Full wwPDB EM Validation Report ⓘ

Apr 22, 2025 – 09:59 AM EDT

PDB ID	:	8VKW / pdb_00008vkw
EMDB ID	:	EMD-43333
Title	:	Structure of Mycobacterium smegmatis 50S ribosomal subunit bound to delNTE-HflX
Authors	:	Majumdar, S.; Koripella, R.K.; Sharma, M.R.; Manjari, S.R.; Banavali, N.K.; Agrawal, R.K.
Deposited on	:	2024-01-10
Resolution	:	3.44 Å(reported)
Based on initial models	:	5O61, 6DZI

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:

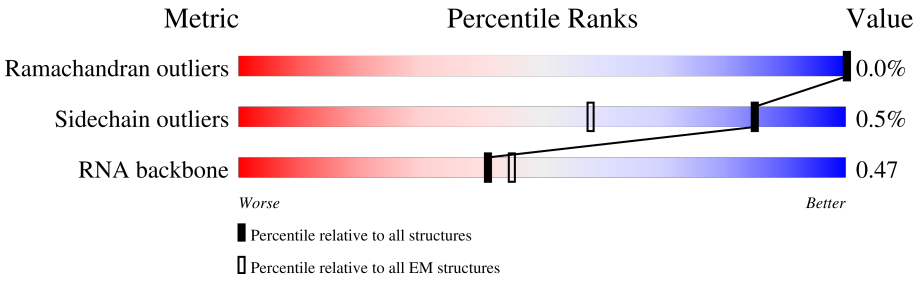
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.44 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 <=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	2	61	97%
2	3	24	96%
3	4	431	12% 99%
4	A	3120	75% 23%
5	B	118	68% 32%
6	C	278	99%
7	D	217	99%
8	E	215	96%

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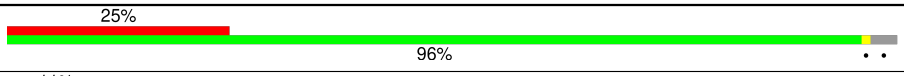
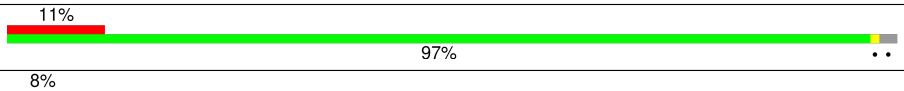
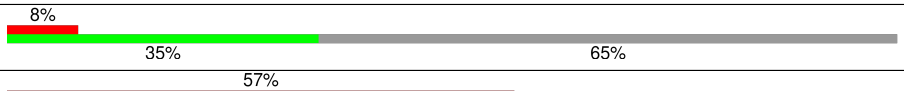
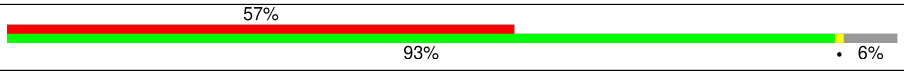
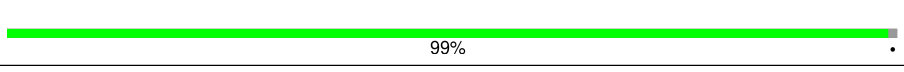
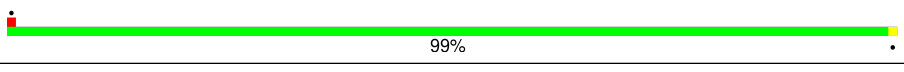
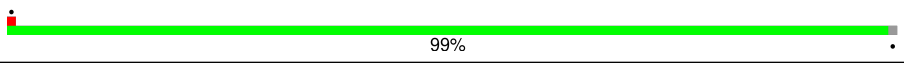
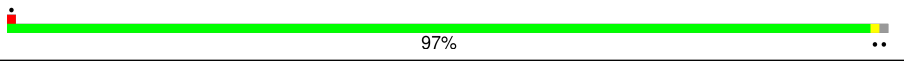
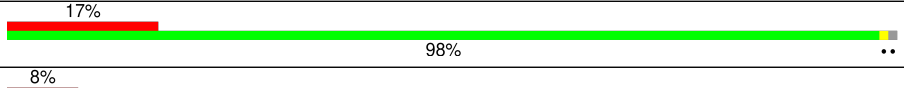
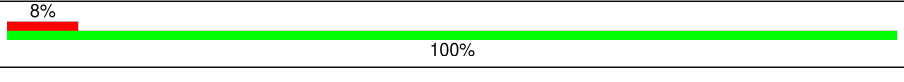
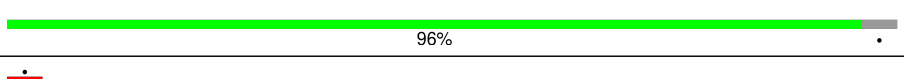
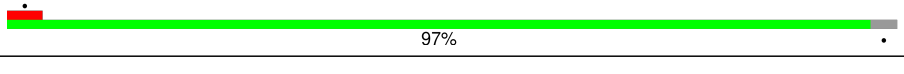
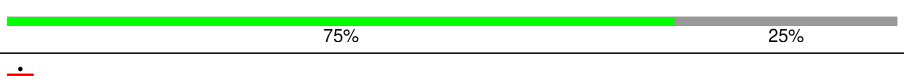
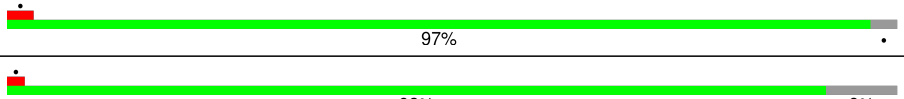
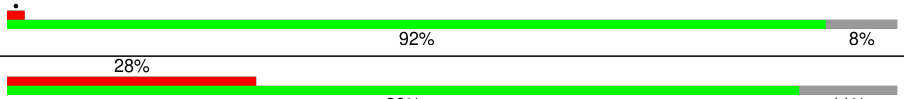
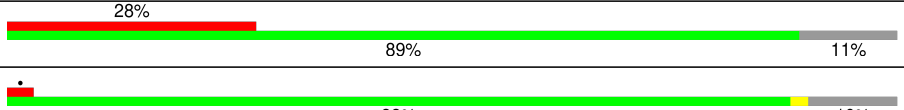
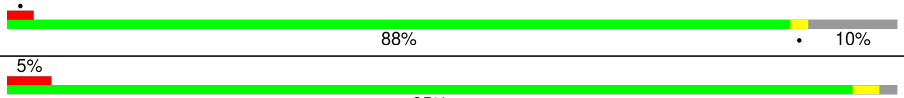
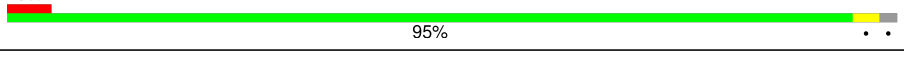
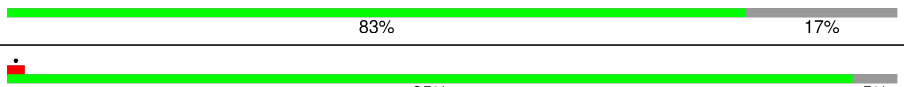
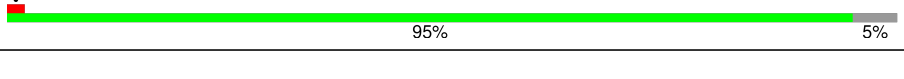
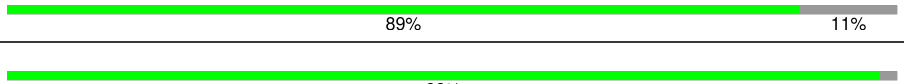
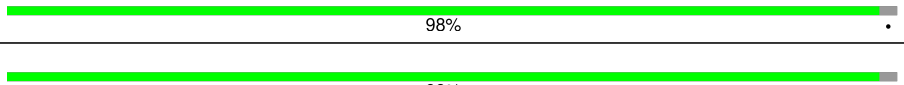
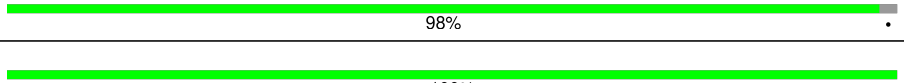
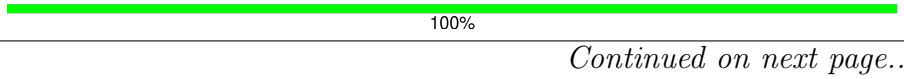
Mol	Chain	Length	Quality of chain
9	F	187	
10	G	179	
11	H	151	
12	J	142	
13	K	147	
14	L	122	
15	M	147	
16	N	138	
17	O	199	
18	P	127	
19	Q	113	
20	R	129	
21	S	103	
22	T	153	
23	U	100	
24	V	105	
25	W	215	
26	X	88	
27	Y	64	
28	Z	77	
29	b	57	
30	c	55	
31	d	47	
32	e	64	
33	f	37	

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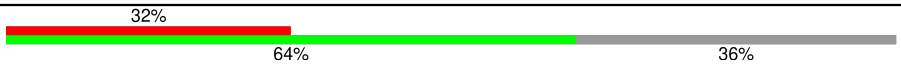
Mol	Chain	Length	Quality of chain
34	g	75	

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 97621 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 L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	2	59	Total	C	N	O	0	0
			474	292	95	87		

- Molecule 2 is a protein called 50S Ribosomal Protein L37.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	3	23	Total	C	N	O	0	0
			189	111	50	28		

- Molecule 3 is a protein called GTPase HflX.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	426	Total	C	N	O	S	0	0
			3224	1995	599	623	7		

- Molecule 4 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	3043	Total	C	N	O	P	0	0
			65348	29127	12020	21158	3043		

- Molecule 5 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	118	Total	C	N	O	P	0	0
			2522	1126	468	810	118		

- Molecule 6 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	275	Total	C	N	O	S	0	0
			2106	1296	437	369	4		

- Molecule 7 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	214	Total	C	N	O	S	0	0
			1587	982	310	290	5		

- Molecule 8 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	209	Total	C	N	O	S	0	0
			1565	967	294	302	2		

- Molecule 9 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	182	Total	C	N	O	S	0	0
			1438	903	270	260	5		

- Molecule 10 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	176	Total	C	N	O	S	0	0
			1346	843	249	253	1		

- Molecule 11 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	53	Total	C	N	O	S	0	0
			367	230	67	69	1		

- Molecule 12 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	133	Total	C	N	O	S	0	0
			990	625	175	187	3		

- Molecule 13 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	146	Total	C	N	O	S	0	0
			1127	719	207	200	1		

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	122	Total 938	C 586	N 179	O 170	S 3	0	0

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	145	Total 1078	C 676	N 205	O 194	S 3	0	0

- Molecule 16 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	136	Total 1089	C 689	N 212	O 186	S 2	0	0

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	118	Total 928	C 583	N 180	O 163	S 2	0	0

- Molecule 18 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	P	126	Total 941	C 576	N 197	O 168	0	0

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	113	Total 907	C 570	N 171	O 165	S 1	0	0

- Molecule 20 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	124	Total 988	C 613	N 203	O 172	0	0

- Molecule 21 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	S	100	Total 754	C 478	N 137	O 139	0	0

- Molecule 22 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	T	114	Total 873	C 543	N 171	O 159	0	0

- Molecule 23 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	U	97	Total 756	C 479	N 138	O 139	0	0

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	97	Total 729	C 455	N 136	O 136	S 2	0	0

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	W	192	Total 1420	C 877	N 253	O 290	0	0

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	X	79	Total 586	C 361	N 123	O 102	0	0

- Molecule 27 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	63	Total 464	C 280	N 100	O 80	S 4	0	0

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	64	Total	C	N	O	S	0	0
			531	324	103	103	1		

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	54	Total	C	N	O	S	0	0
			423	260	93	69	1		

- Molecule 30 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	49	Total	C	N	O	S	0	0
			397	244	79	70	4		

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	46	Total	C	N	O	S	0	0
			377	225	97	54	1		

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	e	63	Total	C	N	O	0	0
			496	300	113	83		

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	37	Total	C	N	O	S	0	0
			299	181	66	47	5		

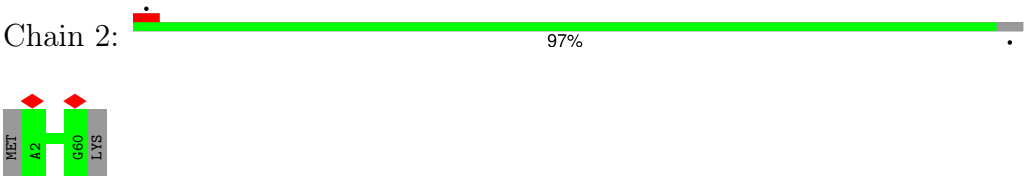
- Molecule 34 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	48	Total	C	N	O	S	0	0
			364	225	63	71	5		

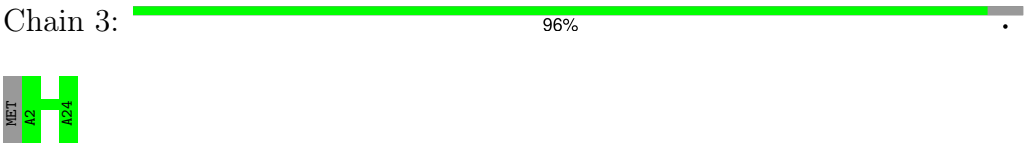
3 Residue-property plots (i)

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.

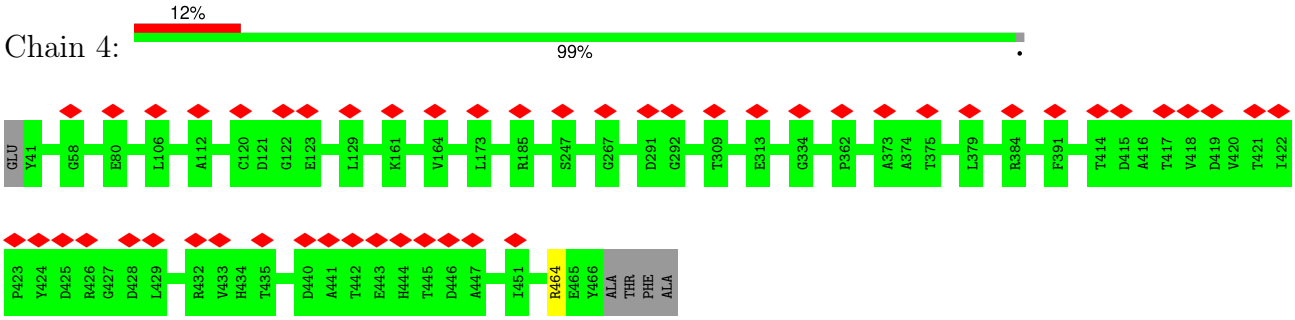
• Molecule 1: 50S ribosomal protein L30



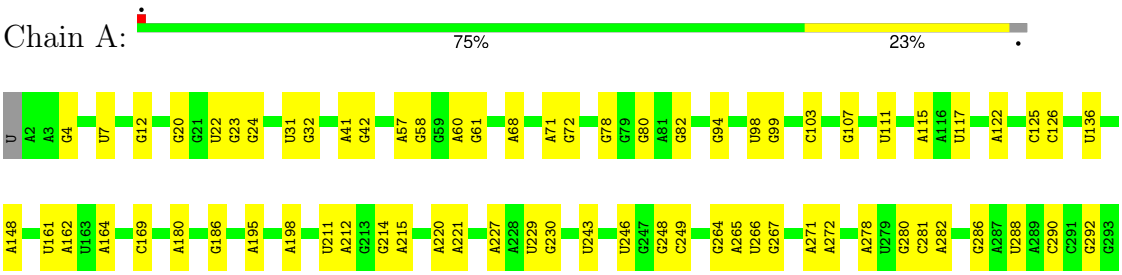
• Molecule 2: 50S Ribosomal Protein L37

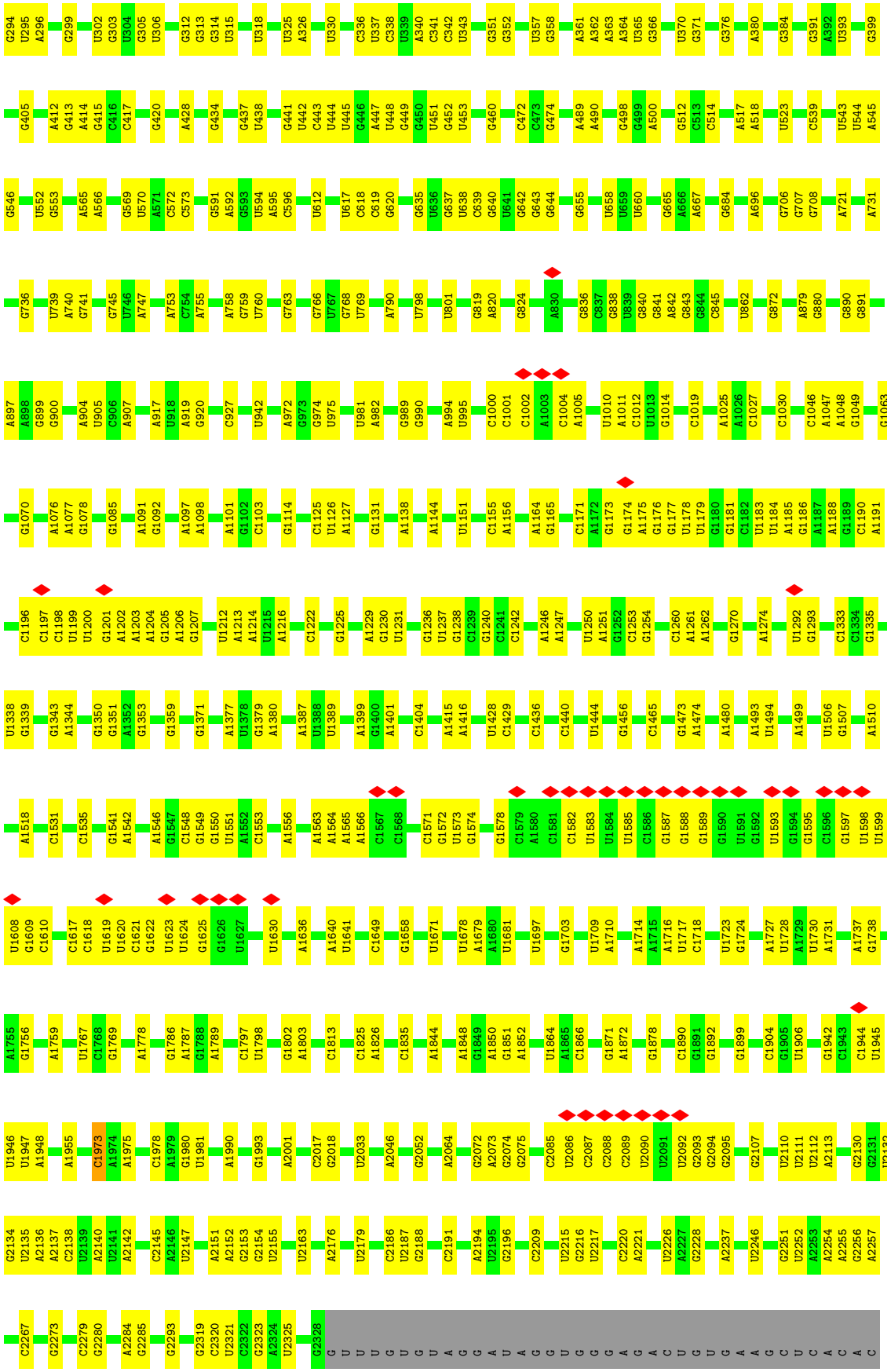


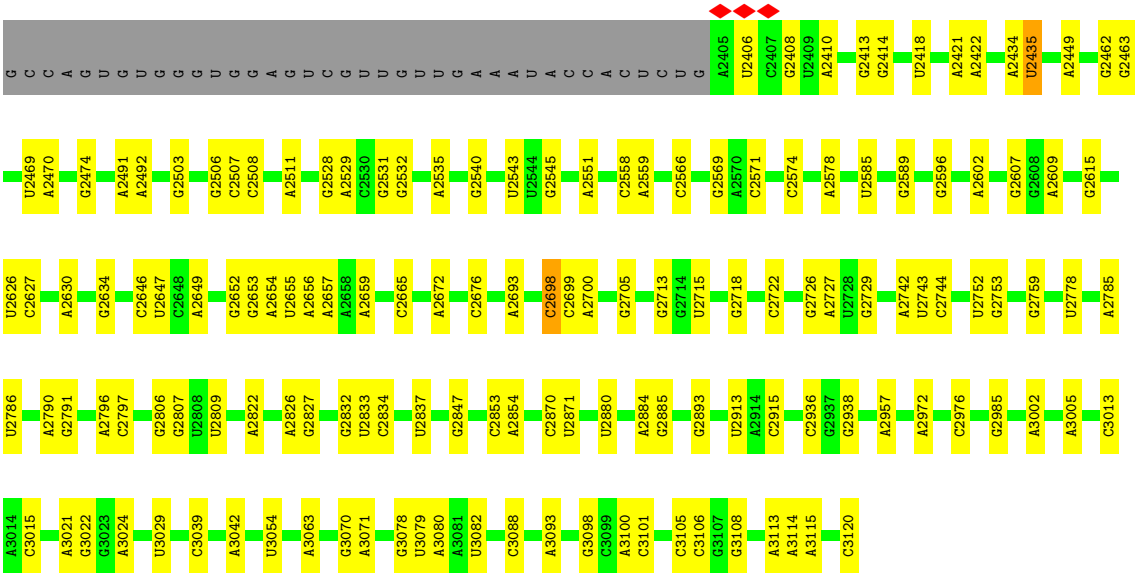
• Molecule 3: GTPase HflX



• Molecule 4: 23S ribosomal RNA

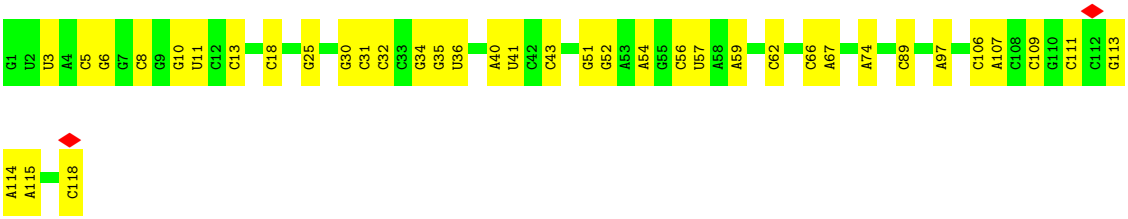






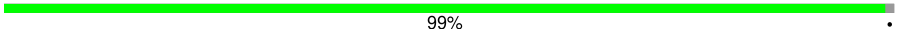
• Molecule 5: 5S ribosomal RNA

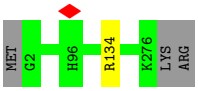
Chain B:



• Molecule 6: 50S ribosomal protein L2

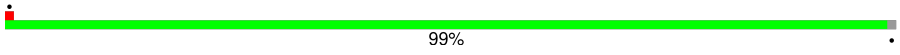
Chain C:

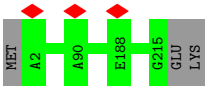




• Molecule 7: 50S ribosomal protein L3

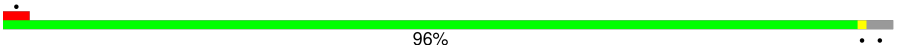
Chain D:

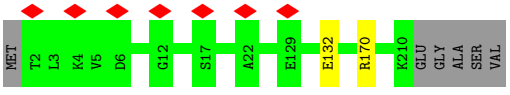




• Molecule 8: 50S Ribosomal Protein L4

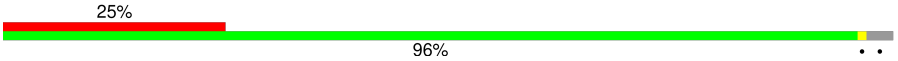
Chain E:

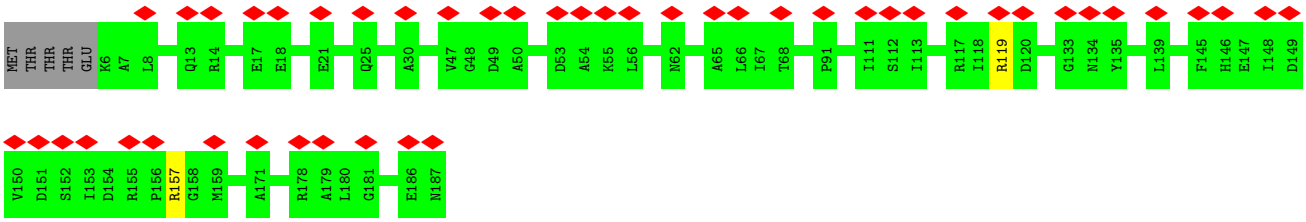




• Molecule 9: 50S Ribosomal Protein L5

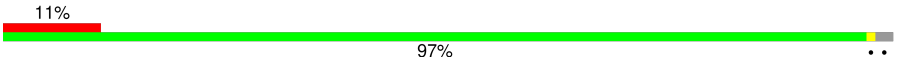
Chain F:

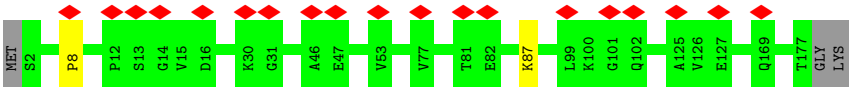




• Molecule 10: 50S ribosomal protein L6

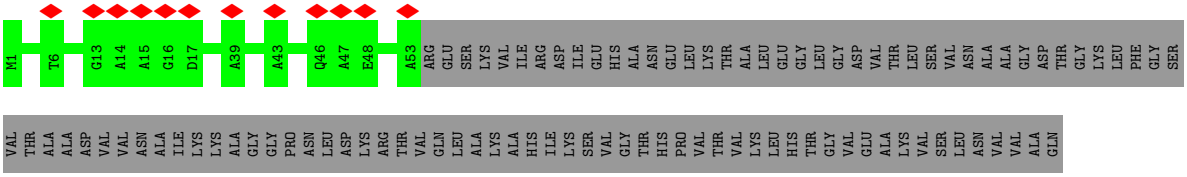
Chain G:





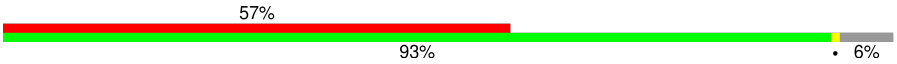
• Molecule 11: 50S ribosomal protein L9

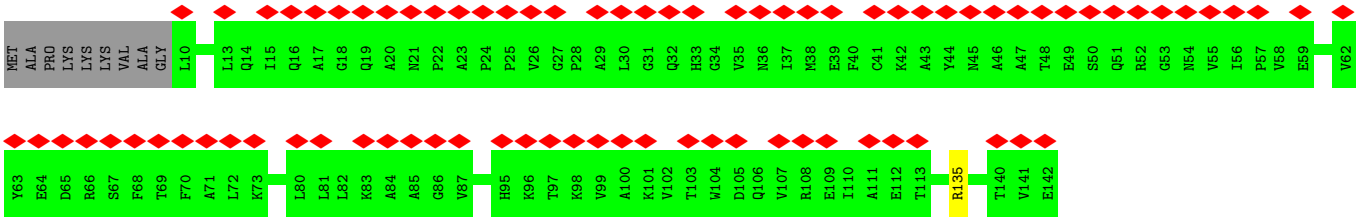
Chain H:



• Molecule 12: 50S ribosomal protein L11

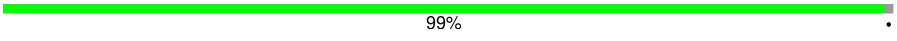
Chain J:





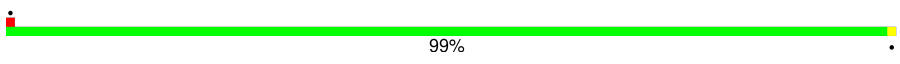
• Molecule 13: 50S Ribosomal Protein L13

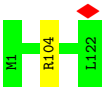
Chain K:



• Molecule 14: 50S ribosomal protein L14

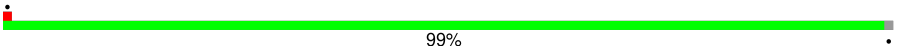
Chain L:

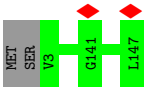




• Molecule 15: 50S ribosomal protein L15

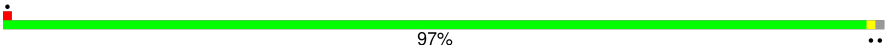
Chain M:

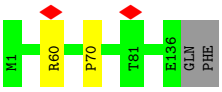




• Molecule 16: Large ribosomal subunit protein uL16

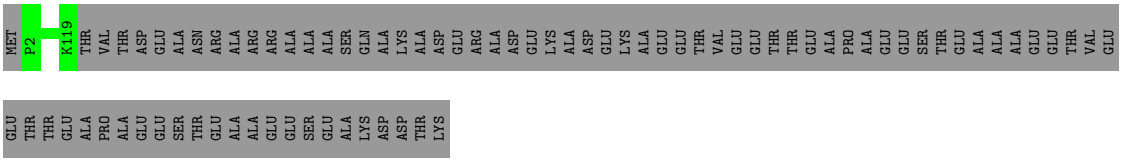
Chain N:





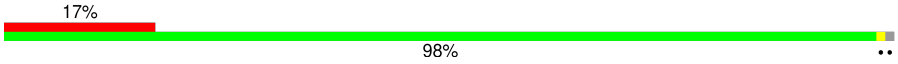
• Molecule 17: 50S ribosomal protein L17

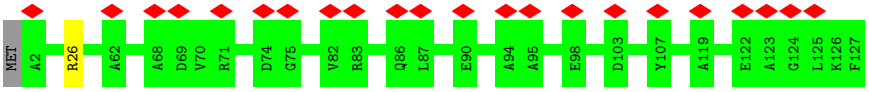
Chain O:



• Molecule 18: 50S Ribosomal Protein L18

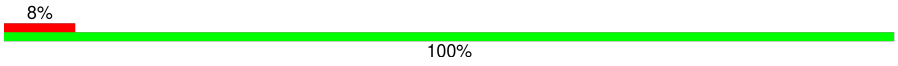
Chain P:

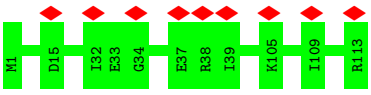




• Molecule 19: 50S ribosomal protein L19

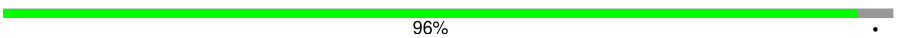
Chain Q:

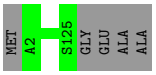




• Molecule 20: 50S Ribosomal Protein L20

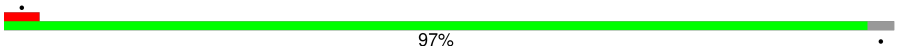
Chain R:

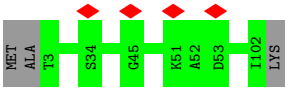




• Molecule 21: 50S Ribosomal Protein L21

Chain S:



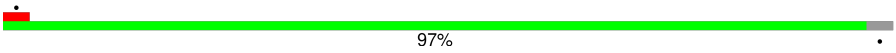


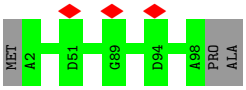
• Molecule 22: 50S Ribosomal Protein L22

Chain T:

• Molecule 23: 50S Ribosomal Protein L23

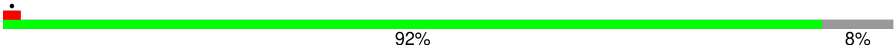
Chain U:

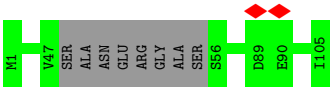




• Molecule 24: 50S ribosomal protein L24

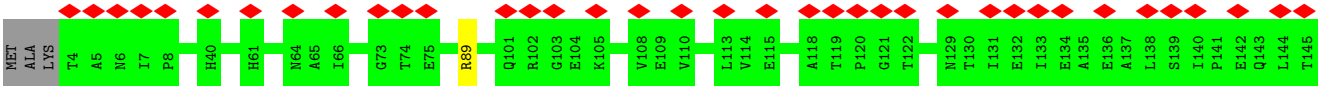
Chain V:

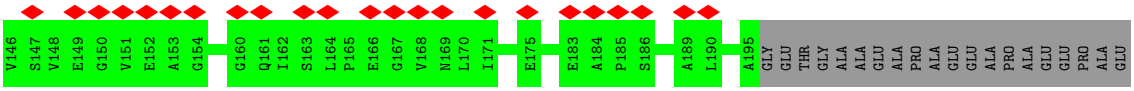




• Molecule 25: 50S ribosomal protein L25

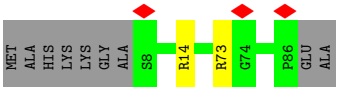
Chain W:





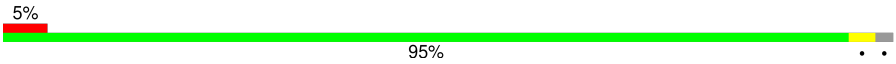
• Molecule 26: 50S ribosomal protein L27

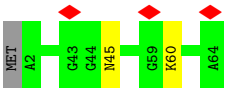
Chain X:



• Molecule 27: 50S Ribosomal Protein L28

Chain Y:



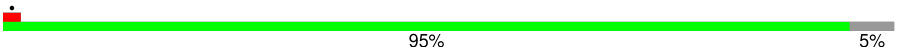


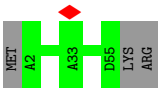
• Molecule 28: 50S ribosomal protein L29

Chain Z:

• Molecule 29: 50S ribosomal protein L32

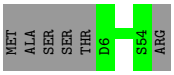
Chain b:





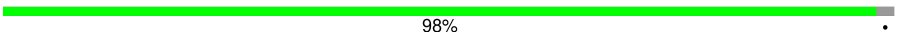
• Molecule 30: 50S Ribosomal Protein L33

Chain c:



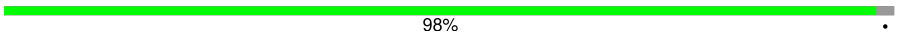
• Molecule 31: 50S ribosomal protein L34

Chain d:



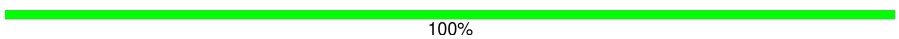
• Molecule 32: 50S ribosomal protein L35

Chain e:



• Molecule 33: 50S ribosomal protein L36

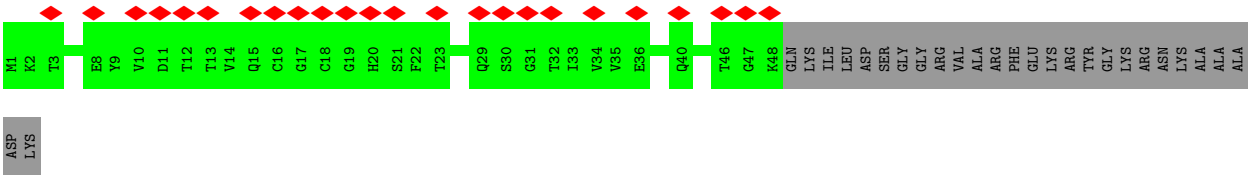
Chain f:



There are no outlier residues recorded for this chain.

• Molecule 34: 50S Ribosomal Protein L31

Chain g:


M1
K2
T3
E8
Y9
V10
D11
T12
T13
V14
Q15
C16
G17
C18
G19
H20
S21
F22
T23
Q29
S30
G31
T32
I33
V34
V35
E36
Q40
T46
G47
K48
GLN
LYS
ILE
LEU
ASP
SER
GLY
GLY
ARG
VAL
ALA
ARG
PHE
GLU
LYS
ARG
TYR
GLY
LYS
ARG
ASN
LYS
ALA
ALA
ALA
ASP
LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27550	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60.64	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.442	Depositor
Minimum map value	-0.335	Depositor
Average map value	0.030	Depositor
Map value standard deviation	0.091	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	338.4, 338.4, 338.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84599996, 0.84599996, 0.84599996	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	2	0.29	0/477	0.57	0/640
2	3	0.29	0/191	0.63	0/247
3	4	0.27	0/3264	0.56	0/4423
4	A	0.57	0/73172	0.79	16/114170 (0.0%)
5	B	0.38	0/2821	0.83	3/4396 (0.1%)
6	C	0.32	0/2149	0.57	0/2890
7	D	0.32	0/1609	0.57	0/2165
8	E	0.31	0/1588	0.52	0/2148
9	F	0.25	0/1460	0.54	0/1965
10	G	0.70	3/1367 (0.2%)	0.95	4/1845 (0.2%)
11	H	0.29	0/370	0.55	0/501
12	J	0.25	0/1006	0.49	0/1364
13	K	0.30	0/1154	0.49	0/1563
14	L	0.31	0/946	0.57	0/1268
15	M	0.32	0/1091	0.53	0/1457
16	N	0.38	1/1115 (0.1%)	0.55	0/1502
17	O	0.30	0/945	0.55	0/1267
18	P	0.38	0/950	0.62	0/1279
19	Q	0.30	0/921	0.56	0/1236
20	R	0.34	0/1000	0.56	0/1341
21	S	0.33	0/764	0.52	0/1030
22	T	0.31	0/887	0.57	0/1204
23	U	0.32	0/766	0.53	0/1030
24	V	0.28	0/735	0.50	0/983
25	W	0.25	0/1435	0.51	0/1960
26	X	0.32	0/595	0.60	0/798
27	Y	0.33	0/472	0.58	0/634
28	Z	0.27	0/534	0.57	0/713
29	b	0.32	0/427	0.60	0/572
30	c	0.29	0/404	0.52	0/541
31	d	0.33	0/380	0.71	0/500
32	e	0.29	0/501	0.64	0/664
33	f	0.30	0/303	0.62	0/401
34	g	0.27	0/372	0.46	0/503

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	0.51	4/106171 (0.0%)	0.75	23/159200 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	8	PRO	N-CD	18.20	1.73	1.47
10	G	8	PRO	CG-CD	-11.84	1.11	1.50
10	G	8	PRO	CB-CG	-7.08	1.14	1.50
16	N	70	PRO	N-CD	6.15	1.56	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	G	8	PRO	N-CD-CG	-20.88	71.88	103.20
10	G	8	PRO	CB-CG-CD	18.82	179.91	106.50
10	G	8	PRO	CA-CB-CG	-14.19	77.03	104.00
10	G	8	PRO	CA-N-CD	-10.40	96.94	111.50
5	B	111	C	N1-C2-O2	7.41	123.35	118.90
5	B	111	C	N3-C2-O2	-7.34	116.76	121.90
4	A	1242	C	N3-C2-O2	-7.14	116.90	121.90
4	A	2698	C	C2-N1-C1'	7.08	126.59	118.80
4	A	1944	C	N3-C2-O2	-6.72	117.20	121.90
4	A	1125	C	N3-C2-O2	-6.72	117.20	121.90
4	A	2698	C	N1-C2-O2	6.67	122.90	118.90
4	A	443	C	N3-C2-O2	-6.54	117.32	121.90
4	A	2698	C	N3-C2-O2	-6.27	117.51	121.90
4	A	1973	C	N3-C2-O2	-6.20	117.56	121.90
4	A	2435	U	C2-N1-C1'	6.05	124.97	117.70
4	A	249	C	C6-N1-C2	5.85	122.64	120.30
4	A	1183	U	C2-N1-C1'	5.72	124.57	117.70
4	A	443	C	N1-C2-O2	5.64	122.28	118.90
4	A	1428	U	C2-N1-C1'	5.60	124.42	117.70
4	A	103	C	N3-C2-O2	-5.37	118.14	121.90
4	A	905	U	C2-N1-C1'	5.25	124.00	117.70
4	A	2698	C	C6-N1-C2	-5.11	118.26	120.30
5	B	62	C	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

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	
1	2	57/61 (93%)	55 (96%)	2 (4%)	0	100	100
2	3	21/24 (88%)	21 (100%)	0	0	100	100
3	4	424/431 (98%)	378 (89%)	46 (11%)	0	100	100
6	C	273/278 (98%)	250 (92%)	23 (8%)	0	100	100
7	D	212/217 (98%)	193 (91%)	19 (9%)	0	100	100
8	E	207/215 (96%)	190 (92%)	16 (8%)	1 (0%)	25	58
9	F	180/187 (96%)	148 (82%)	32 (18%)	0	100	100
10	G	174/179 (97%)	153 (88%)	21 (12%)	0	100	100
11	H	51/151 (34%)	41 (80%)	10 (20%)	0	100	100
12	J	131/142 (92%)	112 (86%)	19 (14%)	0	100	100
13	K	144/147 (98%)	137 (95%)	7 (5%)	0	100	100
14	L	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
15	M	143/147 (97%)	129 (90%)	14 (10%)	0	100	100
16	N	134/138 (97%)	122 (91%)	12 (9%)	0	100	100
17	O	116/199 (58%)	106 (91%)	10 (9%)	0	100	100
18	P	124/127 (98%)	102 (82%)	22 (18%)	0	100	100
19	Q	111/113 (98%)	96 (86%)	15 (14%)	0	100	100
20	R	122/129 (95%)	116 (95%)	6 (5%)	0	100	100
21	S	98/103 (95%)	93 (95%)	5 (5%)	0	100	100
22	T	112/153 (73%)	106 (95%)	6 (5%)	0	100	100
23	U	95/100 (95%)	90 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	V	93/105 (89%)	87 (94%)	6 (6%)	0	100	100
25	W	190/215 (88%)	179 (94%)	11 (6%)	0	100	100
26	X	77/88 (88%)	67 (87%)	10 (13%)	0	100	100
27	Y	61/64 (95%)	55 (90%)	6 (10%)	0	100	100
28	Z	62/77 (80%)	61 (98%)	1 (2%)	0	100	100
29	b	52/57 (91%)	49 (94%)	3 (6%)	0	100	100
30	c	47/55 (86%)	43 (92%)	4 (8%)	0	100	100
31	d	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
32	e	61/64 (95%)	58 (95%)	3 (5%)	0	100	100
33	f	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
34	g	46/75 (61%)	41 (89%)	5 (11%)	0	100	100
All	All	3817/4247 (90%)	3460 (91%)	356 (9%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	E	132	GLU

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	
1	2	52/54 (96%)	52 (100%)	0	100	100
2	3	18/19 (95%)	18 (100%)	0	100	100
3	4	336/340 (99%)	335 (100%)	1 (0%)	91	96
6	C	214/218 (98%)	213 (100%)	1 (0%)	86	92
7	D	160/163 (98%)	160 (100%)	0	100	100
8	E	168/173 (97%)	167 (99%)	1 (1%)	84	91
9	F	149/156 (96%)	147 (99%)	2 (1%)	65	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	G	147/150 (98%)	146 (99%)	1 (1%)	81 89
11	H	31/116 (27%)	31 (100%)	0	100 100
12	J	102/108 (94%)	101 (99%)	1 (1%)	73 84
13	K	118/120 (98%)	118 (100%)	0	100 100
14	L	100/100 (100%)	99 (99%)	1 (1%)	73 84
15	M	112/114 (98%)	112 (100%)	0	100 100
16	N	113/116 (97%)	112 (99%)	1 (1%)	75 86
17	O	97/158 (61%)	97 (100%)	0	100 100
18	P	90/94 (96%)	89 (99%)	1 (1%)	70 82
19	Q	100/100 (100%)	100 (100%)	0	100 100
20	R	97/99 (98%)	97 (100%)	0	100 100
21	S	81/83 (98%)	81 (100%)	0	100 100
22	T	90/117 (77%)	90 (100%)	0	100 100
23	U	83/85 (98%)	83 (100%)	0	100 100
24	V	80/86 (93%)	80 (100%)	0	100 100
25	W	153/168 (91%)	152 (99%)	1 (1%)	81 89
26	X	58/63 (92%)	56 (97%)	2 (3%)	32 60
27	Y	49/51 (96%)	47 (96%)	2 (4%)	26 54
28	Z	58/66 (88%)	58 (100%)	0	100 100
29	b	43/46 (94%)	43 (100%)	0	100 100
30	c	45/52 (86%)	45 (100%)	0	100 100
31	d	35/36 (97%)	35 (100%)	0	100 100
32	e	51/54 (94%)	51 (100%)	0	100 100
33	f	35/35 (100%)	35 (100%)	0	100 100
34	g	43/63 (68%)	43 (100%)	0	100 100
All	All	3108/3403 (91%)	3093 (100%)	15 (0%)	85 92

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	4	464	ARG
6	C	134	ARG
8	E	170	ARG

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Mol	Chain	Res	Type
9	F	119	ARG
9	F	157	ARG
10	G	87	LYS
12	J	135	ARG
14	L	104	ARG
16	N	60	ARG
18	P	26	ARG
25	W	89	ARG
26	X	14	ARG
26	X	73	ARG
27	Y	45	ASN
27	Y	60	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
9	F	58	ASN
9	F	142	GLN
10	G	20	ASN
21	S	85	HIS
25	W	101	GLN
31	d	36	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	A	3041/3120 (97%)	698 (22%)	29 (0%)
5	B	117/118 (99%)	36 (30%)	4 (3%)
All	All	3158/3238 (97%)	734 (23%)	33 (1%)

All (734) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	A	4	G
4	A	7	U
4	A	12	G
4	A	20	G
4	A	23	G
4	A	24	G
4	A	31	U

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Mol	Chain	Res	Type
4	A	32	G
4	A	41	A
4	A	42	G
4	A	57	A
4	A	58	G
4	A	60	A
4	A	61	G
4	A	68	A
4	A	71	A
4	A	72	G
4	A	78	G
4	A	80	G
4	A	82	G
4	A	94	G
4	A	98	U
4	A	99	G
4	A	107	G
4	A	111	U
4	A	115	A
4	A	117	U
4	A	122	A
4	A	125	C
4	A	126	C
4	A	136	U
4	A	148	A
4	A	161	U
4	A	162	A
4	A	164	A
4	A	169	C
4	A	180	A
4	A	186	G
4	A	195	A
4	A	198	A
4	A	211	U
4	A	212	A
4	A	214	G
4	A	215	A
4	A	220	A
4	A	221	A
4	A	227	A
4	A	229	U
4	A	230	G

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Mol	Chain	Res	Type
4	A	243	U
4	A	246	U
4	A	248	G
4	A	264	G
4	A	265	A
4	A	266	U
4	A	267	G
4	A	271	A
4	A	272	A
4	A	278	A
4	A	280	G
4	A	281	C
4	A	282	A
4	A	286	G
4	A	288	U
4	A	290	C
4	A	292	G
4	A	294	G
4	A	295	U
4	A	296	A
4	A	299	G
4	A	302	U
4	A	303	G
4	A	305	G
4	A	306	U
4	A	312	G
4	A	313	G
4	A	314	G
4	A	315	U
4	A	318	U
4	A	325	U
4	A	326	A
4	A	330	U
4	A	337	U
4	A	338	C
4	A	340	A
4	A	341	C
4	A	342	C
4	A	343	U
4	A	351	G
4	A	352	G
4	A	357	U

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Mol	Chain	Res	Type
4	A	358	G
4	A	361	A
4	A	362	A
4	A	363	A
4	A	364	A
4	A	365	U
4	A	366	G
4	A	370	U
4	A	371	G
4	A	376	G
4	A	380	A
4	A	384	G
4	A	391	G
4	A	393	U
4	A	399	G
4	A	405	G
4	A	412	A
4	A	413	G
4	A	414	A
4	A	415	G
4	A	417	C
4	A	420	G
4	A	428	A
4	A	434	G
4	A	437	G
4	A	438	U
4	A	441	G
4	A	442	U
4	A	444	U
4	A	445	U
4	A	447	A
4	A	448	U
4	A	449	G
4	A	451	U
4	A	452	G
4	A	453	U
4	A	460	G
4	A	472	C
4	A	474	G
4	A	489	A
4	A	490	A
4	A	498	G

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Mol	Chain	Res	Type
4	A	500	A
4	A	512	G
4	A	514	C
4	A	518	A
4	A	523	U
4	A	539	C
4	A	543	U
4	A	544	U
4	A	545	A
4	A	546	G
4	A	552	U
4	A	553	G
4	A	565	A
4	A	566	A
4	A	569	G
4	A	570	U
4	A	572	C
4	A	573	C
4	A	591	G
4	A	592	A
4	A	594	U
4	A	595	A
4	A	596	C
4	A	612	U
4	A	617	U
4	A	618	C
4	A	619	C
4	A	620	G
4	A	635	G
4	A	637	G
4	A	638	U
4	A	639	C
4	A	640	G
4	A	642	G
4	A	644	G
4	A	655	G
4	A	658	U
4	A	660	U
4	A	665	G
4	A	667	A
4	A	684	G
4	A	696	A

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Mol	Chain	Res	Type
4	A	706	G
4	A	707	G
4	A	708	G
4	A	721	A
4	A	731	A
4	A	736	G
4	A	739	U
4	A	740	A
4	A	741	G
4	A	745	G
4	A	747	A
4	A	753	A
4	A	755	A
4	A	758	A
4	A	759	G
4	A	760	U
4	A	763	G
4	A	766	G
4	A	768	G
4	A	769	U
4	A	790	A
4	A	798	U
4	A	801	U
4	A	819	G
4	A	820	A
4	A	824	G
4	A	836	G
4	A	838	G
4	A	840	G
4	A	841	G
4	A	842	A
4	A	843	G
4	A	845	C
4	A	862	U
4	A	872	G
4	A	879	A
4	A	880	G
4	A	890	G
4	A	891	G
4	A	897	A
4	A	899	G
4	A	900	G

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Mol	Chain	Res	Type
4	A	904	A
4	A	907	A
4	A	917	A
4	A	919	A
4	A	920	G
4	A	927	C
4	A	942	U
4	A	972	A
4	A	974	G
4	A	975	U
4	A	981	U
4	A	982	A
4	A	989	G
4	A	990	G
4	A	994	A
4	A	995	U
4	A	1000	C
4	A	1001	C
4	A	1002	C
4	A	1004	C
4	A	1005	A
4	A	1010	U
4	A	1011	A
4	A	1012	C
4	A	1014	G
4	A	1019	C
4	A	1025	A
4	A	1027	C
4	A	1030	C
4	A	1046	C
4	A	1047	A
4	A	1048	A
4	A	1049	G
4	A	1063	G
4	A	1070	G
4	A	1076	A
4	A	1078	G
4	A	1085	G
4	A	1091	A
4	A	1092	G
4	A	1097	A
4	A	1098	A

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Mol	Chain	Res	Type
4	A	1101	A
4	A	1103	C
4	A	1114	G
4	A	1126	U
4	A	1127	A
4	A	1131	G
4	A	1138	A
4	A	1144	A
4	A	1151	U
4	A	1155	C
4	A	1156	A
4	A	1164	A
4	A	1165	G
4	A	1171	C
4	A	1173	G
4	A	1174	G
4	A	1175	A
4	A	1176	G
4	A	1177	G
4	A	1178	U
4	A	1179	U
4	A	1181	G
4	A	1184	U
4	A	1185	A
4	A	1186	G
4	A	1188	A
4	A	1190	C
4	A	1191	A
4	A	1196	C
4	A	1197	C
4	A	1198	C
4	A	1199	U
4	A	1200	U
4	A	1201	G
4	A	1202	A
4	A	1203	A
4	A	1204	A
4	A	1205	G
4	A	1206	A
4	A	1207	G
4	A	1212	U
4	A	1213	A

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Mol	Chain	Res	Type
4	A	1214	A
4	A	1216	A
4	A	1222	C
4	A	1225	G
4	A	1229	A
4	A	1230	G
4	A	1231	U
4	A	1236	G
4	A	1237	U
4	A	1238	G
4	A	1240	G
4	A	1246	A
4	A	1247	A
4	A	1250	U
4	A	1251	A
4	A	1253	C
4	A	1254	G
4	A	1260	C
4	A	1261	A
4	A	1262	A
4	A	1270	G
4	A	1274	A
4	A	1292	U
4	A	1293	G
4	A	1333	C
4	A	1335	G
4	A	1339	G
4	A	1343	G
4	A	1344	A
4	A	1351	G
4	A	1353	G
4	A	1359	G
4	A	1371	G
4	A	1377	A
4	A	1379	G
4	A	1380	A
4	A	1387	A
4	A	1389	U
4	A	1399	A
4	A	1401	A
4	A	1404	C
4	A	1415	A

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Mol	Chain	Res	Type
4	A	1416	A
4	A	1429	C
4	A	1436	C
4	A	1440	C
4	A	1444	U
4	A	1456	G
4	A	1465	C
4	A	1474	A
4	A	1480	A
4	A	1493	A
4	A	1494	U
4	A	1499	A
4	A	1506	U
4	A	1507	G
4	A	1510	A
4	A	1518	A
4	A	1531	C
4	A	1535	C
4	A	1541	G
4	A	1542	A
4	A	1546	A
4	A	1548	C
4	A	1549	G
4	A	1550	G
4	A	1551	U
4	A	1553	C
4	A	1556	A
4	A	1563	A
4	A	1564	A
4	A	1565	A
4	A	1566	A
4	A	1571	C
4	A	1572	G
4	A	1573	U
4	A	1574	G
4	A	1578	G
4	A	1582	C
4	A	1583	U
4	A	1585	U
4	A	1587	G
4	A	1588	G
4	A	1589	G

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Mol	Chain	Res	Type
4	A	1593	U
4	A	1595	G
4	A	1597	G
4	A	1598	U
4	A	1599	U
4	A	1600	G
4	A	1603	G
4	A	1607	C
4	A	1608	U
4	A	1609	G
4	A	1610	C
4	A	1617	C
4	A	1618	C
4	A	1619	U
4	A	1620	U
4	A	1621	C
4	A	1622	G
4	A	1623	U
4	A	1624	U
4	A	1625	G
4	A	1630	U
4	A	1636	A
4	A	1640	A
4	A	1641	U
4	A	1649	C
4	A	1658	G
4	A	1671	U
4	A	1678	U
4	A	1679	A
4	A	1681	U
4	A	1697	U
4	A	1703	G
4	A	1709	U
4	A	1710	A
4	A	1714	A
4	A	1716	A
4	A	1717	U
4	A	1718	C
4	A	1723	U
4	A	1724	G
4	A	1727	A
4	A	1728	U

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Mol	Chain	Res	Type
4	A	1730	U
4	A	1731	A
4	A	1737	A
4	A	1738	G
4	A	1754	G
4	A	1756	G
4	A	1759	A
4	A	1767	U
4	A	1769	G
4	A	1778	A
4	A	1786	G
4	A	1787	A
4	A	1789	A
4	A	1797	C
4	A	1798	U
4	A	1802	G
4	A	1803	A
4	A	1813	C
4	A	1825	C
4	A	1826	A
4	A	1835	C
4	A	1844	A
4	A	1848	A
4	A	1850	A
4	A	1851	G
4	A	1852	A
4	A	1864	U
4	A	1866	C
4	A	1871	G
4	A	1872	A
4	A	1878	G
4	A	1890	C
4	A	1892	G
4	A	1899	G
4	A	1904	C
4	A	1906	U
4	A	1942	G
4	A	1945	U
4	A	1946	U
4	A	1947	U
4	A	1948	A
4	A	1955	A

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Mol	Chain	Res	Type
4	A	1973	C
4	A	1975	A
4	A	1978	C
4	A	1980	G
4	A	1981	U
4	A	1990	A
4	A	1993	G
4	A	2001	A
4	A	2017	C
4	A	2018	G
4	A	2033	U
4	A	2046	A
4	A	2052	G
4	A	2064	A
4	A	2072	G
4	A	2073	A
4	A	2074	G
4	A	2075	G
4	A	2085	C
4	A	2086	U
4	A	2087	C
4	A	2088	C
4	A	2089	C
4	A	2090	U
4	A	2092	U
4	A	2093	G
4	A	2094	G
4	A	2095	G
4	A	2107	G
4	A	2110	U
4	A	2111	U
4	A	2112	U
4	A	2113	A
4	A	2130	G
4	A	2132	U
4	A	2133	G
4	A	2134	G
4	A	2135	U
4	A	2136	A
4	A	2137	A
4	A	2138	C
4	A	2140	A

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Mol	Chain	Res	Type
4	A	2142	A
4	A	2145	C
4	A	2147	U
4	A	2151	A
4	A	2152	A
4	A	2153	G
4	A	2154	G
4	A	2155	U
4	A	2163	U
4	A	2176	A
4	A	2179	U
4	A	2187	U
4	A	2188	G
4	A	2191	C
4	A	2194	A
4	A	2196	G
4	A	2209	C
4	A	2215	U
4	A	2216	G
4	A	2217	U
4	A	2220	C
4	A	2221	A
4	A	2226	U
4	A	2228	G
4	A	2237	A
4	A	2246	U
4	A	2251	G
4	A	2252	U
4	A	2254	A
4	A	2255	A
4	A	2256	G
4	A	2257	A
4	A	2267	C
4	A	2273	G
4	A	2279	C
4	A	2280	G
4	A	2284	A
4	A	2285	G
4	A	2293	G
4	A	2319	G
4	A	2321	U
4	A	2323	G

Continued on next page...

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Mol	Chain	Res	Type
4	A	2325	U
4	A	2406	U
4	A	2408	G
4	A	2410	A
4	A	2413	G
4	A	2414	G
4	A	2418	U
4	A	2421	A
4	A	2422	A
4	A	2434	A
4	A	2435	U
4	A	2449	A
4	A	2462	G
4	A	2463	G
4	A	2469	U
4	A	2470	A
4	A	2474	G
4	A	2491	A
4	A	2492	A
4	A	2503	G
4	A	2506	G
4	A	2507	C
4	A	2508	C
4	A	2511	A
4	A	2528	G
4	A	2529	A
4	A	2531	G
4	A	2532	G
4	A	2535	A
4	A	2540	G
4	A	2543	U
4	A	2545	G
4	A	2551	A
4	A	2558	C
4	A	2559	A
4	A	2566	C
4	A	2569	G
4	A	2571	C
4	A	2574	C
4	A	2578	A
4	A	2585	U
4	A	2589	G

Continued on next page...

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Mol	Chain	Res	Type
4	A	2596	G
4	A	2602	A
4	A	2607	G
4	A	2609	A
4	A	2615	G
4	A	2626	U
4	A	2627	C
4	A	2630	A
4	A	2634	G
4	A	2646	C
4	A	2647	U
4	A	2649	A
4	A	2652	G
4	A	2653	G
4	A	2654	A
4	A	2655	U
4	A	2657	A
4	A	2659	A
4	A	2665	C
4	A	2672	A
4	A	2676	C
4	A	2693	A
4	A	2698	C
4	A	2699	C
4	A	2700	A
4	A	2705	G
4	A	2713	G
4	A	2715	U
4	A	2718	G
4	A	2722	C
4	A	2726	G
4	A	2727	A
4	A	2729	G
4	A	2742	A
4	A	2743	U
4	A	2744	C
4	A	2752	U
4	A	2753	G
4	A	2759	G
4	A	2778	U
4	A	2785	A
4	A	2786	U

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Mol	Chain	Res	Type
4	A	2790	A
4	A	2791	G
4	A	2796	A
4	A	2797	C
4	A	2806	G
4	A	2807	G
4	A	2809	U
4	A	2822	A
4	A	2826	A
4	A	2827	G
4	A	2832	G
4	A	2833	U
4	A	2834	C
4	A	2837	U
4	A	2847	G
4	A	2853	C
4	A	2854	A
4	A	2870	C
4	A	2871	U
4	A	2880	U
4	A	2884	A
4	A	2885	G
4	A	2893	G
4	A	2913	U
4	A	2915	C
4	A	2936	C
4	A	2938	G
4	A	2957	A
4	A	2972	A
4	A	2976	C
4	A	2985	G
4	A	3002	A
4	A	3005	A
4	A	3013	C
4	A	3015	C
4	A	3021	A
4	A	3022	G
4	A	3024	A
4	A	3029	U
4	A	3039	C
4	A	3042	A
4	A	3054	U

Continued on next page...

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Mol	Chain	Res	Type
4	A	3063	A
4	A	3070	G
4	A	3071	A
4	A	3078	G
4	A	3079	U
4	A	3080	A
4	A	3082	U
4	A	3088	C
4	A	3093	A
4	A	3098	G
4	A	3100	A
4	A	3101	C
4	A	3105	C
4	A	3106	C
4	A	3108	G
4	A	3113	A
4	A	3114	A
4	A	3115	A
4	A	3120	C
5	B	3	U
5	B	5	C
5	B	6	G
5	B	8	C
5	B	10	G
5	B	11	U
5	B	13	C
5	B	18	C
5	B	25	G
5	B	30	G
5	B	31	C
5	B	32	C
5	B	34	G
5	B	35	G
5	B	36	U
5	B	40	A
5	B	41	U
5	B	43	C
5	B	51	G
5	B	52	G
5	B	54	A
5	B	56	C
5	B	57	U

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Mol	Chain	Res	Type
5	B	59	A
5	B	66	C
5	B	67	A
5	B	74	A
5	B	89	C
5	B	97	A
5	B	106	C
5	B	107	A
5	B	109	C
5	B	113	G
5	B	114	A
5	B	115	A
5	B	118	C

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	A	22	U
4	A	211	U
4	A	305	G
4	A	336	C
4	A	357	U
4	A	517	A
4	A	552	U
4	A	572	C
4	A	643	G
4	A	840	G
4	A	842	A
4	A	919	A
4	A	974	G
4	A	981	U
4	A	1077	A
4	A	1199	U
4	A	1230	G
4	A	1292	U
4	A	1338	U
4	A	1350	G
4	A	1473	G
4	A	1571	C
4	A	2072	G
4	A	2094	G
4	A	2151	A

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Mol	Chain	Res	Type
4	A	2186	C
4	A	2320	C
4	A	2656	A
4	A	2826	A
5	B	10	G
5	B	35	G
5	B	40	A
5	B	66	C

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

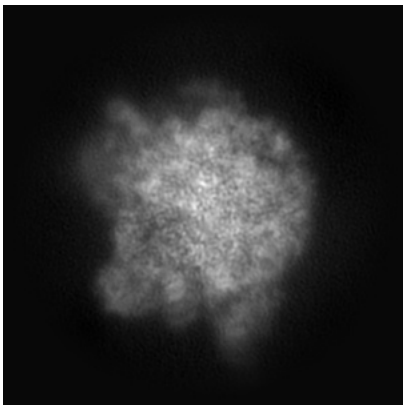
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43333. These allow visual inspection of the internal detail of the map and identification of artifacts.

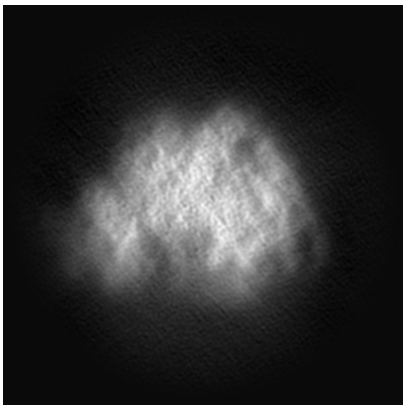
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

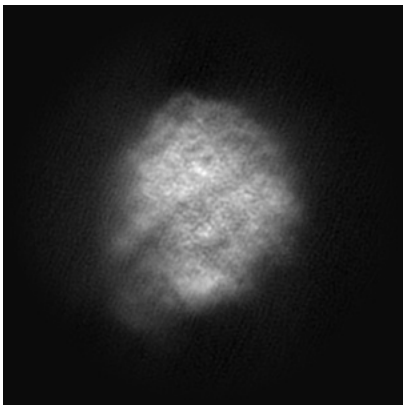
6.1.1 Primary map



X

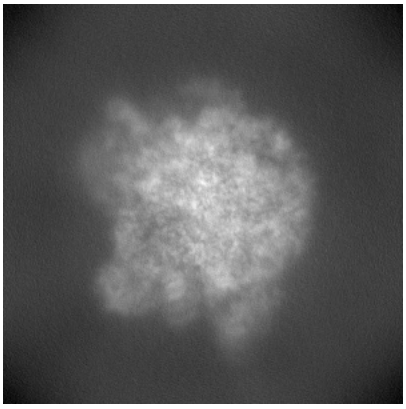


Y

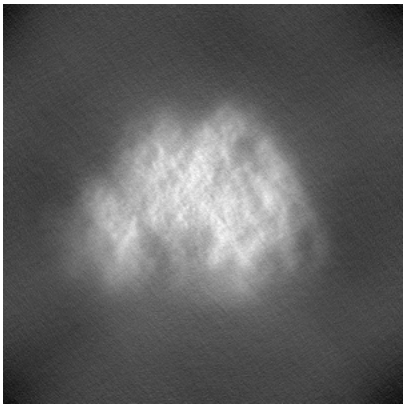


Z

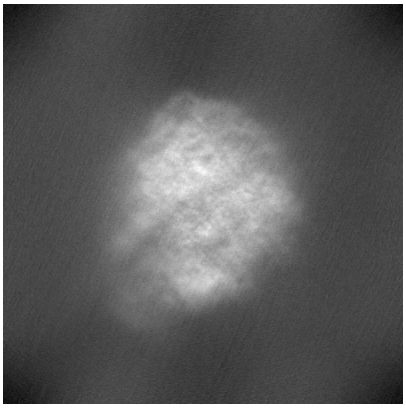
6.1.2 Raw map



X



Y

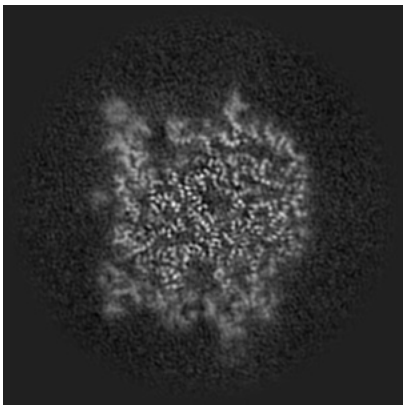


Z

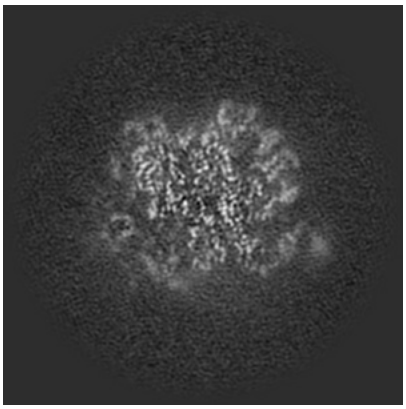
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

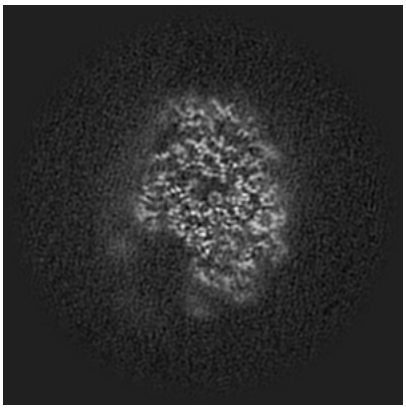
6.2.1 Primary map



X Index: 200

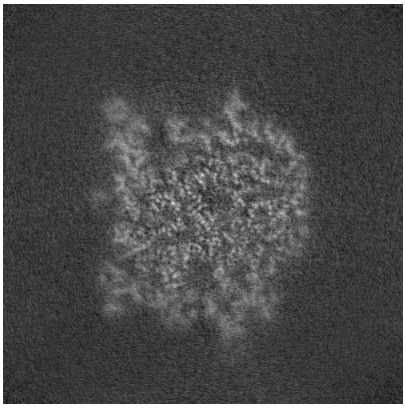


Y Index: 200

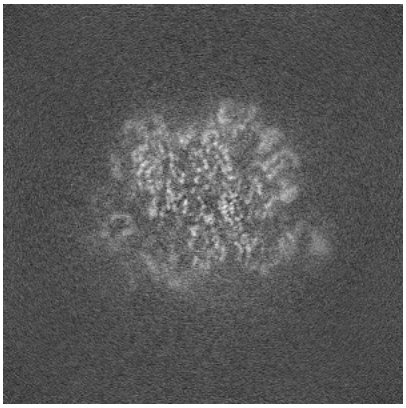


Z Index: 200

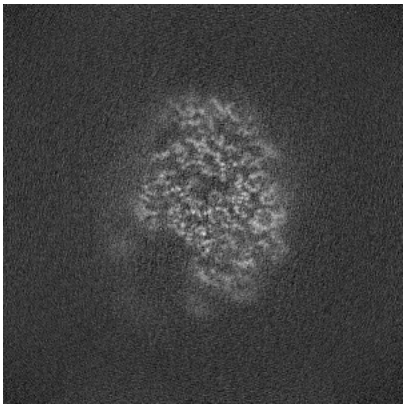
6.2.2 Raw map



X Index: 200



Y Index: 200

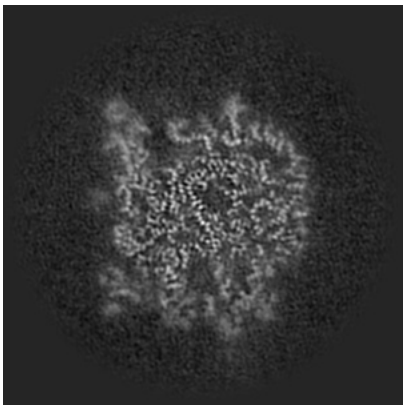


Z Index: 200

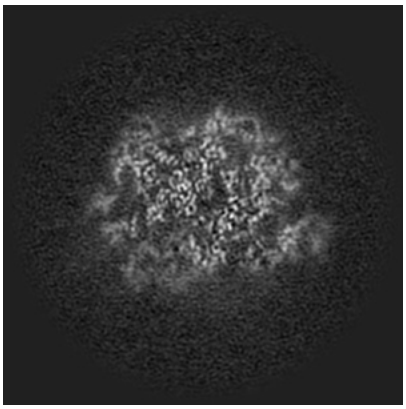
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

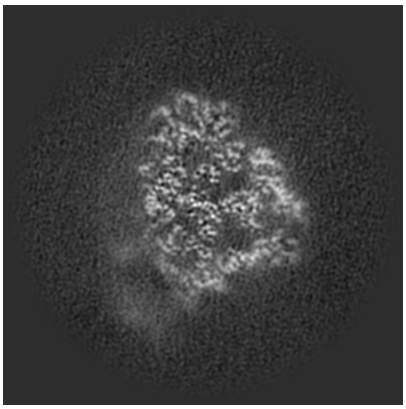
6.3.1 Primary map



X Index: 202

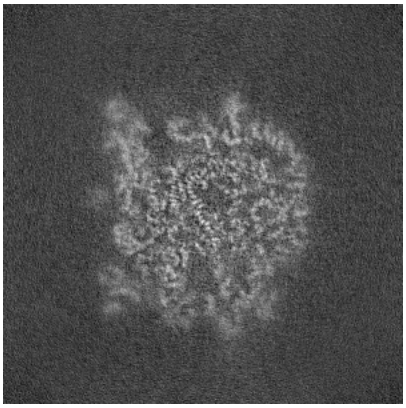


Y Index: 206

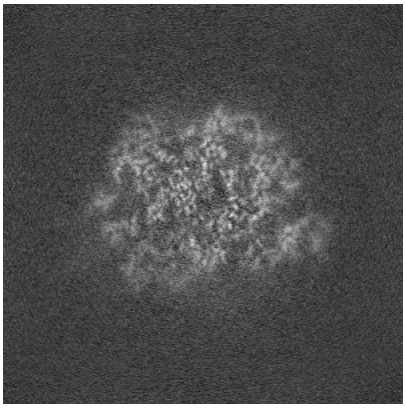


Z Index: 220

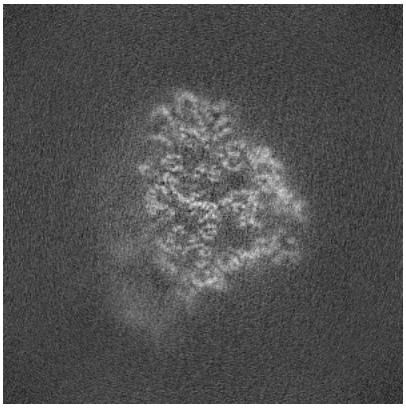
6.3.2 Raw map



X Index: 202



Y Index: 206

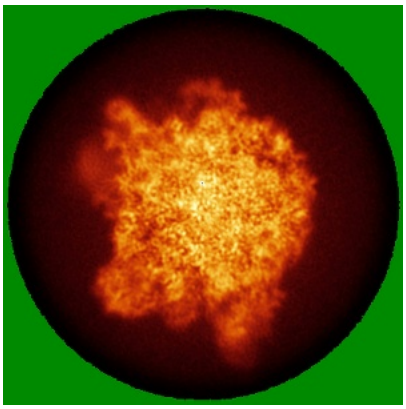


Z Index: 221

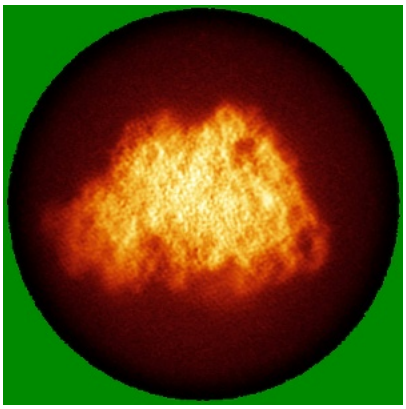
The images above show the largest variance slices of the map in three orthogonal directions.

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

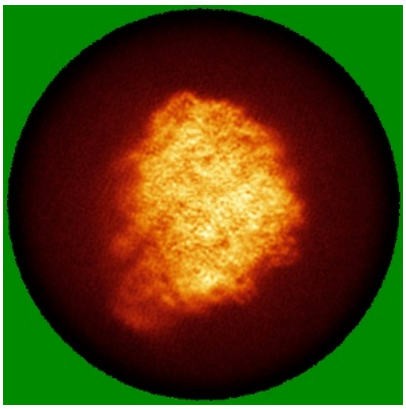
6.4.1 Primary map



X

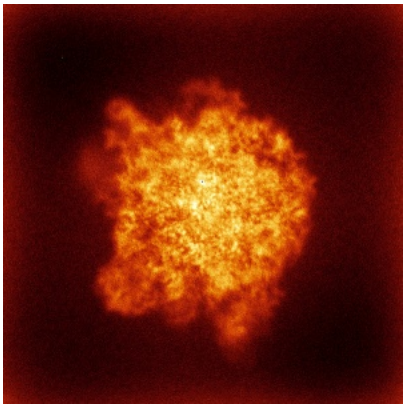


Y

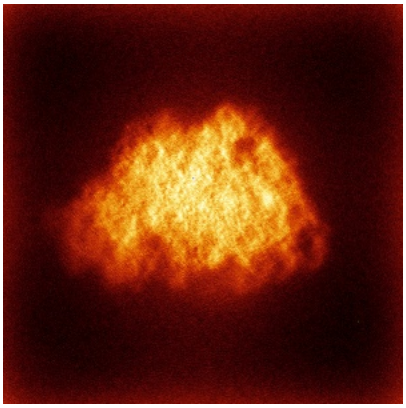


Z

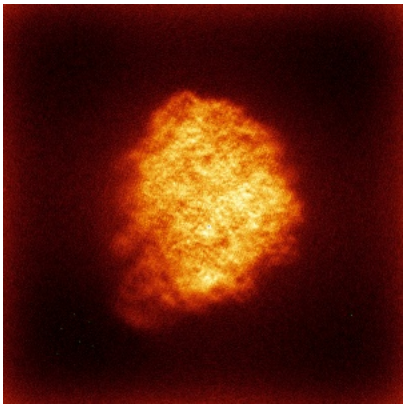
6.4.2 Raw map



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

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.

6.5.2 Raw map

X Y Z

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.

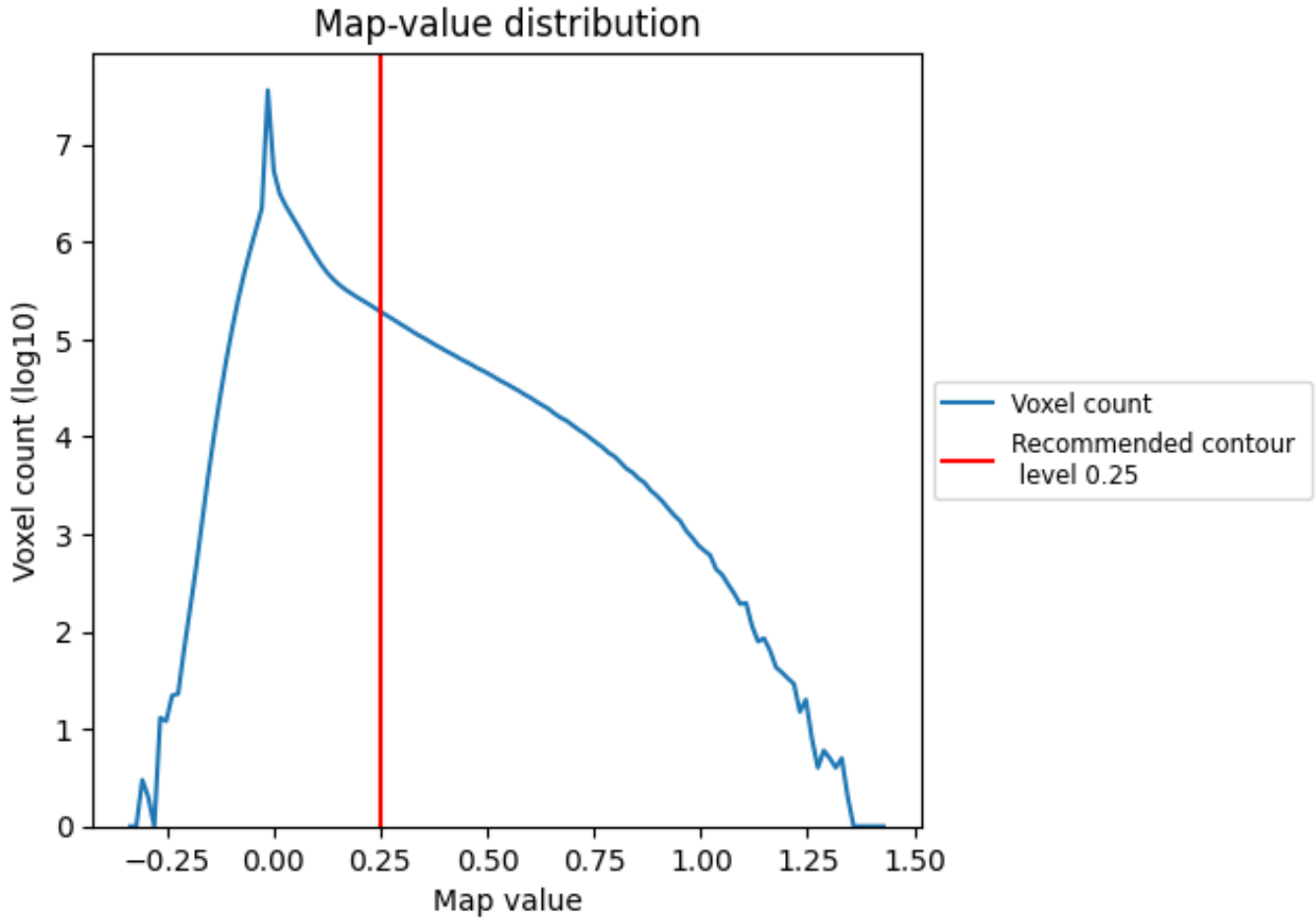
6.6 Mask visualisation (i)

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

7 Map analysis

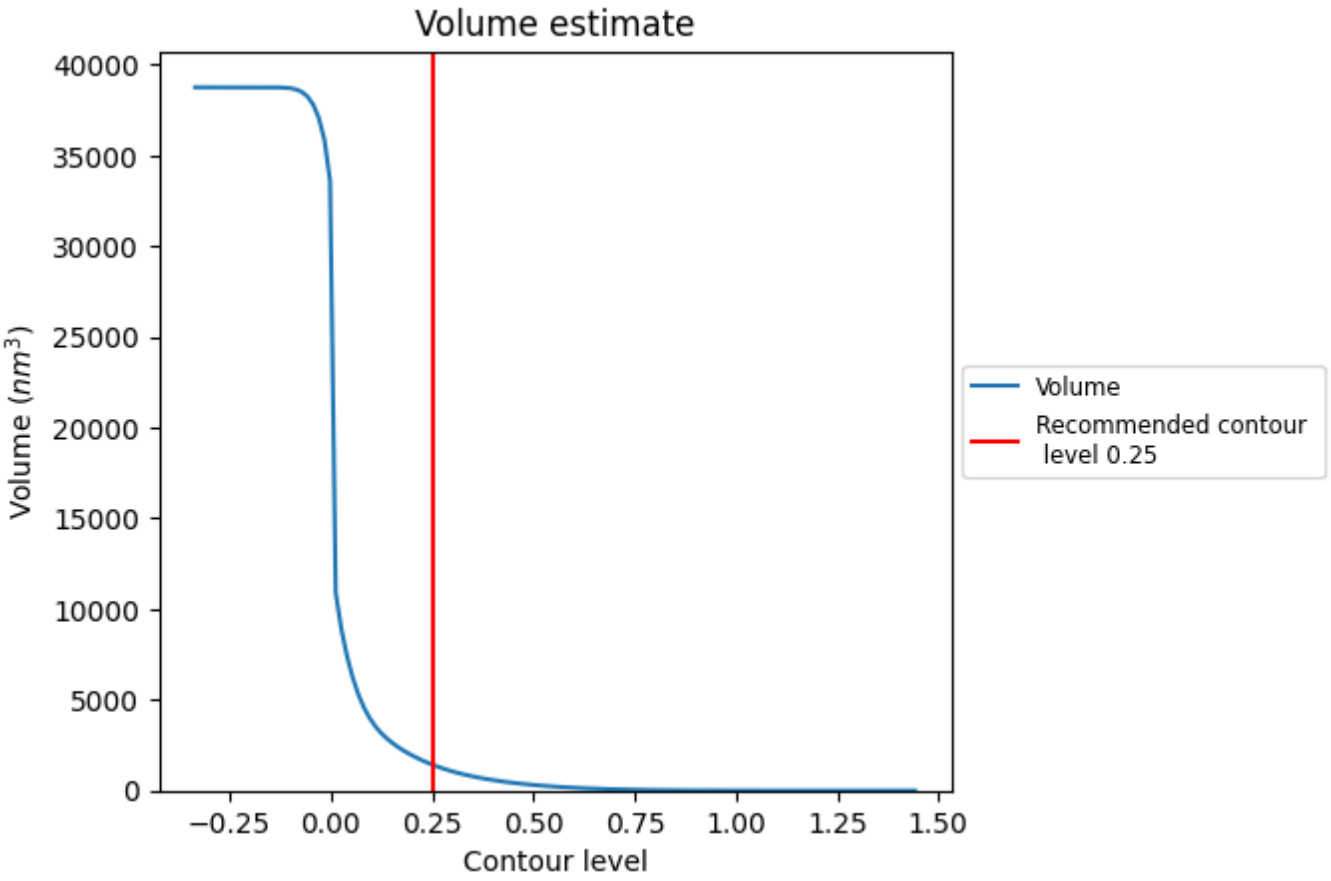
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

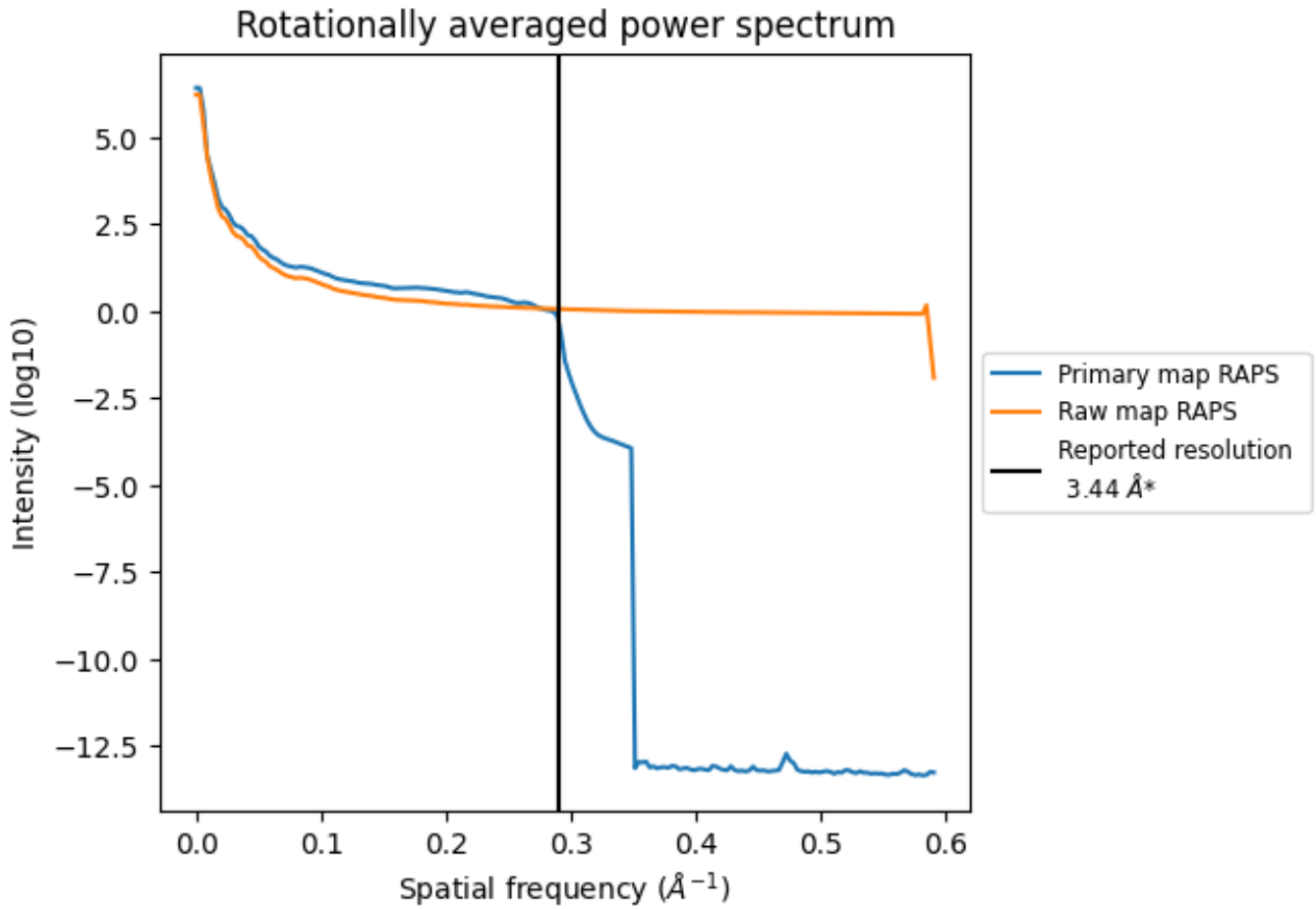
7.2 Volume estimate



The volume at the recommended contour level is 1429 nm^3; this corresponds to an approximate mass of 1291 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)

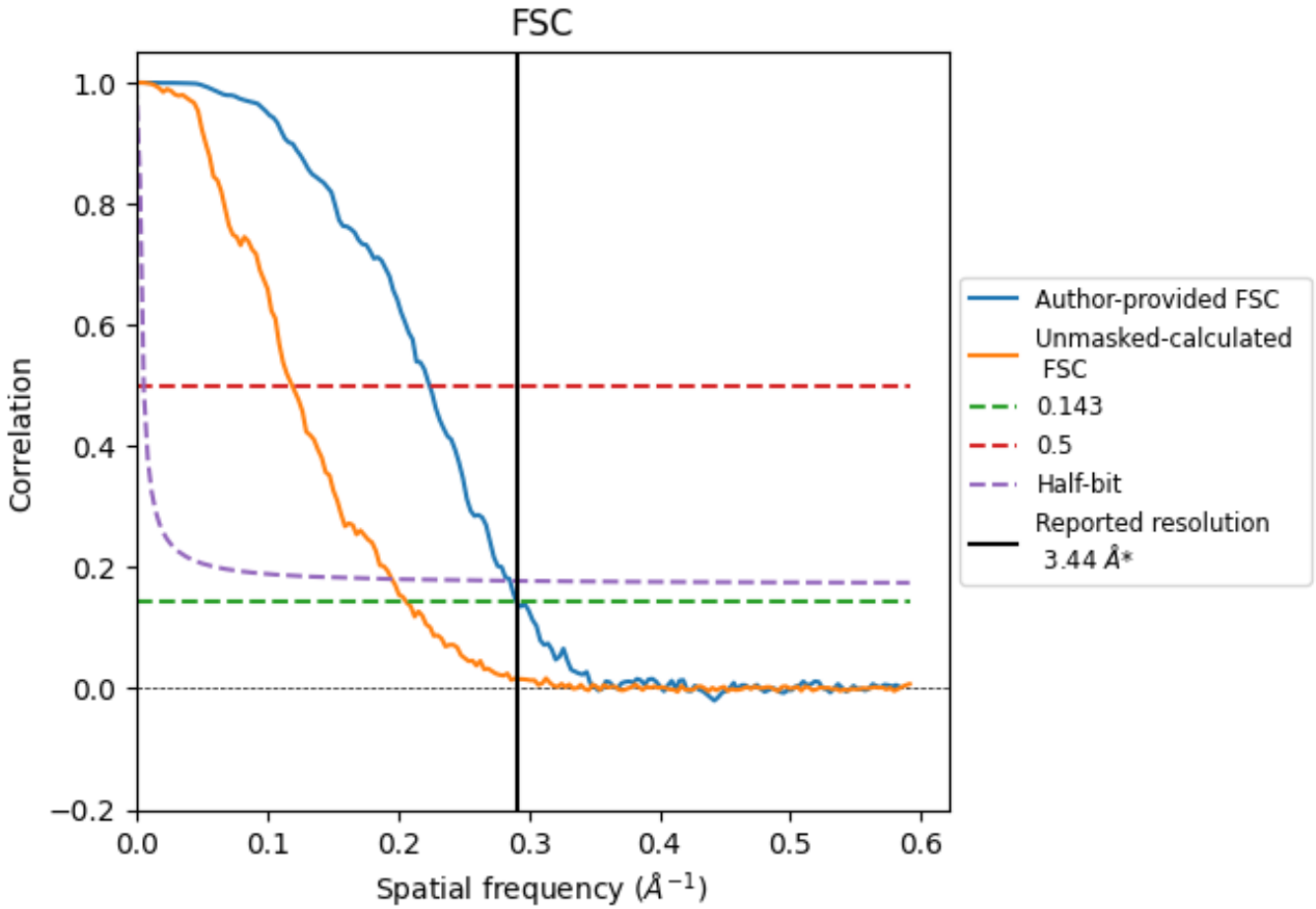


*Reported resolution corresponds to spatial frequency of 0.291 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.291 Å^{-1}

8.2 Resolution estimates (i)

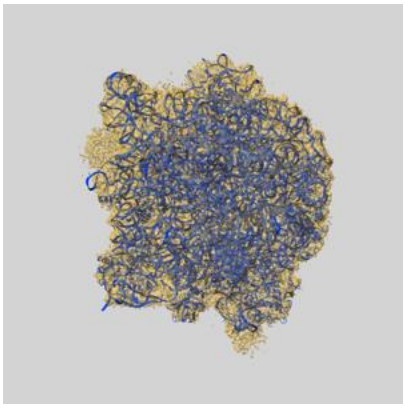
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.44	-	-
Author-provided FSC curve	3.44	4.46	3.50
Unmasked-calculated*	4.85	8.40	5.12

*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 4.85 differs from the reported value 3.44 by more than 10 %

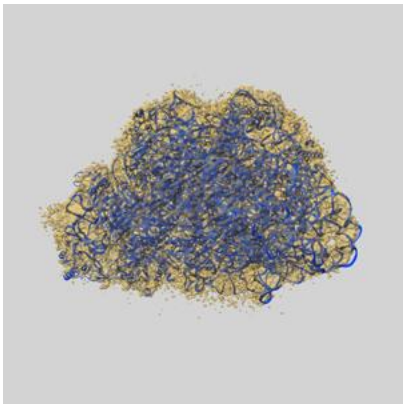
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43333 and PDB model 8VKW. Per-residue inclusion information can be found in section 3 on page 10.

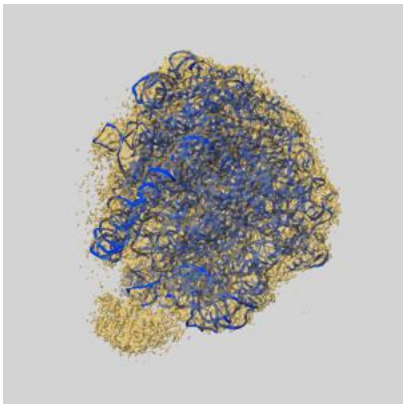
9.1 Map-model overlay



X



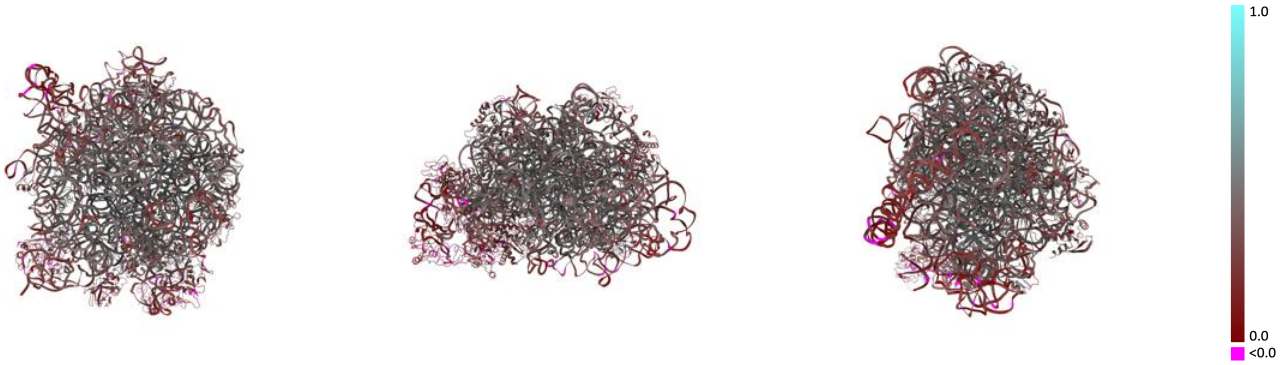
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

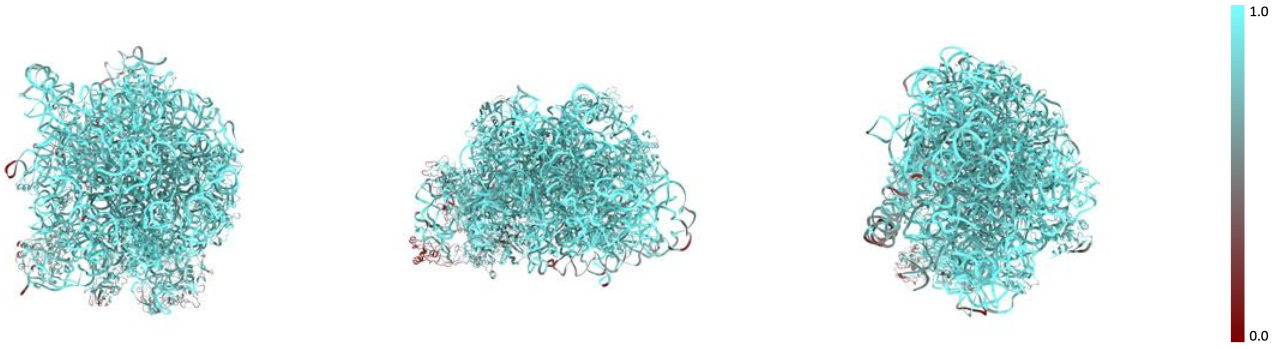
9.2 Q-score mapped to coordinate model



X Y Z

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

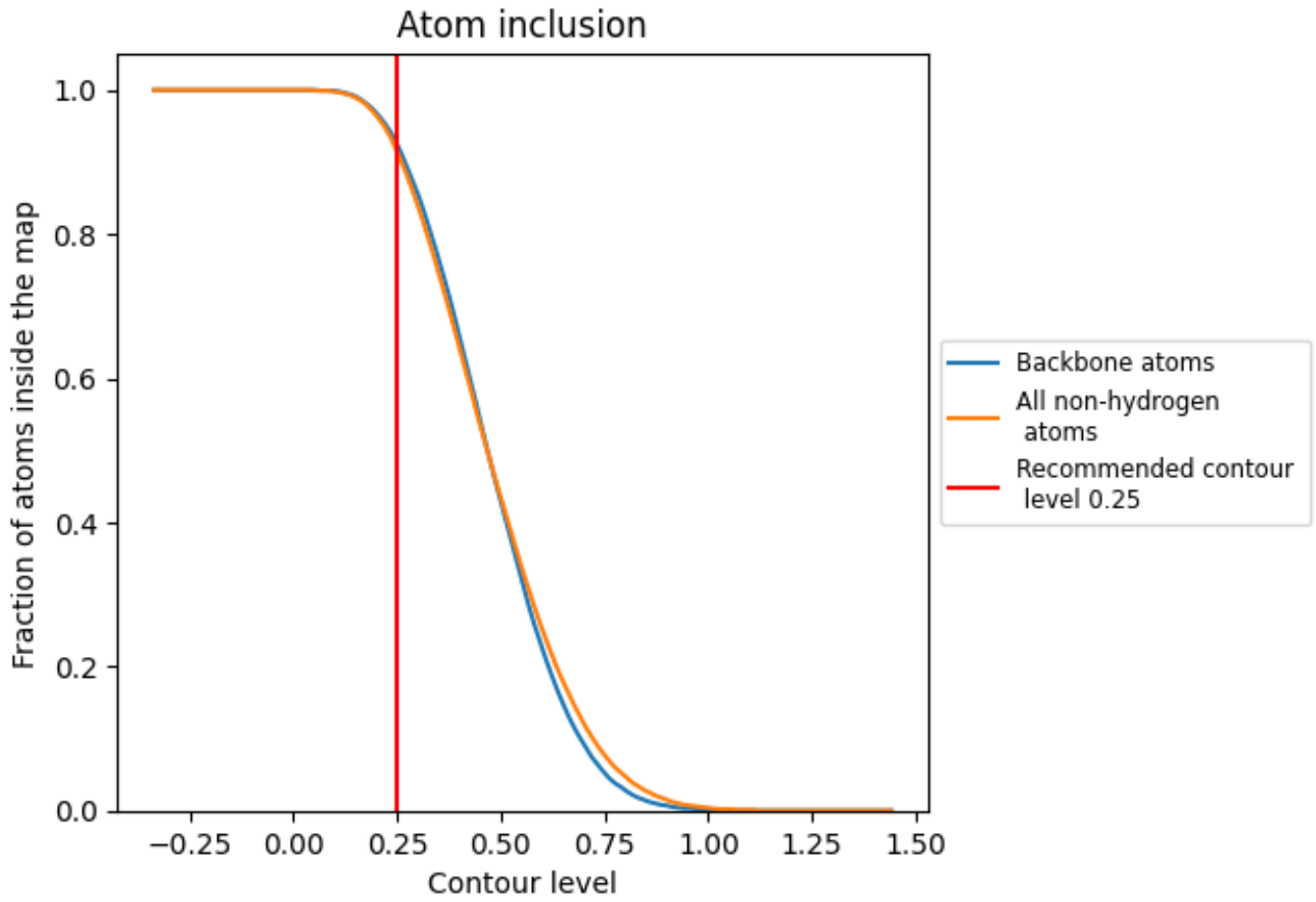
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 92% 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	0.9150	0.3580
2	0.9150	0.4210
3	0.9780	0.4680
4	0.7580	0.2540
A	0.9530	0.3730
B	0.9120	0.2460
C	0.9240	0.4220
D	0.9120	0.4000
E	0.8980	0.3900
F	0.6630	0.1550
G	0.7570	0.2260
H	0.7270	0.2350
J	0.3750	0.1190
K	0.9550	0.4080
L	0.9090	0.3930
M	0.9150	0.4080
N	0.8760	0.3820
O	0.9340	0.4040
P	0.7290	0.1930
Q	0.8240	0.3410
R	0.9620	0.4220
S	0.9020	0.3900
T	0.9480	0.4240
U	0.9320	0.3740
V	0.8950	0.2990
W	0.5830	0.2260
X	0.9030	0.4310
Y	0.9130	0.4170
Z	0.9160	0.3110
b	0.9350	0.4340
c	0.9120	0.3980
d	0.9690	0.4710
e	0.9490	0.4660
f	0.8990	0.3720
g	0.3690	0.1650