



## wwPDB EM Validation Summary Report ⓘ

Apr 19, 2025 – 07:35 am BST

PDB ID : 9HFO / pdb\_00009hfo  
EMDB ID : EMD-52119  
Title : Translation-initiation state of human mitochondrial ribosome small subunit (State G)  
Authors : Finke, A.F.; Heinrichs, M.; Aibara, S.; Richter-Dennerlein, R.; Hillen, H.S.  
Deposited on : 2024-11-18  
Resolution : 3.10 Å(reported)  
Based on initial model : 7PO2

This is a wwPDB EM Validation Summary 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>.

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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

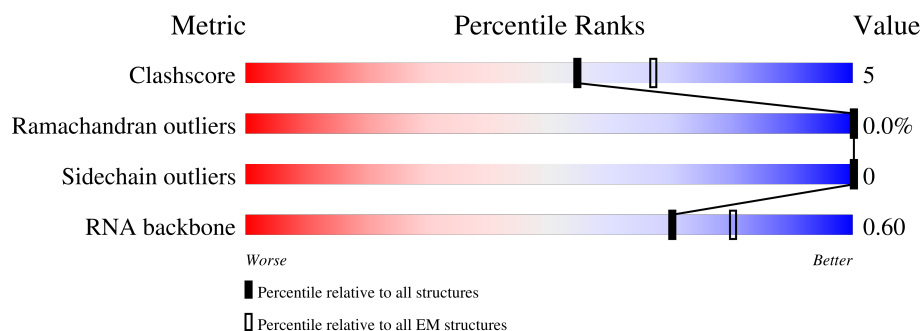
# 1 Overall quality at a glance

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)
Clashscore	210492	15764
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	218	<div> <div>18%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
2	1	323	<div> <div>9%</div> <div>80%</div> <div>6%</div> <div>14%</div> </div>
3	2	117	<div> <div>19%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
4	3	199	<div> <div>.</div> <div>31%</div> <div>5%</div> <div>64%</div> </div>
5	4	689	<div> <div>50%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div>
6	5	71	<div> <div>17%</div> <div>49%</div> <div>37%</div> <div>7%</div> <div>7%</div> </div>
7	6	3	<div> <div>67%</div> <div>33%</div> </div>

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Mol	Chain	Length	Quality of chain
8	7	727	
9	A	955	
10	B	296	
11	C	167	
12	D	430	
13	E	125	
14	F	242	
15	G	396	
16	H	201	
17	I	194	
18	J	138	
19	K	128	
20	L	257	
21	M	137	
22	N	130	
23	O	258	
24	P	142	
25	Q	87	
26	R	360	
27	S	190	
28	T	173	
29	U	205	
30	V	414	
31	W	187	
32	X	398	

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Mol	Chain	Length	Quality of chain
33	Y	395	<div><div><div></div><div></div><div></div></div><div>11%35%62%</div></div>
34	Z	106	<div><div><div></div><div></div><div></div></div><div>9%81%9%9%</div></div>

## 2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 71379 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 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	212	Total	C	N	O	S	0	0
			1765	1116	336	308	5		

- Molecule 2 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	278	Total	C	N	O	S	0	0
			2256	1430	386	429	11		

- Molecule 3 is a protein called Small ribosomal subunit protein mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	116	Total	C	N	O	S	0	0
			927	574	181	164	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	2	ACE	-	acetylation	UNP Q96BP2

- Molecule 4 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	71	Total	C	N	O	S	0	0
			629	403	135	90	1		

- Molecule 5 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	592	Total	C	N	O	S	0	0
			4795	3070	812	885	28		

- Molecule 6 is a RNA chain called fMet-tRNA<sup>Met</sup>.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	66	Total	C	N	O	P	0	0
			1398	626	246	460	66		

- Molecule 7 is a RNA chain called mRNA, start codon.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	3	Total	C	N	O	P	0	0
			65	29	12	21	3		

- Molecule 8 is a protein called Translation initiation factor IF-2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	511	Total	C	N	O	S	0	0
			3924	2469	680	758	17		

- Molecule 9 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	909	Total	C	N	O	P	0	0
			19307	8655	3484	6259	909		

- Molecule 10 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	222	Total	C	N	O	S	0	0
			1806	1151	326	319	10		

- Molecule 11 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	132	Total	C	N	O	S	0	0
			1083	699	195	185	4		

- Molecule 12 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	343	Total	C	N	O	S	0	0
			2731	1713	518	487	13		

- Molecule 13 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	122	Total	C	N	O	S	0	0
			972	614	177	177	4		

- Molecule 14 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	208	Total	C	N	O	S	0	0
			1725	1104	312	298	11		

- Molecule 15 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	326	Total	C	N	O	S	0	0
			2675	1704	472	485	14		

- Molecule 16 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	139	Total	C	N	O	S	0	0
			1138	734	192	209	3		

- Molecule 17 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	137	Total	C	N	O	S	0	0
			1019	641	193	181	4		

- Molecule 18 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	107	Total	C	N	O	S	0	0
			829	515	167	141	6		

- Molecule 19 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	101	Total	C	N	O	S	0	0
			862	537	179	141	5		

- Molecule 20 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	170	Total	C	N	O	S	0	0
			1420	905	263	245	7		

- Molecule 21 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	115	Total	C	N	O	S	0	0
			913	578	181	148	6		

- Molecule 22 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	109	Total	C	N	O	S	0	0
			859	557	155	144	3		

- Molecule 23 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	193	Total	C	N	O	S	0	0
			1592	1014	294	277	7		

- Molecule 24 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	96	Total	C	N	O	S	0	0
			771	496	133	134	8		

- Molecule 25 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	85	Total	C	N	O	S	0	0
			736	455	149	124	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	50	ARG	CYS	variant	UNP P82921

- Molecule 26 is a protein called 28S ribosomal protein S22, mitochondrial.



Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	295	Total	C	N	O	S	0	0
			2409	1533	413	455	8		

- Molecule 27 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	135	Total	C	N	O	S	0	0
			1111	716	198	196	1		

- Molecule 28 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	168	Total	C	N	O	S	0	0
			1371	877	239	244	11		

- Molecule 29 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	176	Total	C	N	O	S	0	0
			1488	916	301	267	4		

- Molecule 30 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	362	Total	C	N	O	S	0	0
			2969	1904	495	558	12		

- Molecule 31 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	99	Total	C	N	O	S	0	0
			783	495	140	144	4		

- Molecule 32 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	X	352	Total	C	N	O	S	0	0
			2849	1822	499	517	11		

- Molecule 33 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y	149	Total	C	N	O	S	0	0
			1246	801	207	234	4		

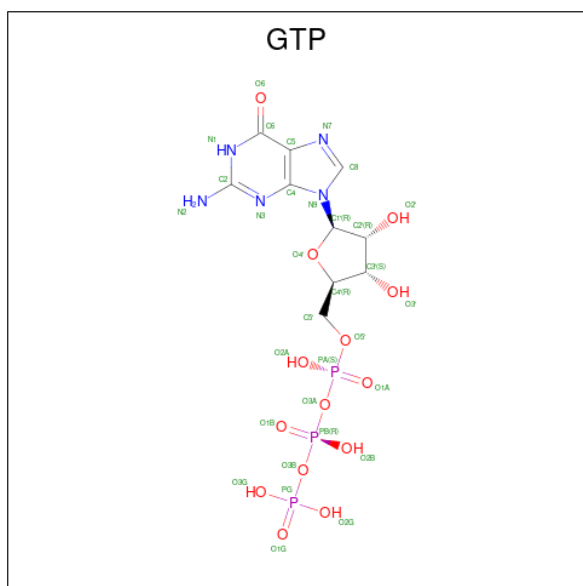
- Molecule 34 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Z	96	Total	C	N	O	S	0	0
			810	517	145	144	4		

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	3	1	Total	Mg	0
			1	1	
35	7	1	Total	Mg	0
			1	1	
35	A	41	Total	Mg	0
			41	41	
35	B	1	Total	Mg	0
			1	1	
35	X	1	Total	Mg	0
			1	1	

- Molecule 36 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					AltConf
36	7	1	Total	C	N	O	P	0
			32	10	5	14	3	

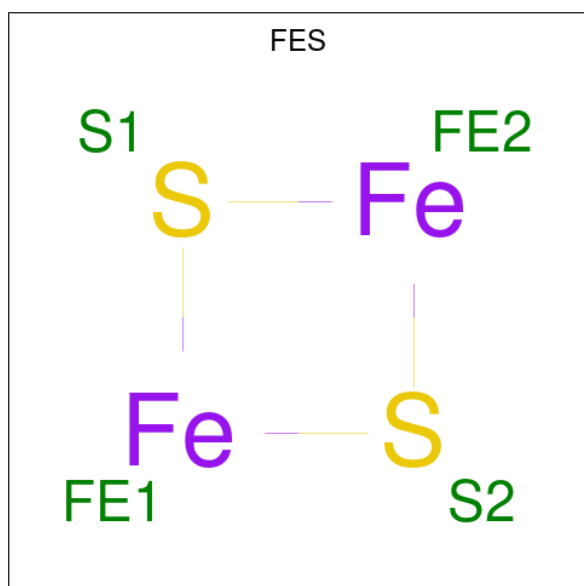
- Molecule 37 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
37	A	1	Total	K	0
			1	1	

- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	O	1	Total	Zn	0
			1	1	

- Molecule 39 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



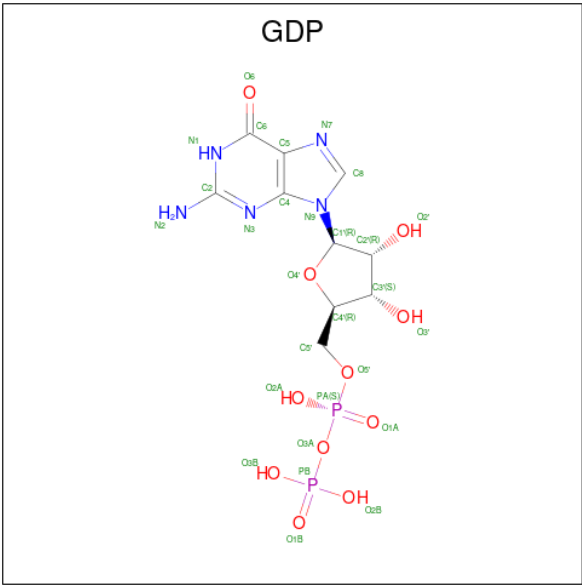
Mol	Chain	Residues	Atoms			AltConf
39	P	1	Total	Fe	S	0
			4	2	2	
39	T	1	Total	Fe	S	0
			4	2	2	

- Molecule 40 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
40	X	1	31	10	5	13	3	0

- Molecule 41 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).

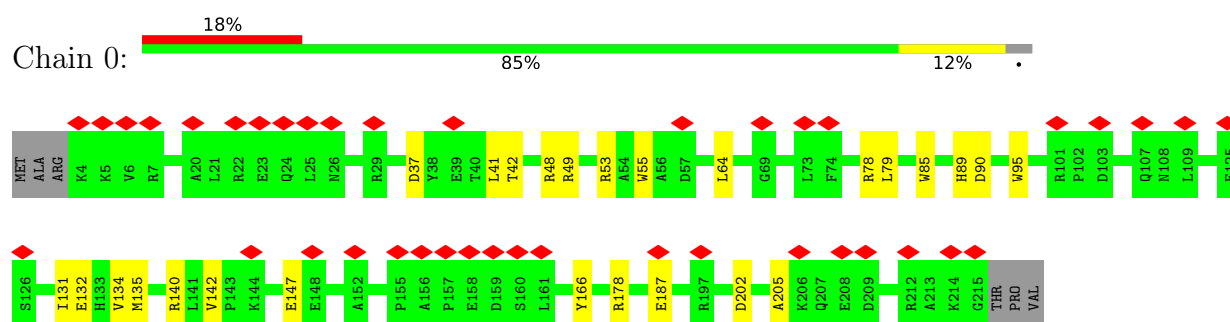


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
41	X	1	28	10	5	11	2	0

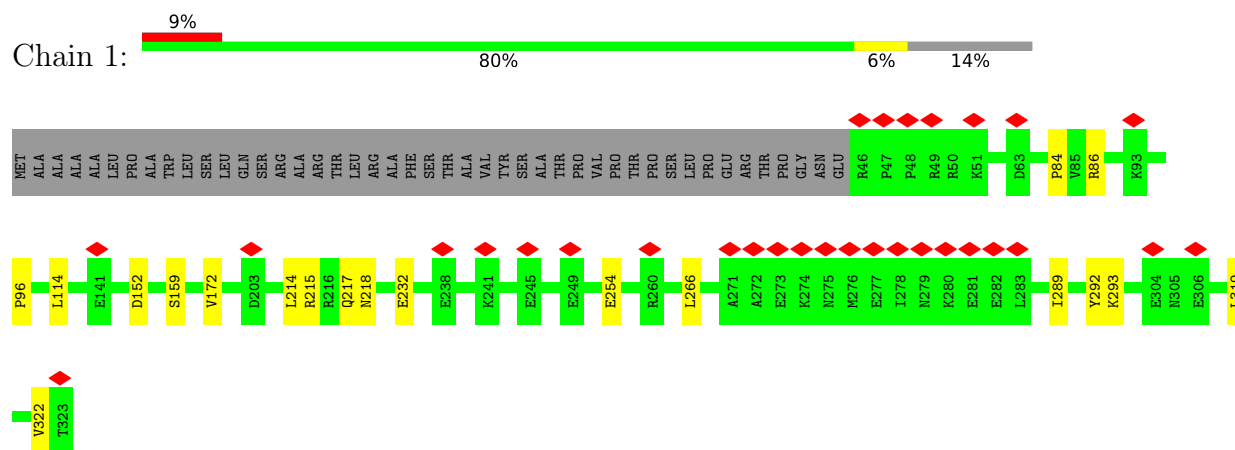
### 3 Residue-property plots [i](#)

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

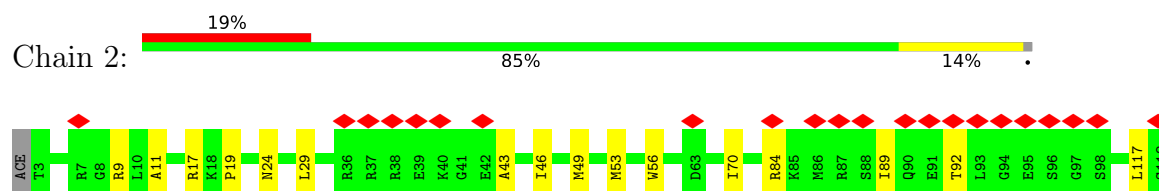
- Molecule 1: 28S ribosomal protein S34, mitochondrial



- Molecule 2: 28S ribosomal protein S35, mitochondrial

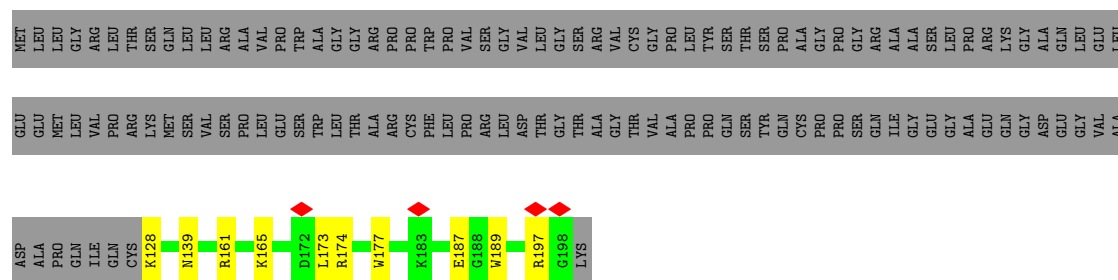


- Molecule 3: Small ribosomal subunit protein mS37

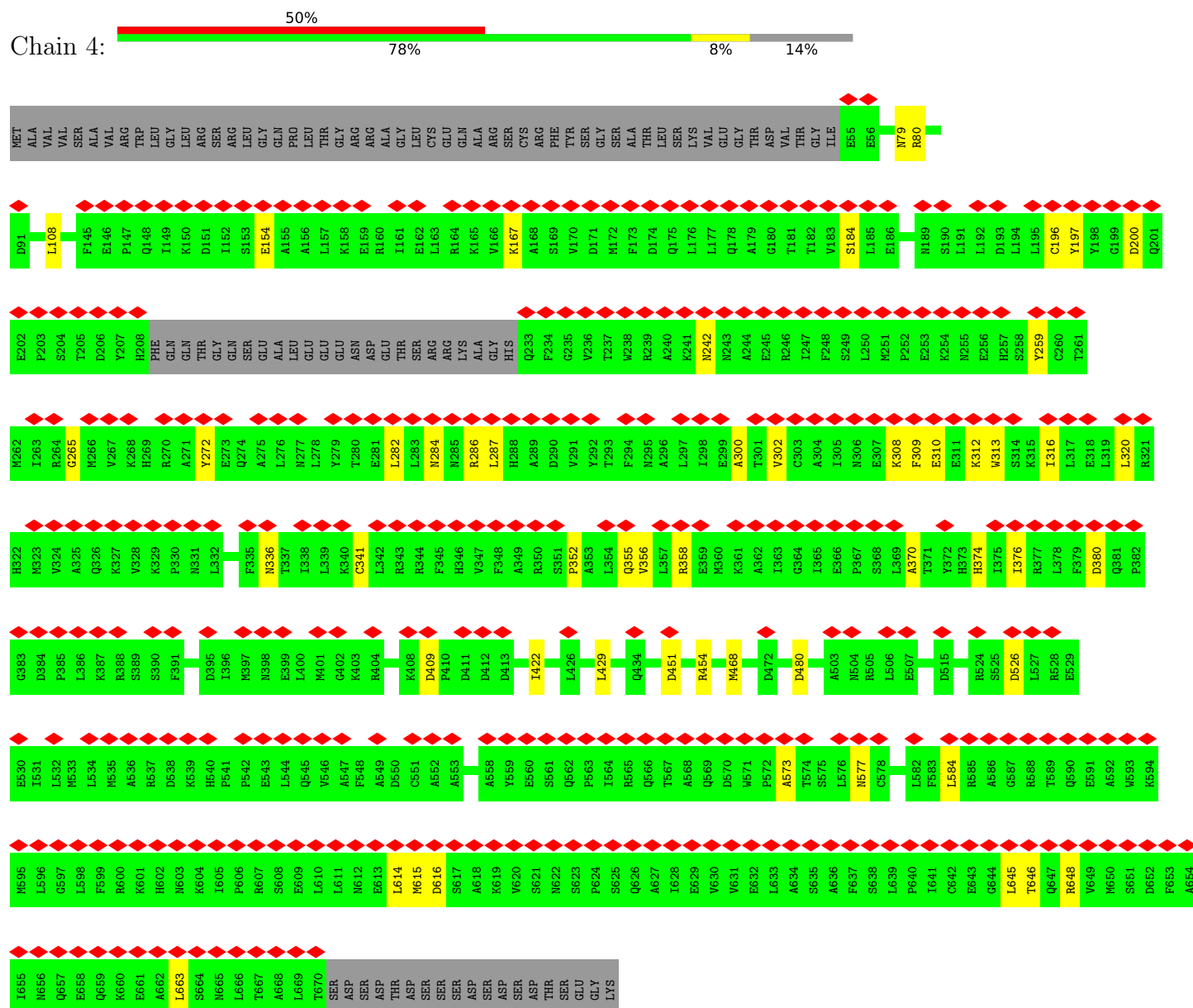


- Molecule 4: Aurora kinase A-interacting protein



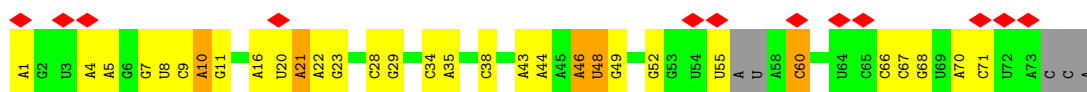


• Molecule 5: Pentatricopeptide repeat domain-containing protein 3, mitochondrial



• Molecule 6: fMet-tRNA<sup>Met</sup>





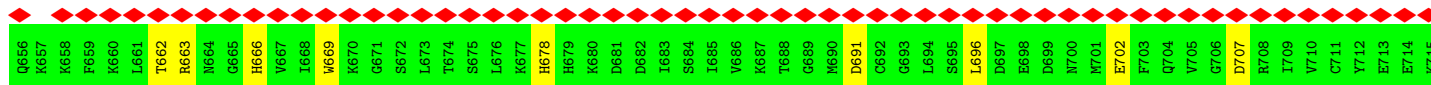
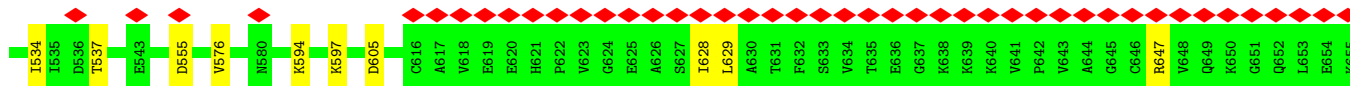
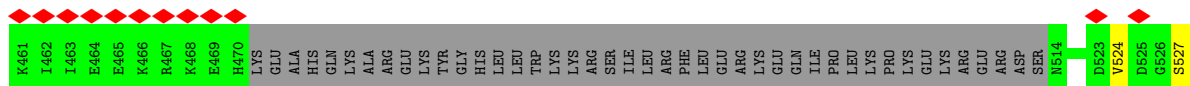
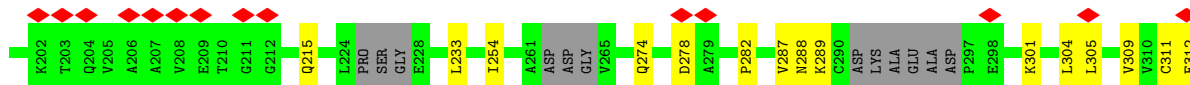
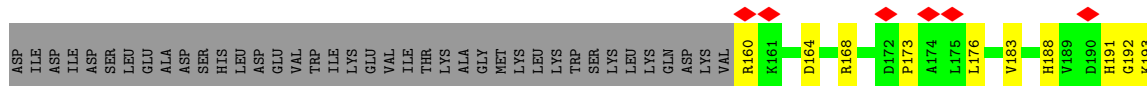
- Molecule 7: mRNA, start codon

Chain 6: 67% 33%



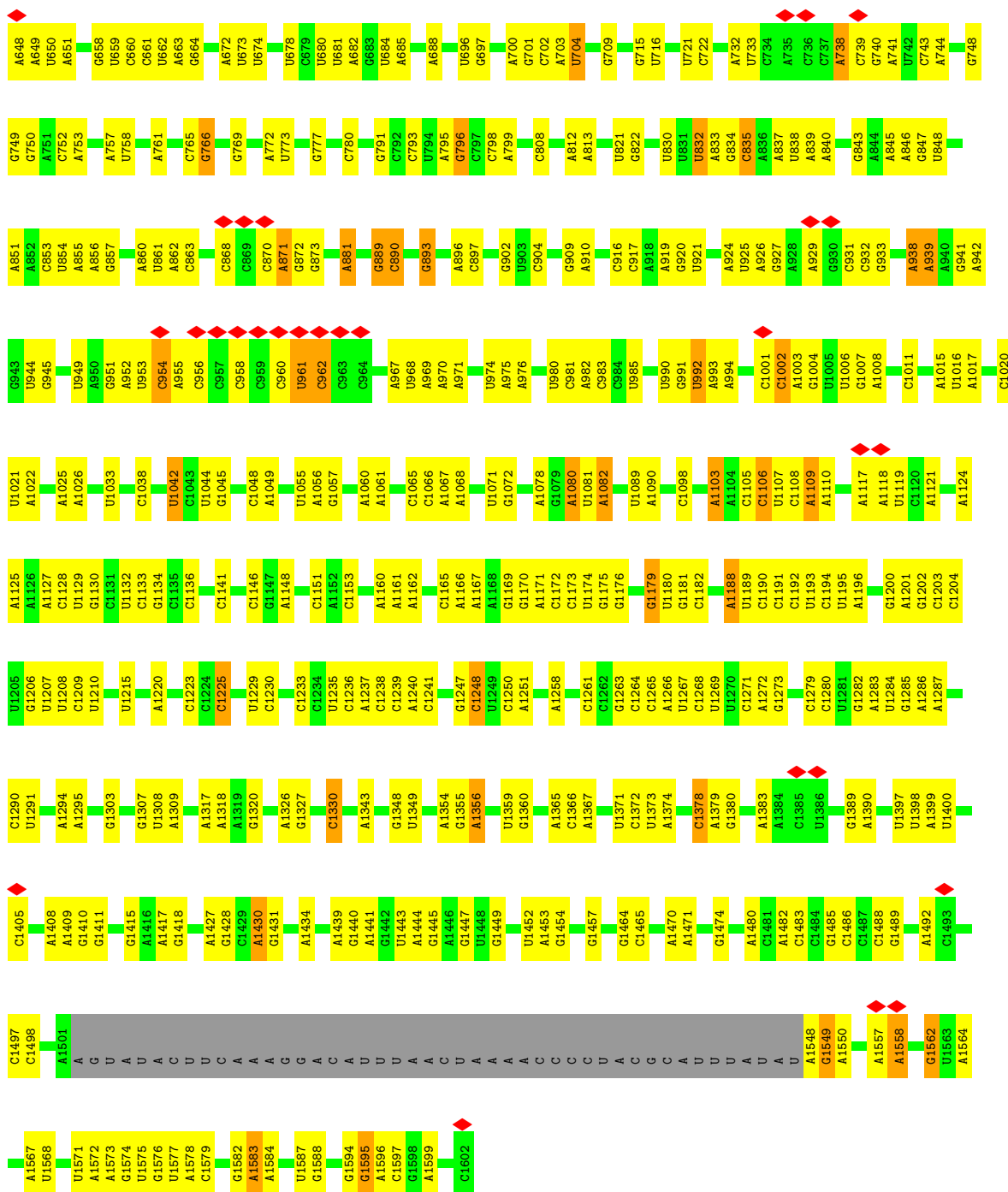
- Molecule 8: Translation initiation factor IF-2, mitochondrial

Chain 7: 21% 61% 9% 30%



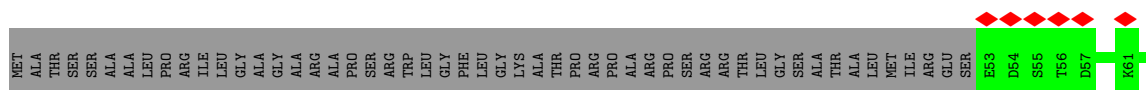
- Molecule 9: 12S mitochondrial rRNA

Chain A: 53% 38% 5%



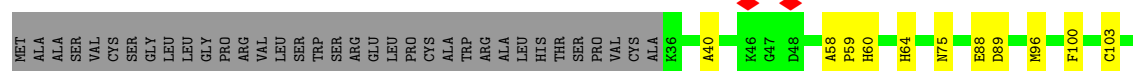
- Molecule 10: 28S ribosomal protein S2, mitochondrial

Chain B:

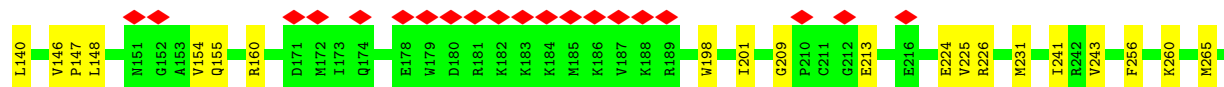
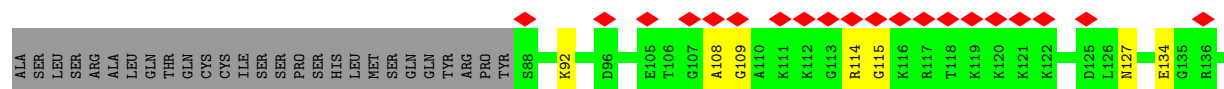
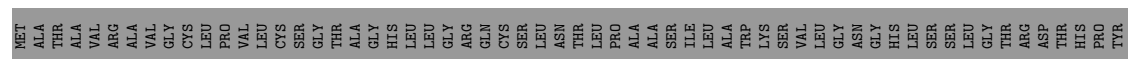




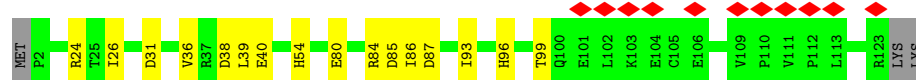
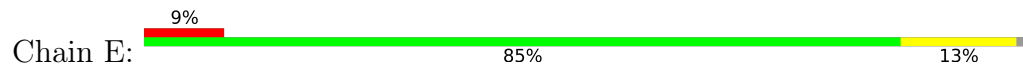
- Molecule 11: 28S ribosomal protein S24, mitochondrial



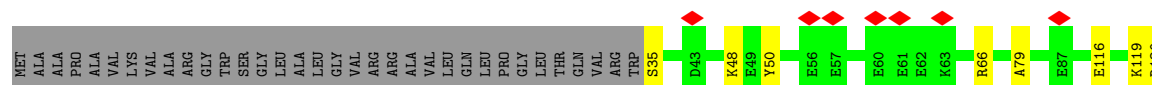
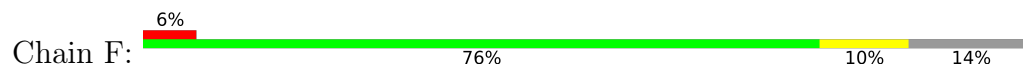
- Molecule 12: 28S ribosomal protein S5, mitochondrial



- Molecule 13: 28S ribosomal protein S6, mitochondrial



- Molecule 14: 28S ribosomal protein S7, mitochondrial







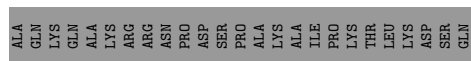
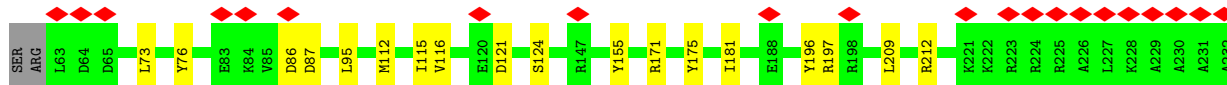
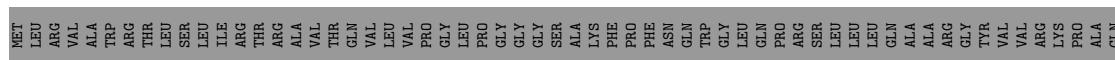
- Molecule 19: 28S ribosomal protein S14, mitochondrial

Chain K: 65% 14% 21%



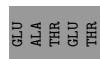
- Molecule 20: 28S ribosomal protein S15, mitochondrial

Chain L: 8% 59% 7% 34%



- Molecule 21: 28S ribosomal protein S16, mitochondrial

Chain M: 70% 14% 16%



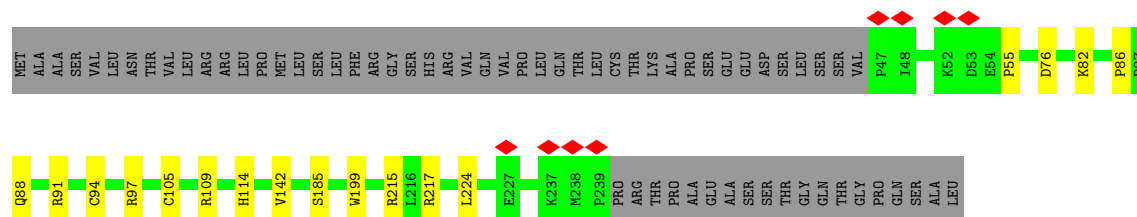
- Molecule 22: 28S ribosomal protein S17, mitochondrial

Chain N: 72% 12% 16%

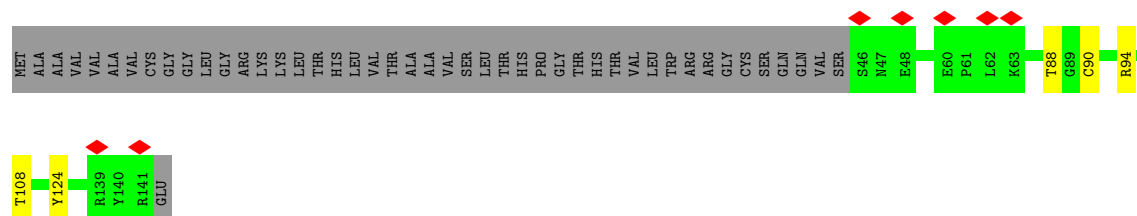


- Molecule 23: 28S ribosomal protein S18b, mitochondrial

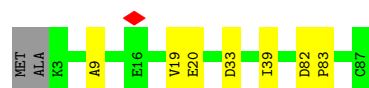
Chain O: 68% 7% 25%



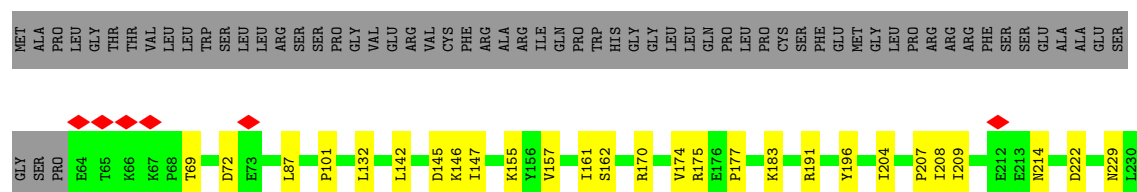
- Molecule 24: 28S ribosomal protein S18c, mitochondrial



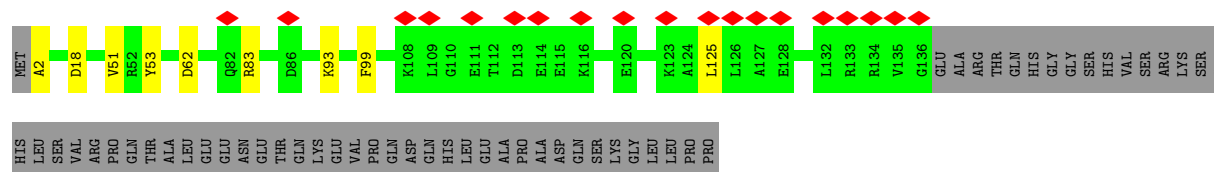
- Molecule 25: 28S ribosomal protein S21, mitochondrial



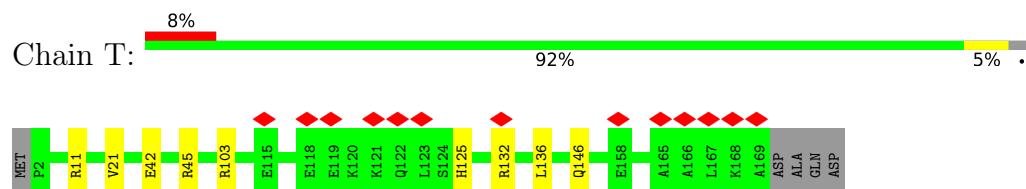
- Molecule 26: 28S ribosomal protein S22, mitochondrial



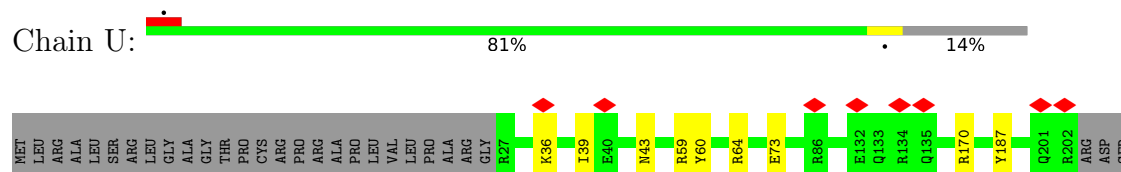
- Molecule 27: 28S ribosomal protein S23, mitochondrial



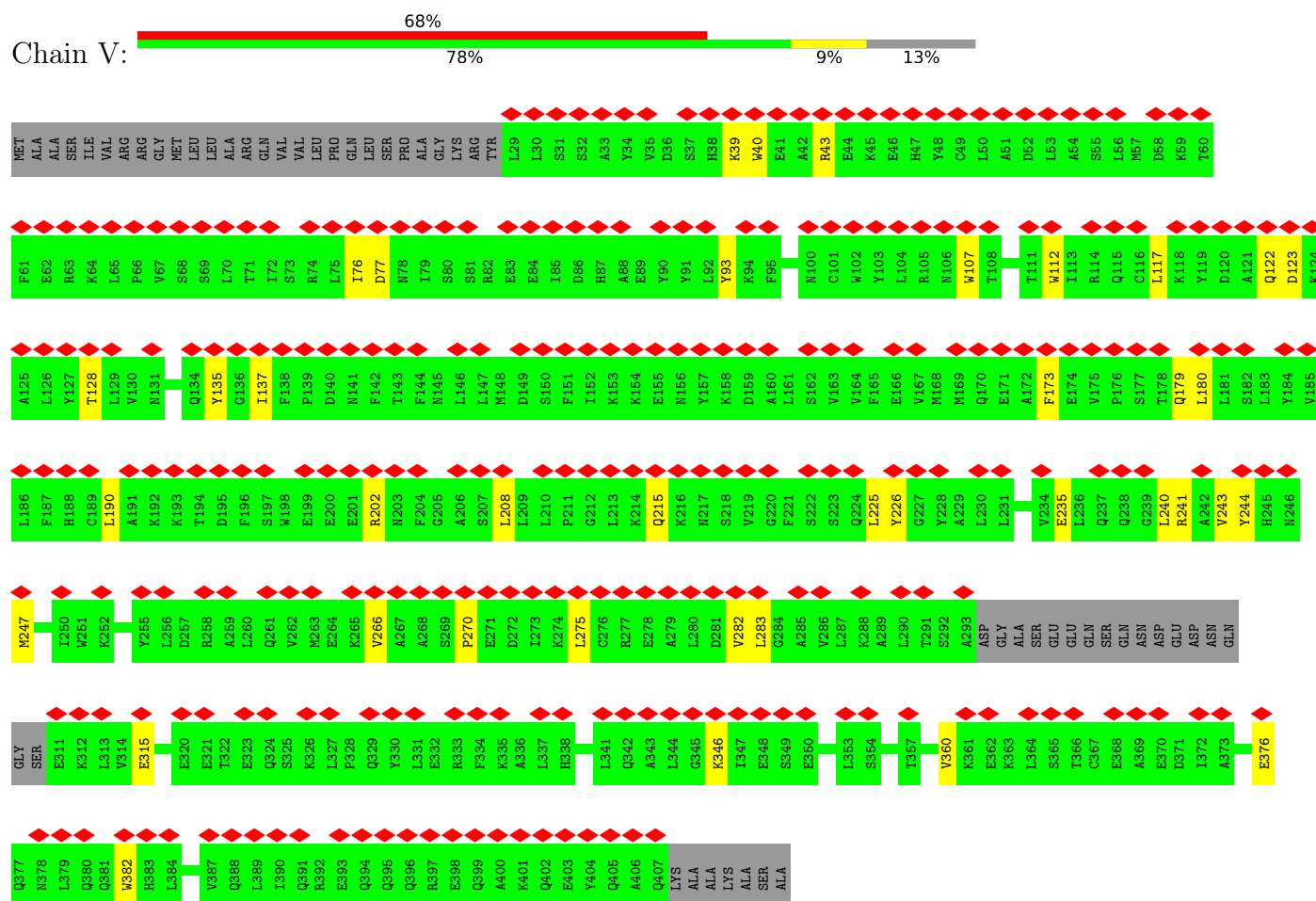
- Molecule 28: 28S ribosomal protein S25, mitochondrial



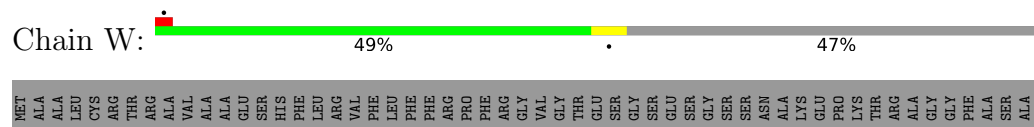
- Molecule 29: 28S ribosomal protein S26, mitochondrial



- Molecule 30: 28S ribosomal protein S27, mitochondrial



- Molecule 31: 28S ribosomal protein S28, mitochondrial





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40824	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.154	Depositor
Minimum map value	-0.709	Depositor
Average map value	0.036	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.496	Depositor
Map size (Å)	461.99997, 461.99997, 461.99997	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, K, MG, ATP, ZN, FES, GDP

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	0.25	0/1811	0.53	0/2452
2	1	0.26	0/2304	0.43	0/3117
3	2	0.25	0/941	0.52	0/1257
4	3	0.27	0/640	0.56	0/844
5	4	0.25	0/4904	0.42	0/6636
6	5	0.35	1/1560 (0.1%)	0.77	0/2422
7	6	0.34	0/72	0.69	0/110
8	7	0.25	0/3979	0.46	0/5371
9	A	0.36	0/21597	0.75	1/33626 (0.0%)
10	B	0.29	0/1849	0.48	0/2503
11	C	0.30	0/1113	0.49	0/1505
12	D	0.28	0/2783	0.51	0/3724
13	E	0.28	0/989	0.51	0/1335
14	F	0.26	0/1767	0.45	0/2373
15	G	0.27	0/2733	0.47	0/3666
16	H	0.29	0/1162	0.48	0/1575
17	I	0.28	0/1039	0.48	0/1400
18	J	0.29	0/845	0.54	0/1137
19	K	0.26	0/880	0.54	0/1182
20	L	0.28	0/1444	0.46	0/1930
21	M	0.28	0/934	0.53	0/1255
22	N	0.29	0/877	0.48	0/1187
23	O	0.29	0/1648	0.48	0/2243
24	P	0.29	0/788	0.43	0/1058
25	Q	0.28	0/748	0.53	0/994
26	R	0.27	0/2456	0.45	0/3317
27	S	0.28	0/1138	0.49	0/1533
28	T	0.29	0/1402	0.46	0/1883
29	U	0.27	0/1510	0.53	0/2025
30	V	0.23	0/3030	0.39	0/4093
31	W	0.28	0/795	0.51	0/1071
32	X	0.25	0/2921	0.44	0/3954



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	Y	0.26	0/1280	0.39	0/1725
34	Z	0.28	0/828	0.45	0/1104
All	All	0.30	1/74767 (0.0%)	0.58	1/105607 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	1	A	OP3-P	-10.60	1.48	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	765	C	C2-N1-Cl1'	5.90	125.29	118.80

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1765	0	1773	18	0
2	1	2256	0	2288	14	0
3	2	927	0	964	11	0
4	3	629	0	702	10	0
5	4	4795	0	4796	37	0
6	5	1398	0	712	19	0
7	6	65	0	33	1	0
8	7	3924	0	3982	40	0
9	A	19307	0	9810	272	0
10	B	1806	0	1791	14	0
11	C	1083	0	1088	14	0
12	D	2731	0	2804	37	0
13	E	972	0	1000	11	0
14	F	1725	0	1769	15	0
15	G	2675	0	2669	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	H	1138	0	1173	12	0
17	I	1019	0	1059	15	0
18	J	829	0	874	8	0
19	K	862	0	885	14	0
20	L	1420	0	1502	15	0
21	M	913	0	943	15	0
22	N	859	0	922	11	0
23	O	1592	0	1557	12	0
24	P	771	0	800	6	0
25	Q	736	0	749	7	0
26	R	2409	0	2428	27	0
27	S	1111	0	1115	7	0
28	T	1371	0	1393	6	0
29	U	1488	0	1499	10	0
30	V	2969	0	2961	25	0
31	W	783	0	797	5	0
32	X	2849	0	2843	33	0
33	Y	1246	0	1197	10	0
34	Z	810	0	824	9	0
35	3	1	0	0	0	0
35	7	1	0	0	0	0
35	A	41	0	0	0	0
35	B	1	0	0	0	0
35	X	1	0	0	0	0
36	7	32	0	12	2	0
37	A	1	0	0	0	0
38	O	1	0	0	0	0
39	P	4	0	0	0	0
39	T	4	0	0	0	0
40	X	31	0	12	1	0
41	X	28	0	12	1	0
All	All	71379	0	61738	647	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 647 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:302:VAL:HG11	5:4:341:CYS:HB3	1.66	0.76
32:X:108:LEU:HD23	32:X:141:VAL:HG21	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5:21:A:H61	6:5:48:U:H5'	1.49	0.76
4:3:139:ASN:ND2	9:A:1141:C:OP1	2.19	0.75
9:A:821:U:H2'	9:A:822:G:H8	1.52	0.75

There are no symmetry-related clashes.

## 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	210/218 (96%)	207 (99%)	3 (1%)	0	100	100
2	1	276/323 (85%)	270 (98%)	6 (2%)	0	100	100
3	2	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
4	3	69/199 (35%)	69 (100%)	0	0	100	100
5	4	588/689 (85%)	583 (99%)	5 (1%)	0	100	100
8	7	499/727 (69%)	495 (99%)	4 (1%)	0	100	100
10	B	220/296 (74%)	218 (99%)	2 (1%)	0	100	100
11	C	130/167 (78%)	128 (98%)	2 (2%)	0	100	100
12	D	341/430 (79%)	334 (98%)	7 (2%)	0	100	100
13	E	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
14	F	206/242 (85%)	205 (100%)	1 (0%)	0	100	100
15	G	322/396 (81%)	314 (98%)	8 (2%)	0	100	100
16	H	137/201 (68%)	135 (98%)	1 (1%)	1 (1%)	19	51
17	I	135/194 (70%)	133 (98%)	2 (2%)	0	100	100
18	J	105/138 (76%)	103 (98%)	2 (2%)	0	100	100
19	K	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
20	L	168/257 (65%)	166 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	M	113/137 (82%)	112 (99%)	1 (1%)	0	100	100
22	N	107/130 (82%)	106 (99%)	1 (1%)	0	100	100
23	O	191/258 (74%)	189 (99%)	2 (1%)	0	100	100
24	P	94/142 (66%)	94 (100%)	0	0	100	100
25	Q	83/87 (95%)	81 (98%)	2 (2%)	0	100	100
26	R	293/360 (81%)	285 (97%)	8 (3%)	0	100	100
27	S	133/190 (70%)	131 (98%)	2 (2%)	0	100	100
28	T	166/173 (96%)	165 (99%)	1 (1%)	0	100	100
29	U	174/205 (85%)	173 (99%)	1 (1%)	0	100	100
30	V	358/414 (86%)	352 (98%)	6 (2%)	0	100	100
31	W	97/187 (52%)	96 (99%)	1 (1%)	0	100	100
32	X	350/398 (88%)	344 (98%)	6 (2%)	0	100	100
33	Y	147/395 (37%)	143 (97%)	4 (3%)	0	100	100
34	Z	94/106 (89%)	93 (99%)	1 (1%)	0	100	100
All	All	6139/8029 (76%)	6052 (99%)	86 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	H	126	ILE

### 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	185/190 (97%)	185 (100%)	0	100	100
2	1	256/291 (88%)	256 (100%)	0	100	100
3	2	100/100 (100%)	100 (100%)	0	100	100
4	3	65/166 (39%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	4	529/609 (87%)	529 (100%)	0	100	100
8	7	428/621 (69%)	428 (100%)	0	100	100
10	B	196/249 (79%)	196 (100%)	0	100	100
11	C	115/143 (80%)	115 (100%)	0	100	100
12	D	286/357 (80%)	286 (100%)	0	100	100
13	E	104/107 (97%)	104 (100%)	0	100	100
14	F	185/209 (88%)	185 (100%)	0	100	100
15	G	283/342 (83%)	283 (100%)	0	100	100
16	H	129/180 (72%)	129 (100%)	0	100	100
17	I	105/147 (71%)	105 (100%)	0	100	100
18	J	92/118 (78%)	92 (100%)	0	100	100
19	K	91/113 (80%)	91 (100%)	0	100	100
20	L	155/226 (69%)	155 (100%)	0	100	100
21	M	94/113 (83%)	94 (100%)	0	100	100
22	N	95/115 (83%)	95 (100%)	0	100	100
23	O	174/230 (76%)	174 (100%)	0	100	100
24	P	87/123 (71%)	87 (100%)	0	100	100
25	Q	78/79 (99%)	78 (100%)	0	100	100
26	R	264/318 (83%)	264 (100%)	0	100	100
27	S	116/164 (71%)	116 (100%)	0	100	100
28	T	153/157 (98%)	153 (100%)	0	100	100
29	U	152/174 (87%)	152 (100%)	0	100	100
30	V	325/364 (89%)	325 (100%)	0	100	100
31	W	86/158 (54%)	86 (100%)	0	100	100
32	X	311/351 (89%)	311 (100%)	0	100	100
33	Y	137/357 (38%)	137 (100%)	0	100	100
34	Z	88/95 (93%)	88 (100%)	0	100	100
All	All	5464/6966 (78%)	5464 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
29	U	188	ASN
30	V	215	GLN
32	X	81	HIS
32	X	67	HIS
16	H	109	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	5	64/71 (90%)	11 (17%)	0
7	6	2/3 (66%)	0	0
9	A	907/955 (94%)	120 (13%)	0
All	All	973/1029 (94%)	131 (13%)	0

5 of 131 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	5	7	G
6	5	8	U
6	5	10	A
6	5	20	U
6	5	21	A

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 52 ligands modelled in this entry, 47 are monoatomic - leaving 5 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	$\# Z  > 2$
36	GTP	7	802	35	26,34,34	1.14	2 (7%)	32,54,54	1.60	7 (21%)
41	GDP	X	403	-	24,30,30	0.98	1 (4%)	30,47,47	1.37	4 (13%)
40	ATP	X	402	35	26,33,33	0.62	0	31,52,52	0.81	2 (6%)
39	FES	P	201	24,13	0,4,4	-	-	-	-	-
39	FES	T	201	28,21	0,4,4	-	-	-	-	-

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
36	GTP	7	802	35	-	5/18/38/38	0/3/3/3
41	GDP	X	403	-	-	3/12/32/32	0/3/3/3
40	ATP	X	402	35	-	4/18/38/38	0/3/3/3
39	FES	P	201	24,13	-	-	0/1/1/1
39	FES	T	201	28,21	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	7	802	GTP	C5-C6	-4.05	1.39	1.47
41	X	403	GDP	C6-N1	-2.52	1.34	1.37
36	7	802	GTP	C2-N3	2.17	1.38	1.33

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	X	403	GDP	PA-O3A-PB	-4.16	118.55	132.83
36	7	802	GTP	PB-O3B-PG	-3.94	119.30	132.83
36	7	802	GTP	C5-C6-N1	3.25	119.68	113.95
36	7	802	GTP	C3'-C2'-C1'	3.05	105.58	100.98
41	X	403	GDP	C3'-C2'-C1'	3.05	105.57	100.98

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

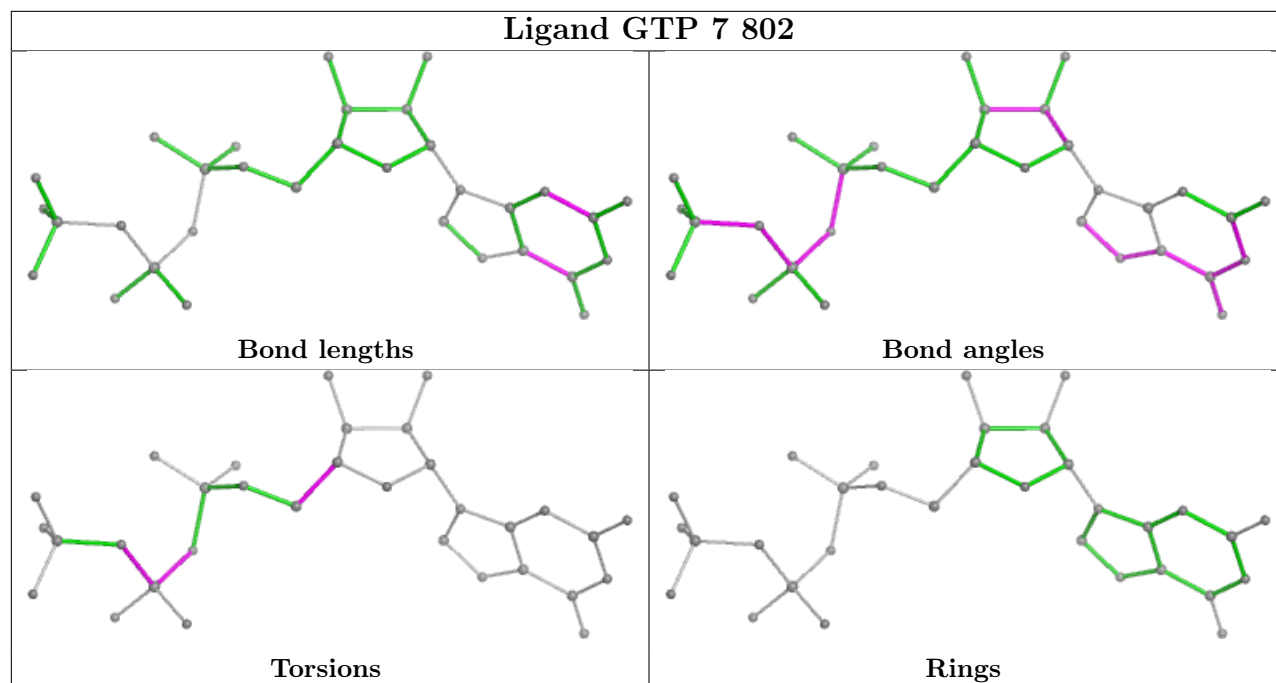
Mol	Chain	Res	Type	Atoms
40	X	402	ATP	PB-O3B-PG-O2G
40	X	402	ATP	PB-O3B-PG-O3G
41	X	403	GDP	O4'-C4'-C5'-O5'
41	X	403	GDP	C3'-C4'-C5'-O5'
36	7	802	GTP	O4'-C4'-C5'-O5'

There are no ring outliers.

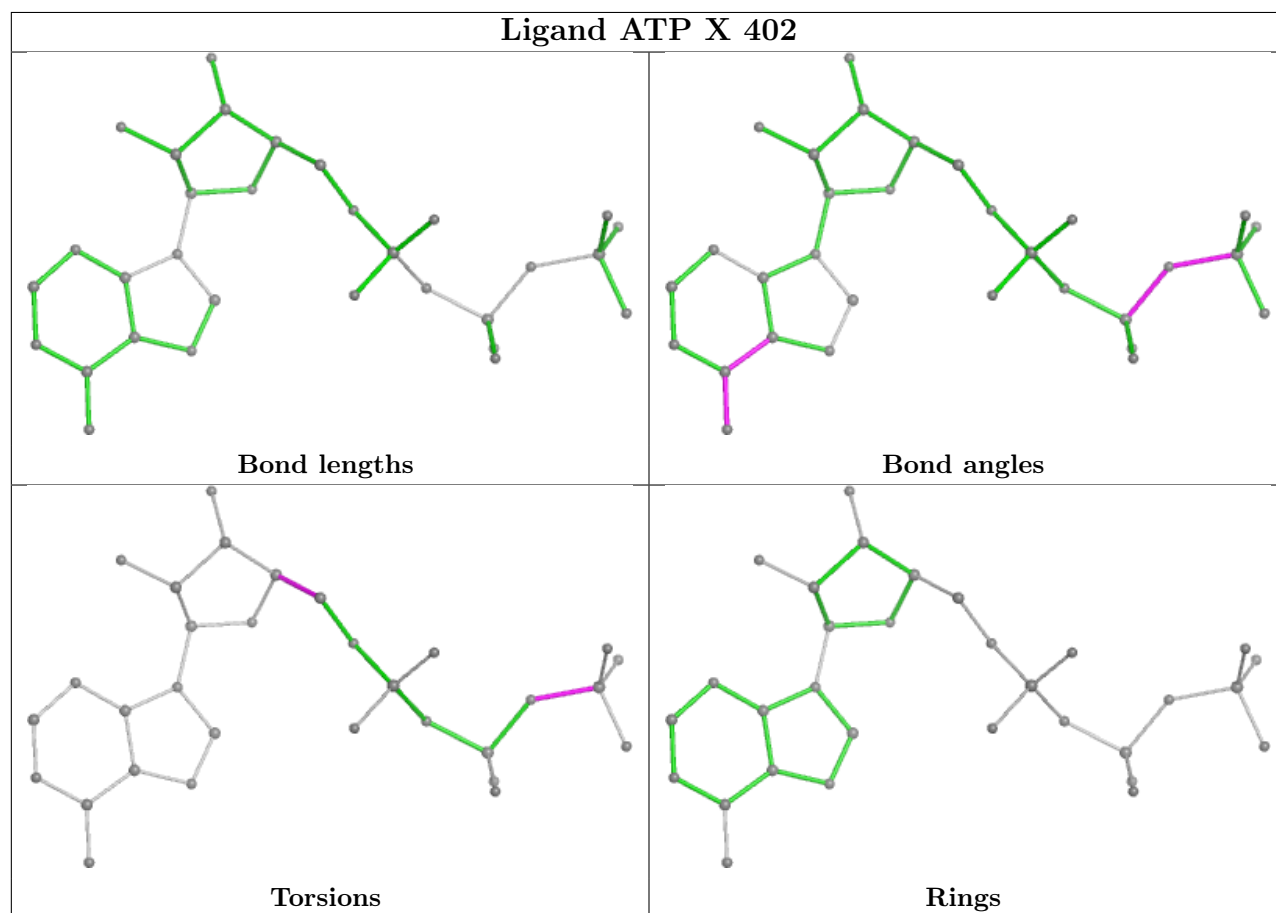
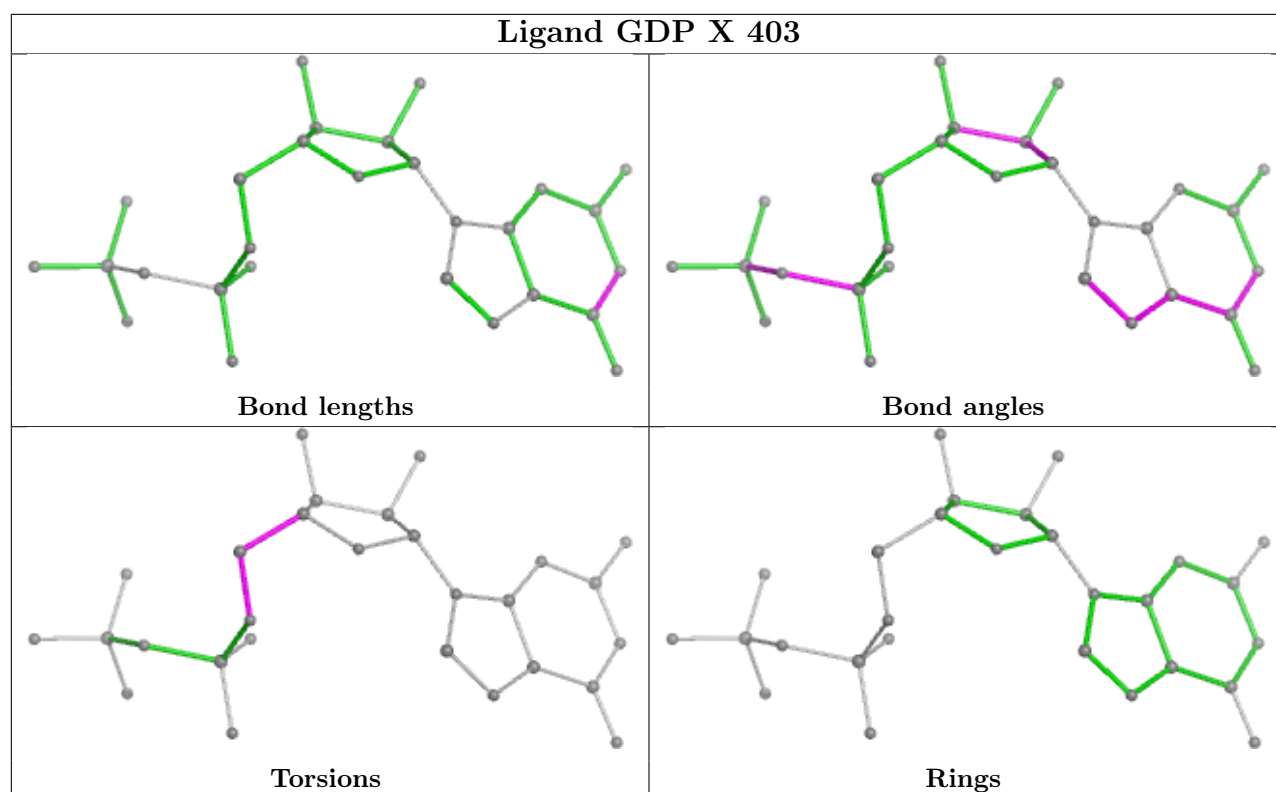
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	7	802	GTP	2	0
41	X	403	GDP	1	0
40	X	402	ATP	1	0

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.

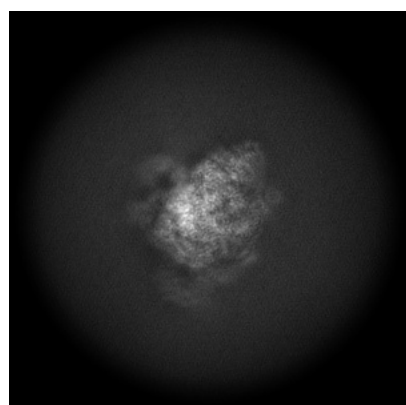
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52119. These allow visual inspection of the internal detail of the map and identification of artifacts.

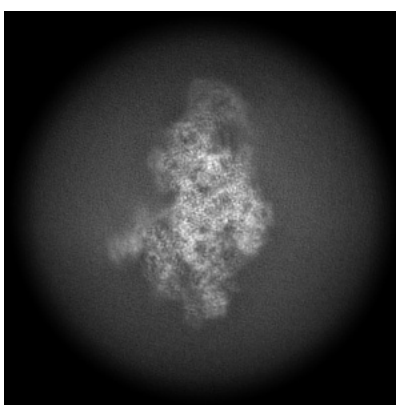
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

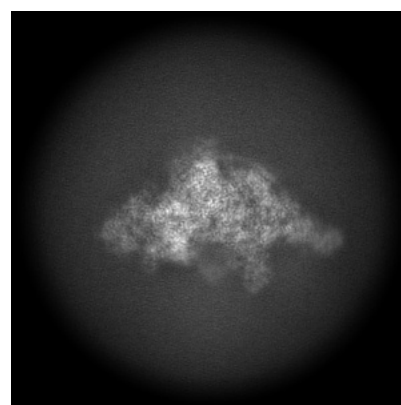
#### 6.1.1 Primary map



X



Y

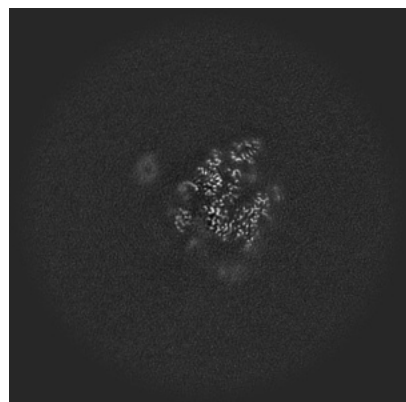


Z

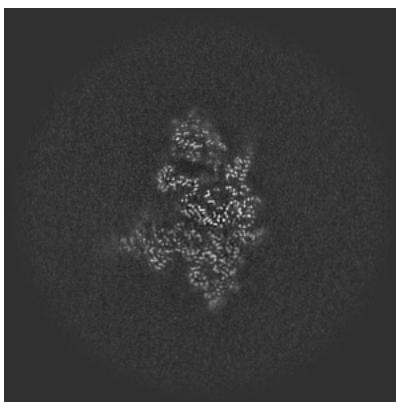
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

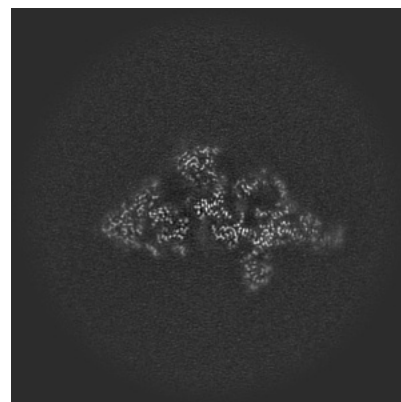
#### 6.2.1 Primary map



X Index: 220



Y Index: 220

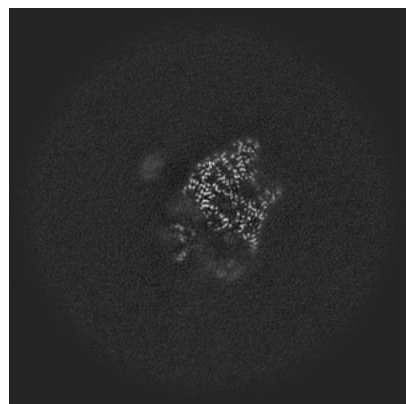


Z Index: 220

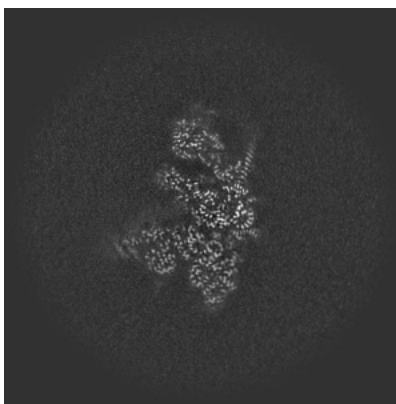
The images above show central slices of the map in three orthogonal directions.

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

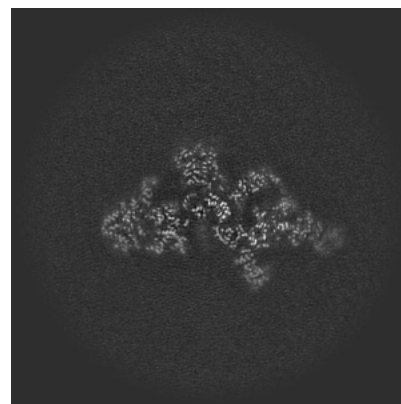
### 6.3.1 Primary map



X Index: 211



Y Index: 216

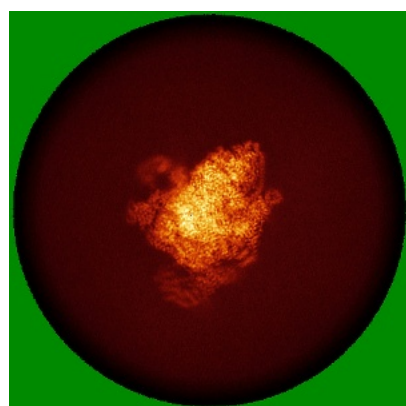


Z Index: 224

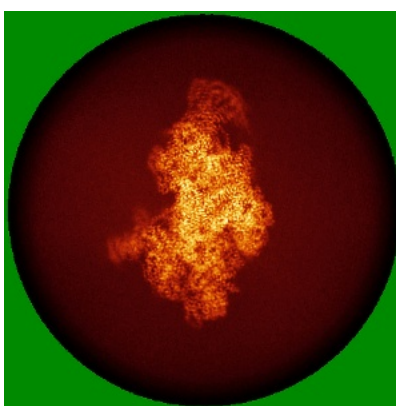
The images above show the largest variance slices of the map in three orthogonal directions.

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

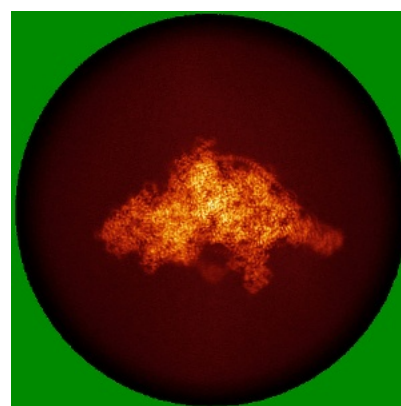
### 6.4.1 Primary map



X



Y

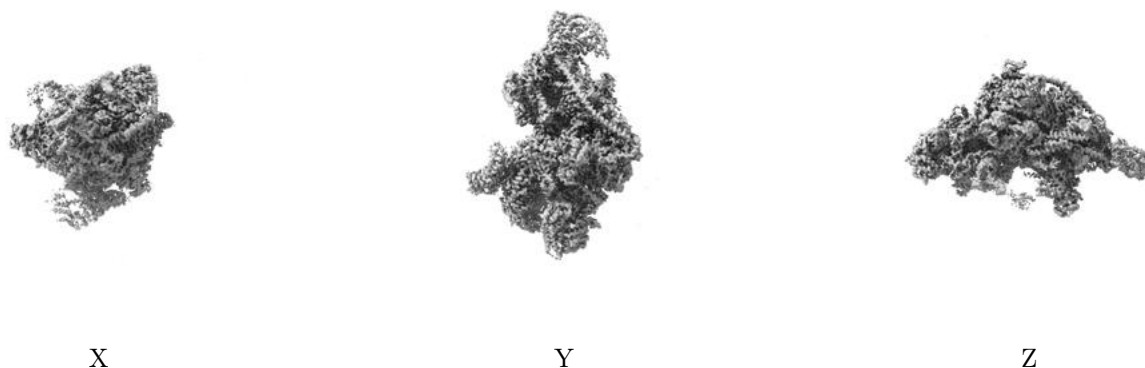


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.496. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

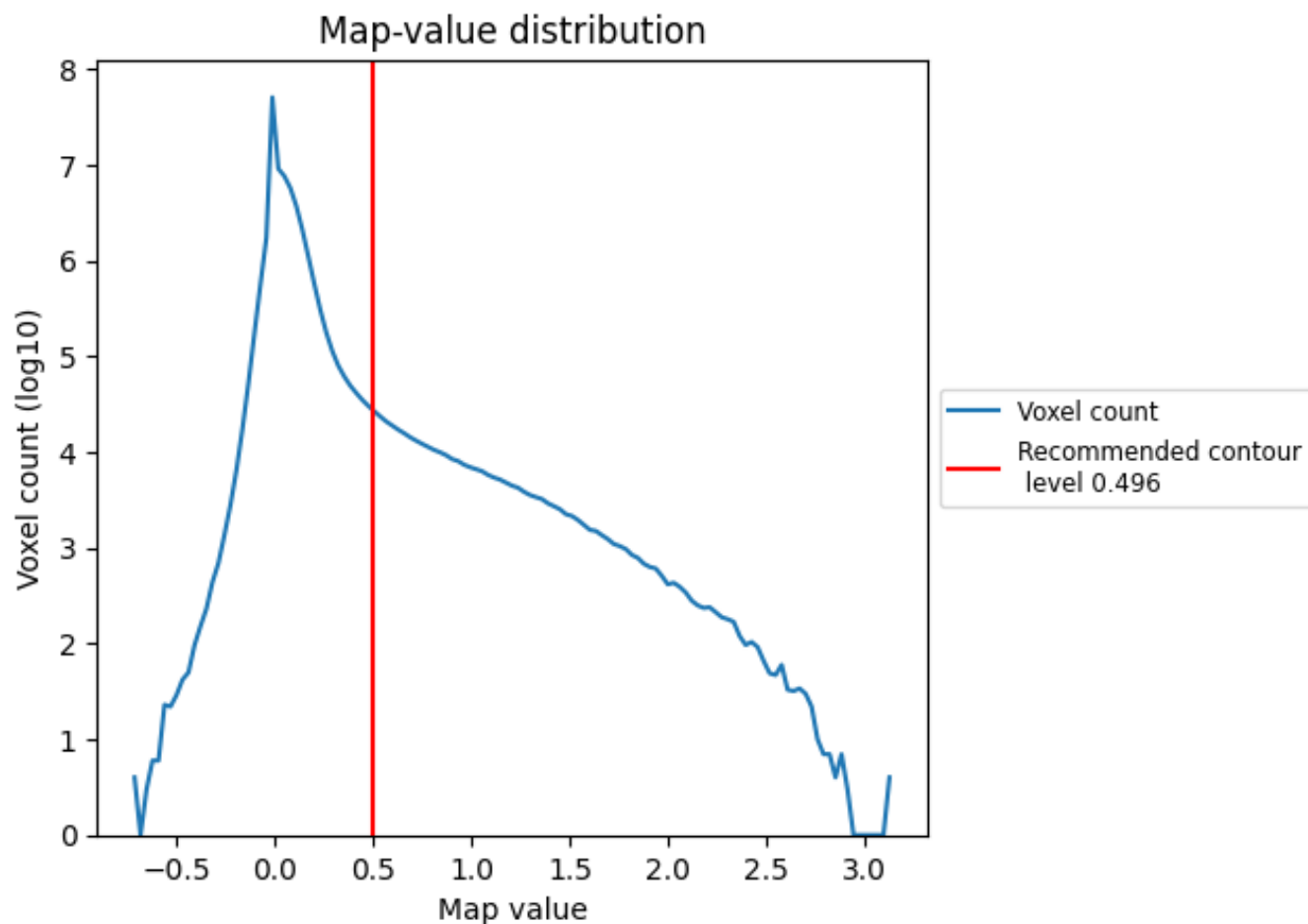
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

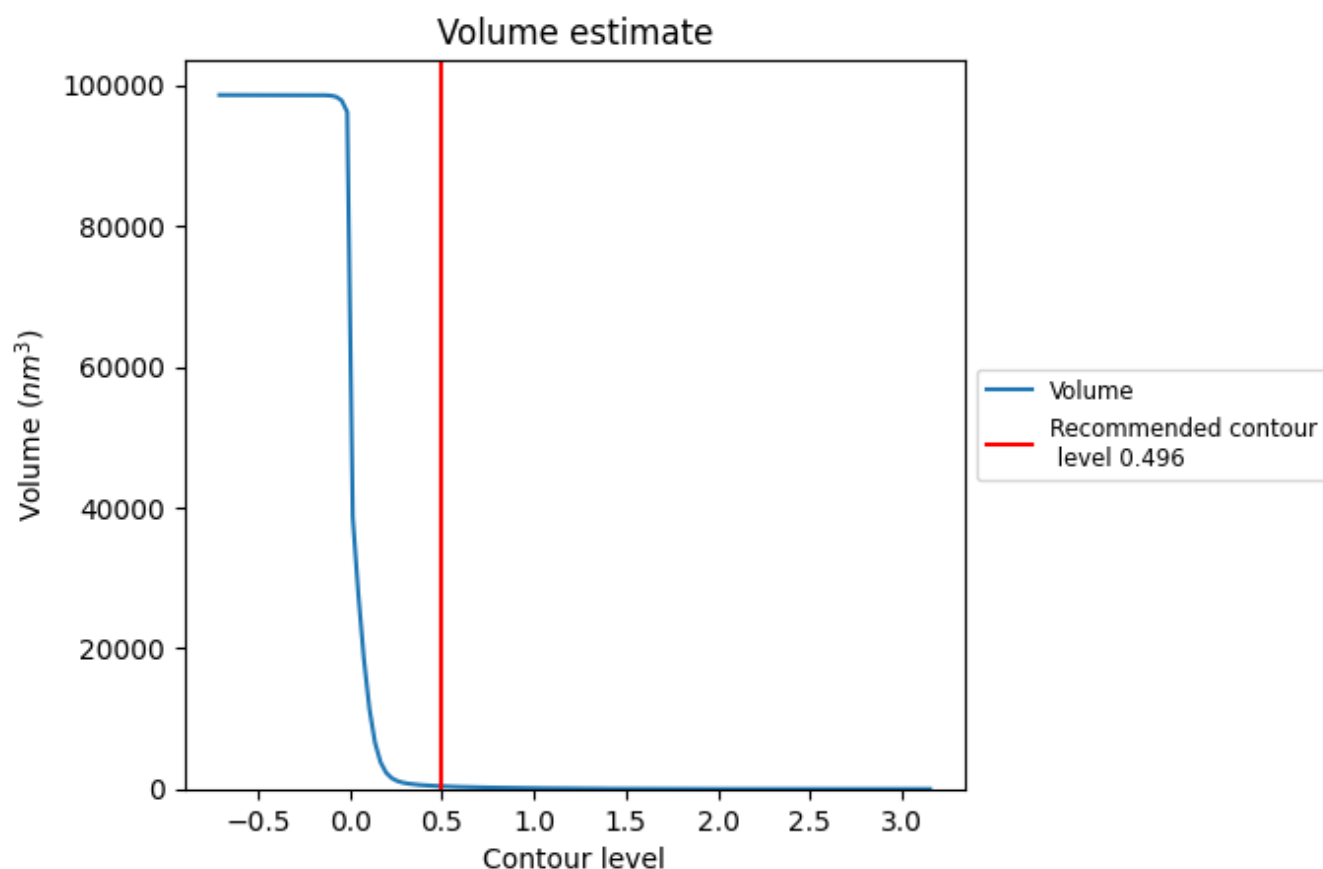
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

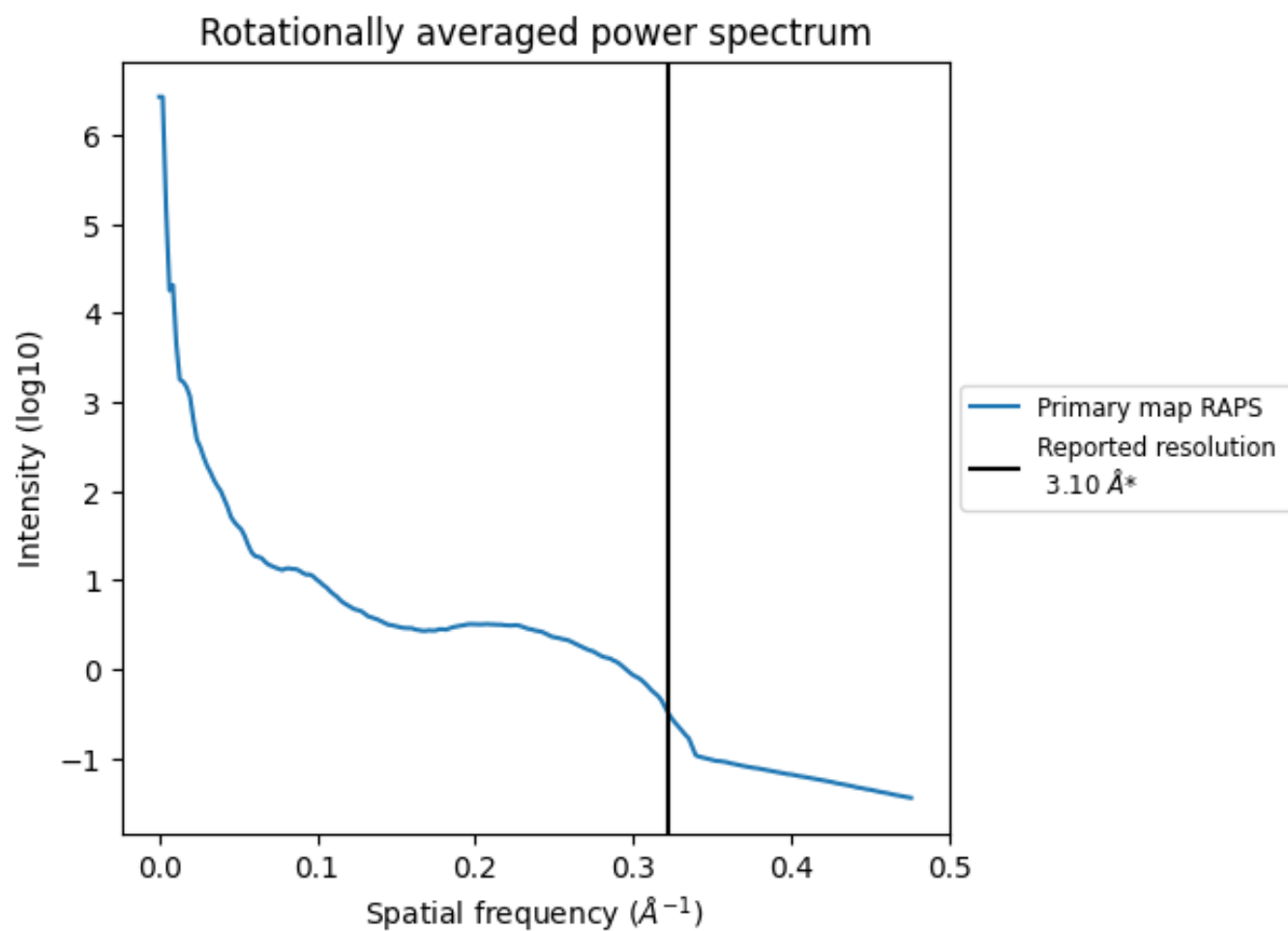
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 390  $\text{nm}^3$ ; this corresponds to an approximate mass of 353 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>



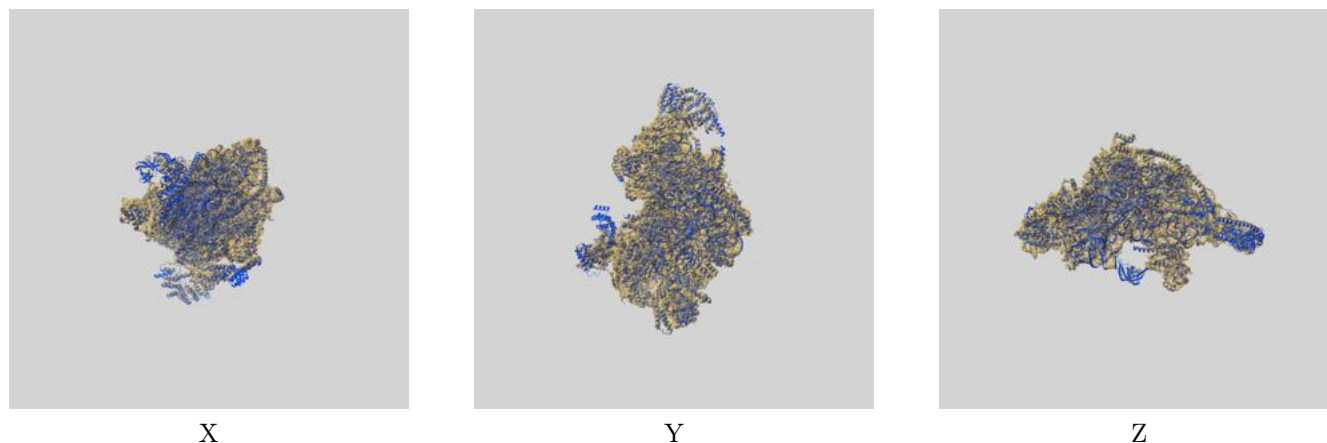
## 8 Fourier-Shell correlation

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

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

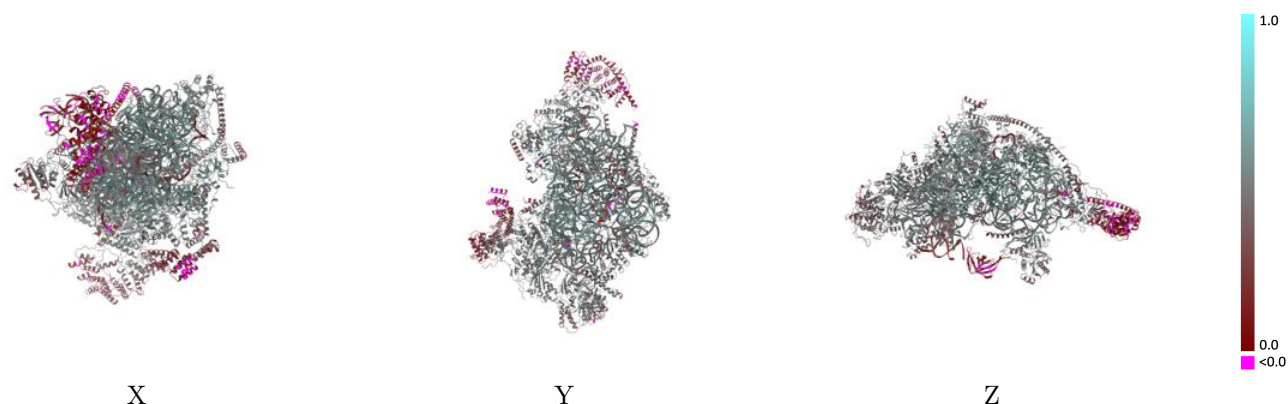
This section contains information regarding the fit between EMDB map EMD-52119 and PDB model 9HFO. Per-residue inclusion information can be found in section 3 on page 13.

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



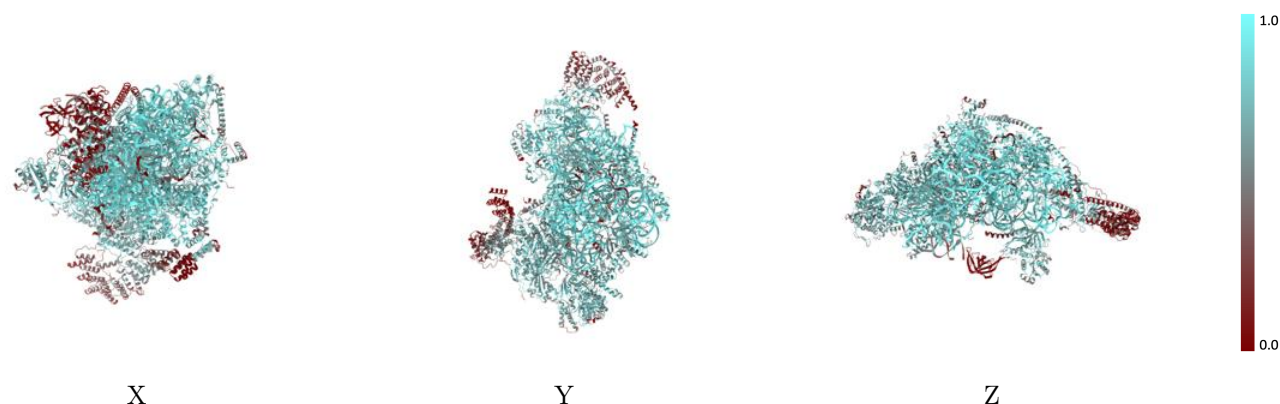
The images above show the 3D surface view of the map at the recommended contour level 0.496 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



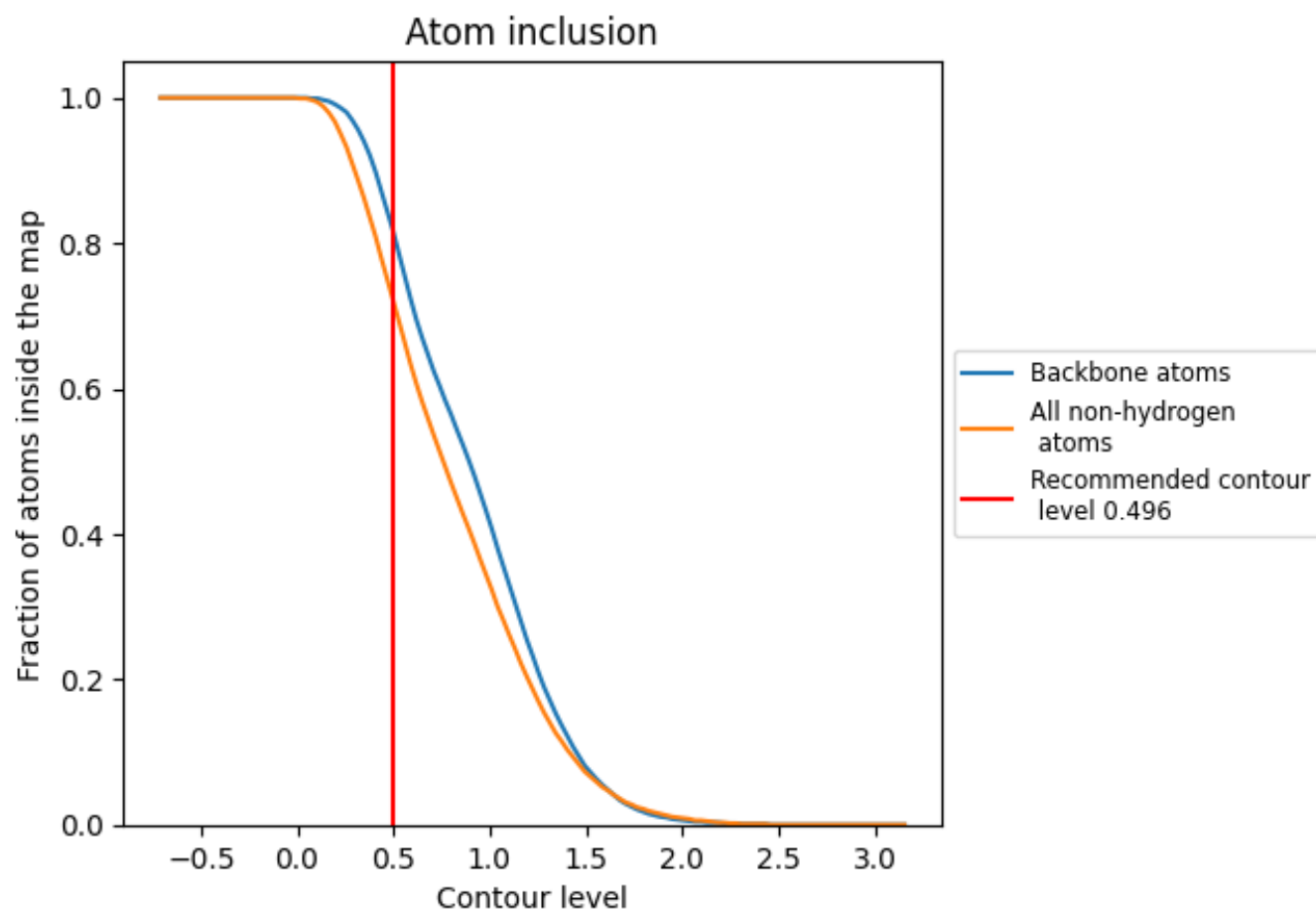
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.496).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 72% 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 (0.496) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7240	 0.4610
0	 0.6330	 0.4290
1	 0.6850	 0.4560
2	 0.6250	 0.4610
3	 0.7680	 0.5150
4	 0.3450	 0.2700
5	 0.6680	 0.3240
6	 0.9230	 0.5390
7	 0.5350	 0.3740
A	 0.9060	 0.5280
B	 0.8640	 0.5420
C	 0.7820	 0.5370
D	 0.7250	 0.5060
E	 0.7500	 0.4970
F	 0.7050	 0.4860
G	 0.6930	 0.4690
H	 0.7200	 0.5050
I	 0.7790	 0.5140
J	 0.7820	 0.5380
K	 0.8290	 0.5370
L	 0.7440	 0.4820
M	 0.8480	 0.5370
N	 0.8440	 0.5450
O	 0.8150	 0.5270
P	 0.8290	 0.5300
Q	 0.8300	 0.5380
R	 0.7590	 0.4780
S	 0.7130	 0.4700
T	 0.8070	 0.5200
U	 0.7210	 0.4580
V	 0.2120	 0.1250
W	 0.8030	 0.5320
X	 0.6910	 0.4480
Y	 0.5720	 0.4070
Z	 0.6900	 0.4830

