wwPDB EM Validation Summary Report

Nov 20, 2022 – 02:00 am GMT

PDB ID	:	6GAZ
EMDB ID	:	EMD-4369
Title	:	Unique features of mammalian mitochondrial translation initiation revealed by cryo-EM. This file contains the 28S ribosomal subunit.
Authors	:	Kummer, E.; Leibundgut, M.; Boehringer, D.; Ban, N.
Deposited on	:	2018-04-13
Resolution	:	3.10 Å(reported)

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 ⓘ symbol.

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

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

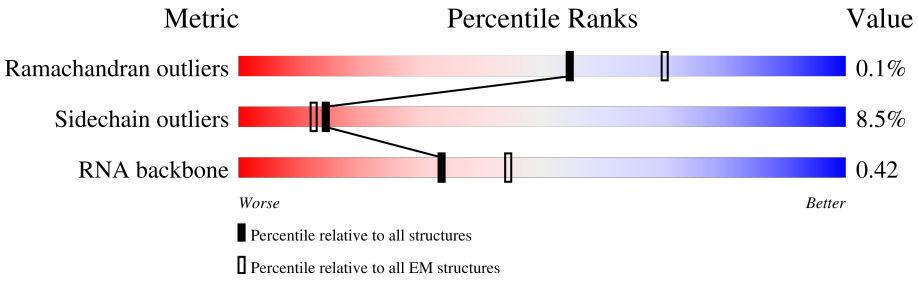
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	BC	657	34% 84% · 13%
2	BT	292	· 5% 94%
3	AA	962	· 70% 28% ·
4	AB	289	· 70% 6% 24%
5	AC	167	· 68% 11% 21%
6	AE	430	9% 73% 7% 20%
7	AF	124	· 89% 10% ·
8	AG	242	6% 79% 7% 14%

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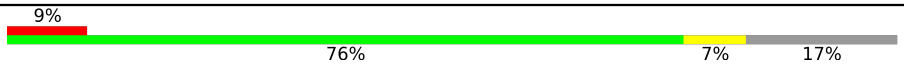
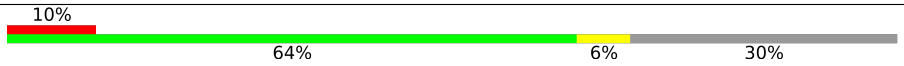
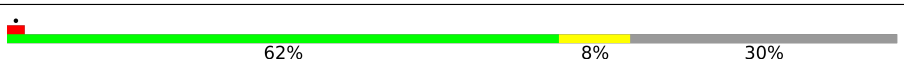
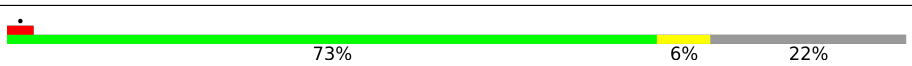
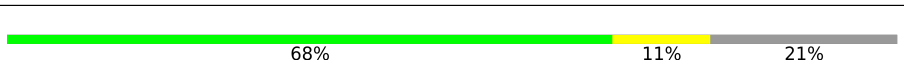
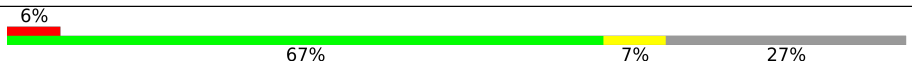
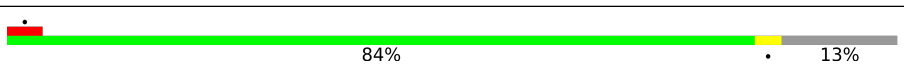
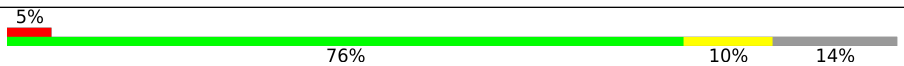
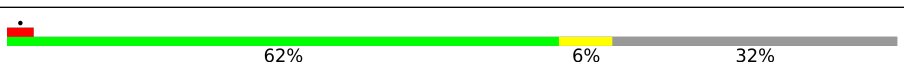
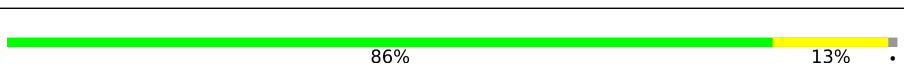
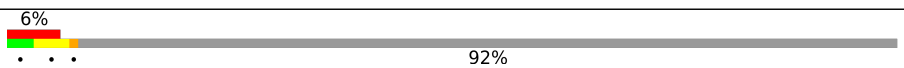
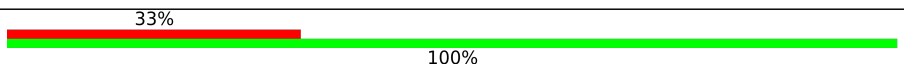
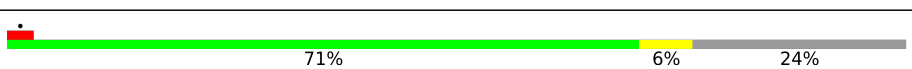
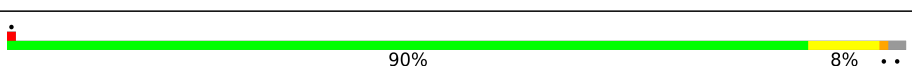
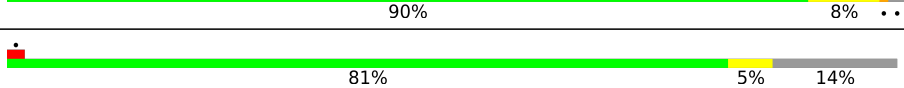
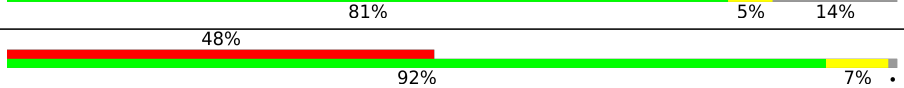
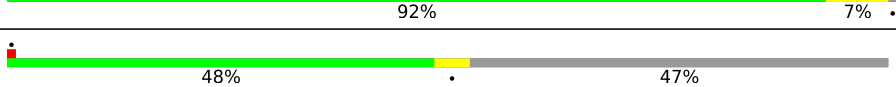
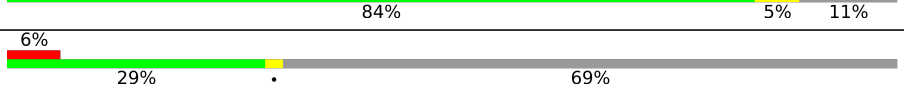
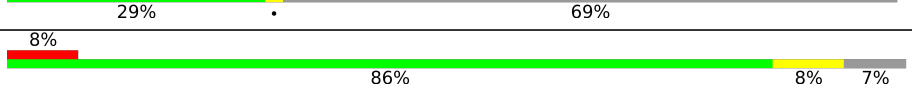
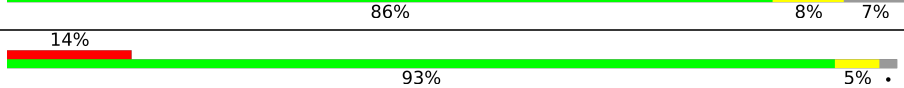
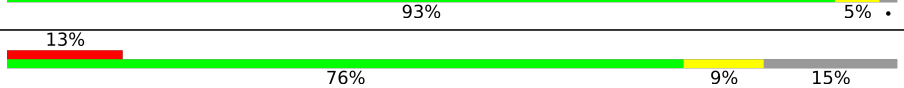
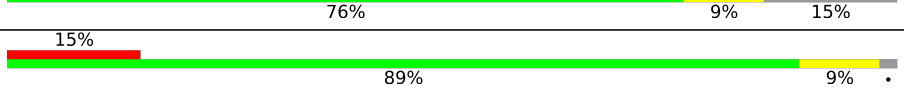
Mol	Chain	Length	Quality of chain
9	AI	397	
10	AJ	201	
11	AK	196	
12	AL	139	
13	AN	128	
14	AO	239	
15	AP	135	
16	AQ	130	
17	AR	143	
18	AU	87	
19	AV	71	
20	AX	201	
21	AZ	18	
22	Aa	382	
23	Ab	190	
24	Ac	173	
25	Ad	205	
26	Ae	390	
27	Af	188	
28	Ag	397	
29	Ah	387	
30	Ai	106	
31	Aj	218	
32	Ak	325	
33	Am	118	

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Mol	Chain	Length	Quality of chain
34	An	199	
35	Ao	692	
36	Ap	258	

2 Entry composition (i)

There are 44 unique types of molecules in this entry. The entry contains 73172 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 Translation initiation factor IF-2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	BC	571	Total	C	N	O	S	0	0
			4364	2743	765	839	17		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	71	SER	-	expression tag	UNP P46199
BC	72	GLY	-	expression tag	UNP P46199
BC	73	GLY	-	expression tag	UNP P46199
BC	74	SER	-	expression tag	UNP P46199
BC	75	GLY	-	expression tag	UNP P46199
BC	76	SER	-	expression tag	UNP P46199
BC	77	GLY	-	expression tag	UNP P46199

- Molecule 2 is a protein called Mitochondrial ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	BT	17	Total	C	N	O	0	0
			109	72	19	18		

- Molecule 3 is a RNA chain called 12S ribosomal RNA, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AA	960	Total	C	N	O	P	0	0
			20411	9162	3708	6581	960		

- Molecule 4 is a protein called Mitochondrial ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AB	220	Total	C	N	O	S	0	0
			1762	1126	326	304	6		

- Molecule 5 is a protein called Mitochondrial ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AC	132	Total	C	N	O	S	0	0
			1075	695	195	181	4		

- Molecule 6 is a protein called Mitochondrial ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AE	343	Total	C	N	O	S	0	0
			2732	1707	527	487	11		

- Molecule 7 is a protein called Mitochondrial ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AF	122	Total	C	N	O	S	0	0
			981	620	178	177	6		

- Molecule 8 is a protein called Mitochondrial ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AG	208	Total	C	N	O	S	0	0
			1721	1097	314	299	11		

- Molecule 9 is a protein called Mitochondrial ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	328	Total	C	N	O	S	0	0
			2650	1678	478	481	13		

- Molecule 10 is a protein called Mitochondrial ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	140	Total	C	N	O	S	0	0
			1155	746	197	208	4		

- Molecule 11 is a protein called Mitochondrial ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	137	Total	C	N	O	S	0	0
			1007	631	193	180	3		

- Molecule 12 is a protein called Mitochondrial ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	109	Total	C	N	O	S	0	0
			840	524	172	138	6		

- Molecule 13 is a protein called Mitochondrial ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AN	101	Total	C	N	O	S	0	0
			858	534	174	144	6		

- Molecule 14 is a protein called Mitochondrial ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AO	175	Total	C	N	O	S	0	0
			1448	919	272	248	9		

- Molecule 15 is a protein called bS16m, MRPS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AP	117	Total	C	N	O	S	0	0
			932	588	184	155	5		

- Molecule 16 is a protein called Mitochondrial ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AQ	112	Total	C	N	O	S	0	0
			875	568	153	151	3		

- Molecule 17 is a protein called Mitochondrial ribosomal protein S18C.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AR	97	Total	C	N	O	S	0	0
			784	507	132	138	7		

- Molecule 18 is a protein called Mitochondrial ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AU	86	Total	C	N	O	S	0	0
			734	453	148	125	8		

- Molecule 19 is a RNA chain called P-site fMet-tRNAMet, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AV	71	Total	C	N	O	P	0	0
			1498	673	264	491	70		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AV	69	C	-	insertion	GB 1208989970
AV	70	C	-	insertion	GB 1208989970
AV	71	A	-	insertion	GB 1208989970

- Molecule 20 is a RNA chain called MT-CO3 mRNA, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AX	17	Total	C	N	O	P	0	0
			354	161	65	112	16		

- Molecule 21 is a protein called unassigned secondary structure elements.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	AZ	18	Total	C	N	O	0	0
			90	54	18	18		

- Molecule 22 is a protein called Mitochondrial ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Aa	292	Total	C	N	O	S	0	0
			2378	1518	409	442	9		

- Molecule 23 is a protein called Mitochondrial ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Ab	135	Total	C	N	O	S	0	0
			1101	709	199	192	1		

- Molecule 24 is a protein called Mitochondrial ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ac	169	Total	C	N	O	S	0	0
			1367	876	236	245	10		

- Molecule 25 is a protein called Mitochondrial ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ad	177	Total	C	N	O	S	0	0
			1467	904	288	273	2		

- Molecule 26 is a protein called Mitochondrial ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Ae	388	Total	C	N	O	S	0	0
			3109	1971	535	589	14		

- Molecule 27 is a protein called Mitoribosomal protein ms28, mrps28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Af	99	Total	C	N	O	S	0	0
			778	494	134	146	4		

- Molecule 28 is a protein called Death associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Ag	353	Total	C	N	O	S	0	0
			2875	1837	515	513	10		

- Molecule 29 is a protein called mS31, MRPS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Ah	120	Total	C	N	O	S	0	0
			1015	659	168	185	3		

- Molecule 30 is a protein called Mitochondrial ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ai	99	Total	C	N	O	S	0	0
			824	522	156	143	3		

- Molecule 31 is a protein called Mitochondrial ribosomal protein S34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Aj	213	Total	C	N	O	S	0	0
			1788	1131	338	311	8		

- Molecule 32 is a protein called Mitochondrial ribosomal protein S35.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ak	275	Total	C	N	O	S	0	0
			2222	1414	380	419	9		

- Molecule 33 is a protein called Mitochondrial ribosomal protein S37.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Am	116	Total	C	N	O	S	0	0
			930	577	185	160	8		

- Molecule 34 is a protein called Aurora kinase A interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	An	72	Total	C	N	O	S	0	0
			639	407	139	92	1		

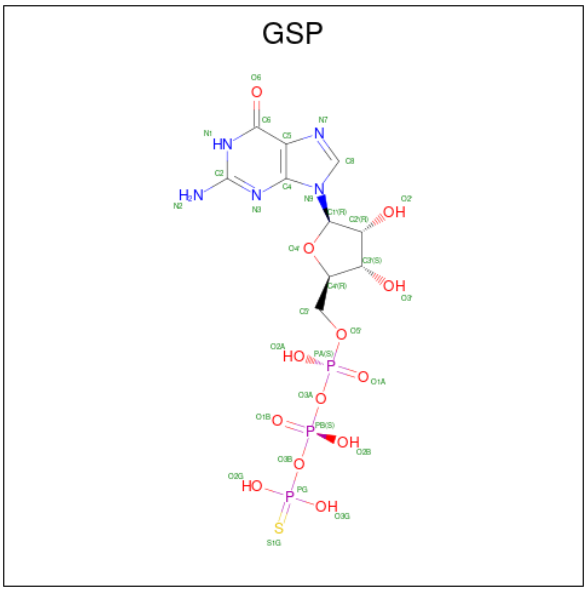
- Molecule 35 is a protein called Mitochondrial ribosomal protein S39.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Ao	572	Total	C	N	O	S	0	0
			4527	2899	770	834	24		

- Molecule 36 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ap	190	Total	C	N	O	S	0	0
			1564	991	292	273	8		

- Molecule 37 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$).



Mol	Chain	Residues	Atoms						AltConf
37	BC	1	Total	C	N	O	P	S	0
			32	10	5	13	3	1	

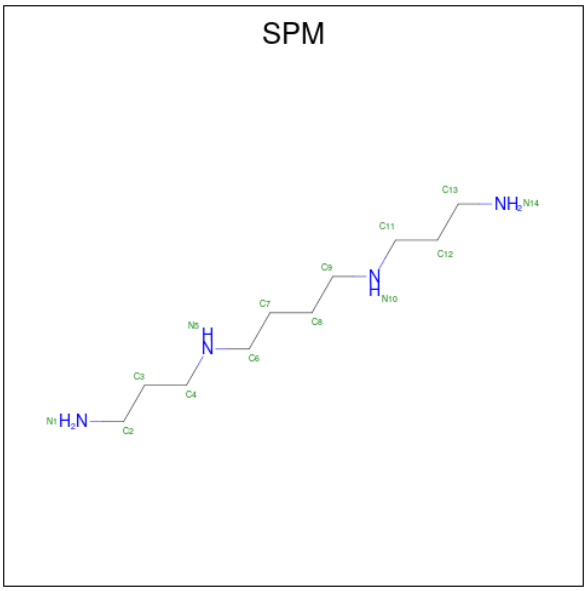
- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	BC	2	Total	Mg	0
			2	2	
38	AA	105	Total	Mg	0
			105	105	
38	AB	1	Total	Mg	0
			1	1	
38	AX	1	Total	Mg	0
			1	1	
38	Ag	1	Total	Mg	0
			1	1	
38	An	1	Total	Mg	0
			1	1	

- Molecule 39 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
39	BC	1	Total	Na	0
			1	1	

- Molecule 40 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).

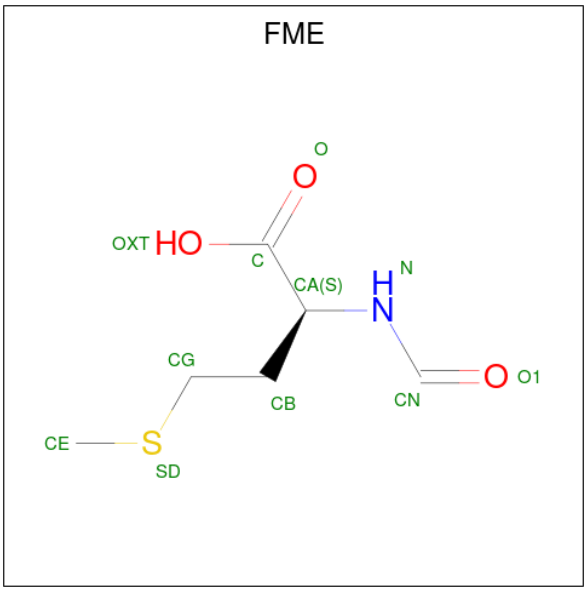


Mol	Chain	Residues	Atoms	AltConf
40	AA	1	Total C N 14 10 4	0

- Molecule 41 is ZINC ION (three-letter code: ZN) (formula: Zn).

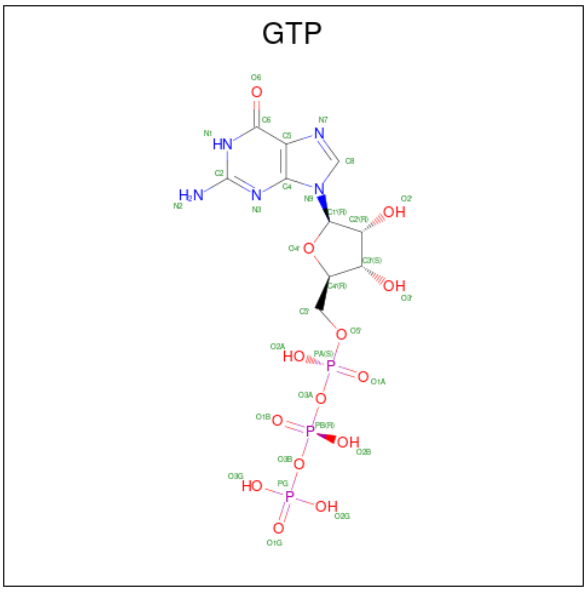
Mol	Chain	Residues	Atoms	AltConf
41	AR	1	Total Zn 1 1	0
41	Ac	1	Total Zn 1 1	0
41	Ap	1	Total Zn 1 1	0

- Molecule 42 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
42	AV	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 43 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 44 is water.

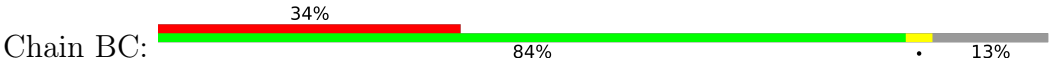
Mol	Chain	Residues	Atoms	AltConf
44	BC	2	Total O 2 2	0
44	Ag	3	Total O 3 3	0

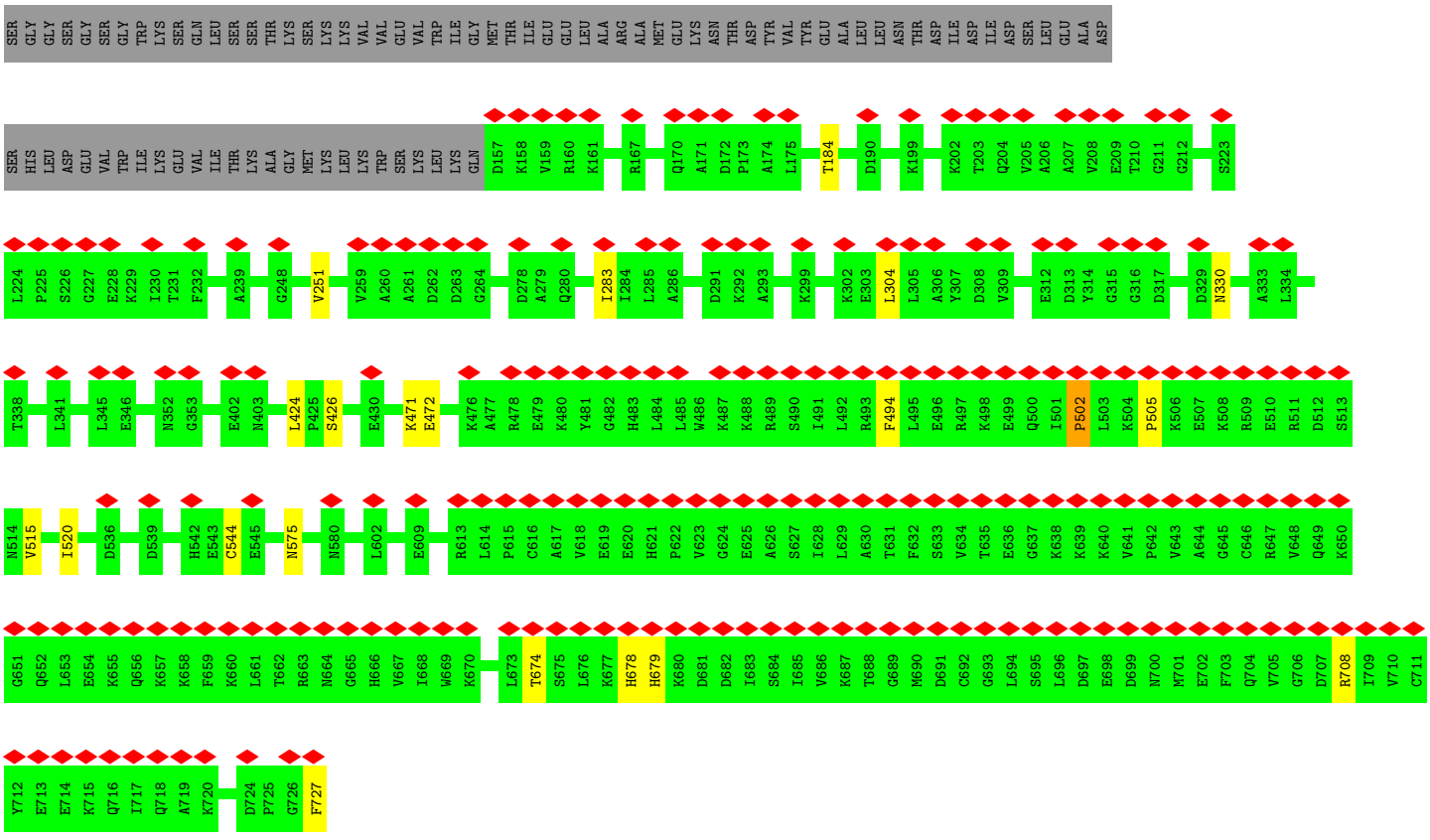
3 Residue-property plots (i)

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: Translation initiation factor IF-2, mitochondrial

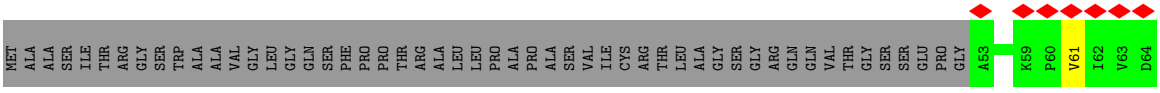
Chain BC:

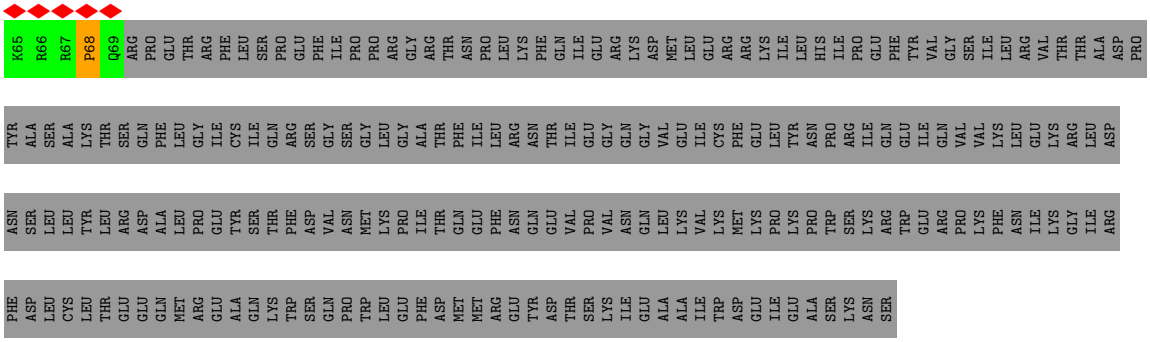




• Molecule 2: Mitochondrial ribosomal protein L19

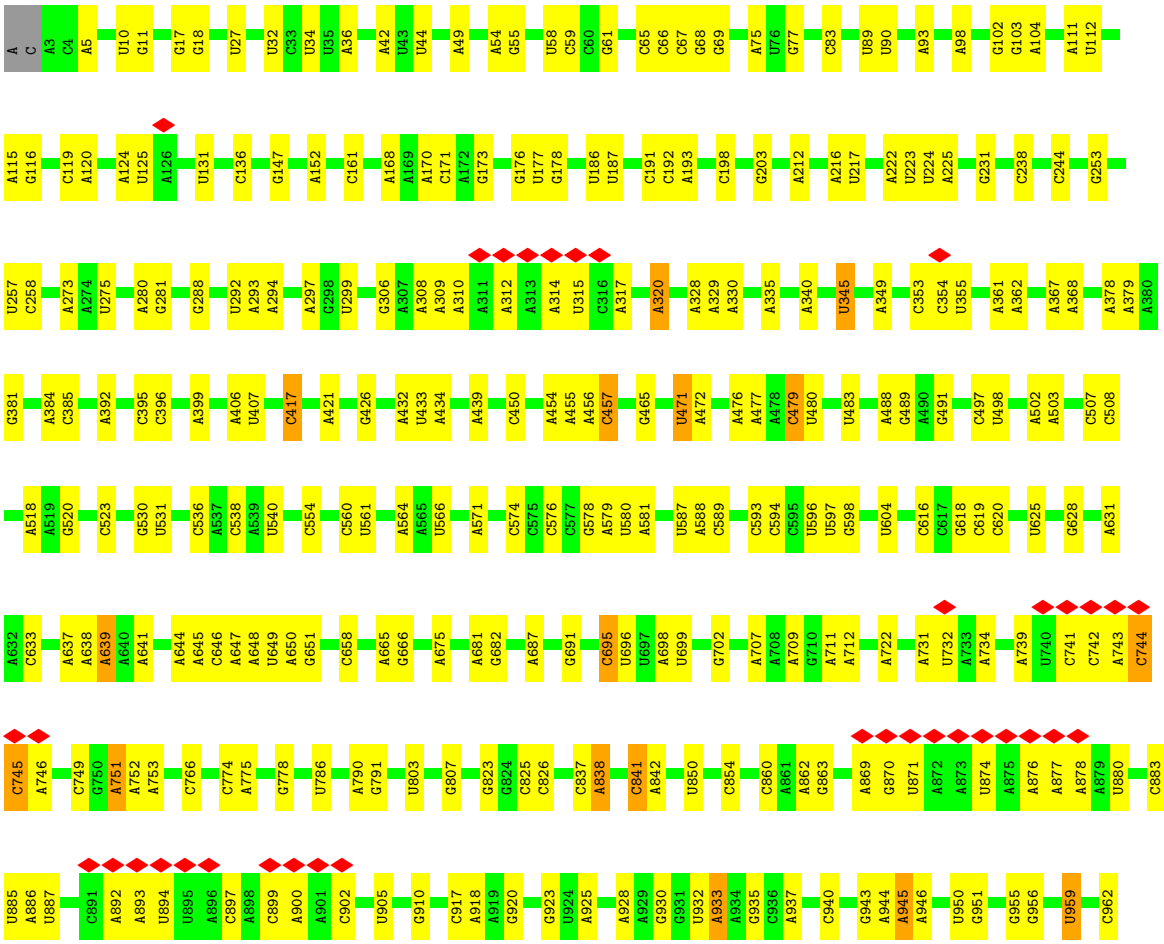
Chain BT:





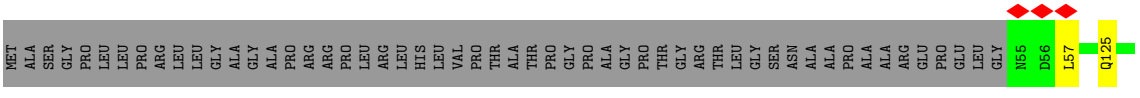
• Molecule 3: 12S ribosomal RNA, mitochondrial

Chain AA:



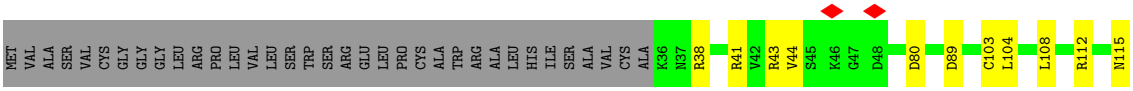
• Molecule 4: Mitochondrial ribosomal protein S2

Chain AB:



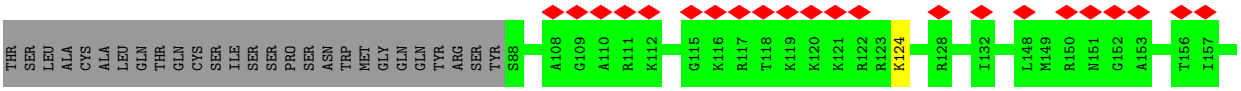
• Molecule 5: Mitochondrial ribosomal protein S24

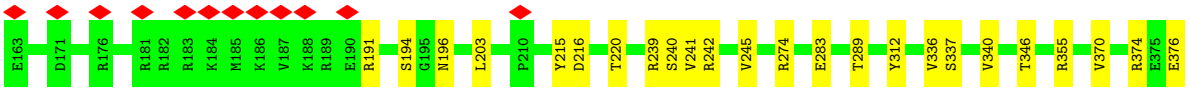
Chain AC:

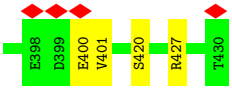


• Molecule 6: Mitochondrial ribosomal protein S5

Chain AE:

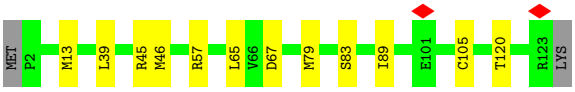






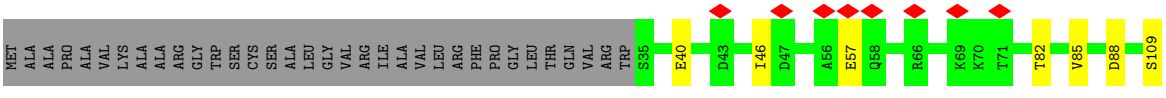
• Molecule 7: Mitochondrial ribosomal protein S6

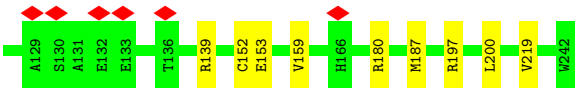
Chain AF:



• Molecule 8: Mitochondrial ribosomal protein S7

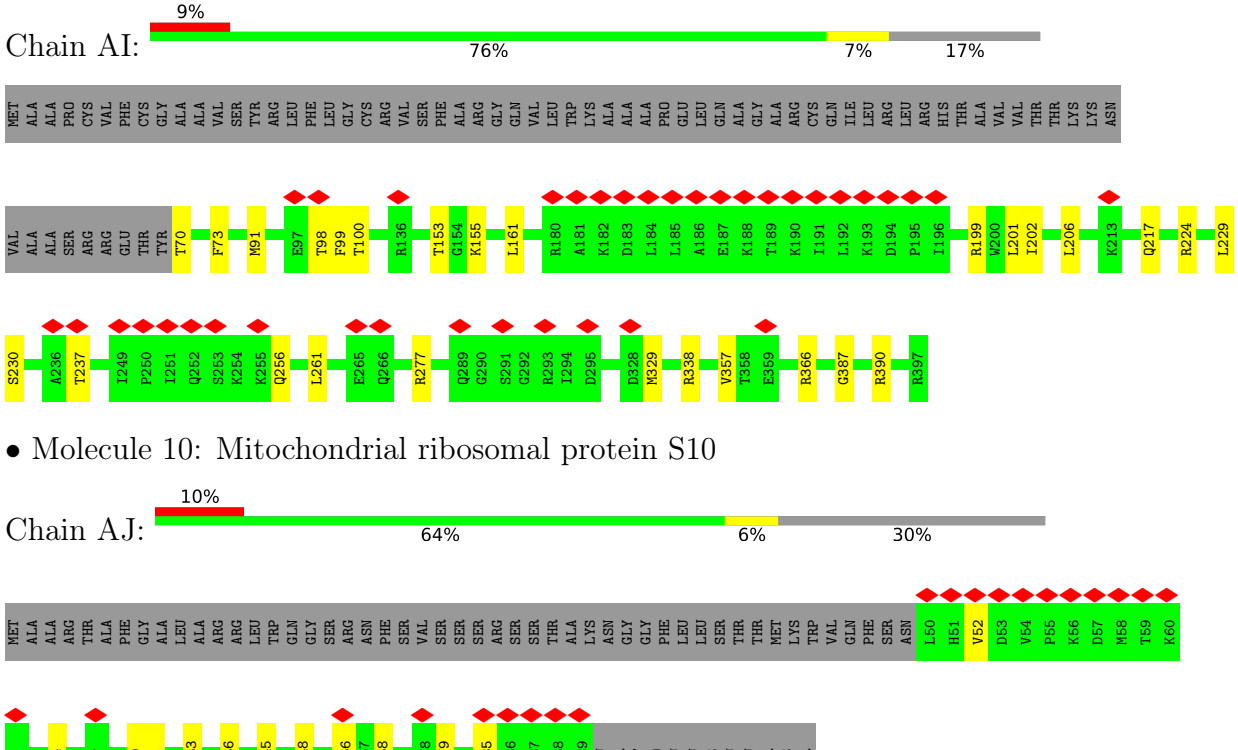
Chain AG:





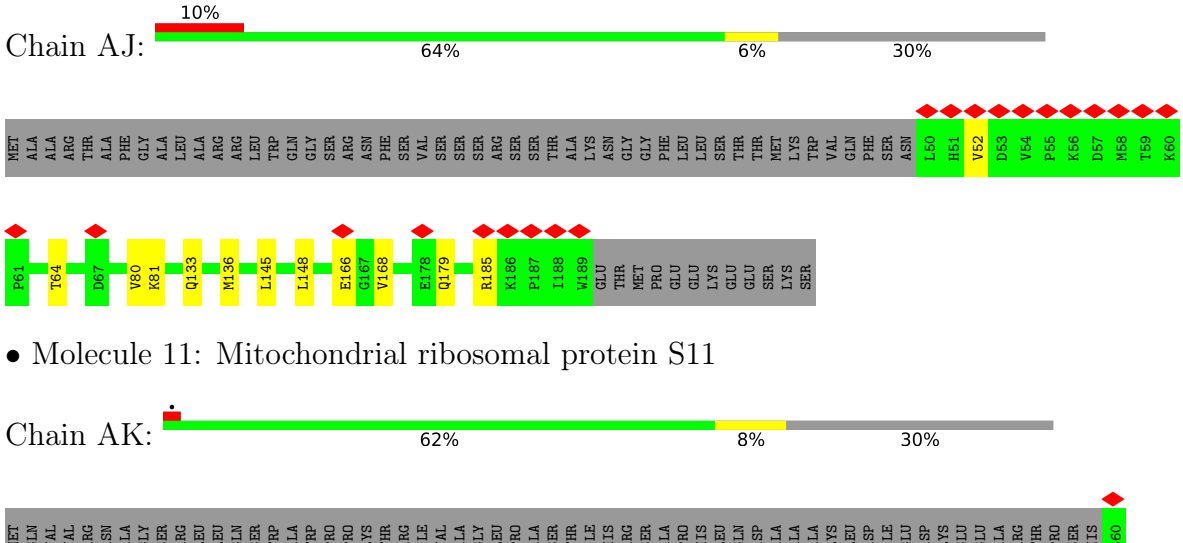
• Molecule 9: Mitochondrial ribosomal protein S9

Chain AI:



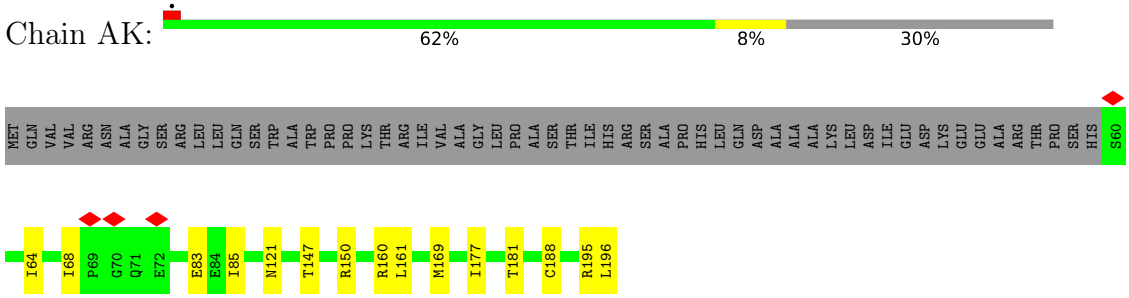
• Molecule 10: Mitochondrial ribosomal protein S10

Chain AJ:



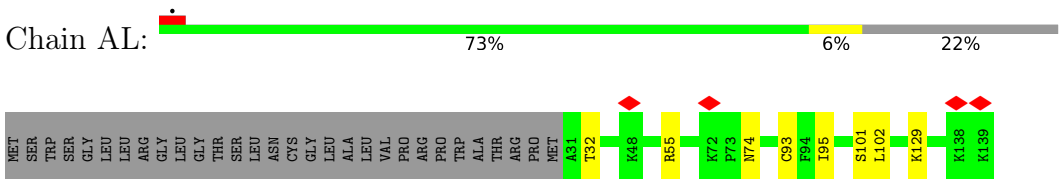
• Molecule 11: Mitochondrial ribosomal protein S11

Chain AK:



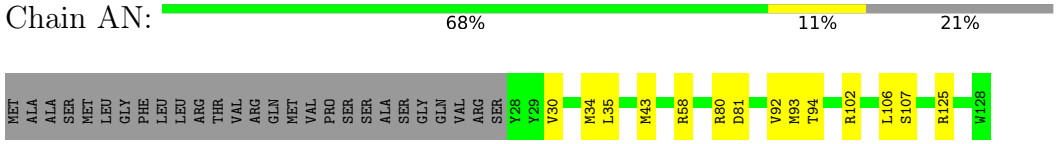
• Molecule 12: Mitochondrial ribosomal protein S12

Chain AL:



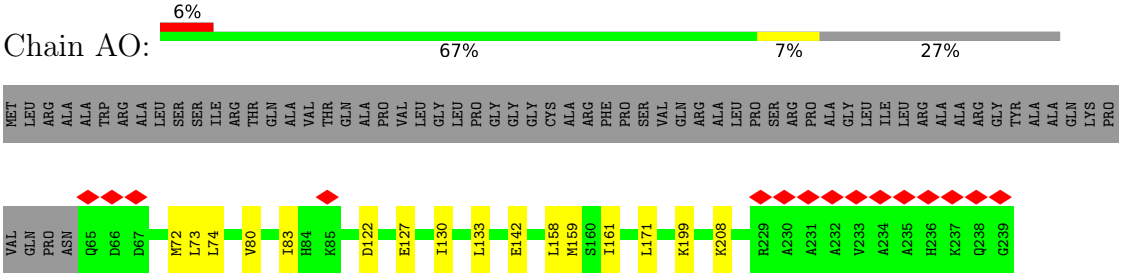
• Molecule 13: Mitochondrial ribosomal protein S14

Chain AN:



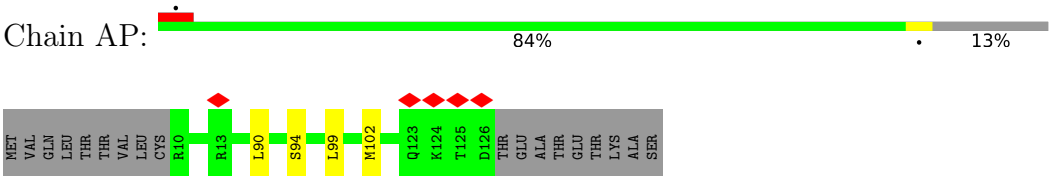
• Molecule 14: Mitochondrial ribosomal protein S15

Chain AO:



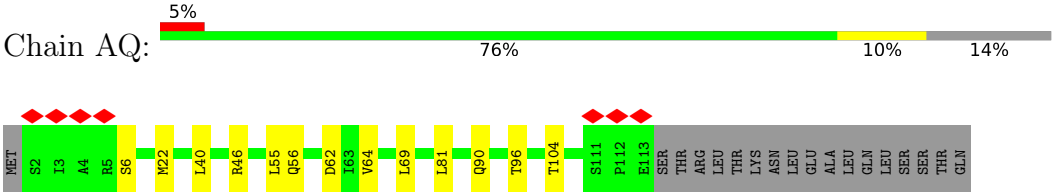
• Molecule 15: bS16m, MRPS16

Chain AP:



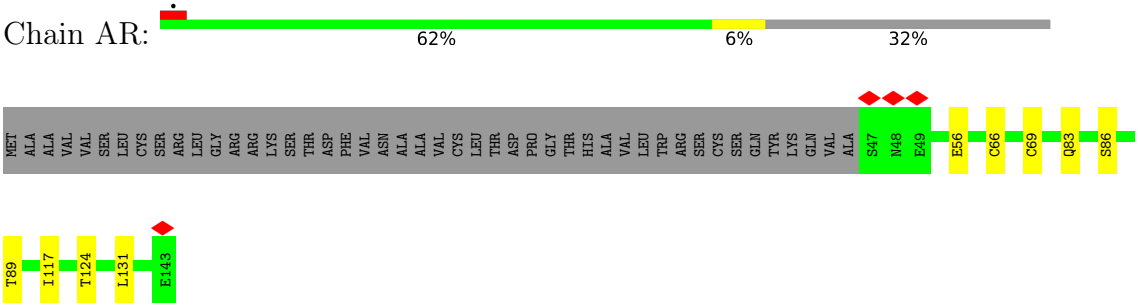
• Molecule 16: Mitochondrial ribosomal protein S17

Chain AQ:



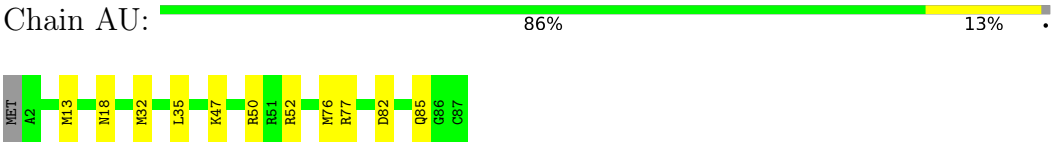
• Molecule 17: Mitochondrial ribosomal protein S18C

Chain AR:



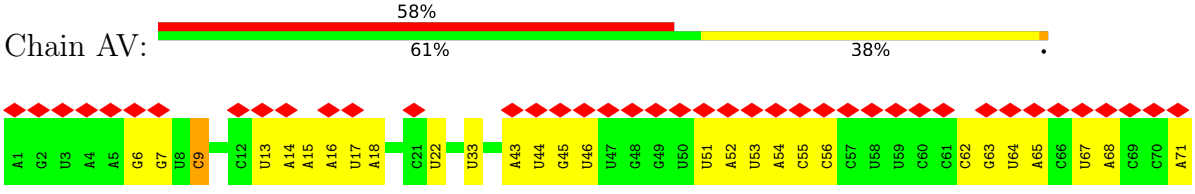
• Molecule 18: Mitochondrial ribosomal protein S21

Chain AU:



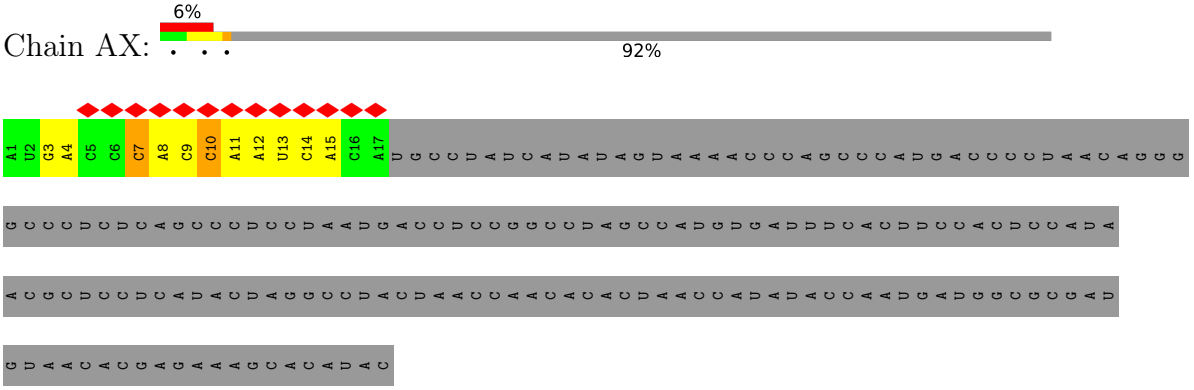
• Molecule 19: P-site fMet-tRNAMet, mitochondrial

Chain AV:



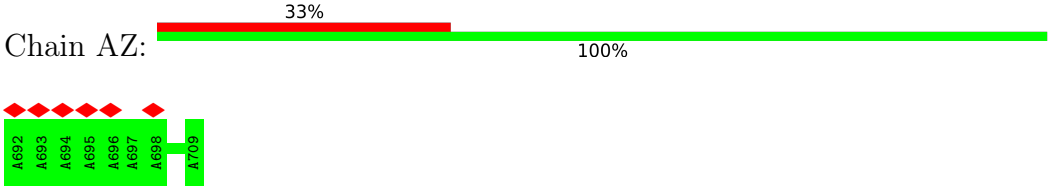
• Molecule 20: MT-CO3 mRNA, mitochondrial

Chain AX:



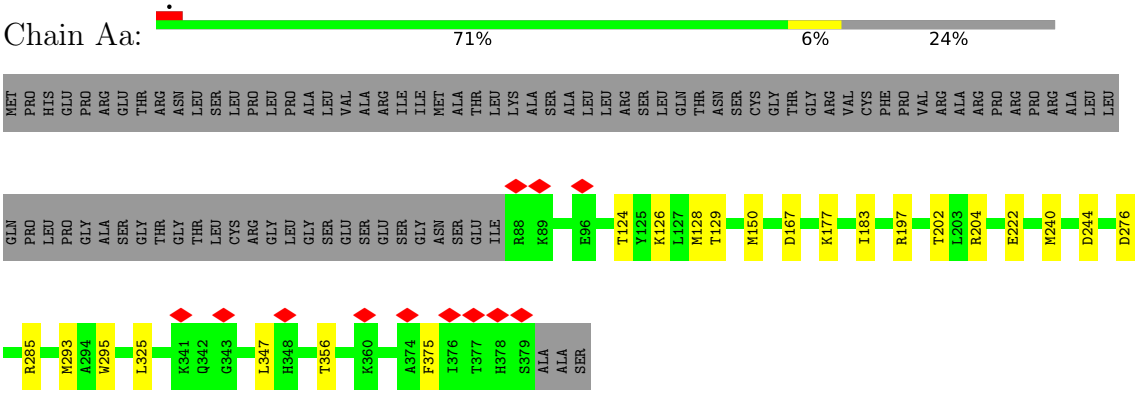
• Molecule 21: unassigned secondary structure elements

Chain AZ:



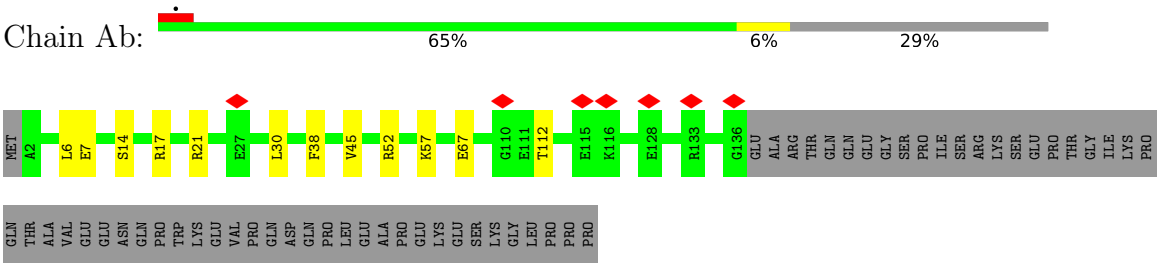
• Molecule 22: Mitochondrial ribosomal protein S22

Chain Aa:



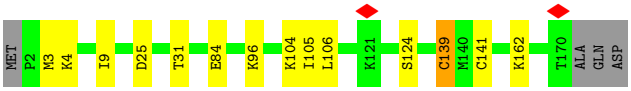
• Molecule 23: Mitochondrial ribosomal protein S23

Chain Ab:

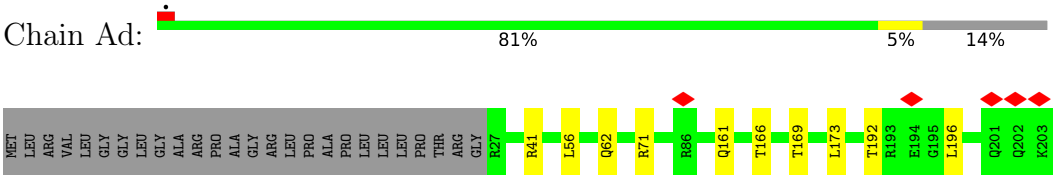


• Molecule 24: Mitochondrial ribosomal protein S25

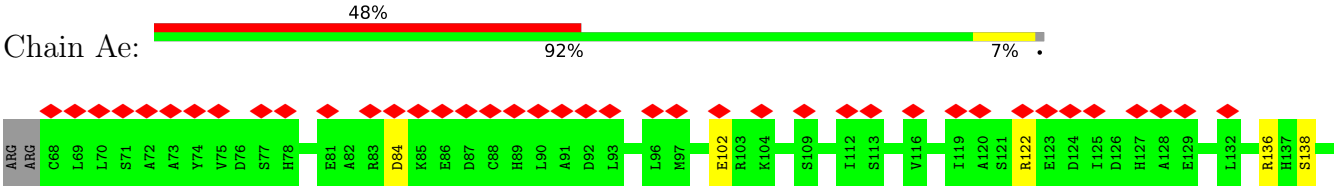
Chain Ac:



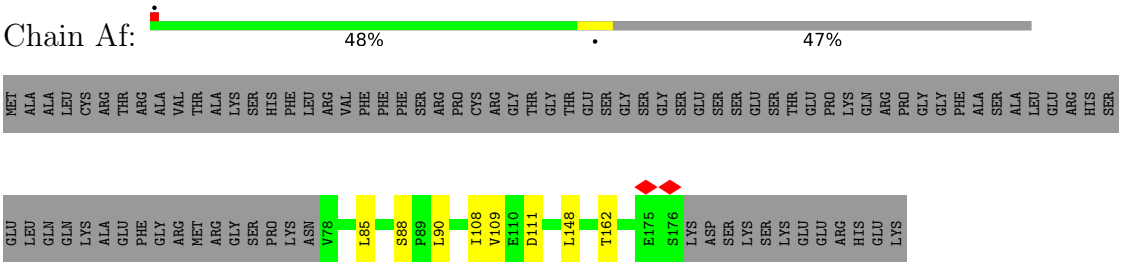
• Molecule 25: Mitochondrial ribosomal protein S26



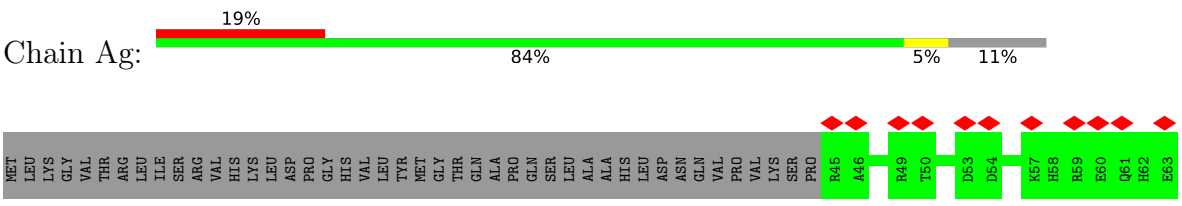
• Molecule 26: Mitochondrial ribosomal protein S27

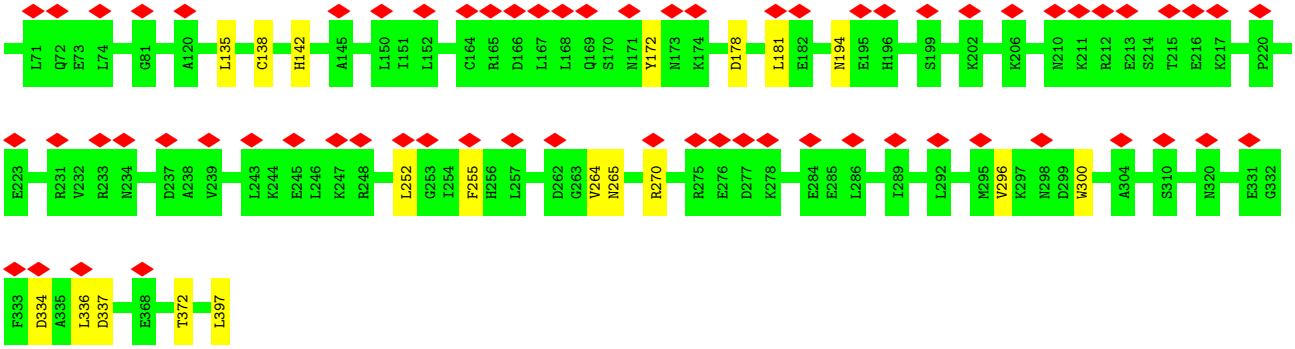


• Molecule 27: Mitoribosomal protein ms28, mrps28

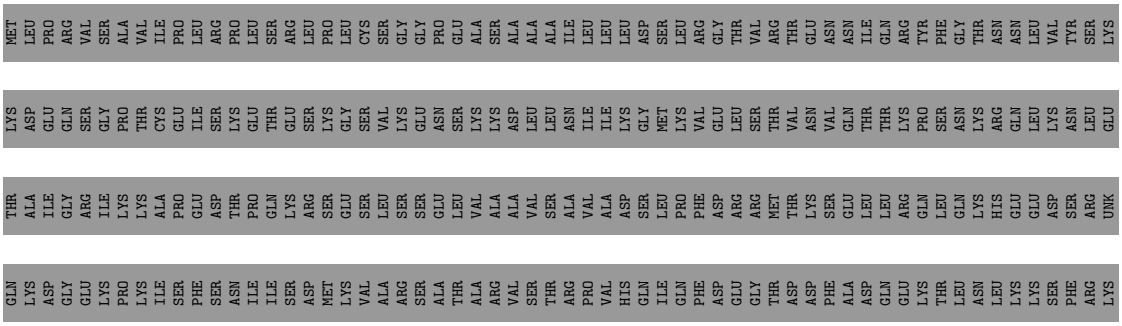


• Molecule 28: Death associated protein 3

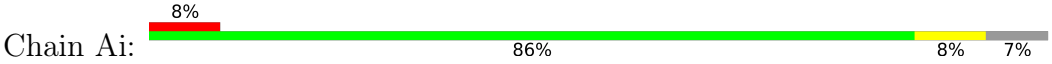




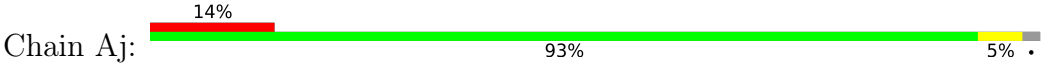
• Molecule 29: mS31, MRPS31

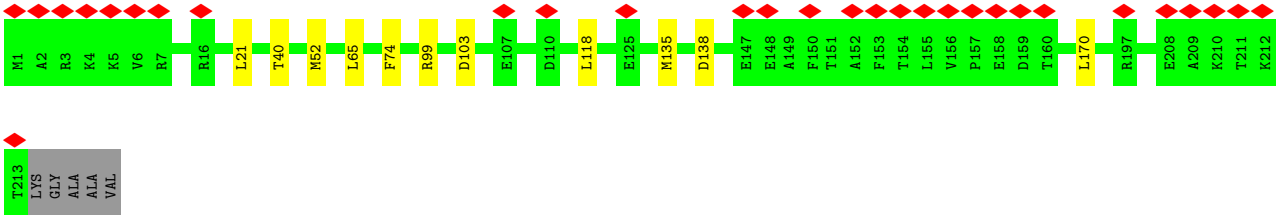


• Molecule 30: Mitochondrial ribosomal protein S33



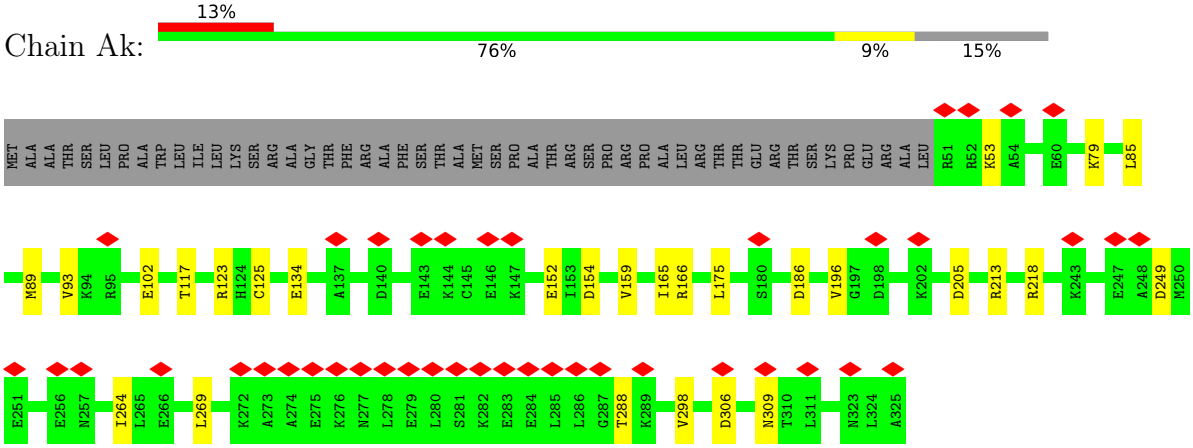
• Molecule 31: Mitochondrial ribosomal protein S34





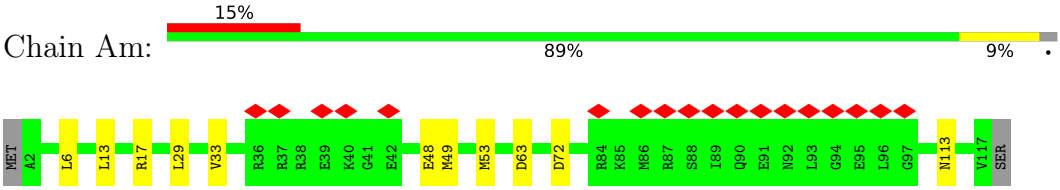
• Molecule 32: Mitochondrial ribosomal protein S35

Chain Ak:



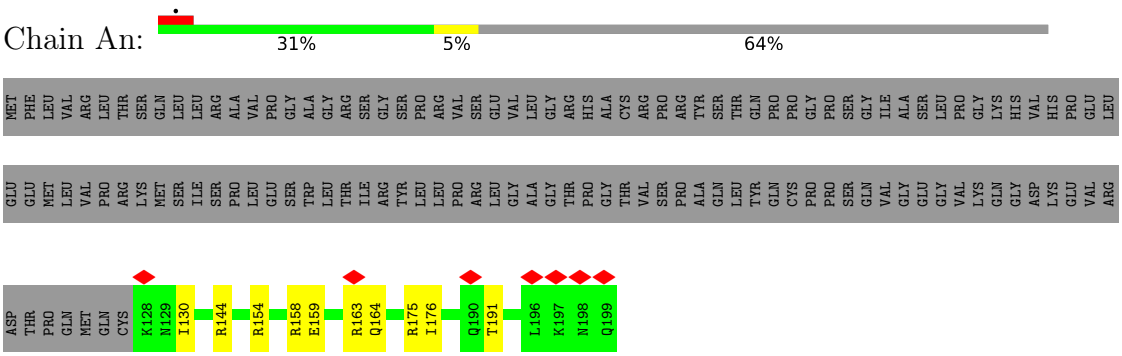
• Molecule 33: Mitochondrial ribosomal protein S37

Chain Am:



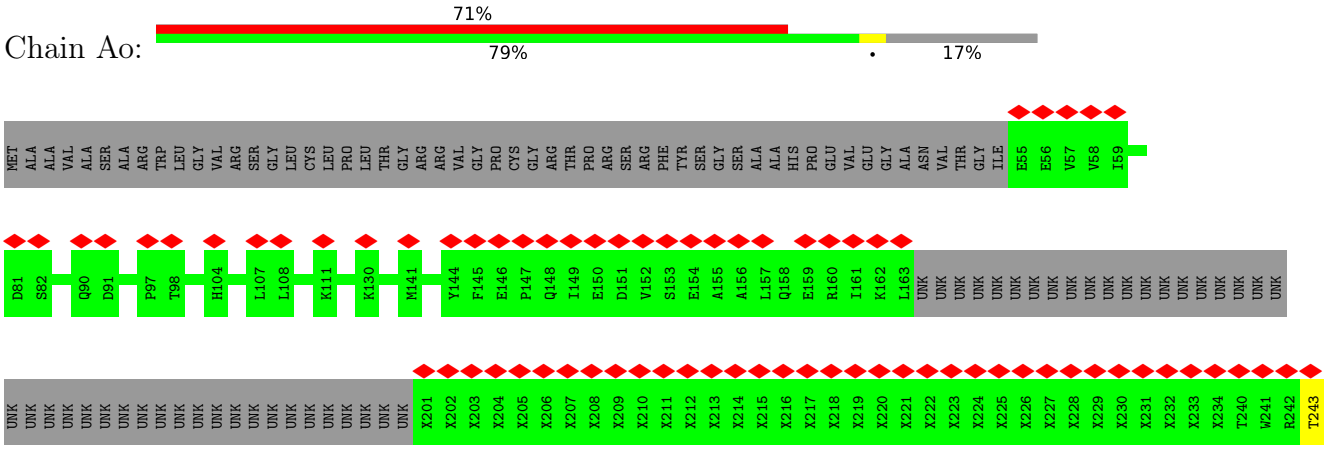
• Molecule 34: Aurora kinase A interacting protein 1

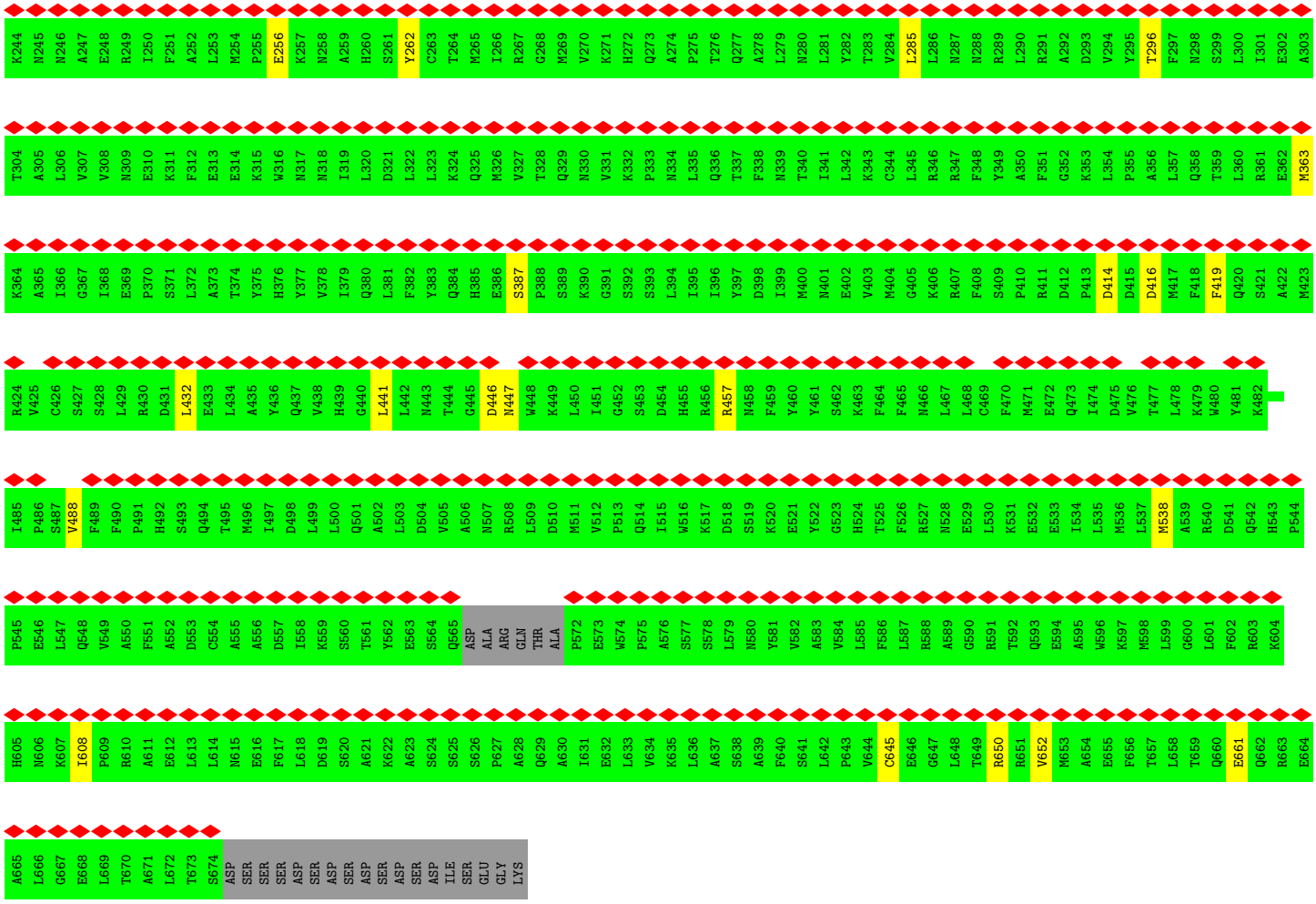
Chain An:



• Molecule 35: Mitochondrial ribosomal protein S39

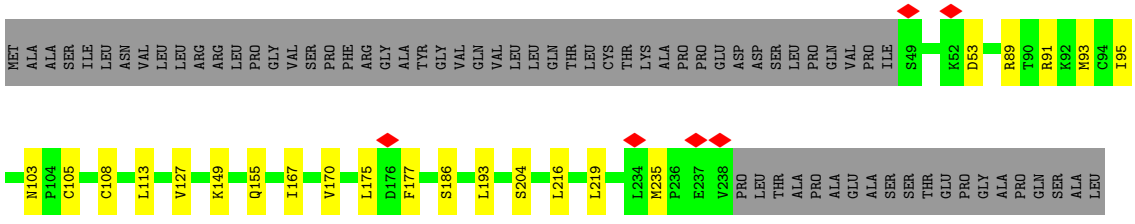
Chain Ao:





• Molecule 36: 28S ribosomal protein S18b, mitochondrial

Chain Ap:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	139206	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.610	Depositor
Minimum map value	-0.242	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.085	Depositor
Map size (Å)	390.59, 390.59, 390.59	wwPDB
Map dimensions	281, 281, 281	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SPM, GTP, FME, NA, GSP, ZN

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	BC	0.35	0/4432	0.53	2/5989 (0.0%)
2	BT	0.35	0/113	0.68	1/157 (0.6%)
3	AA	0.76	8/22852 (0.0%)	1.16	80/35580 (0.2%)
4	AB	0.54	0/1804	0.66	1/2445 (0.0%)
5	AC	0.42	0/1105	0.61	0/1496
6	AE	0.47	0/2785	0.61	0/3735
7	AF	0.51	1/999 (0.1%)	0.64	1/1347 (0.1%)
8	AG	0.36	0/1763	0.52	0/2368
9	AI	0.37	0/2707	0.52	1/3636 (0.0%)
10	AJ	0.43	0/1181	0.63	0/1597
11	AK	0.48	0/1027	0.75	1/1389 (0.1%)
12	AL	0.51	0/858	0.66	0/1152
13	AN	0.44	0/874	0.57	0/1171
14	AO	0.47	0/1473	0.61	0/1970
15	AP	0.55	0/954	0.66	0/1284
16	AQ	0.48	0/894	0.66	0/1213
17	AR	0.68	2/802 (0.2%)	0.74	2/1079 (0.2%)
18	AU	0.53	0/745	0.65	0/993
19	AV	0.43	0/1673	0.98	5/2602 (0.2%)
20	AX	0.55	0/395	1.15	2/612 (0.3%)
21	AZ	0.42	0/89	0.61	0/123
22	Aa	0.42	0/2428	0.60	0/3279
23	Ab	0.43	0/1126	0.58	0/1514
24	Ac	0.55	2/1399 (0.1%)	0.62	1/1881 (0.1%)
25	Ad	0.39	0/1490	0.54	0/2005
26	Ae	0.34	0/3171	0.55	1/4292 (0.0%)
27	Af	0.47	0/790	0.64	0/1064
28	Ag	0.30	0/2945	0.48	0/3984
29	Ah	0.37	0/1045	0.48	0/1409
30	Ai	0.34	0/841	0.52	0/1121
31	Aj	0.34	0/1835	0.52	0/2484
32	Ak	0.32	0/2268	0.49	0/3069

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Am	0.39	0/947	0.54	0/1268
34	An	0.51	0/650	0.65	0/858
35	Ao	0.39	0/4458	0.52	0/6036
36	Ap	0.45	1/1616 (0.1%)	0.59	0/2195
All	All	0.54	14/76534 (0.0%)	0.83	98/108397 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
26	Ae	0	1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Ac	139	CYS	CB-SG	9.52	1.98	1.82
7	AF	105	CYS	CB-SG	8.07	1.96	1.82
17	AR	69	CYS	CB-SG	7.99	1.95	1.82
3	AA	406	A	N9-C4	-7.85	1.33	1.37
24	Ac	141	CYS	CB-SG	7.27	1.94	1.82

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AA	959	U	N1-C2-O2	9.29	129.30	122.80
19	AV	9	C	C2-N1-C1'	8.05	127.66	118.80
3	AA	959	U	N3-C2-O2	-8.01	116.59	122.20
3	AA	476	A	C2-N3-C4	-7.87	106.67	110.60
3	AA	198	C	C6-N1-C2	7.61	123.34	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	Ae	313	GLY	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	BC	569/657 (87%)	549 (96%)	19 (3%)	1 (0%)	47 79
2	BT	15/292 (5%)	14 (93%)	0	1 (7%)	1 7
4	AB	218/289 (75%)	210 (96%)	8 (4%)	0	100 100
5	AC	130/167 (78%)	121 (93%)	9 (7%)	0	100 100
6	AE	341/430 (79%)	330 (97%)	11 (3%)	0	100 100
7	AF	120/124 (97%)	119 (99%)	1 (1%)	0	100 100
8	AG	206/242 (85%)	204 (99%)	2 (1%)	0	100 100
9	AI	326/397 (82%)	312 (96%)	14 (4%)	0	100 100
10	AJ	138/201 (69%)	129 (94%)	7 (5%)	2 (1%)	11 40
11	AK	135/196 (69%)	129 (96%)	5 (4%)	1 (1%)	22 57
12	AL	107/139 (77%)	104 (97%)	3 (3%)	0	100 100
13	AN	99/128 (77%)	99 (100%)	0	0	100 100
14	AO	173/239 (72%)	167 (96%)	6 (4%)	0	100 100
15	AP	115/135 (85%)	113 (98%)	2 (2%)	0	100 100
16	AQ	110/130 (85%)	107 (97%)	3 (3%)	0	100 100
17	AR	95/143 (66%)	95 (100%)	0	0	100 100
18	AU	84/87 (97%)	84 (100%)	0	0	100 100
21	AZ	16/18 (89%)	15 (94%)	1 (6%)	0	100 100
22	Aa	290/382 (76%)	284 (98%)	6 (2%)	0	100 100
23	Ab	133/190 (70%)	128 (96%)	5 (4%)	0	100 100
24	Ac	167/173 (96%)	161 (96%)	5 (3%)	1 (1%)	25 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
25	Ad	175/205 (85%)	169 (97%)	6 (3%)	0	100 100
26	Ae	386/390 (99%)	350 (91%)	33 (8%)	3 (1%)	19 54
27	Af	97/188 (52%)	92 (95%)	5 (5%)	0	100 100
28	Ag	351/397 (88%)	339 (97%)	12 (3%)	0	100 100
29	Ah	118/387 (30%)	115 (98%)	3 (2%)	0	100 100
30	Ai	97/106 (92%)	91 (94%)	6 (6%)	0	100 100
31	Aj	211/218 (97%)	207 (98%)	4 (2%)	0	100 100
32	Ak	273/325 (84%)	267 (98%)	6 (2%)	0	100 100
33	Am	114/118 (97%)	109 (96%)	5 (4%)	0	100 100
34	An	70/199 (35%)	68 (97%)	2 (3%)	0	100 100
35	Ao	532/692 (77%)	505 (95%)	27 (5%)	0	100 100
36	Ap	188/258 (73%)	181 (96%)	7 (4%)	0	100 100
All	All	6199/8242 (75%)	5967 (96%)	223 (4%)	9 (0%)	54 83

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	BT	68	PRO
10	AJ	185	ARG
10	AJ	179	GLN
26	Ae	344	GLU
1	BC	502	PRO

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	BC	464/556 (84%)	445 (96%)	19 (4%)	30 64
2	BT	8/258 (3%)	7 (88%)	1 (12%)	4 18
4	AB	187/233 (80%)	171 (91%)	16 (9%)	10 37
5	AC	115/142 (81%)	97 (84%)	18 (16%)	2 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	AE	282/351 (80%)	253 (90%)	29 (10%)	7 27
7	AF	107/109 (98%)	96 (90%)	11 (10%)	7 27
8	AG	181/205 (88%)	165 (91%)	16 (9%)	10 36
9	AI	273/333 (82%)	247 (90%)	26 (10%)	8 31
10	AJ	130/181 (72%)	120 (92%)	10 (8%)	13 41
11	AK	103/151 (68%)	90 (87%)	13 (13%)	4 18
12	AL	92/116 (79%)	84 (91%)	8 (9%)	10 36
13	AN	92/114 (81%)	78 (85%)	14 (15%)	3 12
14	AO	159/205 (78%)	143 (90%)	16 (10%)	7 28
15	AP	97/113 (86%)	93 (96%)	4 (4%)	30 64
16	AQ	97/114 (85%)	84 (87%)	13 (13%)	4 16
17	AR	89/127 (70%)	82 (92%)	7 (8%)	12 40
18	AU	77/78 (99%)	66 (86%)	11 (14%)	3 14
22	Aa	258/330 (78%)	236 (92%)	22 (8%)	10 37
23	Ab	113/162 (70%)	101 (89%)	12 (11%)	6 26
24	Ac	152/155 (98%)	140 (92%)	12 (8%)	12 40
25	Ad	149/168 (89%)	139 (93%)	10 (7%)	16 46
26	Ae	325/342 (95%)	301 (93%)	24 (7%)	13 42
27	Af	86/160 (54%)	78 (91%)	8 (9%)	9 32
28	Ag	312/350 (89%)	293 (94%)	19 (6%)	18 49
29	Ah	109/346 (32%)	103 (94%)	6 (6%)	21 53
30	Ai	86/93 (92%)	78 (91%)	8 (9%)	9 32
31	Aj	188/190 (99%)	177 (94%)	11 (6%)	19 50
32	Ak	249/289 (86%)	221 (89%)	28 (11%)	6 24
33	Am	100/102 (98%)	89 (89%)	11 (11%)	6 25
34	An	66/174 (38%)	56 (85%)	10 (15%)	3 12
35	Ao	478/538 (89%)	456 (95%)	22 (5%)	27 59
36	Ap	170/225 (76%)	149 (88%)	21 (12%)	4 19
All	All	5394/7010 (77%)	4938 (92%)	456 (8%)	14 37

5 of 456 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	AU	85	GLN
36	Ap	127	VAL
25	Ad	192	THR
36	Ap	93	MET
33	Am	53	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
22	Aa	299	ASN
26	Ae	78	HIS
34	An	164	GLN
22	Aa	327	HIS
24	Ac	69	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	AV	70/71 (98%)	28 (40%)	0
20	AX	16/201 (7%)	10 (62%)	1 (6%)
3	AA	959/962 (99%)	249 (25%)	4 (0%)
All	All	1045/1234 (84%)	287 (27%)	5 (0%)

5 of 287 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	AA	5	A
3	AA	10	U
3	AA	11	G
3	AA	18	G
3	AA	27	U

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	AA	65	C
3	AA	395	C
3	AA	587	U
3	AA	743	A
20	AX	12	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 119 ligands modelled in this entry, 115 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
40	SPM	AA	3001	-	13,13,13	0.34	0	12,12,12	1.03	1 (8%)
37	GSP	BC	901	38	26,34,34	2.12	3 (11%)	27,54,54	1.44	5 (18%)
42	FME	AV	101	19	8,9,10	0.95	0	7,9,11	0.76	0
43	GTP	Ag	500	38	26,34,34	1.11	2 (7%)	32,54,54	1.49	7 (21%)

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
40	SPM	AA	3001	-	-	5/11/11/11	-
37	GSP	BC	901	38	-	0/17/38/38	0/3/3/3
42	FME	AV	101	19	-	4/7/9/11	-
43	GTP	Ag	500	38	-	6/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	BC	901	GSP	PG-S1G	-9.19	1.70	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	Ag	500	GTP	C5-C6	-4.13	1.39	1.47
37	BC	901	GSP	C5-C6	-3.81	1.39	1.47
37	BC	901	GSP	C2-N3	2.29	1.38	1.33
43	Ag	500	GTP	C2-N3	2.08	1.38	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	Ag	500	GTP	PA-O3A-PB	-3.72	120.06	132.83
37	BC	901	GSP	C8-N7-C5	3.18	109.06	102.99
43	Ag	500	GTP	C5-C6-N1	3.00	119.24	113.95
37	BC	901	GSP	C5-C6-N1	2.92	119.11	113.95
43	Ag	500	GTP	C2-N1-C6	-2.73	120.07	125.10

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

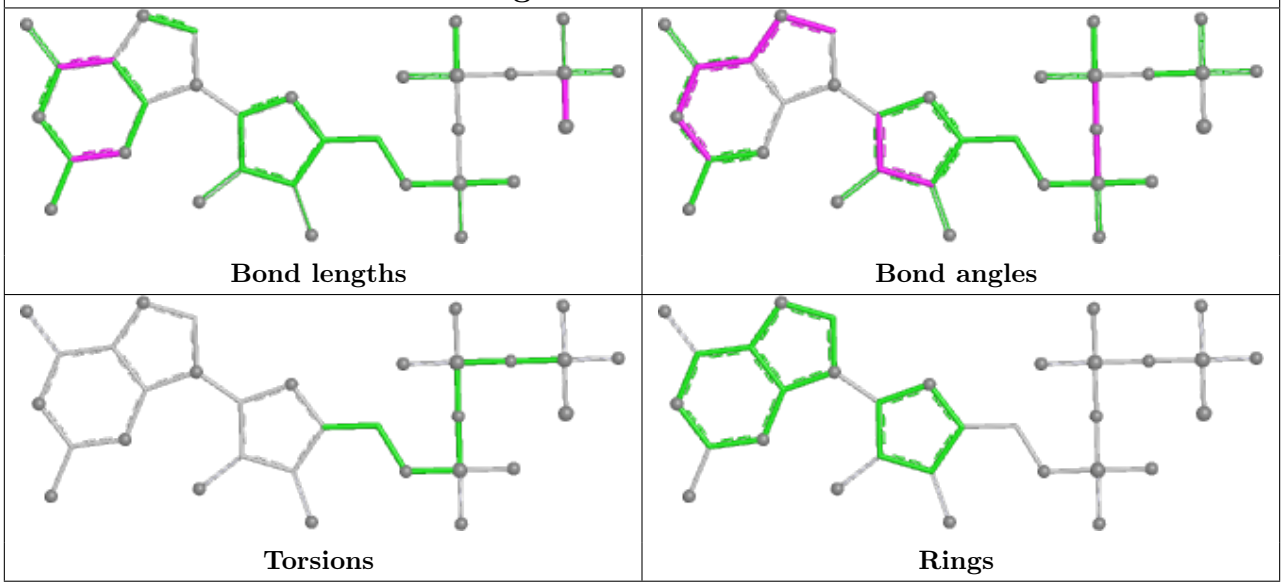
Mol	Chain	Res	Type	Atoms
42	AV	101	FME	C-CA-CB-CG
42	AV	101	FME	CA-CB-CG-SD
43	Ag	500	GTP	C5'-O5'-PA-O3A
40	AA	3001	SPM	C2-C3-C4-N5
40	AA	3001	SPM	C7-C8-C9-N10

There are no ring outliers.

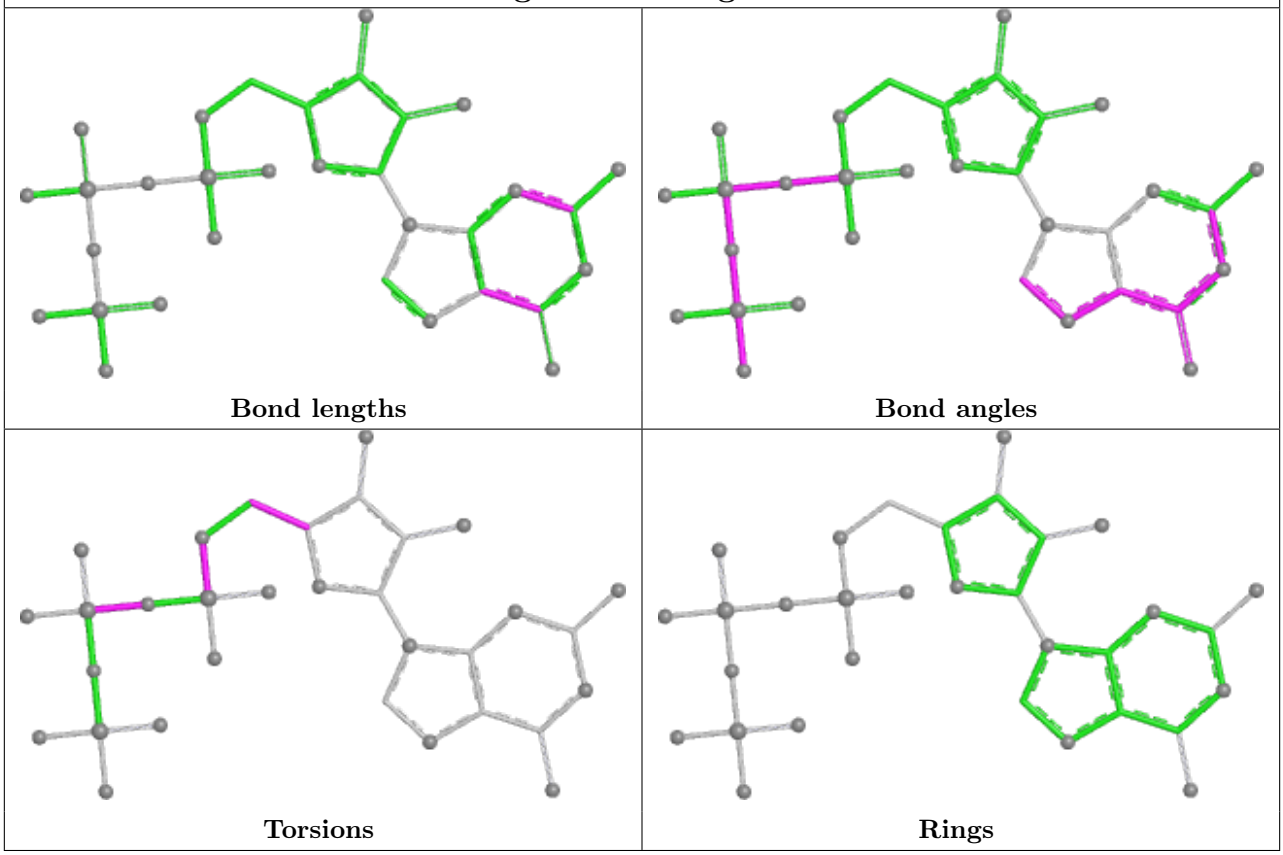
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GSP BC 901



Ligand GTP Ag 500



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
35	Ao	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ao	234:UNK	C	240:THR	N	8.66

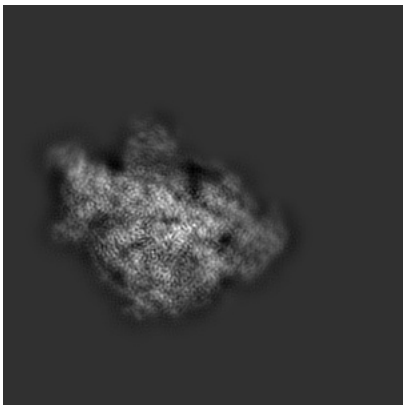
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4369. These allow visual inspection of the internal detail of the map and identification of artifacts.

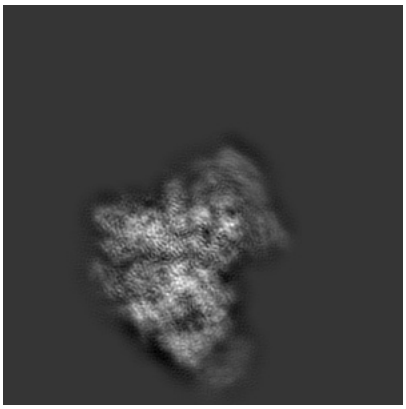
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

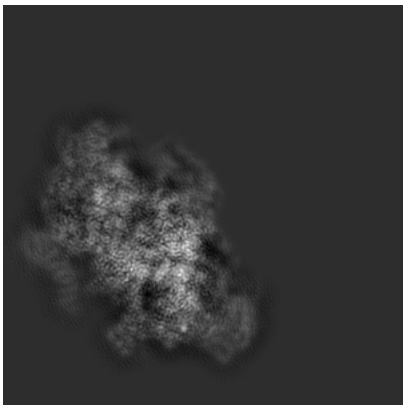
6.1.1 Primary map



X

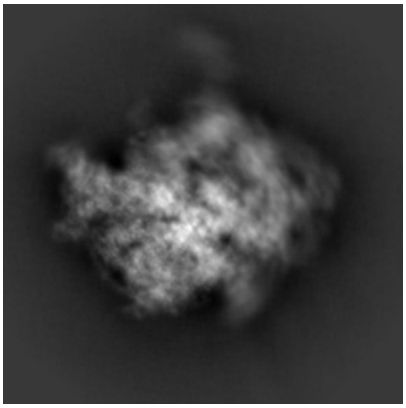


Y

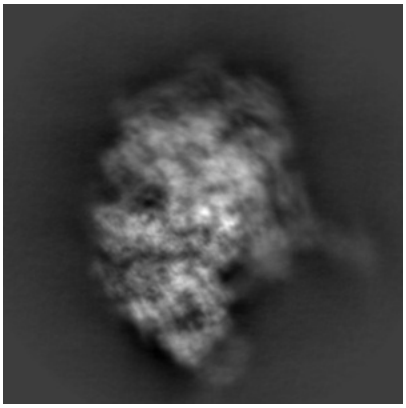


Z

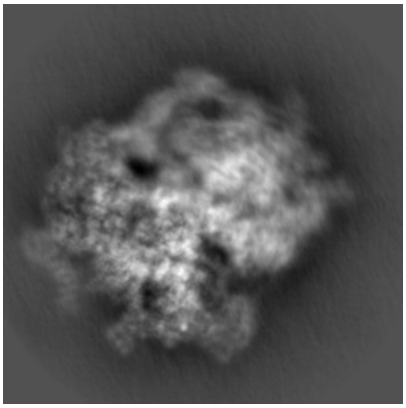
6.1.2 Raw map



X



Y

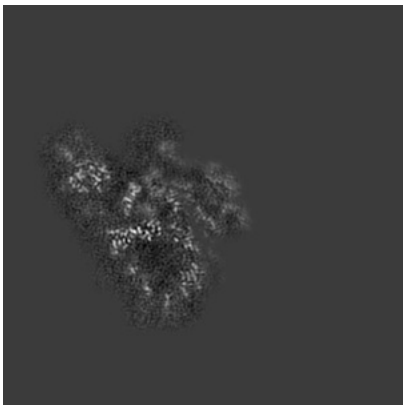


Z

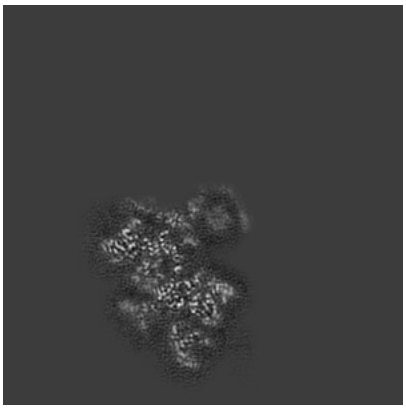
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

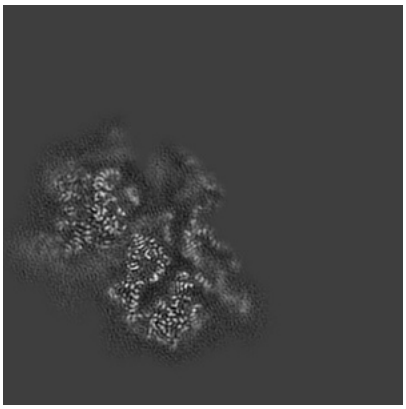
6.2.1 Primary map



X Index: 140

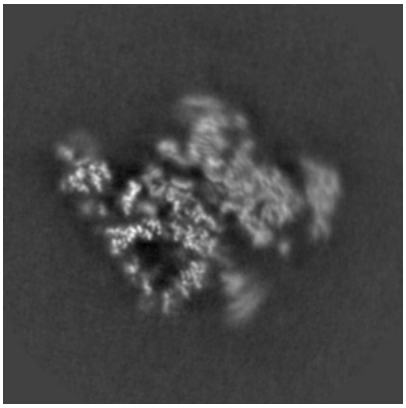


Y Index: 140

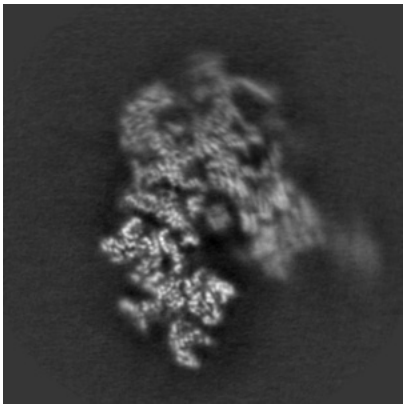


Z Index: 140

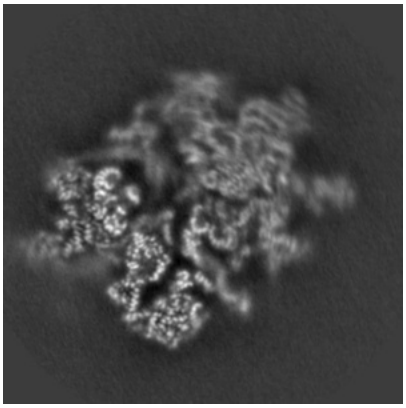
6.2.2 Raw map



X Index: 140



Y Index: 140

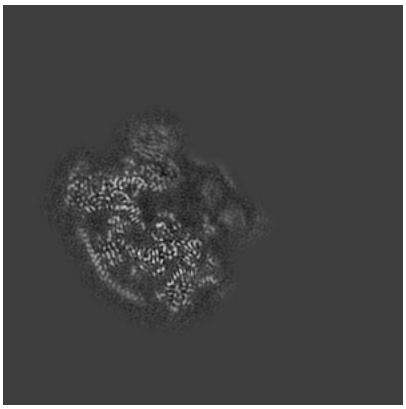


Z Index: 140

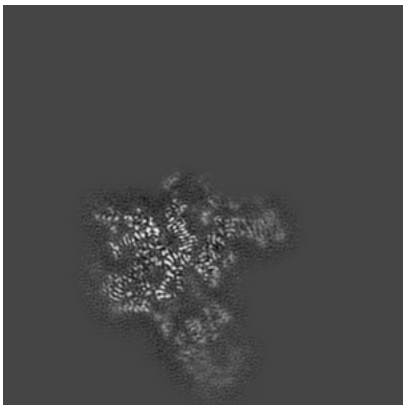
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

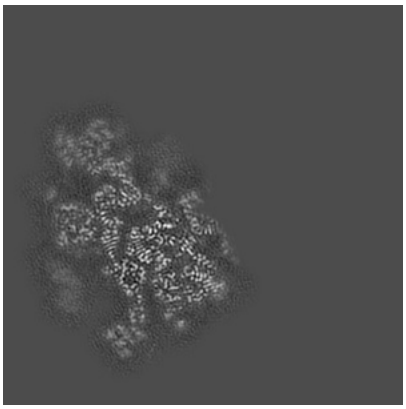
6.3.1 Primary map



X Index: 123

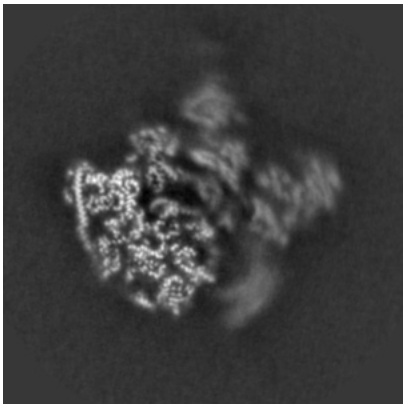


Y Index: 108

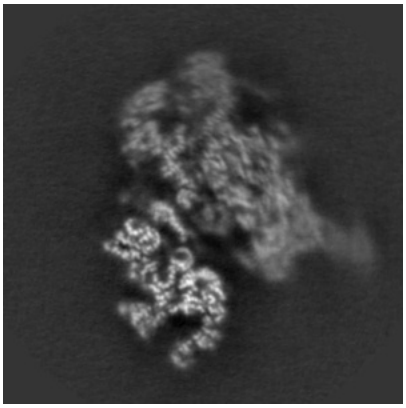


Z Index: 118

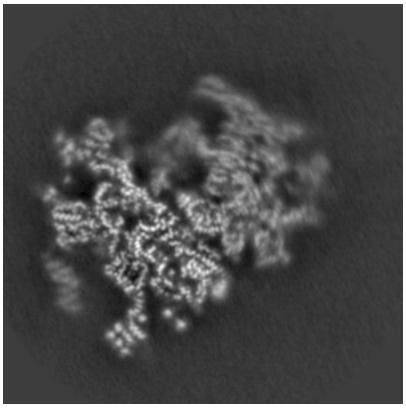
6.3.2 Raw map



X Index: 127



Y Index: 145



Z Index: 120

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

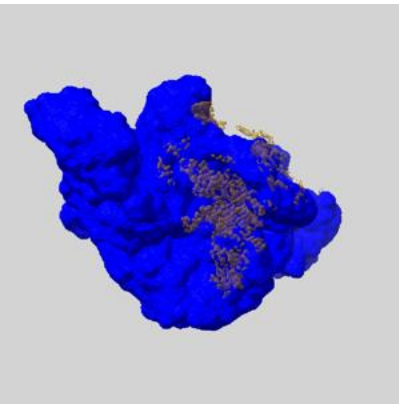
6.5 Mask visualisation (i)

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

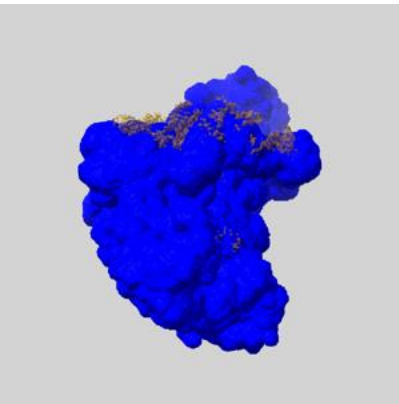
A mask typically either:

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

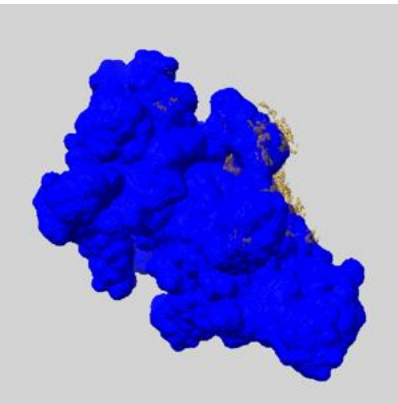
6.5.1 emd_4369_msk_1.map (i)



X



Y

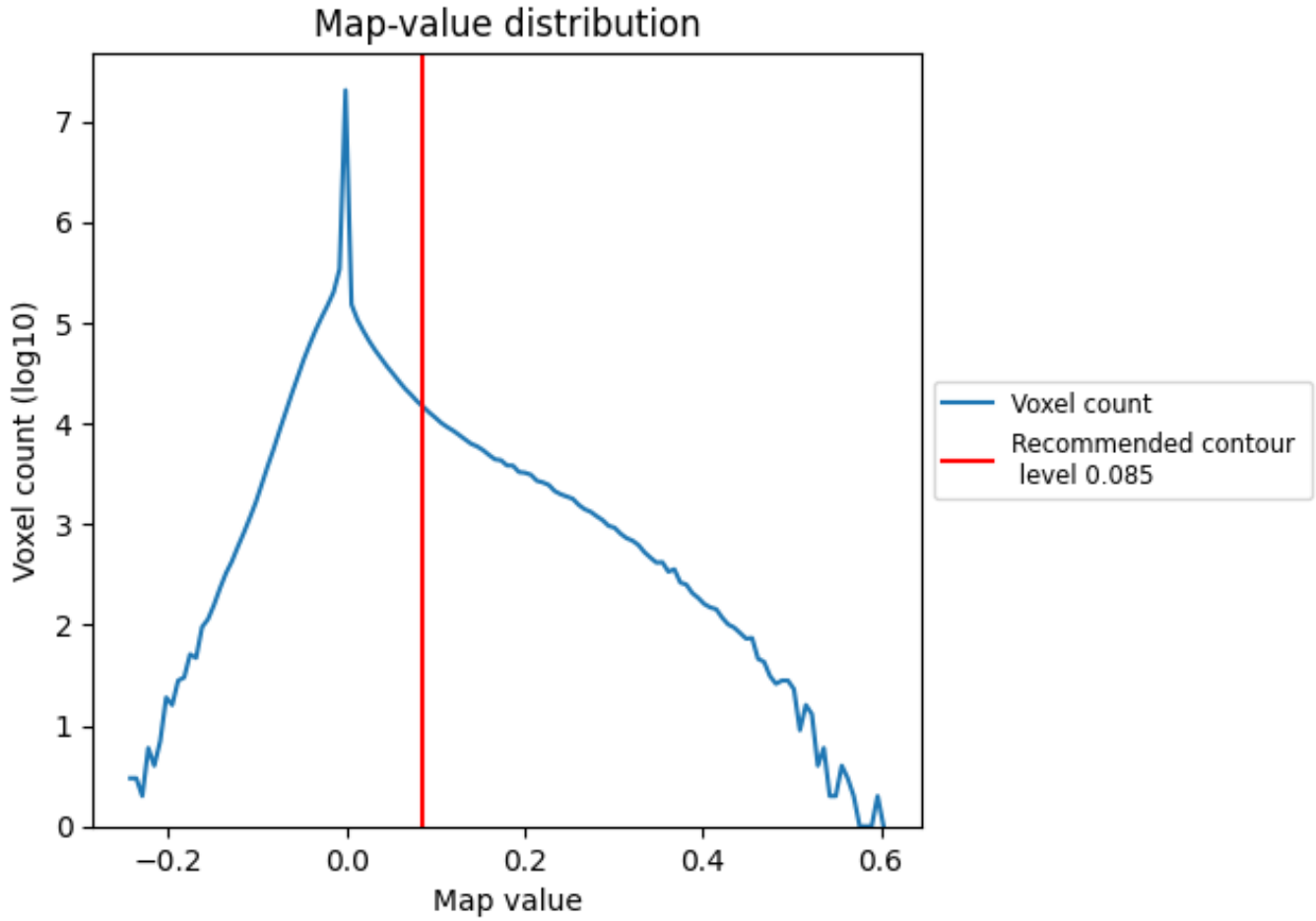


Z

7 Map analysis

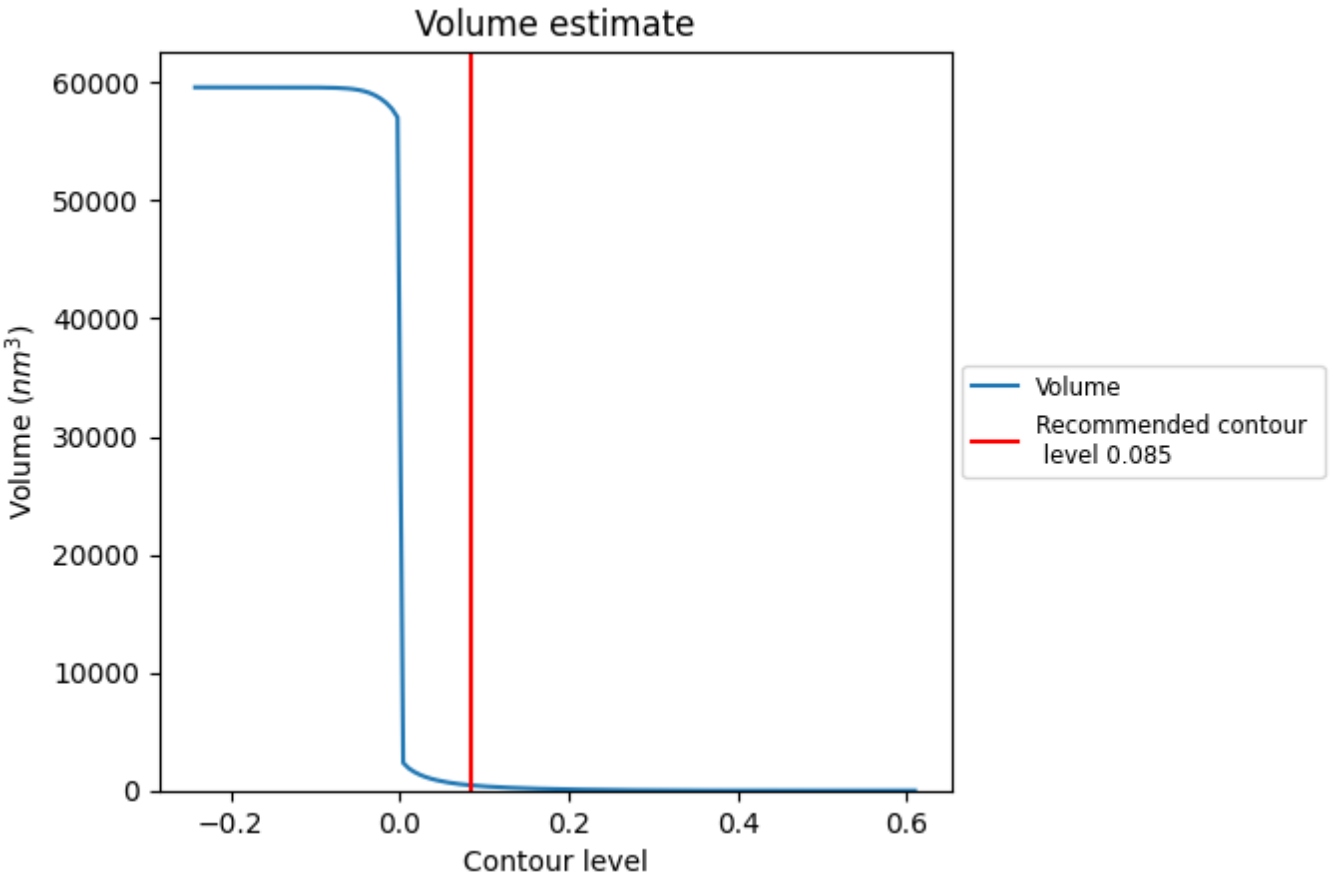
This section contains the results of statistical analysis of the map.

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.

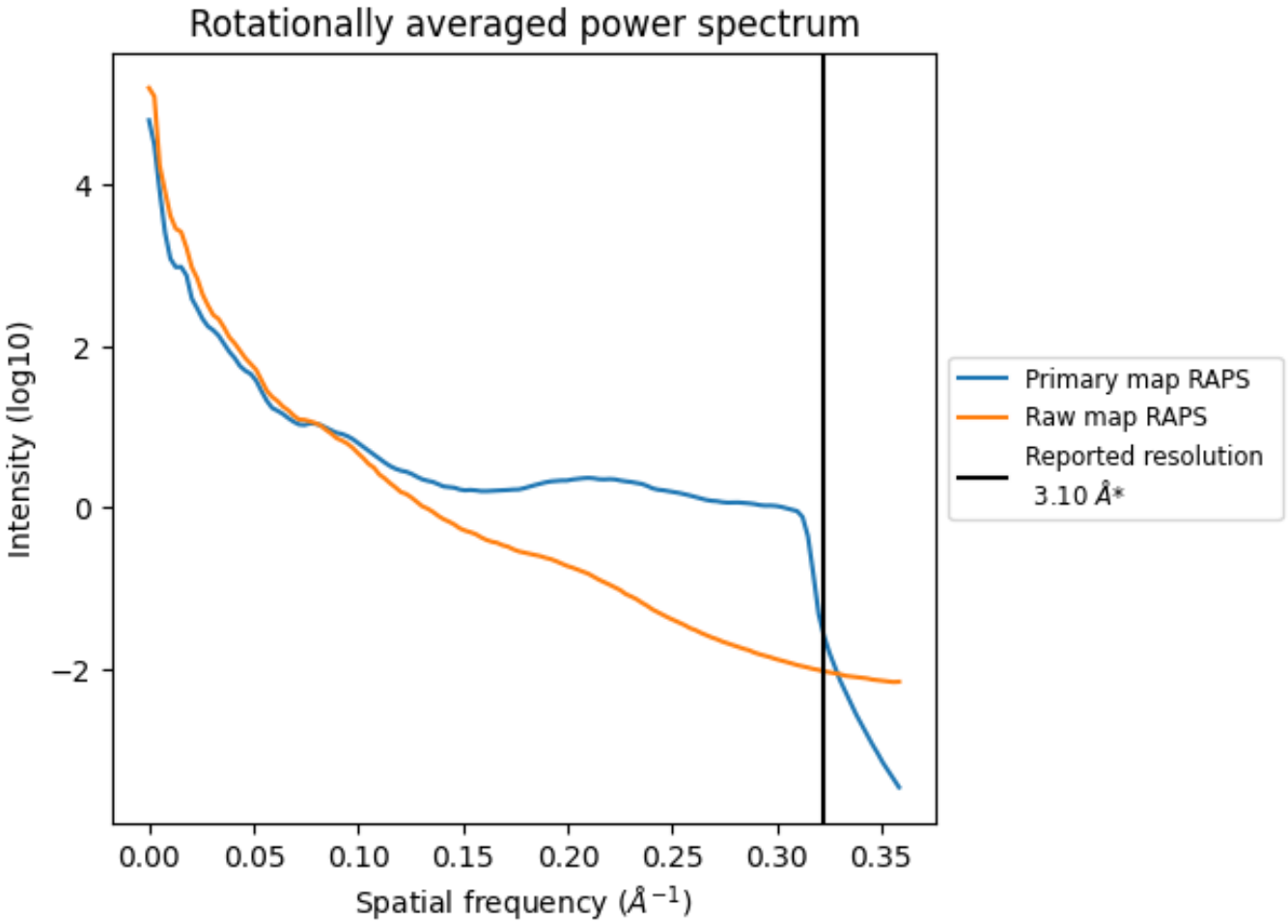
7.2 Volume estimate (i)



The volume at the recommended contour level is 442 nm^3; this corresponds to an approximate mass of 399 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)

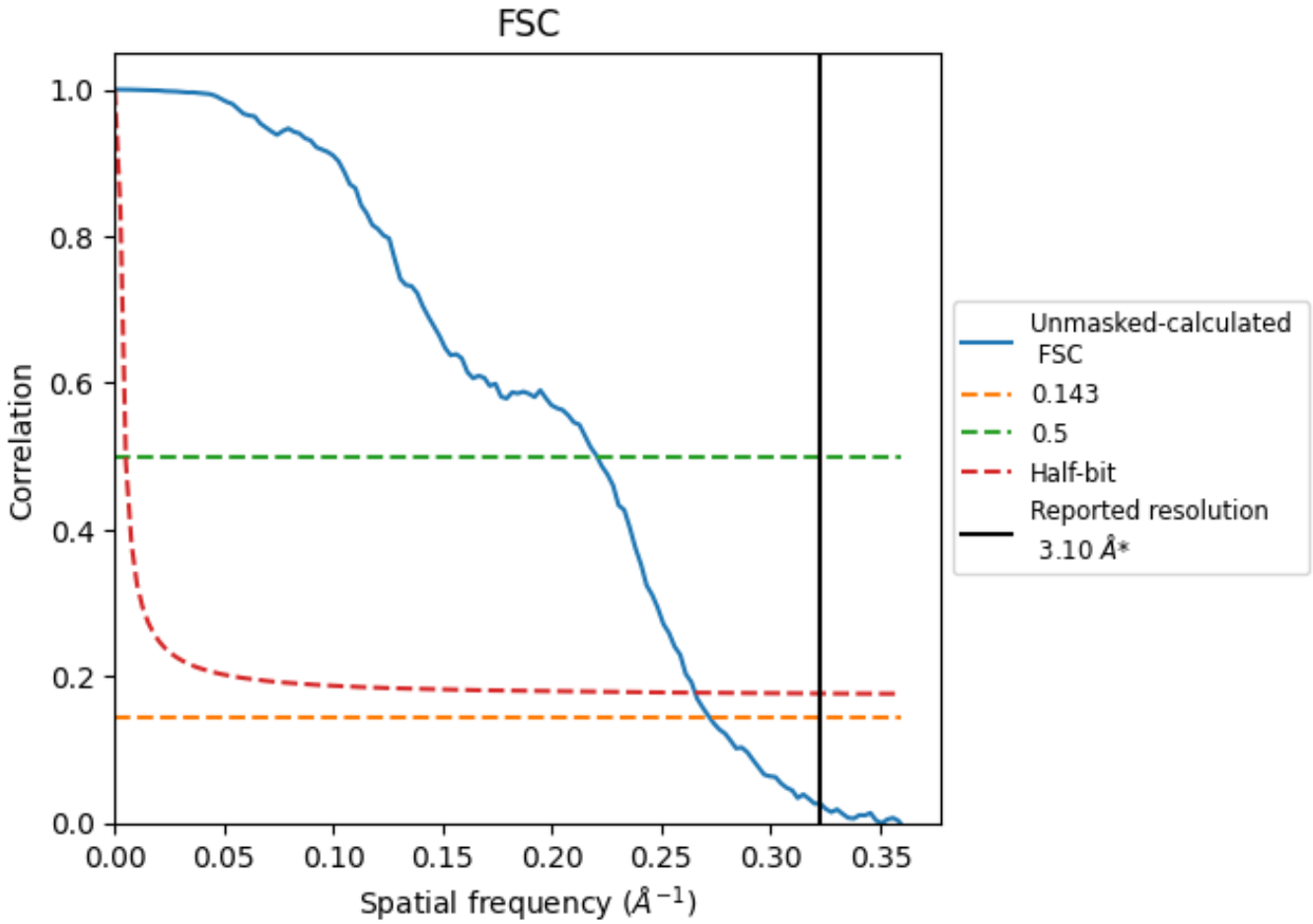


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

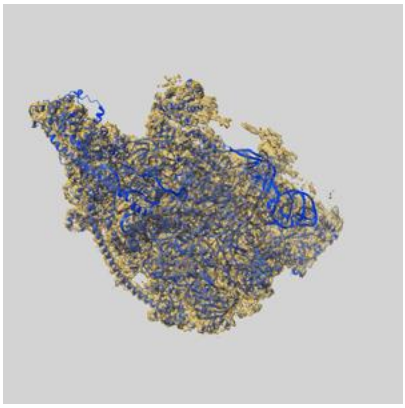
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.68	4.54	3.77

*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 3.68 differs from the reported value 3.1 by more than 10 %

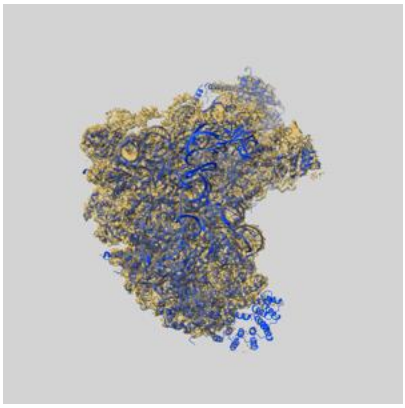
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4369 and PDB model 6GAZ. Per-residue inclusion information can be found in section 3 on page 15.

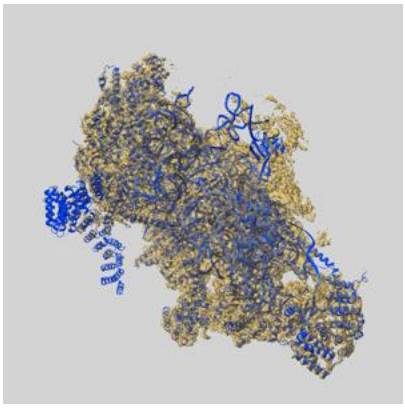
9.1 Map-model overlay



X



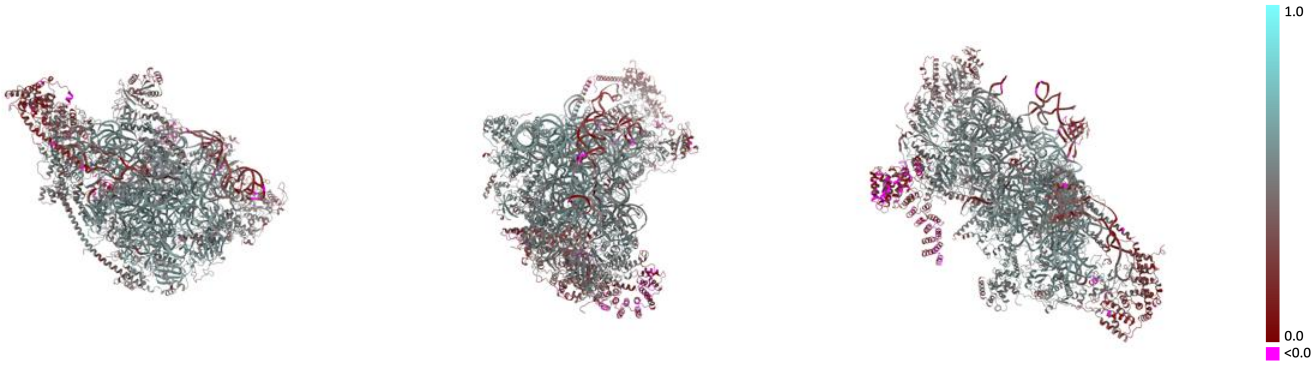
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

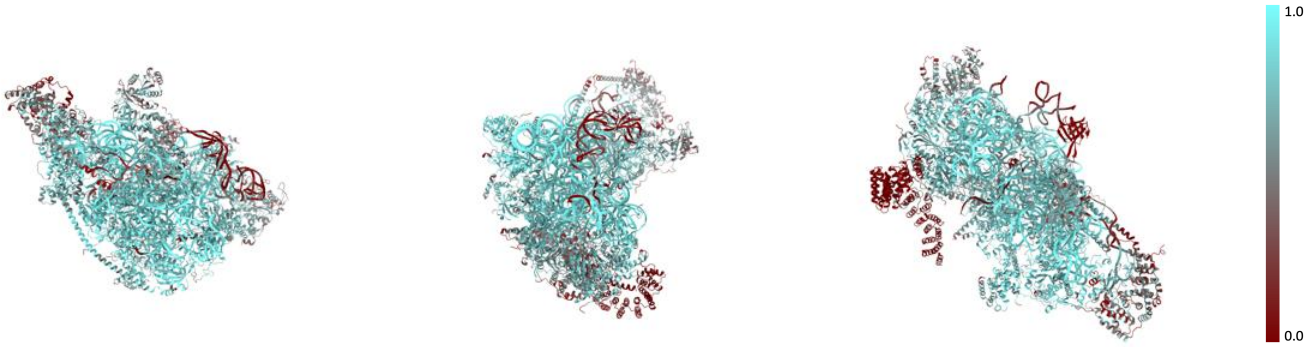
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

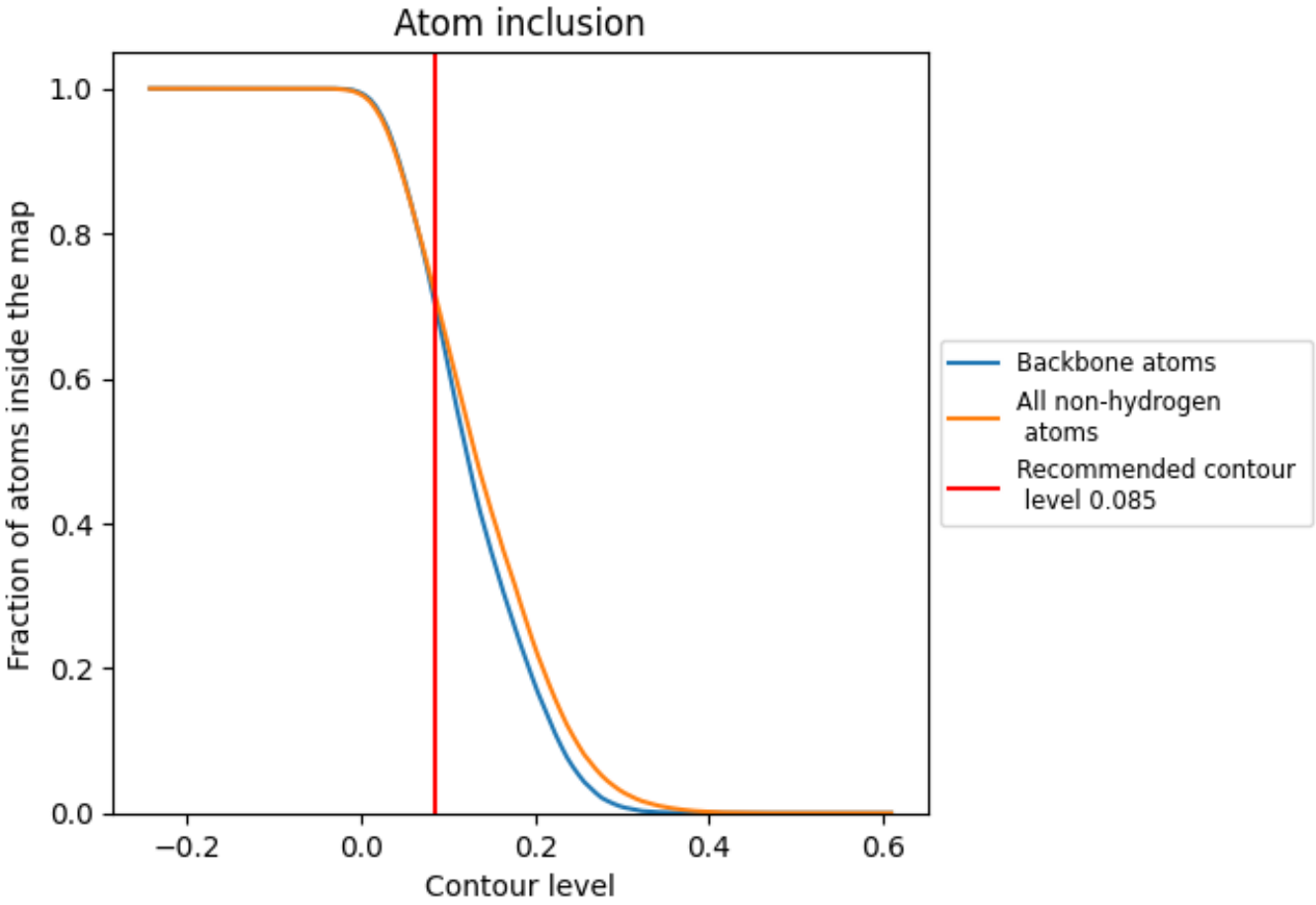
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.085).

9.4 Atom inclusion (i)



At the recommended contour level, 70% 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 (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7168	0.4620
AA	0.9252	0.5370
AB	0.8748	0.5380
AC	0.7655	0.5360
AE	0.7400	0.5130
AF	0.8302	0.5300
AG	0.7597	0.4660
AI	0.7306	0.4680
AJ	0.7073	0.4650
AK	0.8704	0.5250
AL	0.8217	0.5530
AN	0.8687	0.5450
AO	0.7620	0.4980
AP	0.8687	0.5380
AQ	0.8477	0.5410
AR	0.8616	0.5400
AU	0.8883	0.5510
AV	0.4191	0.3250
AX	0.2056	0.2840
AZ	0.5222	0.3510
Aa	0.7918	0.4970
Ab	0.7895	0.4920
Ac	0.8491	0.5310
Ad	0.7866	0.4710
Ae	0.4257	0.2420
Af	0.8521	0.5230
Ag	0.5635	0.3850
Ah	0.6360	0.4240
Ai	0.7280	0.4890
Aj	0.6669	0.4430
Ak	0.6364	0.4190
Am	0.6981	0.4870
An	0.7393	0.5210
Ao	0.1403	0.1860
Ap	0.8316	0.5220

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Chain	Atom inclusion	Q-score
BC	0.4670	0.3780
BT	0.2385	0.3100