wwPDB EM Validation Summary Report (i)

May 5, 2026 – 03:08 pm BST

PDB ID	:	9H55 / pdb_00009h55
EMDB ID	:	EMD-51877
Title	:	Assembly intermediate of human mitochondrial ribosome small subunit in complex with NOA1 and TFB1M (state N3)
Authors	:	Singh, V.; Shiriaev, D.; Khawaja, A.; Rorbach, J.
Deposited on	:	2024-10-22
Resolution	:	3.40 Å(reported)

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

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

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

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

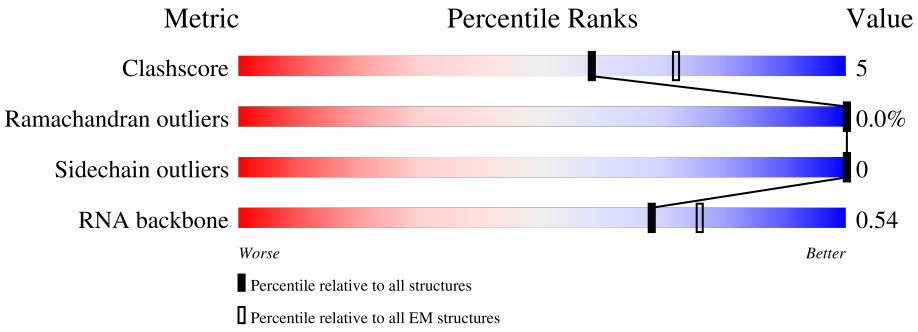
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

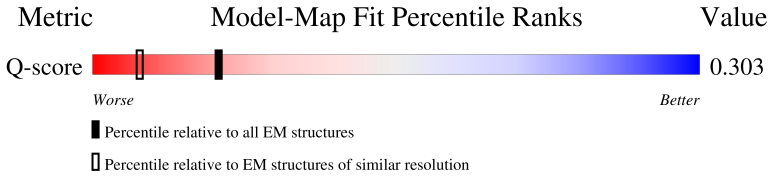
1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	A	955	20%, 63%, 23%, ·, 11%
2	B	296	·, 68%, 8%, 24%
3	C	167	61%, 65%, 14%, 21%

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Mol	Chain	Length	Quality of chain
4	D	430	21% 68% 9% 23%
5	E	125	6% 73% 14% 13%
6	F	242	78% 76% 7% 17%
7	G	396	45% 72% 7% 21%
8	H	201	57% 61% 9% 30%
9	I	194	27% 60% 10% 29%
10	J	138	72% 7% 22%
11	K	128	61% 70% 9% 21%
12	L	257	6% 57% 7% 36%
13	M	137	80% 7% 13%
14	N	130	72% 13% 15%
15	O	258	71% 25%
16	P	142	6% 60% 8% 32%
17	Q	87	21% 95% 5%
18	R	360	75% 7% 18%
19	S	190	62% 9% 29%
20	T	173	89% 8%
21	U	205	78% 8% 14%
22	V	414	72% 15% 13%
23	W	187	43% 11% 47%
24	X	398	84% 77% 11% 12%
25	Y	395	32% 29% 5% 66%
26	Z	106	77% 86% 5% 9%
27	0	215	5% 87% 13%
28	1	323	80% 77% 8% 14%

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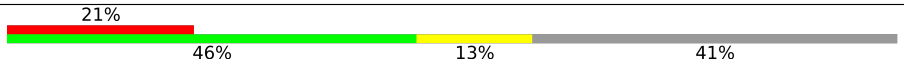
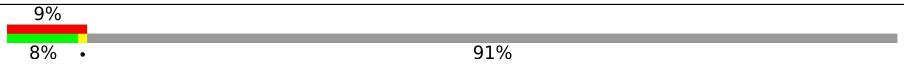
Mol	Chain	Length	Quality of chain
29	4	689	
30	9	698	
31	5	346	
32	a	343	

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 129555 atoms, of which 60710 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 RNA chain called 12S mitochondrial rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	850	27223	8095	9165	3258	5855	850	0	0

- Molecule 2 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	225	3654	1164	1826	331	323	10	0	0

- Molecule 3 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	132	2179	699	1096	195	185	4	0	0

- Molecule 4 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	332	5349	1660	2705	496	475	13	0	0

- Molecule 5 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	109	1747	544	882	158	159	4	0	0

- Molecule 6 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	201	3405	1071	1733	298	292	11	2	0

- Molecule 7 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	313	Total	C	H	N	O	S	0	0
			5147	1637	2570	456	470	14		

- Molecule 8 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	140	Total	C	H	N	O	S	0	0
			2343	745	1191	194	210	3		

- Molecule 9 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	137	Total	C	H	N	O	S	0	0
			2086	642	1066	192	182	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	184	5F0	ASN	variant	UNP P82912

- Molecule 10 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	108	Total	C	H	N	O	S	0	0
			1731	521	892	169	143	6		

- Molecule 11 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	101	Total	C	H	N	O	S	0	0
			1751	537	889	179	141	5		

- Molecule 12 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	164	Total	C	H	N	O	S	0	0
			2851	882	1467	256	239	7		

- Molecule 13 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	119	Total	C	H	N	O	S	0	0
			1914	594	972	185	157	6		

- Molecule 14 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	110	Total	C	H	N	O	S	0	0
			1801	562	933	156	147	3		

- Molecule 15 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	193	Total	C	H	N	O	S	0	0
			3158	1014	1566	294	277	7		

- Molecule 16 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	97	Total	C	H	N	O	S	0	0
			1590	501	809	134	138	8		

- Molecule 17 is a protein called Small ribosomal subunit protein bS21m.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	87	Total	C	H	N	O	S	0	0
			1504	460	760	150	126	8		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1	ACE	-	acetylation	UNP P82921
Q	50	ARG	CYS	conflict	UNP P82921

- Molecule 18 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	295	Total	C	H	N	O	S	0	0
			4845	1533	2436	413	455	8		

- Molecule 19 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	135	Total	C	H	N	O	S	0	0
			2228	716	1117	198	196	1		

- Molecule 20 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	168	Total	C	H	N	O	S	0	0
			2767	877	1396	239	244	11		

- Molecule 21 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	U	176	Total	C	H	N	O	S	0	0
			2993	916	1505	301	267	4		

- Molecule 22 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	362	Total	C	H	N	O	S	0	0
			5941	1904	2972	495	558	12		

- Molecule 23 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	100	Total	C	H	N	O	S	0	0
			1595	498	806	141	146	4		

- Molecule 24 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	X	350	Total	C	H	N	O	S	0	0
			5678	1813	2842	497	515	11		

- Molecule 25 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Y	134	Total	C	H	N	O	S	0	0
			2236	736	1100	191	207	2		

- Molecule 26 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	96	Total	C	H	N	O	S	0	0
			1638	517	828	145	144	4		

- Molecule 27 is a protein called Small ribosomal subunit protein mS34.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	0	215	Total	C	H	N	O	S	0	0
			3589	1130	1802	339	313	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
28	1	277	Total	C	H	N	O	S	0	0
			4526	1424	2281	382	428	11		

- Molecule 29 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	4	586	Total	C	H	N	O	S	0	0
			9502	3035	4761	803	875	28		

- Molecule 30 is a protein called Nitric oxide-associated protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	9	415	Total	C	H	N	O	S	0	0
			6656	2108	3378	574	584	12		

- Molecule 31 is a protein called Dimethyladenosine transferase 1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	5	319	Total	C	H	N	O	S	0	0
			5229	1648	2661	458	451	11		

- Molecule 32 is a protein called Putative ribosome-binding factor A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	32	Total	C	H	N	O	0	0
			520	162	271	42	45		

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
33	A	39	Total Mg 39 39	0
33	B	1	Total Mg 1 1	0
33	X	1	Total Mg 1 1	0

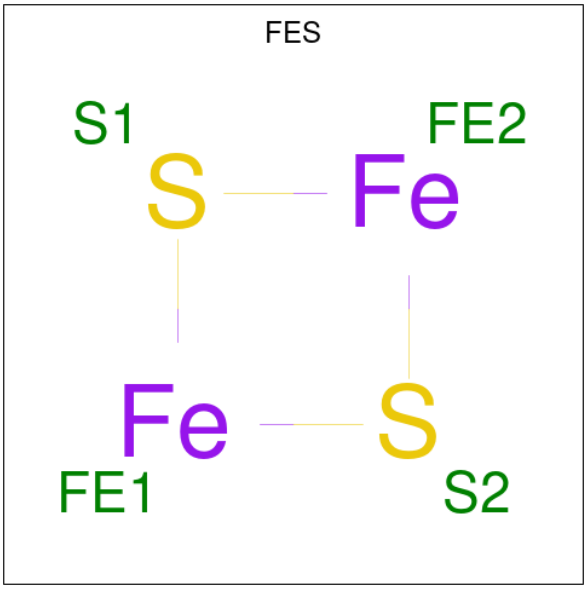
- Molecule 34 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
34	A	10	Total K 10 10	0

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn).

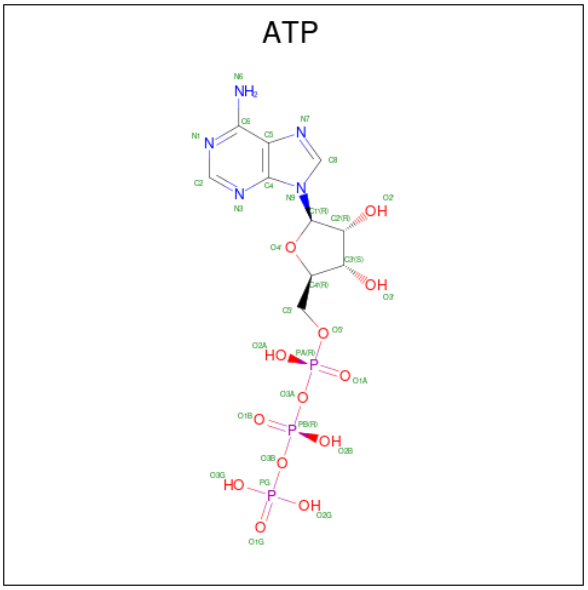
Mol	Chain	Residues	Atoms	AltConf
35	O	1	Total Zn 1 1	0

- Molecule 36 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



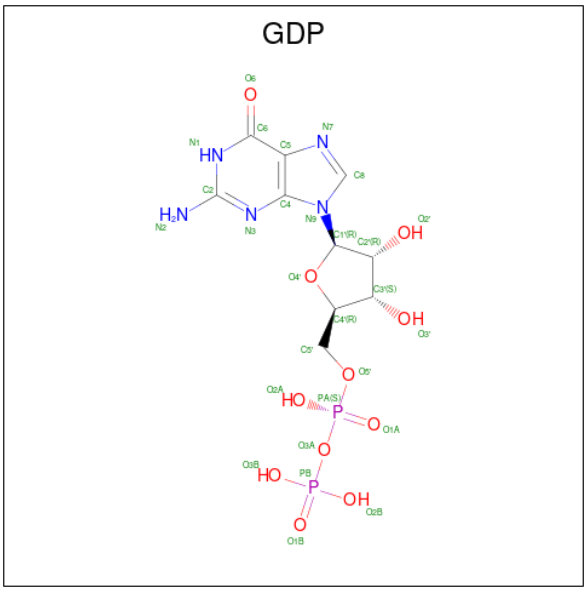
Mol	Chain	Residues	Atoms	AltConf
36	P	1	Total Fe S 4 2 2	0
36	T	1	Total Fe S 4 2 2	0

- Molecule 37 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
37	X	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 38 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



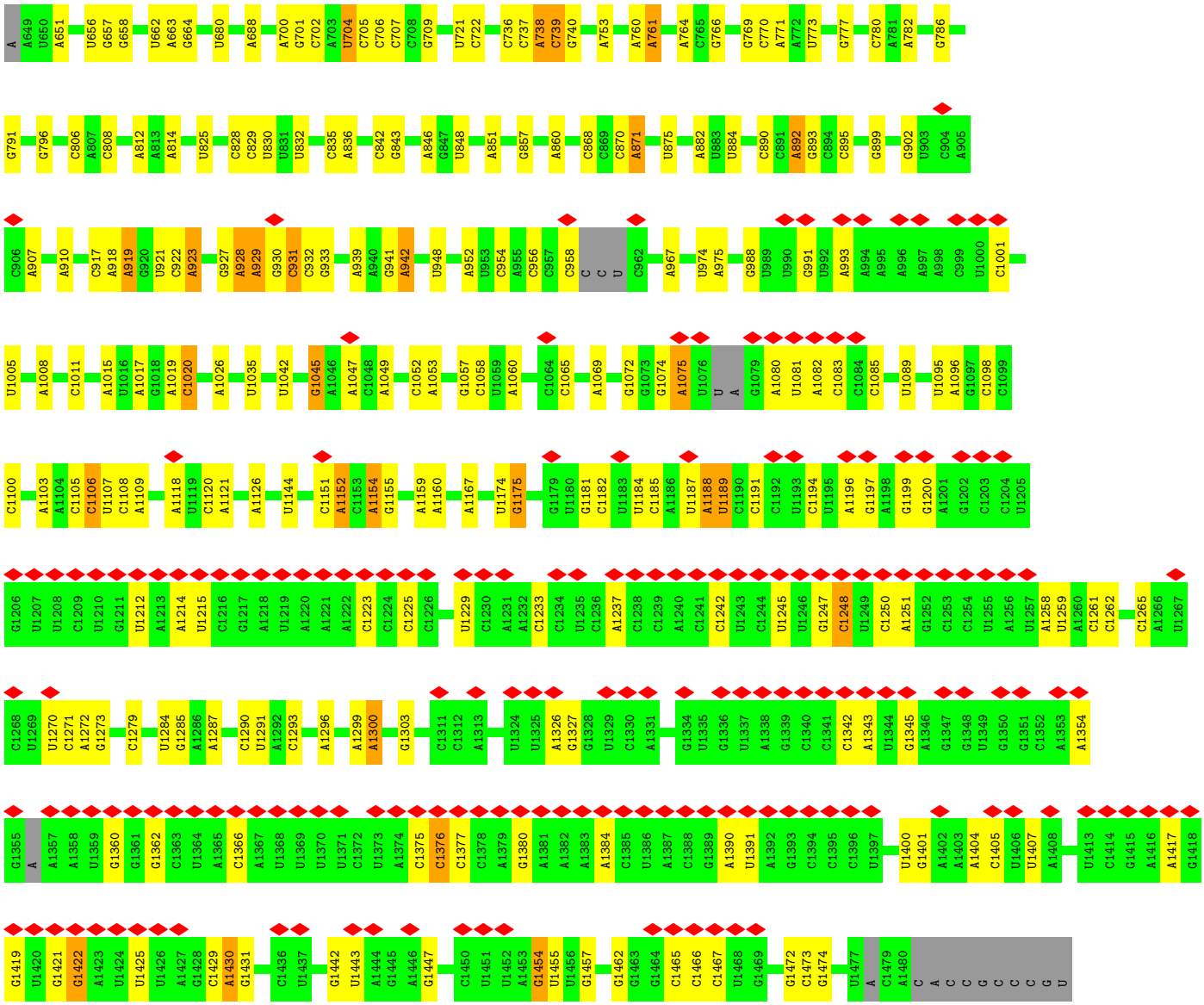
Mol	Chain	Residues	Atoms						AltConf
38	X	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	
38	9	1	Total	C	H	N	O	P	0
			38	10	10	5	11	2	

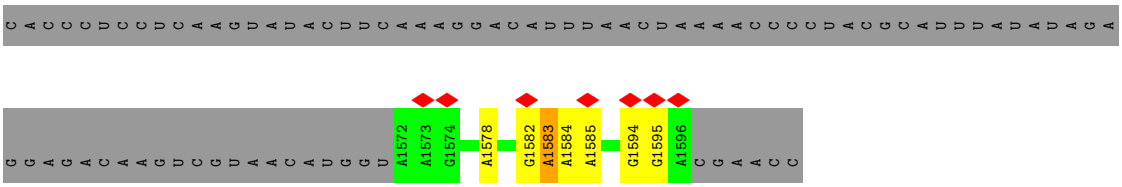
3 Residue-property plots (i)

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: 12S mitochondrial rRNA

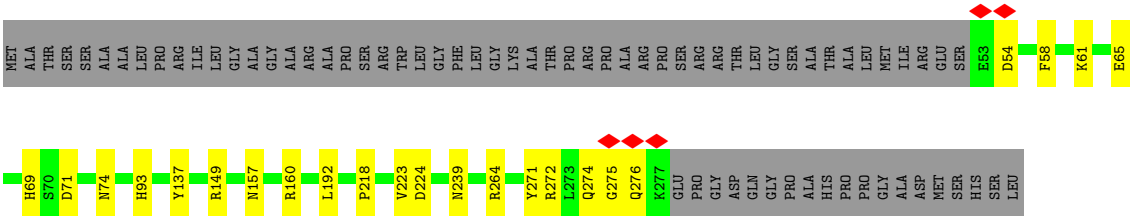
Chain A:





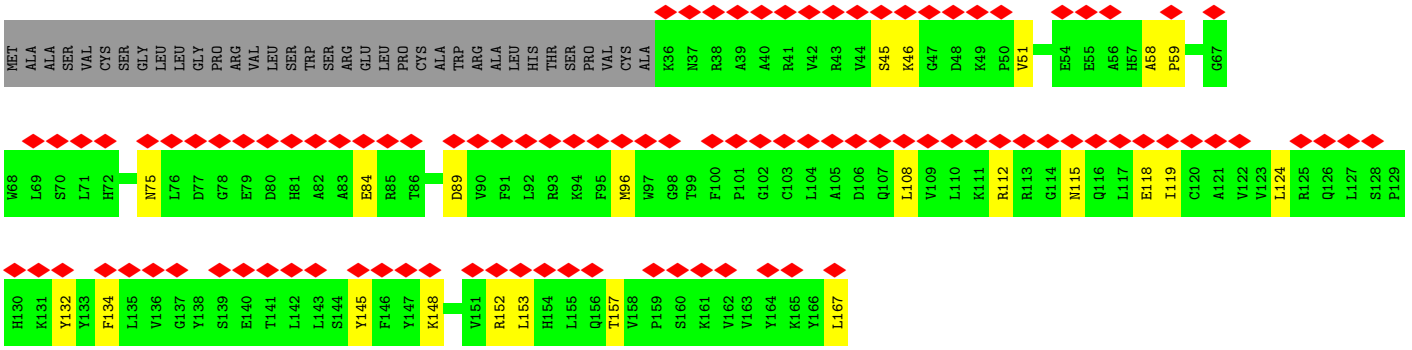
• Molecule 2: 28S ribosomal protein S2, mitochondrial

Chain B:



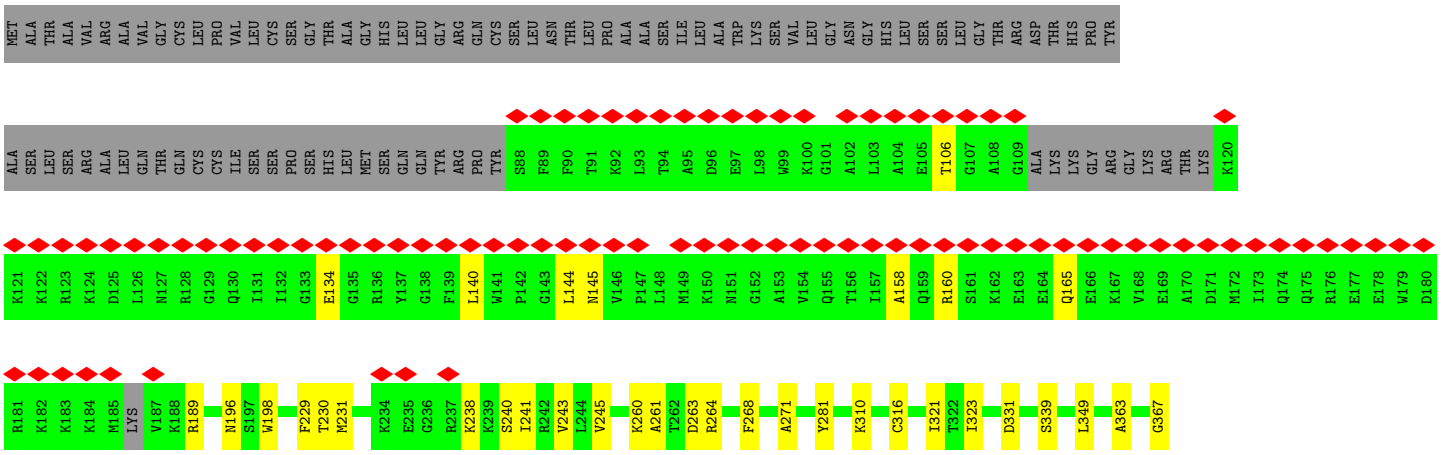
• Molecule 3: 28S ribosomal protein S24, mitochondrial

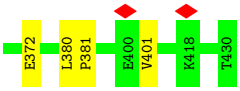
Chain C:



• Molecule 4: 28S ribosomal protein S5, mitochondrial

Chain D:



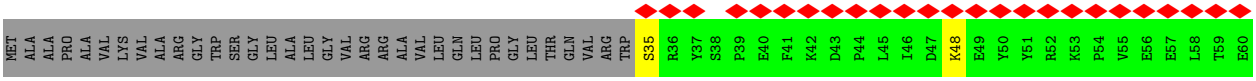


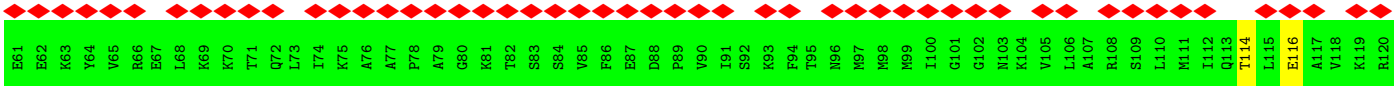
• Molecule 5: 28S ribosomal protein S6, mitochondrial

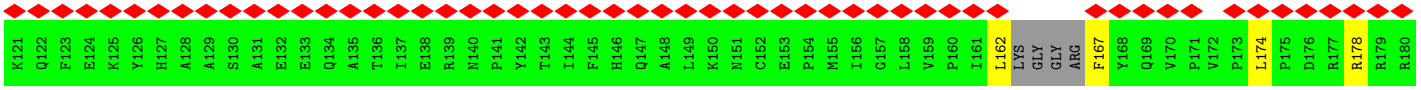
Chain E:

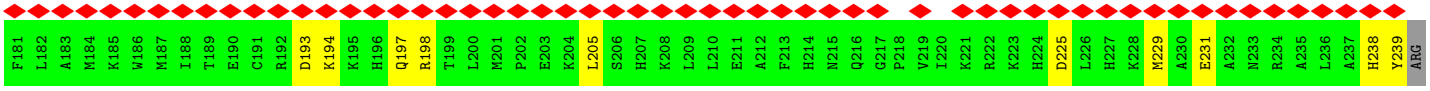
• Molecule 6: 28S ribosomal protein S7, mitochondrial

Chain F:



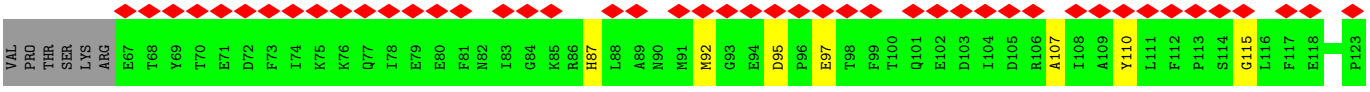


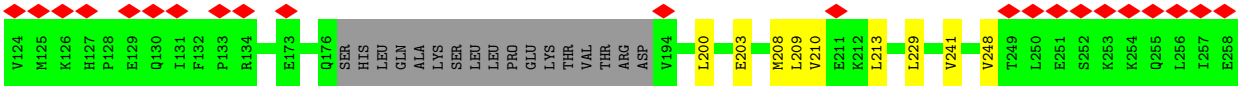


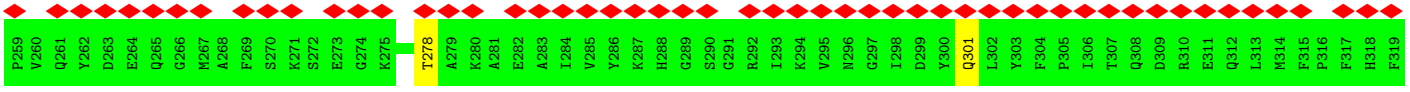


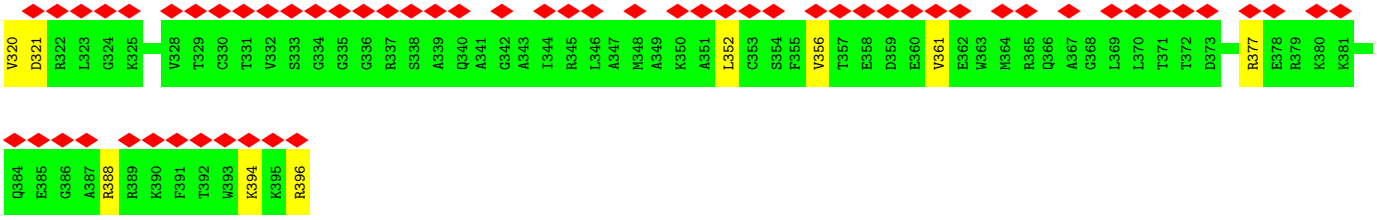
• Molecule 7: 28S ribosomal protein S9, mitochondrial

Chain G:



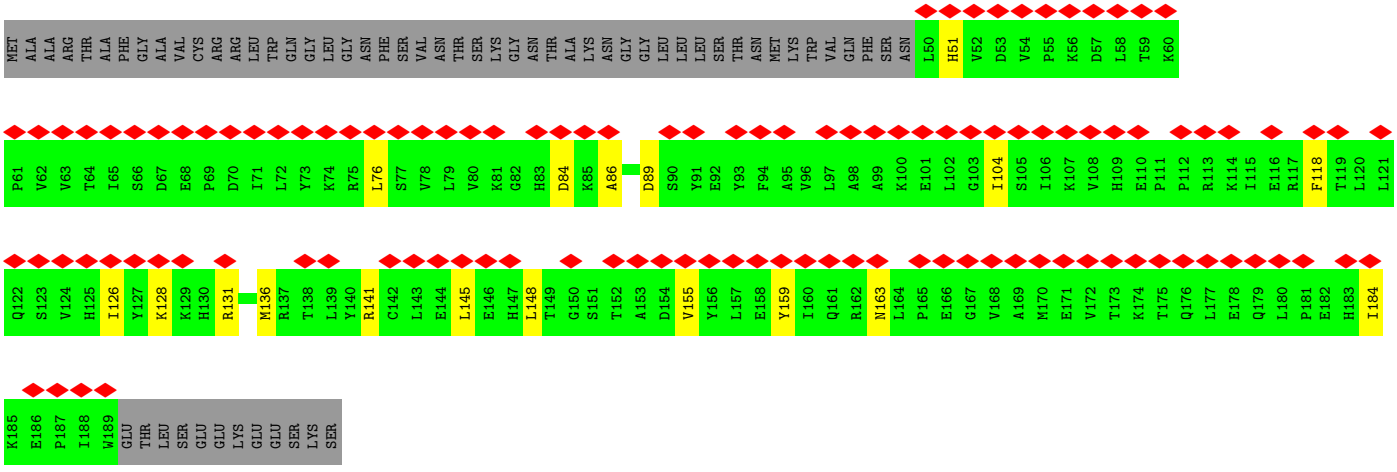






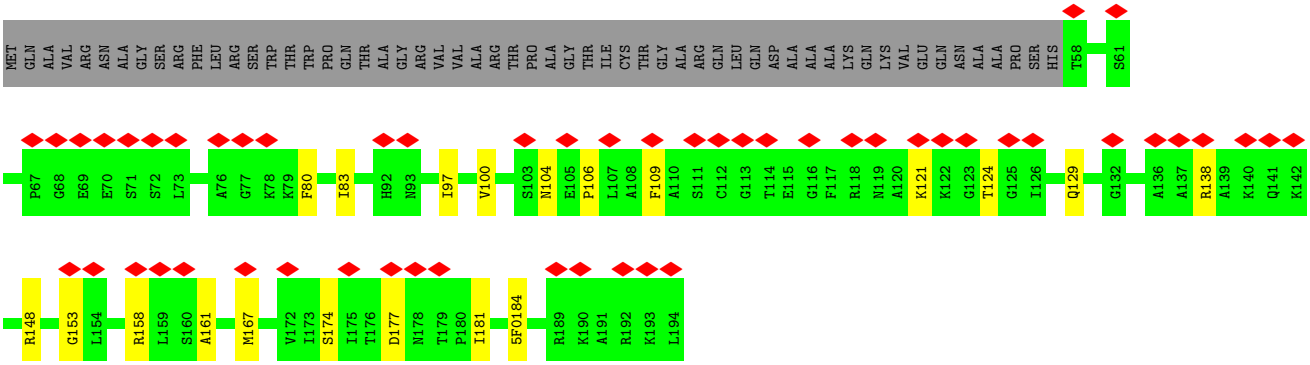
• Molecule 8: 28S ribosomal protein S10, mitochondrial

Chain H:



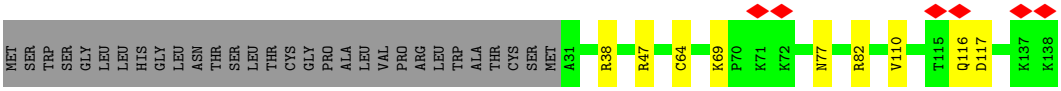
• Molecule 9: 28S ribosomal protein S11, mitochondrial

Chain I:



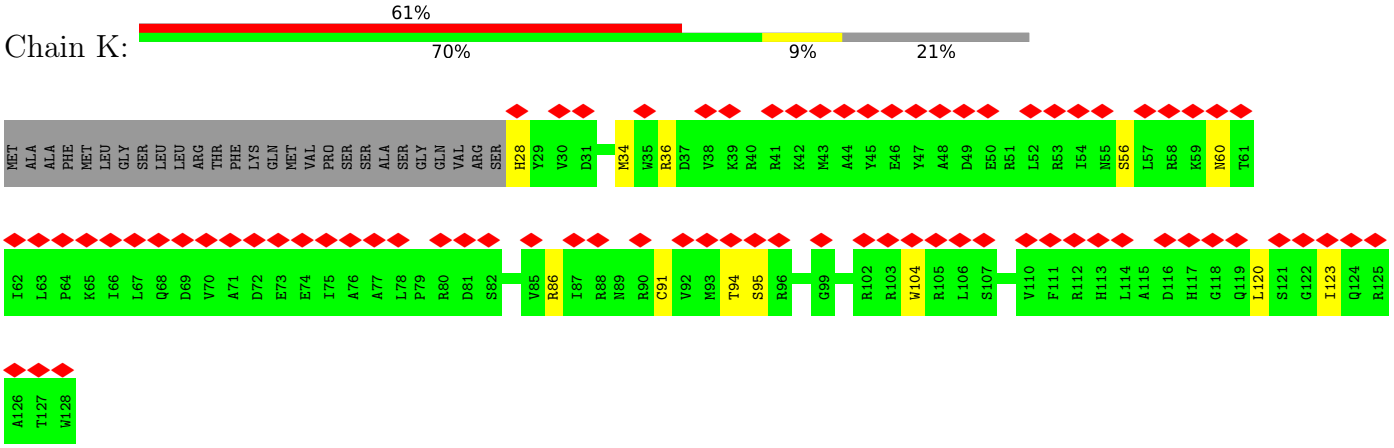
• Molecule 10: 28S ribosomal protein S12, mitochondrial

Chain J:



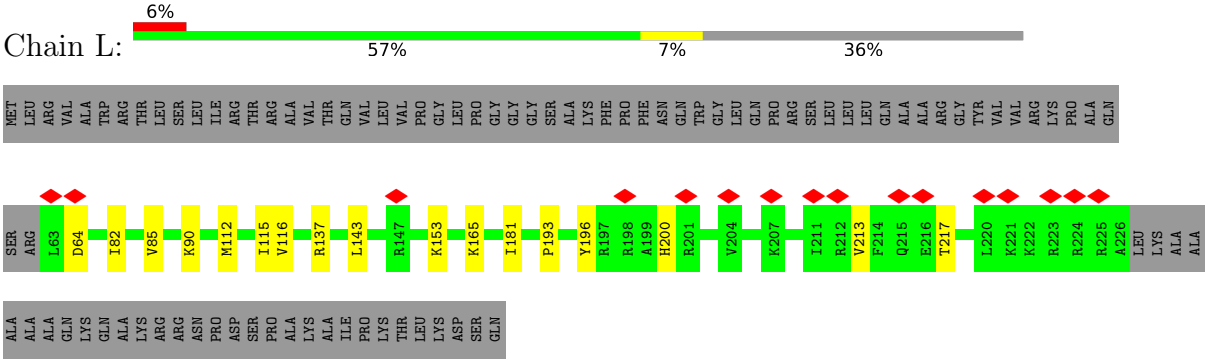
• Molecule 11: 28S ribosomal protein S14, mitochondrial

Chain K:



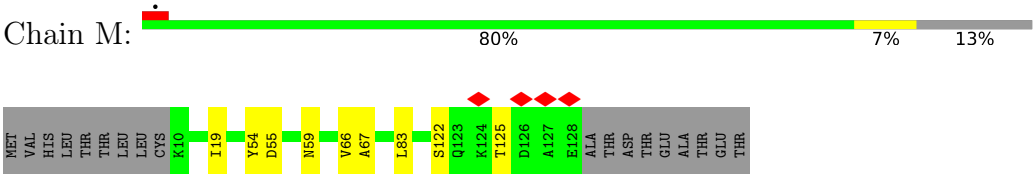
• Molecule 12: 28S ribosomal protein S15, mitochondrial

Chain L:



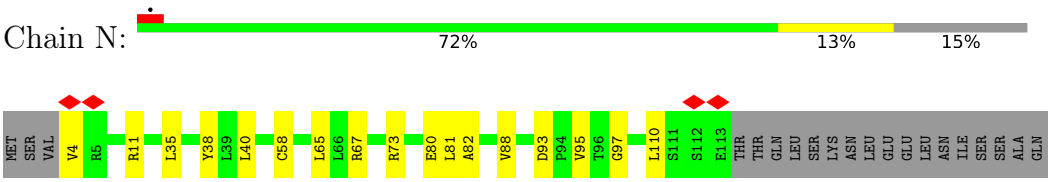
• Molecule 13: 28S ribosomal protein S16, mitochondrial

Chain M:



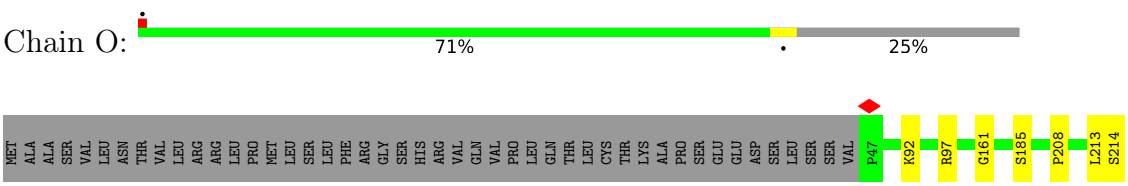
• Molecule 14: 28S ribosomal protein S17, mitochondrial

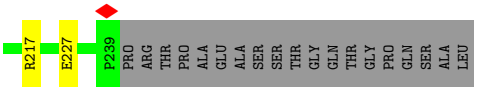
Chain N:



• Molecule 15: 28S ribosomal protein S18b, mitochondrial

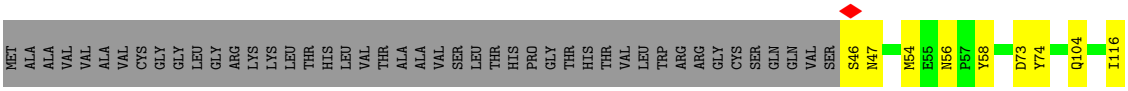
Chain O:

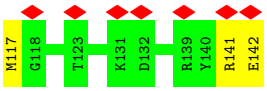




• Molecule 16: 28S ribosomal protein S18c, mitochondrial

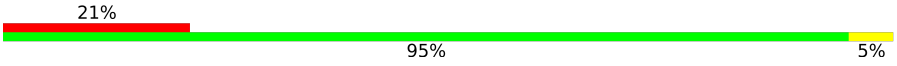
Chain P:

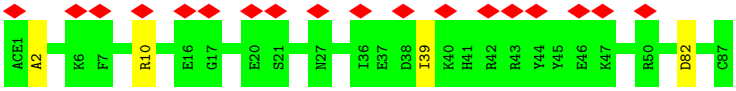




• Molecule 17: Small ribosomal subunit protein bS21m

Chain Q:



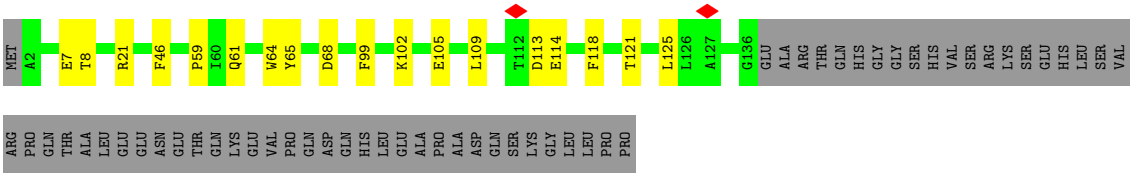


• Molecule 18: 28S ribosomal protein S22, mitochondrial

Chain R:

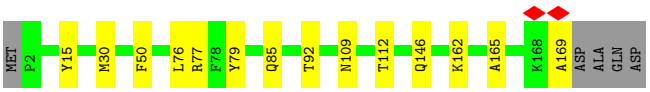
• Molecule 19: 28S ribosomal protein S23, mitochondrial

Chain S:



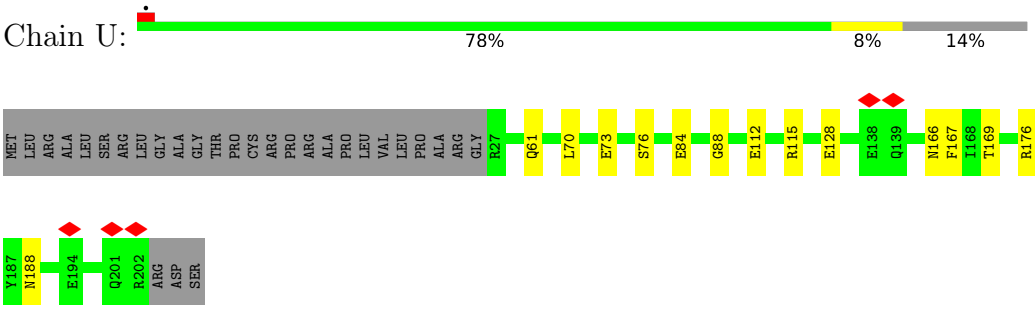
• Molecule 20: 28S ribosomal protein S25, mitochondrial

Chain T:



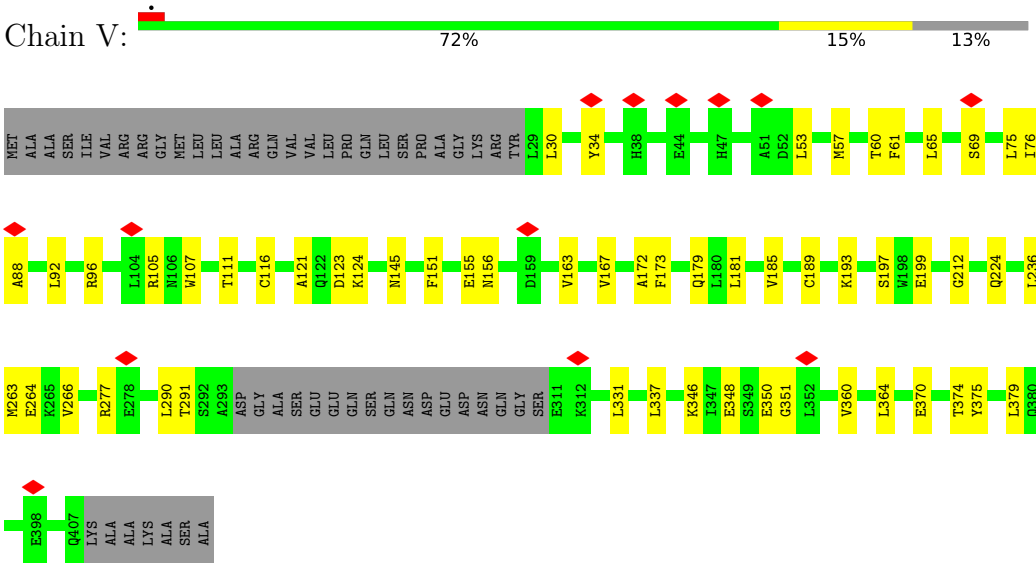
• Molecule 21: 28S ribosomal protein S26, mitochondrial

Chain U:



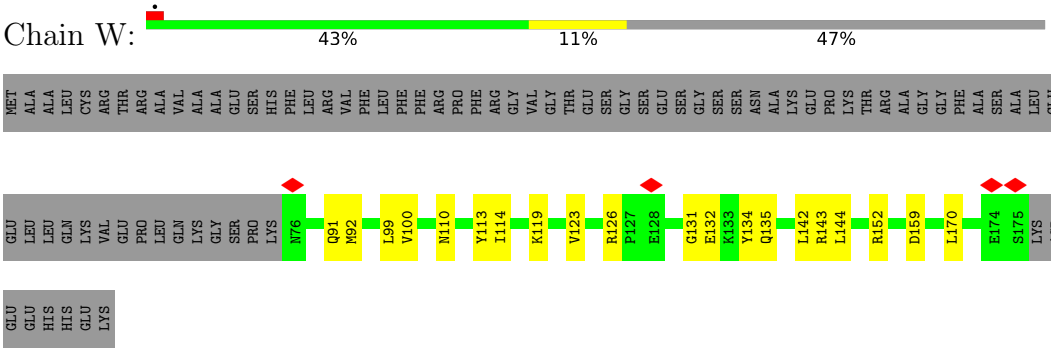
• Molecule 22: 28S ribosomal protein S27, mitochondrial

Chain V:



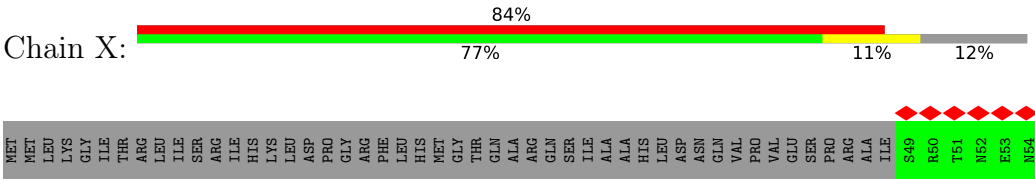
• Molecule 23: 28S ribosomal protein S28, mitochondrial

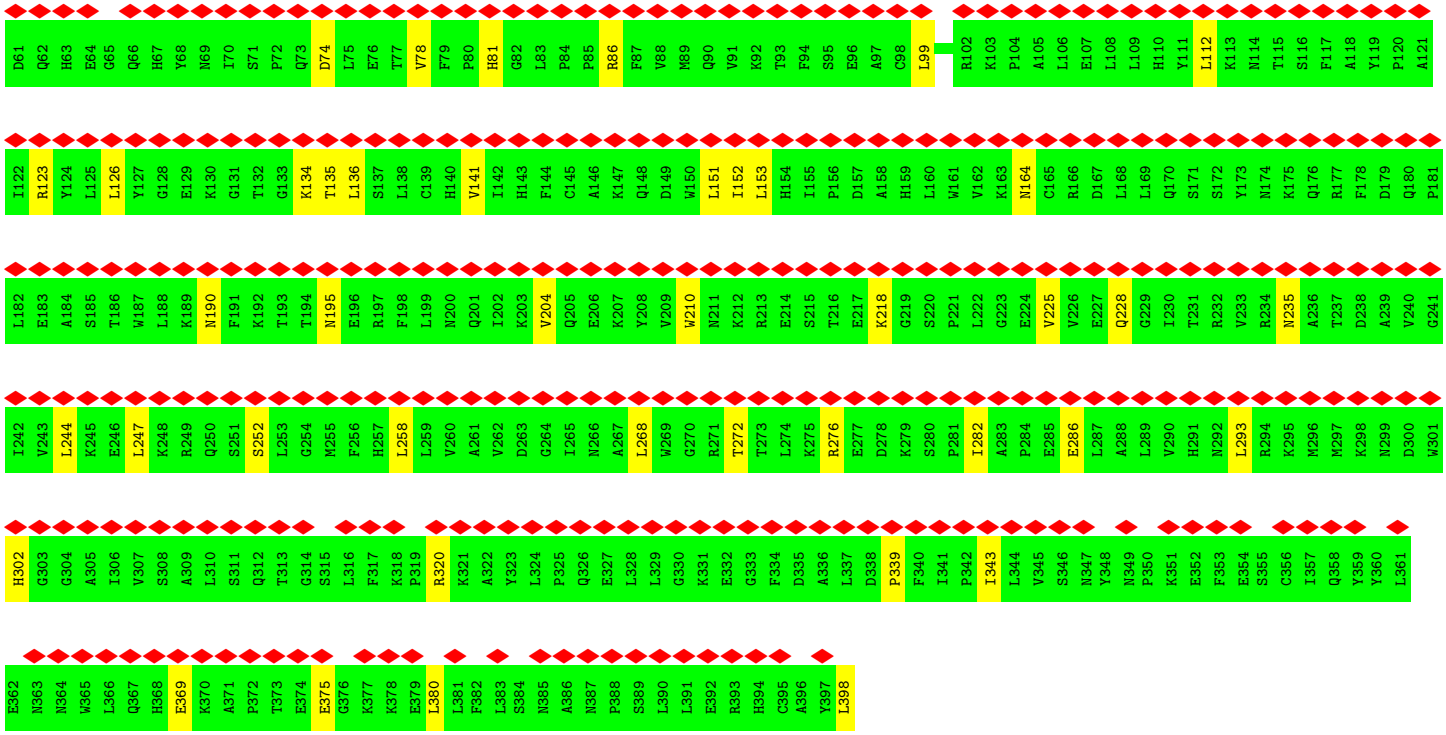
Chain W:



• Molecule 24: 28S ribosomal protein S29, mitochondrial

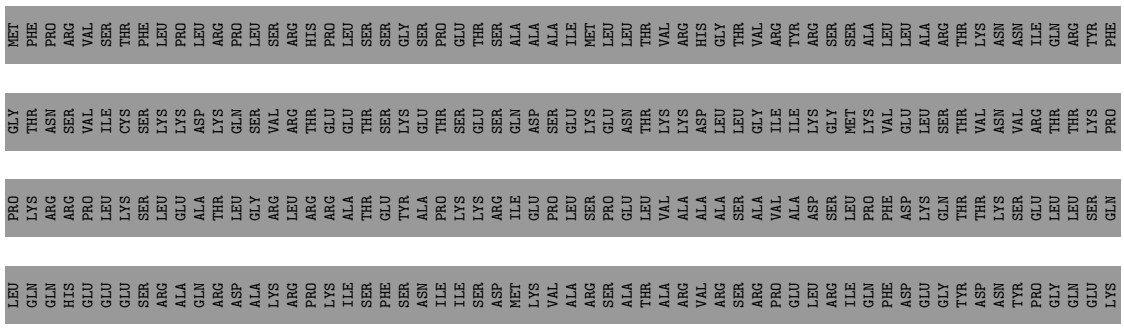
Chain X:

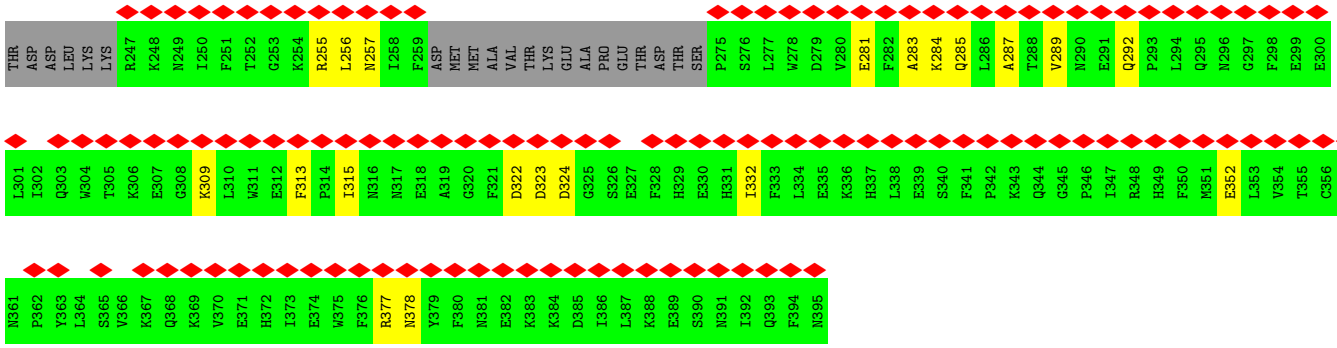




• Molecule 25: 28S ribosomal protein S31, mitochondrial

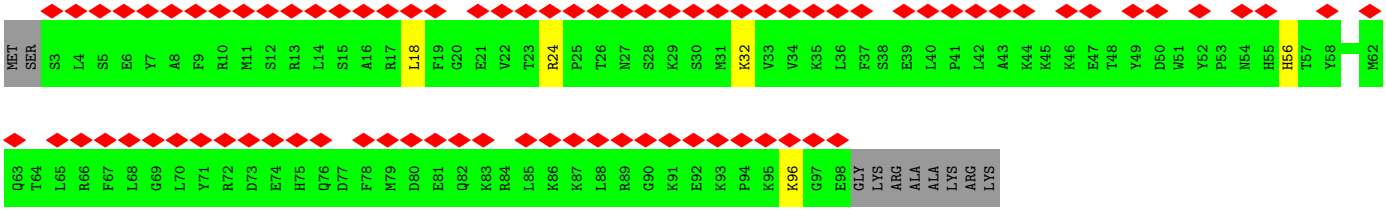
Chain Y:





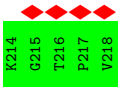
• Molecule 26: 28S ribosomal protein S33, mitochondrial

Chain Z:



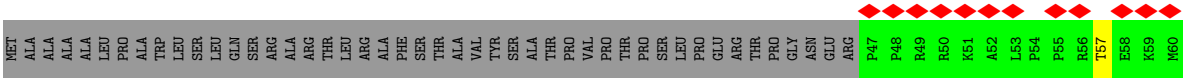
• Molecule 27: Small ribosomal subunit protein mS34

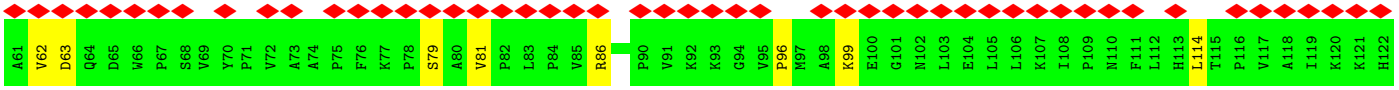
Chain 0:

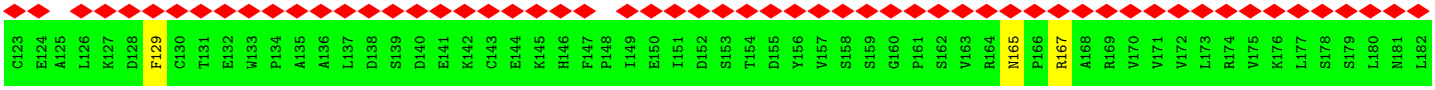


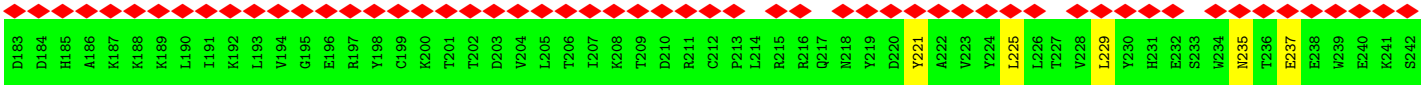
• Molecule 28: 28S ribosomal protein S35, mitochondrial

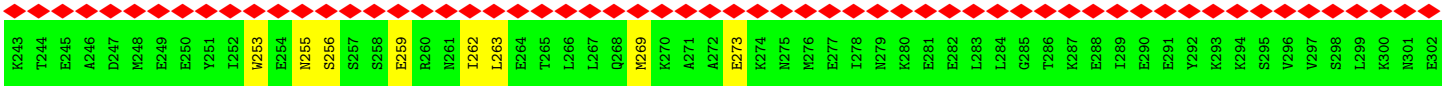
Chain 1:

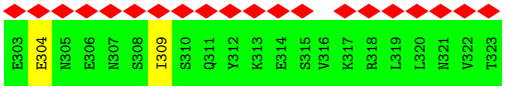






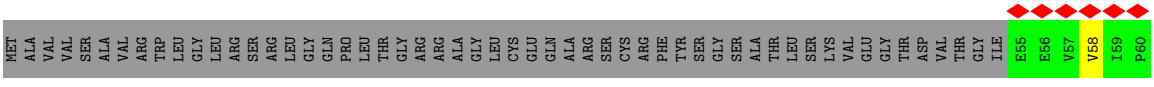


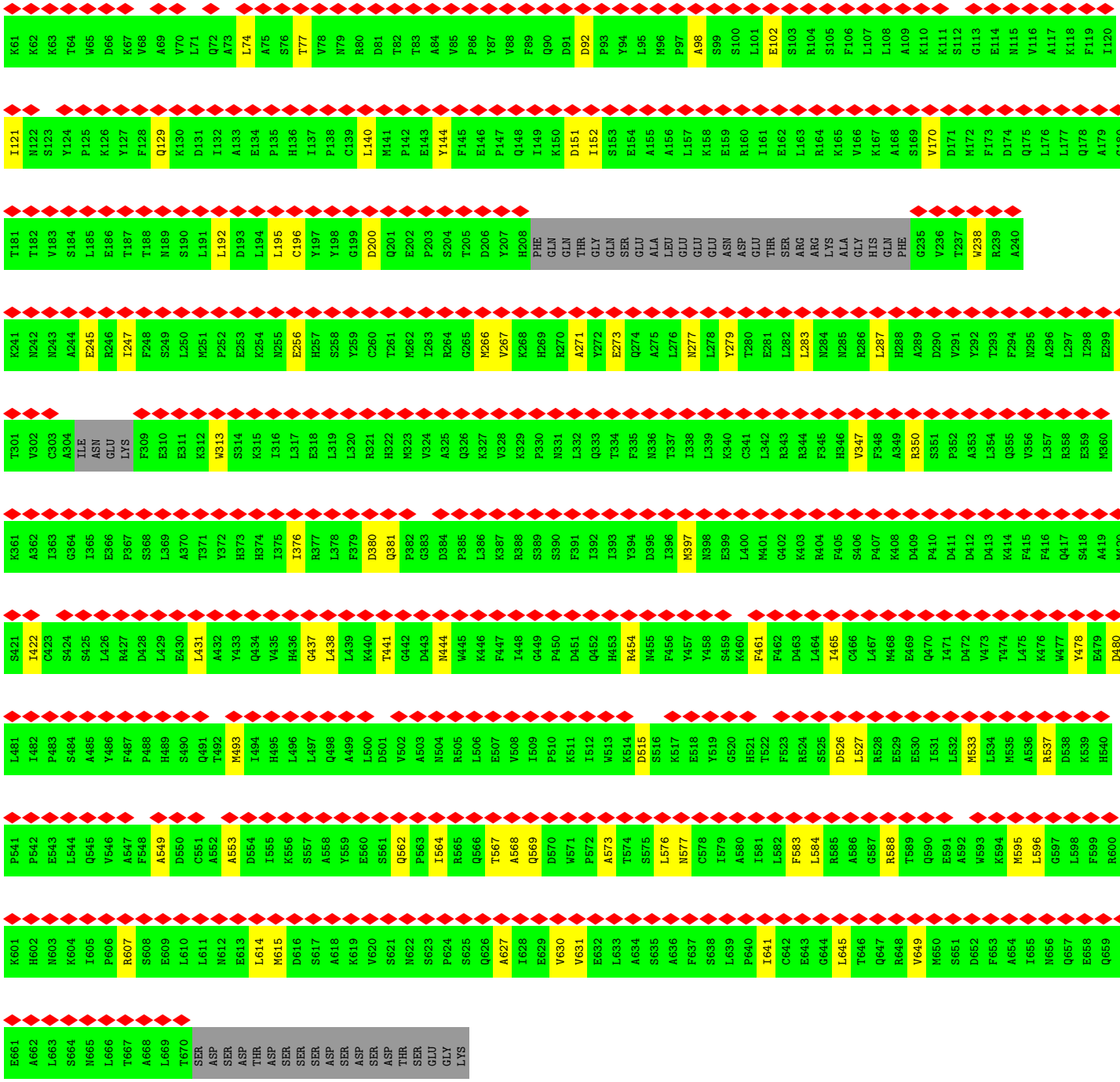




• Molecule 29: Pentatricopeptide repeat domain-containing protein 3, mitochondrial

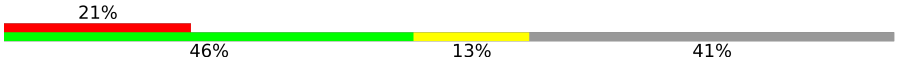
Chain 4:

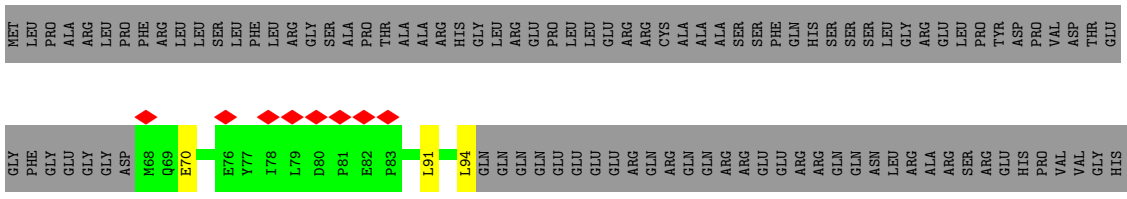


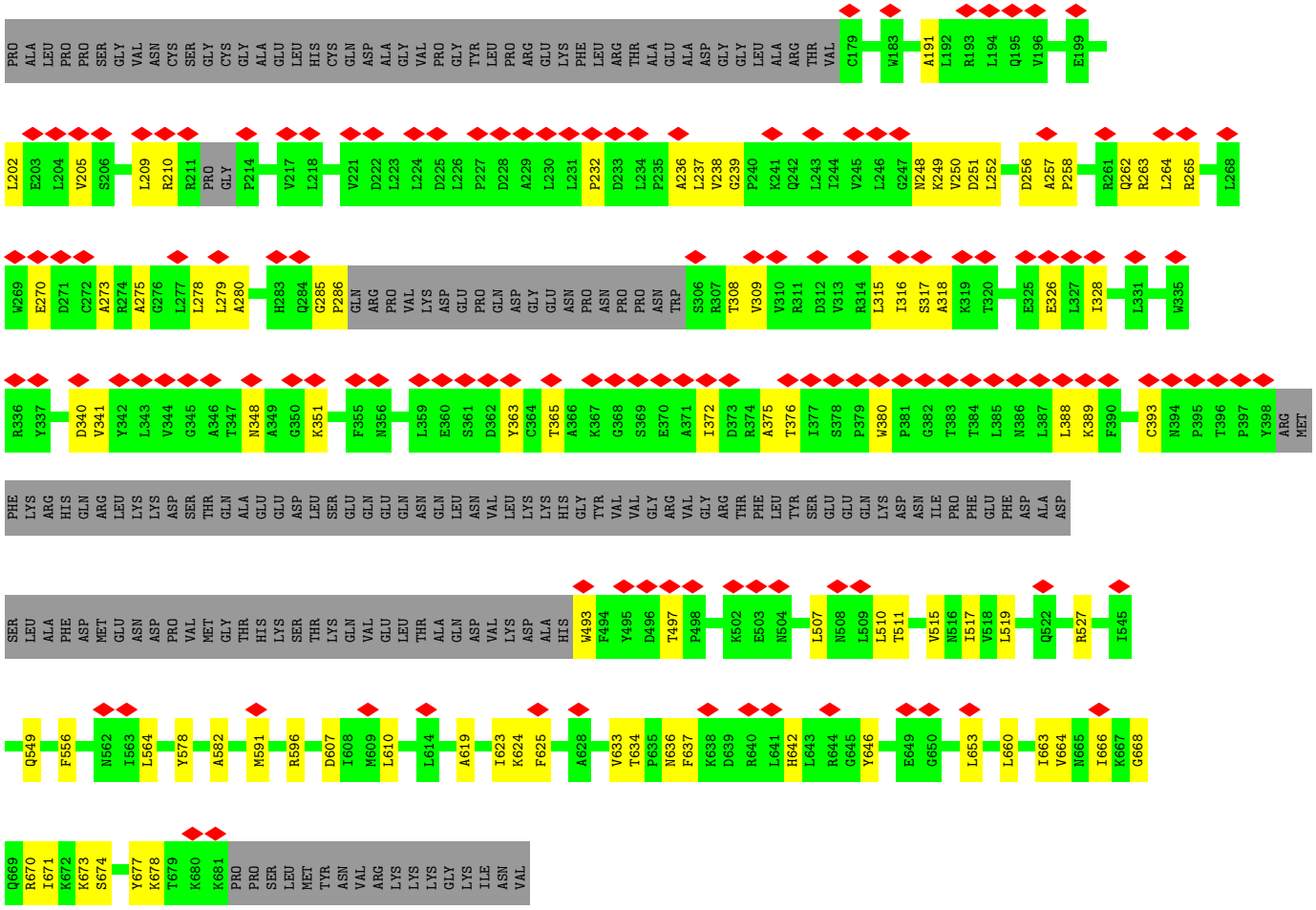


• Molecule 30: Nitric oxide-associated protein 1

Chain 9:

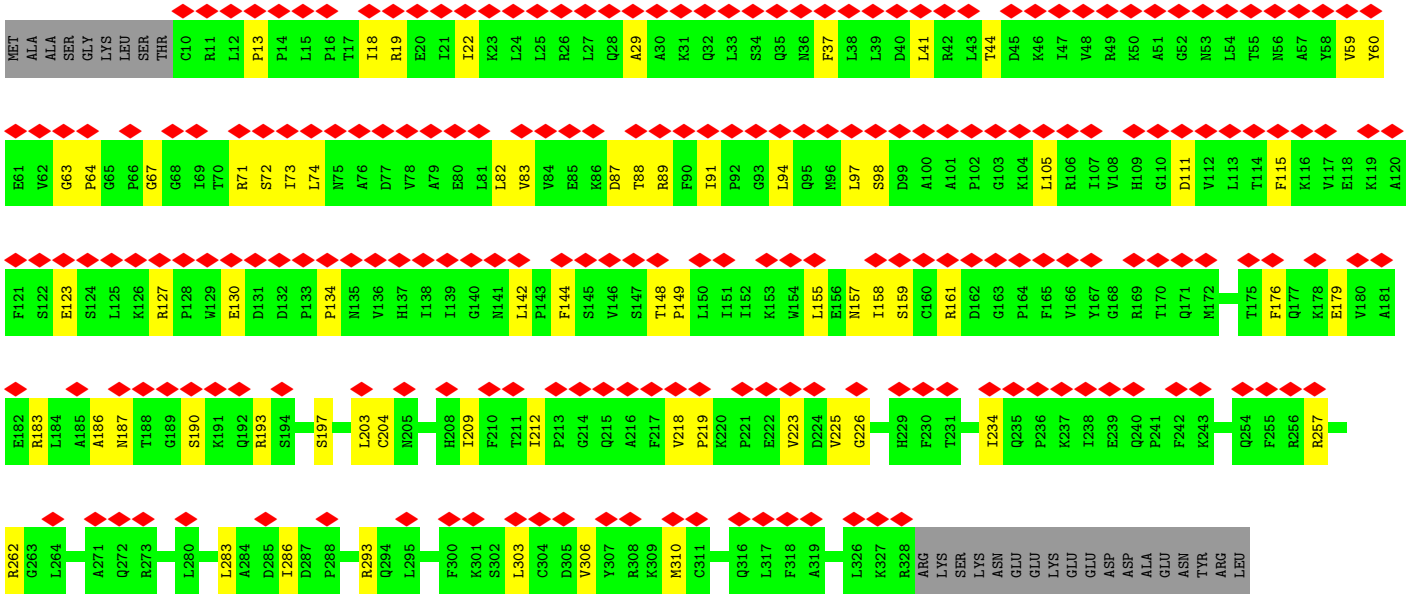






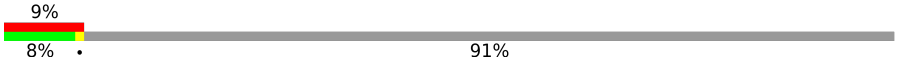
• Molecule 31: Dimethyladenosine transferase 1, mitochondrial

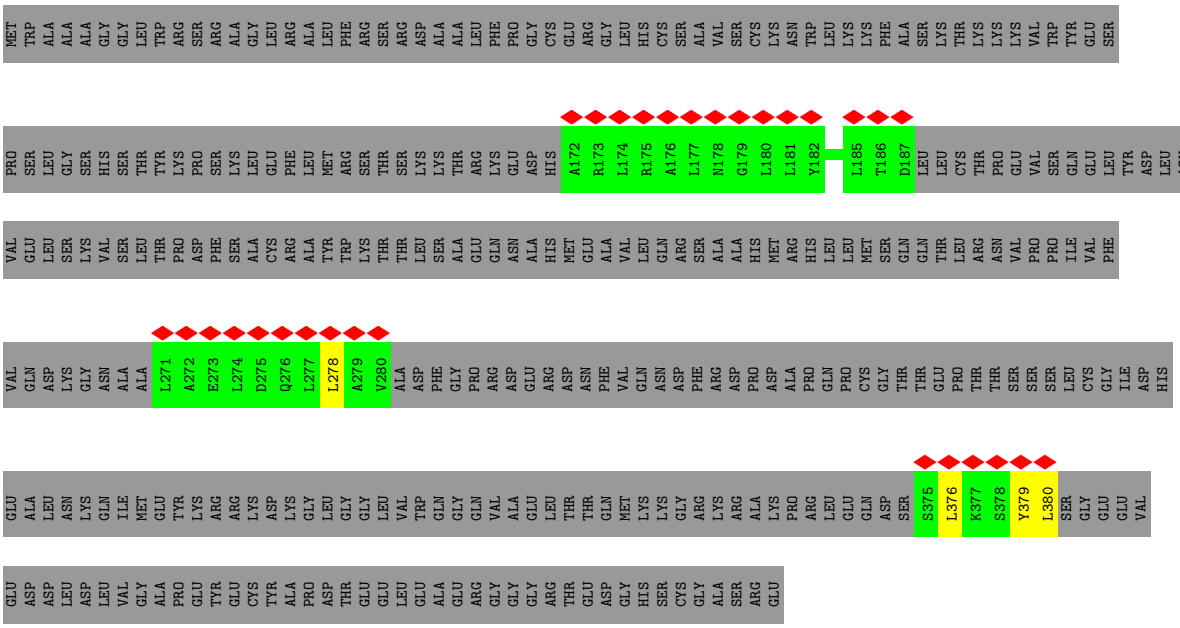
Chain 5:



• Molecule 32: Putative ribosome-binding factor A, mitochondrial

Chain a:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16018	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.037	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0054	Depositor
Map size (Å)	606.0, 606.0, 606.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, ATP, ZN, K, 5F0, FES, MG, 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	A	0.18	0/20197	0.23	0/31437
2	B	0.19	0/1871	0.25	0/2531
3	C	0.16	0/1113	0.22	0/1505
4	D	0.18	0/2694	0.25	0/3608
5	E	0.13	0/880	0.27	0/1189
6	F	0.12	0/1709	0.23	0/2297
7	G	0.15	0/2632	0.23	0/3527
8	H	0.16	0/1178	0.25	0/1598
9	I	0.10	0/1030	0.23	0/1386
10	J	0.15	0/855	0.25	0/1148
11	K	0.14	0/880	0.24	0/1182
12	L	0.14	0/1408	0.25	0/1882
13	M	0.20	0/963	0.26	0/1295
14	N	0.19	0/886	0.25	0/1199
15	O	0.18	0/1648	0.24	0/2243
16	P	0.12	0/798	0.26	0/1070
17	Q	0.15	0/754	0.23	0/1003
18	R	0.18	0/2456	0.23	0/3317
19	S	0.16	0/1138	0.24	0/1533
20	T	0.18	0/1402	0.25	0/1883
21	U	0.14	0/1510	0.22	0/2025
22	V	0.10	0/3030	0.23	0/4093
23	W	0.15	0/801	0.26	0/1079
24	X	0.14	0/2908	0.25	0/3936
25	Y	0.14	0/1168	0.23	0/1570
26	Z	0.14	0/828	0.22	0/1104
27	0	0.14	0/1834	0.26	0/2484
28	1	0.13	0/2293	0.22	0/3102
29	4	0.10	0/4848	0.21	0/6560
30	9	0.12	0/3350	0.28	0/4549
31	5	0.13	0/2624	0.28	0/3552
32	a	0.14	0/248	0.32	0/331

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.15	0/71934	0.24	0/101218

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	18058	9165	9171	105	0
2	B	1828	1826	1815	14	0
3	C	1083	1096	1088	16	0
4	D	2644	2705	2693	29	0
5	E	865	882	878	13	0
6	F	1672	1733	1722	16	0
7	G	2577	2570	2560	21	0
8	H	1152	1191	1183	12	0
9	I	1020	1066	1053	11	0
10	J	839	892	887	8	0
11	K	862	889	885	8	0
12	L	1384	1467	1462	10	0
13	M	942	972	965	6	0
14	N	868	933	928	13	0
15	O	1592	1566	1557	8	0
16	P	781	809	806	8	0
17	Q	744	760	758	3	0
18	R	2409	2436	2428	16	0
19	S	1111	1117	1115	12	0
20	T	1371	1396	1393	10	0
21	U	1488	1505	1499	13	0
22	V	2969	2972	2961	39	0
23	W	789	806	802	12	0
24	X	2836	2842	2827	27	0
25	Y	1136	1100	1094	14	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	Z	810	828	824	5	0
27	0	1787	1802	1796	23	0
28	1	2245	2281	2276	17	0
29	4	4741	4761	4742	51	0
30	9	3278	3378	3371	70	0
31	5	2568	2661	2655	47	0
32	a	249	271	270	6	0
33	A	39	0	0	0	0
33	B	1	0	0	0	0
33	X	1	0	0	0	0
34	A	10	0	0	0	0
35	O	1	0	0	0	0
36	P	4	0	0	0	0
36	T	4	0	0	0	0
37	X	31	12	12	2	0
38	9	28	10	12	1	0
38	X	28	10	12	0	0
All	All	68845	60710	60500	572	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 5.

The worst 5 of 572 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)
30:9:623:ILE:HG22	30:9:653:LEU:HD11	1.46	0.94
1:A:1237:A:OP1	11:K:36:ARG:NH2	2.07	0.87
1:A:1429:C:OP1	7:G:388:ARG:NH1	2.12	0.83
30:9:624:LYS:O	30:9:653:LEU:HD12	1.89	0.72
22:V:167:VAL:HG13	22:V:172:ALA:HB3	1.72	0.71

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	
2	B	223/296 (75%)	220 (99%)	3 (1%)	0	100	100
3	C	130/167 (78%)	127 (98%)	3 (2%)	0	100	100
4	D	326/430 (76%)	320 (98%)	6 (2%)	0	100	100
5	E	107/125 (86%)	104 (97%)	3 (3%)	0	100	100
6	F	199/242 (82%)	198 (100%)	1 (0%)	0	100	100
7	G	309/396 (78%)	303 (98%)	6 (2%)	0	100	100
8	H	138/201 (69%)	135 (98%)	2 (1%)	1 (1%)	18	47
9	I	134/194 (69%)	132 (98%)	2 (2%)	0	100	100
10	J	106/138 (77%)	102 (96%)	4 (4%)	0	100	100
11	K	99/128 (77%)	99 (100%)	0	0	100	100
12	L	162/257 (63%)	160 (99%)	2 (1%)	0	100	100
13	M	117/137 (85%)	117 (100%)	0	0	100	100
14	N	108/130 (83%)	108 (100%)	0	0	100	100
15	O	191/258 (74%)	188 (98%)	3 (2%)	0	100	100
16	P	95/142 (67%)	92 (97%)	3 (3%)	0	100	100
17	Q	85/87 (98%)	82 (96%)	2 (2%)	1 (1%)	10	35
18	R	293/360 (81%)	289 (99%)	4 (1%)	0	100	100
19	S	133/190 (70%)	128 (96%)	5 (4%)	0	100	100
20	T	166/173 (96%)	164 (99%)	2 (1%)	0	100	100
21	U	174/205 (85%)	173 (99%)	1 (1%)	0	100	100
22	V	358/414 (86%)	355 (99%)	3 (1%)	0	100	100
23	W	98/187 (52%)	96 (98%)	2 (2%)	0	100	100
24	X	348/398 (87%)	342 (98%)	6 (2%)	0	100	100
25	Y	130/395 (33%)	128 (98%)	2 (2%)	0	100	100
26	Z	94/106 (89%)	94 (100%)	0	0	100	100
27	0	213/215 (99%)	207 (97%)	6 (3%)	0	100	100
28	1	275/323 (85%)	273 (99%)	2 (1%)	0	100	100
29	4	580/689 (84%)	570 (98%)	10 (2%)	0	100	100
30	9	403/698 (58%)	385 (96%)	18 (4%)	0	100	100
31	5	317/346 (92%)	313 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	a	26/343 (8%)	26 (100%)	0	0	100	100
All	All	6137/8370 (73%)	6030 (98%)	105 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	126	ILE
17	Q	2	ALA

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	
2	B	198/249 (80%)	198 (100%)	0	100	100
3	C	115/143 (80%)	115 (100%)	0	100	100
4	D	278/357 (78%)	278 (100%)	0	100	100
5	E	92/107 (86%)	92 (100%)	0	100	100
6	F	182/209 (87%)	182 (100%)	0	100	100
7	G	272/342 (80%)	272 (100%)	0	100	100
8	H	130/180 (72%)	130 (100%)	0	100	100
9	I	104/146 (71%)	104 (100%)	0	100	100
10	J	93/118 (79%)	93 (100%)	0	100	100
11	K	91/113 (80%)	91 (100%)	0	100	100
12	L	153/226 (68%)	153 (100%)	0	100	100
13	M	97/113 (86%)	97 (100%)	0	100	100
14	N	96/115 (84%)	96 (100%)	0	100	100
15	O	174/230 (76%)	174 (100%)	0	100	100
16	P	88/123 (72%)	88 (100%)	0	100	100
17	Q	78/78 (100%)	78 (100%)	0	100	100
18	R	264/318 (83%)	264 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	S	116/164 (71%)	116 (100%)	0	100	100
20	T	153/157 (98%)	153 (100%)	0	100	100
21	U	152/174 (87%)	152 (100%)	0	100	100
22	V	325/364 (89%)	325 (100%)	0	100	100
23	W	87/158 (55%)	87 (100%)	0	100	100
24	X	310/351 (88%)	310 (100%)	0	100	100
25	Y	124/357 (35%)	124 (100%)	0	100	100
26	Z	88/95 (93%)	88 (100%)	0	100	100
27	0	188/188 (100%)	188 (100%)	0	100	100
28	1	255/291 (88%)	255 (100%)	0	100	100
29	4	523/609 (86%)	523 (100%)	0	100	100
30	9	358/600 (60%)	358 (100%)	0	100	100
31	5	286/309 (93%)	286 (100%)	0	100	100
32	a	26/288 (9%)	26 (100%)	0	100	100
All	All	5496/7272 (76%)	5496 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
20	T	59	ASN
31	5	192	GLN
24	X	180	GLN
31	5	137	HIS
29	4	562	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	844/955 (88%)	132 (15%)	4 (0%)

5 of 132 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	651	A

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Mol	Chain	Res	Type
1	A	657	G
1	A	680	U
1	A	688	A
1	A	704	U

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	928	A
1	A	930	G
1	A	931	C
1	A	1154	A

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
9	5F0	I	184	9	8,8,9	0.58	0	7,9,11	1.09	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	5F0	I	184	9	-	0/9/9/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	184	5F0	O-C-CB	-2.54	118.01	125.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 57 ligands modelled in this entry, 52 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
37	ATP	X	501	33	29,33,33	0.49	0	44,52,52	0.58	0
36	FES	T	201	20,13	0,4,4	-	-	-		
38	GDP	X	502	-	28,30,30	0.43	0	44,47,47	0.41	0
36	FES	P	201	5,16	0,4,4	-	-	-		
38	GDP	9	801	-	28,30,30	0.44	0	44,47,47	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	ATP	X	501	33	-	0/22/38/38	0/3/3/3
36	FES	T	201	20,13	-	-	0/1/1/1
38	GDP	X	502	-	-	3/16/32/32	0/3/3/3
36	FES	P	201	5,16	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	GDP	9	801	-	-	0/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	X	502	GDP	C5'-O5'-PA-O1A
38	X	502	GDP	C5'-O5'-PA-O3A
38	X	502	GDP	C4'-C5'-O5'-PA

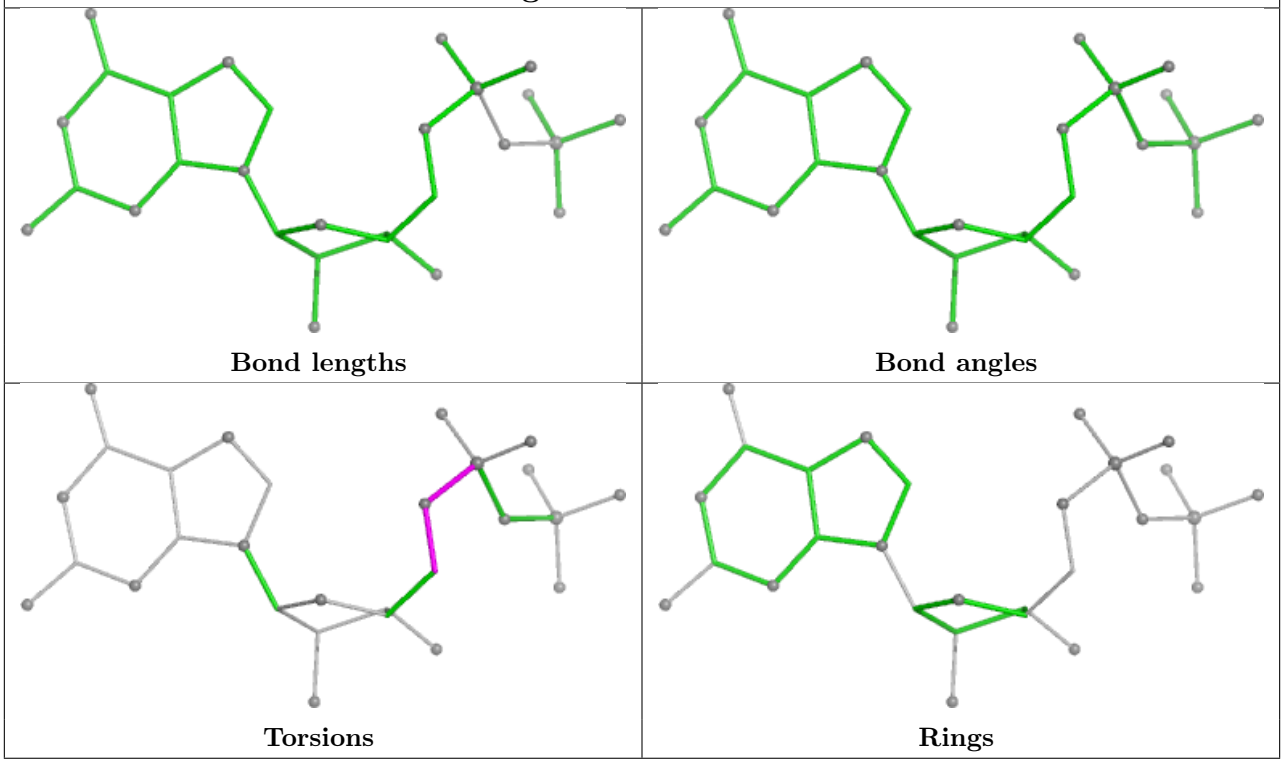
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	X	501	ATP	2	0
38	9	801	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 GDP X 502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
30	9	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	9	279:LEU	C	280:ALA	N	4.87

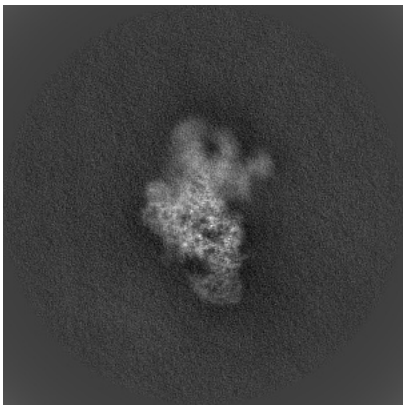
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51877. These allow visual inspection of the internal detail of the map and identification of artifacts.

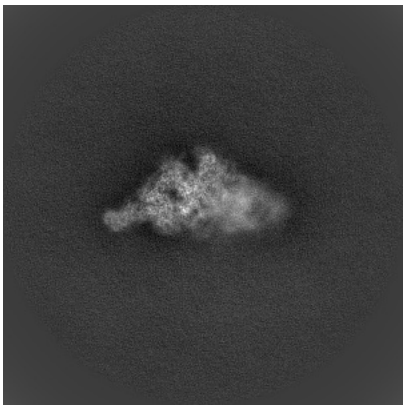
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

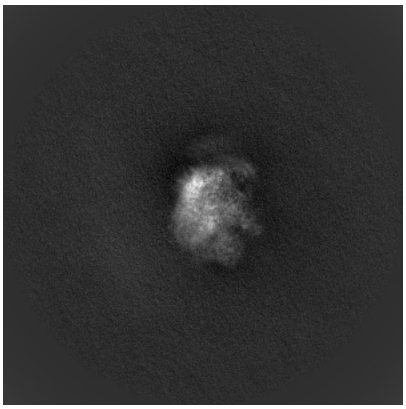
6.1.1 Primary map



X

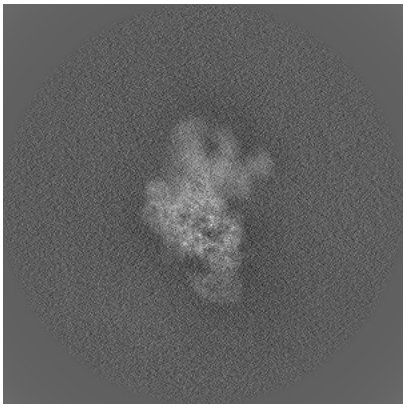


Y

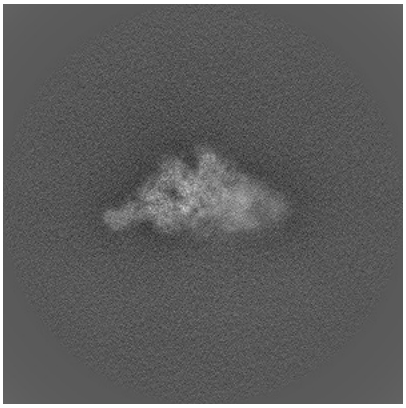


Z

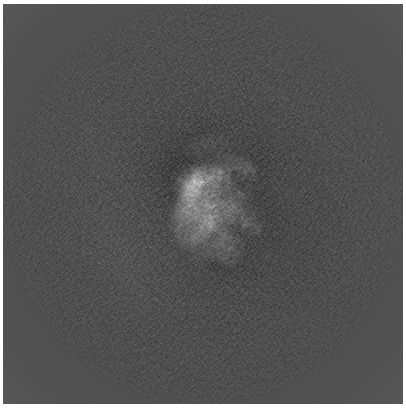
6.1.2 Raw map



X



Y

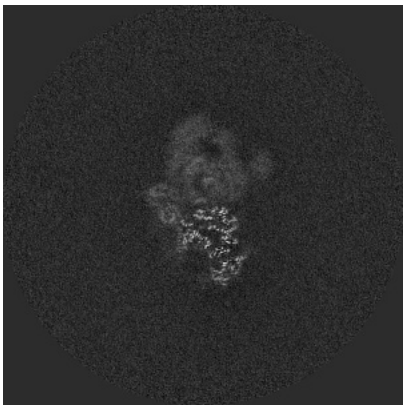


Z

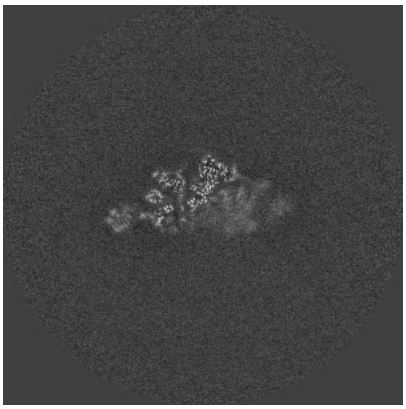
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

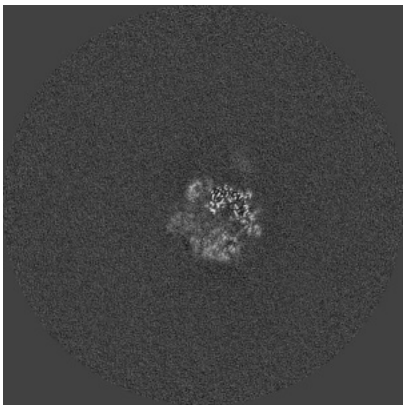
6.2.1 Primary map



X Index: 300

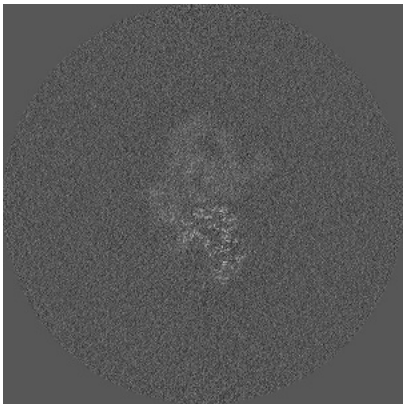


Y Index: 300

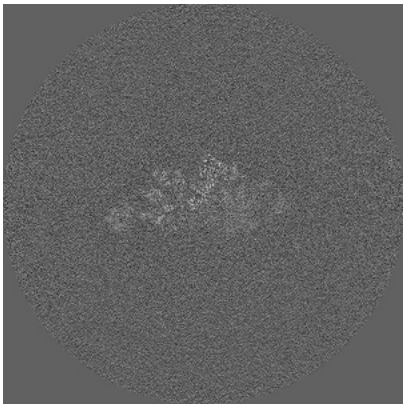


Z Index: 300

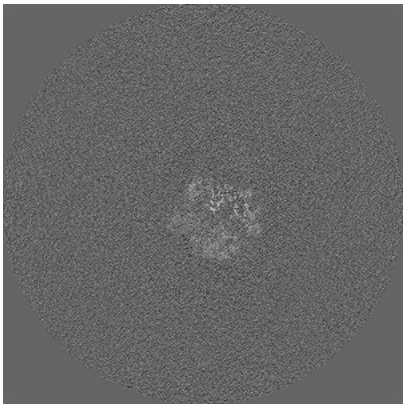
6.2.2 Raw map



X Index: 300



Y Index: 300



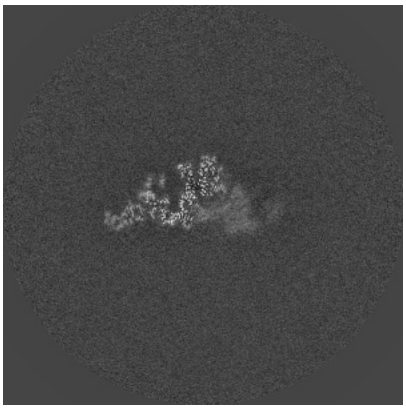
Z Index: 300

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

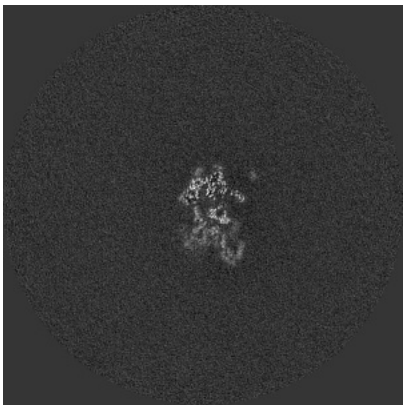
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 314

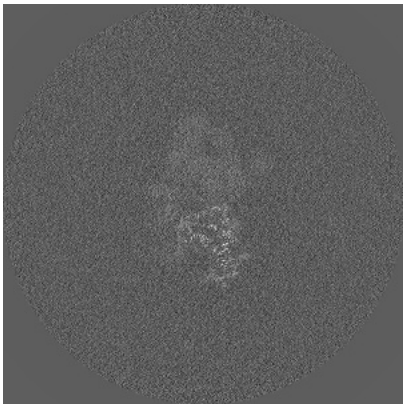


Y Index: 313

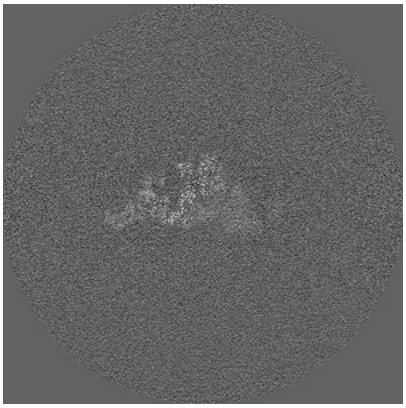


Z Index: 273

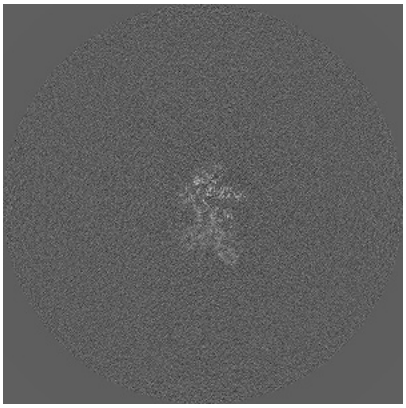
6.3.2 Raw map



X Index: 297



Y Index: 313

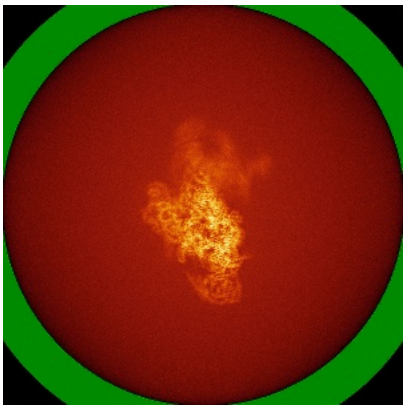


Z Index: 278

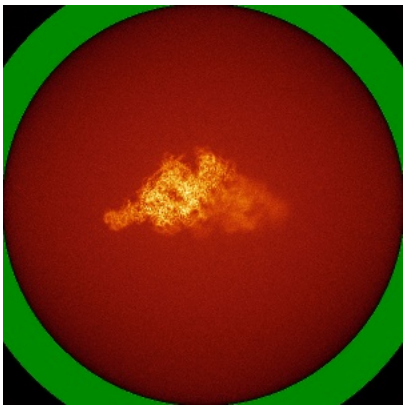
The images above show the largest variance slices of the map in three orthogonal directions.

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

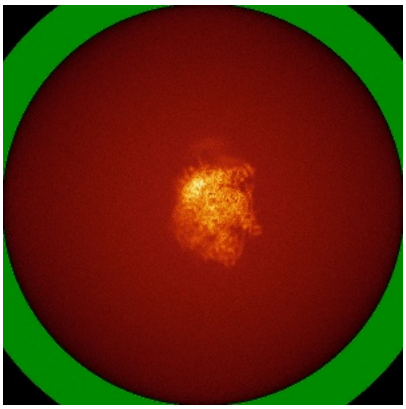
6.4.1 Primary map



X

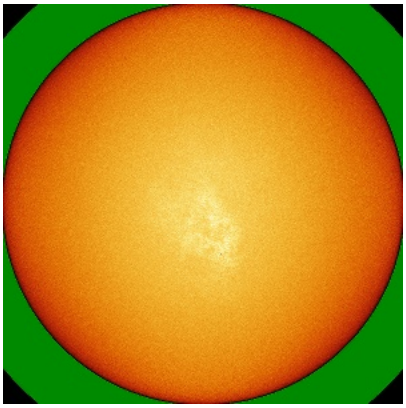


Y

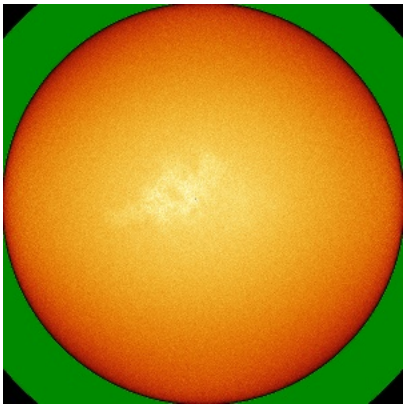


Z

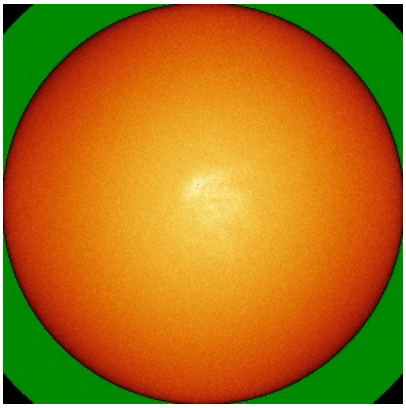
6.4.2 Raw map



X



Y



Z

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

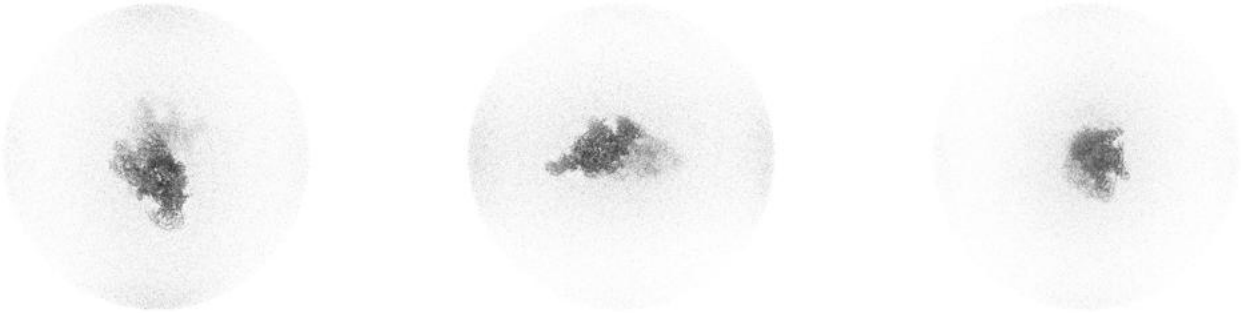
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0054. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

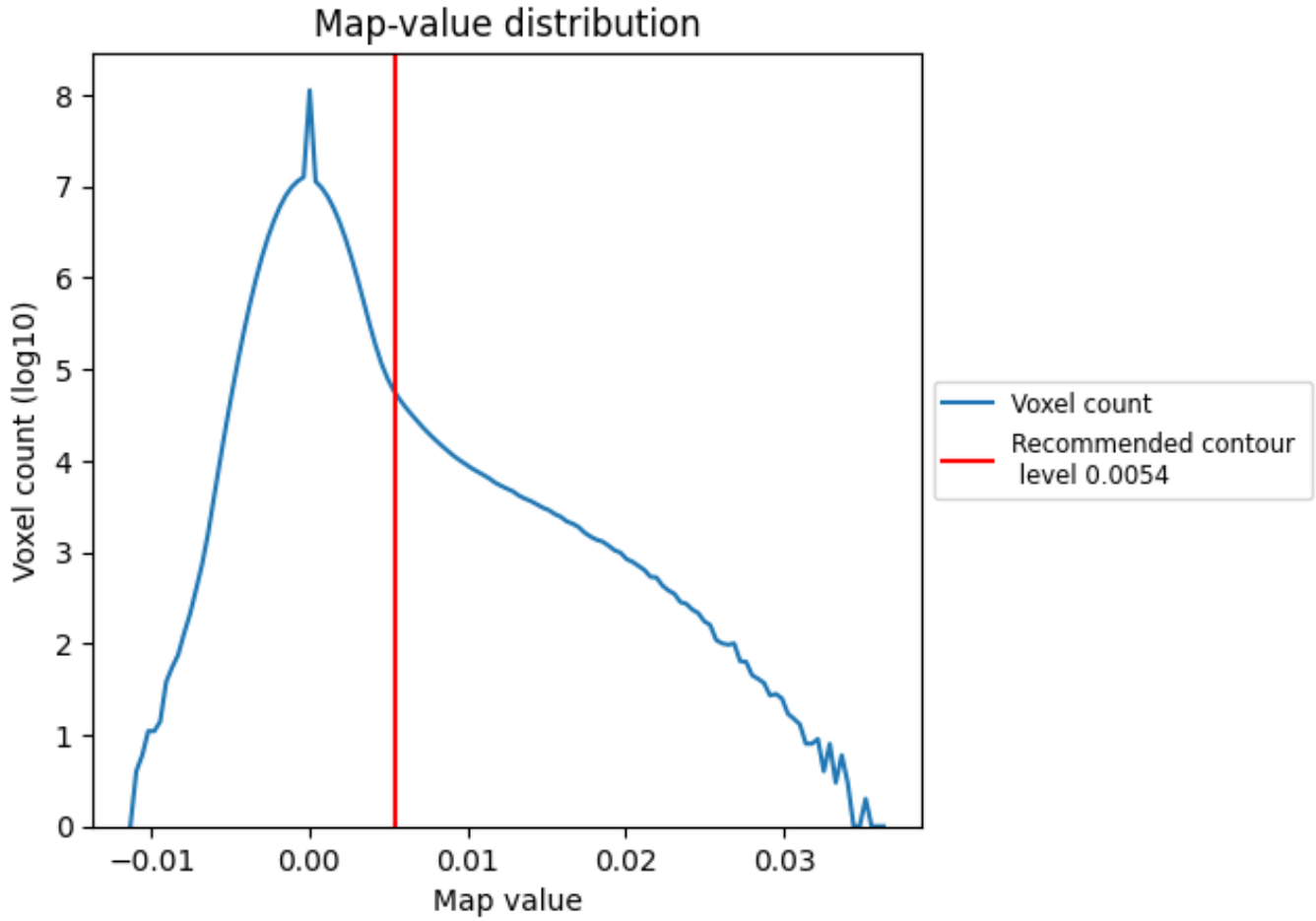
6.6 Mask visualisation (i)

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

7 Map analysis

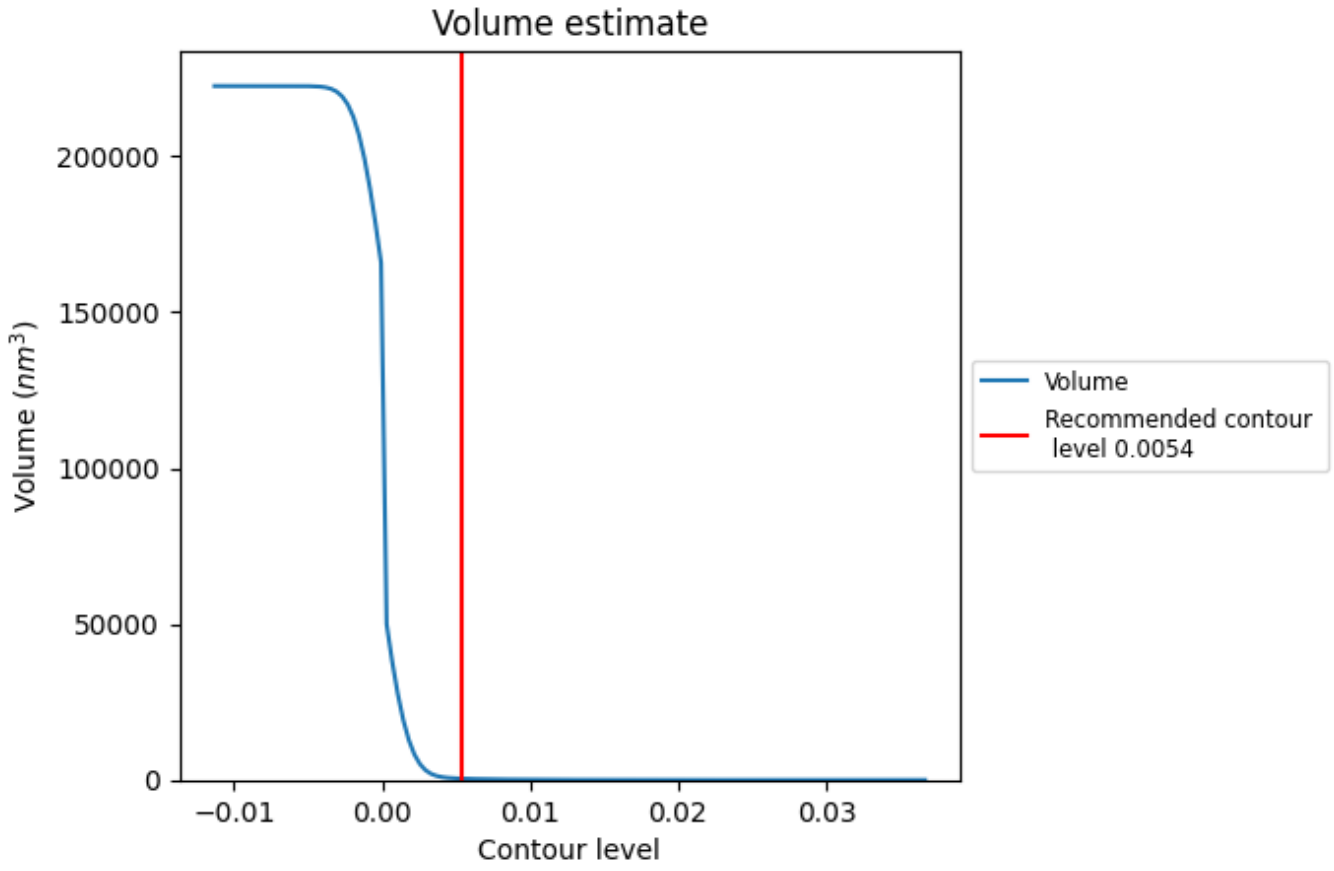
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

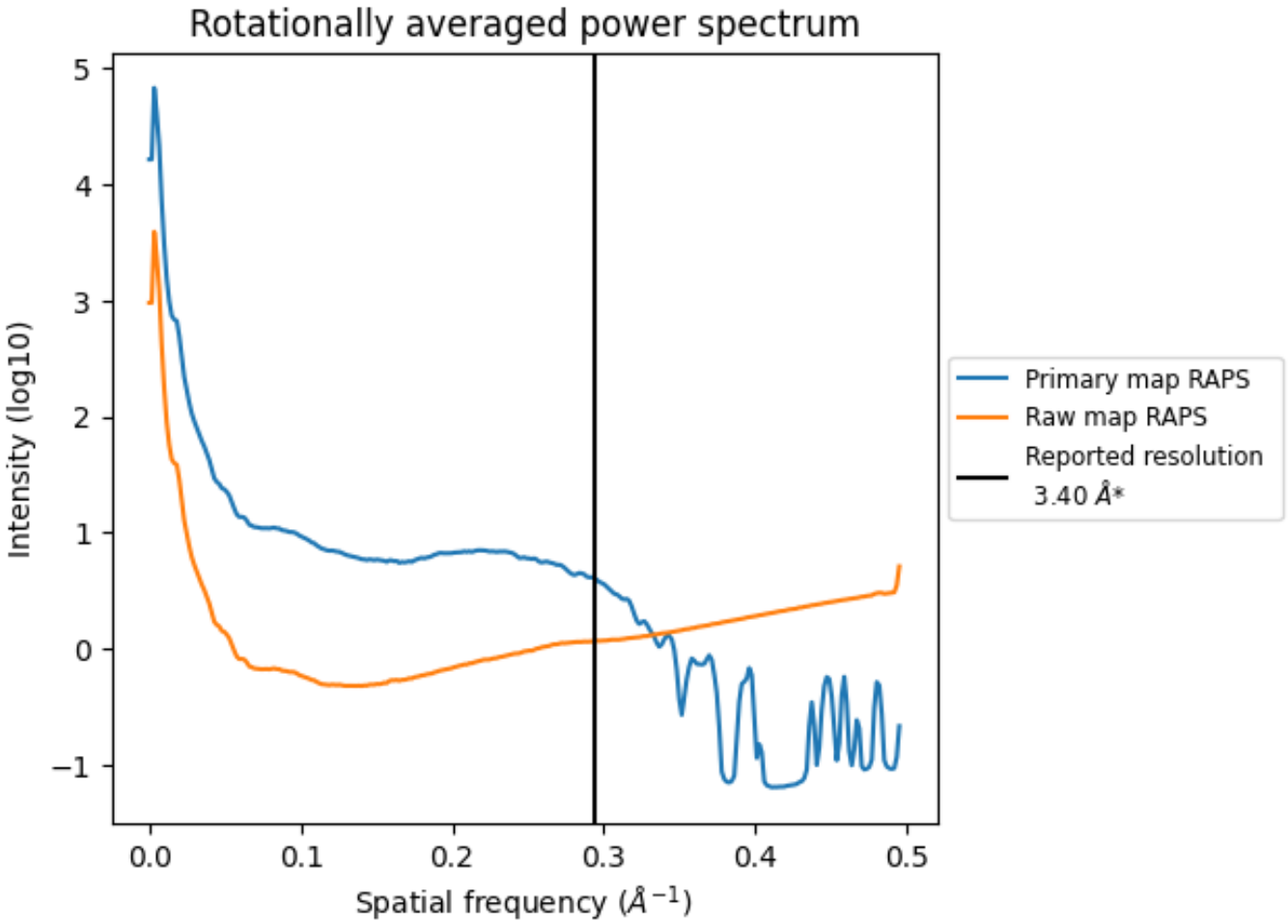
7.2 Volume estimate (i)



The volume at the recommended contour level is 419 nm^3; this corresponds to an approximate mass of 379 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)

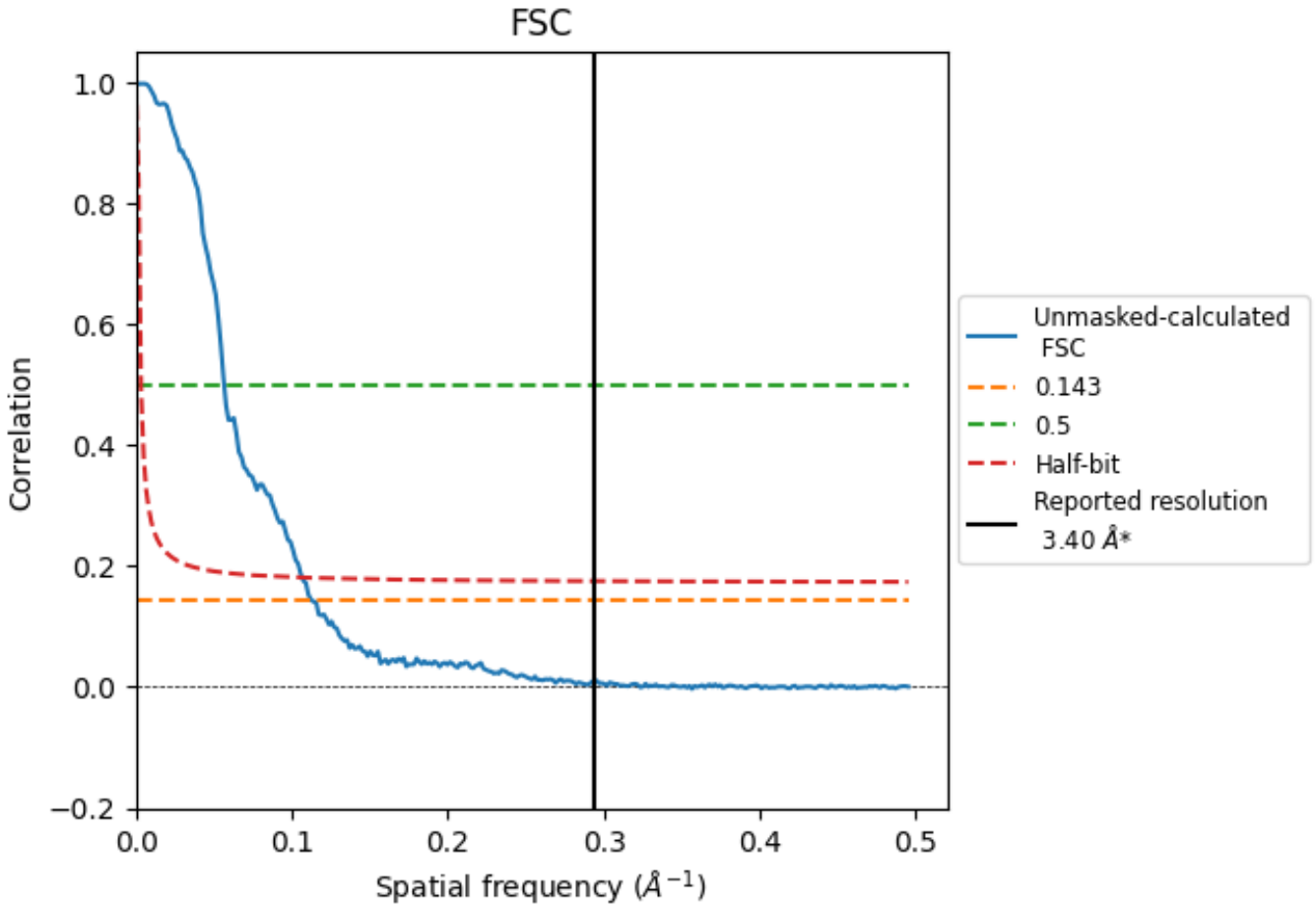


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

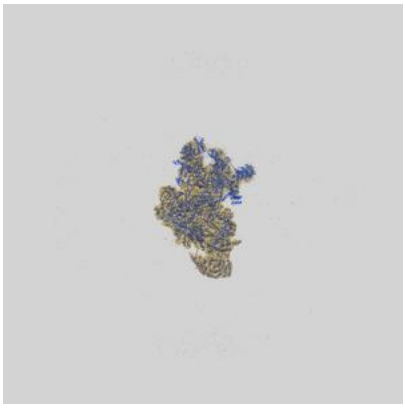
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	3.40	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.87	17.70	9.39

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.5 CUT-OFF 17.70 differs from the reported value 3.4 by more than 10 %

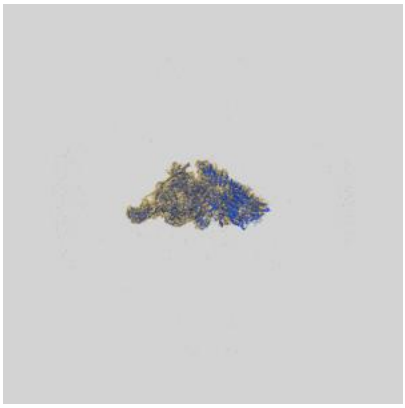
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51877 and PDB model 9H55. Per-residue inclusion information can be found in section 3 on page 12.

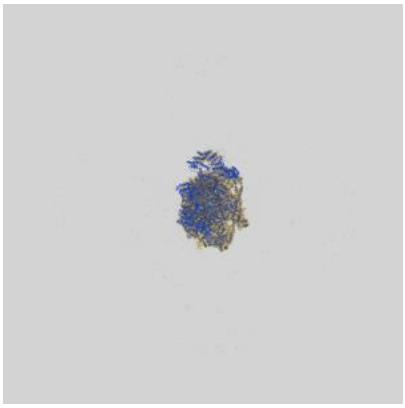
9.1 Map-model overlay



X



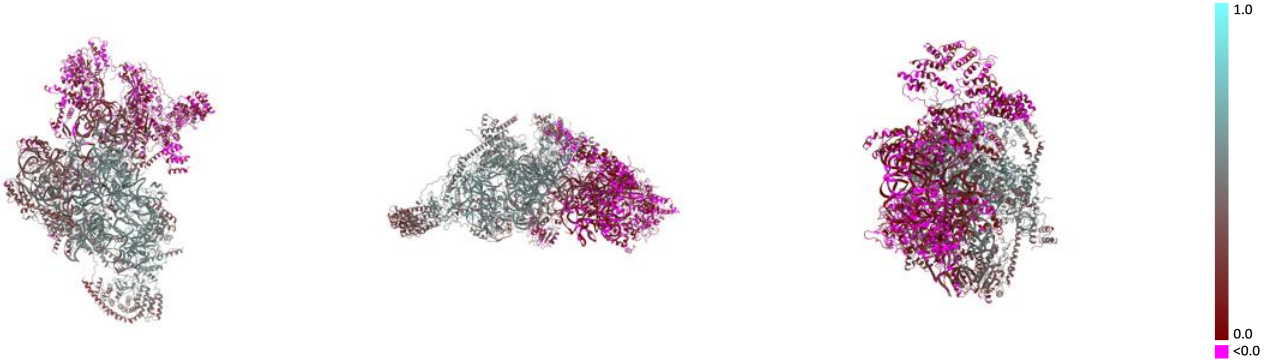
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0054 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

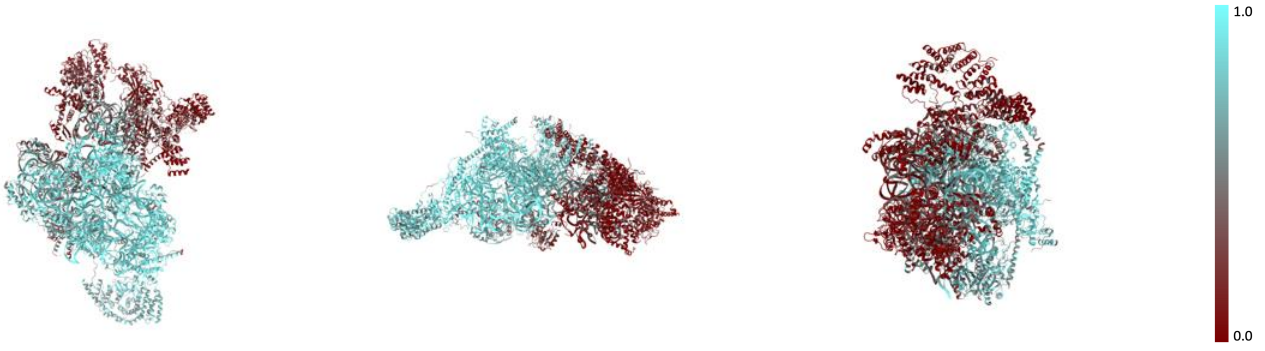
9.2 Q-score mapped to coordinate model



X Y Z

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

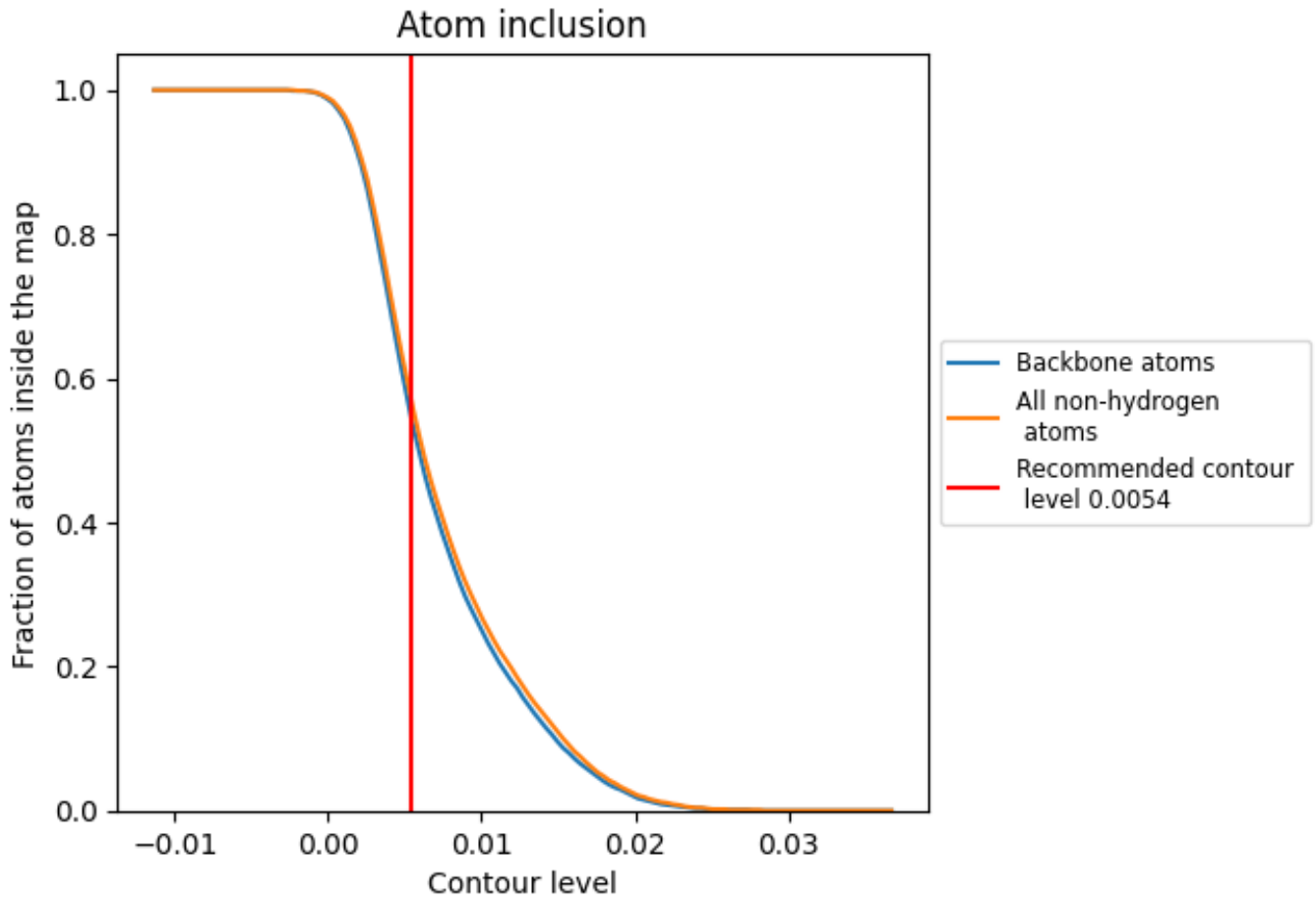
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0054).

9.4 Atom inclusion (i)



At the recommended contour level, 55% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0054) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5710	0.3030
0	0.8260	0.4810
1	0.1190	0.0360
4	0.0860	0.0430
5	0.2970	0.1760
9	0.4940	0.2860
A	0.7210	0.3670
B	0.8910	0.5310
C	0.2420	0.1160
D	0.6660	0.4240
E	0.7240	0.3530
F	0.1110	0.0300
G	0.4150	0.2050
H	0.2110	0.0980
I	0.4950	0.2520
J	0.7880	0.4850
K	0.2530	0.0780
L	0.7280	0.4230
M	0.9070	0.5610
N	0.8720	0.5330
O	0.9030	0.5410
P	0.7320	0.3830
Q	0.6240	0.3680
R	0.8700	0.5130
S	0.8200	0.4500
T	0.8650	0.5210
U	0.7710	0.4110
V	0.7030	0.3220
W	0.8050	0.4860
X	0.0910	0.0340
Y	0.0920	0.0630
Z	0.1700	0.0910
a	0.0950	0.1280