



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 01:51 AM EST

PDB ID : 6NEQ
EMDB ID : EMD-9358
Title : Structure of human mitochondrial translation initiation factor 3 bound to the small ribosomal subunit-Class-II
Authors : Sharma, M.; Koripella, R.; Agrawal, R.
Deposited on : 2018-12-18
Resolution : 3.32 Å(reported)
Based on initial model : 3JD5

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
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) : 2.39

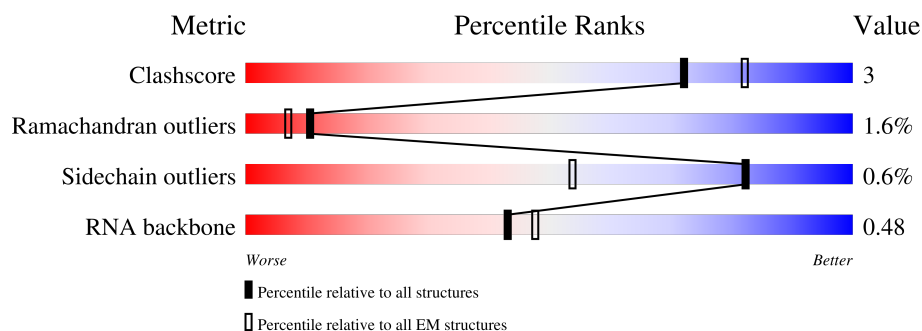
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.32 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



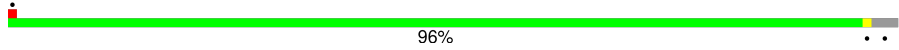

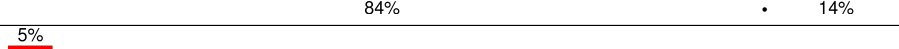
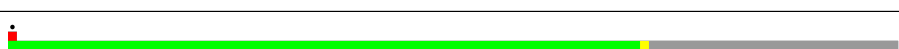



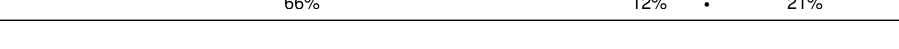



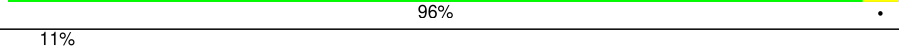

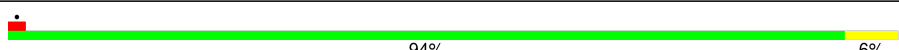


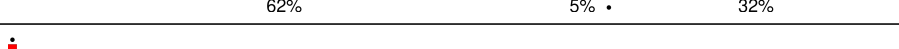

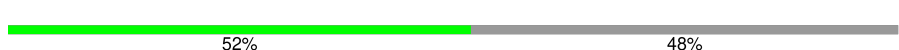





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	955	
2	C	167	
3	E	430	
4	L	139	
5	P	135	
6	Q	130	
7	a	359	

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Mol	Chain	Length	Quality of chain
8	c	173	
9	d	205	
10	e	415	
11	j	218	
12	p	258	
13	G	242	
14	I	396	
15	J	201	
16	N	128	
17	g	351	
18	h	386	
19	i	106	
20	k	325	
21	m	118	
22	o	575	
23	B	293	
24	F	124	
25	K	197	
26	O	256	
27	R	143	
28	U	87	
29	b	190	
30	f	189	
31	n	199	
32	z	247	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 65776 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 28S ribosomal RNA, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	952	Total	C	N	O	P	0	0
			20256	9090	3685	6529	952		

- Molecule 2 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	123	Total	C	N	O	S	0	0
			998	648	177	169	4		

- Molecule 3 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	309	Total	C	N	O	S	0	0
			2464	1535	472	446	11		

- Molecule 4 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	109	Total	C	N	O	S	0	0
			853	534	175	140	4		

- Molecule 5 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	116	Total	C	N	O	S	0	0
			916	580	180	151	5		

- Molecule 6 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	109	Total	C	N	O	S	0	0
			857	555	153	145	4		

- Molecule 7 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	289	Total	C	N	O	S	0	0
			2356	1505	400	443	8		

- Molecule 8 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	c	168	Total	C	N	O	S	0	0
			1374	878	246	241	9		

- Molecule 9 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	d	176	Total	C	N	O	S	0	0
			1463	899	290	272	2		

- Molecule 10 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	e	358	Total	C	N	O	S	0	0
			2950	1886	496	554	14		

- Molecule 11 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	j	213	Total	C	N	O	S	0	0
			1792	1132	346	309	5		

- Molecule 12 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	p	187	Total	C	N	O	S	0	0
			1531	968	288	267	8		

- Molecule 13 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	208	Total	C	N	O	S	0	0
			1721	1093	313	302	13		

- Molecule 14 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	311	Total	C	N	O	S	0	0
			2541	1608	454	467	12		

- Molecule 15 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	128	Total	C	N	O	S	0	0
			1049	676	180	190	3		

- Molecule 16 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	101	Total	C	N	O	S	0	0
			861	538	178	140	5		

- Molecule 17 is a protein called DAP3 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	g	351	Total	C	N	O	S	0	0
			2855	1835	502	508	10		

- Molecule 18 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	h	103	Total	C	N	O	S	0	0
			871	566	141	161	3		

- Molecule 19 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	i	98	Total	C	N	O	S	0	0
			818	519	153	143	3		

- Molecule 20 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	k	275	Total	C	N	O	S	0	0
			2227	1418	377	421	11		

- Molecule 21 is a protein called Coiled-coil-helix-coiled-coil-helix domain containing 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	118	Total	C	N	O	S	0	0
			945	587	185	164	9		

- Molecule 22 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	o	461	Total	C	N	O	S	0	0
			3273	2082	573	605	13		

- Molecule 23 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B	217	Total	C	N	O	S	0	0
			1726	1102	319	298	7		

- Molecule 24 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	F	124	Total	C	N	O	S	0	0
			991	627	179	179	6		

- Molecule 25 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	K	136	Total	C	N	O	S	0	0
			1001	628	193	177	3		

- Molecule 26 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	O	173	Total	C	N	O	S	0	0
			1421	904	258	250	9		

- Molecule 27 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	R	97	Total	C	N	O	S	0	0
			788	507	136	138	7		

- Molecule 28 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	86	Total	C	N	O	S	0	0
			737	457	148	124	8		

- Molecule 29 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	135	Total	C	N	O	S	0	0
			1108	717	195	194	2		

- Molecule 30 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	98	Total	C	N	O	S	0	0
			775	493	135	143	4		

- Molecule 31 is a protein called Aurora kinase A interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	n	72	Total	C	N	O	S	0	0
			642	409	142	89	2		

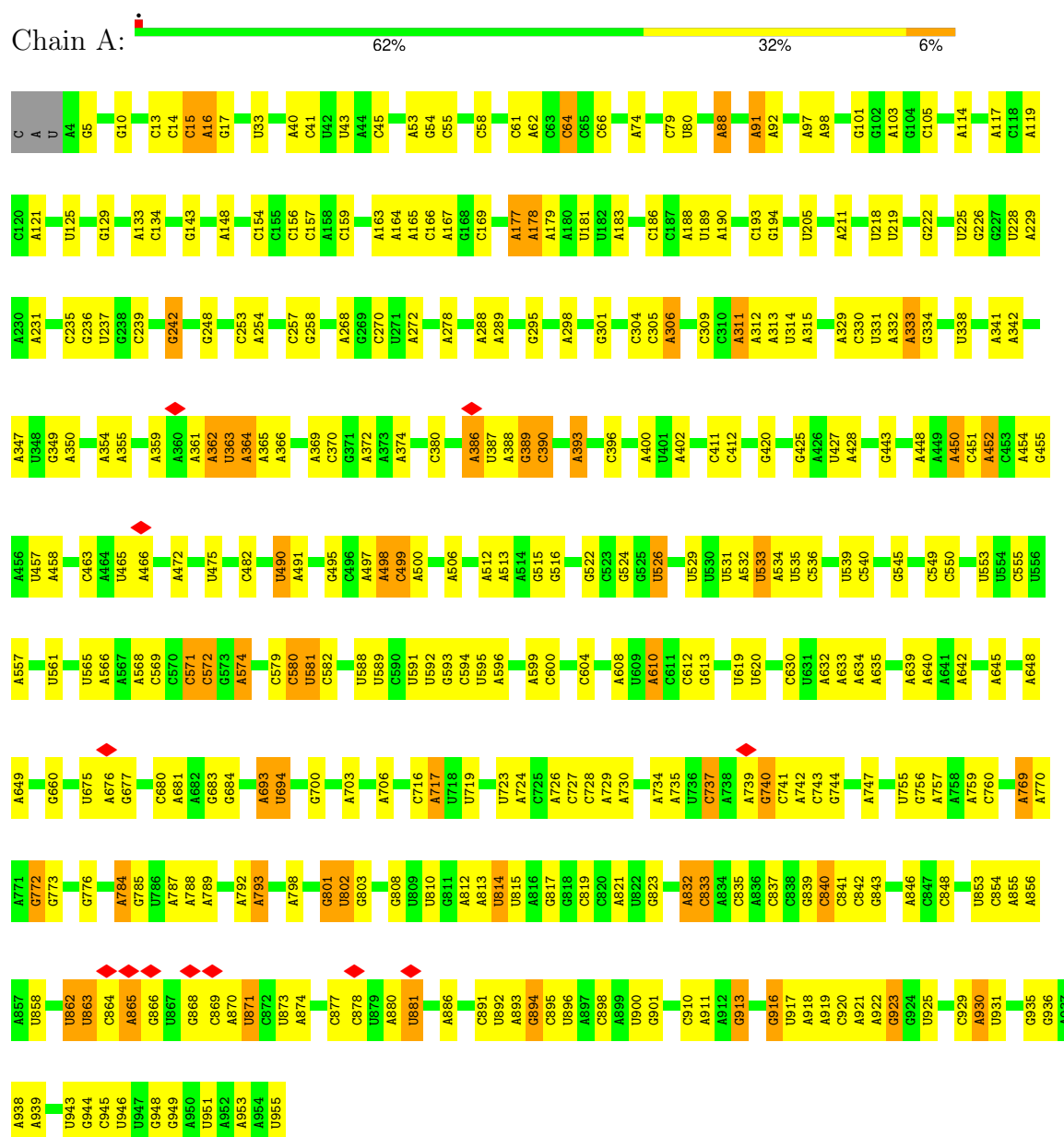
- Molecule 32 is a protein called Translation initiation factor IF-3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	z	207	Total	C	N	O	S	0	0
			1616	998	305	305	8		

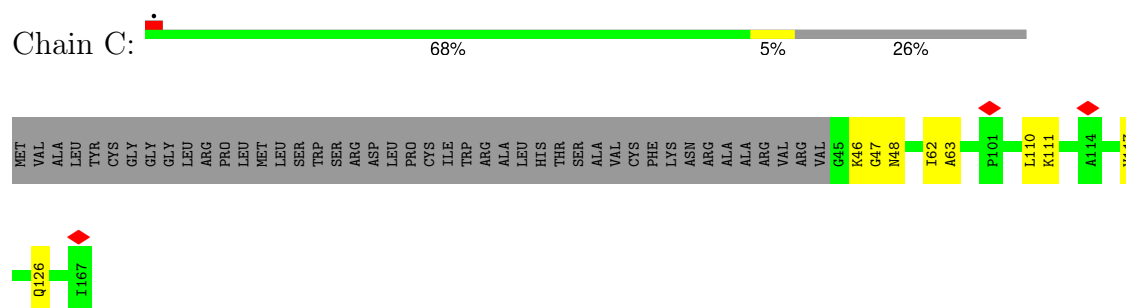
3 Residue-property plots

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

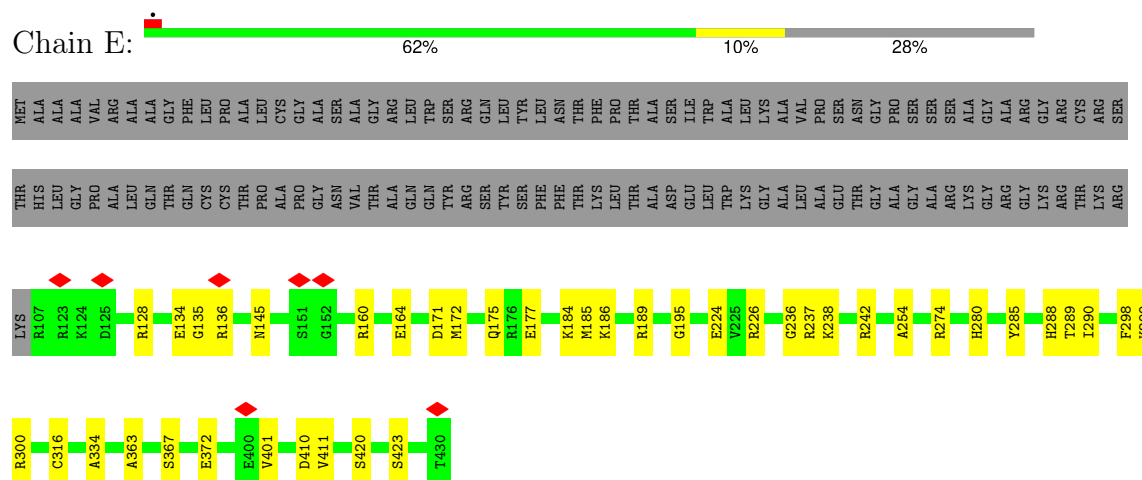
- Molecule 1: 28S ribosomal RNA, mitochondrial



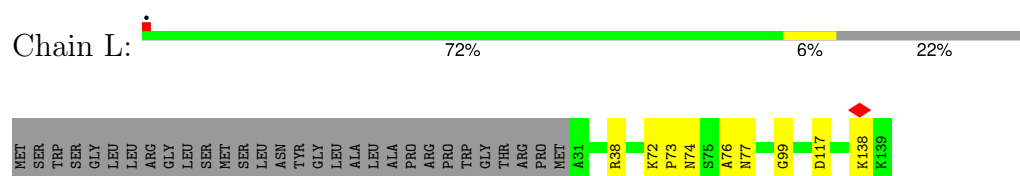
- Molecule 2: 28S ribosomal protein S24, mitochondrial



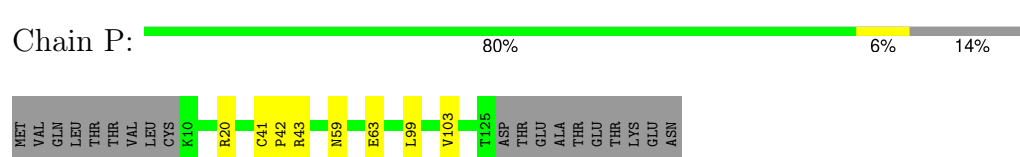
- Molecule 3: 28S ribosomal protein S5, mitochondrial



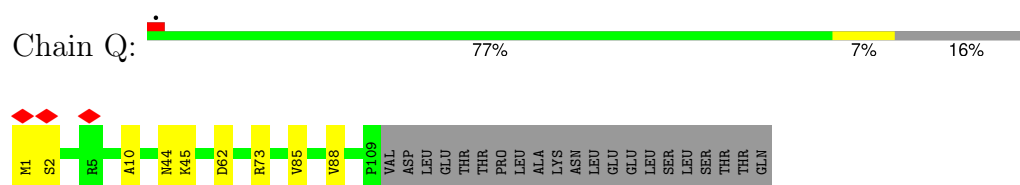
- Molecule 4: 28S ribosomal protein S12, mitochondrial




- Molecule 5: 28S ribosomal protein S16, mitochondrial

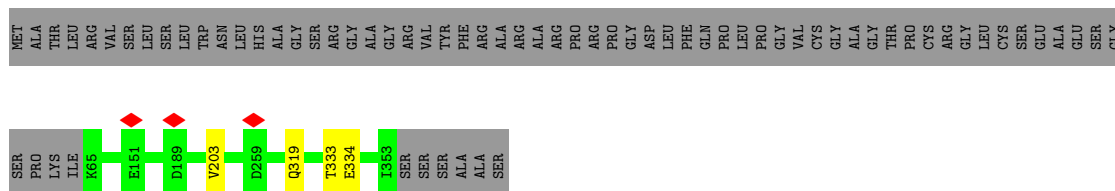


- Molecule 6: 28S ribosomal protein S17, mitochondrial



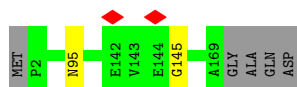
- Molecule 7: 28S ribosomal protein S22, mitochondrial

Chain a:  79% 19%




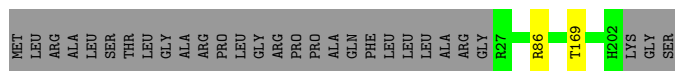
- Molecule 8: 28S ribosomal protein S25, mitochondrial

Chain c:  96%




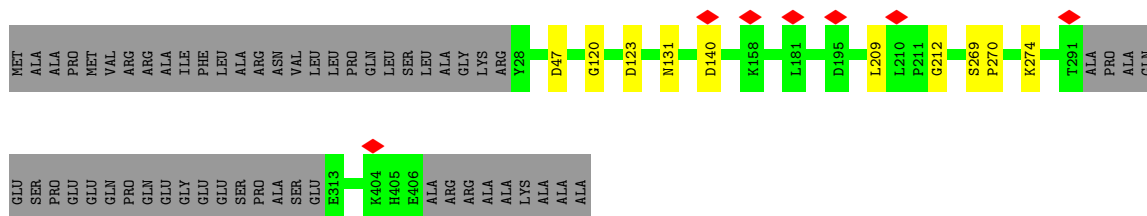
- Molecule 9: 28S ribosomal protein S26, mitochondrial

Chain d:  85% 14%

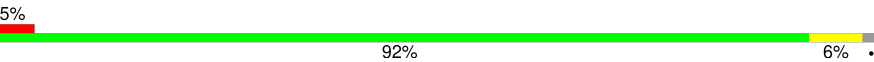


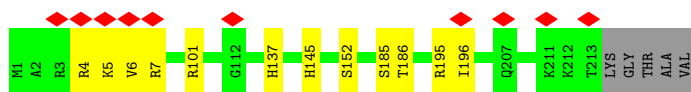
- Molecule 10: 28S ribosomal protein S27, mitochondrial

Chain e:  84% 14%



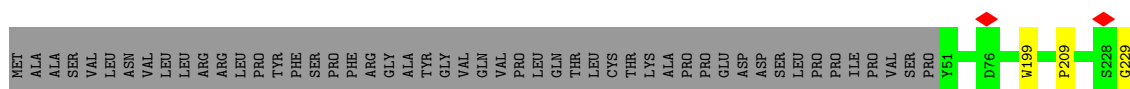
- Molecule 11: 28S ribosomal protein S34, mitochondrial

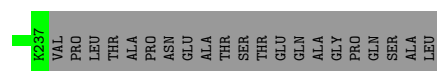
Chain j:  5% 92% 6%



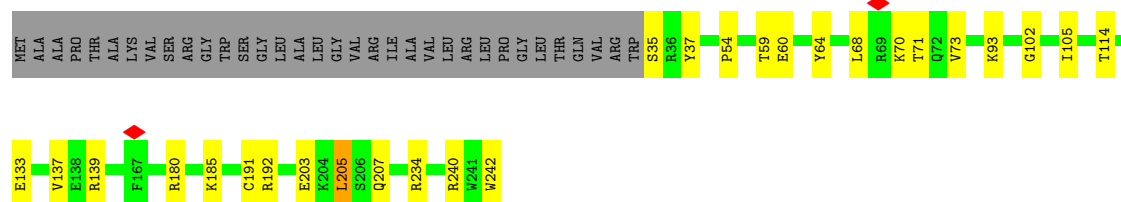
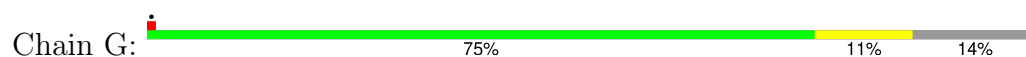
- Molecule 12: 28S ribosomal protein S18b, mitochondrial

Chain p:  71% 28%

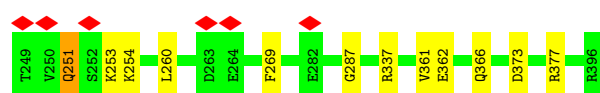
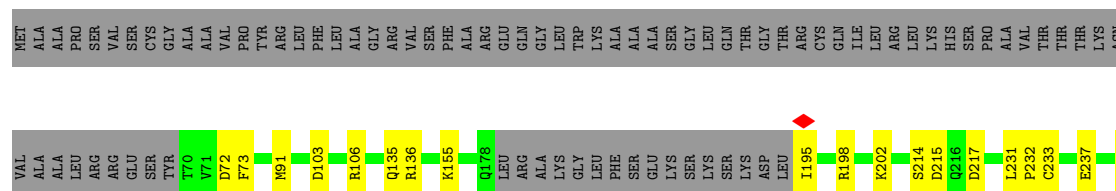




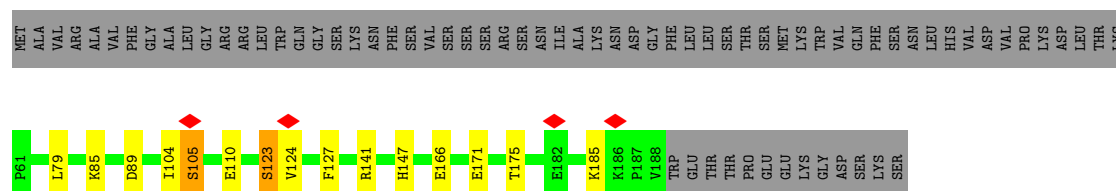
- Molecule 13: 28S ribosomal protein S7, mitochondrial



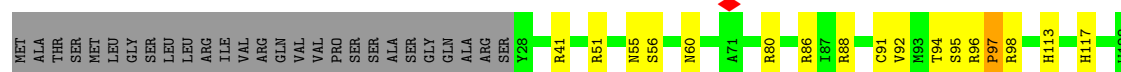
- Molecule 14: 28S ribosomal protein S9, mitochondrial



- Molecule 15: 28S ribosomal protein S10, mitochondrial

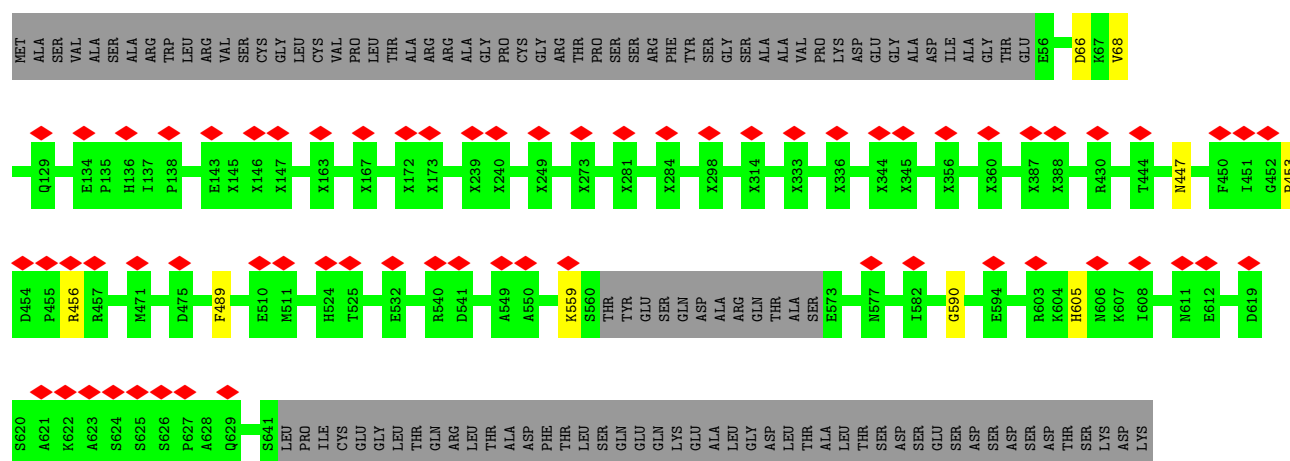


- Molecule 16: 28S ribosomal protein S14, mitochondrial



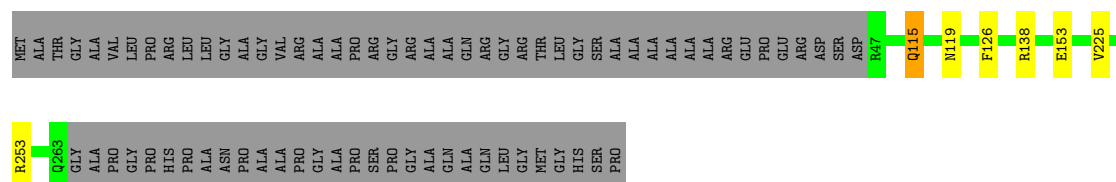
- Molecule 17: DAP3 protein





- Molecule 23: 28S ribosomal protein S2, mitochondrial

Chain B: 72% 26%



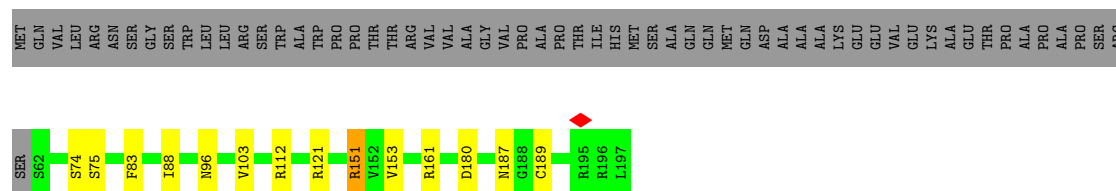
- Molecule 24: 28S ribosomal protein S6, mitochondrial

Chain F: 94% 6%



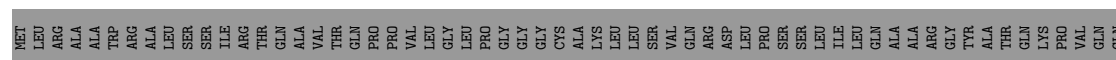
- Molecule 25: 28S ribosomal protein S11, mitochondrial

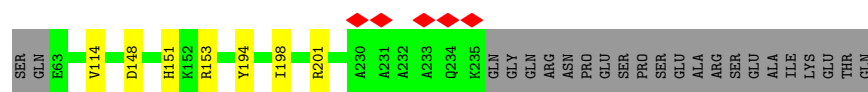
Chain K: 62% 7% 31%



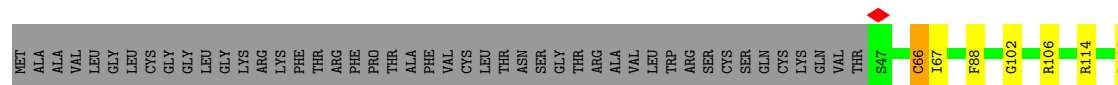
- Molecule 26: 28S ribosomal protein S15, mitochondrial

Chain O: 65% 32%

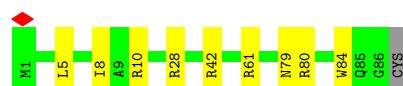
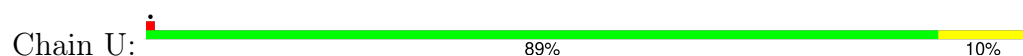




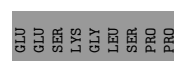
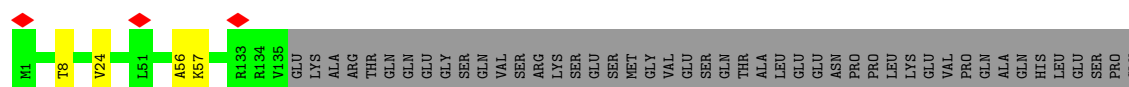
- Molecule 27: 28S ribosomal protein S18c, mitochondrial



- Molecule 28: 28S ribosomal protein S21, mitochondrial



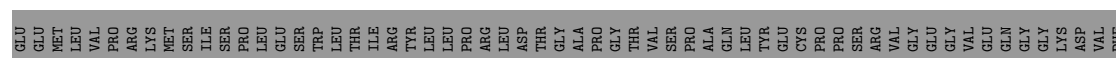
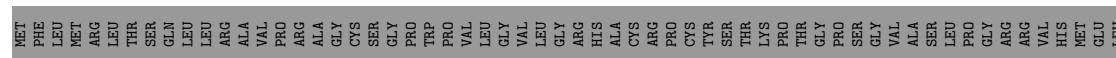
- Molecule 29: 28S ribosomal protein S23, mitochondrial

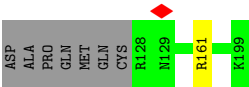


- Molecule 30: 28S ribosomal protein S28, mitochondrial

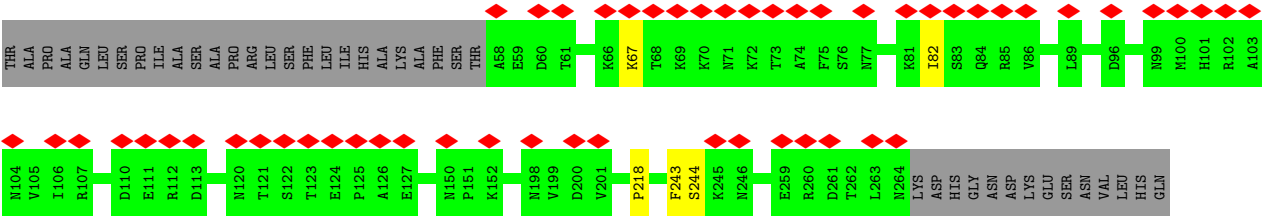
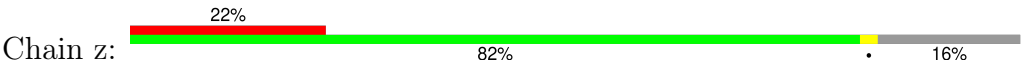


- Molecule 31: Aurora kinase A interacting protein 1





• Molecule 32: Translation initiation factor IF-3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	198355	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.475	Depositor
Minimum map value	-0.896	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.2	Depositor
Map size (\AA)	429.30002, 429.30002, 429.30002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07325, 1.07325, 1.07325	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	A	0.14	0/22681	0.70	2/35318 (0.0%)
2	C	0.23	0/1026	0.37	0/1389
3	E	0.23	0/2511	0.38	0/3369
4	L	0.24	0/872	0.39	0/1171
5	P	0.23	0/937	0.36	0/1262
6	Q	0.23	0/874	0.40	0/1183
7	a	0.23	0/2403	0.36	0/3246
8	c	0.23	0/1406	0.36	0/1894
9	d	0.22	0/1489	0.34	0/2008
10	e	0.23	0/3011	0.35	0/4066
11	j	0.22	0/1841	0.38	0/2493
12	p	0.23	0/1583	0.36	0/2149
13	G	0.25	0/1761	0.38	0/2366
14	I	0.24	0/2597	0.37	0/3487
15	J	0.22	0/1071	0.38	0/1447
16	N	0.22	0/878	0.35	0/1179
17	g	0.24	0/2923	0.38	0/3956
18	h	0.24	0/899	0.31	0/1209
19	i	0.23	0/834	0.34	0/1112
20	k	0.23	0/2275	0.36	0/3075
21	m	0.23	0/961	0.36	0/1284
22	o	0.23	0/2605	0.35	0/3526
23	B	0.24	0/1766	0.37	0/2392
24	F	0.23	0/1009	0.38	0/1362
25	K	0.23	0/1021	0.41	0/1380
26	O	0.23	0/1443	0.33	0/1927
27	R	0.23	0/805	0.37	0/1082
28	U	0.23	0/748	0.35	0/995
29	b	0.24	0/1135	0.35	0/1528
30	f	0.24	0/787	0.40	0/1059
31	n	0.22	0/654	0.34	0/862
32	z	0.22	0/1633	0.38	0/2191
All	All	0.20	0/68439	0.51	2/96967 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	612	C	N3-C2-O2	-5.30	118.19	121.90
1	A	612	C	N1-C2-O2	5.28	122.06	118.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20256	0	10258	140	0
2	C	998	0	1005	3	0
3	E	2464	0	2489	20	0
4	L	853	0	904	5	0
5	P	916	0	944	5	0
6	Q	857	0	920	6	0
7	a	2356	0	2371	0	0
8	c	1374	0	1395	0	0
9	d	1463	0	1438	0	0
10	e	2950	0	2940	0	0
11	j	1792	0	1810	0	0
12	p	1531	0	1495	0	0
13	G	1721	0	1751	18	0
14	I	2541	0	2498	19	0
15	J	1049	0	1088	7	0
16	N	861	0	890	13	0
17	g	2855	0	2894	0	0
18	h	871	0	814	0	0
19	i	818	0	845	0	0
20	k	2227	0	2267	0	0
21	m	945	0	984	0	0
22	o	3273	0	2695	0	0
23	B	1726	0	1747	5	0
24	F	991	0	1034	5	0
25	K	1001	0	1041	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	O	1421	0	1526	4	0
27	R	788	0	823	7	0
28	U	737	0	759	8	0
29	b	1108	0	1124	0	0
30	f	775	0	793	0	0
31	n	642	0	718	0	0
32	z	1616	0	1600	0	0
All	All	65776	0	55860	228	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 228 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:C:O2	1:A:101:G:N2	2.03	0.91
1:A:242:G:HO2'	1:A:257:C:HO2'	1.15	0.87
1:A:580:C:O2'	1:A:581:U:OP1	1.95	0.84
1:A:737:C:O2'	1:A:740:G:N2	2.14	0.80
1:A:755:U:O2'	1:A:798:A:N3	2.14	0.80

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	121/167 (72%)	102 (84%)	15 (12%)	4 (3%)	3	20
3	E	307/430 (71%)	258 (84%)	43 (14%)	6 (2%)	6	29
4	L	107/139 (77%)	97 (91%)	8 (8%)	2 (2%)	6	30
5	P	114/135 (84%)	102 (90%)	12 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Q	107/130 (82%)	92 (86%)	14 (13%)	1 (1%)	14	44
7	a	287/359 (80%)	258 (90%)	25 (9%)	4 (1%)	9	35
8	c	166/173 (96%)	149 (90%)	16 (10%)	1 (1%)	22	53
9	d	174/205 (85%)	169 (97%)	4 (2%)	1 (1%)	22	53
10	e	354/415 (85%)	317 (90%)	30 (8%)	7 (2%)	6	29
11	j	211/218 (97%)	160 (76%)	41 (19%)	10 (5%)	2	13
12	p	185/258 (72%)	161 (87%)	21 (11%)	3 (2%)	8	33
13	G	206/242 (85%)	190 (92%)	15 (7%)	1 (0%)	25	57
14	I	307/396 (78%)	280 (91%)	25 (8%)	2 (1%)	19	50
15	J	126/201 (63%)	108 (86%)	13 (10%)	5 (4%)	2	16
16	N	99/128 (77%)	92 (93%)	6 (6%)	1 (1%)	13	42
17	g	349/351 (99%)	313 (90%)	33 (10%)	3 (1%)	14	44
18	h	101/386 (26%)	87 (86%)	13 (13%)	1 (1%)	13	42
19	i	96/106 (91%)	84 (88%)	10 (10%)	2 (2%)	5	28
20	k	273/325 (84%)	237 (87%)	31 (11%)	5 (2%)	7	31
21	m	116/118 (98%)	95 (82%)	16 (14%)	5 (4%)	2	15
22	o	306/575 (53%)	265 (87%)	32 (10%)	9 (3%)	3	23
23	B	215/293 (73%)	189 (88%)	25 (12%)	1 (0%)	25	57
24	F	122/124 (98%)	114 (93%)	7 (6%)	1 (1%)	16	47
25	K	134/197 (68%)	112 (84%)	22 (16%)	0	100	100
26	O	171/256 (67%)	156 (91%)	13 (8%)	2 (1%)	11	39
27	R	95/143 (66%)	82 (86%)	12 (13%)	1 (1%)	12	41
28	U	84/87 (97%)	78 (93%)	6 (7%)	0	100	100
29	b	133/190 (70%)	116 (87%)	13 (10%)	4 (3%)	3	22
30	f	96/189 (51%)	89 (93%)	7 (7%)	0	100	100
31	n	70/199 (35%)	65 (93%)	5 (7%)	0	100	100
32	z	205/247 (83%)	174 (85%)	26 (13%)	5 (2%)	5	26
All	All	5437/7382 (74%)	4791 (88%)	559 (10%)	87 (2%)	10	33

5 of 87 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	145	ASN

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Mol	Chain	Res	Type
11	j	6	VAL
11	j	145	HIS
20	k	98	PRO
32	z	218	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	106/142 (75%)	106 (100%)	0	100	100
3	E	258/346 (75%)	254 (98%)	4 (2%)	58	76
4	L	94/118 (80%)	94 (100%)	0	100	100
5	P	95/113 (84%)	95 (100%)	0	100	100
6	Q	95/115 (83%)	95 (100%)	0	100	100
7	a	255/307 (83%)	255 (100%)	0	100	100
8	c	152/155 (98%)	151 (99%)	1 (1%)	81	88
9	d	147/168 (88%)	146 (99%)	1 (1%)	81	88
10	e	321/362 (89%)	318 (99%)	3 (1%)	75	85
11	j	190/193 (98%)	188 (99%)	2 (1%)	70	82
12	p	166/226 (74%)	166 (100%)	0	100	100
13	G	183/208 (88%)	177 (97%)	6 (3%)	33	60
14	I	267/333 (80%)	264 (99%)	3 (1%)	70	82
15	J	118/182 (65%)	118 (100%)	0	100	100
16	N	91/113 (80%)	90 (99%)	1 (1%)	70	82
17	g	312/312 (100%)	309 (99%)	3 (1%)	73	84
18	h	94/341 (28%)	94 (100%)	0	100	100
19	i	88/94 (94%)	88 (100%)	0	100	100
20	k	252/292 (86%)	252 (100%)	0	100	100
21	m	102/102 (100%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	o	277/369 (75%)	277 (100%)	0	100	100
23	B	186/230 (81%)	185 (100%)	1 (0%)	86	91
24	F	109/109 (100%)	109 (100%)	0	100	100
25	K	102/151 (68%)	101 (99%)	1 (1%)	73	84
26	O	159/226 (70%)	159 (100%)	0	100	100
27	R	89/126 (71%)	89 (100%)	0	100	100
28	U	77/78 (99%)	76 (99%)	1 (1%)	65	79
29	b	115/163 (71%)	115 (100%)	0	100	100
30	f	85/160 (53%)	85 (100%)	0	100	100
31	n	66/173 (38%)	65 (98%)	1 (2%)	60	77
32	z	168/219 (77%)	168 (100%)	0	100	100
All	All	4819/6226 (77%)	4791 (99%)	28 (1%)	82	90

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	G	191	CYS
31	n	161	ARG
14	I	91	MET
23	B	115	GLN
13	G	234	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
29	b	36	ASN
31	n	178	GLN
14	I	318	HIS
17	g	163	ASN
23	B	115	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	951/955 (99%)	212 (22%)	8 (0%)

5 of 212 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	G
1	A	10	G
1	A	13	C
1	A	15	C
1	A	16	A

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	862	U
1	A	580	C
1	A	363	U
1	A	225	U
1	A	389	G

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	o	13

The worst 5 of 13 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	o	383:TYR	C	386:UNK	N	27.56
1	o	143:GLU	C	145:UNK	N	20.71
1	o	399:UNK	C	417:MET	N	20.68
1	o	173:UNK	C	220:UNK	N	13.81
1	o	300:UNK	C	311:UNK	N	13.34

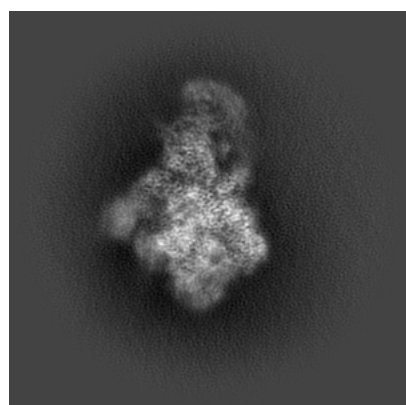
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9358. These allow visual inspection of the internal detail of the map and identification of artifacts.

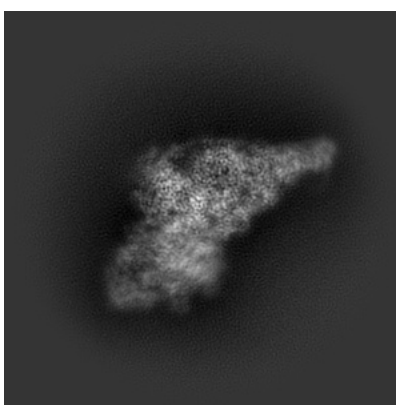
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

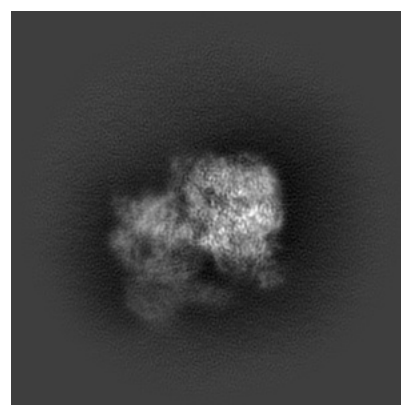
6.1.1 Primary map



X



Y

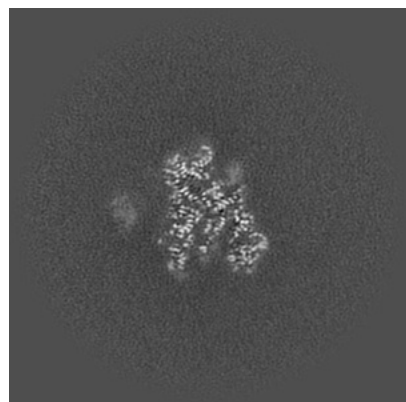


Z

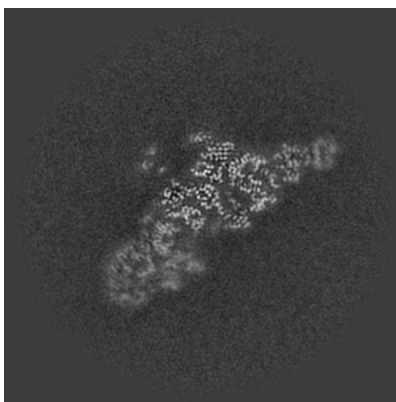
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

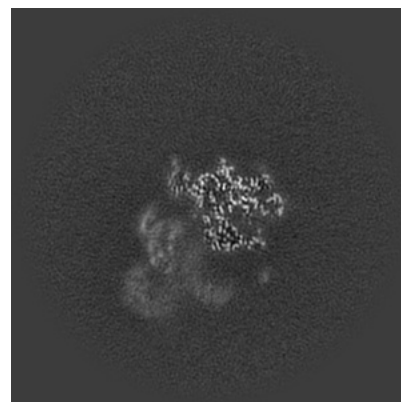
6.2.1 Primary map



X Index: 200



Y Index: 200

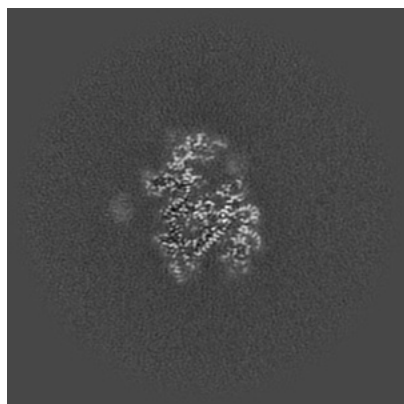


Z Index: 200

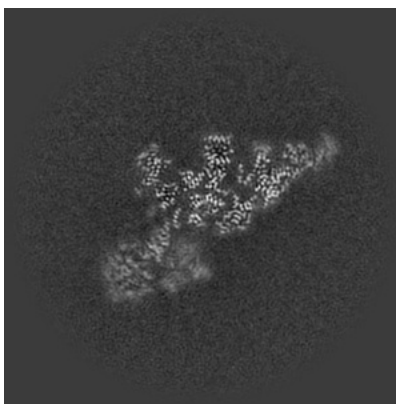
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

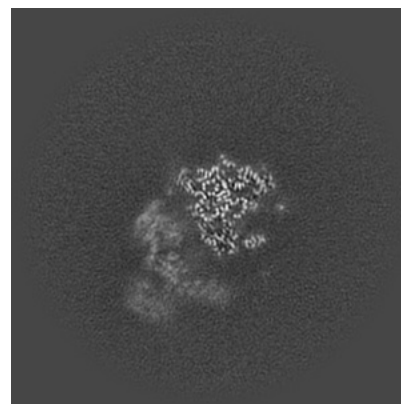
6.3.1 Primary map



X Index: 212



Y Index: 192

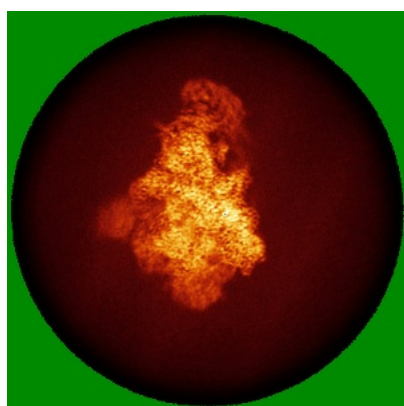


Z Index: 193

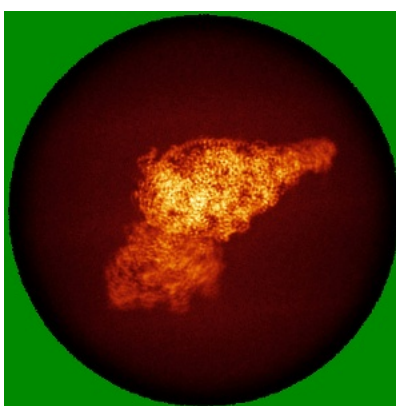
The images above show the largest variance slices of the map in three orthogonal directions.

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

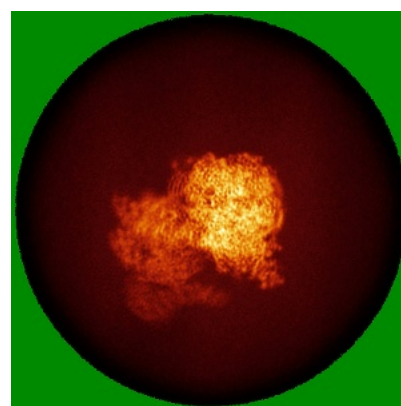
6.4.1 Primary map



X



Y

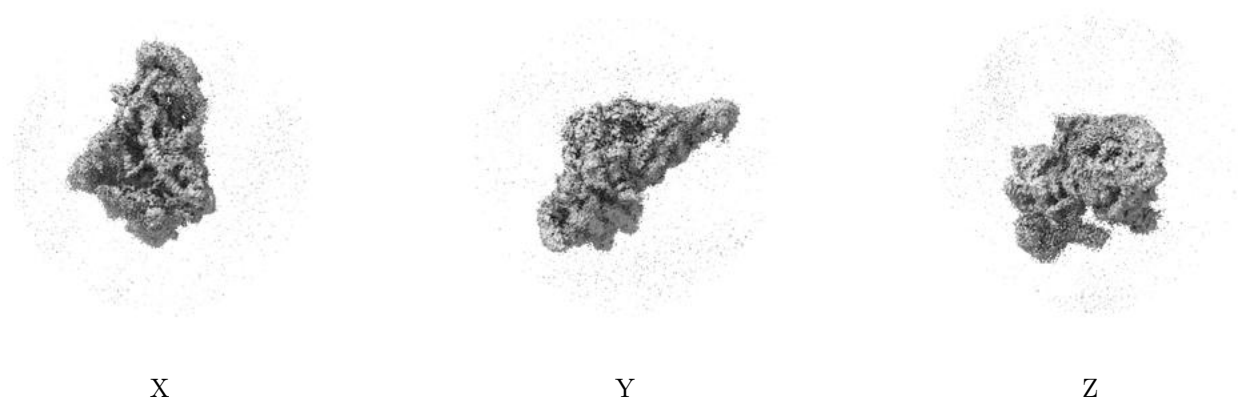


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

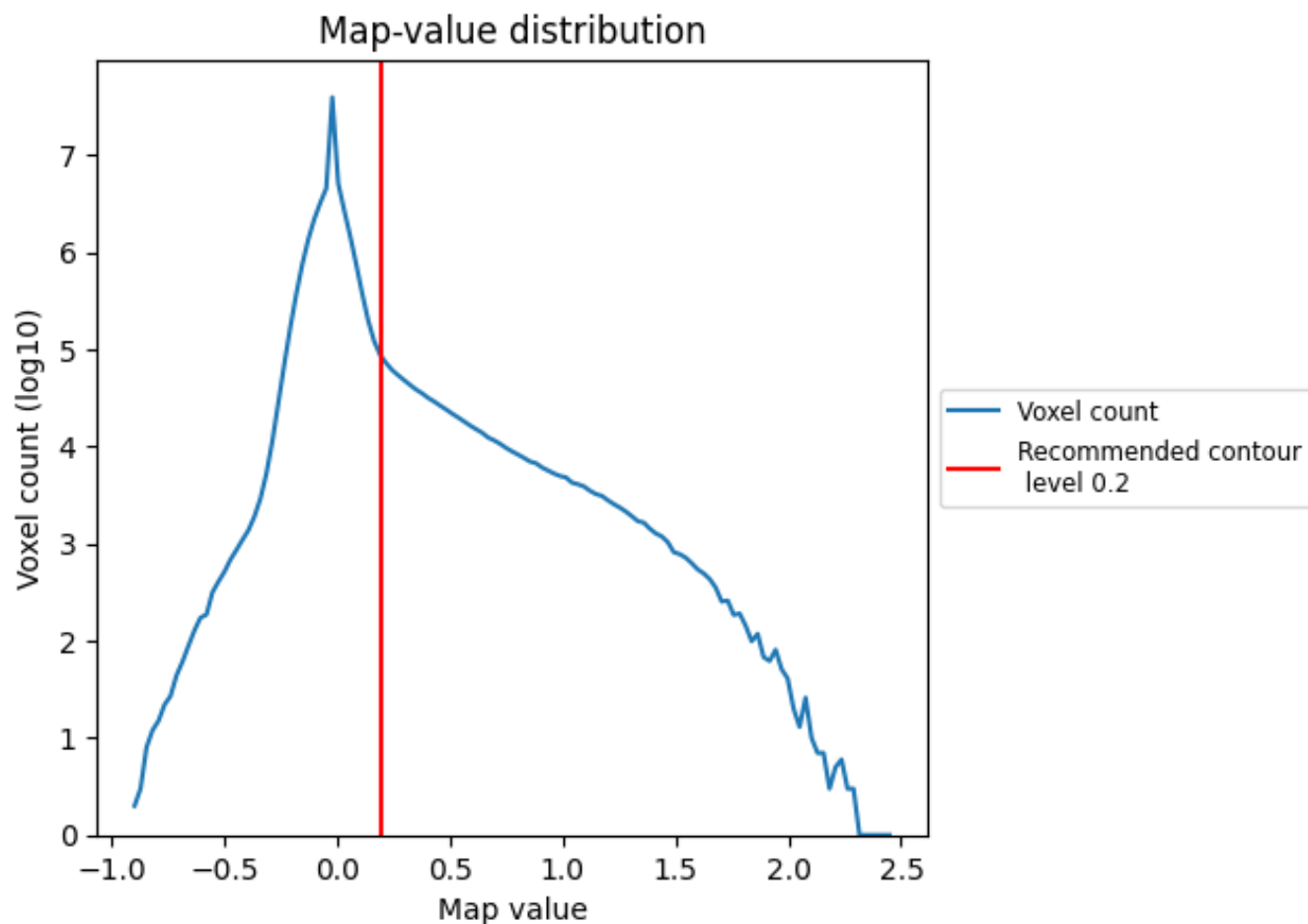
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

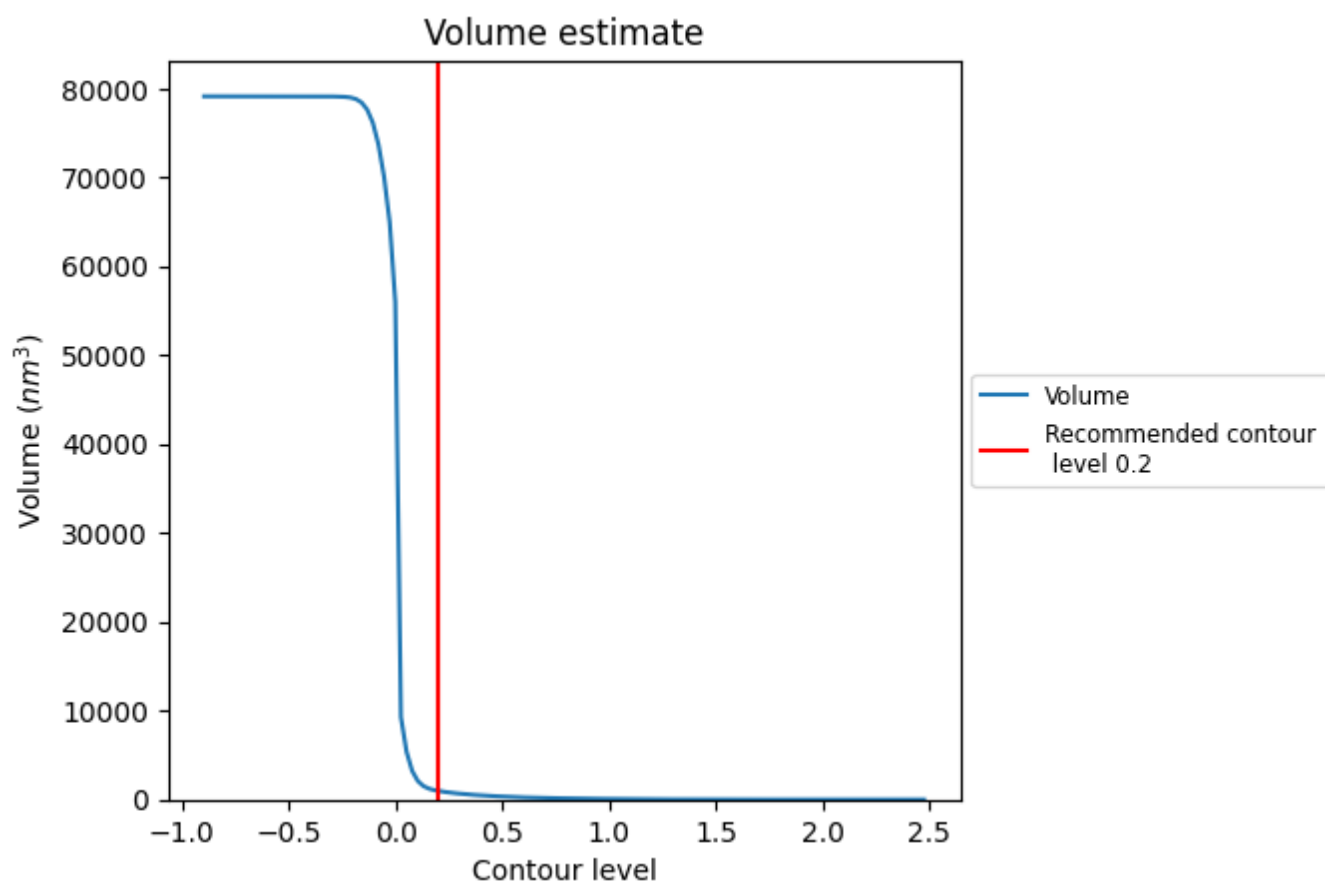
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

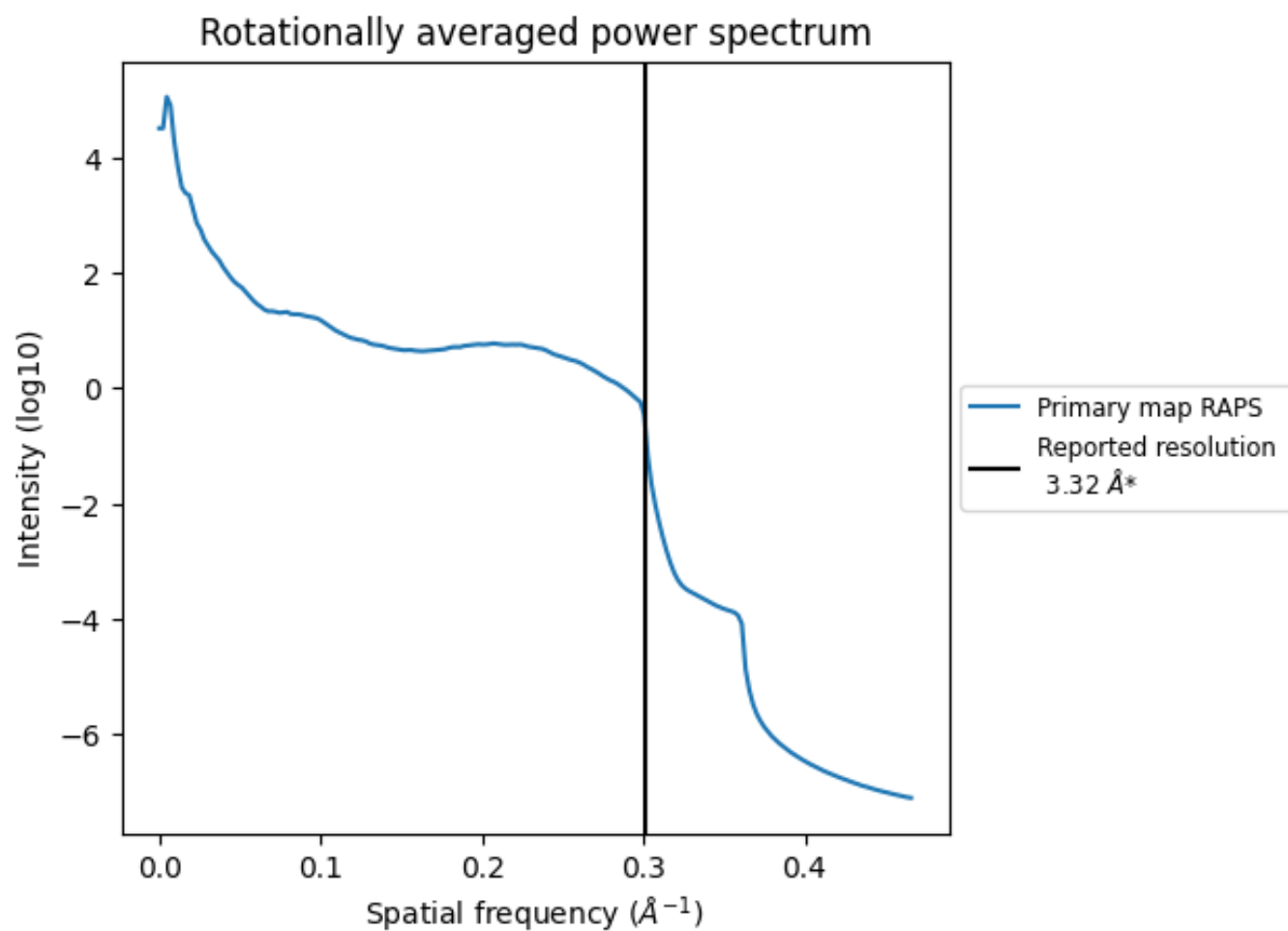
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 980 nm³; this corresponds to an approximate mass of 886 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.301 Å⁻¹

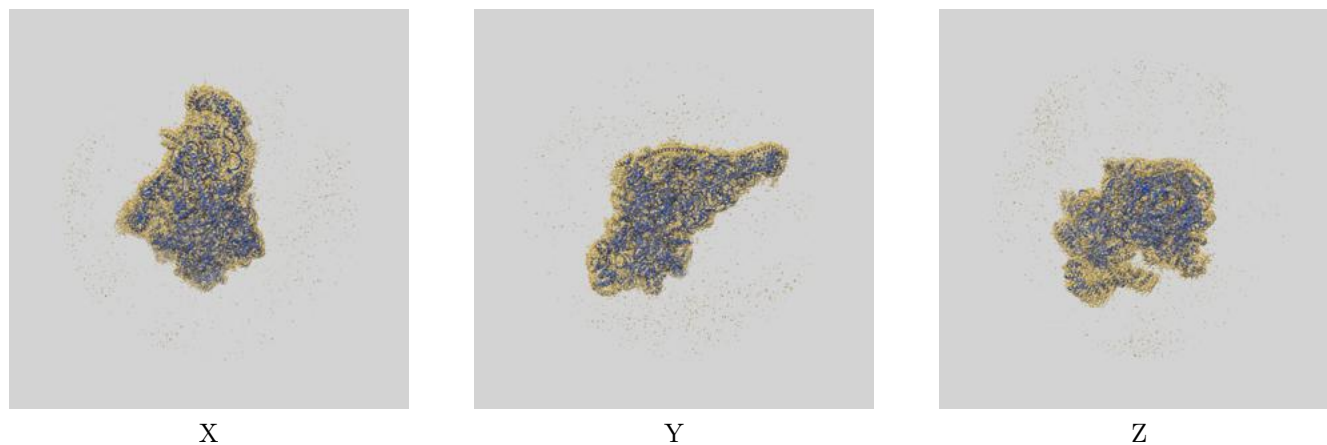
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

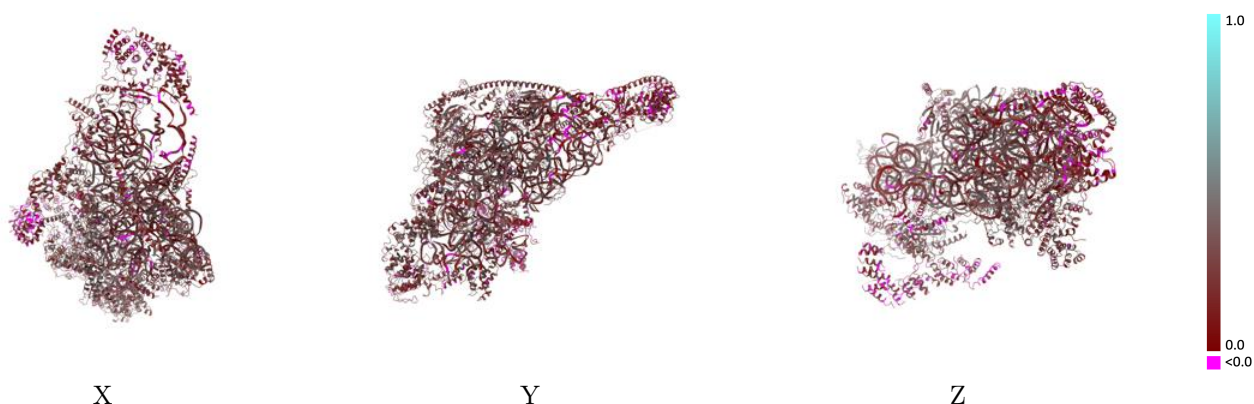
This section contains information regarding the fit between EMDB map EMD-9358 and PDB model 6NEQ. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



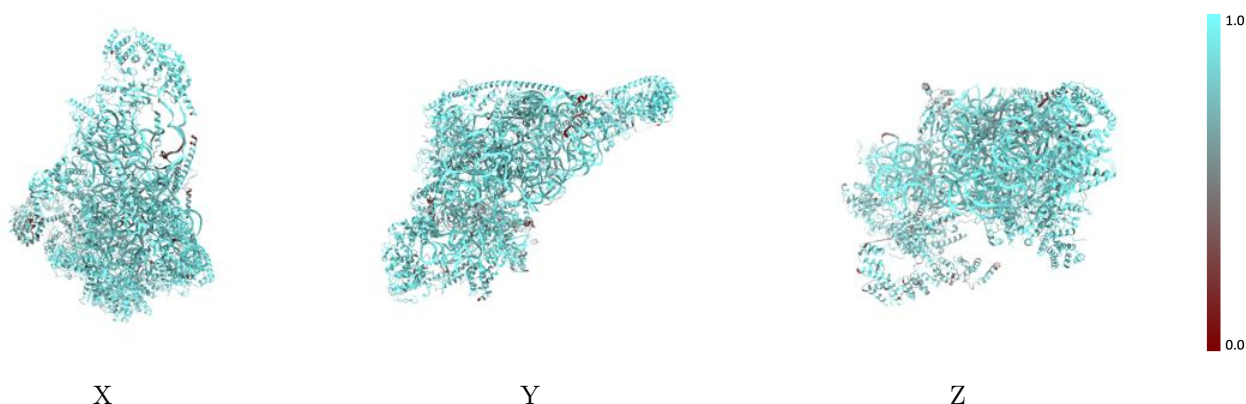
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



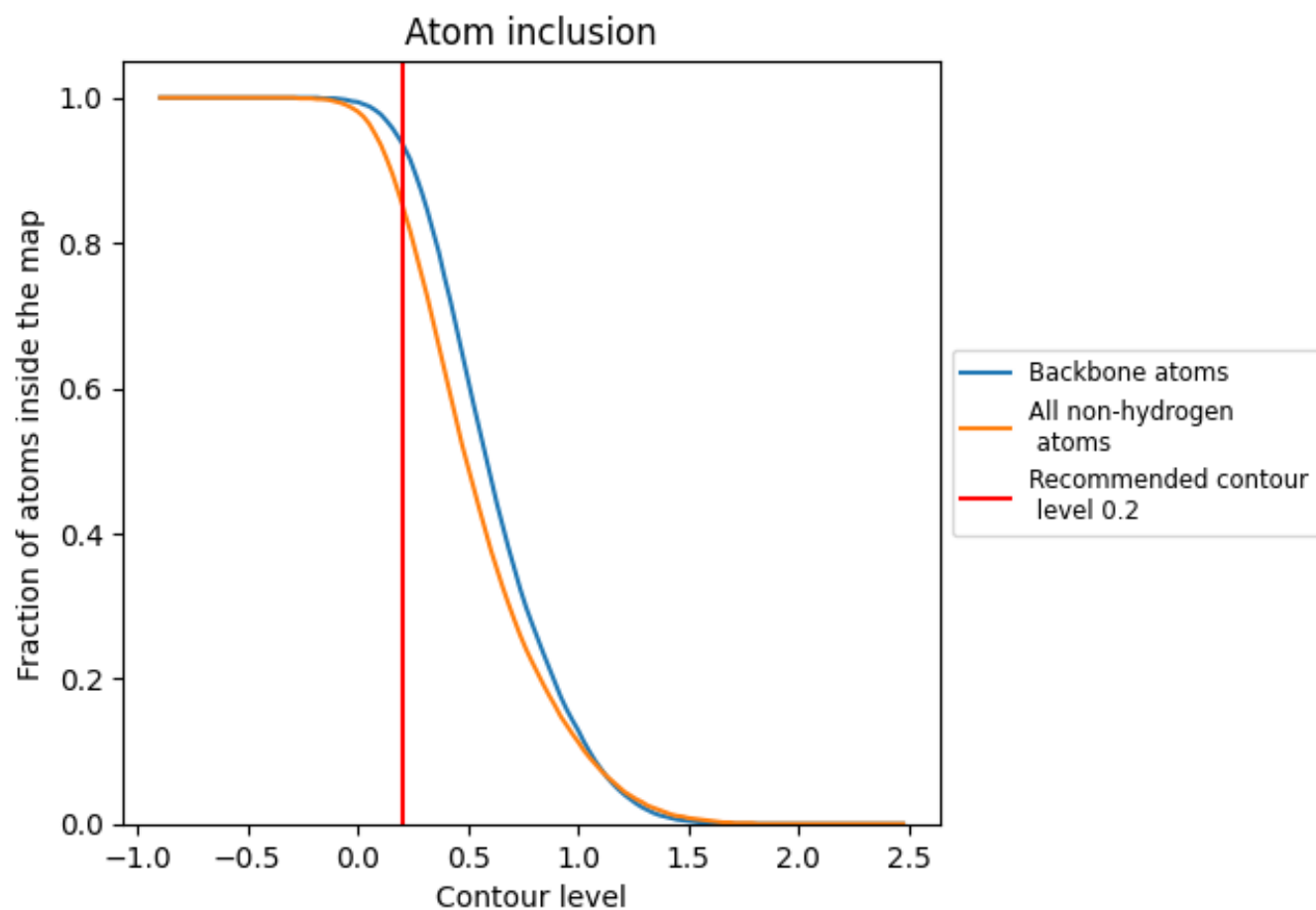
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 86% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8550	 0.2470
A	 0.9150	 0.2470
B	 0.8690	 0.3240
C	 0.8230	 0.2750
E	 0.8210	 0.2840
F	 0.8540	 0.2960
G	 0.8820	 0.2620
I	 0.8590	 0.3220
J	 0.8400	 0.3030
K	 0.8610	 0.2990
L	 0.8470	 0.3080
N	 0.8770	 0.2800
O	 0.8170	 0.2680
P	 0.8380	 0.2560
Q	 0.8210	 0.2880
R	 0.8510	 0.3140
U	 0.8420	 0.2880
a	 0.8350	 0.2550
b	 0.8440	 0.2830
c	 0.8200	 0.2670
d	 0.8590	 0.2530
e	 0.8840	 0.1440
f	 0.8380	 0.3020
g	 0.8980	 0.2730
h	 0.8250	 0.2660
i	 0.7800	 0.1170
j	 0.8180	 0.1760
k	 0.7780	 0.2000
m	 0.7630	 0.2380
n	 0.8220	 0.2480
o	 0.7290	 0.1080
p	 0.8690	 0.2920
z	 0.6200	 0.2160

