Full wwPDB EM Validation Report

Jun 23, 2021 – 06:28 AM BST

PDB ID	:	7OF2
EMDB ID	:	EMD-12867
Title	:	Structure of a human mitochondrial ribosome large subunit assembly intermediate in complex with GTPBP6.
Authors	:	Hillen, H.S.; Lavdovskaia, E.; Nadler, F.; Hanitsch, E.; Linden, A.; Bohnsack, K.E.; Urlaub, H.; Richter-Dennerlein, R.
Deposited on	:	2021-05-04
Resolution	:	2.70 Å(reported)
Based on initial model	:	5OOL

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

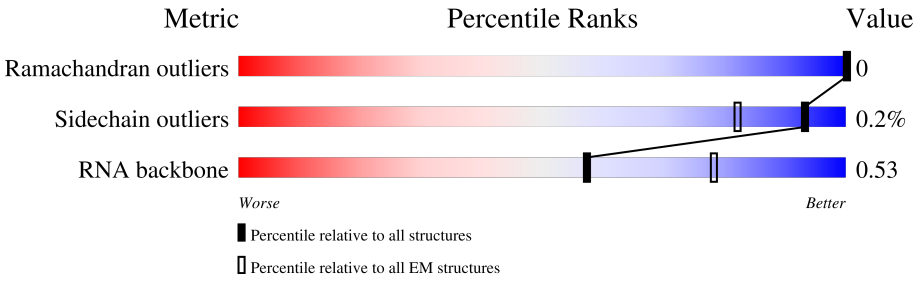
EMDB validation analysis	:	0.0.0.dev75
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	0	188	57% 43%
2	1	65	80% 20%
3	2	92	49% 51%
4	3	188	51% 49%
5	4	103	36% 64%
6	5	423	93% 7%
7	6	380	85% 15%
8	7	338	85% 15%

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Mol	Chain	Length	Quality of chain
9	8	206	8% 37% 63%
10	9	137	85% 15%
11	A	1559	70% 20% 10%
12	B	69	58% 23% 19%
13	C	516	78% 22%
14	D	305	74% 26%
15	E	348	88% 12%
16	F	311	80% 20%
17	H	267	36% 64%
18	I	261	60% 39%
19	J	192	73% 27%
20	K	178	99%
21	L	145	79% 21%
22	M	296	97%
23	N	251	81% 18%
24	O	175	87% 13%
25	P	180	78% 22%
26	Q	292	74% 26%
27	R	149	94% 6%
28	S	205	76% 24%
29	T	206	81% 19%
30	U	153	91% 9%
31	V	216	88% 12%
32	W	148	74% 26%
33	X	256	95% 5%

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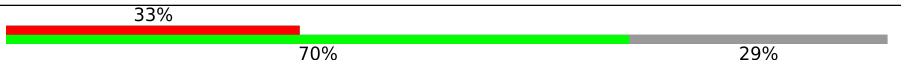
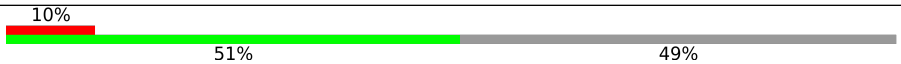
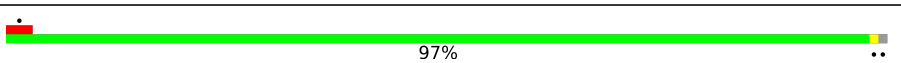
Mol	Chain	Length	Quality of chain
34	Y	250	
35	Z	161	
36	a	142	
37	b	215	
38	c	332	
39	d	306	
40	e	279	
41	f	212	
42	g	166	
43	h	158	
44	i	128	
45	j	123	
46	k	112	
47	l	138	
48	m	128	
49	o	102	
50	p	206	
51	q	222	
52	r	196	
53	s	439	
54	u	234	
55	v	70	
56	w	156	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 101195 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 39S ribosomal protein L32, mitochondrial.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1410	Total	C	N	O	P	0	0
			29940	13436	5400	9694	1410		

- Molecule 12 is a RNA chain called mitochondrial tRNAVal.

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

- Molecule 13 is a protein called Putative GTP-binding protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	401	Total	C	N	O	S	0	0
			3152	1996	579	565	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	227	Total	C	N	O	S	0	0
			1774	1101	358	306	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	305	Total	C	N	O	S	0	0
			2405	1545	418	431	11		

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

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

- Molecule 17 is a protein called 39S ribosomal protein L9, mitochondrial.

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

- Molecule 18 is a protein called 39S ribosomal protein L10, mitochondrial.

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

- Molecule 19 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 20 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 21 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 22 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 23 is a protein called 39S ribosomal protein L16, mitochondrial.

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

- Molecule 24 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 25 is a protein called 39S ribosomal protein L18, mitochondrial.

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

- Molecule 26 is a protein called 39S ribosomal protein L19, mitochondrial.

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

- Molecule 27 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 28 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 29 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 30 is a protein called 39S ribosomal protein L23, mitochondrial.

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

- Molecule 31 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	V	191	Total	C	N	O	S	0	0
			1568	999	280	281	8		

- Molecule 32 is a protein called 39S ribosomal protein L27, mitochondrial.

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

- Molecule 33 is a protein called 39S ribosomal protein L28, mitochondrial.

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

- Molecule 34 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 35 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 36 is a protein called 39S ribosomal protein L42, mitochondrial.

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

- Molecule 37 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 38 is a protein called 39S ribosomal protein L44, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	d	208	Total	C	N	O	S	0	0
			1731	1121	295	306	9		

- Molecule 40 is a protein called 39S ribosomal protein L46, mitochondrial.

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

- Molecule 41 is a protein called 39S ribosomal protein L48, mitochondrial.

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

- Molecule 42 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- Molecule 43 is a protein called 39S ribosomal protein L50, mitochondrial.

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

- Molecule 44 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 45 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	j	84	Total	C	N	O	S	0	0
			679	420	132	125	2		

- Molecule 46 is a protein called 39S ribosomal protein L53, mitochondrial.

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

- Molecule 47 is a protein called 39S ribosomal protein L54, mitochondrial.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	o	94	Total	C	N	O	S	0	0
			797	501	165	128	3		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	r	157	Total	C	N	O	S	0	0
			1287	817	247	215	8		

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

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

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

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

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

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

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

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

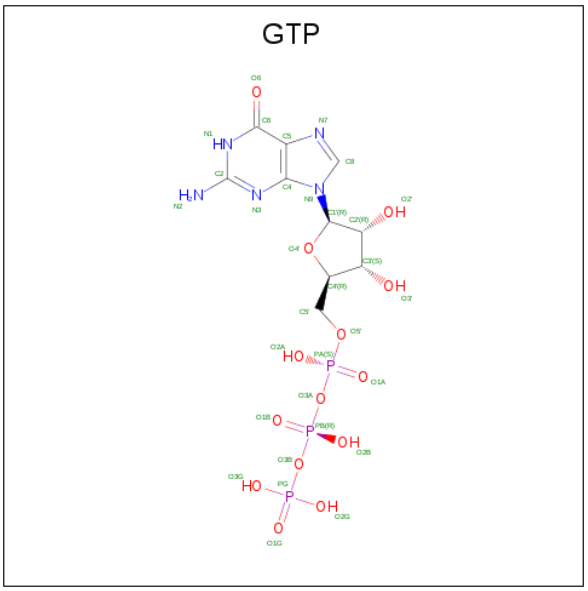
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	0	1	Total	Zn	0
			1	1	
57	4	1	Total	Zn	0
			1	1	
57	r	1	Total	Zn	0
			1	1	

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	A	81	Total	Mg	0
			81	81	
58	C	1	Total	Mg	0
			1	1	
58	E	1	Total	Mg	0
			1	1	
58	W	1	Total	Mg	0
			1	1	
58	g	1	Total	Mg	0
			1	1	

- Molecule 59 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
59	A	1	Total	C	N	O	P	0
			64	20	10	28	6	
59	A	1	Total	C	N	O	P	0
			64	20	10	28	6	
59	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

3 Residue-property plots (i)

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

- Molecule 1: 39S ribosomal protein L32, mitochondrial

Chain 0:

- Molecule 2: 39S ribosomal protein L33, mitochondrial

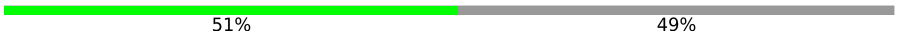
Chain 1:

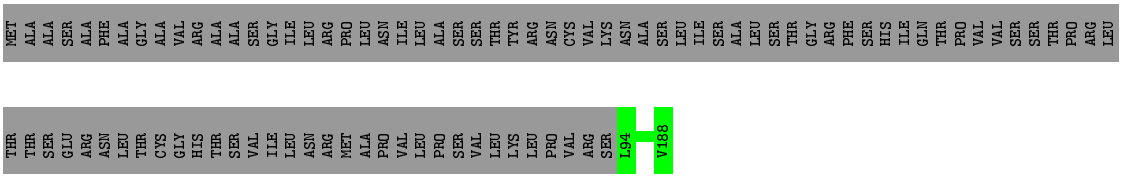
- Molecule 3: 39S ribosomal protein L34, mitochondrial

Chain 2:

- Molecule 4: 39S ribosomal protein L35, mitochondrial

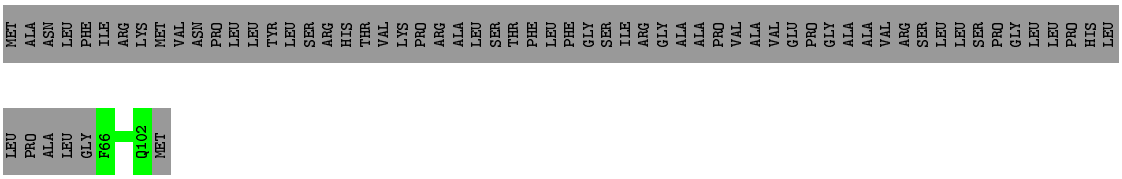
Chain 3:





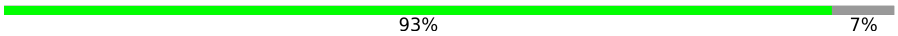
- Molecule 5: 39S ribosomal protein L36, mitochondrial

Chain 4:



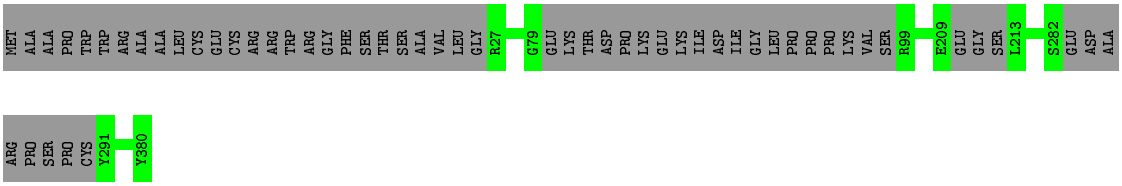
• Molecule 6: 39S ribosomal protein L37, mitochondrial

Chain 5:



• Molecule 7: 39S ribosomal protein L38, mitochondrial

Chain 6:

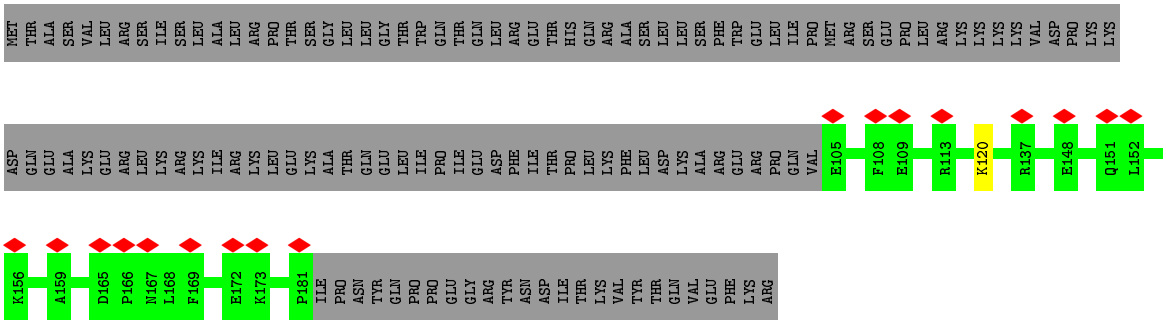


• Molecule 8: 39S ribosomal protein L39, mitochondrial

Chain 7:

• Molecule 9: 39S ribosomal protein L40, mitochondrial

Chain 8:

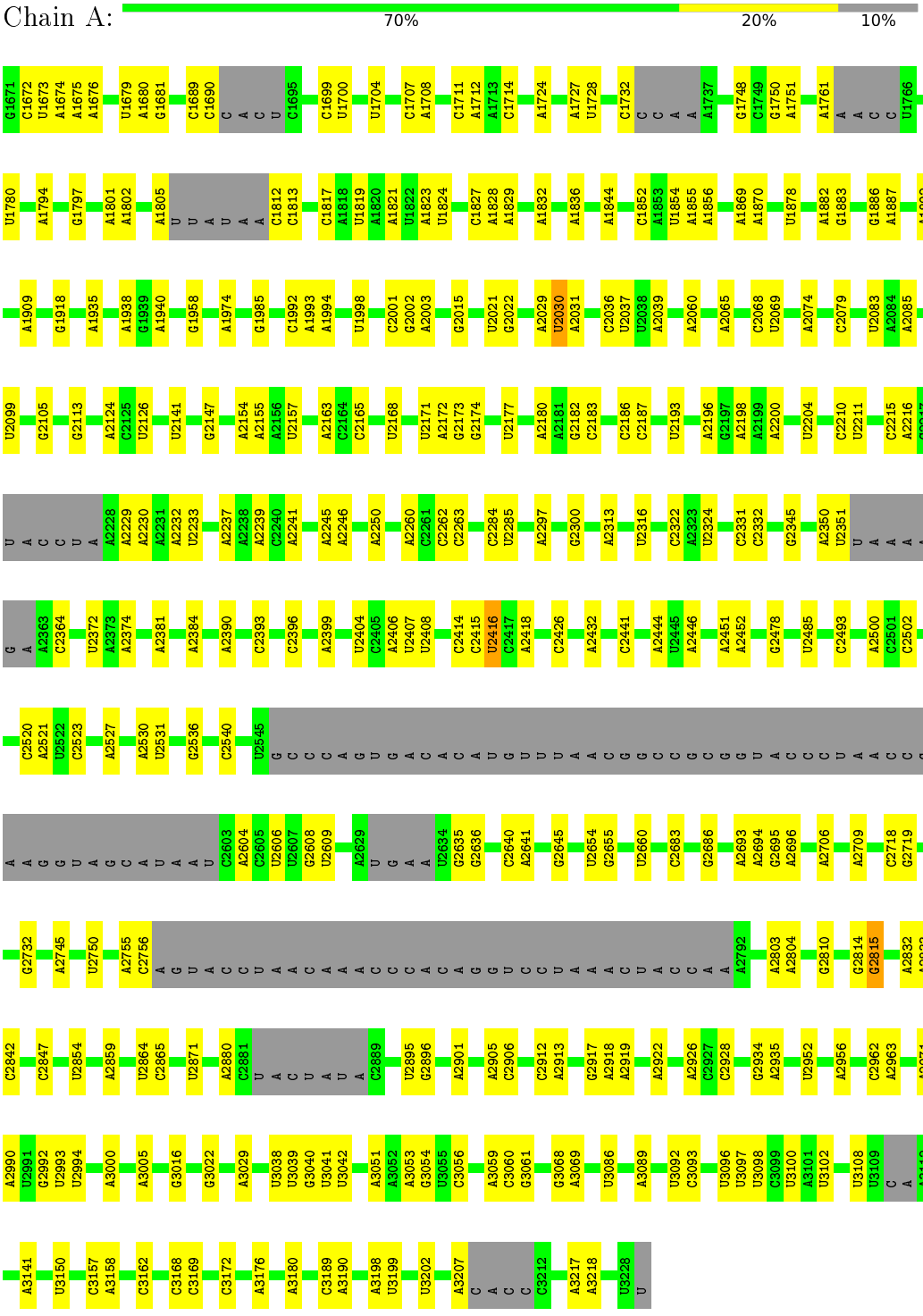


• Molecule 10: 39S ribosomal protein L41, mitochondrial

Chain 9:

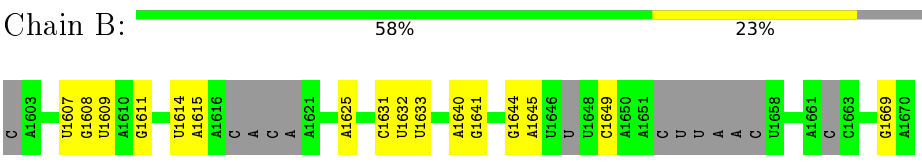
• Molecule 11: 16S ribosomal RNA

Chain A:



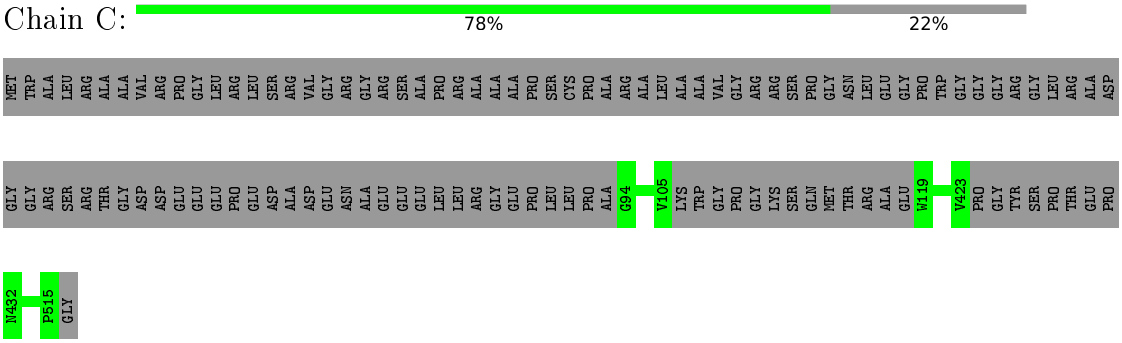
• Molecule 12: mitochondrial tRNAVal

Chain B:



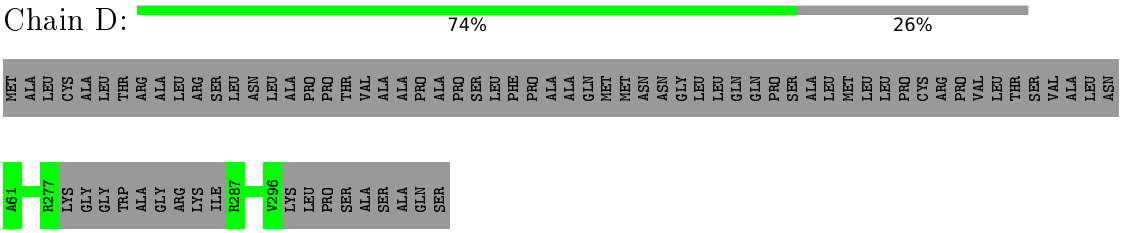
- Molecule 13: Putative GTP-binding protein 6

Chain C:



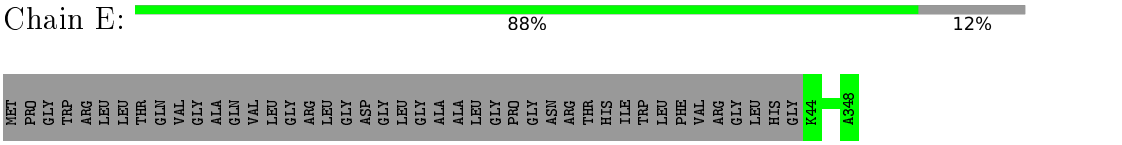
- Molecule 14: 39S ribosomal protein L2, mitochondrial

Chain D:



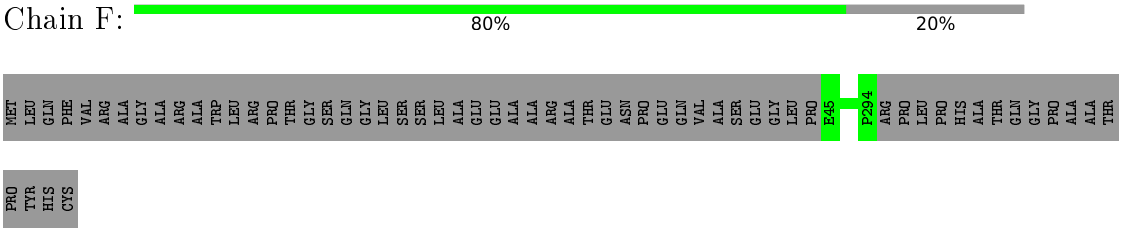
- Molecule 15: 39S ribosomal protein L3, mitochondrial

Chain E:



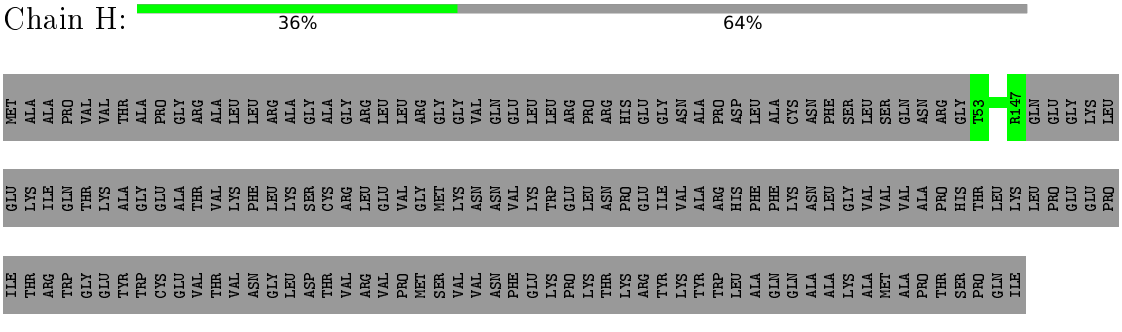
- Molecule 16: 39S ribosomal protein L4, mitochondrial

Chain F:



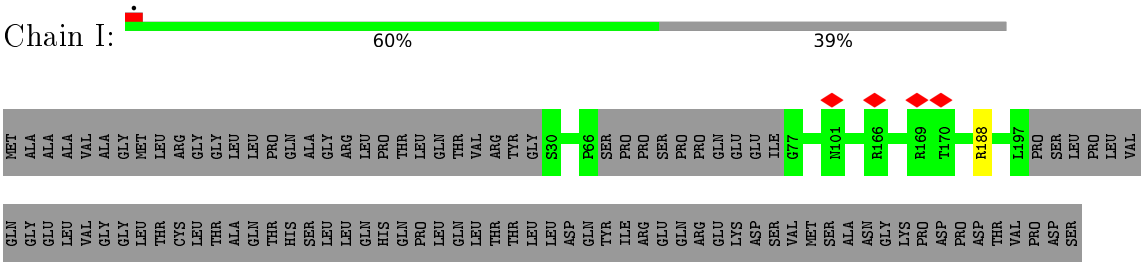
- Molecule 17: 39S ribosomal protein L9, mitochondrial

Chain H:



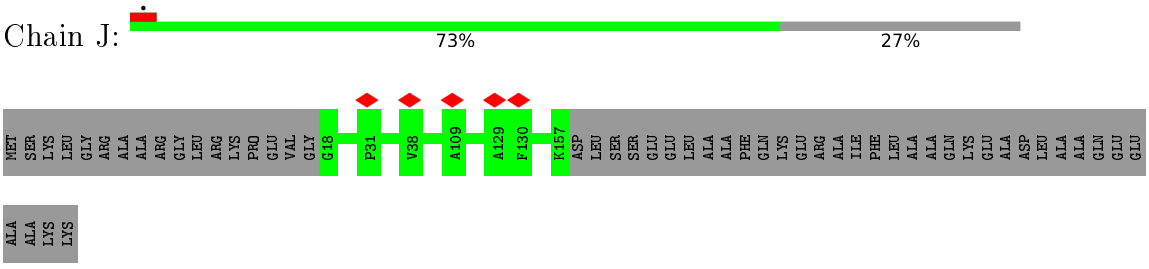
• Molecule 18: 39S ribosomal protein L10, mitochondrial

Chain I:



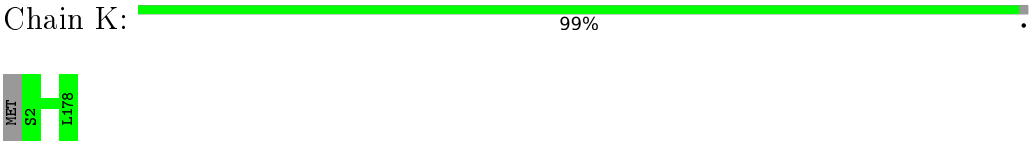
• Molecule 19: 39S ribosomal protein L11, mitochondrial

Chain J:



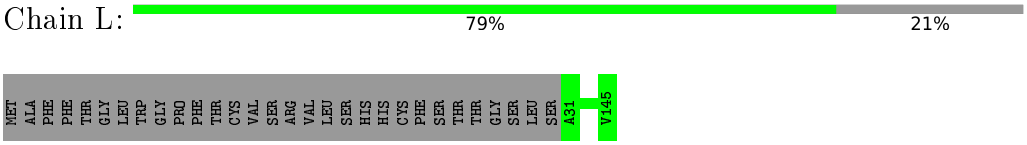
• Molecule 20: 39S ribosomal protein L13, mitochondrial

Chain K:



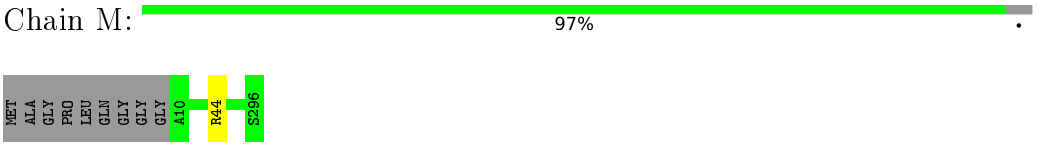
• Molecule 21: 39S ribosomal protein L14, mitochondrial

Chain L:



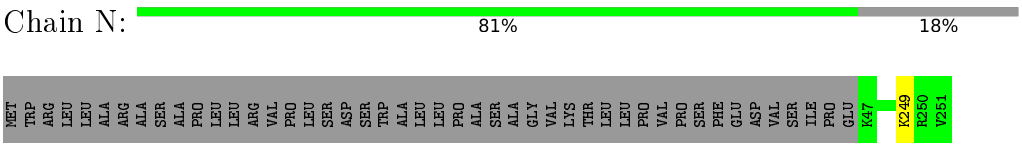
• Molecule 22: 39S ribosomal protein L15, mitochondrial

Chain M:



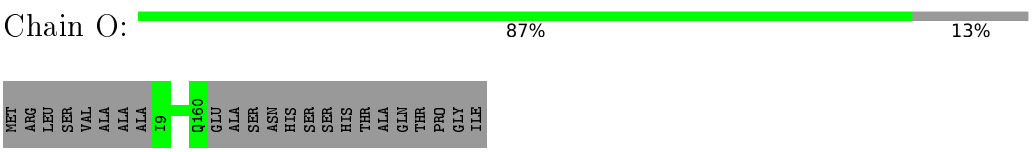
• Molecule 23: 39S ribosomal protein L16, mitochondrial

Chain N:



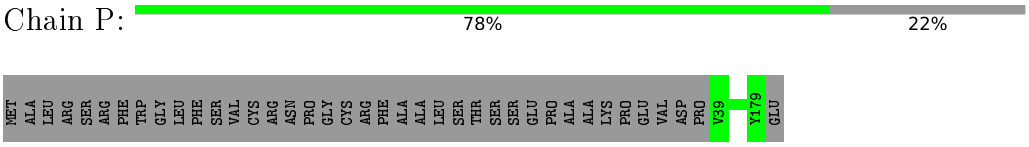
• Molecule 24: 39S ribosomal protein L17, mitochondrial

Chain O:



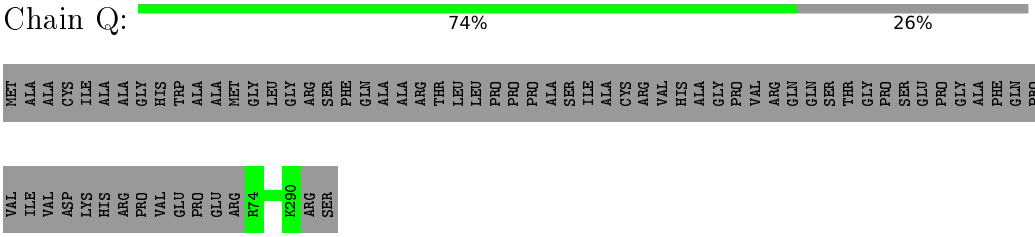
• Molecule 25: 39S ribosomal protein L18, mitochondrial

Chain P:



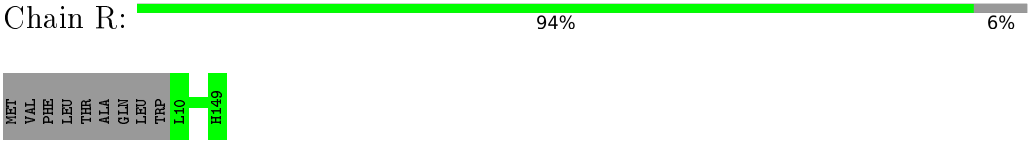
• Molecule 26: 39S ribosomal protein L19, mitochondrial

Chain Q:



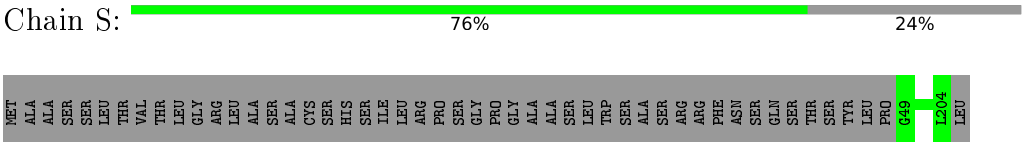
• Molecule 27: 39S ribosomal protein L20, mitochondrial

Chain R:



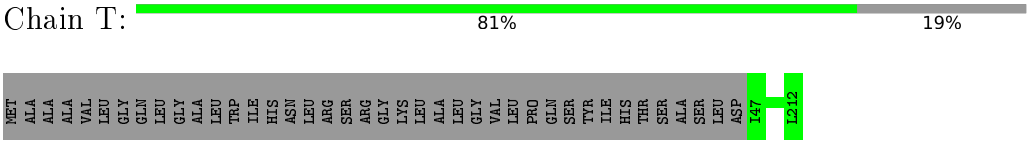
• Molecule 28: 39S ribosomal protein L21, mitochondrial

Chain S:



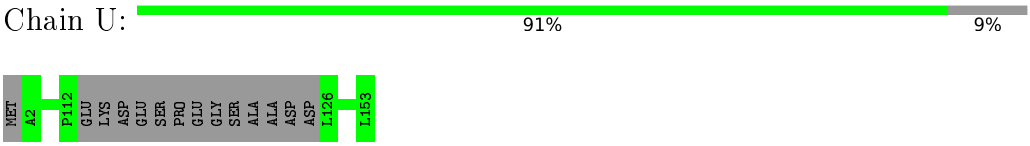
• Molecule 29: 39S ribosomal protein L22, mitochondrial

Chain T:



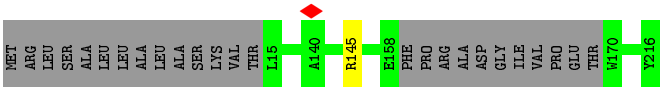
• Molecule 30: 39S ribosomal protein L23, mitochondrial

Chain U:



- Molecule 31: 39S ribosomal protein L24, mitochondrial

Chain V:

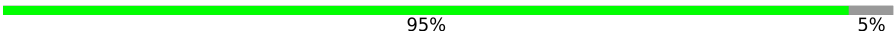


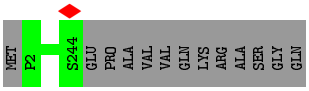
- Molecule 32: 39S ribosomal protein L27, mitochondrial

Chain W:

- Molecule 33: 39S ribosomal protein L28, mitochondrial

Chain X:





- Molecule 34: 39S ribosomal protein L47, mitochondrial

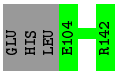
Chain Y:

- Molecule 35: 39S ribosomal protein L30, mitochondrial

Chain Z:

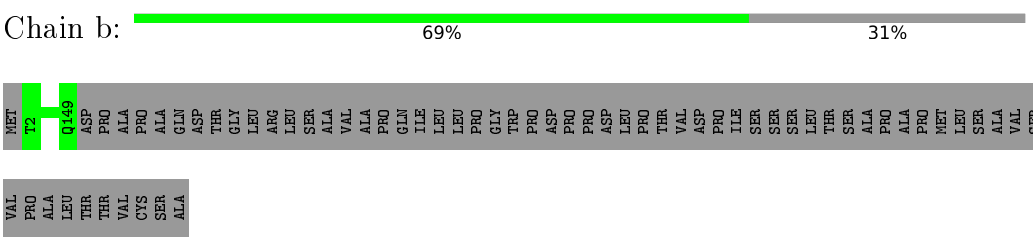
- Molecule 36: 39S ribosomal protein L42, mitochondrial

Chain a:



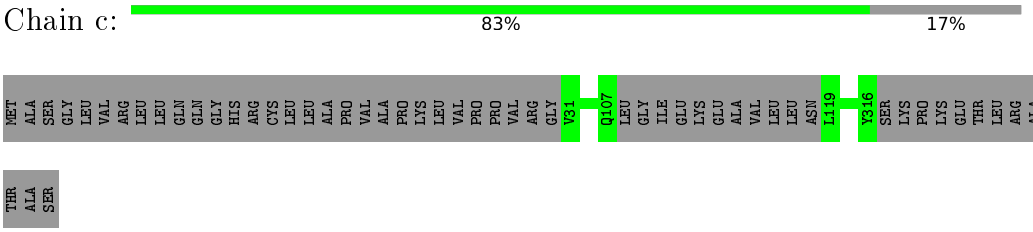
- Molecule 37: 39S ribosomal protein L43, mitochondrial

Chain b:



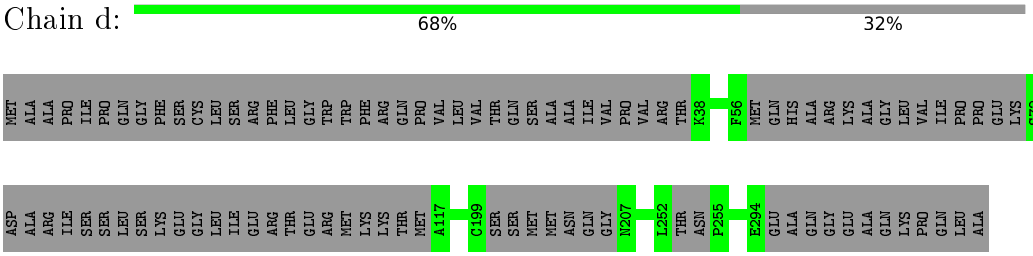
• Molecule 38: 39S ribosomal protein L44, mitochondrial

Chain c:



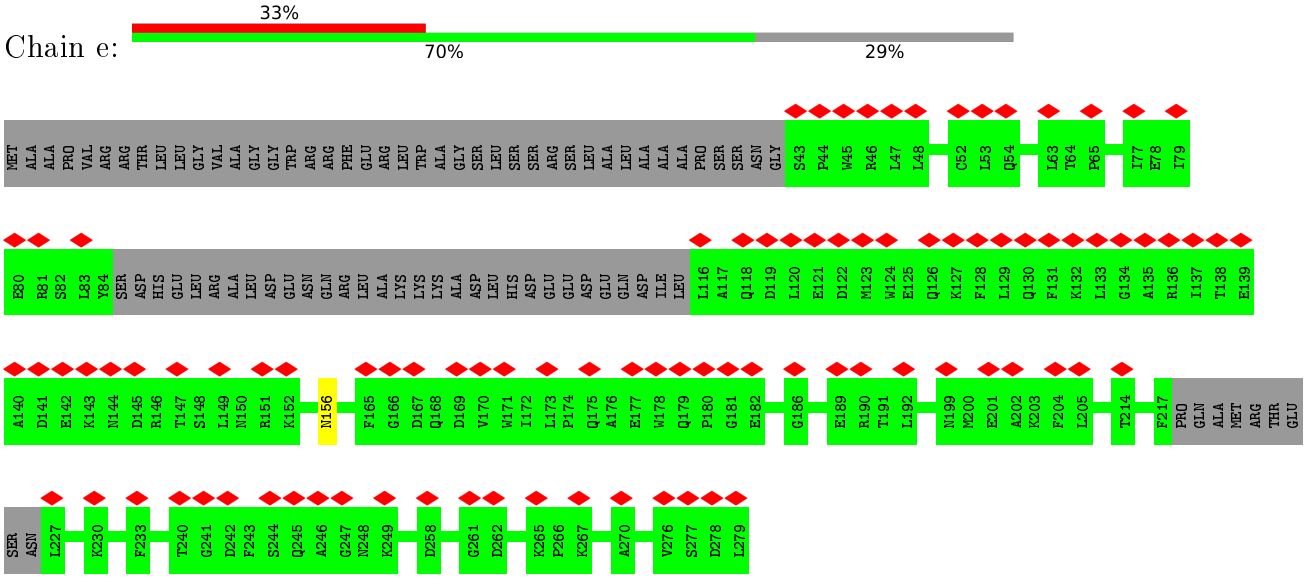
• Molecule 39: 39S ribosomal protein L45, mitochondrial

Chain d:



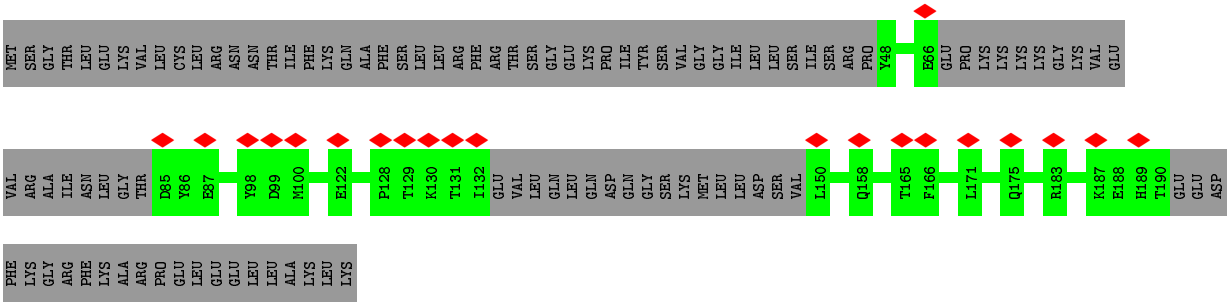
• Molecule 40: 39S ribosomal protein L46, mitochondrial

Chain e:



• Molecule 41: 39S ribosomal protein L48, mitochondrial

Chain f:



- Molecule 42: 39S ribosomal protein L49, mitochondrial

Chain g:

- Molecule 43: 39S ribosomal protein L50, mitochondrial

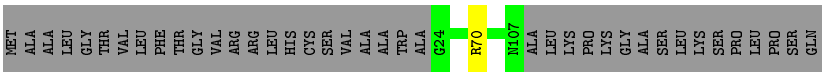
Chain h:

- Molecule 44: 39S ribosomal protein L51, mitochondrial

Chain i:

- Molecule 45: 39S ribosomal protein L52, mitochondrial

Chain j:

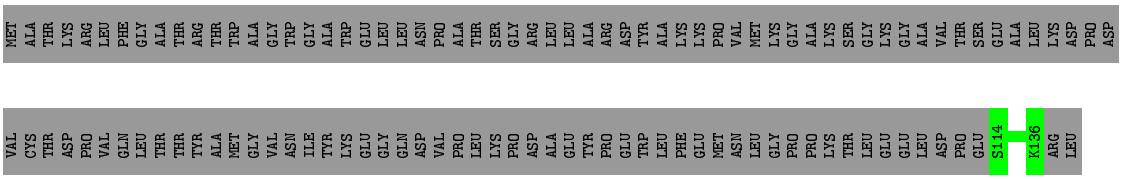


- Molecule 46: 39S ribosomal protein L53, mitochondrial

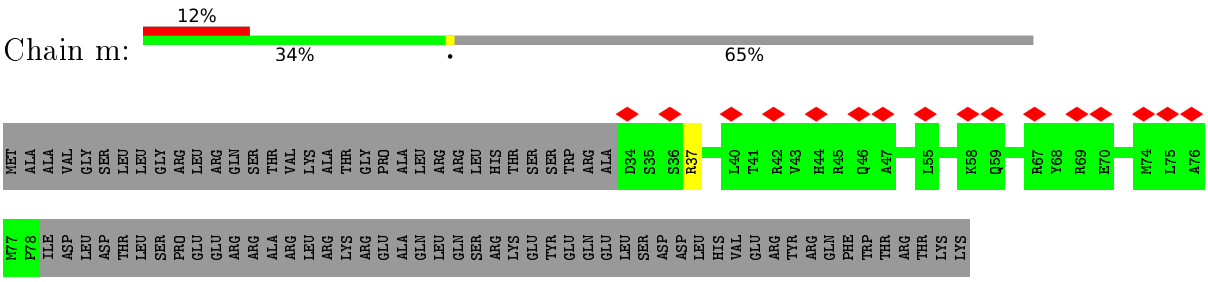
Chain k:

- Molecule 47: 39S ribosomal protein L54, mitochondrial

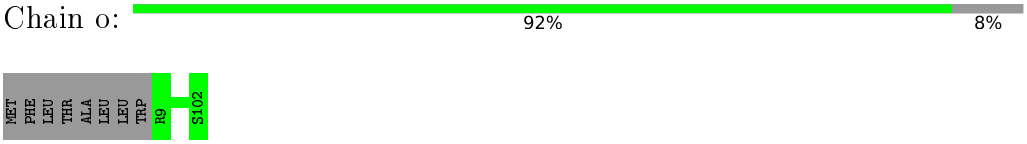
Chain l:



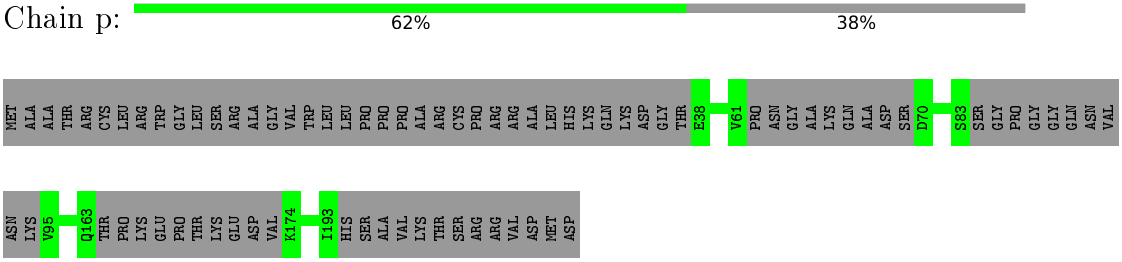
• Molecule 48: 39S ribosomal protein L55, mitochondrial



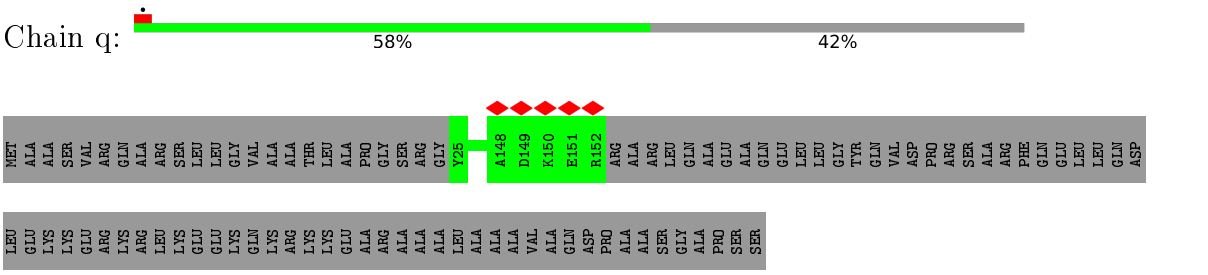
• Molecule 49: Ribosomal protein 63, mitochondrial



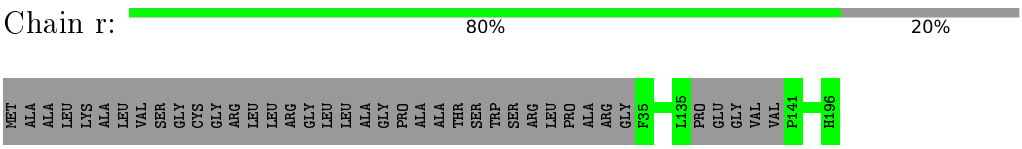
• Molecule 50: Peptidyl-tRNA hydrolase ICT1, mitochondrial



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

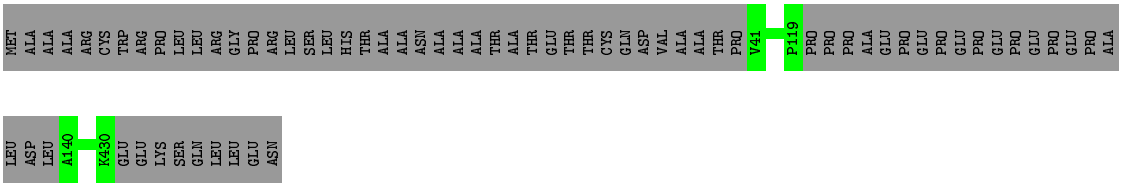


• Molecule 52: 39S ribosomal protein S18a, mitochondrial



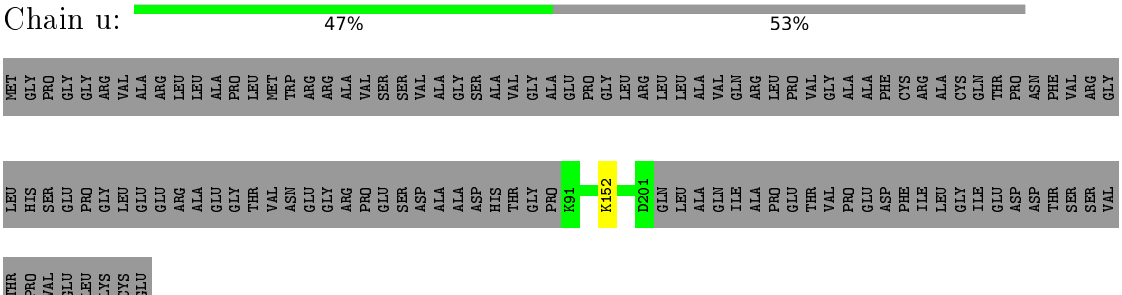
• Molecule 53: 39S ribosomal protein S30, mitochondrial

Chain s:



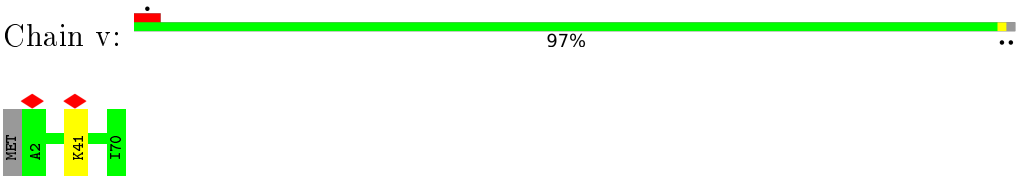
• Molecule 54: Mitochondrial assembly of ribosomal large subunit protein 1

Chain u:



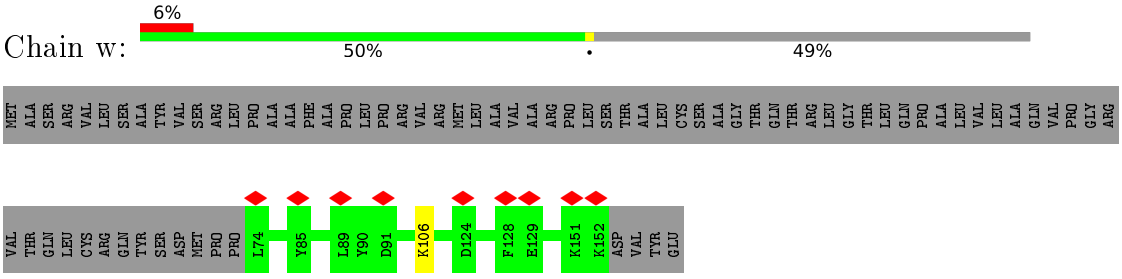
• Molecule 55: MIEF1 upstream open reading frame protein

Chain v:



• Molecule 56: Acyl carrier protein, mitochondrial

Chain w:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	109894	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 ($e^-/Å^2$)	37	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.052	Depositor
Minimum map value	-0.016	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0036	Depositor
Map size (Å)	367.49997, 367.49997, 367.49997	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, ZN, OMU, MG, GTP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	0	0.26	0/895	0.52	0/1201
2	1	0.25	0/438	0.56	0/583
3	2	0.24	0/373	0.55	0/496
4	3	0.26	0/852	0.52	0/1136
5	4	0.27	0/341	0.58	0/451
6	5	0.26	0/3294	0.49	0/4488
7	6	0.26	0/2809	0.52	0/3818
8	7	0.26	0/2391	0.47	0/3234
9	8	0.24	0/665	0.50	0/894
10	9	0.27	0/972	0.47	0/1306
11	A	0.33	0/33413	0.76	5/51989 (0.0%)
12	B	0.20	0/1328	0.75	0/2056
13	C	0.24	0/3205	0.51	0/4336
14	D	0.26	0/1808	0.57	0/2432
15	E	0.27	0/2474	0.46	0/3355
16	F	0.26	0/2071	0.50	0/2817
17	H	0.24	0/798	0.53	0/1073
18	I	0.25	0/1308	0.51	0/1761
19	J	0.25	0/1077	0.50	0/1452
20	K	0.26	0/1495	0.47	0/2029
21	L	0.26	0/904	0.53	0/1218
22	M	0.27	0/2359	0.52	0/3185
23	N	0.27	0/1697	0.52	0/2281
24	O	0.25	0/1269	0.54	0/1708
25	P	0.24	0/1173	0.54	0/1588
26	Q	0.26	0/1846	0.50	0/2487
27	R	0.26	0/1174	0.54	0/1572
28	S	0.26	0/1276	0.52	0/1729
29	T	0.27	0/1402	0.50	0/1886
30	U	0.26	0/1183	0.54	0/1600
31	V	0.25	0/1609	0.51	0/2179
32	W	0.29	0/881	0.48	0/1188

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	X	0.25	0/2090	0.46	0/2825
34	Y	0.25	0/1552	0.50	0/2079
35	Z	0.25	0/1003	0.47	0/1354
36	a	0.27	0/709	0.49	0/963
37	b	0.26	0/1202	0.56	0/1626
38	c	0.26	0/2264	0.47	0/3059
39	d	0.25	0/1781	0.48	0/2410
40	e	0.24	0/1633	0.50	0/2204
41	f	0.25	0/873	0.46	0/1180
42	g	0.27	0/1102	0.50	0/1503
43	h	0.24	0/884	0.47	0/1203
44	i	0.26	0/849	0.53	0/1135
45	j	0.25	0/693	0.51	0/933
46	k	0.24	0/635	0.50	0/855
47	l	0.22	0/226	0.59	0/299
48	m	0.24	0/379	0.67	0/510
49	o	0.26	0/818	0.57	0/1097
50	p	0.24	0/1071	0.53	0/1433
51	q	0.24	0/1107	0.52	0/1498
52	r	0.26	0/1325	0.53	0/1793
53	s	0.26	0/3114	0.51	0/4225
54	u	0.25	0/949	0.48	0/1281
55	v	0.24	0/597	0.60	0/796
56	w	0.25	0/647	0.43	0/871
All	All	0.28	0/106283	0.61	5/150660 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	2523	C	C2-N1-C1'	6.14	125.56	118.80
11	A	2030	U	C2-N1-C1'	5.96	124.85	117.70
11	A	1852	C	C2-N1-C1'	5.24	124.56	118.80
11	A	2523	C	N1-C2-O2	5.11	121.97	118.90
11	A	2416	U	C2-N1-C1'	5.07	123.78	117.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	106/188 (56%)	106 (100%)	0	0	100	100
2	1	50/65 (77%)	50 (100%)	0	0	100	100
3	2	43/92 (47%)	41 (95%)	2 (5%)	0	100	100
4	3	93/188 (50%)	90 (97%)	3 (3%)	0	100	100
5	4	35/103 (34%)	34 (97%)	1 (3%)	0	100	100
6	5	390/423 (92%)	381 (98%)	9 (2%)	0	100	100
7	6	316/380 (83%)	303 (96%)	13 (4%)	0	100	100
8	7	285/338 (84%)	271 (95%)	14 (5%)	0	100	100
9	8	75/206 (36%)	72 (96%)	3 (4%)	0	100	100
10	9	113/137 (82%)	111 (98%)	2 (2%)	0	100	100
13	C	395/516 (77%)	382 (97%)	13 (3%)	0	100	100
14	D	223/305 (73%)	217 (97%)	6 (3%)	0	100	100
15	E	303/348 (87%)	289 (95%)	14 (5%)	0	100	100
16	F	248/311 (80%)	242 (98%)	6 (2%)	0	100	100
17	H	93/267 (35%)	89 (96%)	4 (4%)	0	100	100
18	I	154/261 (59%)	143 (93%)	11 (7%)	0	100	100
19	J	138/192 (72%)	130 (94%)	8 (6%)	0	100	100
20	K	175/178 (98%)	170 (97%)	5 (3%)	0	100	100
21	L	113/145 (78%)	112 (99%)	1 (1%)	0	100	100
22	M	285/296 (96%)	279 (98%)	6 (2%)	0	100	100
23	N	203/251 (81%)	200 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	O	150/175 (86%)	148 (99%)	2 (1%)	0	100	100
25	P	139/180 (77%)	132 (95%)	7 (5%)	0	100	100
26	Q	215/292 (74%)	209 (97%)	6 (3%)	0	100	100
27	R	138/149 (93%)	135 (98%)	3 (2%)	0	100	100
28	S	154/205 (75%)	151 (98%)	3 (2%)	0	100	100
29	T	164/206 (80%)	159 (97%)	5 (3%)	0	100	100
30	U	135/153 (88%)	132 (98%)	3 (2%)	0	100	100
31	V	187/216 (87%)	182 (97%)	5 (3%)	0	100	100
32	W	107/148 (72%)	107 (100%)	0	0	100	100
33	X	241/256 (94%)	238 (99%)	3 (1%)	0	100	100
34	Y	174/250 (70%)	172 (99%)	2 (1%)	0	100	100
35	Z	118/161 (73%)	116 (98%)	2 (2%)	0	100	100
36	a	78/142 (55%)	76 (97%)	2 (3%)	0	100	100
37	b	146/215 (68%)	142 (97%)	4 (3%)	0	100	100
38	c	271/332 (82%)	266 (98%)	5 (2%)	0	100	100
39	d	198/306 (65%)	192 (97%)	6 (3%)	0	100	100
40	e	191/279 (68%)	178 (93%)	13 (7%)	0	100	100
41	f	102/212 (48%)	93 (91%)	9 (9%)	0	100	100
42	g	127/166 (76%)	124 (98%)	3 (2%)	0	100	100
43	h	101/158 (64%)	94 (93%)	7 (7%)	0	100	100
44	i	95/128 (74%)	93 (98%)	2 (2%)	0	100	100
45	j	82/123 (67%)	79 (96%)	3 (4%)	0	100	100
46	k	76/112 (68%)	75 (99%)	1 (1%)	0	100	100
47	l	21/138 (15%)	21 (100%)	0	0	100	100
48	m	43/128 (34%)	36 (84%)	7 (16%)	0	100	100
49	o	92/102 (90%)	89 (97%)	3 (3%)	0	100	100
50	p	119/206 (58%)	116 (98%)	3 (2%)	0	100	100
51	q	126/222 (57%)	125 (99%)	1 (1%)	0	100	100
52	r	153/196 (78%)	149 (97%)	4 (3%)	0	100	100
53	s	366/439 (83%)	359 (98%)	7 (2%)	0	100	100
54	u	109/234 (47%)	103 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	v	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
56	w	77/156 (49%)	72 (94%)	5 (6%)	0	100	100
All	All	8398/11645 (72%)	8140 (97%)	258 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	97/164 (59%)	97 (100%)	0	100	100
2	1	49/60 (82%)	49 (100%)	0	100	100
3	2	39/72 (54%)	39 (100%)	0	100	100
4	3	88/166 (53%)	88 (100%)	0	100	100
5	4	36/89 (40%)	36 (100%)	0	100	100
6	5	353/368 (96%)	353 (100%)	0	100	100
7	6	286/332 (86%)	286 (100%)	0	100	100
8	7	263/303 (87%)	262 (100%)	1 (0%)	91	97
9	8	70/190 (37%)	69 (99%)	1 (1%)	67	86
10	9	99/112 (88%)	99 (100%)	0	100	100
13	C	343/424 (81%)	343 (100%)	0	100	100
14	D	185/245 (76%)	185 (100%)	0	100	100
15	E	260/290 (90%)	260 (100%)	0	100	100
16	F	217/262 (83%)	217 (100%)	0	100	100
17	H	86/228 (38%)	86 (100%)	0	100	100
18	I	145/232 (62%)	144 (99%)	1 (1%)	84	94
19	J	113/150 (75%)	113 (100%)	0	100	100
20	K	155/156 (99%)	155 (100%)	0	100	100
21	L	98/124 (79%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	M	245/249 (98%)	244 (100%)	1 (0%)	91 97
23	N	172/211 (82%)	171 (99%)	1 (1%)	86 95
24	O	133/150 (89%)	133 (100%)	0	100 100
25	P	123/155 (79%)	123 (100%)	0	100 100
26	Q	199/256 (78%)	199 (100%)	0	100 100
27	R	118/126 (94%)	118 (100%)	0	100 100
28	S	141/180 (78%)	141 (100%)	0	100 100
29	T	146/176 (83%)	146 (100%)	0	100 100
30	U	124/135 (92%)	124 (100%)	0	100 100
31	V	171/191 (90%)	170 (99%)	1 (1%)	86 95
32	W	89/119 (75%)	89 (100%)	0	100 100
33	X	219/229 (96%)	219 (100%)	0	100 100
34	Y	159/223 (71%)	159 (100%)	0	100 100
35	Z	111/147 (76%)	110 (99%)	1 (1%)	78 92
36	a	78/133 (59%)	78 (100%)	0	100 100
37	b	130/186 (70%)	130 (100%)	0	100 100
38	c	241/288 (84%)	241 (100%)	0	100 100
39	d	193/274 (70%)	193 (100%)	0	100 100
40	e	171/236 (72%)	170 (99%)	1 (1%)	86 95
41	f	95/188 (50%)	95 (100%)	0	100 100
42	g	119/148 (80%)	119 (100%)	0	100 100
43	h	100/148 (68%)	100 (100%)	0	100 100
44	i	86/110 (78%)	86 (100%)	0	100 100
45	j	68/97 (70%)	67 (98%)	1 (2%)	65 86
46	k	71/90 (79%)	71 (100%)	0	100 100
47	l	23/116 (20%)	23 (100%)	0	100 100
48	m	40/113 (35%)	39 (98%)	1 (2%)	47 76
49	o	80/87 (92%)	80 (100%)	0	100 100
50	p	117/181 (65%)	117 (100%)	0	100 100
51	q	110/178 (62%)	110 (100%)	0	100 100
52	r	143/169 (85%)	143 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
53	s	326/381 (86%)	326 (100%)	0	100 100
54	u	105/200 (52%)	104 (99%)	1 (1%)	76 91
55	v	59/60 (98%)	58 (98%)	1 (2%)	60 84
56	w	73/136 (54%)	72 (99%)	1 (1%)	67 86
All	All	7560/10033 (75%)	7547 (100%)	13 (0%)	93 98

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	7	319	ARG
9	8	120	LYS
18	I	188	ARG
22	M	44	ARG
23	N	249	LYS
31	V	145	ARG
35	Z	44	LYS
40	e	156	ASN
45	j	70	ARG
48	m	37	ARG
54	u	152	LYS
55	v	41	LYS
56	w	106	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
23	N	222	ASN
40	e	156	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1398/1559 (89%)	307 (21%)	23 (1%)
12	B	51/69 (73%)	16 (31%)	1 (1%)
All	All	1449/1628 (89%)	323 (22%)	24 (1%)

All (323) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	A	1672	C
11	A	1673	U
11	A	1674	A
11	A	1675	A
11	A	1676	A
11	A	1679	U
11	A	1680	A
11	A	1681	G
11	A	1689	C
11	A	1690	C
11	A	1699	C
11	A	1700	U
11	A	1704	U
11	A	1707	C
11	A	1708	A
11	A	1711	C
11	A	1712	A
11	A	1714	C
11	A	1724	A
11	A	1727	A
11	A	1728	U
11	A	1732	C
11	A	1748	G
11	A	1750	G
11	A	1751	A
11	A	1761	A
11	A	1770	G
11	A	1777	A
11	A	1780	U
11	A	1794	A
11	A	1797	G
11	A	1801	A
11	A	1802	A
11	A	1805	A
11	A	1813	C
11	A	1817	C
11	A	1819	U
11	A	1821	A
11	A	1823	A
11	A	1824	U
11	A	1827	C
11	A	1828	A
11	A	1829	A

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Mol	Chain	Res	Type
11	A	1832	A
11	A	1836	A
11	A	1844	A
11	A	1854	U
11	A	1855	A
11	A	1856	A
11	A	1869	A
11	A	1870	A
11	A	1878	U
11	A	1882	A
11	A	1883	G
11	A	1886	G
11	A	1887	A
11	A	1892	A
11	A	1893	A
11	A	1902	C
11	A	1903	C
11	A	1909	A
11	A	1918	G
11	A	1935	A
11	A	1938	A
11	A	1940	A
11	A	1958	G
11	A	1974	A
11	A	1985	G
11	A	1992	C
11	A	1993	A
11	A	1994	A
11	A	1998	U
11	A	2001	C
11	A	2002	G
11	A	2003	A
11	A	2015	G
11	A	2021	U
11	A	2022	G
11	A	2029	A
11	A	2030	U
11	A	2031	A
11	A	2036	C
11	A	2037	U
11	A	2039	A
11	A	2060	A

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Mol	Chain	Res	Type
11	A	2065	A
11	A	2068	C
11	A	2069	U
11	A	2074	A
11	A	2079	C
11	A	2083	U
11	A	2085	A
11	A	2093	U
11	A	2097	A
11	A	2098	G
11	A	2099	U
11	A	2105	G
11	A	2113	G
11	A	2124	A
11	A	2126	U
11	A	2141	U
11	A	2147	G
11	A	2154	A
11	A	2155	A
11	A	2157	U
11	A	2163	A
11	A	2165	C
11	A	2168	U
11	A	2171	U
11	A	2172	A
11	A	2173	G
11	A	2174	G
11	A	2177	U
11	A	2180	A
11	A	2182	G
11	A	2183	C
11	A	2187	C
11	A	2193	U
11	A	2196	A
11	A	2198	A
11	A	2200	A
11	A	2204	U
11	A	2210	C
11	A	2211	U
11	A	2215	C
11	A	2216	A
11	A	2229	A

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Mol	Chain	Res	Type
11	A	2230	A
11	A	2232	A
11	A	2233	U
11	A	2237	A
11	A	2239	A
11	A	2241	A
11	A	2245	A
11	A	2246	A
11	A	2250	A
11	A	2260	A
11	A	2262	C
11	A	2263	C
11	A	2284	C
11	A	2285	U
11	A	2297	A
11	A	2300	G
11	A	2313	A
11	A	2316	U
11	A	2322	C
11	A	2324	U
11	A	2331	C
11	A	2332	C
11	A	2345	G
11	A	2350	A
11	A	2351	U
11	A	2364	C
11	A	2372	U
11	A	2374	A
11	A	2381	A
11	A	2384	A
11	A	2390	A
11	A	2393	C
11	A	2396	C
11	A	2399	A
11	A	2404	U
11	A	2406	A
11	A	2407	U
11	A	2408	U
11	A	2414	C
11	A	2415	C
11	A	2416	U
11	A	2418	A

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Mol	Chain	Res	Type
11	A	2426	C
11	A	2432	A
11	A	2441	C
11	A	2444	A
11	A	2446	A
11	A	2451	A
11	A	2452	A
11	A	2478	G
11	A	2485	U
11	A	2493	C
11	A	2500	A
11	A	2502	C
11	A	2507	A
11	A	2508	C
11	A	2511	C
11	A	2520	C
11	A	2521	A
11	A	2527	A
11	A	2531	U
11	A	2536	G
11	A	2540	C
11	A	2604	A
11	A	2606	U
11	A	2608	G
11	A	2609	U
11	A	2635	G
11	A	2636	G
11	A	2640	C
11	A	2641	A
11	A	2645	G
11	A	2654	U
11	A	2655	G
11	A	2660	U
11	A	2683	C
11	A	2686	G
11	A	2693	A
11	A	2694	A
11	A	2695	G
11	A	2696	A
11	A	2706	A
11	A	2709	A
11	A	2718	C

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Mol	Chain	Res	Type
11	A	2719	G
11	A	2722	A
11	A	2723	A
11	A	2724	G
11	A	2725	A
11	A	2732	G
11	A	2745	A
11	A	2750	U
11	A	2755	A
11	A	2756	C
11	A	2803	A
11	A	2804	A
11	A	2810	G
11	A	2814	G
11	A	2815	OMG
11	A	2832	A
11	A	2833	A
11	A	2837	A
11	A	2842	C
11	A	2847	C
11	A	2854	U
11	A	2859	A
11	A	2864	U
11	A	2865	C
11	A	2871	U
11	A	2880	A
11	A	2895	U
11	A	2896	G
11	A	2901	A
11	A	2906	C
11	A	2912	C
11	A	2913	A
11	A	2917	G
11	A	2918	A
11	A	2919	A
11	A	2922	A
11	A	2926	A
11	A	2928	C
11	A	2934	G
11	A	2935	A
11	A	2952	U
11	A	2956	A

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Mol	Chain	Res	Type
11	A	2962	C
11	A	2963	A
11	A	2971	A
11	A	2981	A
11	A	2989	G
11	A	2990	A
11	A	2992	G
11	A	2994	U
11	A	3000	A
11	A	3005	A
11	A	3016	G
11	A	3022	G
11	A	3029	A
11	A	3038	U
11	A	3041	U
11	A	3042	U
11	A	3051	A
11	A	3053	A
11	A	3054	G
11	A	3056	C
11	A	3059	A
11	A	3060	C
11	A	3061	G
11	A	3068	G
11	A	3069	A
11	A	3086	U
11	A	3089	A
11	A	3093	C
11	A	3096	U
11	A	3097	U
11	A	3098	U
11	A	3100	U
11	A	3102	U
11	A	3108	U
11	A	3129	A
11	A	3134	C
11	A	3141	A
11	A	3150	U
11	A	3157	C
11	A	3158	A
11	A	3162	C
11	A	3168	C

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Mol	Chain	Res	Type
11	A	3169	C
11	A	3172	C
11	A	3176	A
11	A	3180	A
11	A	3189	C
11	A	3190	A
11	A	3198	A
11	A	3199	U
11	A	3202	U
11	A	3207	A
11	A	3217	A
11	A	3218	A
12	B	1607	U
12	B	1608	G
12	B	1609	U
12	B	1611	G
12	B	1614	U
12	B	1615	A
12	B	1625	A
12	B	1631	C
12	B	1632	U
12	B	1633	U
12	B	1640	A
12	B	1641	G
12	B	1644	G
12	B	1645	A
12	B	1649	C
12	B	1669	G

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	1812	C
11	A	1823	A
11	A	2030	U
11	A	2186	C
11	A	2245	A
11	A	2284	C
11	A	2507	A
11	A	2530	A
11	A	2608	G
11	A	2635	G

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Mol	Chain	Res	Type
11	A	2693	A
11	A	2694	A
11	A	2814	G
11	A	2836	C
11	A	2895	U
11	A	2905	A
11	A	2993	U
11	A	3041	U
11	A	3059	A
11	A	3060	C
11	A	3092	U
11	A	3097	U
11	A	3198	A
12	B	1607	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	OMG	A	3040	11	18,26,27	1.10	2 (11%)	20,38,41	2.04	5 (25%)
11	OMU	A	3039	11	14,22,23	0.89	1 (7%)	14,31,34	0.88	0
11	OMG	A	2815	11	18,26,27	1.18	2 (11%)	20,38,41	2.13	6 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	OMG	A	3040	11	-	1/5/27/28	0/3/3/3
11	OMU	A	3039	11	-	0/7/27/28	0/2/2/2
11	OMG	A	2815	11	-	1/5/27/28	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	2815	OMG	C6-C5	4.03	1.48	1.41
11	A	3040	OMG	C6-C5	3.61	1.47	1.41
11	A	2815	OMG	C5-C4	2.33	1.47	1.40
11	A	3039	OMU	C2-N3	-2.32	1.33	1.38
11	A	3040	OMG	C5-C4	2.31	1.47	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	2815	OMG	C2-N3-C4	4.88	120.93	115.36
11	A	3040	OMG	C2-N3-C4	4.17	120.11	115.36
11	A	3040	OMG	C6-N1-C2	4.07	122.40	115.93
11	A	3040	OMG	C5-C6-N1	-4.02	117.94	123.43
11	A	2815	OMG	C6-N1-C2	3.92	122.16	115.93
11	A	2815	OMG	C5-C6-N1	-3.92	118.07	123.43
11	A	3040	OMG	C6-C5-C4	-3.91	117.07	120.80
11	A	2815	OMG	C6-C5-C4	-3.63	117.33	120.80
11	A	2815	OMG	N3-C2-N1	-3.14	123.04	127.22
11	A	3040	OMG	N3-C2-N1	-2.96	123.28	127.22
11	A	2815	OMG	C4-C5-N7	-2.66	106.63	109.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	3040	OMG	C1'-C2'-O2'-CM2
11	A	2815	OMG	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 91 ligands modelled in this entry, 88 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
59	GTP	A	3383	-	26,34,34	1.04	1 (3%)	33,54,54	2.10	4 (12%)
59	GTP	A	3382	-	26,34,34	1.05	1 (3%)	33,54,54	2.11	5 (15%)
59	GTP	C	601	58	26,34,34	1.05	1 (3%)	33,54,54	2.12	4 (12%)

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
59	GTP	A	3383	-	-	0/18/38/38	0/3/3/3
59	GTP	A	3382	-	-	0/18/38/38	0/3/3/3
59	GTP	C	601	58	-	2/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	C	601	GTP	C6-N1	4.00	1.40	1.33
59	A	3382	GTP	C6-N1	3.99	1.40	1.33
59	A	3383	GTP	C6-N1	3.97	1.40	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	A	3382	GTP	C5-C6-N1	-8.81	111.38	123.43
59	A	3383	GTP	C5-C6-N1	-8.78	111.43	123.43
59	C	601	GTP	C5-C6-N1	-8.76	111.44	123.43
59	A	3382	GTP	C6-N1-C2	5.89	125.29	115.93
59	C	601	GTP	C6-N1-C2	5.87	125.26	115.93
59	A	3383	GTP	C6-N1-C2	5.86	125.24	115.93
59	C	601	GTP	C2-N3-C4	-2.87	112.08	115.36
59	A	3382	GTP	C2-N3-C4	-2.85	112.10	115.36
59	C	601	GTP	N3-C2-N1	-2.76	123.54	127.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	A	3382	GTP	N3-C2-N1	-2.76	123.54	127.22
59	A	3383	GTP	N3-C2-N1	-2.75	123.56	127.22
59	A	3383	GTP	C2-N3-C4	-2.71	112.26	115.36
59	A	3382	GTP	O4'-C1'-C2'	-2.13	103.82	106.93

There are no chirality outliers.

All (2) torsion outliers are listed below:

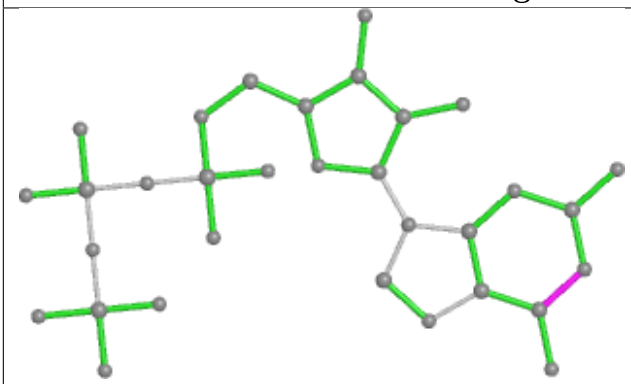
Mol	Chain	Res	Type	Atoms
59	C	601	GTP	O4'-C4'-C5'-O5'
59	C	601	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

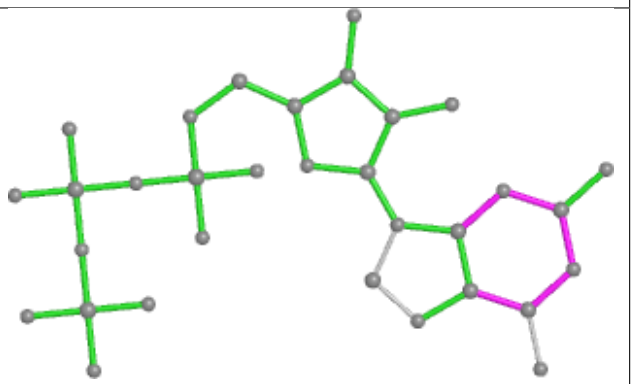
No monomer is involved in short contacts.

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.

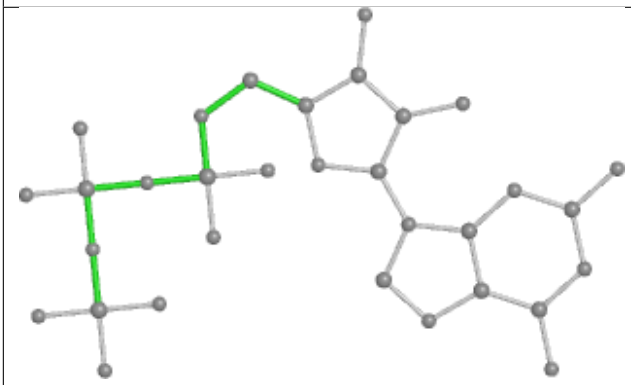
Ligand GTP A 3383



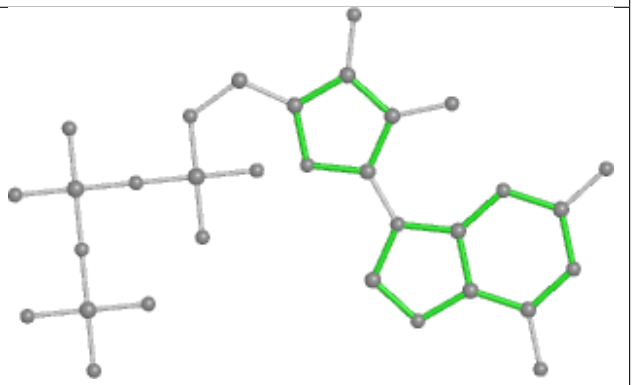
Bond lengths



Bond angles

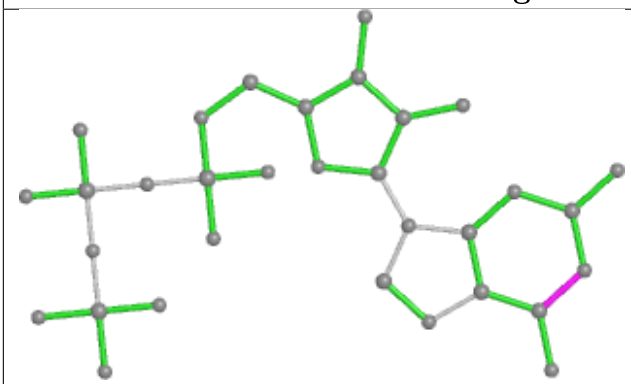


Torsions

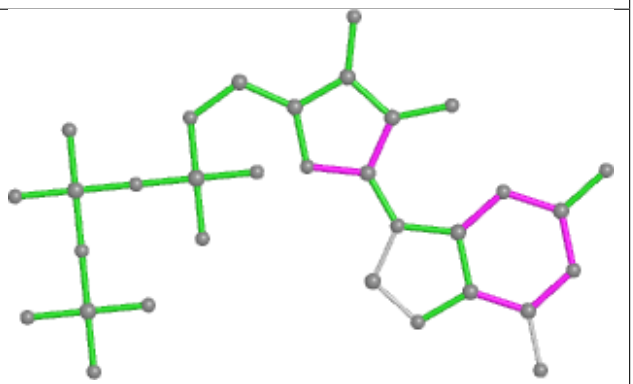


Rings

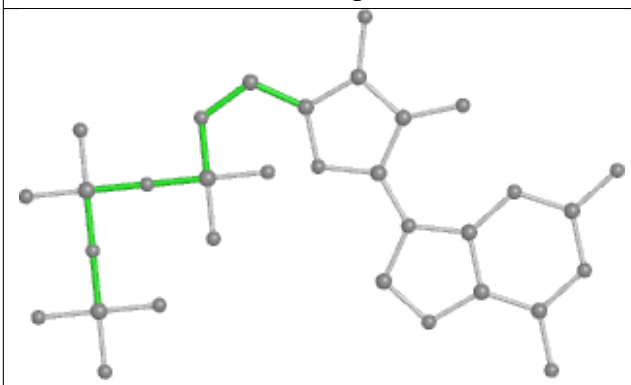
Ligand GTP A 3382



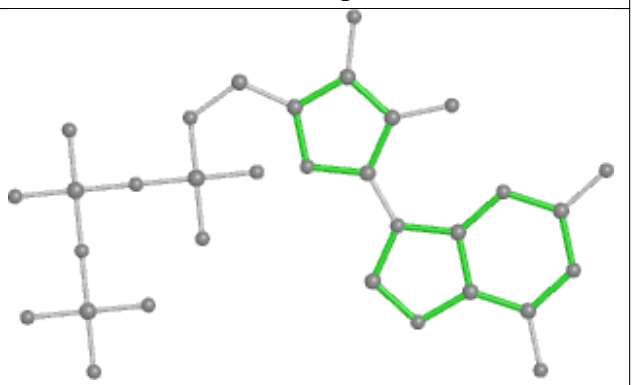
Bond lengths



Bond angles

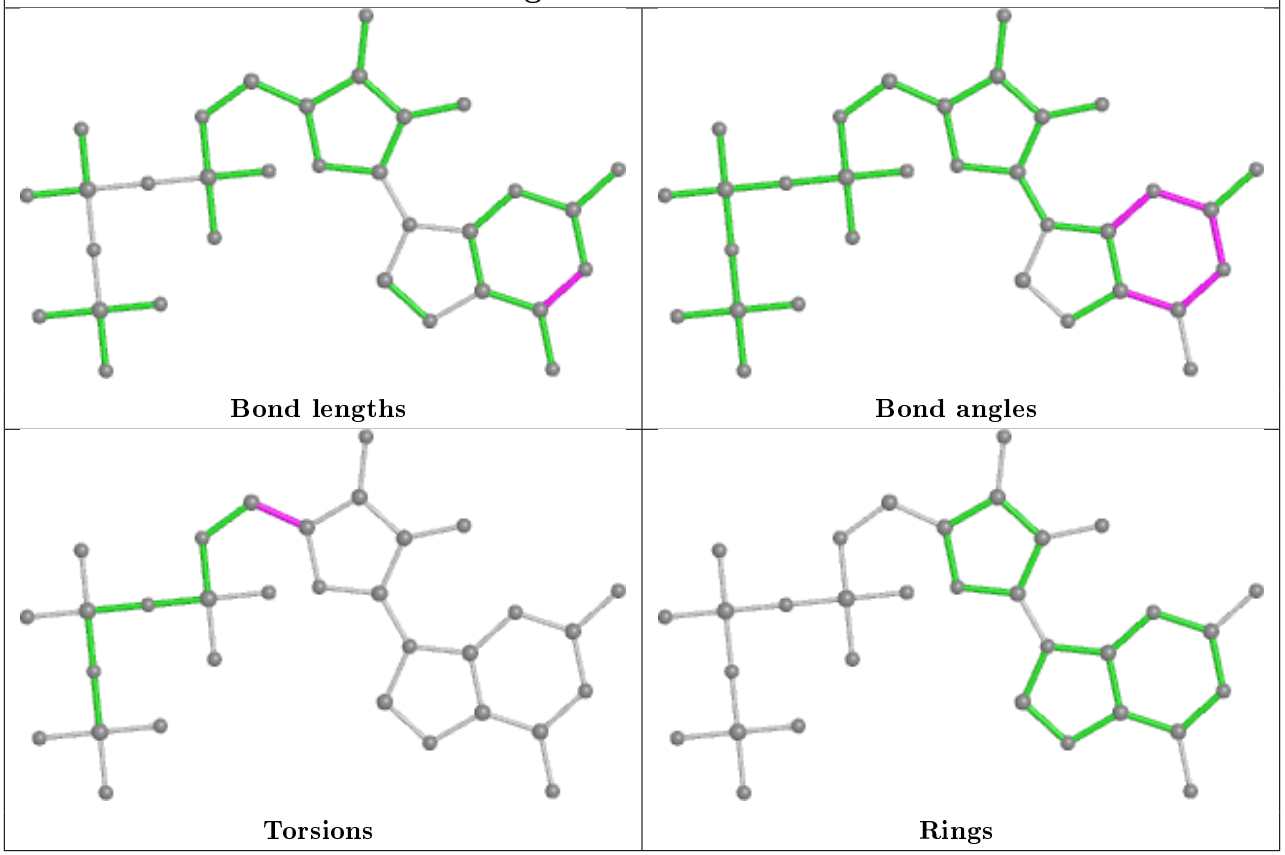


Torsions



Rings

Ligand GTP C 601



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

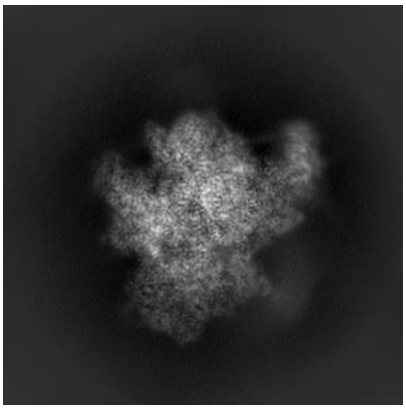
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12867. These allow visual inspection of the internal detail of the map and identification of artifacts.

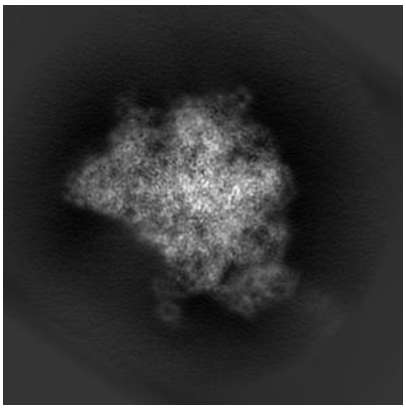
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

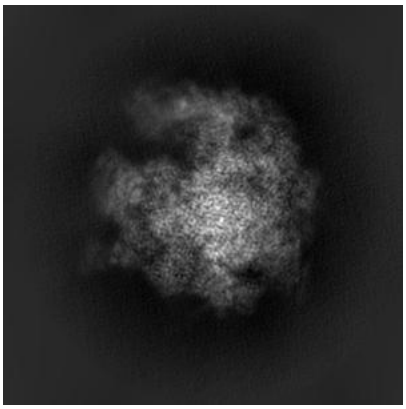
6.1.1 Primary map



X

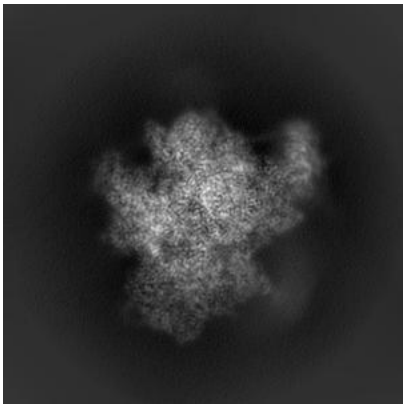


Y

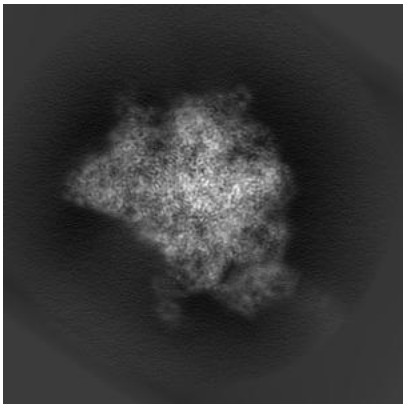


Z

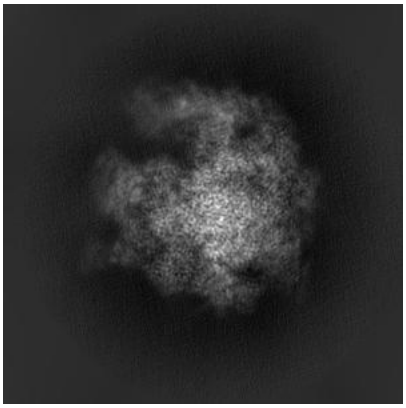
6.1.2 Raw map



X



Y

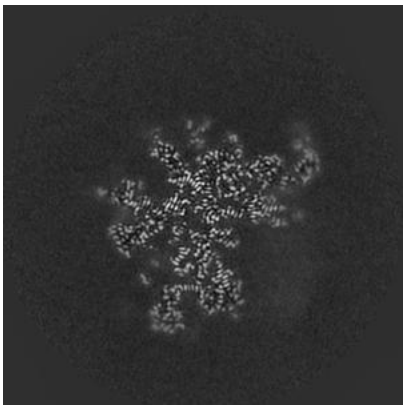


Z

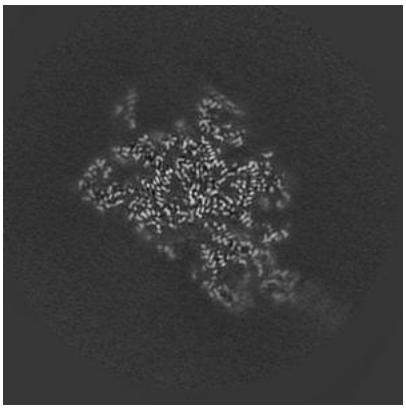
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

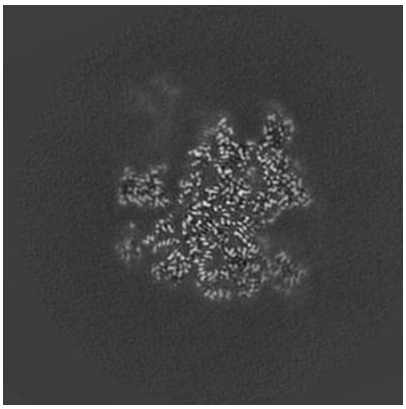
6.2.1 Primary map



X Index: 175

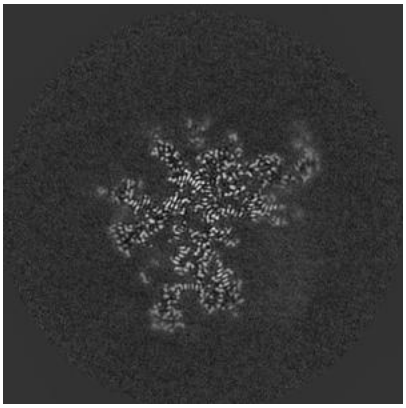


Y Index: 175

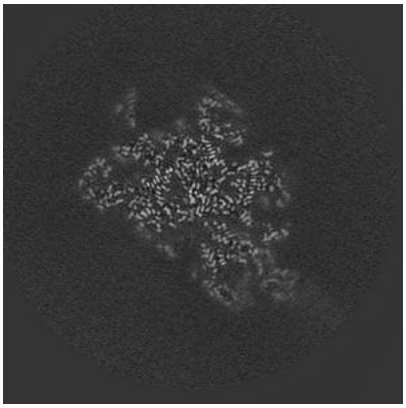


Z Index: 175

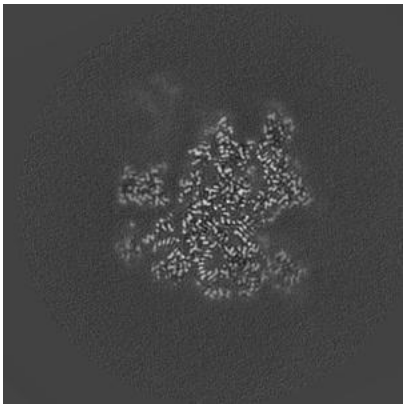
6.2.2 Raw map



X Index: 175



Y Index: 175

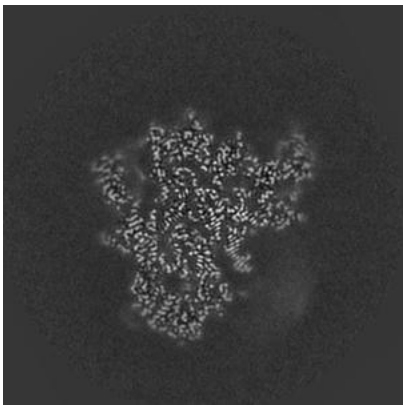


Z Index: 175

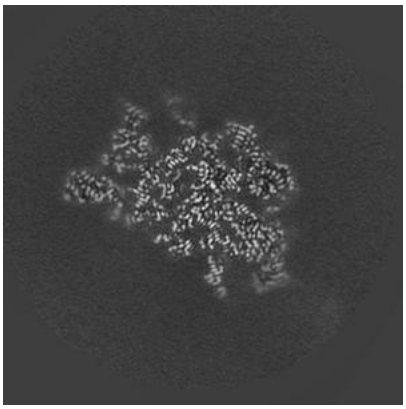
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

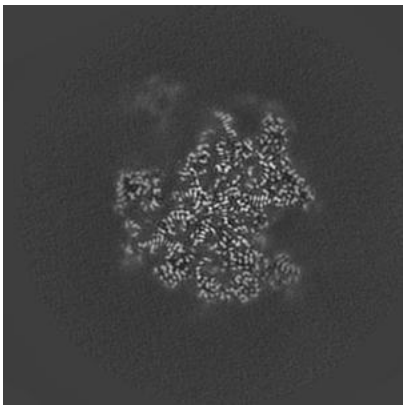
6.3.1 Primary map



X Index: 187

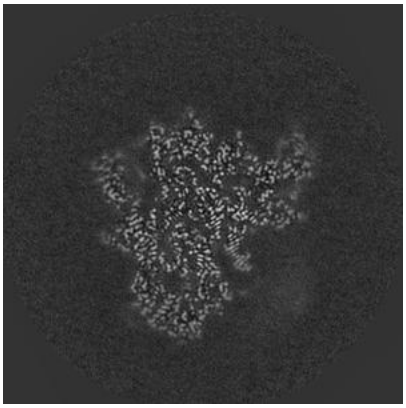


Y Index: 160

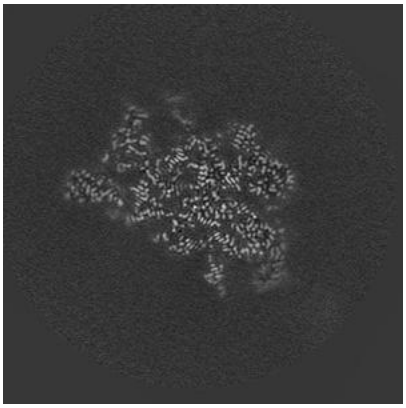


Z Index: 179

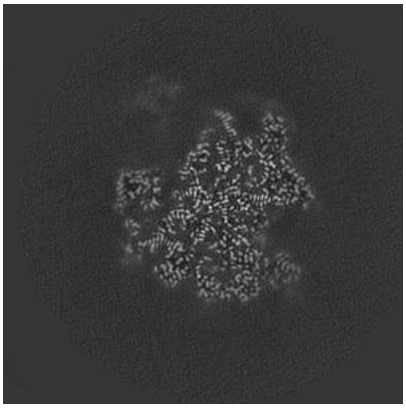
6.3.2 Raw map



X Index: 187



Y Index: 159



Z Index: 179

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

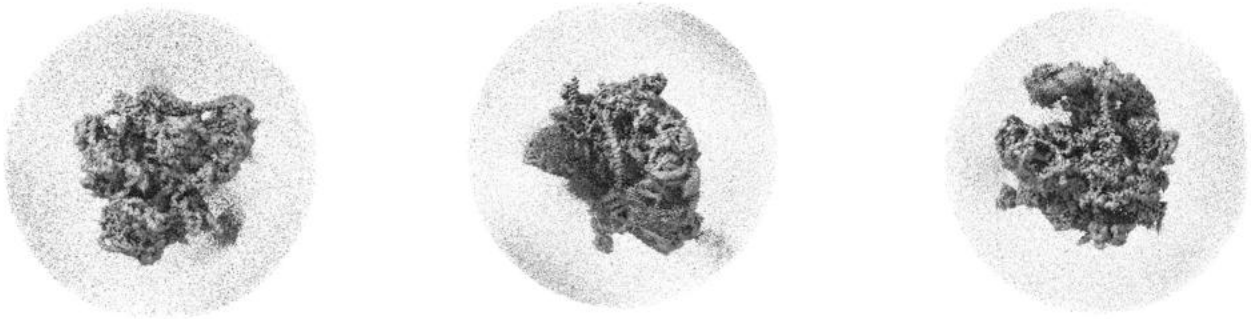
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0036. 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.

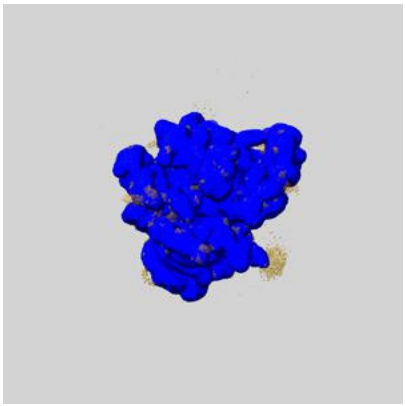
6.5 Mask visualisation

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

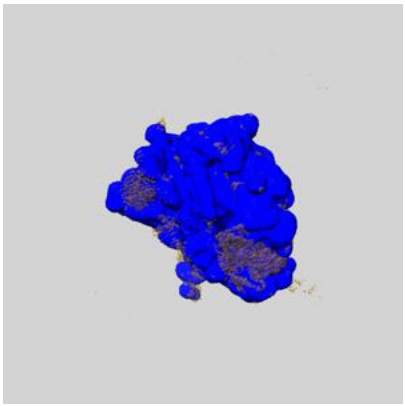
A mask typically either:

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

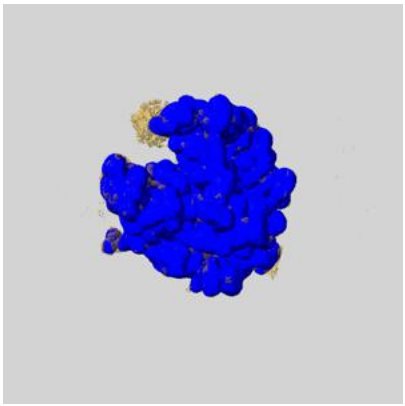
6.5.1 emd_12867_msk_1.map



X



Y

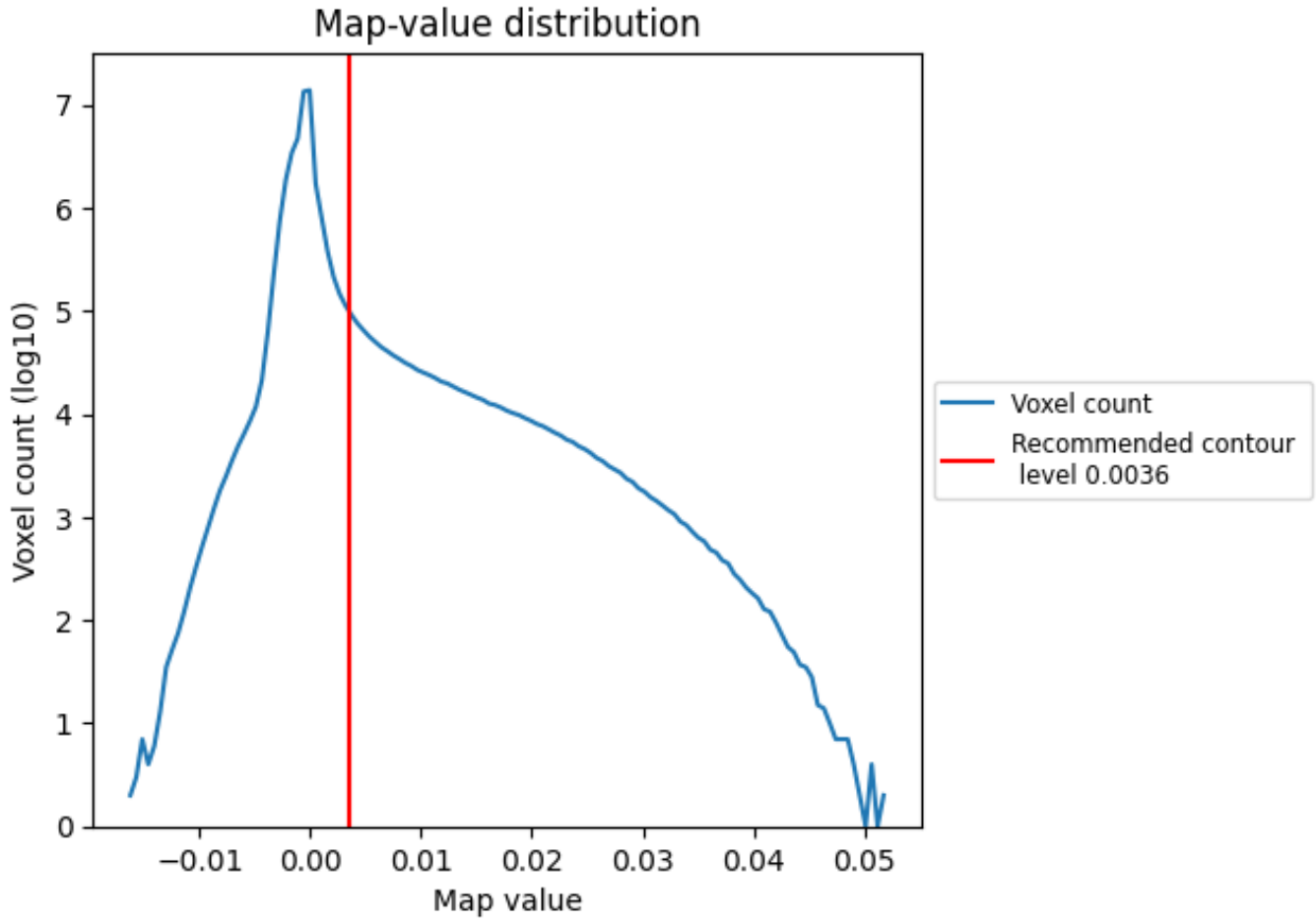


Z

7 Map analysis

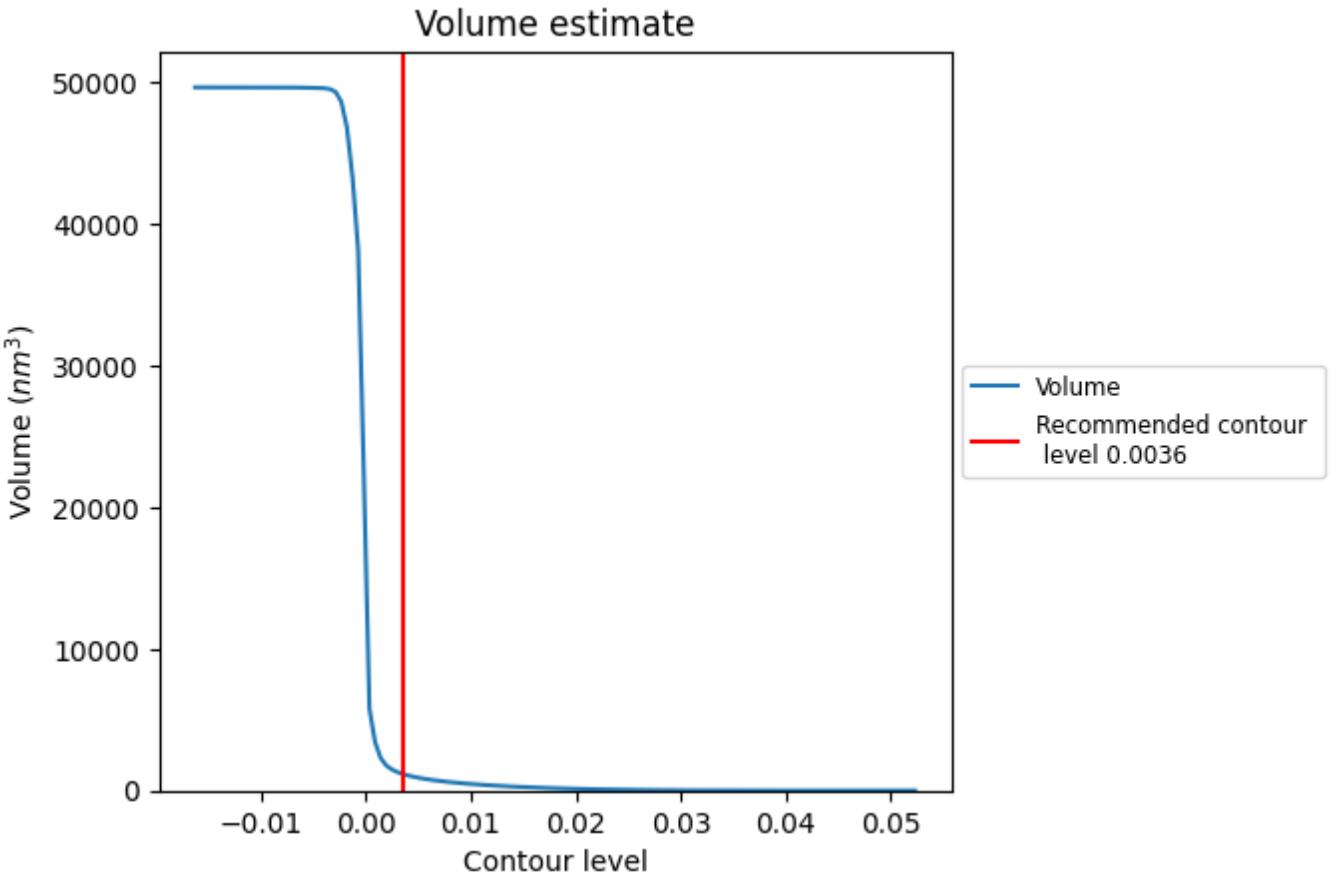
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

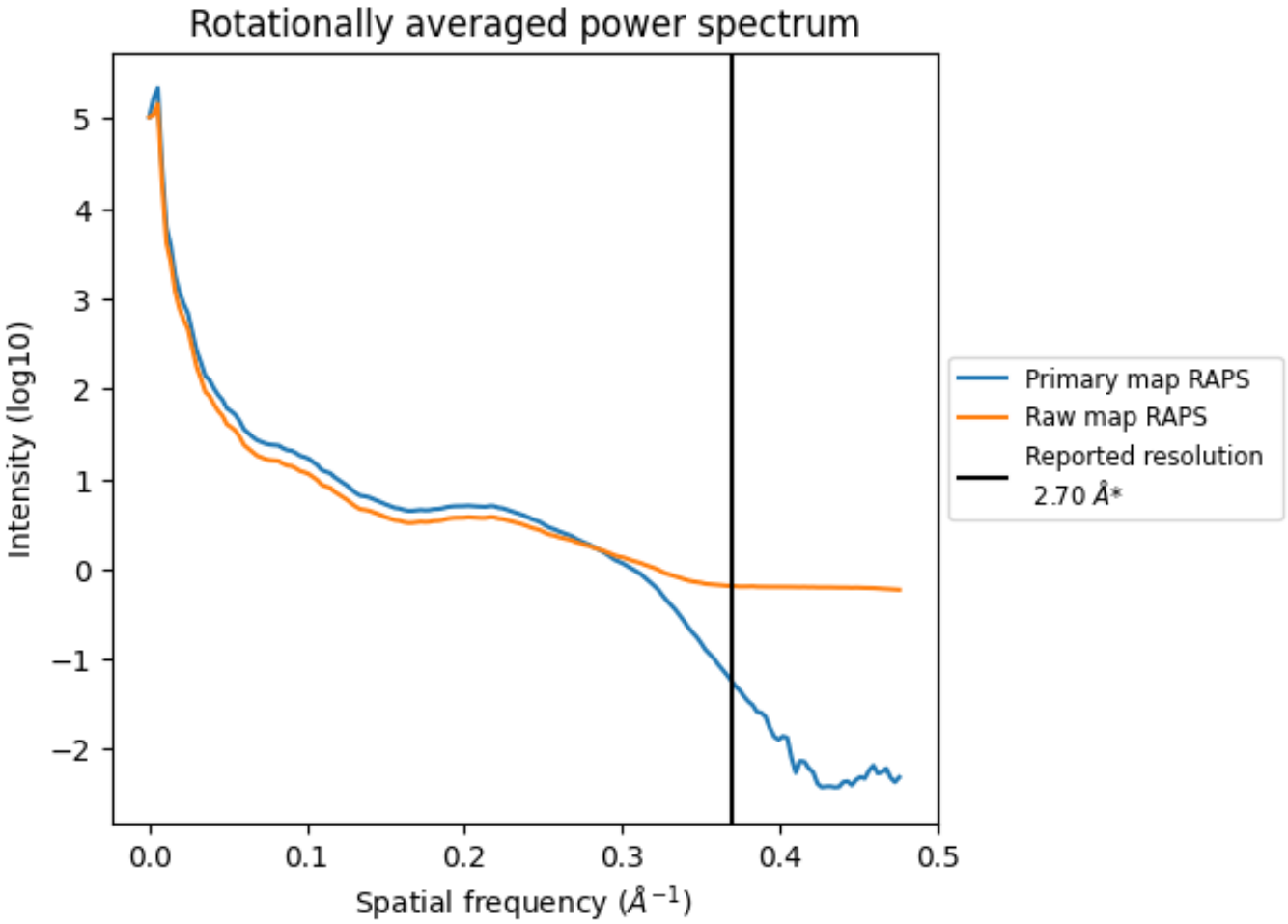
7.2 Volume estimate



The volume at the recommended contour level is 1154 nm^3; this corresponds to an approximate mass of 1043 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)

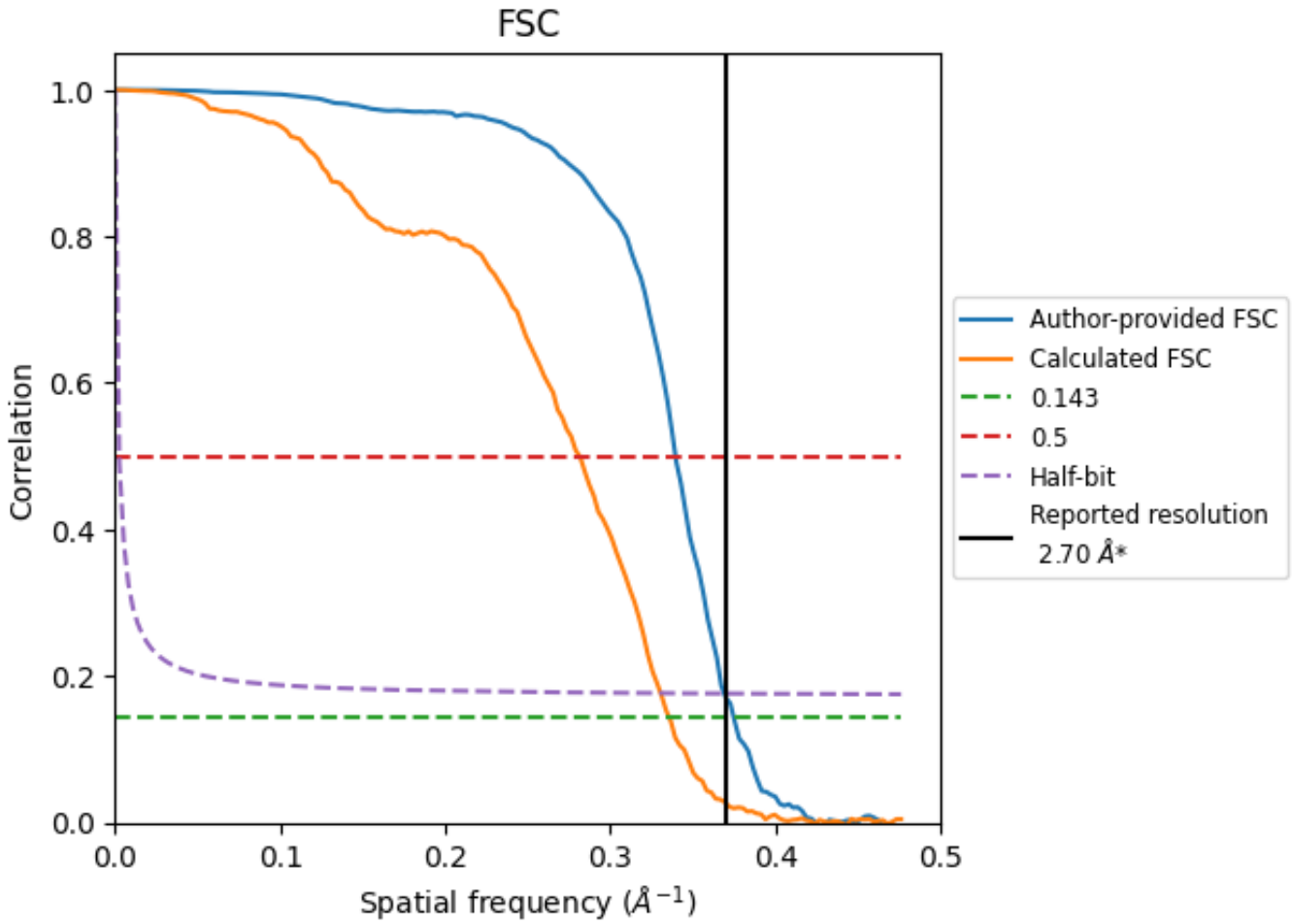


*Reported resolution corresponds to spatial frequency of 0.370 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

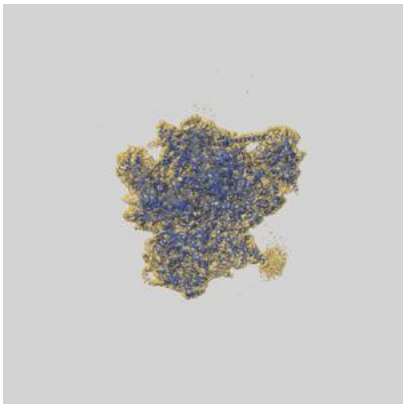
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.67	2.94	2.71
Calculated*	2.98	3.55	3.02

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.98 differs from the reported value 2.7 by more than 10 %

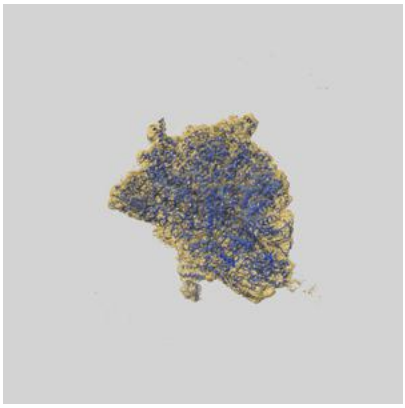
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12867 and PDB model 7OF2. Per-residue inclusion information can be found in section 3 on page 15.

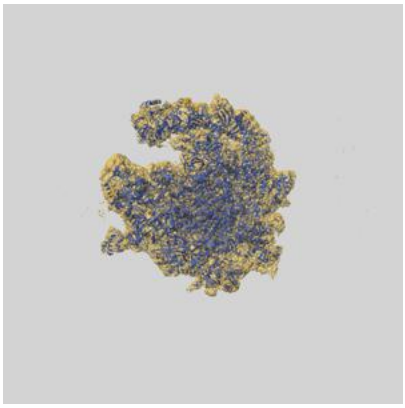
9.1 Map-model overlay



X



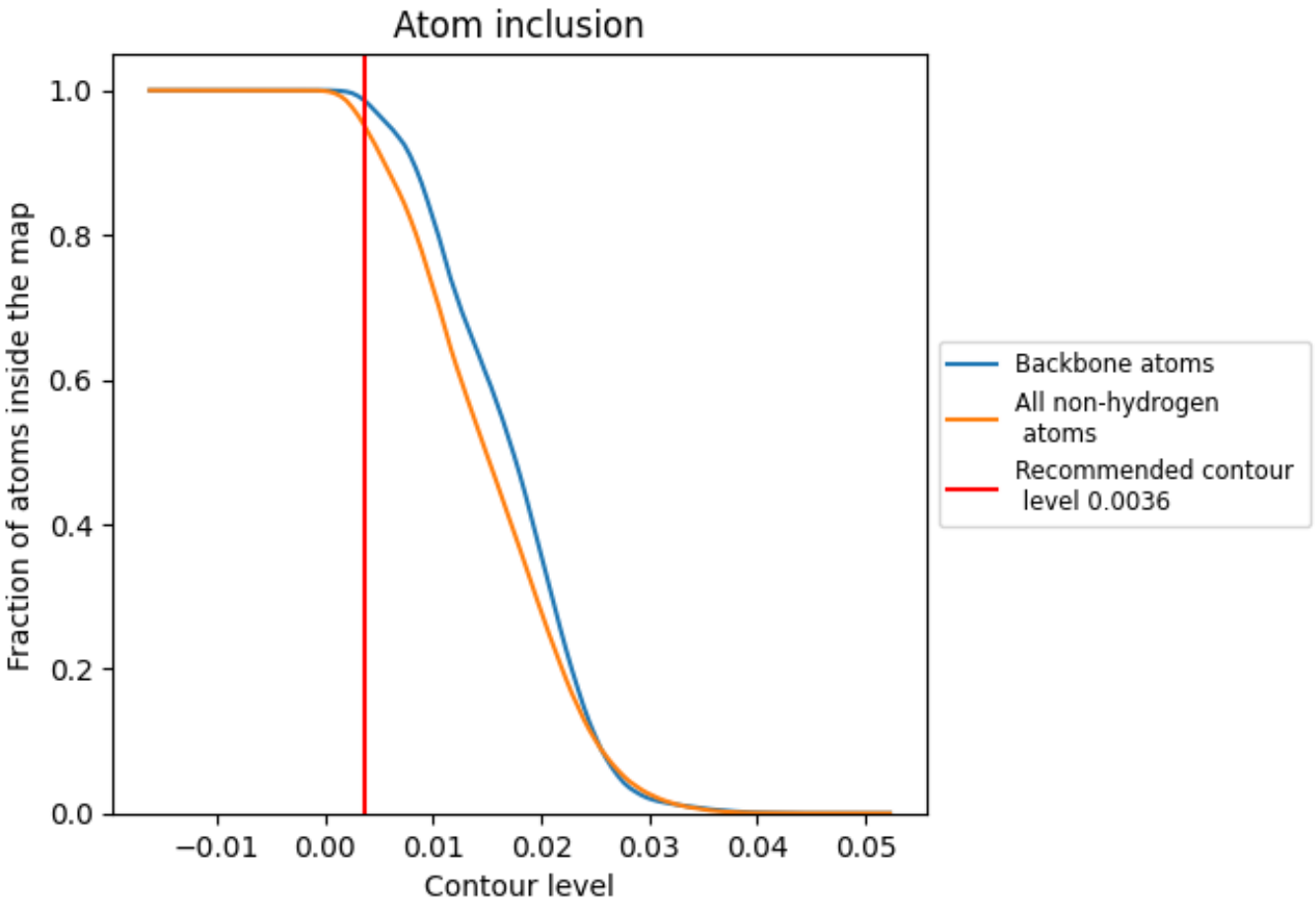
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0036 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 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.