wwPDB EM Validation Summary Report ⓘ

Dec 22, 2022 – 04:53 AM EST

PDB ID	:	8CSS
EMDB ID	:	EMD-26969
Title	:	Human mitochondrial small subunit assembly intermediate (State D)
Authors	:	Harper, N.J.; Burnside, C.; Klinge, S.
Deposited on	:	2022-05-13
Resolution	:	2.36 Å(reported)
Based on initial models	:	6AAX, 6RW4, 2C2N

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

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

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

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

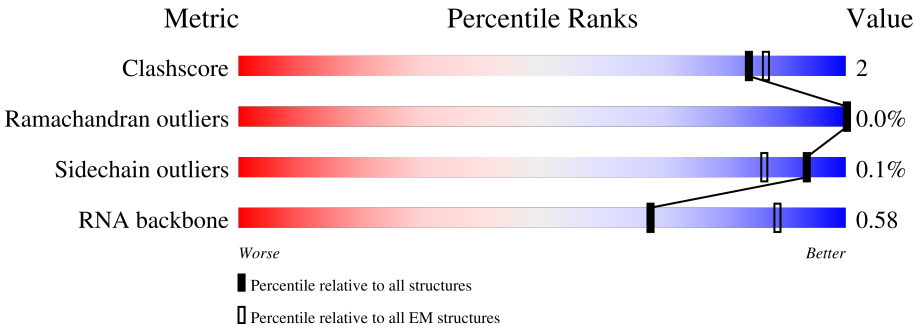
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.36 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	19% 91% 6%
2	1	323	20% 76% 20%
3	3	199	8% 34% 65%
4	4	689	44% 70% 12% 18%
5	6	343	36% 63%
6	7	456	6% 82% 6% 12%
7	8	390	80% 16%

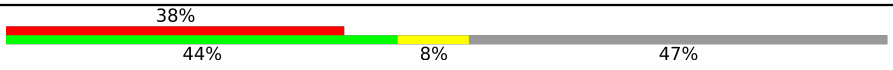
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	A	955	13% 64% 22% 11%
9	B	296	9% 72% 26%
10	C	167	14% 64% 11% 25%
11	D	430	10% 52% 46%
12	E	125	25% 80% 6% 14%
13	F	242	12% 81% 5% 15%
14	G	396	17% 67% 6% 26%
15	H	201	10% 57% 7% 35%
16	I	194	68% 29%
17	J	138	14% 75% 22%
18	K	128	21% 25% 5% 70%
19	L	257	14% 59% 37%
20	M	137	9% 82% 16%
21	N	130	8% 81% 16%
22	O	258	14% 72% 26%
23	P	142	13% 62% 6% 32%
24	Q	87	5% 92% 7%
25	R	360	29% 76% 19%
26	S	190	34% 65% 5% 30%
27	T	173	14% 92% 5%
28	U	205	44% 82% 15%
29	V	414	5% 85% 13%
30	W	187	16% 50% 48%
31	X	398	83% 5% 12%
32	Y	395	11% 26% 5% 69%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	Z	106	

2 Entry composition (i)

There are 43 unique types of molecules in this entry. The entry contains 67466 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	259	2098	1333	353	402	10	0	0

- Molecule 3 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	70	625	401	134	89	1	0	0

- Molecule 4 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

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

- Molecule 5 is a protein called Putative ribosome-binding factor A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	6	126	994	630	177	182	5	0	0

- Molecule 6 is a protein called Methyltransferase-like protein 17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	7	400	3160	2017	581	546	16	0	0

- Molecule 7 is a protein called Malonyl-CoA-acyl carrier protein transacylase, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	326	Total	C	N	O	S	0	0
			2543	1617	463	446	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	846	Total	C	N	O	P	0	0
			17959	8056	3227	5830	846		

- 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	108	Total	C	N	O	S	0	0
			858	539	157	158	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	206	Total	C	N	O	S	0	0
			1696	1082	308	295	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	130	Total	C	N	O	S	0	0
			1064	687	177	197	3		

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	K	38	Total	C	N	O	0	0
			323	199	74	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	161	Total	C	N	O	S	0	0
			1363	869	253	234	7		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	96	Total	C	N	O	S	0	0
			774	498	133	135	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	86	Total	C	N	O	S	0	0
			744	460	150	126	8		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 25 is a protein called 28S ribosomal protein S22, mitochondrial.

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

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

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

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

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

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

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

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

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

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

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

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

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

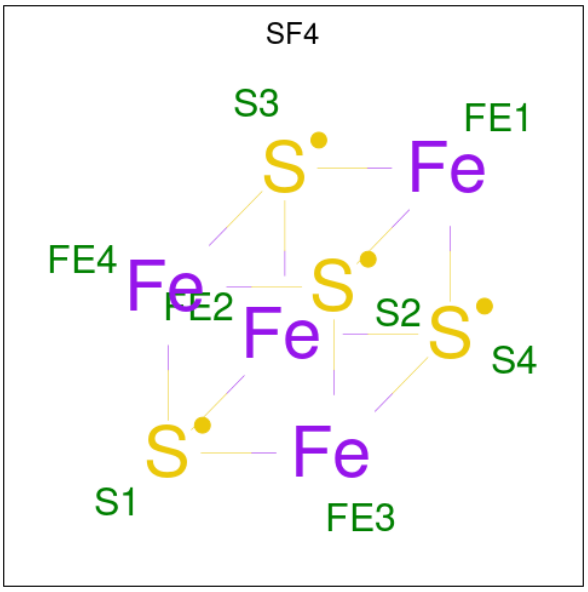
- Molecule 32 is a protein called 28S ribosomal protein S31, mitochondrial.

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

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

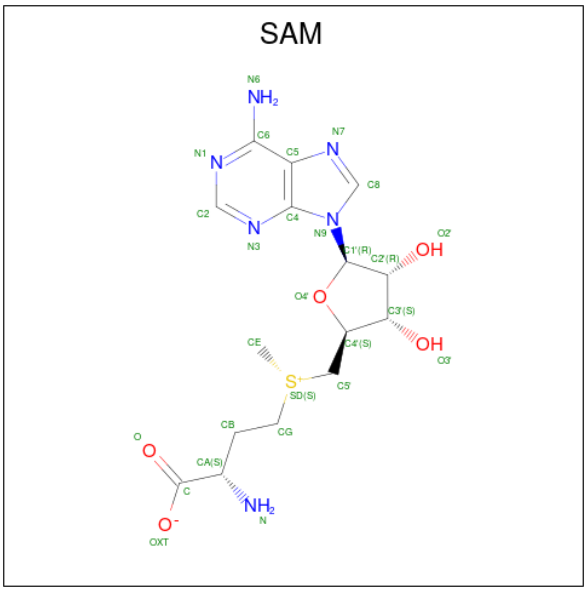
Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	56	Total	C	N	O	S	0	0
			465	298	84	80	3		

- 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	

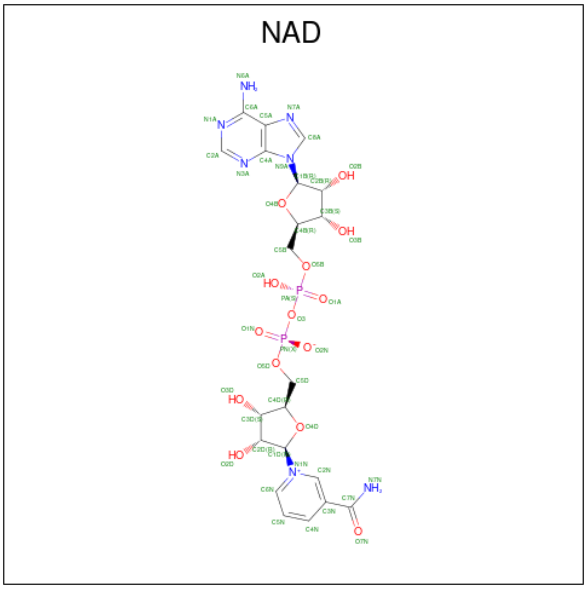
- Molecule 36 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
36	A	7	Total K 7 7	0

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

Mol	Chain	Residues	Atoms	AltConf
37	A	30	Total Mg 30 30	0
37	B	1	Total Mg 1 1	0
37	X	1	Total Mg 1 1	0

- Molecule 38 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).

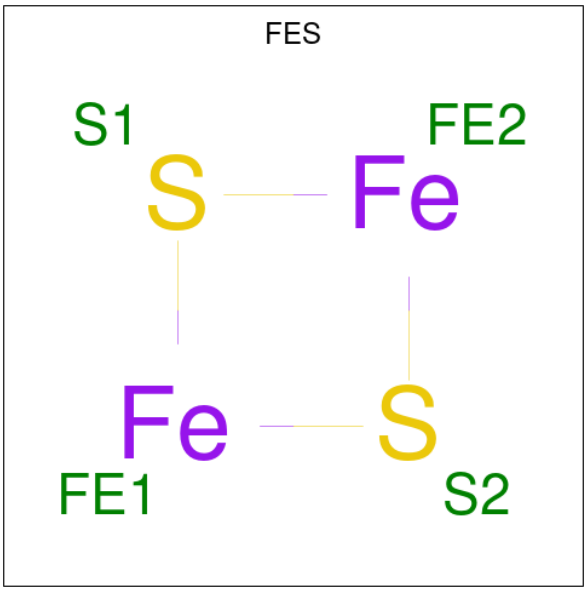


Mol	Chain	Residues	Atoms	AltConf
38	A	1	Total C N O P 44 21 7 14 2	0

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

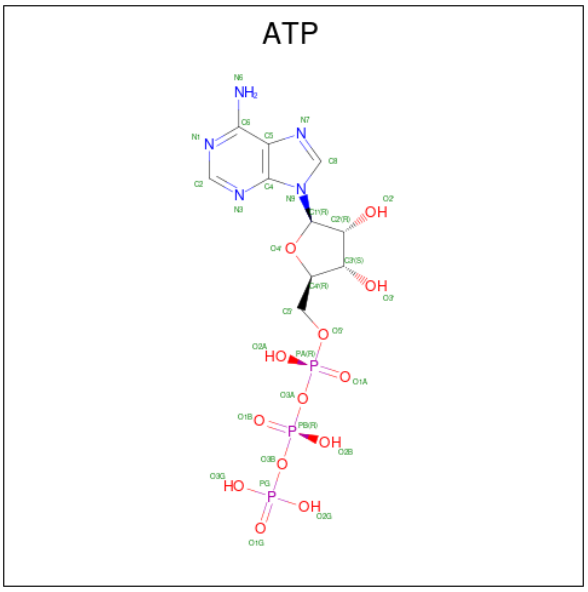
Mol	Chain	Residues	Atoms	AltConf
39	O	1	Total Zn 1 1	0

- Molecule 40 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



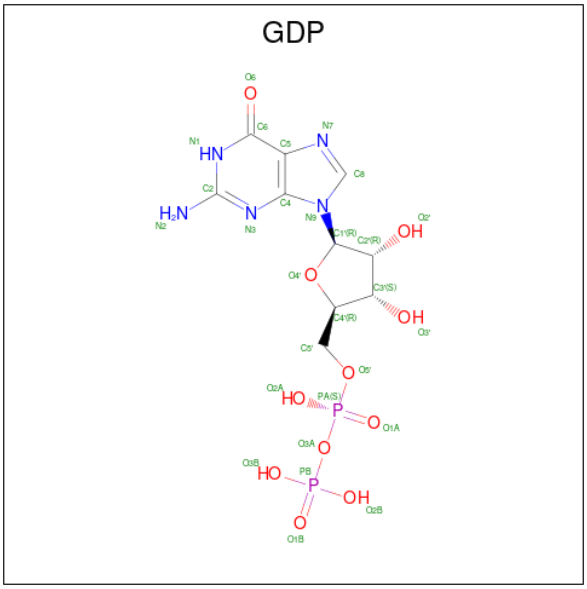
Mol	Chain	Residues	Atoms			AltConf
40	P	1	Total	Fe	S	0
			4	2	2	
40	T	1	Total	Fe	S	0
			4	2	2	

- Molecule 41 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 42 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 43 is water.

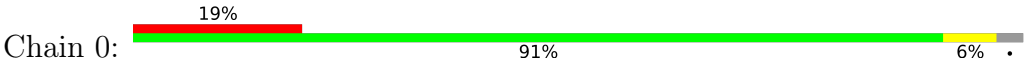
Mol	Chain	Residues	Atoms		AltConf
43	3	1	Total	O	0
			1	1	
43	A	100	Total	O	0
			100	100	
43	M	1	Total	O	0
			1	1	
43	X	2	Total	O	0
			2	2	

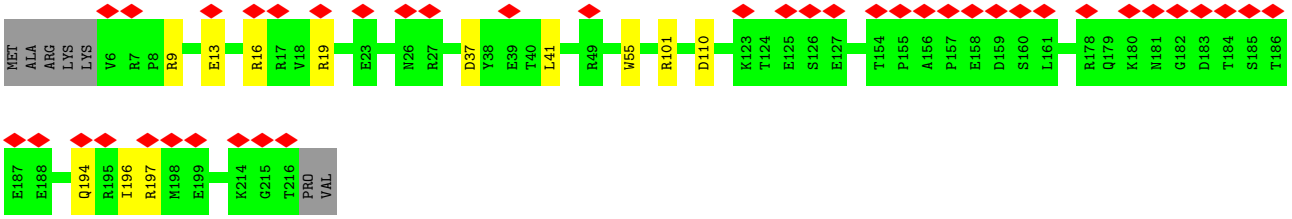
3 Residue-property plots (i)

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

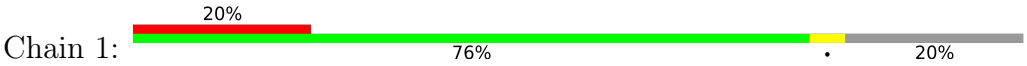
Chain 0:

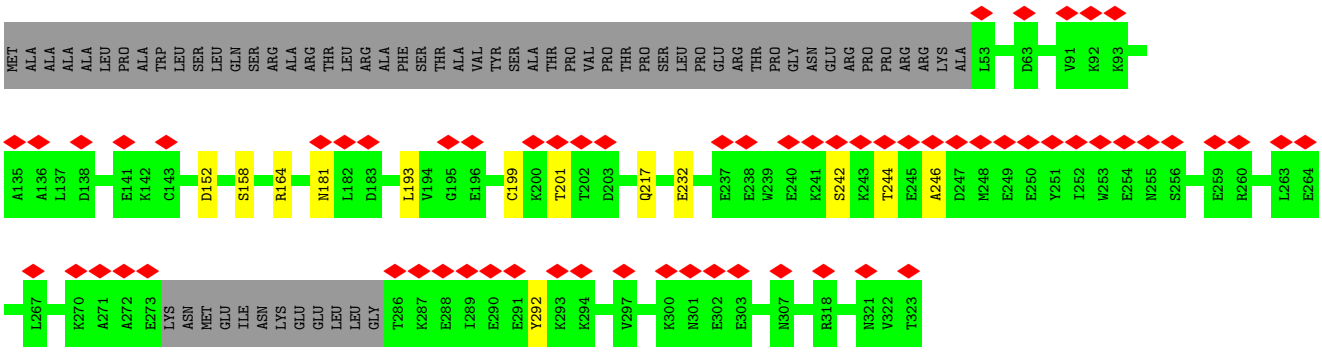




• Molecule 2: 28S ribosomal protein S35, mitochondrial

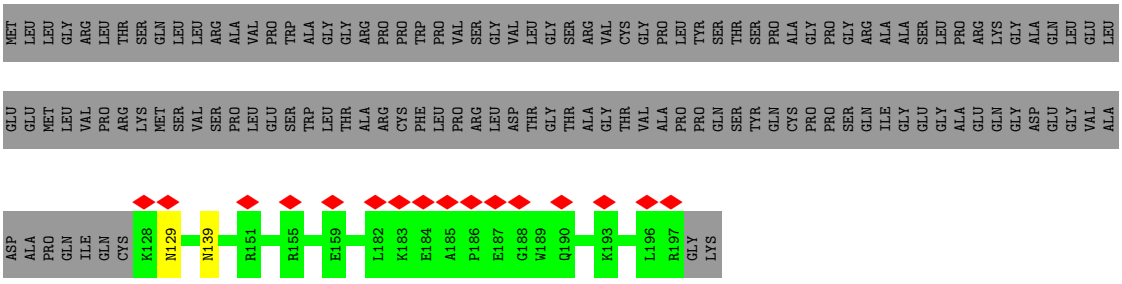
Chain 1:





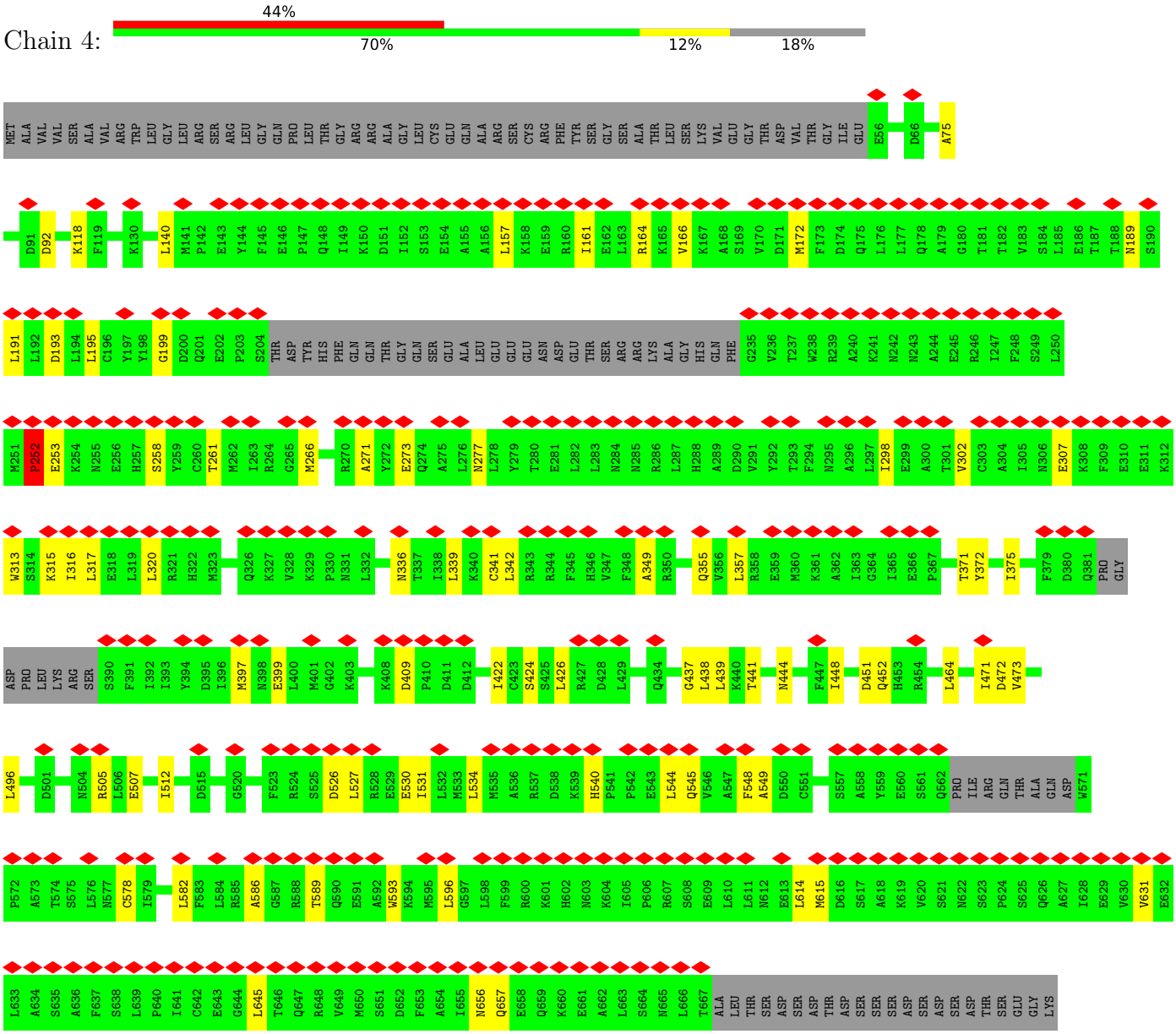
• Molecule 3: Aurora kinase A-interacting protein

Chain 3:



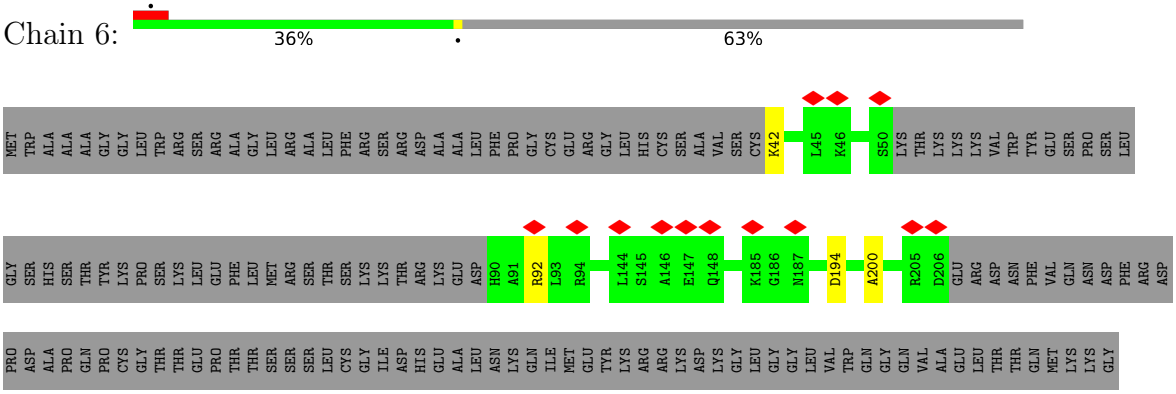
• Molecule 4: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

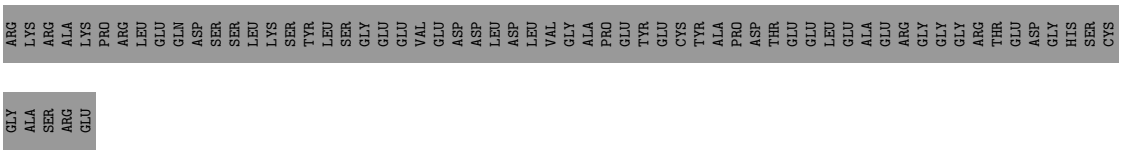
Chain 4:



• Molecule 5: Putative ribosome-binding factor A, mitochondrial

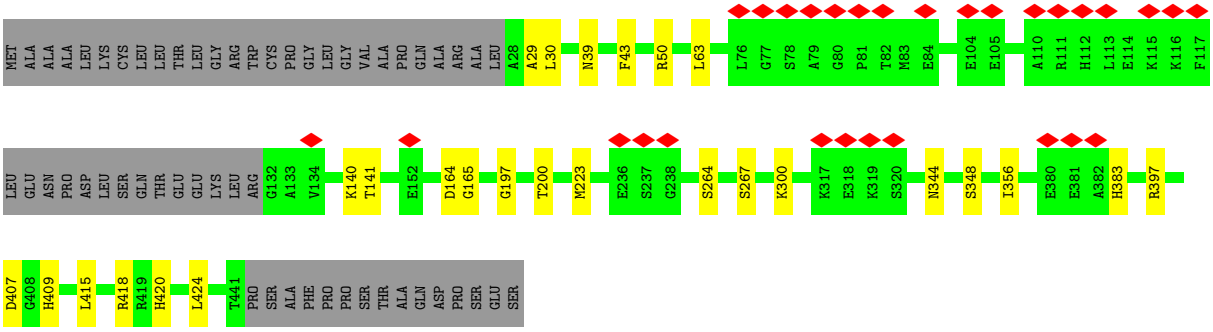
Chain 6:





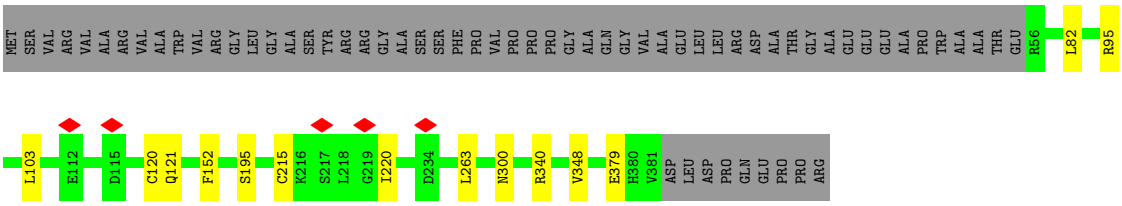
• Molecule 6: Methyltransferase-like protein 17, mitochondrial

Chain 7:



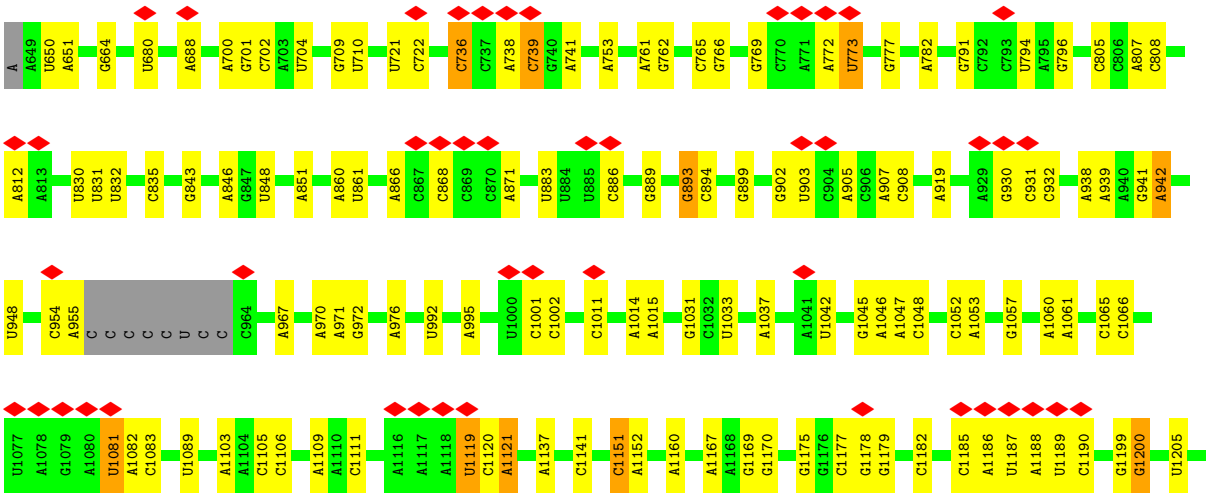
• Molecule 7: Malonyl-CoA-acyl carrier protein transacylase, mitochondrial

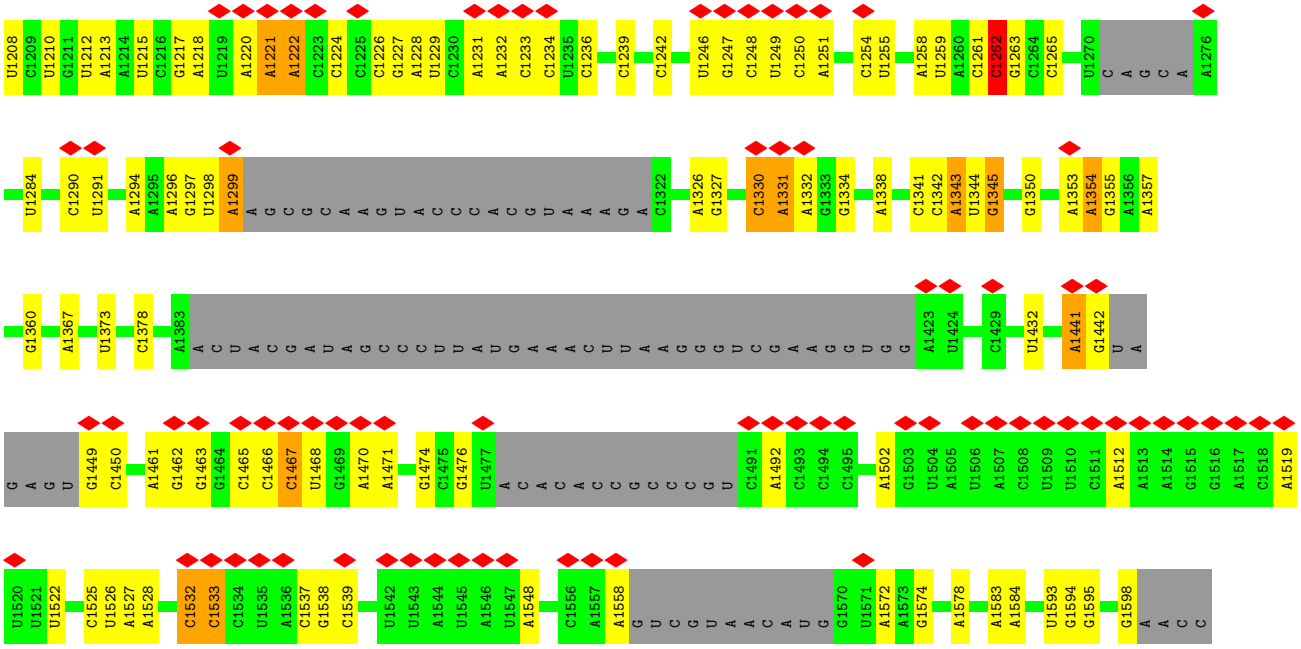
Chain 8:



• Molecule 8: 12S mitochondrial rRNA

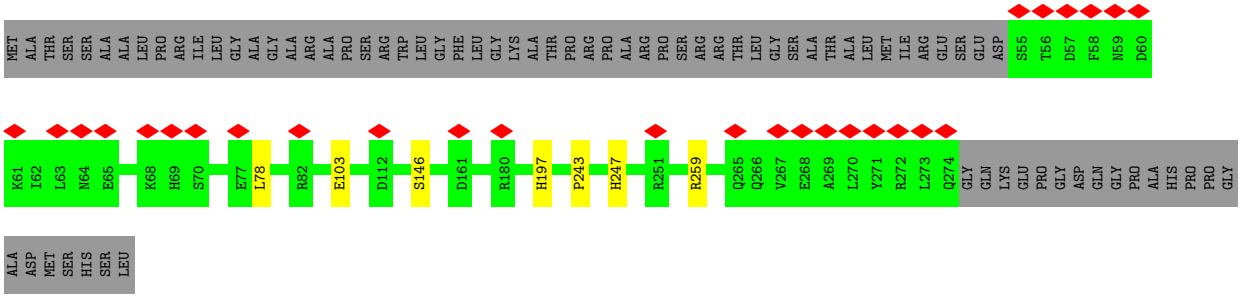
Chain A:





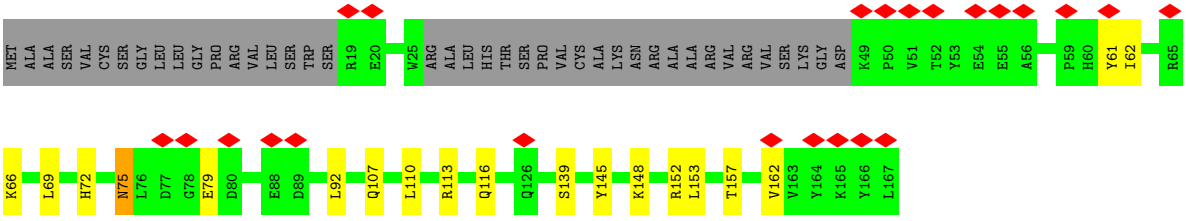
• Molecule 9: 28S ribosomal protein S2, mitochondrial

Chain B:



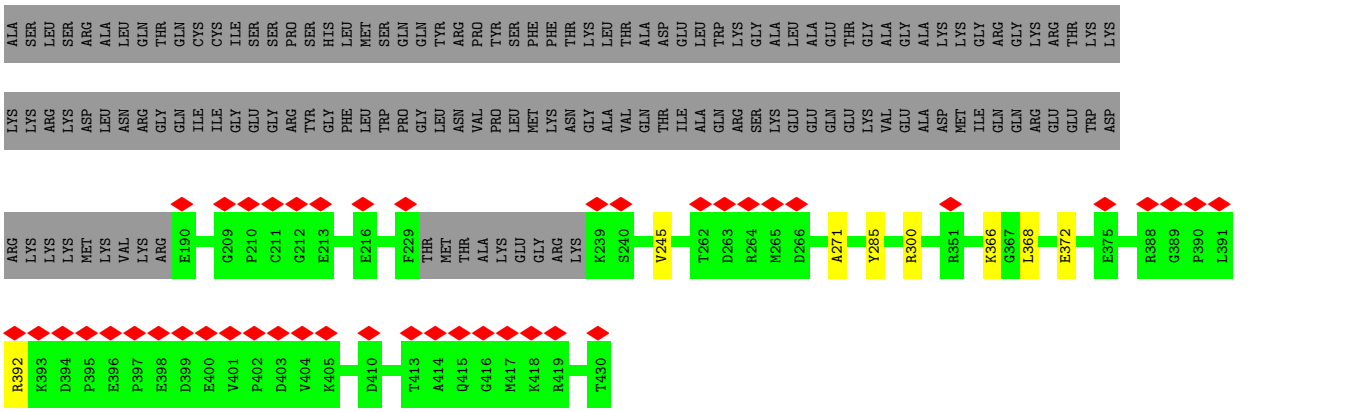
• Molecule 10: 28S ribosomal protein S24, mitochondrial

Chain C:



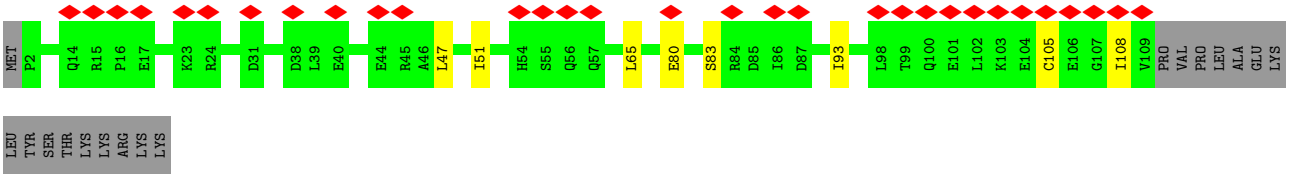
• Molecule 11: 28S ribosomal protein S5, mitochondrial

Chain D:



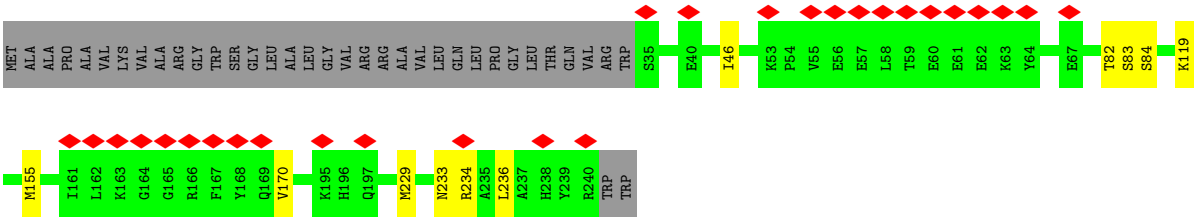
• Molecule 12: 28S ribosomal protein S6, mitochondrial

Chain E:



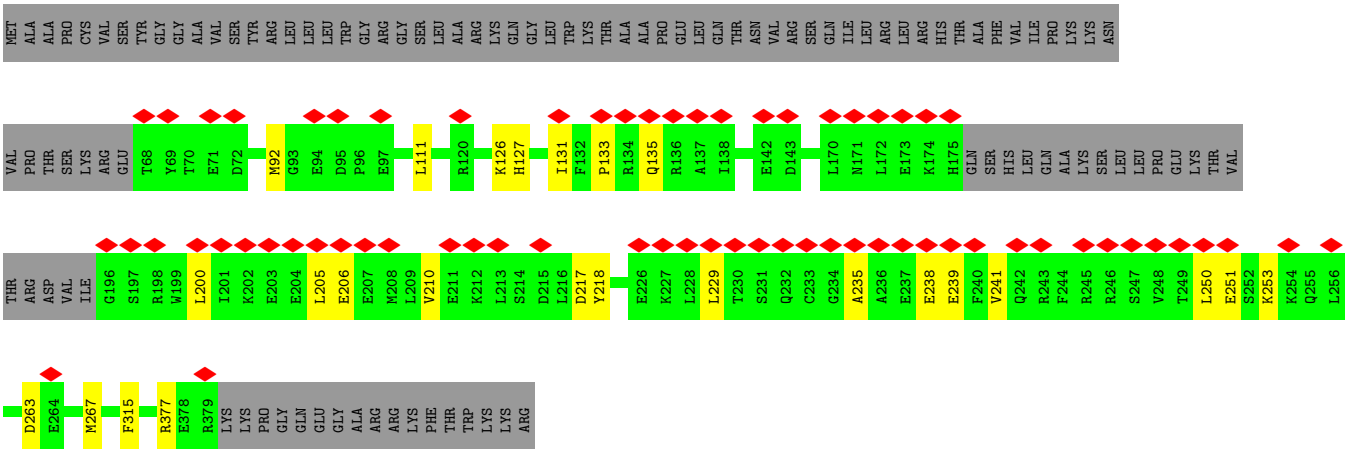
• Molecule 13: 28S ribosomal protein S7, mitochondrial

Chain F:



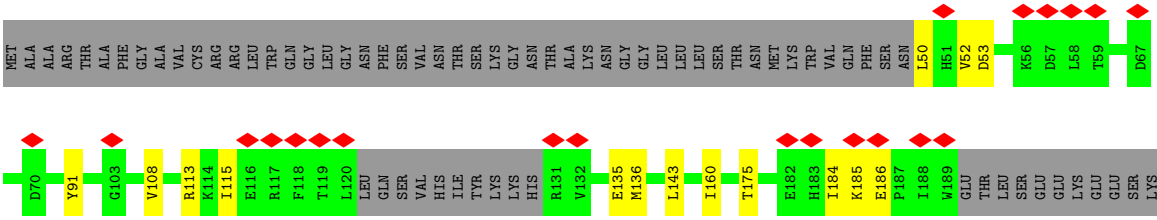
• Molecule 14: 28S ribosomal protein S9, mitochondrial

Chain G:



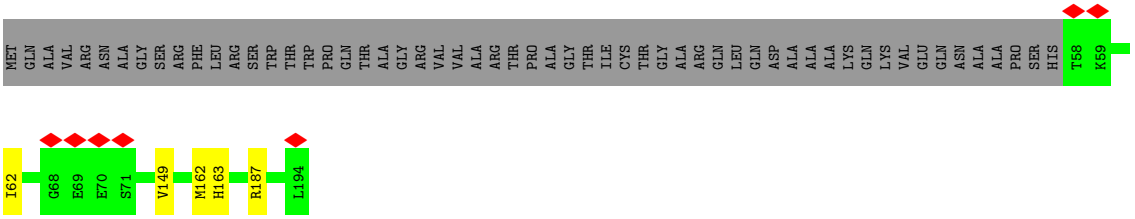
• Molecule 15: 28S ribosomal protein S10, mitochondrial

Chain H:



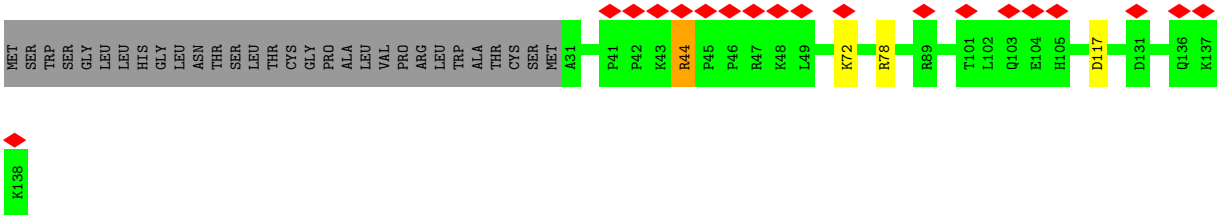
• Molecule 16: 28S ribosomal protein S11, mitochondrial

Chain I:



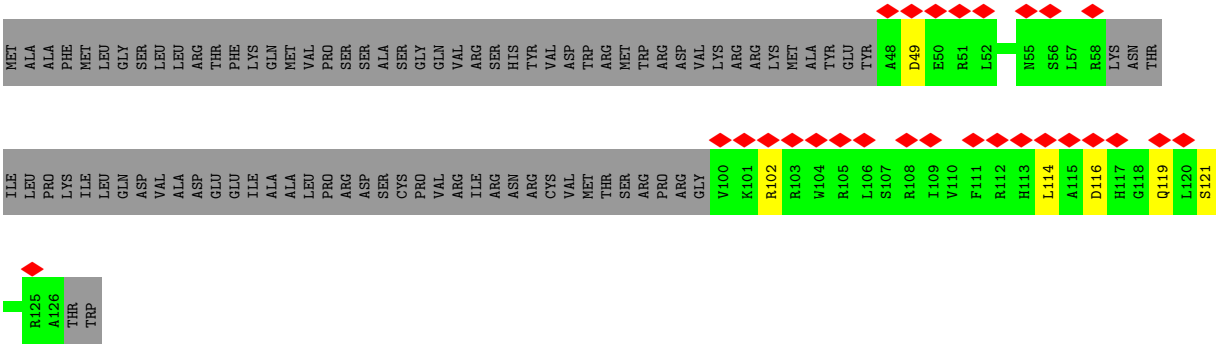
• Molecule 17: 28S ribosomal protein S12, mitochondrial

Chain J:



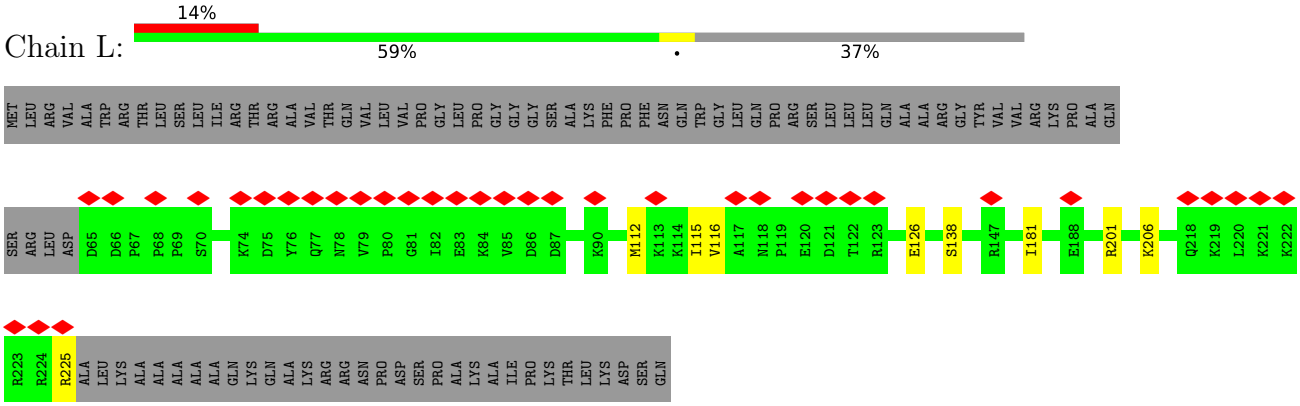
• Molecule 18: 28S ribosomal protein S14, mitochondrial

Chain K:



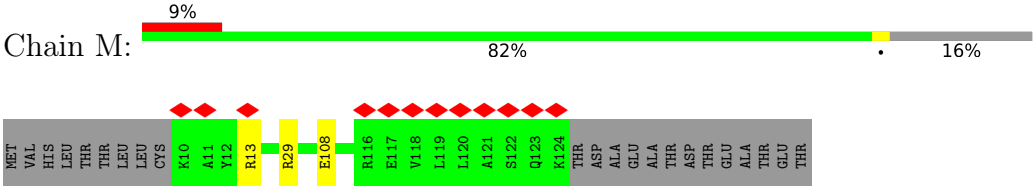
• Molecule 19: 28S ribosomal protein S15, mitochondrial

Chain L:



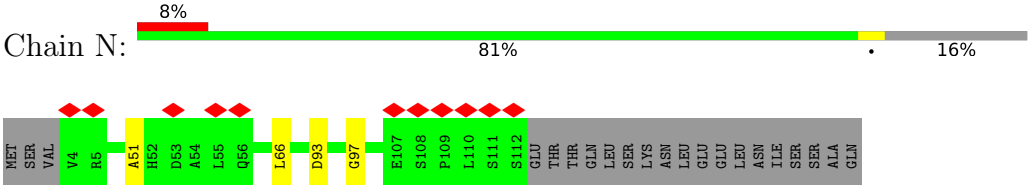
• Molecule 20: 28S ribosomal protein S16, mitochondrial

Chain M:



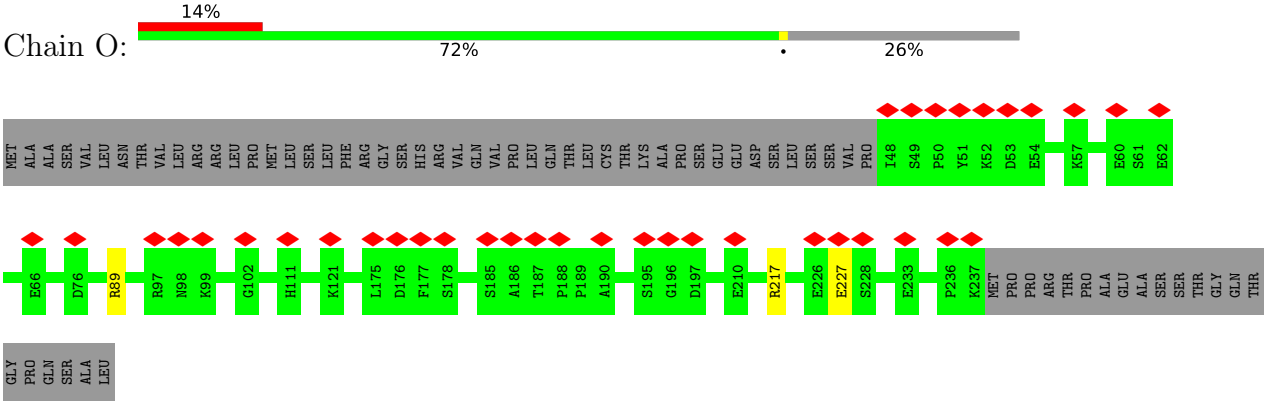
• Molecule 21: 28S ribosomal protein S17, mitochondrial

Chain N:



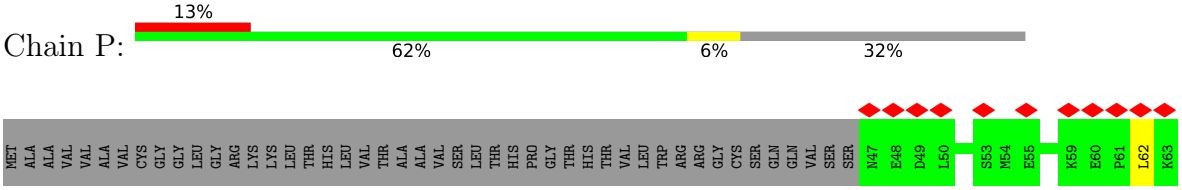
• Molecule 22: 28S ribosomal protein S18b, mitochondrial

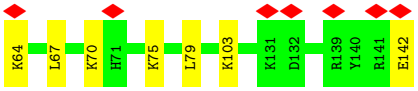
Chain O:



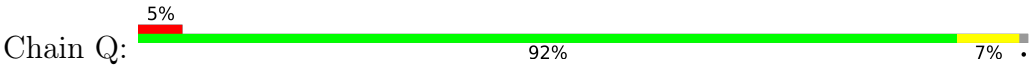
• Molecule 23: 28S ribosomal protein S18c, mitochondrial

Chain P:

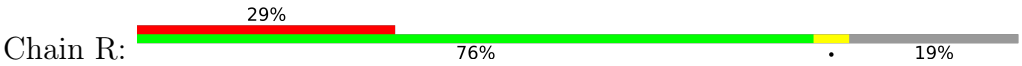


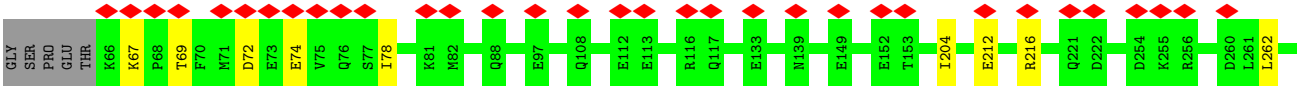


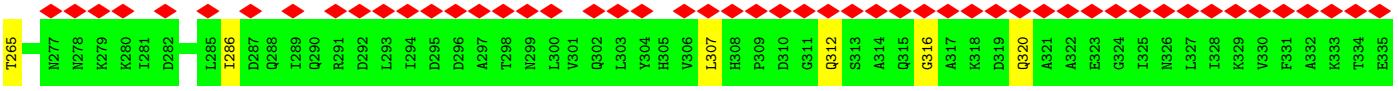
• Molecule 24: 28S ribosomal protein S21, mitochondrial

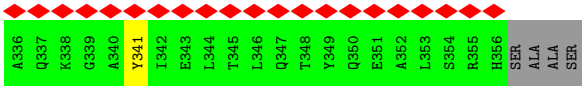


• Molecule 25: 28S ribosomal protein S22, mitochondrial

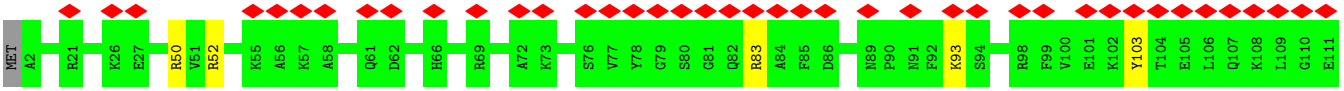


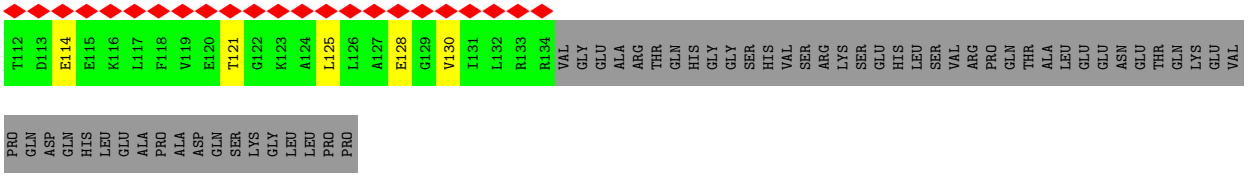




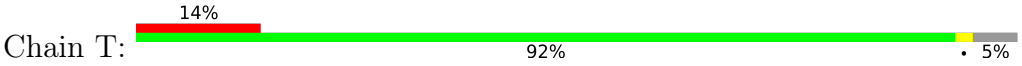


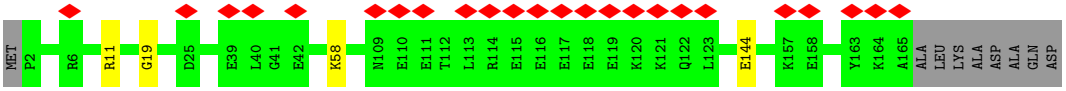
• Molecule 26: 28S ribosomal protein S23, mitochondrial





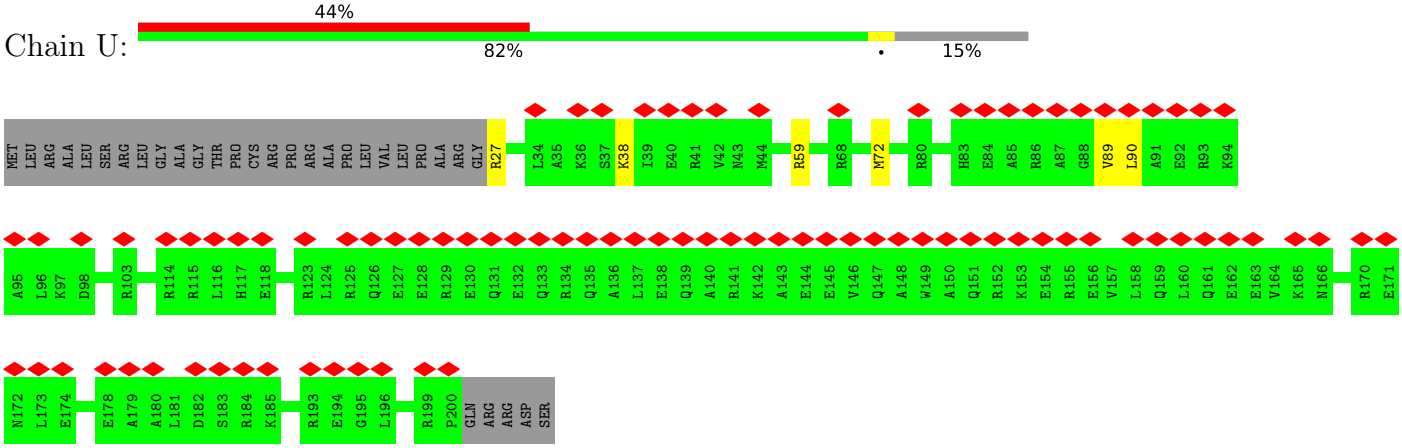
• Molecule 27: 28S ribosomal protein S25, mitochondrial





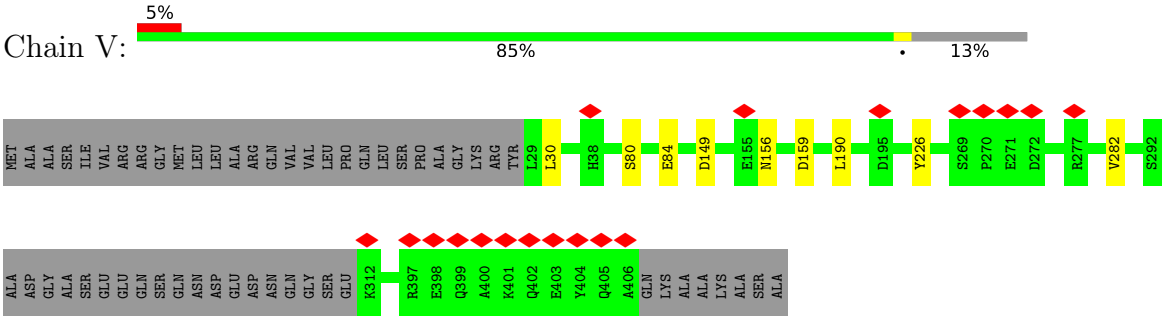
• Molecule 28: 28S ribosomal protein S26, mitochondrial

Chain U:



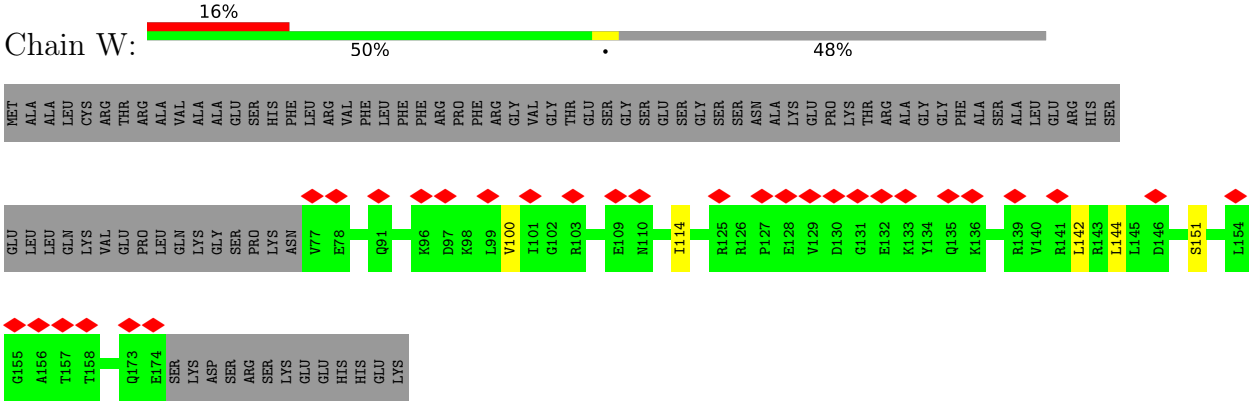
• Molecule 29: 28S ribosomal protein S27, mitochondrial

Chain V:



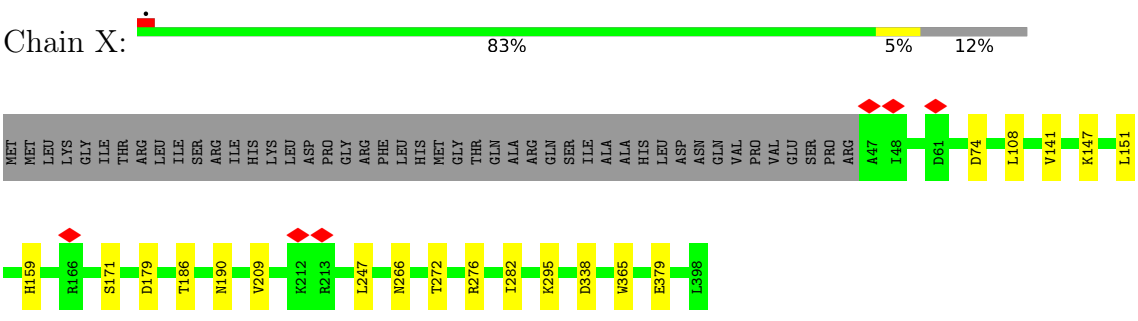
• Molecule 30: 28S ribosomal protein S28, mitochondrial

Chain W:



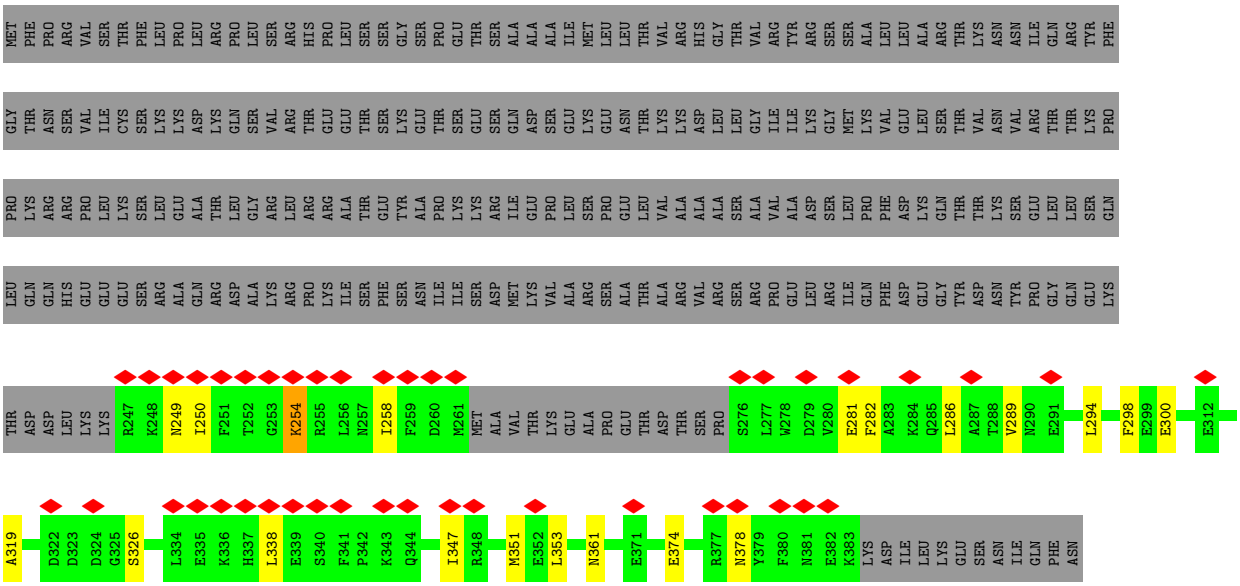
• Molecule 31: 28S ribosomal protein S29, mitochondrial

Chain X:



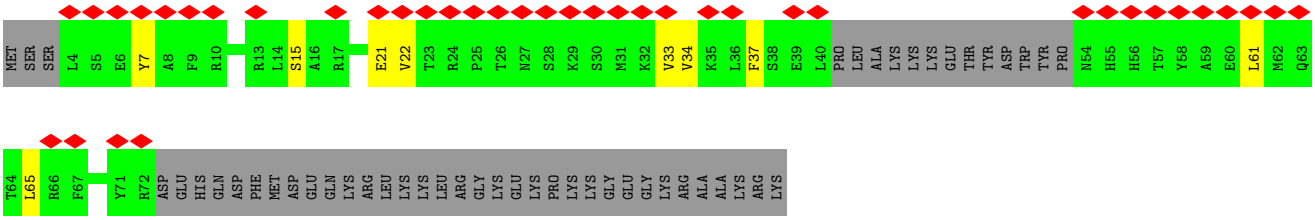
• Molecule 32: 28S ribosomal protein S31, mitochondrial

Chain Y:



• Molecule 33: 28S ribosomal protein S33, mitochondrial

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	368056	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	57.572	Depositor
Minimum map value	-20.751	Depositor
Average map value	0.033	Depositor
Map value standard deviation	1.280	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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ATP, FES, GDP, MG, K, MA6, SAM, AYA, NAD, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	0	0.24	0/1800	0.60	0/2440
2	1	0.25	0/2143	0.48	0/2902
3	3	0.24	0/636	0.65	0/839
4	4	0.27	0/4686	0.52	1/6335 (0.0%)
5	6	0.24	0/1012	0.49	0/1371
6	7	0.24	0/3250	0.52	0/4411
7	8	0.25	0/2603	0.52	0/3520
8	A	0.20	0/20026	0.79	3/31158 (0.0%)
9	B	0.25	0/1832	0.55	0/2480
10	C	0.25	0/1074	0.52	0/1456
11	D	0.25	0/1877	0.57	0/2523
12	E	0.26	0/872	0.59	0/1177
13	F	0.24	0/1734	0.51	0/2327
14	G	0.27	0/2446	0.56	0/3283
15	H	0.25	0/1086	0.51	0/1473
16	I	0.25	0/1039	0.52	0/1400
17	J	0.26	0/855	0.58	0/1148
18	K	0.22	0/326	0.66	0/432
19	L	0.25	0/1387	0.54	0/1853
20	M	0.24	0/934	0.59	0/1255
21	N	0.25	0/877	0.55	0/1187
22	O	0.24	0/1624	0.51	0/2210
23	P	0.26	0/791	0.49	0/1062
24	Q	0.24	0/748	0.59	0/994
25	R	0.25	0/2429	0.50	0/3280
26	S	0.27	0/1127	0.57	0/1518
27	T	0.25	0/1375	0.50	0/1847
28	U	0.26	0/1490	0.60	0/1999
29	V	0.25	0/3007	0.46	0/4062
30	W	0.25	0/787	0.53	0/1060
31	X	0.25	0/2921	0.48	0/3954
32	Y	0.26	0/1073	0.48	0/1444

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	Z	0.29	0/473	0.60	0/631
All	All	0.24	0/70340	0.63	4/99031 (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
17	J	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1081	U	O4'-C1'-N1	-6.53	102.97	108.20
4	4	252	PRO	CA-N-CD	-6.15	102.90	111.50
8	A	765	C	C2-N1-C1'	5.83	125.22	118.80
8	A	1262	C	C6-N1-C2	-5.24	118.20	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	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	9	0
2	1	2098	0	2115	11	0
3	3	625	0	699	3	0
4	4	4585	0	4595	61	0
5	6	994	0	1004	4	0
6	7	3160	0	3171	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	8	2543	0	2561	8	0
8	A	17959	0	9132	60	0
9	B	1789	0	1781	4	0
10	C	1042	0	1033	15	0
11	D	1838	0	1858	5	0
12	E	858	0	871	6	0
13	F	1696	0	1749	9	0
14	G	2395	0	2364	17	0
15	H	1064	0	1089	12	0
16	I	1019	0	1059	4	0
17	J	839	0	887	3	0
18	K	323	0	339	5	0
19	L	1363	0	1442	7	0
20	M	913	0	943	2	0
21	N	859	0	922	2	0
22	O	1570	0	1533	1	0
23	P	774	0	801	6	0
24	Q	744	0	758	4	0
25	R	2382	0	2405	9	0
26	S	1100	0	1103	7	0
27	T	1344	0	1359	3	0
28	U	1468	0	1478	5	0
29	V	2946	0	2942	6	0
30	W	775	0	791	4	0
31	X	2849	0	2843	13	0
32	Y	1043	0	996	20	0
33	Z	465	0	475	10	0
34	7	8	0	0	0	0
35	7	27	0	22	1	0
36	A	7	0	0	0	0
37	A	30	0	0	0	0
37	B	1	0	0	0	0
37	X	1	0	0	0	0
38	A	44	0	26	0	0
39	O	1	0	0	0	0
40	P	4	0	0	0	0
40	T	4	0	0	0	0
41	X	31	0	12	0	0
42	X	28	0	12	1	0
43	3	1	0	0	0	0
43	A	100	0	0	1	0
43	M	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	X	2	0	0	0	0
All	All	67466	0	58924	280	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 2.

The worst 5 of 280 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)
4:4:596:LEU:HD11	4:4:614:LEU:HD21	1.55	0.88
31:X:171:SER:OG	31:X:179:ASP:OD1	1.95	0.82
8:A:736:C:O2'	8:A:738:A:OP2	1.98	0.80
1:0:13:GLU:OE2	1:0:16:ARG:NH2	2.15	0.78
10:C:152:ARG:NH2	32:Y:300:GLU:OE1	2.18	0.77

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%)	207 (99%)	2 (1%)	0	100	100
2	1	255/323 (79%)	252 (99%)	3 (1%)	0	100	100
3	3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
4	4	558/689 (81%)	551 (99%)	6 (1%)	1 (0%)	47	56
5	6	122/343 (36%)	121 (99%)	1 (1%)	0	100	100
6	7	396/456 (87%)	389 (98%)	7 (2%)	0	100	100
7	8	324/390 (83%)	317 (98%)	7 (2%)	0	100	100
9	B	218/296 (74%)	217 (100%)	1 (0%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	C	122/167 (73%)	118 (97%)	4 (3%)	0	100	100
11	D	228/430 (53%)	224 (98%)	4 (2%)	0	100	100
12	E	106/125 (85%)	106 (100%)	0	0	100	100
13	F	204/242 (84%)	203 (100%)	1 (0%)	0	100	100
14	G	288/396 (73%)	281 (98%)	7 (2%)	0	100	100
15	H	126/201 (63%)	125 (99%)	1 (1%)	0	100	100
16	I	135/194 (70%)	131 (97%)	4 (3%)	0	100	100
17	J	106/138 (77%)	102 (96%)	4 (4%)	0	100	100
18	K	34/128 (27%)	34 (100%)	0	0	100	100
19	L	159/257 (62%)	158 (99%)	1 (1%)	0	100	100
20	M	113/137 (82%)	113 (100%)	0	0	100	100
21	N	107/130 (82%)	107 (100%)	0	0	100	100
22	O	188/258 (73%)	186 (99%)	2 (1%)	0	100	100
23	P	94/142 (66%)	92 (98%)	2 (2%)	0	100	100
24	Q	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
25	R	289/360 (80%)	283 (98%)	6 (2%)	0	100	100
26	S	131/190 (69%)	130 (99%)	1 (1%)	0	100	100
27	T	162/173 (94%)	161 (99%)	1 (1%)	0	100	100
28	U	172/205 (84%)	171 (99%)	1 (1%)	0	100	100
29	V	355/414 (86%)	352 (99%)	3 (1%)	0	100	100
30	W	96/187 (51%)	94 (98%)	2 (2%)	0	100	100
31	X	350/398 (88%)	345 (99%)	5 (1%)	0	100	100
32	Y	119/395 (30%)	119 (100%)	0	0	100	100
33	Z	52/106 (49%)	47 (90%)	5 (10%)	0	100	100
All	All	5970/8374 (71%)	5886 (99%)	83 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	4	252	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	184/190 (97%)	184 (100%)	0	100 100
2	1	239/291 (82%)	239 (100%)	0	100 100
3	3	65/166 (39%)	65 (100%)	0	100 100
4	4	506/609 (83%)	506 (100%)	0	100 100
5	6	107/288 (37%)	107 (100%)	0	100 100
6	7	340/385 (88%)	340 (100%)	0	100 100
7	8	270/317 (85%)	269 (100%)	1 (0%)	91 95
9	B	194/249 (78%)	194 (100%)	0	100 100
10	C	111/143 (78%)	110 (99%)	1 (1%)	78 87
11	D	196/357 (55%)	196 (100%)	0	100 100
12	E	91/107 (85%)	91 (100%)	0	100 100
13	F	183/209 (88%)	183 (100%)	0	100 100
14	G	254/342 (74%)	254 (100%)	0	100 100
15	H	120/180 (67%)	120 (100%)	0	100 100
16	I	105/147 (71%)	105 (100%)	0	100 100
17	J	93/118 (79%)	92 (99%)	1 (1%)	73 84
18	K	33/113 (29%)	32 (97%)	1 (3%)	41 50
19	L	151/226 (67%)	151 (100%)	0	100 100
20	M	94/113 (83%)	93 (99%)	1 (1%)	73 84
21	N	95/115 (83%)	95 (100%)	0	100 100
22	O	171/230 (74%)	170 (99%)	1 (1%)	86 93
23	P	87/123 (71%)	87 (100%)	0	100 100
24	Q	78/79 (99%)	78 (100%)	0	100 100
25	R	261/318 (82%)	261 (100%)	0	100 100
26	S	115/164 (70%)	115 (100%)	0	100 100
27	T	151/157 (96%)	151 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
28	U	150/174 (86%)	150 (100%)	0	100 100
29	V	323/364 (89%)	323 (100%)	0	100 100
30	W	85/158 (54%)	85 (100%)	0	100 100
31	X	311/351 (89%)	311 (100%)	0	100 100
32	Y	113/357 (32%)	112 (99%)	1 (1%)	78 87
33	Z	51/95 (54%)	51 (100%)	0	100 100
All	All	5327/7235 (74%)	5320 (100%)	7 (0%)	93 97

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

Mol	Chain	Res	Type
18	K	102	ARG
20	M	29	ARG
32	Y	254	LYS
22	O	89	ARG
17	J	44	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
9	B	167	HIS
11	D	280	HIS
32	Y	378	ASN
25	R	320	GLN
31	X	140	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	A	836/955 (87%)	178 (21%)	3 (0%)

5 of 178 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	650	U
8	A	651	A
8	A	664	G
8	A	680	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	A	688	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	1151	C
8	A	1254	C
8	A	1330	C

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

3 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	$\#\|Z\| > 2$
8	MA6	A	1583	8	19,26,27	1.11	1 (5%)	18,38,41	2.04	3 (16%)
24	AYA	Q	2	24	6,7,8	1.29	1 (16%)	5,8,10	1.33	1 (20%)
8	MA6	A	1584	8	19,26,27	1.10	1 (5%)	18,38,41	2.10	3 (16%)

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
8	MA6	A	1583	8	-	2/7/29/30	0/3/3/3
24	AYA	Q	2	24	-	0/4/6/8	-
8	MA6	A	1584	8	-	3/7/29/30	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1584	MA6	C5-N7	3.42	1.52	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1583	MA6	C5-N7	3.42	1.52	1.39
24	Q	2	AYA	CA-N	-2.47	1.44	1.46

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1583	MA6	C4-C5-N7	-5.52	103.65	109.40
8	A	1584	MA6	C4-C5-N7	-5.35	103.82	109.40
8	A	1584	MA6	N3-C2-N1	-4.97	120.91	128.68
8	A	1583	MA6	N3-C2-N1	-4.86	121.08	128.68
8	A	1584	MA6	C1'-N9-C4	-4.26	119.16	126.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1583	MA6	O4'-C4'-C5'-O5'
8	A	1583	MA6	C3'-C4'-C5'-O5'
8	A	1584	MA6	C5-C6-N6-C9
8	A	1584	MA6	C5-C6-N6-C10
8	A	1584	MA6	N1-C6-N6-C9

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 47 ligands modelled in this entry, 40 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	FES	T	201	27,20	0,4,4	-	-	-		
34	SF4	7	501	6	0,12,12	-	-	-		
42	GDP	X	503	-	24,30,30	3.39	12 (50%)	30,47,47	2.17	8 (26%)
35	SAM	7	502	-	24,29,29	1.18	3 (12%)	23,42,42	1.62	3 (13%)
38	NAD	A	1738	37	42,48,48	2.41	13 (30%)	50,73,73	1.66	10 (20%)
40	FES	P	201	23,12	0,4,4	-	-	-		
41	ATP	X	501	37	26,33,33	0.62	0	31,52,52	1.06	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	FES	T	201	27,20	-	-	0/1/1/1
34	SF4	7	501	6	-	-	0/6/5/5
42	GDP	X	503	-	-	3/12/32/32	0/3/3/3
35	SAM	7	502	-	-	8/12/33/33	0/3/3/3
38	NAD	A	1738	37	-	2/26/62/62	0/5/5/5
40	FES	P	201	23,12	-	-	0/1/1/1
41	ATP	X	501	37	-	2/18/38/38	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	X	503	GDP	O6-C6	9.25	1.42	1.23
42	X	503	GDP	C2-N1	7.55	1.56	1.37
38	A	1738	NAD	C7N-N7N	7.06	1.46	1.33
42	X	503	GDP	C2-N3	5.37	1.46	1.33
38	A	1738	NAD	O4D-C1D	5.26	1.48	1.41

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
42	X	503	GDP	C8-N7-C5	7.06	116.43	102.99
35	7	502	SAM	N3-C2-N1	-5.49	120.10	128.68
38	A	1738	NAD	C4A-C5A-N7A	-5.41	103.76	109.40
38	A	1738	NAD	C1B-N9A-C4A	-4.84	118.14	126.64
42	X	503	GDP	C2-N1-C6	-4.78	116.29	125.10

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	X	503	GDP	C5'-O5'-PA-O3A
42	X	503	GDP	C5'-O5'-PA-O1A
35	7	502	SAM	OXT-C-CA-N
35	7	502	SAM	O-C-CA-CB
35	7	502	SAM	OXT-C-CA-CB

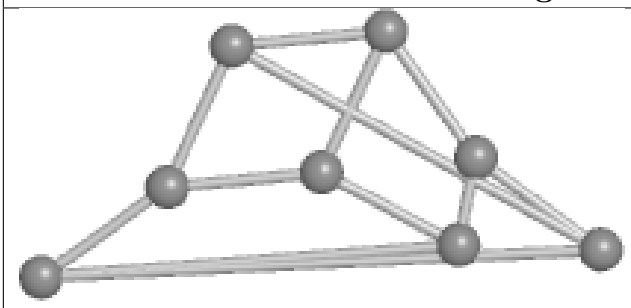
There are no ring outliers.

2 monomers are involved in 2 short contacts:

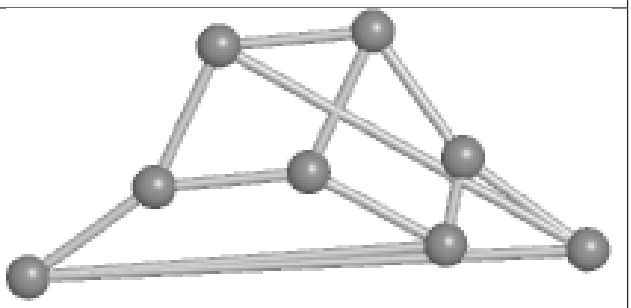
Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	X	503	GDP	1	0
35	7	502	SAM	1	0

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.

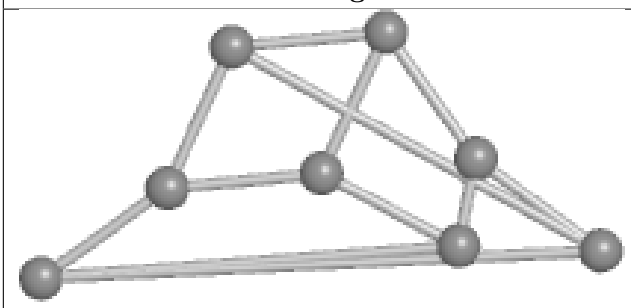
Ligand SF4 7 501



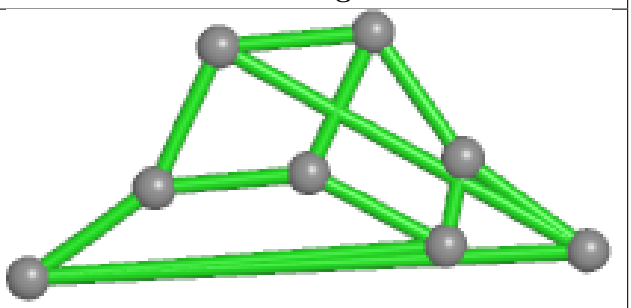
Bond lengths



Bond angles

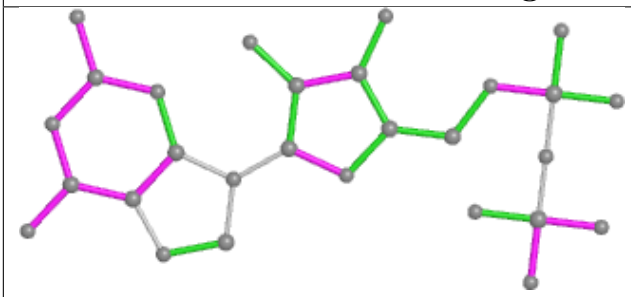


Torsions

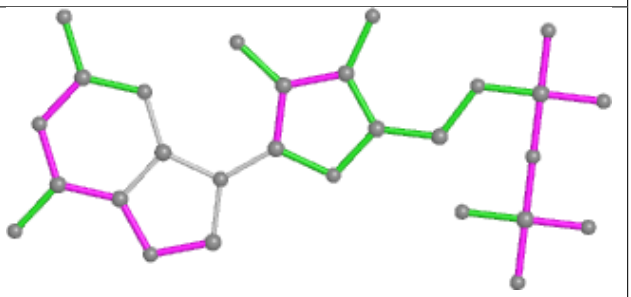


Rings

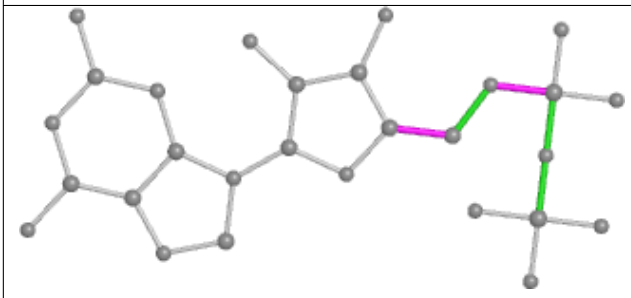
Ligand GDP X 503



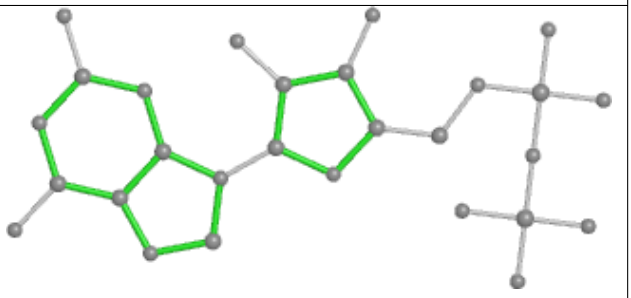
Bond lengths



Bond angles

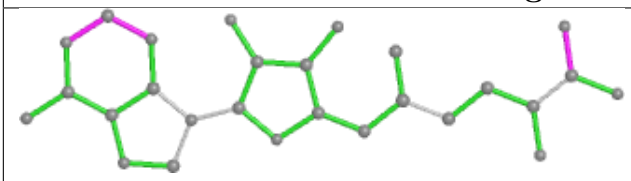


Torsions

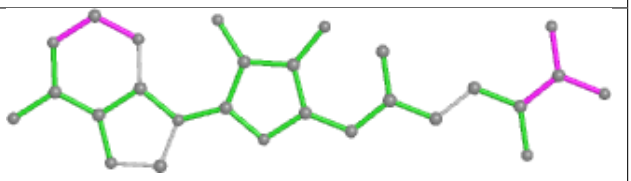


Rings

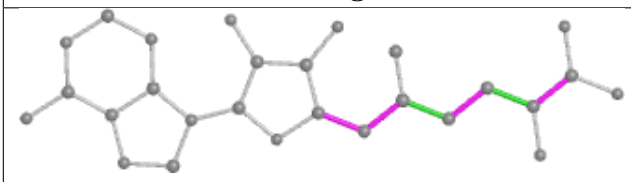
Ligand SAM 7 502



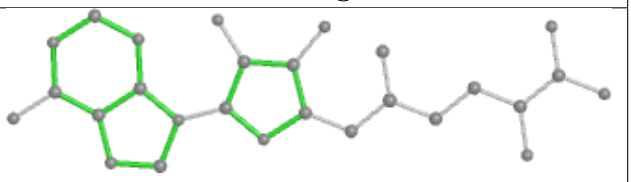
Bond lengths



Bond angles

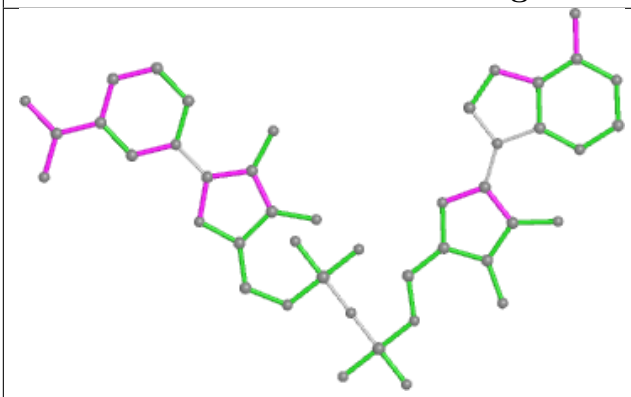


Torsions

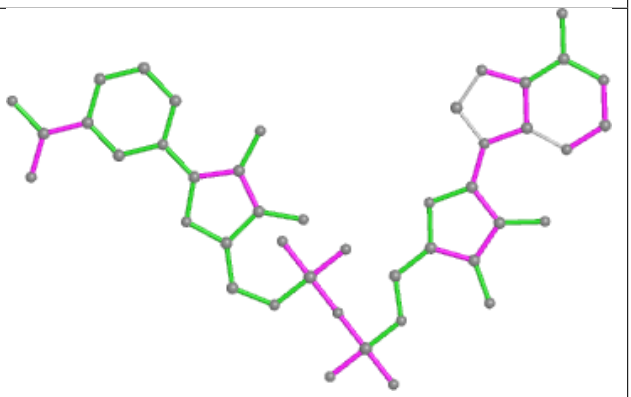


Rings

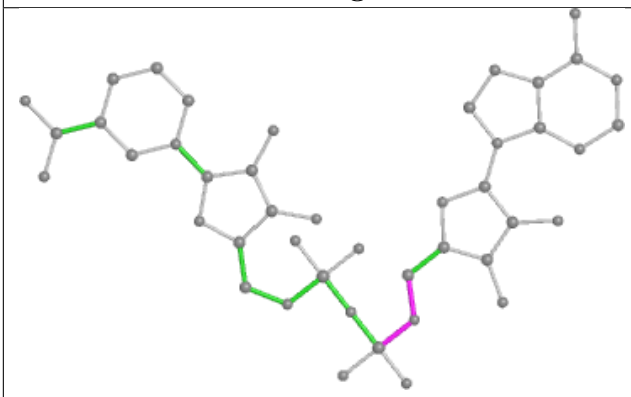
Ligand NAD A 1738



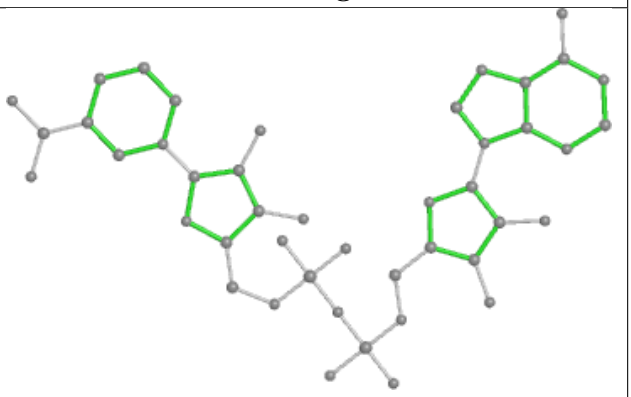
Bond lengths



Bond angles

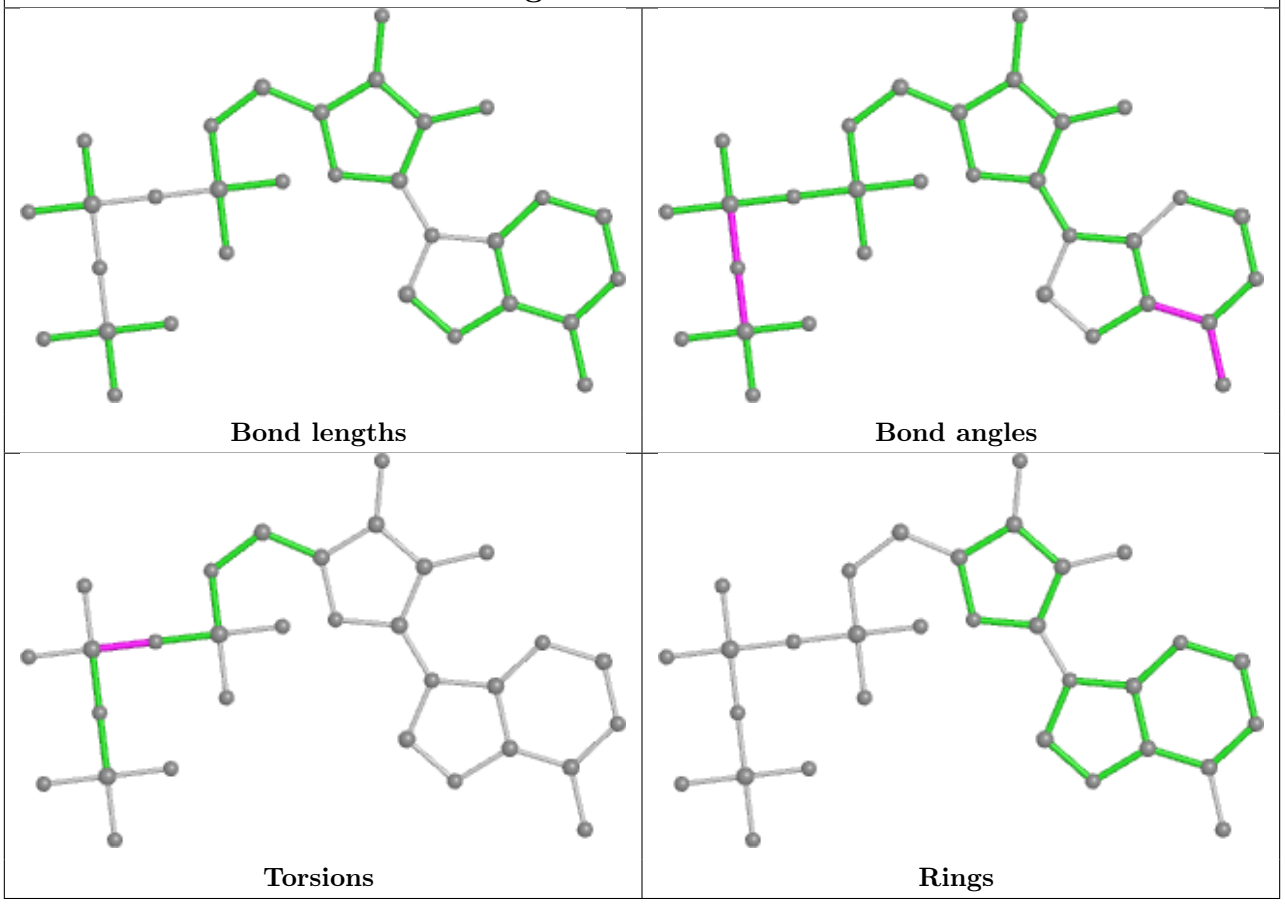


Torsions



Rings

Ligand ATP X 501



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.

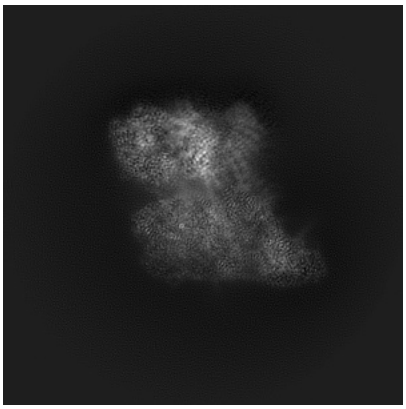
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26969. These allow visual inspection of the internal detail of the map and identification of artifacts.

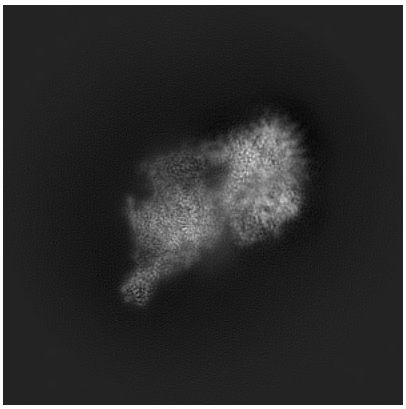
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

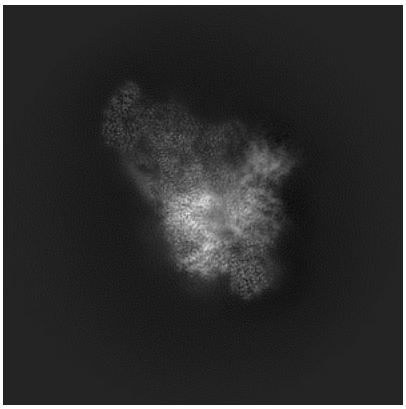
6.1.1 Primary map



X

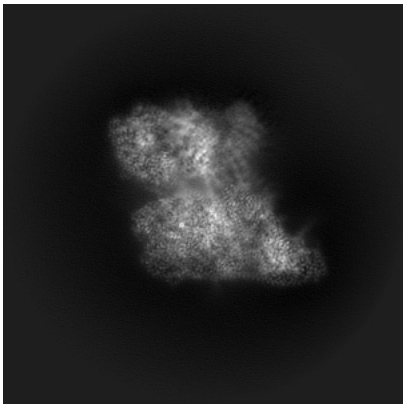


Y

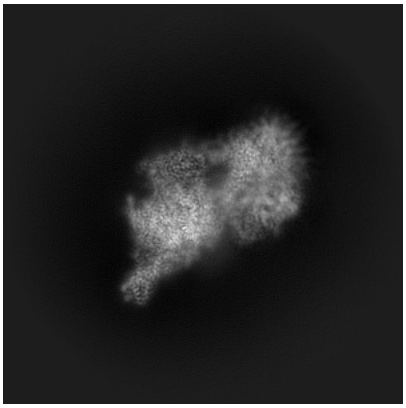


Z

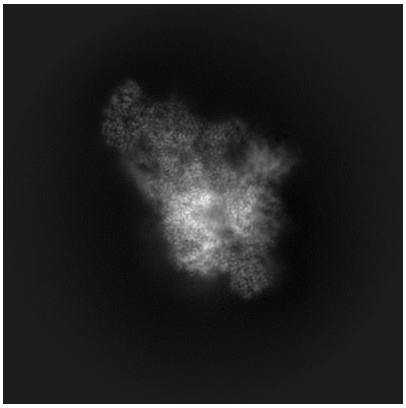
6.1.2 Raw map



X



Y

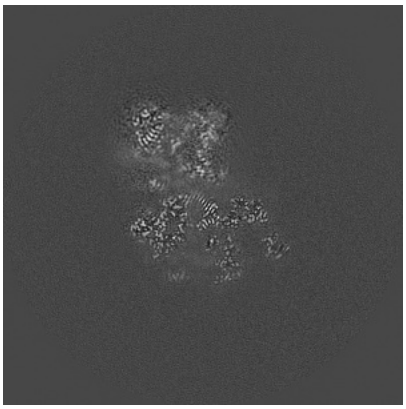


Z

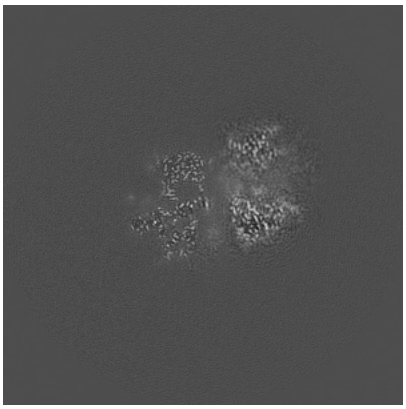
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

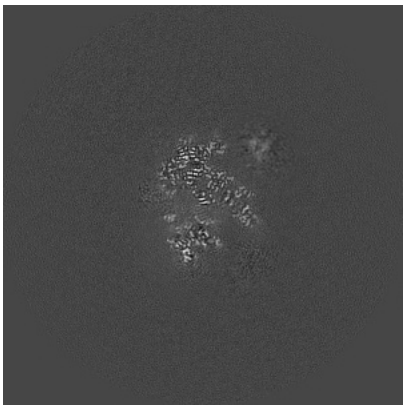
6.2.1 Primary map



X Index: 200

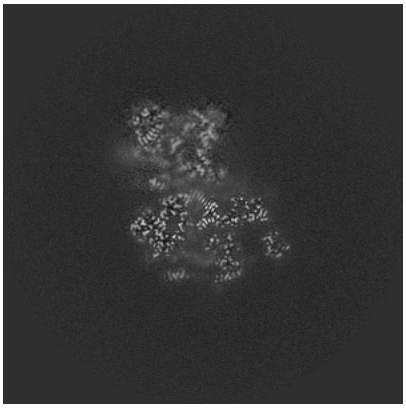


Y Index: 200

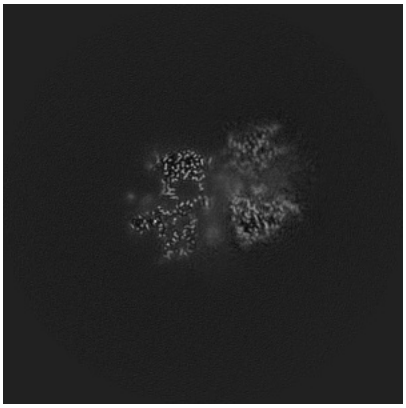


Z Index: 200

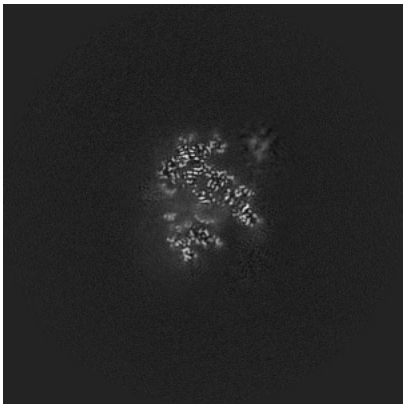
6.2.2 Raw map



X Index: 200



Y Index: 200

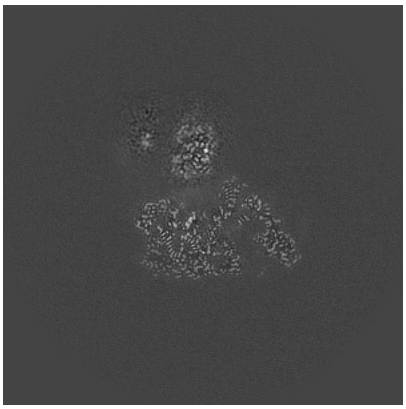


Z Index: 200

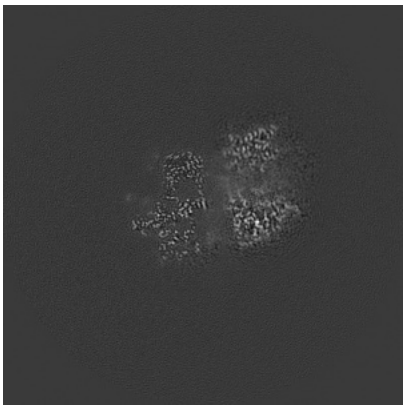
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

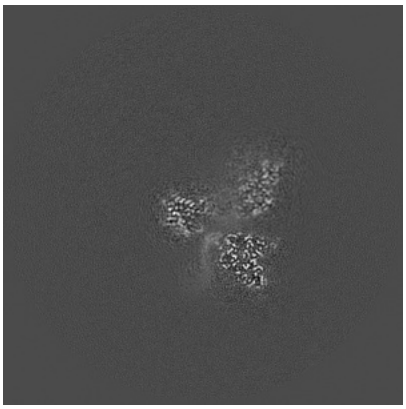
6.3.1 Primary map



X Index: 182

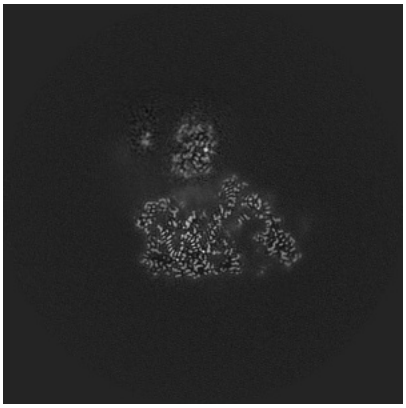


Y Index: 202

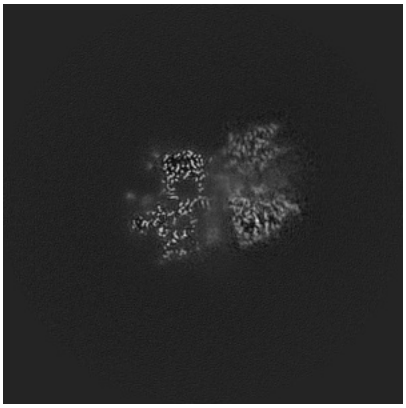


Z Index: 243

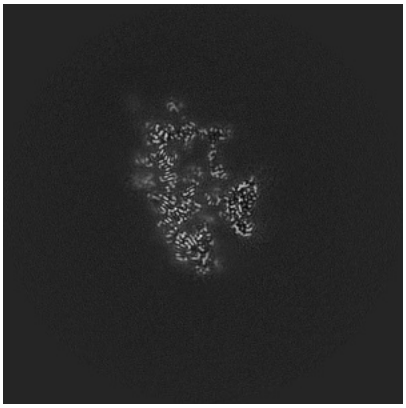
6.3.2 Raw map



X Index: 182



Y Index: 201

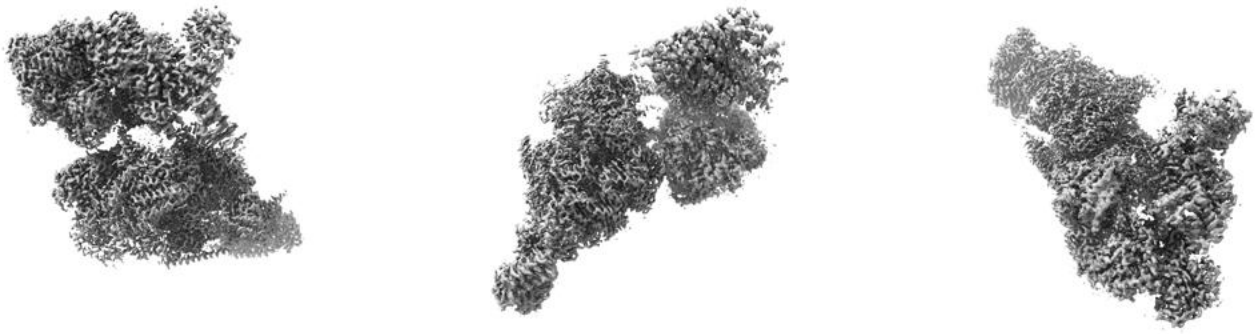


Z Index: 171

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

6.4 Orthogonal surface views (i)

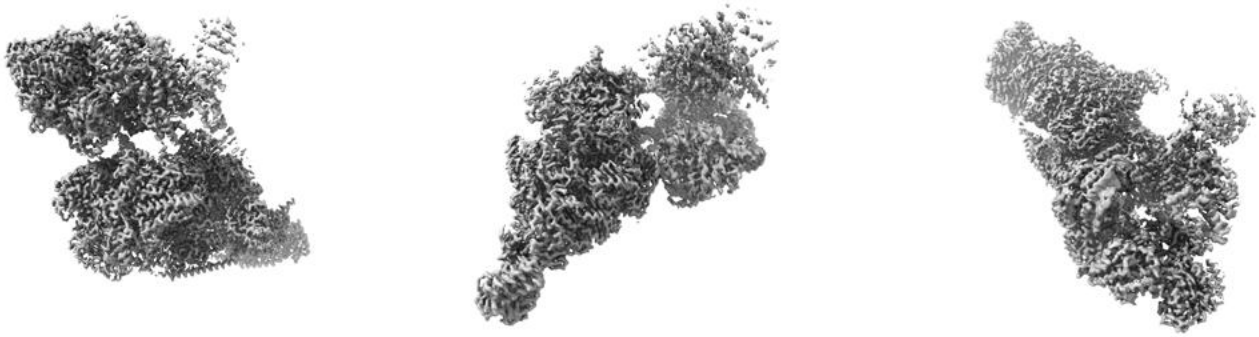
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 8.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

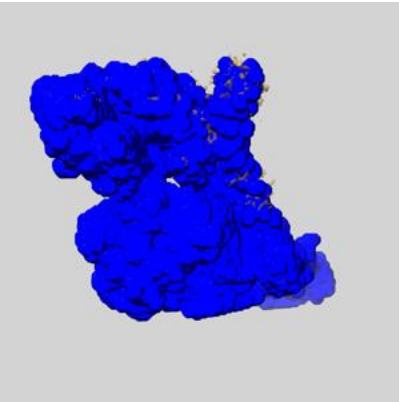
6.5 Mask visualisation (i)

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

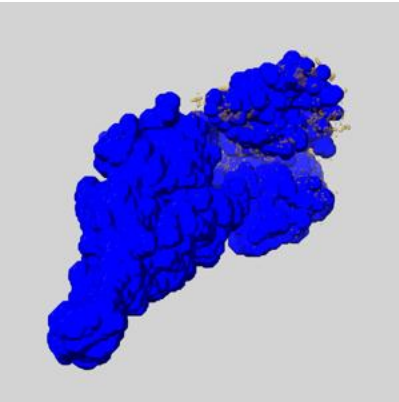
A mask typically either:

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

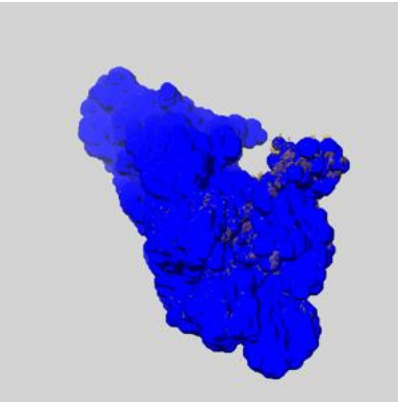
6.5.1 emd_26969_msk_1.map (i)



X



Y

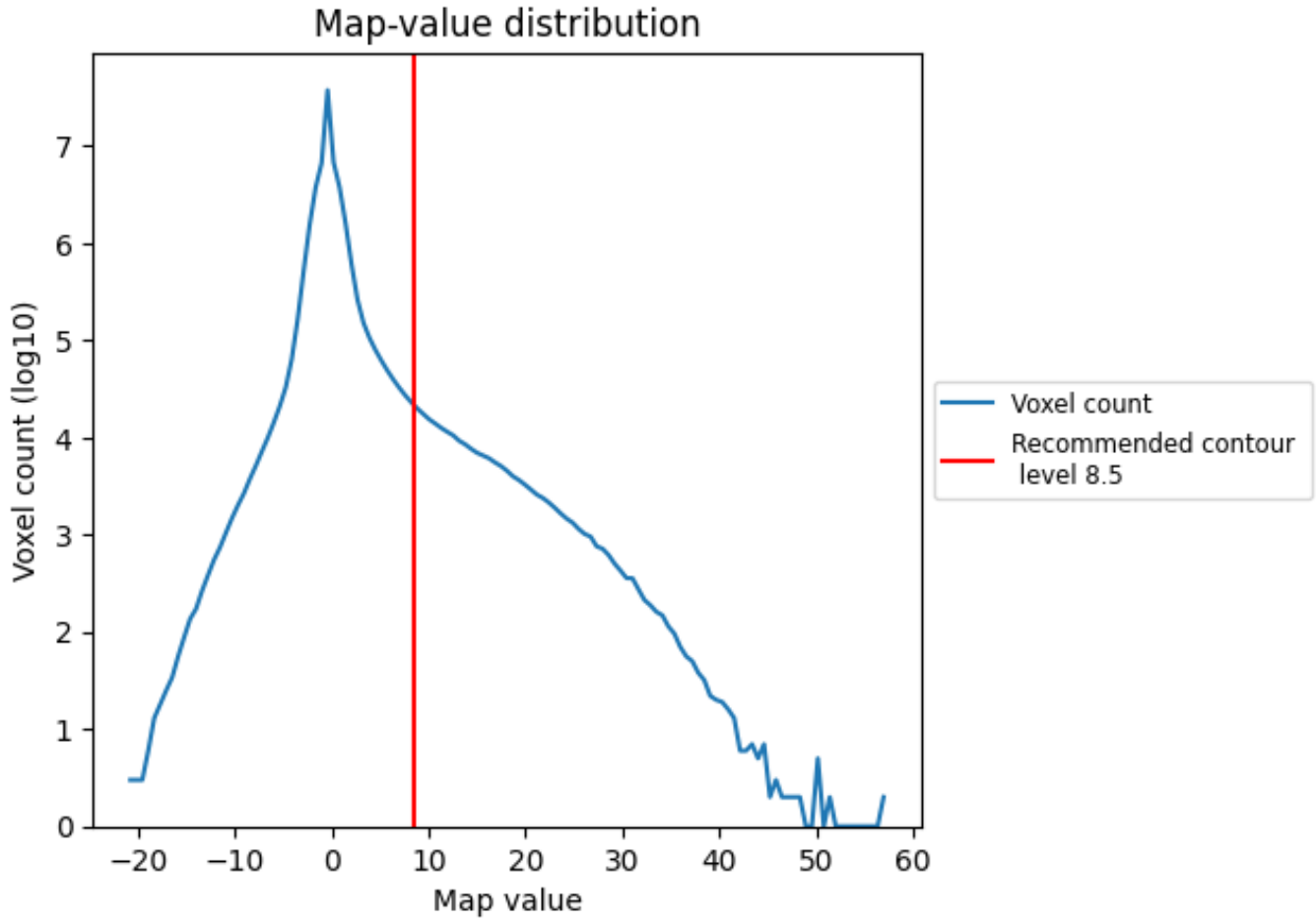


Z

7 Map analysis

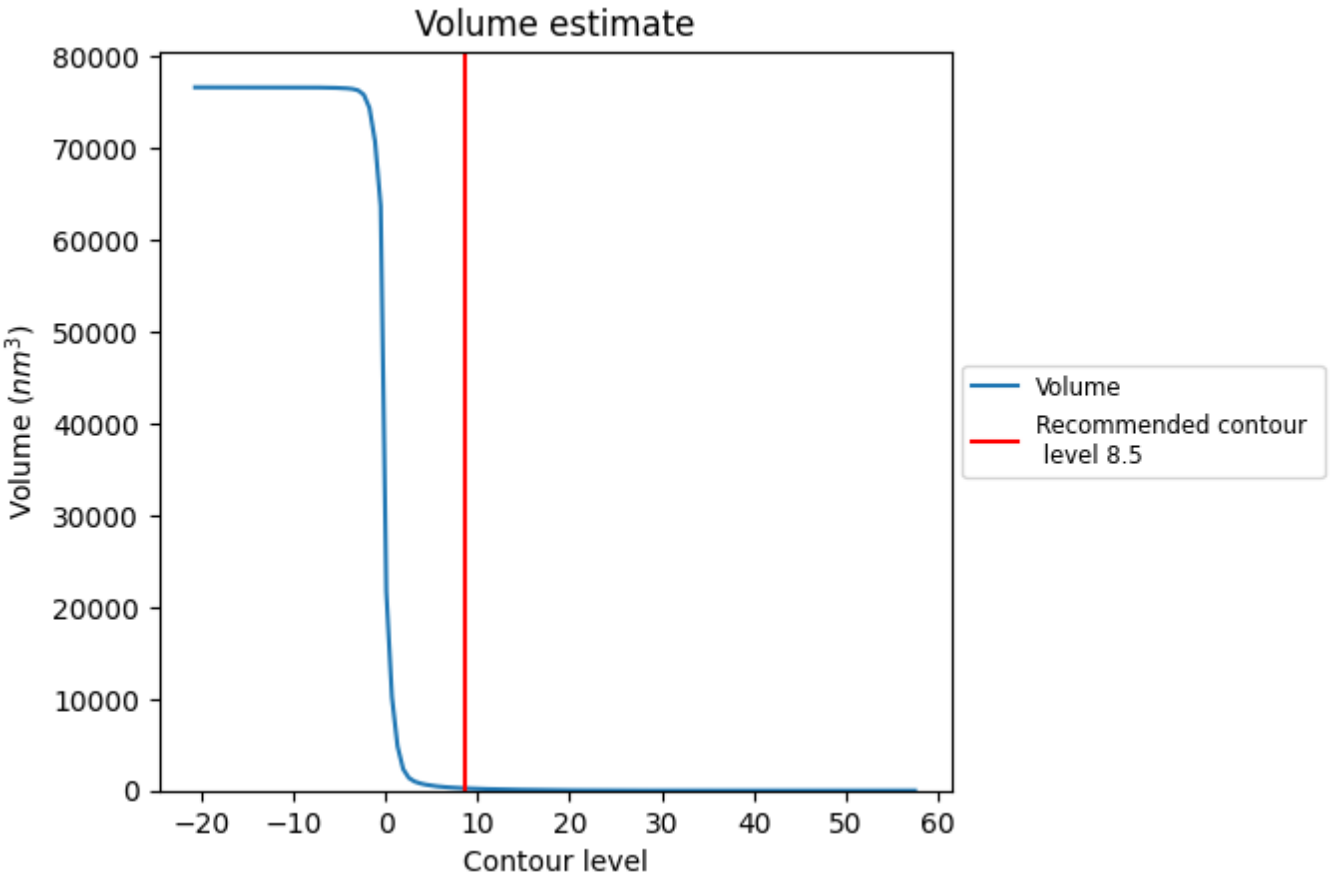
This section contains the results of statistical analysis of the map.

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.

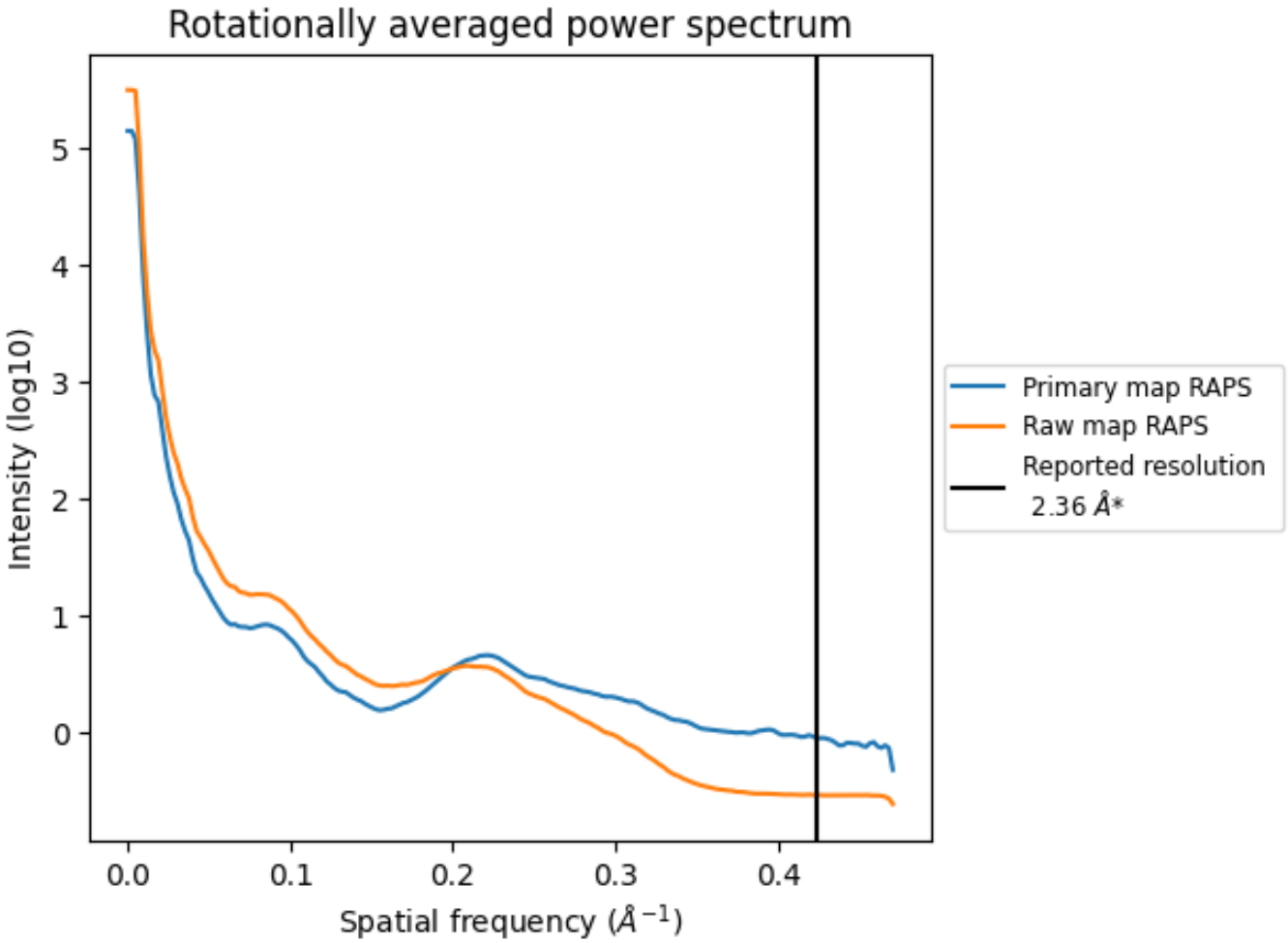
7.2 Volume estimate (i)



The volume at the recommended contour level is 252 nm^3; this corresponds to an approximate mass of 227 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)

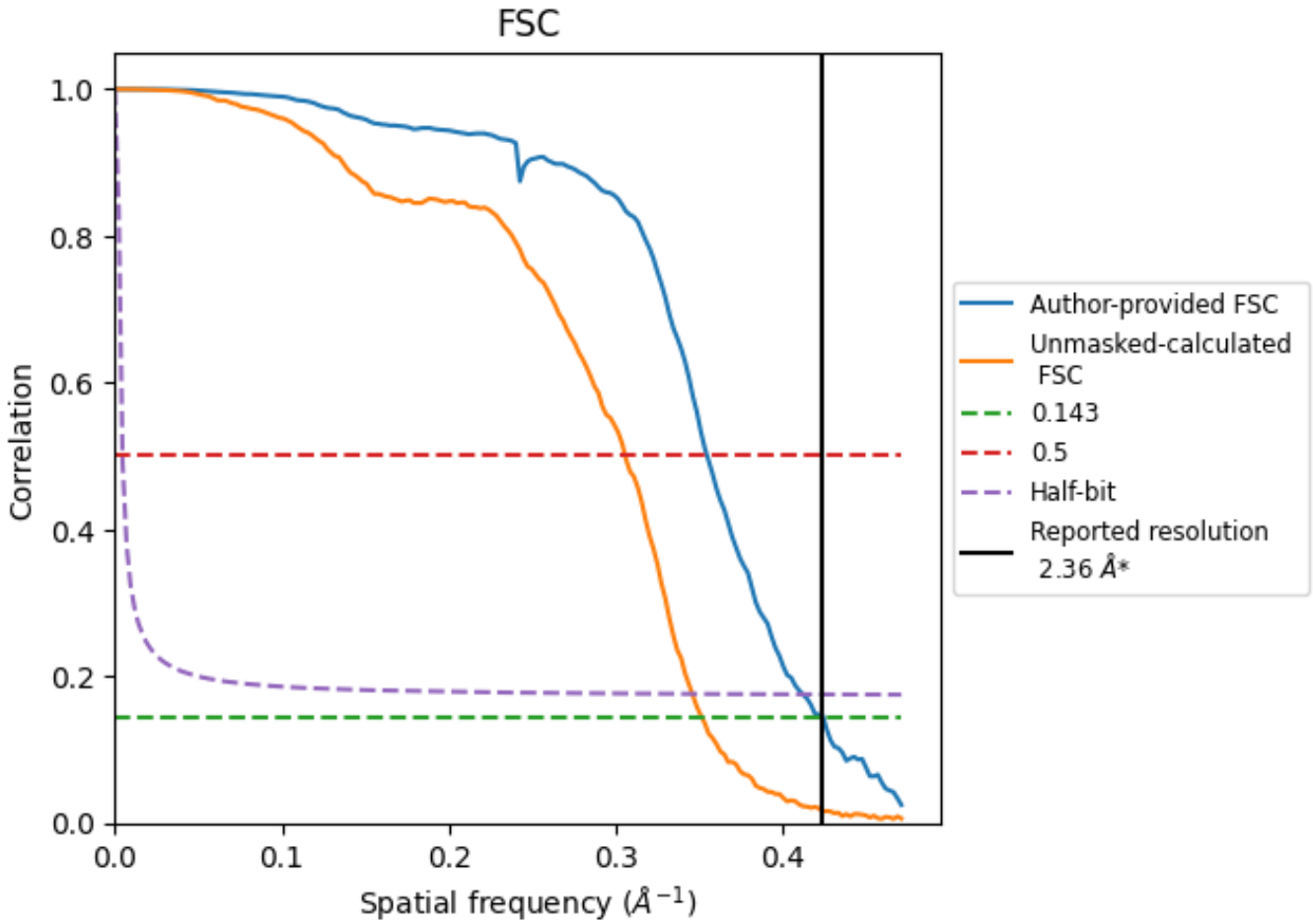


*Reported resolution corresponds to spatial frequency of 0.424 Å^{-1}

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 0.424 Å^{-1}

8.2 Resolution estimates (i)

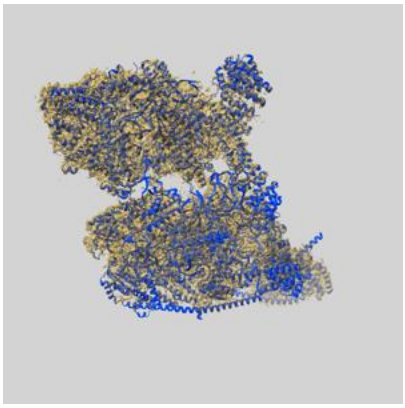
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.36	-	-
Author-provided FSC curve	2.36	2.82	2.43
Unmasked-calculated*	2.84	3.27	2.89

*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 2.84 differs from the reported value 2.36 by more than 10 %

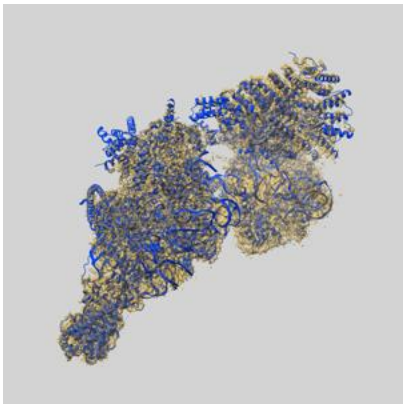
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26969 and PDB model 8CSS. Per-residue inclusion information can be found in section 3 on page 14.

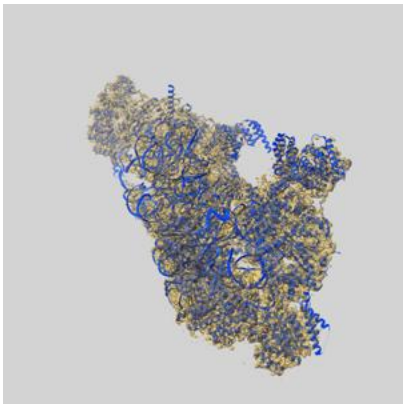
9.1 Map-model overlay



X



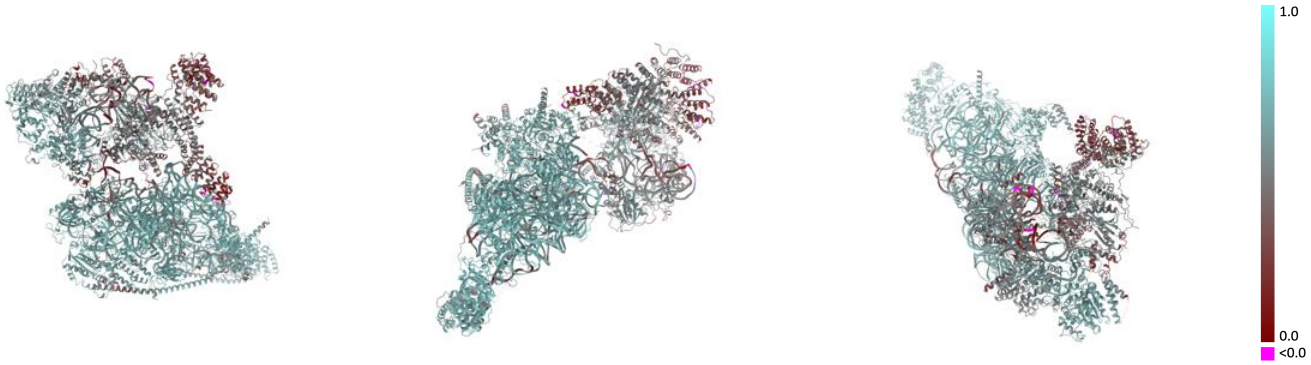
Y



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.

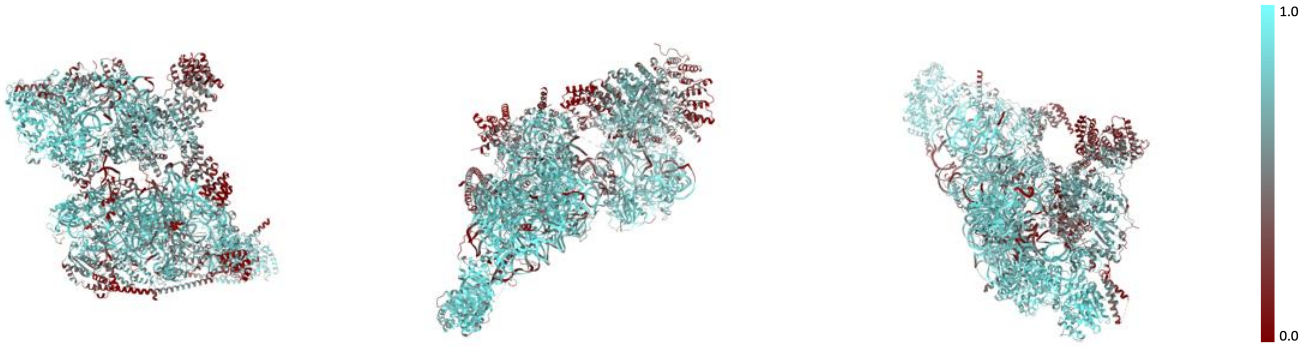
9.2 Q-score mapped to coordinate model (i)



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.

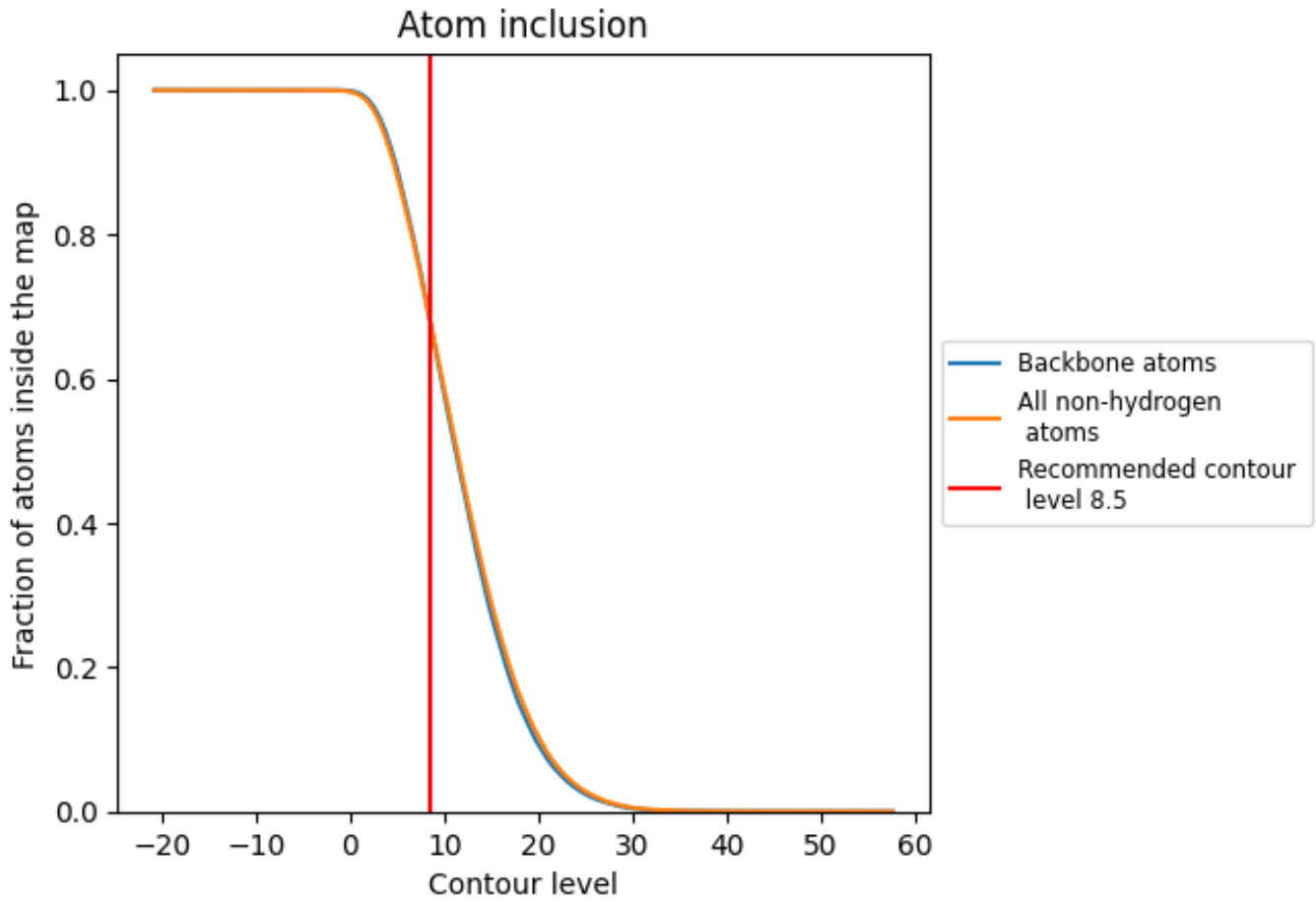
9.3 Atom inclusion mapped to coordinate model (i)



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, 68% of all backbone atoms, 68% 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	0.6791	0.5760
0	0.6977	0.6570
1	0.5802	0.4850
3	0.5933	0.6180
4	0.3802	0.3400
6	0.7282	0.6060
7	0.7703	0.5050
8	0.7924	0.5120
A	0.7585	0.5840
B	0.7474	0.6800
C	0.6105	0.4620
D	0.6982	0.6740
E	0.5647	0.6460
F	0.7317	0.5620
G	0.6455	0.5660
H	0.6180	0.4730
I	0.8472	0.6490
J	0.6544	0.6520
K	0.2961	0.3730
L	0.6289	0.6560
M	0.8256	0.6980
N	0.7619	0.6920
O	0.6995	0.6780
P	0.7094	0.6710
Q	0.8517	0.6740
R	0.5246	0.6370
S	0.4633	0.6140
T	0.7176	0.6760
U	0.4319	0.6060
V	0.7999	0.6480
W	0.5720	0.6490
X	0.8597	0.6290
Y	0.5219	0.4150
Z	0.3089	0.2890