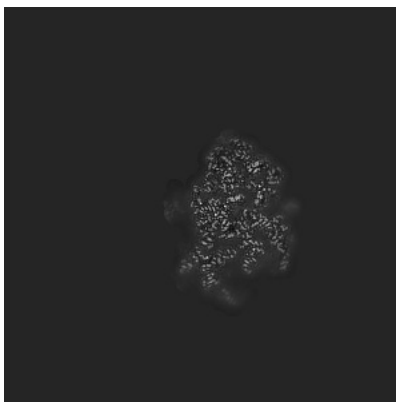
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

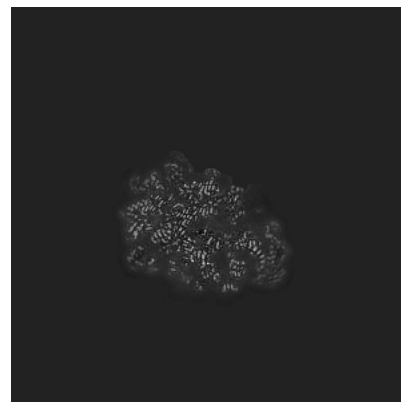
6.2.1 Primary map



X Index: 256

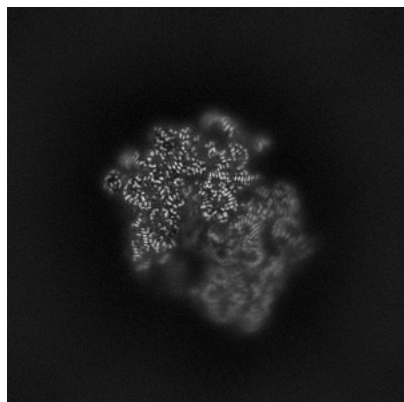


Y Index: 256

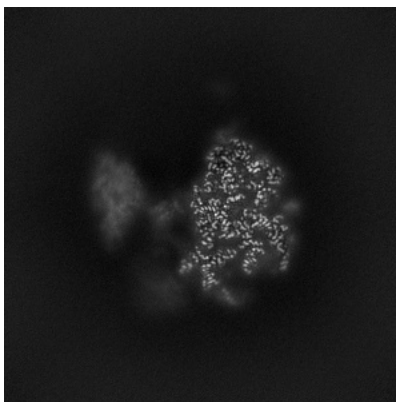


Z Index: 256

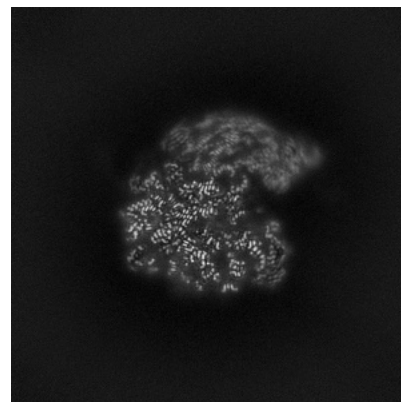
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

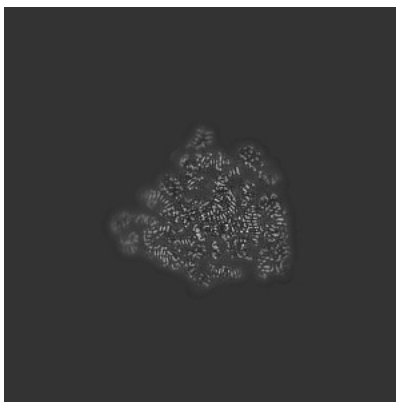
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

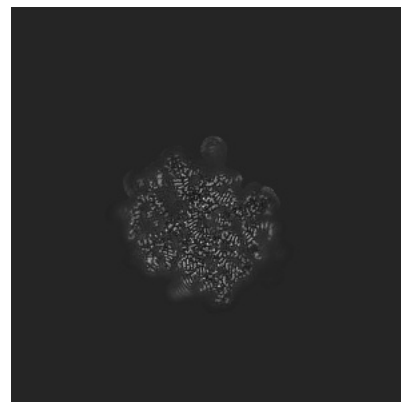
6.3.1 Primary map



X Index: 225

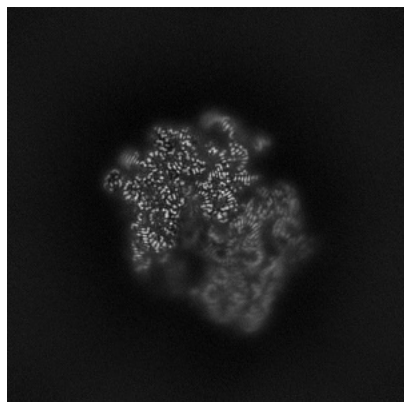


Y Index: 199

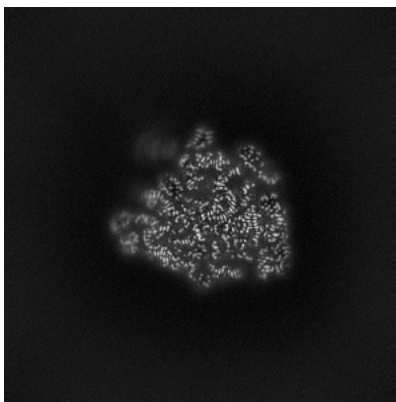


Z Index: 270

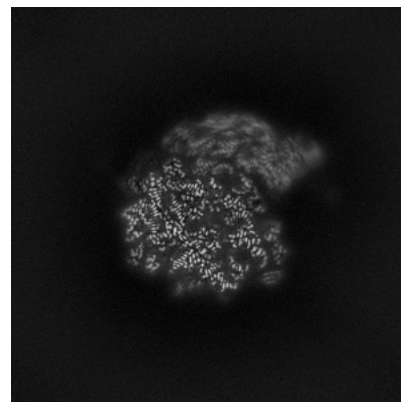
6.3.2 Raw map



X Index: 255



Y Index: 199

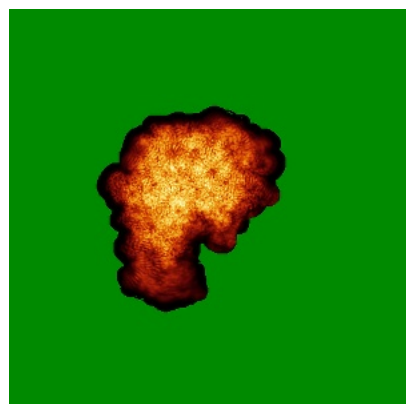


Z Index: 261

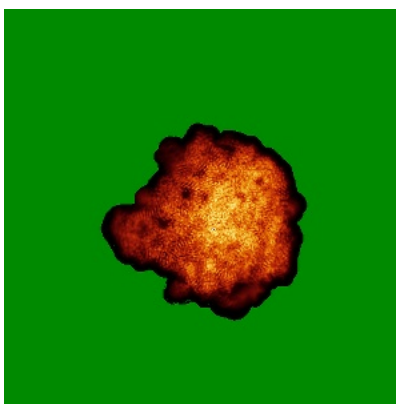
The images above show the largest variance slices of the map in three orthogonal directions.

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

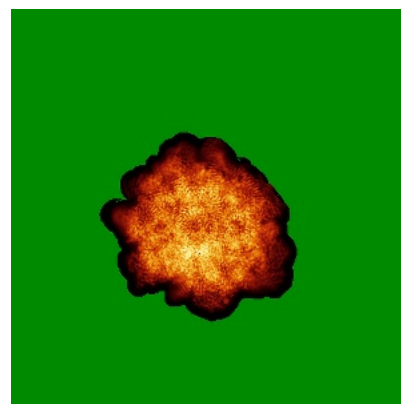
6.4.1 Primary map



X

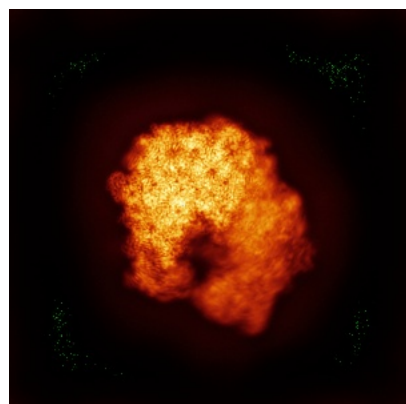


Y

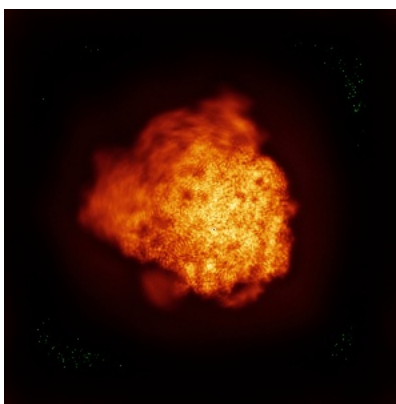


Z

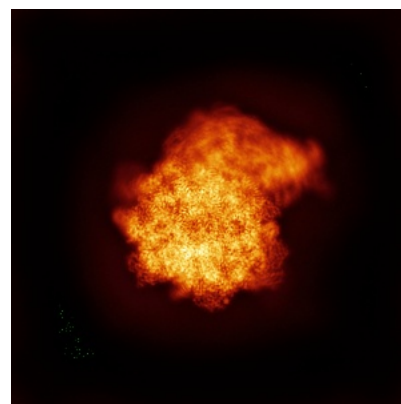
6.4.2 Raw map



X



Y

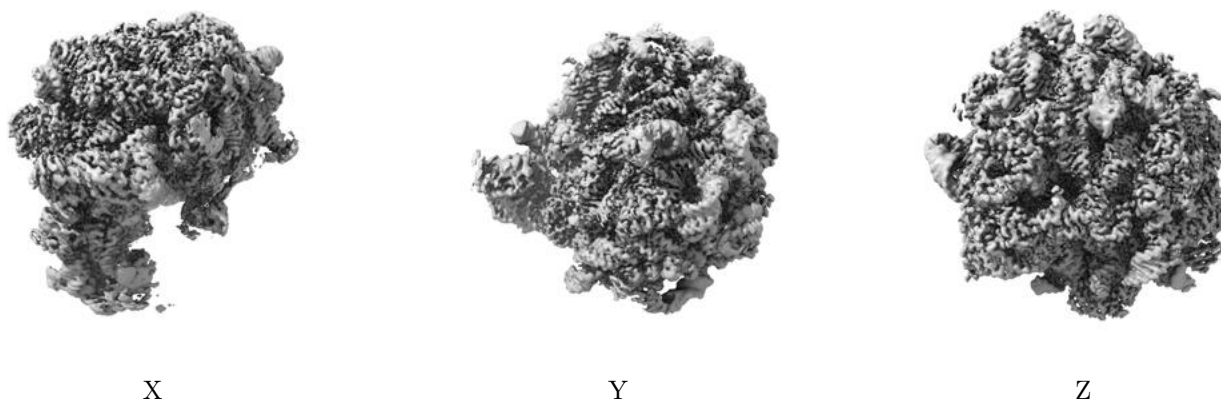


Z

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 1.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

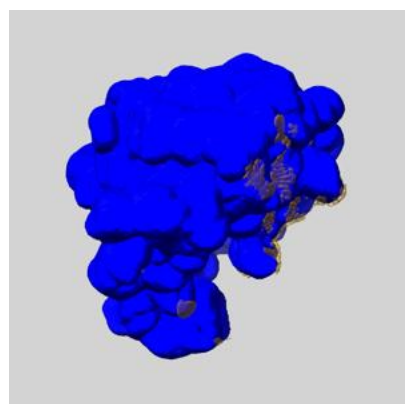
6.6 Mask visualisation [i](#)

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

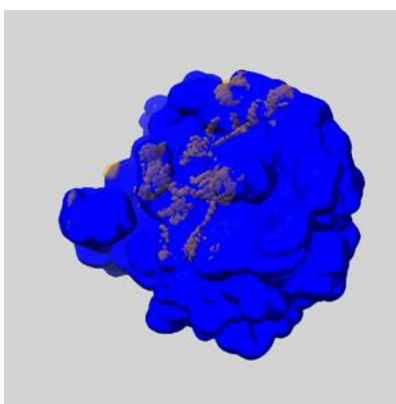
A mask typically either:

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

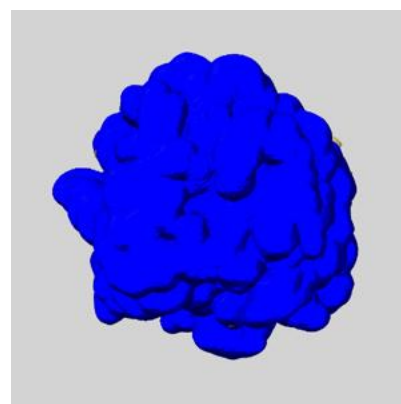
6.6.1 emd_46632_msk_1.map [i](#)



X



Y

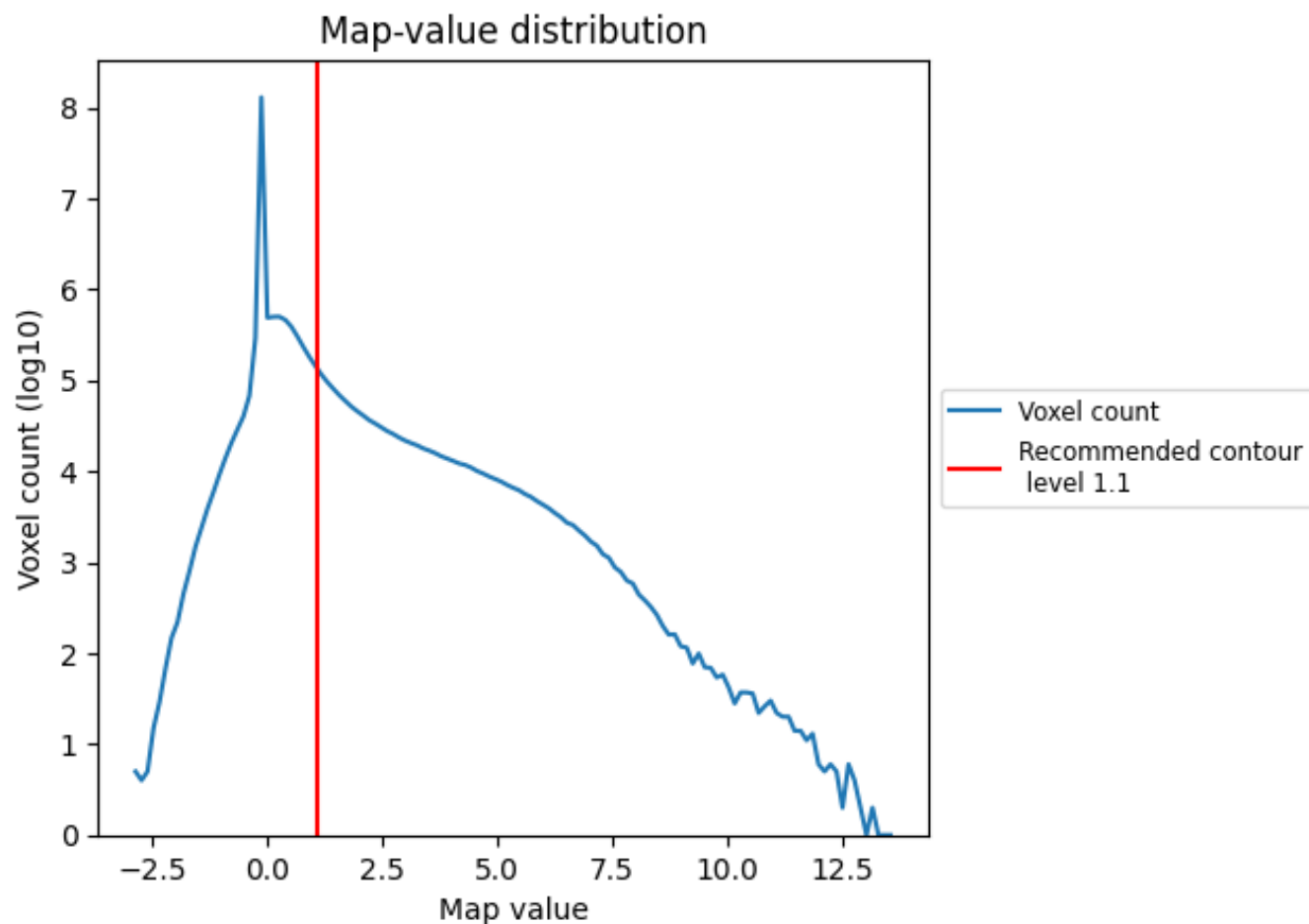


Z

7 Map analysis [i](#)

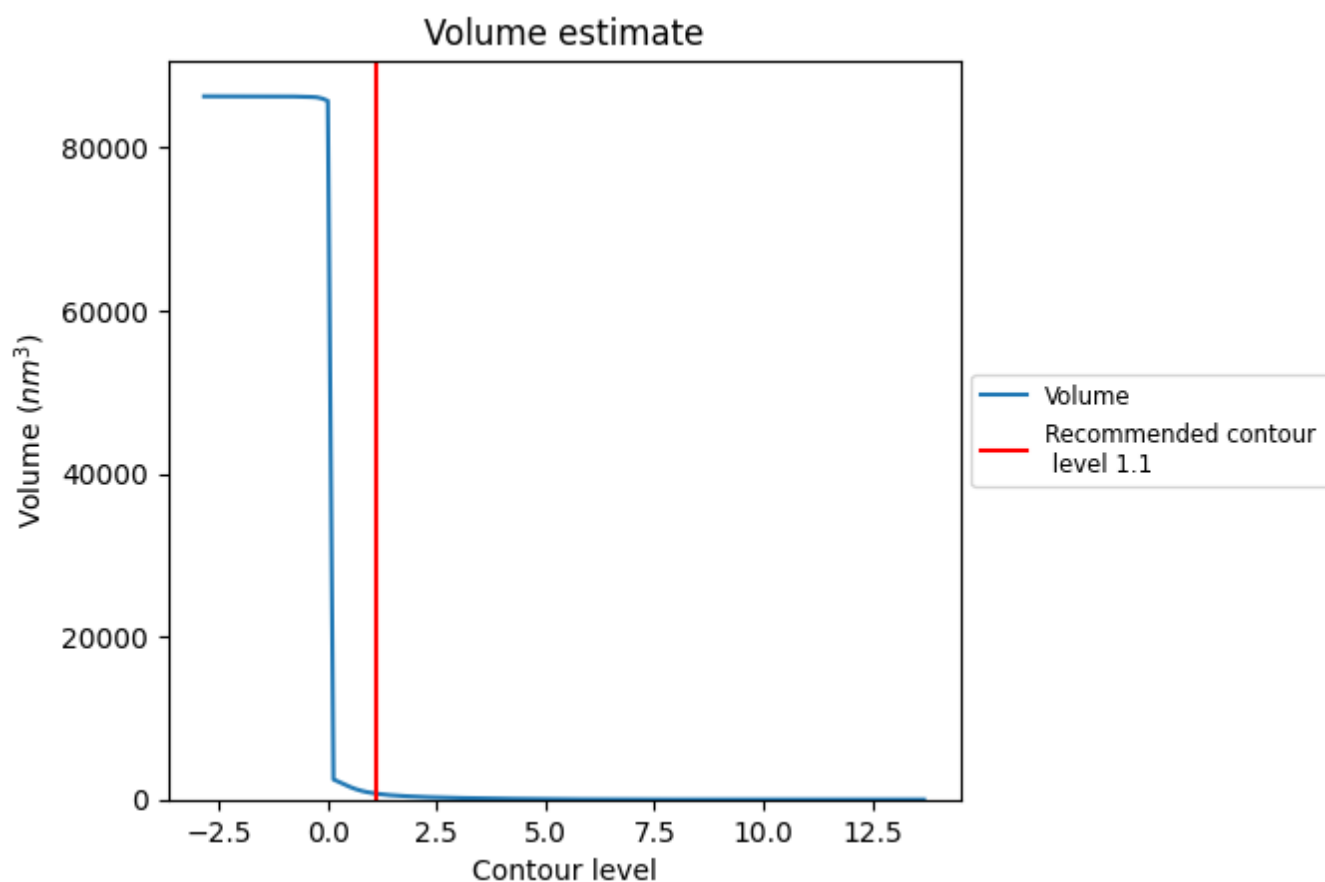
This section contains the results of statistical analysis of the map.

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.

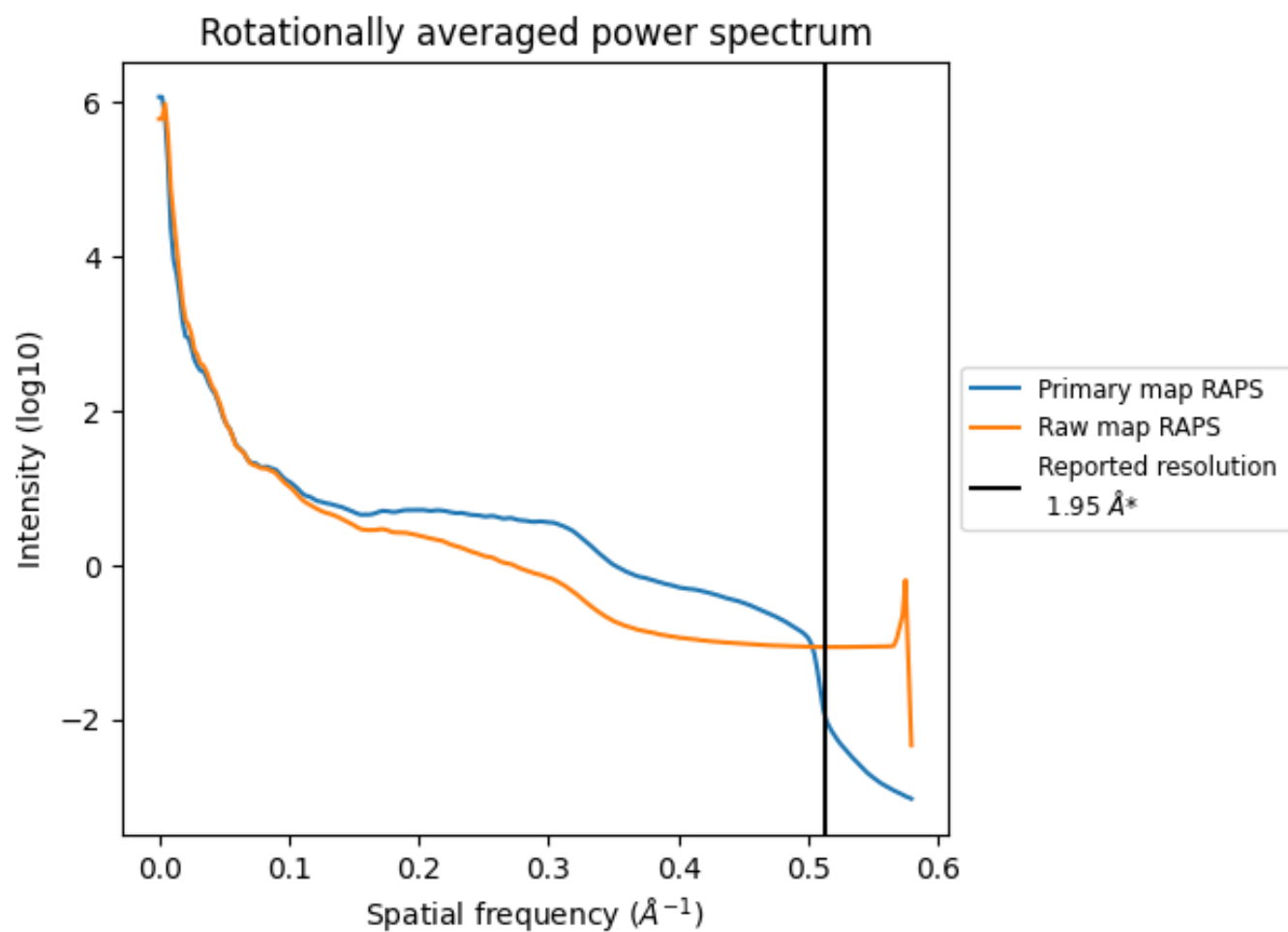
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 734 nm³; this corresponds to an approximate mass of 663 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 ⓘ

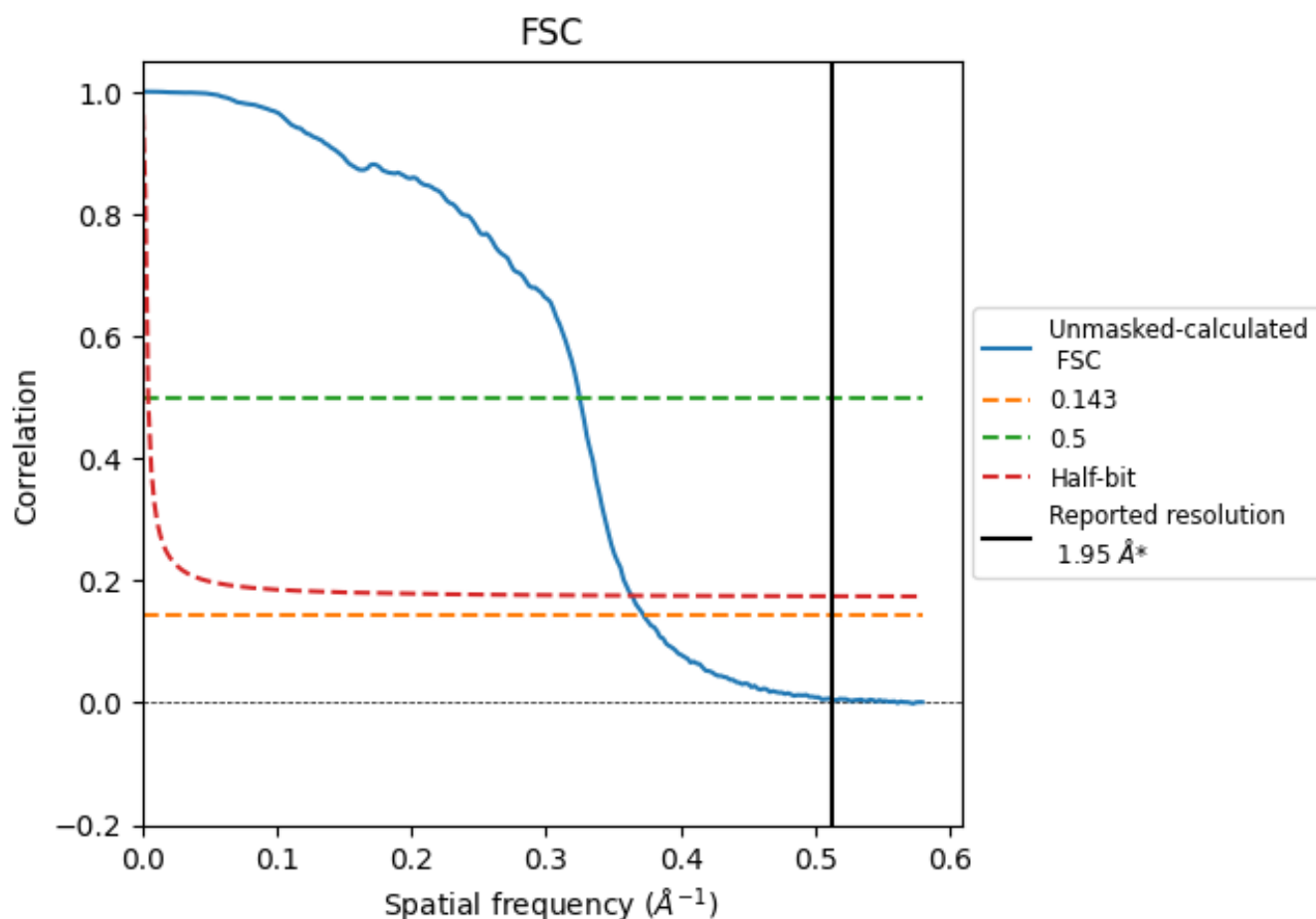


*Reported resolution corresponds to spatial frequency of 0.513 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.513 Å⁻¹

8.2 Resolution estimates [i](#)

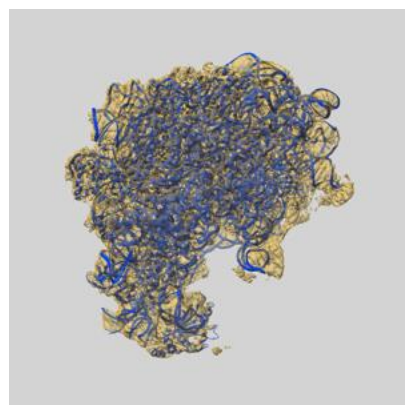
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.95	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.69	3.08	2.75

*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 2.69 differs from the reported value 1.95 by more than 10 %

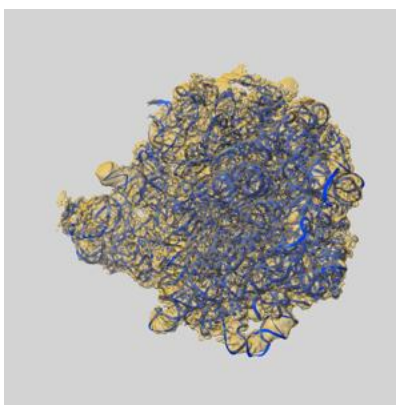
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46632 and PDB model 9D89. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

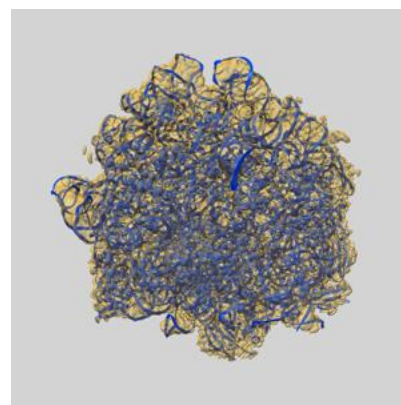
9.1 Map-model overlay [i](#)



X



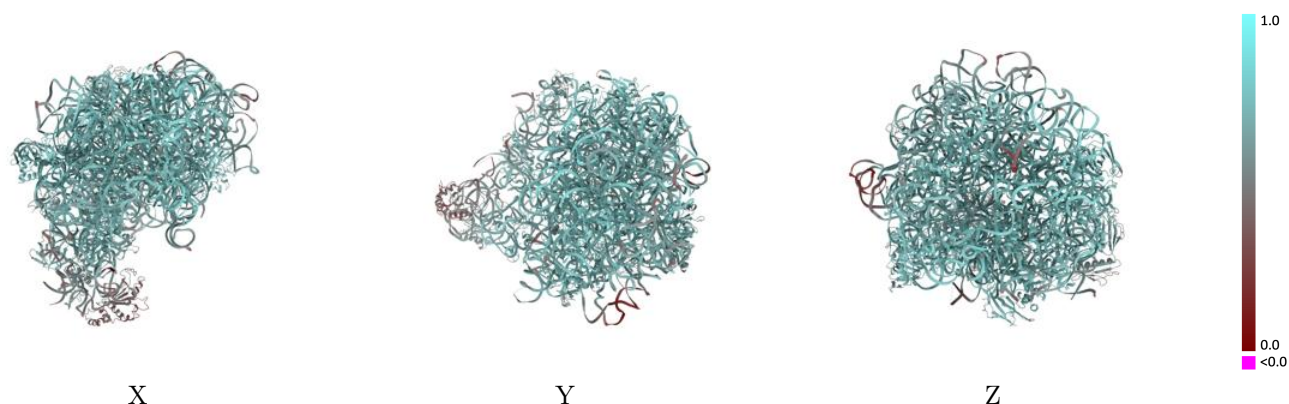
Y



Z

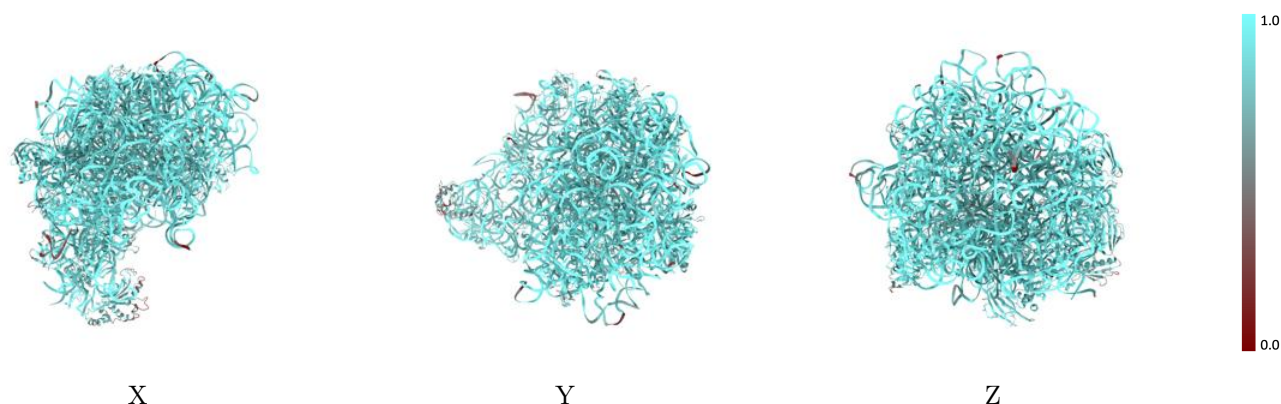
The images above show the 3D surface view of the map at the recommended contour level 1.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



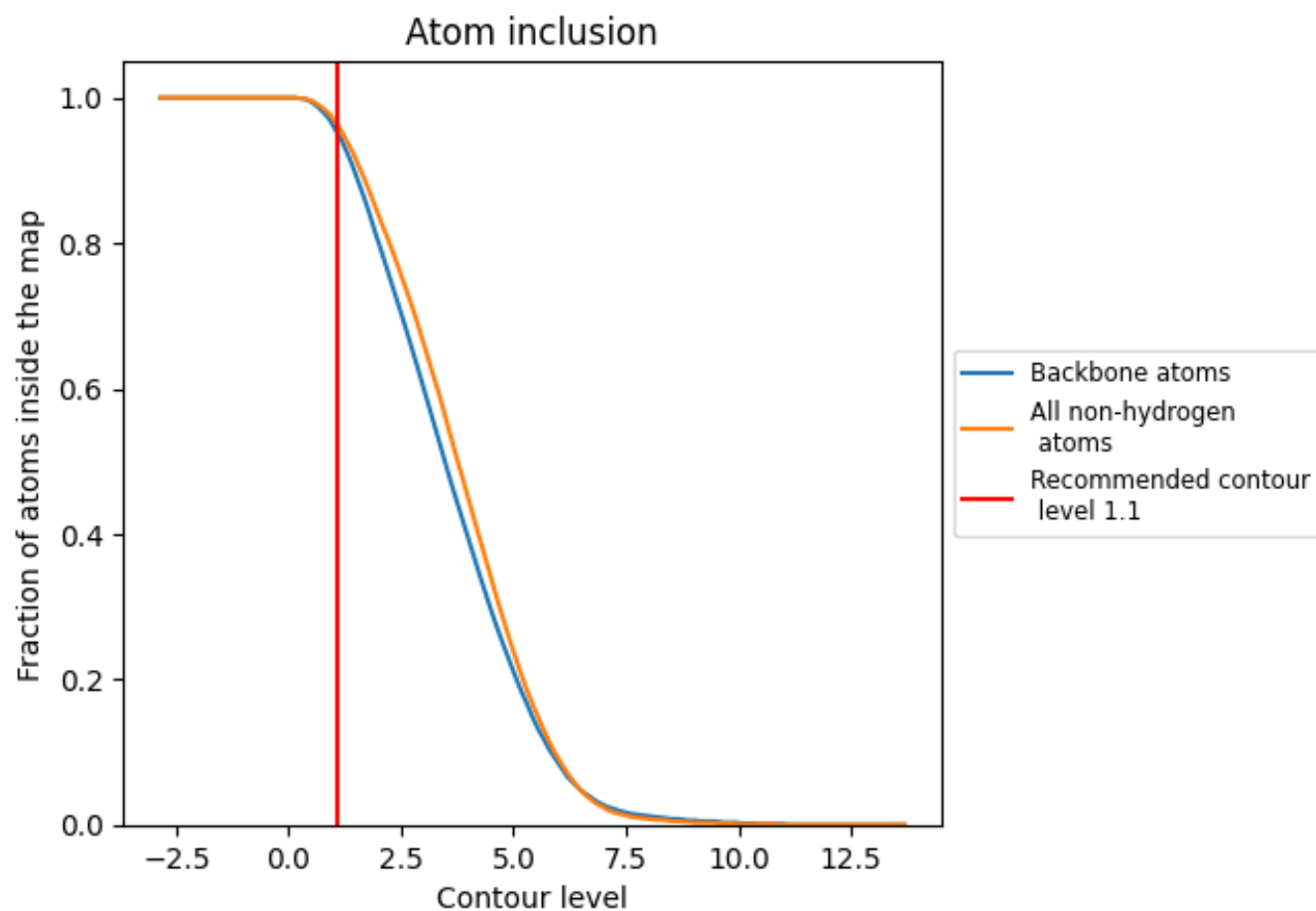
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.1).

































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 96% 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 (1.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9620	 0.6920
0	 0.8700	 0.6750
1	 0.9830	 0.7710
B	 0.9800	 0.7500
C	 0.9490	 0.6780
D	 0.9820	 0.7030
E	 0.9720	 0.5670
F	 0.9700	 0.7390
G	 0.9550	 0.7310
H	 0.9060	 0.6970
I	 0.9500	 0.7180
J	 0.9870	 0.7540
K	 0.9320	 0.6860
L	 0.9340	 0.7110
M	 0.9300	 0.7110
T	 0.9480	 0.6340
f	 0.6500	 0.3860
g	 0.8100	 0.5610
h	 0.7600	 0.6050
i	 0.9590	 0.7320
j	 0.9510	 0.7200
l	 0.9520	 0.7160
n	 0.8880	 0.5800
o	 0.9050	 0.6980
p	 0.9810	 0.7630
q	 0.9250	 0.6980
r	 0.9460	 0.7250
t	 0.8890	 0.6570
u	 0.8650	 0.6340
w	 0.9430	 0.7000
x	 0.8920	 0.6470
y	 0.9180	 0.7170

