Full wwPDB EM Validation Report (i)

Jul 3, 2024 – 07:48 am BST

PDB ID	:	7OI8
EMDB ID	:	EMD-12921
Title	:	Cryo-EM structure of late human 39S mitoribosome assembly intermediates, state 3A
Authors	:	Cheng, J.; Berninghausen, O.; Beckmann, R.
Deposited on	:	2021-05-11
Resolution	:	3.50 Å(reported)

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

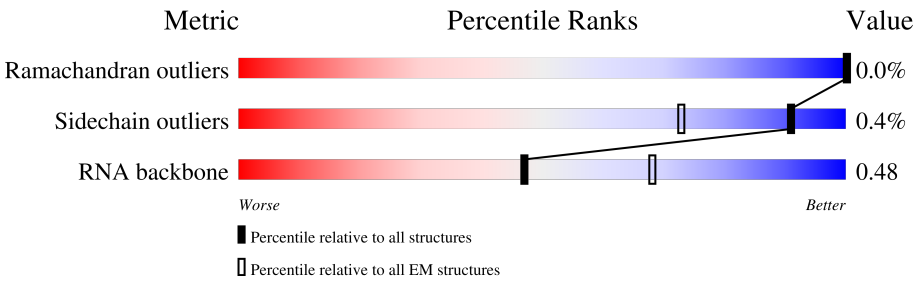
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.50 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	D	305	5% 77% • 23%
2	E	348	5% 87% • 13%
3	F	311	79% • 20%
4	H	267	35% 64%
5	I	261	25% 60% 39%
6	J	192	62% 73% 27%
7	K	178	98% ••
8	L	145	• 79% 21%

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Mol	Chain	Length	Quality of chain
9	M	296	96%
10	N	251	80% 18%
11	O	175	86% 13%
12	P	180	77% 22%
13	Q	292	73% 26%
14	R	149	94% 6%
15	S	205	75% 24%
16	T	206	77% 23%
17	U	153	90% 9%
18	V	216	88% 11%
19	W	148	74% 26%
20	X	256	94% 5%
21	Y	250	70% 30%
22	Z	161	75% 25%
23	0	188	57% 43%
24	1	65	80% 20%
25	2	92	47% 53%
26	3	188	51% 49%
27	5	423	91% 9%
28	6	380	84% 15%
29	7	338	85% 15%
30	8	206	5% 46% 52%
31	9	137	83% 15%
32	a	142	51% 49%
33	b	215	68% 31%

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Mol	Chain	Length	Quality of chain
34	c	332	83% 17%
35	d	306	5% 69% 31%
36	e	279	16% 78% 22%
37	f	212	54% 45%
38	g	166	78% 22%
39	h	158	63% 37%
40	i	128	75% 24%
41	j	123	69% 31%
42	k	112	16% 71% 29%
43	l	138	17% 83%
44	m	128	35% 65%
45	o	102	91% 9%
46	p	206	62% 38%
47	q	222	7% 73% 26%
48	r	196	74% 26%
49	s	439	83% 16%
50	u	234	7% 46% 53%
51	v	70	33% 99%
52	w	156	37% 50% 49%
53	A	1559	51% 18% 30%
54	B	69	58% 23% 19%
55	z	73	32% 51% 47%

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 92769 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 L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D	236	1842	1145	373	315	9	0	0

- Molecule 2 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	304	2396	1539	416	430	11	0	0

- Molecule 3 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 4 is a protein called 39S ribosomal protein L9, mitochondrial.

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

- Molecule 5 is a protein called 39S ribosomal protein L10, mitochondrial.

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

- Molecule 6 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 7 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 8 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 9 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 10 is a protein called 39S ribosomal protein L16, mitochondrial.

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

- Molecule 11 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 12 is a protein called 39S ribosomal protein L18, mitochondrial.

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

- Molecule 13 is a protein called 39S ribosomal protein L19, mitochondrial.

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

- Molecule 14 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 15 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 16 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 17 is a protein called 39S ribosomal protein L23, mitochondrial.

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

- Molecule 18 is a protein called 39S ribosomal protein L24, mitochondrial.

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

- Molecule 19 is a protein called 39S ribosomal protein L27, mitochondrial.

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

- Molecule 20 is a protein called 39S ribosomal protein L28, mitochondrial.

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

- Molecule 21 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 22 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 23 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	0	108	880	545	172	157	6	0	0

- Molecule 24 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	1	52	433	278	83	70	2	0	0

- Molecule 25 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	2	43	351	218	76	56	1	0	0

- Molecule 26 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	3	95	831	539	162	127	3	0	0

- Molecule 27 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	5	387	3156	2039	548	558	11	0	0

- Molecule 28 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	6	324	2640	1694	470	468	8	0	0

- Molecule 29 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	7	287	2334	1495	397	425	17	0	0

- Molecule 30 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	8	99	836	535	144	155	2	0	0

- Molecule 31 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	9	117	947	614	163	168	2	0	0

- Molecule 32 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	a	73	611	385	115	106	5	0	0

- Molecule 33 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 34 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 35 is a protein called 39S ribosomal protein L45, mitochondrial.

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

- Molecule 36 is a protein called 39S ribosomal protein L46, mitochondrial.

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

- Molecule 37 is a protein called 39S ribosomal protein L48, mitochondrial.

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

- Molecule 38 is a protein called 39S ribosomal protein L49, mitochondrial.

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

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

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

- Molecule 40 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 41 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 42 is a protein called 39S ribosomal protein L53, mitochondrial.

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

- Molecule 43 is a protein called 39S ribosomal protein L54, mitochondrial.

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

- Molecule 44 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 45 is a protein called Ribosomal protein 63, mitochondrial.

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

- Molecule 46 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 47 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		
47	q	164	1379	858	267	249	5	0	0

- Molecule 48 is a protein called 39S ribosomal protein S18a, mitochondrial.

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

- Molecule 49 is a protein called 39S ribosomal protein S30, mitochondrial.

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

- Molecule 50 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

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

- Molecule 51 is a protein called MIEF1 upstream open reading frame protein.

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

- Molecule 52 is a protein called Acyl carrier protein, mitochondrial.

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

- Molecule 53 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
53	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	1437	U	UNK	conflict	GB 1025814679

- Molecule 54 is a RNA chain called mitochondrial Val tRNA.

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

- Molecule 55 is a RNA chain called mitochondrial tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
55	z	73	1547	696	280	499	72	0	0

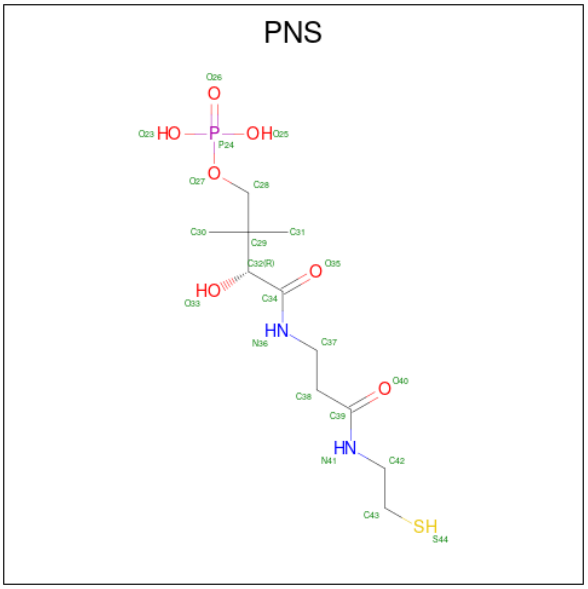
- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
56	E	1	1	1	0
56	A	48	48	48	0

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

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

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



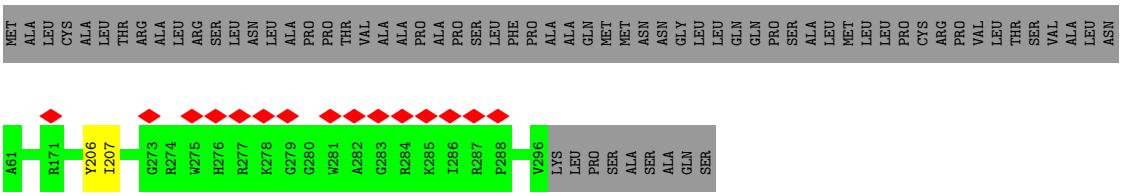
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
58	v	1	21	11	2	6	1	1	0

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.

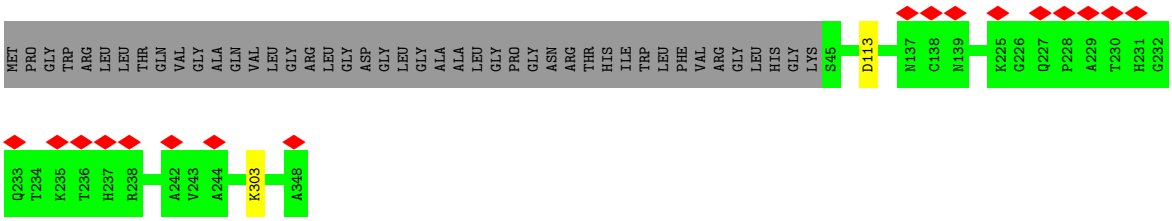
- Molecule 1: 39S ribosomal protein L2, mitochondrial

Chain D:



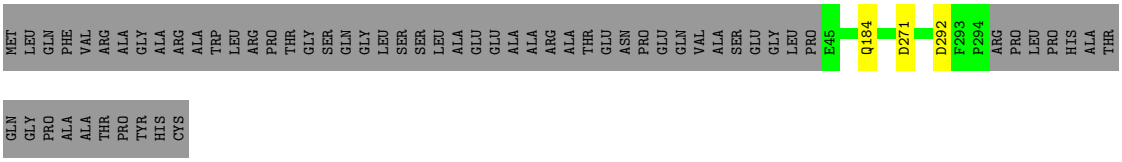
- Molecule 2: 39S ribosomal protein L3, mitochondrial

Chain E:



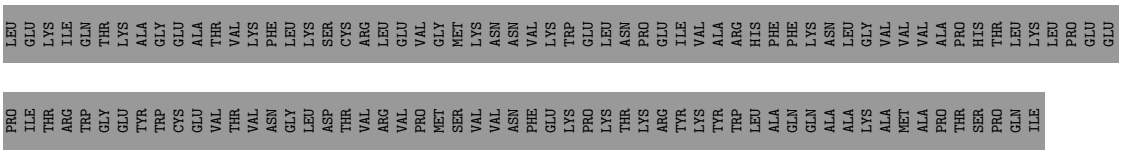
- Molecule 3: 39S ribosomal protein L4, mitochondrial

Chain F:



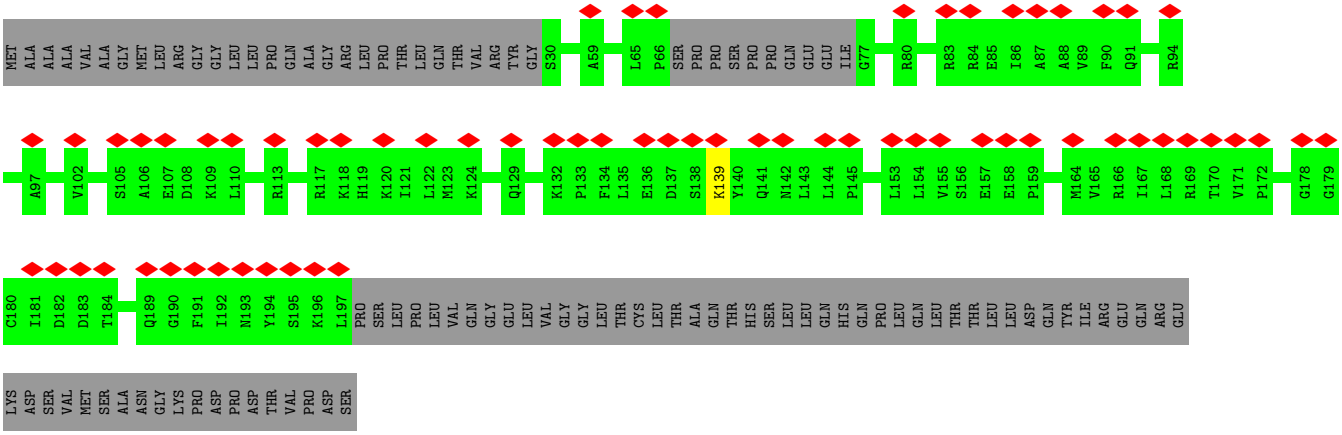
- Molecule 4: 39S ribosomal protein L9, mitochondrial

Chain H:



- Molecule 5: 39S ribosomal protein L10, mitochondrial

Chain I:

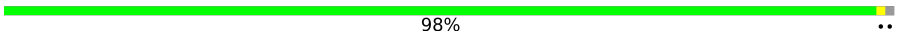


- Molecule 6: 39S ribosomal protein L11, mitochondrial

Chain J:

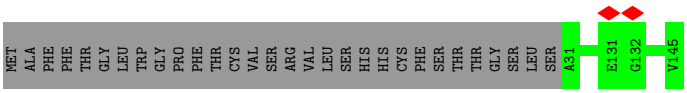
- Molecule 7: 39S ribosomal protein L13, mitochondrial

Chain K:



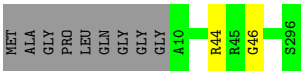
- Molecule 8: 39S ribosomal protein L14, mitochondrial

Chain L:



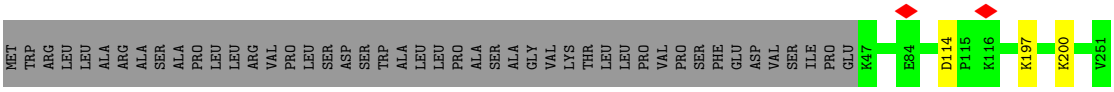
• Molecule 9: 39S ribosomal protein L15, mitochondrial

Chain M: 96%



• Molecule 10: 39S ribosomal protein L16, mitochondrial

Chain N: 80% 18%



• Molecule 11: 39S ribosomal protein L17, mitochondrial

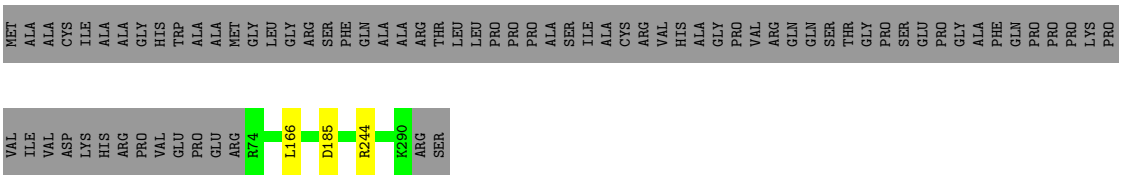
Chain O: 86% 13%

• Molecule 12: 39S ribosomal protein L18, mitochondrial

Chain P: 77% 22%

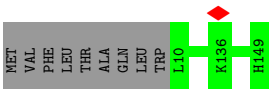
• Molecule 13: 39S ribosomal protein L19, mitochondrial

Chain Q: 73% 26%



• Molecule 14: 39S ribosomal protein L20, mitochondrial

Chain R: 94% 6%



• Molecule 15: 39S ribosomal protein L21, mitochondrial

Chain S: 75% 24%

MET ALA ALA SER SER LEU THR VAL THR LEU GLY ARG LEU ALA SER ALA CYS SER HIS SER ILE LEU ARG PRO SER GLY PRO GLY ALA ALA SER LEU TRP SER ALA SER ARG ARG PHE ASN SER GLN SER THR SER TYR LEU PRO G49 F101 N118 R129 L204 LEU

• Molecule 16: 39S ribosomal protein L22, mitochondrial

Chain T: 77% 23%

MET ALA ALA ALA VAL LEU GLY GLN LEU GLY ALA LEU TRP ILE HIS ASN LEU ARG SER ARG GLY LYS LEU ALA LEU GLY VAL LEU PRO GLN SER TYR ILE HIS THR SER ALA SER LEU ASP I47 R157 TYR HIS GLY ARG GLY ARG PHE G165 L212

• Molecule 17: 39S ribosomal protein L23, mitochondrial

Chain U: 90% 9%

MET A2 R11 P112 GLU LYS ASP GLU SER PRO GLU GLY SER ALA ALA ASP ASP L126 Y127 S128 L153

• Molecule 18: 39S ribosomal protein L24, mitochondrial

Chain V: 88% 11%

MET ARG LEU SER ALA LEU LEU ALA LEU ALA SER LYS VAL THR L115 D103 E139 A140 E158 PHE PRO ARG ALA ASP GLY ILE VAL PRO GLU T169 Y216

• Molecule 19: 39S ribosomal protein L27, mitochondrial

Chain W: 74% 26%

MET ALA SER VAL VAL LEU ALA LEU ARG THR ARG THR ALA VAL THR SER LEU LEU SER PRO THR PRO ALA THR ALA LEU ALA VAL ARG TYR ALA SER LYS LYS SER GLY GLY SER SER K40 L148

• Molecule 20: 39S ribosomal protein L28, mitochondrial

Chain X: 94% 5%

MET P2 D64 D180 S244 GLU PRO ALA VAL VAL GLN LYS ARG ALA SER GLY GLN

• Molecule 21: 39S ribosomal protein L47, mitochondrial

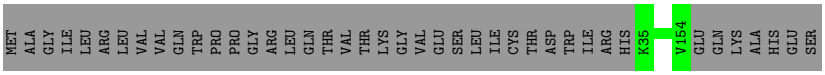
Chain Y: 70% 30%

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

ARG LYS G63 F238 PRO HIS LEU ALA GLU ALA GLN LYS SER SER LEU VAL

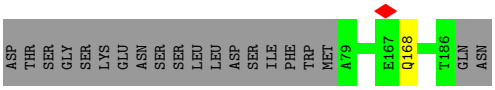
- Molecule 22: 39S ribosomal protein L30, mitochondrial

Chain Z:



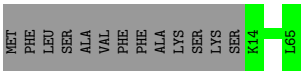
- Molecule 23: 39S ribosomal protein L32, mitochondrial

Chain 0:



- Molecule 24: 39S ribosomal protein L33, mitochondrial

Chain 1:

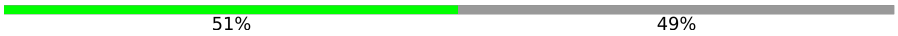


- Molecule 25: 39S ribosomal protein L34, mitochondrial

Chain 2:

- Molecule 26: 39S ribosomal protein L35, mitochondrial

Chain 3:

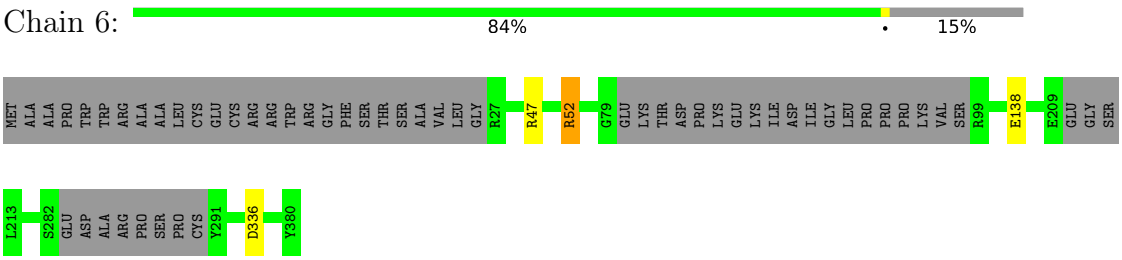


- Molecule 27: 39S ribosomal protein L37, mitochondrial

Chain 5:

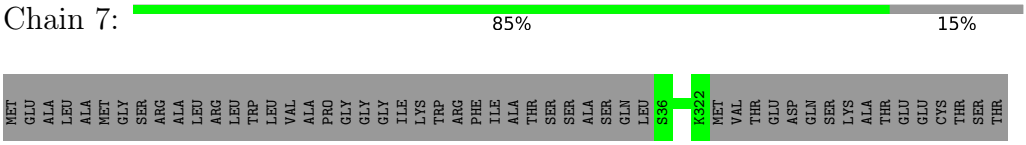
- Molecule 28: 39S ribosomal protein L38, mitochondrial

Chain 6:



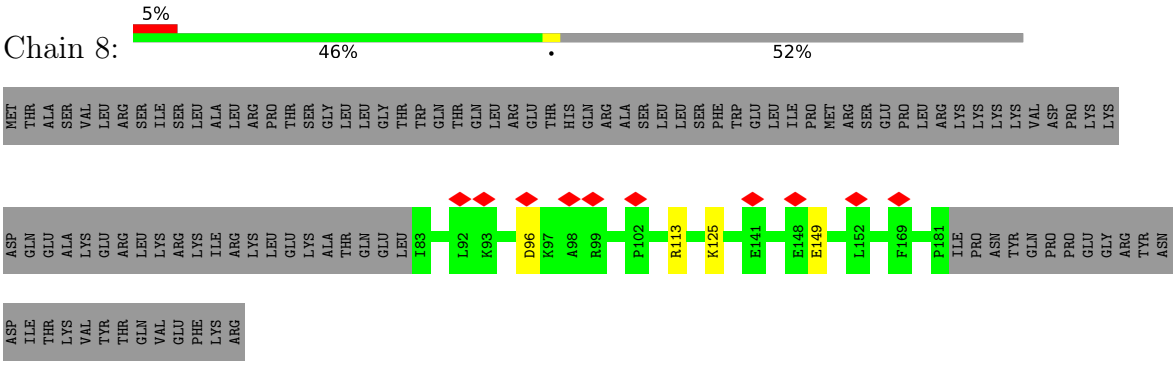
• Molecule 29: 39S ribosomal protein L39, mitochondrial

Chain 7:



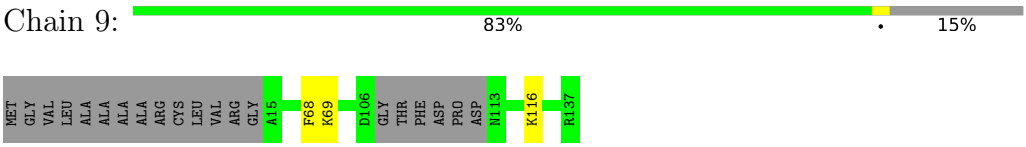
• Molecule 30: 39S ribosomal protein L40, mitochondrial

Chain 8:



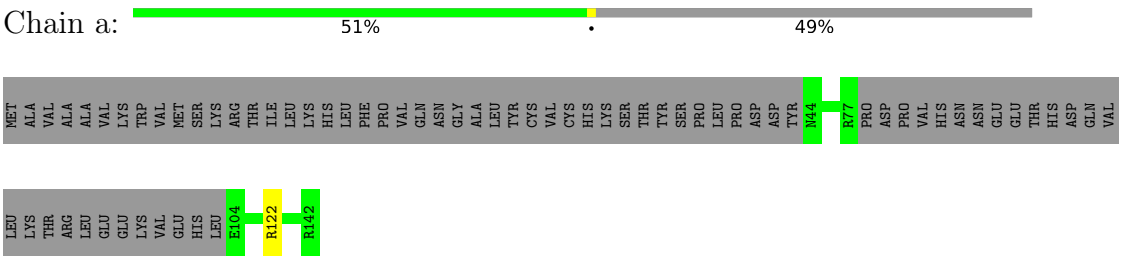
• Molecule 31: 39S ribosomal protein L41, mitochondrial

Chain 9:



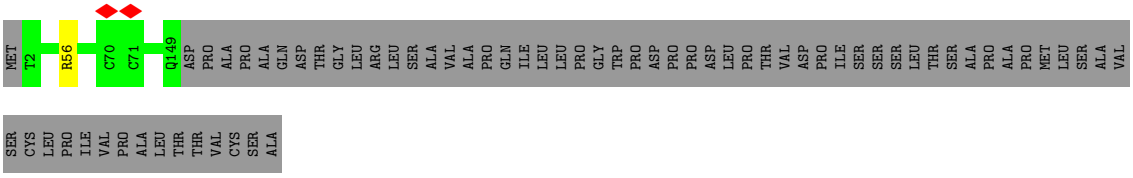
• Molecule 32: 39S ribosomal protein L42, mitochondrial

Chain a:



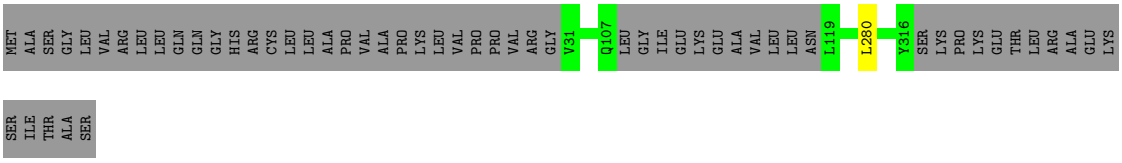
• Molecule 33: 39S ribosomal protein L43, mitochondrial

Chain b:



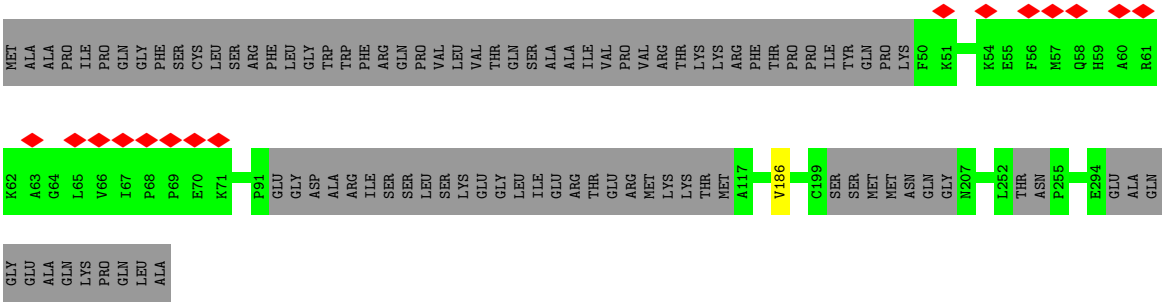
• Molecule 34: 39S ribosomal protein L44, mitochondrial

Chain c:



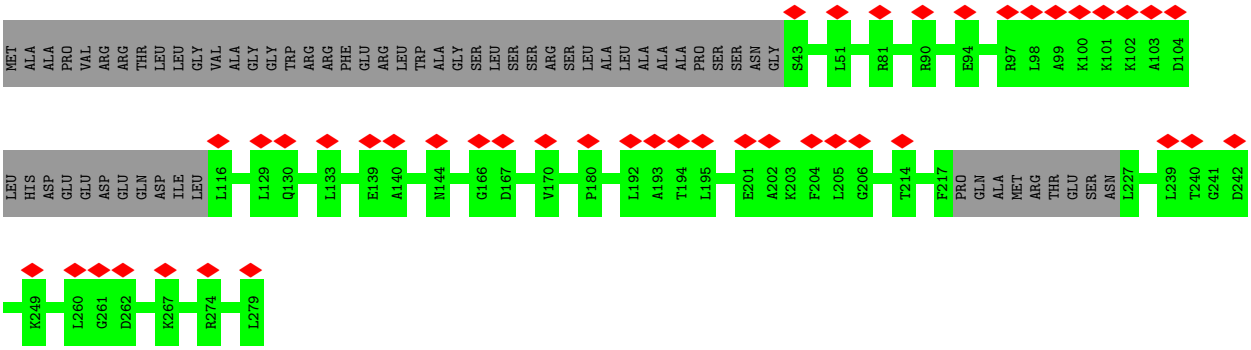
• Molecule 35: 39S ribosomal protein L45, mitochondrial

Chain d:



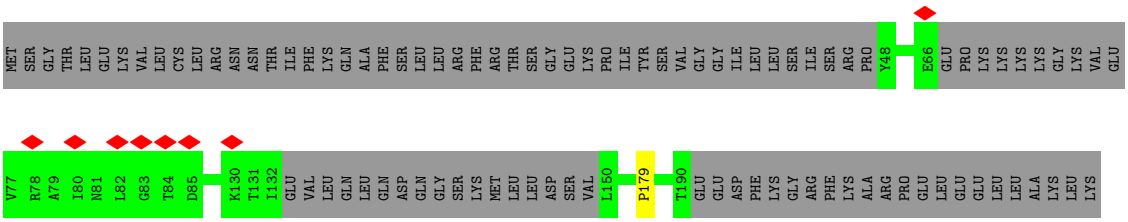
• Molecule 36: 39S ribosomal protein L46, mitochondrial

Chain e:



• Molecule 37: 39S ribosomal protein L48, mitochondrial

Chain f:

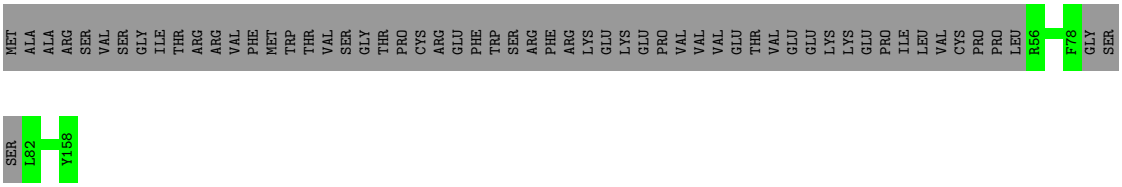


• Molecule 38: 39S ribosomal protein L49, mitochondrial

Chain g:

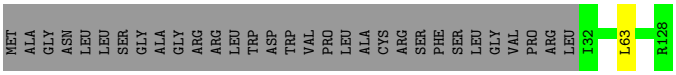
• Molecule 39: 39S ribosomal protein L50, mitochondrial

Chain h:



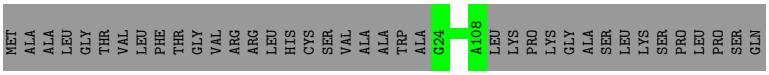
• Molecule 40: 39S ribosomal protein L51, mitochondrial

Chain i:



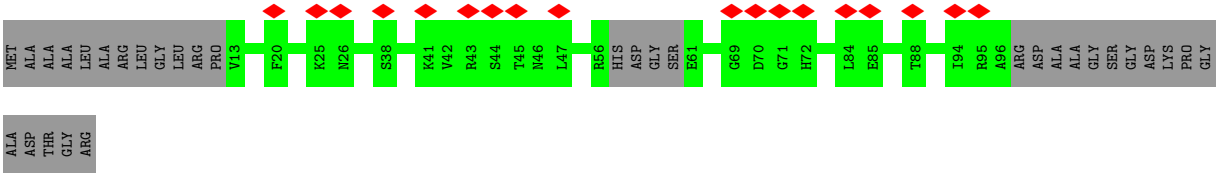
• Molecule 41: 39S ribosomal protein L52, mitochondrial

Chain j:



• Molecule 42: 39S ribosomal protein L53, mitochondrial

Chain k:

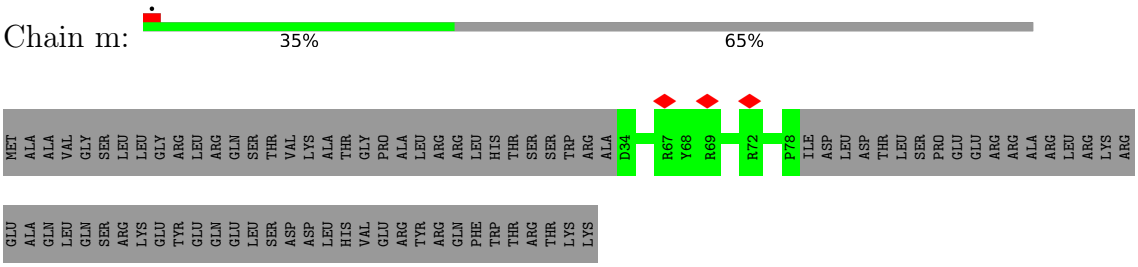


• Molecule 43: 39S ribosomal protein L54, mitochondrial

Chain l:

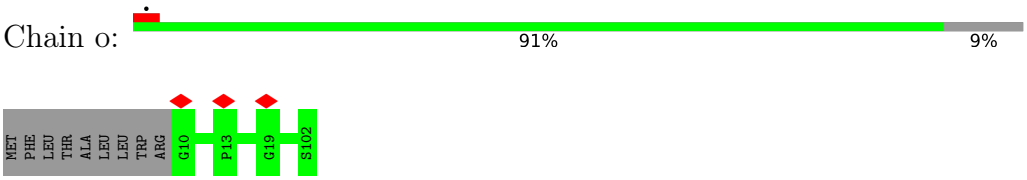
- Molecule 44: 39S ribosomal protein L55, mitochondrial

Chain m:



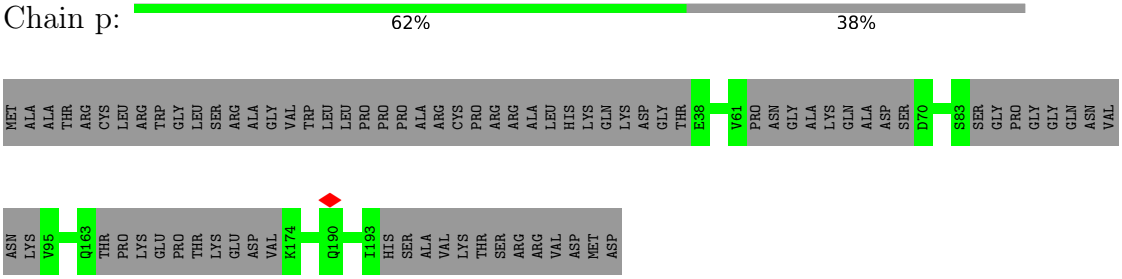
- Molecule 45: Ribosomal protein 63, mitochondrial

Chain o:



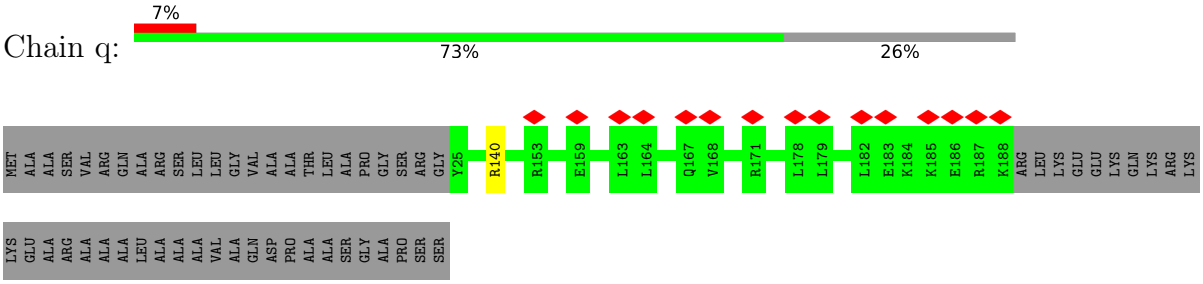
- Molecule 46: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p:



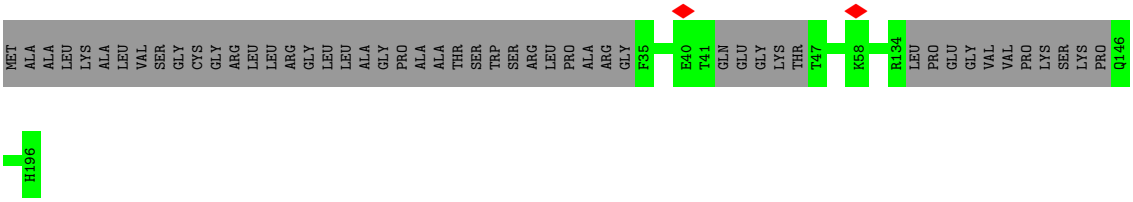
- Molecule 47: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q:



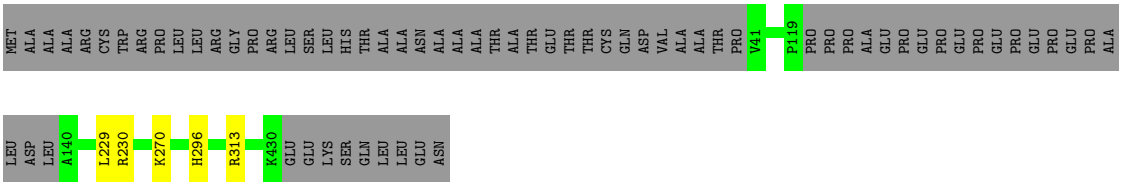
- Molecule 48: 39S ribosomal protein S18a, mitochondrial

Chain r:



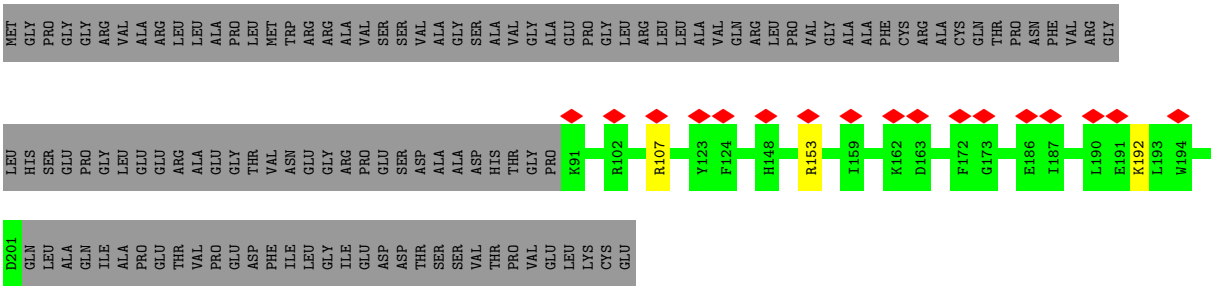
• Molecule 49: 39S ribosomal protein S30, mitochondrial

Chain s:



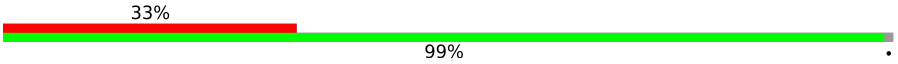
• Molecule 50: Mitochondrial assembly of ribosomal large subunit protein 1

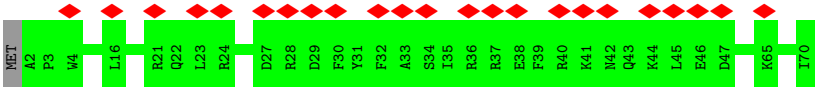
Chain u:



• Molecule 51: MIEF1 upstream open reading frame protein

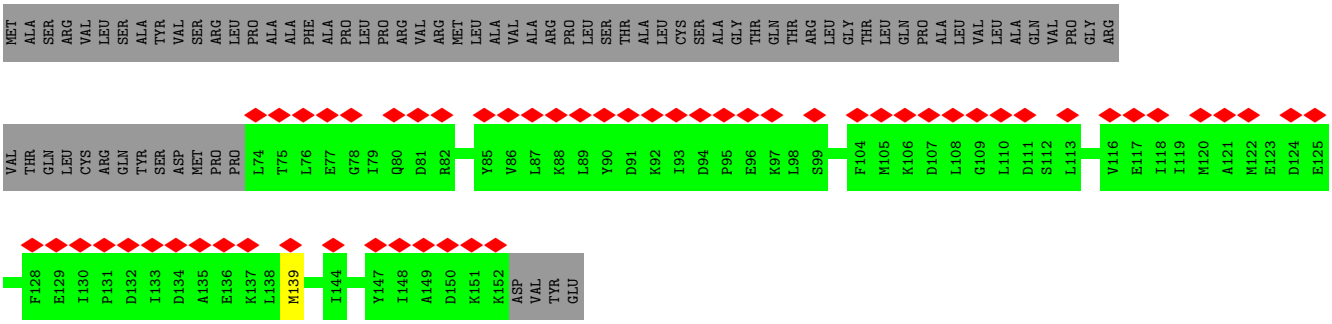
Chain v:





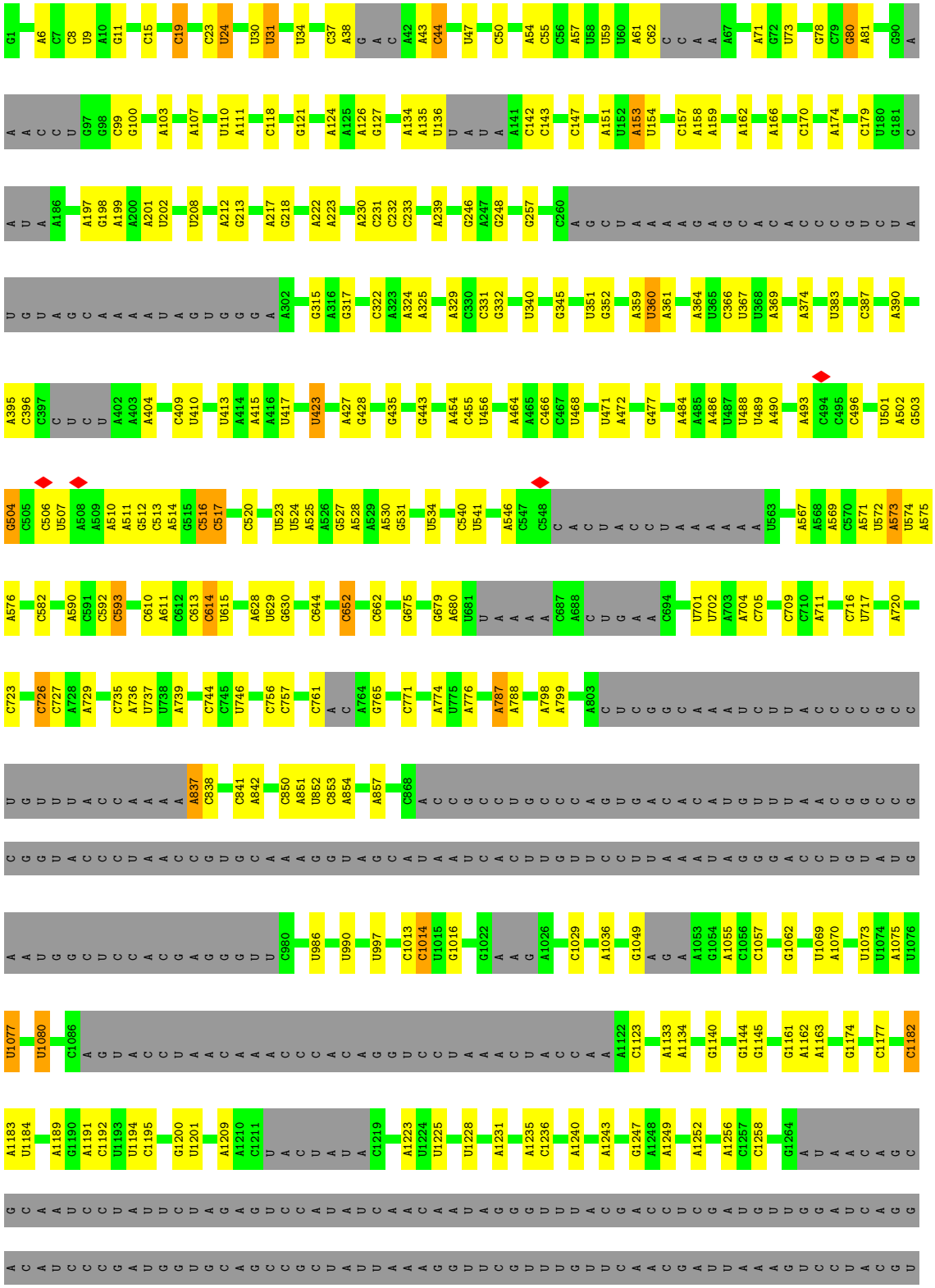
• Molecule 52: Acyl carrier protein, mitochondrial

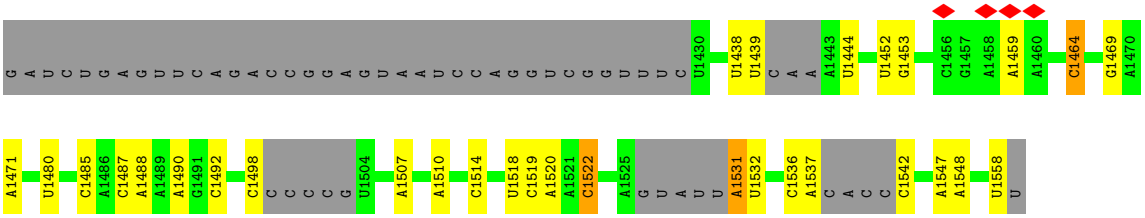
Chain w:



- Molecule 53: 16S rRNA

Chain A: 51% 18% 30%



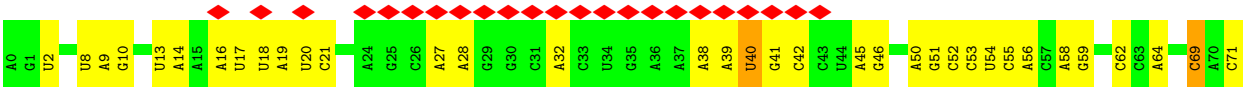


- Molecule 54: mitochondrial Val tRNA

Chain B:

- Molecule 55: mitochondrial tRNA

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59666	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.854	Depositor
Minimum map value	-0.538	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	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: MG, ZN, PNS

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	D	0.31	0/1879	0.57	0/2527
2	E	0.34	0/2465	0.55	1/3344 (0.0%)
3	F	0.42	0/2071	0.65	2/2817 (0.1%)
4	H	0.36	0/798	0.71	1/1073 (0.1%)
5	I	0.30	0/1308	0.63	0/1761
6	J	0.26	0/1077	0.48	0/1452
7	K	0.36	0/1495	0.57	0/2029
8	L	0.28	0/904	0.58	0/1218
9	M	0.43	0/2359	0.64	0/3185
10	N	0.34	0/1697	0.63	1/2281 (0.0%)
11	O	0.40	0/1269	0.71	1/1708 (0.1%)
12	P	0.35	0/1173	0.57	0/1588
13	Q	0.32	0/1846	0.61	2/2487 (0.1%)
14	R	0.47	0/1174	0.56	0/1572
15	S	0.43	0/1276	0.70	0/1729
16	T	0.39	0/1335	0.55	0/1796
17	U	0.40	0/1183	0.60	1/1600 (0.1%)
18	V	0.32	0/1616	0.61	1/2189 (0.0%)
19	W	0.47	0/881	0.59	0/1188
20	X	0.35	0/2090	0.57	2/2825 (0.1%)
21	Y	0.37	0/1552	0.55	0/2079
22	Z	0.40	0/1003	0.65	0/1354
23	0	0.38	0/895	0.55	0/1201
24	1	0.34	0/438	0.70	0/583
25	2	0.42	0/357	0.53	0/475
26	3	0.47	0/852	0.56	0/1136
27	5	0.34	0/3250	0.60	2/4429 (0.0%)
28	6	0.35	0/2726	0.65	3/3715 (0.1%)
29	7	0.34	0/2391	0.58	0/3234
30	8	0.36	0/855	0.83	1/1152 (0.1%)
31	9	0.37	0/972	0.68	1/1306 (0.1%)
32	a	0.36	0/630	0.52	0/852

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	b	0.39	0/1202	0.60	1/1626 (0.1%)
34	c	0.34	0/2264	0.54	1/3059 (0.0%)
35	d	0.32	0/1790	0.58	0/2423
36	e	0.27	0/1797	0.57	0/2422
37	f	0.30	0/931	0.62	0/1259
38	g	0.40	0/1102	0.59	0/1503
39	h	0.31	0/847	0.53	0/1150
40	i	0.42	0/849	0.66	1/1135 (0.1%)
41	j	0.34	0/698	0.54	0/940
42	k	0.29	0/635	0.61	0/855
43	l	0.25	0/226	0.53	0/299
44	m	0.28	0/379	0.72	0/510
45	o	0.35	0/807	0.54	0/1083
46	p	0.28	0/1071	0.54	0/1433
47	q	0.30	0/1413	0.54	0/1906
48	r	0.33	0/1238	0.60	0/1676
49	s	0.38	0/3114	0.59	1/4225 (0.0%)
50	u	0.27	0/949	0.63	0/1281
51	v	0.31	0/597	0.59	0/796
52	w	0.27	0/647	0.66	1/871 (0.1%)
53	A	0.61	2/25926 (0.0%)	1.04	124/40305 (0.3%)
54	B	0.32	0/1328	1.06	2/2056 (0.1%)
55	z	0.30	0/1729	0.97	4/2685 (0.1%)
All	All	0.44	2/97356 (0.0%)	0.77	154/137383 (0.1%)

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
1	D	0	1
7	K	0	1
9	M	0	1
15	S	0	1
28	6	0	1
30	8	0	1
31	9	0	1
35	d	0	1
49	s	0	1
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	A	340	U	N3-C4	-6.28	1.32	1.38
53	A	239	A	C6-N1	-5.44	1.31	1.35

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	A	340	U	C5-C4-O4	21.23	138.64	125.90
53	A	340	U	N3-C4-O4	-17.45	107.18	119.40
53	A	239	A	N1-C6-N6	-13.15	110.71	118.60
53	A	340	U	C2-N3-C4	9.93	132.96	127.00
53	A	652	C	N1-C2-O2	9.90	124.84	118.90
53	A	1522	C	N1-C2-O2	8.37	123.92	118.90
53	A	652	C	N3-C2-O2	-8.36	116.05	121.90
53	A	1542	C	C2-N1-C1'	8.30	127.93	118.80
53	A	652	C	C2-N1-C1'	8.28	127.90	118.80
53	A	517	C	N3-C2-O2	-8.23	116.14	121.90
53	A	239	A	C5-C6-N6	8.21	130.27	123.70
53	A	1542	C	N1-C2-O2	8.13	123.78	118.90
53	A	44	C	N1-C2-O2	8.05	123.73	118.90
53	A	716	C	N1-C2-O2	7.93	123.66	118.90
53	A	716	C	C2-N1-C1'	7.71	127.28	118.80
53	A	516	C	N1-C2-O2	7.64	123.48	118.90
53	A	143	C	C2-N1-C1'	7.56	127.11	118.80
53	A	652	C	C6-N1-C2	-7.45	117.32	120.30
53	A	1522	C	C2-N1-C1'	7.39	126.93	118.80
53	A	143	C	N1-C2-O2	7.34	123.31	118.90
53	A	44	C	C2-N1-C1'	7.30	126.83	118.80
53	A	143	C	N3-C2-O2	-7.29	116.79	121.90
53	A	541	U	N3-C2-O2	-7.23	117.14	122.20
53	A	340	U	N1-C2-N3	-7.16	110.60	114.90
53	A	1228	U	C2-N1-C1'	7.14	126.26	117.70
10	N	114	ASP	CB-CG-OD1	7.09	124.69	118.30
53	A	541	U	N1-C2-O2	7.09	127.76	122.80
53	A	709	C	N1-C2-O2	7.04	123.12	118.90
53	A	702	U	C2-N1-C1'	6.93	126.01	117.70
53	A	44	C	N3-C2-O2	-6.86	117.10	121.90
3	F	271	ASP	CB-CG-OD1	6.83	124.45	118.30
28	6	52	ARG	CA-CB-CG	6.70	128.14	113.40
53	A	118	C	N1-C2-O2	6.69	122.91	118.90
53	A	59	U	N3-C2-O2	-6.58	117.59	122.20
27	5	79	ASP	CB-CG-OD1	6.53	124.17	118.30
53	A	1522	C	N3-C2-O2	-6.52	117.34	121.90
53	A	709	C	C2-N1-C1'	6.51	125.96	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	6	336	ASP	CB-CG-OD1	6.48	124.14	118.30
53	A	1014	C	N1-C2-O2	6.47	122.78	118.90
53	A	153	A	P-O3'-C3'	6.46	127.45	119.70
53	A	746	U	C2-N1-C1'	6.42	125.41	117.70
53	A	1531	A	P-O3'-C3'	6.37	127.34	119.70
54	B	1628	C	C6-N1-C2	-6.37	117.75	120.30
53	A	1464	C	N1-C2-O2	6.36	122.72	118.90
53	A	506	C	N3-C2-O2	-6.33	117.47	121.90
53	A	417	U	C5-C6-N1	6.30	125.85	122.70
55	z	69	C	C2-N1-C1'	6.23	125.65	118.80
53	A	396	C	C2-N1-C1'	6.23	125.65	118.80
53	A	716	C	N3-C2-O2	-6.23	117.54	121.90
53	A	771	C	C2-N1-C1'	6.22	125.65	118.80
27	5	382	LEU	CA-CB-CG	6.15	129.45	115.30
53	A	1542	C	N3-C2-O2	-6.14	117.60	121.90
53	A	23	C	N1-C2-O2	6.13	122.58	118.90
20	X	64	ASP	CB-CG-OD1	6.11	123.80	118.30
53	A	31	U	N1-C2-O2	6.10	127.07	122.80
53	A	702	U	N3-C2-O2	-6.10	117.93	122.20
53	A	23	C	C2-N1-C1'	6.07	125.48	118.80
20	X	180	ASP	CB-CG-OD2	6.06	123.75	118.30
49	s	229	LEU	CA-CB-CG	6.04	129.19	115.30
53	A	31	U	N3-C2-O2	-6.02	117.98	122.20
53	A	396	C	N1-C2-O2	6.02	122.51	118.90
53	A	24	U	N1-C2-O2	6.02	127.02	122.80
53	A	702	U	N1-C2-O2	6.01	127.00	122.80
53	A	787	A	P-O3'-C3'	6.00	126.90	119.70
53	A	573	A	P-O3'-C3'	5.99	126.89	119.70
53	A	19	C	C2-N1-C1'	5.99	125.39	118.80
53	A	360	U	P-O3'-C3'	5.95	126.84	119.70
53	A	1228	U	N3-C2-O2	-5.95	118.03	122.20
53	A	709	C	N3-C2-O2	-5.93	117.75	121.90
40	i	63	LEU	CA-CB-CG	5.92	128.93	115.30
53	A	466	C	C2-N1-C1'	5.92	125.32	118.80
13	Q	185	ASP	CB-CG-OD1	5.91	123.62	118.30
53	A	1522	C	C6-N1-C2	-5.90	117.94	120.30
53	A	652	C	C5-C6-N1	5.89	123.95	121.00
31	9	69	LYS	CA-CB-CG	5.89	126.36	113.40
18	V	103	ASP	CB-CG-OD1	5.86	123.57	118.30
53	A	374	A	N3-C4-N9	5.82	132.06	127.40
3	F	292	ASP	CB-CG-OD1	5.82	123.54	118.30
17	U	11	ARG	NE-CZ-NH1	5.81	123.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	A	1228	U	N1-C2-O2	5.80	126.86	122.80
53	A	374	A	N9-C4-C5	-5.80	103.48	105.80
53	A	19	C	N1-C2-O2	5.78	122.37	118.90
53	A	55	C	N1-C2-O2	5.74	122.34	118.90
53	A	986	U	C2-N1-C1'	5.73	124.58	117.70
53	A	37	C	N1-C2-O2	5.73	122.34	118.90
53	A	1542	C	C6-N1-C1'	-5.71	113.94	120.80
55	z	40	U	N3-C2-O2	-5.71	118.20	122.20
53	A	31	U	C2-N1-C1'	5.70	124.54	117.70
53	A	504	G	N1-C2-N2	-5.69	111.08	116.20
53	A	44	C	C6-N1-C2	-5.68	118.03	120.30
4	H	146	LEU	CA-CB-CG	5.66	128.32	115.30
53	A	423	U	N3-C2-O2	-5.66	118.24	122.20
53	A	726	C	N1-C2-O2	5.65	122.29	118.90
53	A	573	A	OP2-P-O3'	5.64	117.60	105.20
53	A	614	C	C2-N1-C1'	5.64	125.00	118.80
30	8	96	ASP	CB-CG-OD2	5.63	123.36	118.30
53	A	517	C	N1-C2-O2	5.63	122.28	118.90
53	A	516	C	C5-C6-N1	5.60	123.80	121.00
53	A	170	C	C5-C6-N1	5.60	123.80	121.00
28	6	52	ARG	CB-CA-C	5.59	121.59	110.40
53	A	143	C	C6-N1-C2	-5.59	118.07	120.30
53	A	80	G	O4'-C1'-N9	5.58	112.66	108.20
53	A	1014	C	C2-N1-C1'	5.57	124.93	118.80
53	A	1464	C	N3-C2-O2	-5.57	118.00	121.90
55	z	40	U	C2-N1-C1'	5.54	124.34	117.70
53	A	1123	C	N1-C2-O2	5.51	122.21	118.90
53	A	73	U	C5-C6-N1	5.51	125.45	122.70
53	A	1542	C	C6-N1-C2	-5.48	118.11	120.30
53	A	727	C	N1-C2-O2	5.47	122.18	118.90
53	A	716	C	C6-N1-C2	-5.47	118.11	120.30
53	A	24	U	N3-C2-O2	-5.46	118.38	122.20
55	z	40	U	N1-C2-O2	5.46	126.62	122.80
53	A	986	U	N3-C2-O2	-5.45	118.38	122.20
53	A	1080	U	C2-N1-C1'	5.45	124.24	117.70
53	A	516	C	C2-N1-C1'	5.44	124.78	118.80
53	A	410	U	N1-C2-O2	5.41	126.58	122.80
53	A	986	U	N1-C2-O2	5.41	126.58	122.80
53	A	396	C	N3-C2-O2	-5.40	118.12	121.90
53	A	593	C	C6-N1-C2	-5.40	118.14	120.30
52	w	139	MET	CA-CB-CG	5.40	122.47	113.30
53	A	387	C	C6-N1-C2	-5.38	118.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	A	37	C	C2-N1-C1'	5.38	124.71	118.80
53	A	466	C	C5-C6-N1	5.37	123.68	121.00
53	A	716	C	C6-N1-C1'	-5.36	114.37	120.80
53	A	1077	U	C2-N1-C1'	5.33	124.10	117.70
53	A	1542	C	C5-C6-N1	5.32	123.66	121.00
53	A	1522	C	C5-C6-N1	5.29	123.64	121.00
11	O	75	MET	CB-CG-SD	-5.27	96.59	112.40
33	b	56	ARG	NE-CZ-NH1	5.27	122.94	120.30
53	A	50	C	N1-C2-O2	5.26	122.06	118.90
53	A	55	C	N3-C2-O2	-5.22	118.25	121.90
53	A	468	U	N3-C2-O2	-5.22	118.55	122.20
53	A	705	C	C2-N1-C1'	5.19	124.51	118.80
53	A	410	U	N3-C2-O2	-5.19	118.57	122.20
54	B	1635	C	N1-C2-O2	5.18	122.01	118.90
53	A	837	A	P-O3'-C3'	5.13	125.85	119.70
34	c	280	LEU	CA-CB-CG	5.12	127.08	115.30
53	A	423	U	C2-N1-C1'	5.12	123.84	117.70
53	A	541	U	C2-N1-C1'	5.11	123.83	117.70
53	A	143	C	C6-N1-C1'	-5.10	114.68	120.80
53	A	374	A	C6-C5-N7	-5.10	128.73	132.30
53	A	423	U	N1-C2-O2	5.10	126.37	122.80
53	A	506	C	C6-N1-C2	-5.10	118.26	120.30
53	A	997	U	N1-C2-O2	5.08	126.35	122.80
53	A	516	C	N3-C2-O2	-5.07	118.35	121.90
53	A	1057	C	C5-C6-N1	5.06	123.53	121.00
53	A	239	A	N1-C2-N3	-5.04	126.78	129.30
53	A	1080	U	N1-C2-O2	5.03	126.32	122.80
13	Q	166	LEU	CA-CB-CG	5.03	126.86	115.30
53	A	466	C	N1-C2-O2	5.02	121.91	118.90
53	A	652	C	C6-N1-C1'	-5.02	114.77	120.80
53	A	1182	C	C2-N1-C1'	5.02	124.33	118.80
53	A	23	C	C6-N1-C2	-5.01	118.30	120.30
2	E	113	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	6	138	GLU	Peptide
30	8	149	GLU	Peptide
31	9	68	PHE	Peptide
1	D	206	TYR	Peptide

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Mol	Chain	Res	Type	Group
7	K	168	ARG	Peptide
9	M	46	GLY	Peptide
15	S	101	PHE	Peptide
35	d	186	VAL	Peptide
49	s	270	LYS	Peptide

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	D	234/305 (77%)	213 (91%)	20 (8%)	1 (0%)	34	72
2	E	302/348 (87%)	279 (92%)	23 (8%)	0	100	100
3	F	248/311 (80%)	239 (96%)	9 (4%)	0	100	100
4	H	93/267 (35%)	89 (96%)	4 (4%)	0	100	100
5	I	154/261 (59%)	142 (92%)	12 (8%)	0	100	100
6	J	138/192 (72%)	127 (92%)	11 (8%)	0	100	100
7	K	175/178 (98%)	169 (97%)	6 (3%)	0	100	100
8	L	113/145 (78%)	105 (93%)	8 (7%)	0	100	100
9	M	285/296 (96%)	268 (94%)	17 (6%)	0	100	100
10	N	203/251 (81%)	195 (96%)	8 (4%)	0	100	100
11	O	150/175 (86%)	144 (96%)	6 (4%)	0	100	100
12	P	139/180 (77%)	134 (96%)	5 (4%)	0	100	100
13	Q	215/292 (74%)	202 (94%)	13 (6%)	0	100	100
14	R	138/149 (93%)	135 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	S	154/205 (75%)	143 (93%)	11 (7%)	0	100	100
16	T	155/206 (75%)	152 (98%)	3 (2%)	0	100	100
17	U	135/153 (88%)	129 (96%)	6 (4%)	0	100	100
18	V	188/216 (87%)	182 (97%)	6 (3%)	0	100	100
19	W	107/148 (72%)	102 (95%)	5 (5%)	0	100	100
20	X	241/256 (94%)	235 (98%)	6 (2%)	0	100	100
21	Y	174/250 (70%)	170 (98%)	4 (2%)	0	100	100
22	Z	118/161 (73%)	110 (93%)	8 (7%)	0	100	100
23	0	106/188 (56%)	103 (97%)	3 (3%)	0	100	100
24	1	50/65 (77%)	50 (100%)	0	0	100	100
25	2	41/92 (45%)	41 (100%)	0	0	100	100
26	3	93/188 (50%)	90 (97%)	3 (3%)	0	100	100
27	5	383/423 (90%)	367 (96%)	15 (4%)	1 (0%)	41	75
28	6	316/380 (83%)	303 (96%)	13 (4%)	0	100	100
29	7	285/338 (84%)	268 (94%)	17 (6%)	0	100	100
30	8	97/206 (47%)	89 (92%)	8 (8%)	0	100	100
31	9	113/137 (82%)	108 (96%)	5 (4%)	0	100	100
32	a	69/142 (49%)	67 (97%)	2 (3%)	0	100	100
33	b	146/215 (68%)	133 (91%)	13 (9%)	0	100	100
34	c	271/332 (82%)	265 (98%)	6 (2%)	0	100	100
35	d	203/306 (66%)	195 (96%)	8 (4%)	0	100	100
36	e	211/279 (76%)	194 (92%)	17 (8%)	0	100	100
37	f	110/212 (52%)	100 (91%)	9 (8%)	1 (1%)	17	56
38	g	127/166 (76%)	123 (97%)	4 (3%)	0	100	100
39	h	96/158 (61%)	94 (98%)	2 (2%)	0	100	100
40	i	95/128 (74%)	92 (97%)	3 (3%)	0	100	100
41	j	83/123 (68%)	81 (98%)	2 (2%)	0	100	100
42	k	76/112 (68%)	68 (90%)	8 (10%)	0	100	100
43	l	21/138 (15%)	21 (100%)	0	0	100	100
44	m	43/128 (34%)	38 (88%)	5 (12%)	0	100	100
45	o	91/102 (89%)	87 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	p	119/206 (58%)	116 (98%)	3 (2%)	0	100	100
47	q	162/222 (73%)	157 (97%)	5 (3%)	0	100	100
48	r	140/196 (71%)	131 (94%)	9 (6%)	0	100	100
49	s	366/439 (83%)	356 (97%)	10 (3%)	0	100	100
50	u	109/234 (47%)	99 (91%)	10 (9%)	0	100	100
51	v	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
52	w	77/156 (49%)	71 (92%)	6 (8%)	0	100	100
All	All	8025/11026 (73%)	7635 (95%)	387 (5%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	5	216	GLU
37	f	179	PRO
1	D	207	ILE

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	D	190/245 (78%)	190 (100%)	0	100	100
2	E	259/290 (89%)	258 (100%)	1 (0%)	91	96
3	F	217/262 (83%)	216 (100%)	1 (0%)	88	94
4	H	86/228 (38%)	86 (100%)	0	100	100
5	I	145/232 (62%)	144 (99%)	1 (1%)	84	93
6	J	113/150 (75%)	113 (100%)	0	100	100
7	K	155/156 (99%)	154 (99%)	1 (1%)	86	94
8	L	98/124 (79%)	98 (100%)	0	100	100
9	M	245/249 (98%)	244 (100%)	1 (0%)	91	96
10	N	172/211 (82%)	170 (99%)	2 (1%)	71	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	O	133/150 (89%)	133 (100%)	0	100	100
12	P	123/155 (79%)	120 (98%)	3 (2%)	49	76
13	Q	199/256 (78%)	198 (100%)	1 (0%)	88	94
14	R	118/126 (94%)	118 (100%)	0	100	100
15	S	141/180 (78%)	139 (99%)	2 (1%)	67	85
16	T	141/176 (80%)	141 (100%)	0	100	100
17	U	124/135 (92%)	124 (100%)	0	100	100
18	V	172/191 (90%)	172 (100%)	0	100	100
19	W	89/119 (75%)	89 (100%)	0	100	100
20	X	219/229 (96%)	219 (100%)	0	100	100
21	Y	159/223 (71%)	159 (100%)	0	100	100
22	Z	111/147 (76%)	111 (100%)	0	100	100
23	0	97/164 (59%)	96 (99%)	1 (1%)	76	88
24	1	49/60 (82%)	49 (100%)	0	100	100
25	2	38/72 (53%)	38 (100%)	0	100	100
26	3	88/166 (53%)	88 (100%)	0	100	100
27	5	348/368 (95%)	348 (100%)	0	100	100
28	6	265/332 (80%)	263 (99%)	2 (1%)	81	91
29	7	263/303 (87%)	263 (100%)	0	100	100
30	8	91/190 (48%)	89 (98%)	2 (2%)	52	78
31	9	99/112 (88%)	98 (99%)	1 (1%)	76	88
32	a	69/133 (52%)	68 (99%)	1 (1%)	67	85
33	b	130/186 (70%)	130 (100%)	0	100	100
34	c	241/288 (84%)	241 (100%)	0	100	100
35	d	193/274 (70%)	193 (100%)	0	100	100
36	e	188/236 (80%)	188 (100%)	0	100	100
37	f	101/188 (54%)	101 (100%)	0	100	100
38	g	119/148 (80%)	119 (100%)	0	100	100
39	h	95/148 (64%)	95 (100%)	0	100	100
40	i	86/110 (78%)	86 (100%)	0	100	100
41	j	68/97 (70%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	k	71/90 (79%)	71 (100%)	0	100	100
43	l	23/116 (20%)	23 (100%)	0	100	100
44	m	40/113 (35%)	40 (100%)	0	100	100
45	o	79/87 (91%)	79 (100%)	0	100	100
46	p	117/181 (65%)	117 (100%)	0	100	100
47	q	141/178 (79%)	140 (99%)	1 (1%)	84	93
48	r	133/169 (79%)	133 (100%)	0	100	100
49	s	326/381 (86%)	323 (99%)	3 (1%)	78	90
50	u	105/200 (52%)	102 (97%)	3 (3%)	42	71
51	v	59/60 (98%)	59 (100%)	0	100	100
52	w	73/136 (54%)	73 (100%)	0	100	100
All	All	7204/9520 (76%)	7177 (100%)	27 (0%)	91	96

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	303	LYS
3	F	184	GLN
5	I	139	LYS
7	K	6	ARG
9	M	44	ARG
10	N	197	LYS
10	N	200	LYS
12	P	108	ARG
12	P	142	ASN
12	P	144	MET
13	Q	244	ARG
15	S	118	ASN
15	S	129	ARG
23	0	168	GLN
28	6	47	ARG
28	6	52	ARG
30	8	113	ARG
30	8	125	LYS
31	9	116	LYS
32	a	122	ARG
47	q	140	ARG
49	s	230	ARG

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Mol	Chain	Res	Type
49	s	296	HIS
49	s	313	ARG
50	u	107	ARG
50	u	153	ARG
50	u	192	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
10	N	210	GLN
11	O	91	GLN
12	P	142	ASN
21	Y	88	GLN
21	Y	89	GLN
21	Y	183	GLN
29	7	285	ASN
34	c	310	ASN
37	f	111	HIS
37	f	115	ASN
41	j	63	GLN
49	s	296	HIS
49	s	319	GLN
52	w	142	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	A	1071/1559 (68%)	264 (24%)	12 (1%)
54	B	51/69 (73%)	14 (27%)	1 (1%)
55	z	70/73 (95%)	36 (51%)	0
All	All	1192/1701 (70%)	314 (26%)	13 (1%)

All (314) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
53	A	6	A
53	A	8	C
53	A	9	U
53	A	11	G
53	A	15	C

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Mol	Chain	Res	Type
53	A	19	C
53	A	24	U
53	A	30	U
53	A	31	U
53	A	34	U
53	A	38	A
53	A	44	C
53	A	47	U
53	A	54	A
53	A	57	A
53	A	61	A
53	A	62	C
53	A	71	A
53	A	78	G
53	A	80	G
53	A	81	A
53	A	99	C
53	A	100	G
53	A	103	A
53	A	107	A
53	A	110	U
53	A	111	A
53	A	121	G
53	A	124	A
53	A	126	A
53	A	127	G
53	A	134	A
53	A	135	A
53	A	136	U
53	A	142	C
53	A	147	C
53	A	151	A
53	A	153	A
53	A	154	U
53	A	157	C
53	A	158	A
53	A	159	A
53	A	162	A
53	A	166	A
53	A	174	A
53	A	179	C
53	A	197	A

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Mol	Chain	Res	Type
53	A	198	G
53	A	199	A
53	A	201	A
53	A	202	U
53	A	208	U
53	A	212	A
53	A	213	G
53	A	217	A
53	A	218	G
53	A	222	A
53	A	223	A
53	A	230	A
53	A	231	C
53	A	232	C
53	A	233	C
53	A	246	G
53	A	248	G
53	A	257	G
53	A	315	G
53	A	317	G
53	A	322	C
53	A	324	A
53	A	325	A
53	A	329	A
53	A	331	C
53	A	332	G
53	A	345	G
53	A	351	U
53	A	352	G
53	A	359	A
53	A	360	U
53	A	361	A
53	A	364	A
53	A	366	C
53	A	367	U
53	A	369	A
53	A	383	U
53	A	390	A
53	A	395	A
53	A	404	A
53	A	409	C
53	A	413	U

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Mol	Chain	Res	Type
53	A	415	A
53	A	423	U
53	A	427	A
53	A	428	G
53	A	435	G
53	A	443	G
53	A	454	A
53	A	455	C
53	A	456	U
53	A	464	A
53	A	471	U
53	A	472	A
53	A	477	G
53	A	484	A
53	A	486	A
53	A	488	U
53	A	489	U
53	A	490	A
53	A	493	A
53	A	496	C
53	A	501	U
53	A	502	A
53	A	503	G
53	A	504	G
53	A	507	U
53	A	510	A
53	A	511	A
53	A	512	G
53	A	513	C
53	A	514	A
53	A	517	C
53	A	520	C
53	A	523	U
53	A	524	U
53	A	525	A
53	A	527	G
53	A	528	A
53	A	530	A
53	A	531	G
53	A	534	U
53	A	540	C
53	A	546	A

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Mol	Chain	Res	Type
53	A	567	A
53	A	569	A
53	A	571	A
53	A	572	U
53	A	573	A
53	A	574	U
53	A	575	A
53	A	576	A
53	A	582	C
53	A	590	A
53	A	592	C
53	A	593	C
53	A	610	C
53	A	611	A
53	A	613	C
53	A	614	C
53	A	615	U
53	A	628	A
53	A	629	U
53	A	630	G
53	A	644	C
53	A	652	C
53	A	662	C
53	A	675	G
53	A	679	G
53	A	680	A
53	A	701	U
53	A	704	A
53	A	711	A
53	A	717	U
53	A	720	A
53	A	723	C
53	A	726	C
53	A	729	A
53	A	735	C
53	A	736	A
53	A	737	U
53	A	739	A
53	A	744	C
53	A	756	C
53	A	757	C
53	A	761	C

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Mol	Chain	Res	Type
53	A	765	G
53	A	774	A
53	A	776	A
53	A	788	A
53	A	798	A
53	A	799	A
53	A	838	C
53	A	841	C
53	A	842	A
53	A	850	C
53	A	851	A
53	A	852	U
53	A	853	C
53	A	854	A
53	A	857	A
53	A	990	U
53	A	1013	C
53	A	1014	C
53	A	1016	G
53	A	1029	C
53	A	1036	A
53	A	1049	G
53	A	1055	A
53	A	1062	G
53	A	1069	U
53	A	1070	A
53	A	1073	U
53	A	1075	A
53	A	1077	U
53	A	1080	U
53	A	1133	A
53	A	1134	A
53	A	1140	G
53	A	1144	G
53	A	1145	G
53	A	1161	G
53	A	1162	A
53	A	1163	A
53	A	1174	G
53	A	1177	C
53	A	1182	C
53	A	1183	A

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Mol	Chain	Res	Type
53	A	1184	U
53	A	1189	A
53	A	1191	A
53	A	1192	C
53	A	1194	U
53	A	1195	C
53	A	1200	G
53	A	1201	U
53	A	1209	A
53	A	1223	A
53	A	1225	U
53	A	1231	A
53	A	1236	C
53	A	1240	A
53	A	1243	A
53	A	1247	G
53	A	1249	A
53	A	1252	A
53	A	1256	A
53	A	1258	C
53	A	1438	U
53	A	1439	U
53	A	1444	U
53	A	1452	U
53	A	1453	G
53	A	1459	A
53	A	1464	C
53	A	1469	G
53	A	1471	A
53	A	1480	U
53	A	1485	C
53	A	1487	C
53	A	1488	A
53	A	1490	A
53	A	1492	C
53	A	1498	C
53	A	1507	A
53	A	1510	A
53	A	1514	C
53	A	1518	U
53	A	1519	C
53	A	1520	A

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Mol	Chain	Res	Type
53	A	1522	C
53	A	1532	U
53	A	1536	C
53	A	1537	A
53	A	1547	A
53	A	1548	A
53	A	1558	U
54	B	1607	U
54	B	1608	G
54	B	1611	G
54	B	1614	U
54	B	1615	A
54	B	1625	A
54	B	1629	A
54	B	1637	C
54	B	1640	A
54	B	1641	G
54	B	1643	A
54	B	1644	G
54	B	1645	A
54	B	1649	C
55	z	2	U
55	z	8	U
55	z	9	A
55	z	10	G
55	z	13	U
55	z	14	A
55	z	16	A
55	z	17	U
55	z	18	U
55	z	19	A
55	z	20	U
55	z	21	C
55	z	27	A
55	z	28	A
55	z	32	A
55	z	38	A
55	z	39	A
55	z	40	U
55	z	41	G
55	z	42	C
55	z	45	A

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Mol	Chain	Res	Type
55	z	46	G
55	z	50	A
55	z	51	G
55	z	52	C
55	z	53	C
55	z	54	U
55	z	55	C
55	z	56	A
55	z	58	A
55	z	59	G
55	z	62	C
55	z	64	A
55	z	69	C
55	z	71	C
55	z	72	C

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	A	43	A
53	A	135	A
53	A	153	A
53	A	360	U
53	A	502	A
53	A	516	C
53	A	573	A
53	A	787	A
53	A	837	A
53	A	1235	A
53	A	1438	U
53	A	1531	A
54	B	1607	U

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	-	13,20,21	2.40	4 (30%)	18,26,29	1.16	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	-	-	11/24/26/27	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	v	101	PNS	C34-N36	5.51	1.45	1.33
58	v	101	PNS	C39-N41	5.43	1.45	1.33
58	v	101	PNS	O35-C34	-2.21	1.19	1.23
58	v	101	PNS	O40-C39	-2.10	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	C38-C39-N41	2.12	120.00	116.42

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	v	101	PNS	C28-C29-C32-O33
58	v	101	PNS	C31-C29-C32-O33
58	v	101	PNS	N41-C42-C43-S44

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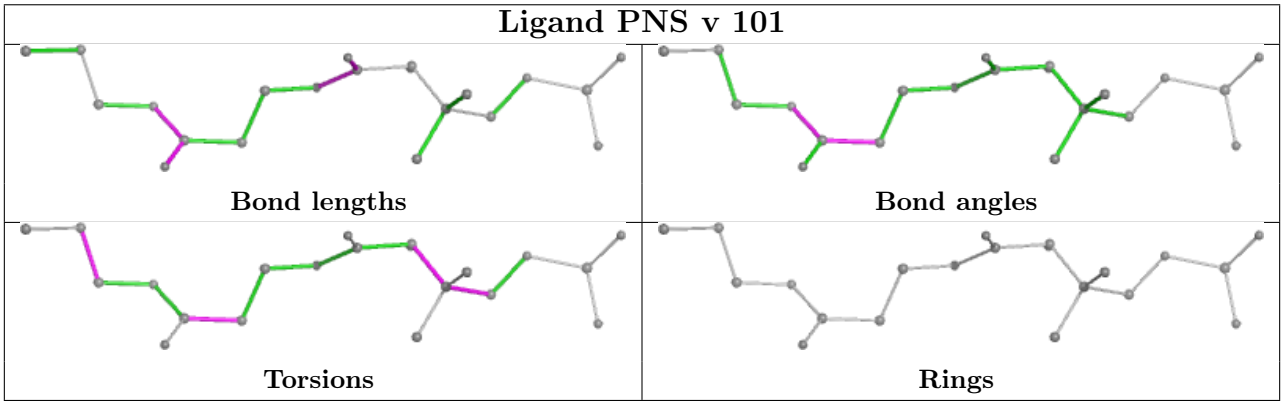
Mol	Chain	Res	Type	Atoms
58	v	101	PNS	C37-C38-C39-O40
58	v	101	PNS	C30-C29-C32-O33
58	v	101	PNS	C31-C29-C32-C34
58	v	101	PNS	C28-C29-C32-C34
58	v	101	PNS	C37-C38-C39-N41
58	v	101	PNS	O27-C28-C29-C30
58	v	101	PNS	O27-C28-C29-C31
58	v	101	PNS	C30-C29-C32-C34

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
55	z	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	z	4:A	O3'	6:U	P	8.95

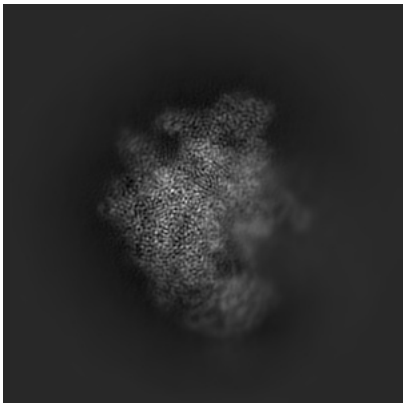
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12921. These allow visual inspection of the internal detail of the map and identification of artifacts.

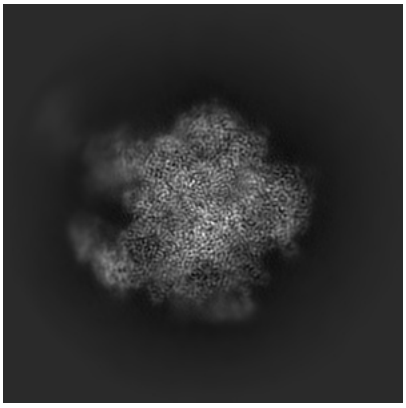
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

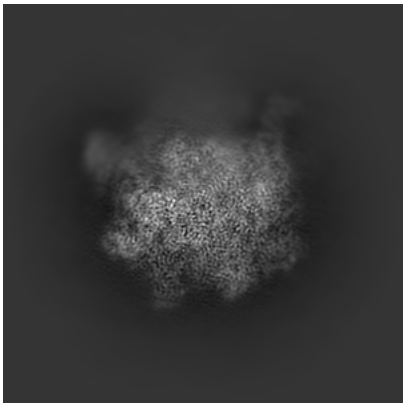
6.1.1 Primary map



X



Y

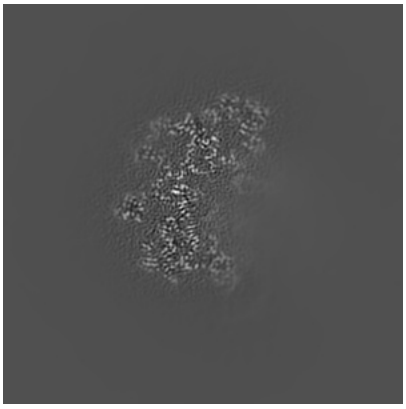


Z

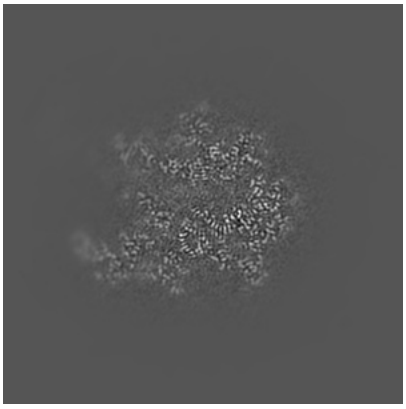
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

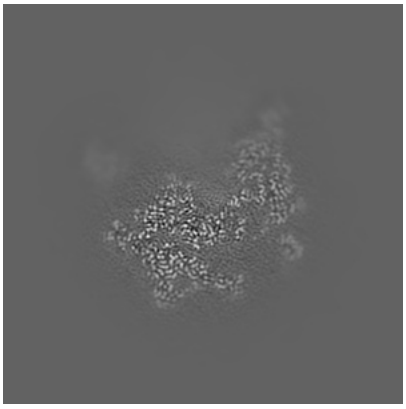
6.2.1 Primary map



X Index: 180



Y Index: 180

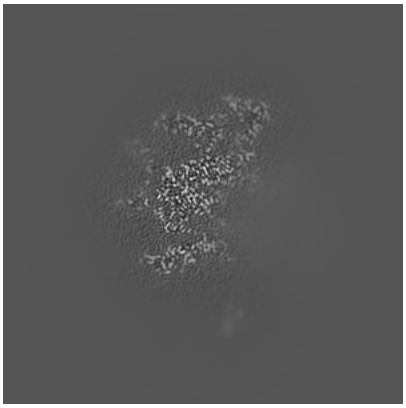


Z Index: 180

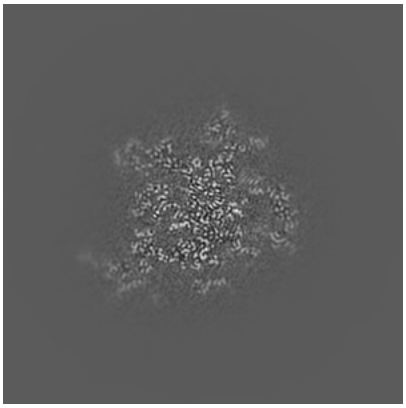
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

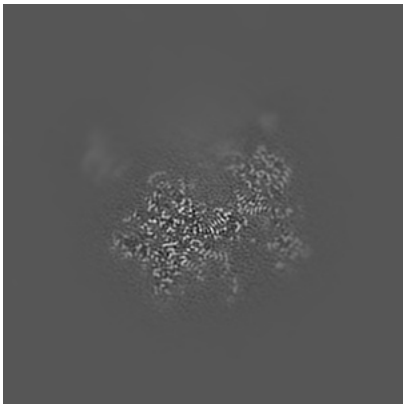
6.3.1 Primary map



X Index: 169



Y Index: 161

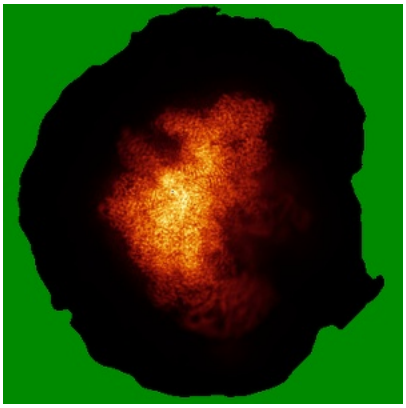


Z Index: 188

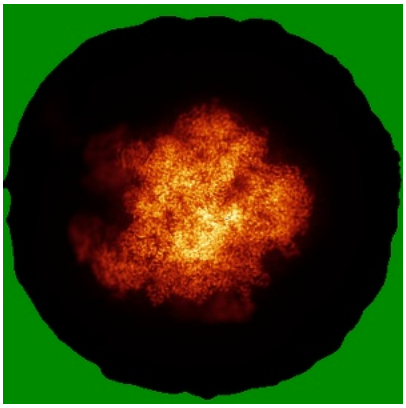
The images above show the largest variance slices of the map in three orthogonal directions.

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

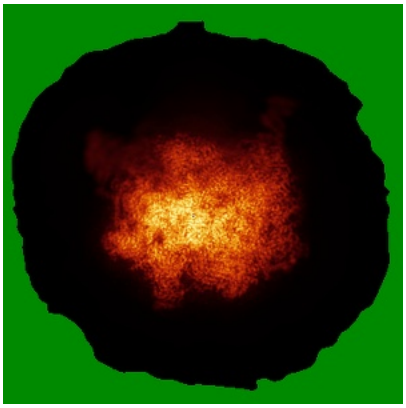
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

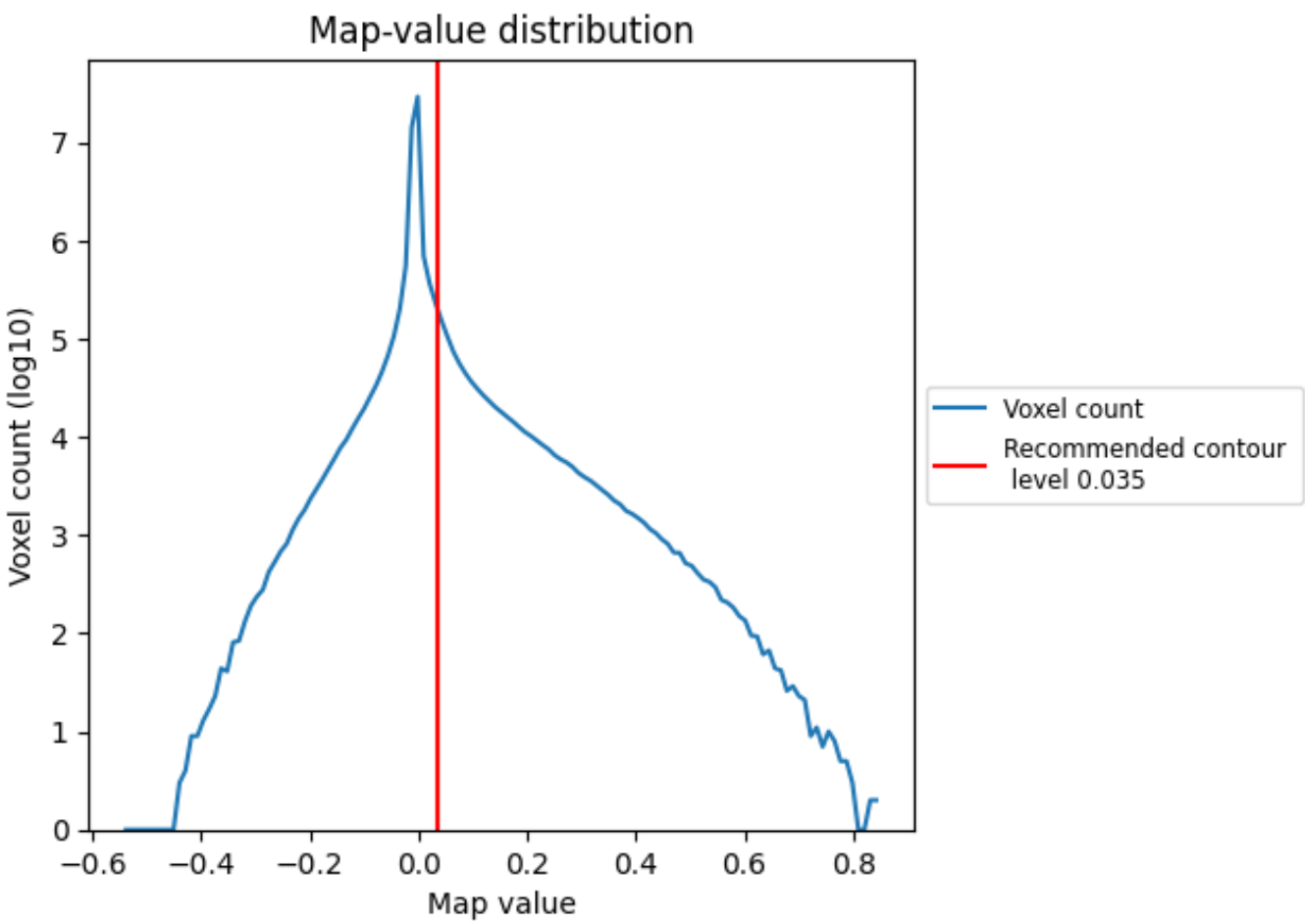
6.6 Mask visualisation (i)

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

7 Map analysis (i)

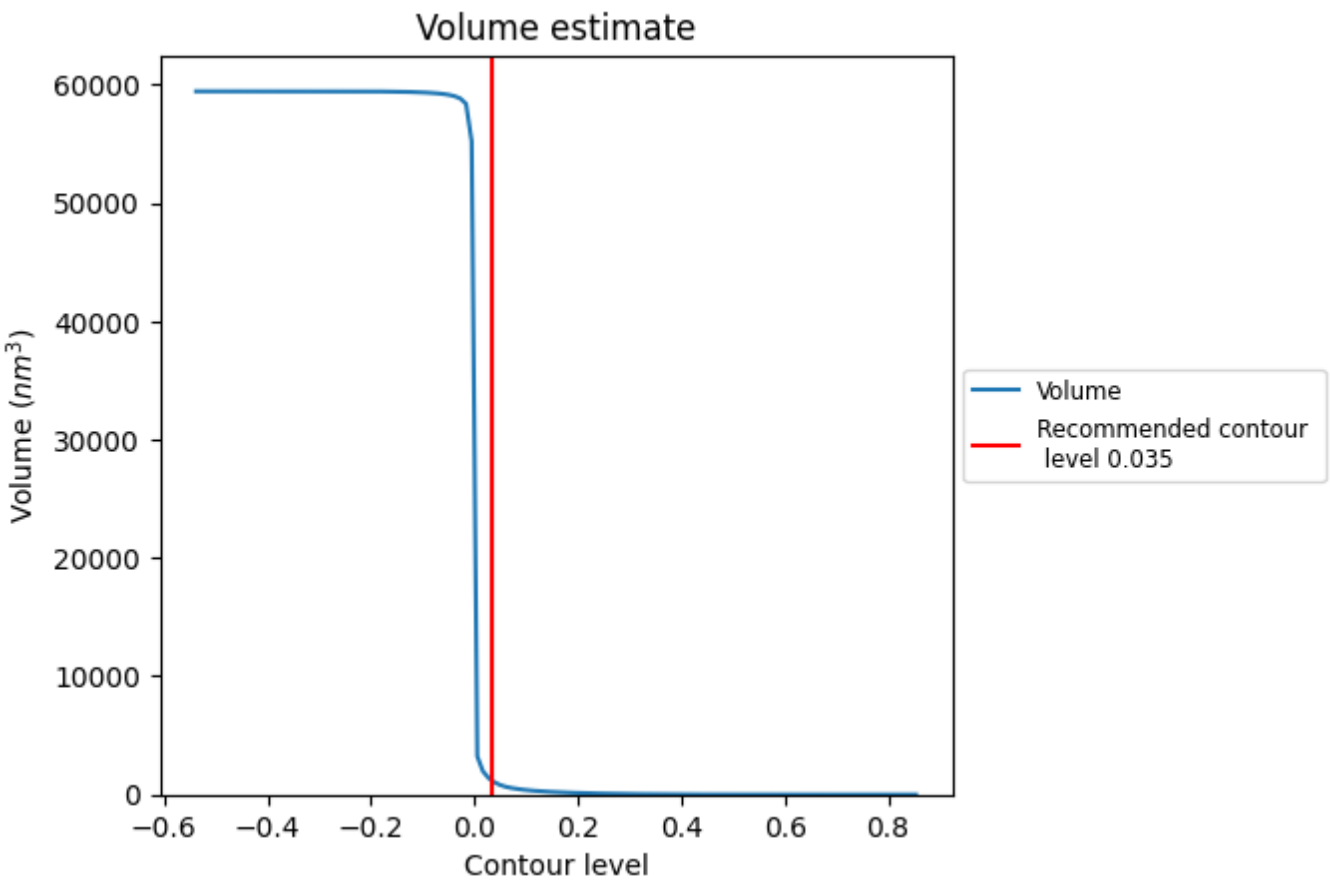
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

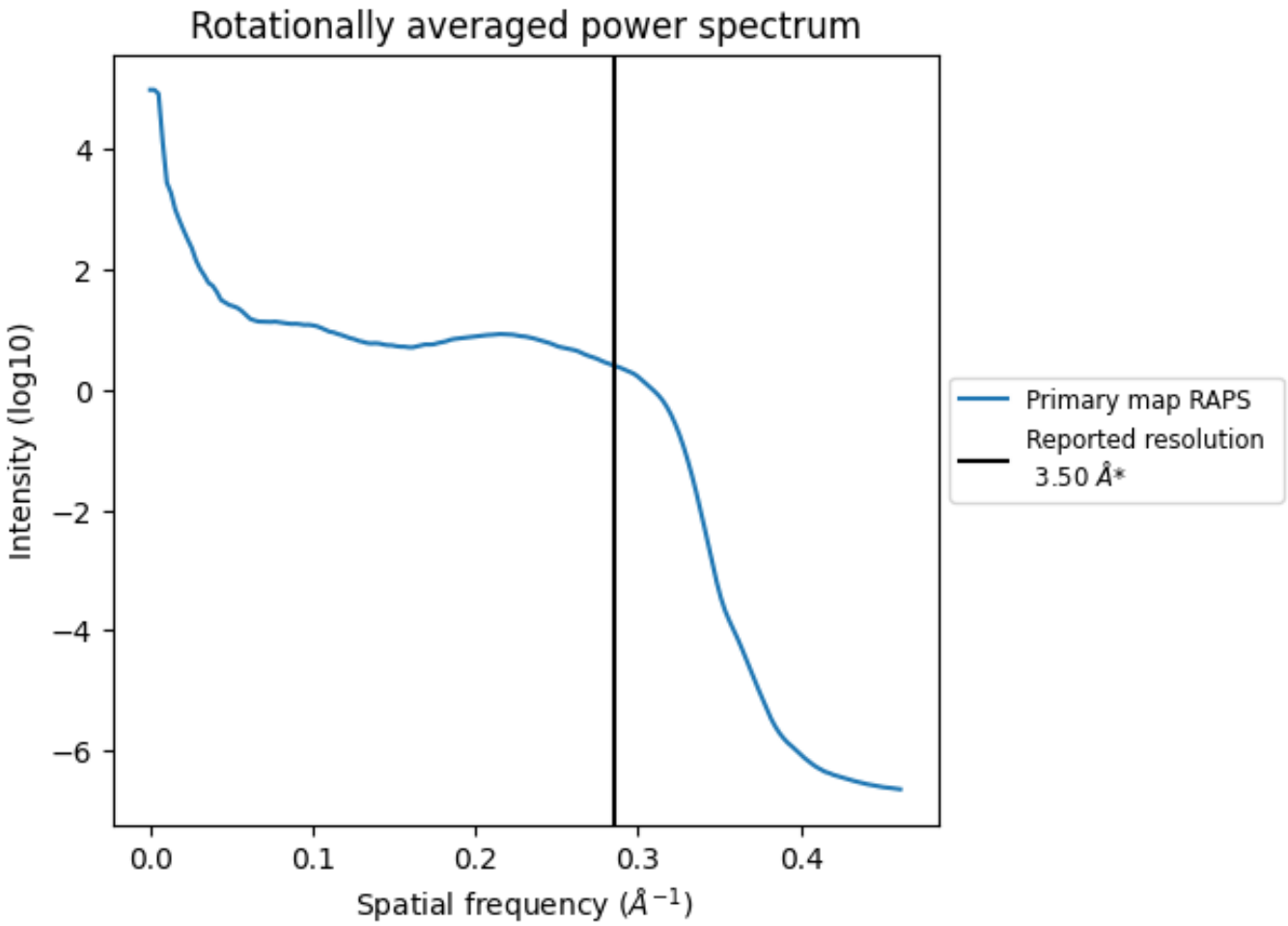
7.2 Volume estimate (i)



The volume at the recommended contour level is 1148 nm^3; this corresponds to an approximate mass of 1037 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)

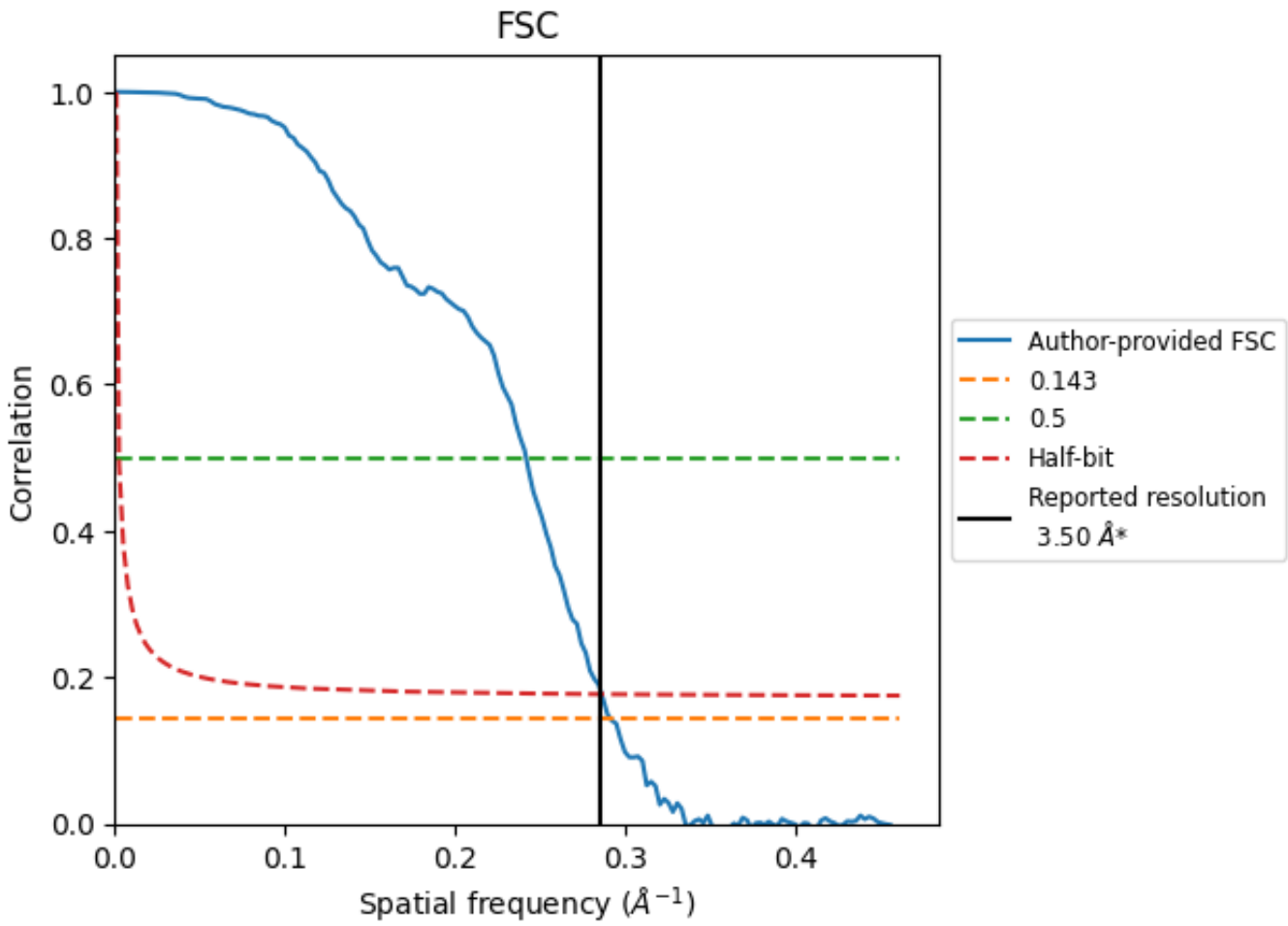


*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

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 0.286 Å^{-1}

8.2 Resolution estimates (i)

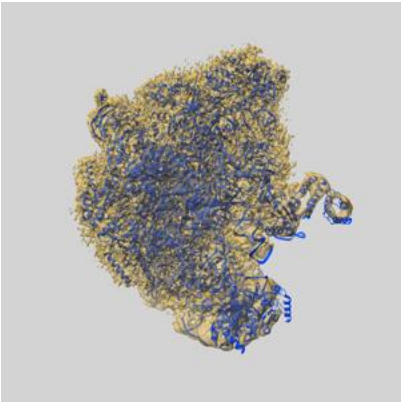
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.43	4.14	3.50
Unmasked-calculated*	-	-	-

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

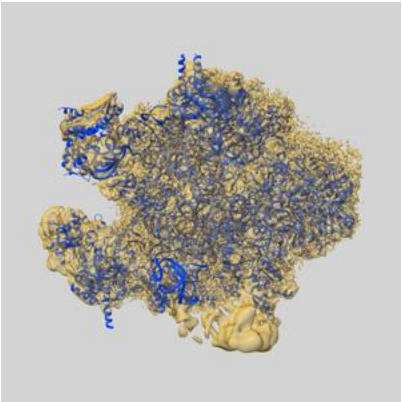
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12921 and PDB model 7OI8. Per-residue inclusion information can be found in section 3 on page 14.

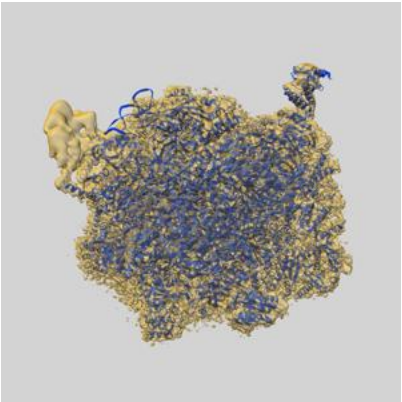
9.1 Map-model overlay (i)



X



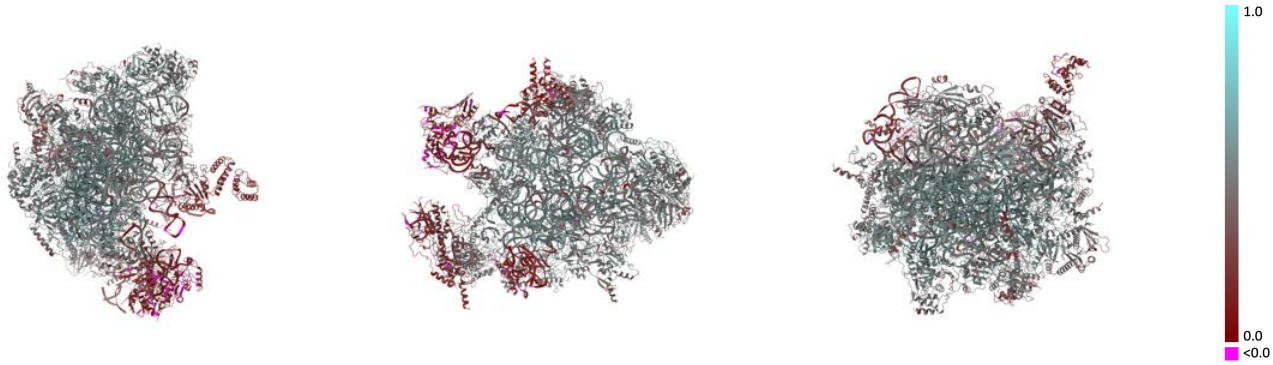
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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.

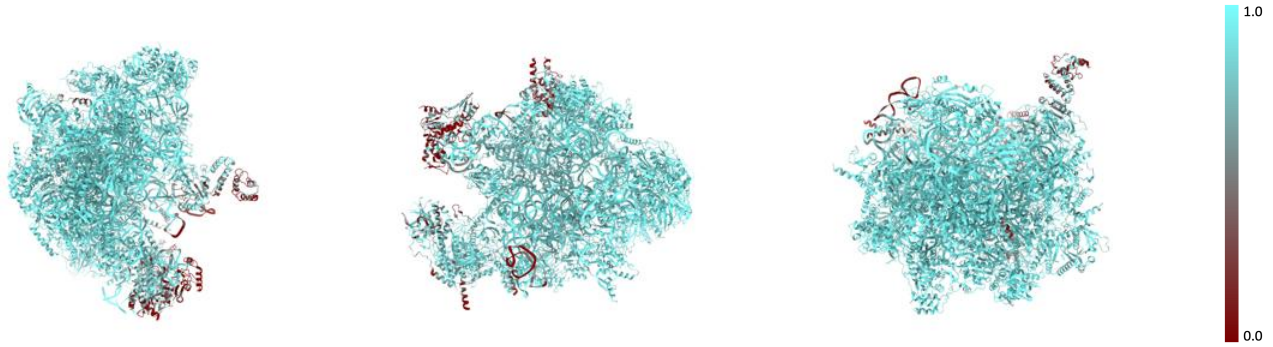
9.2 Q-score mapped to coordinate model (i)



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.

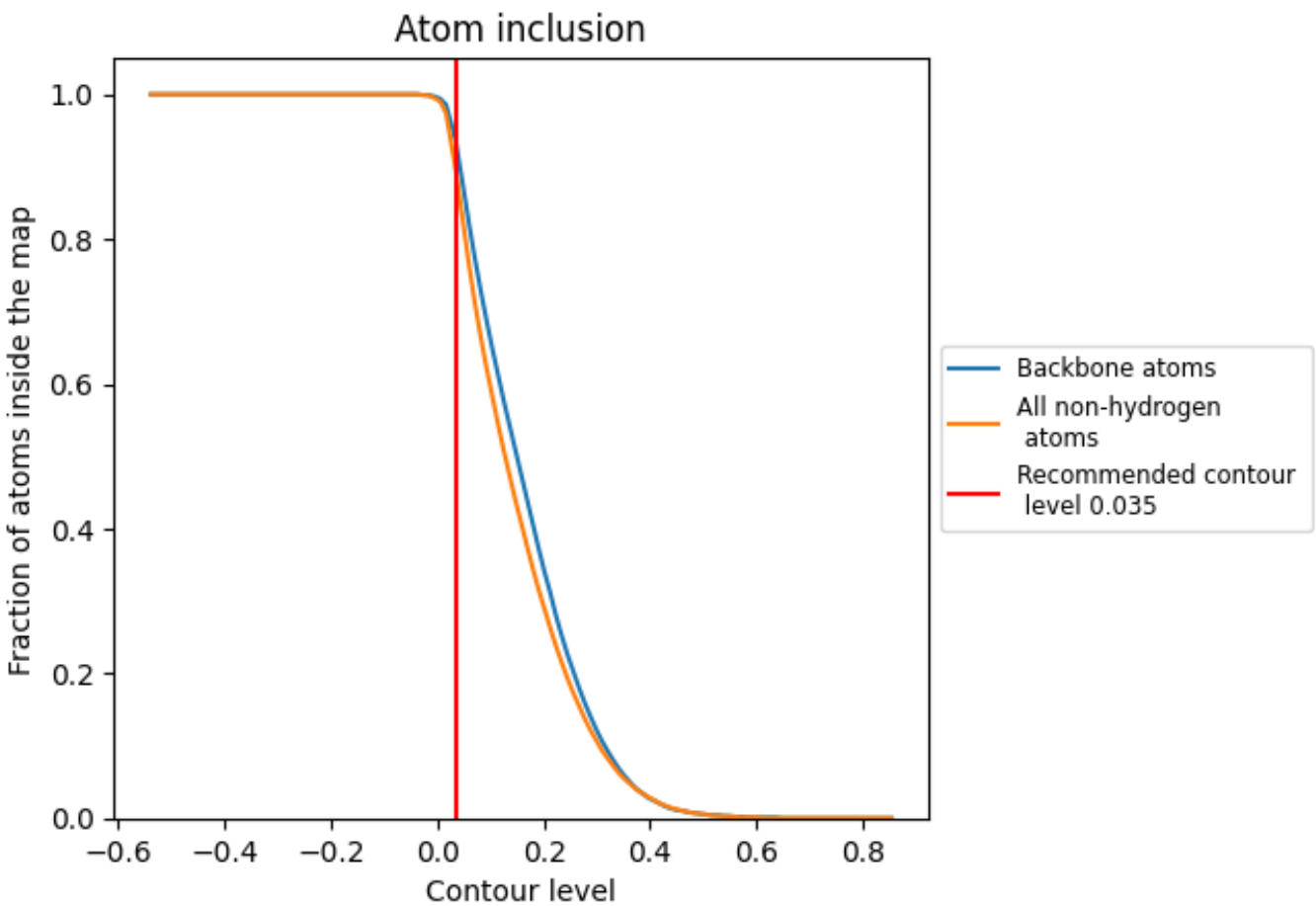
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 89% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8940	0.4580
0	0.9380	0.5180
1	0.9360	0.4830
2	0.9850	0.5910
3	0.9740	0.5880
5	0.9370	0.4760
6	0.9280	0.4420
7	0.8960	0.4320
8	0.6920	0.2360
9	0.9450	0.5000
A	0.9650	0.5050
B	0.9610	0.3140
D	0.8630	0.4470
E	0.8880	0.4650
F	0.9620	0.5500
H	0.9130	0.4680
I	0.4990	0.2210
J	0.1280	0.0900
K	0.9460	0.5240
L	0.8870	0.4120
M	0.9620	0.5470
N	0.9100	0.4560
O	0.9430	0.5170
P	0.9340	0.4780
Q	0.9120	0.4480
R	0.9510	0.5550
S	0.9440	0.5250
T	0.9600	0.5520
U	0.9390	0.5130
V	0.8950	0.4430
W	0.9620	0.5520
X	0.9350	0.5070
Y	0.9620	0.5330
Z	0.9440	0.5330
a	0.9510	0.5290

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Chain	Atom inclusion	Q-score
b	0.9570	0.5370
c	0.9420	0.5020
d	0.8350	0.4000
e	0.6130	0.1830
f	0.7840	0.3500
g	0.9640	0.5380
h	0.9440	0.4650
i	0.9660	0.5760
j	0.9260	0.4940
k	0.6100	0.2040
l	0.8400	0.2030
m	0.7340	0.2360
o	0.9120	0.5020
p	0.9340	0.4710
q	0.8440	0.3830
r	0.9140	0.4510
s	0.9480	0.5130
u	0.6680	0.2430
v	0.5700	0.1950
w	0.2460	0.1390
z	0.5430	0.1510