wwPDB EM Validation Summary Report ⓘ

Jun 2, 2024 – 08:54 AM EDT

PDB ID	:	8CSP
EMDB ID	:	EMD-26966
Title	:	Human mitochondrial small subunit assembly intermediate (State A)
Authors	:	Harper, N.J.; Burnside, C.; Klinge, S.
Deposited on	:	2022-05-13
Resolution	:	2.66 Å(reported)
Based on initial models	:	2C2N, 6RW4, 6AAX

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:

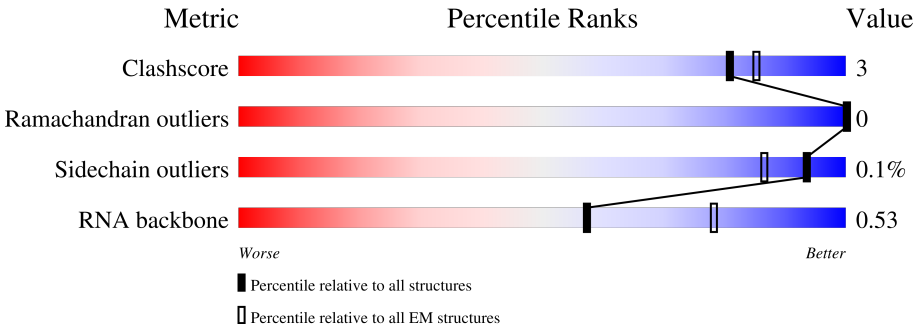
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.66 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
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	0	218	13% 89% 7%
2	1	323	10% 77% 7% 16%
3	4	689	28% 73% 9% 18%
4	5	346	86% 7% 8%
5	7	456	82% 5% 13%
6	8	390	5% 75% 8% 16%
7	9	698	7% 59% 5% 36%

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Mol	Chain	Length	Quality of chain
8	A	955	13% 54% 20% 23%
9	B	296	71% 26%
10	C	167	64% 11% 25%
11	D	430	9% 53% 46%
12	E	125	74% 10% 16%
13	F	242	5% 83% 14%
14	G	396	16% 67% 6% 26%
15	H	201	57% 6% 36%
16	J	138	30% 74% 22%
17	K	128	11% 21% 5% 74%
18	L	257	45% 6% 49%
19	M	137	7% 82% 16%
20	N	130	17% 82% 16%
21	O	258	9% 70% 26%
22	P	142	7% 58% 7% 35%
23	Q	87	7% 7% 93%
24	R	360	18% 77% 19%
25	S	190	13% 68% 30%
26	T	173	23% 89% 6% 5%
27	U	205	30% 80% 15%
28	V	414	81% 6% 13%
29	W	187	5% 50% 48%
30	X	398	83% 6% 12%
31	Y	395	5% 28% 69%
32	Z	106	14% 44% 8% 47%

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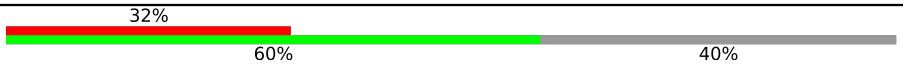
Mol	Chain	Length	Quality of chain
33	a	437	

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 69302 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	211	1754	1108	333	308	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	271	2195	1393	369	422	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	566	4585	2940	774	843	28	0	0

- Molecule 4 is a protein called Dimethyladenosine transferase 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	319	2568	1648	458	451	11	0	0

- Molecule 5 is a protein called Methyltransferase-like protein 17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	7	398	3145	2006	579	544	16	0	0

- Molecule 6 is a protein called Malonyl-CoA-acyl carrier protein transacylase, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	8	326	2543	1617	463	446	17	0	0

- Molecule 7 is a protein called Nitric oxide-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	446	Total	C	N	O	S	0	0
			3558	2271	637	637	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	737	Total	C	N	O	P	0	0
			15655	7018	2818	5082	737		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	126	Total	C	N	O	S	0	0
			1042	679	181	177	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	232	Total	C	N	O	S	0	0
			1838	1155	345	329	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	105	Total	C	N	O	S	0	0
			839	526	154	155	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	208	Total	C	N	O	S	0	0
			1724	1104	312	297	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	292	Total	C	N	O	S	0	0
			2395	1522	418	441	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	128	Total	C	N	O	S	0	0
			1045	675	172	195	3		

- Molecule 16 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	108	Total	C	N	O	S	0	0
			839	521	169	143	6		

- Molecule 17 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	K	33	Total	C	N	O	0	0
			283	173	66	44		

- Molecule 18 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	131	Total	C	N	O	S	0	0
			1091	698	190	197	6		

- Molecule 19 is a protein called 28S ribosomal protein S16, mitochondrial.

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

- Molecule 20 is a protein called 28S ribosomal protein S17, mitochondrial.

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

- Molecule 21 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	190	Total	C	N	O	S	0	0
			1570	999	291	274	6		

- Molecule 22 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	92	Total	C	N	O	S	0	0
			731	472	123	128	8		

- Molecule 23 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	6	Total	C	N	O	S	0	0
			49	30	8	10	1		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 24 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	291	Total	C	N	O	S	0	0
			2382	1518	409	447	8		

- Molecule 25 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	133	Total	C	N	O	S	0	0
			1100	709	196	194	1		

- Molecule 26 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	164	Total	C	N	O	S	0	0
			1344	859	234	240	11		

- Molecule 27 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	174	Total	C	N	O	S	0	0
			1468	905	295	264	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	359	Total	C	N	O	S	0	0
			2946	1891	491	552	12		

- Molecule 29 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	98	Total	C	N	O	S	0	0
			775	491	138	142	4		

- Molecule 30 is a protein called 28S ribosomal protein S29, mitochondrial.

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

- Molecule 31 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	123	Total	C	N	O	S	0	0
			1043	676	175	189	3		

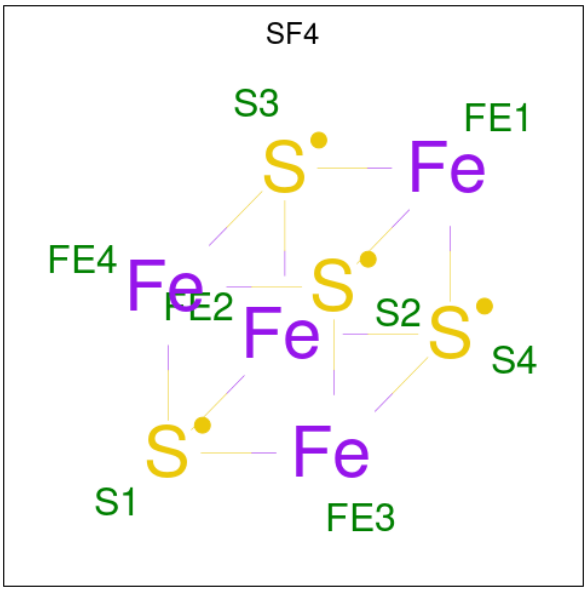
- Molecule 32 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	56	Total	C	N	O	S	0	0
			465	298	84	80	3		

- Molecule 33 is a protein called GTPase Era, mitochondrial.

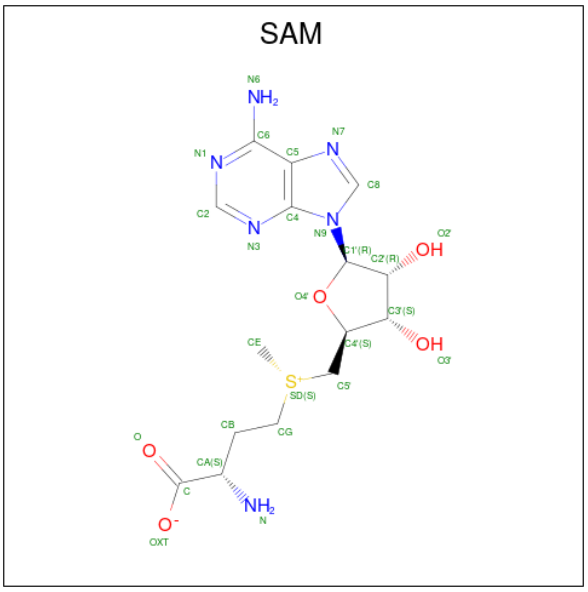
Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	263	Total	C	N	O	S	0	0
			1785	1121	323	335	6		

- Molecule 34 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
34	7	1	Total	Fe	S	0
			8	4	4	

- Molecule 35 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
35	7	1	Total	C	N	O	S	0
			27	15	6	5	1	

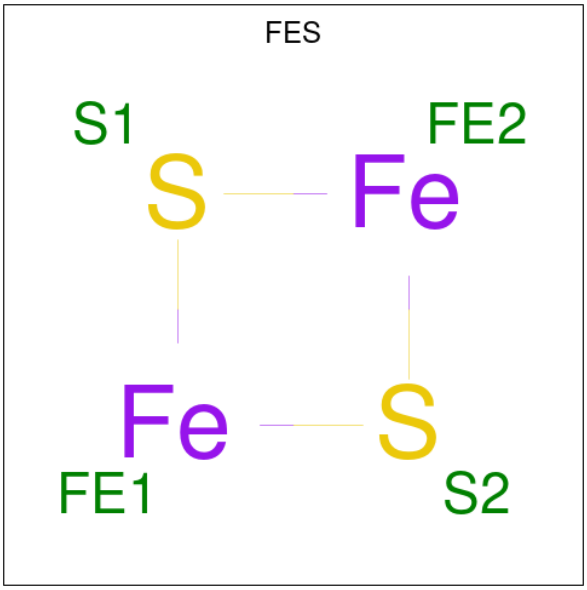
- Molecule 36 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
36	A	4	Total K 4 4	0

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

Mol	Chain	Residues	Atoms	AltConf
37	A	26	Total Mg 26 26	0
37	B	1	Total Mg 1 1	0
37	X	1	Total Mg 1 1	0

- Molecule 38 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).

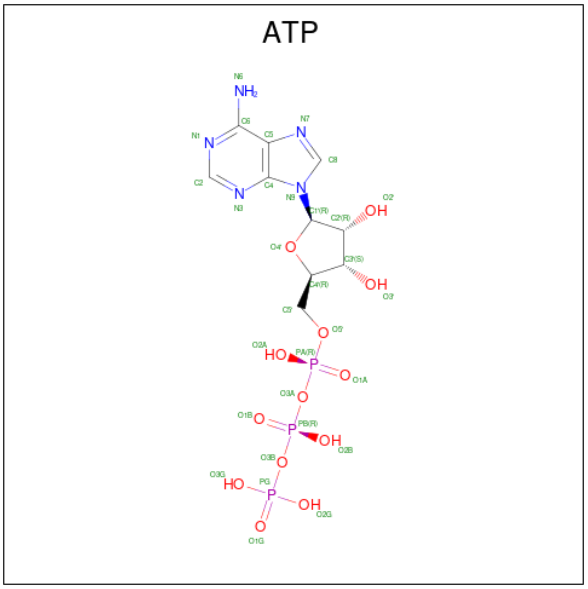


Mol	Chain	Residues	Atoms	AltConf
38	E	1	Total Fe S 4 2 2	0
38	T	1	Total Fe S 4 2 2	0

- Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

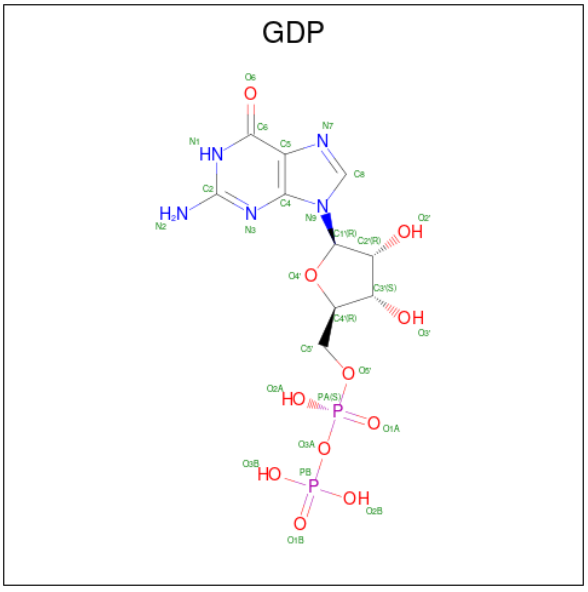
Mol	Chain	Residues	Atoms	AltConf
39	O	1	Total Zn 1 1	0

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



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

- Molecule 41 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

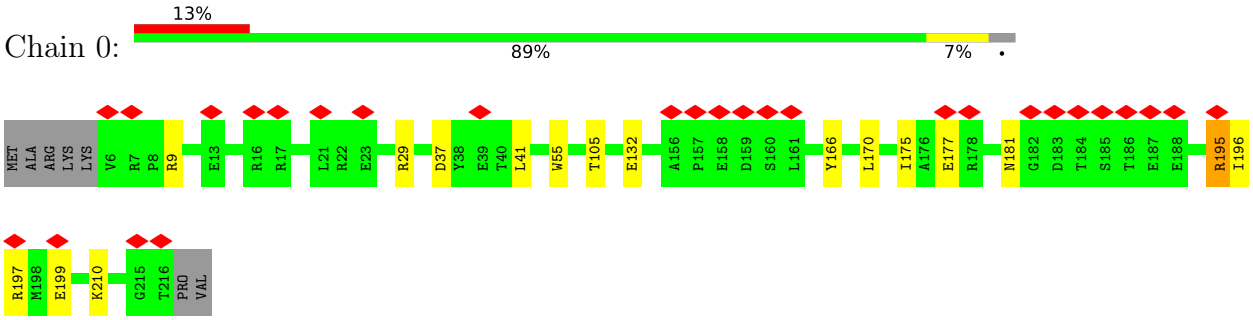


Mol	Chain	Residues	Atoms					AltConf
41	X	1	Total	C	N	O	P	0
			28	10	5	11	2	

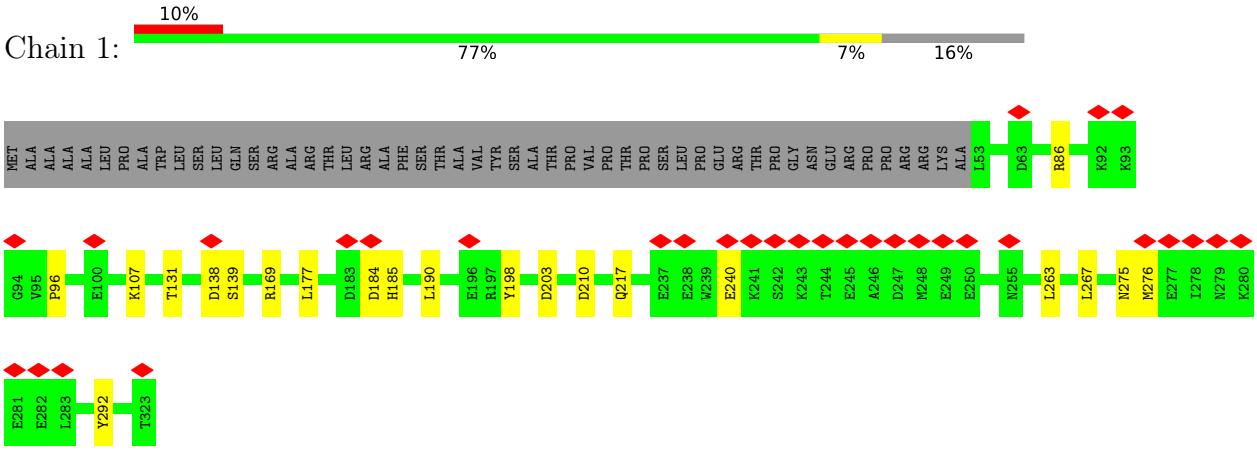
3 Residue-property plots (i)

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

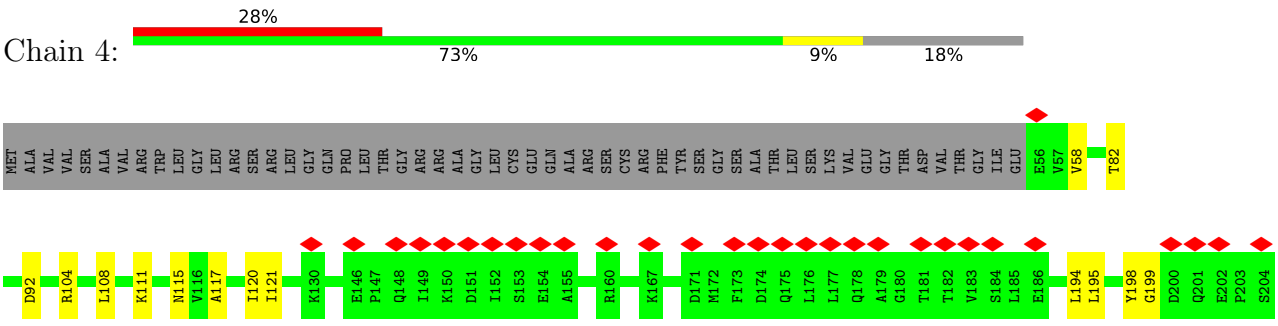
• Molecule 1: 28S ribosomal protein S34, mitochondrial

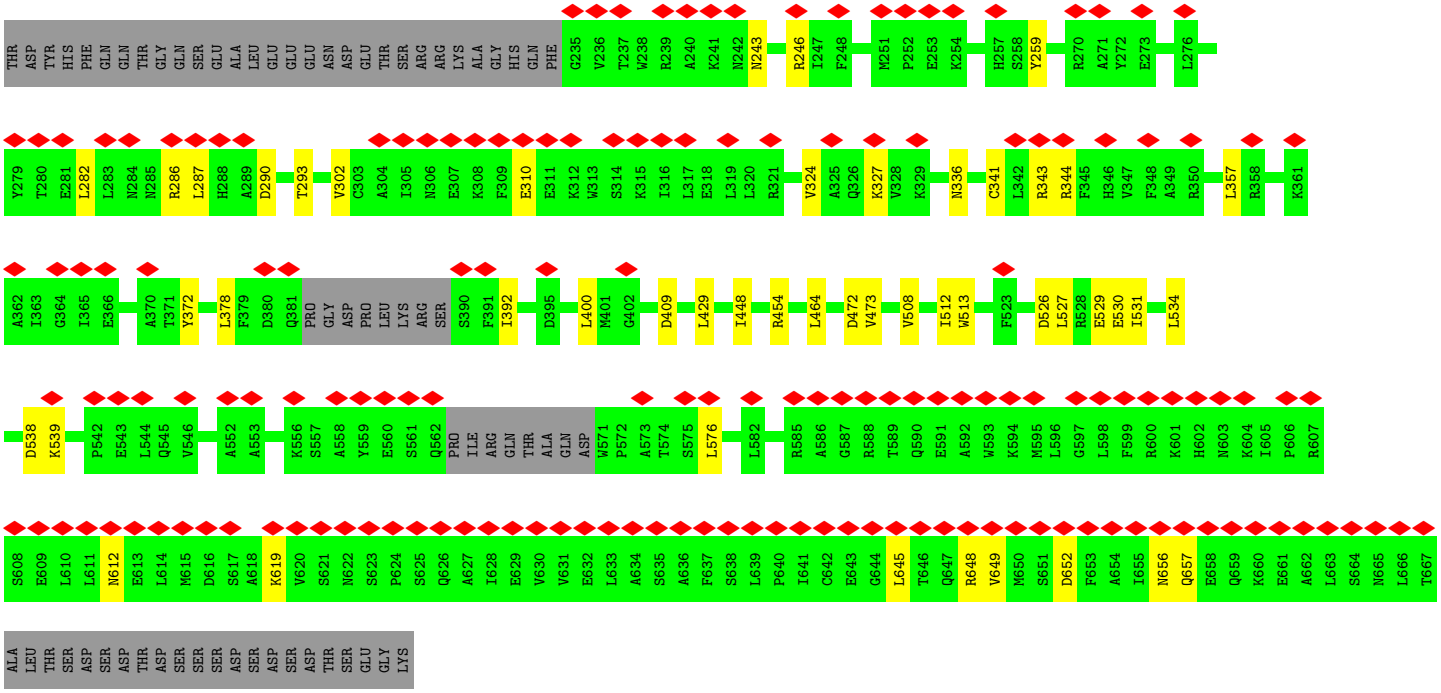


• Molecule 2: 28S ribosomal protein S35, mitochondrial



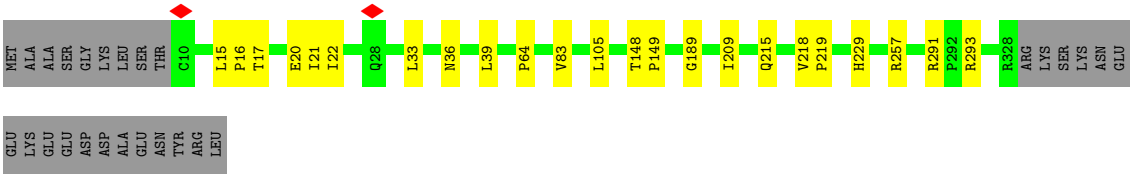
• Molecule 3: Pentatricopeptide repeat domain-containing protein 3, mitochondrial





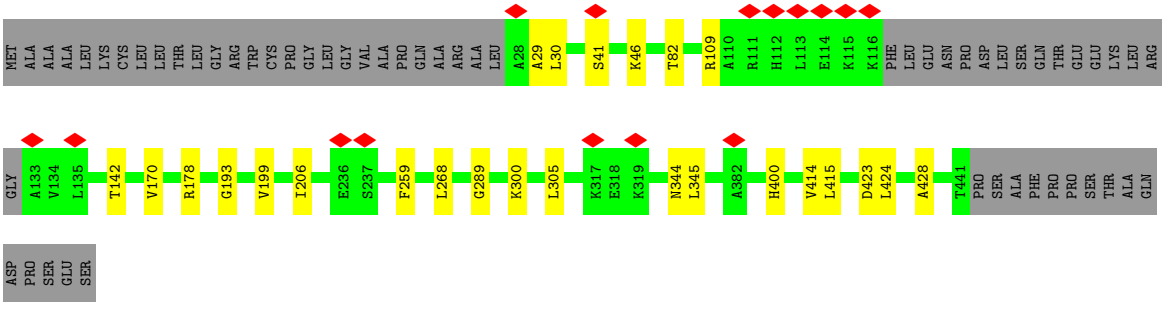
• Molecule 4: Dimethyladenosine transferase 1, mitochondrial

Chain 5:



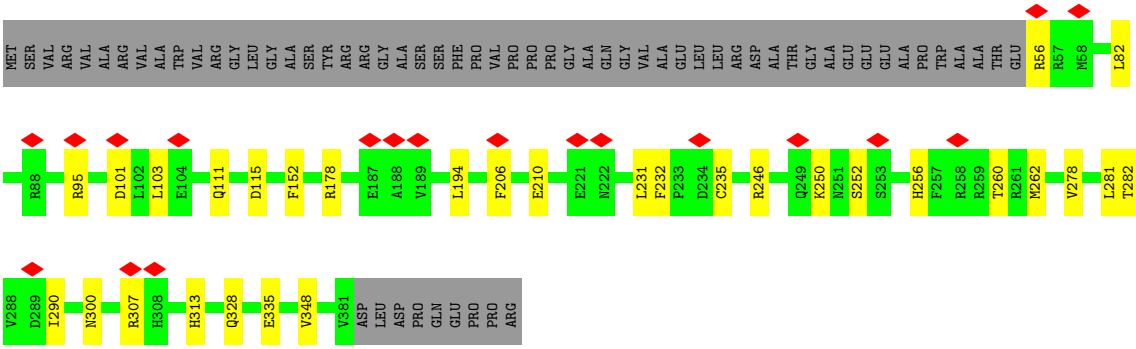
• Molecule 5: Methyltransferase-like protein 17, mitochondrial

Chain 7:

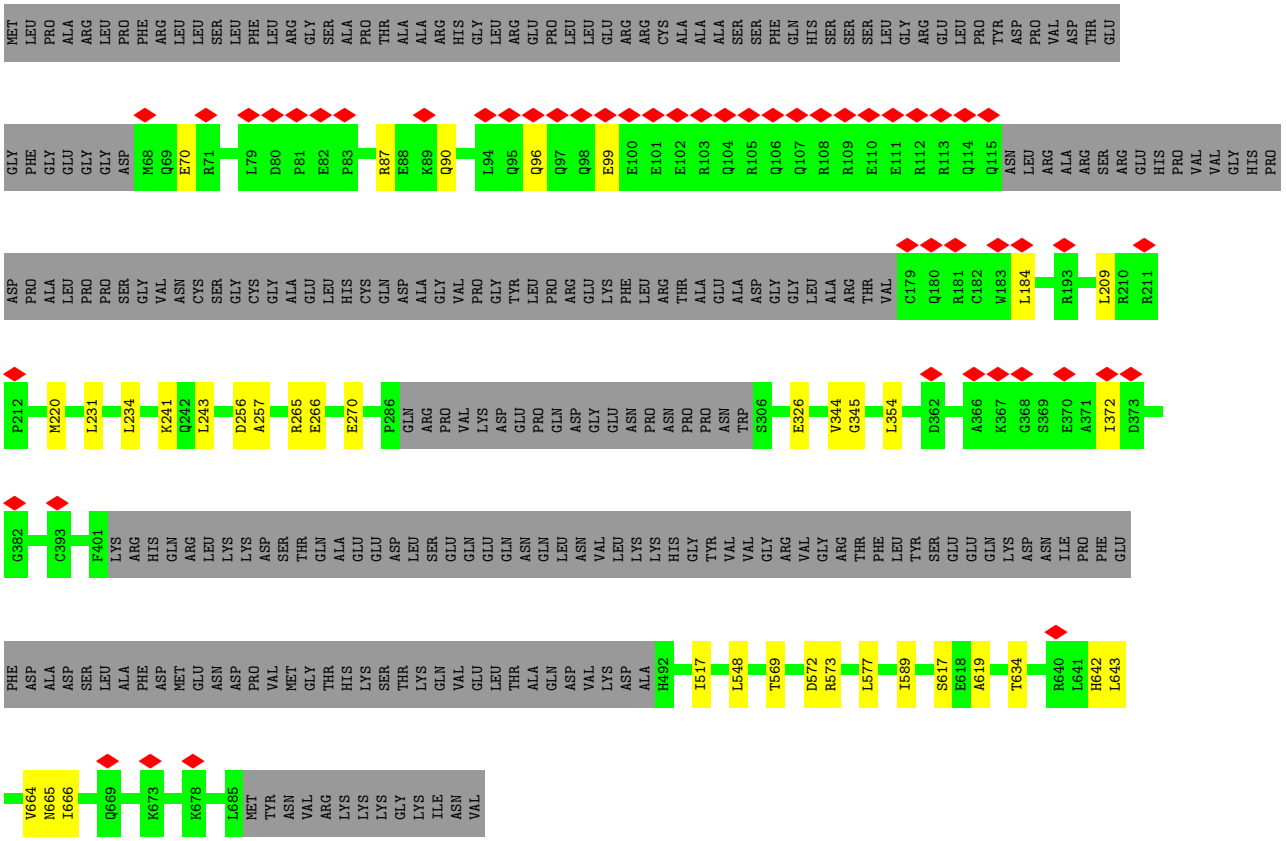


• Molecule 6: Malonyl-CoA-acyl carrier protein transacylase, mitochondrial

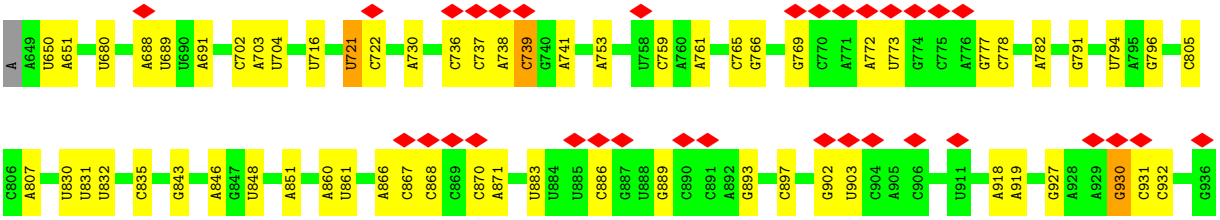
Chain 8:

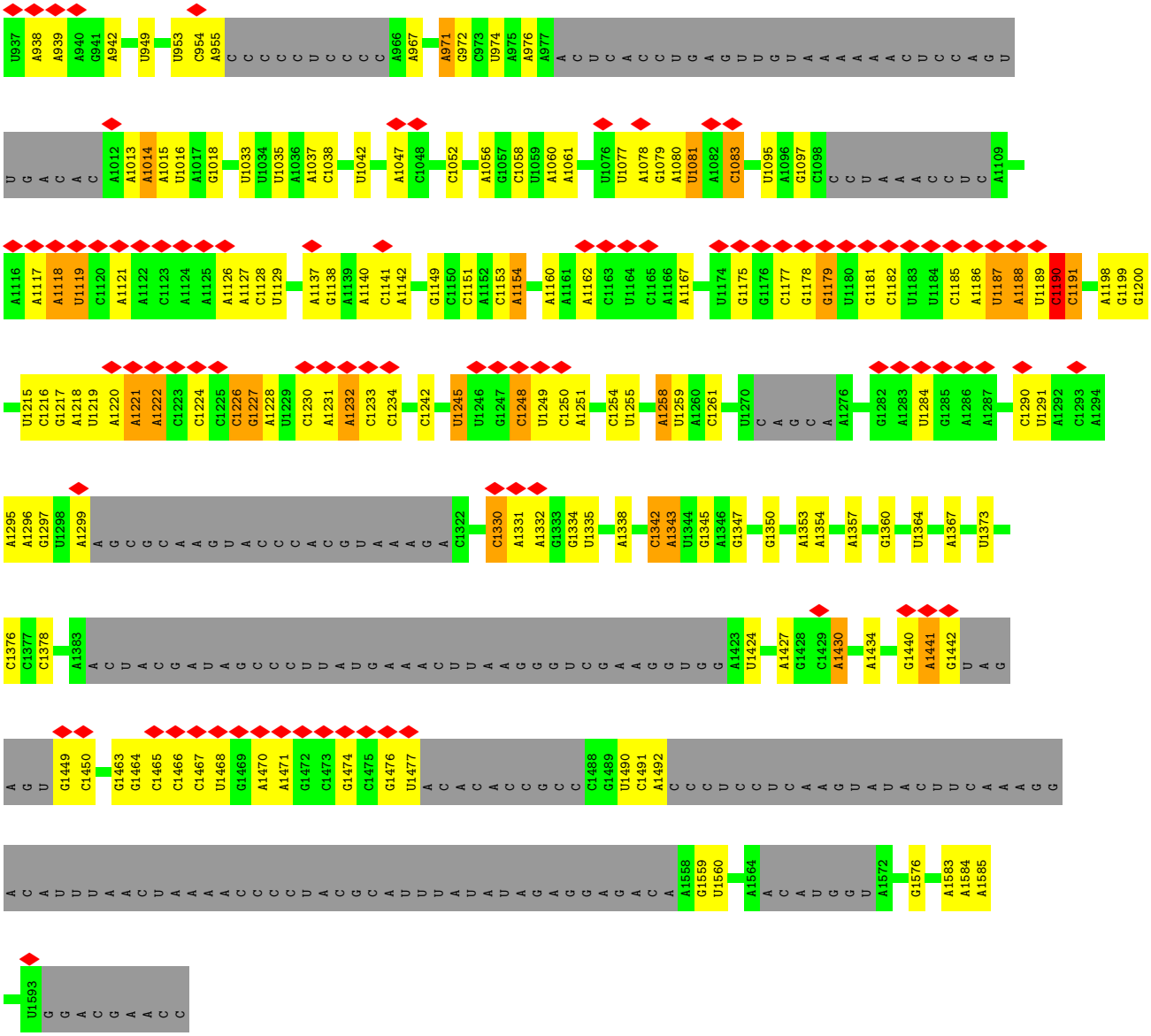


• Molecule 7: Nitric oxide-associated protein 1



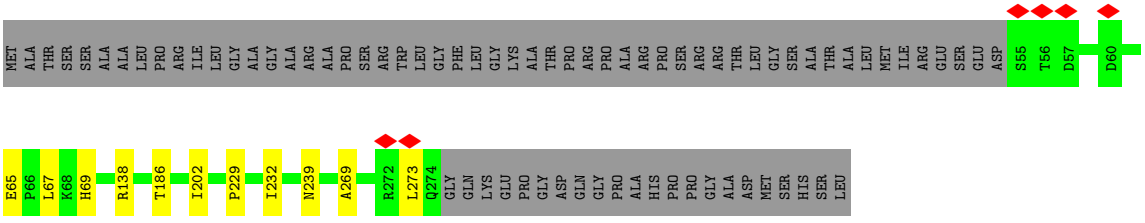
• Molecule 8: 12S mitochondrial rRNA





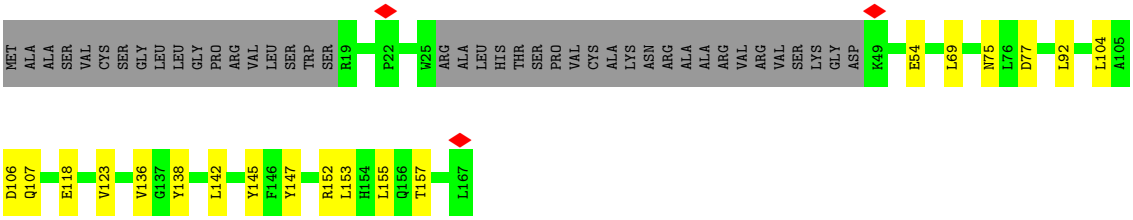
• Molecule 9: 28S ribosomal protein S2, mitochondrial

Chain B:



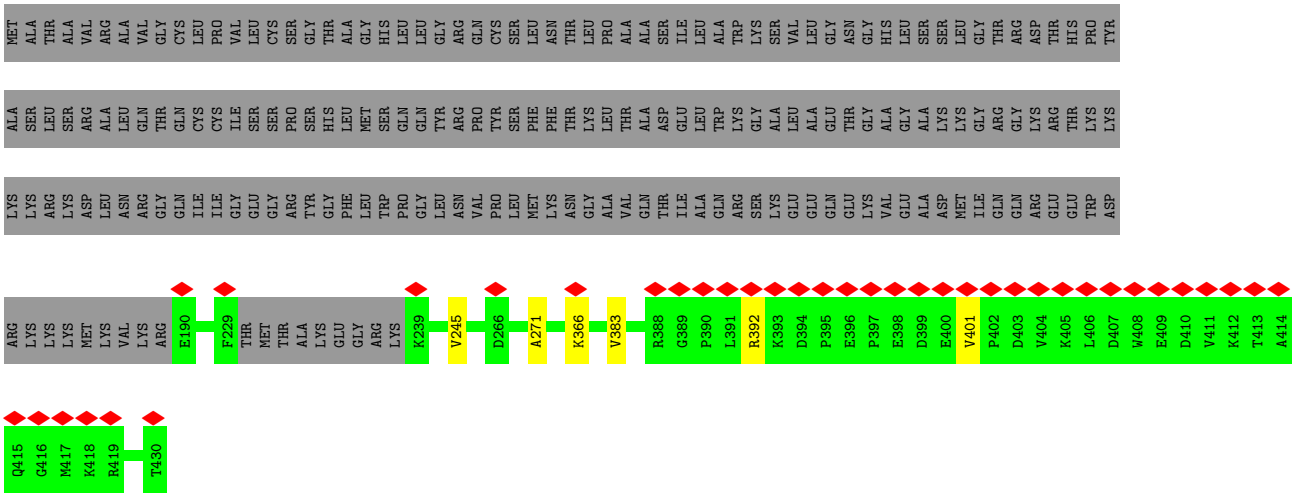
• Molecule 10: 28S ribosomal protein S24, mitochondrial

Chain C:



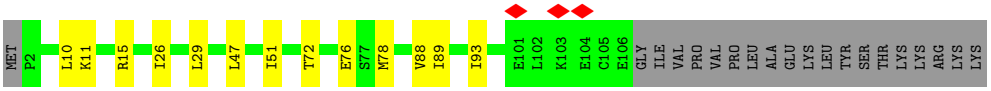
• Molecule 11: 28S ribosomal protein S5, mitochondrial

Chain D:



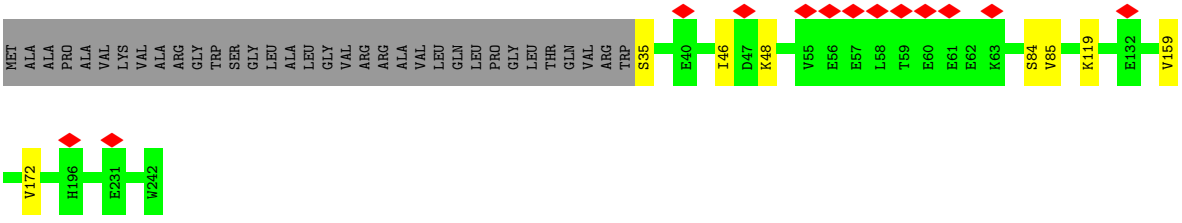
• Molecule 12: 28S ribosomal protein S6, mitochondrial

Chain E:



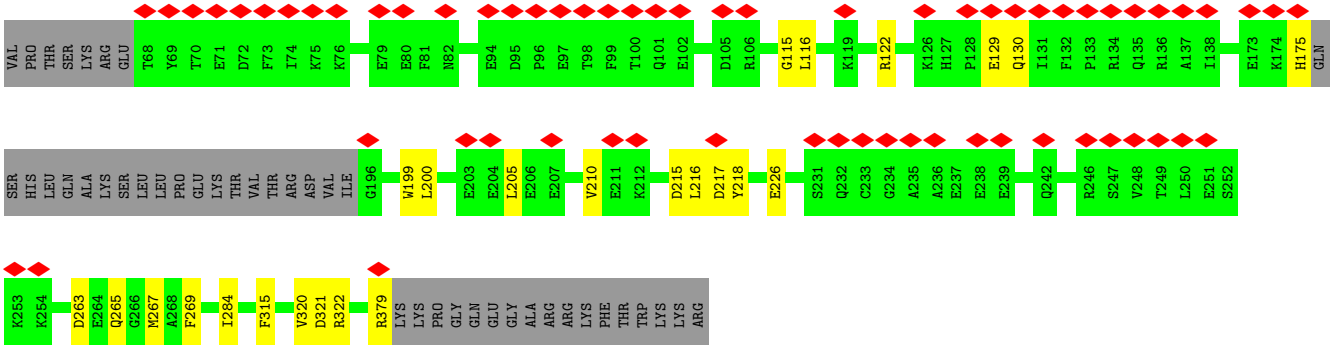
• Molecule 13: 28S ribosomal protein S7, mitochondrial

Chain F:



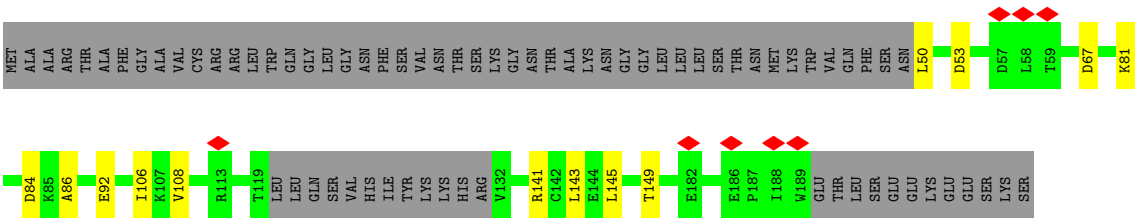
• Molecule 14: 28S ribosomal protein S9, mitochondrial

Chain G:



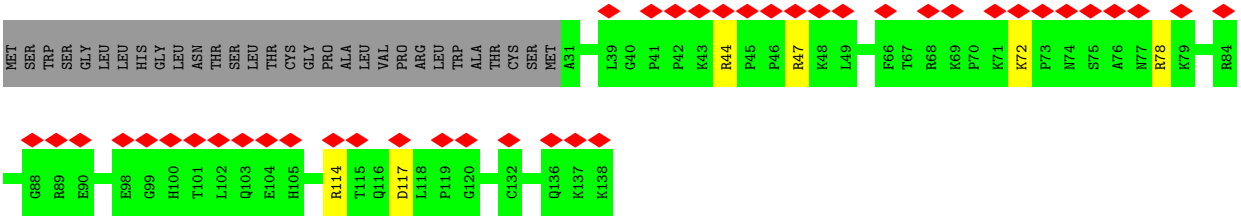
• Molecule 15: 28S ribosomal protein S10, mitochondrial

Chain H:



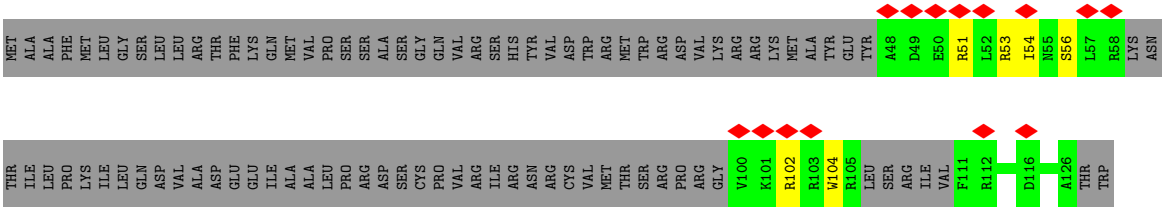
• Molecule 16: 28S ribosomal protein S12, mitochondrial

Chain J:



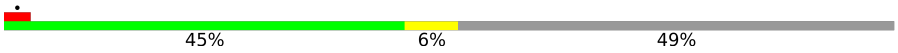
• Molecule 17: 28S ribosomal protein S14, mitochondrial

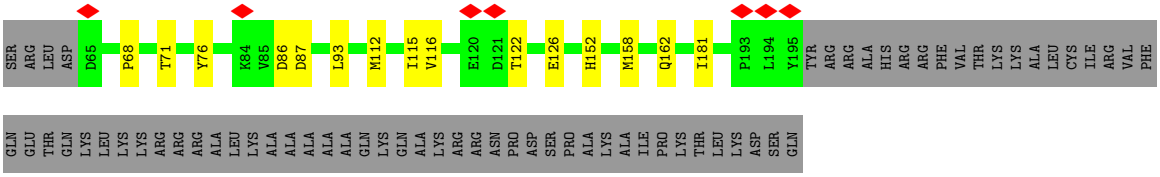
Chain K:



• Molecule 18: 28S ribosomal protein S15, mitochondrial

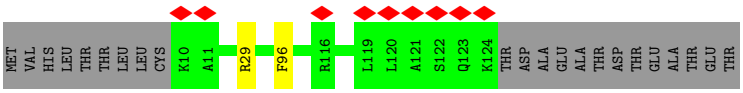
Chain L:





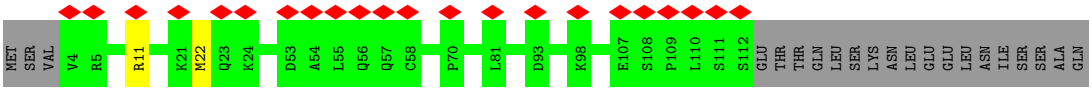
• Molecule 19: 28S ribosomal protein S16, mitochondrial

Chain M:



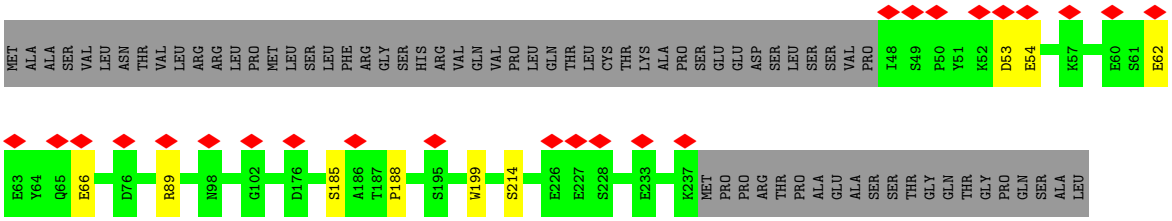
• Molecule 20: 28S ribosomal protein S17, mitochondrial

Chain N:



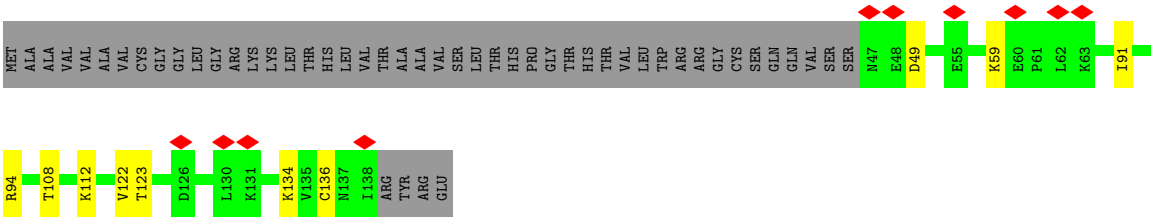
• Molecule 21: 28S ribosomal protein S18b, mitochondrial

Chain O:



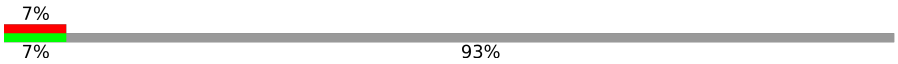
• Molecule 22: 28S ribosomal protein S18c, mitochondrial

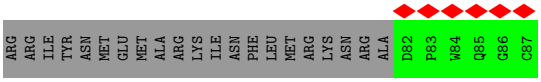
Chain P:



• Molecule 23: 28S ribosomal protein S21, mitochondrial

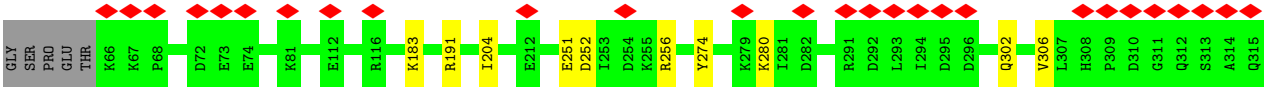
Chain Q:

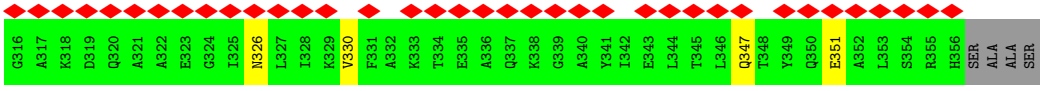




• Molecule 24: 28S ribosomal protein S22, mitochondrial

Chain R:



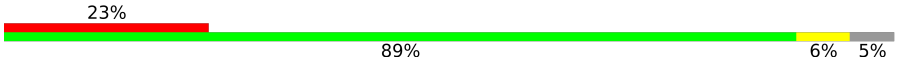


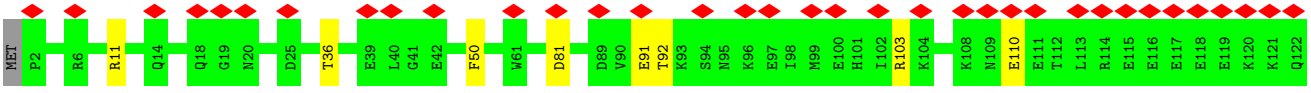
• Molecule 25: 28S ribosomal protein S23, mitochondrial

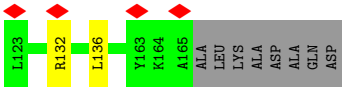
Chain S:

• Molecule 26: 28S ribosomal protein S25, mitochondrial

Chain T:

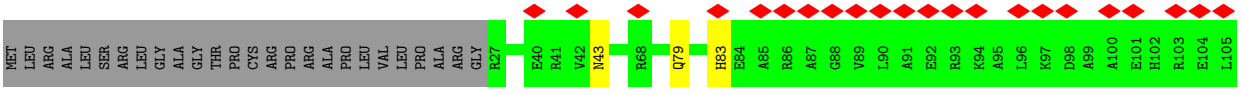


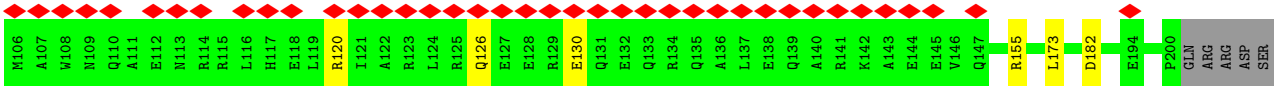




• Molecule 27: 28S ribosomal protein S26, mitochondrial

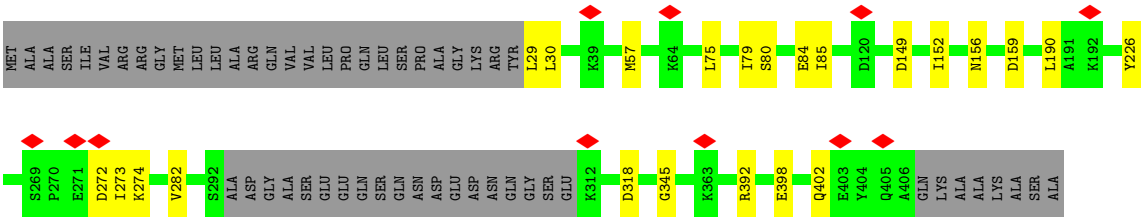
Chain U:





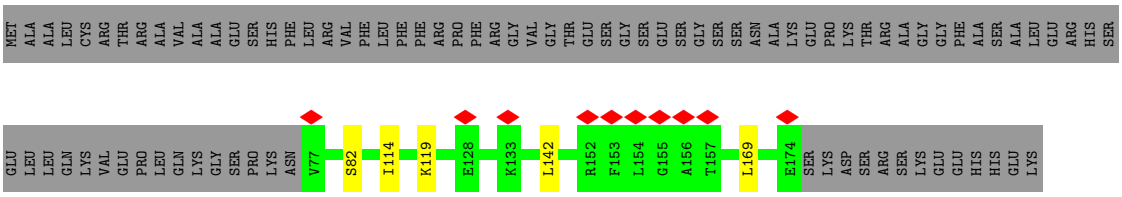
• Molecule 28: 28S ribosomal protein S27, mitochondrial

Chain V:



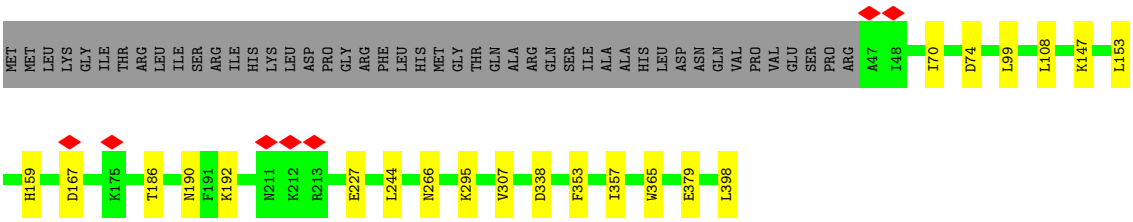
• Molecule 29: 28S ribosomal protein S28, mitochondrial

Chain W:



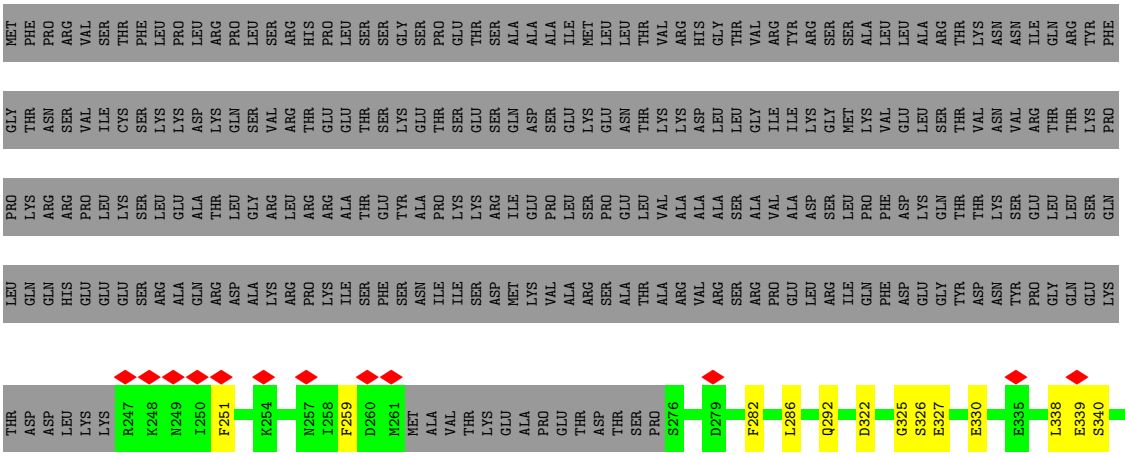
• Molecule 30: 28S ribosomal protein S29, mitochondrial

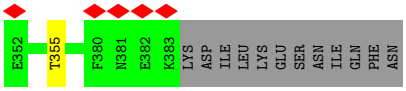
Chain X:



• Molecule 31: 28S ribosomal protein S31, mitochondrial

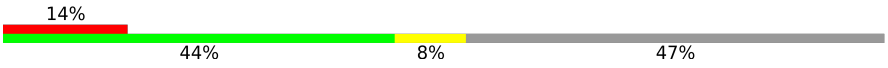
Chain Y:

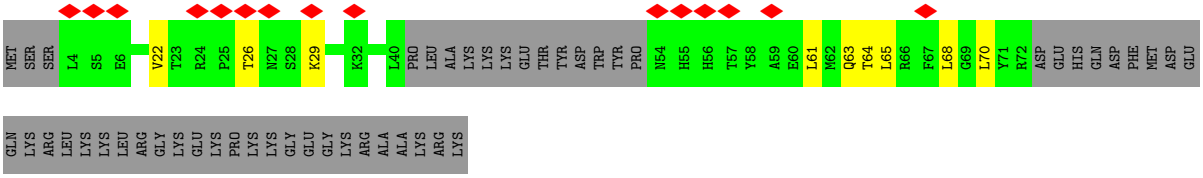




• Molecule 32: 28S ribosomal protein S33, mitochondrial

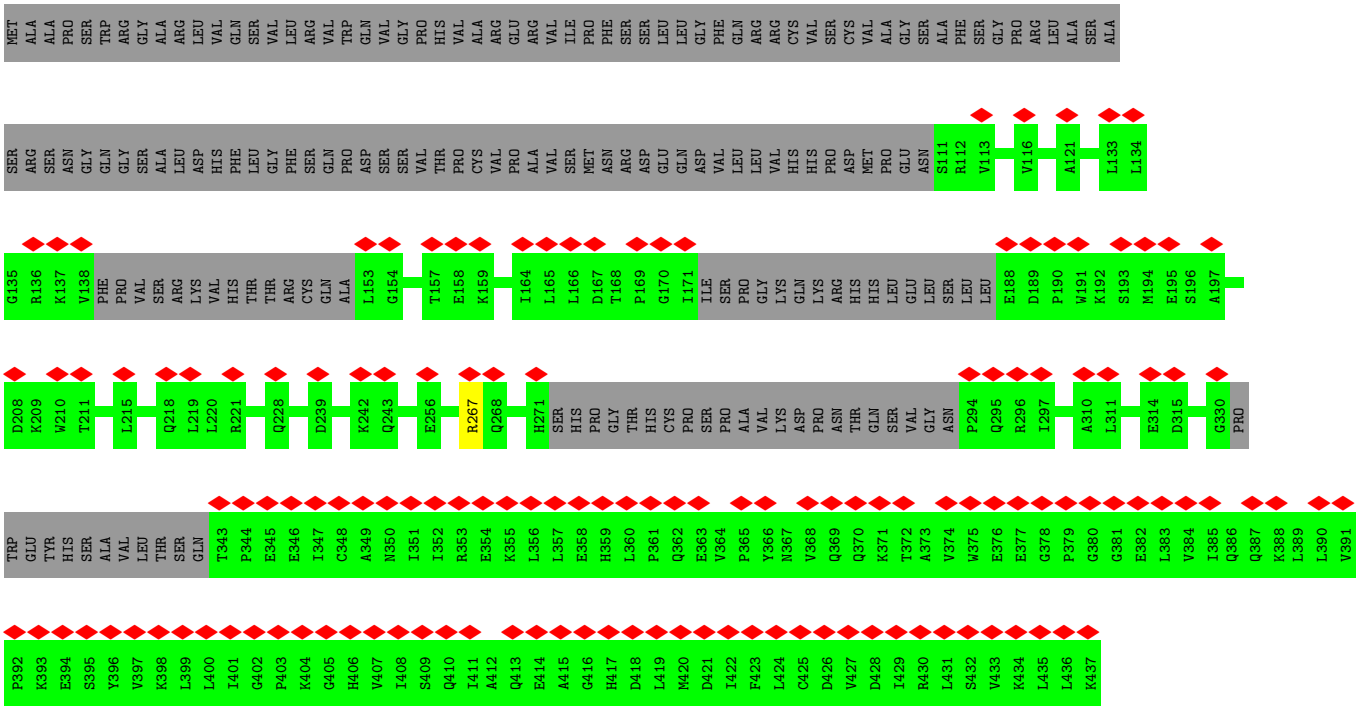
Chain Z:





• Molecule 33: GTPase Era, mitochondrial

Chain a:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	263184	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 ($e^-/Å^2$)	51	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	66.216	Depositor
Minimum map value	-26.873	Depositor
Average map value	0.045	Depositor
Map value standard deviation	1.467	Depositor
Recommended contour level	8.5	Depositor
Map size (Å)	424.80002, 424.80002, 424.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.062, 1.062, 1.062	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, SF4, SAM, ATP, MG, ZN, K, GDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	0	0.27	0/1800	0.61	0/2440
2	1	0.28	0/2241	0.50	0/3033
3	4	0.28	0/4686	0.51	1/6335 (0.0%)
4	5	0.29	0/2624	0.58	0/3552
5	7	0.28	0/3234	0.55	0/4390
6	8	0.29	0/2603	0.55	0/3520
7	9	0.28	0/3637	0.57	0/4935
8	A	0.30	0/17503	0.81	5/27229 (0.0%)
9	B	0.28	0/1832	0.56	0/2480
10	C	0.29	0/1074	0.52	0/1456
11	D	0.26	0/1877	0.56	0/2523
12	E	0.28	0/853	0.59	0/1151
13	F	0.26	0/1766	0.52	0/2373
14	G	0.29	0/2446	0.55	0/3283
15	H	0.28	0/1067	0.51	0/1448
16	J	0.25	0/855	0.58	0/1148
17	K	0.23	0/285	0.66	0/375
18	L	0.28	0/1111	0.51	0/1490
19	M	0.26	0/934	0.60	0/1255
20	N	0.25	0/877	0.54	0/1187
21	O	0.28	0/1624	0.54	0/2210
22	P	0.27	0/747	0.45	0/1004
23	Q	0.22	0/51	0.33	0/68
24	R	0.26	0/2429	0.50	0/3280
25	S	0.29	0/1127	0.59	0/1518
26	T	0.27	0/1375	0.51	0/1847
27	U	0.28	0/1490	0.61	0/1999
28	V	0.28	0/3007	0.48	0/4062
29	W	0.27	0/787	0.56	0/1060
30	X	0.28	0/2921	0.50	0/3954
31	Y	0.27	0/1073	0.45	0/1444
32	Z	0.27	0/473	0.60	0/631

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	a	0.25	0/1801	0.50	0/2447
All	All	0.28	0/72210	0.62	6/101127 (0.0%)

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
1	0	0	1
16	J	0	1
All	All	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1190	C	N1-C2-O2	7.72	123.53	118.90
8	A	721	U	C2-N1-C1'	6.95	126.04	117.70
8	A	1190	C	N3-C2-O2	-6.66	117.24	121.90
8	A	1191	C	C2-N1-C1'	5.32	124.66	118.80
8	A	765	C	C2-N1-C1'	5.21	124.53	118.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	195	ARG	Sidechain
16	J	72	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1754	0	1754	12	0
2	1	2195	0	2217	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	4	4585	0	4595	44	0
4	5	2568	0	2655	17	0
5	7	3145	0	3159	16	0
6	8	2543	0	2561	26	0
7	9	3558	0	3636	24	0
8	A	15655	0	7953	48	0
9	B	1789	0	1781	7	0
10	C	1042	0	1033	17	0
11	D	1838	0	1858	4	0
12	E	839	0	848	10	0
13	F	1724	0	1769	9	0
14	G	2395	0	2364	15	0
15	H	1045	0	1065	13	0
16	J	839	0	887	4	0
17	K	283	0	289	3	0
18	L	1091	0	1137	9	0
19	M	913	0	943	1	0
20	N	859	0	922	2	0
21	O	1570	0	1533	7	0
22	P	731	0	761	6	0
23	Q	49	0	36	0	0
24	R	2382	0	2405	8	0
25	S	1100	0	1103	6	0
26	T	1344	0	1359	8	0
27	U	1468	0	1478	6	0
28	V	2946	0	2942	16	0
29	W	775	0	791	4	0
30	X	2849	0	2843	16	0
31	Y	1043	0	996	10	0
32	Z	465	0	475	6	0
33	a	1785	0	1599	0	0
34	7	8	0	0	0	0
35	7	27	0	22	1	0
36	A	4	0	0	0	0
37	A	26	0	0	0	0
37	B	1	0	0	0	0
37	X	1	0	0	0	0
38	E	4	0	0	0	0
38	T	4	0	0	0	0
39	O	1	0	0	0	0
40	X	31	0	12	0	0
41	X	28	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	69302	0	61793	324	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 324 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:198:TYR:OH	2:1:203:ASP:OD1	1.96	0.84
4:5:17:THR:OG1	4:5:20:GLU:OE1	1.96	0.82
2:1:185:HIS:NE2	2:1:240:GLU:OE2	2.13	0.82
8:A:1081:U:O2'	8:A:1083:C:OP2	1.99	0.79
3:4:243:ASN:OD1	3:4:246:ARG:NH2	2.16	0.78

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	209/218 (96%)	206 (99%)	3 (1%)	0	100	100
2	1	269/323 (83%)	263 (98%)	6 (2%)	0	100	100
3	4	558/689 (81%)	550 (99%)	8 (1%)	0	100	100
4	5	317/346 (92%)	313 (99%)	4 (1%)	0	100	100
5	7	394/456 (86%)	383 (97%)	11 (3%)	0	100	100
6	8	324/390 (83%)	315 (97%)	9 (3%)	0	100	100
7	9	438/698 (63%)	425 (97%)	13 (3%)	0	100	100
9	B	218/296 (74%)	216 (99%)	2 (1%)	0	100	100
10	C	122/167 (73%)	119 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	D	228/430 (53%)	224 (98%)	4 (2%)	0	100	100
12	E	103/125 (82%)	100 (97%)	3 (3%)	0	100	100
13	F	206/242 (85%)	204 (99%)	2 (1%)	0	100	100
14	G	288/396 (73%)	282 (98%)	6 (2%)	0	100	100
15	H	124/201 (62%)	121 (98%)	3 (2%)	0	100	100
16	J	106/138 (77%)	101 (95%)	5 (5%)	0	100	100
17	K	27/128 (21%)	27 (100%)	0	0	100	100
18	L	129/257 (50%)	129 (100%)	0	0	100	100
19	M	113/137 (82%)	113 (100%)	0	0	100	100
20	N	107/130 (82%)	107 (100%)	0	0	100	100
21	O	188/258 (73%)	187 (100%)	1 (0%)	0	100	100
22	P	90/142 (63%)	88 (98%)	2 (2%)	0	100	100
23	Q	4/87 (5%)	4 (100%)	0	0	100	100
24	R	289/360 (80%)	283 (98%)	6 (2%)	0	100	100
25	S	131/190 (69%)	130 (99%)	1 (1%)	0	100	100
26	T	162/173 (94%)	160 (99%)	2 (1%)	0	100	100
27	U	172/205 (84%)	170 (99%)	2 (1%)	0	100	100
28	V	355/414 (86%)	351 (99%)	4 (1%)	0	100	100
29	W	96/187 (51%)	95 (99%)	1 (1%)	0	100	100
30	X	350/398 (88%)	346 (99%)	4 (1%)	0	100	100
31	Y	119/395 (30%)	118 (99%)	1 (1%)	0	100	100
32	Z	52/106 (49%)	52 (100%)	0	0	100	100
33	a	253/437 (58%)	247 (98%)	6 (2%)	0	100	100
All	All	6541/9119 (72%)	6429 (98%)	112 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	184/190 (97%)	184 (100%)	0	100	100
2	1	250/291 (86%)	250 (100%)	0	100	100
3	4	506/609 (83%)	506 (100%)	0	100	100
4	5	286/309 (93%)	286 (100%)	0	100	100
5	7	339/385 (88%)	339 (100%)	0	100	100
6	8	270/317 (85%)	270 (100%)	0	100	100
7	9	388/600 (65%)	388 (100%)	0	100	100
9	B	194/249 (78%)	194 (100%)	0	100	100
10	C	111/143 (78%)	111 (100%)	0	100	100
11	D	196/357 (55%)	196 (100%)	0	100	100
12	E	89/107 (83%)	89 (100%)	0	100	100
13	F	185/209 (88%)	185 (100%)	0	100	100
14	G	254/342 (74%)	253 (100%)	1 (0%)	91	95
15	H	118/180 (66%)	118 (100%)	0	100	100
16	J	93/118 (79%)	93 (100%)	0	100	100
17	K	28/113 (25%)	27 (96%)	1 (4%)	35	51
18	L	123/226 (54%)	123 (100%)	0	100	100
19	M	94/113 (83%)	93 (99%)	1 (1%)	73	85
20	N	95/115 (83%)	95 (100%)	0	100	100
21	O	171/230 (74%)	171 (100%)	0	100	100
22	P	83/123 (68%)	82 (99%)	1 (1%)	71	84
23	Q	5/79 (6%)	5 (100%)	0	100	100
24	R	261/318 (82%)	261 (100%)	0	100	100
25	S	115/164 (70%)	115 (100%)	0	100	100
26	T	151/157 (96%)	151 (100%)	0	100	100
27	U	150/174 (86%)	149 (99%)	1 (1%)	84	91
28	V	323/364 (89%)	323 (100%)	0	100	100
29	W	85/158 (54%)	85 (100%)	0	100	100
30	X	311/351 (89%)	311 (100%)	0	100	100
31	Y	113/357 (32%)	113 (100%)	0	100	100
32	Z	51/95 (54%)	50 (98%)	1 (2%)	55	73
33	a	151/386 (39%)	150 (99%)	1 (1%)	84	91

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5773/7929 (73%)	5766 (100%)	7 (0%)	93 97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	P	59	LYS
27	U	155	ARG
33	a	267	ARG
32	Z	29	LYS
19	M	29	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
10	C	57	HIS
27	U	62	HIS
30	X	140	HIS
30	X	110	HIS
5	7	412	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	A	726/955 (76%)	184 (25%)	3 (0%)

5 of 184 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	650	U
8	A	651	A
8	A	680	U
8	A	688	A
8	A	689	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	1077	U
8	A	1226	C
8	A	1330	C

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 39 ligands modelled in this entry, 33 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	FES	E	201	22,12	0,4,4	-	-	-		
34	SF4	7	501	5	0,12,12	-	-	-		
38	FES	T	201	26,19	0,4,4	-	-	-		
35	SAM	7	502	-	24,29,29	1.19	3 (12%)	23,42,42	1.59	3 (13%)
40	ATP	X	501	37	26,33,33	0.66	0	31,52,52	1.06	2 (6%)
41	GDP	X	503	-	24,30,30	3.36	12 (50%)	30,47,47	2.19	7 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	FES	E	201	22,12	-	-	0/1/1/1
34	SF4	7	501	5	-	-	0/6/5/5
38	FES	T	201	26,19	-	-	0/1/1/1
35	SAM	7	502	-	-	6/12/33/33	0/3/3/3
40	ATP	X	501	37	-	2/18/38/38	0/3/3/3
41	GDP	X	503	-	-	5/12/32/32	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	X	503	GDP	O6-C6	9.25	1.42	1.23
41	X	503	GDP	C2-N1	7.44	1.56	1.37
41	X	503	GDP	C2-N3	5.21	1.45	1.33
41	X	503	GDP	C2-N2	5.08	1.46	1.34
35	7	502	SAM	C2-N3	3.85	1.38	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	X	503	GDP	C8-N7-C5	7.04	116.41	102.99
35	7	502	SAM	N3-C2-N1	-5.44	120.18	128.68
41	X	503	GDP	C2-N1-C6	-4.72	116.40	125.10
41	X	503	GDP	C3'-C2'-C1'	3.73	106.60	100.98
41	X	503	GDP	O3B-PB-O3A	2.98	114.62	104.64

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	X	503	GDP	C5'-O5'-PA-O3A
41	X	503	GDP	C5'-O5'-PA-O1A
40	X	501	ATP	PA-O3A-PB-O1B
35	7	502	SAM	CB-CG-SD-C5'
35	7	502	SAM	O4'-C4'-C5'-SD

There are no ring outliers.

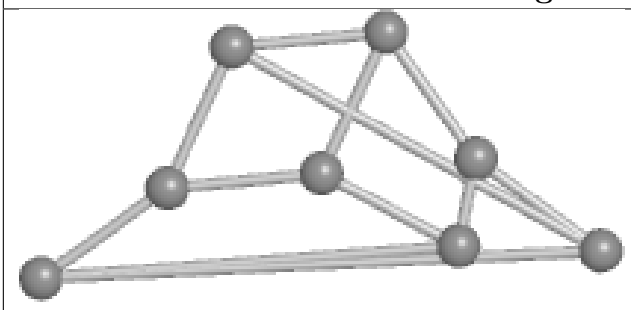
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	7	502	SAM	1	0
41	X	503	GDP	1	0

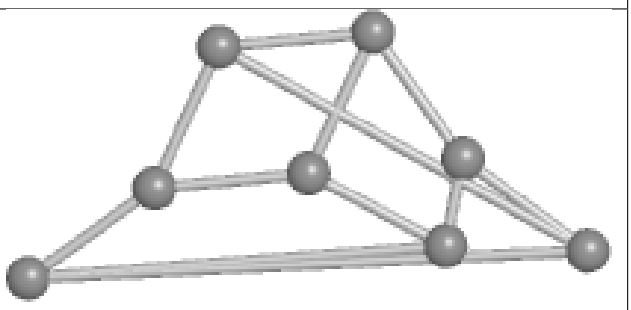
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

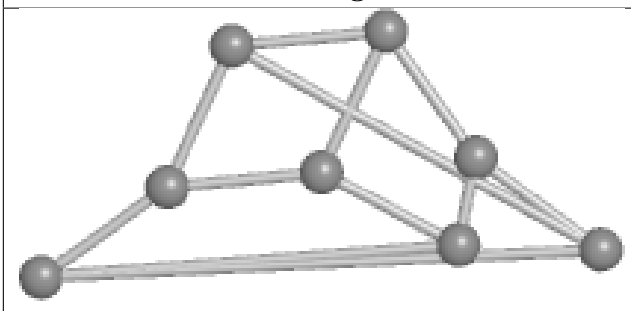
Ligand SF4 7 501



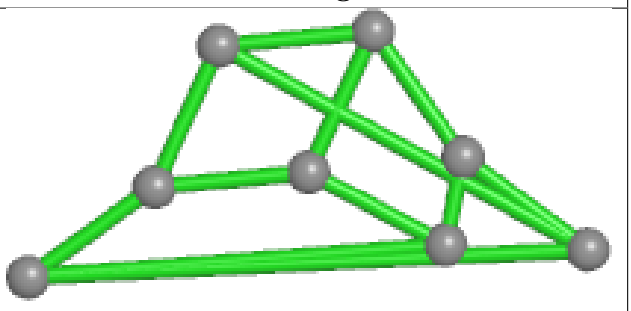
Bond lengths



Bond angles

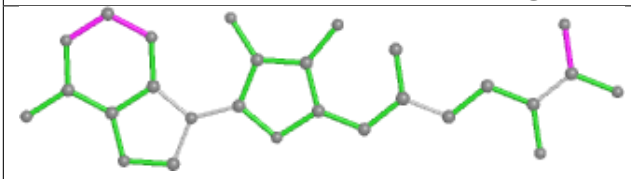


Torsions

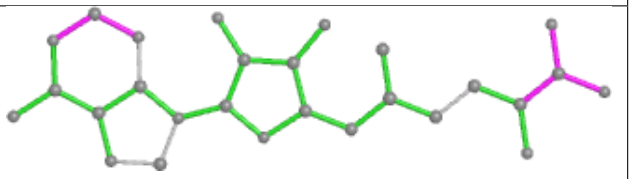


Rings

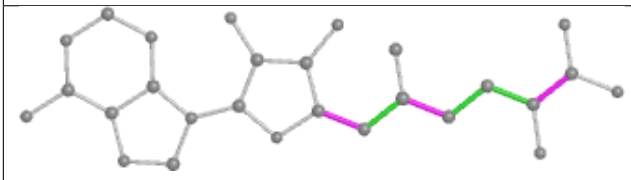
Ligand SAM 7 502



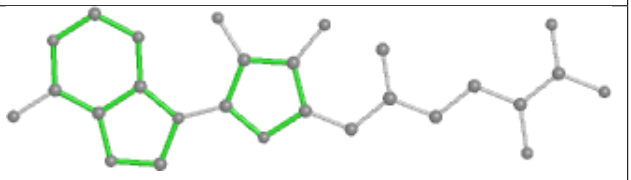
Bond lengths



Bond angles

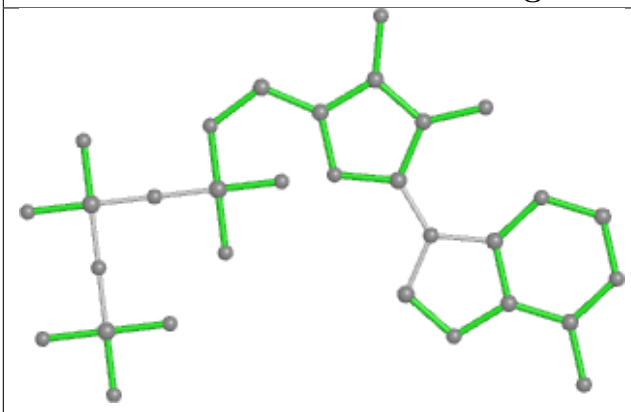


Torsions

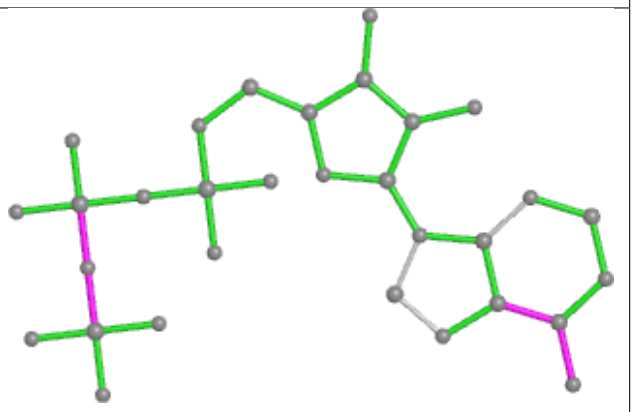


Rings

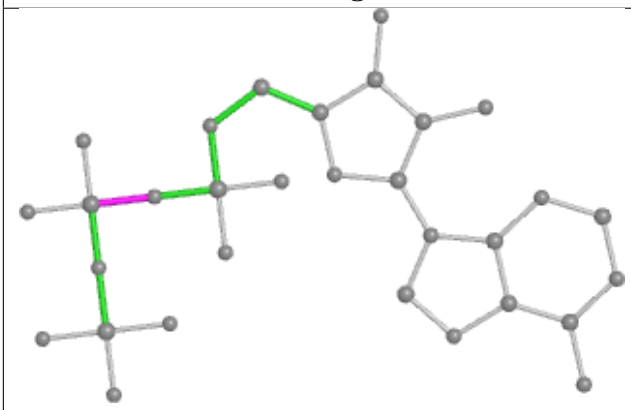
Ligand ATP X 501



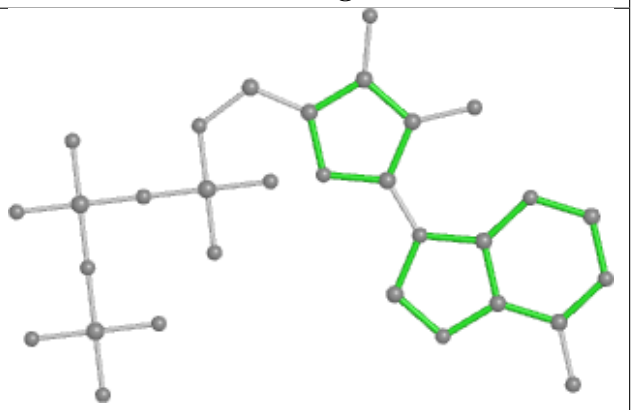
Bond lengths



Bond angles

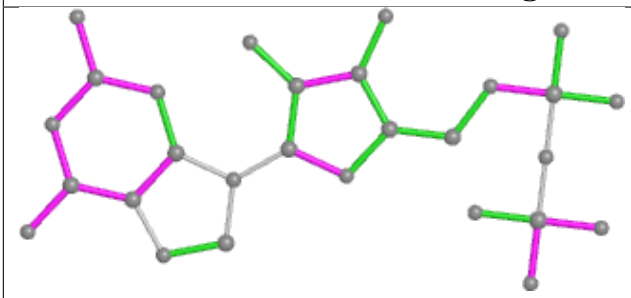


Torsions

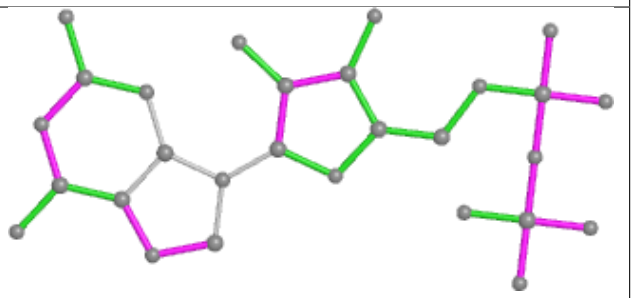


Rings

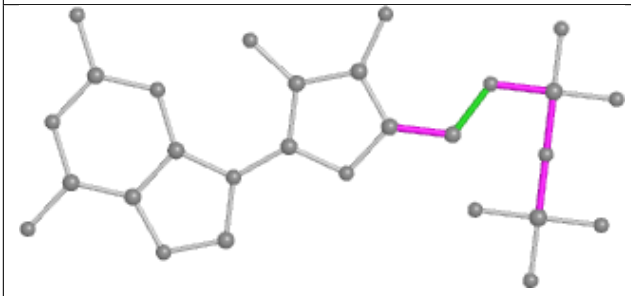
Ligand GDP X 503



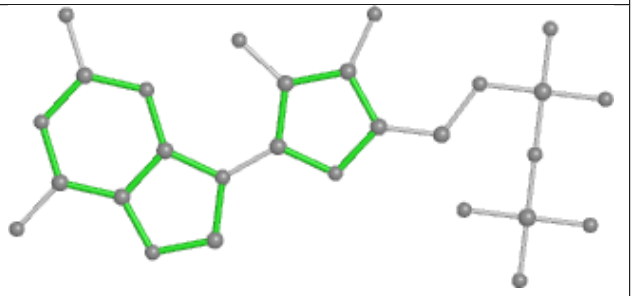
Bond lengths



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.

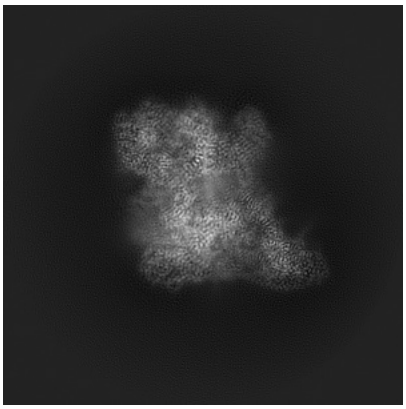
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26966. These allow visual inspection of the internal detail of the map and identification of artifacts.

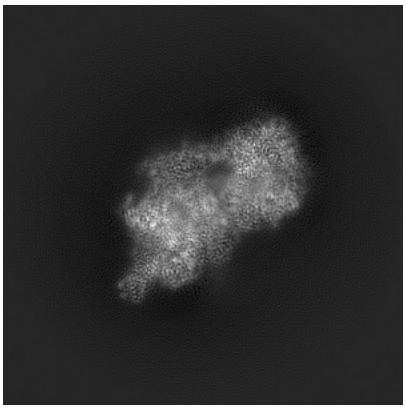
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

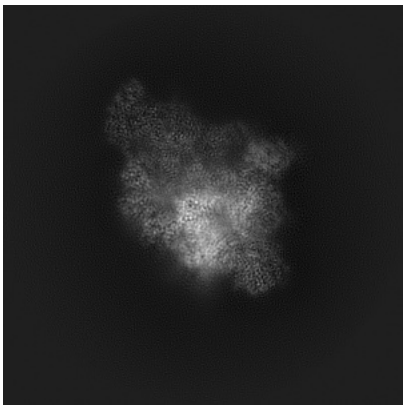
6.1.1 Primary map



X

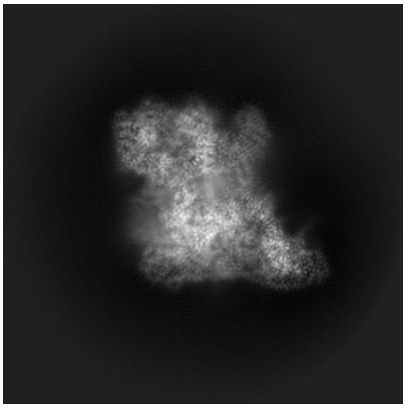


Y

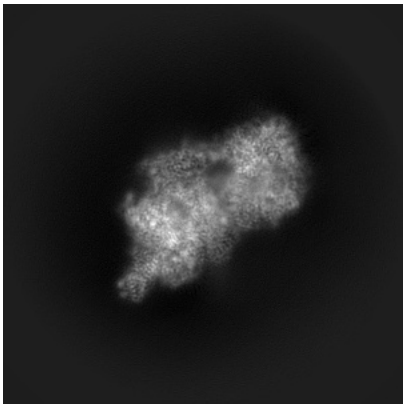


Z

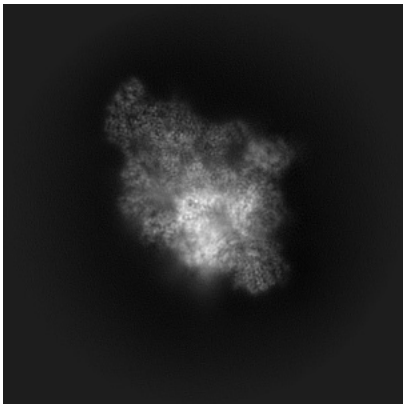
6.1.2 Raw map



X



Y

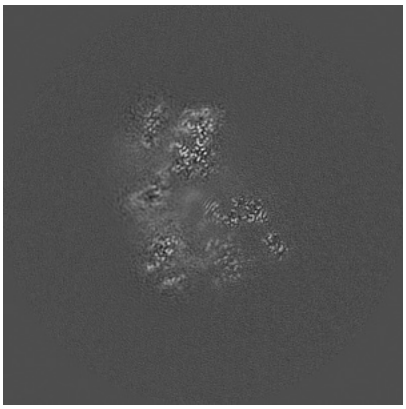


Z

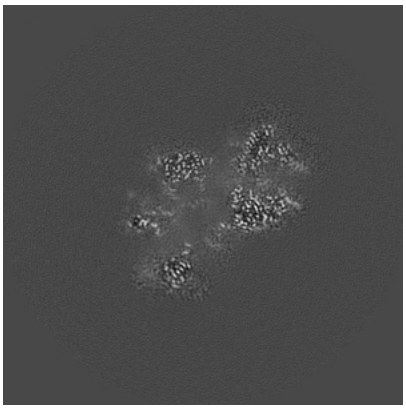
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

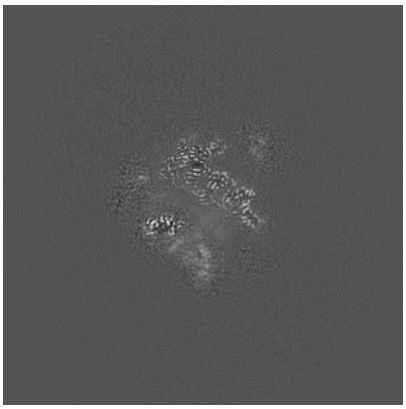
6.2.1 Primary map



X Index: 200

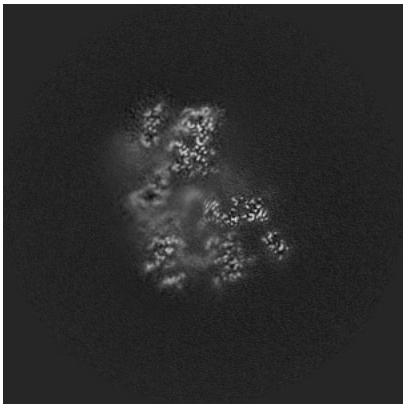


Y Index: 200

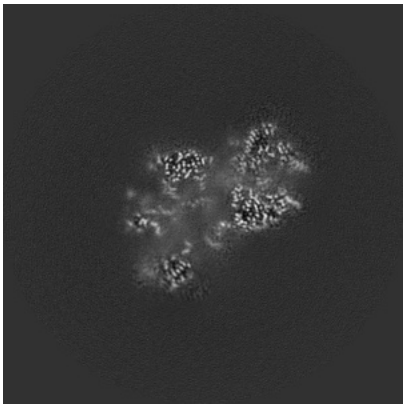


Z Index: 200

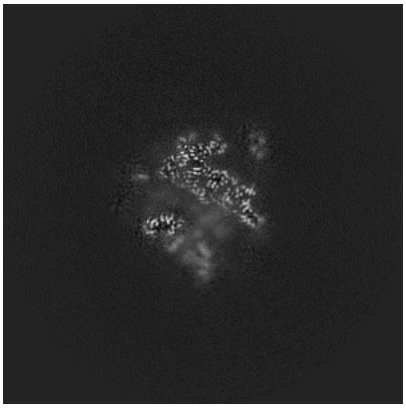
6.2.2 Raw map



X Index: 200



Y Index: 200

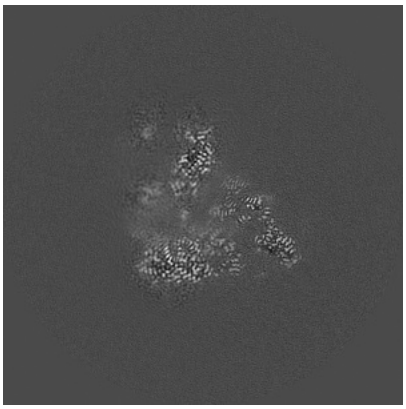


Z Index: 200

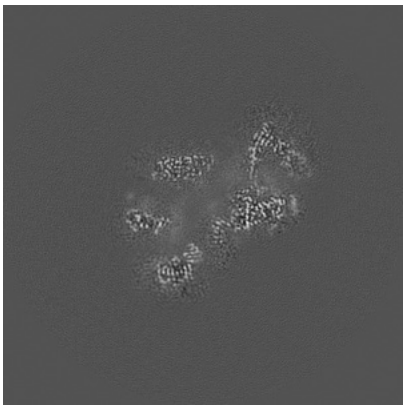
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

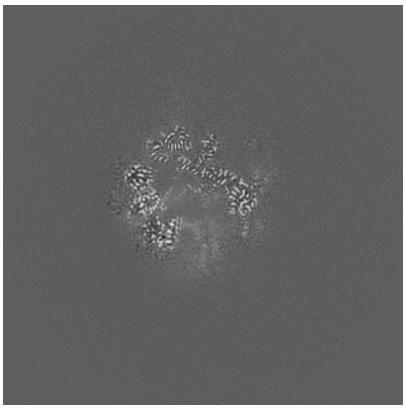
6.3.1 Primary map



X Index: 185

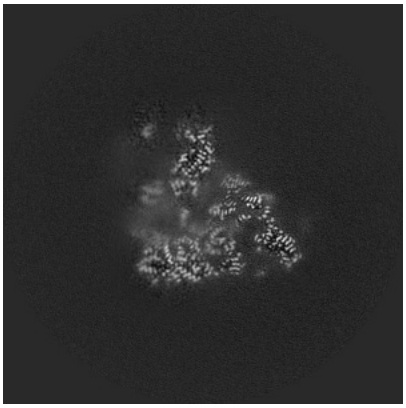


Y Index: 194

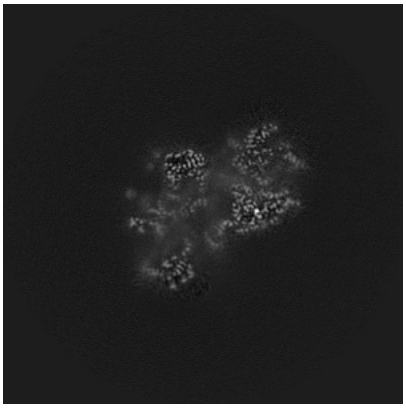


Z Index: 185

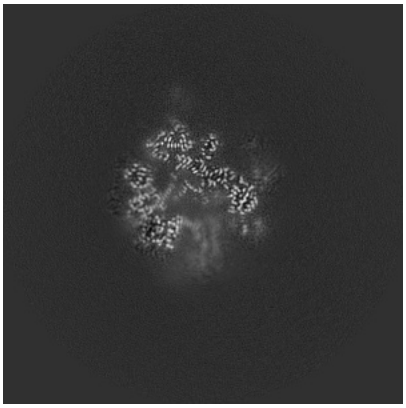
6.3.2 Raw map



X Index: 185



Y Index: 202

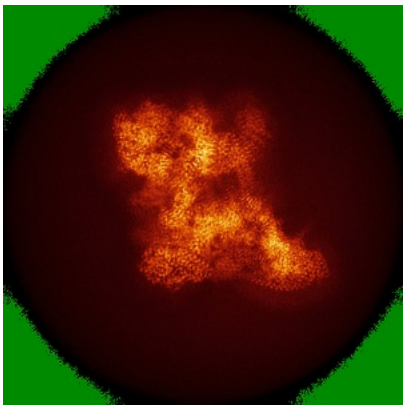


Z Index: 186

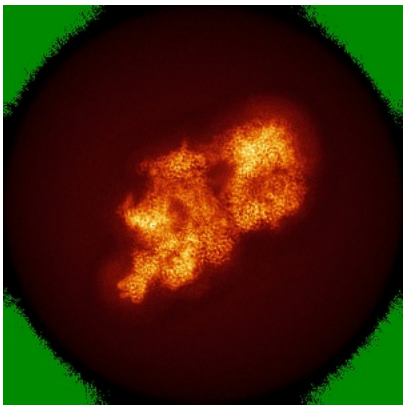
The images above show the largest variance slices of the map in three orthogonal directions.

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

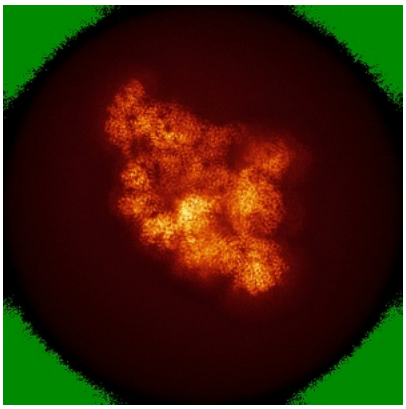
6.4.1 Primary map



X



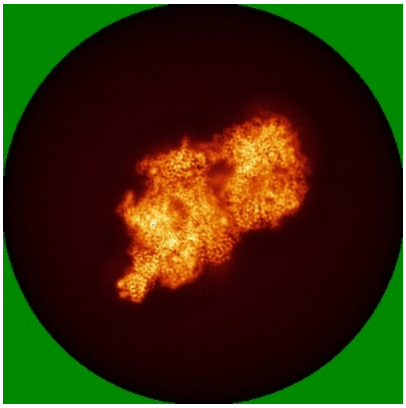
Y



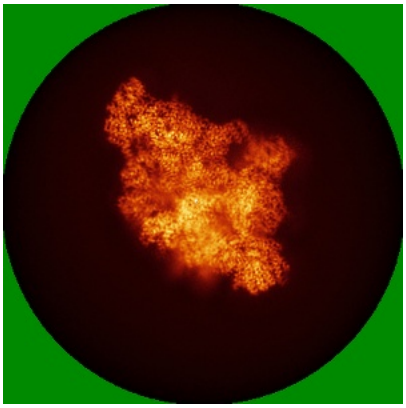
Z

6.4.2 Raw map

X



Y

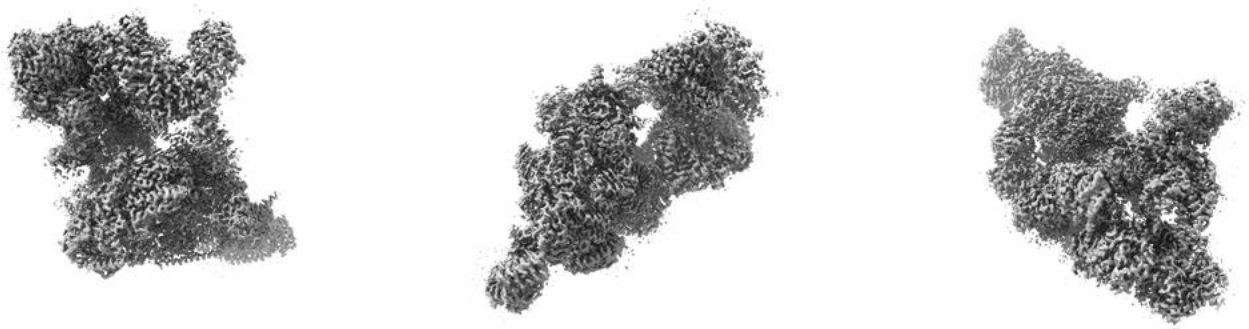


Z

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)

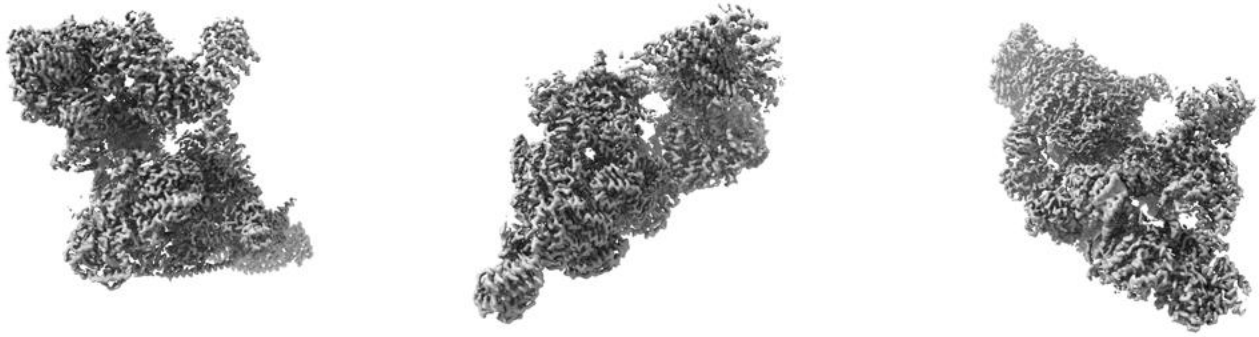
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 8.5. 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.

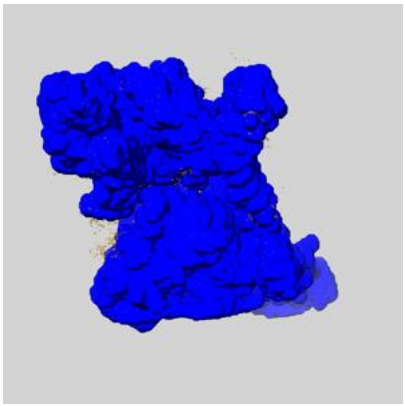
6.6 Mask visualisation (i)

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

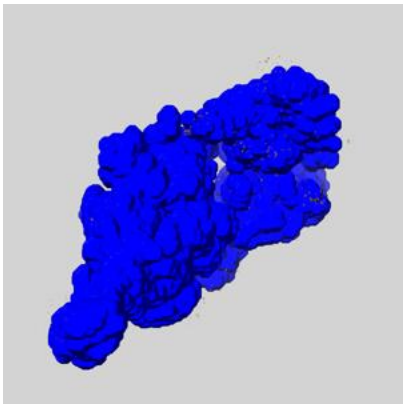
A mask typically either:

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

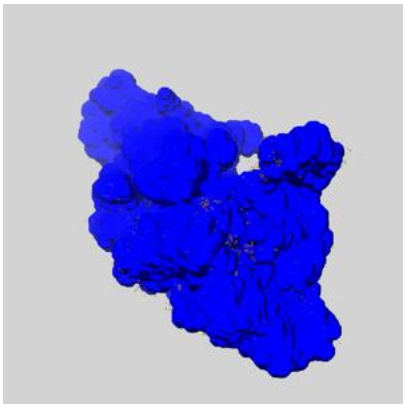
6.6.1 emd_26966_msk_1.map (i)



X



Y

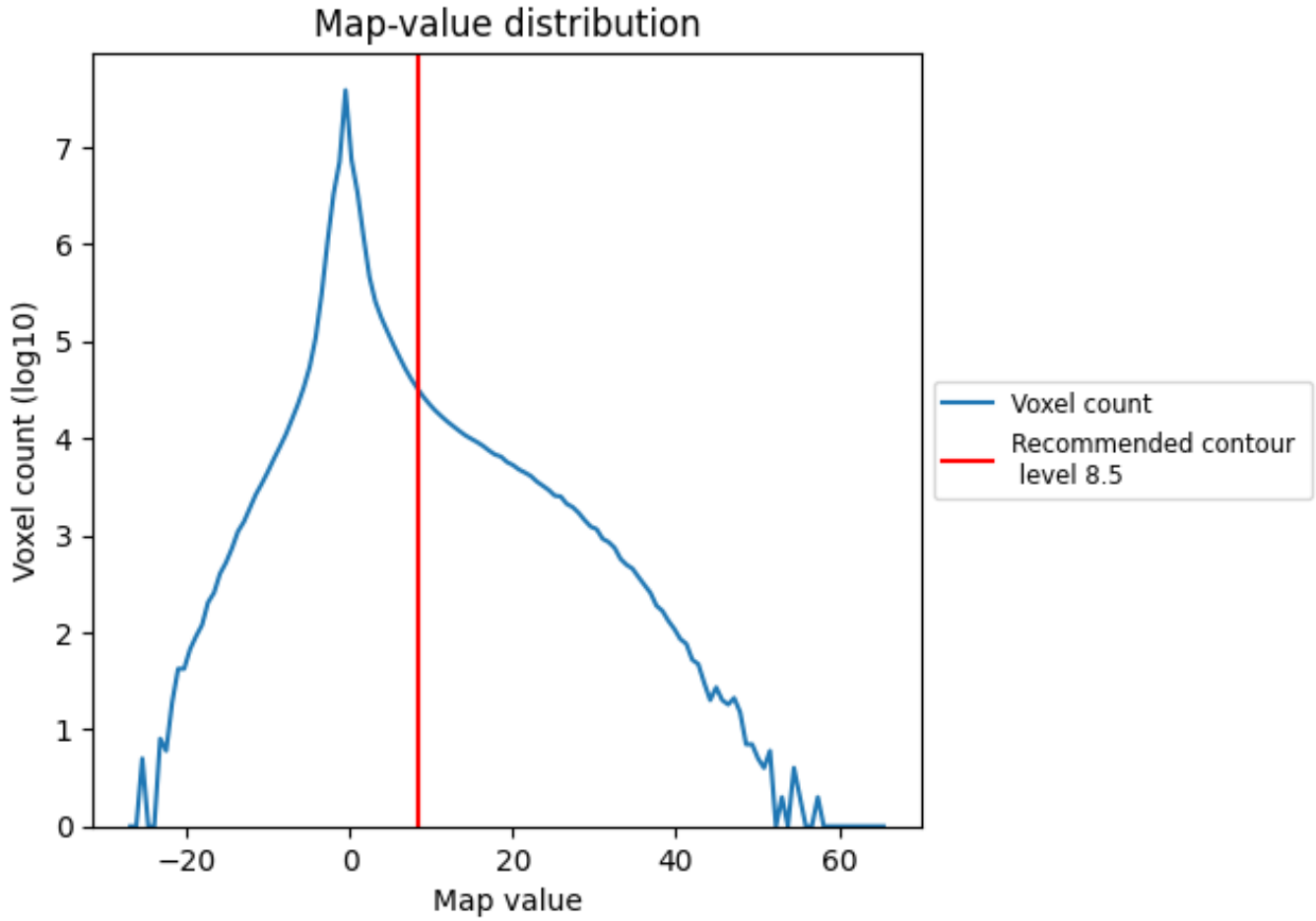


Z

7 Map analysis

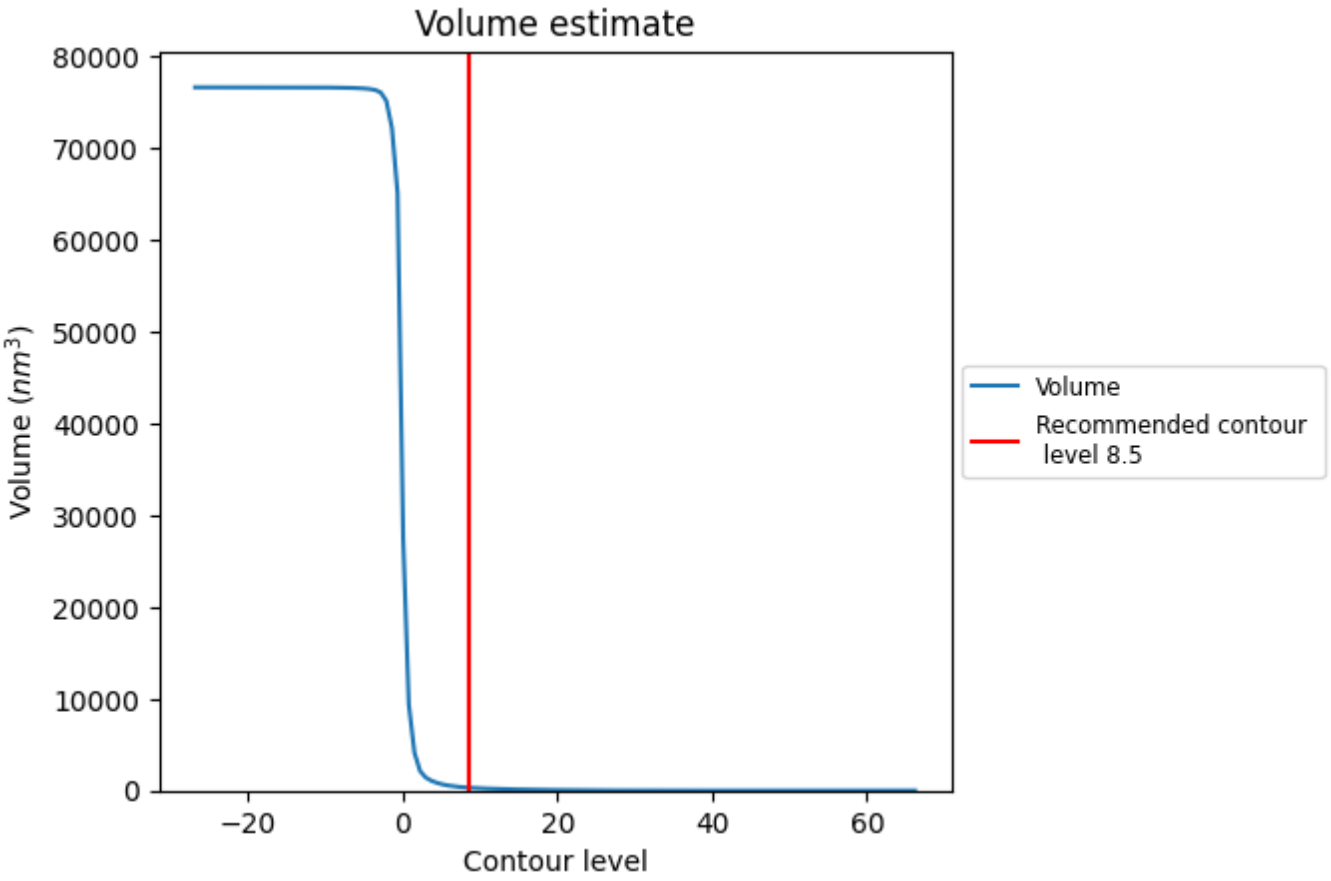
This section contains the results of statistical analysis of the map.

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.

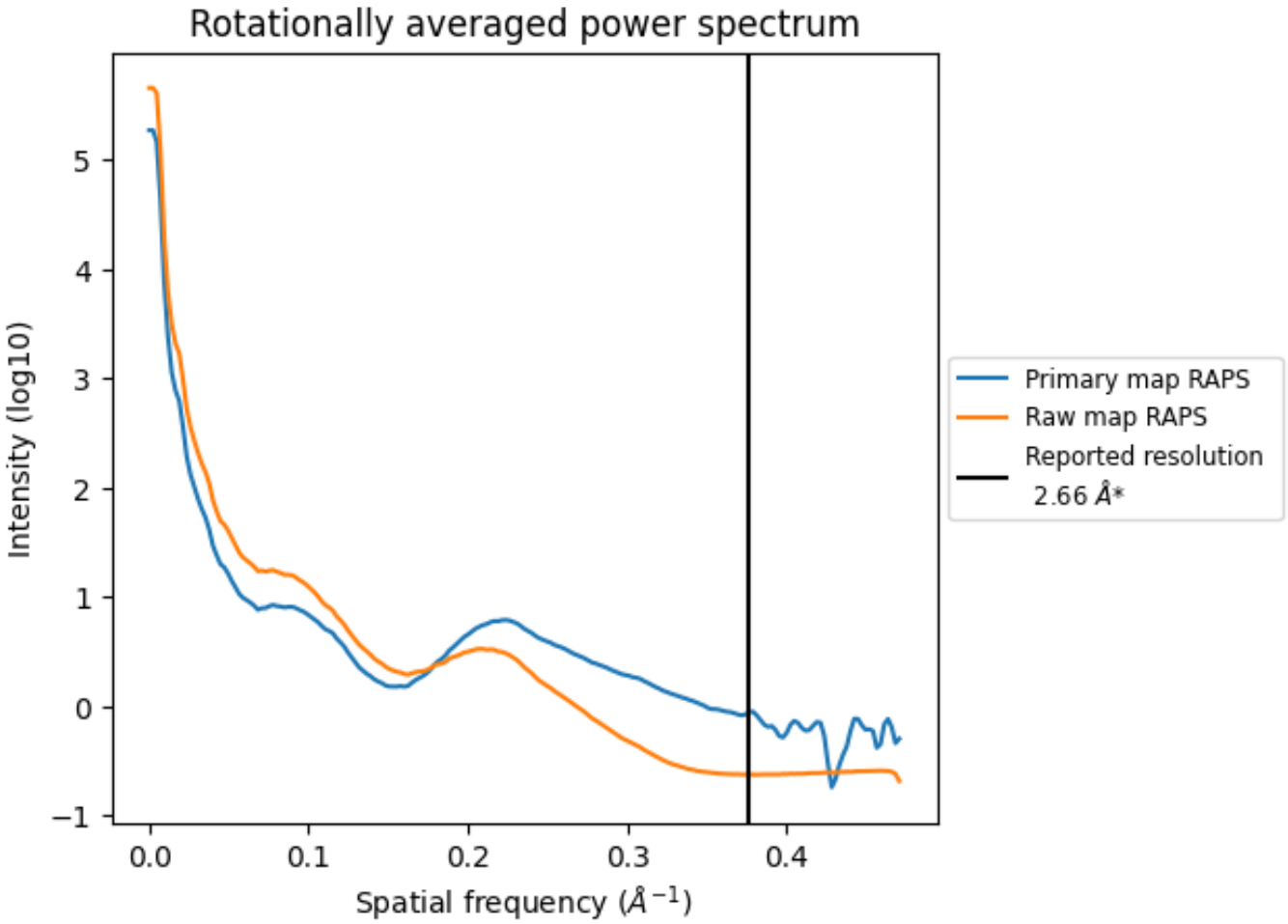
7.2 Volume estimate (i)



The volume at the recommended contour level is 315 nm^3; this corresponds to an approximate mass of 285 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)

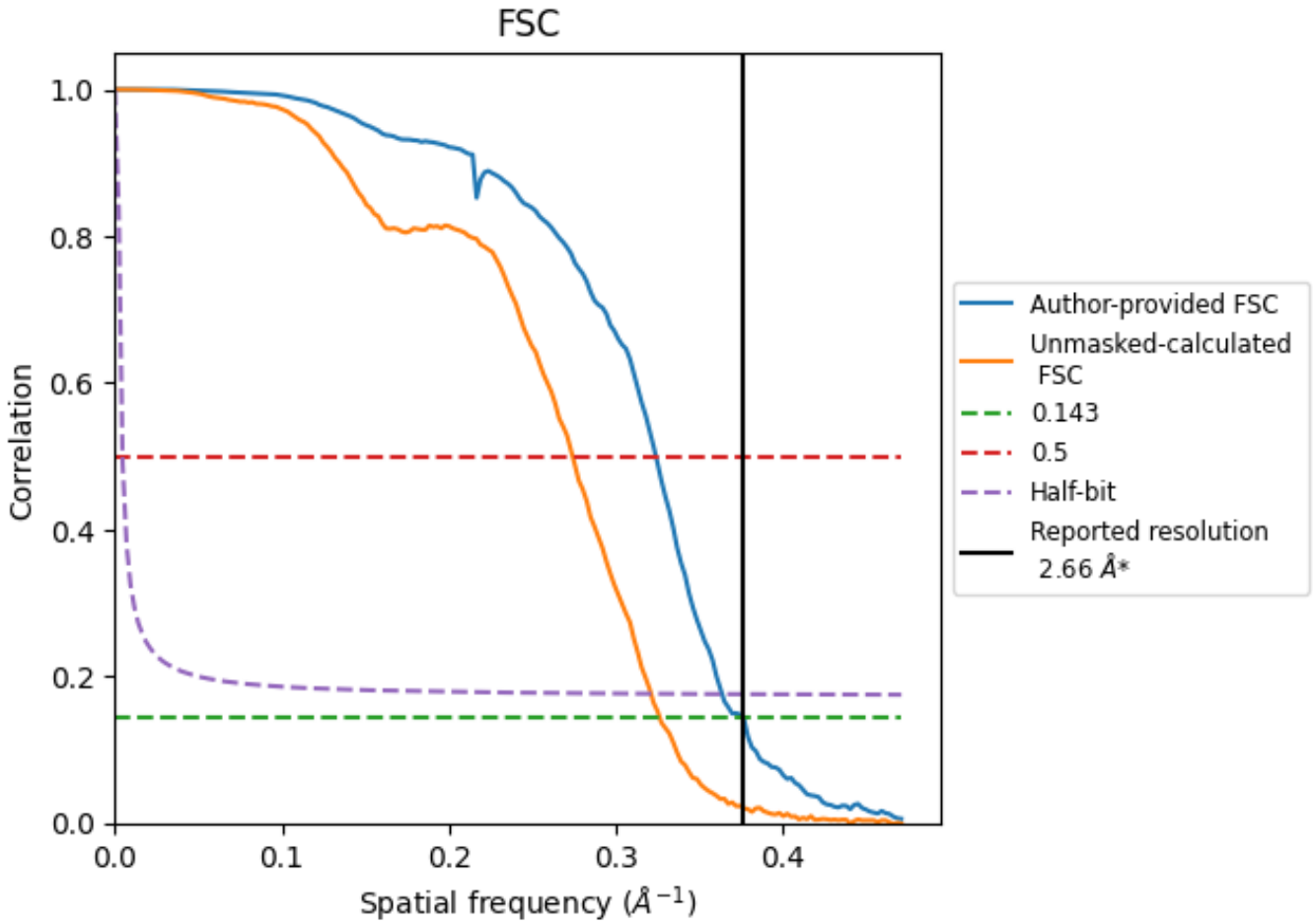


*Reported resolution corresponds to spatial frequency of 0.376 Å^{-1}

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 0.376 Å^{-1}

8.2 Resolution estimates (i)

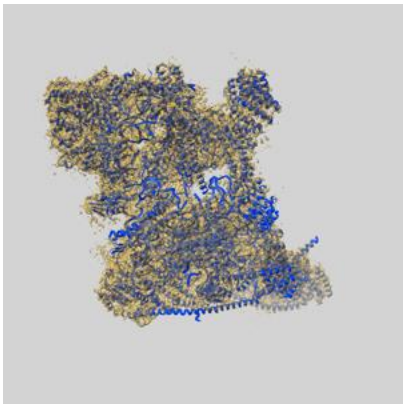
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	2.66	3.09	2.75
Unmasked-calculated*	3.07	3.65	3.12

*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 3.07 differs from the reported value 2.66 by more than 10 %

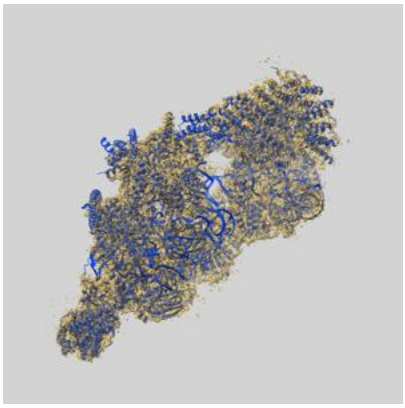
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26966 and PDB model 8CSP. Per-residue inclusion information can be found in section 3 on page 13.

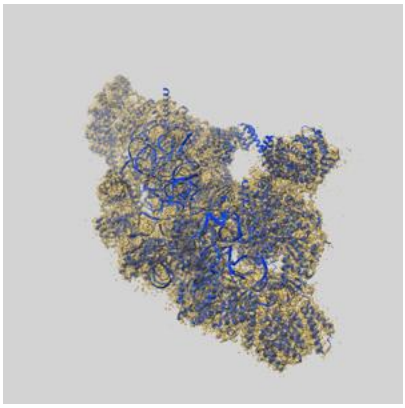
9.1 Map-model overlay



X



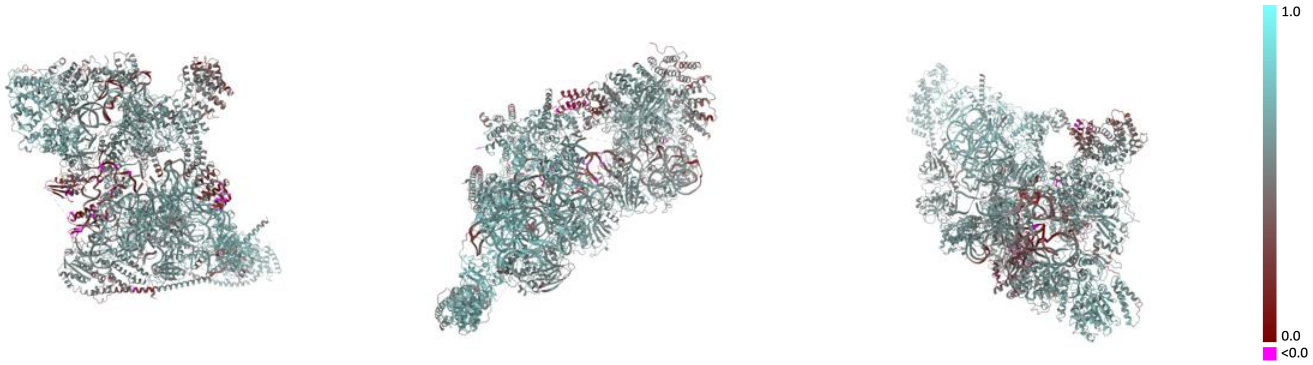
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 8.5 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.

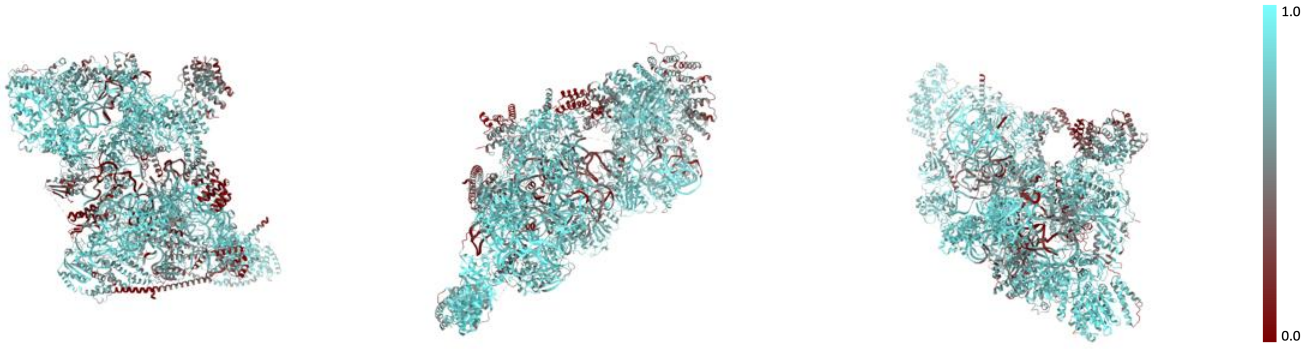
9.2 Q-score mapped to coordinate model (i)



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.

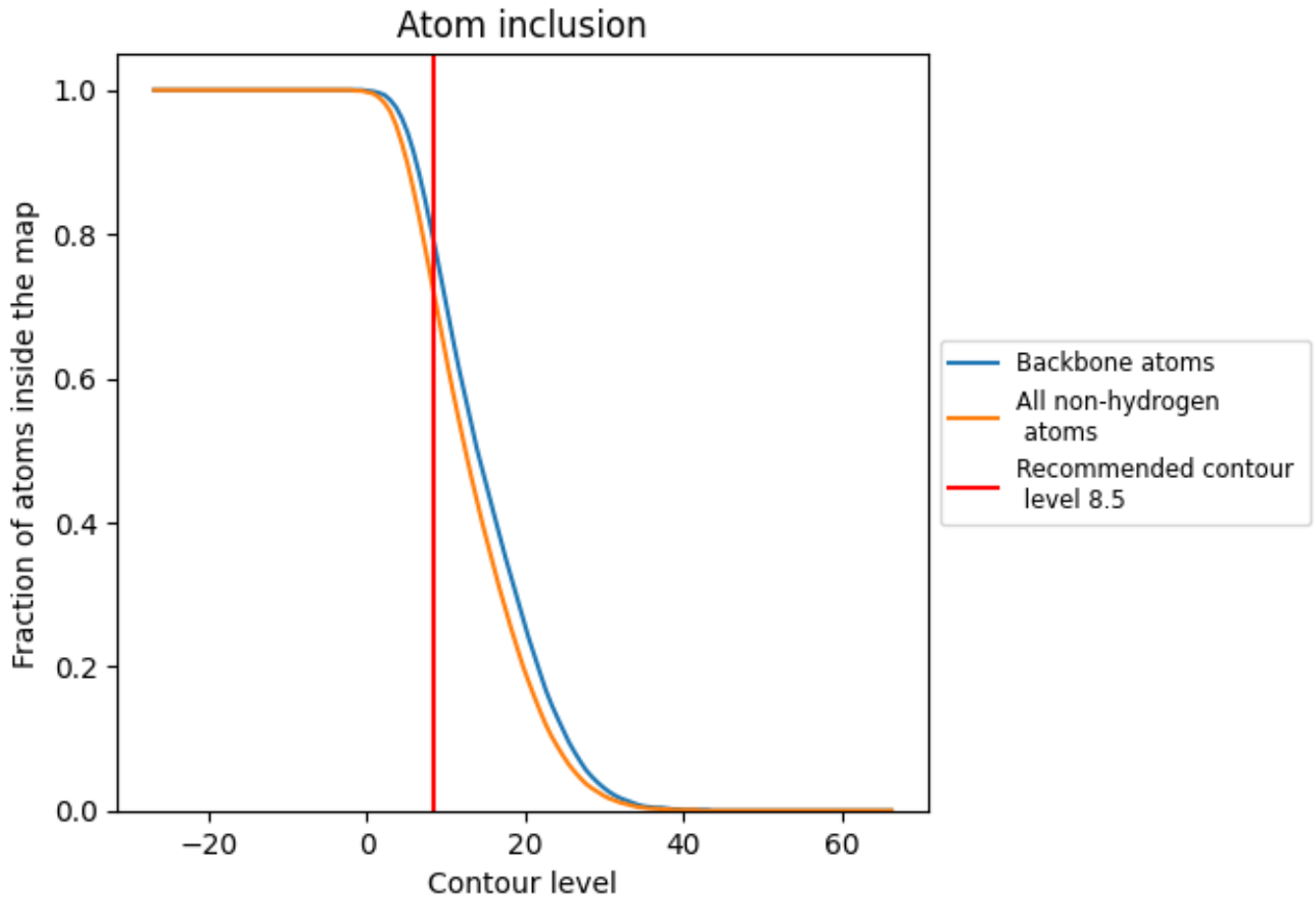
9.3 Atom inclusion mapped to coordinate model (i)



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 (8.5).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 71% 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 (8.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7140	0.5480
0	0.7930	0.6370
1	0.7310	0.5570
4	0.5240	0.4470
5	0.8610	0.5750
7	0.8520	0.5670
8	0.7250	0.5320
9	0.7320	0.5100
A	0.7140	0.5260
B	0.8760	0.6230
C	0.8070	0.5810
D	0.6980	0.6110
E	0.7980	0.5240
F	0.7780	0.5580
G	0.6860	0.5470
H	0.7530	0.5760
J	0.4840	0.5870
K	0.4960	0.4670
L	0.7660	0.5230
M	0.8680	0.6740
N	0.6130	0.6040
O	0.7640	0.6500
P	0.7470	0.5070
Q	0.1250	0.4210
R	0.6380	0.6180
S	0.6580	0.5420
T	0.6300	0.6060
U	0.5520	0.5220
V	0.8010	0.6160
W	0.7320	0.5690
X	0.8690	0.6220
Y	0.6530	0.5240
Z	0.4890	0.4550
a	0.3870	0.2740