Full wwPDB EM Validation Report (i)

Jul 3, 2024 – 07:44 am BST

PDB ID	:	7OF7
EMDB ID	:	EMD-12872
Title	:	Structure of a human mitochondrial ribosome large subunit assembly intermediate in complex with MTERF4-NSUN4 and GTPBP5 (dataset1).
Authors	:	Hillen, H.S.; Lavdovskaia, E.; Nadler, F.; Hanitsch, E.; Linden, A.; Bohnsack, K.E.; Urlaub, H.; Richter-Dennerlein, R.
Deposited on	:	2021-05-04
Resolution	:	2.50 Å(reported)
Based on initial model	:	5OOL

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 (i) 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 (i)) were used in the production of this report:

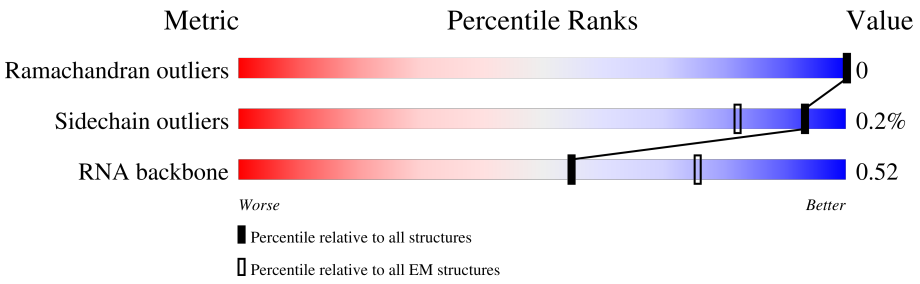
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.50 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 <=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	108	100%
2	1	65	80% 20%
3	2	92	49% 51%
4	3	188	51% 49%
5	4	103	36% 64%
6	5	423	92% 7%
7	6	380	85% 15%
8	7	338	85% 15%

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Mol	Chain	Length	Quality of chain
9	8	206	25% 37% 63%
10	9	137	85% 15%
11	A	1559	68% 20% 12%
12	B	69	58% 23% 19%
13	C	384	88% 12%
14	D	305	78% 21%
15	E	348	89% 11%
16	F	311	80% 20%
17	G	381	62% 38%
18	H	267	36% 64%
19	I	261	61% 39%
20	J	192	20% 73% 27%
21	K	178	99%
22	L	145	79% 21%
23	M	296	96%
24	N	251	81% 18%
25	O	175	87% 13%
26	P	180	78% 22%
27	Q	292	74% 26%
28	R	149	78% 22%
29	S	205	76% 24%
30	T	206	81% 19%
31	U	153	9% 91% 9%
32	V	216	22% 78%
33	W	148	74% 26%

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Mol	Chain	Length	Quality of chain
34	X	256	95% 5%
35	Y	250	70% 30%
36	Z	161	71% 29%
37	a	142	50% 50%
38	b	215	69% 31%
39	c	332	83% 17%
40	d	306	13% 65% 35%
41	e	279	59% 71% 29%
42	f	212	26% 51% 49%
43	g	166	78% 22%
44	h	158	66% 34%
45	i	128	76% 24%
46	j	85	100%
47	k	112	71% 29%
48	m	128	17% 22% 78%
49	o	102	90% 9%
50	p	206	62% 38%
51	q	222	58% 42%
52	r	196	74% 26%
53	s	439	84% 16%
54	u	234	47% 53%
55	v	70	97%
56	w	156	6% 50% 49%
57	x	406	36% 64%

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 101032 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 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	108	880	545	172	157	6	0	0

- Molecule 2 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	52	433	278	83	70	2	0	0

- Molecule 3 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	45	367	227	81	58	1	0	0

- Molecule 4 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	95	831	539	162	127	3	0	0

- Molecule 5 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	37	333	212	71	47	3	0	0

- Molecule 6 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	392	3199	2067	558	563	11	0	0

- Molecule 7 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	324	2723	1743	488	484	8	0	0

- Molecule 8 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	7	287	2334	1495	397	425	17	0	0

- Molecule 9 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	8	77	651	413	113	123	2	0	0

- Molecule 10 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	9	117	947	614	163	168	2	0	0

- Molecule 11 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	A	1376	29222	13113	5273	9460	1376	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3107	U	N	conflict	GB 1025814679

- Molecule 12 is a RNA chain called mitochondrial tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
12	B	56	1191	534	214	387	56	0	0

- Molecule 13 is a protein called 5-methylcytosine rRNA methyltransferase NSUN4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	C	338	2690	1715	470	489	16	1	0

- Molecule 14 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	D	240	1872	1165	378	320	9	0	0

- Molecule 15 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	E	308	2427	1559	423	434	11	0	0

- Molecule 16 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	F	250	2013	1294	365	348	6	0	0

- Molecule 17 is a protein called Transcription termination factor 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	G	238	1943	1243	336	352	12	0	0

- Molecule 18 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	H	95	784	498	152	134	0	0

- Molecule 19 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	I	158	1283	828	235	210	10	0	0

- Molecule 20 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	J	140	1061	680	192	187	2	0	0

- Molecule 21 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	K	177	1451	934	259	251	7	0	0

- Molecule 22 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	L	115	889	559	171	154	5	0	0

- Molecule 23 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	M	287	2305	1472	425	402	6	0	0

- Molecule 24 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	N	205	1654	1056	308	280	10	0	0

- Molecule 25 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	O	152	1245	784	239	215	7	0	0

- Molecule 26 is a protein called 39S ribosomal protein L18, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	P	141	1148	719	221	203	5	0	0

- Molecule 27 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Q	217	1805	1159	317	320	9	0	0

- Molecule 28 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	R	116	971	616	200	151	4	0	0

- Molecule 29 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	S	156	1251	806	222	219	4	0	0

- Molecule 30 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	T	166	1368	875	254	232	7	0	0

- Molecule 31 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	U	139	1154	734	220	197	3	0	0

- Molecule 32 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	V	47	395	255	62	75	3	0	0

- Molecule 33 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	W	109	859	552	162	142	3	0	0

- Molecule 34 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	X	243	2035	1317	351	362	5	0	0

- Molecule 35 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	Y	176	1517	970	291	252	4	0	0

- Molecule 36 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	Z	115	937	598	175	161	3	0	0

- Molecule 37 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	a	71	597	378	112	103	4	0	0

- Molecule 38 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	b	148	1178	733	229	213	3	0	0

- Molecule 39 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	c	275	2217	1415	383	410	9	0	0

- Molecule 40 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	d	199	1653	1075	276	293	9	0	0

- Molecule 41 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	e	197	1599	1027	277	290	5	0	0

- Molecule 42 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	f	108	857	549	140	165	3	0	0

- Molecule 43 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	g	129	1067	690	185	190	2	0	0

- Molecule 44 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	h	105	862	548	151	160	3	0	0

- Molecule 45 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	i	97	827	532	165	126	4	0	0

- Molecule 46 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	j	85	684	423	133	126	2	0	0

- Molecule 47 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	k	80	627	392	116	114	5	0	0

- Molecule 48 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	m	28	234	151	44	37	2	0	0

- Molecule 49 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	o	93	786	495	161	127	3	0	0

- Molecule 50 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	p	127	1058	661	201	192	4	0	0

- Molecule 51 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	q	128	1076	671	208	192	5	0	0

- Molecule 52 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	r	146	1203	764	232	199	8	0	0

- Molecule 53 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	s	370	3036	1946	542	534	14	0	0

- Molecule 54 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	u	111	927	595	155	167	10	0	0

- Molecule 55 is a protein called MIEF1 upstream open reading frame protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
55	v	69	588	372	116	100	0	0

- Molecule 56 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	w	79	638	410	95	128	5	0	0

- Molecule 57 is a protein called Mitochondrial ribosome-associated GTPase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	x	148	1073	659	205	204	5	0	0

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
58	0	1	1	1	0
58	4	1	1	1	0
58	r	1	1	1	0

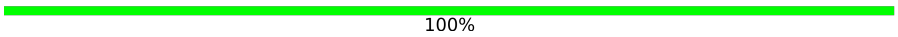
- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
59	A	71	71	71	0
59	E	1	1	1	0
59	W	1	1	1	0
59	g	1	1	1	0

3 Residue-property plots (i)

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

• Molecule 1: 39S ribosomal protein L32, mitochondrial

Chain 0: 

There are no outlier residues recorded for this chain.

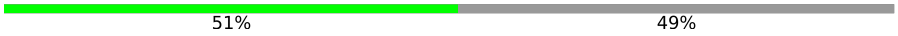
• Molecule 2: 39S ribosomal protein L33, mitochondrial

Chain 1:

• Molecule 3: 39S ribosomal protein L34, mitochondrial

Chain 2:

• Molecule 4: 39S ribosomal protein L35, mitochondrial

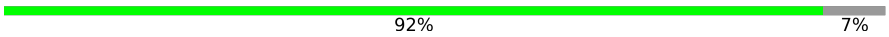
Chain 3: 

• Molecule 5: 39S ribosomal protein L36, mitochondrial

Chain 4:

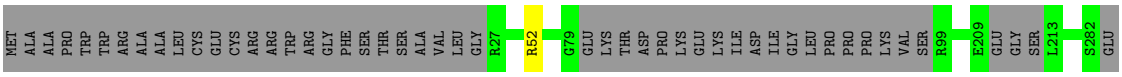
• Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5:



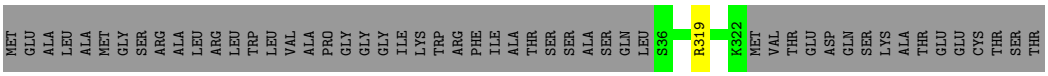
• Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6:



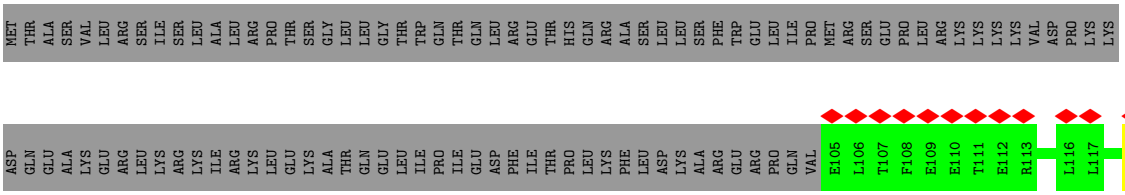
• Molecule 8: 39S ribosomal protein L39, mitochondrial

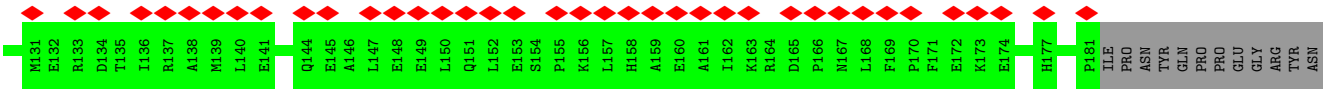
Chain 7:



• Molecule 9: 39S ribosomal protein L40, mitochondrial

Chain 8:



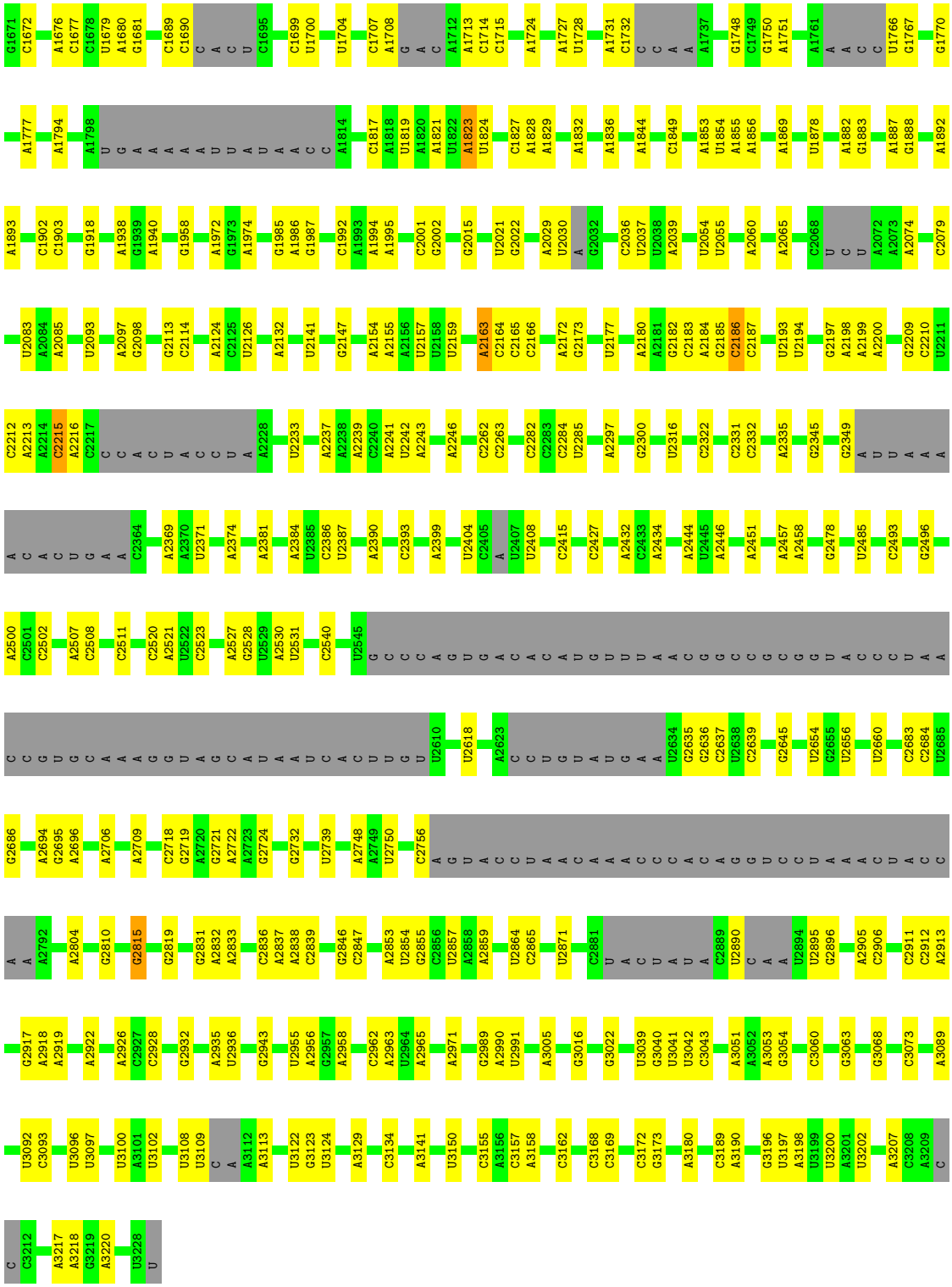


• Molecule 10: 39S ribosomal protein L41, mitochondrial

Chain 9:

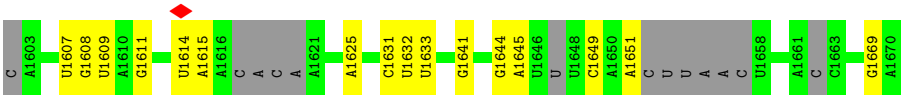
• Molecule 11: 16S ribosomal RNA

Chain A: 68% 20% 12%



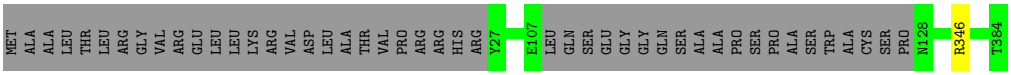
• Molecule 12: mitochondrial tRNAVal

Chain B: 58% 23% 19%



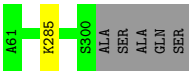
- Molecule 13: 5-methylcytosine rRNA methyltransferase NSUN4

Chain C:



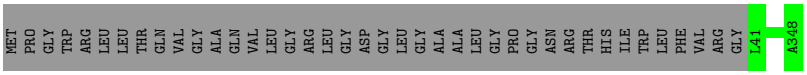
- Molecule 14: 39S ribosomal protein L2, mitochondrial

Chain D:



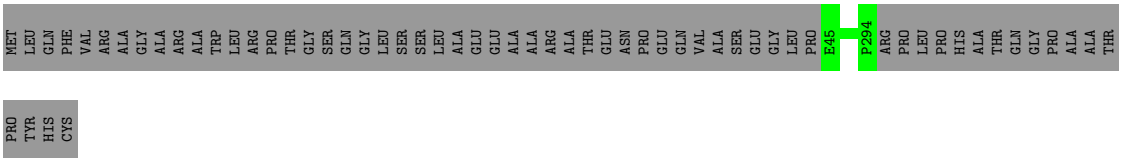
- Molecule 15: 39S ribosomal protein L3, mitochondrial

Chain E:



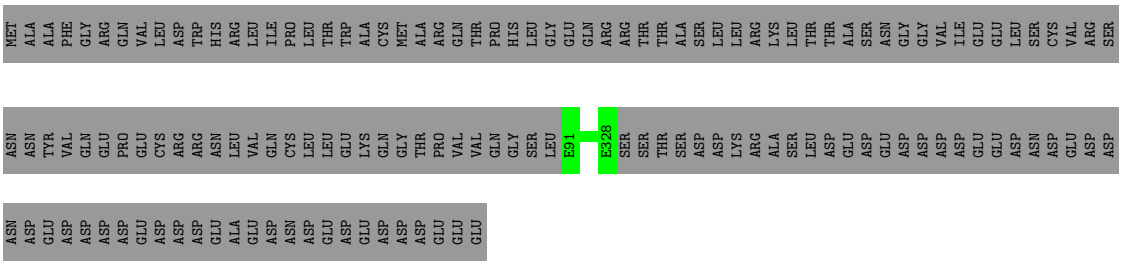
- Molecule 16: 39S ribosomal protein L4, mitochondrial

Chain F:



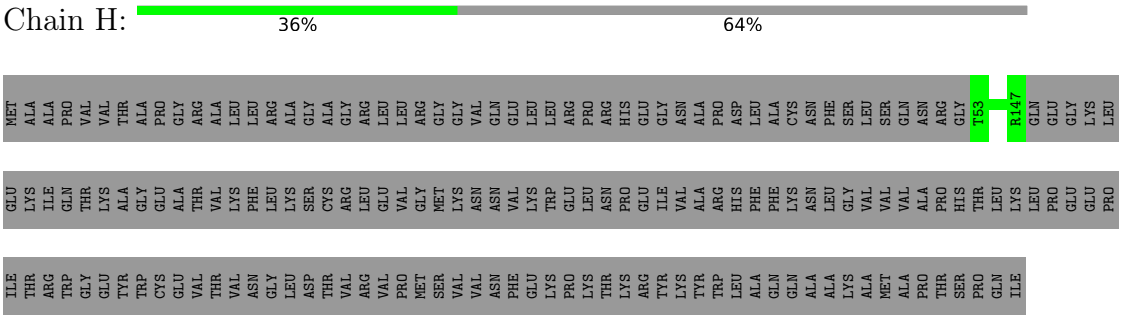
- Molecule 17: Transcription termination factor 4, mitochondrial

Chain G:



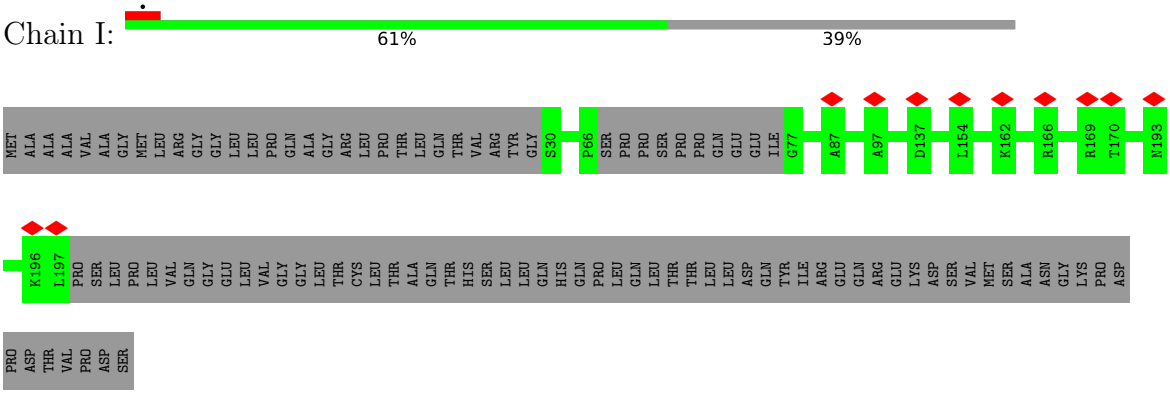
- Molecule 18: 39S ribosomal protein L9, mitochondrial

Chain H:



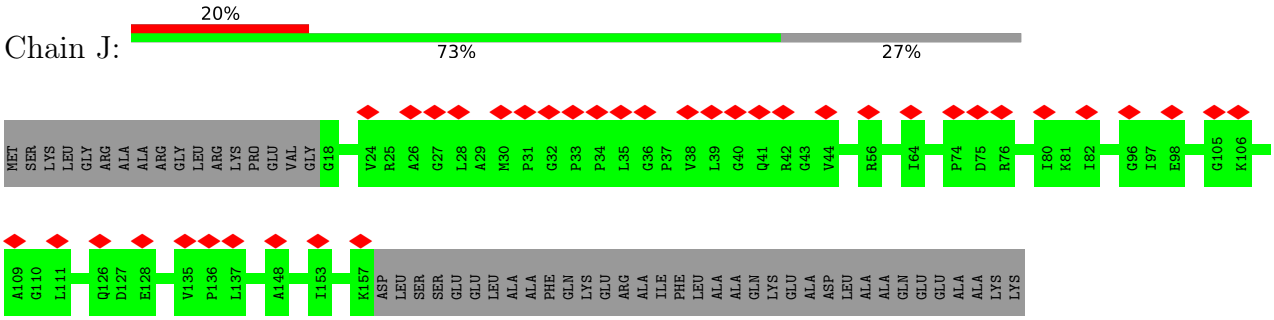
- Molecule 19: 39S ribosomal protein L10, mitochondrial

Chain I:



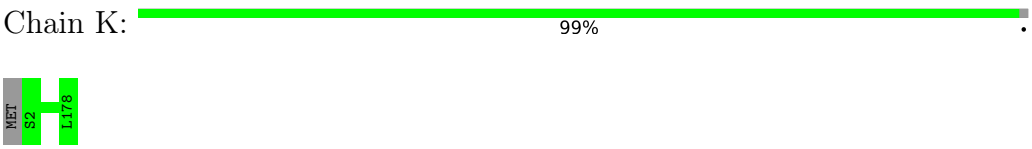
- Molecule 20: 39S ribosomal protein L11, mitochondrial

Chain J:



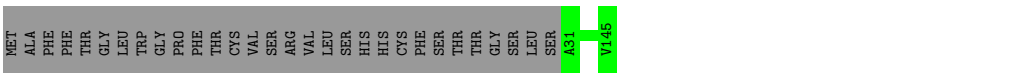
- Molecule 21: 39S ribosomal protein L13, mitochondrial

Chain K:



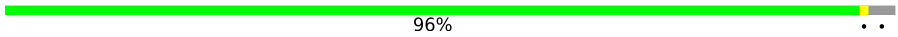
- Molecule 22: 39S ribosomal protein L14, mitochondrial

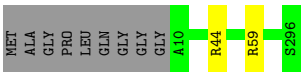
Chain L:



- Molecule 23: 39S ribosomal protein L15, mitochondrial

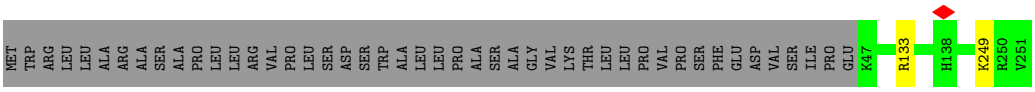
Chain M:





• Molecule 24: 39S ribosomal protein L16, mitochondrial

Chain N:



• Molecule 25: 39S ribosomal protein L17, mitochondrial

Chain O:

• Molecule 26: 39S ribosomal protein L18, mitochondrial

Chain P:

• Molecule 27: 39S ribosomal protein L19, mitochondrial

Chain Q:

• Molecule 28: 39S ribosomal protein L20, mitochondrial

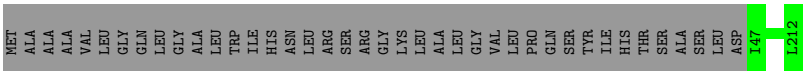
Chain R:

• Molecule 29: 39S ribosomal protein L21, mitochondrial

Chain S:

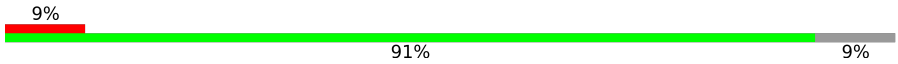
- Molecule 30: 39S ribosomal protein L22, mitochondrial

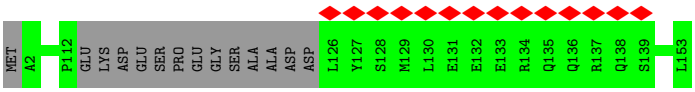
Chain T:



- Molecule 31: 39S ribosomal protein L23, mitochondrial

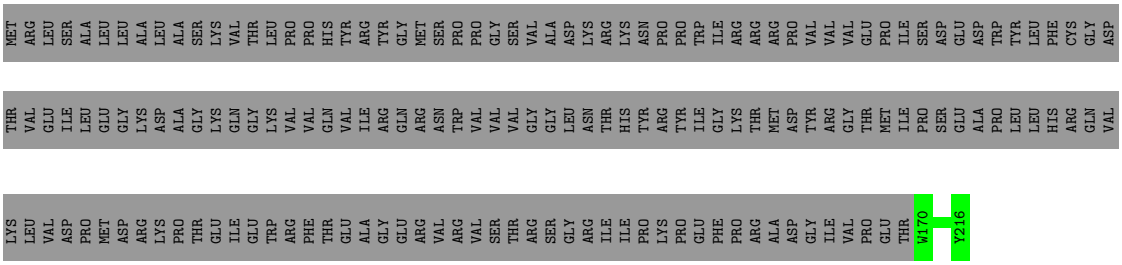
Chain U:





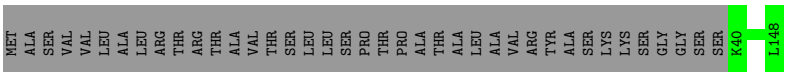
- Molecule 32: 39S ribosomal protein L24, mitochondrial

Chain V:



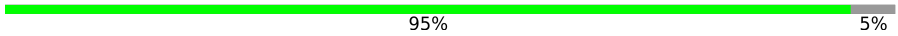
- Molecule 33: 39S ribosomal protein L27, mitochondrial

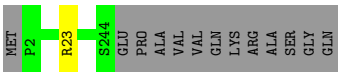
Chain W:



- Molecule 34: 39S ribosomal protein L28, mitochondrial

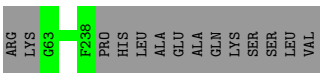
Chain X:





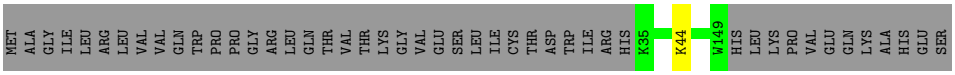
- Molecule 35: 39S ribosomal protein L47, mitochondrial

Chain Y:



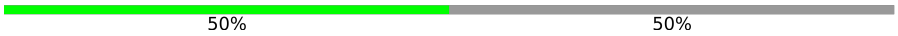
• Molecule 36: 39S ribosomal protein L30, mitochondrial

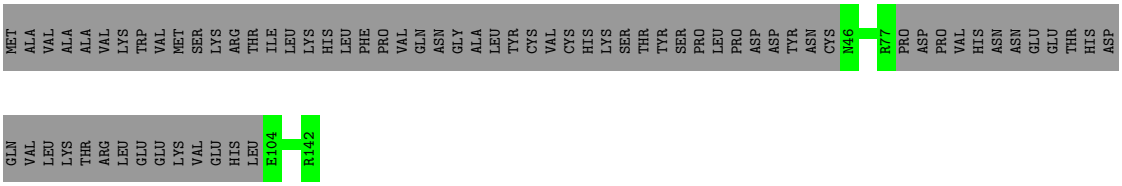
Chain Z:



• Molecule 37: 39S ribosomal protein L42, mitochondrial

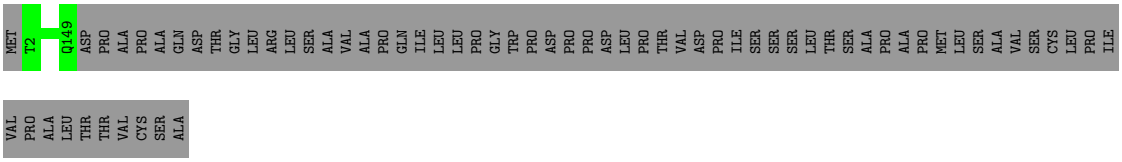
Chain a:





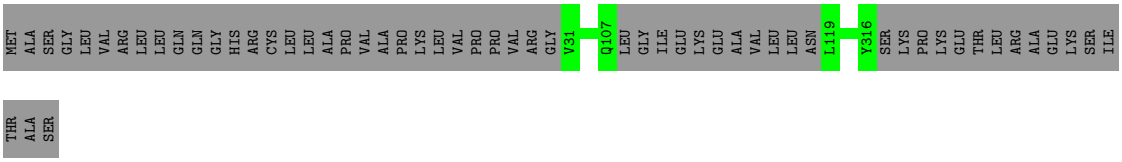
• Molecule 38: 39S ribosomal protein L43, mitochondrial

Chain b:



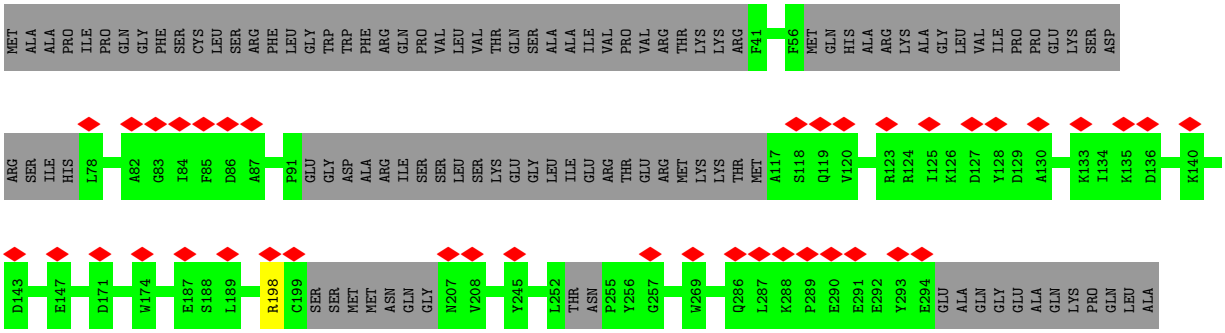
• Molecule 39: 39S ribosomal protein L44, mitochondrial

Chain c:



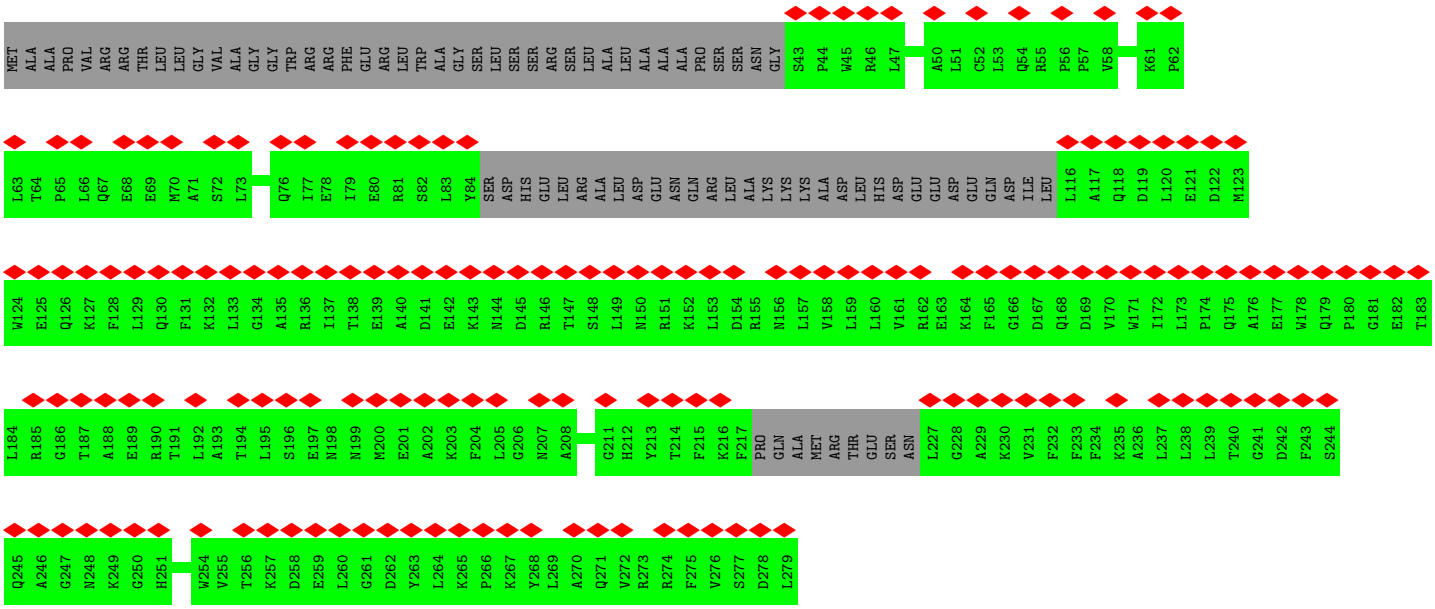
• Molecule 40: 39S ribosomal protein L45, mitochondrial

Chain d:



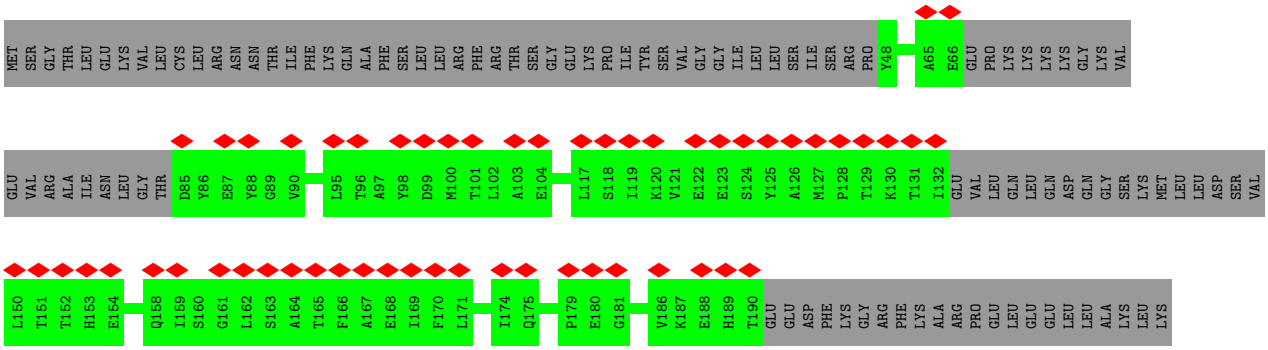
• Molecule 41: 39S ribosomal protein L46, mitochondrial

Chain e: 59% 71% 29%



• Molecule 42: 39S ribosomal protein L48, mitochondrial

Chain f: 26% 51% 49%

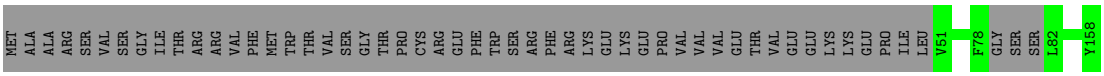


• Molecule 43: 39S ribosomal protein L49, mitochondrial

Chain g: 78% 22%

• Molecule 44: 39S ribosomal protein L50, mitochondrial

Chain h: 66% 34%

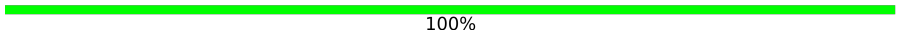


• Molecule 45: 39S ribosomal protein L51, mitochondrial

Chain i:

• Molecule 46: 39S ribosomal protein L52, mitochondrial

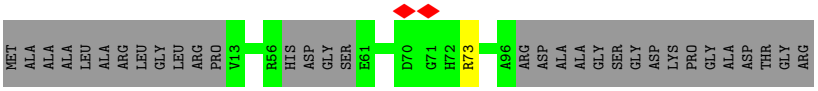
Chain j:



There are no outlier residues recorded for this chain.

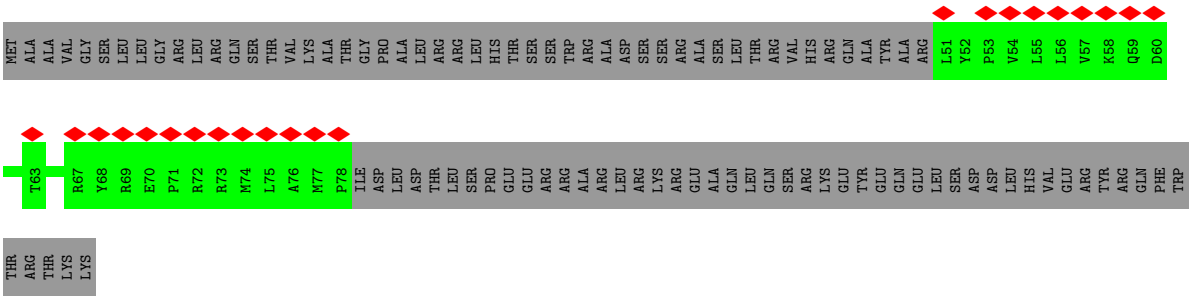
• Molecule 47: 39S ribosomal protein L53, mitochondrial

Chain k:



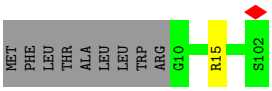
• Molecule 48: 39S ribosomal protein L55, mitochondrial

Chain m:



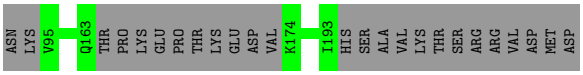
• Molecule 49: Ribosomal protein 63, mitochondrial

Chain o:



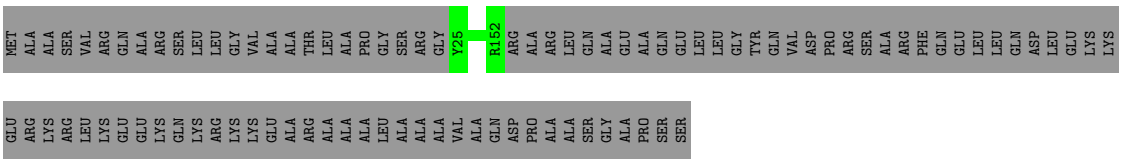
• Molecule 50: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p:



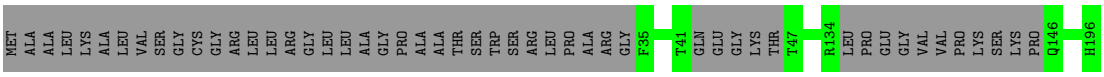
• Molecule 51: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:



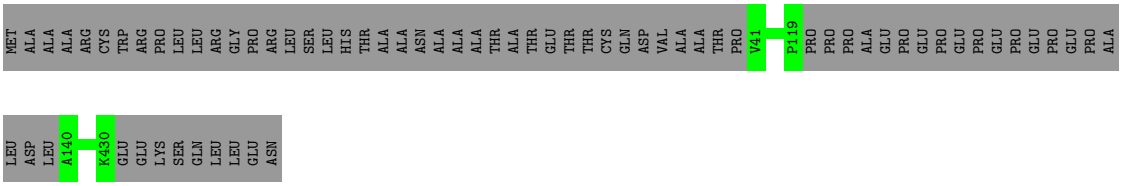
• Molecule 52: 39S ribosomal protein S18a, mitochondrial

Chain r:



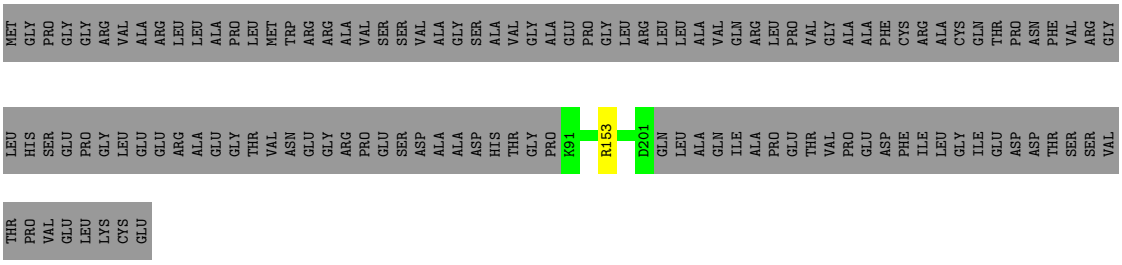
• Molecule 53: 39S ribosomal protein S30, mitochondrial

Chain s:



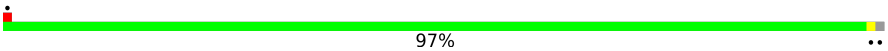
• Molecule 54: Mitochondrial assembly of ribosomal large subunit protein 1

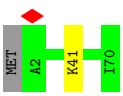
Chain u:



• Molecule 55: MIEF1 upstream open reading frame protein

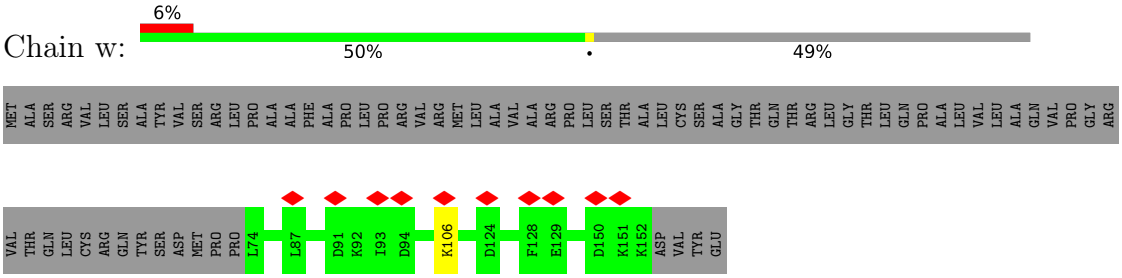
Chain v:





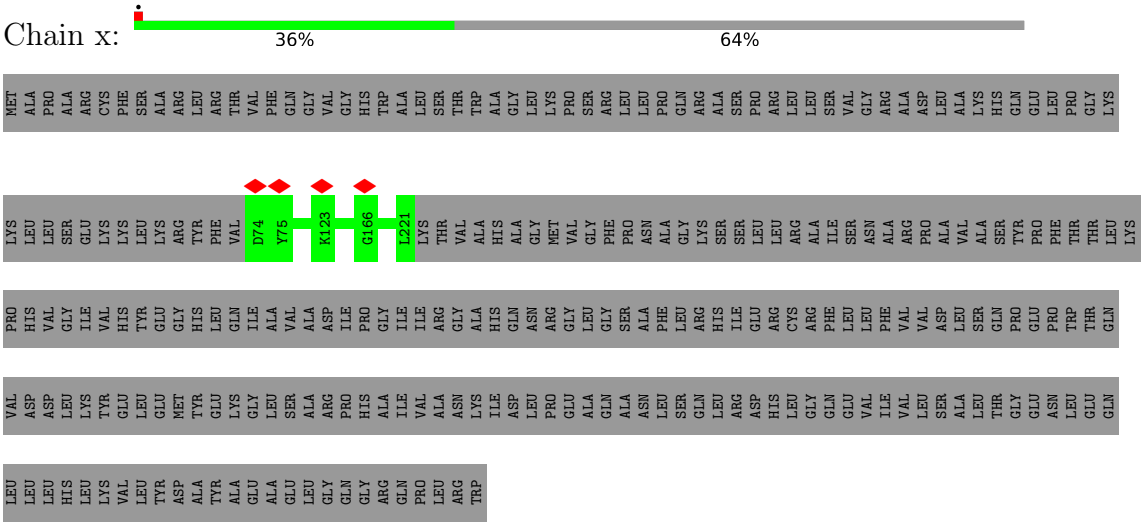
• Molecule 56: Acyl carrier protein, mitochondrial

Chain w:



• Molecule 57: Mitochondrial ribosome-associated GTPase 2

Chain x:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98227	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 ($e^-/Å^2$)	36	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.113	Depositor
Minimum map value	-0.035	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	367.49997, 367.49997, 367.49997	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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, OMG, MG, OMU

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	0.36	0/895	0.54	0/1201
2	1	0.26	0/438	0.54	0/583
3	2	0.41	0/373	0.58	0/496
4	3	0.42	0/852	0.54	0/1136
5	4	0.39	0/341	0.59	0/451
6	5	0.33	0/3294	0.50	0/4488
7	6	0.34	0/2809	0.54	0/3818
8	7	0.32	0/2391	0.47	0/3234
9	8	0.25	0/665	0.51	0/894
10	9	0.37	0/972	0.50	0/1306
11	A	0.78	0/32605	0.80	8/50720 (0.0%)
12	B	0.26	0/1328	0.75	0/2056
13	C	0.27	0/2754	0.49	0/3734
14	D	0.37	0/1910	0.58	0/2569
15	E	0.41	0/2497	0.49	0/3386
16	F	0.40	0/2071	0.53	0/2817
17	G	0.28	0/1974	0.48	0/2652
18	H	0.33	0/798	0.55	0/1073
19	I	0.27	0/1308	0.51	0/1761
20	J	0.25	0/1077	0.50	0/1452
21	K	0.40	0/1495	0.49	0/2029
22	L	0.37	0/904	0.56	0/1218
23	M	0.41	0/2359	0.54	0/3185
24	N	0.35	0/1697	0.54	0/2281
25	O	0.37	0/1269	0.57	0/1708
26	P	0.33	0/1173	0.55	0/1588
27	Q	0.37	0/1846	0.52	0/2487
28	R	0.42	0/987	0.57	0/1320
29	S	0.38	0/1276	0.53	0/1729
30	T	0.42	0/1402	0.53	0/1886
31	U	0.38	0/1183	0.55	0/1600
32	V	0.36	0/404	0.45	0/545

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	W	0.44	0/881	0.52	0/1188
34	X	0.36	0/2090	0.48	0/2825
35	Y	0.36	0/1552	0.52	0/2079
36	Z	0.36	0/960	0.49	0/1295
37	a	0.38	0/616	0.52	0/833
38	b	0.38	0/1202	0.59	0/1626
39	c	0.35	0/2264	0.49	0/3059
40	d	0.27	0/1702	0.48	0/2307
41	e	0.25	0/1633	0.49	0/2204
42	f	0.28	0/873	0.47	0/1180
43	g	0.40	0/1102	0.51	0/1503
44	h	0.27	0/884	0.48	0/1203
45	i	0.43	0/849	0.56	0/1135
46	j	0.33	0/698	0.51	0/940
47	k	0.24	0/635	0.53	0/855
48	m	0.23	0/239	0.59	0/322
49	o	0.37	0/807	0.58	0/1083
50	p	0.28	0/1071	0.54	0/1433
51	q	0.30	0/1107	0.53	0/1498
52	r	0.35	0/1238	0.53	0/1676
53	s	0.39	0/3114	0.53	0/4225
54	u	0.31	0/949	0.50	0/1281
55	v	0.26	0/597	0.61	0/796
56	w	0.26	0/647	0.44	0/871
57	x	0.33	0/1091	0.56	0/1467
All	All	0.52	0/106148	0.63	8/150287 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	2215	C	C2-N1-C1'	8.26	127.88	118.80
11	A	2186	C	N1-C2-O2	6.16	122.59	118.90
11	A	2215	C	C6-N1-C1'	-6.16	113.41	120.80
11	A	2215	C	N1-C2-O2	5.99	122.49	118.90
11	A	2163	A	O4'-C1'-N9	5.46	112.57	108.20
11	A	2185	G	N1-C6-O6	-5.39	116.67	119.90
11	A	2523	C	C2-N1-C1'	5.36	124.70	118.80
11	A	1823	A	P-O3'-C3'	5.08	125.80	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	106/108 (98%)	105 (99%)	1 (1%)	0	100	100
2	1	50/65 (77%)	49 (98%)	1 (2%)	0	100	100
3	2	43/92 (47%)	42 (98%)	1 (2%)	0	100	100
4	3	93/188 (50%)	90 (97%)	3 (3%)	0	100	100
5	4	35/103 (34%)	34 (97%)	1 (3%)	0	100	100
6	5	390/423 (92%)	376 (96%)	14 (4%)	0	100	100
7	6	316/380 (83%)	303 (96%)	13 (4%)	0	100	100
8	7	285/338 (84%)	268 (94%)	17 (6%)	0	100	100
9	8	75/206 (36%)	72 (96%)	3 (4%)	0	100	100
10	9	113/137 (82%)	112 (99%)	1 (1%)	0	100	100
13	C	335/384 (87%)	317 (95%)	18 (5%)	0	100	100
14	D	238/305 (78%)	232 (98%)	6 (2%)	0	100	100
15	E	306/348 (88%)	296 (97%)	10 (3%)	0	100	100
16	F	248/311 (80%)	242 (98%)	6 (2%)	0	100	100
17	G	236/381 (62%)	225 (95%)	11 (5%)	0	100	100
18	H	93/267 (35%)	88 (95%)	5 (5%)	0	100	100
19	I	154/261 (59%)	146 (95%)	8 (5%)	0	100	100
20	J	138/192 (72%)	126 (91%)	12 (9%)	0	100	100
21	K	175/178 (98%)	171 (98%)	4 (2%)	0	100	100
22	L	113/145 (78%)	109 (96%)	4 (4%)	0	100	100
23	M	285/296 (96%)	282 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	N	203/251 (81%)	191 (94%)	12 (6%)	0	100	100
25	O	150/175 (86%)	147 (98%)	3 (2%)	0	100	100
26	P	139/180 (77%)	134 (96%)	5 (4%)	0	100	100
27	Q	215/292 (74%)	212 (99%)	3 (1%)	0	100	100
28	R	114/149 (76%)	113 (99%)	1 (1%)	0	100	100
29	S	154/205 (75%)	151 (98%)	3 (2%)	0	100	100
30	T	164/206 (80%)	161 (98%)	3 (2%)	0	100	100
31	U	135/153 (88%)	133 (98%)	2 (2%)	0	100	100
32	V	45/216 (21%)	45 (100%)	0	0	100	100
33	W	107/148 (72%)	105 (98%)	2 (2%)	0	100	100
34	X	241/256 (94%)	236 (98%)	5 (2%)	0	100	100
35	Y	174/250 (70%)	170 (98%)	4 (2%)	0	100	100
36	Z	113/161 (70%)	110 (97%)	3 (3%)	0	100	100
37	a	67/142 (47%)	67 (100%)	0	0	100	100
38	b	146/215 (68%)	141 (97%)	5 (3%)	0	100	100
39	c	271/332 (82%)	267 (98%)	4 (2%)	0	100	100
40	d	189/306 (62%)	183 (97%)	6 (3%)	0	100	100
41	e	191/279 (68%)	179 (94%)	12 (6%)	0	100	100
42	f	102/212 (48%)	94 (92%)	8 (8%)	0	100	100
43	g	127/166 (76%)	120 (94%)	7 (6%)	0	100	100
44	h	101/158 (64%)	99 (98%)	2 (2%)	0	100	100
45	i	95/128 (74%)	94 (99%)	1 (1%)	0	100	100
46	j	83/85 (98%)	83 (100%)	0	0	100	100
47	k	76/112 (68%)	70 (92%)	6 (8%)	0	100	100
48	m	26/128 (20%)	20 (77%)	6 (23%)	0	100	100
49	o	91/102 (89%)	89 (98%)	2 (2%)	0	100	100
50	p	119/206 (58%)	116 (98%)	3 (2%)	0	100	100
51	q	126/222 (57%)	126 (100%)	0	0	100	100
52	r	140/196 (71%)	133 (95%)	7 (5%)	0	100	100
53	s	366/439 (83%)	358 (98%)	8 (2%)	0	100	100
54	u	109/234 (47%)	100 (92%)	9 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	v	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
56	w	77/156 (49%)	73 (95%)	4 (5%)	0	100	100
57	x	146/406 (36%)	138 (94%)	8 (6%)	0	100	100
All	All	8496/12044 (70%)	8208 (97%)	288 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	97/97 (100%)	97 (100%)	0	100	100
2	1	49/60 (82%)	49 (100%)	0	100	100
3	2	39/72 (54%)	39 (100%)	0	100	100
4	3	88/166 (53%)	88 (100%)	0	100	100
5	4	36/89 (40%)	36 (100%)	0	100	100
6	5	353/368 (96%)	352 (100%)	1 (0%)	92	97
7	6	286/332 (86%)	285 (100%)	1 (0%)	92	97
8	7	263/303 (87%)	262 (100%)	1 (0%)	91	97
9	8	70/190 (37%)	69 (99%)	1 (1%)	67	86
10	9	99/112 (88%)	99 (100%)	0	100	100
13	C	293/328 (89%)	292 (100%)	1 (0%)	92	97
14	D	194/245 (79%)	193 (100%)	1 (0%)	88	96
15	E	262/290 (90%)	262 (100%)	0	100	100
16	F	217/262 (83%)	217 (100%)	0	100	100
17	G	221/350 (63%)	221 (100%)	0	100	100
18	H	86/228 (38%)	86 (100%)	0	100	100
19	I	145/232 (62%)	145 (100%)	0	100	100
20	J	113/150 (75%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	K	155/156 (99%)	155 (100%)	0	100	100
22	L	98/124 (79%)	98 (100%)	0	100	100
23	M	245/249 (98%)	243 (99%)	2 (1%)	81	93
24	N	172/211 (82%)	170 (99%)	2 (1%)	71	88
25	O	133/150 (89%)	133 (100%)	0	100	100
26	P	123/155 (79%)	123 (100%)	0	100	100
27	Q	199/256 (78%)	199 (100%)	0	100	100
28	R	101/126 (80%)	101 (100%)	0	100	100
29	S	141/180 (78%)	141 (100%)	0	100	100
30	T	146/176 (83%)	146 (100%)	0	100	100
31	U	124/135 (92%)	124 (100%)	0	100	100
32	V	43/191 (22%)	43 (100%)	0	100	100
33	W	89/119 (75%)	89 (100%)	0	100	100
34	X	219/229 (96%)	218 (100%)	1 (0%)	88	96
35	Y	159/223 (71%)	159 (100%)	0	100	100
36	Z	106/147 (72%)	105 (99%)	1 (1%)	78	92
37	a	67/133 (50%)	67 (100%)	0	100	100
38	b	130/186 (70%)	130 (100%)	0	100	100
39	c	241/288 (84%)	241 (100%)	0	100	100
40	d	184/274 (67%)	183 (100%)	1 (0%)	88	96
41	e	171/236 (72%)	171 (100%)	0	100	100
42	f	95/188 (50%)	95 (100%)	0	100	100
43	g	119/148 (80%)	119 (100%)	0	100	100
44	h	100/148 (68%)	100 (100%)	0	100	100
45	i	86/110 (78%)	86 (100%)	0	100	100
46	j	68/68 (100%)	68 (100%)	0	100	100
47	k	71/90 (79%)	70 (99%)	1 (1%)	67	86
48	m	26/113 (23%)	26 (100%)	0	100	100
49	o	79/87 (91%)	78 (99%)	1 (1%)	69	87
50	p	117/181 (65%)	117 (100%)	0	100	100
51	q	110/178 (62%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	r	133/169 (79%)	133 (100%)	0	100	100
53	s	326/381 (86%)	326 (100%)	0	100	100
54	u	105/200 (52%)	104 (99%)	1 (1%)	76	90
55	v	59/60 (98%)	58 (98%)	1 (2%)	60	82
56	w	73/136 (54%)	72 (99%)	1 (1%)	67	86
57	x	109/320 (34%)	109 (100%)	0	100	100
All	All	7633/10395 (73%)	7615 (100%)	18 (0%)	93	98

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	5	412	ARG
7	6	52	ARG
8	7	319	ARG
9	8	120	LYS
13	C	346	ARG
14	D	285	LYS
23	M	44	ARG
23	M	59	ARG
24	N	133	ARG
24	N	249	LYS
34	X	23	ARG
36	Z	44	LYS
40	d	198	ARG
47	k	73	ARG
49	o	15	ARG
54	u	153	ARG
55	v	41	LYS
56	w	106	LYS

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

Mol	Chain	Res	Type
13	C	46	GLN
22	L	33	GLN
23	M	26	ASN
29	S	118	ASN
47	k	19	GLN
51	q	130	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1359/1559 (87%)	294 (21%)	21 (1%)
12	B	51/69 (73%)	16 (31%)	1 (1%)
All	All	1410/1628 (86%)	310 (21%)	22 (1%)

All (310) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	1672	C
11	A	1676	A
11	A	1677	C
11	A	1679	U
11	A	1680	A
11	A	1681	G
11	A	1689	C
11	A	1690	C
11	A	1699	C
11	A	1700	U
11	A	1704	U
11	A	1708	A
11	A	1714	C
11	A	1715	C
11	A	1724	A
11	A	1727	A
11	A	1728	U
11	A	1731	A
11	A	1732	C
11	A	1748	G
11	A	1750	G
11	A	1751	A
11	A	1767	G
11	A	1770	G
11	A	1777	A
11	A	1794	A
11	A	1817	C
11	A	1819	U
11	A	1821	A
11	A	1823	A
11	A	1824	U
11	A	1827	C
11	A	1828	A
11	A	1829	A

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Mol	Chain	Res	Type
11	A	1832	A
11	A	1836	A
11	A	1844	A
11	A	1849	C
11	A	1853	A
11	A	1854	U
11	A	1855	A
11	A	1856	A
11	A	1869	A
11	A	1878	U
11	A	1882	A
11	A	1883	G
11	A	1887	A
11	A	1888	G
11	A	1892	A
11	A	1893	A
11	A	1902	C
11	A	1903	C
11	A	1918	G
11	A	1938	A
11	A	1940	A
11	A	1958	G
11	A	1972	A
11	A	1974	A
11	A	1985	G
11	A	1987	G
11	A	1992	C
11	A	1994	A
11	A	1995	A
11	A	2001	C
11	A	2002	G
11	A	2015	G
11	A	2021	U
11	A	2022	G
11	A	2029	A
11	A	2030	U
11	A	2036	C
11	A	2037	U
11	A	2039	A
11	A	2054	U
11	A	2055	U
11	A	2060	A

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Mol	Chain	Res	Type
11	A	2065	A
11	A	2074	A
11	A	2079	C
11	A	2083	U
11	A	2085	A
11	A	2093	U
11	A	2097	A
11	A	2098	G
11	A	2113	G
11	A	2114	C
11	A	2124	A
11	A	2126	U
11	A	2132	A
11	A	2141	U
11	A	2147	G
11	A	2154	A
11	A	2155	A
11	A	2157	U
11	A	2159	U
11	A	2163	A
11	A	2164	C
11	A	2165	C
11	A	2166	C
11	A	2172	A
11	A	2173	G
11	A	2177	U
11	A	2180	A
11	A	2182	G
11	A	2183	C
11	A	2184	A
11	A	2187	C
11	A	2193	U
11	A	2194	U
11	A	2197	G
11	A	2198	A
11	A	2199	A
11	A	2200	A
11	A	2210	C
11	A	2212	C
11	A	2213	A
11	A	2215	C
11	A	2216	A

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Mol	Chain	Res	Type
11	A	2233	U
11	A	2237	A
11	A	2239	A
11	A	2241	A
11	A	2242	U
11	A	2243	A
11	A	2246	A
11	A	2262	C
11	A	2263	C
11	A	2282	C
11	A	2285	U
11	A	2297	A
11	A	2300	G
11	A	2316	U
11	A	2322	C
11	A	2331	C
11	A	2332	C
11	A	2335	A
11	A	2345	G
11	A	2349	G
11	A	2369	A
11	A	2371	U
11	A	2374	A
11	A	2381	A
11	A	2384	A
11	A	2386	C
11	A	2387	U
11	A	2390	A
11	A	2393	C
11	A	2399	A
11	A	2404	U
11	A	2408	U
11	A	2415	C
11	A	2427	C
11	A	2432	A
11	A	2434	A
11	A	2444	A
11	A	2446	A
11	A	2451	A
11	A	2458	A
11	A	2478	G
11	A	2485	U

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Mol	Chain	Res	Type
11	A	2493	C
11	A	2496	G
11	A	2500	A
11	A	2502	C
11	A	2507	A
11	A	2508	C
11	A	2511	C
11	A	2520	C
11	A	2521	A
11	A	2527	A
11	A	2528	G
11	A	2531	U
11	A	2540	C
11	A	2618	U
11	A	2635	G
11	A	2636	G
11	A	2637	C
11	A	2639	C
11	A	2645	G
11	A	2654	U
11	A	2656	U
11	A	2660	U
11	A	2683	C
11	A	2684	C
11	A	2686	G
11	A	2694	A
11	A	2696	A
11	A	2706	A
11	A	2709	A
11	A	2718	C
11	A	2719	G
11	A	2721	G
11	A	2722	A
11	A	2724	G
11	A	2732	G
11	A	2739	U
11	A	2748	A
11	A	2750	U
11	A	2756	C
11	A	2804	A
11	A	2810	G
11	A	2815	OMG

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Mol	Chain	Res	Type
11	A	2819	G
11	A	2831	G
11	A	2832	A
11	A	2833	A
11	A	2836	C
11	A	2837	A
11	A	2838	A
11	A	2839	C
11	A	2846	G
11	A	2847	C
11	A	2853	A
11	A	2854	U
11	A	2855	G
11	A	2857	U
11	A	2859	A
11	A	2864	U
11	A	2865	C
11	A	2871	U
11	A	2890	U
11	A	2895	U
11	A	2896	G
11	A	2906	C
11	A	2911	C
11	A	2912	C
11	A	2913	A
11	A	2917	G
11	A	2918	A
11	A	2919	A
11	A	2922	A
11	A	2926	A
11	A	2928	C
11	A	2932	G
11	A	2935	A
11	A	2936	U
11	A	2943	G
11	A	2955	U
11	A	2956	A
11	A	2958	A
11	A	2962	C
11	A	2963	A
11	A	2965	A
11	A	2971	A

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Mol	Chain	Res	Type
11	A	2989	G
11	A	2990	A
11	A	2991	U
11	A	3005	A
11	A	3016	G
11	A	3022	G
11	A	3041	U
11	A	3042	U
11	A	3043	C
11	A	3051	A
11	A	3053	A
11	A	3054	G
11	A	3060	C
11	A	3063	G
11	A	3068	G
11	A	3073	C
11	A	3089	A
11	A	3093	C
11	A	3096	U
11	A	3097	U
11	A	3100	U
11	A	3102	U
11	A	3108	U
11	A	3109	U
11	A	3113	A
11	A	3123	G
11	A	3124	U
11	A	3129	A
11	A	3134	C
11	A	3141	A
11	A	3150	U
11	A	3155	C
11	A	3157	C
11	A	3158	A
11	A	3162	C
11	A	3168	C
11	A	3169	C
11	A	3172	C
11	A	3173	G
11	A	3180	A
11	A	3189	C
11	A	3190	A

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Mol	Chain	Res	Type
11	A	3197	U
11	A	3198	A
11	A	3200	U
11	A	3202	U
11	A	3207	A
11	A	3217	A
11	A	3218	A
11	A	3220	A
12	B	1607	U
12	B	1608	G
12	B	1609	U
12	B	1611	G
12	B	1614	U
12	B	1615	A
12	B	1625	A
12	B	1631	C
12	B	1632	U
12	B	1633	U
12	B	1641	G
12	B	1644	G
12	B	1645	A
12	B	1649	C
12	B	1651	A
12	B	1669	G

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	1707	C
11	A	1713	A
11	A	1766	U
11	A	1823	A
11	A	1986	A
11	A	2164	C
11	A	2182	G
11	A	2186	C
11	A	2209	G
11	A	2284	C
11	A	2457	A
11	A	2507	A
11	A	2530	A
11	A	2635	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	A	2695	G
11	A	2836	C
11	A	2837	A
11	A	2905	A
11	A	3092	U
11	A	3122	U
11	A	3196	G
12	B	1607	U

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	OMU	A	3039	11	19,22,23	1.30	3 (15%)	26,31,34	1.96	5 (19%)
11	OMG	A	3040	11	18,26,27	1.04	1 (5%)	19,38,41	1.10	2 (10%)
11	OMG	A	2815	11	18,26,27	0.99	1 (5%)	19,38,41	1.16	2 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	OMU	A	3039	11	-	0/9/27/28	0/2/2/2
11	OMG	A	3040	11	-	0/5/27/28	0/3/3/3
11	OMG	A	2815	11	-	2/5/27/28	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	3039	OMU	C4-N3	-3.01	1.33	1.38

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	3040	OMG	C6-N1	-2.81	1.33	1.37
11	A	3039	OMU	C2-N3	-2.70	1.33	1.38
11	A	2815	OMG	C6-N1	-2.41	1.34	1.37
11	A	3039	OMU	C5-C4	-2.34	1.38	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	3039	OMU	C4-N3-C2	-4.57	120.55	126.58
11	A	3039	OMU	N3-C2-N1	4.14	120.39	114.89
11	A	3039	OMU	C5-C4-N3	4.04	120.89	114.84
11	A	3039	OMU	C2'-C1'-N1	-3.70	107.03	114.22
11	A	3039	OMU	O4-C4-C5	-2.95	119.97	125.16
11	A	3040	OMG	C5-C6-N1	2.49	118.34	113.95
11	A	2815	OMG	C8-N7-C5	2.38	107.53	102.99
11	A	2815	OMG	C5-C6-N1	2.38	118.15	113.95
11	A	3040	OMG	C8-N7-C5	2.25	107.27	102.99

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	2815	OMG	O4'-C4'-C5'-O5'
11	A	2815	OMG	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 77 ligands modelled in this entry, 77 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)

There are no chain breaks in this entry.

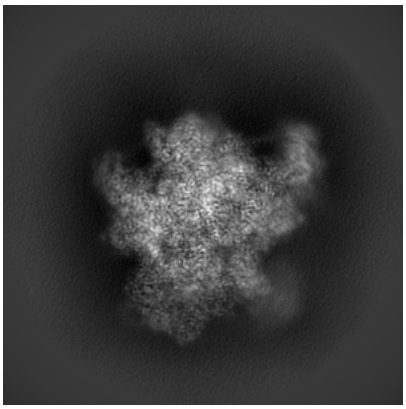
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12872. These allow visual inspection of the internal detail of the map and identification of artifacts.

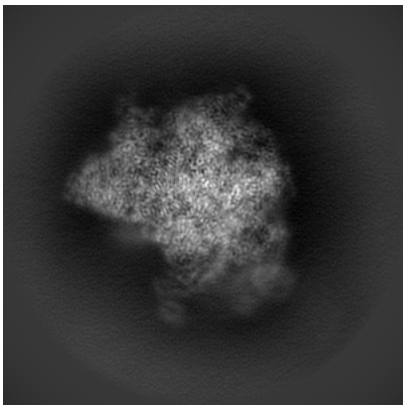
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

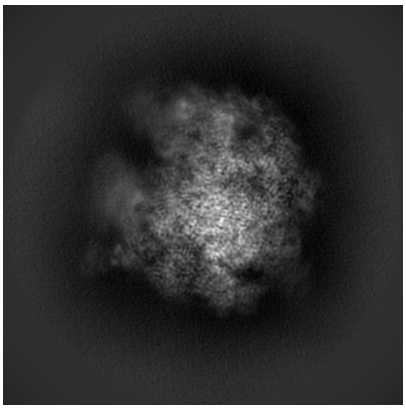
6.1.1 Primary map



X

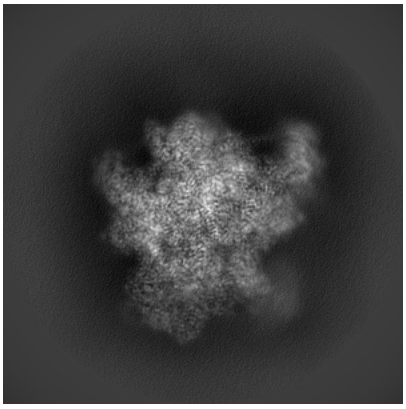


Y

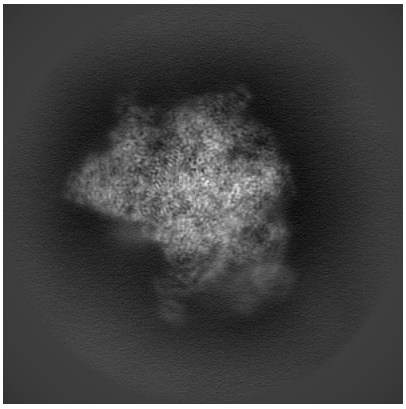


Z

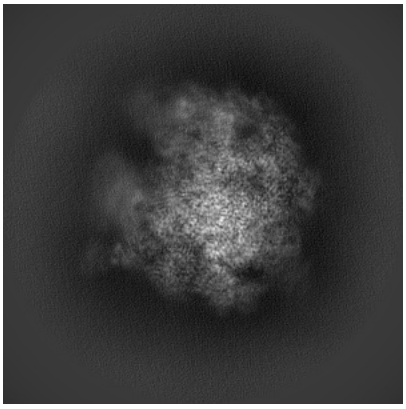
6.1.2 Raw map



X



Y

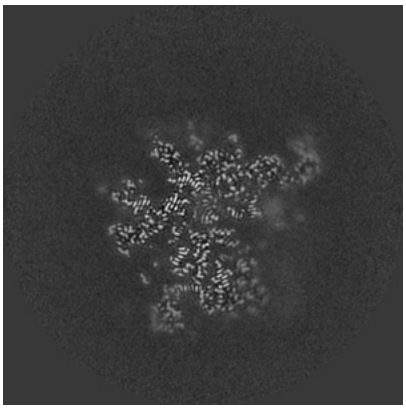


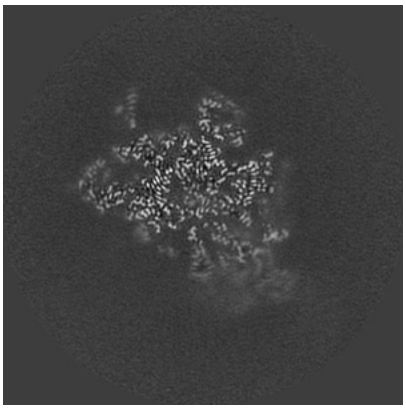
Z

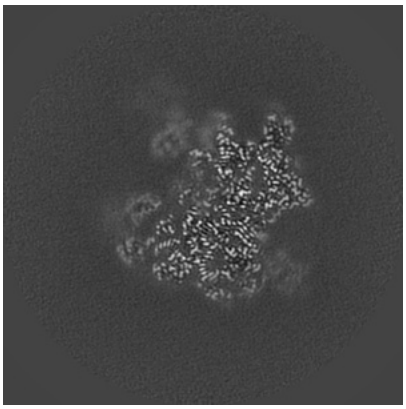
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

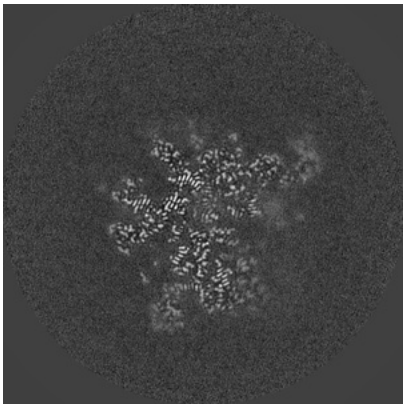
6.2.1 Primary map

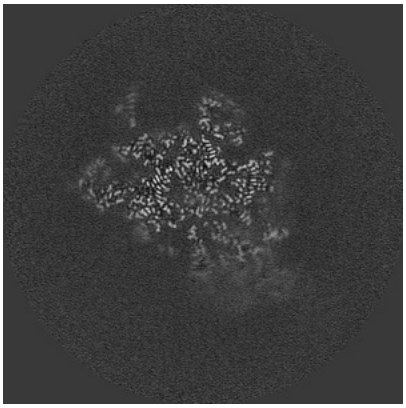

X Index: 175

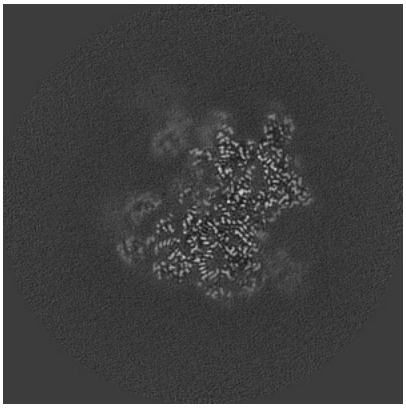

Y Index: 175


Z Index: 175

6.2.2 Raw map


X Index: 175

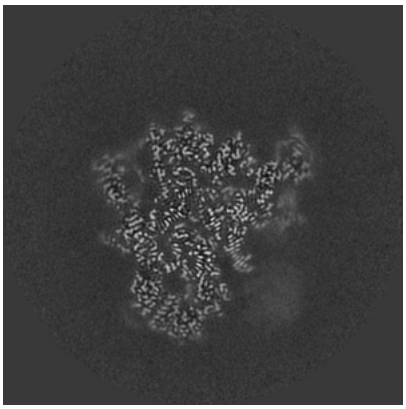

Y Index: 175


Z Index: 175

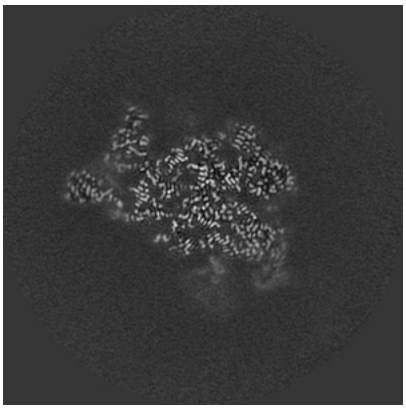
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

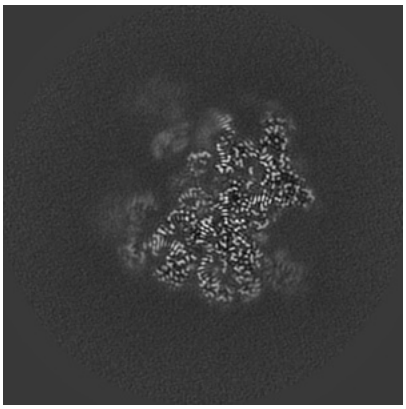
6.3.1 Primary map



X Index: 188

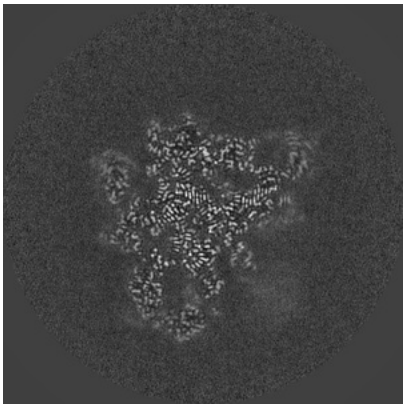


Y Index: 159

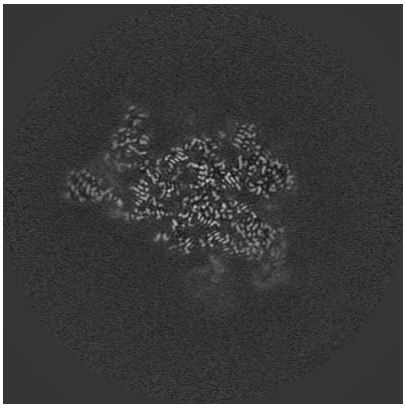


Z Index: 178

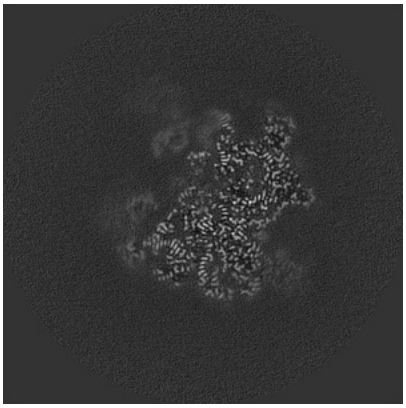
6.3.2 Raw map



X Index: 192



Y Index: 159

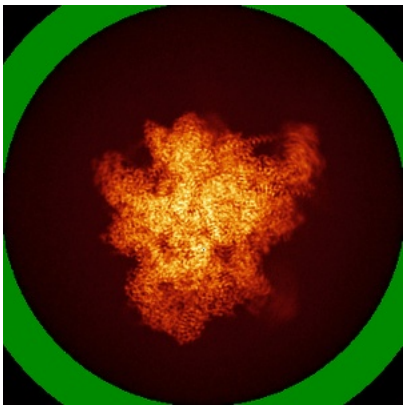


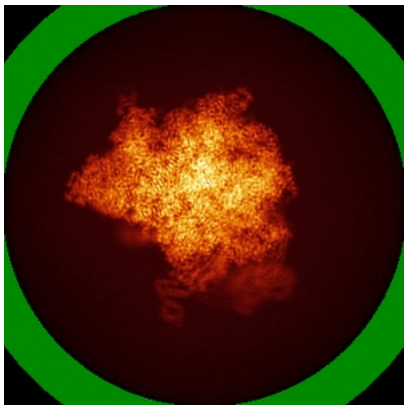
Z Index: 177

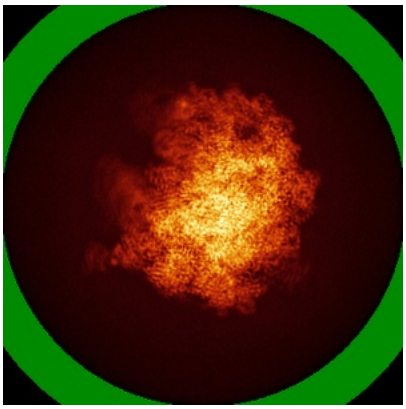
The images above show the largest variance slices of the map in three orthogonal directions.

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

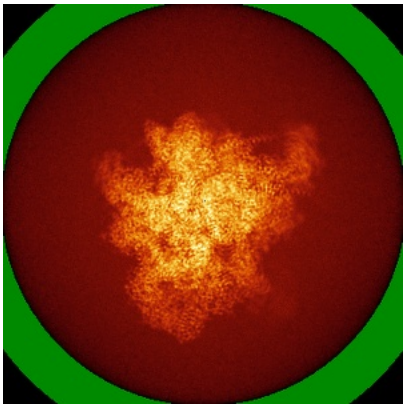
6.4.1 Primary map

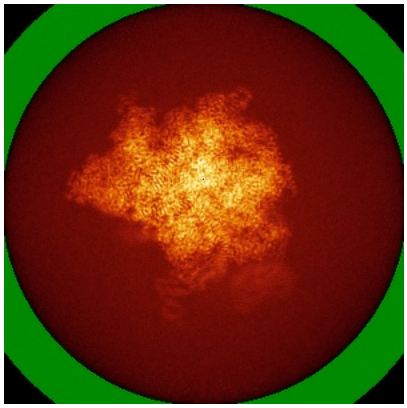

X

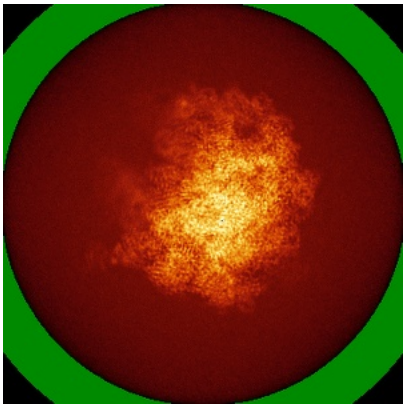

Y


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.

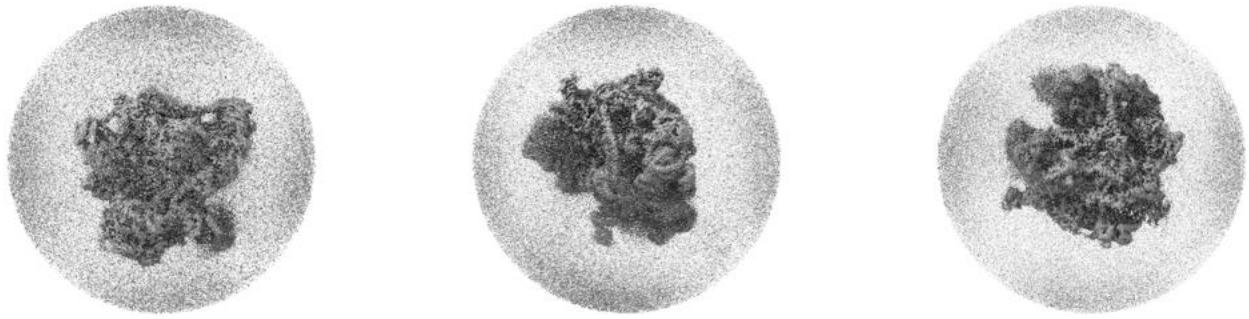
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. 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.

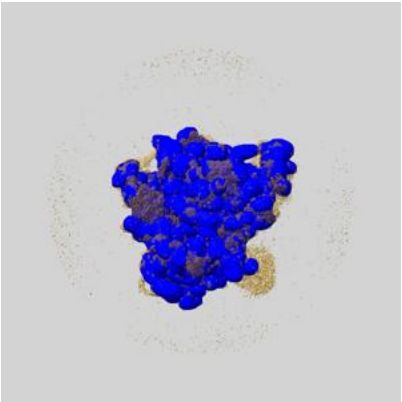
6.6 Mask visualisation (i)

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

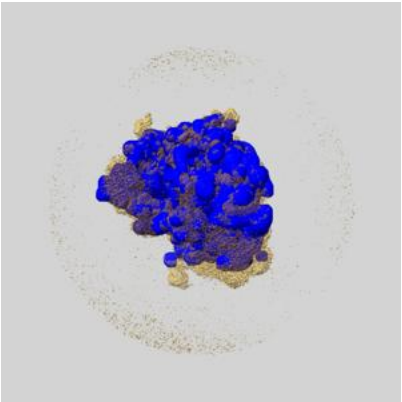
A mask typically either:

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

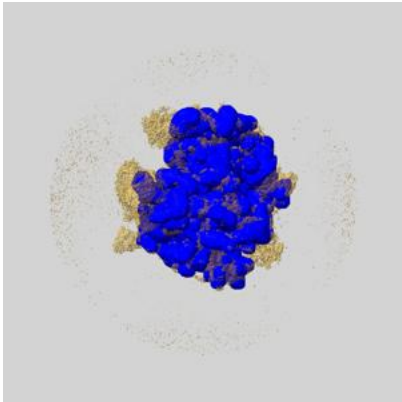
6.6.1 emd_12872_msk_1.map (i)



X



Y

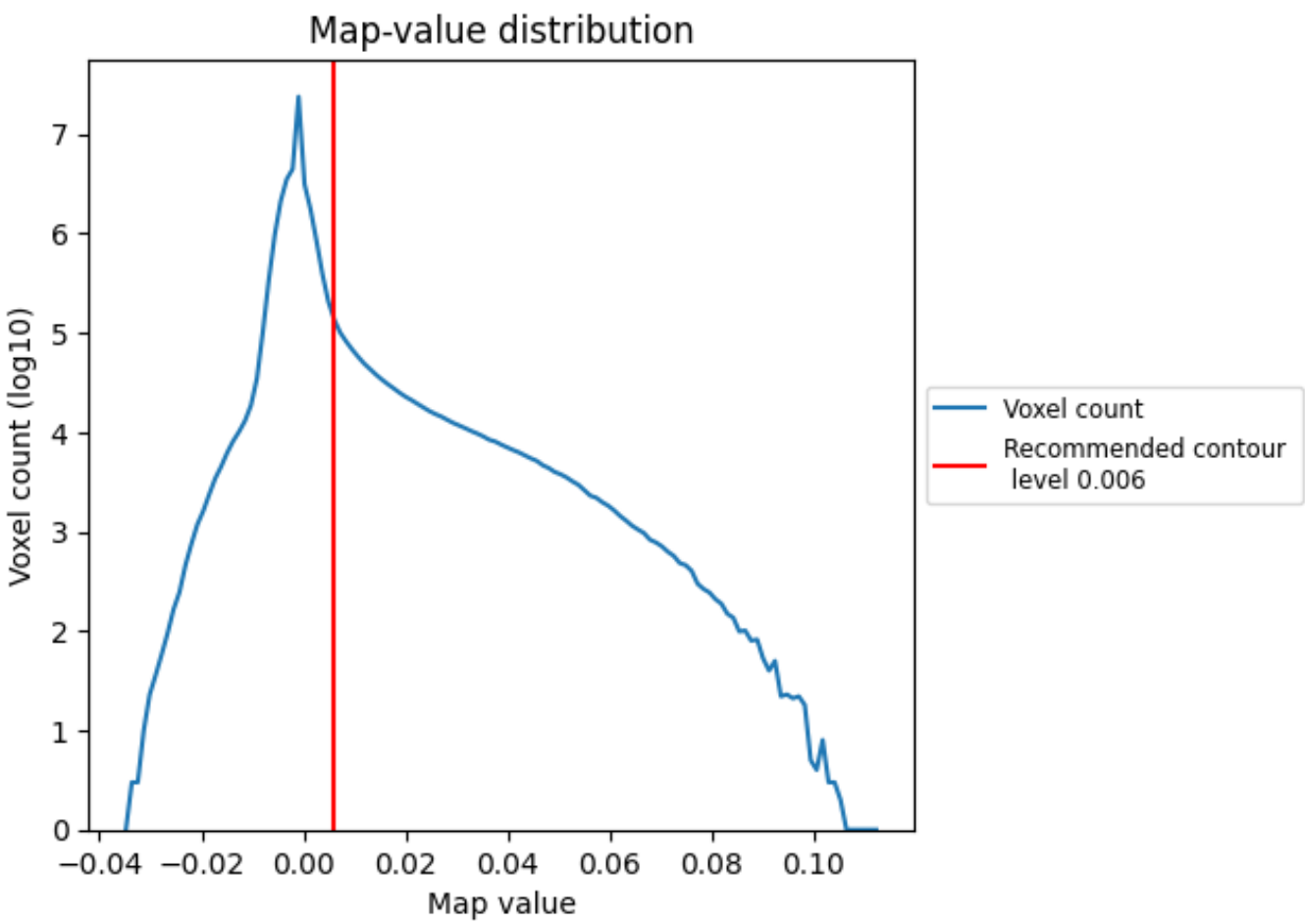


Z

7 Map analysis (i)

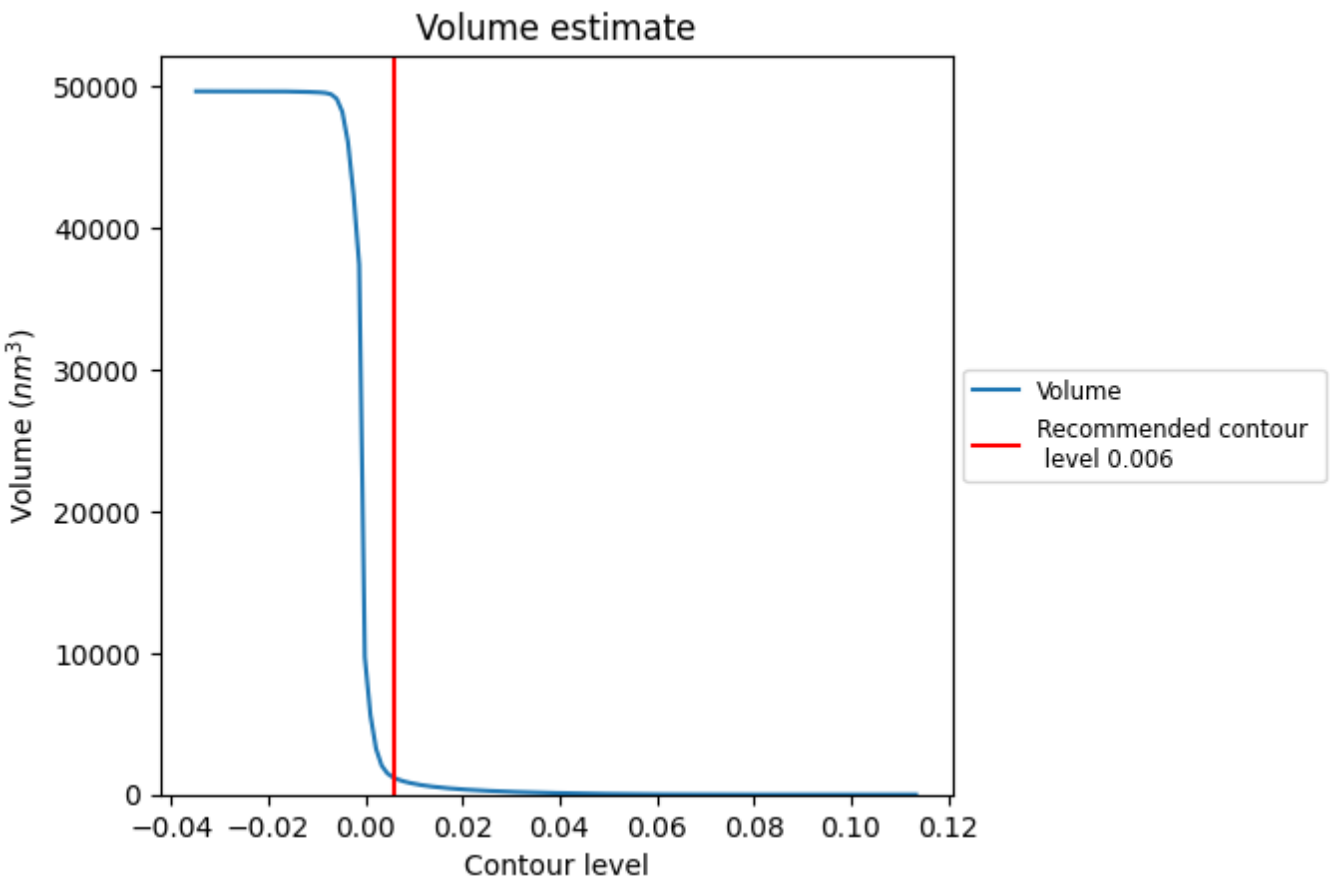
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

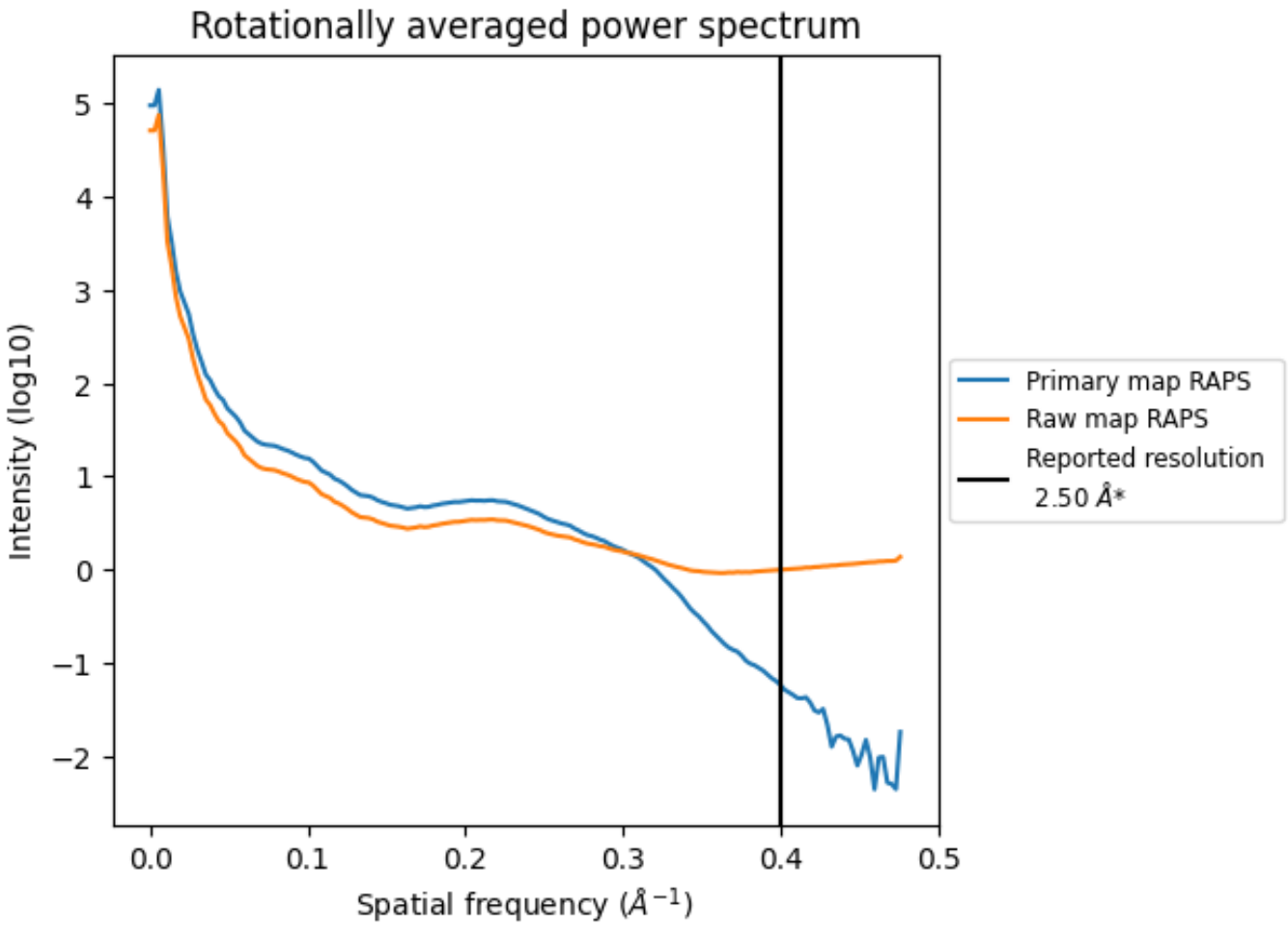
7.2 Volume estimate (i)



The volume at the recommended contour level is 1175 nm^3; this corresponds to an approximate mass of 1062 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)

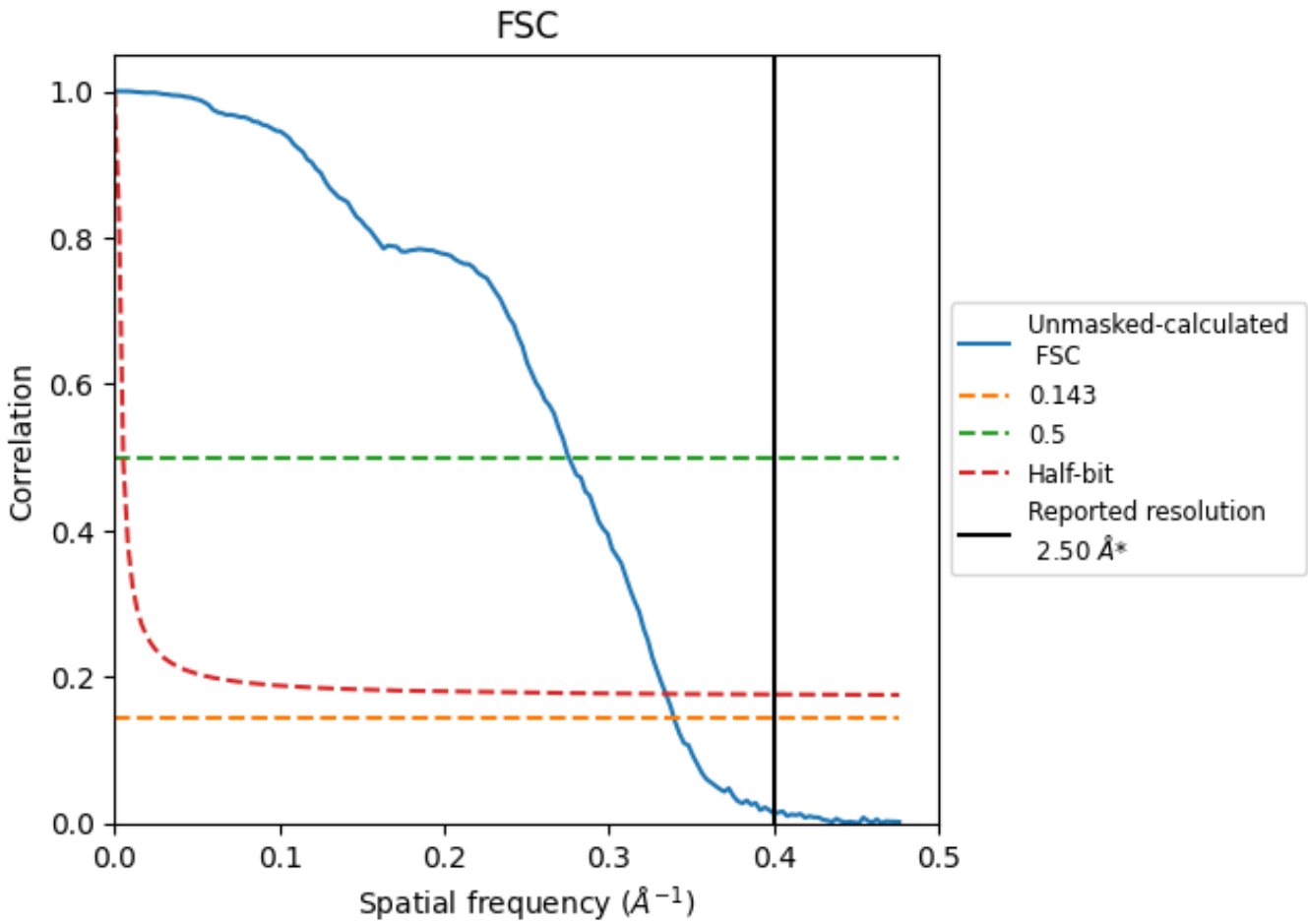


*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.400 Å^{-1}

8.2 Resolution estimates (i)

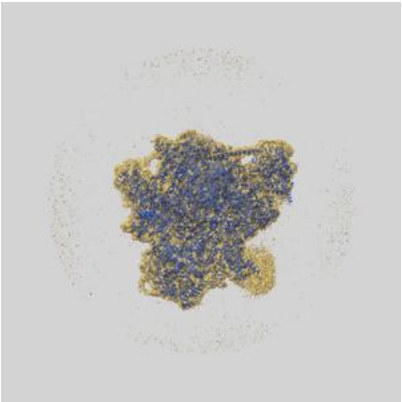
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.94	3.63	2.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.94 differs from the reported value 2.5 by more than 10 %

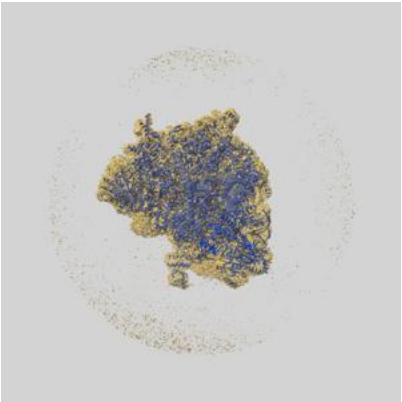
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12872 and PDB model 7OF7. Per-residue inclusion information can be found in section 3 on page 14.

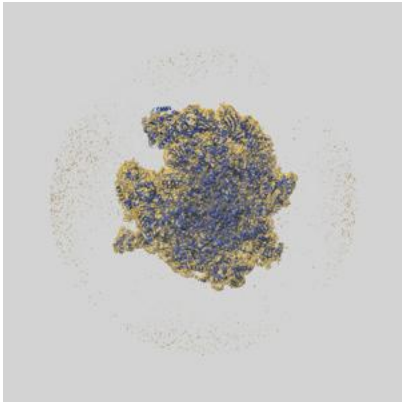
9.1 Map-model overlay (i)



X



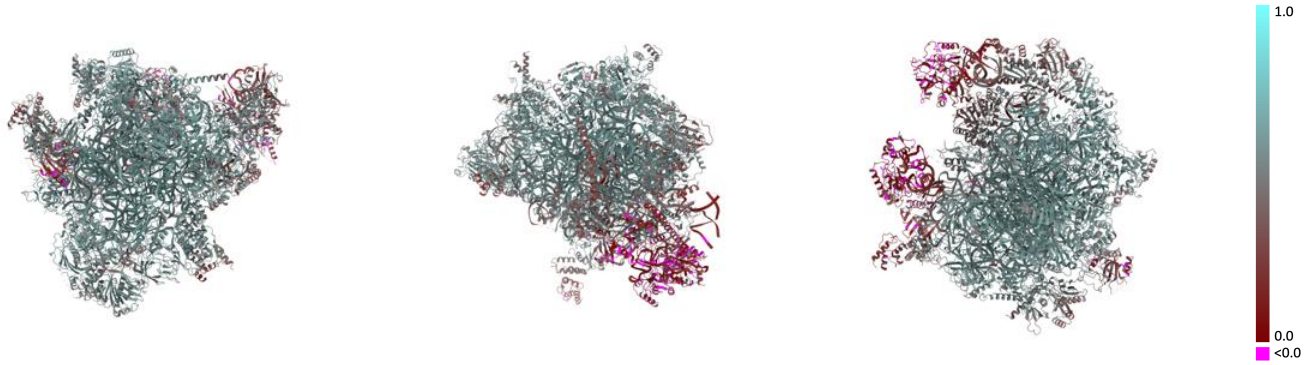
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 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.

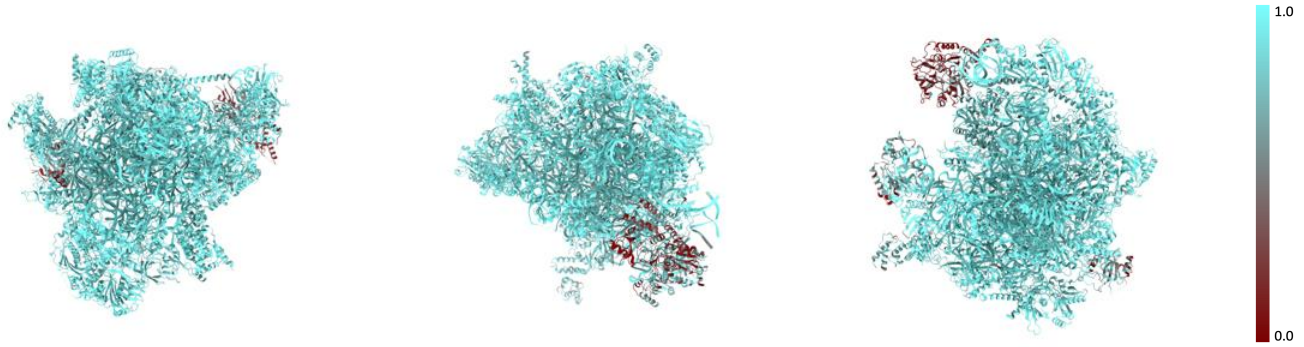
9.2 Q-score mapped to coordinate model (i)



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.

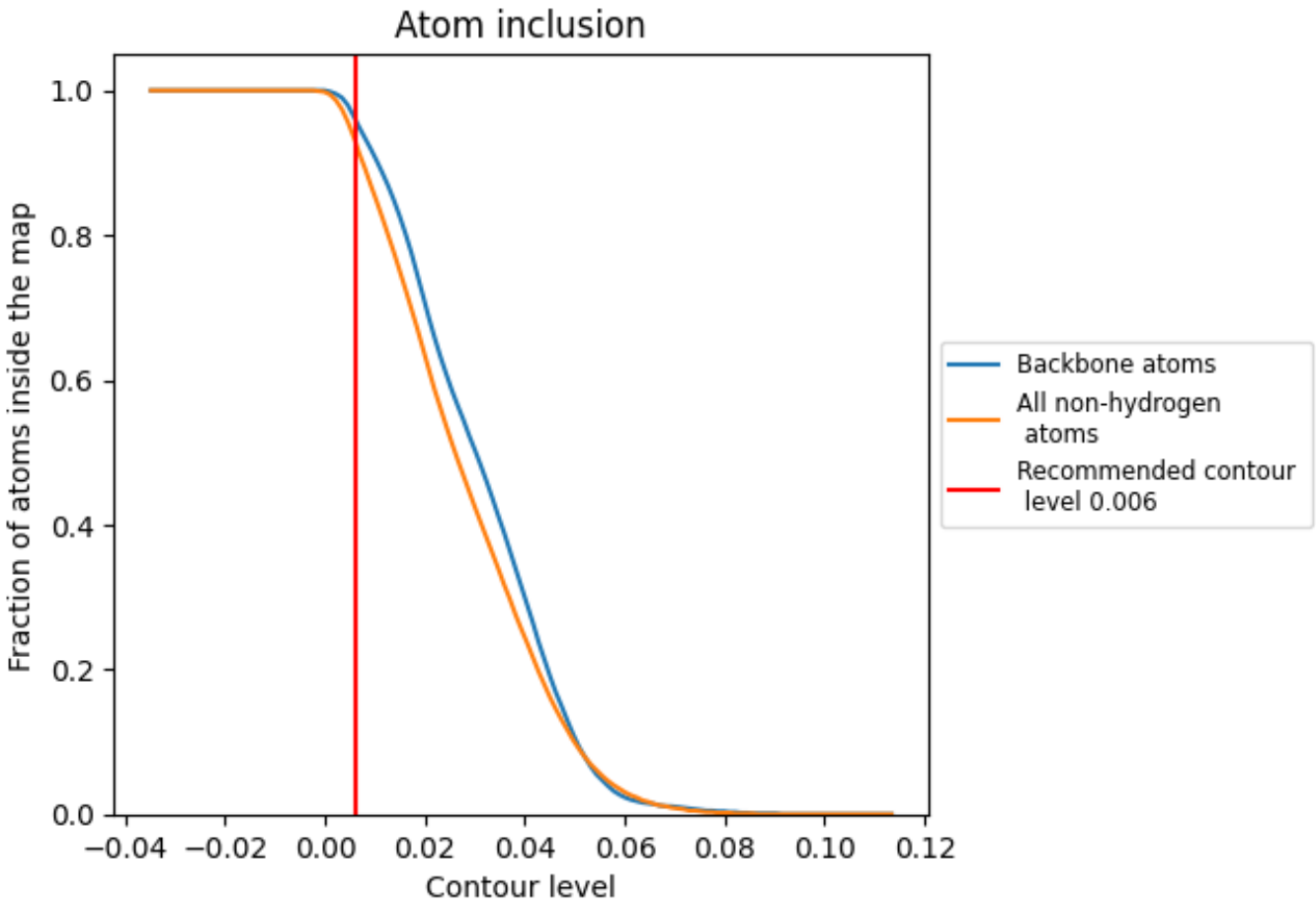
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9310	0.5230
0	0.9640	0.5670
1	0.8860	0.3710
2	1.0000	0.6420
3	0.9840	0.6260
4	0.9750	0.5650
5	0.9590	0.5370
6	0.9460	0.4560
7	0.9360	0.4950
8	0.3370	0.1560
9	0.9510	0.5530
A	0.9950	0.5800
B	0.9350	0.2930
C	0.9100	0.4110
D	0.9610	0.5800
E	0.9720	0.5880
F	0.9840	0.6080
G	0.9000	0.4410
H	0.9260	0.5320
I	0.8200	0.2460
J	0.5860	0.0940
K	0.9840	0.6050
L	0.9690	0.5830
M	0.9740	0.5980
N	0.9480	0.5390
O	0.9800	0.5950
P	0.9670	0.5120
Q	0.9610	0.5710
R	0.9870	0.6170
S	0.9690	0.5900
T	0.9740	0.6050
U	0.8710	0.5420
V	0.9560	0.5360
W	0.9790	0.5970
X	0.9570	0.5700

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Chain	Atom inclusion	Q-score
Y	0.9630	0.5840
Z	0.9660	0.5910
a	0.9690	0.5940
b	0.9800	0.5990
c	0.9590	0.5590
d	0.6550	0.3280
e	0.1900	0.0940
f	0.4250	0.2540
g	0.9830	0.5930
h	0.9300	0.4890
i	0.9870	0.6300
j	0.9620	0.5720
k	0.8780	0.2730
m	0.2140	0.1370
o	0.9730	0.6040
p	0.9240	0.4990
q	0.8860	0.4520
r	0.9700	0.5440
s	0.9680	0.5800
u	0.9450	0.4580
v	0.8790	0.3490
w	0.6790	0.1820
x	0.8820	0.3910