



## Full wwPDB EM Validation Report ⓘ

Apr 1, 2025 – 10:45 pm BST

PDB ID : 7O9K / pdb\_00007o9k  
EMDB ID : EMD-12763  
Title : Human mitochondrial ribosome large subunit assembly intermediate with MTERF4-NSUN4, MRM2, MTG1, the MALSU module, GTPBP5 and mtEF-Tu  
Authors : Valentin Gese, G.; Hallberg, B.M.  
Deposited on : 2021-04-16  
Resolution : 3.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

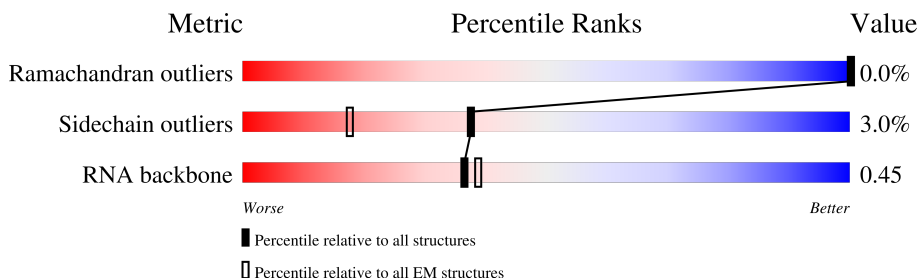
EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42

# 1 Overall quality at a glance

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









The reported resolution of this entry is 3.10 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.





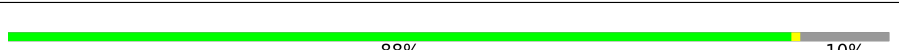
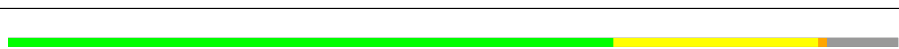

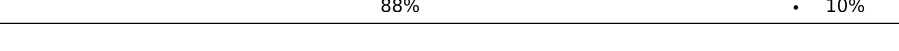
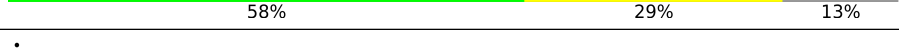





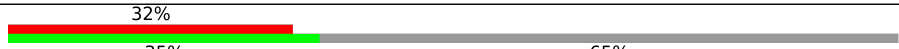


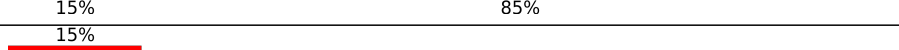








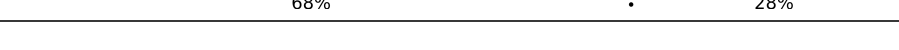
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	0	188	
2	a	142	
3	1	65	
4	2	92	
5	3	188	
6	4	103	
7	5	423	
8	6	380	



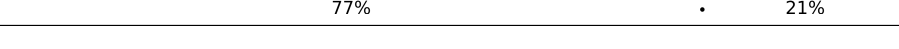
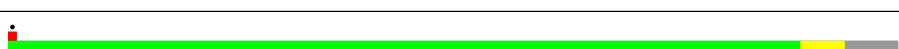



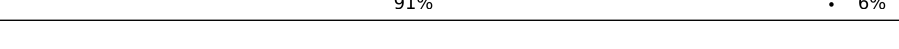


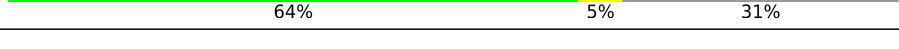

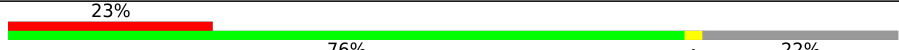

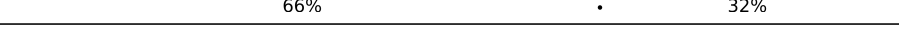







Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	7	338	
10	8	206	
11	9	137	
12	A	1559	
13	A1	384	
14	B	69	
15	A2	381	
16	C	334	
17	D	305	
18	E	348	
19	F	311	
20	FF	198	
20	t1	198	
20	t2	198	
20	t3	198	
20	t4	198	
20	t5	198	
20	t6	198	
21	G	414	
22	H	267	
23	I	261	
24	J	192	
25	K	178	
26	L	145	
27	M	296	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	N	251	
29	O	175	
30	P	179	
31	Q	292	
32	R	149	
33	S	205	
34	T	212	
35	U	153	
36	V	216	
37	W	148	
38	X	256	
39	Y	250	
40	Z	161	
41	b	215	
42	c	332	
43	d	306	
44	e	279	
45	f	212	
46	g	166	
47	h	158	
48	i	128	
49	j	123	
50	k	112	
51	l	138	
52	m	128	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
53	n	246	
54	o	102	
55	p	206	
56	q	222	
57	r	196	
58	s	439	
59	t	452	
60	u	234	
61	v	70	
62	w	156	
63	UNK	28	

## 2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 115679 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
1	0	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 2 is a protein called 39S ribosomal protein L42, mitochondrial.

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

- Molecule 3 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 4 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	45	Total	C	N	O	S	0	0
			367	227	81	58	1		

- Molecule 5 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 6 is a protein called 39S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4	38	Total	C	N	O	S	0	0
			342	217	72	49	4		

- Molecule 7 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	5	392	Total	C	N	O	S	0	0
			3199	2067	558	563	11		

- Molecule 8 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	6	331	Total	C	N	O	S	0	0
			2692	1723	480	480	9		

- Molecule 9 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	7	290	Total	C	N	O	S	0	0
			2356	1509	400	429	18		

- Molecule 10 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	8	85	Total	C	N	O	S	0	0
			719	454	129	134	2		

- Molecule 11 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	9	123	Total	C	N	O	S	0	0
			992	642	169	179	2		

- Molecule 12 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	1436	Total	C	N	O	P	0	0
			30486	13680	5498	9872	1436		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A1	344	Total	C	N	O	S	0	0
			2731	1743	476	495	17		

- Molecule 14 is a RNA chain called MT-TRNAVAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	60	Total	C	N	O	P	0	0
			1275	572	230	413	60		

- Molecule 15 is a protein called Transcription termination factor 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A2	238	Total	C	N	O	S	0	0
			1942	1244	336	350	12		

- Molecule 16 is a protein called Mitochondrial ribosome-associated GTPase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	C	255	Total	C	N	O	S	0	0
			1990	1267	349	360	14		

- Molecule 17 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	D	237	Total	C	N	O	S	0	0
			1851	1151	375	316	9		

- Molecule 18 is a protein called 39S ribosomal protein L3, mitochondrial.

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

- Molecule 19 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 20 is a protein called 39S ribosomal protein L12, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	FF	70	Total	C	N	O	0	0
			540	348	92	100		
20	t1	46	Total	C	N	O	0	0
			354	228	56	70		
20	t2	30	Total	C	N	O	0	0
			238	154	38	46		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf	Trace
20	t3	30	Total	C	N	O	0	0
			238	154	38	46		
20	t4	29	Total	C	N	O	0	0
			229	148	36	45		
20	t5	29	Total	C	N	O	0	0
			229	148	36	45		
20	t6	27	Total	C	N	O	0	0
			214	137	34	43		

- Molecule 21 is a protein called Mitochondrial ribosome-associated GTPase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	337	Total	C	N	O	S	0	0
			2549	1608	466	467	8		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	407	ASP	-	expression tag	UNP Q9H4K7
G	408	TYR	-	expression tag	UNP Q9H4K7
G	409	LYS	-	expression tag	UNP Q9H4K7
G	410	ASP	-	expression tag	UNP Q9H4K7
G	411	ASP	-	expression tag	UNP Q9H4K7
G	412	ASP	-	expression tag	UNP Q9H4K7
G	413	ASP	-	expression tag	UNP Q9H4K7
G	414	LYS	-	expression tag	UNP Q9H4K7

- Molecule 22 is a protein called 39S ribosomal protein L9, mitochondrial.

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

- Molecule 23 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	I	212	Total	C	N	O	S	0	0
			1695	1088	304	292	11		

- Molecule 24 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	J	138	Total	C	N	O	S	0	0
			1050	673	190	185	2		

- Molecule 25 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 26 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 27 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 28 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	N	179	Total	C	N	O	S	0	0
			1457	930	267	251	9		

- Molecule 29 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 30 is a protein called Mitochondrial ribosomal protein L18, isoform CRA\_b.

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

- Molecule 31 is a protein called 39S ribosomal protein L19, mitochondrial.

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

- Molecule 32 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 33 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 34 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 35 is a protein called 39S ribosomal protein L23, mitochondrial.

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

- Molecule 36 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	V	202	Total	C	N	O	S	0	0
			1652	1053	294	297	8		

- Molecule 37 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	W	101	Total	C	N	O	S	0	0
			805	520	151	131	3		

- Molecule 38 is a protein called 39S ribosomal protein L28, mitochondrial.

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

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

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

- Molecule 40 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 41 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 42 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 43 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	d	223	Total	C	N	O	S	0	0
			1847	1187	317	330	13		

- Molecule 44 is a protein called 39S ribosomal protein L46, mitochondrial.

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

- Molecule 45 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	f	123	Total	C	N	O	S	0	0
			979	625	164	187	3		

- Molecule 46 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- Molecule 47 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	h	107	Total	C	N	O	S	0	0
			871	551	153	164	3		

- Molecule 48 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 49 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 50 is a protein called 39S ribosomal protein L53, mitochondrial.

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

- Molecule 51 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	l	44	Total	C	N	O	S	0	0
			395	251	76	67	1		

- Molecule 52 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	m	35	Total	C	N	O	0	0
			287	180	57	50		

- Molecule 53 is a protein called rRNA methyltransferase 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	n	189	Total	C	N	O	S	0	0
			1450	917	259	268	6		

- Molecule 54 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	o	91	Total	C	N	O	S	0	0
			771	487	156	125	3		

- Molecule 55 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 56 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	q	135	Total	C	N	O	S	0	0
			1134	705	222	202	5		

- Molecule 57 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	r	155	Total	C	N	O	S	0	0
			1268	806	243	211	8		

- Molecule 58 is a protein called 39S ribosomal protein S30, mitochondrial.

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

- Molecule 59 is a protein called Elongation factor Tu, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	t	381	Total	C	N	O	S	0	0
			2939	1860	519	545	15		

- Molecule 60 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	u	133	Total	C	N	O	S	0	0
			1092	702	181	199	10		

- Molecule 61 is a protein called MIEF1 upstream open reading frame protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	v	68	Total	C	N	O		0	0
			584	369	115	100			

- Molecule 62 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	w	87	Total	C	N	O	S	0	0
			705	452	103	144	6		

- Molecule 63 is a protein called UNK.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	UNK	26	Total	C	N	O		0	0
			130	78	26	26			

- Molecule 64 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
64	0	1	Total	Zn	0
			1	1	
64	4	1	Total	Zn	0
			1	1	

- Molecule 65 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

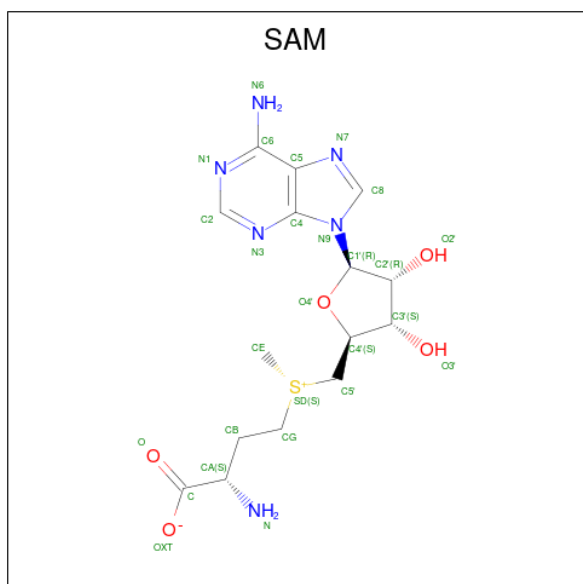
Mol	Chain	Residues	Atoms		AltConf
65	A	85	Total	Mg	0
			85	85	
65	D	1	Total	Mg	0
			1	1	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
65	E	1	Total	Mg	0
			1	1	
65	G	2	Total	Mg	0
			2	2	
65	M	1	Total	Mg	0
			1	1	
65	W	1	Total	Mg	0
			1	1	
65	g	1	Total	Mg	0
			1	1	
65	t	1	Total	Mg	0
			1	1	

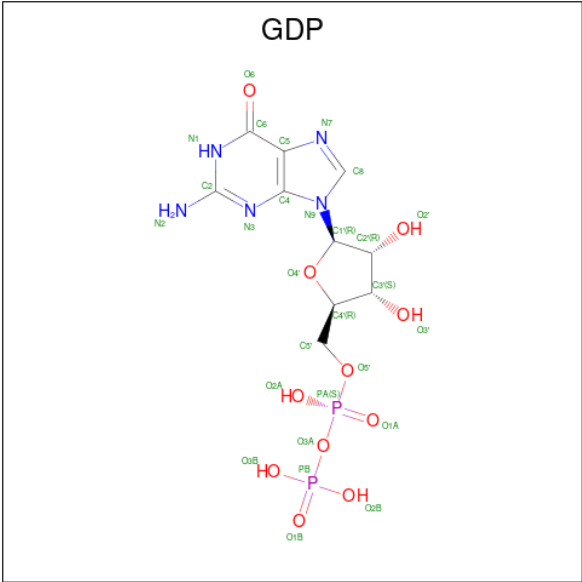
- Molecule 66 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula:  $C_{15}H_{22}N_6O_5S$ ).



Mol	Chain	Residues	Atoms					AltConf
66	A1	1	Total	C	N	O	S	0
			27	15	6	5	1	

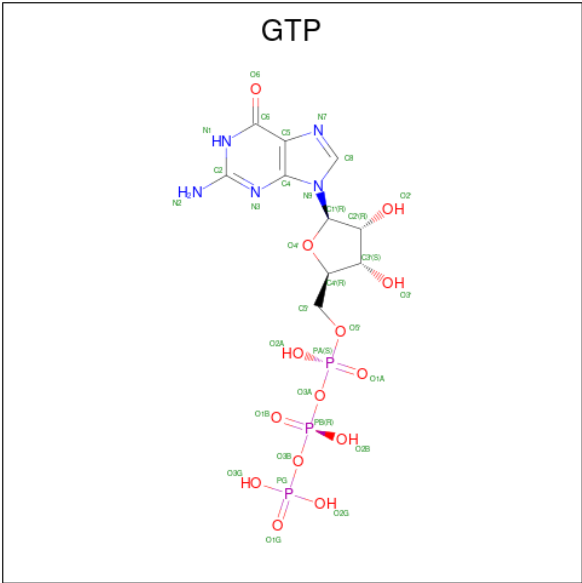
- Molecule 67 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).





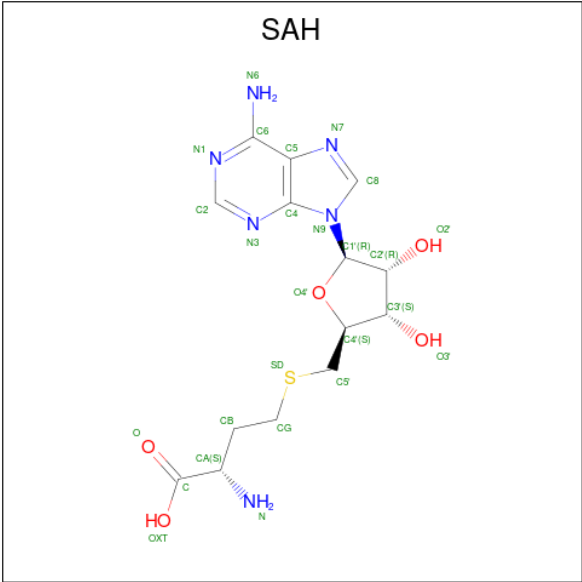
Mol	Chain	Residues	Atoms					AltConf
67	C	1	Total	C	N	O	P	0
			28	10	5	11	2	
67	t	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 68 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



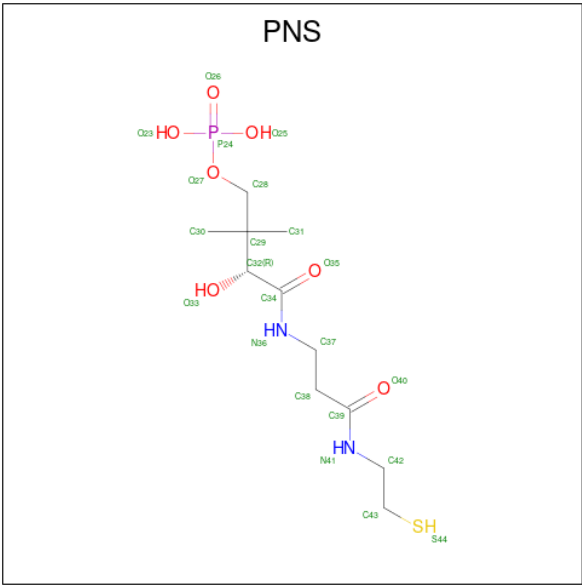
Mol	Chain	Residues	Atoms					AltConf
68	G	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 69 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).



Mol	Chain	Residues	Atoms					AltConf
69	n	1	Total	C	N	O	S	0
			26	14	6	5	1	

- Molecule 70 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: C<sub>11</sub>H<sub>23</sub>N<sub>2</sub>O<sub>7</sub>PS).

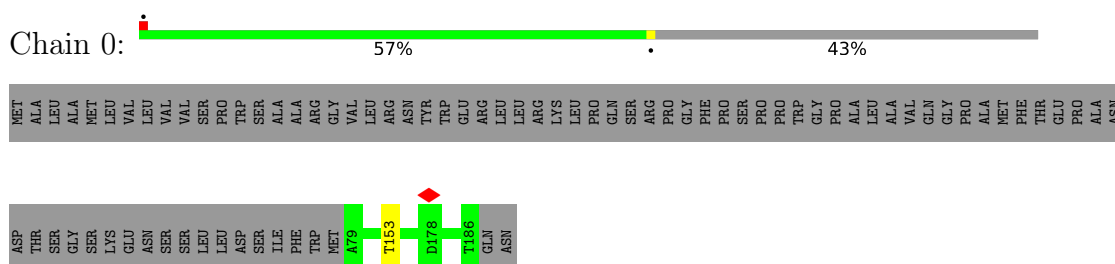


Mol	Chain	Residues	Atoms						AltConf
70	w	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	

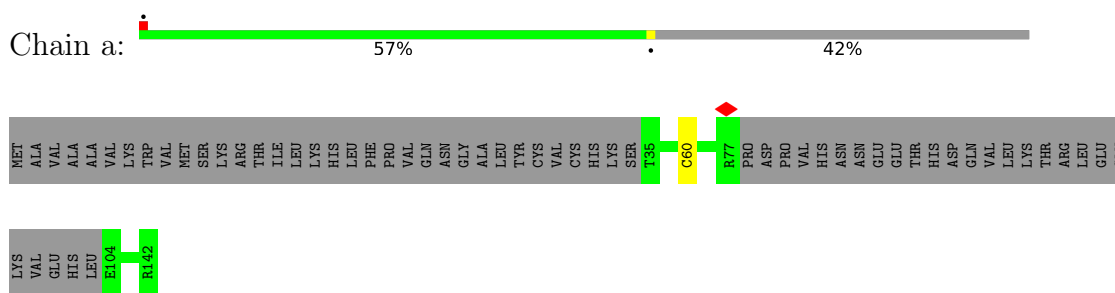
### 3 Residue-property plots [i](#)

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.

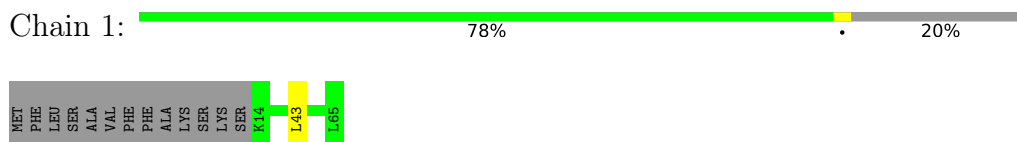
- Molecule 1: 39S ribosomal protein L32, mitochondrial



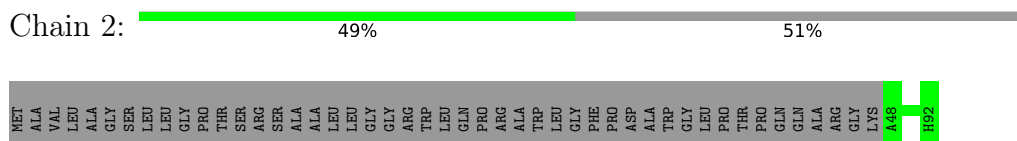
- Molecule 2: 39S ribosomal protein L42, mitochondrial



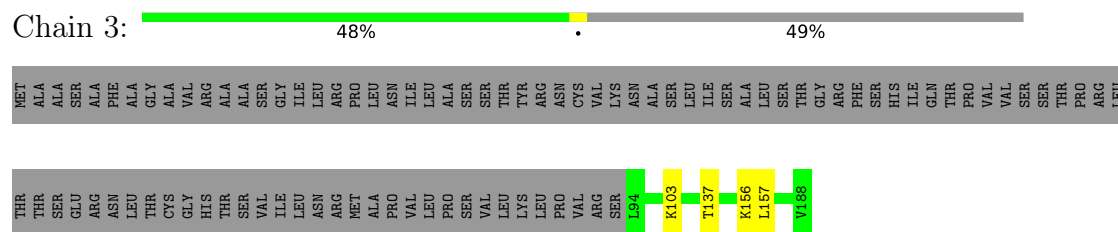
- Molecule 3: 39S ribosomal protein L33, mitochondrial



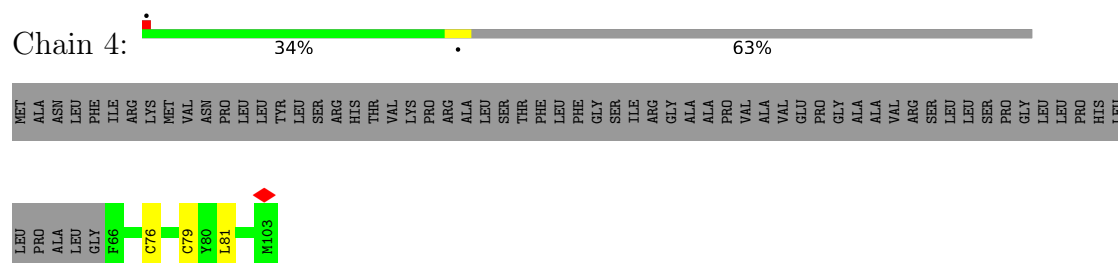
- Molecule 4: 39S ribosomal protein L34, mitochondrial



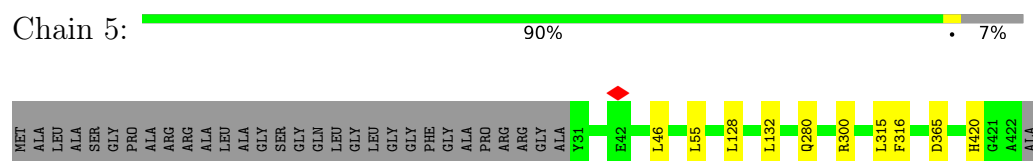
- Molecule 5: 39S ribosomal protein L35, mitochondrial



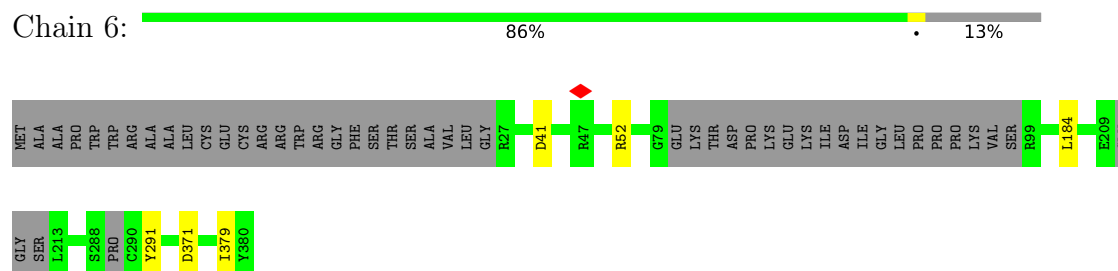
- Molecule 6: 39S ribosomal protein L36, mitochondrial



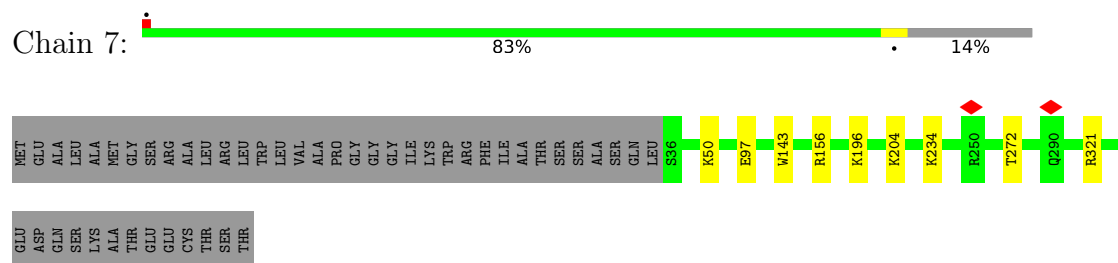
- Molecule 7: 39S ribosomal protein L37, mitochondrial



- Molecule 8: 39S ribosomal protein L38, mitochondrial



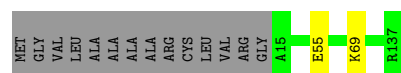
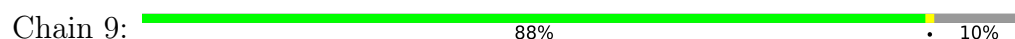
- Molecule 9: 39S ribosomal protein L39, mitochondrial



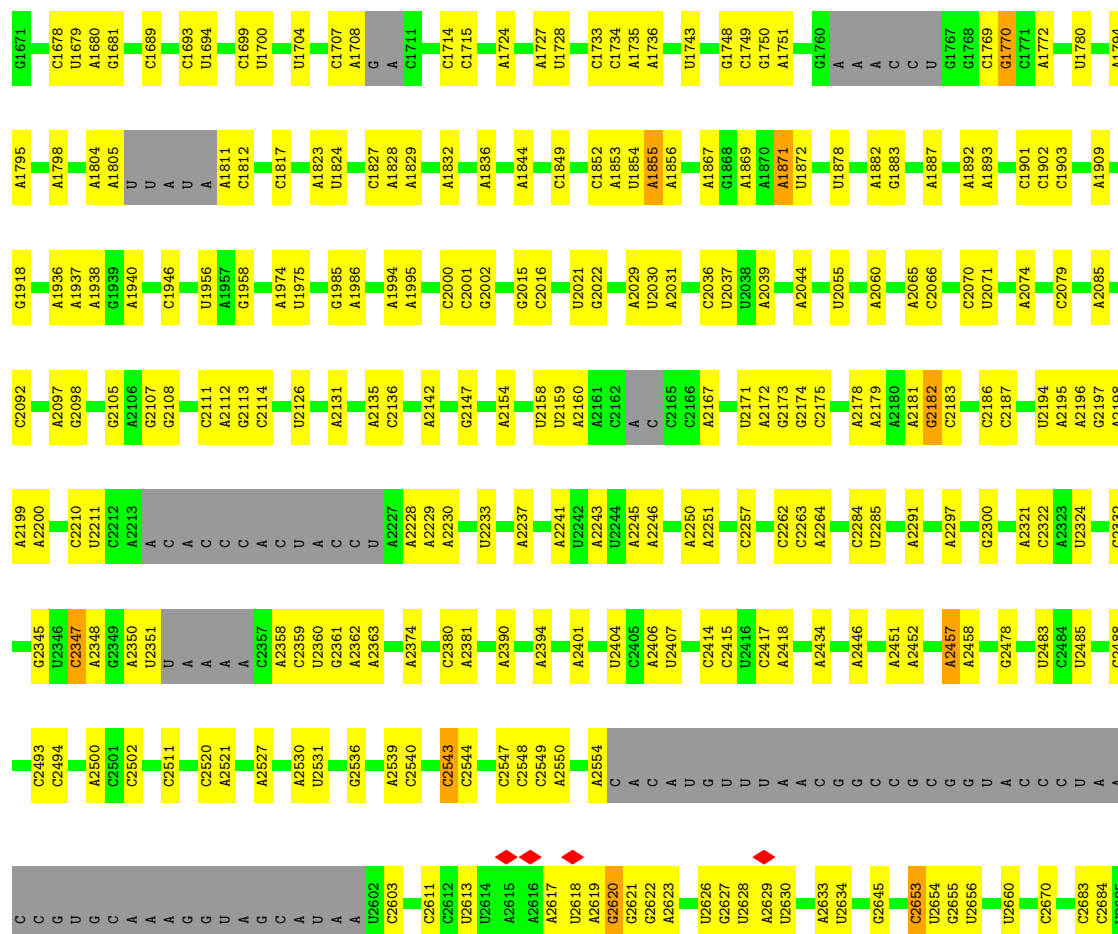
- Molecule 10: 39S ribosomal protein L40, mitochondrial

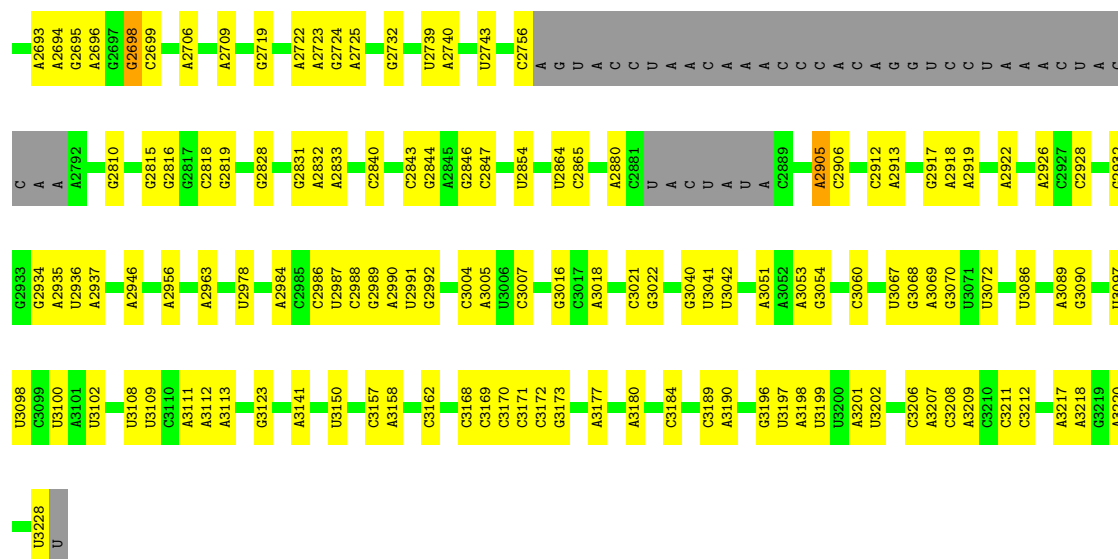


- Molecule 11: 39S ribosomal protein L41, mitochondrial

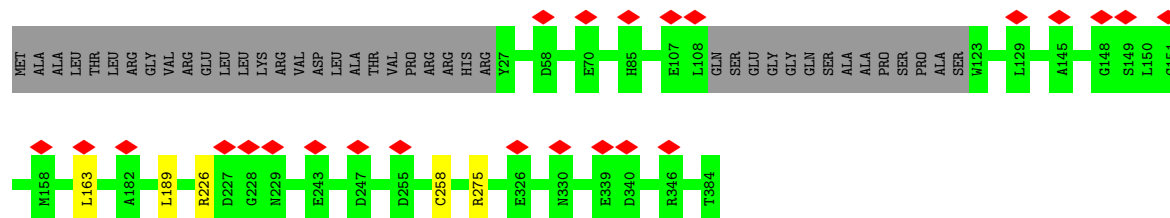


- Molecule 12: 16S rRNA





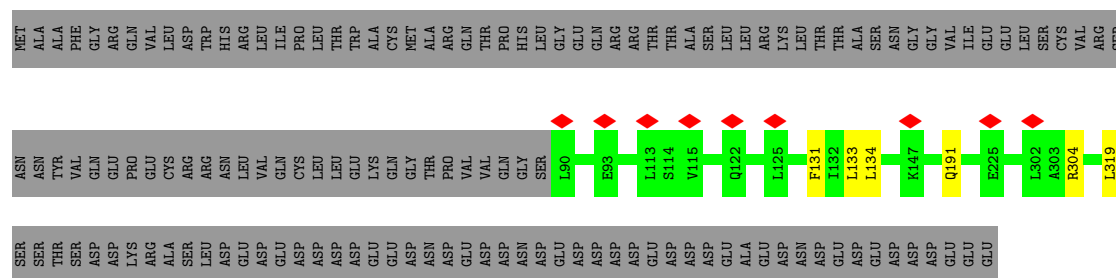
- Molecule 13: 5-methylcytosine rRNA methyltransferase NSUN4



- Molecule 14: MT-TRNAVAL



- Molecule 15: Transcription termination factor 4, mitochondrial

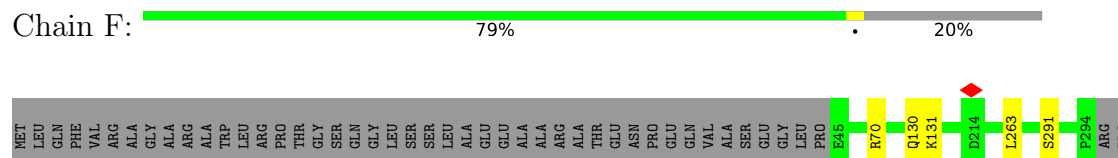


- Molecule 16: Mitochondrial ribosome-associated GTPase 1

- Molecule 17: 39S ribosomal protein L2, mitochondrial

- Molecule 18: 39S ribosomal protein L3, mitochondrial

- Molecule 19: 39S ribosomal protein L4, mitochondrial



LEU  
PRO  
HIS  
ALA  
ALA  
THR  
GLY  
PRO  
ALA  
ALA  
THR  
THR  
PRO  
TVR  
HIS  
CYS

- Molecule 20: 39S ribosomal protein L12, mitochondrial



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

PRO  
PRO  
LYS  
ILE  
ALA  
GLN  
LEU  
VAL  
GLN  
THR  
HIS  
H129  
F130  
F131  
V132  
R133  
L134  
T135  
E136  
A137  
K138  
P139  
V140  
D141  
K142  
V143  
K144  
L145  
I146  
K147  
E148  
I149  
K150  
N151  
Y152  
I153  
Q154  
G155  
I156  
N157  
L158  
V159  
Q160  
A161  
K162  
L163  
L164  
V165  
E166  
S167  
L168  
P169  
Q170  
E171  
I172  
K173  
A174  
N175  
V176  
A177  
K178  
A179  
E180

A181  
E182  
K183  
I184  
K185  
A186  
A187  
L188  
E189  
A190  
V191  
T194  
V195  
V196  
L197  
E198

- Molecule 20: 39S ribosomal protein L12, mitochondrial



MET  
LEU  
PRO  
HIS  
ALA  
ALA  
ARG  
PRO  
TRP  
GLY  
PRO  
CYS  
LEU  
GLY  
ARG  
ALA  
ALA  
PHE  
LEU  
LEU  
ALA  
ARG  
ARG  
GLN  
VAL  
PRO  
CYS  
VAL  
CYS  
ALA  
VAL  
ARG  
HIS  
MET  
ARG  
SER  
SER  
GLY  
HIS  
GLN  
ARG  
CYS  
E-15  
A-14  
L-13  
A-12  
P-9  
N-6  
A-5  
P-4  
K-3  
E-2  
Y-1  
P0  
P1

K2  
I3  
Q4  
Q5  
L6  
V7  
Q8  
D9  
I10  
A11  
S12  
L13  
T14  
L15  
L16  
E17  
I18  
S19  
D20  
L21  
N22  
E23  
L24  
L25  
K26  
K27  
T28  
L29  
K30  
ILE  
GLN  
ASP  
VAL  
VAL  
LEU  
VAL  
VAL  
PRO  
MET  
GLY  
GLY  
VAL  
MET  
ILE  
SER  
GLY  
ALA  
VAL  
PRO  
ASN  
VAL  
VAL  
ALA  
ALA  
LYS  
ALA  
ALA  
GLN  
GLU  
VAL  
GLU  
GLU  
ASP  
ILE  
PRO

LYS  
ILE  
LYS  
ALA  
ALA  
LEU  
GLU  
ALA  
PHE  
HIS  
THR  
VAL  
GLY  
GLY  
THR  
VAL  
VAL  
GLU

- Molecule 20: 39S ribosomal protein L12, mitochondrial



MET  
LEU  
PRO  
HIS  
ALA  
ALA  
ARG  
PRO  
TRP  
GLY  
LEU  
CYS  
LEU  
GLY  
ARG  
ALA  
ALA  
PHE  
ARG  
LEU  
ALA  
ARG  
ARG  
GLN  
VAL  
PRO  
CYS  
VAL  
CYS  
ALA  
VAL  
ARG  
HIS  
MET  
ARG  
SER  
SER  
GLY  
HIS  
GLN  
ARG  
CYS  
GLY  
ALA  
ALA  
VAL  
PRO  
ASN  
ASP  
LEU  
LEU  
VAL  
ASN  
ALA  
ALA  
GLN  
PRO  
LYS  
TYR

PRO  
P1  
K2  
I3  
Q4  
L6  
V7  
Q8  
D9  
I10  
A11  
S12  
L13  
L14  
L15  
L16  
E17  
E23  
L24  
L25  
K26  
K27  
T28  
L29  
K30  
GLN  
ASP  
VAL  
GLY  
LEU  
VAL  
VAL  
PRO  
MET  
GLY  
GLY  
VAL  
MET  
SER  
GLY  
ALA  
ALA  
VAL  
PRO  
ALA  
ALA  
ASN  
ALA  
ALA  
GLN  
GLU  
VAL  
GLU  
ASP  
ILE  
PRO  
ILE  
ALA

LYS  
GLU  
ARG  
THR  
HIS  
PHE  
THR  
VAL  
ARG  
LEU  
THR  
GLU  
ALA  
LYS  
PRO  
VAL  
ASP  
LYS  
VAL  
LYS  
LEU  
ILE  
LYS  
ILE  
GLU  
LYS  
ASN  
TYR  
ILE  
GLN  
GLY  
ILE  
ASN  
VAL  
VAL  
GLN  
ALA  
LYS  
LYS  
LEU  
VAL  
VAL  
ALA  
GLU  
GLU  
LYS  
ILE

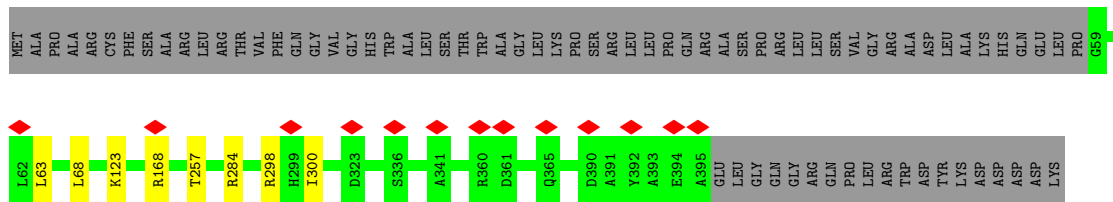
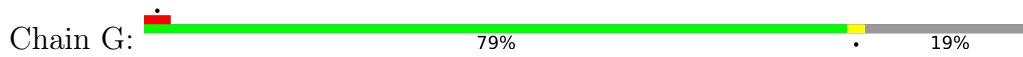
LYS  
ALA  
ALA  
LEU  
GLU  
ALA  
VAL  
GLY  
GLY  
THR  
VAL  
VAL  
LEU  
GLU

- Molecule 20: 39S ribosomal protein L12, mitochondrial

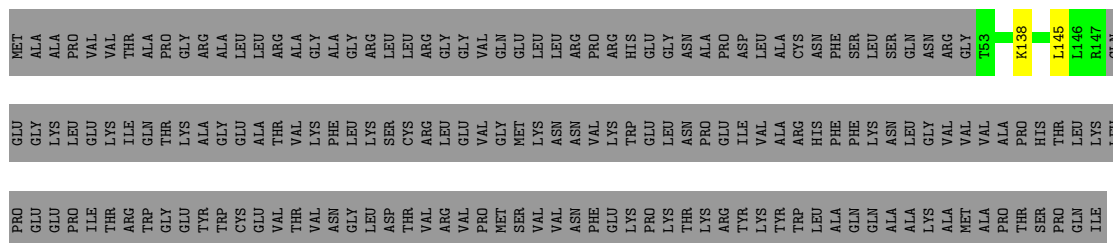




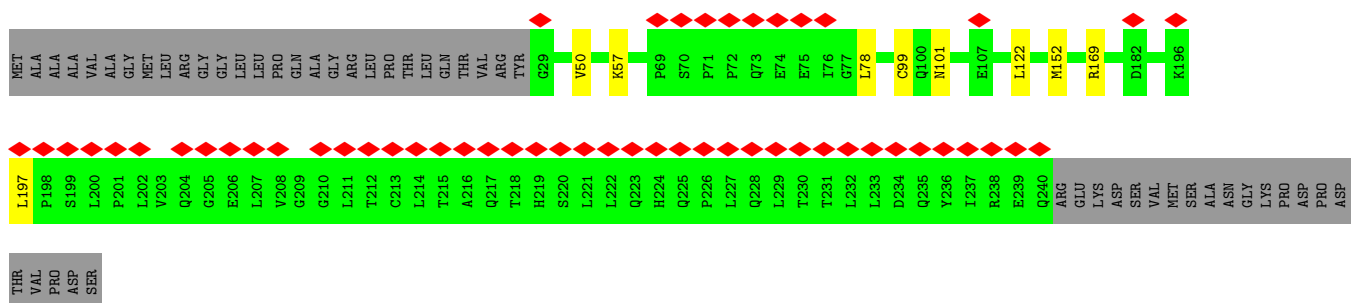
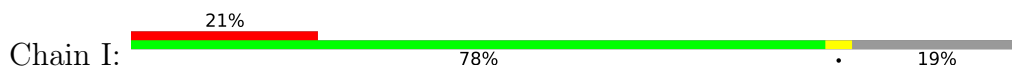
- Molecule 21: Mitochondrial ribosome-associated GTPase 2



- Molecule 22: 39S ribosomal protein L9, mitochondrial

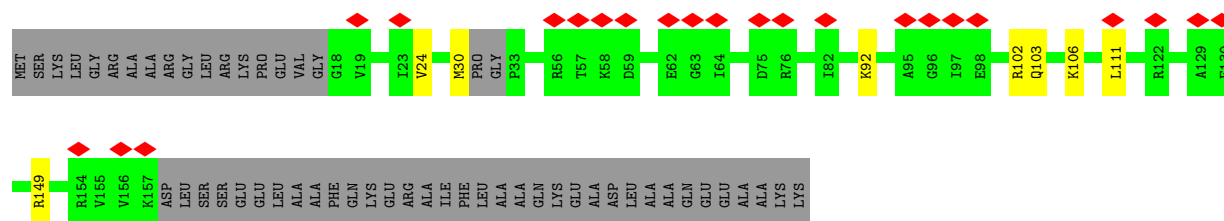


- Molecule 23: 39S ribosomal protein L10, mitochondrial



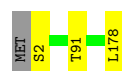
- Molecule 24: 39S ribosomal protein L11, mitochondrial





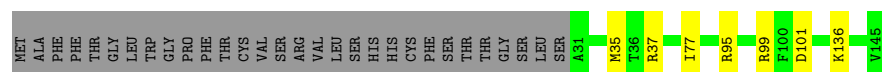
- Molecule 25: 39S ribosomal protein L13, mitochondrial

Chain K: 98%



- Molecule 26: 39S ribosomal protein L14, mitochondrial

Chain L: 74% 5% 21%



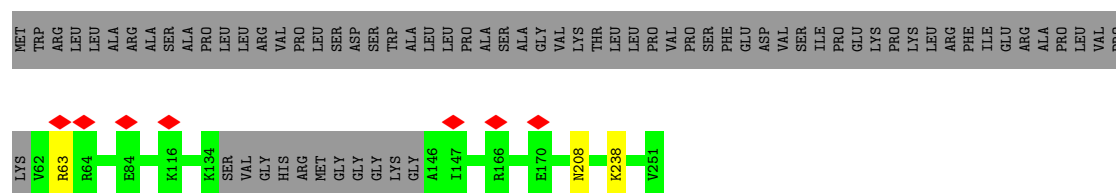
- Molecule 27: 39S ribosomal protein L15, mitochondrial

Chain M: 94%



- Molecule 28: 39S ribosomal protein L16, mitochondrial

Chain N: 70% 29%



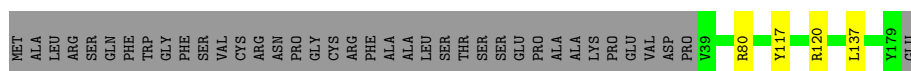
- Molecule 29: 39S ribosomal protein L17, mitochondrial

Chain O: 82% 5% 13%



- Molecule 30: Mitochondrial ribosomal protein L18, isoform CRA\_b

Chain P: 77% 21%



- Molecule 31: 39S ribosomal protein L19, mitochondrial

Chain Q: 72% 26%



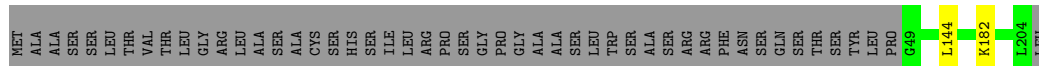
- Molecule 32: 39S ribosomal protein L20, mitochondrial

Chain R: 89% 5% 6%



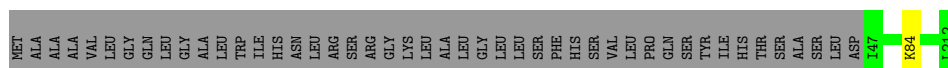
- Molecule 33: 39S ribosomal protein L21, mitochondrial

Chain S: 75% 24%



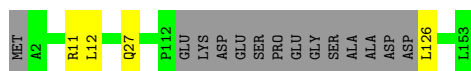
- Molecule 34: 39S ribosomal protein L22, mitochondrial

Chain T: 78% 22%



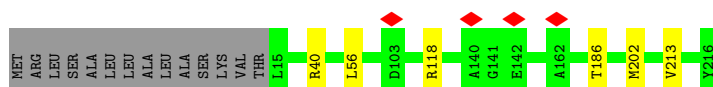
- Molecule 35: 39S ribosomal protein L23, mitochondrial

Chain U: 88% 9%



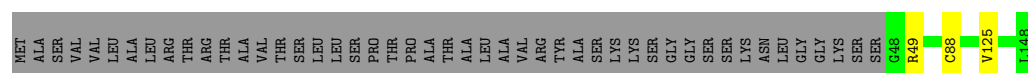
- Molecule 36: 39S ribosomal protein L24, mitochondrial

Chain V: 91% 6%



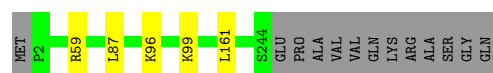
- Molecule 37: 39S ribosomal protein L27, mitochondrial

Chain W:  66% 32%



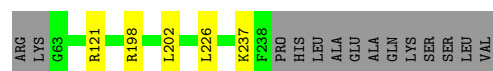
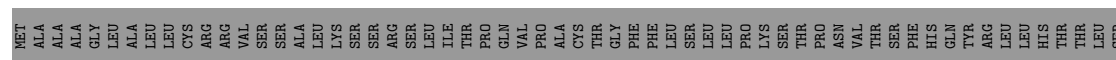
- Molecule 38: 39S ribosomal protein L28, mitochondrial

Chain X:  93% 5%



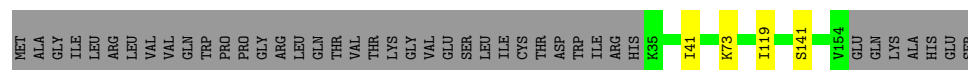
- Molecule 39: 39S ribosomal protein L47, mitochondrial

Chain Y:  68% 30%



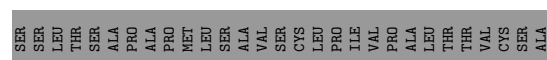
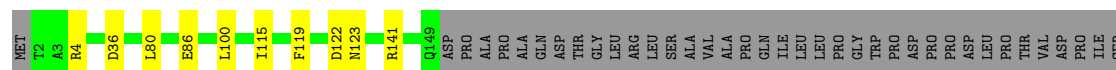
- Molecule 40: 39S ribosomal protein L30, mitochondrial

Chain Z:  72% 25%




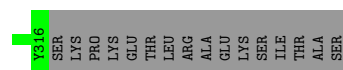
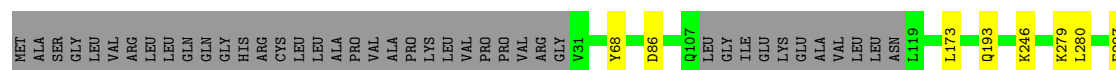
- Molecule 41: 39S ribosomal protein L43, mitochondrial

Chain b:  64% 5% 31%



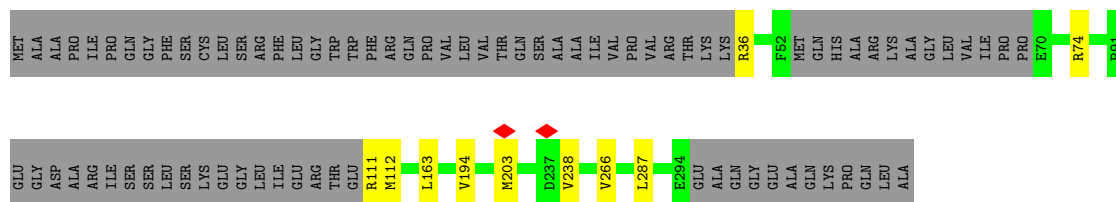
- Molecule 42: 39S ribosomal protein L44, mitochondrial

Chain c:  80% 17%




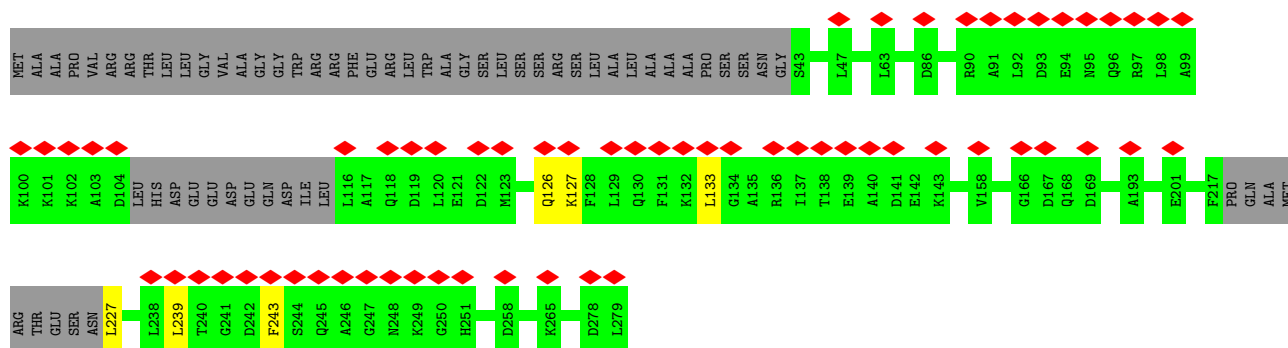
- Molecule 43: 39S ribosomal protein L45, mitochondrial

Chain d:  70% 27%



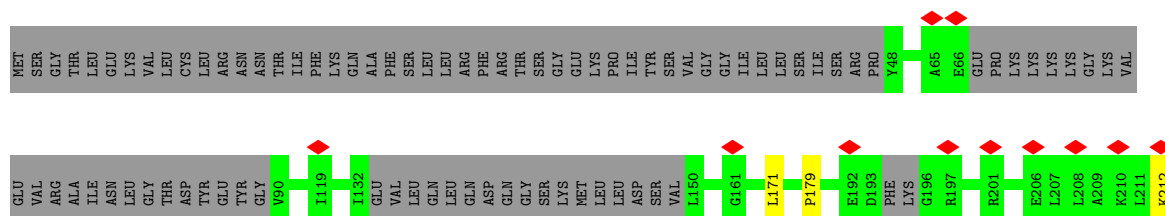
- Molecule 44: 39S ribosomal protein L46, mitochondrial

Chain e:  23% 76% 22%




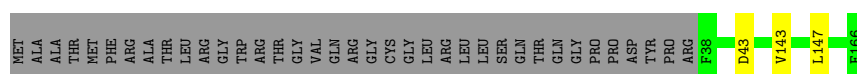
- Molecule 45: 39S ribosomal protein L48, mitochondrial

Chain f:  5% 57% 42%



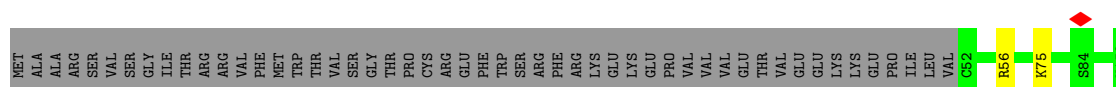
- Molecule 46: 39S ribosomal protein L49, mitochondrial

Chain g:  76% 22%

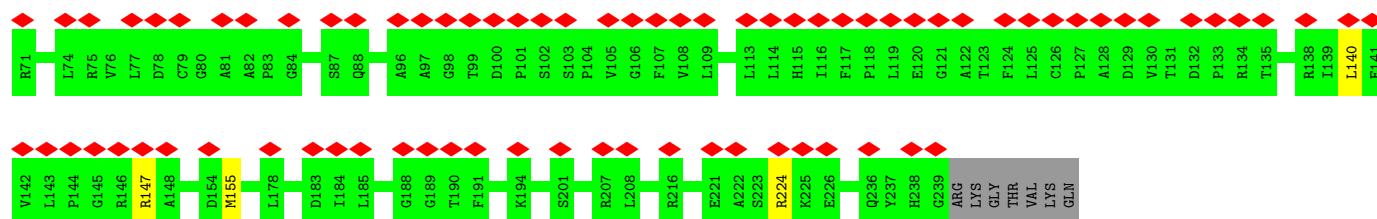


- Molecule 47: 39S ribosomal protein L50, mitochondrial

Chain h:  66% 32%

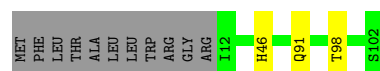


- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ALA | GLY | TYR | LEU | LYS | LEU | VAL | CYS | VAL | SER | PHE | GLN | ARG | GLN | GLY | PHE | HIS | THR | VAL | VAL | GLY | SER | ARG | CYS | LYS | ASN | ARG | THR | GLY | ALA | GLU | HIS | HIS | LEU | TRP | LEU | LEU | THR | ARG | HIS | HIS | LEU | ASP | ARG | PRO | PHE | VAL | LYS | ALA | ALA | LYS | VAL | VAL | GLU | S51 | Y52 | R55 | F58 | E65 | R66 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



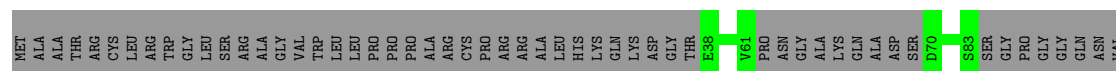
- Molecule 54: Ribosomal protein 63, mitochondrial

Chain o: 86% 11%



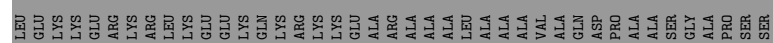
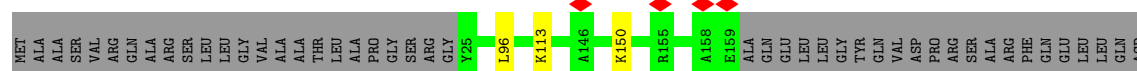
- Molecule 55: Peptidyl-tRNA hydrolase ICT1, mitochondrial

Chain p: 61% 38%



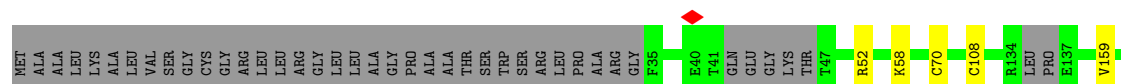
- Molecule 56: Growth arrest and DNA damage-inducible proteins-interacting protein 1

Chain q: 59% 39%



- Molecule 57: 39S ribosomal protein S18a, mitochondrial

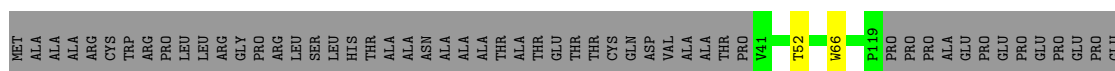
Chain r: 76% 21%



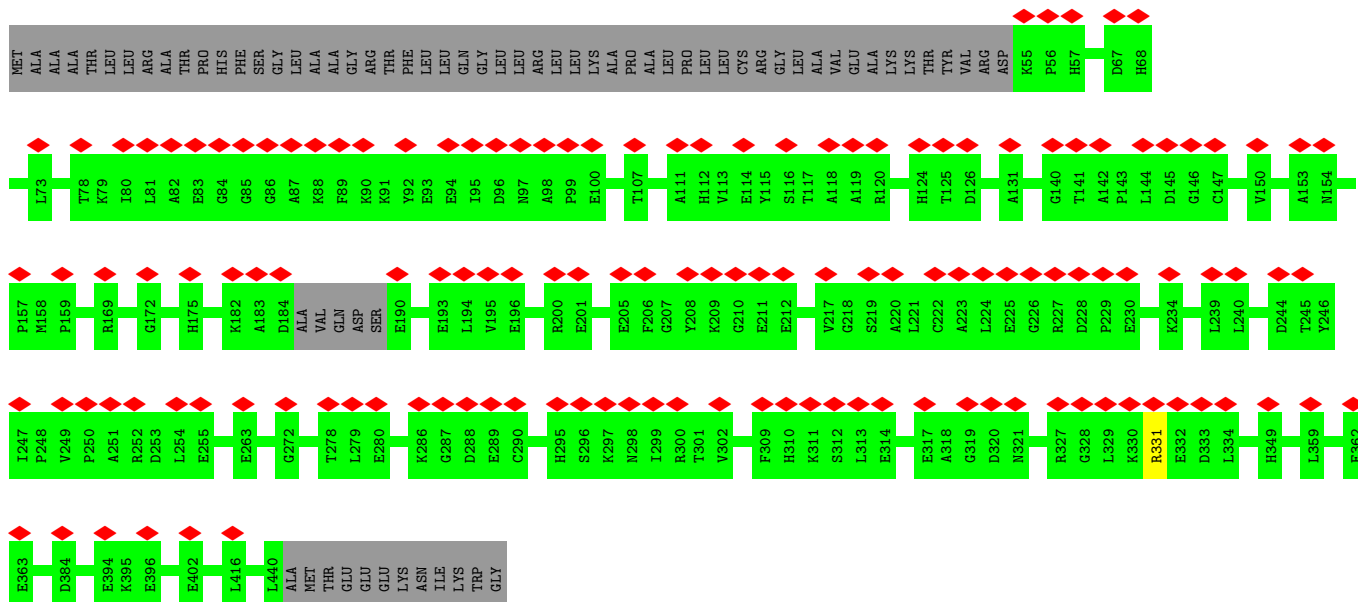
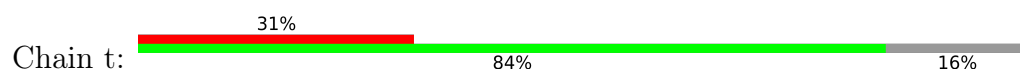
- Molecule 58: 39S ribosomal protein S30, mitochondrial

Chain s: 83% 16%

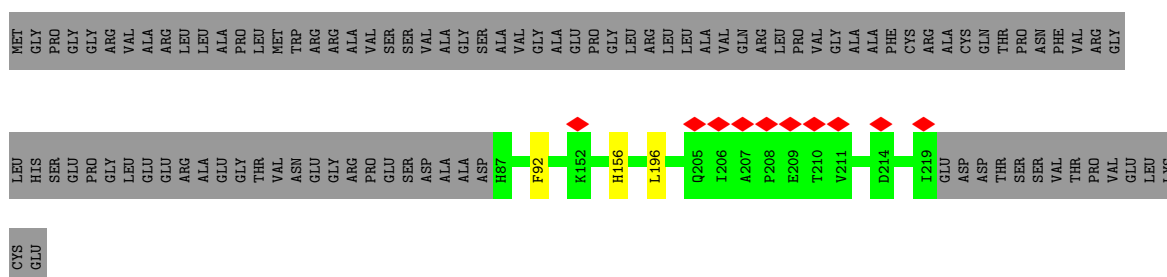




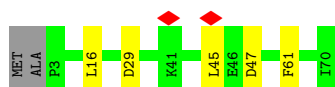
• Molecule 59: Elongation factor Tu, mitochondrial



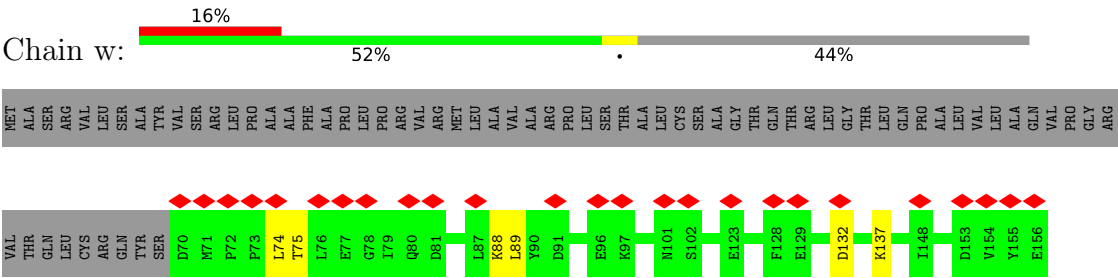
• Molecule 60: Mitochondrial assembly of ribosomal large subunit protein 1



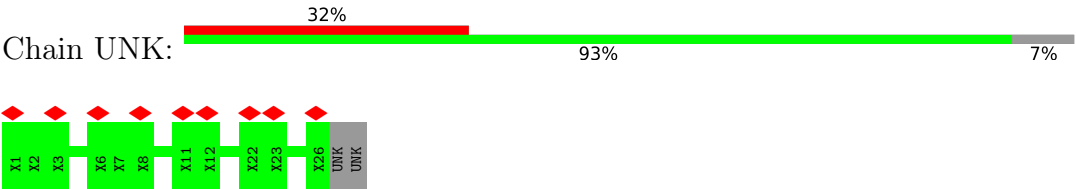
• Molecule 61: MIEF1 upstream open reading frame protein



• Molecule 62: Acyl carrier protein, mitochondrial



• Molecule 63: UNK



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39495	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	49.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.935	Depositor
Minimum map value	-0.278	Depositor
Average map value	0.025	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	221.34, 280.5, 250.92	wwPDB
Map dimensions	246, 275, 217	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.02, 1.02, 1.02	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.34	0/895	0.66	0/1201
2	a	0.29	0/709	0.63	0/963
3	1	0.26	0/438	0.69	0/583
4	2	0.33	0/373	0.68	0/496
5	3	0.27	0/852	0.63	0/1136
6	4	0.39	0/350	0.77	1/461 (0.2%)
7	5	0.27	0/3294	0.62	0/4488
8	6	0.27	0/2779	0.62	0/3787
9	7	0.26	0/2413	0.61	0/3264
10	8	0.26	0/734	0.65	0/986
11	9	0.30	0/1020	0.66	0/1374
12	A	0.49	0/34076	0.76	12/53028 (0.0%)
13	A1	0.27	0/2795	0.62	0/3792
14	B	0.46	0/1423	0.72	0/2206
15	A2	0.26	0/1973	0.62	0/2651
16	C	0.35	0/2020	0.55	0/2724
17	D	0.29	0/1888	0.69	0/2538
18	E	0.28	0/2465	0.63	0/3344
19	F	0.29	0/2071	0.64	0/2817
20	FF	0.25	0/544	0.66	0/730
20	t1	0.44	0/358	0.54	0/486
20	t2	0.22	0/238	0.36	0/319
20	t3	0.21	0/238	0.35	0/319
20	t4	0.22	0/229	0.34	0/308
20	t5	0.21	0/229	0.41	0/308
20	t6	0.22	0/213	0.39	0/286
21	G	0.28	0/2600	0.63	0/3513
22	H	0.27	0/798	0.71	0/1073
23	I	0.28	0/1731	0.62	0/2345
24	J	0.28	0/1064	0.68	0/1431
25	K	0.28	0/1495	0.63	0/2029
26	L	0.28	0/904	0.64	0/1218

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
27	M	0.28	0/2359	0.66	0/3185
28	N	0.27	0/1494	0.64	0/2010
29	O	0.28	0/1269	0.64	0/1708
30	P	0.28	0/1173	0.65	0/1588
31	Q	0.27	0/1846	0.64	0/2487
32	R	0.28	0/1174	0.64	0/1572
33	S	0.27	0/1276	0.68	0/1729
34	T	0.28	0/1402	0.63	0/1886
35	U	0.28	0/1183	0.66	0/1600
36	V	0.27	0/1697	0.64	0/2302
37	W	0.28	0/827	0.65	0/1118
38	X	0.26	0/2090	0.62	0/2825
39	Y	0.26	0/1552	0.63	0/2079
40	Z	0.28	0/1003	0.66	0/1354
41	b	0.30	0/1202	0.67	0/1626
42	c	0.28	0/2264	0.62	0/3059
43	d	0.27	0/1899	0.64	0/2569
44	e	0.27	0/1797	0.66	0/2422
45	f	0.28	0/994	0.62	0/1336
46	g	0.28	0/1102	0.63	0/1503
47	h	0.29	0/894	0.63	0/1217
48	i	0.29	0/849	0.66	0/1135
49	j	0.32	0/698	0.64	0/940
50	k	0.28	0/635	0.68	0/855
51	l	0.26	0/407	0.62	0/547
52	m	0.28	0/292	0.67	0/394
53	n	0.27	0/1480	0.61	0/2013
54	o	0.26	0/792	0.63	0/1064
55	p	0.28	0/1071	0.64	0/1433
56	q	0.27	0/1165	0.62	0/1575
57	r	0.29	0/1305	0.65	0/1767
58	s	0.27	0/3114	0.62	0/4225
59	t	0.26	0/2992	0.63	0/4047
60	u	0.25	0/1119	0.63	0/1516
61	v	0.25	0/593	0.64	0/788
62	w	0.26	0/717	0.60	0/967
All	All	0.35	0/120935	0.67	13/170645 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1855	A	C2'-C3'-O3'	7.67	126.38	109.50
12	A	2182	G	C2'-C3'-O3'	7.49	125.97	109.50
12	A	1871	A	C2'-C3'-O3'	6.95	124.82	113.70
12	A	2457	A	C2'-C3'-O3'	6.63	124.31	113.70
12	A	2905	A	C2'-C3'-O3'	6.48	124.07	113.70
12	A	2653	C	C4'-C3'-O3'	6.38	125.75	113.00
6	4	79	CYS	CA-CB-SG	-6.16	102.91	114.00
12	A	2620	G	C2'-C3'-O3'	5.90	123.14	113.70
12	A	2543	C	C2'-C3'-O3'	5.75	122.91	113.70
12	A	2347	C	C2'-C3'-O3'	5.72	122.85	113.70
12	A	1958	G	C1'-O4'-C4'	-5.35	105.62	109.90
12	A	2698	G	O4'-C1'-N9	5.35	112.48	108.20
12	A	1770	G	C4'-C3'-C2'	-5.01	97.59	102.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	106/188 (56%)	103 (97%)	3 (3%)	0	100	100
2	a	78/142 (55%)	75 (96%)	3 (4%)	0	100	100
3	1	50/65 (77%)	50 (100%)	0	0	100	100
4	2	43/92 (47%)	42 (98%)	1 (2%)	0	100	100
5	3	93/188 (50%)	89 (96%)	4 (4%)	0	100	100
6	4	36/103 (35%)	36 (100%)	0	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	5	390/423 (92%)	376 (96%)	14 (4%)	0	100	100
8	6	323/380 (85%)	310 (96%)	13 (4%)	0	100	100
9	7	288/338 (85%)	274 (95%)	14 (5%)	0	100	100
10	8	83/206 (40%)	75 (90%)	8 (10%)	0	100	100
11	9	121/137 (88%)	117 (97%)	4 (3%)	0	100	100
13	A1	340/384 (88%)	330 (97%)	10 (3%)	0	100	100
15	A2	236/381 (62%)	233 (99%)	3 (1%)	0	100	100
16	C	251/334 (75%)	245 (98%)	6 (2%)	0	100	100
17	D	235/305 (77%)	225 (96%)	10 (4%)	0	100	100
18	E	302/348 (87%)	288 (95%)	14 (5%)	0	100	100
19	F	248/311 (80%)	243 (98%)	5 (2%)	0	100	100
20	FF	68/198 (34%)	65 (96%)	3 (4%)	0	100	100
20	t1	44/198 (22%)	38 (86%)	4 (9%)	2 (4%)	2	12
20	t2	28/198 (14%)	28 (100%)	0	0	100	100
20	t3	28/198 (14%)	28 (100%)	0	0	100	100
20	t4	27/198 (14%)	27 (100%)	0	0	100	100
20	t5	27/198 (14%)	27 (100%)	0	0	100	100
20	t6	25/198 (13%)	24 (96%)	1 (4%)	0	100	100
21	G	335/414 (81%)	316 (94%)	19 (6%)	0	100	100
22	H	93/267 (35%)	91 (98%)	2 (2%)	0	100	100
23	I	210/261 (80%)	207 (99%)	3 (1%)	0	100	100
24	J	134/192 (70%)	127 (95%)	7 (5%)	0	100	100
25	K	175/178 (98%)	173 (99%)	2 (1%)	0	100	100
26	L	113/145 (78%)	107 (95%)	6 (5%)	0	100	100
27	M	285/296 (96%)	279 (98%)	6 (2%)	0	100	100
28	N	175/251 (70%)	170 (97%)	5 (3%)	0	100	100
29	O	150/175 (86%)	144 (96%)	6 (4%)	0	100	100
30	P	139/179 (78%)	137 (99%)	2 (1%)	0	100	100
31	Q	215/292 (74%)	209 (97%)	6 (3%)	0	100	100
32	R	138/149 (93%)	137 (99%)	1 (1%)	0	100	100
33	S	154/205 (75%)	149 (97%)	5 (3%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	T	164/212 (77%)	161 (98%)	3 (2%)	0	100	100
35	U	135/153 (88%)	131 (97%)	4 (3%)	0	100	100
36	V	200/216 (93%)	196 (98%)	4 (2%)	0	100	100
37	W	99/148 (67%)	99 (100%)	0	0	100	100
38	X	241/256 (94%)	239 (99%)	2 (1%)	0	100	100
39	Y	174/250 (70%)	170 (98%)	4 (2%)	0	100	100
40	Z	118/161 (73%)	113 (96%)	5 (4%)	0	100	100
41	b	146/215 (68%)	138 (94%)	8 (6%)	0	100	100
42	c	271/332 (82%)	267 (98%)	4 (2%)	0	100	100
43	d	217/306 (71%)	207 (95%)	10 (5%)	0	100	100
44	e	211/279 (76%)	202 (96%)	9 (4%)	0	100	100
45	f	115/212 (54%)	107 (93%)	7 (6%)	1 (1%)	14	45
46	g	127/166 (76%)	125 (98%)	2 (2%)	0	100	100
47	h	105/158 (66%)	101 (96%)	4 (4%)	0	100	100
48	i	95/128 (74%)	92 (97%)	3 (3%)	0	100	100
49	j	83/123 (68%)	82 (99%)	1 (1%)	0	100	100
50	k	76/112 (68%)	73 (96%)	3 (4%)	0	100	100
51	l	42/138 (30%)	42 (100%)	0	0	100	100
52	m	33/128 (26%)	31 (94%)	2 (6%)	0	100	100
53	n	187/246 (76%)	186 (100%)	1 (0%)	0	100	100
54	o	89/102 (87%)	84 (94%)	5 (6%)	0	100	100
55	p	119/206 (58%)	115 (97%)	4 (3%)	0	100	100
56	q	133/222 (60%)	132 (99%)	1 (1%)	0	100	100
57	r	149/196 (76%)	143 (96%)	6 (4%)	0	100	100
58	s	366/439 (83%)	353 (96%)	13 (4%)	0	100	100
59	t	377/452 (83%)	368 (98%)	9 (2%)	0	100	100
60	u	131/234 (56%)	124 (95%)	7 (5%)	0	100	100
61	v	66/70 (94%)	61 (92%)	5 (8%)	0	100	100
62	w	85/156 (54%)	83 (98%)	2 (2%)	0	100	100
All	All	10140/14731 (69%)	9819 (97%)	318 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
20	t1	-3	LYS
45	f	179	PRO
20	t1	1	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	97/164 (59%)	96 (99%)	1 (1%)	73	86
2	a	78/133 (59%)	77 (99%)	1 (1%)	65	82
3	1	49/60 (82%)	48 (98%)	1 (2%)	50	74
4	2	39/72 (54%)	39 (100%)	0	100	100
5	3	88/166 (53%)	84 (96%)	4 (4%)	23	53
6	4	37/89 (42%)	35 (95%)	2 (5%)	18	47
7	5	353/368 (96%)	343 (97%)	10 (3%)	38	66
8	6	271/332 (82%)	265 (98%)	6 (2%)	47	71
9	7	266/303 (88%)	257 (97%)	9 (3%)	32	62
10	8	77/190 (40%)	71 (92%)	6 (8%)	10	35
11	9	104/112 (93%)	102 (98%)	2 (2%)	52	75
13	A1	297/328 (90%)	292 (98%)	5 (2%)	56	78
15	A2	221/350 (63%)	215 (97%)	6 (3%)	40	67
16	C	224/287 (78%)	219 (98%)	5 (2%)	47	71
17	D	191/245 (78%)	189 (99%)	2 (1%)	73	86
18	E	259/290 (89%)	255 (98%)	4 (2%)	60	80
19	F	217/262 (83%)	212 (98%)	5 (2%)	45	70
20	FF	58/158 (37%)	58 (100%)	0	100	100
20	t1	40/158 (25%)	38 (95%)	2 (5%)	20	50
20	t2	29/158 (18%)	29 (100%)	0	100	100
20	t3	29/158 (18%)	28 (97%)	1 (3%)	32	62
20	t4	28/158 (18%)	28 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	t5	28/158 (18%)	28 (100%)	0	100	100
20	t6	26/158 (16%)	26 (100%)	0	100	100
21	G	264/328 (80%)	256 (97%)	8 (3%)	36	64
22	H	86/228 (38%)	84 (98%)	2 (2%)	45	70
23	I	194/232 (84%)	185 (95%)	9 (5%)	23	52
24	J	112/150 (75%)	104 (93%)	8 (7%)	12	39
25	K	155/156 (99%)	152 (98%)	3 (2%)	52	75
26	L	98/124 (79%)	91 (93%)	7 (7%)	12	39
27	M	245/249 (98%)	235 (96%)	10 (4%)	26	57
28	N	152/211 (72%)	149 (98%)	3 (2%)	50	74
29	O	133/150 (89%)	124 (93%)	9 (7%)	13	40
30	P	123/154 (80%)	119 (97%)	4 (3%)	33	62
31	Q	199/256 (78%)	193 (97%)	6 (3%)	36	64
32	R	118/126 (94%)	111 (94%)	7 (6%)	16	44
33	S	141/180 (78%)	139 (99%)	2 (1%)	62	81
34	T	146/182 (80%)	145 (99%)	1 (1%)	81	90
35	U	124/135 (92%)	120 (97%)	4 (3%)	34	63
36	V	180/191 (94%)	174 (97%)	6 (3%)	33	62
37	W	83/119 (70%)	80 (96%)	3 (4%)	30	60
38	X	219/229 (96%)	214 (98%)	5 (2%)	45	70
39	Y	159/223 (71%)	154 (97%)	5 (3%)	35	63
40	Z	111/147 (76%)	107 (96%)	4 (4%)	30	60
41	b	130/186 (70%)	120 (92%)	10 (8%)	10	35
42	c	241/288 (84%)	233 (97%)	8 (3%)	33	62
43	d	207/274 (76%)	197 (95%)	10 (5%)	21	51
44	e	188/236 (80%)	182 (97%)	6 (3%)	34	63
45	f	108/188 (57%)	106 (98%)	2 (2%)	52	75
46	g	119/148 (80%)	116 (98%)	3 (2%)	42	69
47	h	101/148 (68%)	99 (98%)	2 (2%)	50	74
48	i	86/110 (78%)	81 (94%)	5 (6%)	17	45
49	j	68/97 (70%)	65 (96%)	3 (4%)	24	54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	k	71/90 (79%)	68 (96%)	3 (4%)	25	56
51	l	43/116 (37%)	41 (95%)	2 (5%)	22	52
52	m	31/113 (27%)	29 (94%)	2 (6%)	14	41
53	n	157/209 (75%)	152 (97%)	5 (3%)	34	63
54	o	78/87 (90%)	75 (96%)	3 (4%)	28	59
55	p	117/181 (65%)	116 (99%)	1 (1%)	75	88
56	q	115/178 (65%)	112 (97%)	3 (3%)	41	68
57	r	141/169 (83%)	135 (96%)	6 (4%)	25	55
58	s	326/381 (86%)	319 (98%)	7 (2%)	48	72
59	t	317/371 (85%)	316 (100%)	1 (0%)	91	95
60	u	123/200 (62%)	120 (98%)	3 (2%)	44	70
61	v	59/60 (98%)	54 (92%)	5 (8%)	8	32
62	w	81/136 (60%)	75 (93%)	6 (7%)	11	36
All	All	9055/12593 (72%)	8781 (97%)	274 (3%)	37	64

All (274) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	153	THR
2	a	60	CYS
3	1	43	LEU
5	3	103	LYS
5	3	137	THR
5	3	156	LYS
5	3	157	LEU
6	4	76	CYS
6	4	81	LEU
7	5	46	LEU
7	5	55	LEU
7	5	128	LEU
7	5	132	LEU
7	5	280	GLN
7	5	300	ARG
7	5	315	LEU
7	5	316	PHE
7	5	365	ASP
7	5	420	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	6	41	ASP
8	6	52	ARG
8	6	184	LEU
8	6	291	TYR
8	6	371	ASP
8	6	379	ILE
9	7	50	LYS
9	7	97	GLU
9	7	143	TRP
9	7	156	ARG
9	7	196	LYS
9	7	204	LYS
9	7	234	LYS
9	7	272	THR
9	7	321	ARG
10	8	97	LYS
10	8	113	ARG
10	8	117	LEU
10	8	125	LYS
10	8	156	LYS
10	8	163	LYS
11	9	55	GLU
11	9	69	LYS
13	A1	163	LEU
13	A1	189	LEU
13	A1	226	ARG
13	A1	258	CYS
13	A1	275	ARG
15	A2	131	PHE
15	A2	133	LEU
15	A2	134	LEU
15	A2	191	GLN
15	A2	304	ARG
15	A2	319	LEU
16	C	60	ILE
16	C	120	LYS
16	C	216	THR
16	C	317	VAL
16	C	318	MET
17	D	187	LEU
17	D	281	TRP
18	E	152	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	E	245	THR
18	E	303	LYS
18	E	346	THR
19	F	70	ARG
19	F	130	GLN
19	F	131	LYS
19	F	263	LEU
19	F	291	SER
21	G	63	LEU
21	G	68	LEU
21	G	123	LYS
21	G	168	ARG
21	G	257	THR
21	G	284	ARG
21	G	298	ARG
21	G	300	ILE
22	H	138	LYS
22	H	145	LEU
23	I	50	VAL
23	I	57	LYS
23	I	78	LEU
23	I	99	CYS
23	I	101	ASN
23	I	122	LEU
23	I	152	MET
23	I	169	ARG
23	I	197	LEU
24	J	24	VAL
24	J	30	MET
24	J	92	LYS
24	J	102	ARG
24	J	103	GLN
24	J	106	LYS
24	J	111	LEU
24	J	149	ARG
25	K	2	SER
25	K	91	THR
25	K	178	LEU
26	L	35	MET
26	L	37	ARG
26	L	77	ILE
26	L	95	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
26	L	99	ARG
26	L	101	ASP
26	L	136	LYS
27	M	43	ARG
27	M	44	ARG
27	M	98	LEU
27	M	134	ARG
27	M	146	ASP
27	M	222	TYR
27	M	239	LYS
27	M	269	LEU
27	M	277	MET
27	M	292	LYS
28	N	63	ARG
28	N	208	ASN
28	N	238	LYS
29	O	14	VAL
29	O	20	LEU
29	O	26	ILE
29	O	28	LEU
29	O	123	ILE
29	O	144	LEU
29	O	149	LEU
29	O	155	ASP
29	O	156	LEU
30	P	80	ARG
30	P	117	TYR
30	P	120	ARG
30	P	137	LEU
31	Q	139	GLN
31	Q	214	LYS
31	Q	215	VAL
31	Q	227	LYS
31	Q	247	LEU
31	Q	271	ARG
32	R	11	ARG
32	R	32	ARG
32	R	40	ARG
32	R	82	LYS
32	R	87	ILE
32	R	104	ASP
32	R	119	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
33	S	144	LEU
33	S	182	LYS
34	T	84	LYS
35	U	11	ARG
35	U	12	LEU
35	U	27	GLN
35	U	126	LEU
36	V	40	ARG
36	V	56	LEU
36	V	118	ARG
36	V	186	THR
36	V	202	MET
36	V	213	VAL
37	W	49	ARG
37	W	88	CYS
37	W	125	VAL
38	X	59	ARG
38	X	87	LEU
38	X	96	LYS
38	X	99	LYS
38	X	161	LEU
39	Y	121	ARG
39	Y	198	ARG
39	Y	202	LEU
39	Y	226	LEU
39	Y	237	LYS
40	Z	41	ILE
40	Z	73	LYS
40	Z	119	ILE
40	Z	141	SER
41	b	4	ARG
41	b	36	ASP
41	b	80	LEU
41	b	86	GLU
41	b	100	LEU
41	b	115	ILE
41	b	119	PHE
41	b	122	ASP
41	b	123	ASN
41	b	141	ARG
42	c	68	TYR
42	c	86	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
42	c	173	LEU
42	c	193	GLN
42	c	246	LYS
42	c	279	LYS
42	c	280	LEU
42	c	287	GLU
43	d	36	ARG
43	d	74	ARG
43	d	111	ARG
43	d	112	MET
43	d	163	LEU
43	d	194	VAL
43	d	203	MET
43	d	238	VAL
43	d	266	VAL
43	d	287	LEU
44	e	126	GLN
44	e	127	LYS
44	e	133	LEU
44	e	227	LEU
44	e	239	LEU
44	e	243	PHE
45	f	171	LEU
45	f	212	LYS
46	g	43	ASP
46	g	143	VAL
46	g	147	LEU
47	h	56	ARG
47	h	75	LYS
48	i	36	LEU
48	i	37	THR
48	i	80	LEU
48	i	105	ASP
48	i	107	LEU
49	j	67	LYS
49	j	93	LEU
49	j	103	ARG
50	k	34	LEU
50	k	41	LYS
50	k	56	ARG
51	l	110	LEU
51	l	128	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
52	m	40	LEU
52	m	51	LEU
53	n	55	ARG
53	n	140	LEU
53	n	147	ARG
53	n	155	MET
53	n	224	ARG
54	o	46	HIS
54	o	91	GLN
54	o	98	THR
55	p	179	ARG
56	q	96	LEU
56	q	113	LYS
56	q	150	LYS
57	r	52	ARG
57	r	58	LYS
57	r	70	CYS
57	r	108	CYS
57	r	159	VAL
57	r	164	LYS
58	s	52	THR
58	s	66	TRP
58	s	150	LEU
58	s	200	LEU
58	s	230	ARG
58	s	279	GLU
58	s	379	LEU
59	t	331	ARG
20	t1	-3	LYS
20	t1	3	ILE
20	t3	27	LYS
60	u	92	PHE
60	u	156	HIS
60	u	196	LEU
61	v	16	LEU
61	v	29	ASP
61	v	45	LEU
61	v	47	ASP
61	v	61	PHE
62	w	74	LEU
62	w	75	THR
62	w	88	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
62	w	89	LEU
62	w	132	ASP
62	w	137	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
4	2	77	GLN
5	3	154	GLN
7	5	96	HIS
7	5	108	HIS
7	5	165	GLN
7	5	385	HIS
8	6	66	GLN
8	6	354	GLN
9	7	298	GLN
10	8	143	GLN
13	A1	317	ASN
13	A1	367	ASN
15	A2	191	GLN
15	A2	255	GLN
16	C	295	GLN
16	C	297	ASN
19	F	103	GLN
23	I	101	ASN
23	I	225	GLN
25	K	26	GLN
25	K	126	HIS
25	K	147	GLN
27	M	26	ASN
27	M	30	ASN
27	M	92	GLN
27	M	264	GLN
28	N	210	GLN
29	O	69	ASN
30	P	147	GLN
32	R	79	HIS
32	R	94	GLN
33	S	84	ASN
34	T	132	HIS
35	U	103	GLN
35	U	138	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
38	X	15	GLN
39	Y	99	HIS
39	Y	183	GLN
41	b	120	HIS
42	c	122	ASN
42	c	172	ASN
42	c	193	GLN
43	d	149	HIS
44	e	175	GLN
45	f	111	HIS
45	f	153	HIS
48	i	59	ASN
49	j	63	GLN
53	n	214	ASN
54	o	33	GLN
54	o	94	HIS
58	s	87	GLN
58	s	101	ASN
58	s	239	ASN
60	u	156	HIS
62	w	103	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	A	1427/1559 (91%)	355 (24%)	54 (3%)
14	B	56/69 (81%)	19 (33%)	2 (3%)
All	All	1483/1628 (91%)	374 (25%)	56 (3%)

All (374) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	A	1678	C
12	A	1679	U
12	A	1680	A
12	A	1681	G
12	A	1689	C
12	A	1693	C
12	A	1694	U
12	A	1699	C
12	A	1700	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	A	1704	U
12	A	1707	C
12	A	1708	A
12	A	1714	C
12	A	1715	C
12	A	1724	A
12	A	1728	U
12	A	1733	C
12	A	1734	C
12	A	1735	A
12	A	1736	A
12	A	1743	U
12	A	1748	G
12	A	1750	G
12	A	1751	A
12	A	1769	C
12	A	1770	G
12	A	1780	U
12	A	1794	A
12	A	1795	A
12	A	1798	A
12	A	1804	A
12	A	1805	A
12	A	1812	C
12	A	1817	C
12	A	1824	U
12	A	1827	C
12	A	1828	A
12	A	1829	A
12	A	1832	A
12	A	1836	A
12	A	1844	A
12	A	1849	C
12	A	1852	C
12	A	1853	A
12	A	1854	U
12	A	1855	A
12	A	1856	A
12	A	1867	A
12	A	1869	A
12	A	1872	U
12	A	1878	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	A	1882	A
12	A	1883	G
12	A	1887	A
12	A	1892	A
12	A	1893	A
12	A	1901	C
12	A	1902	C
12	A	1903	C
12	A	1909	A
12	A	1918	G
12	A	1936	A
12	A	1937	A
12	A	1938	A
12	A	1940	A
12	A	1946	C
12	A	1974	A
12	A	1975	U
12	A	1985	G
12	A	1986	A
12	A	1994	A
12	A	1995	A
12	A	2000	C
12	A	2001	C
12	A	2002	G
12	A	2015	G
12	A	2016	C
12	A	2021	U
12	A	2022	G
12	A	2029	A
12	A	2030	U
12	A	2031	A
12	A	2036	C
12	A	2037	U
12	A	2039	A
12	A	2044	A
12	A	2055	U
12	A	2060	A
12	A	2065	A
12	A	2066	C
12	A	2070	C
12	A	2071	U
12	A	2074	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	A	2079	C
12	A	2085	A
12	A	2092	C
12	A	2097	A
12	A	2098	G
12	A	2105	G
12	A	2107	G
12	A	2108	G
12	A	2111	C
12	A	2112	A
12	A	2113	G
12	A	2114	C
12	A	2126	U
12	A	2131	A
12	A	2135	A
12	A	2136	C
12	A	2142	A
12	A	2147	G
12	A	2154	A
12	A	2158	U
12	A	2159	U
12	A	2160	A
12	A	2167	A
12	A	2171	U
12	A	2172	A
12	A	2173	G
12	A	2174	G
12	A	2175	C
12	A	2178	A
12	A	2179	A
12	A	2181	A
12	A	2182	G
12	A	2183	C
12	A	2187	C
12	A	2194	U
12	A	2195	A
12	A	2196	A
12	A	2197	G
12	A	2198	A
12	A	2199	A
12	A	2200	A
12	A	2210	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	A	2211	U
12	A	2228	A
12	A	2229	A
12	A	2230	A
12	A	2233	U
12	A	2237	A
12	A	2241	A
12	A	2243	A
12	A	2245	A
12	A	2246	A
12	A	2250	A
12	A	2251	A
12	A	2257	C
12	A	2262	C
12	A	2263	C
12	A	2264	A
12	A	2284	C
12	A	2285	U
12	A	2297	A
12	A	2300	G
12	A	2321	A
12	A	2322	C
12	A	2324	U
12	A	2332	C
12	A	2345	G
12	A	2348	A
12	A	2350	A
12	A	2351	U
12	A	2358	A
12	A	2359	C
12	A	2360	U
12	A	2361	G
12	A	2362	A
12	A	2363	A
12	A	2374	A
12	A	2381	A
12	A	2390	A
12	A	2394	A
12	A	2401	A
12	A	2404	U
12	A	2406	A
12	A	2407	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	A	2414	C
12	A	2415	C
12	A	2418	A
12	A	2434	A
12	A	2446	A
12	A	2451	A
12	A	2452	A
12	A	2457	A
12	A	2458	A
12	A	2478	G
12	A	2483	U
12	A	2485	U
12	A	2488	C
12	A	2493	C
12	A	2494	C
12	A	2500	A
12	A	2502	C
12	A	2511	C
12	A	2520	C
12	A	2521	A
12	A	2527	A
12	A	2530	A
12	A	2531	U
12	A	2536	G
12	A	2539	A
12	A	2540	C
12	A	2544	C
12	A	2547	C
12	A	2548	C
12	A	2549	C
12	A	2550	A
12	A	2554	A
12	A	2603	C
12	A	2611	C
12	A	2613	U
12	A	2617	A
12	A	2618	U
12	A	2619	A
12	A	2620	G
12	A	2621	G
12	A	2622	G
12	A	2623	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
12	A	2626	U
12	A	2627	G
12	A	2628	U
12	A	2629	A
12	A	2630	U
12	A	2633	A
12	A	2634	U
12	A	2645	G
12	A	2654	U
12	A	2655	G
12	A	2656	U
12	A	2660	U
12	A	2670	C
12	A	2683	C
12	A	2684	C
12	A	2686	G
12	A	2693	A
12	A	2694	A
12	A	2695	G
12	A	2696	A
12	A	2698	G
12	A	2699	C
12	A	2706	A
12	A	2709	A
12	A	2719	G
12	A	2722	A
12	A	2723	A
12	A	2724	G
12	A	2725	A
12	A	2732	G
12	A	2739	U
12	A	2740	A
12	A	2743	U
12	A	2756	C
12	A	2810	G
12	A	2815	G
12	A	2816	G
12	A	2819	G
12	A	2828	G
12	A	2831	G
12	A	2832	A
12	A	2833	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	A	2840	C
12	A	2843	C
12	A	2844	G
12	A	2847	C
12	A	2854	U
12	A	2864	U
12	A	2865	C
12	A	2880	A
12	A	2906	C
12	A	2912	C
12	A	2913	A
12	A	2917	G
12	A	2918	A
12	A	2919	A
12	A	2922	A
12	A	2926	A
12	A	2928	C
12	A	2932	G
12	A	2934	G
12	A	2935	A
12	A	2936	U
12	A	2937	A
12	A	2946	A
12	A	2956	A
12	A	2963	A
12	A	2978	U
12	A	2984	A
12	A	2986	C
12	A	2987	U
12	A	2988	C
12	A	2989	G
12	A	2990	A
12	A	2991	U
12	A	2992	G
12	A	3005	A
12	A	3007	C
12	A	3016	G
12	A	3018	A
12	A	3021	C
12	A	3022	G
12	A	3041	U
12	A	3042	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	A	3051	A
12	A	3053	A
12	A	3054	G
12	A	3060	C
12	A	3067	U
12	A	3069	A
12	A	3070	G
12	A	3072	U
12	A	3086	U
12	A	3089	A
12	A	3090	G
12	A	3097	U
12	A	3098	U
12	A	3100	U
12	A	3102	U
12	A	3108	U
12	A	3109	U
12	A	3111	A
12	A	3112	A
12	A	3113	A
12	A	3123	G
12	A	3141	A
12	A	3150	U
12	A	3157	C
12	A	3158	A
12	A	3162	C
12	A	3168	C
12	A	3169	C
12	A	3170	C
12	A	3171	C
12	A	3172	C
12	A	3173	G
12	A	3177	A
12	A	3180	A
12	A	3184	C
12	A	3189	C
12	A	3190	A
12	A	3196	G
12	A	3197	U
12	A	3198	A
12	A	3199	U
12	A	3201	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	A	3202	U
12	A	3207	A
12	A	3208	C
12	A	3209	A
12	A	3211	C
12	A	3212	C
12	A	3217	A
12	A	3218	A
12	A	3220	A
12	A	3228	U
14	B	1604	G
14	B	1608	G
14	B	1609	U
14	B	1610	A
14	B	1611	G
14	B	1614	U
14	B	1615	A
14	B	1617	C
14	B	1618	A
14	B	1620	A
14	B	1621	A
14	B	1622	A
14	B	1628	C
14	B	1632	U
14	B	1633	U
14	B	1644	G
14	B	1645	A
14	B	1646	U
14	B	1670	A

All (56) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	A	1727	A
12	A	1749	C
12	A	1772	A
12	A	1811	A
12	A	1823	A
12	A	1824	U
12	A	1853	A
12	A	1854	U
12	A	1855	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	A	1871	A
12	A	1936	A
12	A	1956	U
12	A	1974	A
12	A	1994	A
12	A	2001	C
12	A	2015	G
12	A	2021	U
12	A	2030	U
12	A	2065	A
12	A	2097	A
12	A	2135	A
12	A	2158	U
12	A	2182	G
12	A	2186	C
12	A	2245	A
12	A	2291	A
12	A	2347	C
12	A	2361	G
12	A	2380	C
12	A	2417	C
12	A	2457	A
12	A	2527	A
12	A	2530	A
12	A	2543	C
12	A	2619	A
12	A	2620	G
12	A	2628	U
12	A	2629	A
12	A	2630	U
12	A	2653	C
12	A	2723	A
12	A	2724	G
12	A	2739	U
12	A	2818	C
12	A	2832	A
12	A	2846	G
12	A	2905	A
12	A	2926	A
12	A	2935	A
12	A	2991	U
12	A	3004	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	A	3041	U
12	A	3068	G
12	A	3206	C
14	B	1607	U
14	B	1614	U

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

1 non-standard protein/DNA/RNA residue is 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
12	OMG	A	3040	12	18,26,27	1.01	1 (5%)	19,38,41	1.09	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
12	OMG	A	3040	12	-	0/5/27/28	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	3040	OMG	C5-C4	2.18	1.48	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	3040	OMG	C5-C6-N1	2.17	117.78	113.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 101 ligands modelled in this entry, 95 are monoatomic - leaving 6 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	$\# Z  > 2$
69	SAH	n	301	-	24,28,28	0.69	1 (4%)	25,40,40	1.20	4 (16%)
67	GDP	C	401	-	24,30,30	0.95	1 (4%)	30,47,47	1.30	4 (13%)
68	GTP	G	502	65	26,34,34	0.93	2 (7%)	32,54,54	0.71	0
67	GDP	t	501	65	24,30,30	0.94	0	30,47,47	1.27	4 (13%)
70	PNS	w	201	62	13,20,21	0.30	0	18,26,29	0.73	0
66	SAM	A1	401	-	24,29,29	0.69	1 (4%)	23,42,42	1.20	4 (17%)

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
69	SAH	n	301	-	-	7/11/31/31	0/3/3/3
67	GDP	C	401	-	-	0/12/32/32	0/3/3/3
68	GTP	G	502	65	-	2/18/38/38	0/3/3/3
67	GDP	t	501	65	-	0/12/32/32	0/3/3/3
70	PNS	w	201	62	-	16/24/26/27	-
66	SAM	A1	401	-	-	3/12/33/33	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
68	G	502	GTP	C5-C6	-2.51	1.42	1.47
67	C	401	GDP	C6-N1	-2.36	1.34	1.37
69	n	301	SAH	OXT-C	-2.11	1.23	1.30
68	G	502	GTP	C8-N7	-2.07	1.31	1.35
66	A1	401	SAM	OXT-C	-2.04	1.23	1.30

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	C	401	GDP	PA-O3A-PB	-3.62	120.40	132.83
69	n	301	SAH	OXT-C-O	-3.61	115.90	124.09
67	C	401	GDP	C3'-C2'-C1'	3.15	105.73	100.98
66	A1	401	SAM	OXT-C-O	-3.07	117.12	124.09
69	n	301	SAH	OXT-C-CA	3.01	123.65	113.38
67	t	501	GDP	C3'-C2'-C1'	2.84	105.26	100.98
67	t	501	GDP	PA-O3A-PB	-2.62	123.83	132.83
66	A1	401	SAM	OXT-C-CA	2.54	122.02	113.38
67	t	501	GDP	C5-C6-N1	2.54	118.43	113.95
67	t	501	GDP	C8-N7-C5	2.33	107.42	102.99
67	C	401	GDP	C8-N7-C5	2.28	107.33	102.99
67	C	401	GDP	C5-C6-N1	2.25	117.93	113.95
69	n	301	SAH	C3'-C2'-C1'	2.17	104.25	100.98
66	A1	401	SAM	C3'-C2'-C1'	2.10	104.14	100.98
69	n	301	SAH	C5-C6-N6	2.01	123.40	120.35
66	A1	401	SAM	C5-C6-N6	2.00	123.40	120.35

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
66	A1	401	SAM	N-CA-CB-CG
66	A1	401	SAM	CA-CB-CG-SD
69	n	301	SAH	O-C-CA-N
70	w	201	PNS	O27-C28-C29-C31
70	w	201	PNS	O27-C28-C29-C32
70	w	201	PNS	C28-C29-C32-C34
70	w	201	PNS	O33-C32-C34-N36
70	w	201	PNS	C32-C34-N36-C37
70	w	201	PNS	O35-C34-N36-C37
70	w	201	PNS	N36-C37-C38-C39
69	n	301	SAH	OXT-C-CA-N

*Continued on next page...*



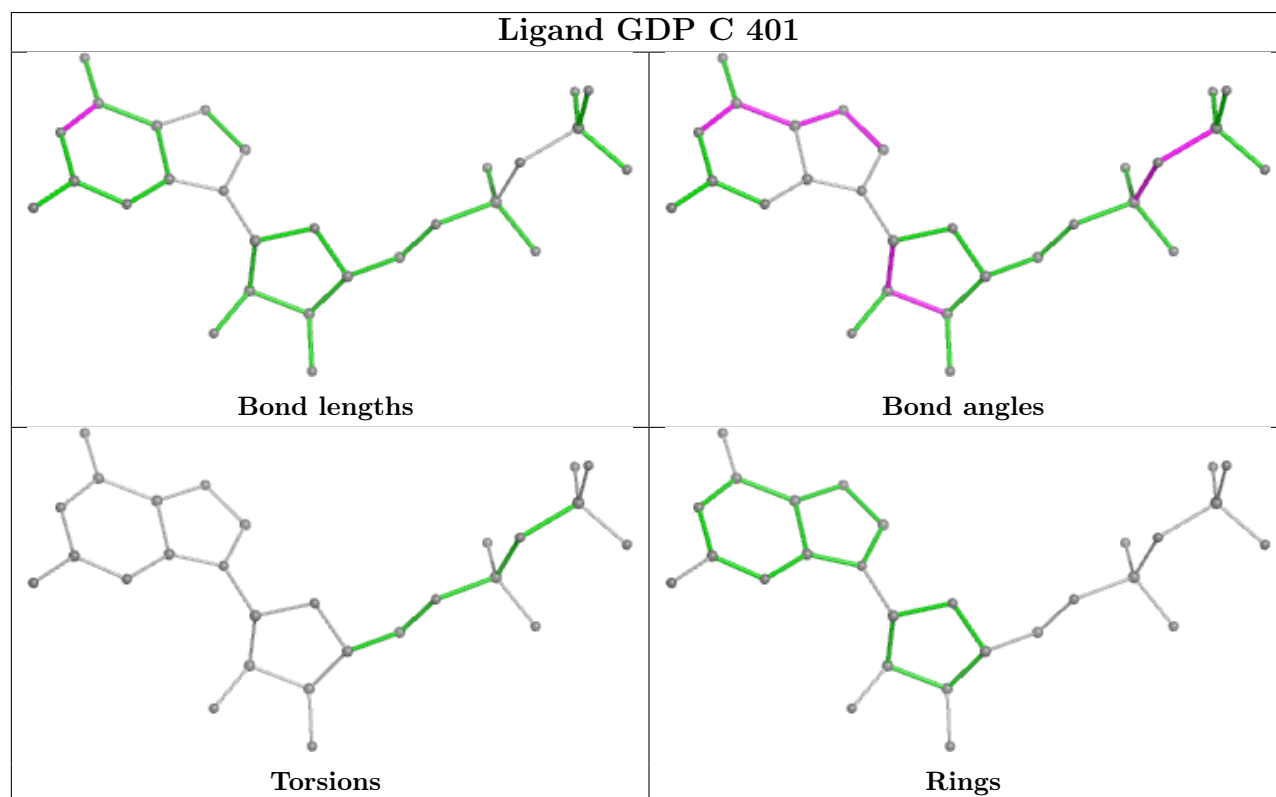
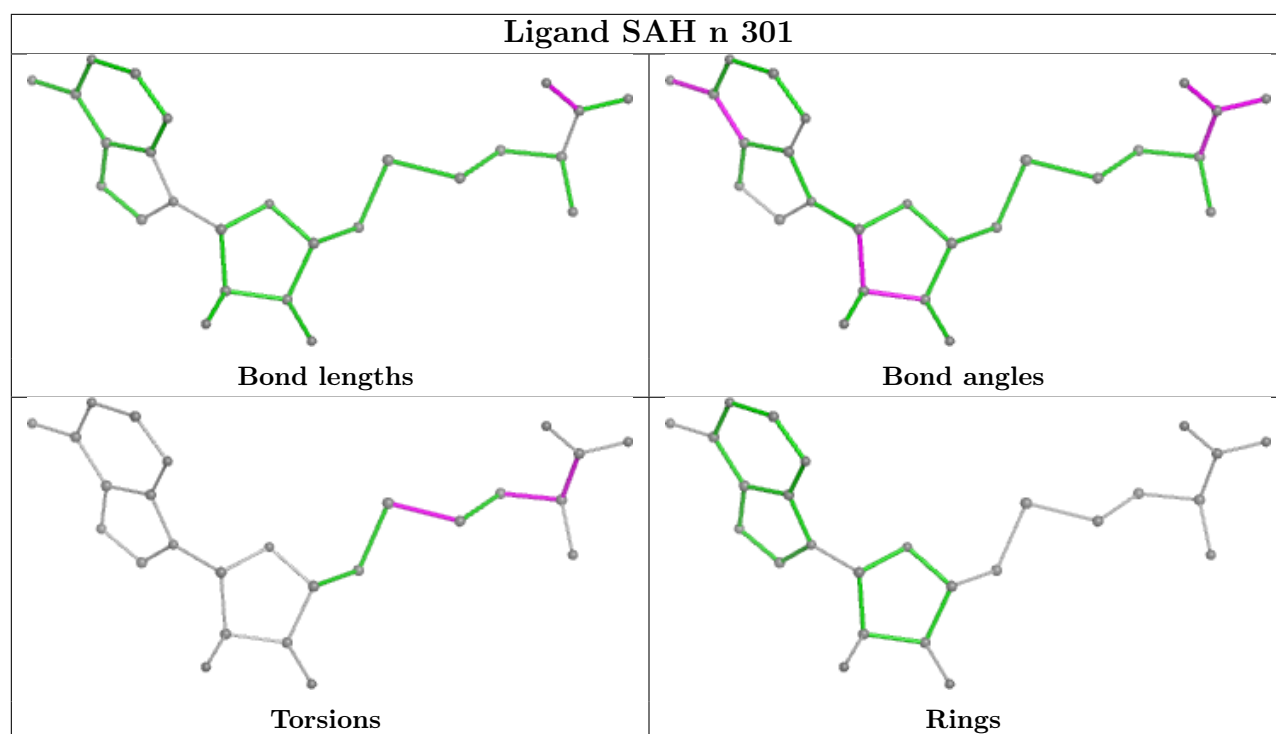
*Continued from previous page...*

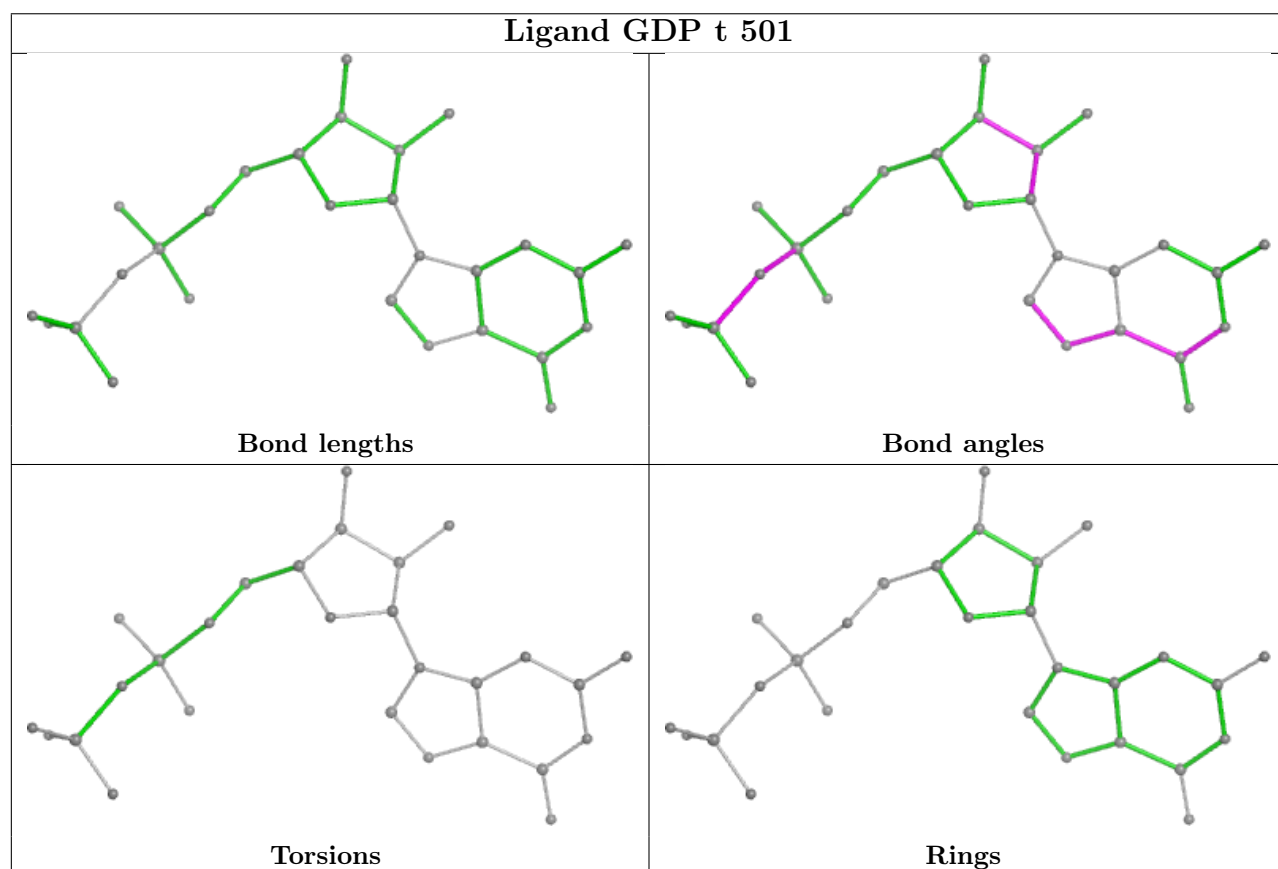
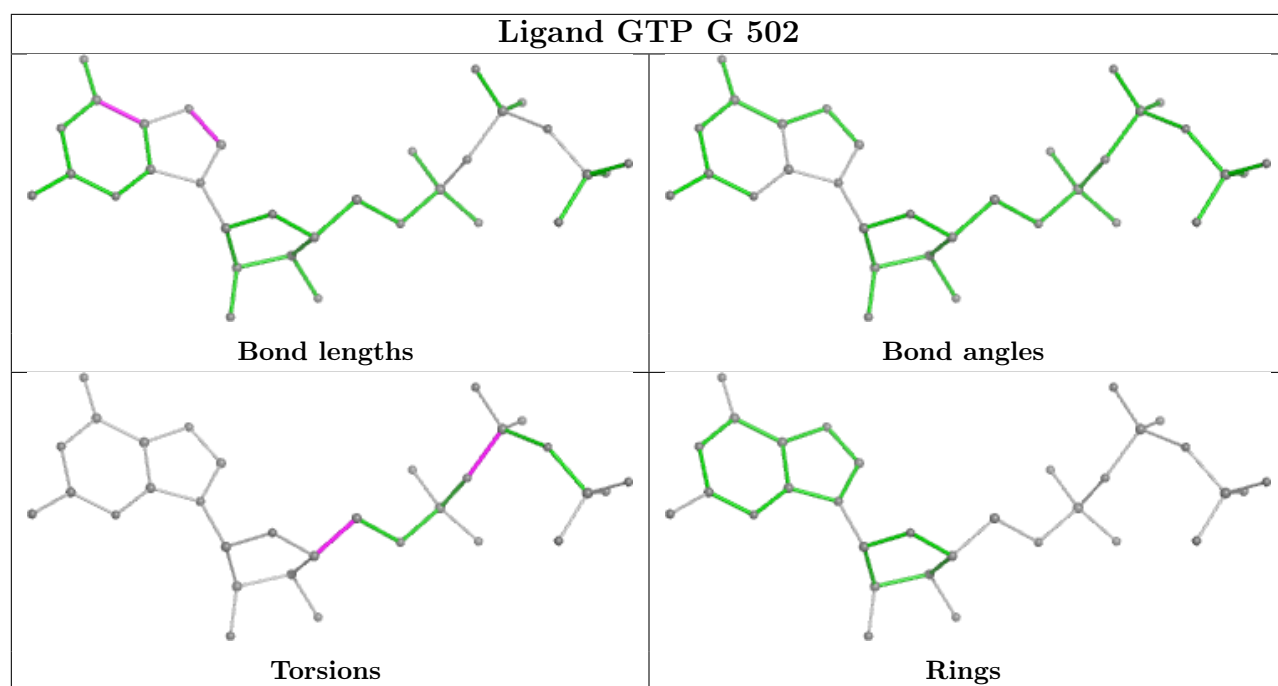
Mol	Chain	Res	Type	Atoms
70	w	201	PNS	O40-C39-N41-C42
70	w	201	PNS	O27-C28-C29-C30
70	w	201	PNS	C38-C39-N41-C42
66	A1	401	SAM	C-CA-CB-CG
69	n	301	SAH	C-CA-CB-CG
70	w	201	PNS	O33-C32-C34-O35
69	n	301	SAH	OXT-C-CA-CB
70	w	201	PNS	N41-C42-C43-S44
69	n	301	SAH	O-C-CA-CB
70	w	201	PNS	C30-C29-C32-C34
70	w	201	PNS	C31-C29-C32-C34
69	n	301	SAH	N-CA-CB-CG
69	n	301	SAH	CB-CG-SD-C5'
68	G	502	GTP	O4'-C4'-C5'-O5'
68	G	502	GTP	PA-O3A-PB-O2B
70	w	201	PNS	C37-C38-C39-O40
70	w	201	PNS	C37-C38-C39-N41

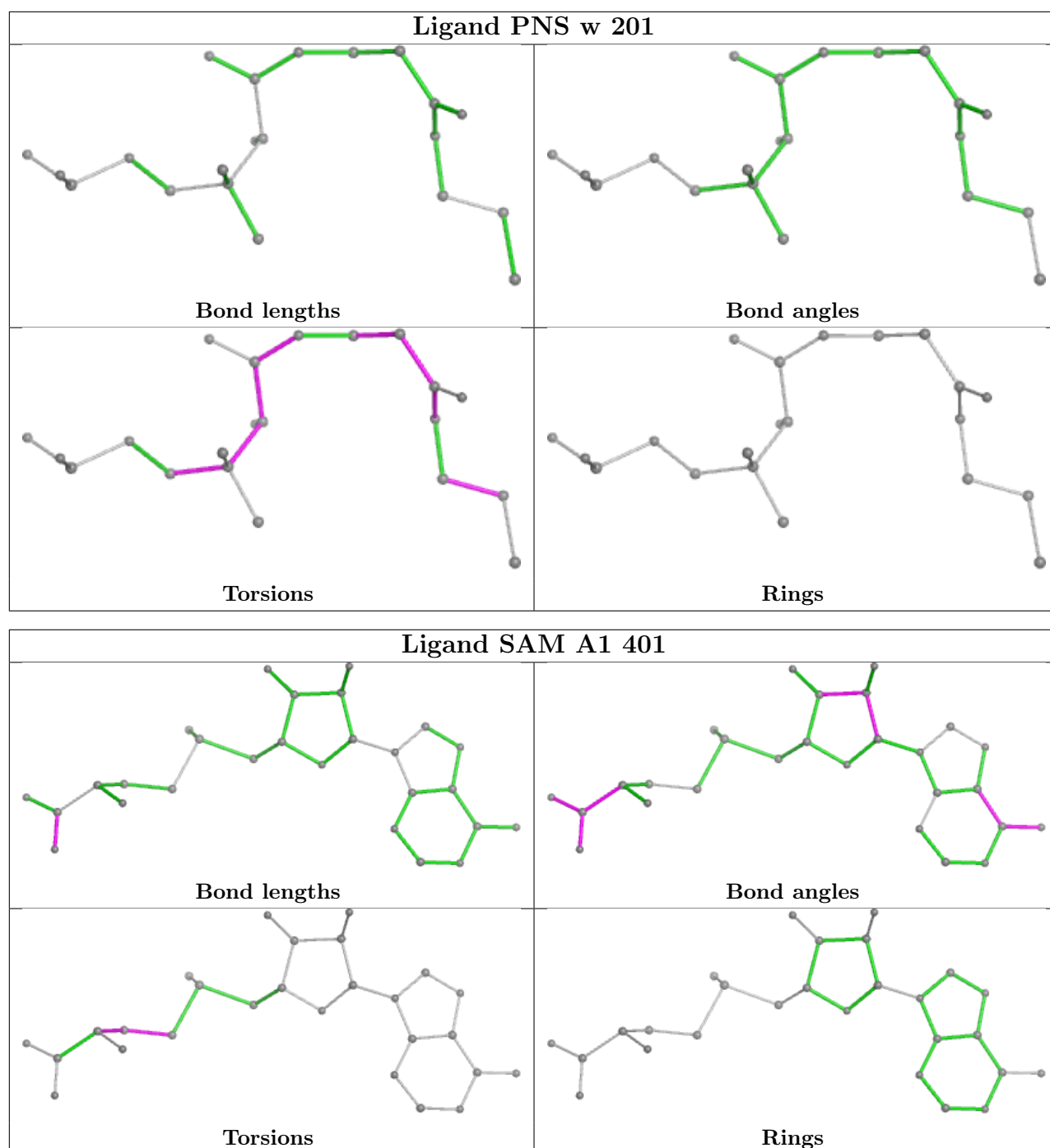
There are no ring outliers.

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 than 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](#)

There are no chain breaks in this entry.

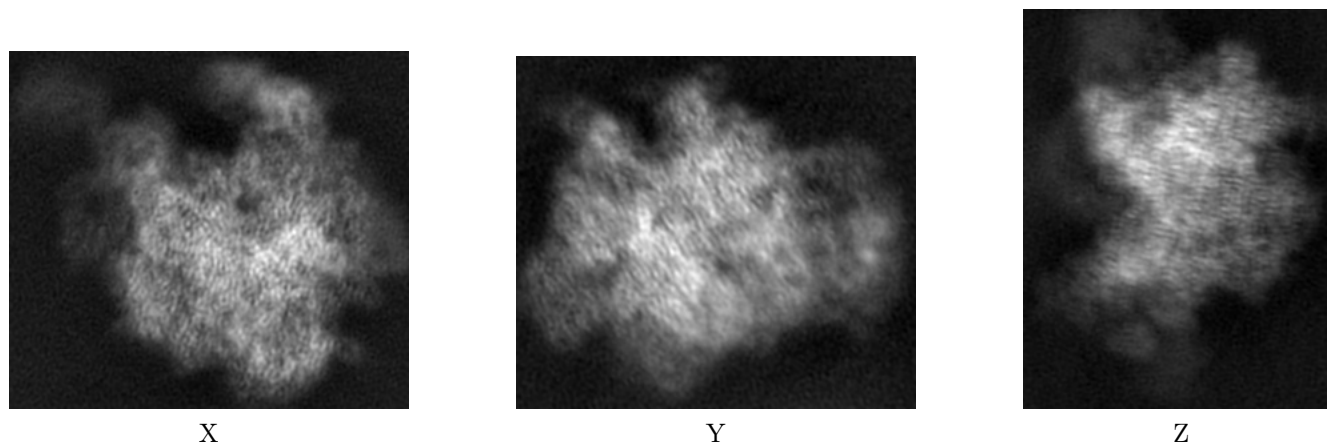
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12763. These allow visual inspection of the internal detail of the map and identification of artifacts.

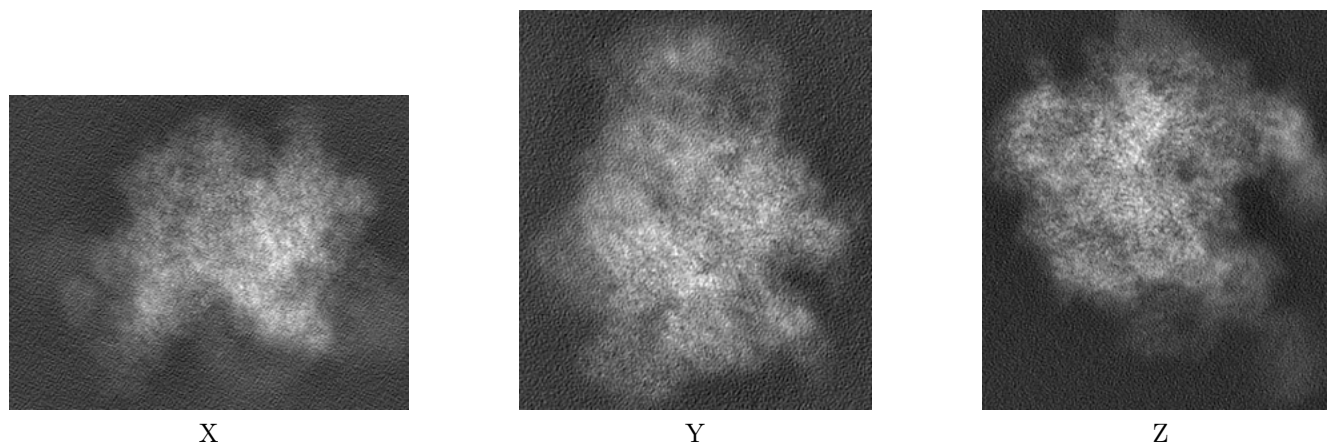
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



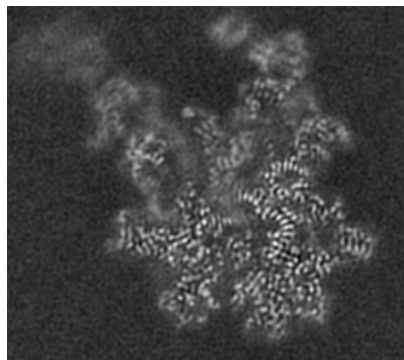
#### 6.1.2 Raw map



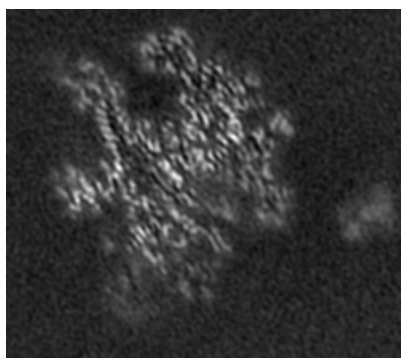
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

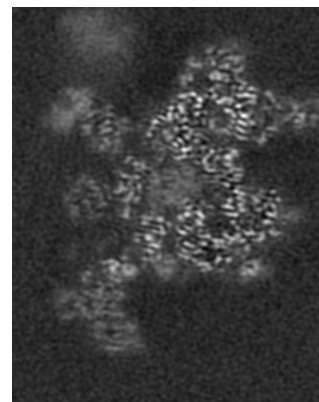
### 6.2.1 Primary map



X Index: 108

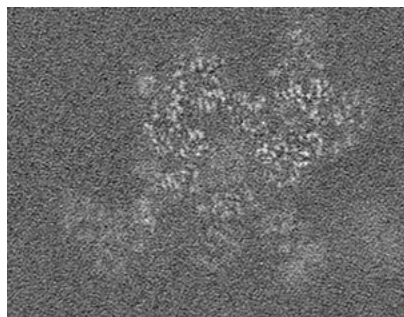


Y Index: 137

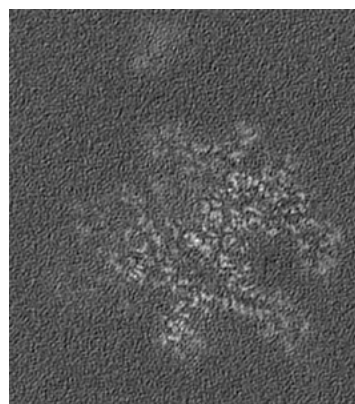


Z Index: 123

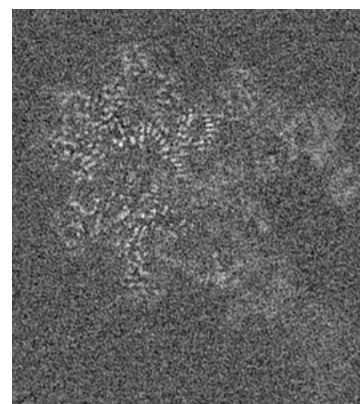
### 6.2.2 Raw map



X Index: 123



Y Index: 138



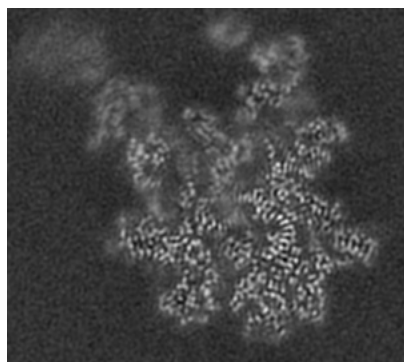
Z Index: 108

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

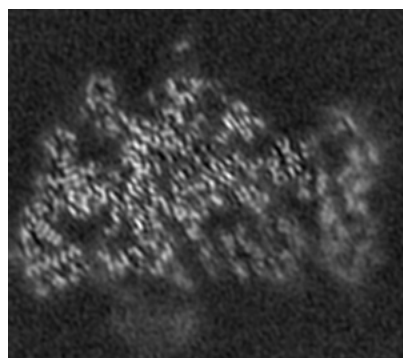


## 6.3 Largest variance slices [i](#)

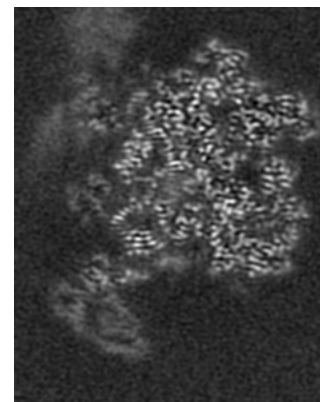
### 6.3.1 Primary map



X Index: 106

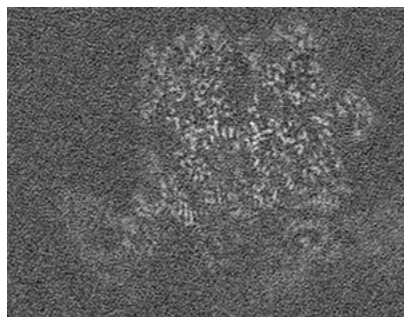


Y Index: 181

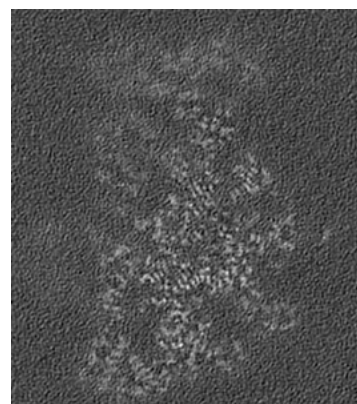


Z Index: 113

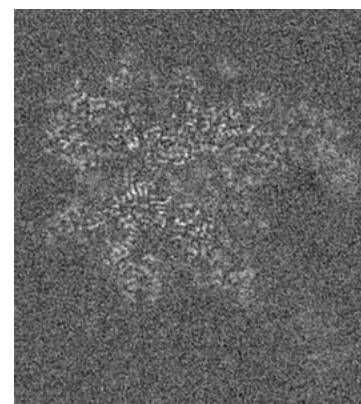
### 6.3.2 Raw map



X Index: 110



Y Index: 182

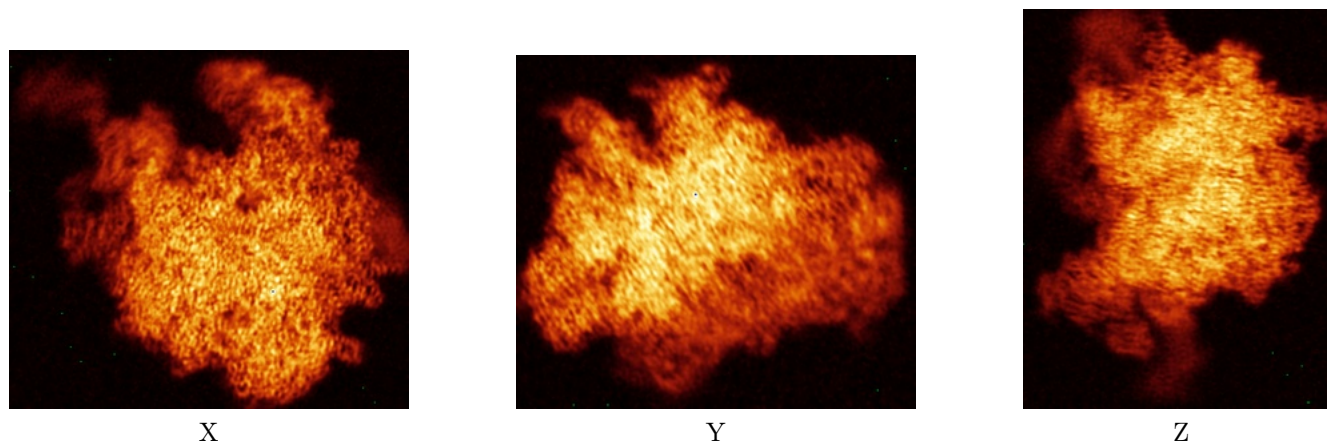


Z Index: 117

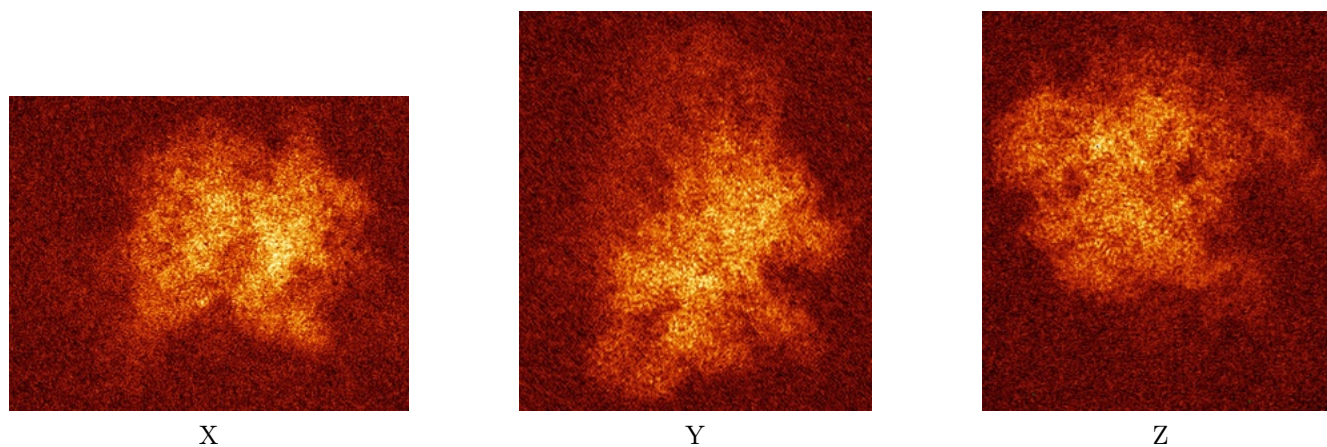
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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



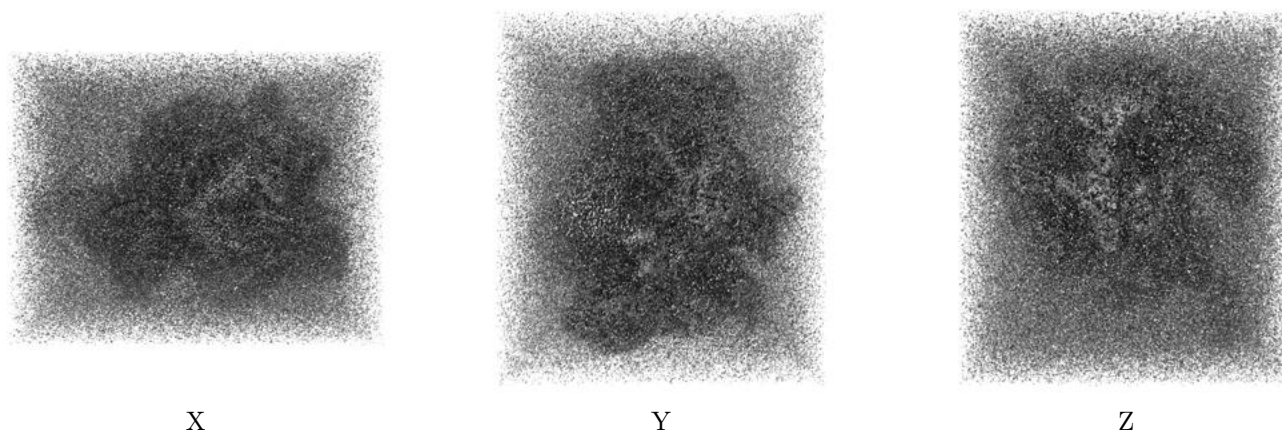
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

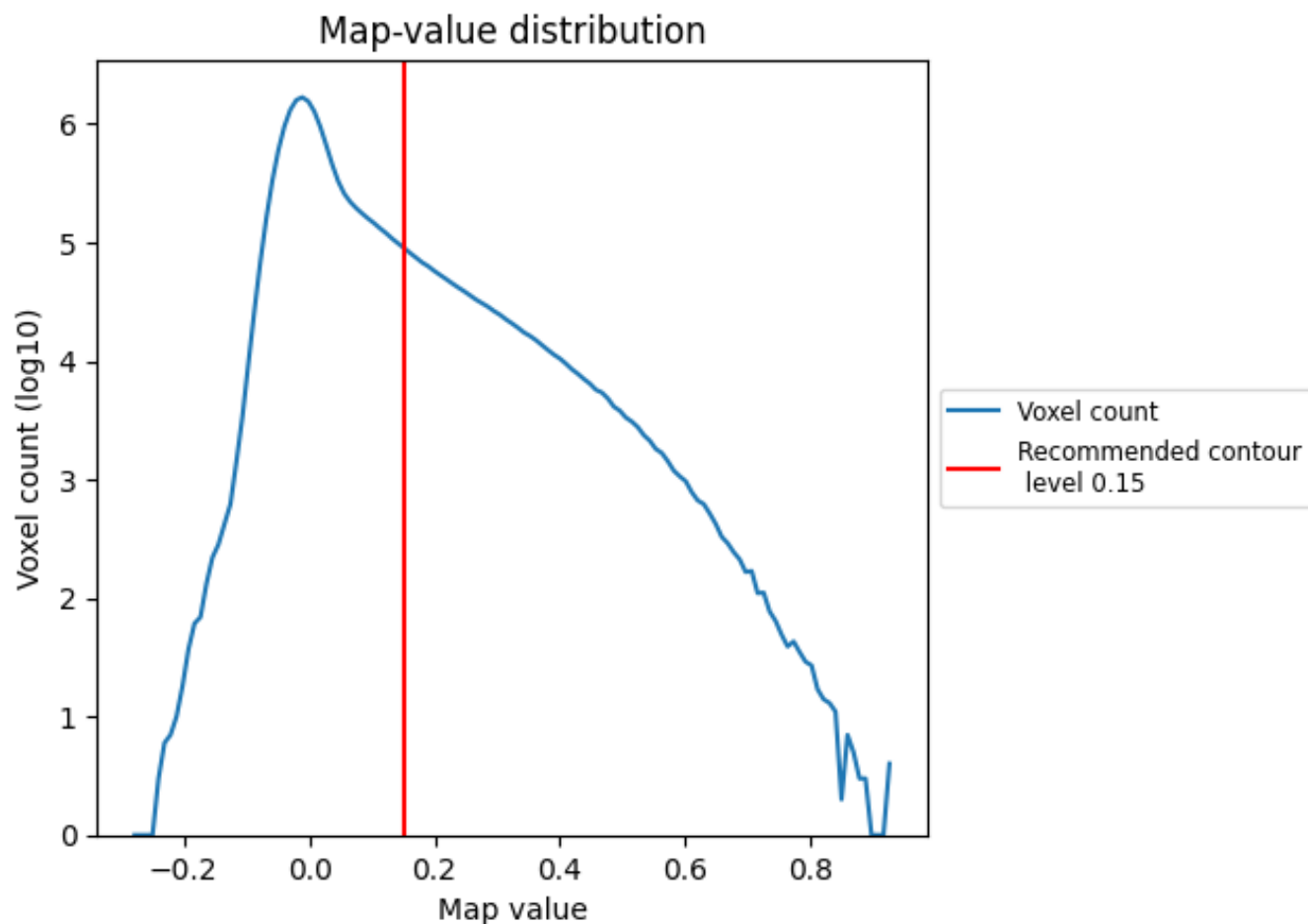
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

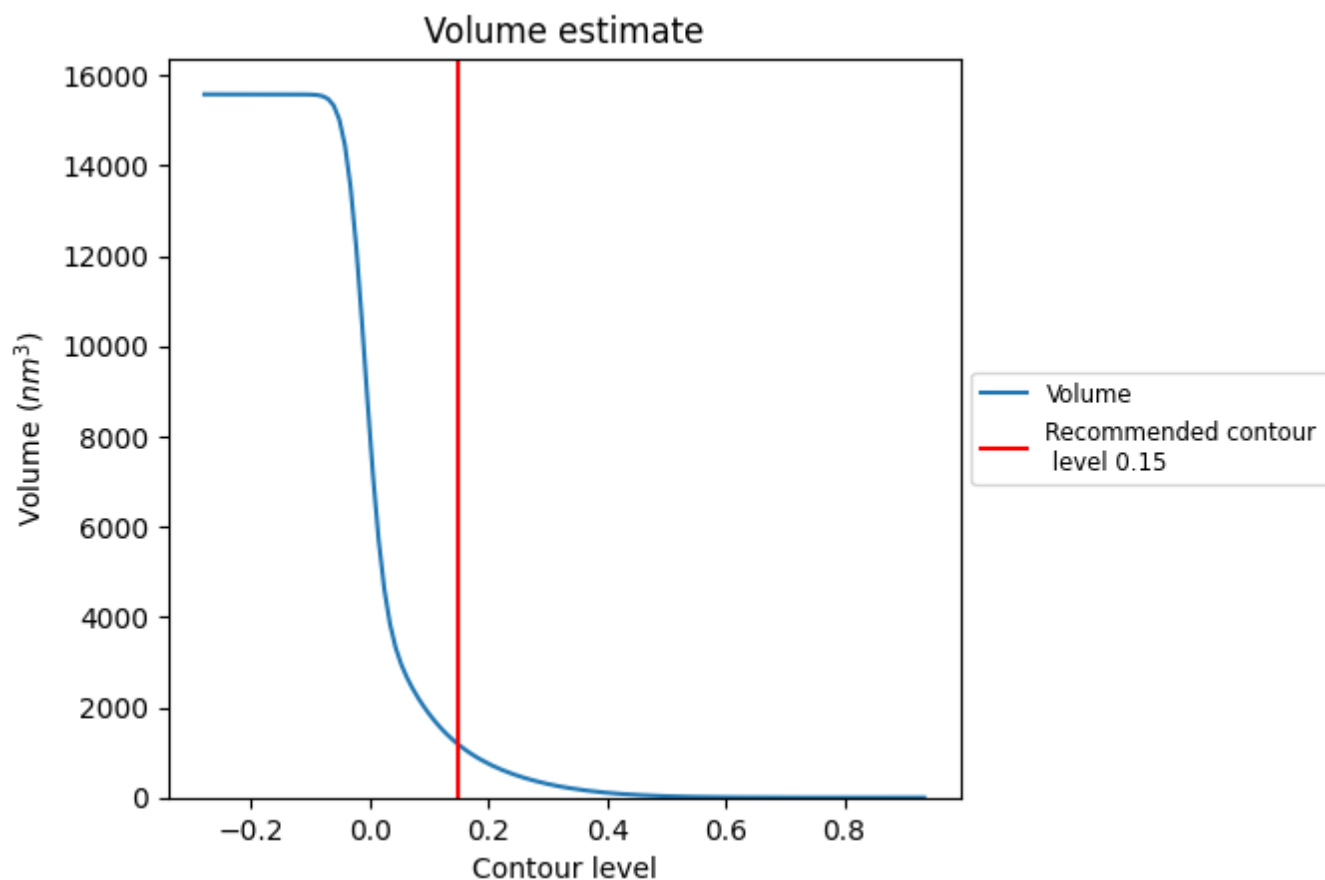
This section contains the results of statistical analysis of the map.

### 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 1174 nm<sup>3</sup>; this corresponds to an approximate mass of 1061 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

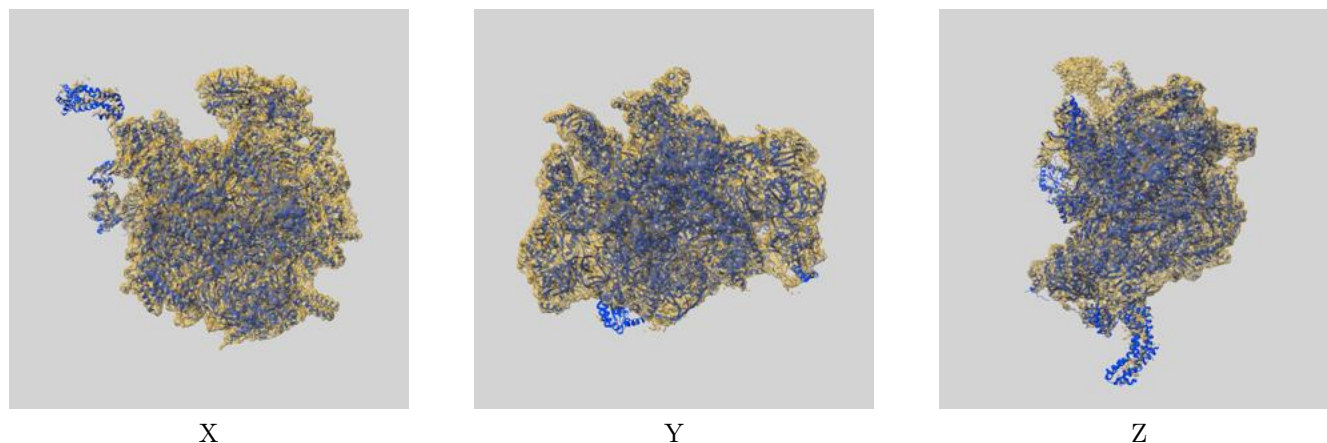
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

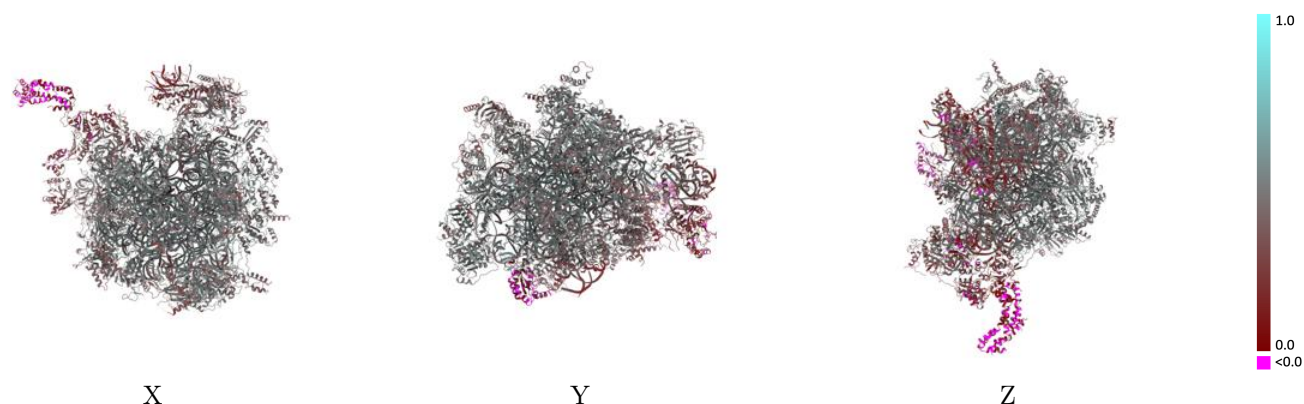
This section contains information regarding the fit between EMDB map EMD-12763 and PDB model 7O9K. Per-residue inclusion information can be found in section 3 on page 19.

### 9.1 Map-model overlay [i](#)



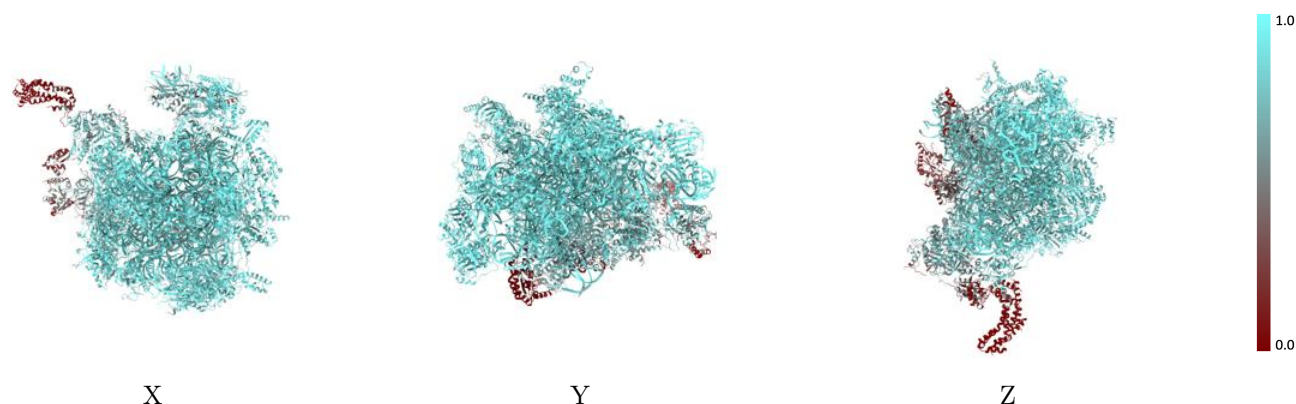
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



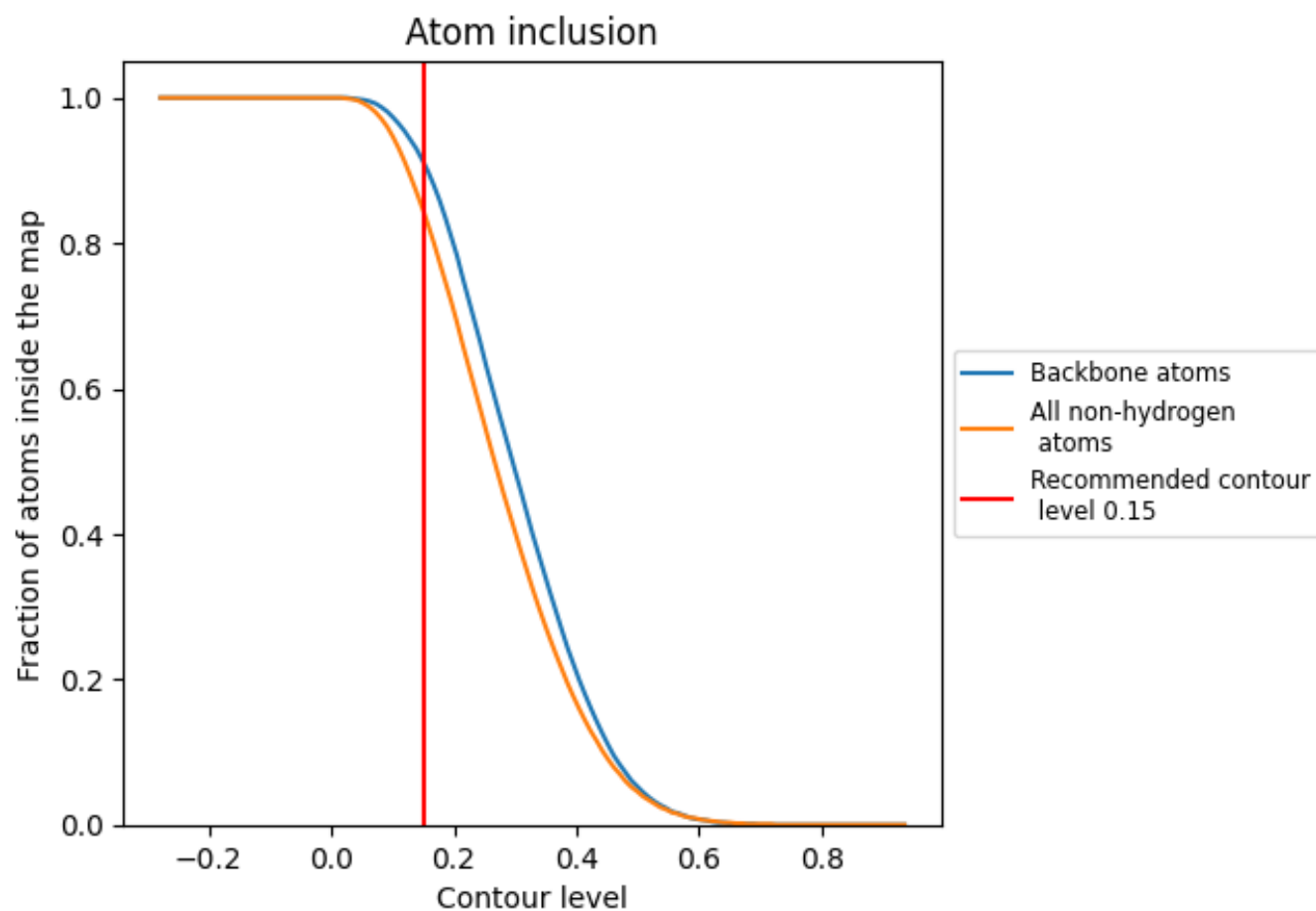
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.







































































Chain	Atom inclusion	Q-score
All	 0.8450	 0.4280
0	 0.9100	 0.4650
1	 0.8620	 0.4650
2	 0.9540	 0.5310
3	 0.9510	 0.5170
4	 0.8870	 0.4770
5	 0.9150	 0.4760
6	 0.9120	 0.4280
7	 0.8580	 0.4310
8	 0.6190	 0.2450
9	 0.9060	 0.4700
A	 0.9740	 0.4660
A1	 0.7460	 0.4070
A2	 0.7390	 0.4000
B	 0.9570	 0.3150
C	 0.1210	 0.1320
D	 0.9000	 0.4820
E	 0.9110	 0.4810
F	 0.9200	 0.4910
FF	 0.1140	 0.1840
G	 0.7600	 0.4150
H	 0.8470	 0.4470
I	 0.5970	 0.2430
J	 0.6770	 0.1950
K	 0.9350	 0.4990
L	 0.8630	 0.4870
M	 0.9310	 0.4880
N	 0.8120	 0.3930
O	 0.9360	 0.4960
P	 0.9200	 0.4410
Q	 0.8980	 0.4750
R	 0.9350	 0.5020
S	 0.8990	 0.4880
T	 0.9120	 0.5010
U	 0.9310	 0.4860



*Continued on next page...*



Continued from previous page...

Chain	Atom inclusion	Q-score
UNK	 0.6080	 0.2820
V	 0.8450	 0.4210
W	 0.8990	 0.4920
X	 0.8850	 0.4680
Y	 0.9160	 0.4760
Z	 0.9120	 0.4900
a	 0.9140	 0.4930
b	 0.9200	 0.4970
c	 0.8740	 0.4610
d	 0.8420	 0.4170
e	 0.5650	 0.2060
f	 0.6870	 0.3080
g	 0.9360	 0.4810
h	 0.8560	 0.4230
i	 0.9420	 0.5120
j	 0.8910	 0.4660
k	 0.8240	 0.3110
l	 0.7390	 0.2770
m	 0.5150	 0.1920
n	 0.4320	 0.4110
o	 0.9070	 0.4640
p	 0.8880	 0.4230
q	 0.8270	 0.3940
r	 0.9100	 0.4670
s	 0.9390	 0.4910
t	 0.4820	 0.3220
t1	 0.2380	 0.1210
t2	 0.2230	 0.1260
t3	 0.0500	 0.0150
t4	 0.0220	 0.0060
t5	 0.0040	 0.0220
t6	 0.0050	 -0.0020
u	 0.7700	 0.4430
v	 0.7520	 0.4020
w	 0.5010	 0.2740