



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 06:55 pm GMT

PDB ID : 4CE4
EMDB ID : EMD-2490
Title : 39S large subunit of the porcine mitochondrial ribosome
Authors : Greber, B.J.; Boehringer, D.; Leitner, A.; Bieri, P.; Voigts-Hoffmann, F.;
Erzberger, J.P.; Leibundgut, M.; Aebersold, R.; Ban, N.
Deposited on : 2013-11-08
Resolution : 4.90 Å (reported)
Based on initial models : 1J26, 1S3A, 2CW9, 1O0W, 1R73, 2QYQ, 2XZN, 1QF6, 3V2D

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

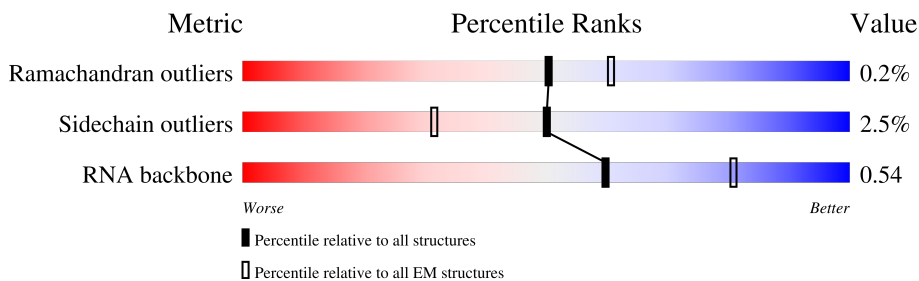
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 4.90 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	0	148	
2	1	256	
3	2	252	
4	3	161	
5	5	146	
6	6	65	
7	7	95	
8	8	188	


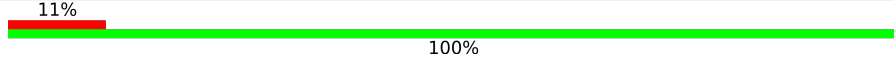
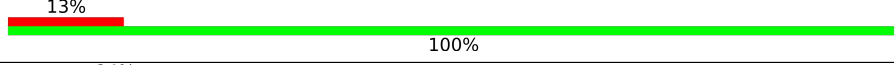
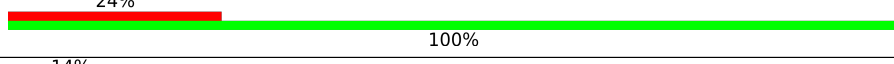
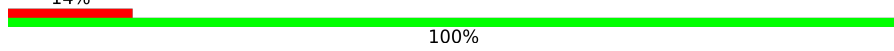
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Mol	Chain	Length	Quality of chain
9	9	100	
10	A	1570	
11	B	29	
12	D	306	
13	E	399	
14	F	224	
15	I	268	
16	N	178	
17	O	145	
18	P	288	
19	Q	208	
20	R	169	
21	S	180	
22	T	292	
23	U	132	
24	V	207	
25	W	134	
26	X	87	
27	Y	216	
28	b	380	
29	c	301	
30	h	298	
31	i	312	
32	l	166	
33	o	56	

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Mol	Chain	Length	Quality of chain
34	u	205	
35	v	91	
35	w	91	
36	x	85	
37	z	426	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 65473 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 MRPL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	76	607	392	114	99	2	0	0

- Molecule 2 is a protein called MRPL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	58	489	312	90	85	2	0	0

- Molecule 3 is a protein called MRPL47.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	76	633	394	116	119	4	0	0

- Molecule 4 is a protein called MRPL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	59	491	321	95	74	1	0	0

- Molecule 5 is a protein called MRPL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	68	508	317	103	83	5	0	0

- Molecule 6 is a protein called MRPL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	48	391	253	70	66	2	0	0

- Molecule 7 is a protein called MRPL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	7	43	362	224	82	55	1	0	0

- Molecule 8 is a protein called MRPL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	8	60	520	338	106	74	2	0	0

- Molecule 9 is a protein called MRPL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	9	36	316	200	68	45	3	0	0

- Molecule 10 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	A	1444	30656	13760	5548	9904	1444	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127A	G	-	insertion	GB AJ002189

- Molecule 11 is a RNA chain called UNASSIGNED RNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	O	P		
11	B	29	348	145	174	29	0	0

- Molecule 12 is a protein called MRPL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	D	200	1531	944	309	269	9	0	0

- Molecule 13 is a protein called MRPL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	208	Total	C	N	O	S	0	0
			1621	1040	300	274	7		

- Molecule 14 is a protein called MRPL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	224	Total	C	N	O	S	0	0
			1713	1101	310	298	4		

- Molecule 15 is a protein called MRPL9.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	I	57	Total	C	N	O	0	0
			447	282	79	86		

- Molecule 16 is a protein called MRPL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	147	Total	C	N	O	S	0	0
			1178	756	210	204	8		

- Molecule 17 is a protein called MRPL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	114	Total	C	N	O	S	0	0
			891	559	175	153	4		

- Molecule 18 is a protein called MRPL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	169	Total	C	N	O	S	0	0
			1309	816	258	233	2		

- Molecule 19 is a protein called MRPL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	154	Total	C	N	O	S	0	0
			1179	758	218	195	8		

- Molecule 20 is a protein called MRPL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	120	Total	C	N	O	S	0	0
			982	619	187	172	4		

- Molecule 21 is a protein called MRPL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	94	Total	C	N	O	S	0	0
			748	467	146	131	4		

- Molecule 22 is a protein called MRPL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	119	Total	C	N	O	S	0	0
			962	615	166	177	4		

- Molecule 23 is a protein called MRPL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	123	Total	C	N	O	S	0	0
			1018	647	212	156	3		

- Molecule 24 is a protein called MRPL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	109	Total	C	N	O	S	0	0
			877	565	156	154	2		

- Molecule 25 is a protein called MRPL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	134	Total	C	N	O	S	0	0
			1058	679	191	182	6		

- Molecule 26 is a protein called MRPL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	87	Total	C	N	O	S	0	0
			689	436	133	118	2		

- Molecule 27 is a protein called MRPL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	103	Total	C	N	O	S	0	0
			835	526	156	151	2		

- Molecule 28 is a protein called MRPL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	192	Total	C	N	O	S	0	0
			1562	1006	266	284	6		

- Molecule 29 is a protein called MRPL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	292	Total	C	N	O	S	0	0
			2310	1489	391	415	15		

- Molecule 30 is a protein called MRPL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	272	Total	C	N	O	S	0	0
			2075	1333	344	391	7		

- Molecule 31 is a protein called MRPL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	161	Total	C	N	O	S	0	0
			1335	845	243	239	8		

- Molecule 32 is a protein called MRPL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	l	76	Total	C	N	O	S	0	0
			619	398	108	111	2		

- Molecule 33 is a protein called MRPL52.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	o	56	Total	C	N	O	0	0
			336	224	56	56		

- Molecule 34 is a protein called ICT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	u	90	Total	C	N	O	S	0	0
			717	444	137	132	4		

- Molecule 35 is a protein called UNASSIGNED HELICES.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	v	91	Total	C	N	O	0	0
			546	364	91	91		
35	w	91	Total	C	N	O	0	0
			546	364	91	91		

- Molecule 36 is a protein called THIOREDOXIN FOLD.

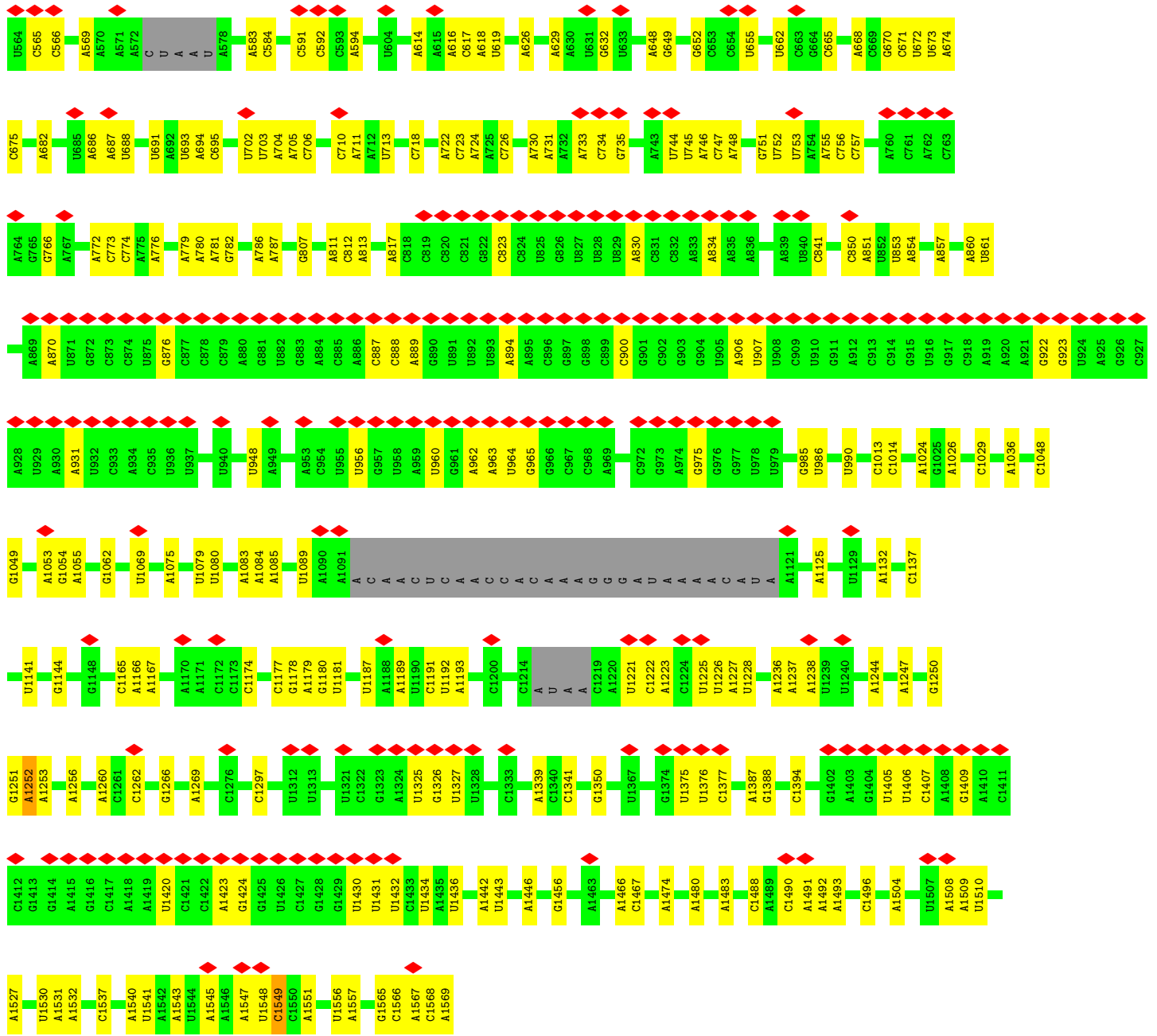
Mol	Chain	Residues	Atoms				AltConf	Trace
36	x	85	Total	C	N	O	0	0
			510	340	85	85		

- Molecule 37 is a protein called UNASSIGNED HELICES.

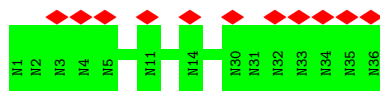
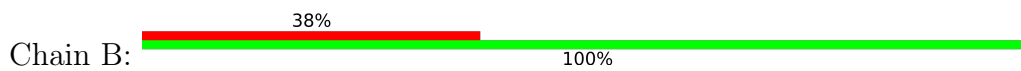
Mol	Chain	Residues	Atoms				AltConf	Trace
37	z	426	Total	C	N	O	0	0
			2556	1704	426	426		

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	5	1	Total	Zn	0
			1	1	
38	9	1	Total	Zn	0
			1	1	

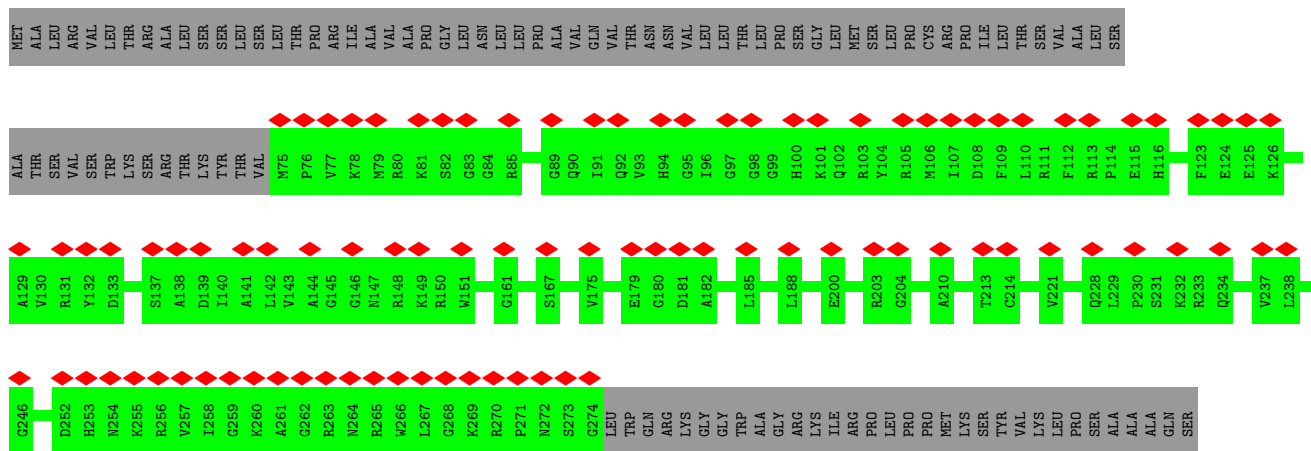


• Molecule 11: UNASSIGNED RNA

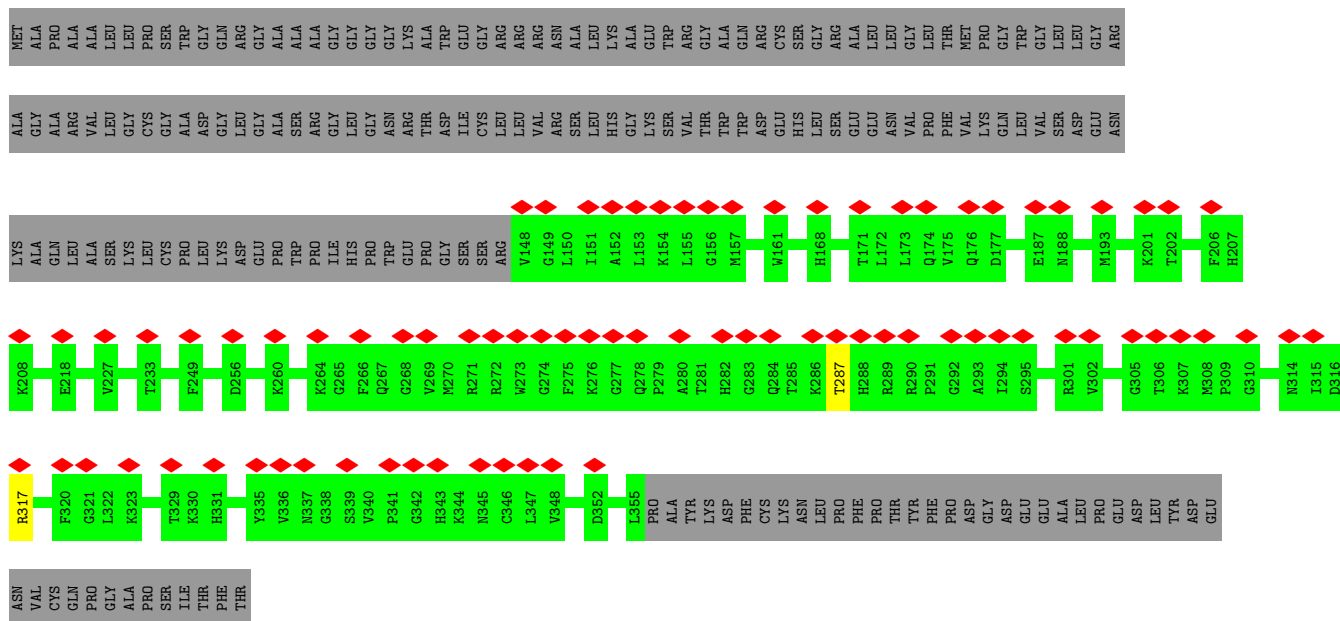


• Molecule 12: MRPL2

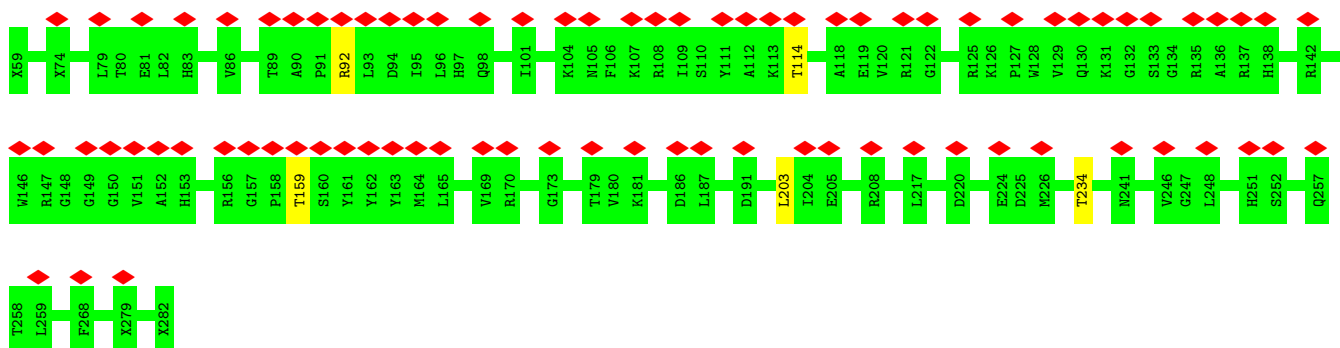


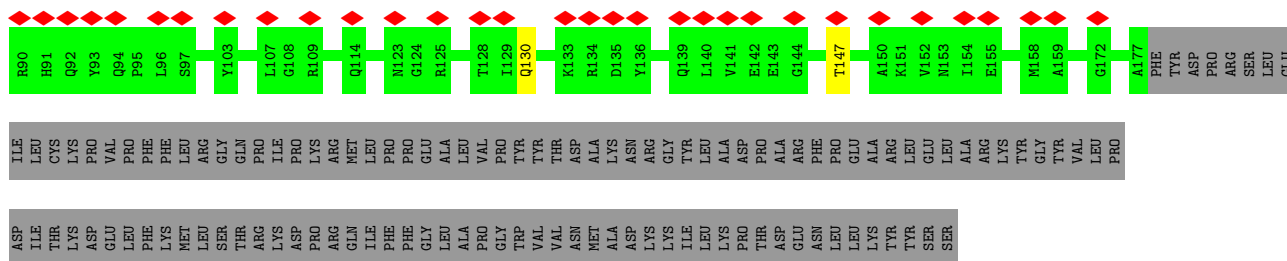


• Molecule 13: MRPL3

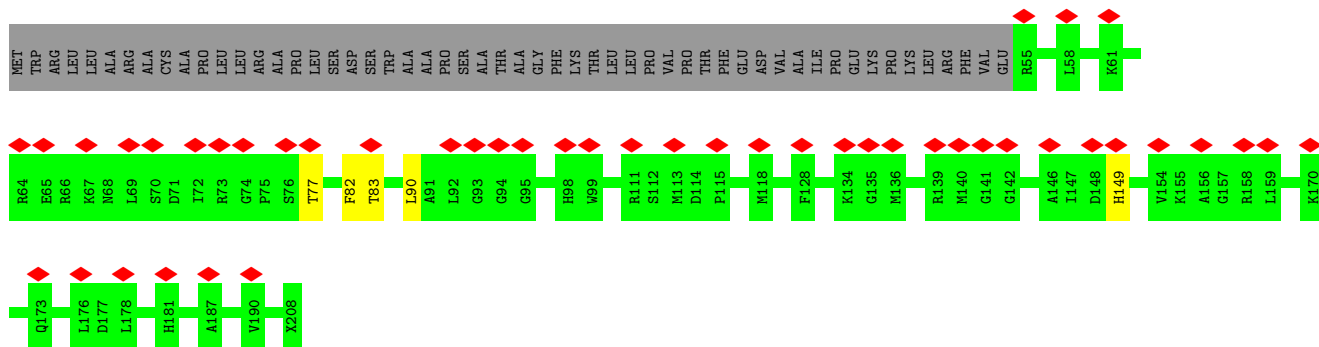
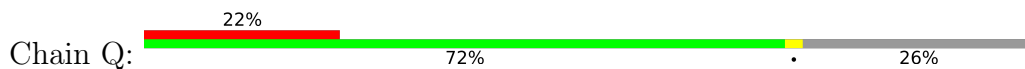


• Molecule 14: MRPL4

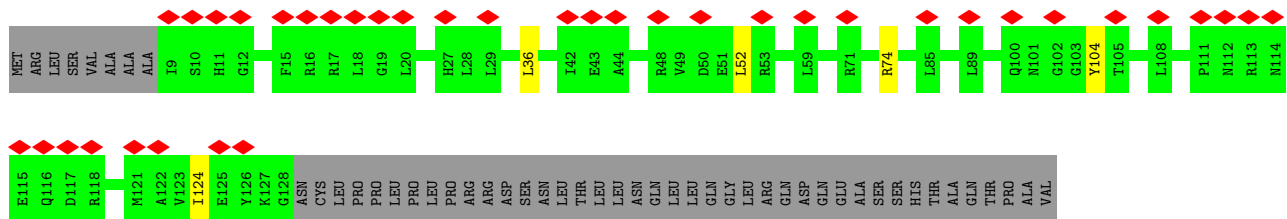




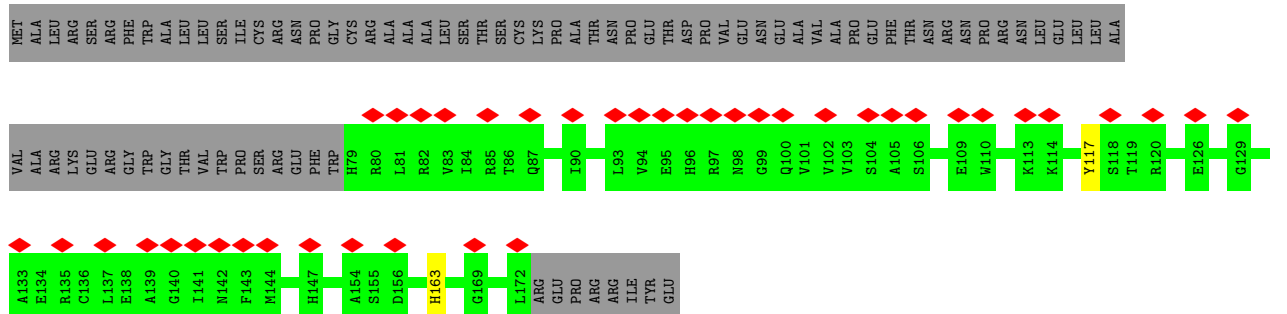
• Molecule 19: MRPL16



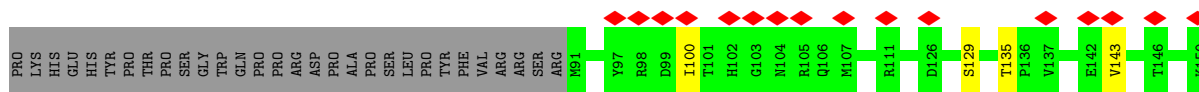
• Molecule 20: MRPL17



• Molecule 21: MRPL18



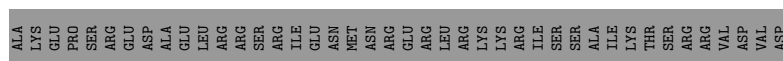
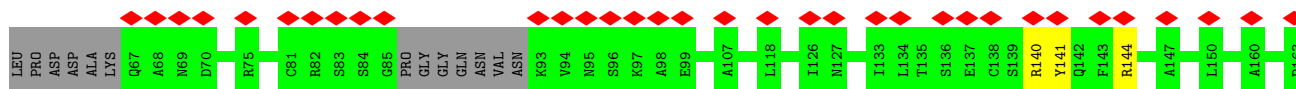
• Molecule 22: MRPL19



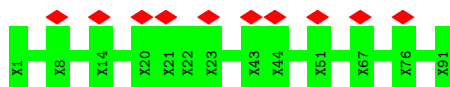
- Molecule 33: MRPL52



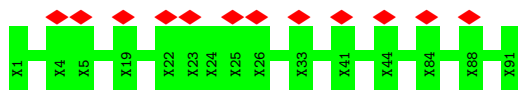
- Molecule 34: ICT1



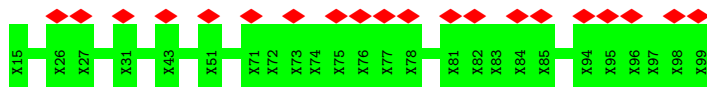
- Molecule 35: UNASSIGNED HELICES



- Molecule 35: UNASSIGNED HELICES

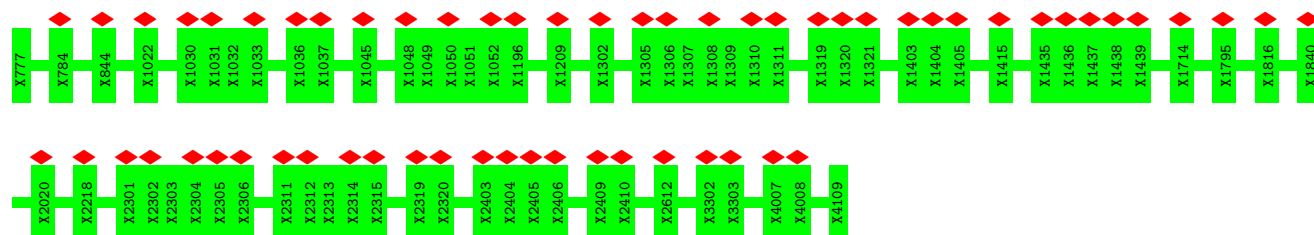


- Molecule 36: THIOREDOXIN FOLD



- Molecule 37: UNASSIGNED HELICES

Chain z:  14% 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	232181	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PER DETECTOR FRAME	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	48.929	Depositor
Minimum map value	-45.891	Depositor
Average map value	-0.047	Depositor
Map value standard deviation	3.830	Depositor
Recommended contour level	11.0	Depositor
Map size (\AA)	360.96, 360.96, 360.96	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.41, 1.41, 1.41	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	0.20	0/624	0.34	0/836
2	1	0.20	0/498	0.41	0/670
3	2	0.19	0/641	0.32	0/862
4	3	0.19	0/501	0.40	0/671
5	5	0.19	0/393	0.37	0/524
6	6	0.21	0/396	0.36	0/526
7	7	0.19	0/370	0.35	0/492
8	8	0.21	0/529	0.33	0/698
9	9	0.20	0/322	0.32	0/424
10	A	0.16	0/34230	0.72	8/53284 (0.0%)
12	D	0.19	0/1557	0.36	0/2093
13	E	0.21	0/1662	0.37	0/2246
14	F	0.20	0/1582	0.38	0/2148
15	I	0.20	0/450	0.37	0/603
16	N	0.21	0/1211	0.40	0/1639
17	O	0.21	0/907	0.40	0/1224
18	P	0.21	0/1254	0.40	0/1686
19	Q	0.21	0/1104	0.36	0/1483
20	R	0.21	0/1000	0.38	0/1342
21	S	0.18	0/763	0.36	0/1033
22	T	0.22	0/978	0.39	0/1318
23	U	0.21	0/986	0.36	0/1319
24	V	0.21	0/866	0.41	0/1168
25	W	0.20	0/931	0.33	0/1241
26	X	0.20	0/585	0.37	0/788
27	Y	0.20	0/853	0.40	0/1155
28	b	0.21	0/1616	0.39	0/2205
29	c	0.29	1/2171 (0.0%)	0.43	1/2937 (0.0%)
30	h	0.23	0/1918	0.38	0/2597
31	i	0.21	0/1366	0.41	0/1844
32	l	0.22	0/632	0.42	0/855
34	u	0.20	0/726	0.38	0/975

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.19	1/63622 (0.0%)	0.60	9/92886 (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
29	c	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	141	ARG	C-N	6.05	1.48	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	753	U	C2-N1-C1'	7.69	126.93	117.70
10	A	1549	C	N3-C2-O2	-7.49	116.66	121.90
10	A	753	U	N1-C2-O2	7.31	127.92	122.80
10	A	753	U	N3-C2-O2	-6.98	117.31	122.20
10	A	1549	C	C6-N1-C2	-6.66	117.64	120.30
10	A	1549	C	N1-C2-O2	5.79	122.37	118.90
29	c	100	SER	O-C-N	5.52	131.54	122.70
10	A	1252	A	C2-N3-C4	5.46	113.33	110.60
10	A	64	C	N1-C2-O2	5.29	122.08	118.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	c	70	THR	Peptide

5.2 Too-close contacts

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	72/148 (49%)	69 (96%)	3 (4%)	0	100	100
2	1	56/256 (22%)	51 (91%)	5 (9%)	0	100	100
3	2	74/252 (29%)	73 (99%)	1 (1%)	0	100	100
4	3	57/161 (35%)	56 (98%)	1 (2%)	0	100	100
5	5	47/146 (32%)	44 (94%)	3 (6%)	0	100	100
6	6	46/65 (71%)	43 (94%)	3 (6%)	0	100	100
7	7	41/95 (43%)	41 (100%)	0	0	100	100
8	8	58/188 (31%)	58 (100%)	0	0	100	100
9	9	34/100 (34%)	34 (100%)	0	0	100	100
12	D	198/306 (65%)	188 (95%)	10 (5%)	0	100	100
13	E	206/399 (52%)	194 (94%)	12 (6%)	0	100	100
14	F	196/224 (88%)	188 (96%)	8 (4%)	0	100	100
15	I	55/268 (20%)	47 (86%)	8 (14%)	0	100	100
16	N	145/178 (82%)	132 (91%)	13 (9%)	0	100	100
17	O	112/145 (77%)	109 (97%)	3 (3%)	0	100	100
18	P	155/288 (54%)	144 (93%)	10 (6%)	1 (1%)	25	65
19	Q	136/208 (65%)	131 (96%)	5 (4%)	0	100	100
20	R	118/169 (70%)	107 (91%)	11 (9%)	0	100	100
21	S	92/180 (51%)	87 (95%)	5 (5%)	0	100	100
22	T	117/292 (40%)	113 (97%)	4 (3%)	0	100	100
23	U	114/132 (86%)	110 (96%)	3 (3%)	1 (1%)	17	56
24	V	104/207 (50%)	97 (93%)	7 (7%)	0	100	100
25	W	109/134 (81%)	106 (97%)	3 (3%)	0	100	100
26	X	68/87 (78%)	68 (100%)	0	0	100	100
27	Y	101/216 (47%)	95 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	b	190/380 (50%)	179 (94%)	10 (5%)	1 (0%)	29	68
29	c	259/301 (86%)	246 (95%)	12 (5%)	1 (0%)	34	72
30	h	239/298 (80%)	220 (92%)	18 (8%)	1 (0%)	34	72
31	i	159/312 (51%)	148 (93%)	11 (7%)	0	100	100
32	l	74/166 (45%)	70 (95%)	3 (4%)	1 (1%)	11	46
34	u	86/205 (42%)	77 (90%)	9 (10%)	0	100	100
All	All	3518/6506 (54%)	3325 (94%)	187 (5%)	6 (0%)	50	81

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	l	143	VAL
23	U	14	VAL
28	b	187	VAL
18	P	47	ARG
30	h	223	MET
29	c	71	ASP

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	0	62/115 (54%)	60 (97%)	2 (3%)	39	61
2	1	54/229 (24%)	51 (94%)	3 (6%)	21	48
3	2	72/228 (32%)	72 (100%)	0	100	100
4	3	56/147 (38%)	56 (100%)	0	100	100
5	5	44/108 (41%)	43 (98%)	1 (2%)	50	70
6	6	45/60 (75%)	45 (100%)	0	100	100
7	7	39/78 (50%)	39 (100%)	0	100	100
8	8	54/162 (33%)	52 (96%)	2 (4%)	34	58
9	9	34/77 (44%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	D	158/248 (64%)	158 (100%)	0	100	100
13	E	173/320 (54%)	171 (99%)	2 (1%)	71	84
14	F	166/166 (100%)	161 (97%)	5 (3%)	41	63
15	I	50/228 (22%)	48 (96%)	2 (4%)	31	56
16	N	127/157 (81%)	126 (99%)	1 (1%)	81	89
17	O	99/123 (80%)	97 (98%)	2 (2%)	55	73
18	P	129/235 (55%)	125 (97%)	4 (3%)	40	62
19	Q	111/155 (72%)	106 (96%)	5 (4%)	27	53
20	R	101/143 (71%)	96 (95%)	5 (5%)	24	50
21	S	80/153 (52%)	78 (98%)	2 (2%)	47	68
22	T	107/258 (42%)	105 (98%)	2 (2%)	57	75
23	U	100/109 (92%)	98 (98%)	2 (2%)	55	73
24	V	94/173 (54%)	92 (98%)	2 (2%)	53	72
25	W	95/95 (100%)	94 (99%)	1 (1%)	73	85
26	X	62/62 (100%)	61 (98%)	1 (2%)	62	79
27	Y	91/192 (47%)	88 (97%)	3 (3%)	38	61
28	b	165/328 (50%)	158 (96%)	7 (4%)	30	54
29	c	236/244 (97%)	228 (97%)	8 (3%)	37	60
30	h	206/230 (90%)	203 (98%)	3 (2%)	65	80
31	i	148/281 (53%)	143 (97%)	5 (3%)	37	60
32	l	68/147 (46%)	63 (93%)	5 (7%)	13	40
34	u	79/177 (45%)	76 (96%)	3 (4%)	33	57
All	All	3105/5428 (57%)	3027 (98%)	78 (2%)	50	68

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	50	ARG
1	0	83	LEU
2	1	96	LYS
2	1	125	VAL
2	1	126	THR
5	5	121	ILE
8	8	129	TYR

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Mol	Chain	Res	Type
8	8	134	TRP
13	E	287	THR
13	E	317	ARG
14	F	92	ARG
14	F	114	THR
14	F	159	THR
14	F	203	LEU
14	F	234	THR
15	I	130	VAL
15	I	136	ASN
16	N	11	TRP
17	O	75	LEU
17	O	77	ILE
18	P	61	THR
18	P	81	TYR
18	P	130	GLN
18	P	147	THR
19	Q	77	THR
19	Q	82	PHE
19	Q	83	THR
19	Q	90	LEU
19	Q	149	HIS
20	R	36	LEU
20	R	52	LEU
20	R	74	ARG
20	R	104	TYR
20	R	124	ILE
21	S	117	TYR
21	S	163	HIS
22	T	166	LEU
22	T	177	VAL
23	U	30	HIS
23	U	81	LEU
24	V	148	LEU
24	V	158	VAL
25	W	119	LEU
26	X	56	TYR
27	Y	85	TRP
27	Y	138	THR
27	Y	153	ILE
28	b	179	VAL
28	b	206	TYR

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Mol	Chain	Res	Type
28	b	258	PHE
28	b	297	THR
28	b	298	PHE
28	b	304	TYR
28	b	308	GLN
29	c	69	LYS
29	c	70	THR
29	c	126	THR
29	c	165	ARG
29	c	180	VAL
29	c	207	ILE
29	c	280	VAL
29	c	305	HIS
30	h	184	PHE
30	h	230	GLU
30	h	233	THR
31	i	116	VAL
31	i	149	HIS
31	i	249	GLU
31	i	253	VAL
31	i	256	TYR
32	l	100	ILE
32	l	129	SER
32	l	135	THR
32	l	153	PHE
32	l	157	LEU
34	u	140	ARG
34	u	141	TYR
34	u	144	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	41	ASN
1	0	72	HIS
3	2	119	GLN
5	5	83	ASN
8	8	151	ASN
8	8	154	GLN
9	9	99	GLN
12	D	234	GLN
13	E	231	ASN

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Mol	Chain	Res	Type
16	N	26	GLN
16	N	48	HIS
17	O	33	GLN
18	P	26	ASN
18	P	53	HIS
18	P	71	GLN
20	R	31	ASN
23	U	36	ASN
23	U	79	HIS
23	U	89	ASN
24	V	122	ASN
25	W	73	HIS
25	W	130	HIS
25	W	157	HIS
25	W	171	HIS
26	X	73	GLN
26	X	84	ASN
26	X	98	GLN
27	Y	118	ASN
28	b	147	HIS
28	b	191	ASN
28	b	307	HIS
28	b	320	GLN
32	l	92	HIS
32	l	141	ASN
34	u	103	HIS
34	u	122	HIS
34	u	124	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	1431/1570 (91%)	368 (25%)	25 (1%)
11	B	0/29	-	-
All	All	1431/1599 (89%)	368 (25%)	25 (1%)

All (368) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	2	C
10	A	5	A

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Mol	Chain	Res	Type
10	A	7	G
10	A	8	C
10	A	46	A
10	A	48	U
10	A	49	A
10	A	50	A
10	A	56	A
10	A	59	A
10	A	64	C
10	A	65	C
10	A	66	U
10	A	67	A
10	A	69	C
10	A	70	A
10	A	73	A
10	A	82	G
10	A	95	U
10	A	96	U
10	A	97	A
10	A	100	C
10	A	101	U
10	A	102	G
10	A	105	G
10	A	108	A
10	A	109	U
10	A	112	A
10	A	116	A
10	A	117	G
10	A	128	A
10	A	131	G
10	A	132	A
10	A	133	U
10	A	138	G
10	A	139	A
10	A	140	A
10	A	142	A
10	A	144	A
10	A	145	A
10	A	147	A
10	A	148	A
10	A	149	A
10	A	150	A

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Mol	Chain	Res	Type
10	A	152	U
10	A	153	A
10	A	154	A
10	A	156	A
10	A	157	A
10	A	160	A
10	A	161	G
10	A	162	C
10	A	163	A
10	A	164	A
10	A	169	U
10	A	171	C
10	A	172	C
10	A	174	C
10	A	179	A
10	A	188	A
10	A	189	U
10	A	191	A
10	A	203	G
10	A	204	A
10	A	205	A
10	A	206	A
10	A	217	A
10	A	218	A
10	A	221	G
10	A	222	A
10	A	227	U
10	A	228	A
10	A	237	C
10	A	238	C
10	A	253	G
10	A	266	A
10	A	270	U
10	A	271	A
10	A	272	A
10	A	273	A
10	A	274	A
10	A	275	G
10	A	293	G
10	A	299	A
10	A	310	A
10	A	321	G

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Mol	Chain	Res	Type
10	A	322	A
10	A	323	G
10	A	328	A
10	A	330	A
10	A	331	G
10	A	338	G
10	A	351	G
10	A	357	U
10	A	358	G
10	A	365	A
10	A	372	U
10	A	379	C
10	A	381	A
10	A	382	C
10	A	390	A
10	A	391	U
10	A	393	C
10	A	394	C
10	A	395	C
10	A	398	A
10	A	399	A
10	A	400	A
10	A	409	U
10	A	413	A
10	A	414	A
10	A	415	U
10	A	417	U
10	A	418	A
10	A	419	U
10	A	421	U
10	A	422	U
10	A	427	A
10	A	432	G
10	A	439	A
10	A	444	A
10	A	445	C
10	A	447	G
10	A	457	A
10	A	458	A
10	A	459	C
10	A	466	A
10	A	468	C

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Mol	Chain	Res	Type
10	A	472	G
10	A	474	C
10	A	478	A
10	A	487	C
10	A	489	U
10	A	490	A
10	A	492	U
10	A	494	C
10	A	560	A
10	A	561	U
10	A	565	C
10	A	566	C
10	A	569	A
10	A	583	A
10	A	584	C
10	A	591	C
10	A	592	C
10	A	594	A
10	A	614	A
10	A	616	A
10	A	617	C
10	A	618	A
10	A	619	U
10	A	626	A
10	A	629	A
10	A	632	G
10	A	648	A
10	A	649	G
10	A	652	G
10	A	655	U
10	A	662	U
10	A	665	C
10	A	668	A
10	A	670	G
10	A	671	C
10	A	673	U
10	A	674	A
10	A	675	C
10	A	682	A
10	A	686	A
10	A	687	A
10	A	688	U

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Mol	Chain	Res	Type
10	A	691	U
10	A	693	U
10	A	694	A
10	A	695	C
10	A	702	U
10	A	703	U
10	A	704	A
10	A	705	A
10	A	706	C
10	A	710	C
10	A	711	A
10	A	713	U
10	A	718	C
10	A	722	A
10	A	723	C
10	A	724	A
10	A	726	C
10	A	731	A
10	A	733	A
10	A	734	C
10	A	735	G
10	A	744	U
10	A	745	U
10	A	746	A
10	A	747	C
10	A	748	A
10	A	752	U
10	A	755	A
10	A	757	C
10	A	766	G
10	A	772	A
10	A	773	C
10	A	774	C
10	A	776	A
10	A	779	A
10	A	780	A
10	A	781	A
10	A	782	G
10	A	787	A
10	A	807	G
10	A	811	A
10	A	812	C

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Mol	Chain	Res	Type
10	A	813	A
10	A	817	A
10	A	823	C
10	A	830	A
10	A	834	A
10	A	841	C
10	A	850	C
10	A	851	A
10	A	853	U
10	A	854	A
10	A	857	A
10	A	861	U
10	A	870	A
10	A	876	G
10	A	887	C
10	A	888	C
10	A	889	A
10	A	894	A
10	A	900	C
10	A	906	A
10	A	907	U
10	A	922	G
10	A	923	G
10	A	931	A
10	A	948	U
10	A	956	U
10	A	960	U
10	A	962	A
10	A	963	A
10	A	964	U
10	A	965	G
10	A	975	G
10	A	985	G
10	A	986	U
10	A	990	U
10	A	1013	C
10	A	1014	C
10	A	1024	A
10	A	1026	A
10	A	1029	C
10	A	1036	A
10	A	1048	C

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Mol	Chain	Res	Type
10	A	1049	G
10	A	1053	A
10	A	1054	G
10	A	1055	A
10	A	1062	G
10	A	1069	U
10	A	1075	A
10	A	1080	U
10	A	1083	A
10	A	1084	A
10	A	1085	A
10	A	1089	U
10	A	1125	A
10	A	1132	A
10	A	1137	C
10	A	1141	U
10	A	1144	G
10	A	1165	C
10	A	1166	A
10	A	1167	A
10	A	1174	C
10	A	1177	C
10	A	1178	G
10	A	1179	A
10	A	1180	G
10	A	1181	U
10	A	1187	U
10	A	1189	A
10	A	1191	C
10	A	1192	U
10	A	1193	A
10	A	1221	U
10	A	1222	C
10	A	1223	A
10	A	1225	U
10	A	1226	U
10	A	1227	A
10	A	1228	U
10	A	1236	A
10	A	1237	A
10	A	1238	A
10	A	1244	A

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Mol	Chain	Res	Type
10	A	1247	A
10	A	1250	G
10	A	1251	G
10	A	1252	A
10	A	1253	A
10	A	1256	A
10	A	1260	A
10	A	1262	C
10	A	1266	G
10	A	1269	A
10	A	1297	C
10	A	1325	U
10	A	1326	G
10	A	1327	U
10	A	1339	A
10	A	1341	C
10	A	1350	G
10	A	1376	U
10	A	1377	C
10	A	1387	A
10	A	1388	G
10	A	1394	C
10	A	1405	U
10	A	1406	U
10	A	1407	C
10	A	1409	G
10	A	1420	U
10	A	1423	A
10	A	1424	G
10	A	1430	U
10	A	1431	U
10	A	1432	U
10	A	1434	U
10	A	1436	U
10	A	1442	A
10	A	1443	U
10	A	1446	A
10	A	1456	G
10	A	1466	A
10	A	1467	C
10	A	1474	A
10	A	1480	A

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Mol	Chain	Res	Type
10	A	1483	A
10	A	1488	C
10	A	1490	C
10	A	1491	A
10	A	1492	A
10	A	1493	A
10	A	1496	C
10	A	1504	A
10	A	1508	A
10	A	1509	A
10	A	1510	U
10	A	1527	A
10	A	1530	U
10	A	1531	A
10	A	1532	A
10	A	1537	C
10	A	1540	A
10	A	1541	U
10	A	1543	A
10	A	1545	A
10	A	1547	A
10	A	1548	U
10	A	1549	C
10	A	1551	A
10	A	1556	U
10	A	1557	A
10	A	1565	G
10	A	1567	A
10	A	1568	C
10	A	1569	A

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	1	A
10	A	66	U
10	A	72	U
10	A	115	U
10	A	273	A
10	A	298	A
10	A	418	A
10	A	618	A

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Mol	Chain	Res	Type
10	A	672	U
10	A	702	U
10	A	730	A
10	A	746	A
10	A	751	G
10	A	756	C
10	A	786	A
10	A	860	A
10	A	985	G
10	A	1013	C
10	A	1079	U
10	A	1166	A
10	A	1236	A
10	A	1252	A
10	A	1375	U
10	A	1566	C
10	A	1568	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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
37	z	20
35	v	4
35	w	4
10	A	2
11	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	z	3019:UNK	C	3301:UNK	N	179.35
1	z	1718:UNK	C	1795:UNK	N	178.65
1	z	1325:UNK	C	1403:UNK	N	151.39
1	z	844:UNK	C	1001:UNK	N	141.39
1	z	2220:UNK	C	2301:UNK	N	132.08
1	z	4008:UNK	C	4101:UNK	N	128.55
1	z	2719:UNK	C	3004:UNK	N	119.93
1	z	1225:UNK	C	1302:UNK	N	101.25
1	z	2022:UNK	C	2201:UNK	N	100.33
1	z	1052:UNK	C	1196:UNK	N	80.72
1	z	3316:UNK	C	4000:UNK	N	74.67
1	z	2613:UNK	C	2703:UNK	N	73.14
1	z	1439:UNK	C	1704:UNK	N	68.39
1	z	1939:UNK	C	1977:UNK	N	49.60
1	v	25:UNK	C	26:UNK	N	44.67
1	z	1997:UNK	C	2003:UNK	N	44.67
1	w	25:UNK	C	26:UNK	N	43.96
1	z	1847:UNK	C	1926:UNK	N	43.50
1	z	2413:UNK	C	2601:UNK	N	40.26
1	A	37:N	O3'	45:A	P	29.60
1	v	80:UNK	C	81:UNK	N	27.95
1	w	50:UNK	C	51:UNK	N	27.75
1	w	80:UNK	C	81:UNK	N	26.67
1	v	50:UNK	C	51:UNK	N	25.67
1	z	2321:UNK	C	2401:UNK	N	25.50
1	w	67:UNK	C	68:UNK	N	13.96

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	27:N	O3'	35:N	P	12.68
1	v	67:UNK	C	68:UNK	N	12.57
1	B	22:N	O3'	30:N	P	11.59
1	z	1814:UNK	C	1816:UNK	N	8.48
1	z	787:UNK	C	829:UNK	N	8.09

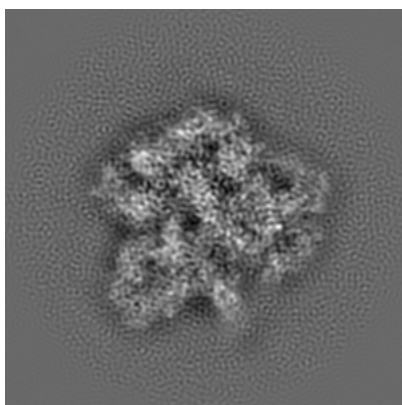
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2490. These allow visual inspection of the internal detail of the map and identification of artifacts.

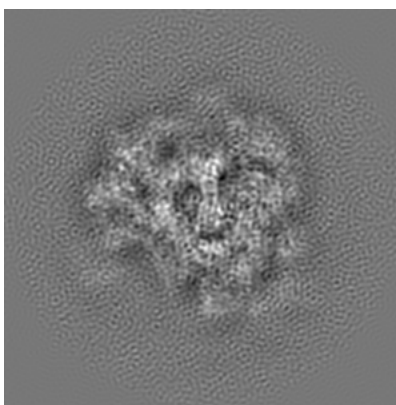
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

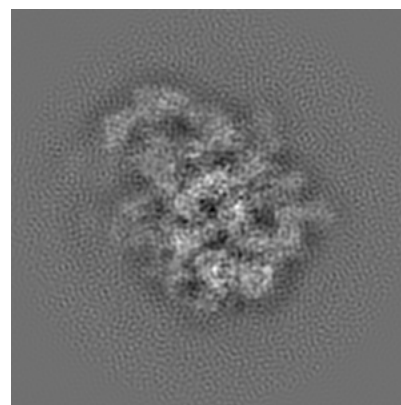
6.1.1 Primary map



X



Y

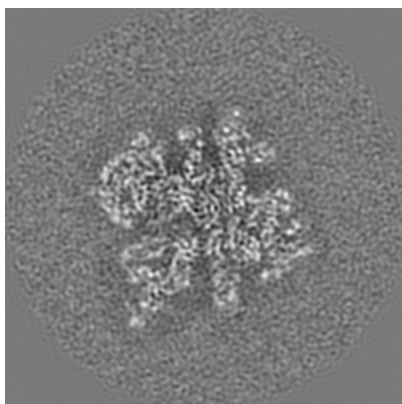


Z

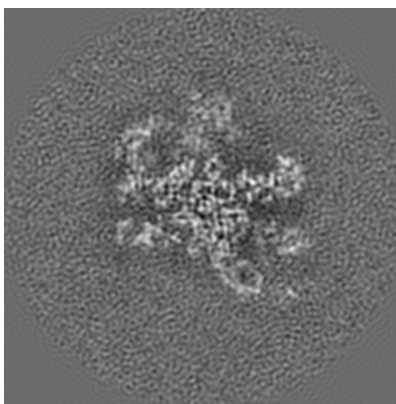
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

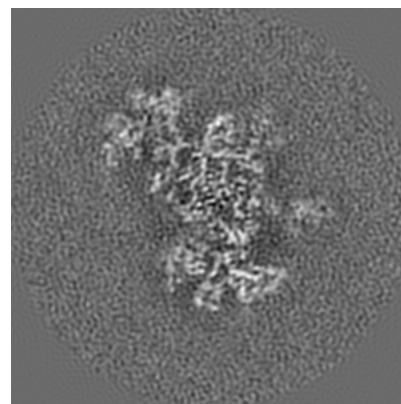
6.2.1 Primary map



X Index: 128



Y Index: 128

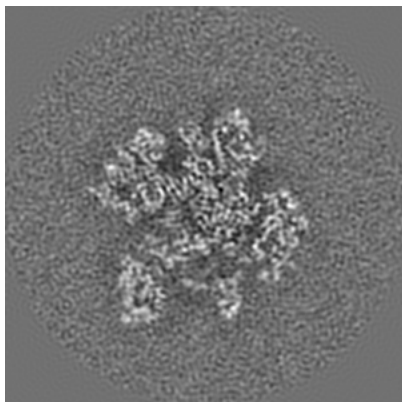


Z Index: 128

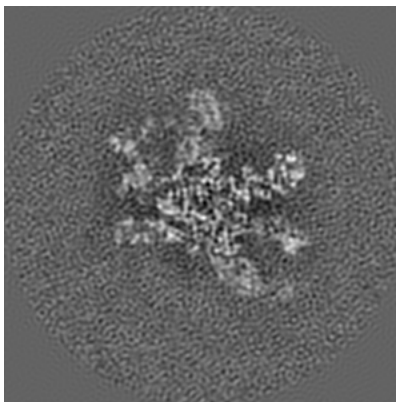
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

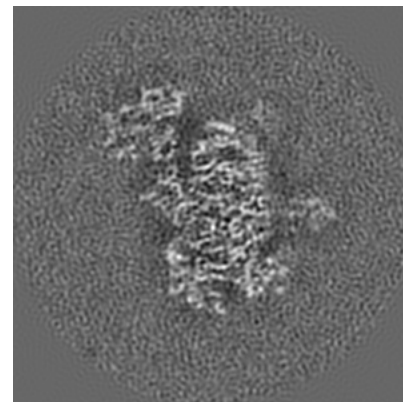
6.3.1 Primary map



X Index: 132



Y Index: 130



Z Index: 134

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 11.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

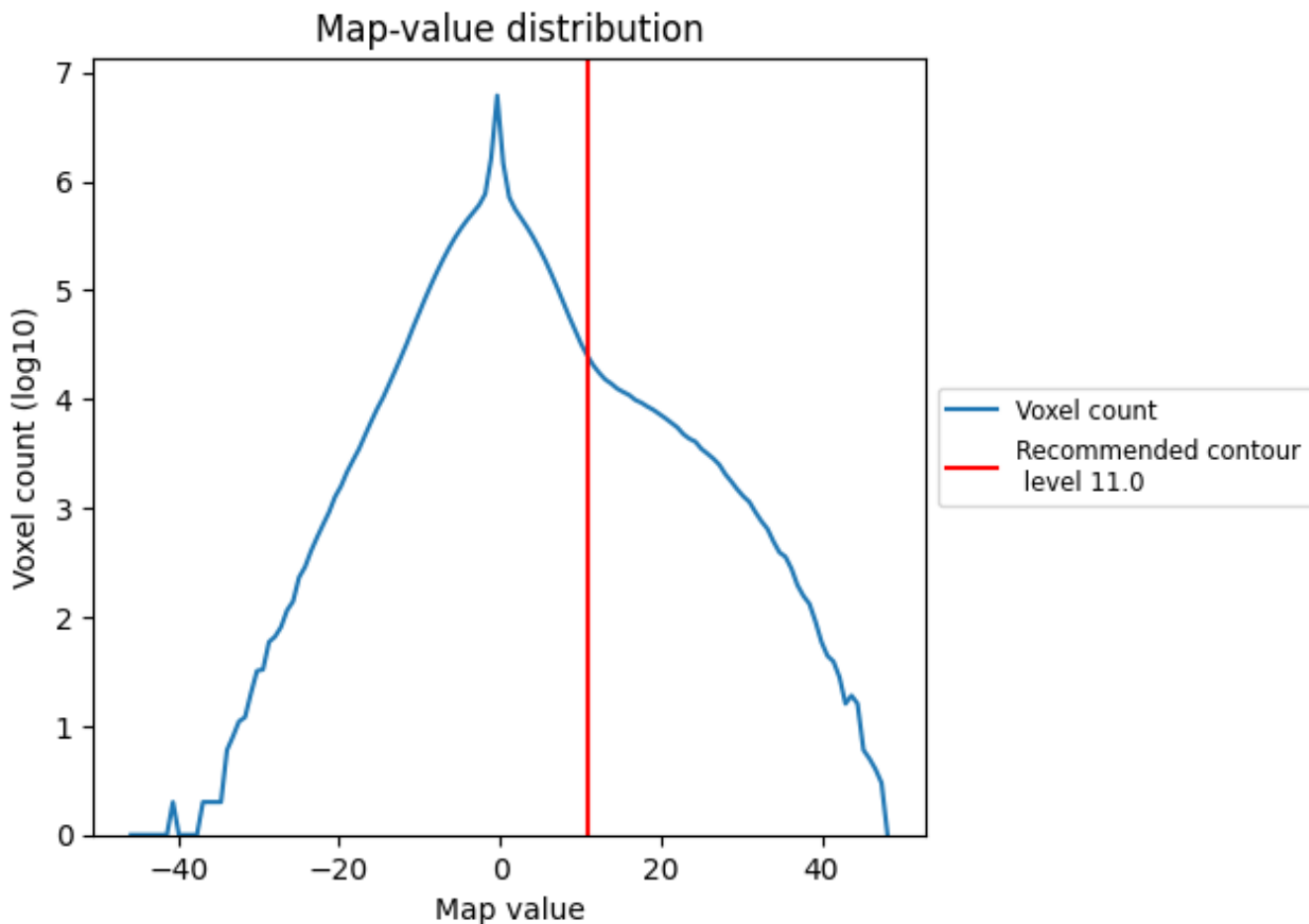
6.5 Mask visualisation

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

7 Map analysis [i](#)

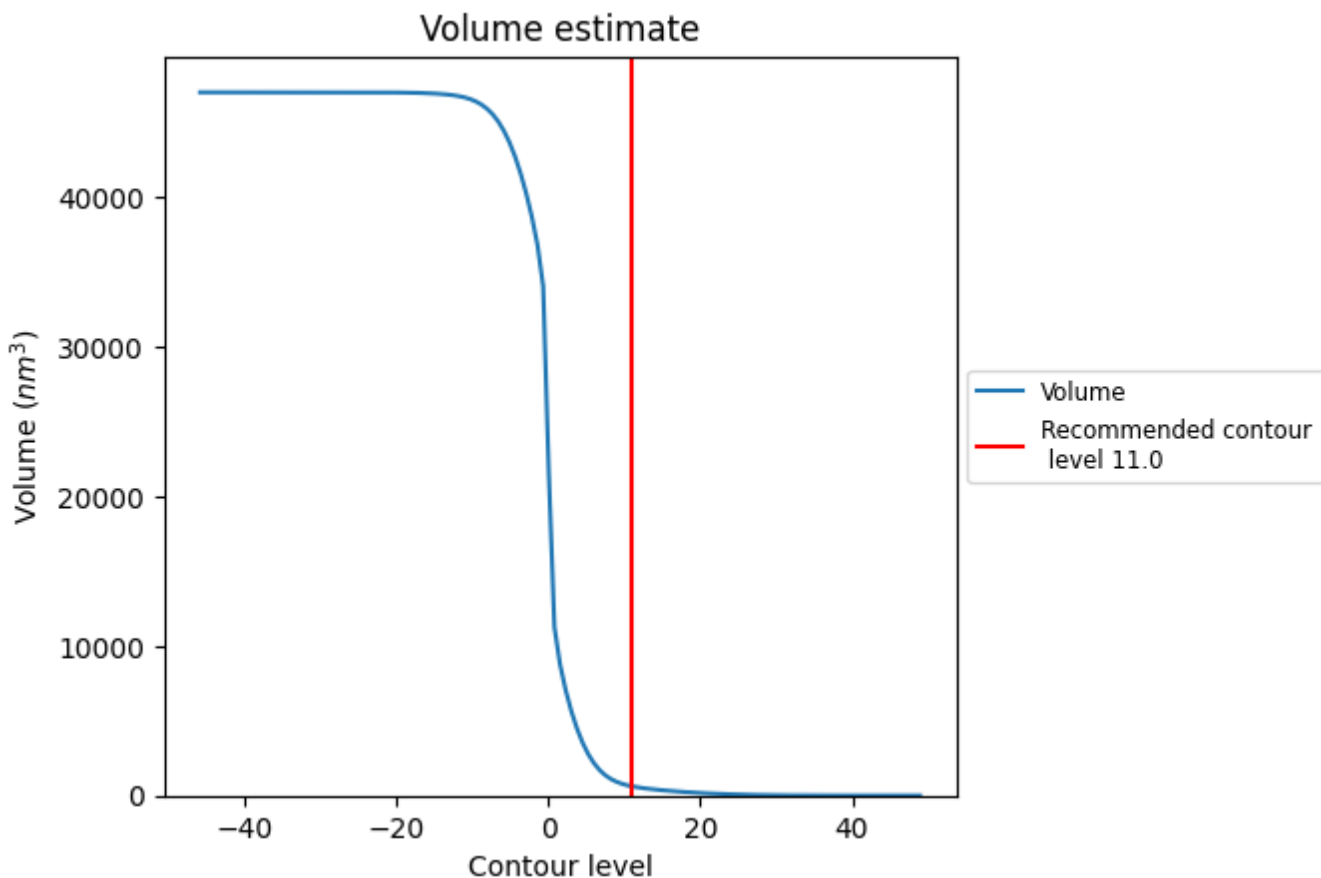
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

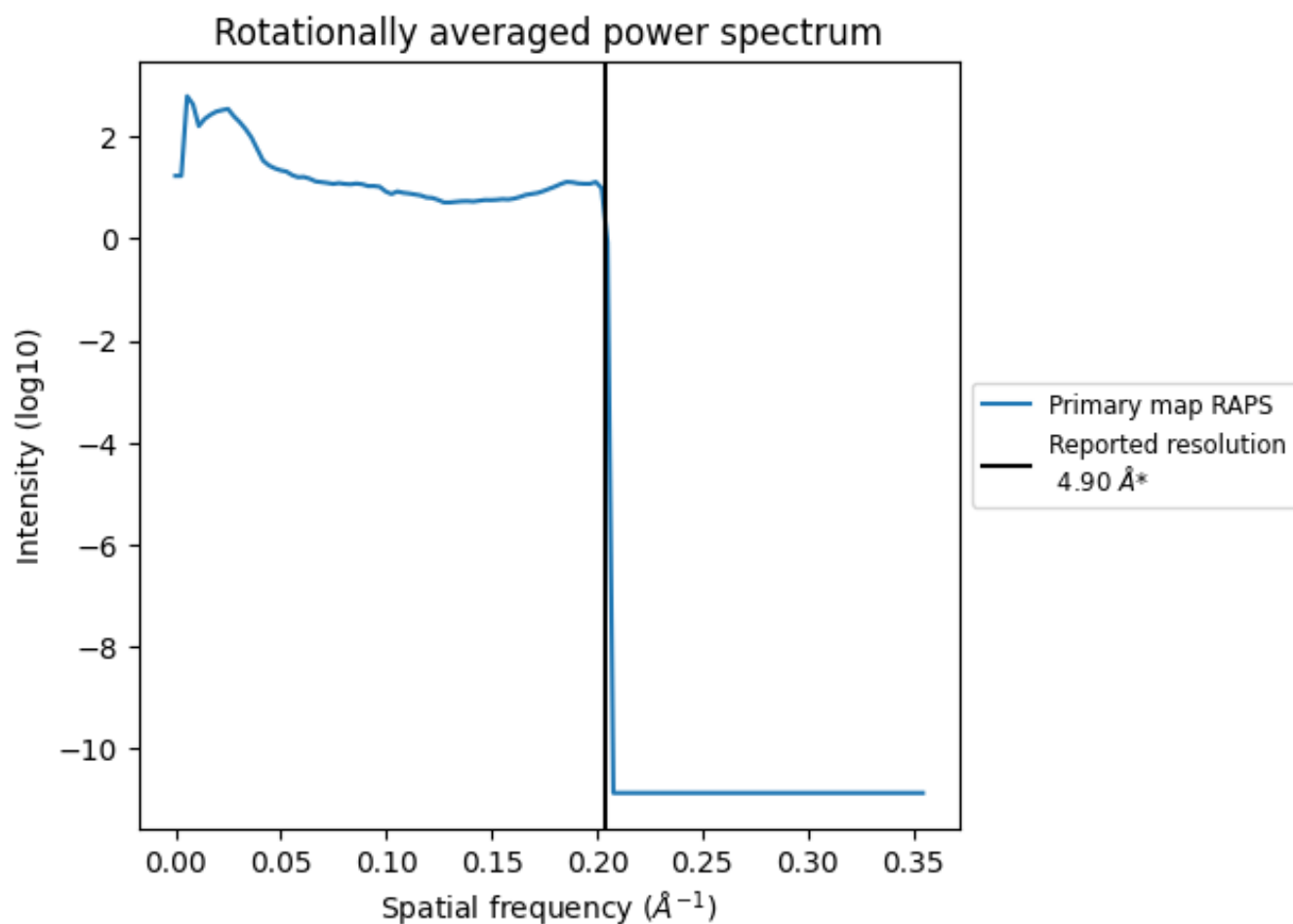
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 619 nm³; this corresponds to an approximate mass of 559 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 0.204 Å⁻¹

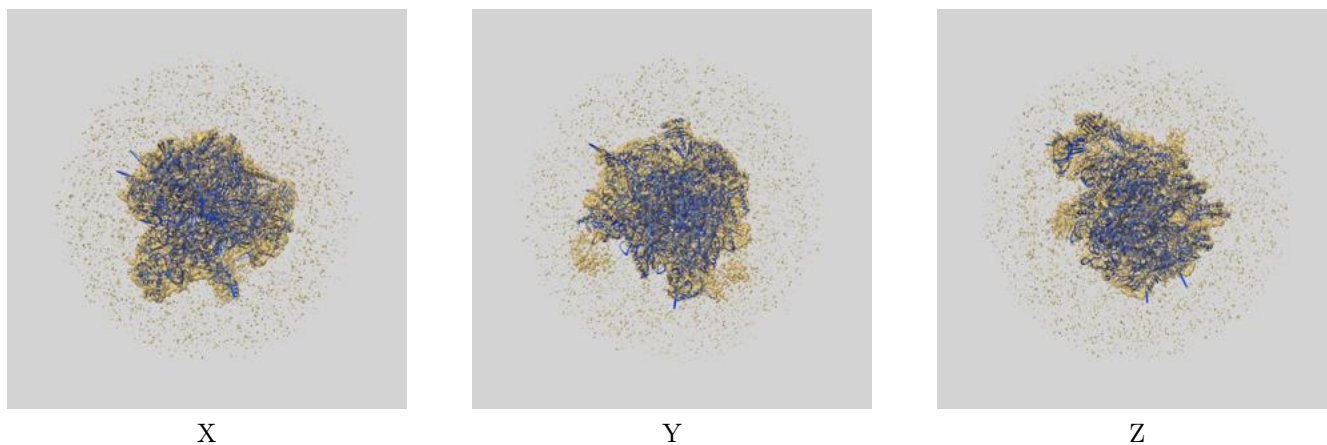
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

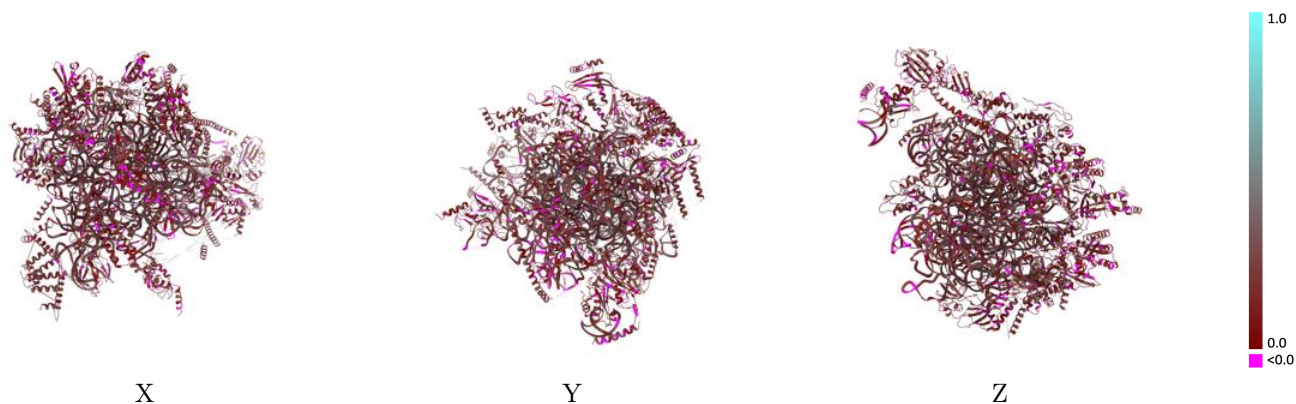
This section contains information regarding the fit between EMDB map EMD-2490 and PDB model 4CE4. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



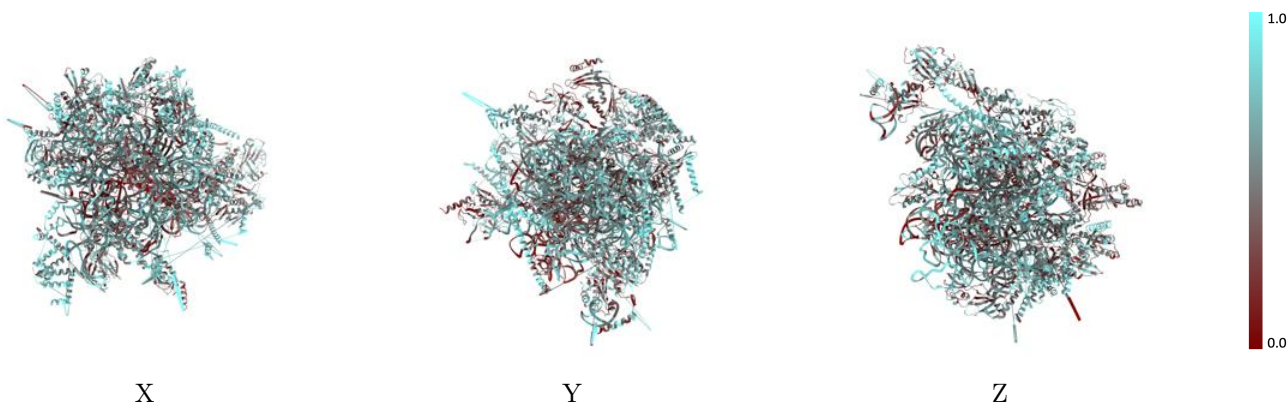
The images above show the 3D surface view of the map at the recommended contour level 11.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



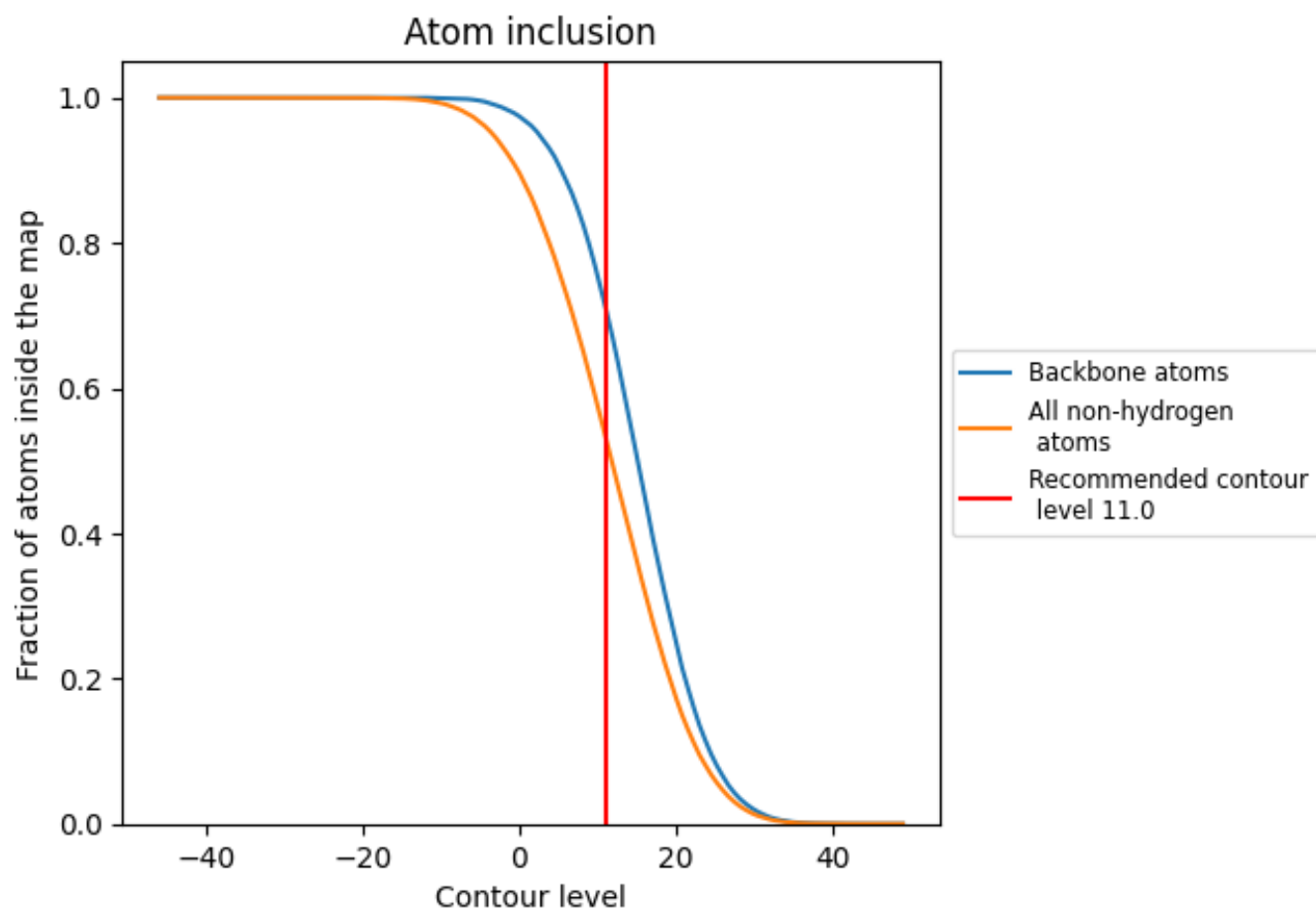
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (11.0).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 53% 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 (11.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5338	 0.2120
0	 0.4132	 0.2170
1	 0.4630	 0.1570
2	 0.5698	 0.1350
3	 0.4595	 0.2120
5	 0.5343	 0.2220
6	 0.1927	 0.0790
7	 0.4277	 0.2160
8	 0.3735	 0.2070
9	 0.3477	 0.2100
A	 0.5763	 0.2430
B	 0.5086	 0.1790
D	 0.4178	 0.1520
E	 0.4686	 0.1920
F	 0.4794	 0.1970
I	 0.2420	 0.1430
N	 0.4870	 0.2170
O	 0.4277	 0.2010
P	 0.4139	 0.1780
Q	 0.5091	 0.2000
R	 0.5105	 0.1860
S	 0.4601	 0.1730
T	 0.5335	 0.1820
U	 0.4227	 0.2040
V	 0.4547	 0.2230
W	 0.4689	 0.2180
X	 0.4562	 0.2160
Y	 0.2769	 0.1180
b	 0.5409	 0.1730
c	 0.5256	 0.1590
h	 0.5850	 0.1590
i	 0.3652	 0.1510
l	 0.5354	 0.1460
o	 0.7619	 0.1880
u	 0.4641	 0.1450



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Chain	Atom inclusion	Q-score
v	 0.7161	 0.2320
w	 0.6832	 0.2250
x	 0.6431	 0.2130
z	 0.6839	 0.2170