wwPDB EM Validation Summary Report (i)

Apr 16, 2024 – 01:45 pm BST

PDB ID	:	8OIP
EMDB ID	:	EMD-16895
Title	:	28S mammalian mitochondrial small ribosomal subunit with mtRF1 and P-site tRNA
Authors	:	Saurer, M.; Leibundgut, M.; Scaiola, A.; Schoenhut, T.; Ban, N.
Deposited on	:	2023-03-23
Resolution	:	3.60 Å(reported)
Based on initial models	:	7QI4, ., 7NQH

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:

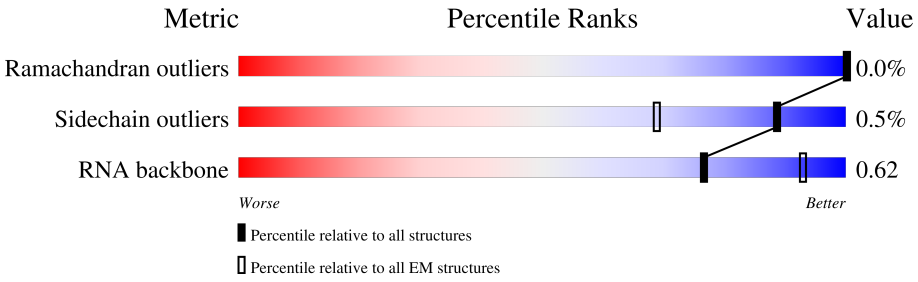
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.60 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	BX	303	5% 95%
2	Bd	126	12% 17% 82%
3	AA	962	5% 84% 15%
4	AB	366	9% 75% 25%
5	AC	167	79% 21%
6	AD	199	36% 64%
7	AE	376	32% 68%
8	AF	242	7% 86% 14%

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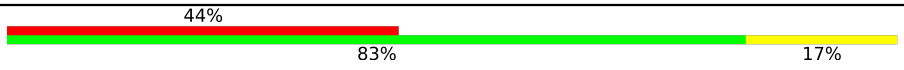
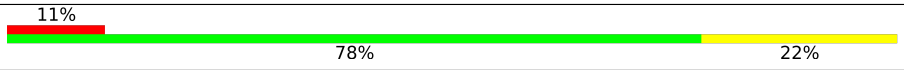
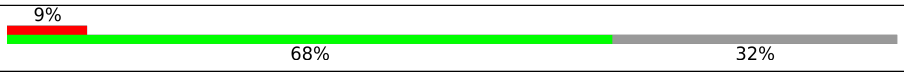
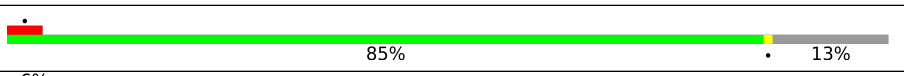
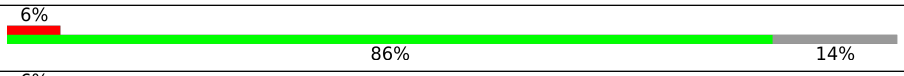
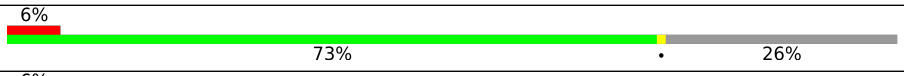
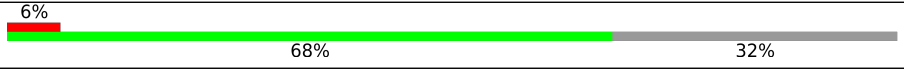
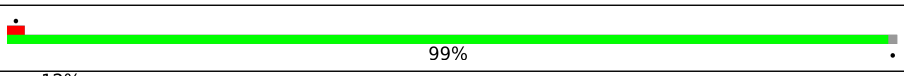
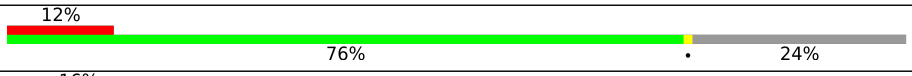
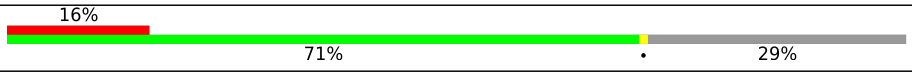
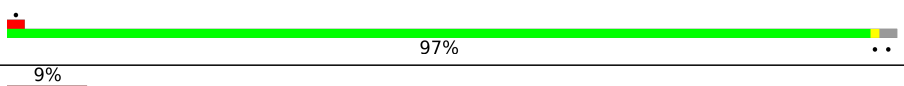
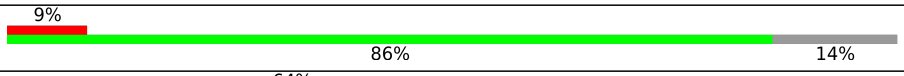
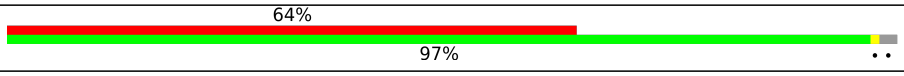
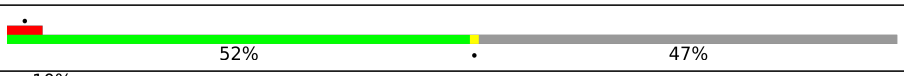
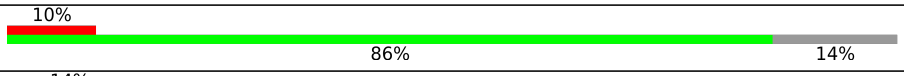
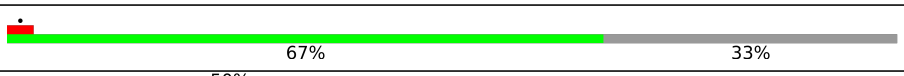
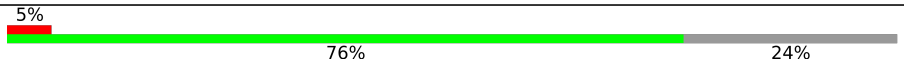
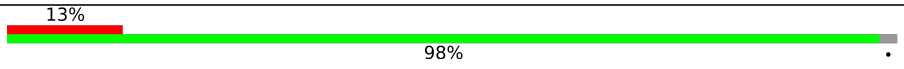
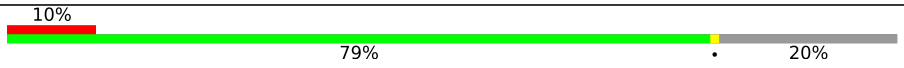
Mol	Chain	Length	Quality of chain
9	AG	72	
10	AH	200	
11	AI	9	
12	AJ	139	
13	AK	128	
14	AL	259	
15	AM	135	
16	AN	130	
17	AO	258	
18	AP	143	
19	AQ	87	
20	AR	382	
21	AS	190	
22	AT	173	
23	AU	205	
24	AV	395	
25	AW	188	
26	AX	410	
27	AY	381	
28	AZ	148	
29	Aa	474	
30	Ab	289	
31	Ac	118	
32	Ad	430	
33	Ae	692	

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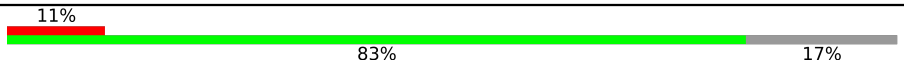
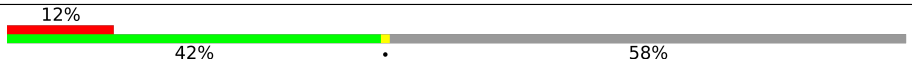
Mol	Chain	Length	Quality of chain
34	Ag	397	
35	Ai	196	
36	Aj	505	

2 Entry composition (i)

There are 45 unique types of molecules in this entry. The entry contains 72369 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	BX	15	99	66	17	16	0	0

- Molecule 2 is a protein called bL31m.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	Bd	23	192	124	31	37	0	0

- Molecule 3 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	AA	960	20418	9169	3708	6581	960	0	0

- Molecule 4 is a protein called 28S ribosomal protein S35, mitochondrial isoform 1.

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

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

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

- Molecule 6 is a protein called Aurora kinase A interacting protein 1.

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

- Molecule 7 is a protein called bS6m,Mitochondrial ribosomal protein S6.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	-22	SER	PRO	conflict	UNP A0A4X1TSM9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AF	208	Total	C	N	O	S	0	0
			1722	1097	314	300	11		

- Molecule 9 is a RNA chain called P-site Met-tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
9	AG	72	Total	C	N	O	P	S	0	0
			1512	679	265	496	71	1		

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

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

- Molecule 11 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AI	9	Total	C	N	O	P	0	0
			193	88	40	57	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AJ	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	AK	101	Total	C	N	O	S	0	0
			858	534	174	144	6		

- Molecule 14 is a protein called 28S ribosomal protein S15, mitochondrial.

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

- Molecule 15 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 16 is a protein called uS17m.

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

- Molecule 17 is a protein called 28S ribosomal protein S18b, mitochondrial.

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

- Molecule 18 is a protein called Mitochondrial ribosomal protein S18C.

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

- Molecule 19 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AQ	86	Total	C	N	O	S	0	0
			737	455	148	126	8		

- Molecule 20 is a protein called Mitochondrial ribosomal protein S22.

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

- Molecule 21 is a protein called mS23.

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

- Molecule 22 is a protein called Mitochondrial ribosomal protein S25.

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

- Molecule 23 is a protein called Mitochondrial ribosomal protein S26.

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

- Molecule 24 is a protein called Mitochondrial ribosomal protein S27.

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

- Molecule 25 is a protein called Mitoribosomal protein ms28, mrps28.

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

- Molecule 26 is a protein called Death associated protein 3.

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

- Molecule 27 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AY	149	Total	C	N	O	S	0	0
			1250	807	211	229	3		

- Molecule 28 is a protein called Mitochondrial ribosomal protein S33.

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

- Molecule 29 is a protein called Peptide chain release factor 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Aa	381	Total	C	N	O	S	1	0
			3120	1943	572	592	13		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aa	446	GLY	-	expression tag	UNP O75570
Aa	447	GLY	-	expression tag	UNP O75570
Aa	448	SER	-	expression tag	UNP O75570
Aa	449	GLY	-	expression tag	UNP O75570
Aa	450	GLY	-	expression tag	UNP O75570
Aa	451	SER	-	expression tag	UNP O75570
Aa	452	GLY	-	expression tag	UNP O75570
Aa	453	ASP	-	expression tag	UNP O75570
Aa	454	TYR	-	expression tag	UNP O75570
Aa	455	LYS	-	expression tag	UNP O75570
Aa	456	ASP	-	expression tag	UNP O75570
Aa	457	HIS	-	expression tag	UNP O75570
Aa	458	ASP	-	expression tag	UNP O75570
Aa	459	GLY	-	expression tag	UNP O75570
Aa	460	ASP	-	expression tag	UNP O75570
Aa	461	TYR	-	expression tag	UNP O75570
Aa	462	LYS	-	expression tag	UNP O75570
Aa	463	ASP	-	expression tag	UNP O75570
Aa	464	HIS	-	expression tag	UNP O75570
Aa	465	ASP	-	expression tag	UNP O75570
Aa	466	ILE	-	expression tag	UNP O75570
Aa	467	ASP	-	expression tag	UNP O75570
Aa	468	TYR	-	expression tag	UNP O75570
Aa	469	LYS	-	expression tag	UNP O75570
Aa	470	ASP	-	expression tag	UNP O75570

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Chain	Residue	Modelled	Actual	Comment	Reference
Aa	471	ASP	-	expression tag	UNP O75570
Aa	472	ASP	-	expression tag	UNP O75570
Aa	473	ASP	-	expression tag	UNP O75570
Aa	474	LYS	-	expression tag	UNP O75570

- Molecule 30 is a protein called Mitochondrial ribosomal protein S2.

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

- Molecule 31 is a protein called Coiled-coil-helix-coiled-coil-helix domain containing 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ac	116	Total	C	N	O	S	0	0
			933	579	185	161	8		

- Molecule 32 is a protein called 28S ribosomal protein S5, mitochondrial isoform X2.

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

- Molecule 33 is a protein called mS39.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ae	588	Total	C	N	O	S	0	0
			4748	3039	804	879	26		

- Molecule 34 is a protein called uS9m.

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

- Molecule 35 is a protein called Mitochondrial ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Ai	137	Total	C	N	O	S	0	0
			1008	632	192	181	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ai	186	5F0	ASN	variant	UNP A0A286ZJJ6

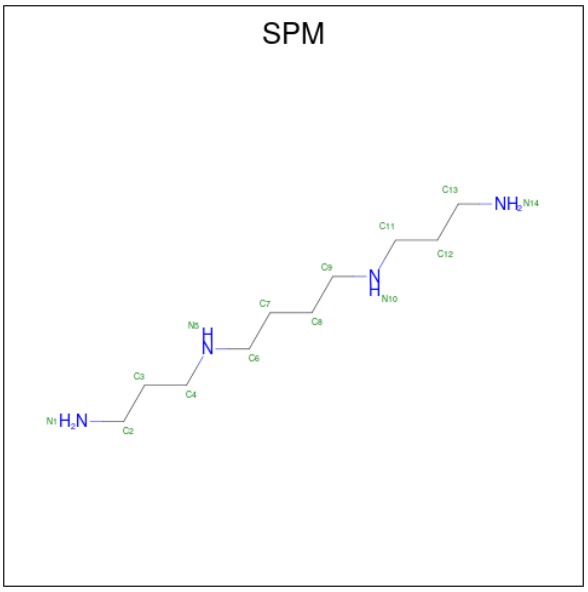
- Molecule 36 is a protein called Mitochondrial ribosomal protein S34.

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

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

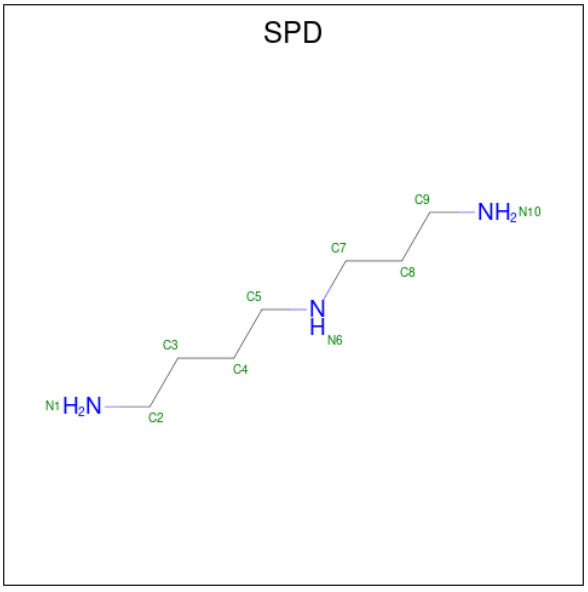
Mol	Chain	Residues	Atoms		AltConf
37	AA	120	Total	Mg	0
			120	120	
37	AD	1	Total	Mg	0
			1	1	
37	AG	1	Total	Mg	0
			1	1	
37	AI	1	Total	Mg	0
			1	1	
37	AJ	2	Total	Mg	0
			2	2	
37	AX	1	Total	Mg	0
			1	1	
37	Ab	1	Total	Mg	0
			1	1	

- Molecule 38 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



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

- Molecule 39 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
39	AA	1	Total	C	N	0
			10	7	3	

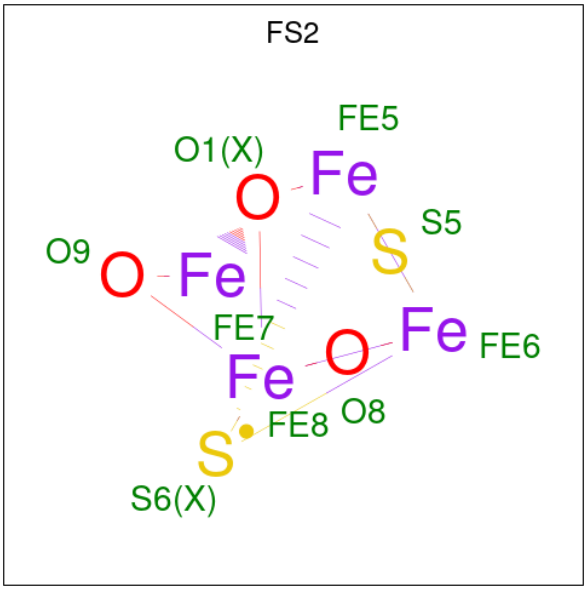
- Molecule 40 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
40	AA	11	Total K 11 11	0

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

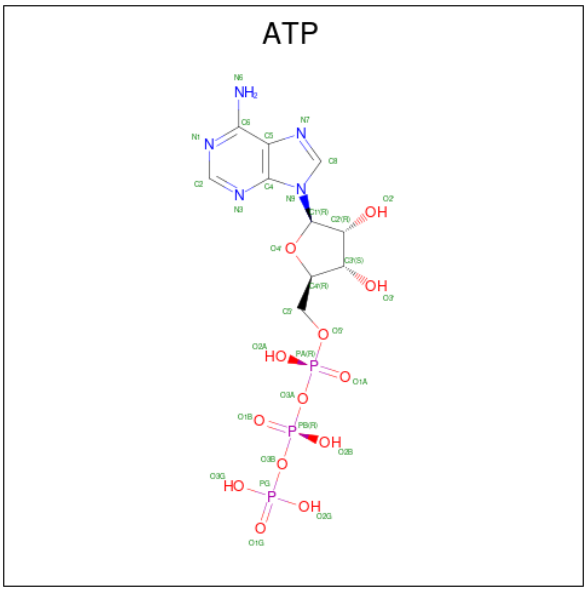
Mol	Chain	Residues	Atoms	AltConf
41	AO	1	Total Zn 1 1	0

- Molecule 42 is FE-S-O HYBRID CLUSTER (three-letter code: FS2) (formula: $Fe_4O_3S_2$).



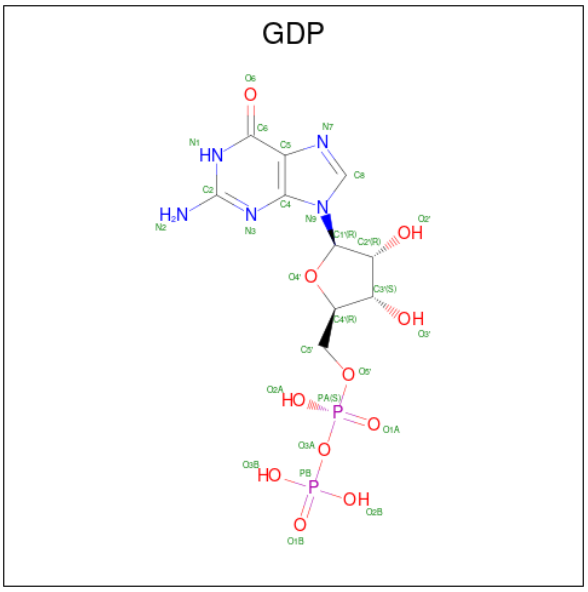
Mol	Chain	Residues	Atoms	AltConf
42	AP	1	Total Fe S 4 2 2	0
42	AT	1	Total Fe S 4 2 2	0

- Molecule 43 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 44 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 45 is water.

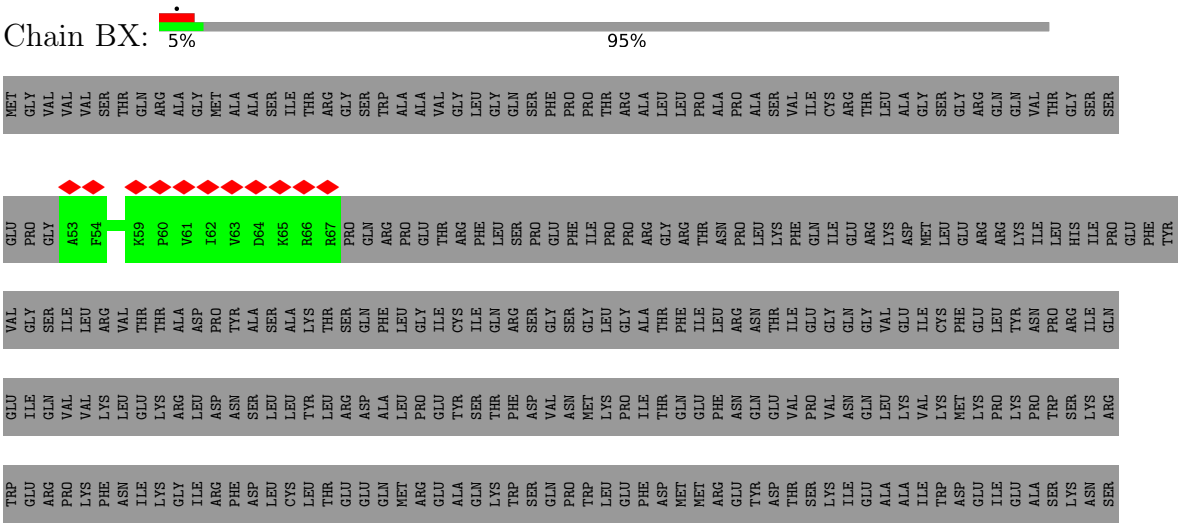
Mol	Chain	Residues	Atoms		AltConf
45	AX	3	Total	O	0
			3	3	

3 Residue-property plots (i)

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

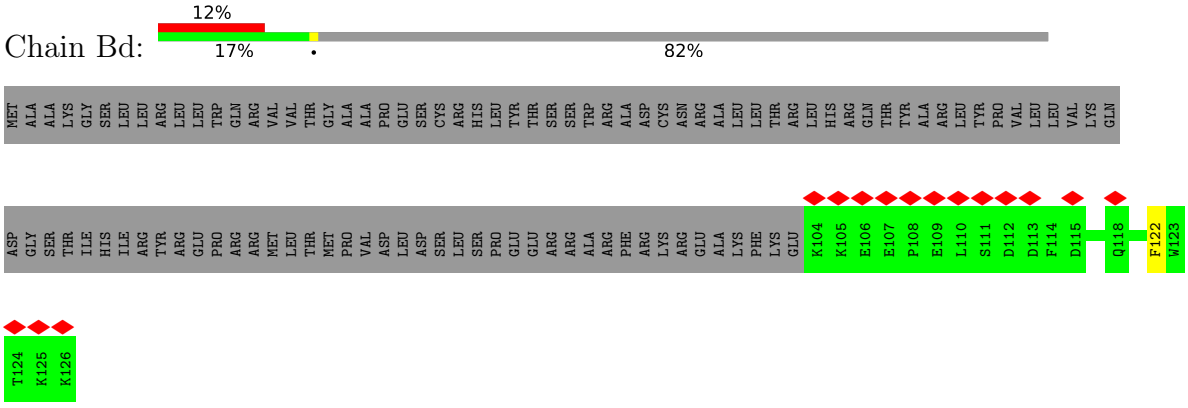
• Molecule 1: 39S ribosomal protein L19, mitochondrial

Chain BX:



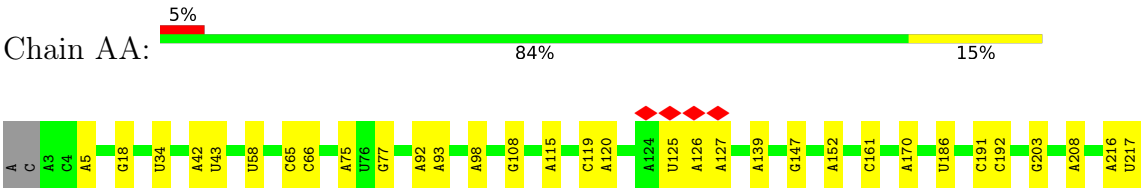
• Molecule 2: bL31m

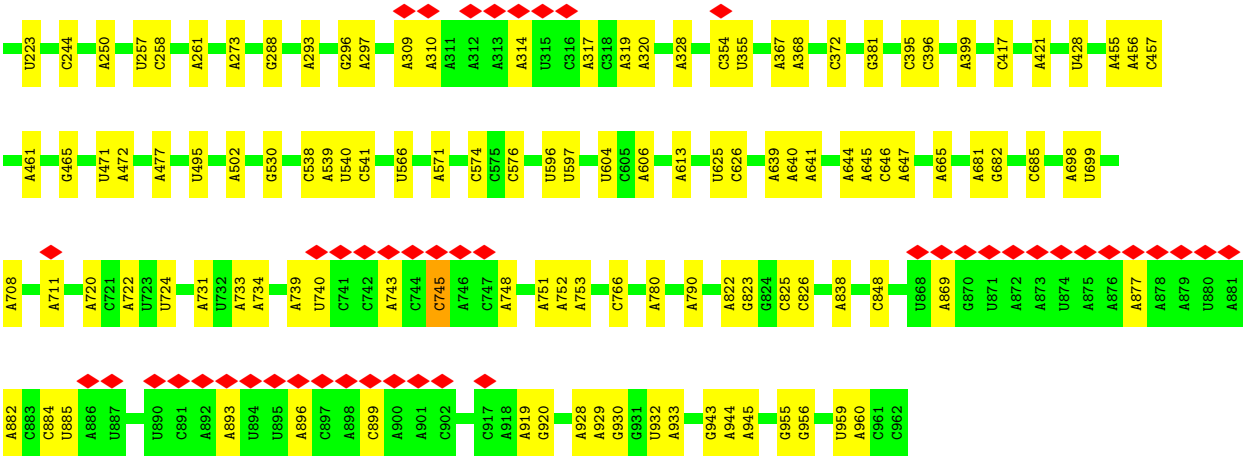
Chain Bd:



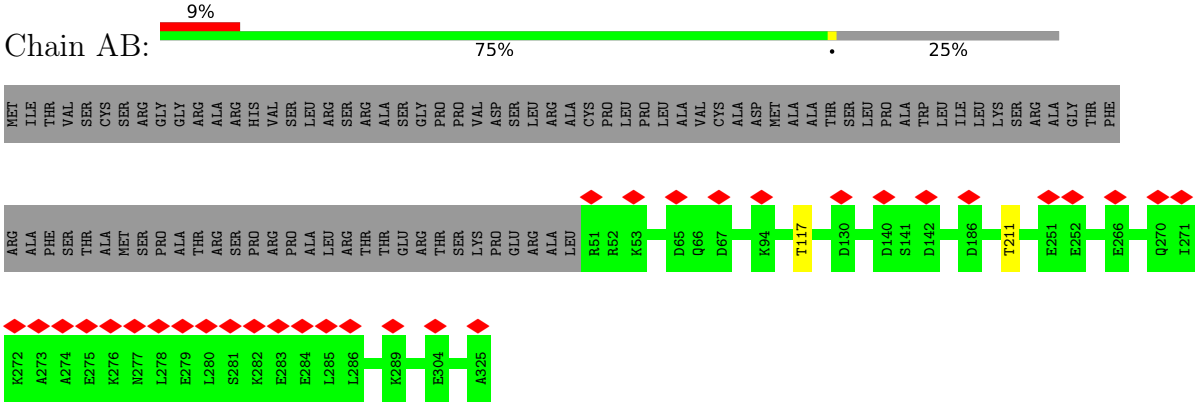
• Molecule 3: 12S rRNA

Chain AA:

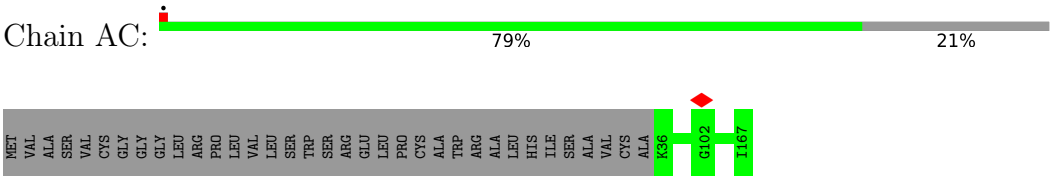




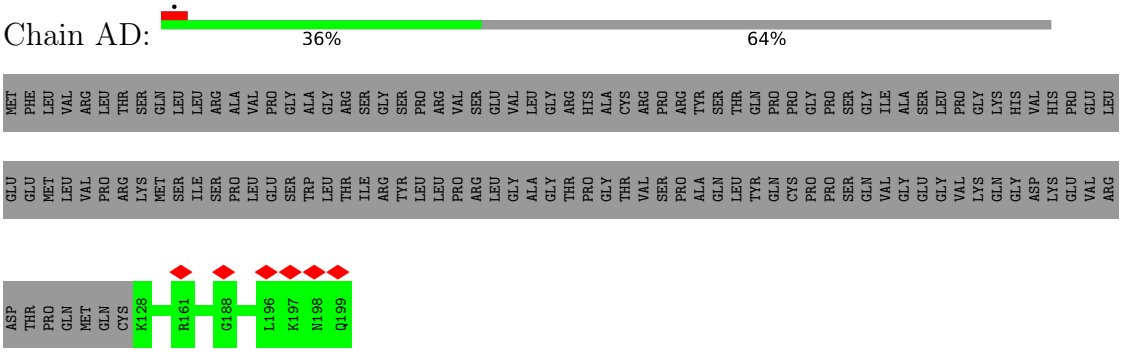
• Molecule 4: 28S ribosomal protein S35, mitochondrial isoform 1



• Molecule 5: Mitochondrial ribosomal protein S24

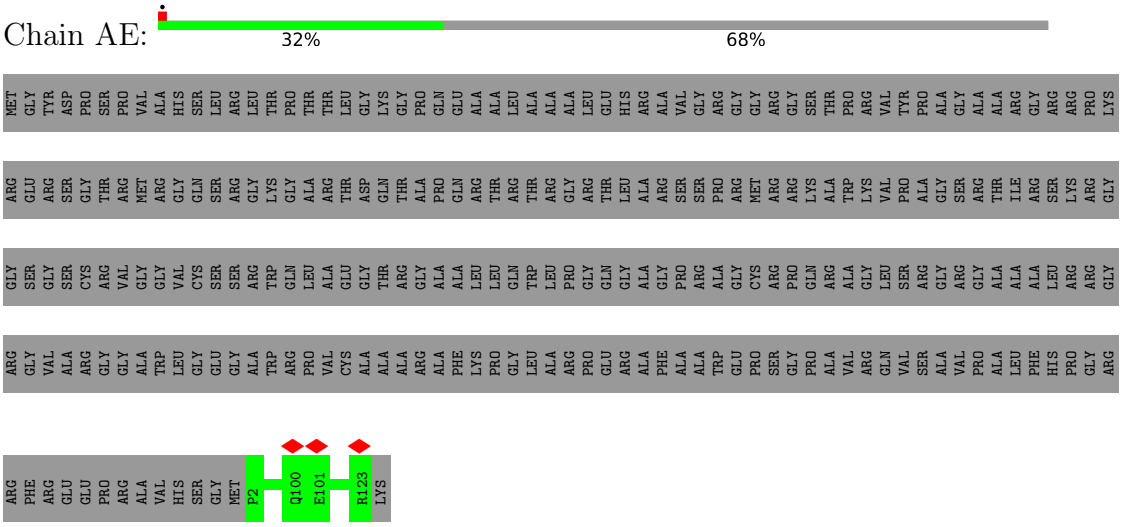


• Molecule 6: Aurora kinase A interacting protein 1



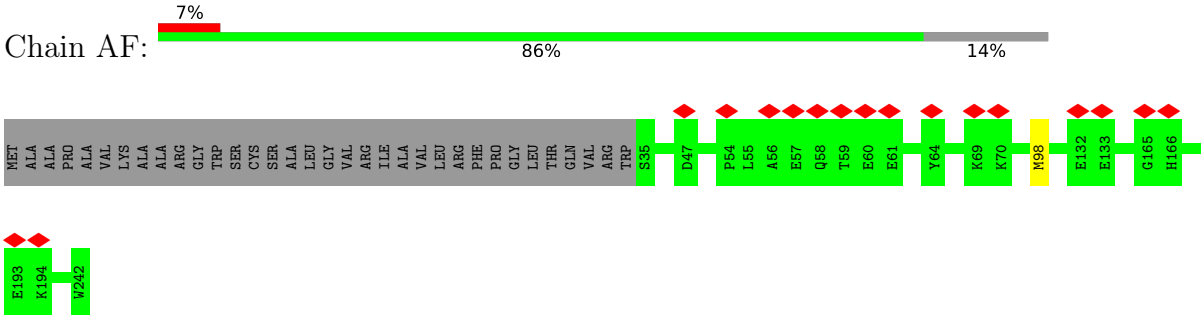
• Molecule 7: bS6m,Mitochondrial ribosomal protein S6

Chain AE:



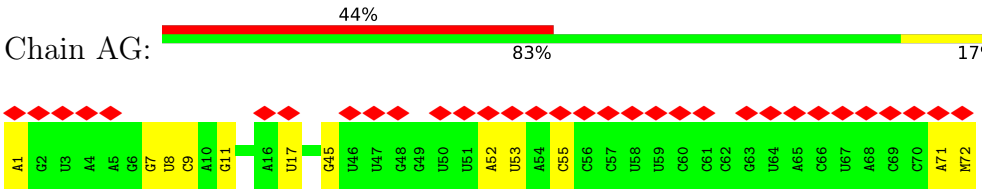
• Molecule 8: Mitochondrial ribosomal protein S7

Chain AF:



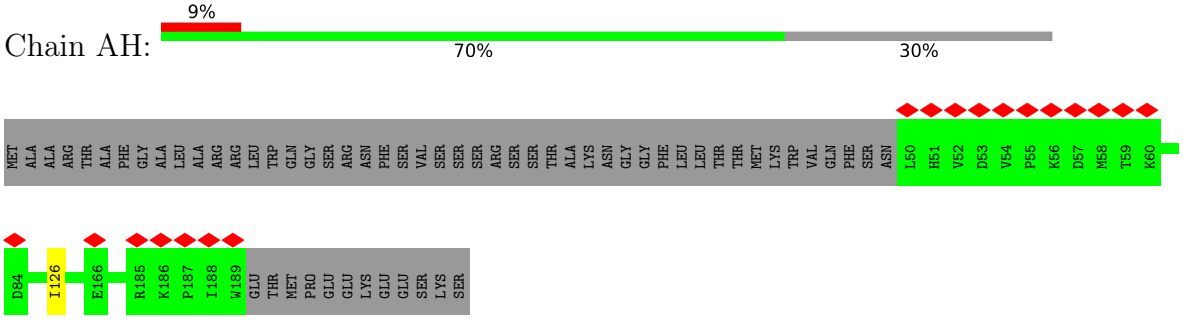
• Molecule 9: P-site Met-tRNA(fMet)

Chain AG:



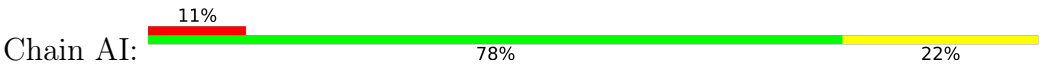
• Molecule 10: Mitochondrial ribosomal protein S10

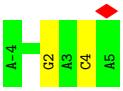
Chain AH:



• Molecule 11: mRNA

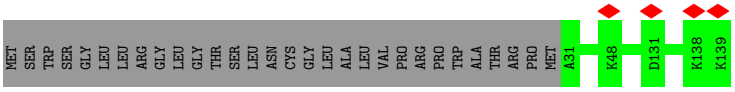
Chain AI:





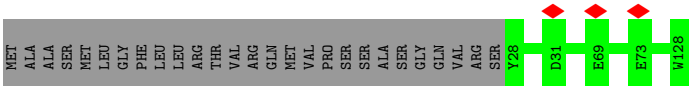
• Molecule 12: Mitochondrial ribosomal protein S12

Chain AJ:



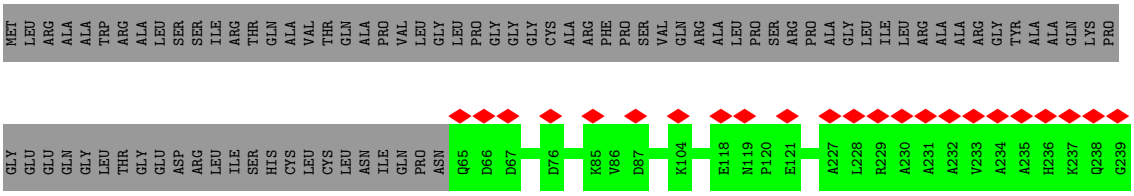
• Molecule 13: Mitochondrial ribosomal protein S14

Chain AK:



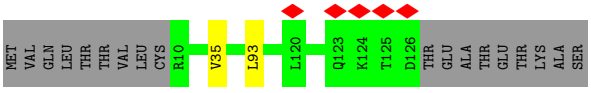
• Molecule 14: 28S ribosomal protein S15, mitochondrial

Chain AL:



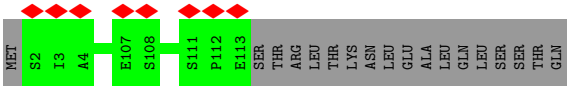
• Molecule 15: 28S ribosomal protein S16, mitochondrial

Chain AM:



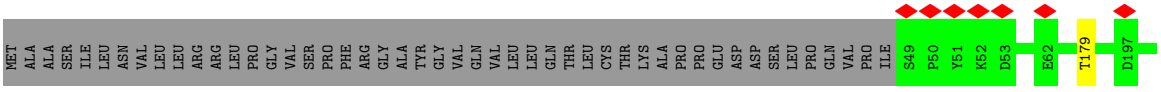
• Molecule 16: uS17m

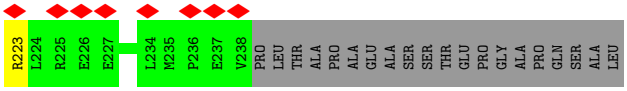
Chain AN:



• Molecule 17: 28S ribosomal protein S18b, mitochondrial

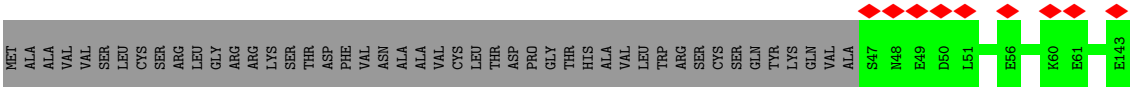
Chain AO:





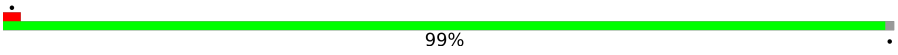
• Molecule 18: Mitochondrial ribosomal protein S18C

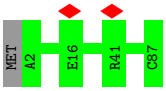
Chain AP:



• Molecule 19: 28S ribosomal protein S21, mitochondrial

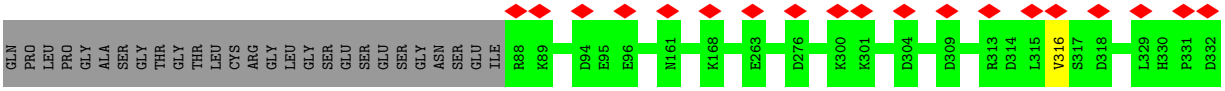
Chain AQ:

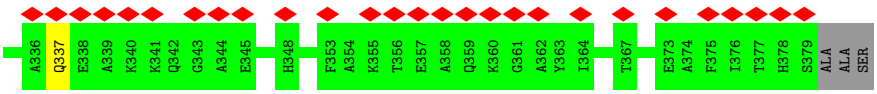




• Molecule 20: Mitochondrial ribosomal protein S22

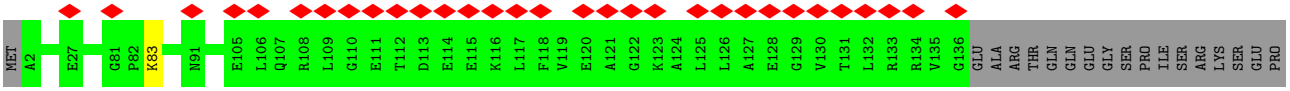
Chain AR:





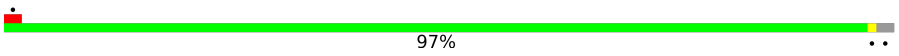
• Molecule 21: mS23

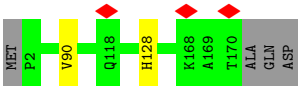
Chain AS:



• Molecule 22: Mitochondrial ribosomal protein S25

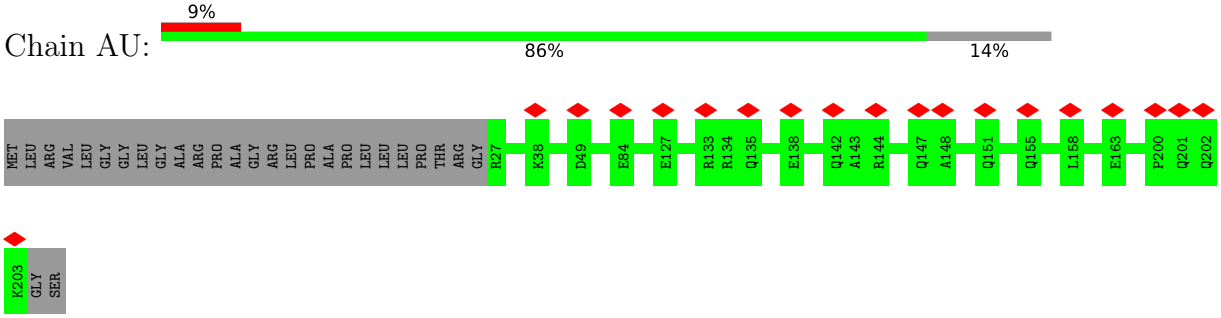
Chain AT:





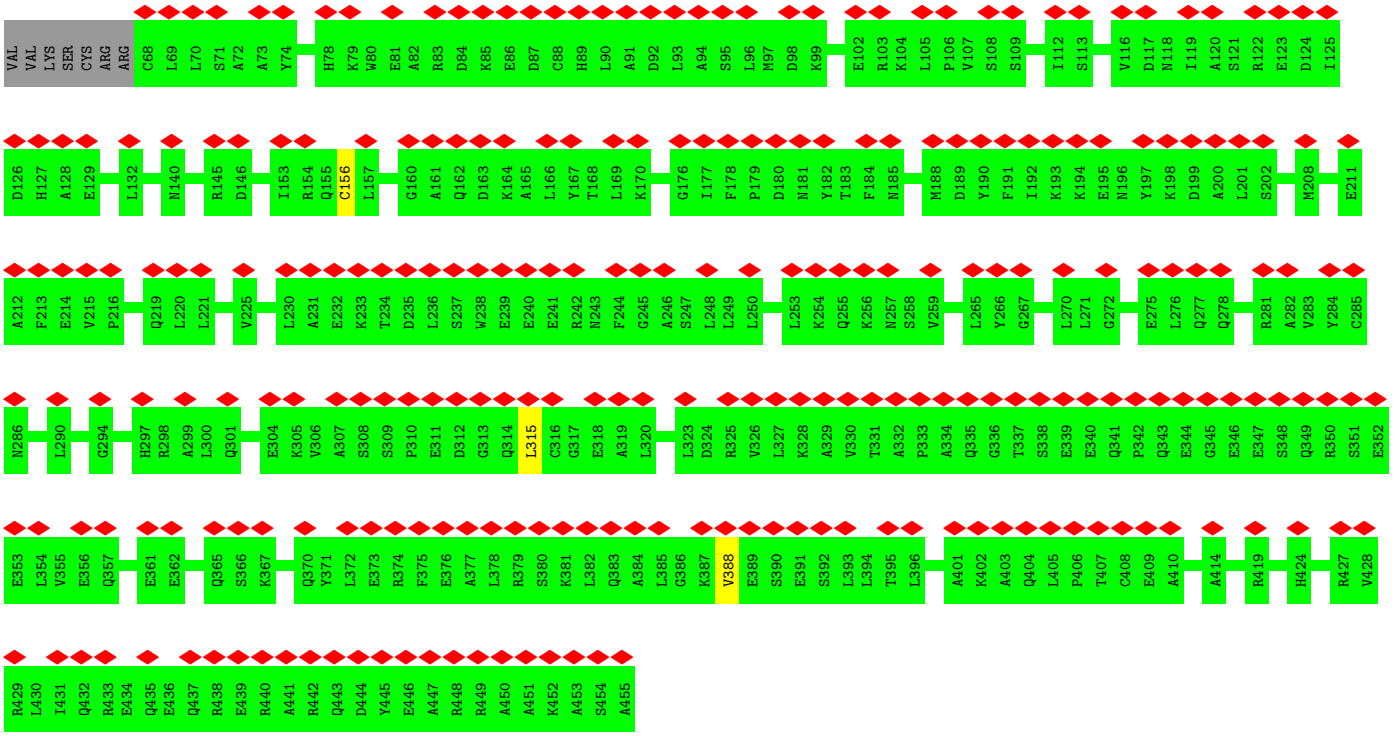
• Molecule 23: Mitochondrial ribosomal protein S26

Chain AU:



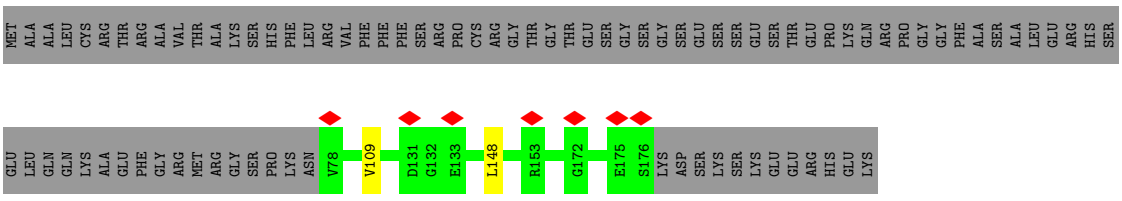
• Molecule 24: Mitochondrial ribosomal protein S27

Chain AV:



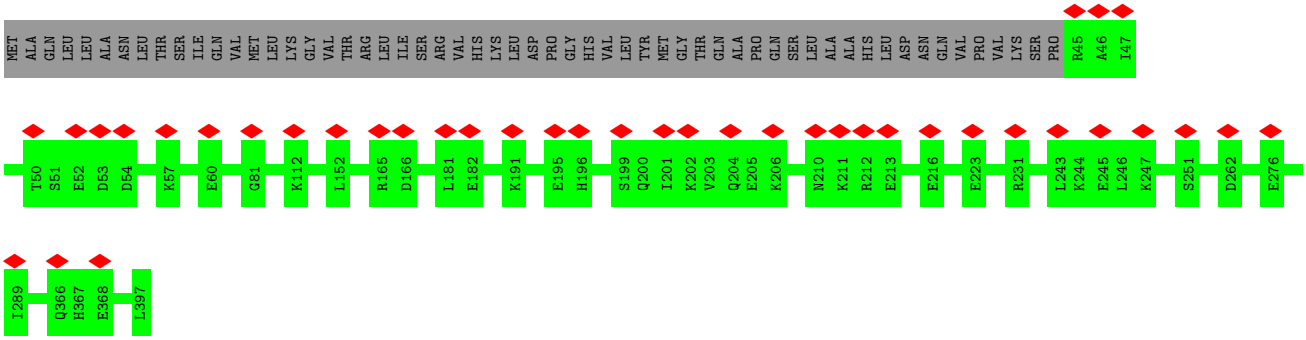
• Molecule 25: Mitoribosomal protein ms28, mrps28

Chain AW:



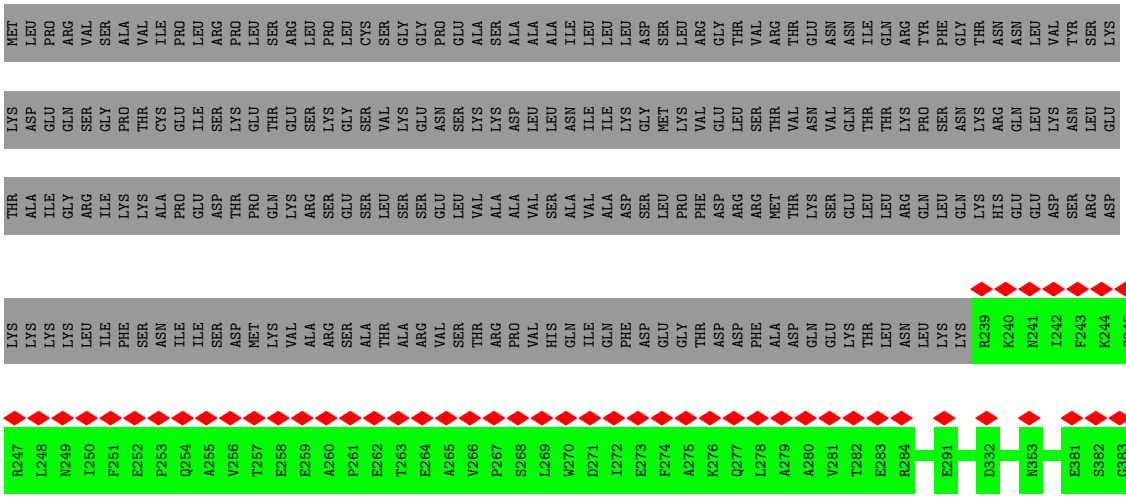
• Molecule 26: Death associated protein 3

Chain AX:



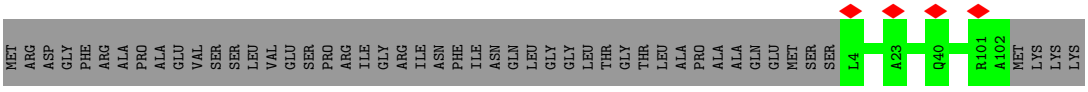
• Molecule 27: 28S ribosomal protein S31, mitochondrial

Chain AY:



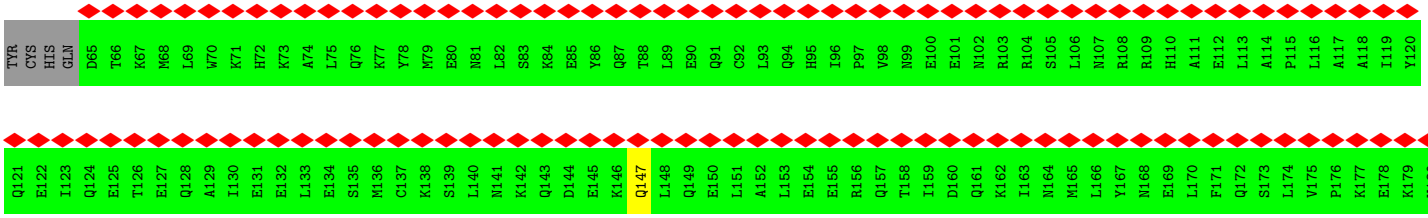
• Molecule 28: Mitochondrial ribosomal protein S33

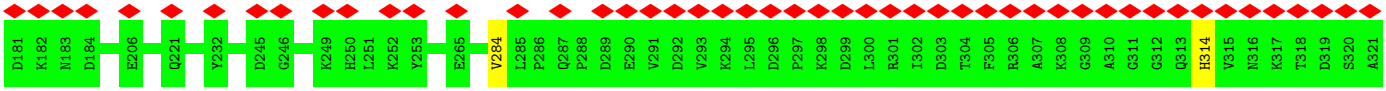
Chain AZ:

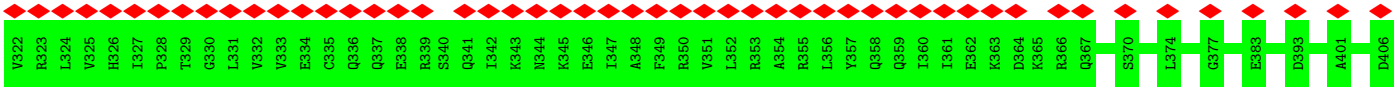


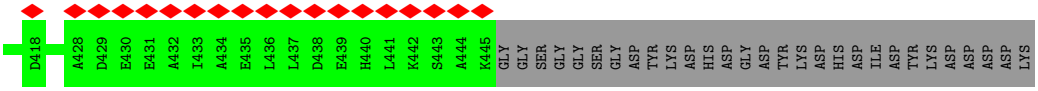
• Molecule 29: Peptide chain release factor 1, mitochondrial

Chain Aa:



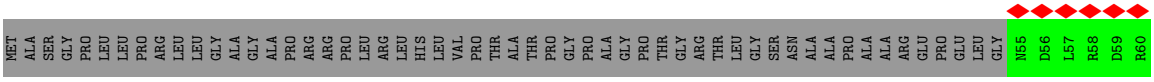


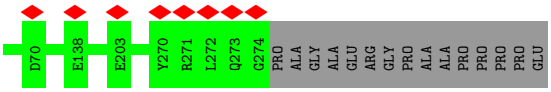




• Molecule 30: Mitochondrial ribosomal protein S2

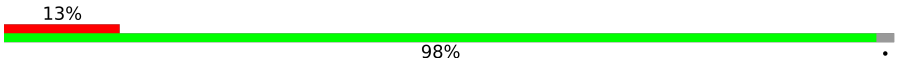
Chain Ab:

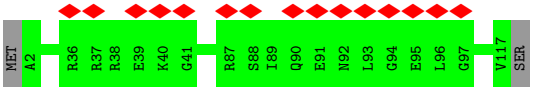




• Molecule 31: Coiled-coil-helix-coiled-coil-helix domain containing 1

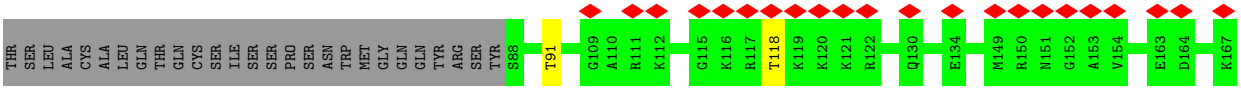
Chain Ac:

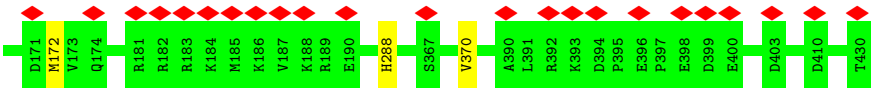




• Molecule 32: 28S ribosomal protein S5, mitochondrial isoform X2

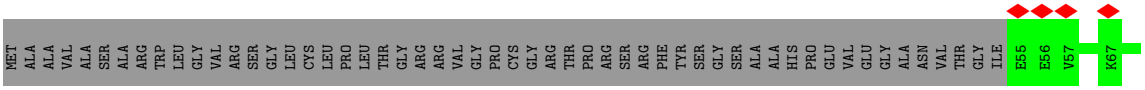
Chain Ad:

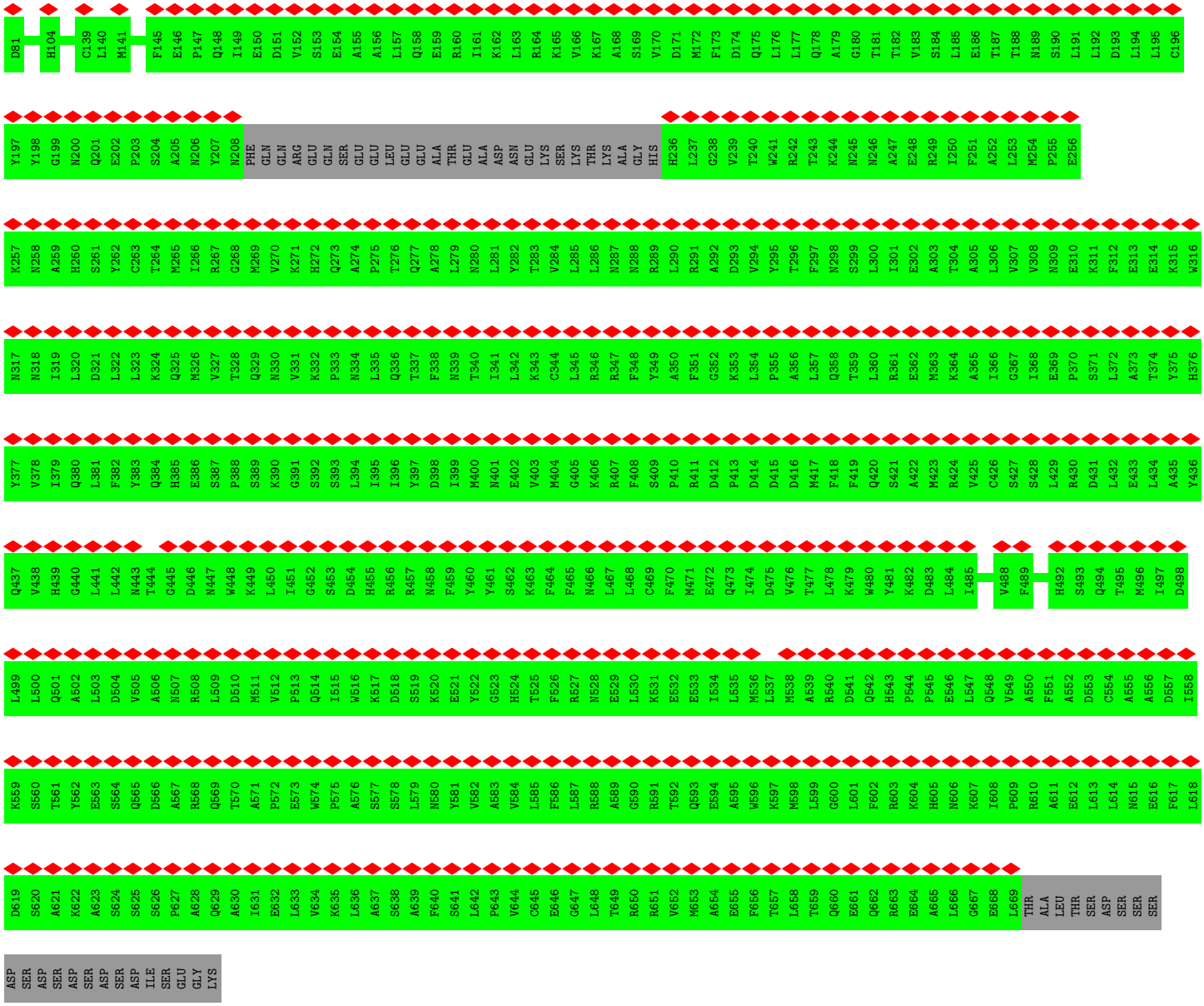




• Molecule 33: mS39

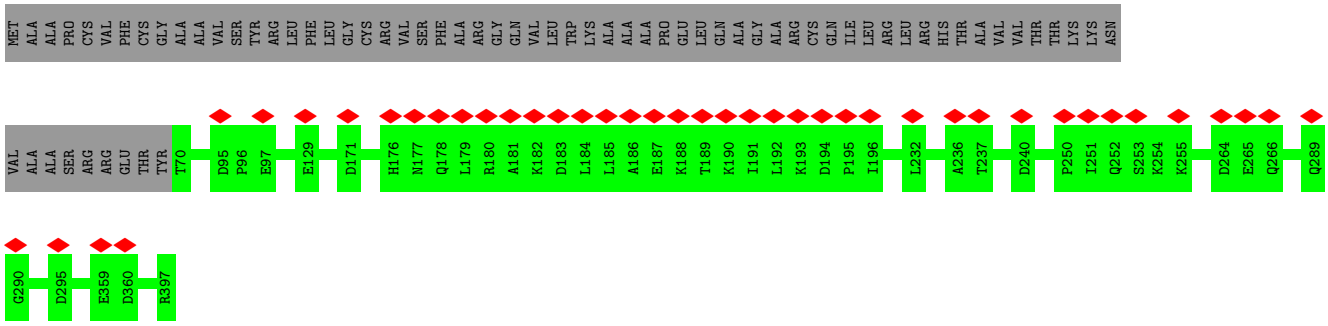
Chain Ae:





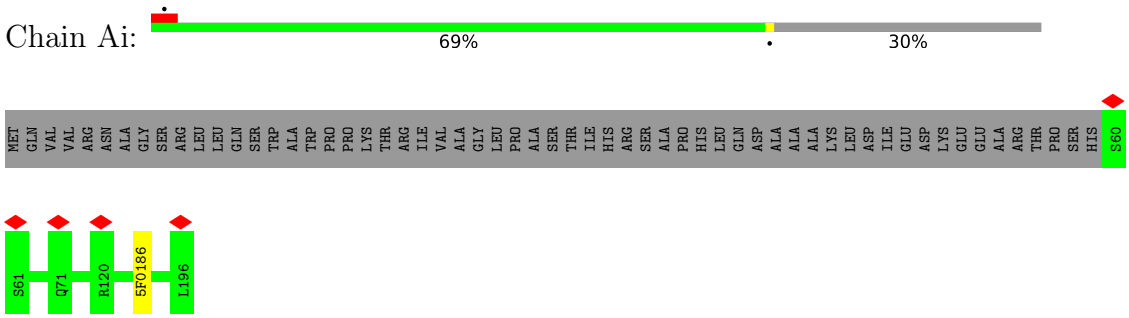
• Molecule 34: uS9m

Chain Ag:



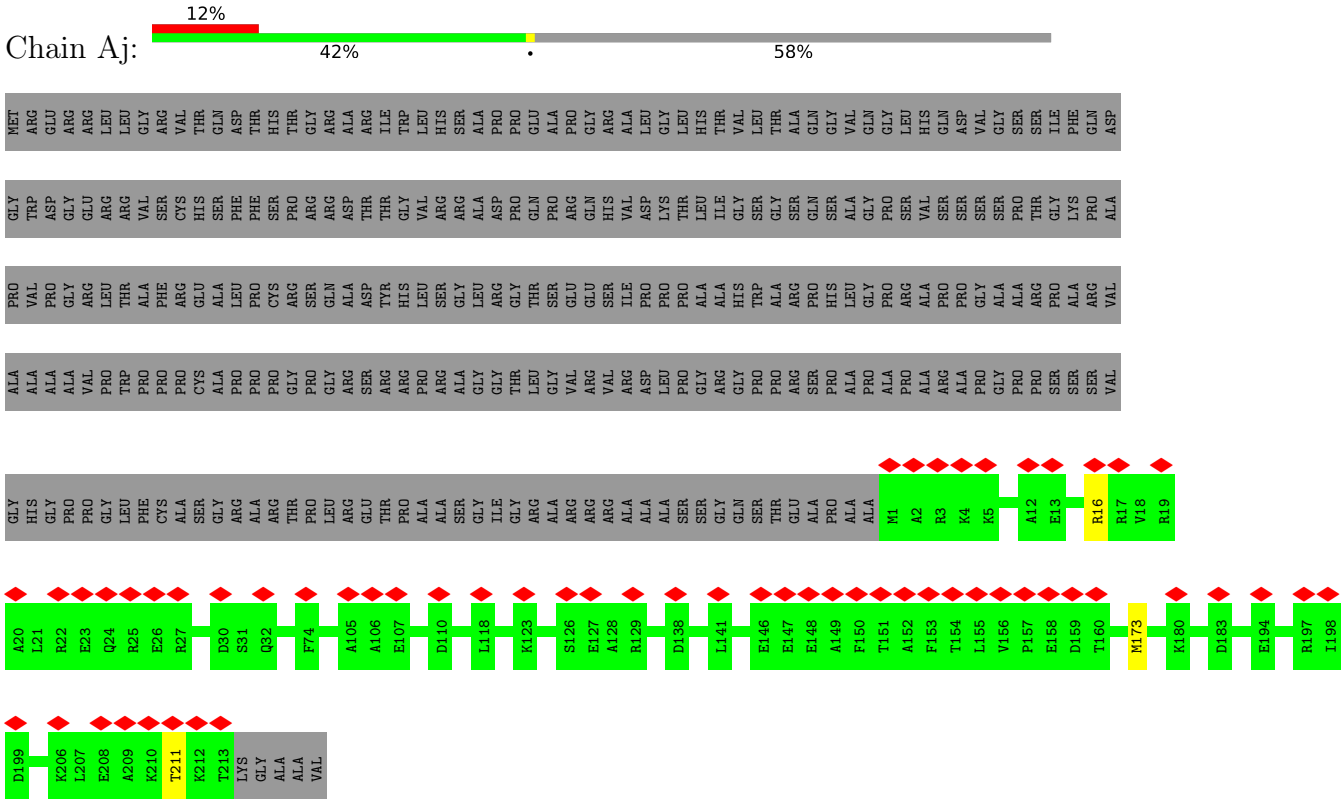
• Molecule 35: Mitochondrial ribosomal protein S11

Chain Ai:



• Molecule 36: Mitochondrial ribosomal protein S34

Chain Aj:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50622	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.185	Depositor
Minimum map value	-1.749	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	532.5, 532.5, 532.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	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: GDP, 5MU, 5F0, AYA, FS2, K, FME, MG, MA6, ZN, ATP, SPD, SPM, 5MC, B8T

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	BX	0.29	0/103	0.37	0/143
2	Bd	0.27	0/197	0.42	0/265
3	AA	0.20	0/22734	0.67	4/35392 (0.0%)
4	AB	0.24	0/2268	0.44	0/3069
5	AC	0.25	0/1105	0.47	0/1496
6	AD	0.23	0/650	0.53	0/858
7	AE	0.25	0/999	0.50	0/1347
8	AF	0.24	0/1764	0.45	0/2368
9	AG	0.30	1/1677 (0.1%)	0.69	0/2606
10	AH	0.24	0/1181	0.47	0/1597
11	AI	0.19	0/217	0.67	0/337
12	AJ	0.25	0/858	0.52	0/1152
13	AK	0.23	0/874	0.53	0/1171
14	AL	0.24	0/1473	0.44	0/1970
15	AM	0.24	0/954	0.52	0/1284
16	AN	0.25	0/894	0.47	0/1213
17	AO	0.25	0/1616	0.47	0/2195
18	AP	0.25	0/802	0.42	0/1079
19	AQ	0.25	0/740	0.54	0/986
20	AR	0.24	0/2428	0.44	0/3279
21	AS	0.25	0/1126	0.49	0/1514
22	AT	0.25	0/1399	0.45	0/1881
23	AU	0.24	0/1490	0.50	0/2005
24	AV	0.23	0/3171	0.44	0/4292
25	AW	0.25	0/790	0.49	0/1064
26	AX	0.24	0/2945	0.45	0/3984
27	AY	0.25	0/1285	0.42	0/1734
28	AZ	0.24	0/841	0.49	0/1121
29	Aa	0.23	0/3171	0.45	0/4263
30	Ab	0.25	0/1804	0.48	0/2445
31	Ac	0.24	0/942	0.50	0/1261
32	Ad	0.24	0/2785	0.50	0/3735

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Ae	0.24	0/4856	0.40	0/6579
34	Ag	0.24	0/2707	0.47	0/3636
35	Ai	0.25	0/1018	0.48	0/1375
36	Aj	0.23	0/1835	0.52	0/2484
All	All	0.23	1/75699 (0.0%)	0.55	4/107180 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	AG	1	A	OP3-P	-10.53	1.48	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AA	119	C	C2-N1-C1'	5.63	125.00	118.80
3	AA	745	C	C2-N1-C1'	5.30	124.64	118.80
3	AA	745	C	N1-C2-O2	5.22	122.03	118.90
3	AA	119	C	N1-C2-O2	5.04	121.93	118.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BX	13/303 (4%)	12 (92%)	1 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Bd	21/126 (17%)	20 (95%)	1 (5%)	0	100	100
4	AB	273/366 (75%)	268 (98%)	5 (2%)	0	100	100
5	AC	130/167 (78%)	125 (96%)	5 (4%)	0	100	100
6	AD	70/199 (35%)	70 (100%)	0	0	100	100
7	AE	120/376 (32%)	118 (98%)	2 (2%)	0	100	100
8	AF	206/242 (85%)	201 (98%)	5 (2%)	0	100	100
10	AH	138/200 (69%)	129 (94%)	8 (6%)	1 (1%)	22	61
12	AJ	107/139 (77%)	105 (98%)	2 (2%)	0	100	100
13	AK	99/128 (77%)	99 (100%)	0	0	100	100
14	AL	173/259 (67%)	169 (98%)	4 (2%)	0	100	100
15	AM	115/135 (85%)	112 (97%)	3 (3%)	0	100	100
16	AN	110/130 (85%)	106 (96%)	4 (4%)	0	100	100
17	AO	188/258 (73%)	185 (98%)	3 (2%)	0	100	100
18	AP	95/143 (66%)	95 (100%)	0	0	100	100
19	AQ	84/87 (97%)	84 (100%)	0	0	100	100
20	AR	290/382 (76%)	283 (98%)	7 (2%)	0	100	100
21	AS	133/190 (70%)	130 (98%)	3 (2%)	0	100	100
22	AT	167/173 (96%)	165 (99%)	2 (1%)	0	100	100
23	AU	175/205 (85%)	174 (99%)	1 (1%)	0	100	100
24	AV	386/395 (98%)	369 (96%)	17 (4%)	0	100	100
25	AW	97/188 (52%)	96 (99%)	1 (1%)	0	100	100
26	AX	351/410 (86%)	341 (97%)	10 (3%)	0	100	100
27	AY	147/381 (39%)	146 (99%)	1 (1%)	0	100	100
28	AZ	97/148 (66%)	95 (98%)	2 (2%)	0	100	100
29	Aa	380/474 (80%)	372 (98%)	8 (2%)	0	100	100
30	Ab	218/289 (75%)	209 (96%)	9 (4%)	0	100	100
31	Ac	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
32	Ad	341/430 (79%)	331 (97%)	10 (3%)	0	100	100
33	Ae	584/692 (84%)	576 (99%)	8 (1%)	0	100	100
34	Ag	326/397 (82%)	323 (99%)	3 (1%)	0	100	100
35	Ai	134/196 (68%)	130 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	Aj	211/505 (42%)	208 (99%)	3 (1%)	0	100	100
All	All	6093/8831 (69%)	5957 (98%)	135 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	AH	126	ILE

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	BX	8/266 (3%)	8 (100%)	0	100	100
2	Bd	19/114 (17%)	18 (95%)	1 (5%)	22	58
4	AB	249/322 (77%)	247 (99%)	2 (1%)	81	91
5	AC	115/142 (81%)	115 (100%)	0	100	100
6	AD	66/174 (38%)	66 (100%)	0	100	100
7	AE	107/283 (38%)	107 (100%)	0	100	100
8	AF	181/205 (88%)	180 (99%)	1 (1%)	86	94
10	AH	130/180 (72%)	130 (100%)	0	100	100
12	AJ	92/116 (79%)	92 (100%)	0	100	100
13	AK	92/114 (81%)	92 (100%)	0	100	100
14	AL	159/222 (72%)	159 (100%)	0	100	100
15	AM	97/113 (86%)	95 (98%)	2 (2%)	53	78
16	AN	97/114 (85%)	97 (100%)	0	100	100
17	AO	170/225 (76%)	168 (99%)	2 (1%)	71	87
18	AP	89/127 (70%)	89 (100%)	0	100	100
19	AQ	77/78 (99%)	77 (100%)	0	100	100
20	AR	258/330 (78%)	256 (99%)	2 (1%)	81	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	AS	113/162 (70%)	112 (99%)	1 (1%)	78 90
22	AT	152/155 (98%)	150 (99%)	2 (1%)	69 86
23	AU	149/168 (89%)	149 (100%)	0	100 100
24	AV	325/347 (94%)	322 (99%)	3 (1%)	78 90
25	AW	86/160 (54%)	84 (98%)	2 (2%)	50 76
26	AX	312/361 (86%)	312 (100%)	0	100 100
27	AY	134/342 (39%)	134 (100%)	0	100 100
28	AZ	86/125 (69%)	86 (100%)	0	100 100
29	Aa	339/424 (80%)	336 (99%)	3 (1%)	78 90
30	Ab	187/233 (80%)	187 (100%)	0	100 100
31	Ac	100/102 (98%)	100 (100%)	0	100 100
32	Ad	282/351 (80%)	277 (98%)	5 (2%)	59 81
33	Ae	521/604 (86%)	521 (100%)	0	100 100
34	Ag	273/333 (82%)	273 (100%)	0	100 100
35	Ai	102/150 (68%)	102 (100%)	0	100 100
36	Aj	188/404 (46%)	185 (98%)	3 (2%)	62 83
All	All	5355/7546 (71%)	5326 (100%)	29 (0%)	89 95

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	AV	315	LEU
36	Aj	173	MET
25	AW	148	LEU
32	Ad	288	HIS
25	AW	109	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
26	AX	169	GLN
35	Ai	107	GLN
29	Aa	202	GLN
35	Ai	73	ASN
33	Ae	380	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	AI	8/9 (88%)	2 (25%)	0
3	AA	956/962 (99%)	143 (14%)	0
9	AG	70/72 (97%)	10 (14%)	0
All	All	1034/1043 (99%)	155 (14%)	0

5 of 155 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	AA	5	A
3	AA	18	G
3	AA	34	U
3	AA	42	A
3	AA	43	U

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	AYA	AQ	2	19	6,7,8	0.77	0	5,8,10	0.29	0
3	MA6	AA	945	3	18,26,27	1.10	1 (5%)	19,38,41	1.93	3 (15%)
3	MA6	AA	944	3	18,26,27	1.10	2 (11%)	19,38,41	2.03	3 (15%)
9	FME	AG	72	9	8,9,10	0.55	0	7,9,11	0.98	1 (14%)
31	AYA	Ac	2	31	6,7,8	0.78	0	5,8,10	0.27	0
3	5MU	AA	428	3	19,22,23	1.38	5 (26%)	28,32,35	1.98	6 (21%)
35	5F0	Ai	186	35	8,8,9	1.46	2 (25%)	7,9,11	1.69	1 (14%)
3	B8T	AA	846	3	19,22,23	0.43	0	26,31,34	0.37	0
3	5MC	AA	848	3	18,22,23	0.93	2 (11%)	26,32,35	1.05	2 (7%)

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
19	AYA	AQ	2	19	-	2/4/6/8	-
3	MA6	AA	945	3	-	4/7/29/30	0/3/3/3
3	MA6	AA	944	3	-	0/7/29/30	0/3/3/3
9	FME	AG	72	9	-	1/7/9/11	-
31	AYA	Ac	2	31	-	2/4/6/8	-
3	5MU	AA	428	3	-	0/7/25/26	0/2/2/2
35	5F0	Ai	186	35	-	4/9/9/10	-
3	B8T	AA	846	3	-	0/7/27/28	0/2/2/2
3	5MC	AA	848	3	-	0/7/25/26	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AA	944	MA6	C5-N7	3.33	1.51	1.39
3	AA	945	MA6	C5-N7	3.31	1.51	1.39
35	Ai	186	5F0	OD1-C1	2.92	1.40	1.33
3	AA	428	5MU	C6-C5	2.66	1.39	1.34
3	AA	428	5MU	C4-N3	-2.62	1.34	1.38

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AA	944	MA6	C4-C5-N7	-5.65	103.51	109.40
3	AA	945	MA6	C4-C5-N7	-5.22	103.96	109.40
3	AA	428	5MU	C4-N3-C2	-4.88	121.04	127.35
3	AA	944	MA6	C1'-N9-C4	-4.84	118.13	126.64
3	AA	428	5MU	N3-C2-N1	4.57	120.95	114.89

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AA	945	MA6	C5-C6-N6-C9
3	AA	945	MA6	C5-C6-N6-C10
9	AG	72	FME	O1-CN-N-CA
35	Ai	186	5F0	OD1-C1-CA-CB
19	AQ	2	AYA	OT-CT-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 145 ligands modelled in this entry, 139 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
38	SPM	AA	1120	-	13,13,13	0.35	0	12,12,12	0.94	0
39	SPD	AA	1121	-	9,9,9	0.33	0	8,8,8	0.85	0
44	GDP	AX	503	-	24,30,30	0.94	1 (4%)	30,47,47	1.30	4 (13%)
43	ATP	AX	501	37	26,33,33	0.61	0	31,52,52	0.73	2 (6%)
42	FS2	AT	201	22,15	0,5,14	-	-	-		
42	FS2	AP	201	7,18	0,5,14	-	-	-		

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
42	FS2	AT	201	22,15	-	-	0/2/2/6
38	SPM	AA	1120	-	-	2/11/11/11	-
39	SPD	AA	1121	-	-	0/7/7/7	-
43	ATP	AX	501	37	-	2/18/38/38	0/3/3/3
44	GDP	AX	503	-	-	3/12/32/32	0/3/3/3
42	FS2	AP	201	7,18	-	-	0/2/2/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	AX	503	GDP	C6-N1	-2.31	1.34	1.37

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	AX	503	GDP	PA-O3A-PB	-3.59	120.49	132.83
44	AX	503	GDP	C3'-C2'-C1'	3.05	105.58	100.98
44	AX	503	GDP	C8-N7-C5	2.37	107.50	102.99
43	AX	501	ATP	C5-C6-N6	2.28	123.81	120.35
44	AX	503	GDP	C5-C6-N1	2.26	117.94	113.95

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

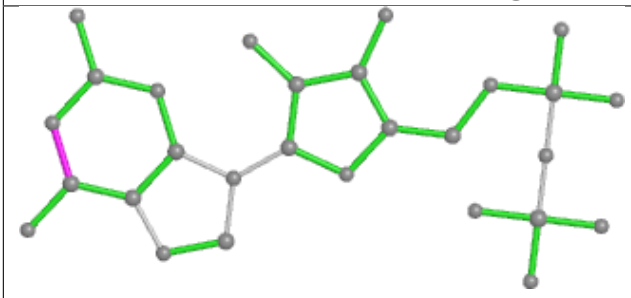
Mol	Chain	Res	Type	Atoms
43	AX	501	ATP	O4'-C4'-C5'-O5'
44	AX	503	GDP	O4'-C4'-C5'-O5'
43	AX	501	ATP	C3'-C4'-C5'-O5'
44	AX	503	GDP	C3'-C4'-C5'-O5'
38	AA	1120	SPM	N5-C6-C7-C8

There are no ring outliers.

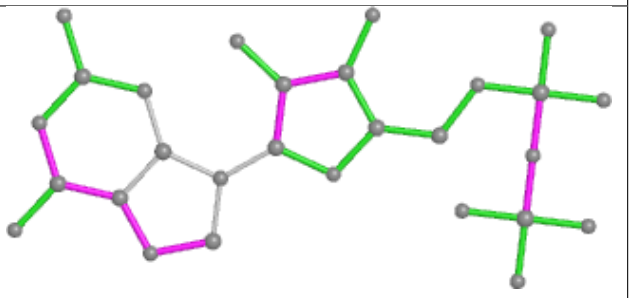
No monomer is involved in short contacts.

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.

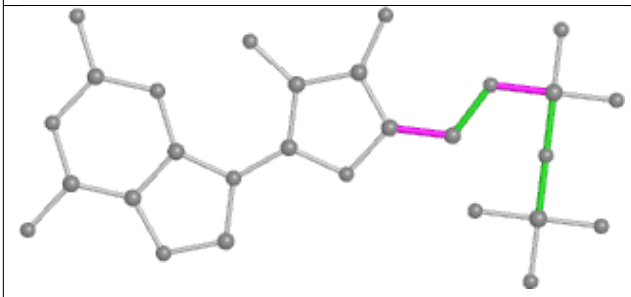
Ligand GDP AX 503



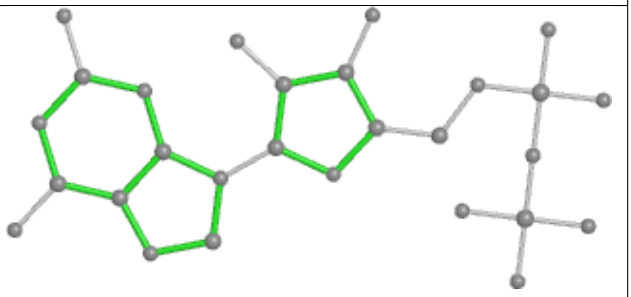
Bond lengths



Bond angles

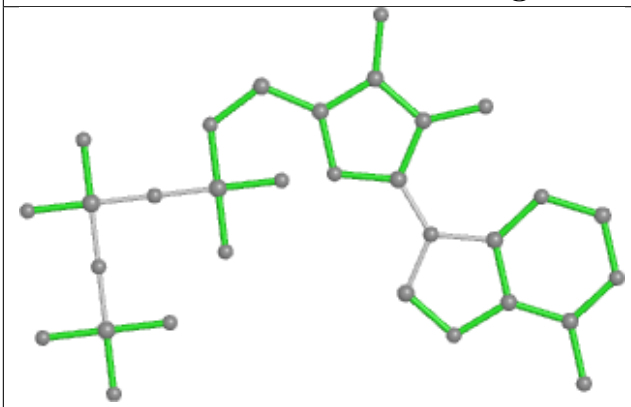


Torsions

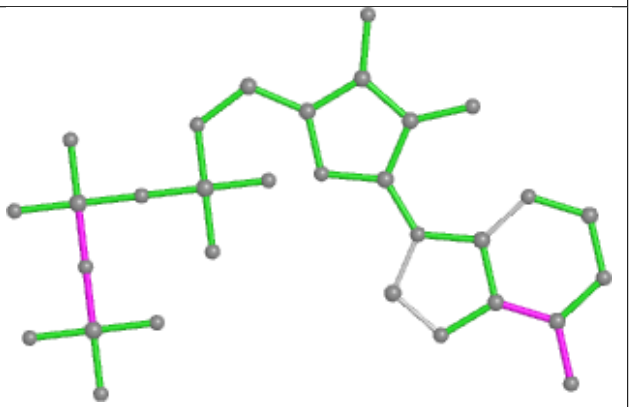


Rings

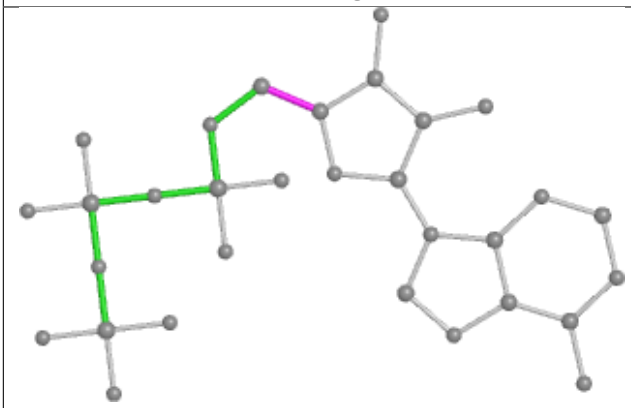
Ligand ATP AX 501



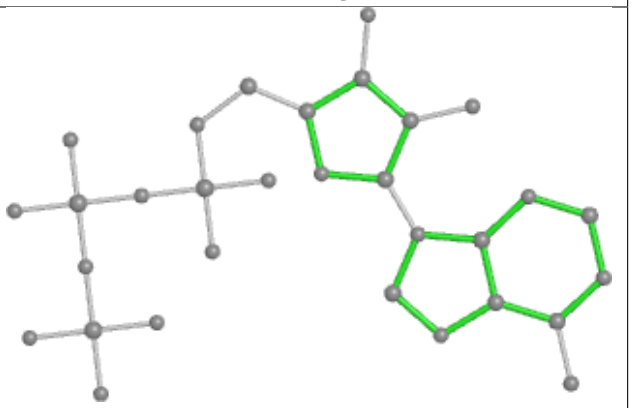
Bond lengths



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.

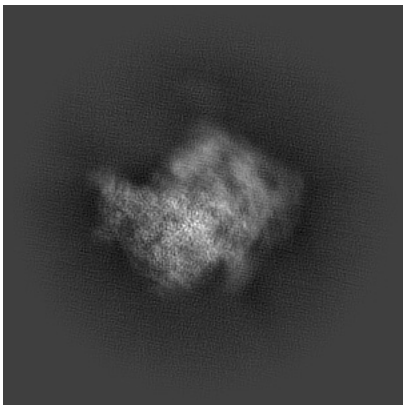
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16895. These allow visual inspection of the internal detail of the map and identification of artifacts.

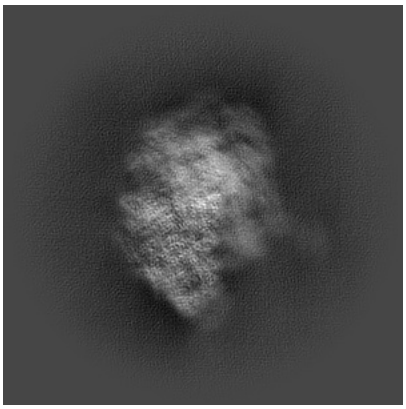
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

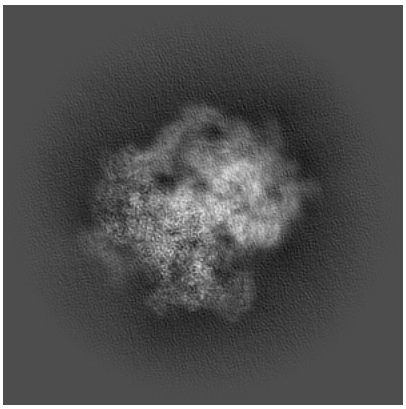
6.1.1 Primary map



X

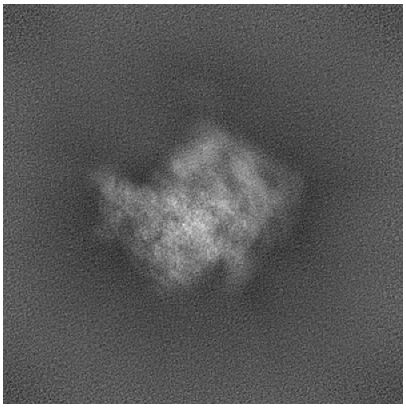


Y

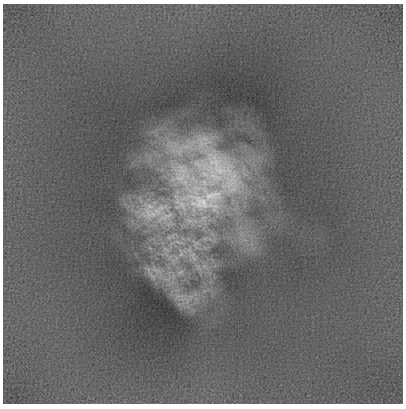


Z

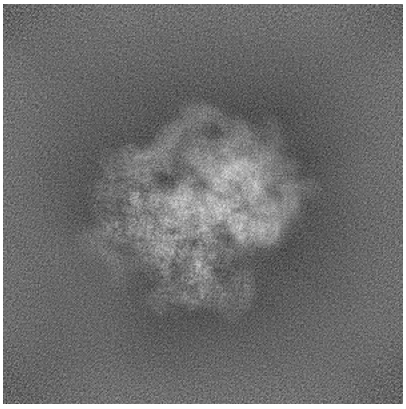
6.1.2 Raw map



X



Y

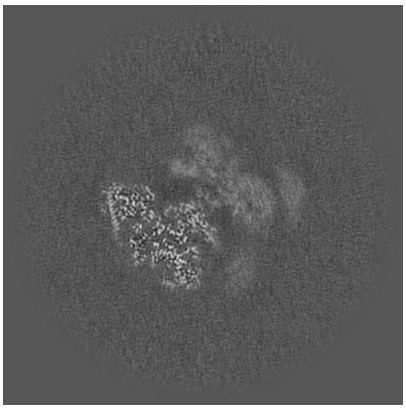


Z

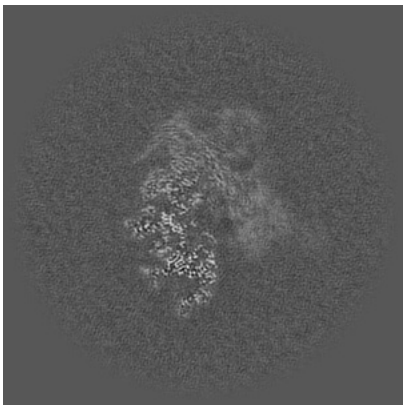
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

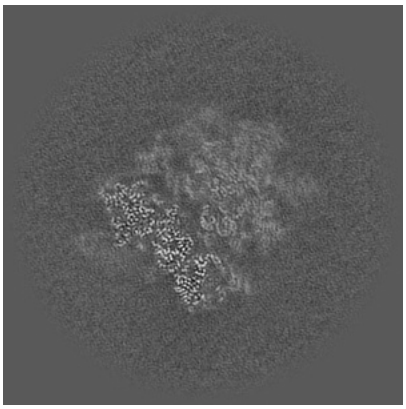
6.2.1 Primary map



X Index: 250

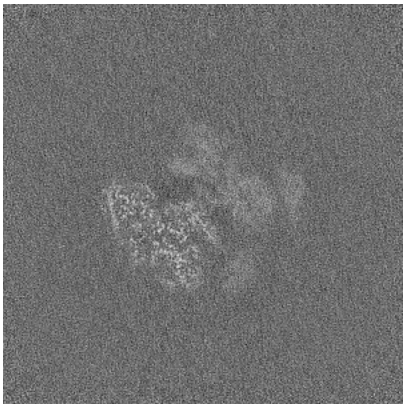


Y Index: 250

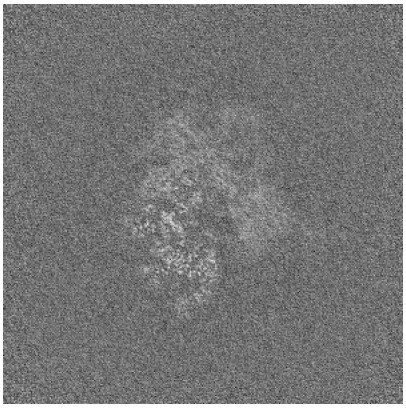


Z Index: 250

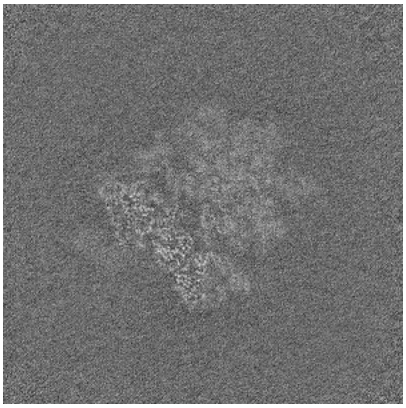
6.2.2 Raw map



X Index: 250



Y Index: 250

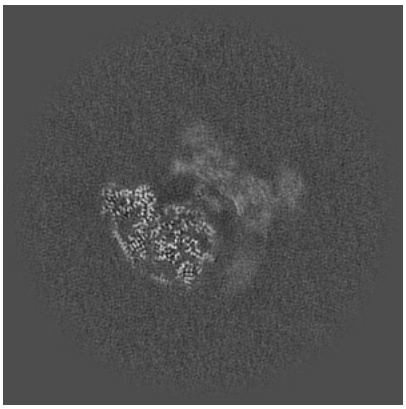


Z Index: 250

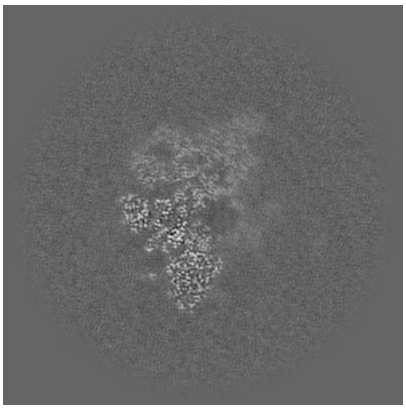
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

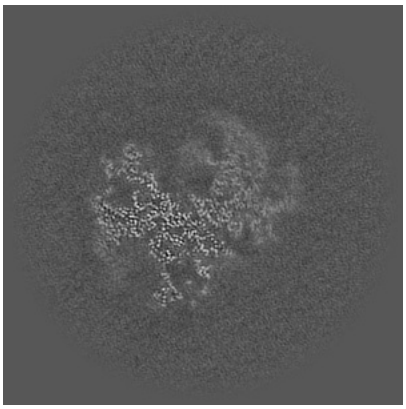
6.3.1 Primary map



X Index: 246

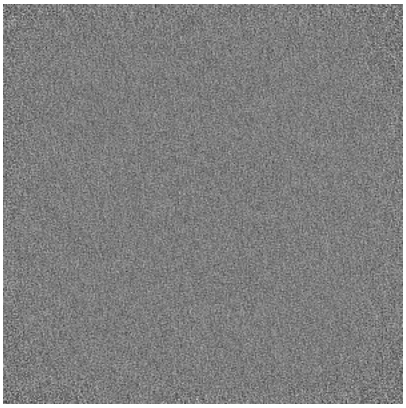


Y Index: 228

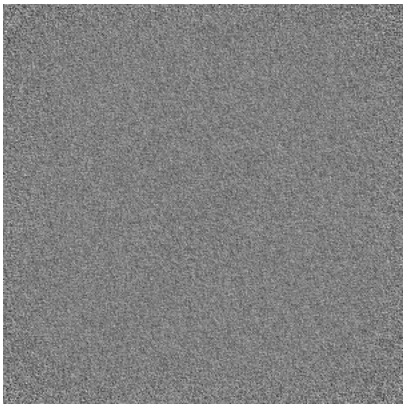


Z Index: 224

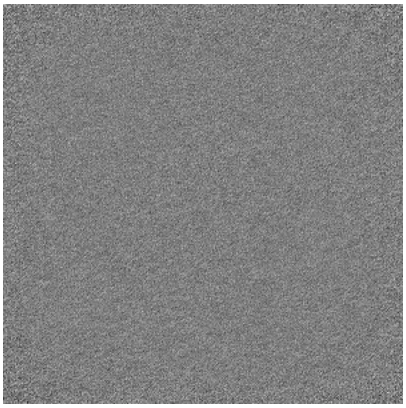
6.3.2 Raw map



X Index: 0



Y Index: 0

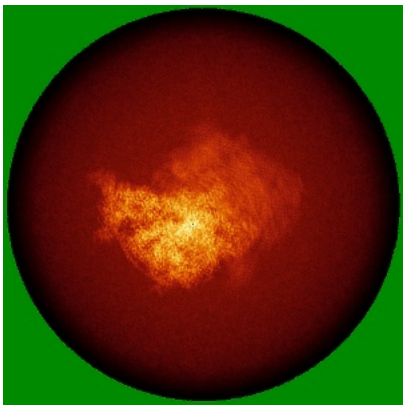


Z Index: 0

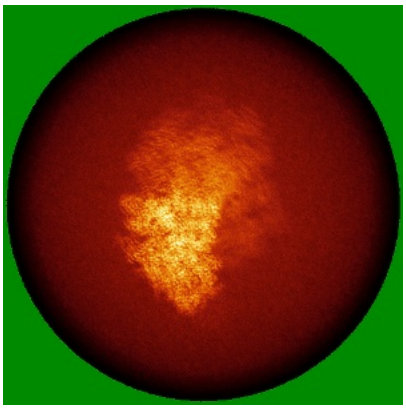
The images above show the largest variance slices of the map in three orthogonal directions.

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

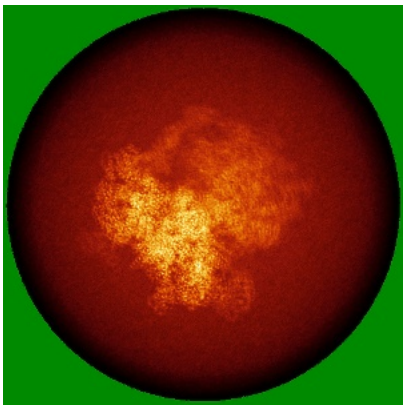
6.4.1 Primary map



X

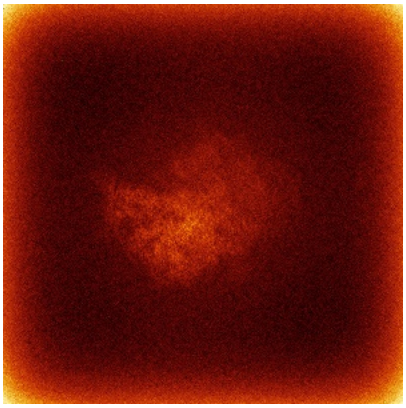


Y

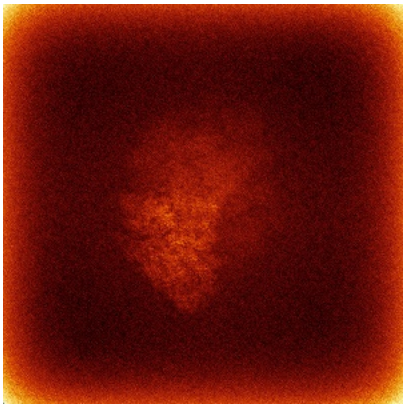


Z

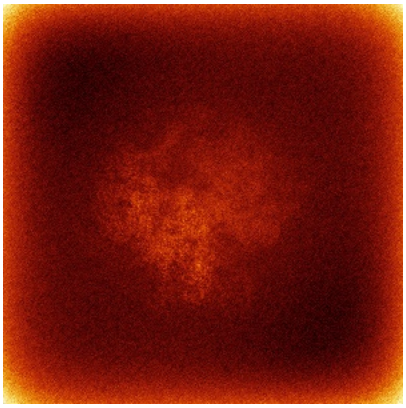
6.4.2 Raw map



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.

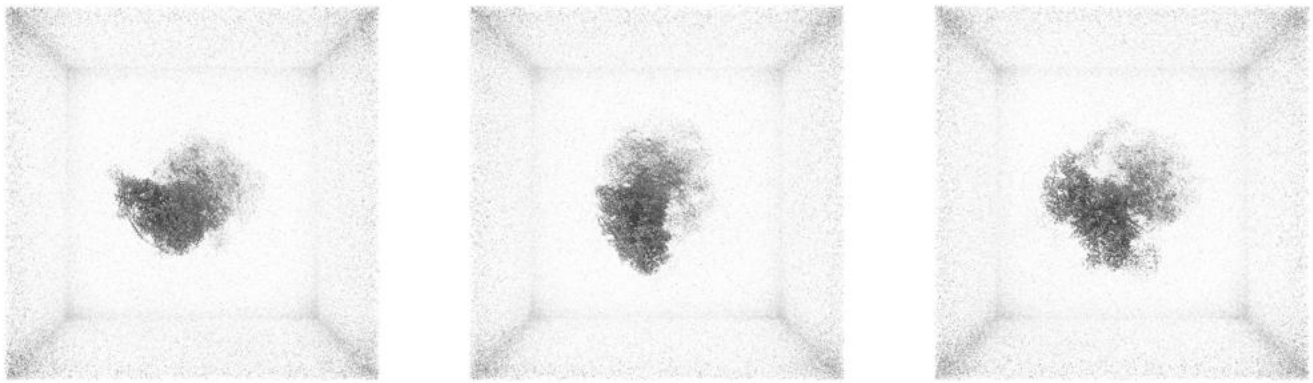
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

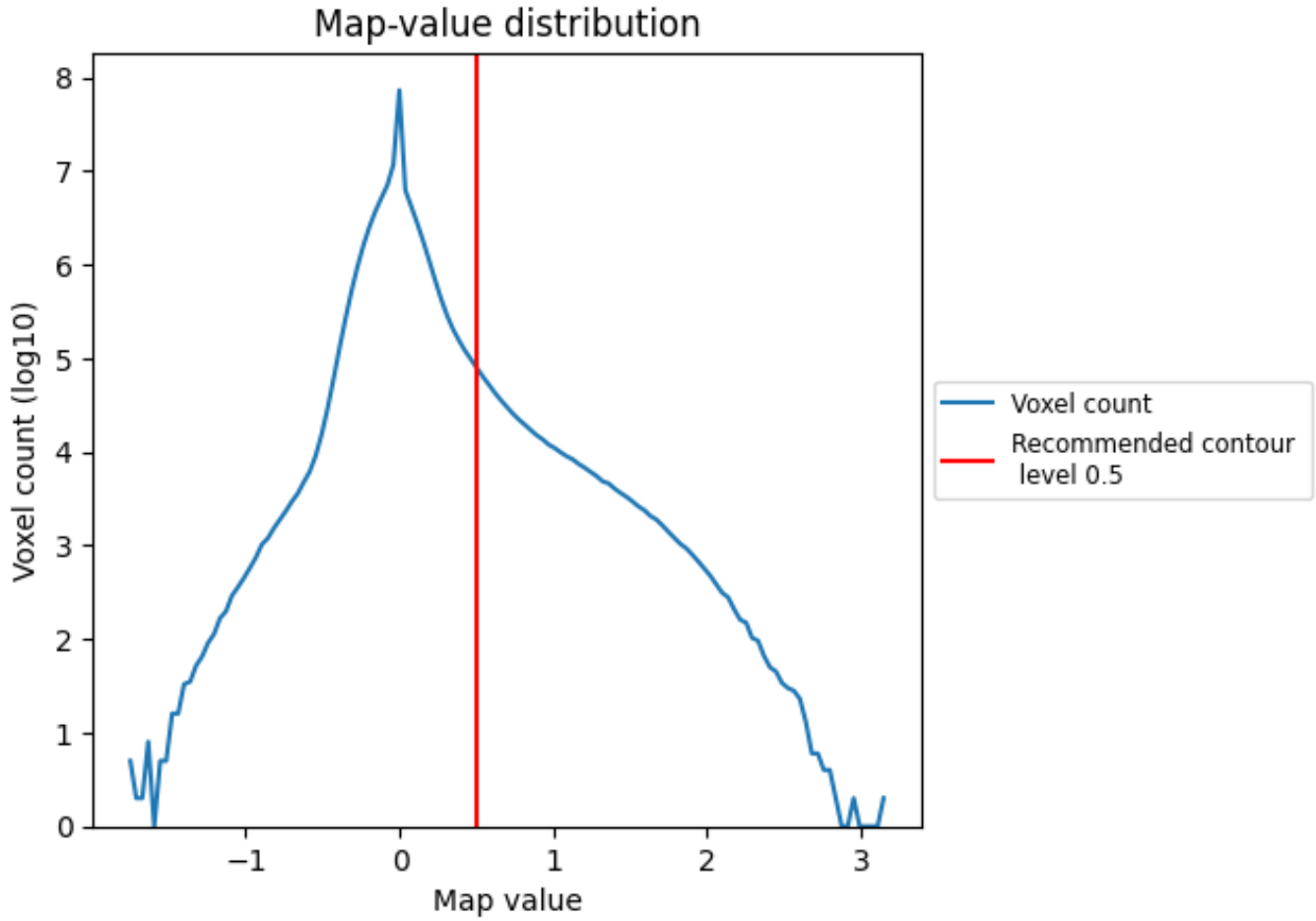
6.6 Mask visualisation (i)

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

7 Map analysis

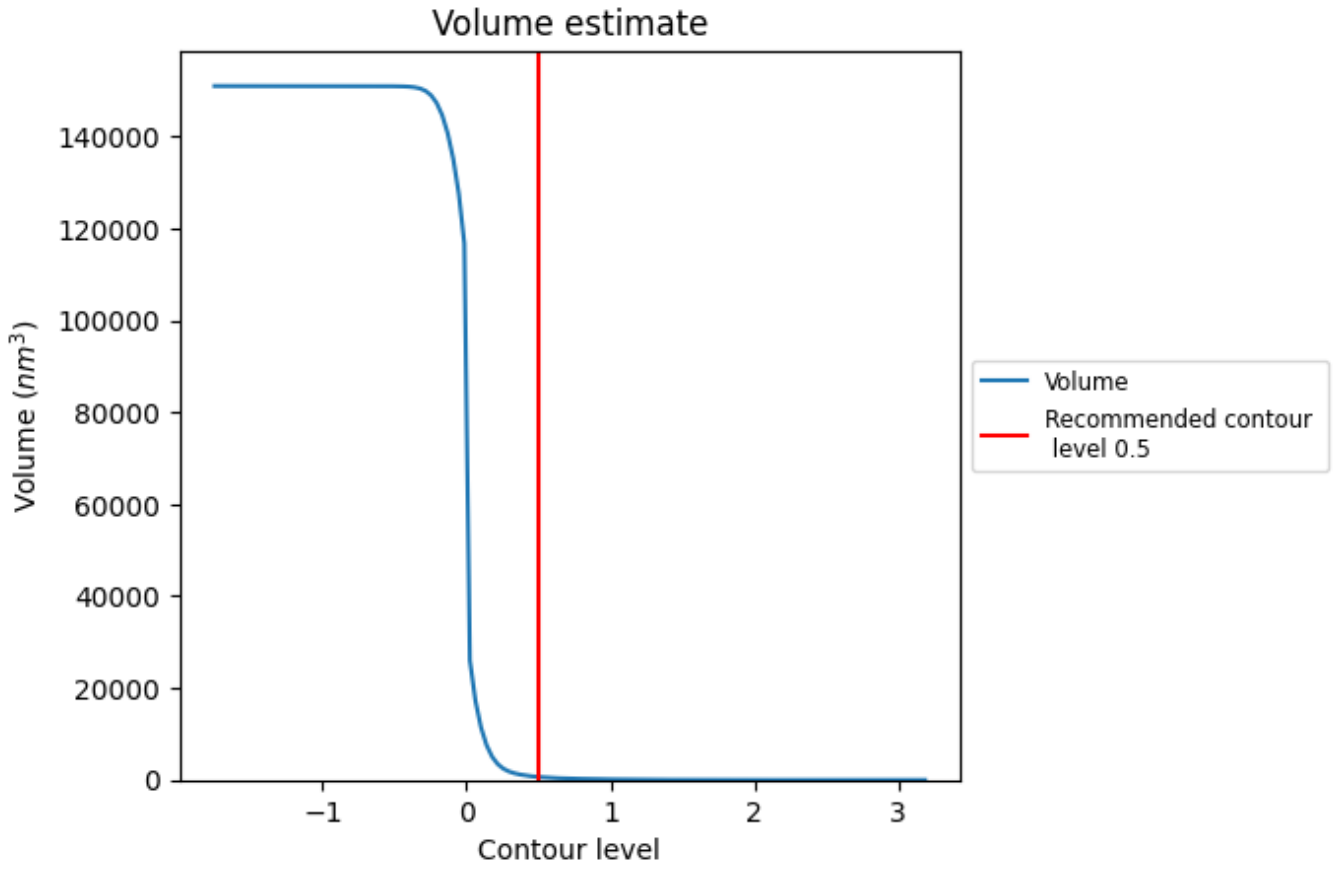
This section contains the results of statistical analysis of the map.

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.

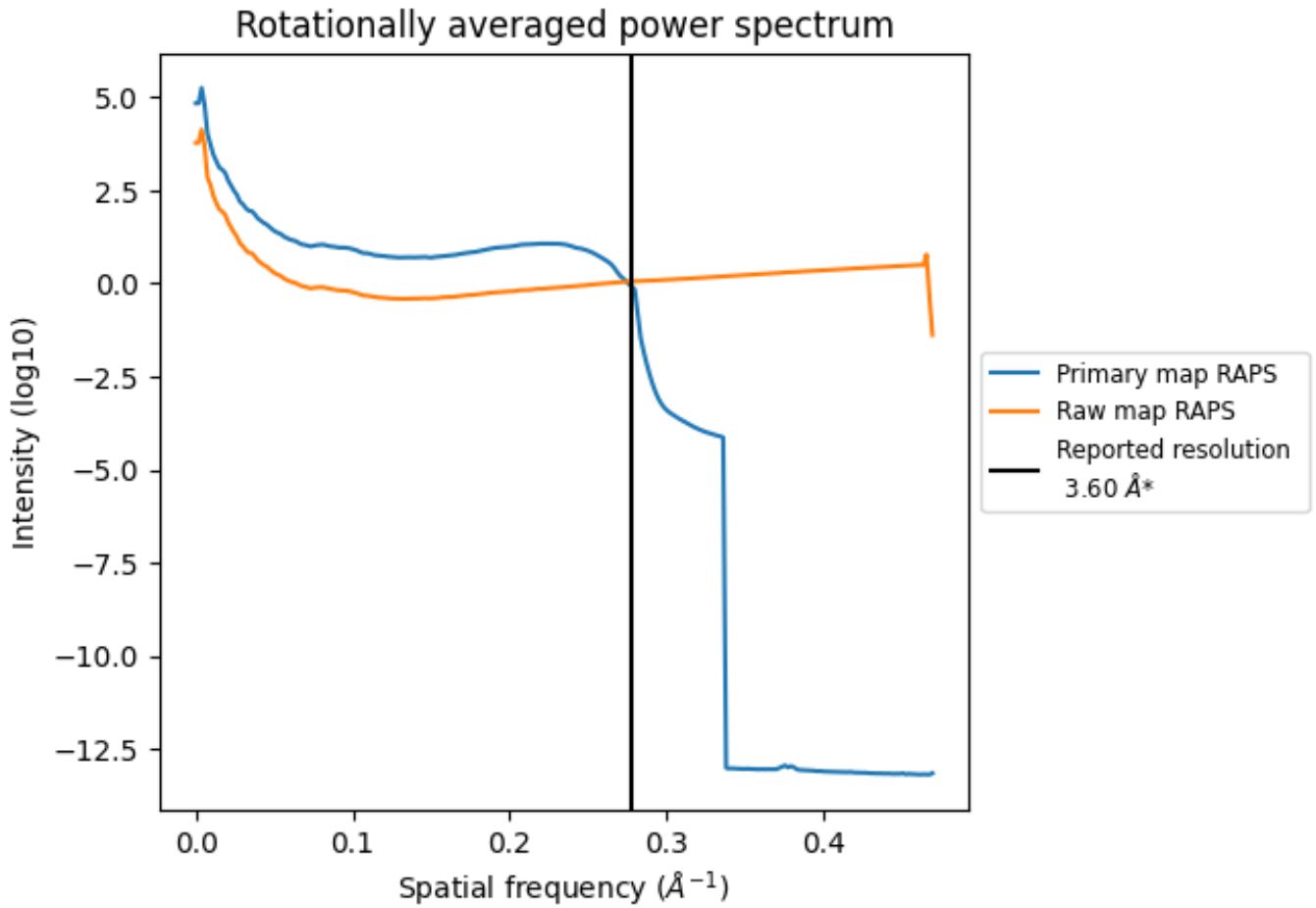
7.2 Volume estimate (i)



The volume at the recommended contour level is 657 nm^3; this corresponds to an approximate mass of 593 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)

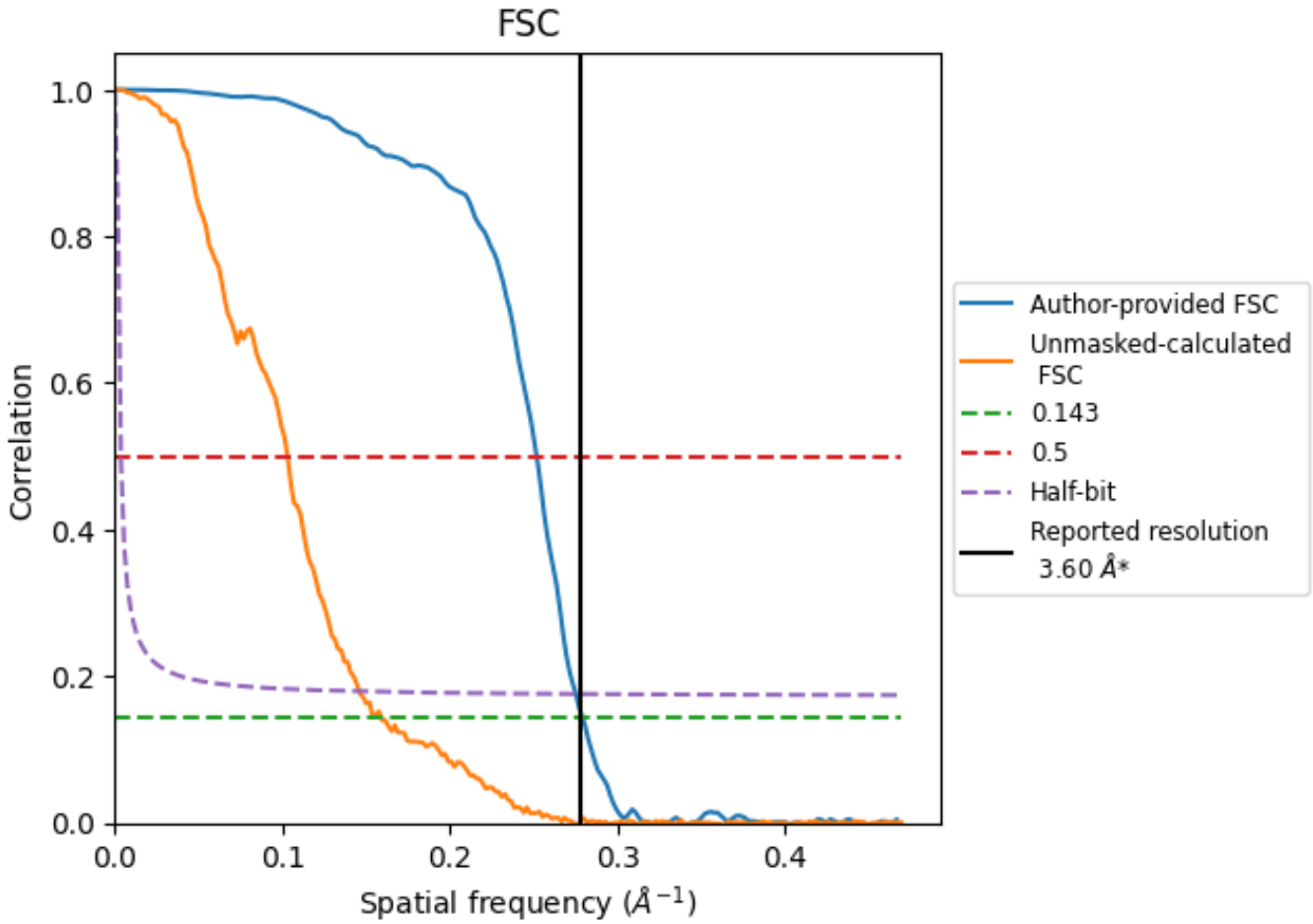


*Reported resolution corresponds to spatial frequency of 0.278 $Å^{-1}$

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 0.278 Å^{-1}

8.2 Resolution estimates (i)

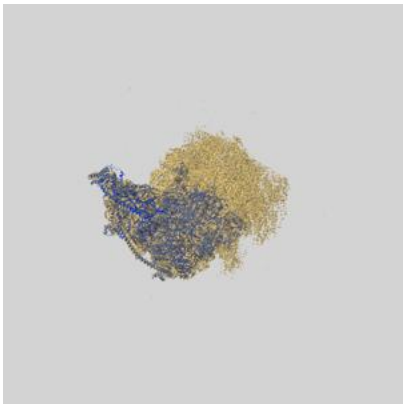
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	3.97	3.63
Unmasked-calculated*	6.29	9.70	6.85

*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 6.29 differs from the reported value 3.6 by more than 10 %

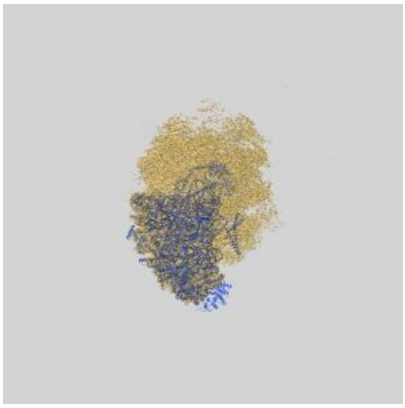
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16895 and PDB model 8OIP. Per-residue inclusion information can be found in section 3 on page 16.

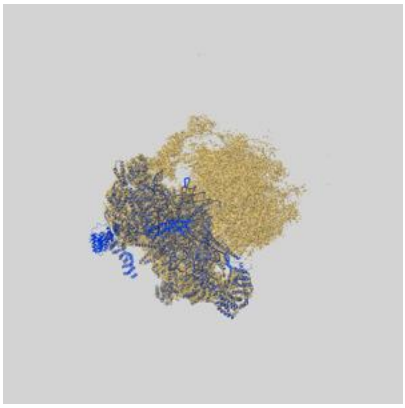
9.1 Map-model overlay



X



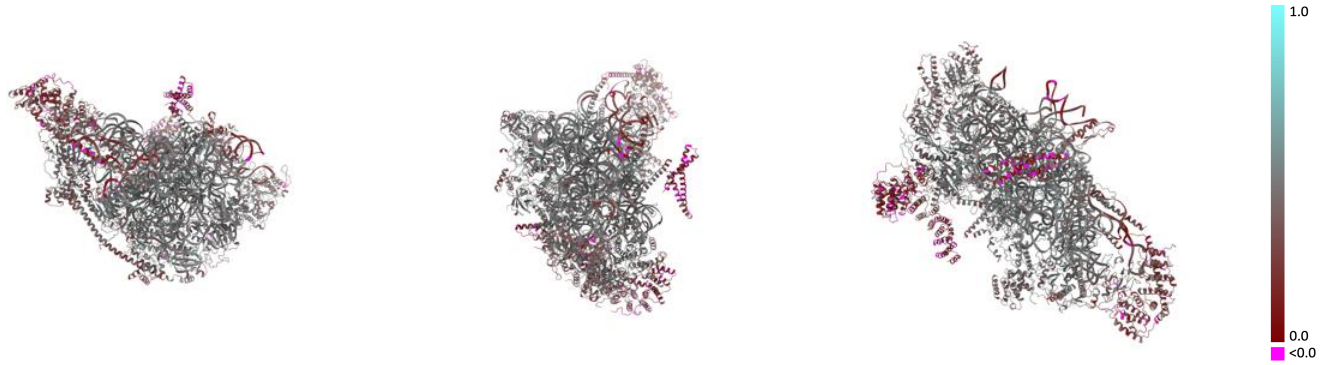
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

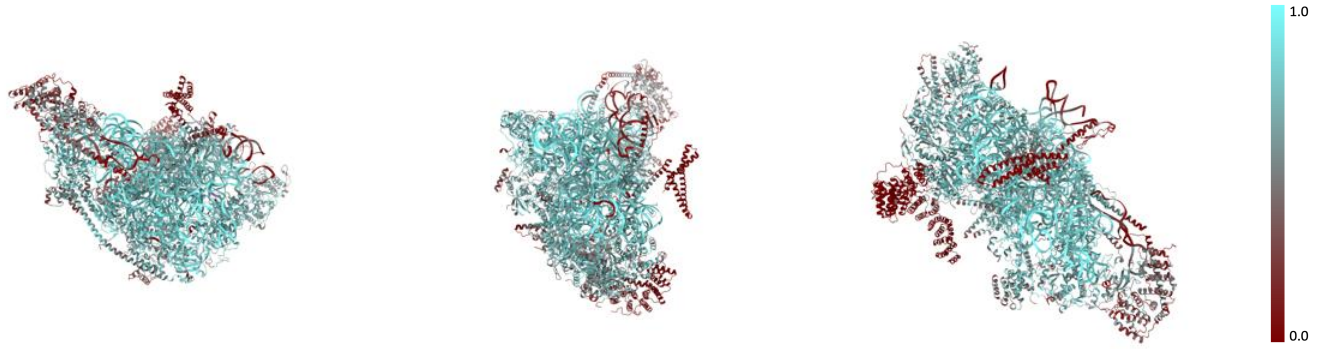
9.2 Q-score mapped to coordinate model (i)



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.

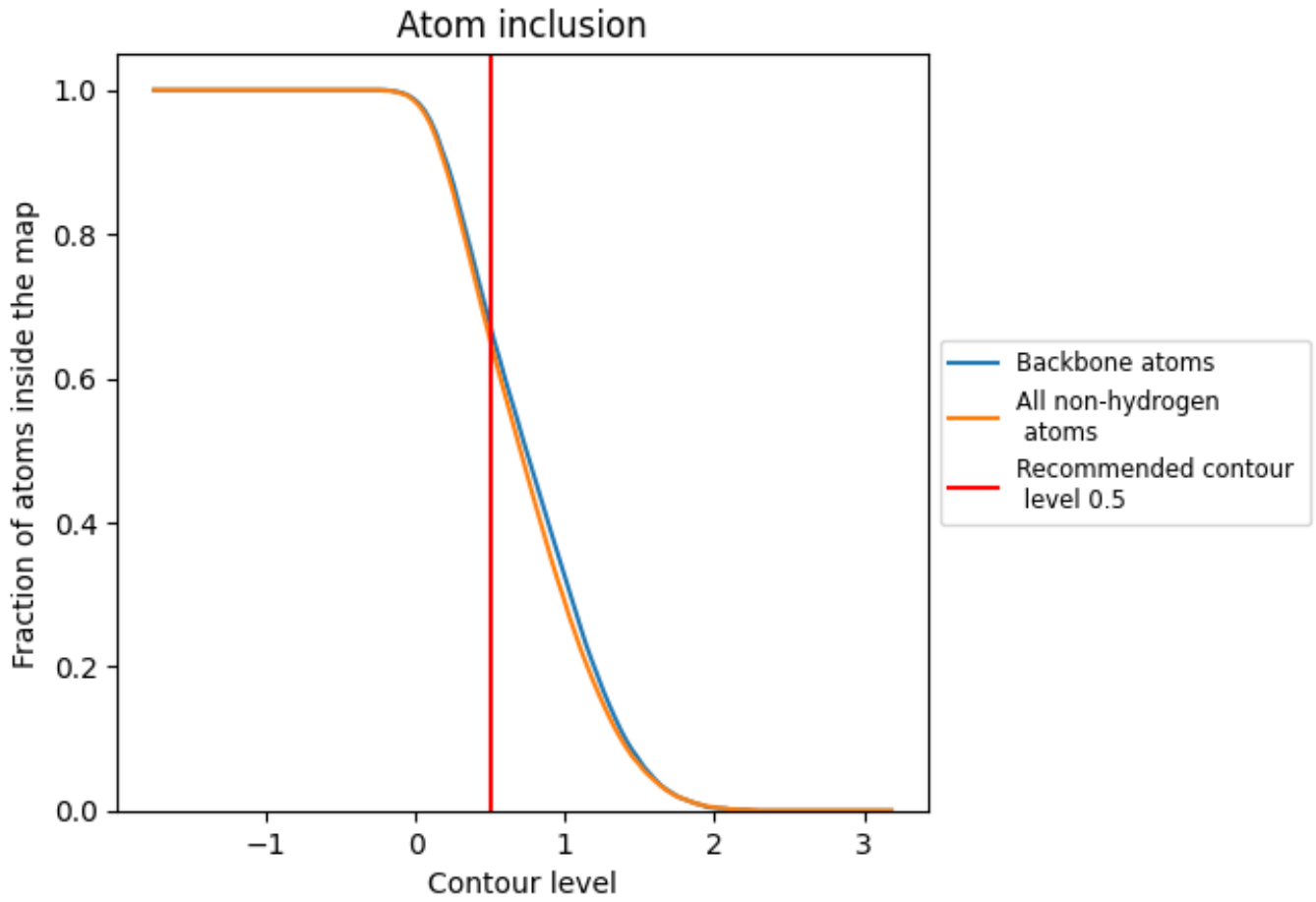
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 67% of all backbone atoms, 65% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6520	0.4180
AA	0.8450	0.4580
AB	0.6500	0.4330
AC	0.7640	0.4920
AD	0.7230	0.4690
AE	0.7220	0.4620
AF	0.7030	0.4340
AG	0.4860	0.3220
AH	0.6680	0.4500
AI	0.7630	0.4740
AJ	0.7200	0.4980
AK	0.7860	0.4910
AL	0.6510	0.4470
AM	0.7590	0.4740
AN	0.7450	0.4690
AO	0.7150	0.4560
AP	0.7380	0.4770
AQ	0.7920	0.4810
AR	0.6260	0.4280
AS	0.6120	0.4160
AT	0.7660	0.4770
AU	0.6680	0.4120
AV	0.3250	0.2600
AW	0.6990	0.4640
AX	0.6530	0.4120
AY	0.4790	0.3500
AZ	0.7150	0.4670
Aa	0.2980	0.3230
Ab	0.7590	0.4620
Ac	0.6560	0.4550
Ad	0.6800	0.4790
Ae	0.1270	0.2150
Ag	0.6790	0.4220
Ai	0.7500	0.4680
Aj	0.5540	0.4000

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Chain	Atom inclusion	Q-score
BX	0.1720	0.2790
Bd	0.3460	0.3870