wwPDB EM Validation Summary Report (i)

Mar 9, 2023 – 04:08 pm GMT

PDB ID	:	5OOM
EMDB ID	:	EMD-3843
Title	:	Structure of a native assembly intermediate of the human mitochondrial ribosome with unfolded interfacial rRNA
Authors	:	Brown, A.; Rathore, S.; Kimanius, D.; Aibara, S.; Bai, X.C.; Rorbach, J.; Amunts, A.; Ramakrishnan, V.
Deposited on	:	2017-08-08
Resolution	:	3.03 Å(reported)
Based on initial model	:	3J9M

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

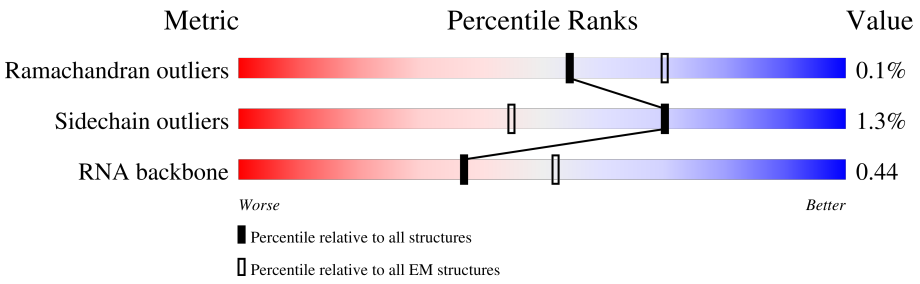
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 3.03 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	A	1559	6%; 35%, 29%, 6%, 30%
2	B	69	6%; 52%, 28%, •, 19%
3	D	305	28%; 71%, •, 28%
4	E	348	13%; 81%, •, 18%
5	F	311	12%; 78%, •, 20%
6	H	267	11%; 35%, 64%
7	I	261	51%; 59%, •, 39%
8	J	192	73%; 72%, •, 27%

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Mol	Chain	Length	Quality of chain
9	K	178	12% 98%
10	L	145	24% 78% 21%
11	M	296	17% 94%
12	N	251	39% 80% 18%
13	O	175	14% 85% 13%
14	P	180	14% 77% 22%
15	Q	292	15% 74% 26%
16	R	149	19% 90% 6%
17	S	205	5% 75% 24%
18	T	206	11% 76% 23%
19	U	153	12% 89% 9%
20	V	216	15% 87% 11%
21	W	148	19% 72% 26%
22	X	256	20% 93% 5%
23	Y	250	11% 69% 30%
24	Z	161	7% 74% 25%
25	0	188	6% 56% 43%
26	1	65	22% 74% 6% 20%
27	2	92	11% 46% 53%
28	3	188	11% 49% 49%
29	5	423	16% 89% 9%
30	6	380	18% 84% 15%
31	7	338	8% 83% 15%
32	8	206	32% 48% 52%
33	9	137	18% 85% 15%

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Mol	Chain	Length	Quality of chain
34	a	142	6% 56% 42%
35	b	215	6% 67% 31%
36	c	332	5% 82% 17%
37	d	306	17% 68% 31%
38	e	279	67% 76% 22%
39	f	212	38% 54% 45%
40	g	166	6% 75% 22%
41	h	158	9% 62% 37%
42	i	128	16% 71% 5% 24%
43	j	123	8% 69% 31%
44	k	112	63% 71% 29%
45	l	138	14% 17% 83%
46	m	128	30% 33% 65%
47	o	102	6% 77% 23%
48	p	206	19% 61% 38%
49	q	222	12% 56% 42%
50	r	196	15% 73% 26%
51	s	439	10% 82% 16%
52	t	28	100% 100%
53	u	234	10% 47% 53%
54	v	70	50% 97%
55	w	156	47% 50% 49%

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 90739 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1092	23184	10409	4202	7481	1092	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a RNA chain called mitochondrial tRNAVal.

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

- Molecule 3 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	220	1706	1059	339	299	9	0	0

- Molecule 4 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	285	2258	1457	384	406	11	0	0

- Molecule 5 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 6 is a protein called 39S ribosomal protein L9, mitochondrial.

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

- Molecule 7 is a protein called 39S ribosomal protein L10, mitochondrial.

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

- Molecule 8 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 9 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 10 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 11 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 12 is a protein called 39S ribosomal protein L16, mitochondrial.

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

- Molecule 13 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 14 is a protein called 39S ribosomal protein L18, mitochondrial.

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

- Molecule 15 is a protein called 39S ribosomal protein L19, mitochondrial.

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

- Molecule 16 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	R	140	1153	732	231	186	4	0	0

- Molecule 17 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 18 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	T	159	1305	835	239	224	7	0	0

- Molecule 19 is a protein called 39S ribosomal protein L23, mitochondrial.

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

- Molecule 20 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	V	192	1575	1003	281	283	8	0	0

- Molecule 21 is a protein called 39S ribosomal protein L27, mitochondrial.

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

- Molecule 22 is a protein called 39S ribosomal protein L28, mitochondrial.

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

- Molecule 23 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 24 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Z	120	978	626	183	166	3	0	0

- Molecule 25 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	0	108	880	545	172	157	6	0	0

- Molecule 26 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	1	52	433	278	83	70	2	0	0

- Molecule 27 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	2	43	351	218	76	56	1	0	0

- Molecule 28 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	3	95	831	539	162	127	3	0	0

- Molecule 29 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	5	387	3156	2039	548	558	11	0	0

- Molecule 30 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	6	324	2640	1694	470	468	8	0	0

- Molecule 31 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	7	287	2334	1495	397	425	17	0	0

- Molecule 32 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	8	99	836	535	144	155	2	0	0

- Molecule 33 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	9	117	947	614	163	168	2	0	0

- Molecule 34 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	a	82	686	434	124	123	5	0	0

- Molecule 35 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 36 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 37 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	d	211	1741	1123	299	309	10	0	0

- Molecule 38 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	e	217	1762	1124	310	323	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	f	116	915	585	152	175	3	0	0

- Molecule 40 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- Molecule 41 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	h	100	827	524	146	155	2	0	0

- Molecule 42 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 43 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 44 is a protein called 39S ribosomal protein L53, mitochondrial.

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

- Molecule 45 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
45	l	23	221	137	52	32	0	0

- Molecule 46 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	m	45	372	232	76	62	2	0	0

- Molecule 47 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	o	79	665	420	130	112	3	0	0

- Molecule 48 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 49 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		
49	q	128	1076	671	208	192	5	0	0

- Molecule 50 is a protein called 39S ribosomal protein S18a, mitochondrial.

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

- Molecule 51 is a protein called 39S ribosomal protein S30, mitochondrial.

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

- Molecule 52 is a protein called Unknown protein or protein extension.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	t	28	140	84	28	28	0	0

- Molecule 53 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

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

- Molecule 54 is a protein called MIEF1 upstream open reading frame protein.

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

- Molecule 55 is a protein called Acyl carrier protein, mitochondrial.

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

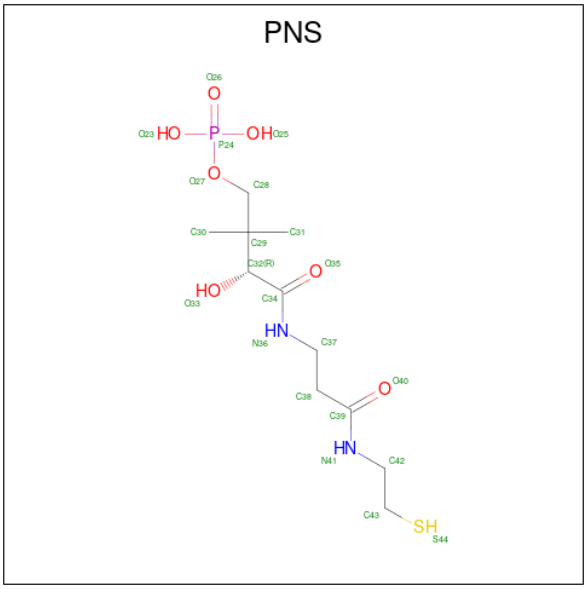
- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
56	A	47	47	47	0
56	W	1	1	1	0
56	g	1	1	1	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
57	I	1	1	1	0
57	0	1	1	1	0

- Molecule 58 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).



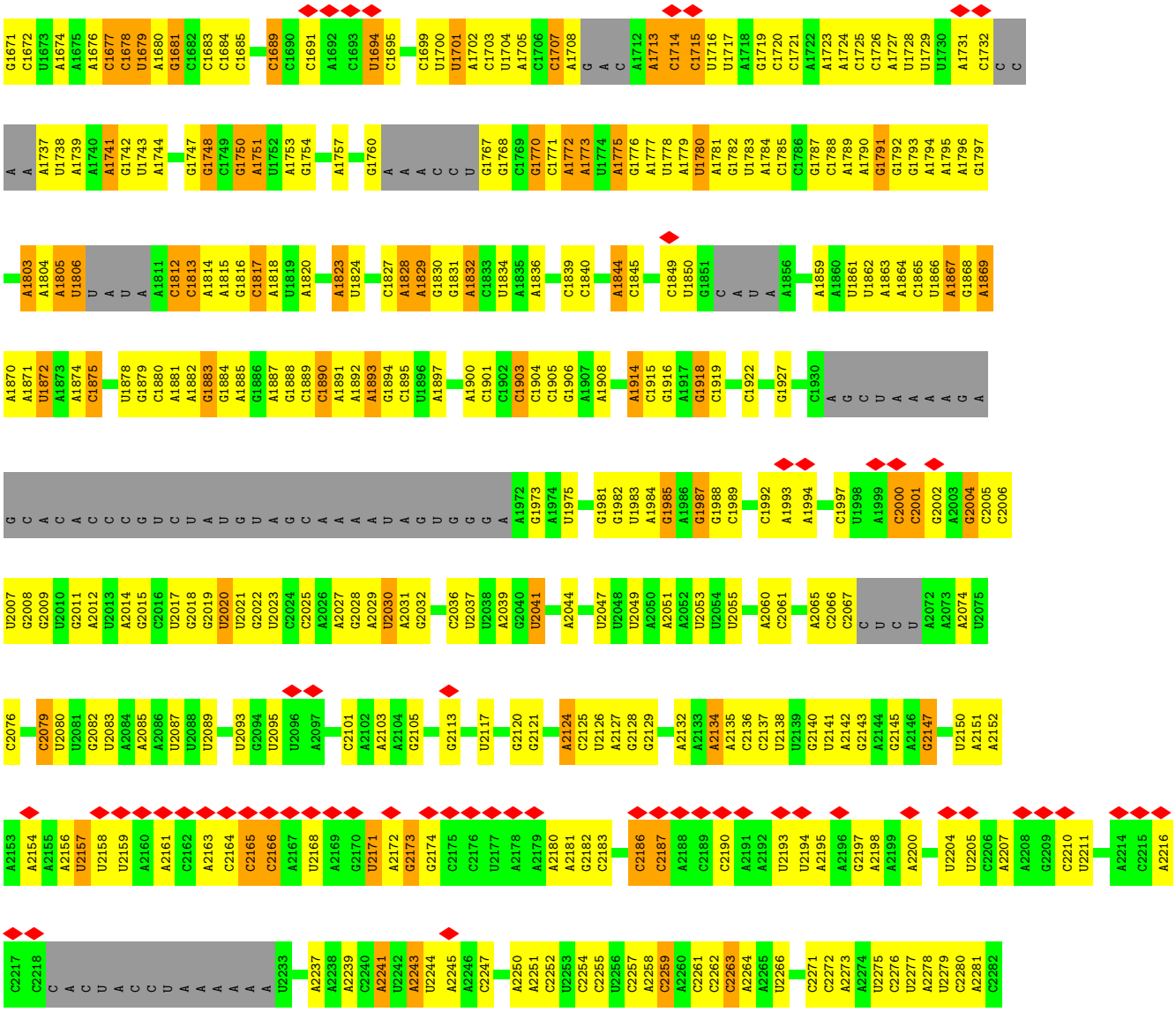
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
58	v	1	21	11	2	6	1	1	0

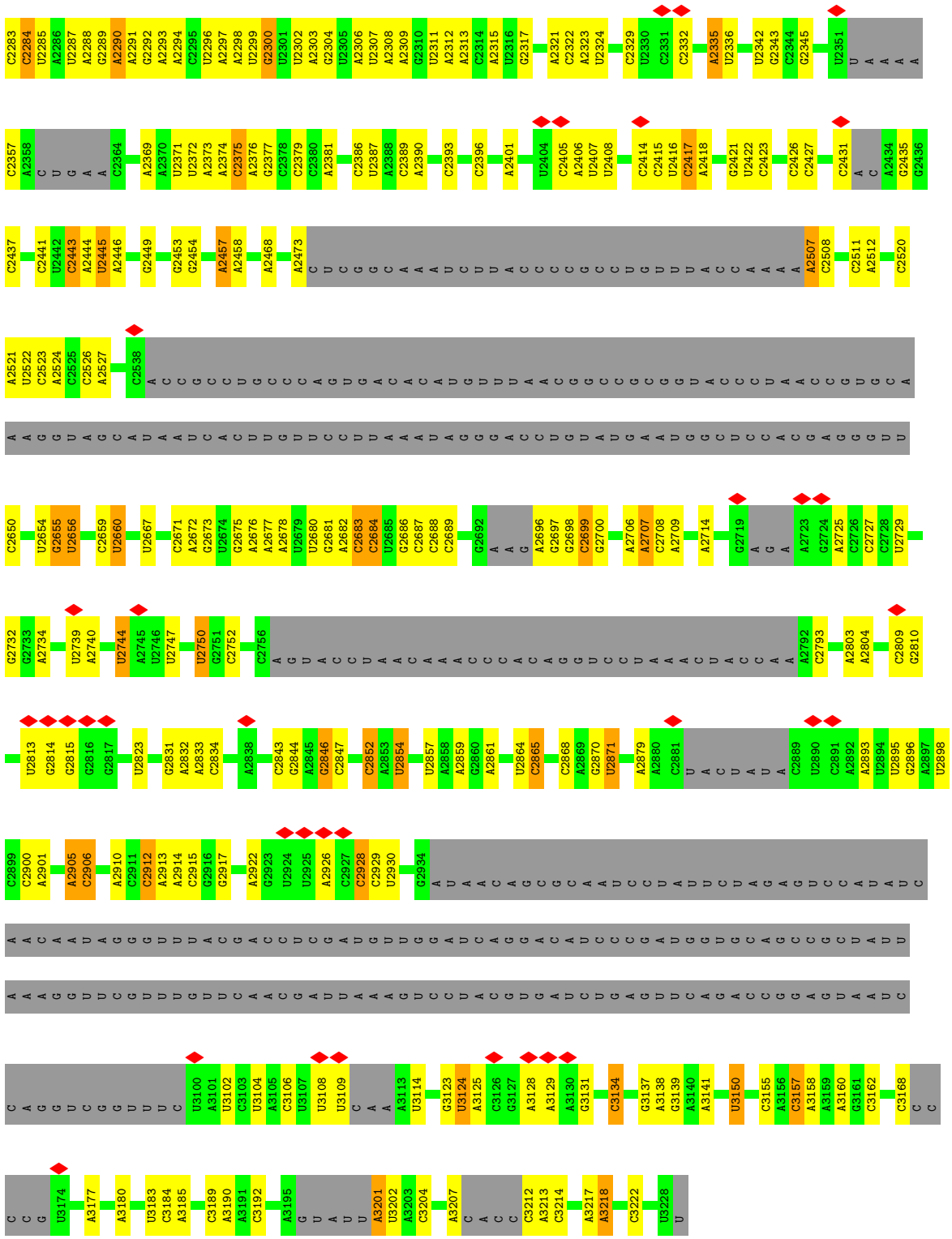
3 Residue-property plots (i)

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: 16S ribosomal RNA

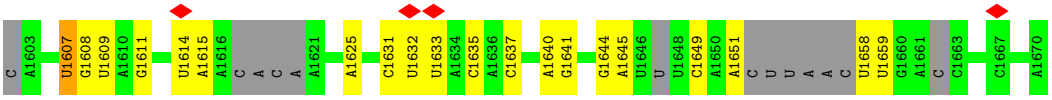
Chain A: 6% 35% 29% 6% 30%





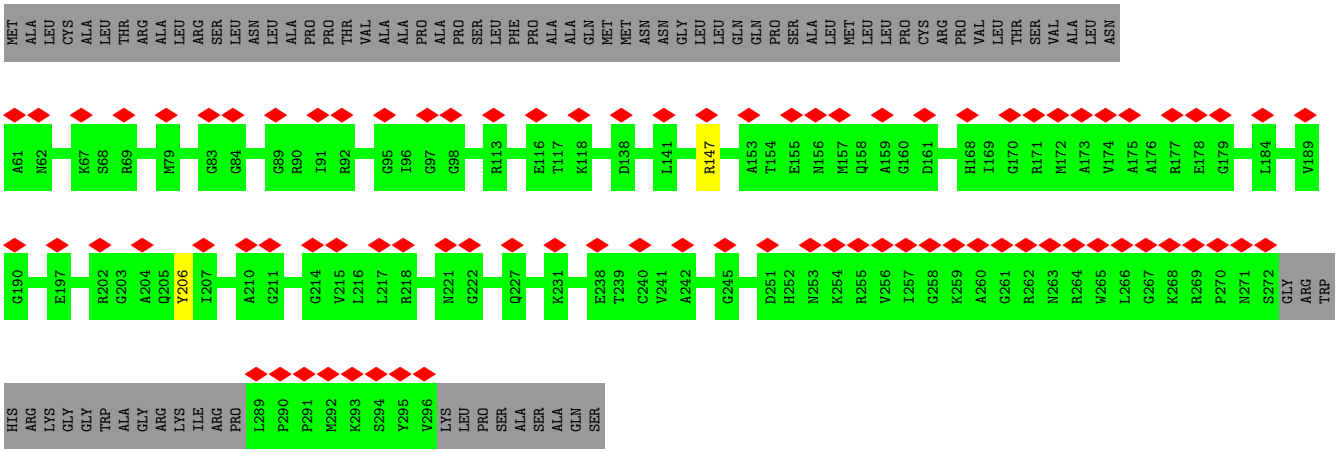
• Molecule 2: mitochondrial tRNAVal

Chain B:



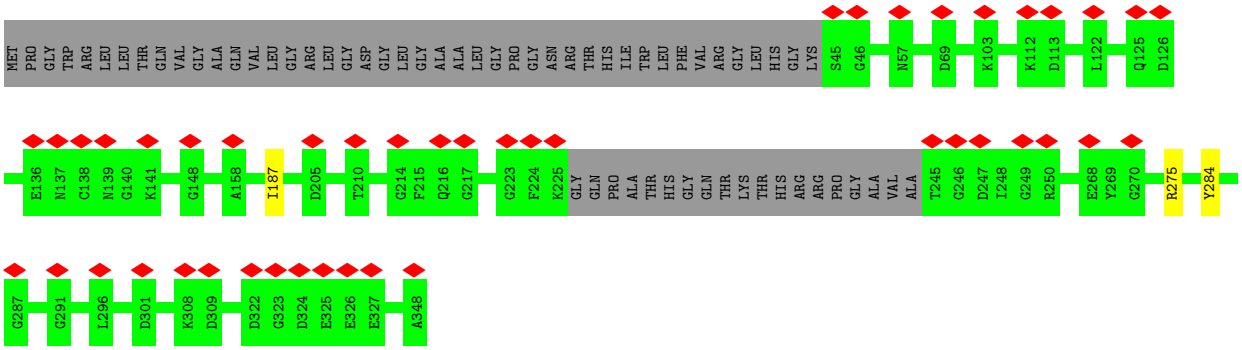
- Molecule 3: 39S ribosomal protein L2, mitochondrial

Chain D:



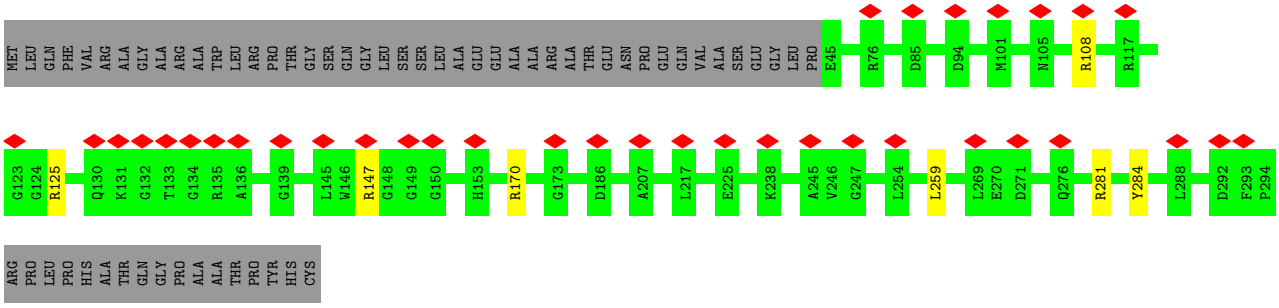
- Molecule 4: 39S ribosomal protein L3, mitochondrial

Chain E:



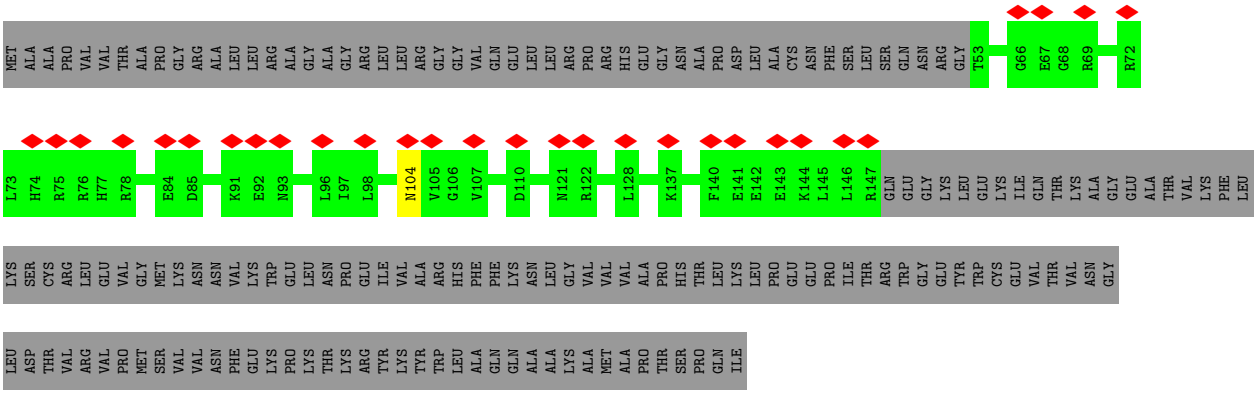
- Molecule 5: 39S ribosomal protein L4, mitochondrial

Chain F:



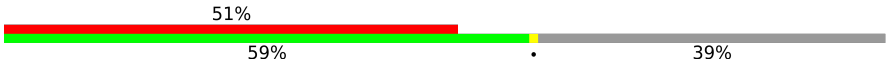
- Molecule 6: 39S ribosomal protein L9, mitochondrial

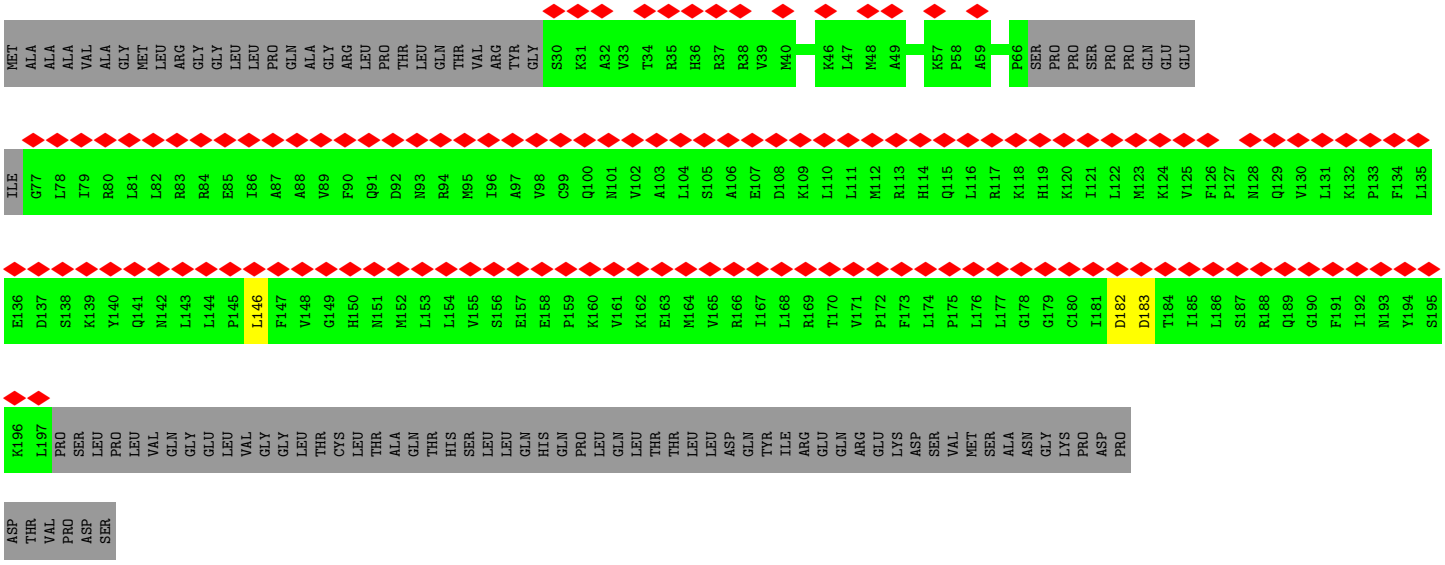
Chain H:



- Molecule 7: 39S ribosomal protein L10, mitochondrial

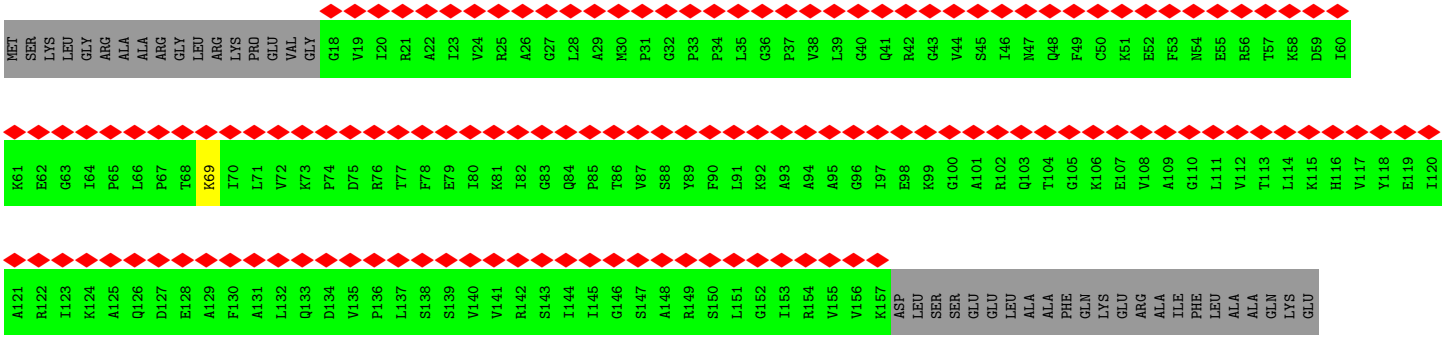
Chain I:





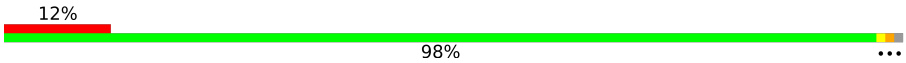
- Molecule 8: 39S ribosomal protein L11, mitochondrial

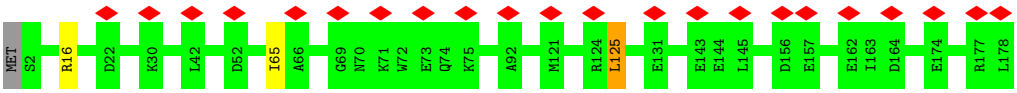
Chain J:



• Molecule 9: 39S ribosomal protein L13, mitochondrial

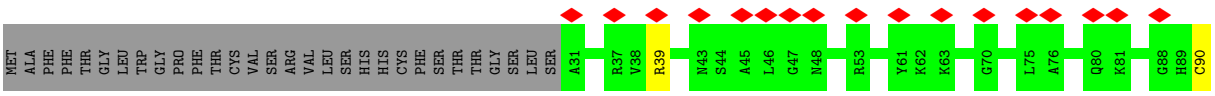
Chain K:

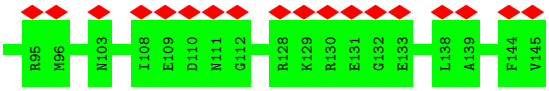




• Molecule 10: 39S ribosomal protein L14, mitochondrial

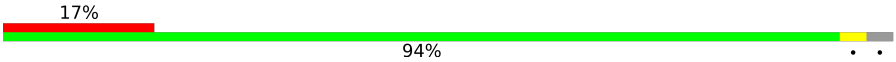
Chain L:

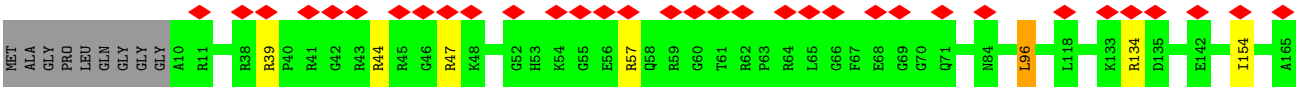


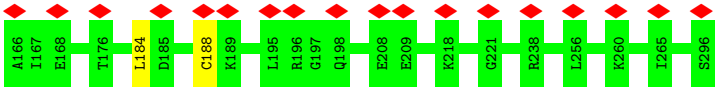


• Molecule 11: 39S ribosomal protein L15, mitochondrial

Chain M:

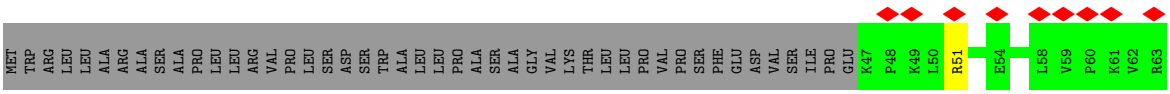


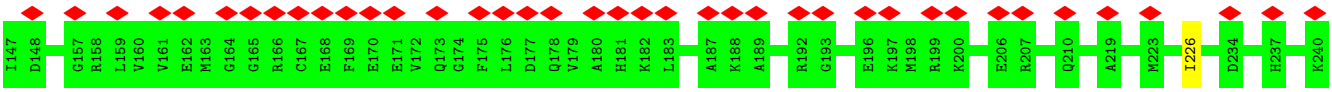


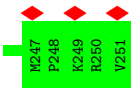


• Molecule 12: 39S ribosomal protein L16, mitochondrial

Chain N:

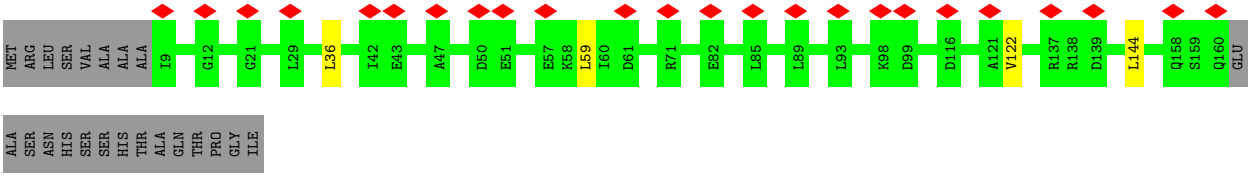






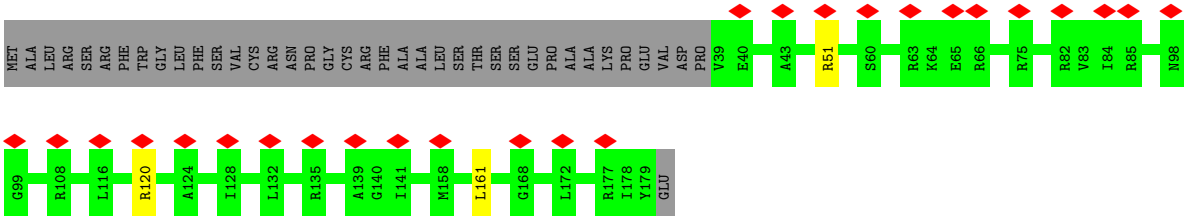
- Molecule 13: 39S ribosomal protein L17, mitochondrial

Chain O:



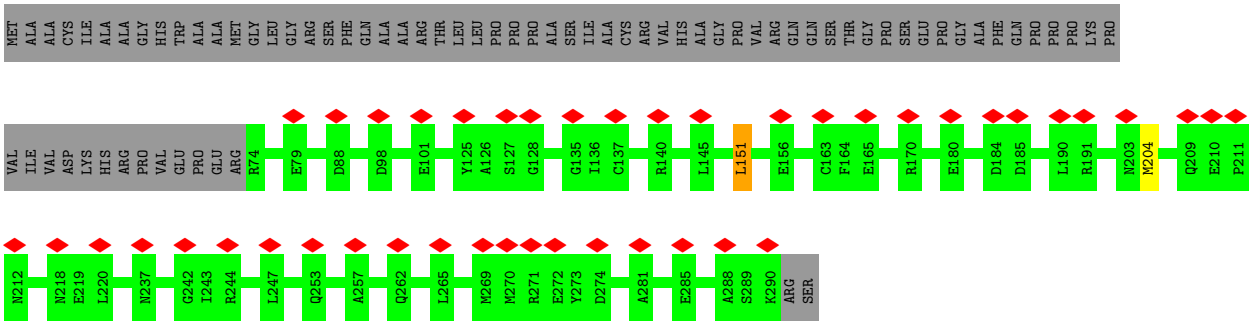
- Molecule 14: 39S ribosomal protein L18, mitochondrial

Chain P:



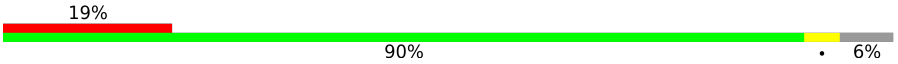
- Molecule 15: 39S ribosomal protein L19, mitochondrial

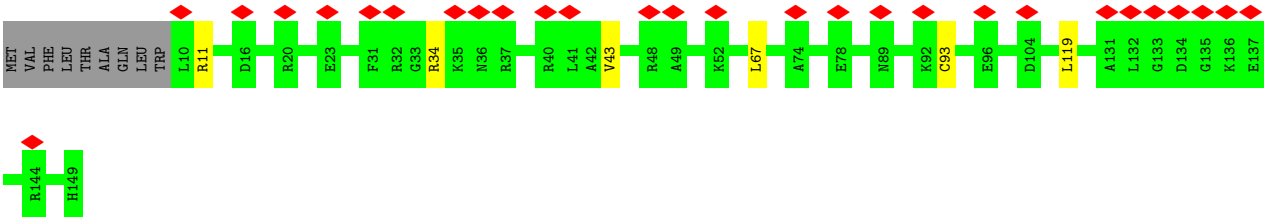
Chain Q:



- Molecule 16: 39S ribosomal protein L20, mitochondrial

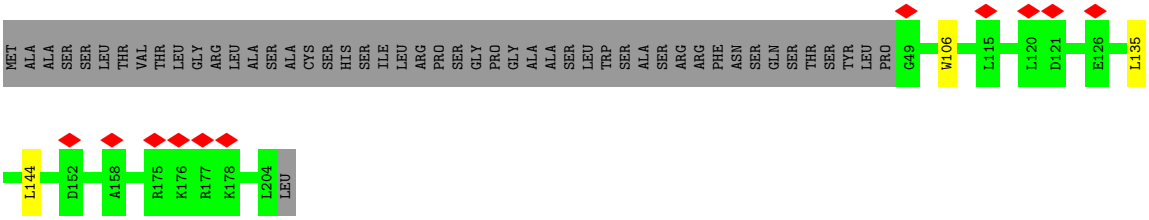
Chain R:





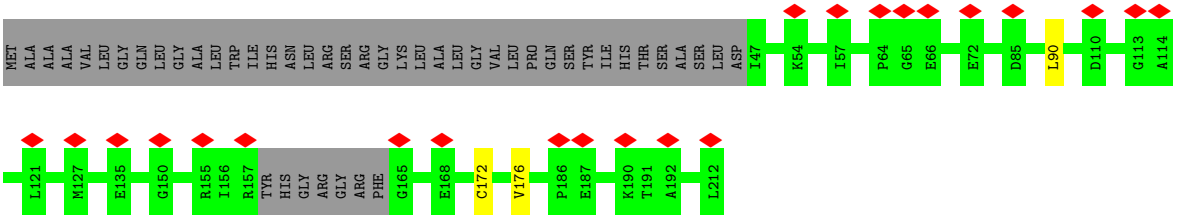
- Molecule 17: 39S ribosomal protein L21, mitochondrial

Chain S:



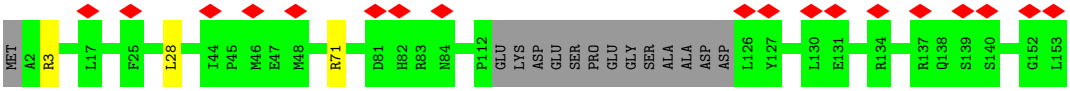
• Molecule 18: 39S ribosomal protein L22, mitochondrial

Chain T:



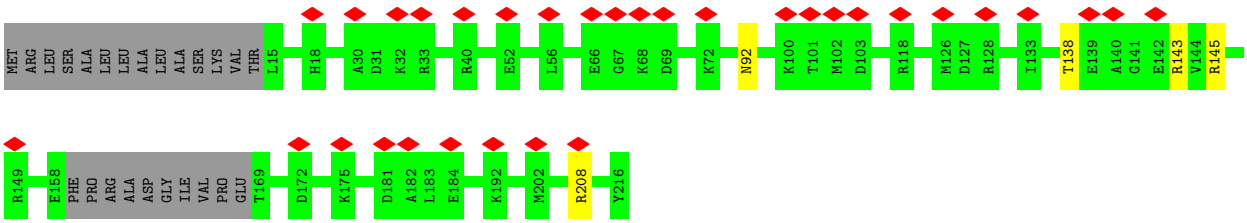
• Molecule 19: 39S ribosomal protein L23, mitochondrial

Chain U:



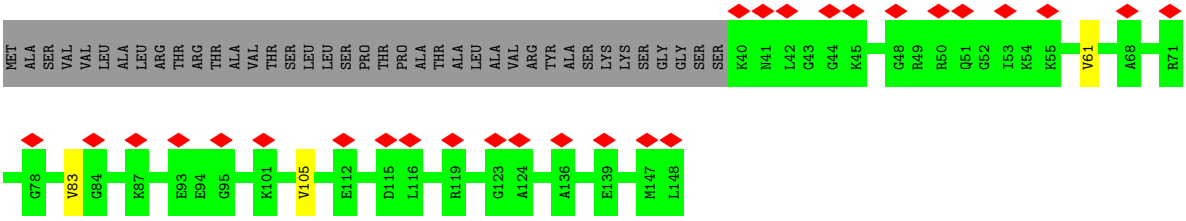
• Molecule 20: 39S ribosomal protein L24, mitochondrial

Chain V:



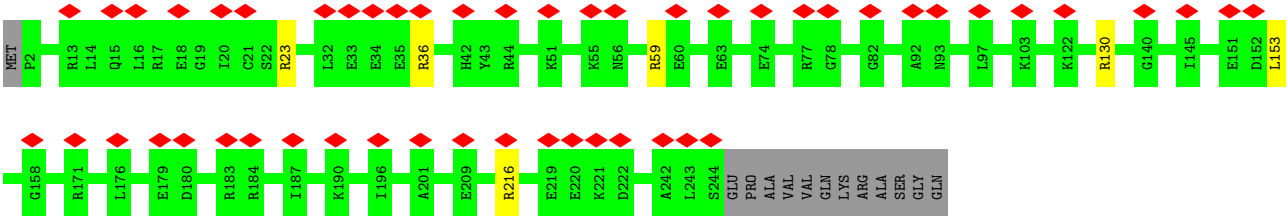
• Molecule 21: 39S ribosomal protein L27, mitochondrial

Chain W:



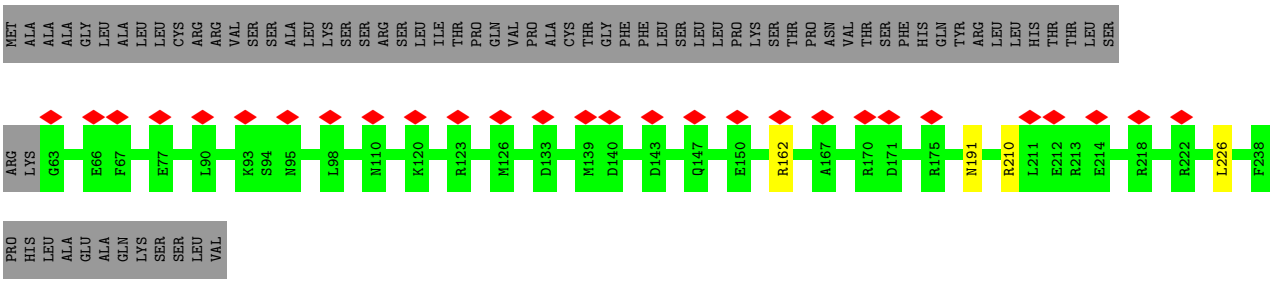
• Molecule 22: 39S ribosomal protein L28, mitochondrial

Chain X: 20% 93% • 5%



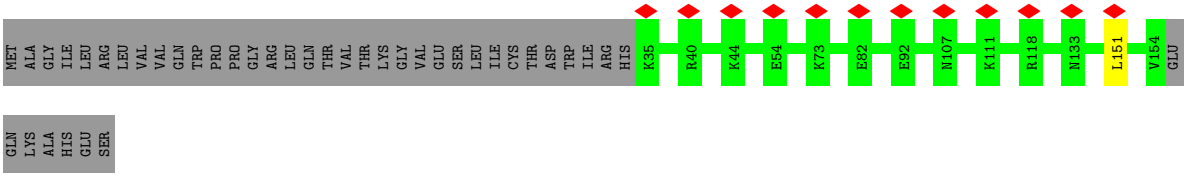
• Molecule 23: 39S ribosomal protein L47, mitochondrial

Chain Y: 11% 69% • 30%



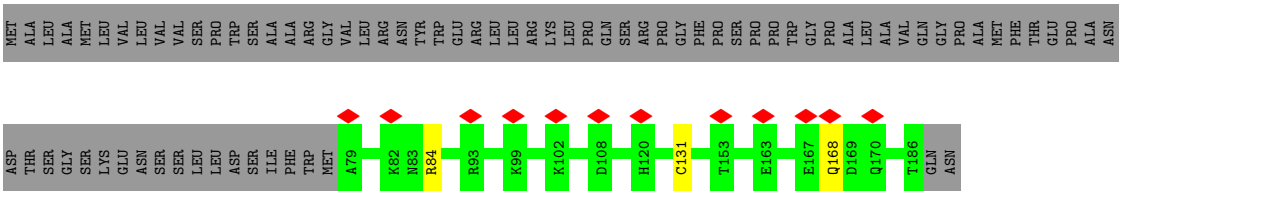
• Molecule 24: 39S ribosomal protein L30, mitochondrial

Chain Z: 7% 74% • 25%



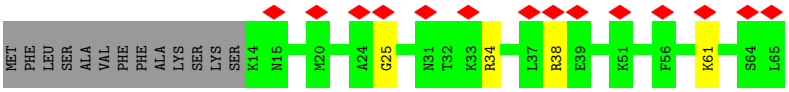
• Molecule 25: 39S ribosomal protein L32, mitochondrial

Chain 0: 6% 56% • 43%



• Molecule 26: 39S ribosomal protein L33, mitochondrial

Chain 1: 22% 74% 6% 20%



• Molecule 27: 39S ribosomal protein L34, mitochondrial

Chain 2: 11% 46% • 53%

MET ALA VAL LEU ALA GLY SER LEU LEU LEU GLY PRO THR SER ARG SER ALA ALA ALA LEU LEU GLY GLY ARG TRP LEU GLN PRO ARG ALA TRP LEU GLY PHE PRO ASP ALA TRP GLY LEU PRO THR PRO GLN GLN ALA ARG GLY LYS ALA ARG G50 N51 E52 Y53 Q54 K59 G65 A74

G75 V76 Q77 R81 R87 H92

• Molecule 28: 39S ribosomal protein L35, mitochondrial

Chain 3: 11% 49% • 49%

MET ALA ALA SER ALA PHE ALA GLY ALA VAL ARG ALA ALA SER GLY ILE LEU ARG PRO LEU ASN ILE LEU ALA SER SER THR TYR ARG ASN CYS VAL LYS ASN ALA SER LEU ILE SER ALA LEU SER THR GLY ARG PHE SER HIS ILE GLN THR PRO VAL VAL SER SER THR PRO ARG LEU

THR THR SER GLU ARG ASN LEU THR CYS GLY HIS THR SER VAL ILE LEU ASN ARG MET ALA PRO VAL LEU PRO SER VAL LEU LYS LEU PRO VAL ARG SER L94 R100 A109 V110 R113 R125 K126 A127 K131 K132 K135 R140 R143 E146 K156 L157 L158

M161 R168 D174 Y177 Y180 H181 D182 K187 V188

• Molecule 29: 39S ribosomal protein L37, mitochondrial

Chain 5: 16% 89% • 9%

MET ALA LEU ALA SER GLY PRO ALA ARG ARG ALA LEU ALA GLY SER GLY GLN LEU GLY LEU GLY GLY PHE GLY ALA PRO ARG ARG GLY ALA Y31 R36 R39 K40 S41 E42 P43 R48 L55 Y82 L98 D101 Q102 A103 I106 R112 E115 G116 L128

E134 D141 D142 P143 R144 M145 N149 Q150 D151 E152 L155 E169 M183 L187 L198 C203 S217 L218 R223 G224 S225 G226 G227 A228 R229 D234 I239 A240 E243 E244 N250 E254 I263 D264 I270 K274 N275 D276 T277 G278

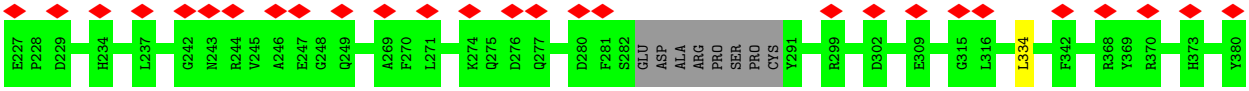
V292 L293 L294 D295 R303 F318 G330 N331 D332 A333 L336 E337 T347 D348 G349 R350 L359 L364 K371 N372 L373 A374 D377 S378 D379 I392 LYS LYS ARG VAL VAL V398 E399 K407 L415 A422 ALA

• Molecule 30: 39S ribosomal protein L38, mitochondrial

Chain 6: 18% 84% • 15%

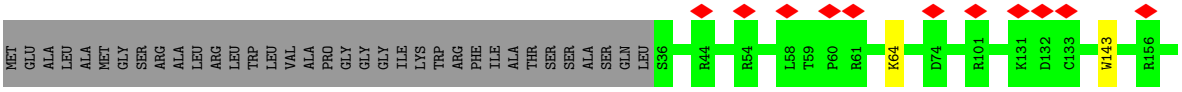
MET ALA ALA PRO TRP TRP ARG ALA ALA LEU CYS GLU CYS ARG ARG TRP ARG GLY PHE SER THR SER ALA VAL LEU GLY R27 R28 M35 S38 D39 I40 D41 L42 S43 N44 L45 E46 R47 L48 R52 R56 R60 E64 E76 G79 GLU LYS THR ASP PRO LYS

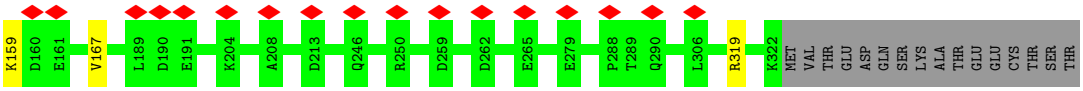
GLU LYS ILE ASP ILE GLY LEU PRO PRO PRO LYS VAL SER R99 A115 R124 L125 R126 T127 A128 A134 R141 A152 Y158 R159 A165 R170 G180 E181 D182 D183 L184 C189 G190 E197 E207 A208 E209 GLU GLY SER L213 L216 L217 L221



• Molecule 31: 39S ribosomal protein L39, mitochondrial

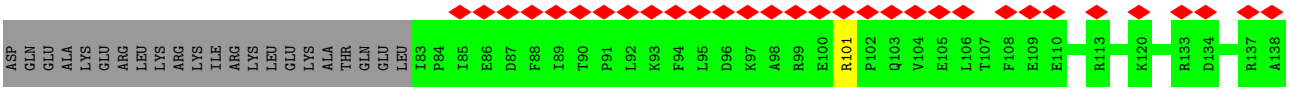
Chain 7:

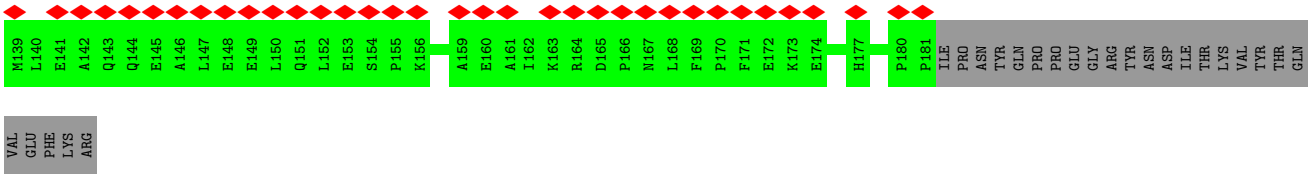




• Molecule 32: 39S ribosomal protein L40, mitochondrial

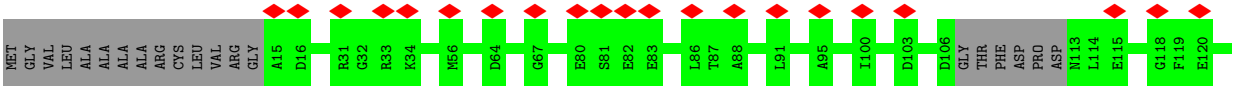
Chain 8:

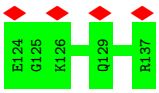




• Molecule 33: 39S ribosomal protein L41, mitochondrial

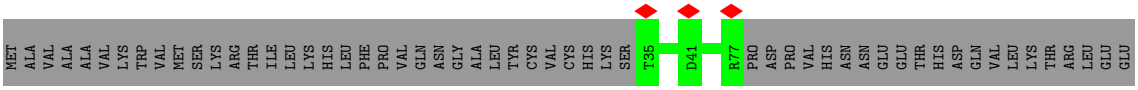
Chain 9:

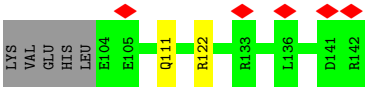




• Molecule 34: 39S ribosomal protein L42, mitochondrial

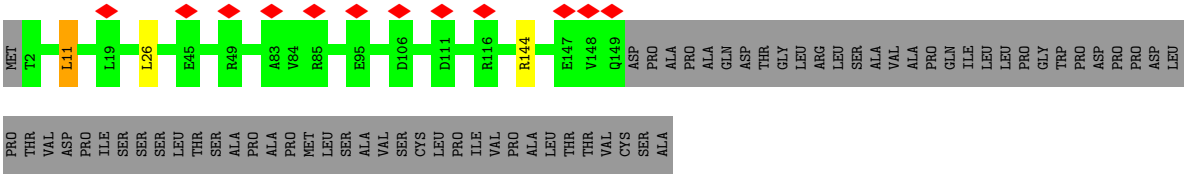
Chain a:





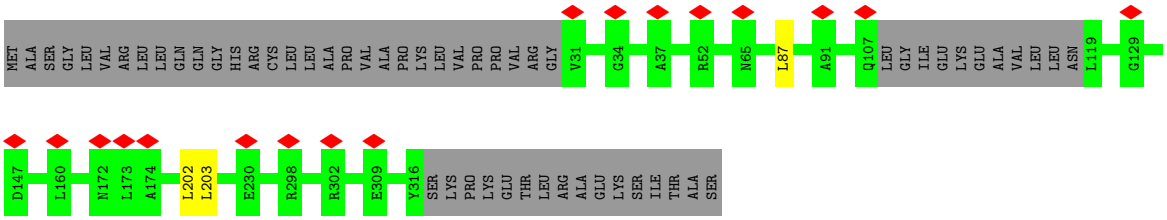
• Molecule 35: 39S ribosomal protein L43, mitochondrial

Chain b:



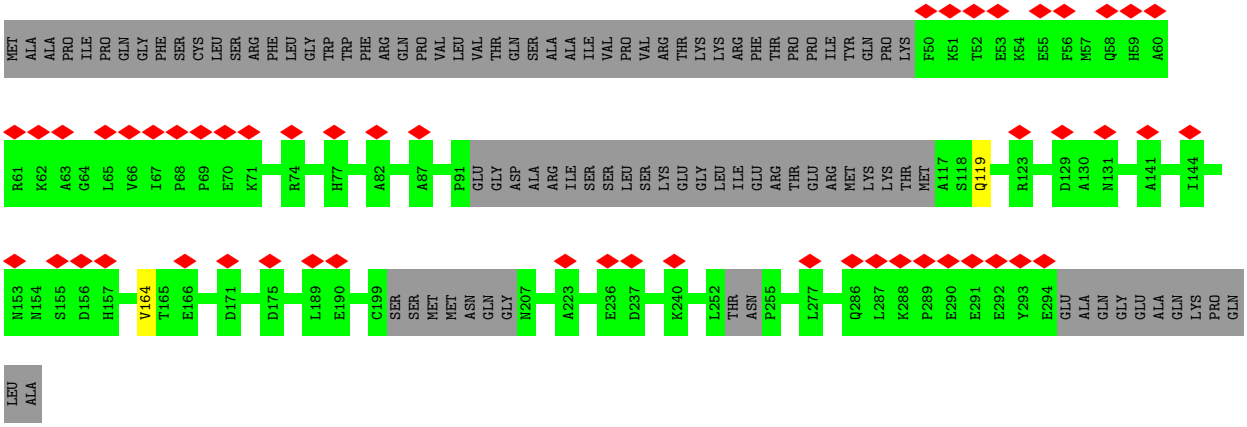
• Molecule 36: 39S ribosomal protein L44, mitochondrial

Chain c:



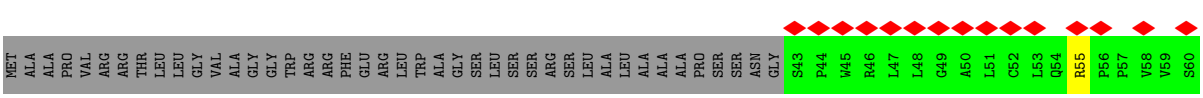
• Molecule 37: 39S ribosomal protein L45, mitochondrial

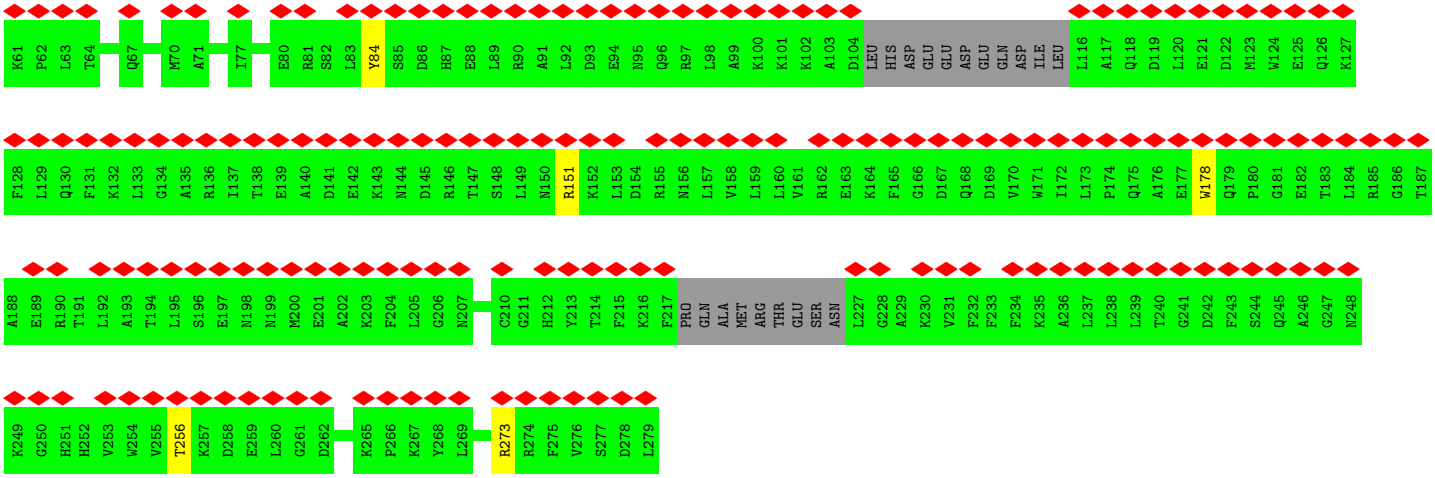
Chain d:



• Molecule 38: 39S ribosomal protein L46, mitochondrial

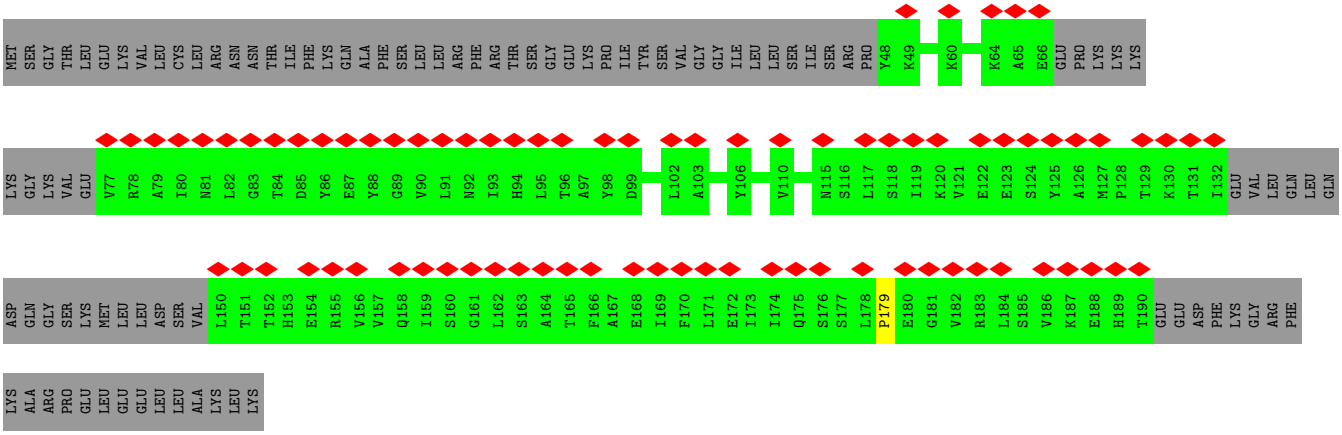
Chain e:





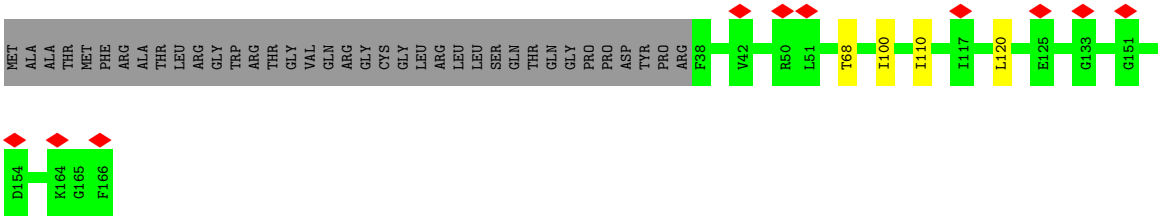
- Molecule 39: 39S ribosomal protein L48, mitochondrial

Chain f:



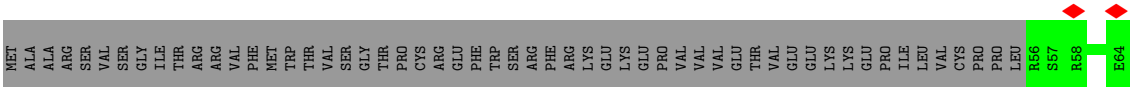
- Molecule 40: 39S ribosomal protein L49, mitochondrial

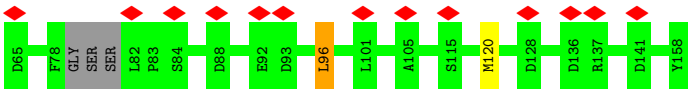
Chain g:



- Molecule 41: 39S ribosomal protein L50, mitochondrial

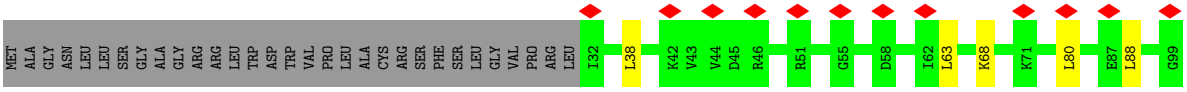
Chain h:

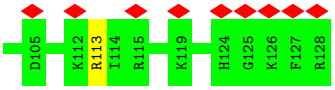




• Molecule 42: 39S ribosomal protein L51, mitochondrial

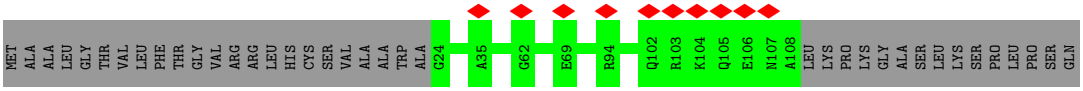
Chain i:





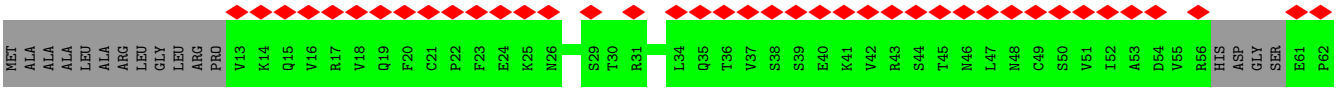
• Molecule 43: 39S ribosomal protein L52, mitochondrial

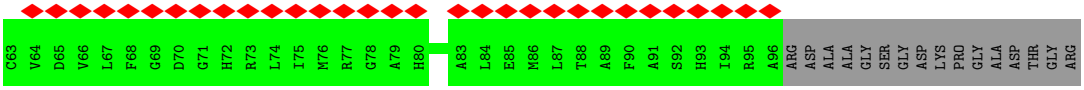
Chain j:



• Molecule 44: 39S ribosomal protein L53, mitochondrial

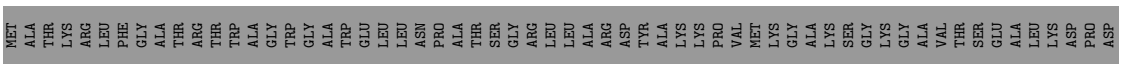
Chain k:

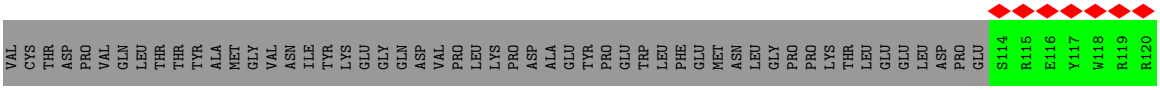


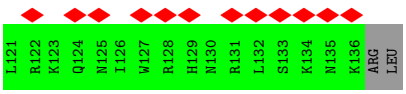


• Molecule 45: 39S ribosomal protein L54, mitochondrial

Chain l:

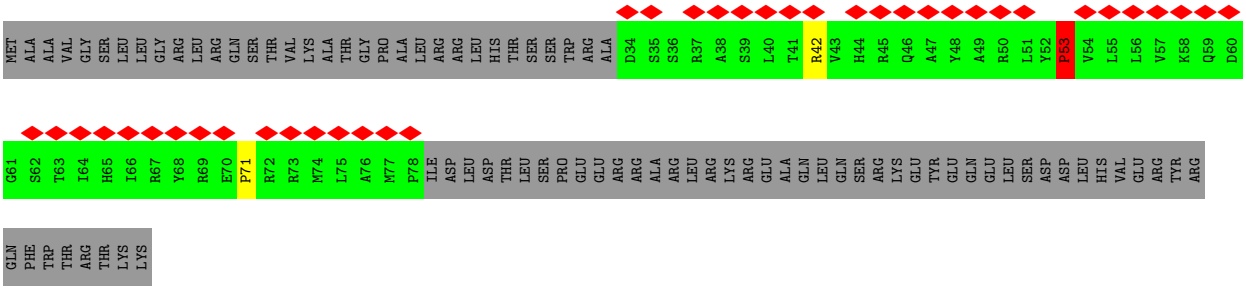






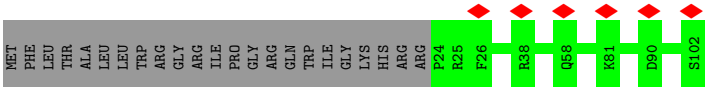
• Molecule 46: 39S ribosomal protein L55, mitochondrial

Chain m:



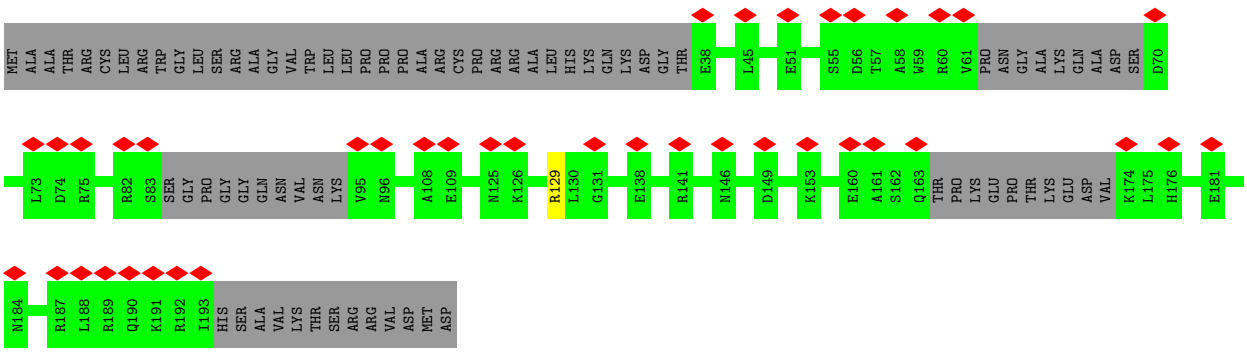
- Molecule 47: Ribosomal protein 63, mitochondrial

Chain o:



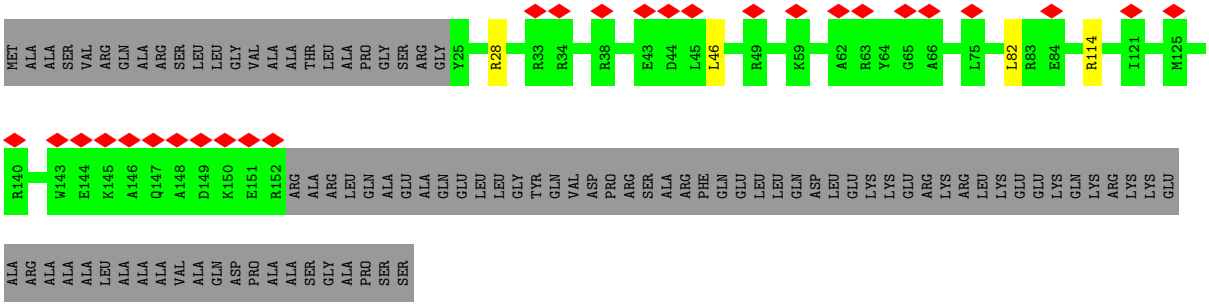
- Molecule 48: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p:



- Molecule 49: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:



- Molecule 50: 39S ribosomal protein S18a, mitochondrial

Chain r: 15% 73% • 26%

MET ALA ALA LEU LYS ALA LEU VAL SER GLY CYS GLY ARG LEU LEU ARG GLY LEU LEU ALA GLY PRO ALA ALA THR SER TRP SER ARG LEU PRO ALA ARG GLY F35 R36 E37 V38 V39 E40 T41 GLN GLU GLY LYS THR T47 I48 I49 E50 G51 R52 I53 T54 A55 T56 P57 K58 R74

D84 G97 I104 E111 M121 L127 R132 P133 R134 LEU PRO GLU GLY VAL VAL PRO LYS SER LYS PRO Q146 R171 V172 R173 L180 R189 H196

- Molecule 51: 39S ribosomal protein S30, mitochondrial

Chain s: 10% 82% • 16%

MET ALA ALA ARG CYS TRP ARG PRO LEU LEU ARG GLY PRO ARG LEU SER LEU HIS THR ALA ALA ASN ALA ALA ALA THR ALA THR GLU THR THR CYS GLN ASP VAL ALA ALA THR PRO V41 A42 R43 A58 D77 R81 K85 P119 PRO PRO PRO ALA GLU PRO GLU

PRO GLU PRO GLU PRO GLU PRO GLU PRO ALA LEU ASP LEU A140 A141 L142 C149 E153 R159 R160 R161 E167 E170 L174 D178 S182 L188 S189 A197 A198 A199 L200 D201 Y202 R203 E215 D227 D228 L229 R230 D235 N238 I259 D269

K270 N280 F299 H300 L301 L306 C316 A330 A334 A338 M341 E348 A349 D350 V360 I361 T362 D363 G364 L374 L379 Q382 N386 G395 D409 I421 K430 GLU GLU LYS SER GLN LEU LEU GLU ASN

- Molecule 52: Unknown protein or protein extension

Chain t: 100% 100%

X1 X2 X3 X4 X5 X6 X7 X8 X9 X10 X11 X12 X13 X14 X15 X16 X17 X18 X19 X20 X21 X22 X23 X24 X25 X26 X27 X28

- Molecule 53: Mitochondrial assembly of ribosomal large subunit protein 1

Chain u: 10% 47% 53%

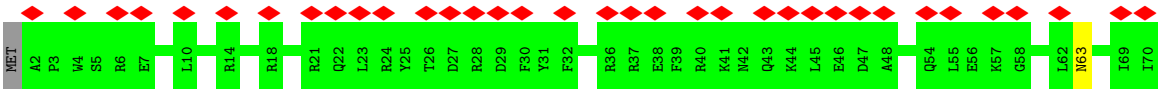
MET GLY PRO GLY GLY ARG VAL ALA ARG LEU LEU ALA PRO LEU MET TRP ARG ARG ARG ALA VAL SER SER VAL ALA ALA GLY SER ALA VAL GLY ALA GLU PRO GLY LEU ARG LEU LEU ALA VAL GLN ARG LEU PRO VAL GLY ALA ALA PHE CYS ARG ALA CYS GLN THR PRO ASN PHE VAL ARG GLY

LEU HIS SER GLU PRO GLY LEU GLU GLU ARG ALA GLU GLY THR VAL ASN GLU GLY ARG PRO GLU SER ASP ALA ALA ASP HIS THR GLY PRO K91 S99 Q103 R107 M118 R119 R133 A137 Y141 H148 K152 R153 D154 K158 I159 K162 D163 T164 D165

D166 D171 F172 G173 Y188 E191 R197 D201 GLN LEU ALA GLN ILE ALA PRO GLU THR VAL PRO GLU ASP PHE ILE LEU GLY ILE GLU ASP ASP THR SER SER VAL THR PRO VAL GLU LEU LYS CYS GLU

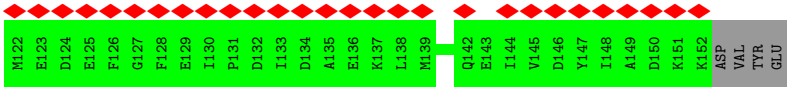
- Molecule 54: MIEF1 upstream open reading frame protein

Chain v: 50% 97% ••



- Molecule 55: Acyl carrier protein, mitochondrial

Chain w:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	379869	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 ($e^-/Å^2$)	1.56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130841	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.350	Depositor
Minimum map value	-0.156	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	373.12, 373.12, 373.12	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: PNS, ZN, MG

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	1.77	301/25926 (1.2%)	1.45	433/40305 (1.1%)
2	B	0.71	0/1328	1.26	10/2056 (0.5%)
3	D	0.58	0/1736	0.65	0/2335
4	E	0.74	0/2322	0.71	1/3148 (0.0%)
5	F	0.94	1/2071 (0.0%)	0.81	0/2817
6	H	0.65	0/798	0.71	0/1073
7	I	0.41	0/1308	0.68	2/1761 (0.1%)
8	J	0.30	0/1077	0.58	0/1452
9	K	0.84	0/1495	0.76	2/2029 (0.1%)
10	L	0.51	0/904	0.63	1/1218 (0.1%)
11	M	0.88	1/2359 (0.0%)	0.80	4/3185 (0.1%)
12	N	0.56	0/1697	0.63	0/2281
13	O	0.84	1/1269 (0.1%)	0.83	2/1708 (0.1%)
14	P	0.68	0/1173	0.71	1/1588 (0.1%)
15	Q	0.60	1/1846 (0.1%)	0.69	2/2487 (0.1%)
16	R	1.04	3/1174 (0.3%)	0.89	5/1572 (0.3%)
17	S	0.91	1/1276 (0.1%)	0.82	2/1729 (0.1%)
18	T	1.00	1/1335 (0.1%)	0.76	2/1796 (0.1%)
19	U	0.87	0/1183	0.78	1/1600 (0.1%)
20	V	0.73	0/1616	0.64	0/2189
21	W	0.92	2/881 (0.2%)	0.72	0/1188
22	X	0.68	0/2090	0.69	1/2825 (0.0%)
23	Y	0.83	0/1552	0.71	1/2079 (0.0%)
24	Z	0.82	1/1003 (0.1%)	0.74	0/1354
25	0	0.85	1/895 (0.1%)	0.74	0/1201
26	1	0.63	0/438	0.81	0/583
27	2	1.05	1/357 (0.3%)	0.84	0/475
28	3	1.03	0/852	0.79	1/1136 (0.1%)
29	5	0.65	0/3250	0.70	2/4429 (0.0%)
30	6	0.66	0/2726	0.65	2/3715 (0.1%)
31	7	0.67	1/2391 (0.0%)	0.67	0/3234
32	8	0.39	0/855	0.55	0/1152

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	9	0.75	0/972	0.68	0/1306
34	a	0.84	0/709	0.65	0/963
35	b	0.92	0/1202	0.78	2/1626 (0.1%)
36	c	0.78	0/2264	0.71	1/3059 (0.0%)
37	d	0.64	0/1790	0.66	0/2423
38	e	0.30	0/1797	0.59	2/2422 (0.1%)
39	f	0.47	0/931	0.58	0/1259
40	g	0.91	0/1102	0.77	1/1503 (0.1%)
41	h	0.63	0/847	0.71	1/1150 (0.1%)
42	i	1.05	1/849 (0.1%)	0.87	5/1135 (0.4%)
43	j	0.75	0/698	0.64	0/940
44	k	0.32	0/635	0.60	0/855
45	l	0.29	0/226	0.43	0/299
46	m	0.29	0/379	0.75	1/510 (0.2%)
47	o	0.74	0/682	0.66	0/916
48	p	0.53	0/1071	0.62	0/1433
49	q	0.58	0/1107	0.59	0/1498
50	r	0.69	0/1238	0.67	0/1676
51	s	0.80	0/3114	0.77	5/4225 (0.1%)
53	u	0.40	0/949	0.59	0/1281
54	v	0.35	0/597	0.58	0/796
55	w	0.31	0/647	0.61	0/871
All	All	1.11	317/94989 (0.3%)	1.00	493/133846 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
8	J	0	1
26	1	0	1
31	7	0	1
40	g	0	1
46	m	0	1
51	s	0	1
All	All	0	6

The worst 5 of 317 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1789	A	N9-C4	-9.69	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2308	A	N9-C4	-8.74	1.32	1.37
1	A	1751	A	N9-C8	-7.99	1.31	1.37
1	A	1864	A	C5-C4	-7.96	1.33	1.38
42	i	68	LYS	C-N	-7.79	1.16	1.34

The worst 5 of 493 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2066	C	N1-C2-O2	10.36	125.12	118.90
1	A	2322	C	N1-C2-O2	10.29	125.08	118.90
1	A	2252	C	C5-C6-N1	10.02	126.01	121.00
38	e	178	TRP	C-N-CA	10.01	146.71	121.70
1	A	2372	U	N3-C2-O2	-9.99	115.21	122.20

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	1	25	GLY	Peptide
31	7	159	LYS	Peptide
8	J	69	LYS	Peptide
40	g	110	ILE	Peptide
46	m	53	PRO	Mainchain

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	
3	D	216/305 (71%)	203 (94%)	13 (6%)	0	100	100
4	E	281/348 (81%)	273 (97%)	8 (3%)	0	100	100
5	F	248/311 (80%)	234 (94%)	14 (6%)	0	100	100
6	H	93/267 (35%)	85 (91%)	7 (8%)	1 (1%)	14	47
7	I	154/261 (59%)	141 (92%)	13 (8%)	0	100	100
8	J	138/192 (72%)	120 (87%)	18 (13%)	0	100	100
9	K	175/178 (98%)	166 (95%)	9 (5%)	0	100	100
10	L	113/145 (78%)	106 (94%)	7 (6%)	0	100	100
11	M	285/296 (96%)	275 (96%)	10 (4%)	0	100	100
12	N	203/251 (81%)	192 (95%)	11 (5%)	0	100	100
13	O	150/175 (86%)	145 (97%)	5 (3%)	0	100	100
14	P	139/180 (77%)	130 (94%)	9 (6%)	0	100	100
15	Q	215/292 (74%)	200 (93%)	15 (7%)	0	100	100
16	R	138/149 (93%)	133 (96%)	5 (4%)	0	100	100
17	S	154/205 (75%)	147 (96%)	7 (4%)	0	100	100
18	T	155/206 (75%)	152 (98%)	3 (2%)	0	100	100
19	U	135/153 (88%)	126 (93%)	9 (7%)	0	100	100
20	V	188/216 (87%)	183 (97%)	5 (3%)	0	100	100
21	W	107/148 (72%)	103 (96%)	4 (4%)	0	100	100
22	X	241/256 (94%)	233 (97%)	8 (3%)	0	100	100
23	Y	174/250 (70%)	170 (98%)	4 (2%)	0	100	100
24	Z	118/161 (73%)	110 (93%)	8 (7%)	0	100	100
25	0	106/188 (56%)	101 (95%)	5 (5%)	0	100	100
26	1	50/65 (77%)	49 (98%)	1 (2%)	0	100	100
27	2	41/92 (45%)	40 (98%)	1 (2%)	0	100	100
28	3	93/188 (50%)	87 (94%)	6 (6%)	0	100	100
29	5	383/423 (90%)	363 (95%)	20 (5%)	0	100	100
30	6	316/380 (83%)	300 (95%)	16 (5%)	0	100	100
31	7	285/338 (84%)	262 (92%)	23 (8%)	0	100	100
32	8	97/206 (47%)	88 (91%)	9 (9%)	0	100	100
33	9	113/137 (82%)	109 (96%)	4 (4%)	0	100	100
34	a	78/142 (55%)	74 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	b	146/215 (68%)	130 (89%)	16 (11%)	0	100	100
36	c	271/332 (82%)	264 (97%)	7 (3%)	0	100	100
37	d	203/306 (66%)	191 (94%)	12 (6%)	0	100	100
38	e	211/279 (76%)	179 (85%)	31 (15%)	1 (0%)	29	65
39	f	110/212 (52%)	98 (89%)	11 (10%)	1 (1%)	17	52
40	g	127/166 (76%)	115 (91%)	12 (9%)	0	100	100
41	h	96/158 (61%)	93 (97%)	3 (3%)	0	100	100
42	i	95/128 (74%)	90 (95%)	5 (5%)	0	100	100
43	j	83/123 (68%)	81 (98%)	2 (2%)	0	100	100
44	k	76/112 (68%)	71 (93%)	5 (7%)	0	100	100
45	l	21/138 (15%)	21 (100%)	0	0	100	100
46	m	43/128 (34%)	37 (86%)	4 (9%)	2 (5%)	2	12
47	o	77/102 (76%)	76 (99%)	1 (1%)	0	100	100
48	p	119/206 (58%)	114 (96%)	5 (4%)	0	100	100
49	q	126/222 (57%)	124 (98%)	2 (2%)	0	100	100
50	r	140/196 (71%)	134 (96%)	6 (4%)	0	100	100
51	s	366/439 (83%)	354 (97%)	12 (3%)	0	100	100
53	u	109/234 (47%)	100 (92%)	9 (8%)	0	100	100
54	v	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
55	w	77/156 (49%)	69 (90%)	8 (10%)	0	100	100
All	All	7945/11026 (72%)	7507 (94%)	433 (5%)	5 (0%)	54	84

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
46	m	71	PRO
6	H	104	ASN
38	e	256	THR
39	f	179	PRO
46	m	53	PRO

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	
3	D	179/245 (73%)	177 (99%)	2 (1%)	73	90
4	E	246/290 (85%)	244 (99%)	2 (1%)	81	92
5	F	217/262 (83%)	211 (97%)	6 (3%)	43	75
6	H	86/228 (38%)	86 (100%)	0	100	100
7	I	145/232 (62%)	144 (99%)	1 (1%)	84	93
8	J	113/150 (75%)	113 (100%)	0	100	100
9	K	155/156 (99%)	153 (99%)	2 (1%)	69	88
10	L	98/124 (79%)	97 (99%)	1 (1%)	76	91
11	M	245/249 (98%)	240 (98%)	5 (2%)	55	81
12	N	172/211 (82%)	169 (98%)	3 (2%)	60	84
13	O	133/150 (89%)	132 (99%)	1 (1%)	81	92
14	P	123/155 (79%)	121 (98%)	2 (2%)	62	85
15	Q	199/256 (78%)	198 (100%)	1 (0%)	88	95
16	R	118/126 (94%)	118 (100%)	0	100	100
17	S	141/180 (78%)	141 (100%)	0	100	100
18	T	141/176 (80%)	141 (100%)	0	100	100
19	U	124/135 (92%)	122 (98%)	2 (2%)	62	85
20	V	172/191 (90%)	167 (97%)	5 (3%)	42	74
21	W	89/119 (75%)	88 (99%)	1 (1%)	73	90
22	X	219/229 (96%)	214 (98%)	5 (2%)	50	78
23	Y	159/223 (71%)	156 (98%)	3 (2%)	57	82
24	Z	111/147 (76%)	111 (100%)	0	100	100
25	0	97/164 (59%)	95 (98%)	2 (2%)	53	80
26	1	49/60 (82%)	46 (94%)	3 (6%)	18	50
27	2	38/72 (53%)	38 (100%)	0	100	100
28	3	88/166 (53%)	86 (98%)	2 (2%)	50	78
29	5	348/368 (95%)	341 (98%)	7 (2%)	55	81
30	6	265/332 (80%)	262 (99%)	3 (1%)	73	90
31	7	263/303 (87%)	260 (99%)	3 (1%)	73	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	8	91/190 (48%)	90 (99%)	1 (1%)	73	90
33	9	99/112 (88%)	99 (100%)	0	100	100
34	a	78/133 (59%)	76 (97%)	2 (3%)	46	76
35	b	130/186 (70%)	128 (98%)	2 (2%)	65	86
36	c	241/288 (84%)	239 (99%)	2 (1%)	81	92
37	d	193/274 (70%)	191 (99%)	2 (1%)	76	91
38	e	188/236 (80%)	185 (98%)	3 (2%)	62	85
39	f	101/188 (54%)	101 (100%)	0	100	100
40	g	119/148 (80%)	117 (98%)	2 (2%)	60	84
41	h	95/148 (64%)	93 (98%)	2 (2%)	53	80
42	i	86/110 (78%)	85 (99%)	1 (1%)	71	89
43	j	68/97 (70%)	68 (100%)	0	100	100
44	k	71/90 (79%)	71 (100%)	0	100	100
45	l	23/116 (20%)	23 (100%)	0	100	100
46	m	40/113 (35%)	39 (98%)	1 (2%)	47	77
47	o	68/87 (78%)	68 (100%)	0	100	100
48	p	117/181 (65%)	116 (99%)	1 (1%)	78	91
49	q	110/178 (62%)	106 (96%)	4 (4%)	35	68
50	r	133/169 (79%)	131 (98%)	2 (2%)	65	86
51	s	326/381 (86%)	320 (98%)	6 (2%)	59	83
53	u	105/200 (52%)	105 (100%)	0	100	100
54	v	59/60 (98%)	58 (98%)	1 (2%)	60	84
55	w	73/136 (54%)	72 (99%)	1 (1%)	67	86
All	All	7147/9520 (75%)	7052 (99%)	95 (1%)	70	88

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	6	159	ARG
38	e	55	ARG
31	7	64	LYS
35	b	11	LEU
40	g	100	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
38	e	212	HIS
51	s	238	ASN
39	f	112	ASN
42	i	124	HIS
54	v	63	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1071/1559 (68%)	302 (28%)	17 (1%)
2	B	51/69 (73%)	15 (29%)	1 (1%)
All	All	1122/1628 (68%)	317 (28%)	18 (1%)

5 of 317 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1676	A
1	A	1677	C
1	A	1678	C
1	A	1679	U
1	A	1681	G

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2507	A
2	B	1607	U
1	A	3201	A
1	A	2165	C
1	A	2457	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 52 ligands modelled in this entry, 51 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	PNS	v	101	55	13,20,21	2.39	4 (30%)	18,26,29	1.11	1 (5%)

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
58	PNS	v	101	55	-	7/24/26/27	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	v	101	PNS	C34-N36	5.55	1.45	1.33
58	v	101	PNS	C39-N41	5.32	1.45	1.33
58	v	101	PNS	O40-C39	-2.18	1.18	1.23
58	v	101	PNS	O35-C34	-2.13	1.19	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	v	101	PNS	C31-C29-C32	2.55	113.25	108.82

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	v	101	PNS	C28-C29-C32-O33
58	v	101	PNS	C28-C29-C32-C34
58	v	101	PNS	C31-C29-C32-O33

Continued on next page...

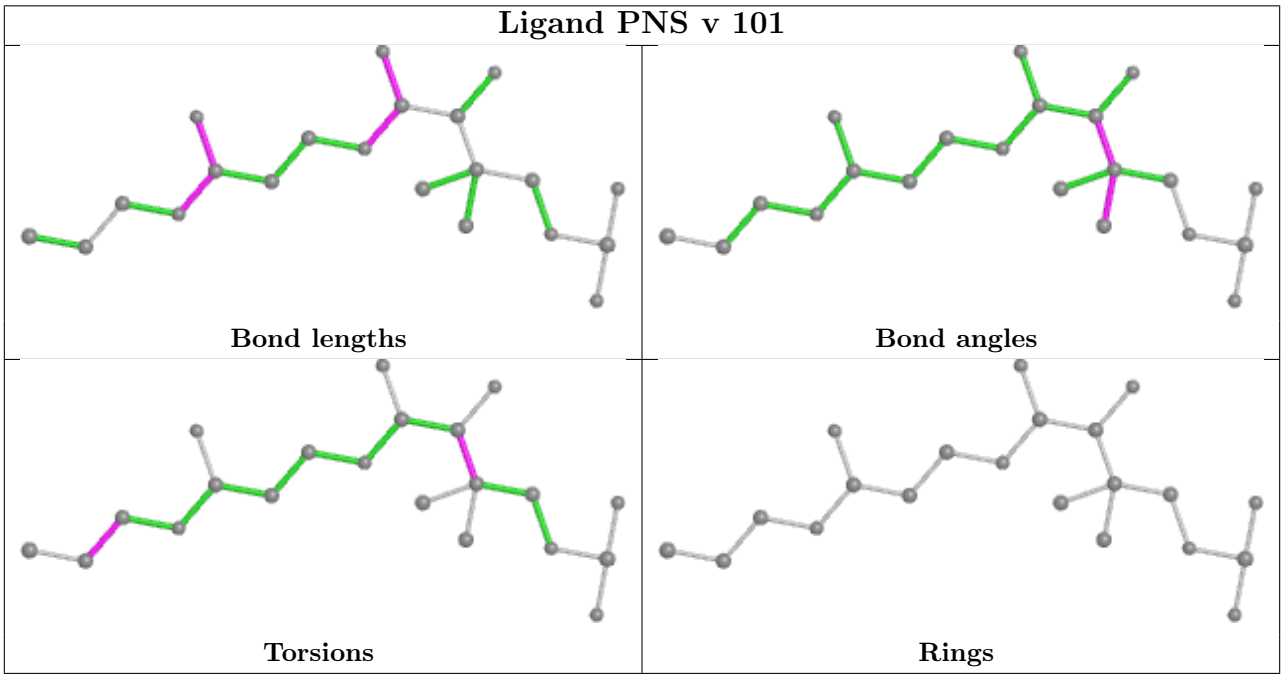
Continued from previous page...

Mol	Chain	Res	Type	Atoms
58	v	101	PNS	N41-C42-C43-S44
58	v	101	PNS	C30-C29-C32-O33

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	Z	1
42	i	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	151:LEU	C	152:LYS	N	1.17
1	i	68:LYS	C	69:HIS	N	1.16

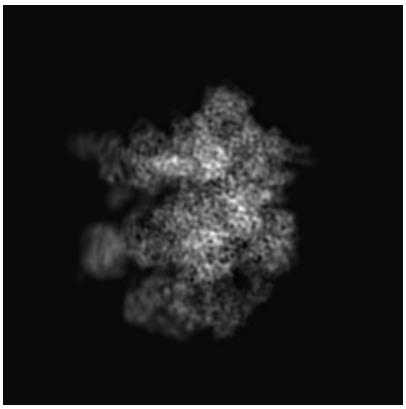
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3843. These allow visual inspection of the internal detail of the map and identification of artifacts.

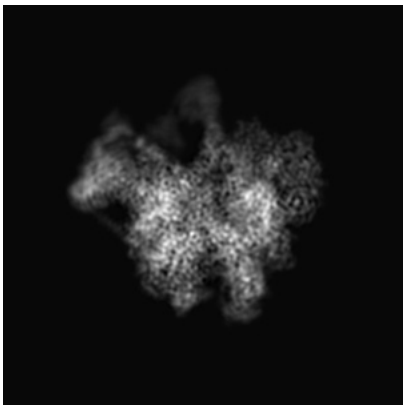
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

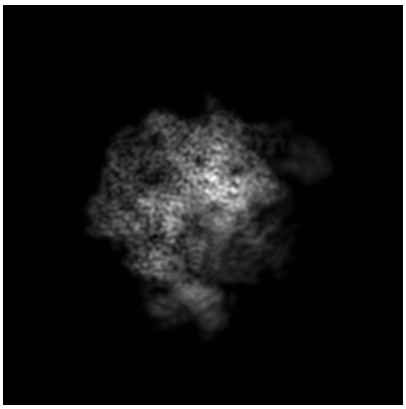
6.1.1 Primary map



X

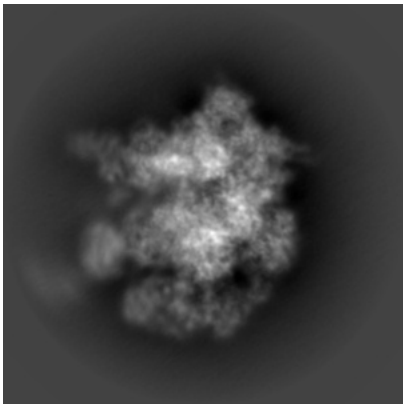


Y

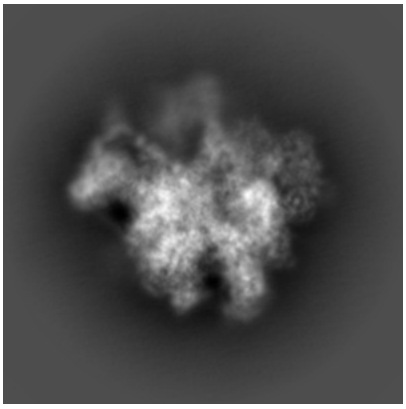


Z

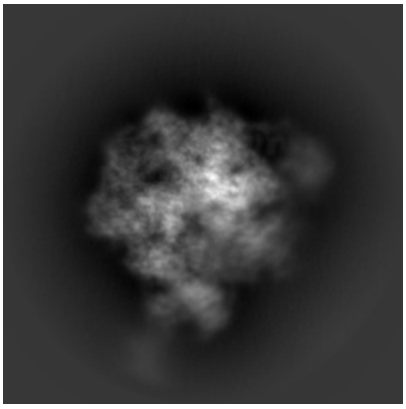
6.1.2 Raw map



X



Y

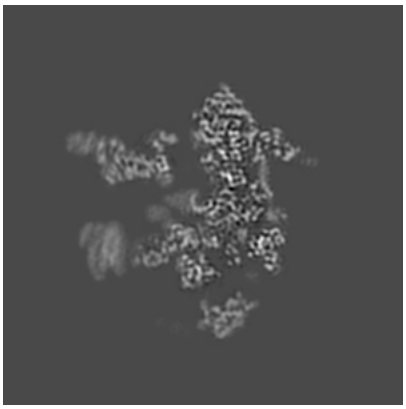


Z

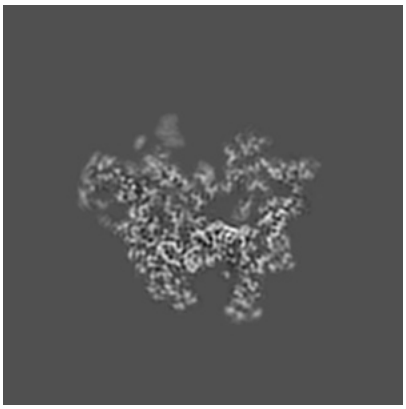
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

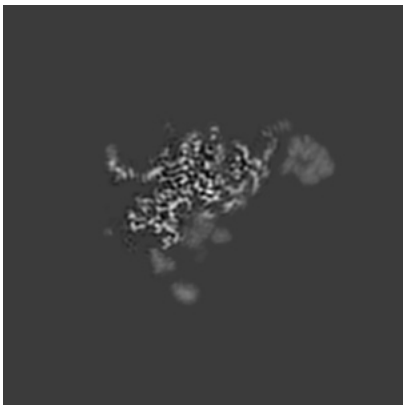
6.2.1 Primary map



X Index: 176

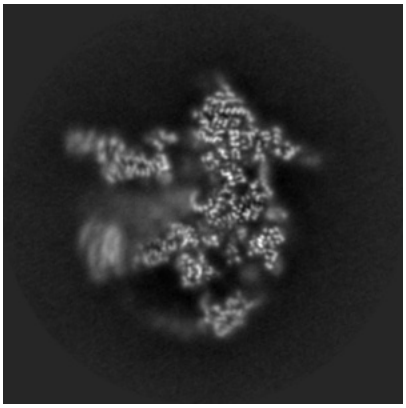


Y Index: 176

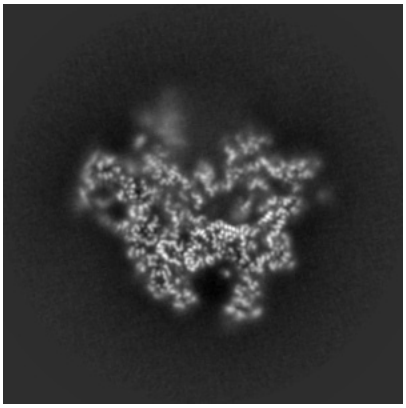


Z Index: 176

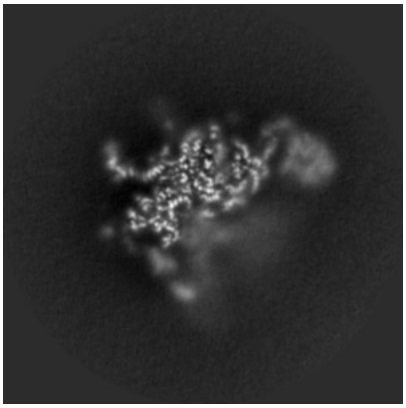
6.2.2 Raw map



X Index: 176



Y Index: 176

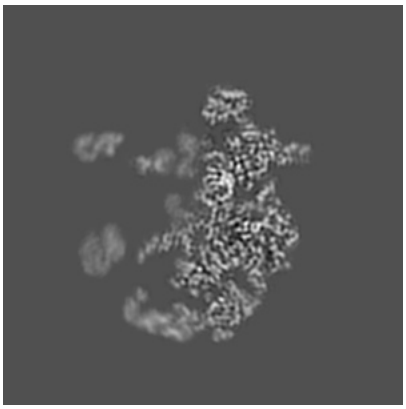


Z Index: 176

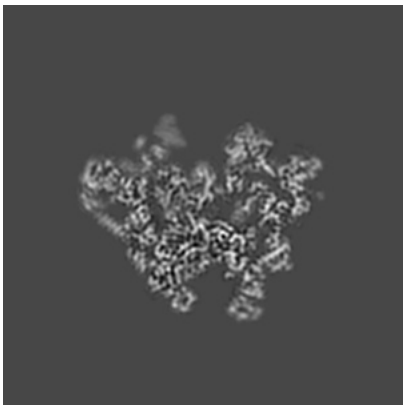
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

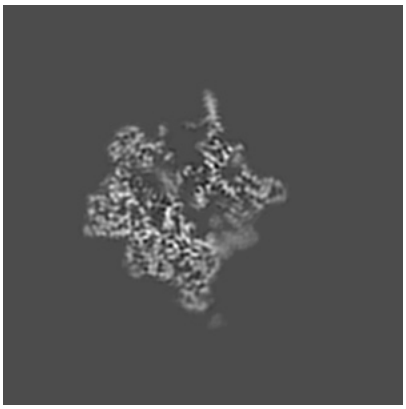
6.3.1 Primary map



X Index: 188

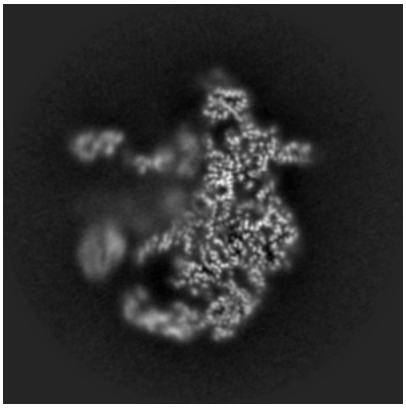


Y Index: 179

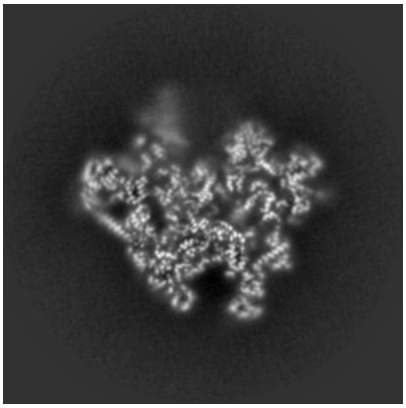


Z Index: 214

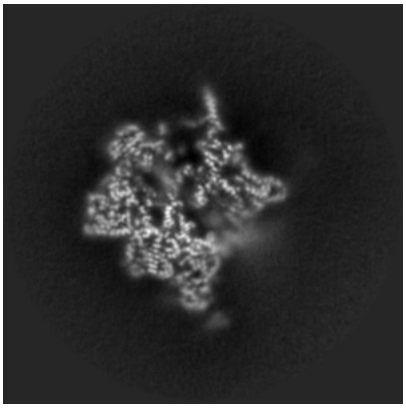
6.3.2 Raw map



X Index: 187



Y Index: 180



Z Index: 214

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

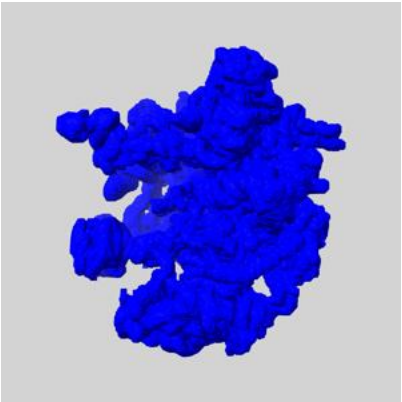
6.5 Mask visualisation (i)

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

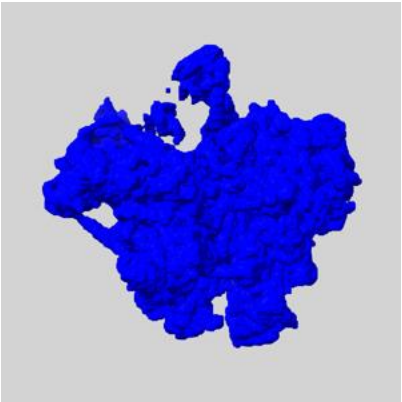
A mask typically either:

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

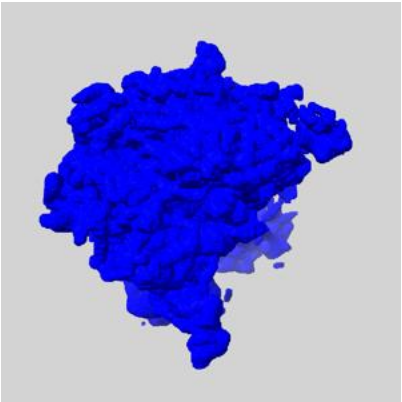
6.5.1 emd_3843_msk_1.map (i)



X



Y

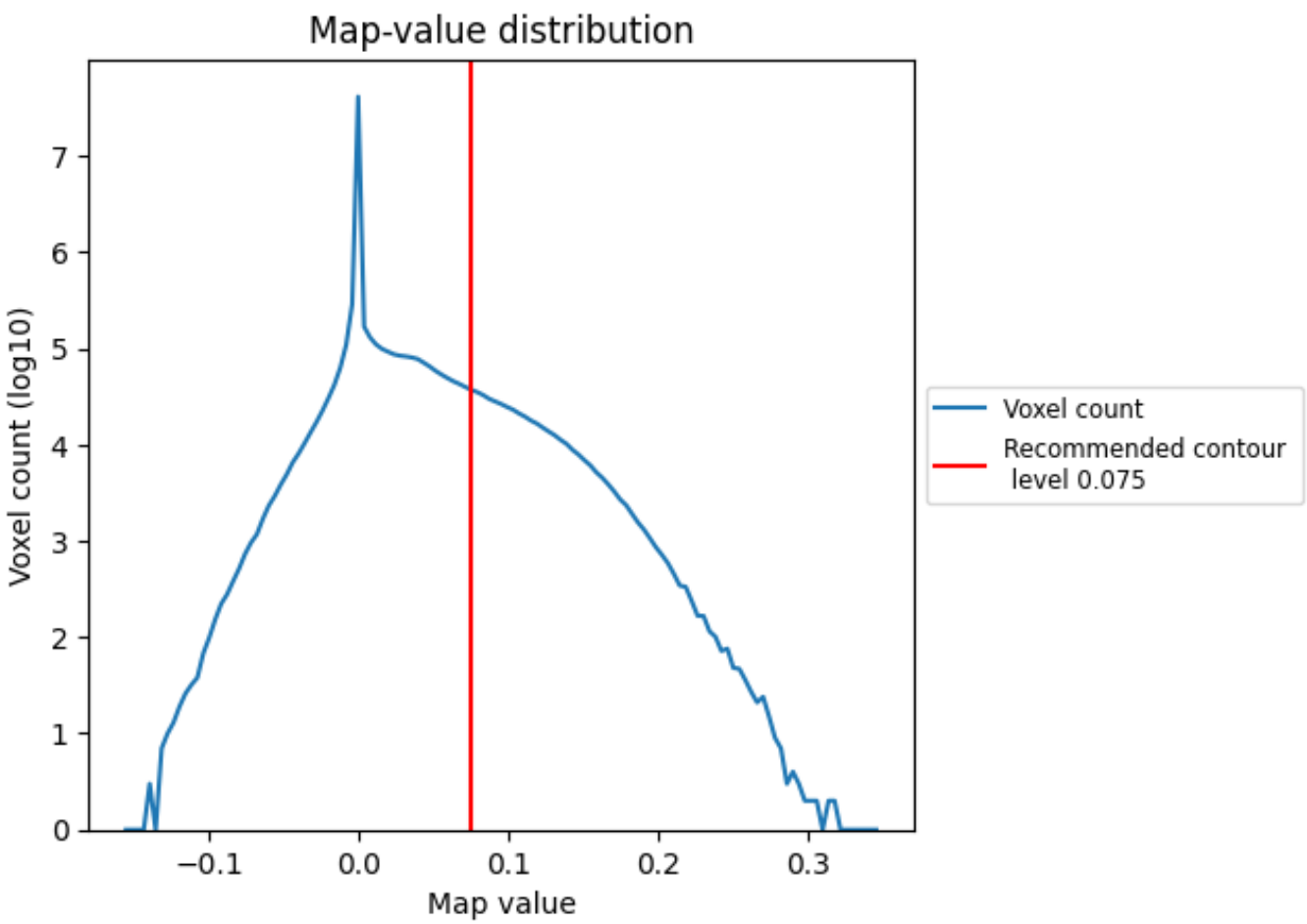


Z

7 Map analysis (i)

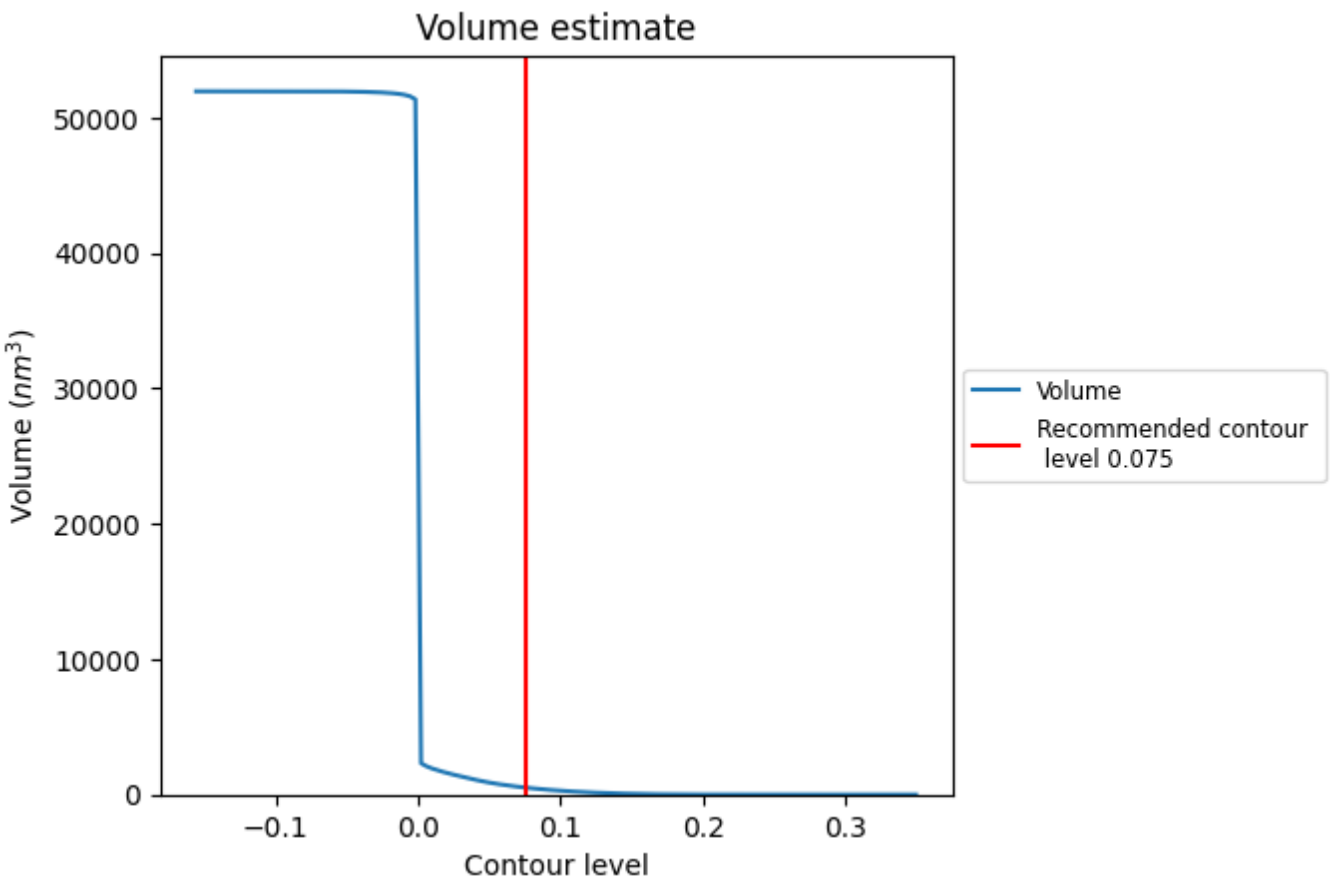
This section contains the results of statistical analysis of the map.

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.

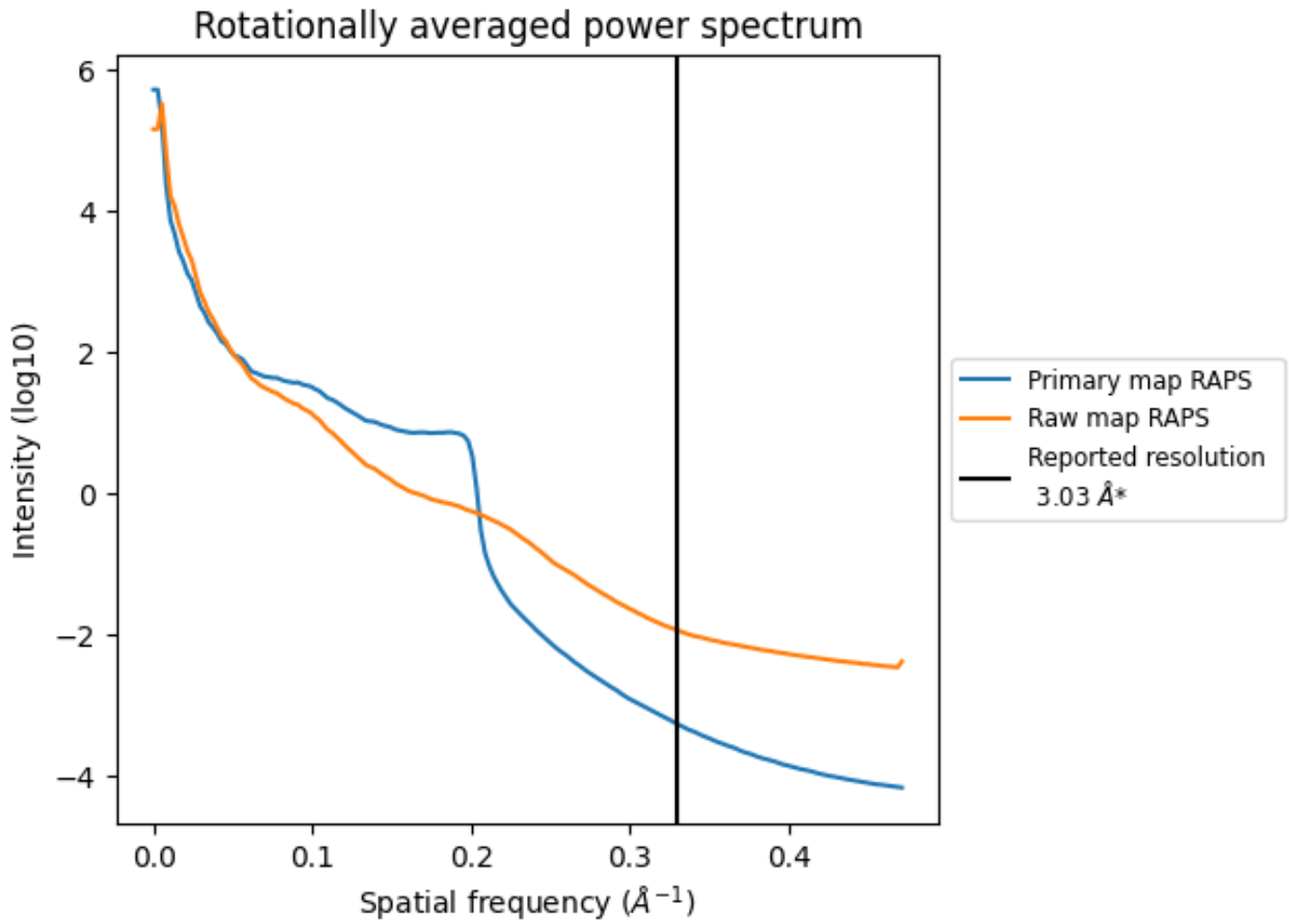
7.2 Volume estimate (i)



The volume at the recommended contour level is 519 nm^3; this corresponds to an approximate mass of 469 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)

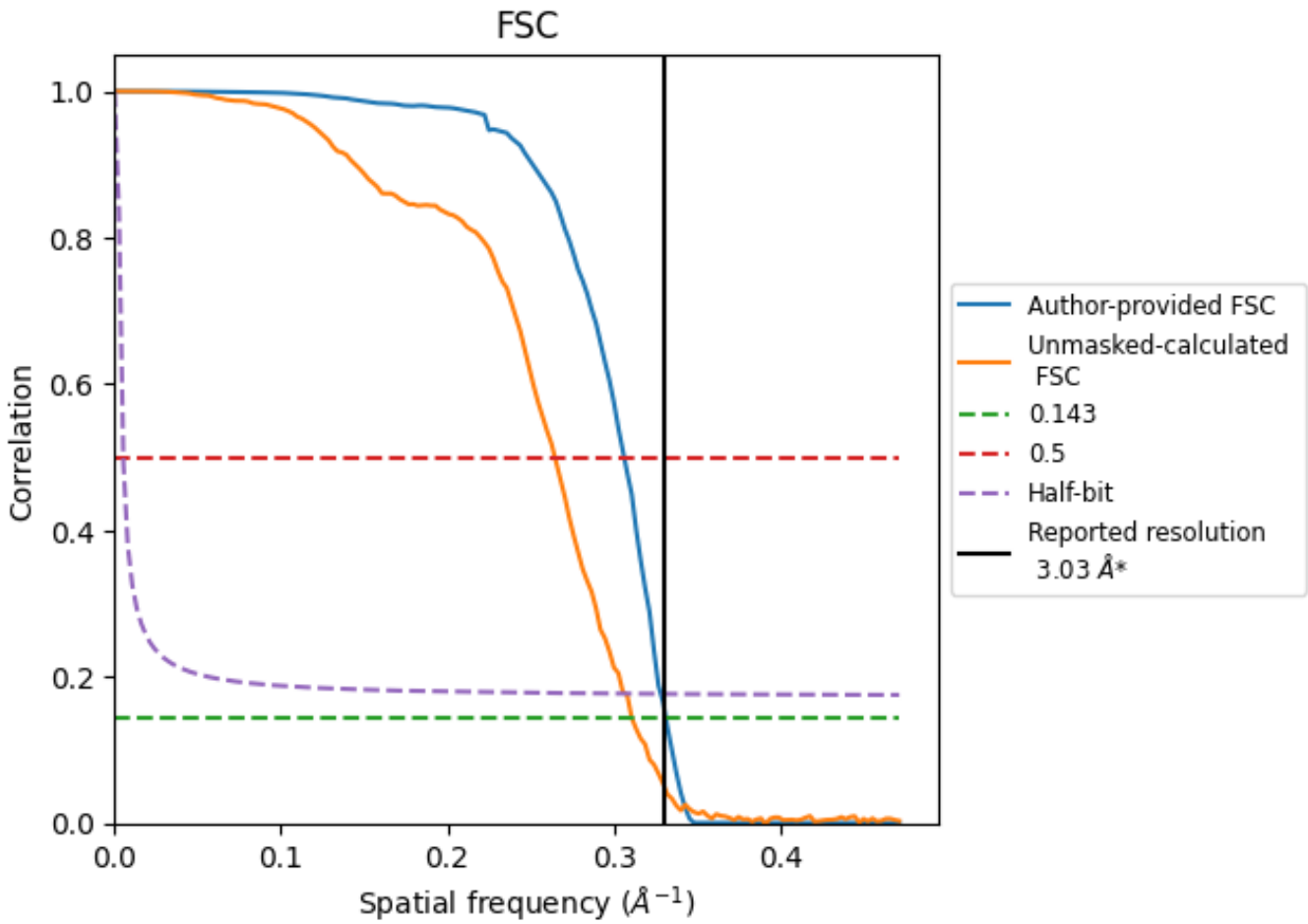


*Reported resolution corresponds to spatial frequency of 0.330 Å^{-1}

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 0.330 Å^{-1}

8.2 Resolution estimates (i)

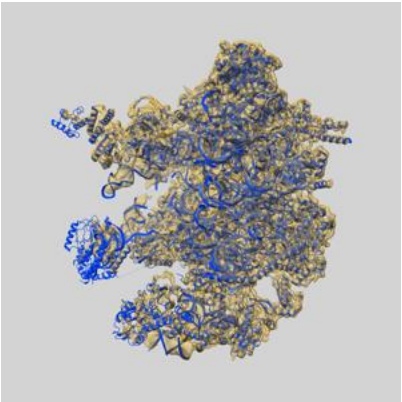
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	3.02	3.26	3.05
Unmasked-calculated*	3.22	3.78	3.26

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

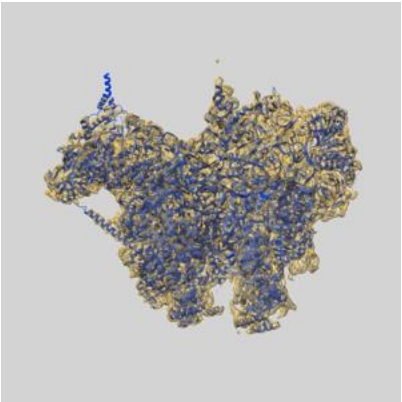
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3843 and PDB model 5OOM. Per-residue inclusion information can be found in section 3 on page 14.

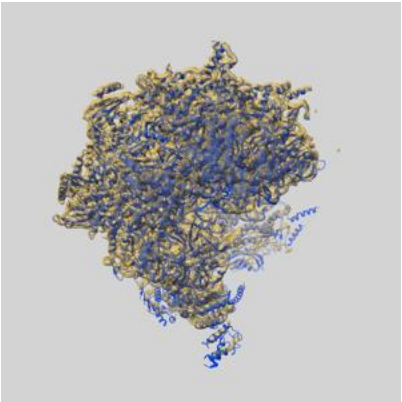
9.1 Map-model overlay (i)



X



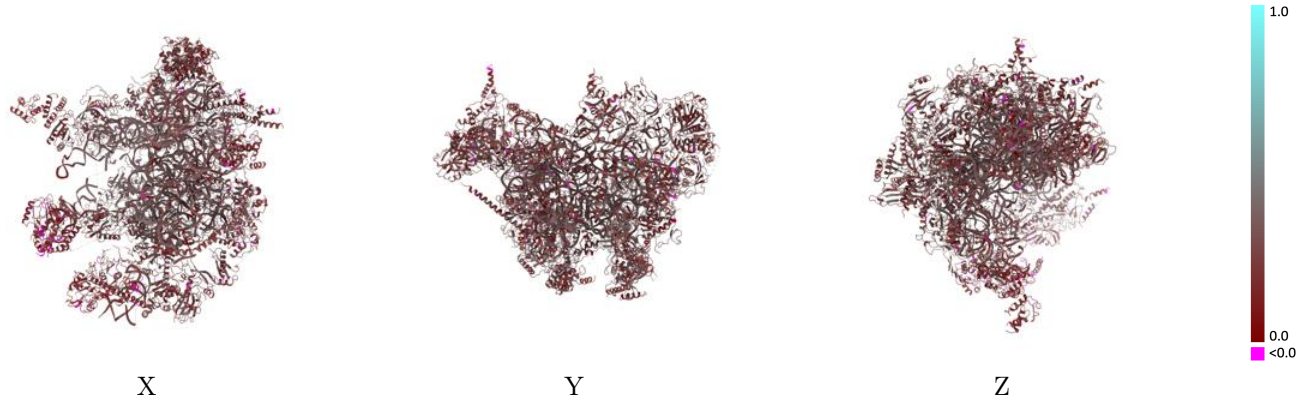
Y



Z

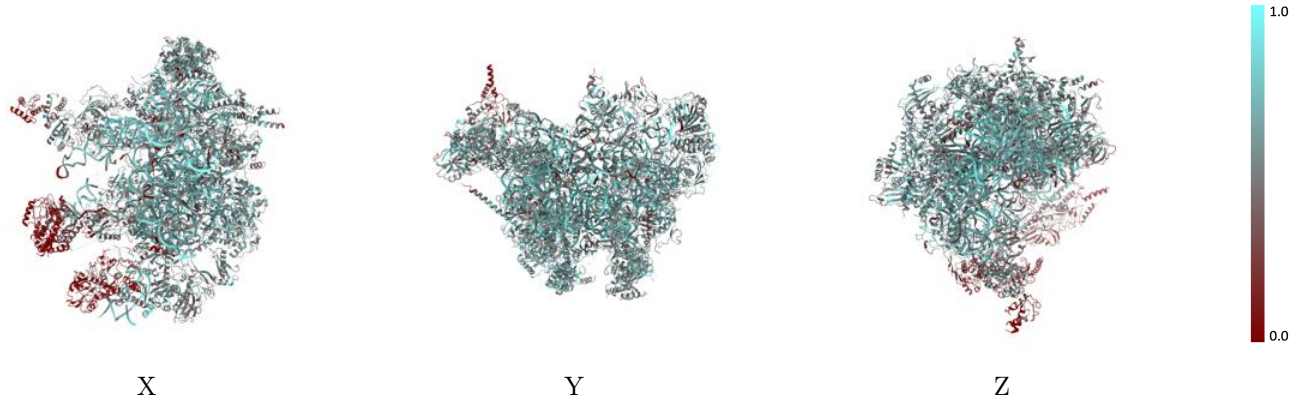
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



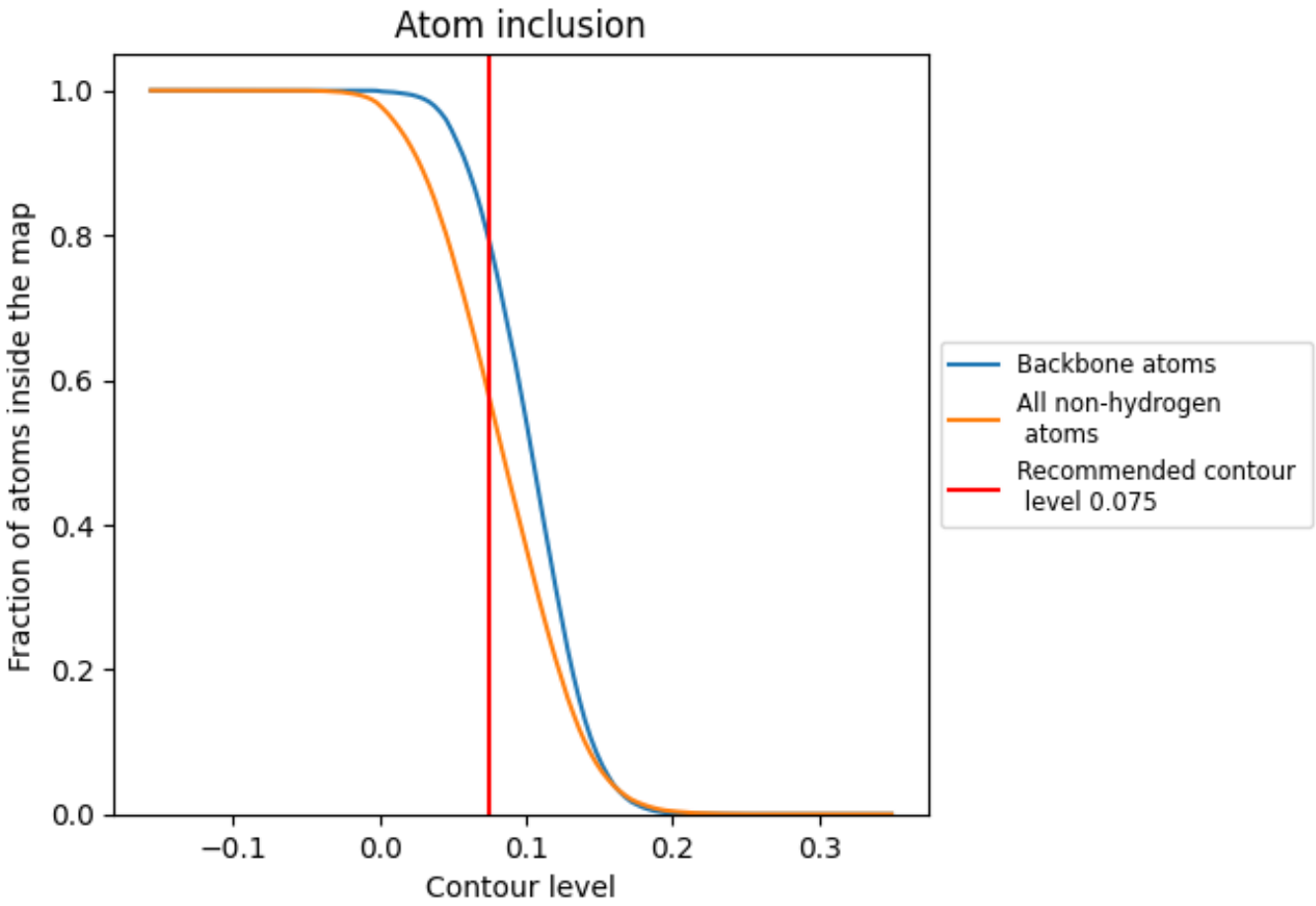
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.075).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 58% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5758	0.2900
0	0.5826	0.2950
1	0.5190	0.2800
2	0.5727	0.2750
3	0.5401	0.2880
5	0.5636	0.2750
6	0.5637	0.2930
7	0.5813	0.2940
8	0.2815	0.2180
9	0.5796	0.2950
A	0.7380	0.3310
B	0.7364	0.2960
D	0.4552	0.2710
E	0.5671	0.3030
F	0.5890	0.2970
H	0.5053	0.2710
I	0.1410	0.1770
J	0.0000	0.1210
K	0.6001	0.2990
L	0.4677	0.2880
M	0.5742	0.2790
N	0.4275	0.2890
O	0.6000	0.2980
P	0.5564	0.2740
Q	0.5535	0.2920
R	0.5641	0.2810
S	0.6023	0.3110
T	0.5800	0.2970
U	0.5892	0.2890
V	0.5719	0.3020
W	0.5131	0.2790
X	0.5499	0.2680
Y	0.5891	0.2640
Z	0.5750	0.3070
a	0.5955	0.3120

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Chain	Atom inclusion	Q-score
b	0.6265	0.3150
c	0.6150	0.2960
d	0.5282	0.3020
e	0.1525	0.1760
f	0.2930	0.2410
g	0.6430	0.3100
h	0.5752	0.2920
i	0.5597	0.2750
j	0.5961	0.2910
k	0.1664	0.2010
l	0.2427	0.1580
m	0.1870	0.2490
o	0.6318	0.2870
p	0.5196	0.2680
q	0.5552	0.2740
r	0.5650	0.3100
s	0.5971	0.2770
t	0.0000	0.1400
u	0.5094	0.2500
v	0.4010	0.1980
w	0.0821	0.1790