wwPDB EM Validation Summary Report (i)

Aug 23, 2026 – 03:54 pm BST

PDB ID	:	9HFN / pdb_00009hfn
EMDB ID	:	EMD-52118
Title	:	Translation-initiation state of human mitochondrial ribosome small subunit (State E)
Authors	:	Finke, A.F.; Heinrichs, M.; Aibara, S.; Richter-Dennerlein, R.; Hillen, H.S.
Deposited on	:	2024-11-18
Resolution	:	3.30 Å(reported)
Based on initial models	:	7PO1, 7PO2

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

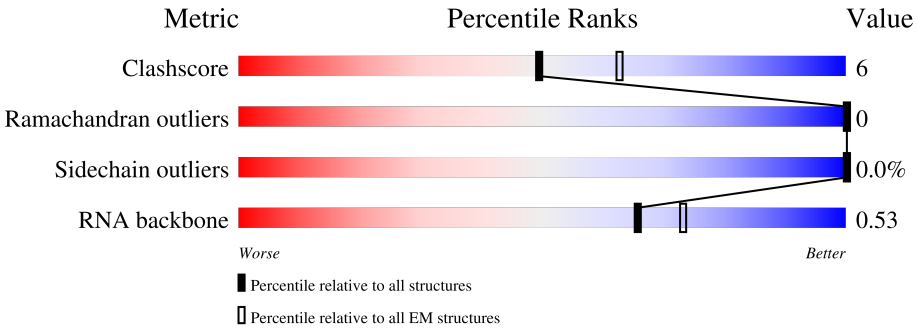
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

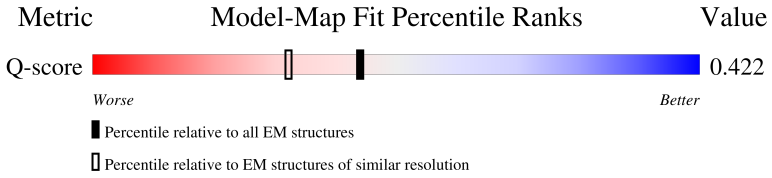
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	0	218	19% 78% 19% .
2	1	323	9% 75% 11% 15%
3	2	118	35% 75% 16% 8%

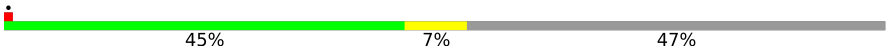
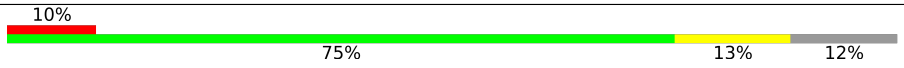
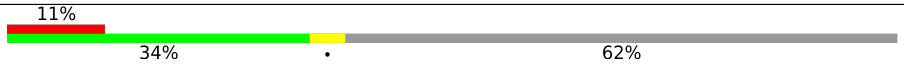
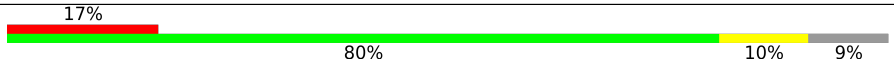
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Mol	Chain	Length	Quality of chain
4	3	199	31% 5% 64%
5	4	689	47% 74% 11% 14%
6	7	727	13% 47% 10% 43%
7	8	278	17% 29% 67%
8	A	955	57% 33% 5% 6%
9	B	296	66% 8% 26%
10	C	167	9% 66% 13% 21%
11	D	430	15% 72% 7% 21%
12	E	125	15% 86% 12%
13	F	242	18% 73% 13% 14%
14	G	396	8% 64% 13% 23%
15	H	201	6% 59% 10% 31%
16	I	194	7% 60% 11% 29%
17	J	138	5% 70% 7% 22%
18	K	128	65% 14% 21%
19	L	257	7% 57% 9% 34%
20	M	137	69% 15% 16%
21	N	130	71% 13% 16%
22	O	258	5% 68% 7% 25%
23	P	142	60% 8% 32%
24	Q	87	85% 13%
25	R	360	70% 11% 19%
26	S	190	7% 62% 9% 29%
27	T	173	88% 9%
28	U	205	76% 10% 14%

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Mol	Chain	Length	Quality of chain
29	V	414	
30	W	187	
31	X	398	
32	Y	395	
33	Z	106	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	GTP	7	802	-	-	X	-
40	ATP	X	403	-	-	X	-

2 Entry composition (i)

There are 40 unique types of molecules in this entry. The entry contains 69310 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
			Total	C	N	O	S		
1	0	212	1765	1116	336	308	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	276	2238	1419	381	427	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	108	867	540	171	148	8	0	0

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
			Total	C	N	O	S		
4	3	71	629	403	135	90	1	0	0

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

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

- Molecule 6 is a protein called Translation initiation factor IF-2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	416	Total	C	N	O	S	0	0
			3185	2000	550	624	11		

- Molecule 7 is a protein called Translation initiation factor IF-3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	93	Total	C	N	O	S	0	0
			752	473	134	141	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	243	LEU	PHE	variant	UNP Q9H2K0

- Molecule 8 is a RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	896	Total	C	N	O	P	0	0
			19041	8535	3441	6169	896		

- Molecule 9 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	220	Total	C	N	O	S	0	0
			1789	1142	324	313	10		

- Molecule 10 is a protein called 28S ribosomal protein S24, mitochondrial.

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

- Molecule 11 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	338	Total	C	N	O	S	0	0
			2691	1689	508	481	13		

- Molecule 12 is a protein called 28S ribosomal protein S6, mitochondrial.

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

- Molecule 13 is a protein called 28S ribosomal protein S7, mitochondrial.

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

- Molecule 14 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	303	Total	C	N	O	S	0	0
			2491	1584	442	451	14		

- Molecule 15 is a protein called 28S ribosomal protein S10, mitochondrial.

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

- Molecule 16 is a protein called 28S ribosomal protein S11, mitochondrial.

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

- Molecule 17 is a protein called 28S ribosomal protein S12, mitochondrial.

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

- Molecule 18 is a protein called 28S ribosomal protein S14, mitochondrial.

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

- Molecule 19 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	170	Total	C	N	O	S	0	0
			1421	906	263	245	7		

- Molecule 20 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 21 is a protein called 28S ribosomal protein S17, mitochondrial.

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

- Molecule 22 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 23 is a protein called 28S ribosomal protein S18c, mitochondrial.

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

- Molecule 24 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	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 25 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	293	Total	C	N	O	S	0	0
			2393	1524	411	450	8		

- Molecule 26 is a protein called 28S ribosomal protein S23, mitochondrial.

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

- Molecule 27 is a protein called 28S ribosomal protein S25, mitochondrial.

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

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

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

- Molecule 29 is a protein called 28S ribosomal protein S27, mitochondrial.

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

- Molecule 30 is a protein called 28S ribosomal protein S28, mitochondrial.

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

- Molecule 31 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	349	Total	C	N	O	S	0	0
			2830	1810	496	513	11		

- Molecule 32 is a protein called 28S ribosomal protein S31, mitochondrial.

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

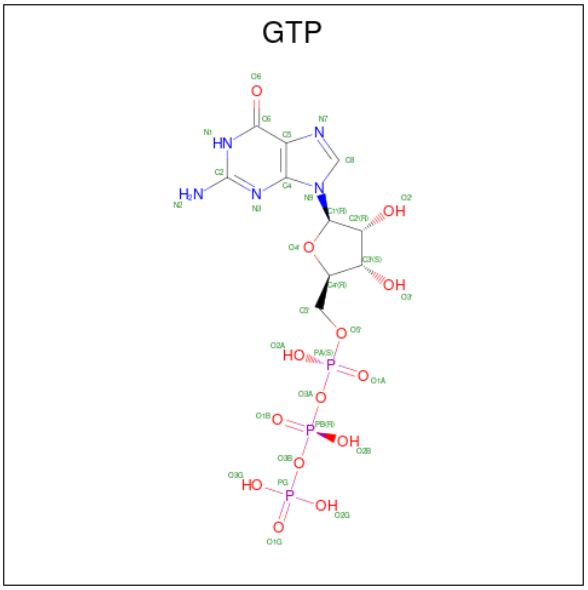
- Molecule 33 is a protein called 28S ribosomal protein S33, mitochondrial.

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

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
34	3	1	Total	Mg	0
			1	1	
34	7	1	Total	Mg	0
			1	1	
34	A	41	Total	Mg	0
			41	41	
34	B	1	Total	Mg	0
			1	1	
34	X	1	Total	Mg	0
			1	1	

- Molecule 35 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
35	7	1	Total	C	N	O	P	0
			32	10	5	14	3	

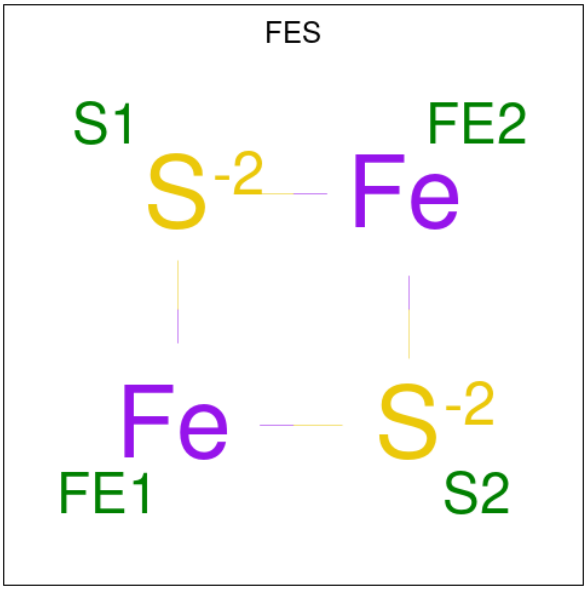
- Molecule 36 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

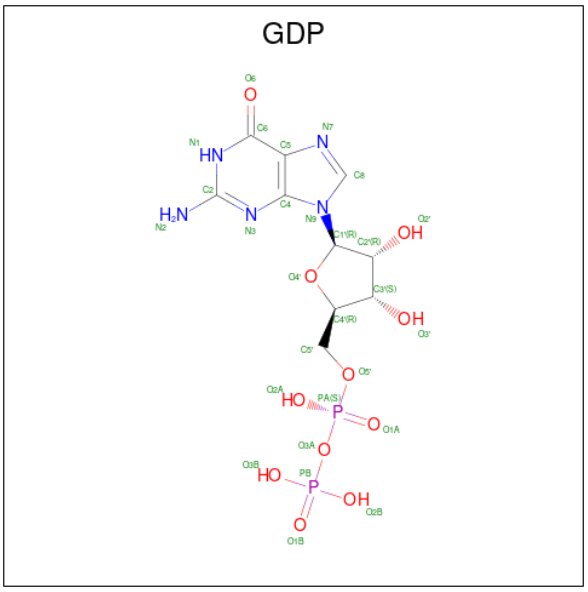
Mol	Chain	Residues	Atoms		AltConf
37	O	1	Total	Zn	0
			1	1	

- Molecule 38 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



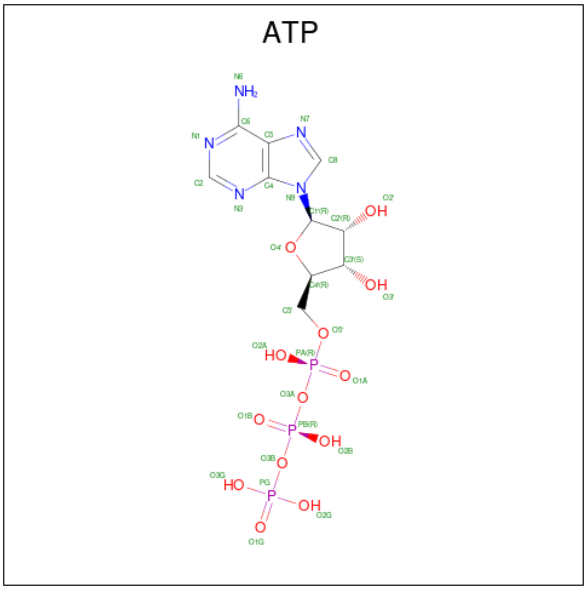
Mol	Chain	Residues	Atoms			AltConf
38	P	1	Total	Fe	S	0
			4	2	2	
38	T	1	Total	Fe	S	0
			4	2	2	

- Molecule 39 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 40 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

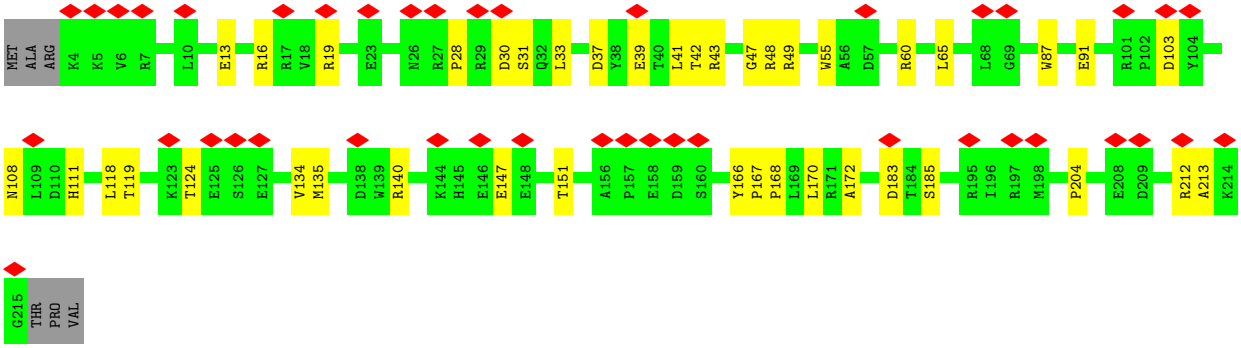
3 Residue-property plots (i)

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

• Molecule 1: 28S ribosomal protein S34, mitochondrial

Chain 0:

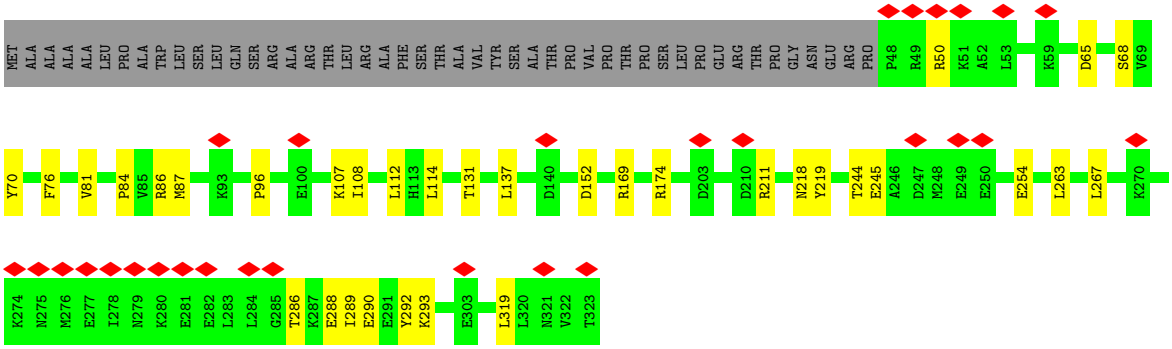




• Molecule 2: 28S ribosomal protein S35, mitochondrial

Chain 1:

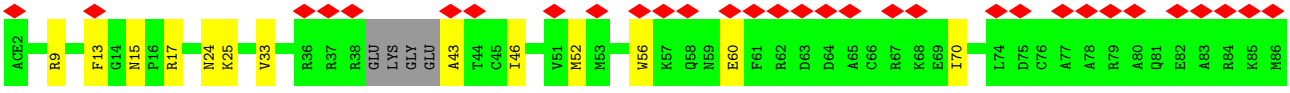


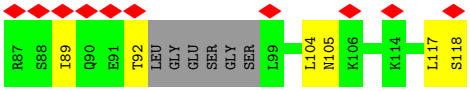


• Molecule 3: Small ribosomal subunit protein mS37

Chain 2:



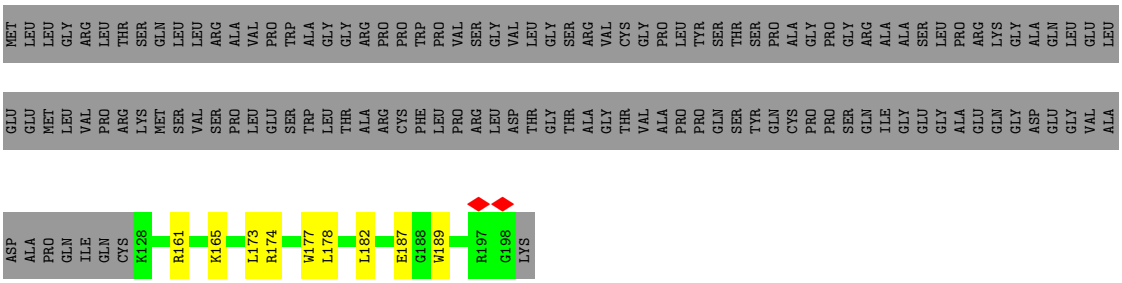




• Molecule 4: Aurora kinase A-interacting protein

Chain 3:

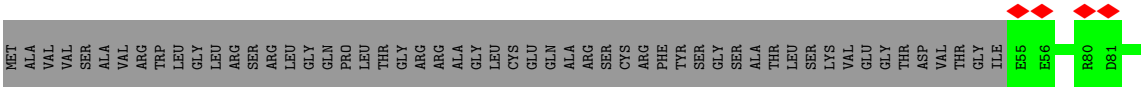


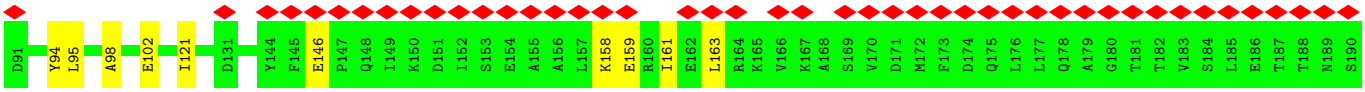


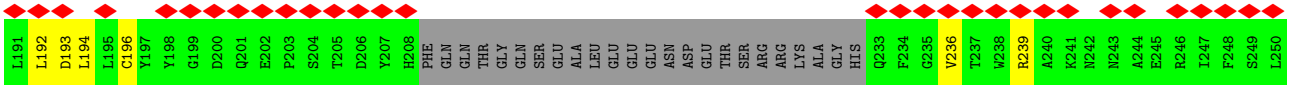
• Molecule 5: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

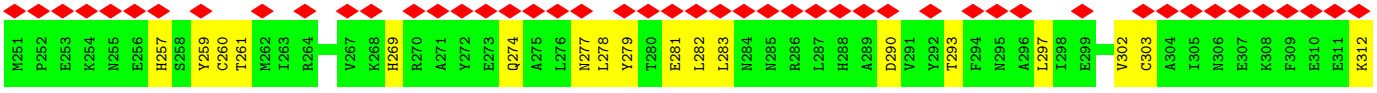
Chain 4:

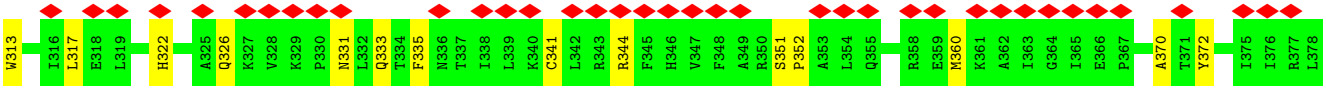


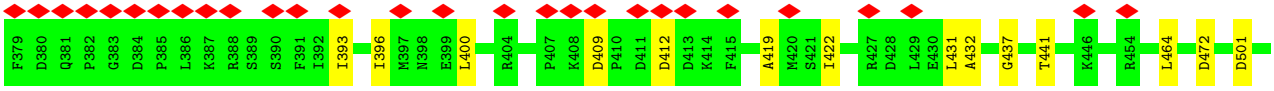


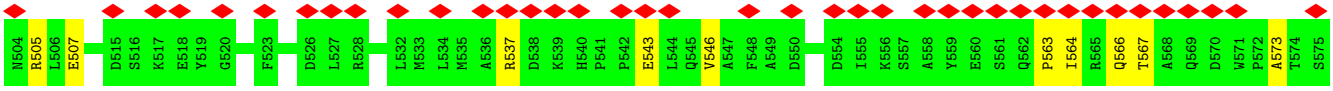


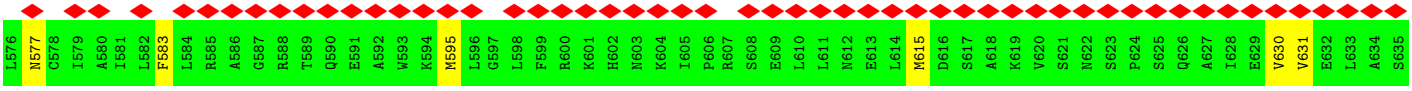


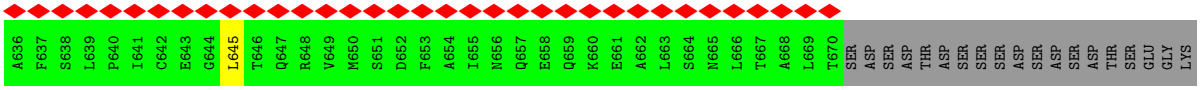






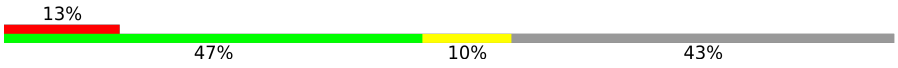


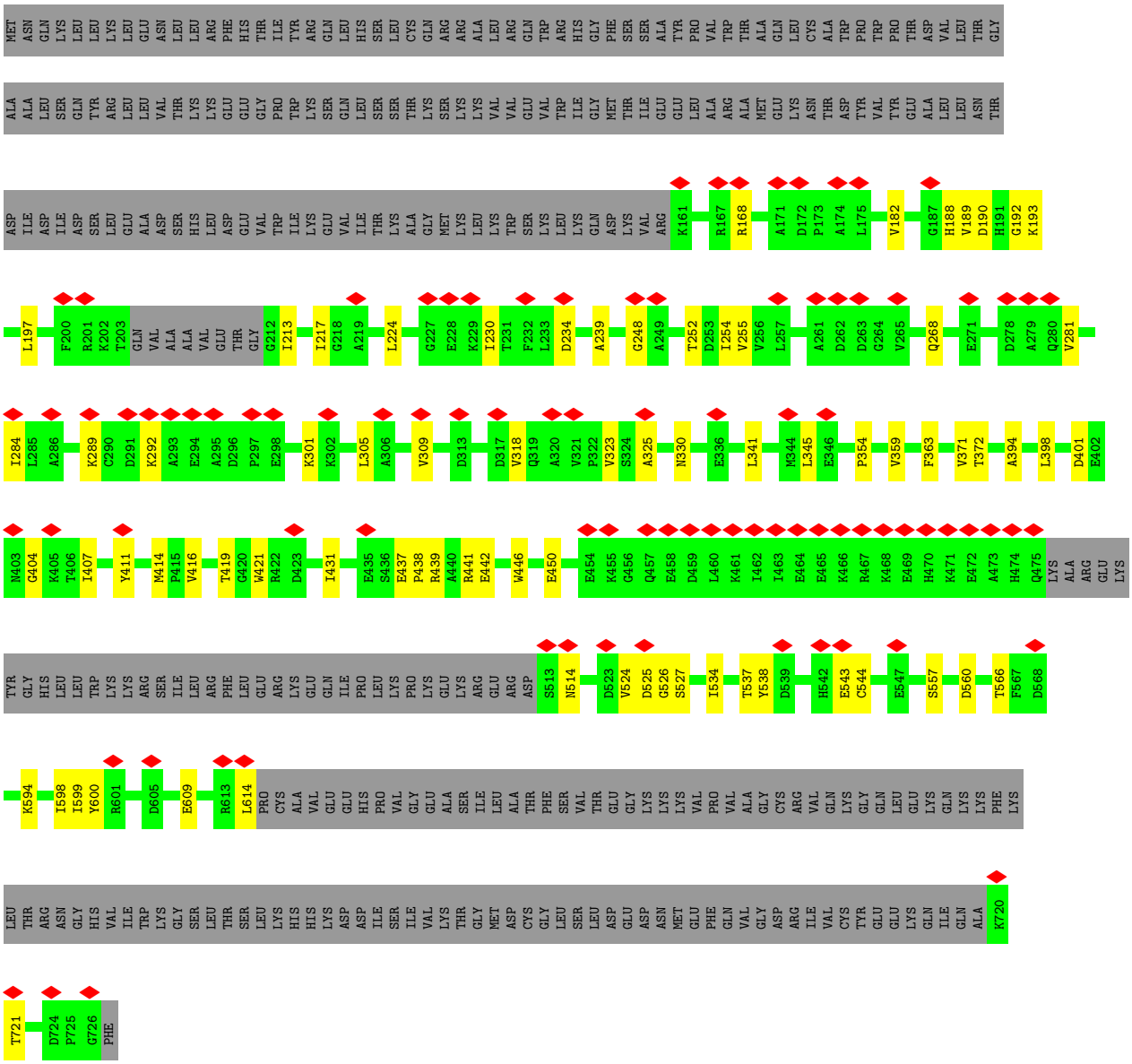




• Molecule 6: Translation initiation factor IF-2, mitochondrial

Chain 7:

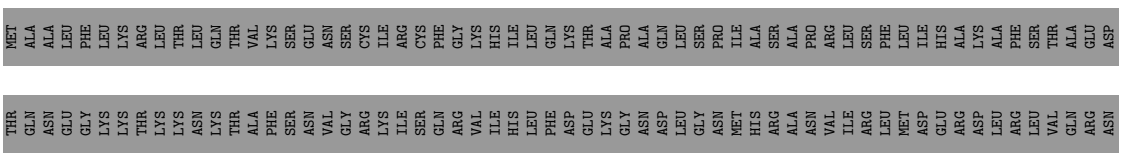


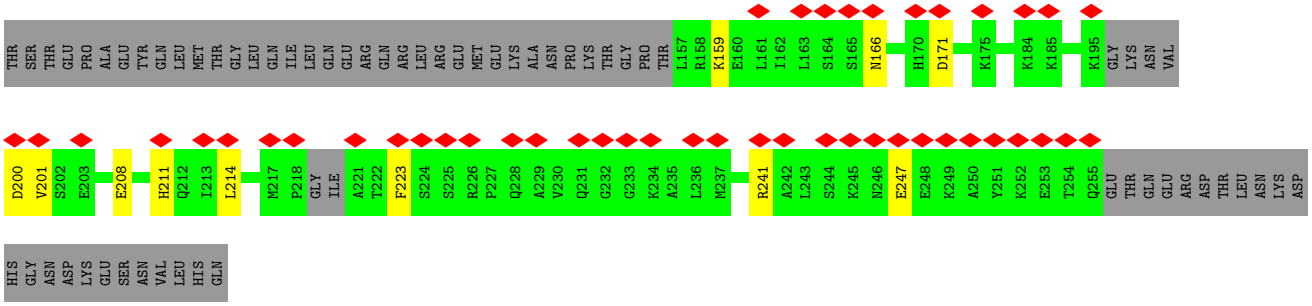


• Molecule 7: Translation initiation factor IF-3, mitochondrial

Chain 8:



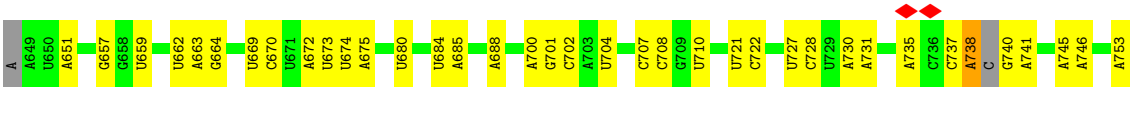




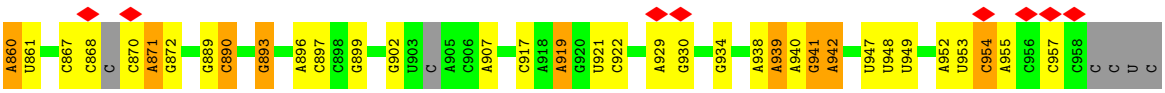
• Molecule 8: 12S mitochondrial rRNA

Chain A:

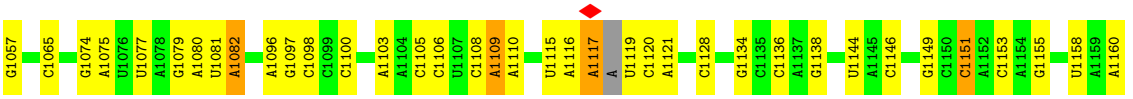


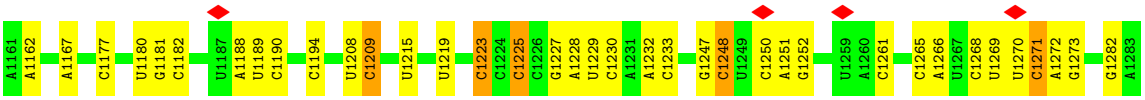


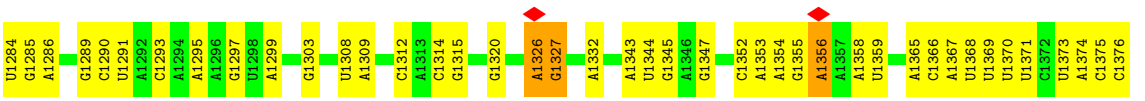


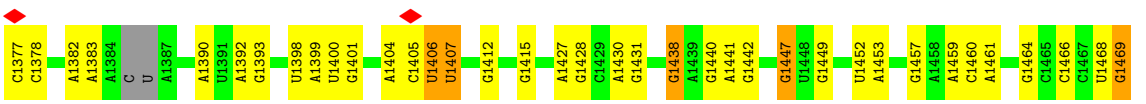




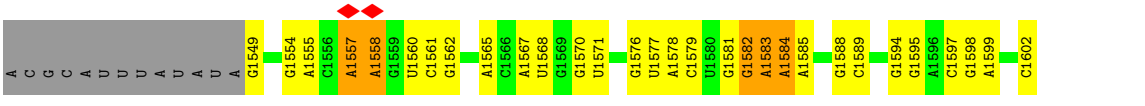






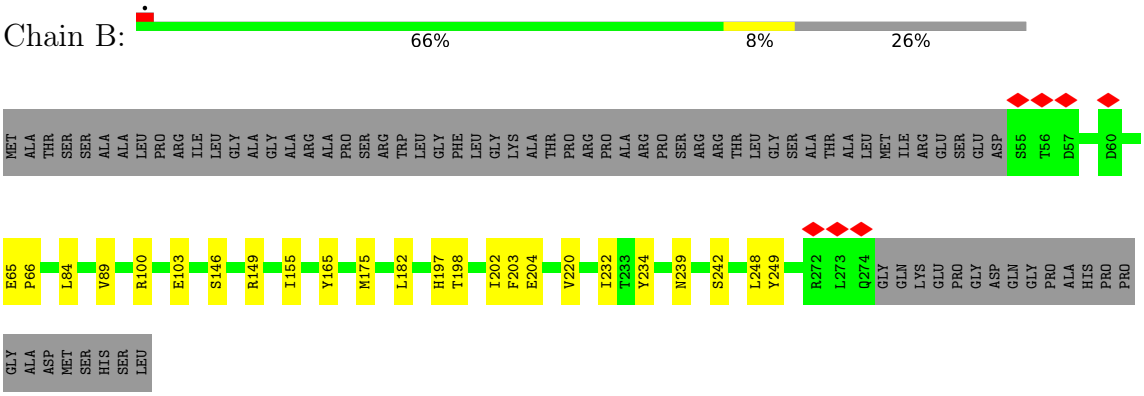






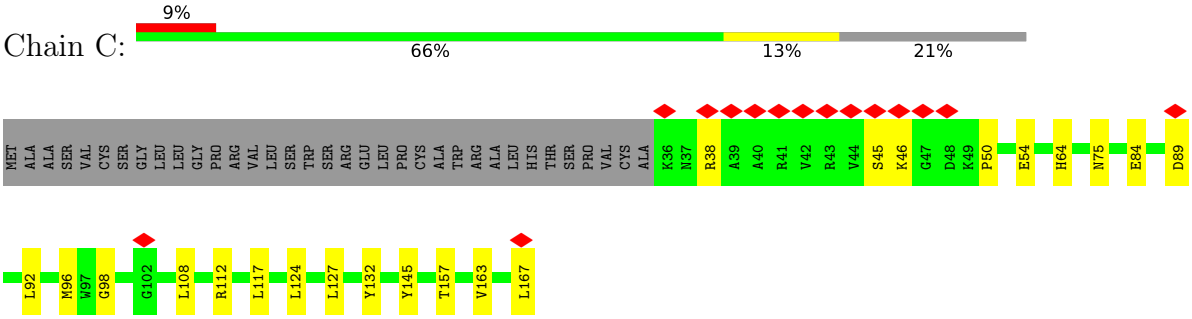
• Molecule 9: 28S ribosomal protein S2, mitochondrial

Chain B:



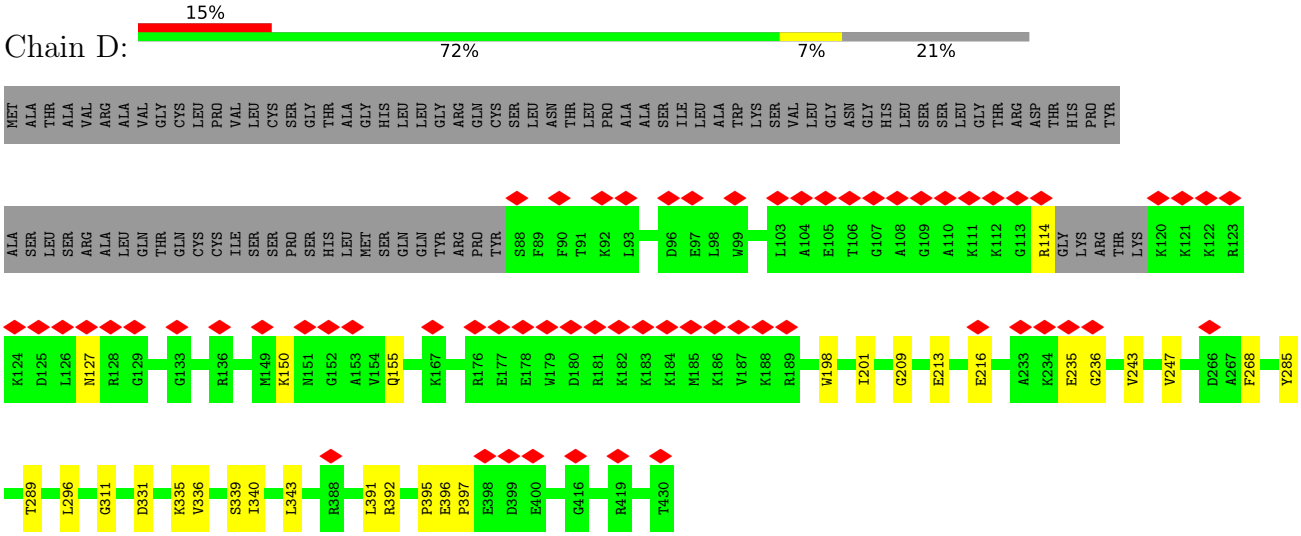
• Molecule 10: 28S ribosomal protein S24, mitochondrial

Chain C:



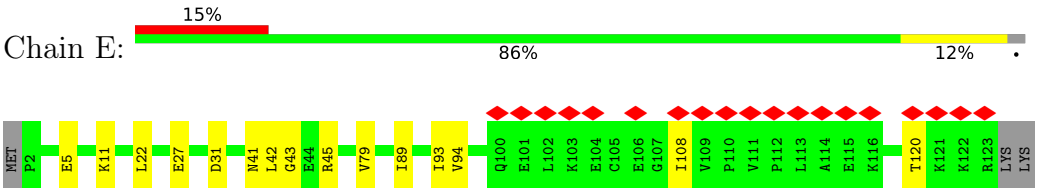
• Molecule 11: 28S ribosomal protein S5, mitochondrial

Chain D:



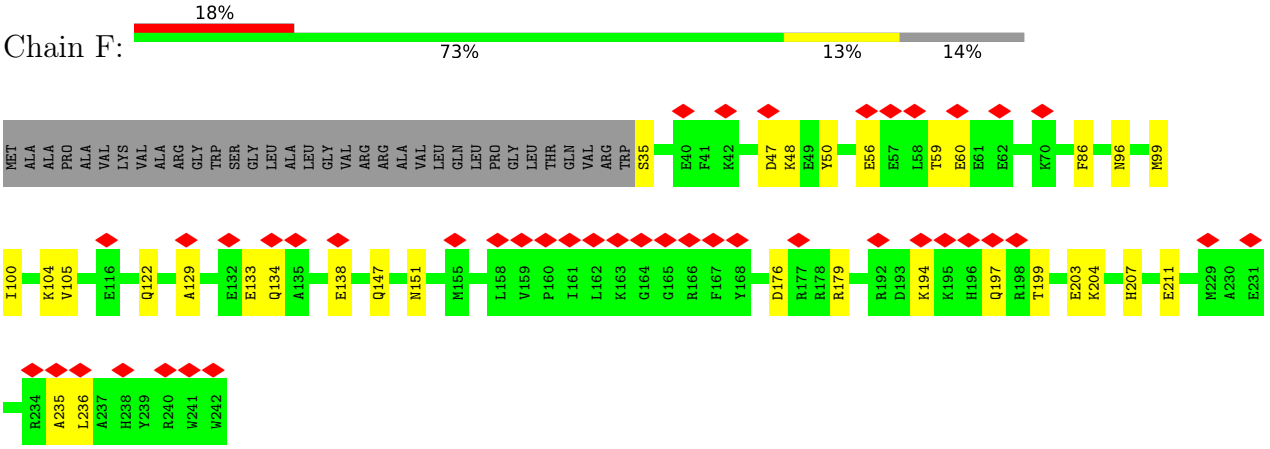
• Molecule 12: 28S ribosomal protein S6, mitochondrial

Chain E:



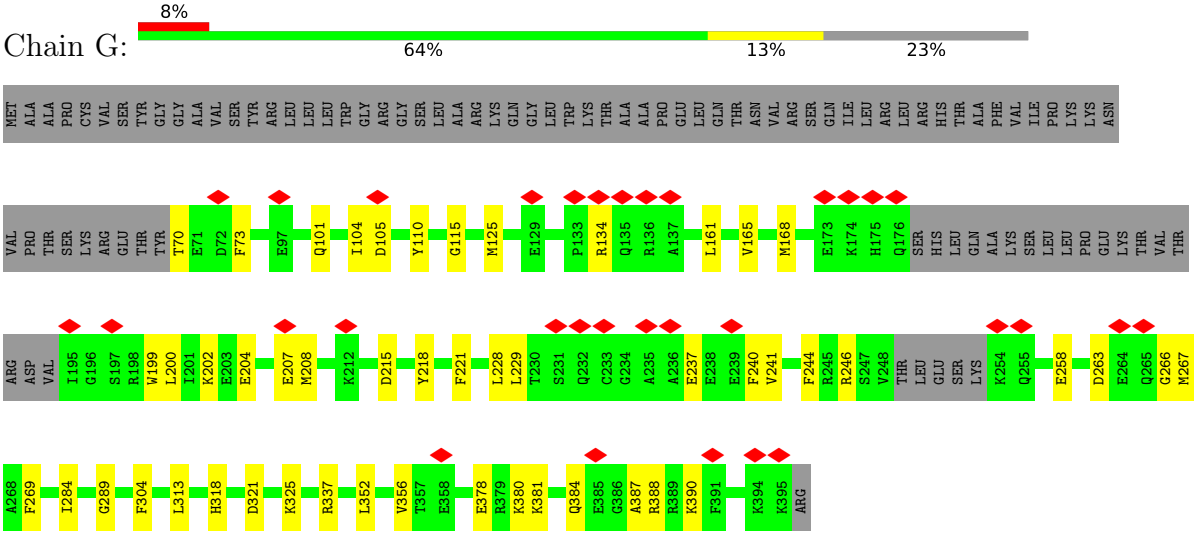
• Molecule 13: 28S ribosomal protein S7, mitochondrial

Chain F:



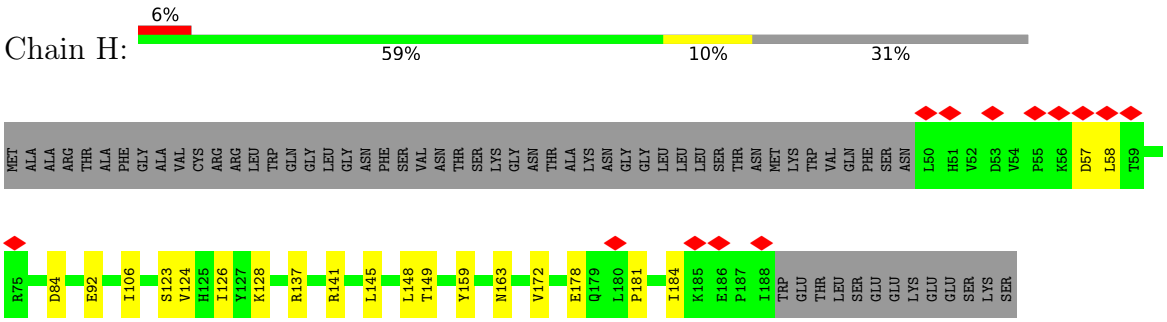
• Molecule 14: 28S ribosomal protein S9, mitochondrial

Chain G:



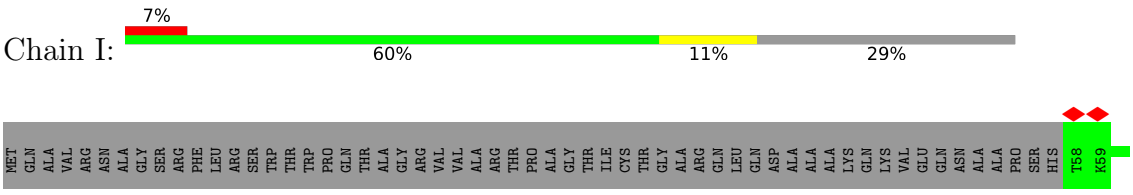
• Molecule 15: 28S ribosomal protein S10, mitochondrial

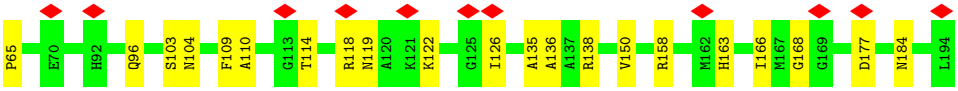
Chain H:



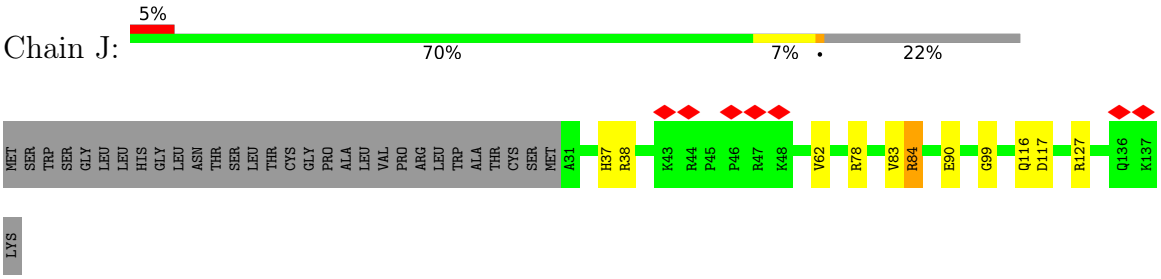
• Molecule 16: 28S ribosomal protein S11, mitochondrial

Chain I:

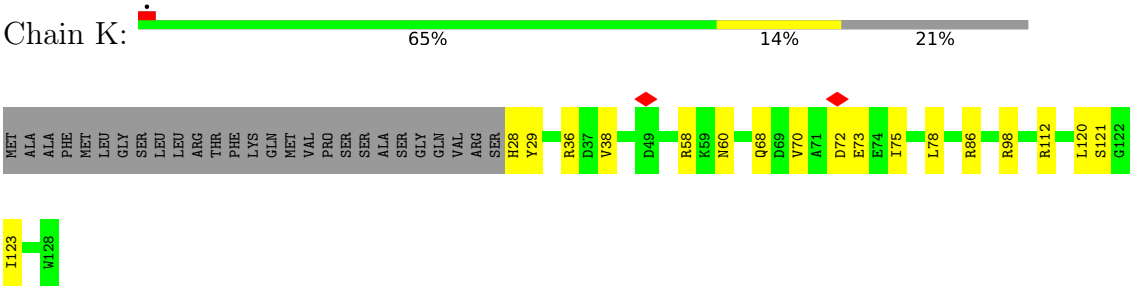




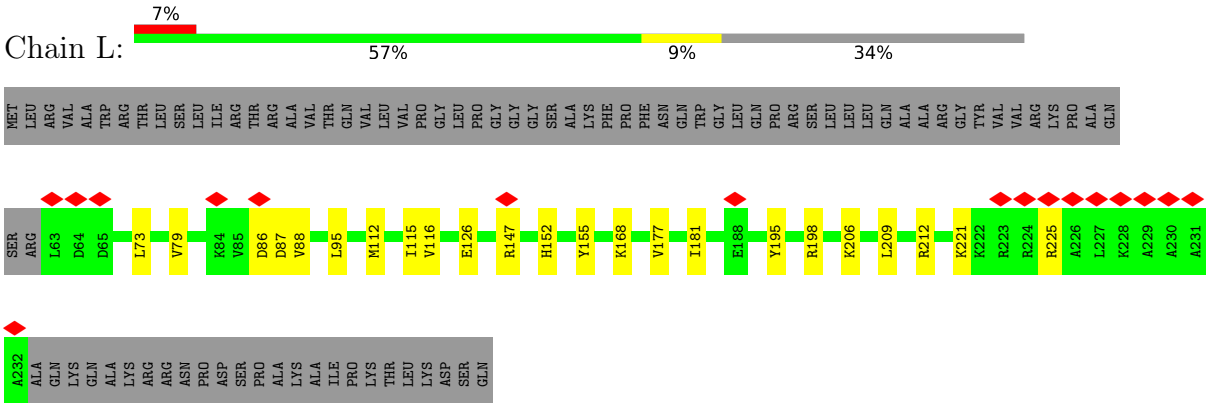
• Molecule 17: 28S ribosomal protein S12, mitochondrial



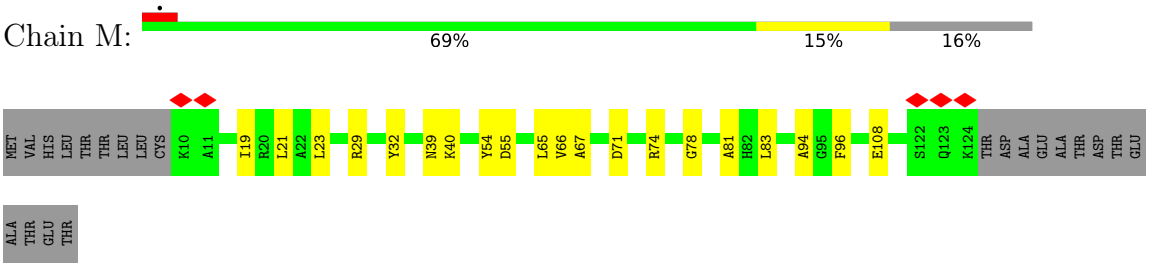
• Molecule 18: 28S ribosomal protein S14, mitochondrial



• Molecule 19: 28S ribosomal protein S15, mitochondrial

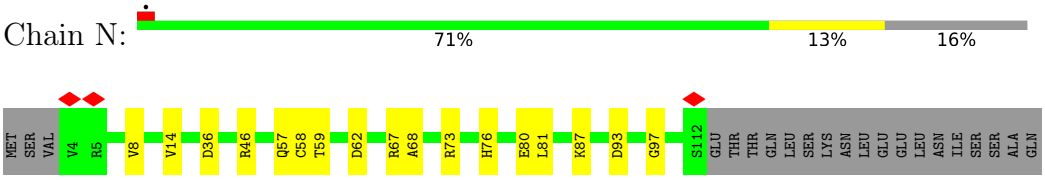


• Molecule 20: 28S ribosomal protein S16, mitochondrial



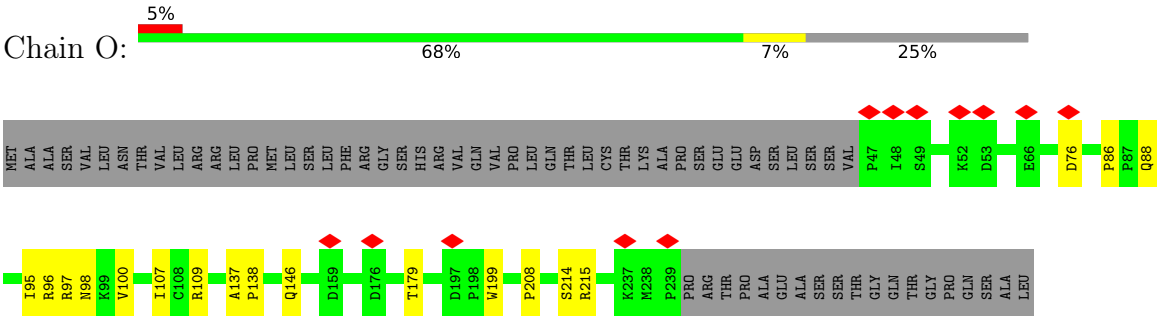
• Molecule 21: 28S ribosomal protein S17, mitochondrial

Chain N:



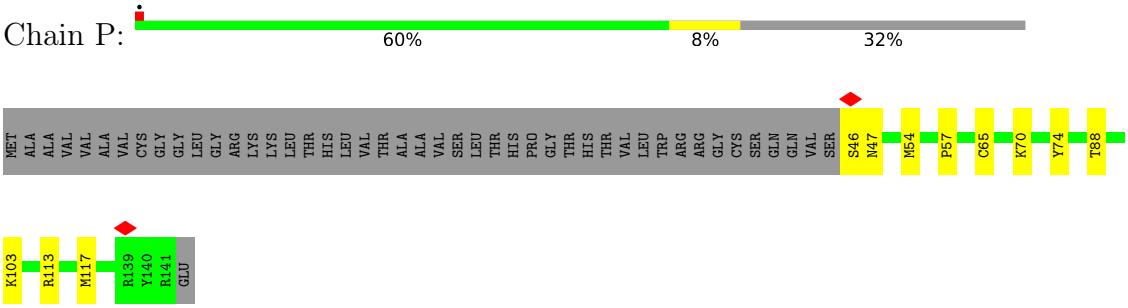
• Molecule 22: 28S ribosomal protein S18b, mitochondrial

Chain O:



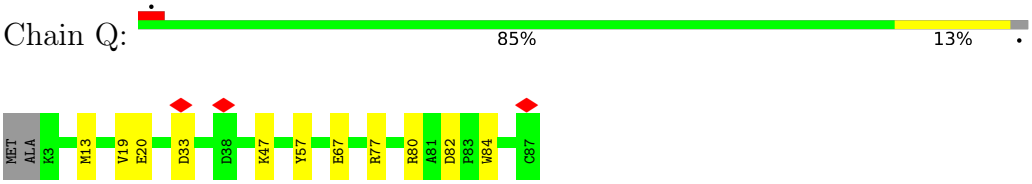
• Molecule 23: 28S ribosomal protein S18c, mitochondrial

Chain P:



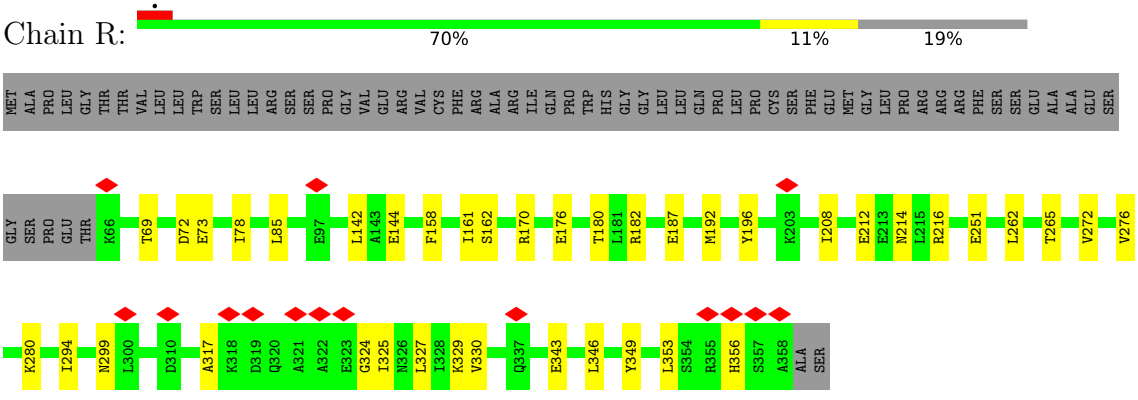
• Molecule 24: 28S ribosomal protein S21, mitochondrial

Chain Q:



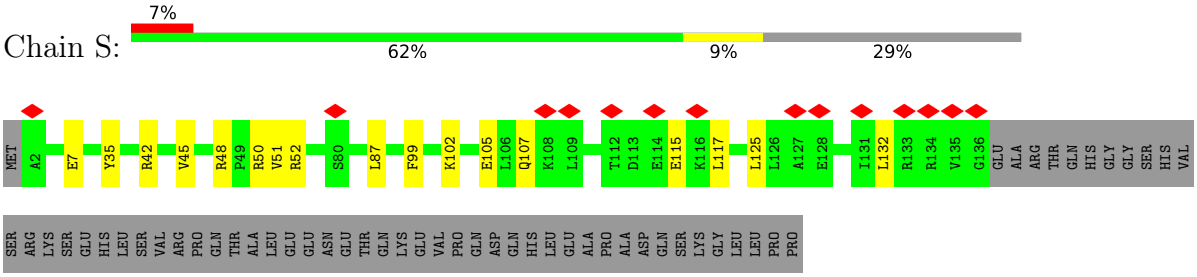
• Molecule 25: 28S ribosomal protein S22, mitochondrial

Chain R:



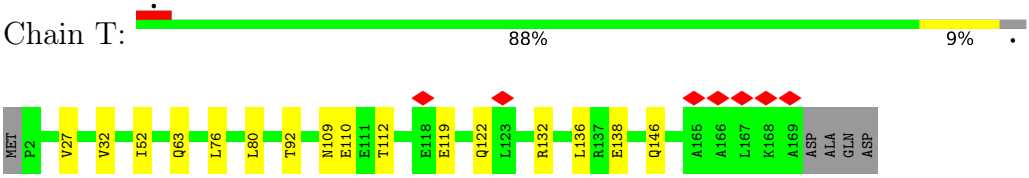
• Molecule 26: 28S ribosomal protein S23, mitochondrial

Chain S:



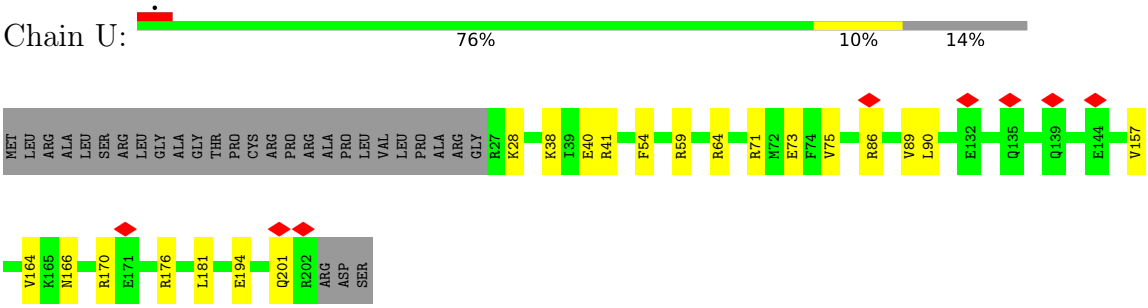
• Molecule 27: 28S ribosomal protein S25, mitochondrial

Chain T:



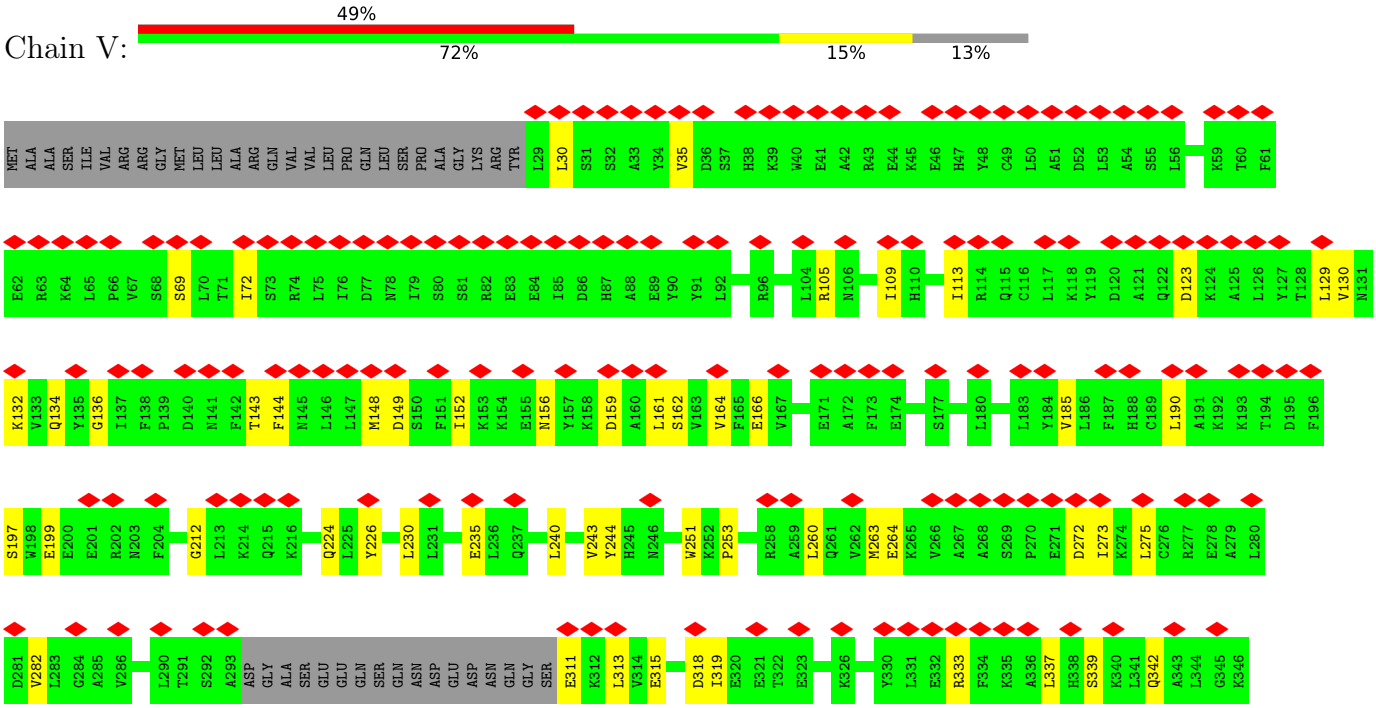
• Molecule 28: 28S ribosomal protein S26, mitochondrial

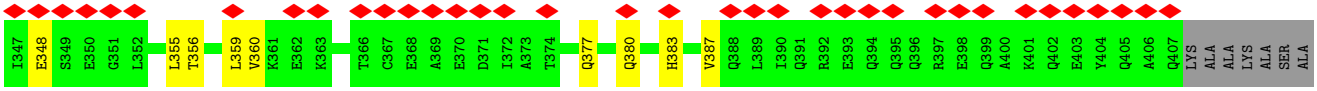
Chain U:



• Molecule 29: 28S ribosomal protein S27, mitochondrial

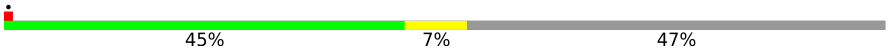
Chain V:

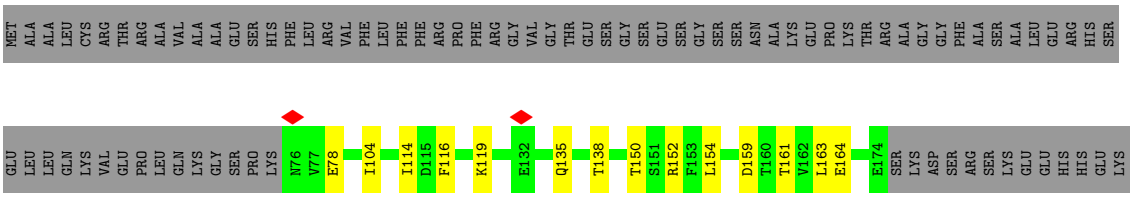




• Molecule 30: 28S ribosomal protein S28, mitochondrial

Chain W:

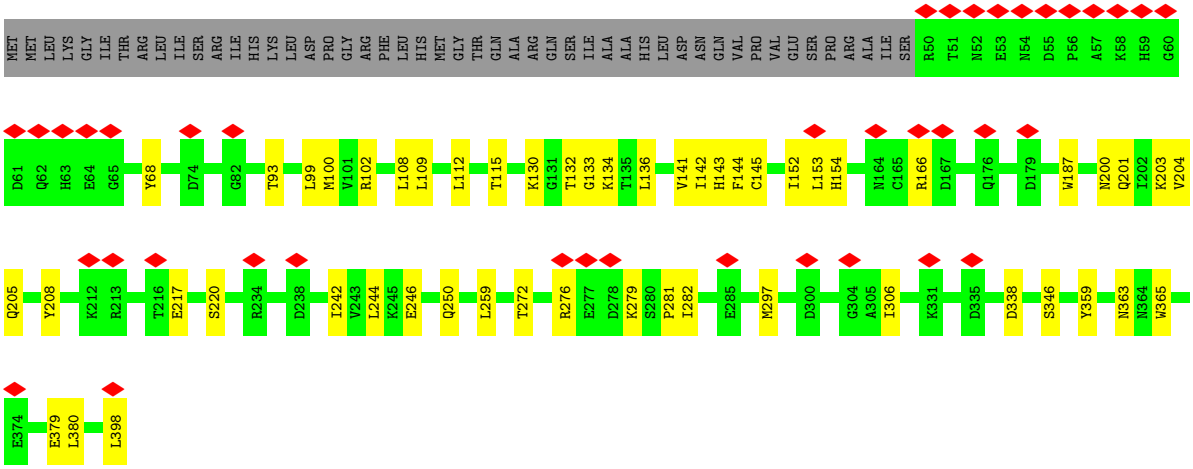




• Molecule 31: 28S ribosomal protein S29, mitochondrial

Chain X:

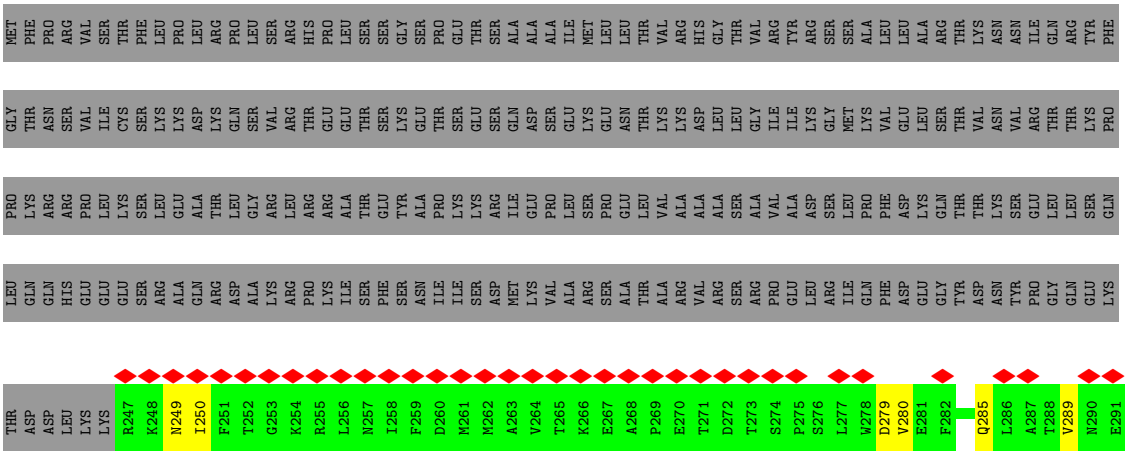


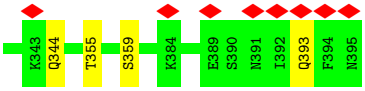


• Molecule 32: 28S ribosomal protein S31, mitochondrial

Chain Y:



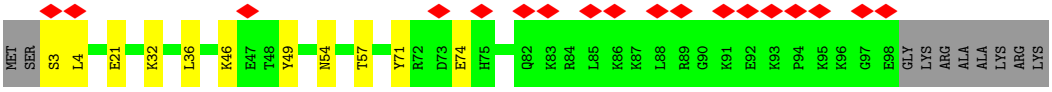




• Molecule 33: 28S ribosomal protein S33, mitochondrial

Chain Z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18003	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 ($e^-/Å^2$)	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	2.240	Depositor
Minimum map value	-0.393	Depositor
Average map value	0.022	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.43	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	0	0.15	0/1811	0.25	0/2452
2	1	0.15	0/2285	0.25	0/3090
3	2	0.15	0/877	0.25	0/1171
4	3	0.17	0/640	0.28	0/844
5	4	0.12	0/4904	0.24	0/6636
6	7	0.15	0/3231	0.25	0/4370
7	8	0.12	0/759	0.24	0/1012
8	A	0.23	0/21295	0.27	2/33141 (0.0%)
9	B	0.23	0/1832	0.27	0/2480
10	C	0.19	0/1113	0.27	0/1505
11	D	0.20	0/2742	0.27	0/3670
12	E	0.19	0/989	0.26	0/1335
13	F	0.14	0/1767	0.24	0/2373
14	G	0.16	0/2544	0.25	0/3408
15	H	0.18	0/1162	0.28	0/1575
16	I	0.16	0/1039	0.25	0/1400
17	J	0.20	0/845	0.25	0/1137
18	K	0.19	0/880	0.26	0/1182
19	L	0.19	0/1445	0.28	0/1932
20	M	0.22	0/934	0.29	0/1255
21	N	0.20	0/877	0.24	0/1187
22	O	0.20	0/1648	0.25	0/2243
23	P	0.21	0/788	0.25	0/1058
24	Q	0.21	0/748	0.24	0/994
25	R	0.19	0/2440	0.26	0/3295
26	S	0.18	0/1138	0.24	0/1533
27	T	0.20	0/1402	0.26	0/1883
28	U	0.17	0/1510	0.23	0/2025
29	V	0.12	0/3030	0.26	0/4093
30	W	0.20	0/795	0.25	0/1071
31	X	0.14	0/2902	0.25	0/3928
32	Y	0.15	0/1280	0.24	0/1725

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	Z	0.16	0/828	0.24	0/1104
All	All	0.19	0/72480	0.26	2/102107 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1582	G	P-O3'-C3'	-8.08	108.09	120.20
8	A	1581	G	P-O3'-C3'	-6.60	110.30	120.20

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	33	0
2	1	2238	0	2269	24	0
3	2	867	0	908	15	0
4	3	629	0	702	10	0
5	4	4795	0	4796	55	0
6	7	3185	0	3209	62	0
7	8	752	0	783	7	0
8	A	19041	0	9676	197	0
9	B	1789	0	1781	19	0
10	C	1083	0	1088	17	0
11	D	2691	0	2754	20	0
12	E	972	0	1000	13	0
13	F	1725	0	1769	23	0
14	G	2491	0	2473	35	0
15	H	1138	0	1173	16	0
16	I	1019	0	1059	17	0
17	J	829	0	874	11	0
18	K	862	0	885	12	0
19	L	1421	0	1506	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	M	913	0	943	17	0
21	N	859	0	922	11	0
22	O	1592	0	1557	14	0
23	P	771	0	800	10	0
24	Q	736	0	749	15	0
25	R	2393	0	2415	28	0
26	S	1111	0	1115	15	0
27	T	1371	0	1393	12	0
28	U	1488	0	1499	22	0
29	V	2969	0	2961	44	0
30	W	783	0	797	10	0
31	X	2830	0	2823	46	0
32	Y	1246	0	1197	10	0
33	Z	810	0	824	7	0
34	3	1	0	0	0	0
34	7	1	0	0	0	0
34	A	41	0	0	0	0
34	B	1	0	0	0	0
34	X	1	0	0	0	0
35	7	32	0	12	21	0
36	A	1	0	0	0	0
37	O	1	0	0	0	0
38	P	4	0	0	1	0
38	T	4	0	0	0	0
39	X	28	0	12	5	0
40	X	31	0	12	13	0
All	All	69310	0	60509	730	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 6.

The worst 5 of 730 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)
31:X:136:LEU:HD12	40:X:403:ATP:H5'2	1.39	1.04
8:A:1598:G:OP1	24:Q:57:TYR:OH	1.84	0.94
5:4:260:CYS:SG	5:4:293:THR:OG1	2.26	0.92
8:A:1382:A:OP1	31:X:166:ARG:NH2	2.04	0.90
6:7:213:ILE:HA	35:7:802:GTP:O1G	1.74	0.87

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	274/323 (85%)	267 (97%)	7 (3%)	0	100	100
3	2	102/118 (86%)	96 (94%)	6 (6%)	0	100	100
4	3	69/199 (35%)	67 (97%)	2 (3%)	0	100	100
5	4	588/689 (85%)	569 (97%)	19 (3%)	0	100	100
6	7	408/727 (56%)	397 (97%)	11 (3%)	0	100	100
7	8	87/278 (31%)	81 (93%)	6 (7%)	0	100	100
9	B	218/296 (74%)	213 (98%)	5 (2%)	0	100	100
10	C	130/167 (78%)	125 (96%)	5 (4%)	0	100	100
11	D	334/430 (78%)	320 (96%)	14 (4%)	0	100	100
12	E	120/125 (96%)	118 (98%)	2 (2%)	0	100	100
13	F	206/242 (85%)	205 (100%)	1 (0%)	0	100	100
14	G	297/396 (75%)	293 (99%)	4 (1%)	0	100	100
15	H	137/201 (68%)	132 (96%)	5 (4%)	0	100	100
16	I	135/194 (70%)	129 (96%)	6 (4%)	0	100	100
17	J	105/138 (76%)	97 (92%)	8 (8%)	0	100	100
18	K	99/128 (77%)	97 (98%)	2 (2%)	0	100	100
19	L	168/257 (65%)	162 (96%)	6 (4%)	0	100	100
20	M	113/137 (82%)	108 (96%)	5 (4%)	0	100	100
21	N	107/130 (82%)	105 (98%)	2 (2%)	0	100	100
22	O	191/258 (74%)	189 (99%)	2 (1%)	0	100	100
23	P	94/142 (66%)	91 (97%)	3 (3%)	0	100	100
24	Q	83/87 (95%)	83 (100%)	0	0	100	100
25	R	291/360 (81%)	275 (94%)	16 (6%)	0	100	100
26	S	133/190 (70%)	132 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	T	166/173 (96%)	165 (99%)	1 (1%)	0	100	100
28	U	174/205 (85%)	172 (99%)	2 (1%)	0	100	100
29	V	358/414 (86%)	346 (97%)	12 (3%)	0	100	100
30	W	97/187 (52%)	93 (96%)	4 (4%)	0	100	100
31	X	347/398 (87%)	335 (96%)	12 (4%)	0	100	100
32	Y	147/395 (37%)	142 (97%)	5 (3%)	0	100	100
33	Z	94/106 (89%)	92 (98%)	2 (2%)	0	100	100
All	All	6082/8308 (73%)	5903 (97%)	179 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	185/190 (97%)	185 (100%)	0	100	100
2	1	254/291 (87%)	254 (100%)	0	100	100
3	2	93/100 (93%)	93 (100%)	0	100	100
4	3	65/166 (39%)	65 (100%)	0	100	100
5	4	529/609 (87%)	529 (100%)	0	100	100
6	7	345/621 (56%)	345 (100%)	0	100	100
7	8	85/247 (34%)	85 (100%)	0	100	100
9	B	194/249 (78%)	194 (100%)	0	100	100
10	C	115/143 (80%)	115 (100%)	0	100	100
11	D	282/357 (79%)	282 (100%)	0	100	100
12	E	104/107 (97%)	104 (100%)	0	100	100
13	F	185/209 (88%)	185 (100%)	0	100	100
14	G	262/342 (77%)	262 (100%)	0	100	100
15	H	129/180 (72%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	I	105/147 (71%)	105 (100%)	0	100	100
17	J	92/118 (78%)	91 (99%)	1 (1%)	65	76
18	K	91/113 (80%)	91 (100%)	0	100	100
19	L	155/226 (69%)	155 (100%)	0	100	100
20	M	94/113 (83%)	94 (100%)	0	100	100
21	N	95/115 (83%)	95 (100%)	0	100	100
22	O	174/230 (76%)	174 (100%)	0	100	100
23	P	87/123 (71%)	87 (100%)	0	100	100
24	Q	78/79 (99%)	78 (100%)	0	100	100
25	R	262/318 (82%)	262 (100%)	0	100	100
26	S	116/164 (71%)	116 (100%)	0	100	100
27	T	153/157 (98%)	153 (100%)	0	100	100
28	U	152/174 (87%)	152 (100%)	0	100	100
29	V	325/364 (89%)	325 (100%)	0	100	100
30	W	86/158 (54%)	86 (100%)	0	100	100
31	X	309/351 (88%)	309 (100%)	0	100	100
32	Y	137/357 (38%)	137 (100%)	0	100	100
33	Z	88/95 (93%)	88 (100%)	0	100	100
All	All	5426/7213 (75%)	5425 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	J	84	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
29	V	145	ASN
31	X	195	ASN
29	V	324	GLN
29	V	388	GLN
32	Y	257	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	A	887/955 (92%)	131 (14%)	1 (0%)

5 of 131 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	651	A
8	A	680	U
8	A	688	A
8	A	704	U
8	A	721	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	1406	U

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
38	FES	P	201	12,23	0,4,4	-	-	-		
38	FES	T	201	27,20	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	GTP	7	802	34	30,34,34	0.50	0	46,54,54	0.72	1 (2%)
40	ATP	X	403	34	29,33,33	0.50	0	44,52,52	0.60	0
39	GDP	X	402	-	28,30,30	0.48	0	44,47,47	0.50	0

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
38	FES	P	201	12,23	-	-	0/1/1/1
38	FES	T	201	27,20	-	-	0/1/1/1
35	GTP	7	802	34	-	4/22/38/38	0/3/3/3
40	ATP	X	403	34	-	5/22/38/38	0/3/3/3
39	GDP	X	402	-	-	1/16/32/32	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	7	802	GTP	PB-O3B-PG	-2.93	122.76	132.83

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	7	802	GTP	C5'-O5'-PA-O3A
40	X	403	ATP	PB-O3B-PG-O3G
35	7	802	GTP	C5'-O5'-PA-O2A
40	X	403	ATP	C4'-C5'-O5'-PA
40	X	403	ATP	PB-O3B-PG-O1G

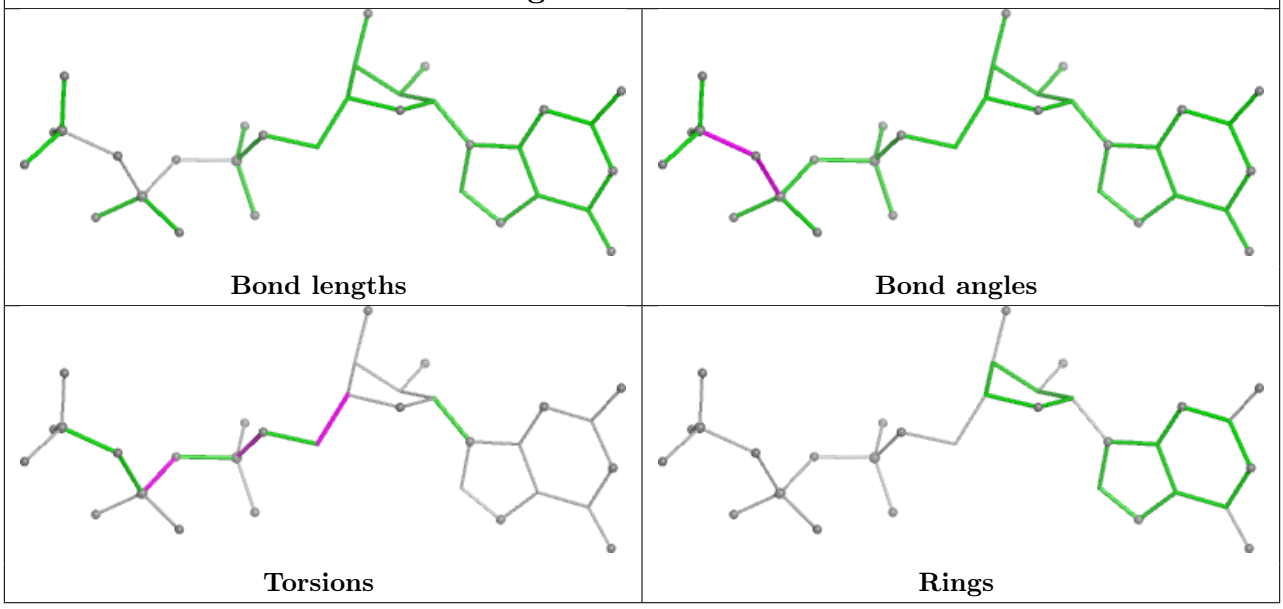
There are no ring outliers.

4 monomers are involved in 40 short contacts:

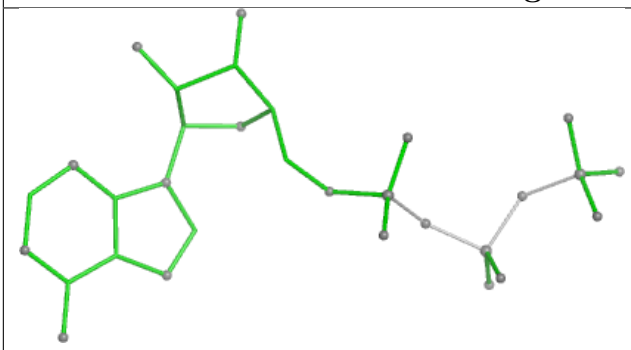
Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	P	201	FES	1	0
35	7	802	GTP	21	0
40	X	403	ATP	13	0
39	X	402	GDP	5	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

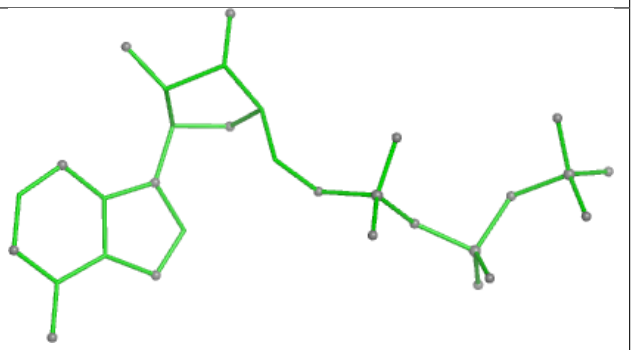
Ligand GTP 7 802



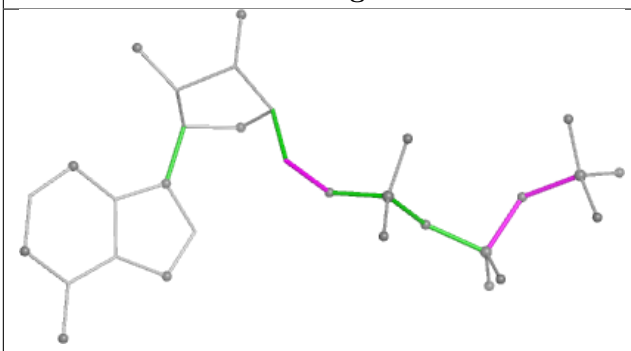
Ligand ATP X 403



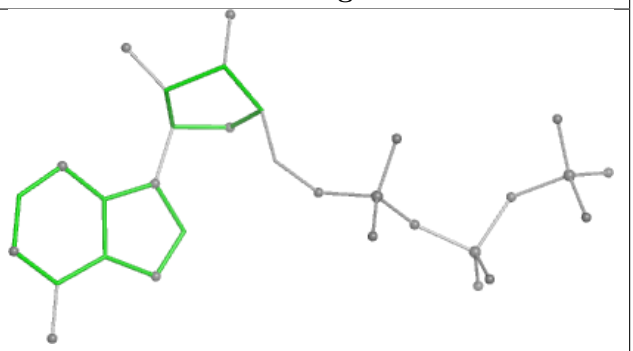
Bond lengths



Bond angles

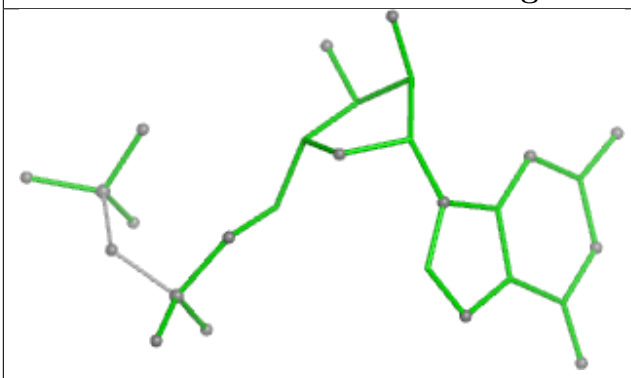


Torsions

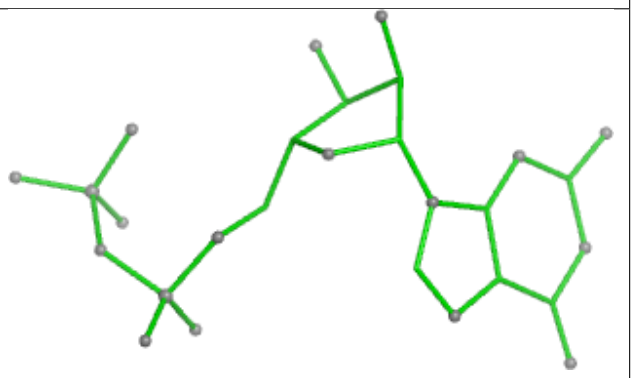


Rings

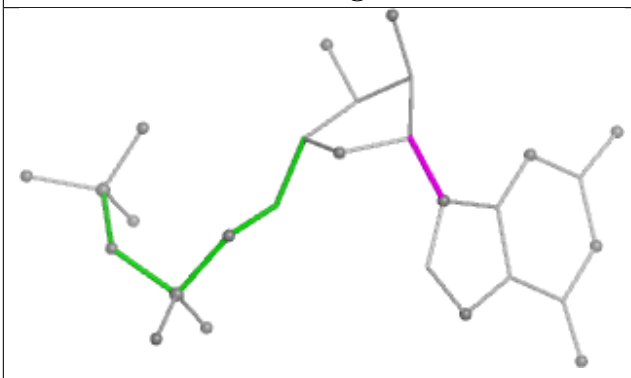
Ligand GDP X 402



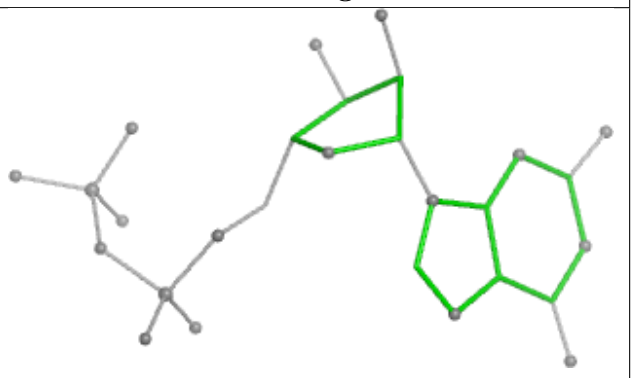
Bond lengths



Bond angles



Torsions



Rings

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.

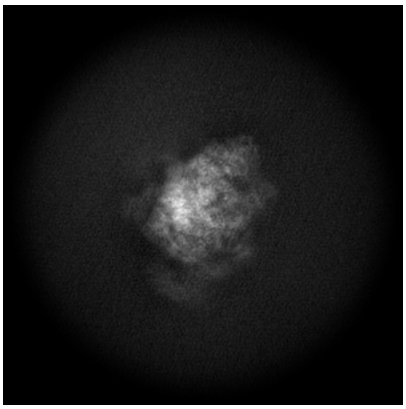
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-52118. These allow visual inspection of the internal detail of the map and identification of artifacts.

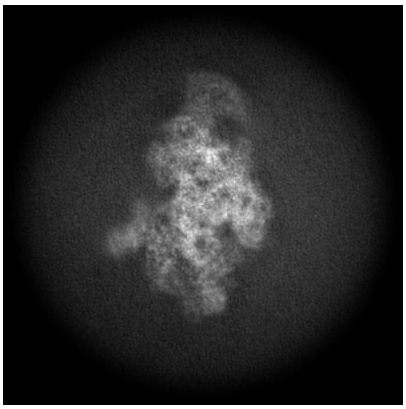
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

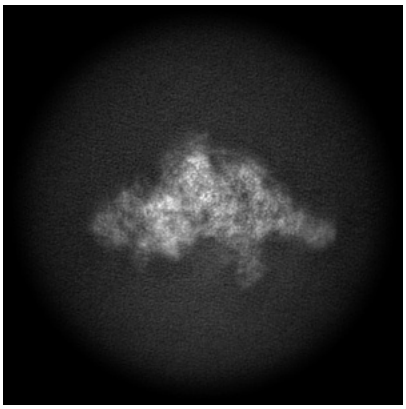
6.1.1 Primary map



X

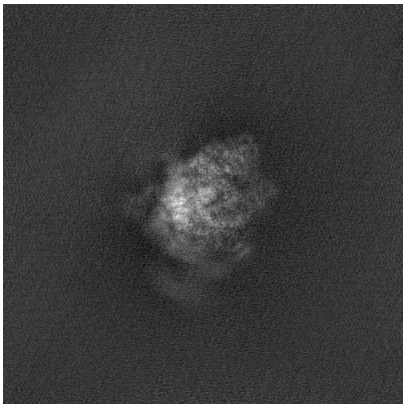


Y

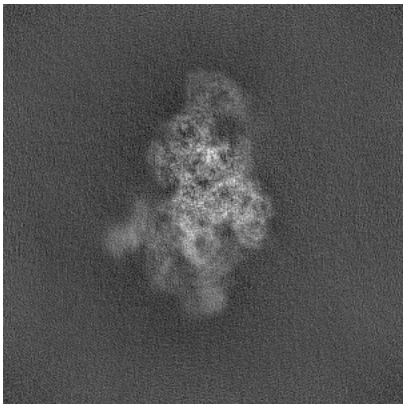


Z

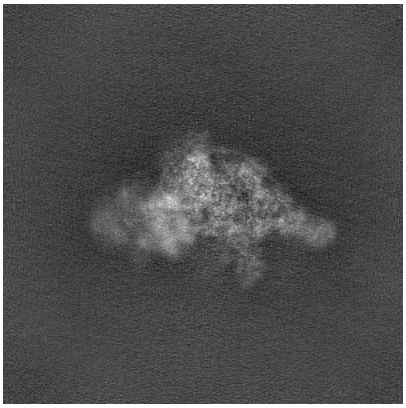
6.1.2 Raw map



X



Y

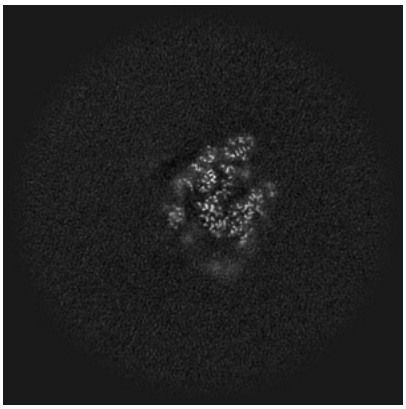


Z

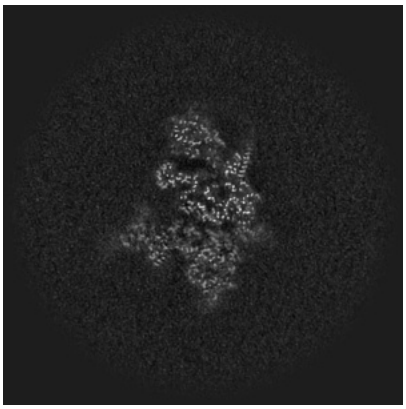
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

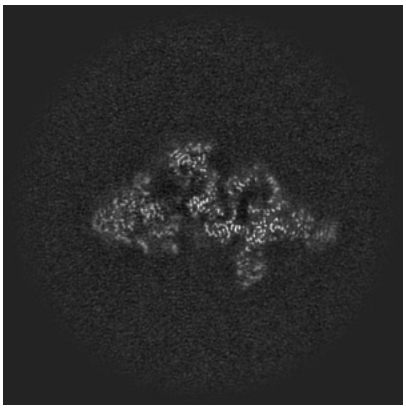
6.2.1 Primary map



X Index: 220

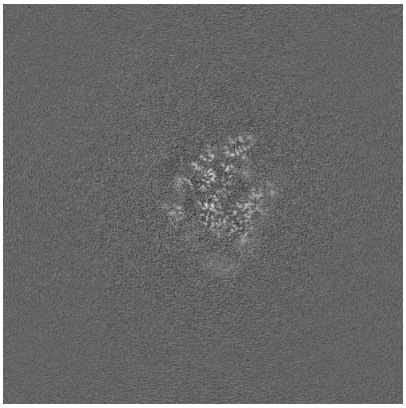


Y Index: 220

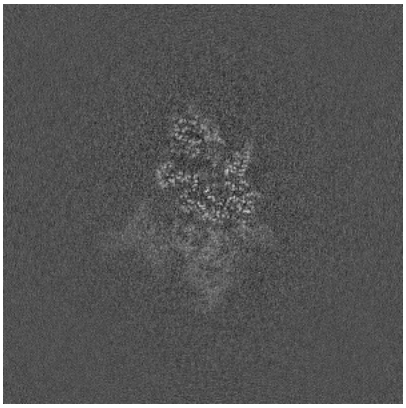


Z Index: 220

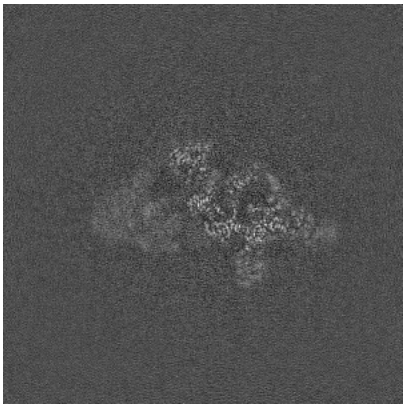
6.2.2 Raw map



X Index: 220



Y Index: 220

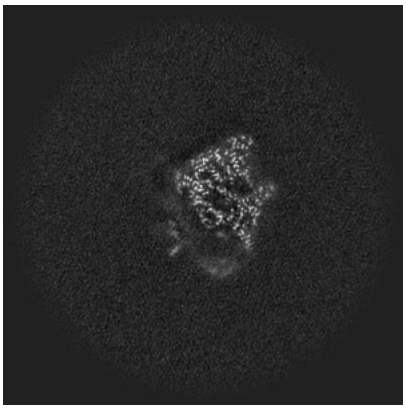


Z Index: 220

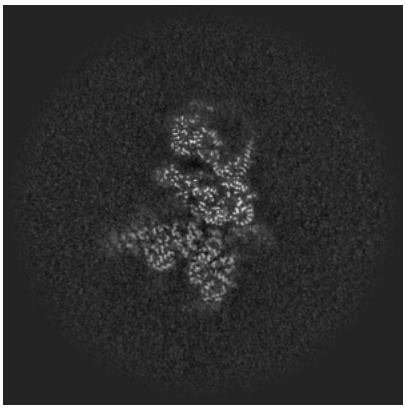
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

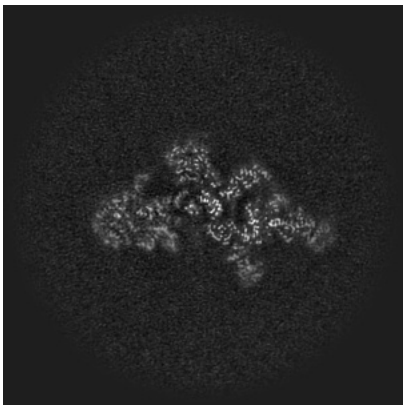
6.3.1 Primary map



X Index: 212

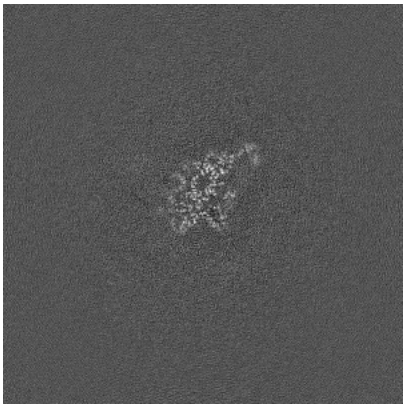


Y Index: 216

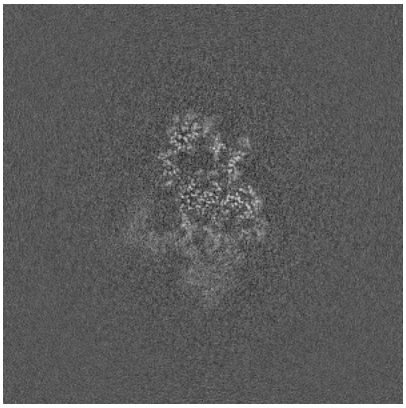


Z Index: 225

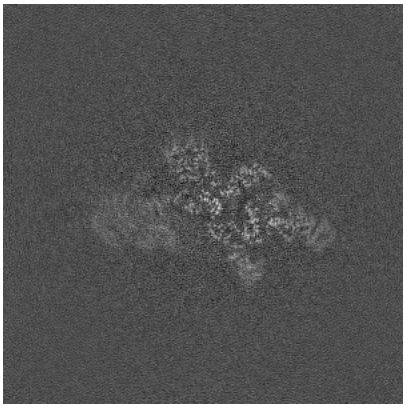
6.3.2 Raw map



X Index: 235



Y Index: 226

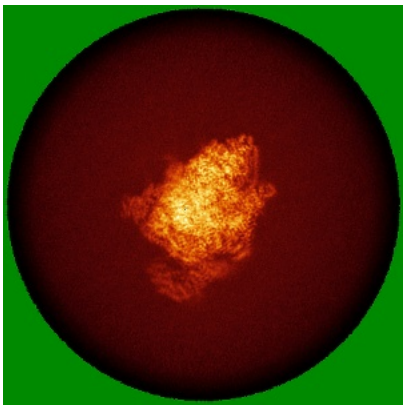


Z Index: 225

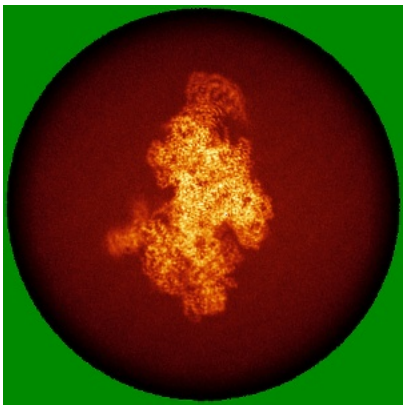
The images above show the largest variance slices of the map in three orthogonal directions.

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

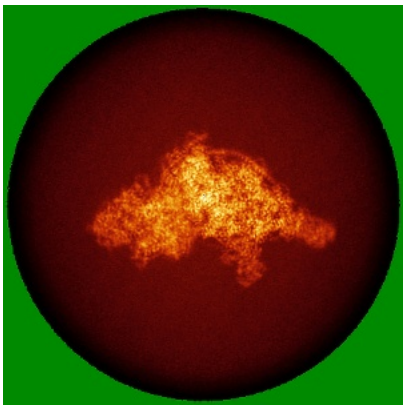
6.4.1 Primary map



X

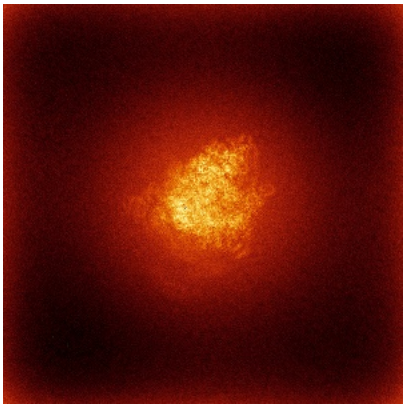


Y

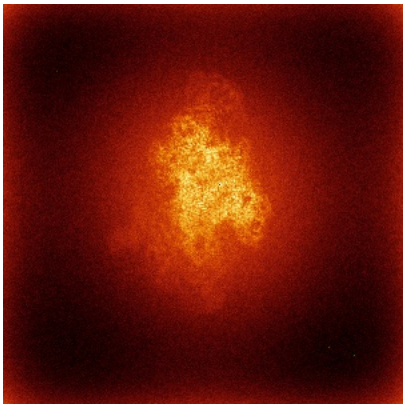


Z

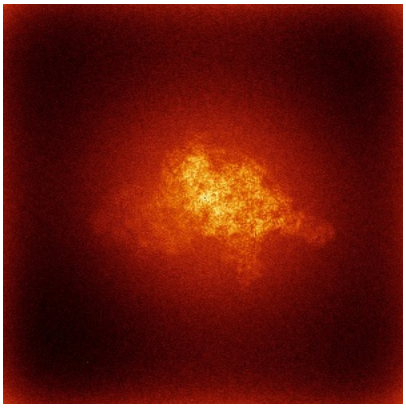
6.4.2 Raw map



X



Y

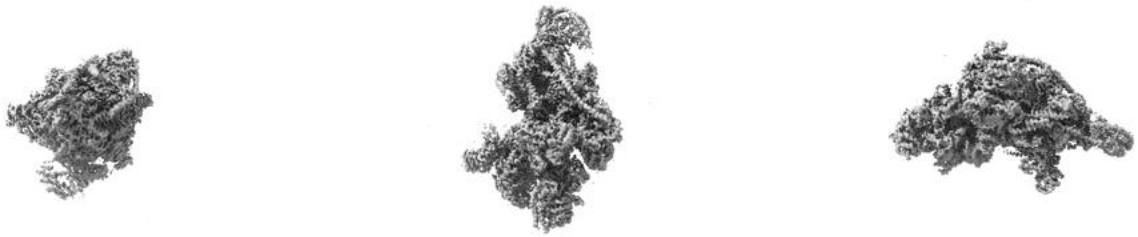


Z

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

6.5 Orthogonal surface views (i)

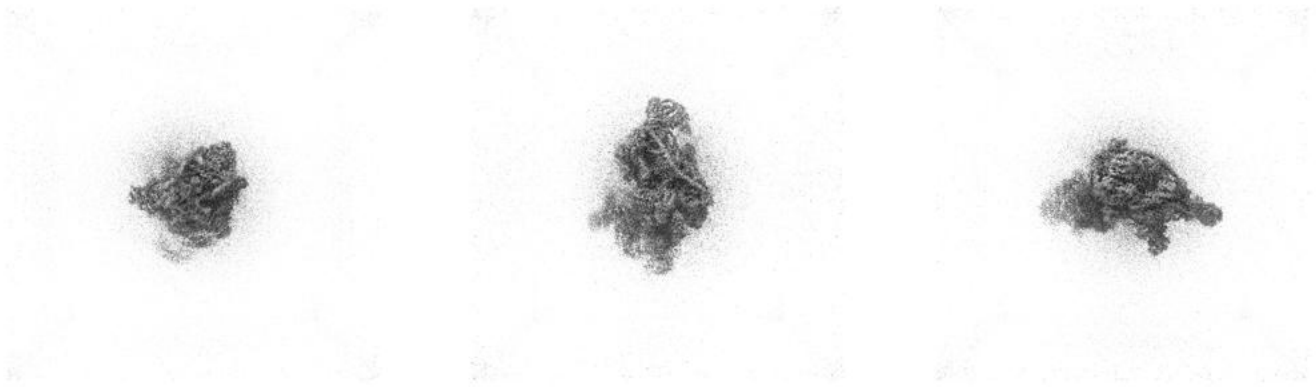
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.43. 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



X Y Z

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

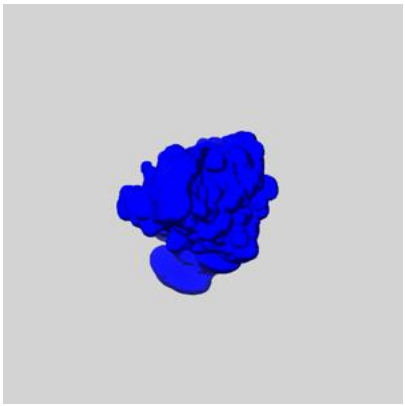
6.6 Mask visualisation (i)

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

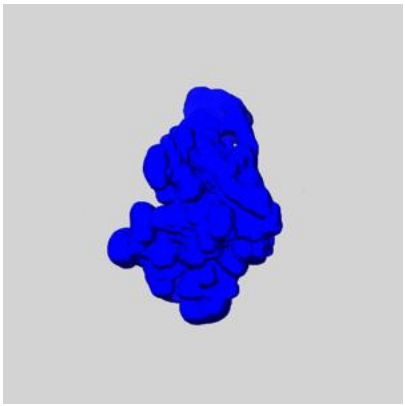
A mask typically either:

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

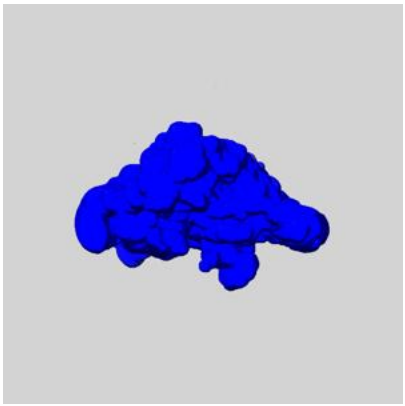
6.6.1 emd_52118_msk_1.map (i)



X



Y

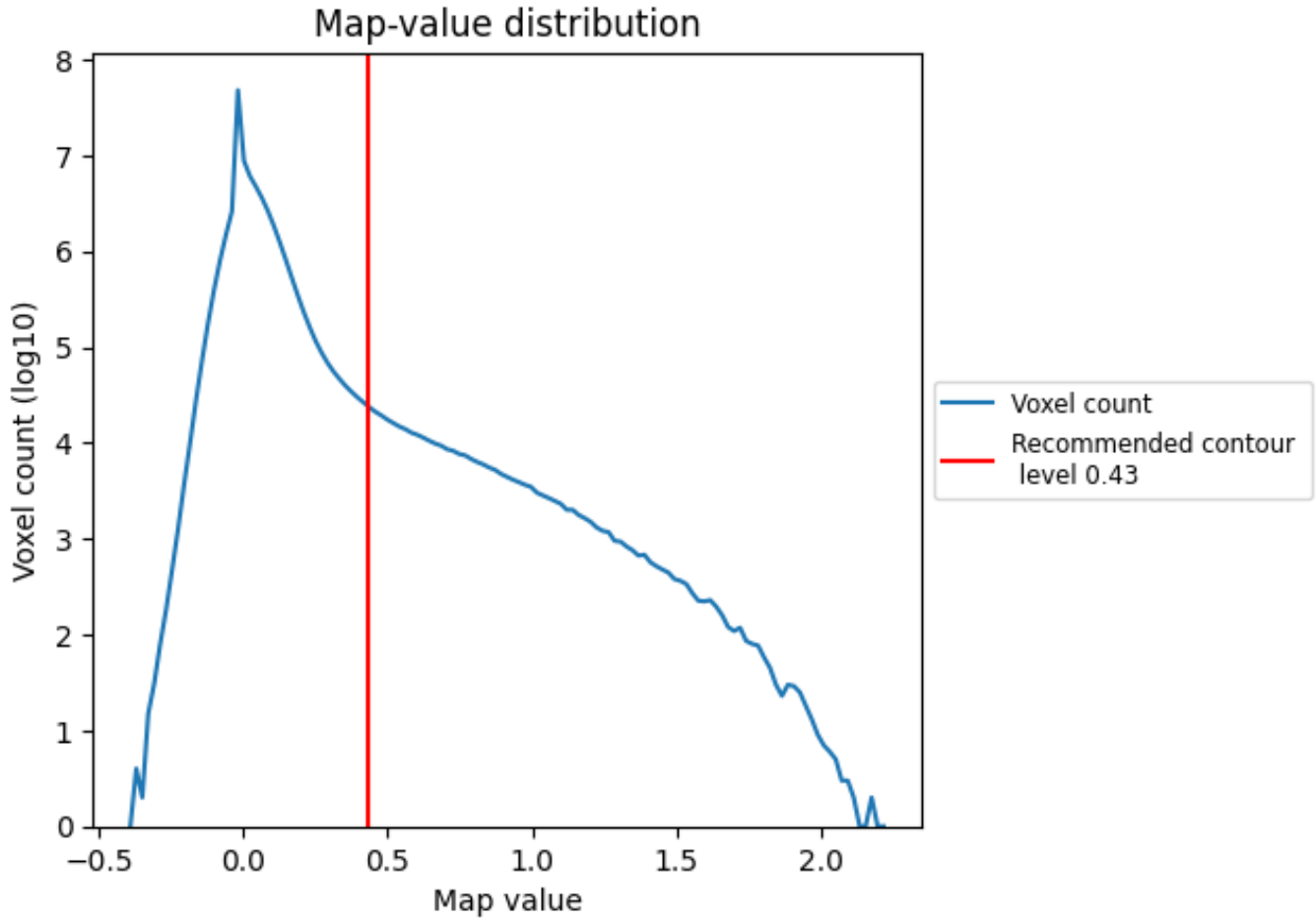


Z

7 Map analysis

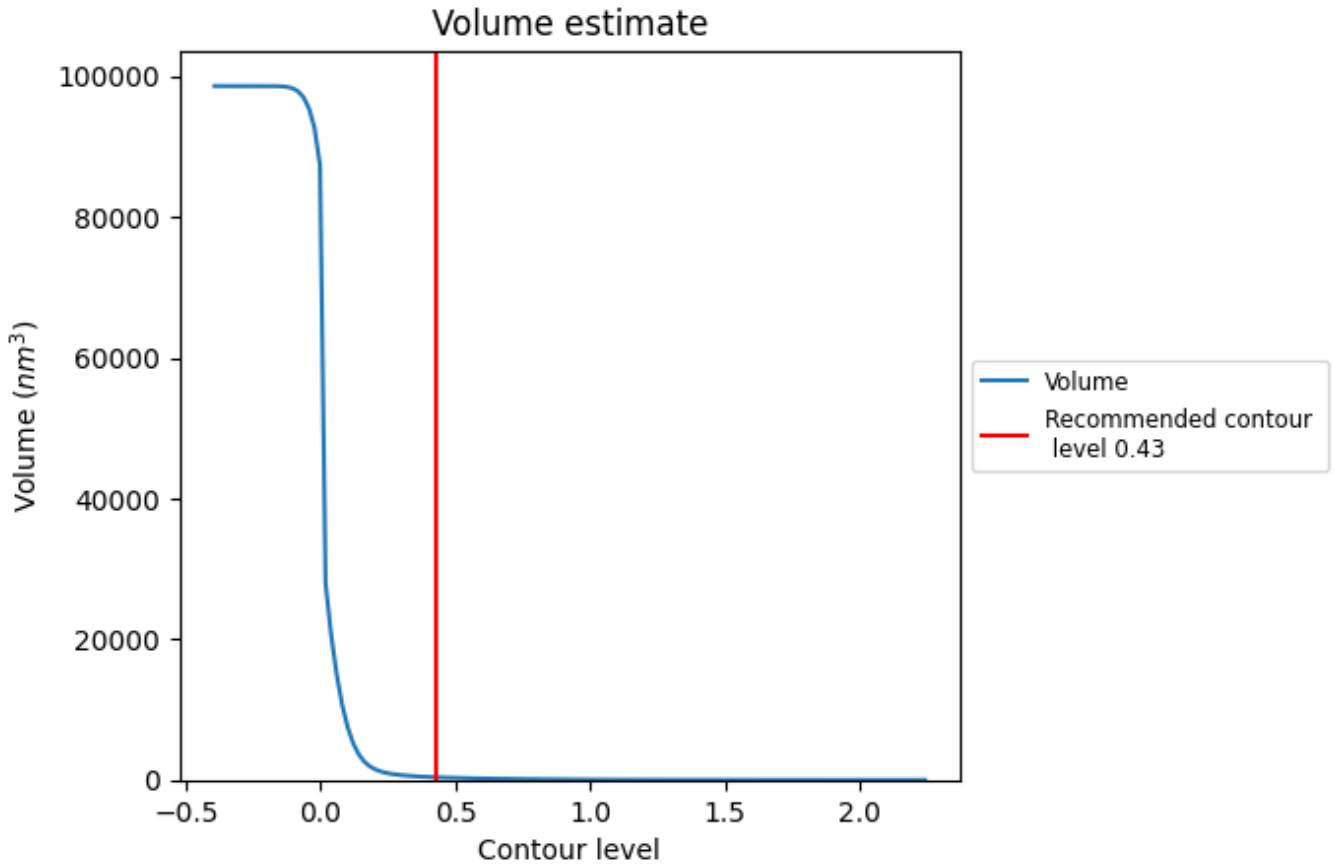
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

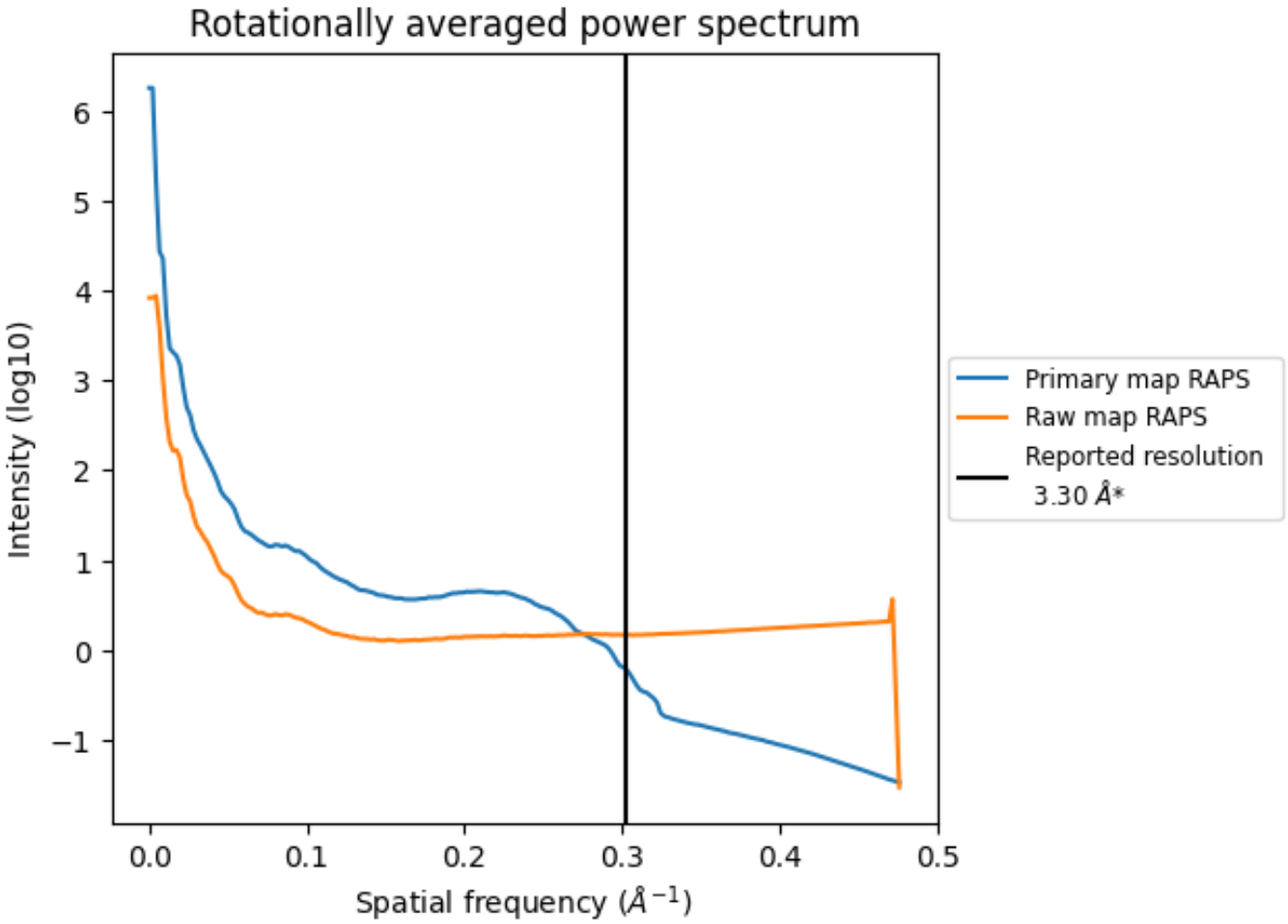
7.2 Volume estimate (i)



The volume at the recommended contour level is 373 nm^3; this corresponds to an approximate mass of 337 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

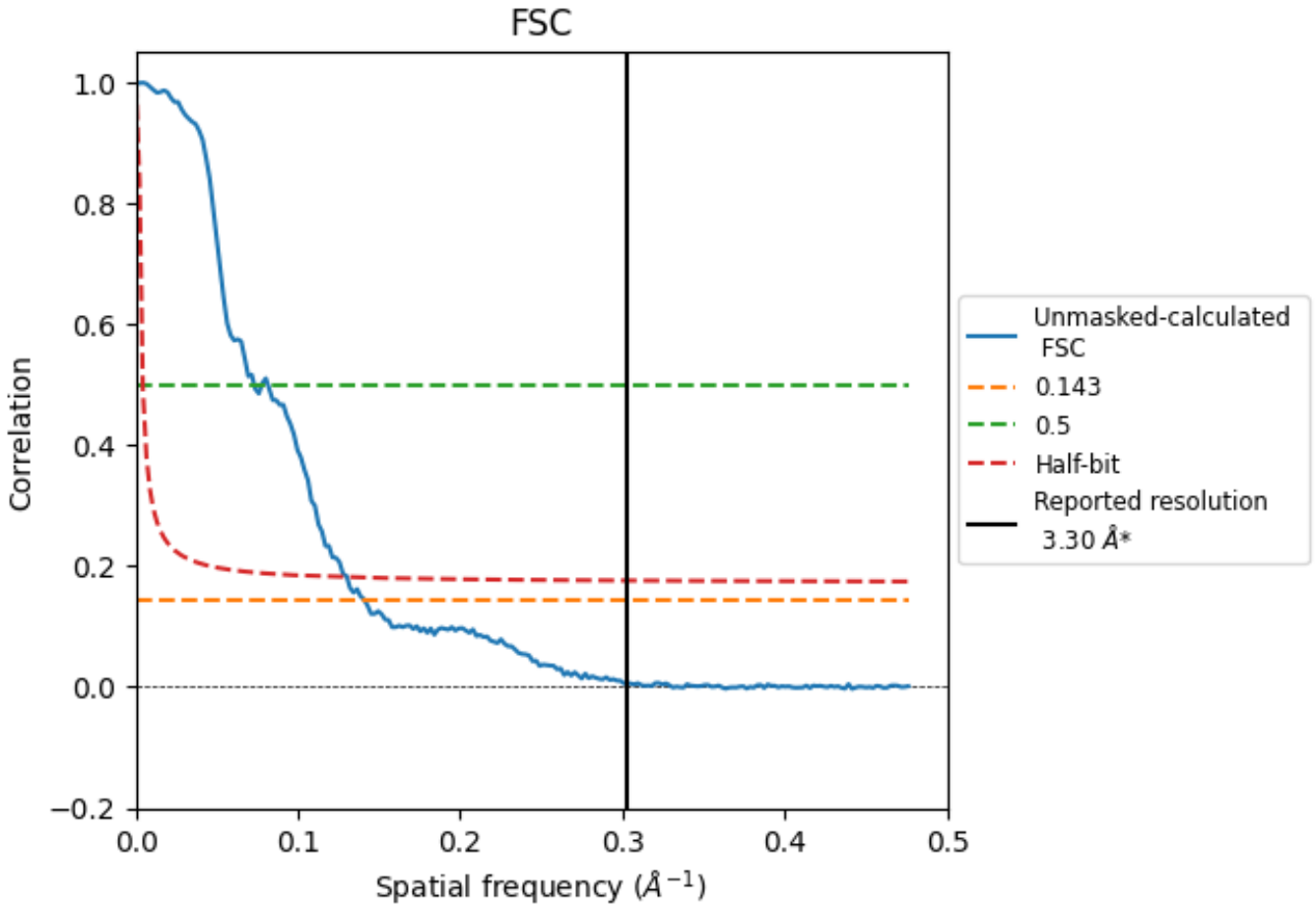


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

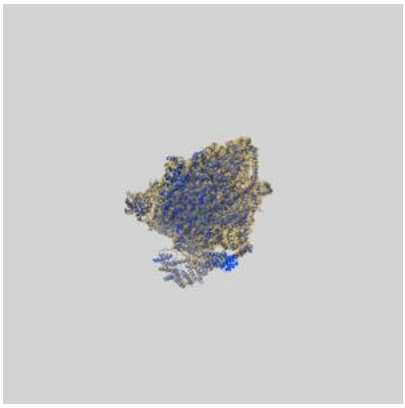
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.09	13.72	7.69

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.09 differs from the reported value 3.3 by more than 10 %

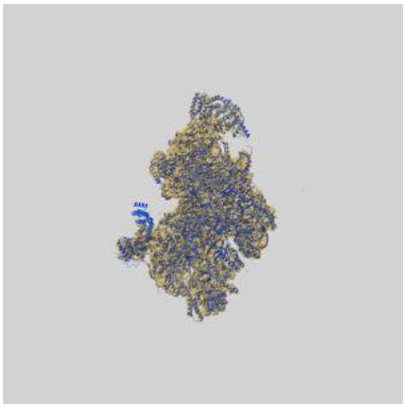
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52118 and PDB model 9HFN. Per-residue inclusion information can be found in section 3 on page 13.

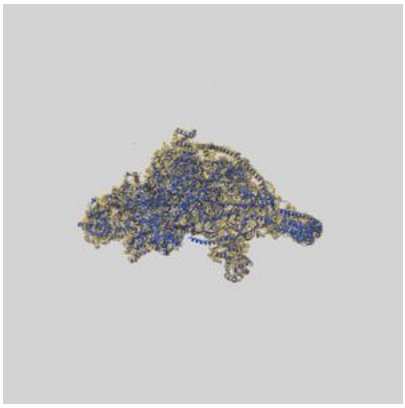
9.1 Map-model overlay



X



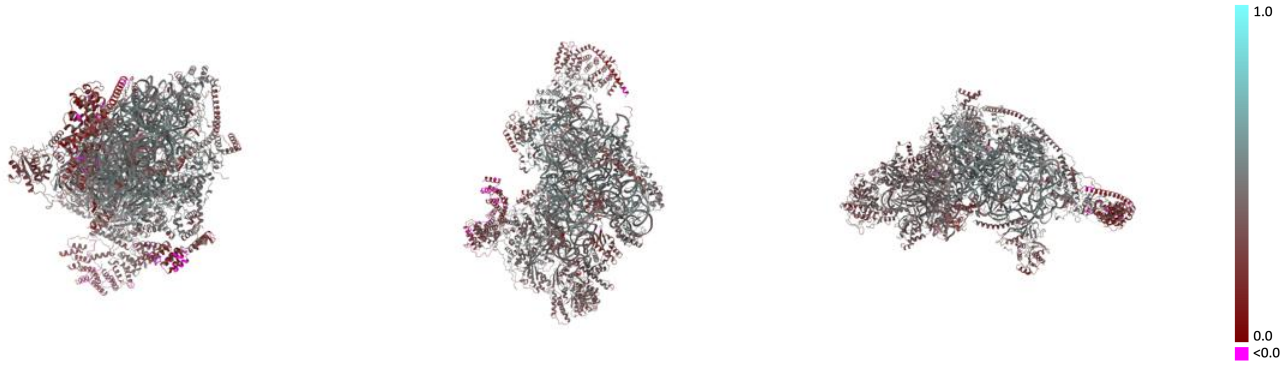
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.43 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.

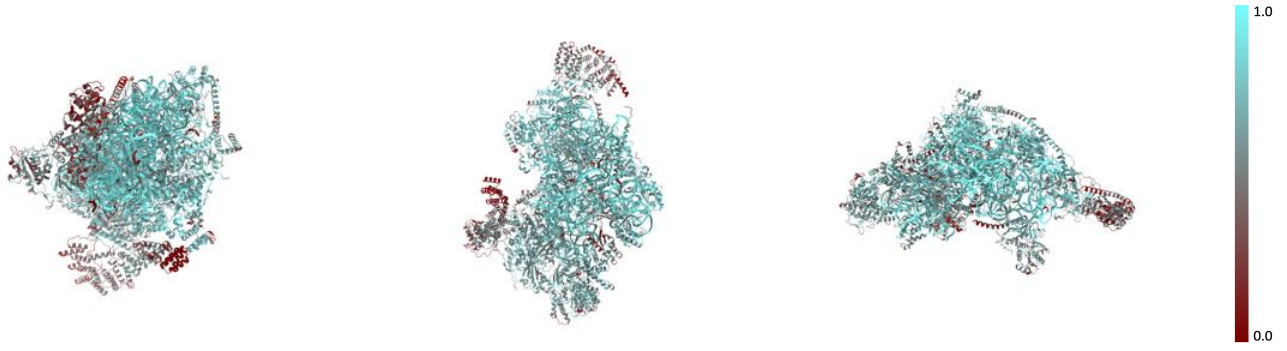
9.2 Q-score mapped to coordinate model



X Y Z

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

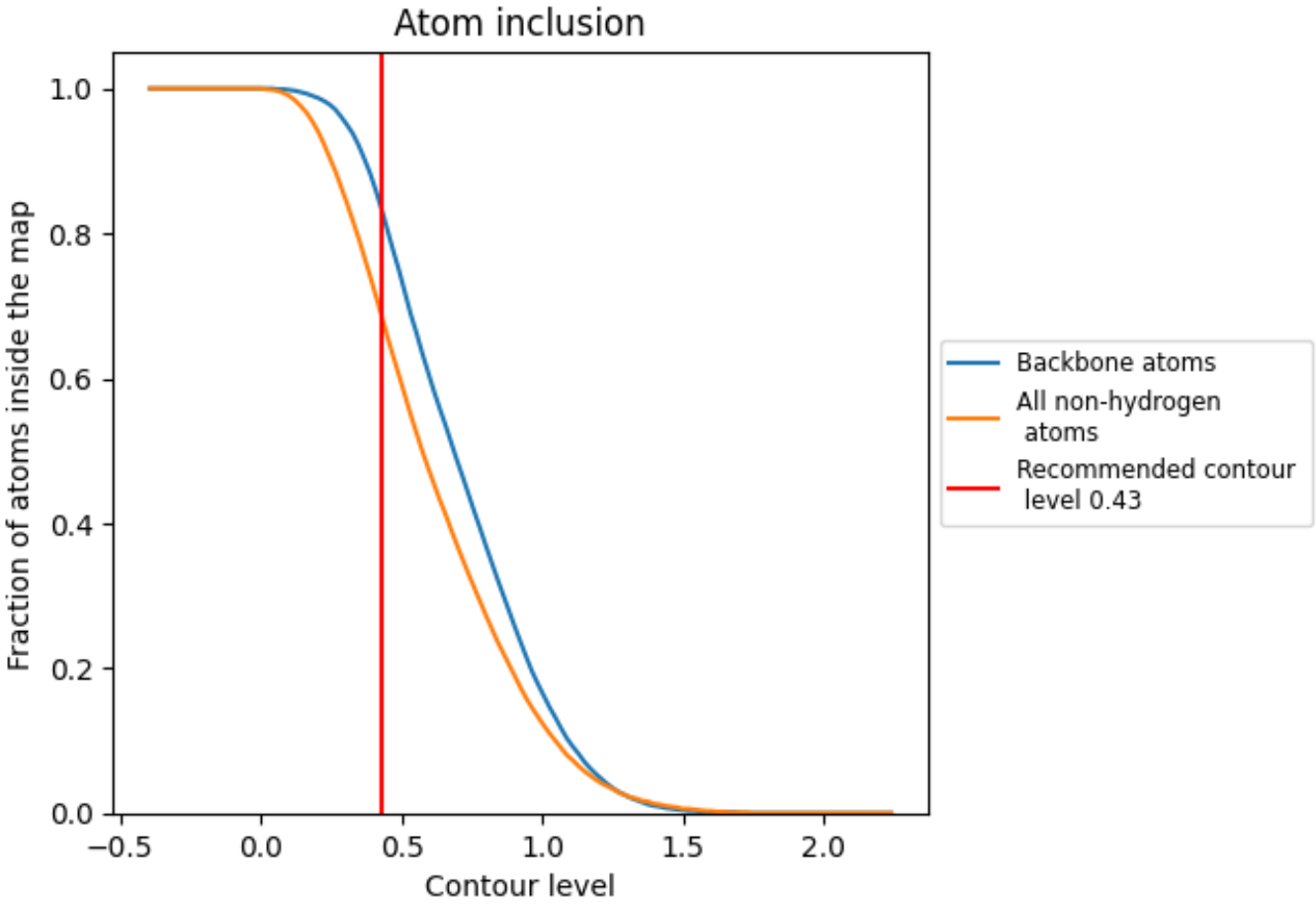
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.43).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 69% 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 (0.43) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6860	0.4220
0	0.6170	0.4220
1	0.6230	0.3980
2	0.4680	0.3830
3	0.6750	0.4530
4	0.3600	0.2560
7	0.5540	0.3690
8	0.3980	0.2780
A	0.8720	0.4770
B	0.8070	0.4890
C	0.6440	0.4690
D	0.6430	0.4610
E	0.6660	0.4400
F	0.5730	0.3760
G	0.6610	0.4130
H	0.6230	0.4430
I	0.6890	0.4340
J	0.6850	0.4880
K	0.7370	0.4540
L	0.7080	0.4480
M	0.7920	0.4910
N	0.7760	0.5040
O	0.7870	0.4870
P	0.7660	0.4800
Q	0.7570	0.4900
R	0.7290	0.4380
S	0.6850	0.4250
T	0.7600	0.4830
U	0.6950	0.4160
V	0.3680	0.2480
W	0.7560	0.4760
X	0.6100	0.3820
Y	0.5080	0.3470
Z	0.5760	0.3890

