wwPDB EM Validation Summary Report

Feb 13, 2024 – 06:17 PM EST

PDB ID	:	3J6B
EMDB ID	:	EMD-2566
Title	:	Structure of the yeast mitochondrial large ribosomal subunit
Authors	:	Amunts, A.; Brown, A.; Bai, X.C.; Llacer, J.L.; Hussain, T.; Emsley, P.; Long, F.; Murshudov, G.; Scheres, S.H.W.; Ramakrishnan, V.
Deposited on	:	2014-01-22
Resolution	:	3.20 Å(reported)

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

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

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

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

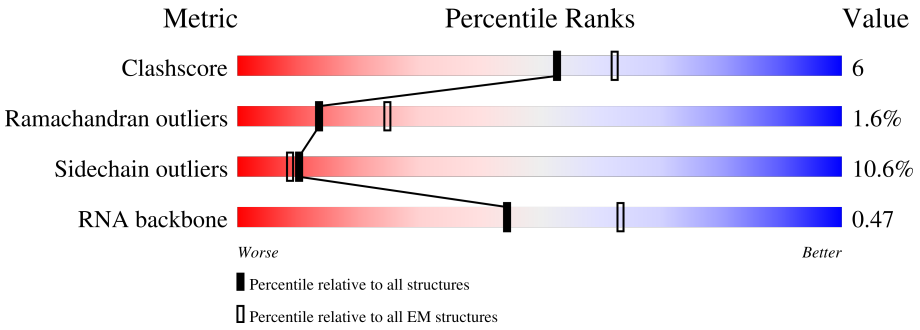
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	A	3296	48% 26% 8% 18%
2	B	393	55% 18% • 25%
3	C	269	74% 16% • 7%
4	D	286	62% 18% • 16%
5	E	292	78% 15% • 6%
6	F	214	66% 17% • 14%
7	G	139	35% 5% 60%

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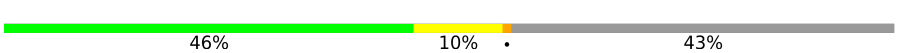
Mol	Chain	Length	Quality of chain
8	H	163	
9	I	138	
10	J	322	
11	K	232	
12	L	238	
13	M	169	
14	N	161	
15	O	309	
16	P	263	
17	Q	297	
18	R	371	
19	S	258	
20	T	319	
21	U	86	
22	V	177	
23	W	183	
24	X	70	
25	Y	105	
26	Z	115	
27	0	93	
28	1	367	
29	2	147	
30	3	146	
31	4	140	
32	5	390	

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Mol	Chain	Length	Quality of chain
33	6	281	62% 11% 26%
34	7	146	53% 19% 27%
35	8	264	58% 10% 31%
36	9	253	62% 13% 23%
37	a	195	77% 12% 10%
38	b	157	84% 14%
39	c	131	84% 6% 10%
40	d	226	78% 12% 10%
41	e	20	70% 65% 35%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
44	ZN	0	100	-	-	X	-

2 Entry composition (i)

There are 44 unique types of molecules in this entry. The entry contains 195137 atoms, of which 83818 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 21S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	2713	86569	25948	28898	10265	18752	2706	0	0

- Molecule 2 is a protein called 54S ribosomal protein RML2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	B	295	4603	1405	2343	459	387	9	0	0

- Molecule 3 is a protein called 54S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	249	3906	1217	1976	360	343	10	0	0

- Molecule 4 is a protein called 54S ribosomal protein YmL6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	239	3780	1187	1914	337	339	3	0	0

- Molecule 5 is a protein called 54S ribosomal protein L7, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	274	4294	1363	2169	387	369	6	0	0

- Molecule 6 is a protein called 54S ribosomal protein L6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	185	2747	870	1392	236	246	3	0	0

- Molecule 7 is a protein called 54S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	55	Total	C	H	N	O	S	0	0
			929	293	471	86	78	1		

- Molecule 8 is a protein called 54S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	148	Total	C	H	N	O	S	0	0
			2394	742	1218	225	205	4		

- Molecule 9 is a protein called 54S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	125	Total	C	H	N	O	S	0	0
			1952	583	1015	175	168	11		

- Molecule 10 is a protein called 54S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	220	Total	C	H	N	O	S	0	0
			3555	1109	1828	325	290	3		

- Molecule 11 is a protein called 54S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	195	Total	C	H	N	O	S	0	0
			3208	1001	1635	297	270	5		

- Molecule 12 is a protein called 54S ribosomal protein L8, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	229	Total	C	H	N	O	S	0	0
			3698	1139	1883	333	335	8		

- Molecule 13 is a protein called 54S ribosomal protein IMG1, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	151	Total	C	H	N	O	S	0	0
			2492	766	1286	220	217	3		

- Molecule 14 is a protein called 54S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	118	Total	C	H	N	O	S	0	0
			1958	598	1010	177	171	2		

- Molecule 15 is a protein called 54S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	223	Total	C	H	N	O	S	0	0
			3684	1147	1895	328	309	5		

- Molecule 16 is a protein called 54S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	207	Total	C	H	N	O	S	0	0
			3450	1101	1728	310	305	6		

- Molecule 17 is a protein called 54S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	279	Total	C	H	N	O	S	0	0
			4287	1368	2161	375	375	8		

- Molecule 18 is a protein called 54S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	318	Total	C	H	N	O	S	0	0
			4981	1571	2500	452	454	4		

- Molecule 19 is a protein called 54S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	146	Total	C	H	N	O	S	0	0
			2440	763	1249	220	207	1		

- Molecule 20 is a protein called 54S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	209	Total	C	H	N	O	S	0	0
			3264	1044	1618	307	292	3		

- Molecule 21 is a protein called 54S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	82	Total	C	H	N	O	0	0
			1341	410	702	116	113		

- Molecule 22 is a protein called 54S ribosomal protein L36, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	V	64	Total	C	H	N	O	S	0	0
			1083	332	555	105	90	1		

- Molecule 23 is a protein called 54S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	W	112	Total	C	H	N	O	S	0	0
			1922	587	985	181	163	6		

- Molecule 24 is a protein called 54S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	64	Total	C	H	N	O	0	0
			1077	330	565	96	86		

- Molecule 25 is a protein called 54S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	45	Total	C	H	N	O	0	0
			788	239	412	80	57		

- Molecule 26 is a protein called mitochondrial ribosomal protein YNL122C.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	62	Total	C	H	N	O	S	0	0
			1054	322	546	111	74	1		

- Molecule 27 is a protein called 54S ribosomal protein RTC6, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	0	38	Total	C	H	N	O	S	0	0
			673	205	349	66	50	3		

- Molecule 28 is a protein called 54S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	1	332	Total	C	H	N	O	S	0	0
			5397	1744	2690	467	490	6		

- Molecule 29 is a protein called 54S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	2	113	Total	C	H	N	O	S	0	0
			1858	583	939	169	162	5		

- Molecule 30 is a protein called 54S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	3	126	Total	C	H	N	O	S	0	0
			2025	643	1030	181	168	3		

- Molecule 31 is a protein called 54S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	4	138	Total	C	H	N	O	S	0	0
			2263	700	1146	219	193	5		

- Molecule 32 is a protein called 54S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	5	326	Total	C	H	N	O	S	0	0
			5026	1596	2541	425	453	11		

- Molecule 33 is a protein called 54S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	6	209	Total	C	H	N	O	S	0	0
			3187	1046	1595	273	271	2		

- Molecule 34 is a protein called 54S ribosomal protein IMG2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	7	106	Total	C	H	N	O	S	0	0
			1755	550	901	150	152	2		

- Molecule 35 is a protein called 54S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	8	182	Total	C	H	N	O	S	0	0
			2829	898	1416	241	271	3		

- Molecule 36 is a protein called 54S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	9	195	Total	C	H	N	O	S	0	0
			2865	919	1437	250	254	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	169	GLY	ASP	conflict	UNP P36523

- Molecule 37 is a protein called 54S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	a	176	Total	C	H	N	O	S	0	0
			2882	898	1455	264	259	6		

- Molecule 38 is a protein called 54S ribosomal protein L25, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	b	155	Total	C	H	N	O	S	0	0
			2671	850	1372	225	221	3		

- Molecule 39 is a protein called 54S ribosomal protein L31, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	c	118	Total	C	H	N	O	S	0	0
			2066	643	1066	190	163	4		

- Molecule 40 is a protein called Mitochondrial homologous recombination protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	d	204	Total	C	H	N	O	S	0	0
			3423	1099	1706	313	299	6		

- Molecule 41 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	e	20	Total	C	H	N	O	P	0	0
			648	191	221	81	136	19		

- Molecule 42 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
42	A	109	Total	Mg	0
			109	109	
42	N	1	Total	Mg	0
			1	1	

- Molecule 43 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
43	B	1	Total	Na	0
			1	1	

- Molecule 44 is ZINC ION (three-letter code: ZN) (formula: Zn).

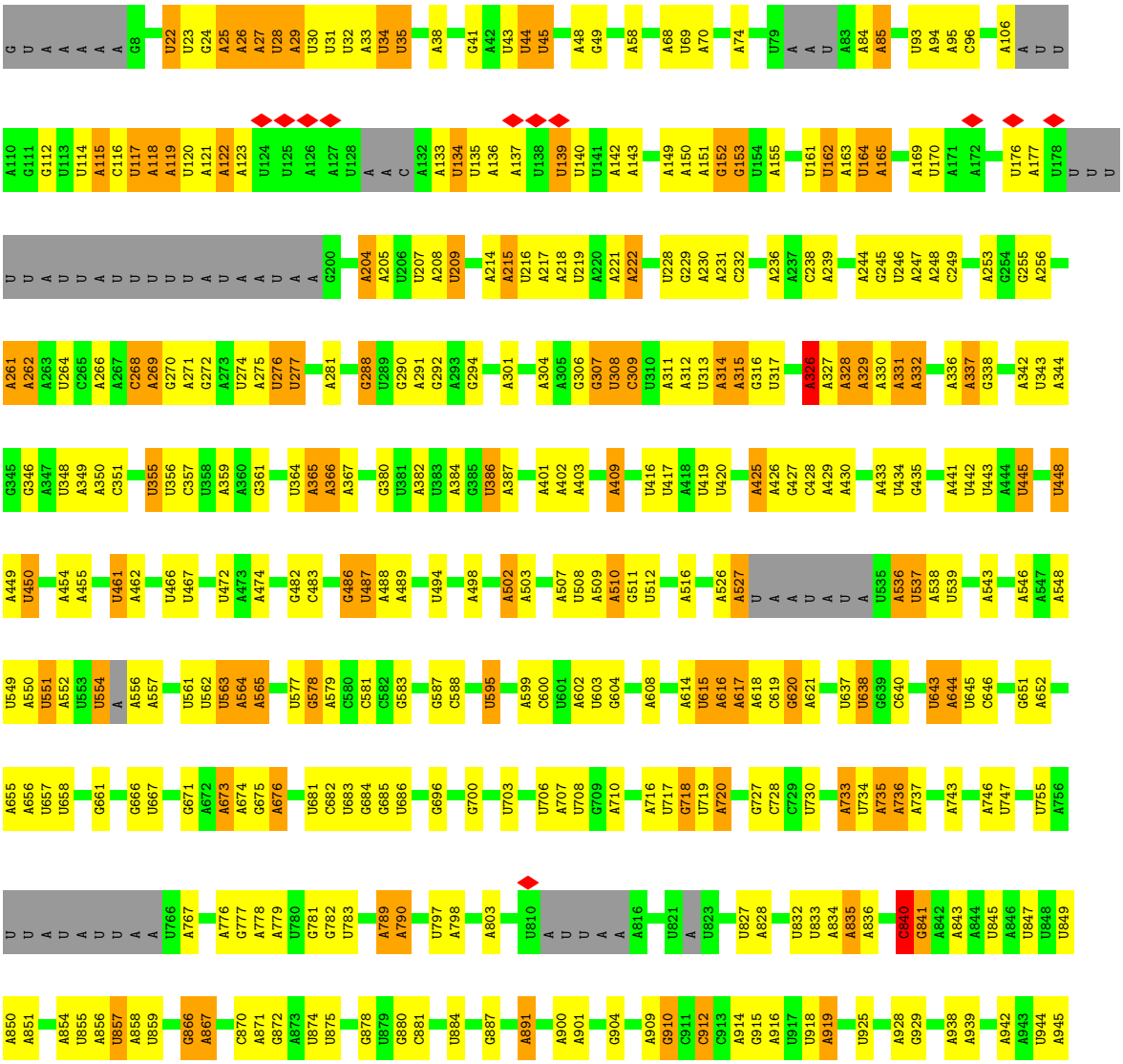
Mol	Chain	Residues	Atoms		AltConf
44	W	1	Total	Zn	0
			1	1	
44	0	1	Total	Zn	0
			1	1	

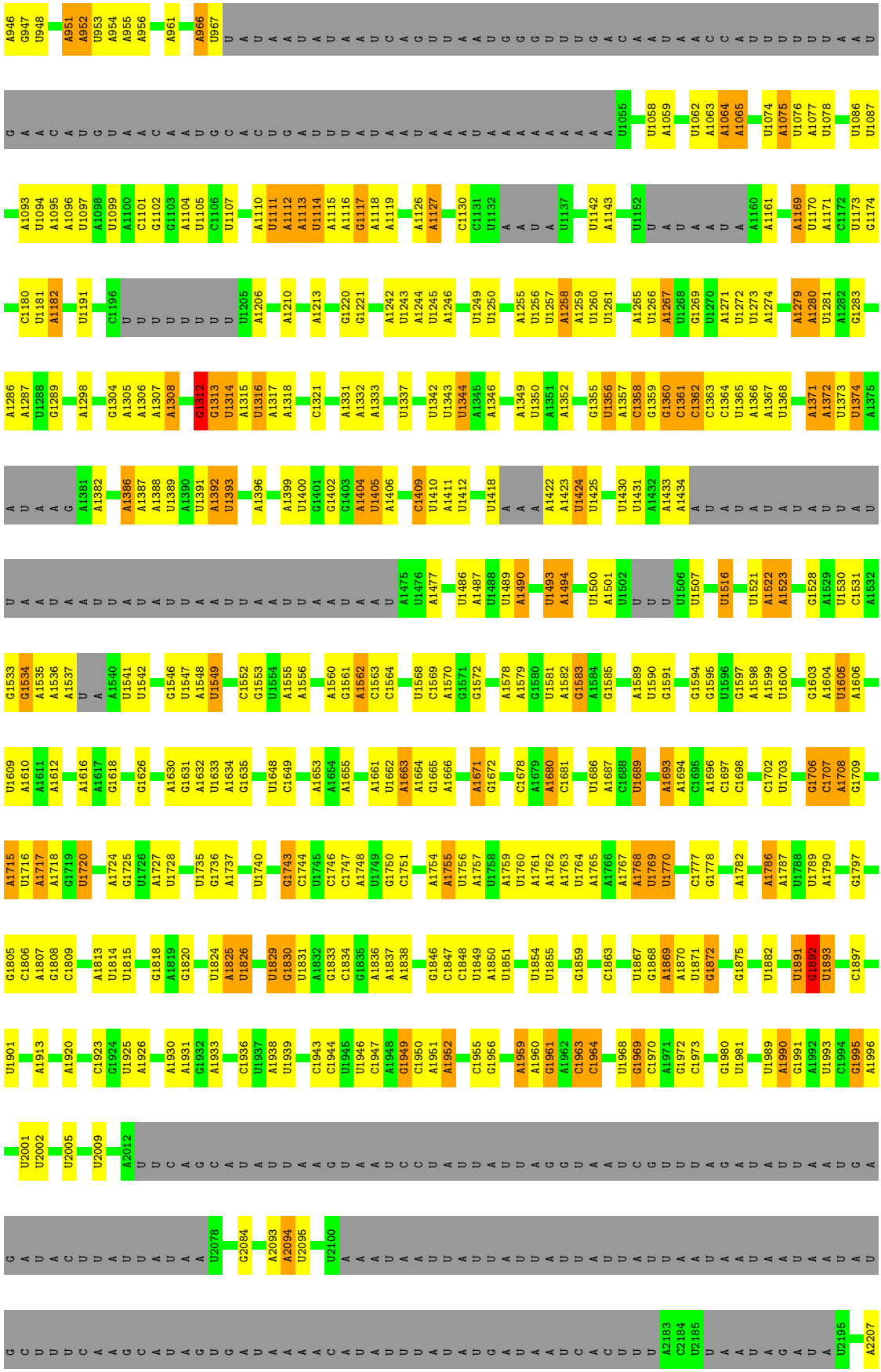
3 Residue-property plots (i)

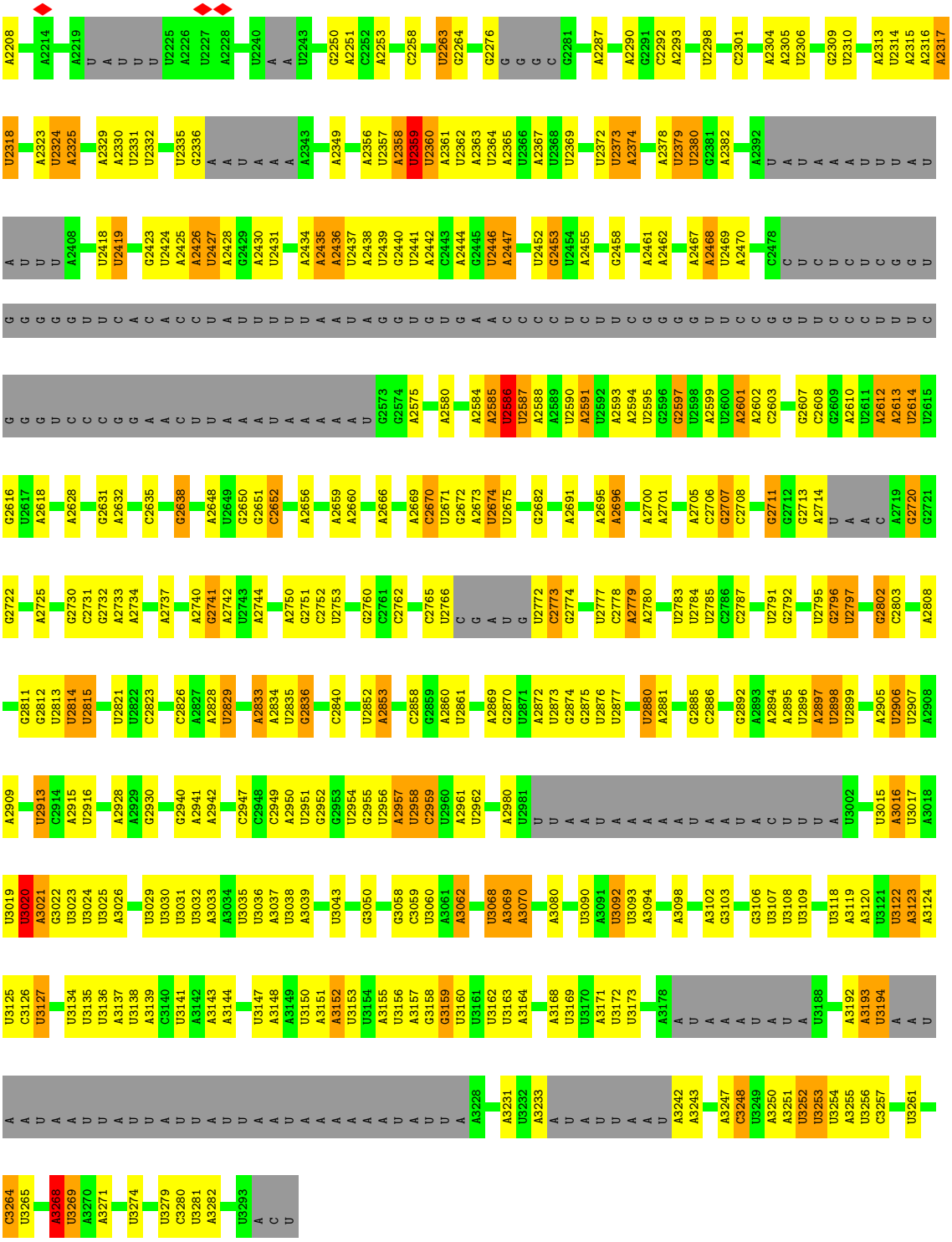
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 21S ribosomal RNA

Chain A:

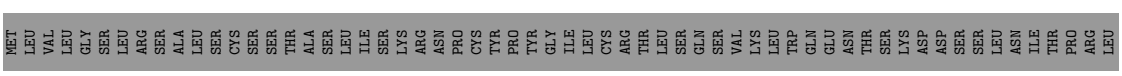


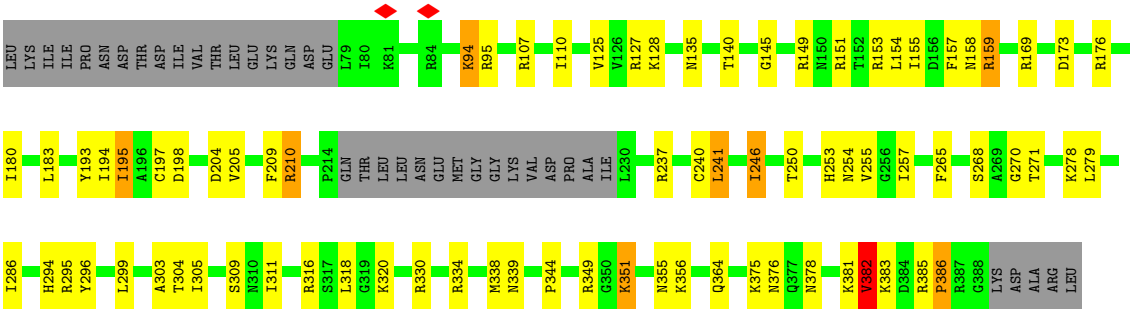




• Molecule 2: 54S ribosomal protein RML2, mitochondrial

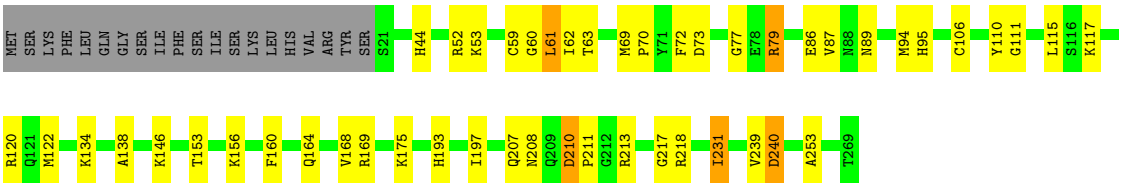
Chain B:





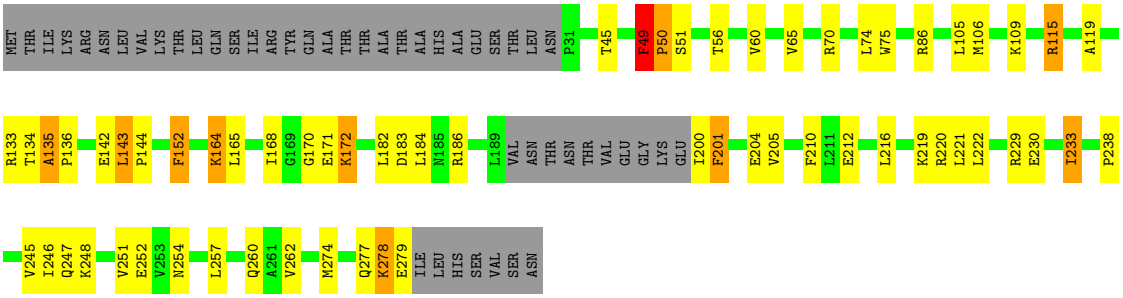
• Molecule 3: 54S ribosomal protein L9, mitochondrial

Chain C:



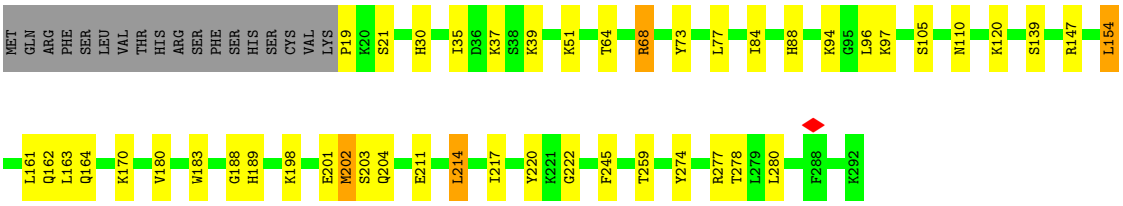
• Molecule 4: 54S ribosomal protein YmL6, mitochondrial

Chain D:



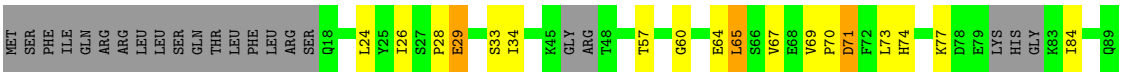
• Molecule 5: 54S ribosomal protein L7, mitochondrial

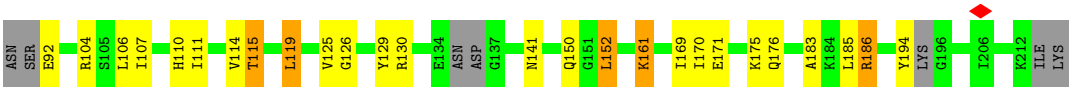
Chain E:



• Molecule 6: 54S ribosomal protein L6, mitochondrial

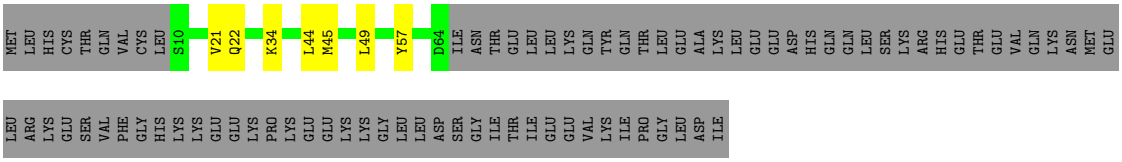
Chain F:





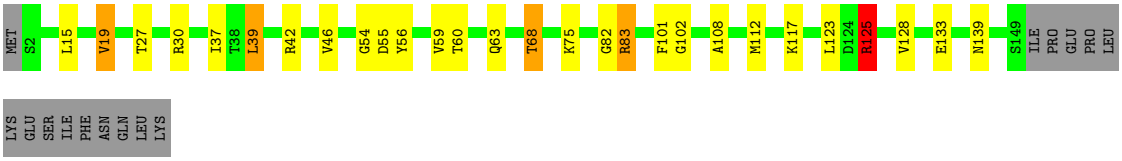
• Molecule 7: 54S ribosomal protein L50, mitochondrial

Chain G:



• Molecule 8: 54S ribosomal protein L23, mitochondrial

Chain H:

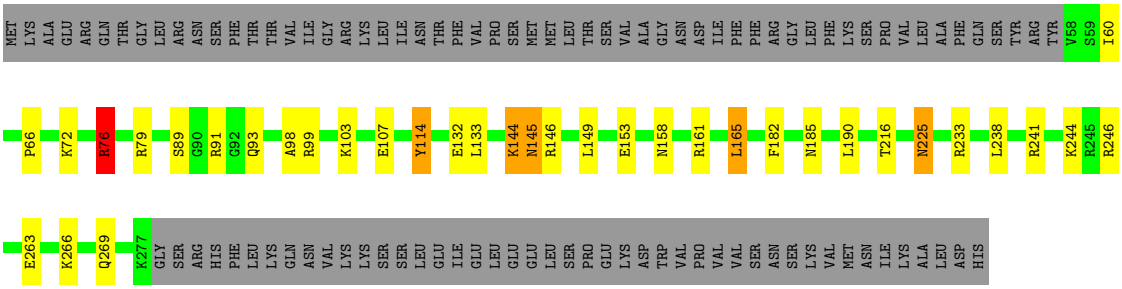


• Molecule 9: 54S ribosomal protein L38, mitochondrial

Chain I:

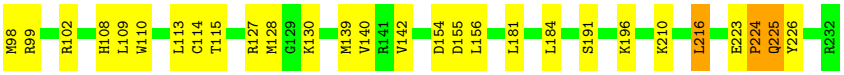
• Molecule 10: 54S ribosomal protein L10, mitochondrial

Chain J:



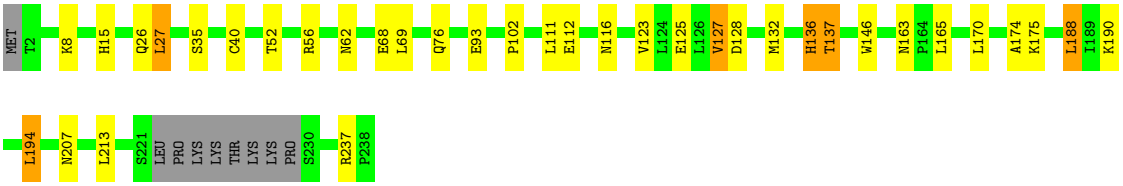
• Molecule 11: 54S ribosomal protein L16, mitochondrial

Chain K:



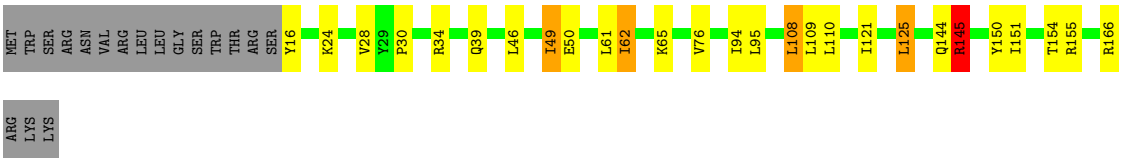
• Molecule 12: 54S ribosomal protein L8, mitochondrial

Chain L:



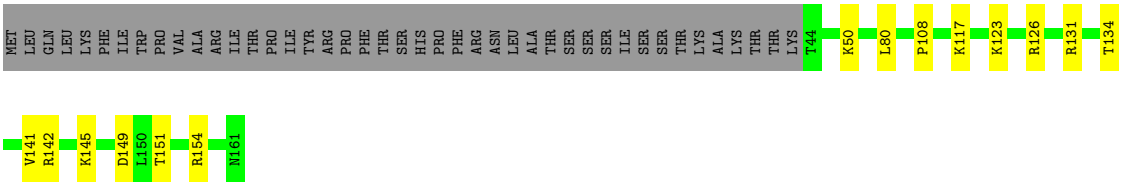
• Molecule 13: 54S ribosomal protein IMG1, mitochondrial

Chain M:



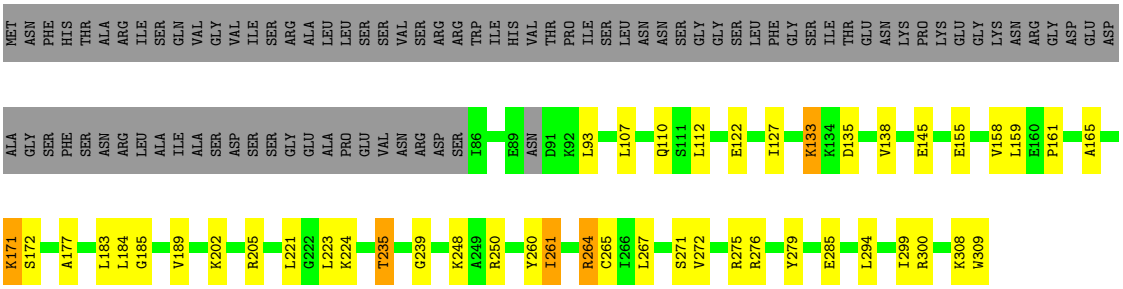
• Molecule 14: 54S ribosomal protein L49, mitochondrial

Chain N:



• Molecule 15: 54S ribosomal protein L22, mitochondrial

Chain O:

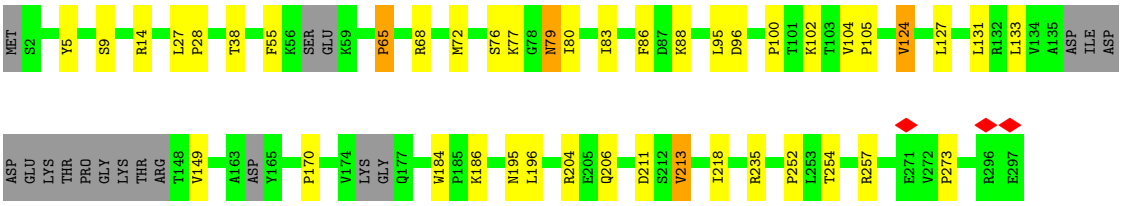


• Molecule 16: 54S ribosomal protein L41, mitochondrial

Chain P:

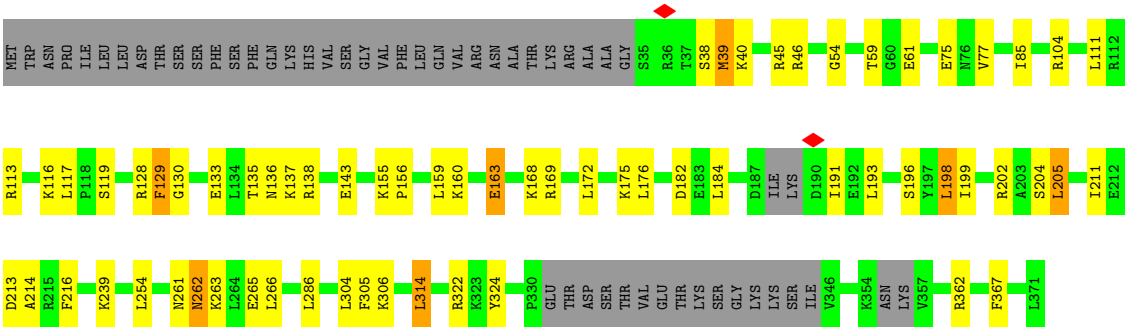
• Molecule 17: 54S ribosomal protein L40, mitochondrial

Chain Q:



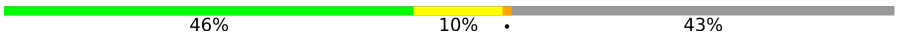
• Molecule 18: 54S ribosomal protein L2, mitochondrial

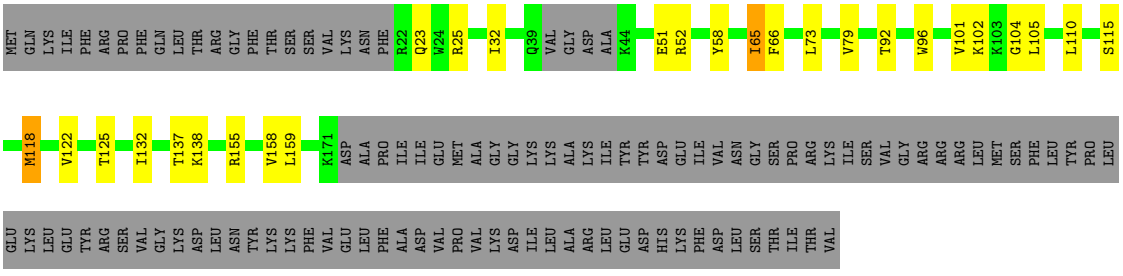
Chain R:



• Molecule 19: 54S ribosomal protein L24, mitochondrial

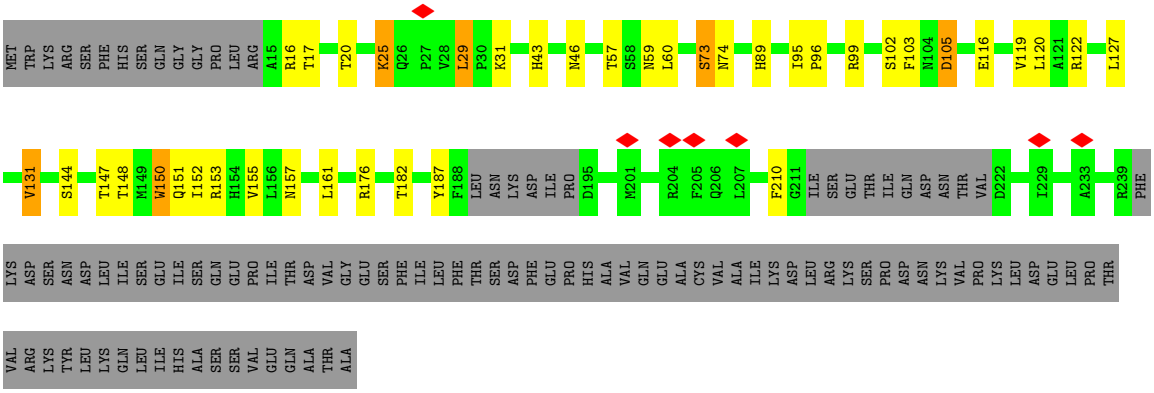
Chain S:





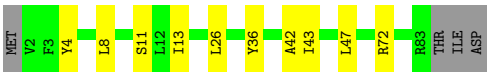
• Molecule 20: 54S ribosomal protein L4, mitochondrial

Chain T:



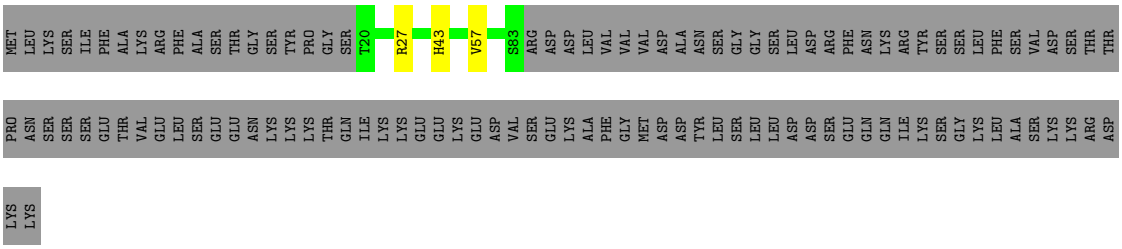
• Molecule 21: 54S ribosomal protein L33, mitochondrial

Chain U:



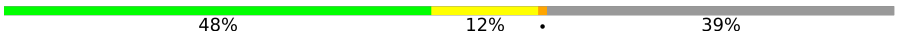
• Molecule 22: 54S ribosomal protein L36, mitochondrial

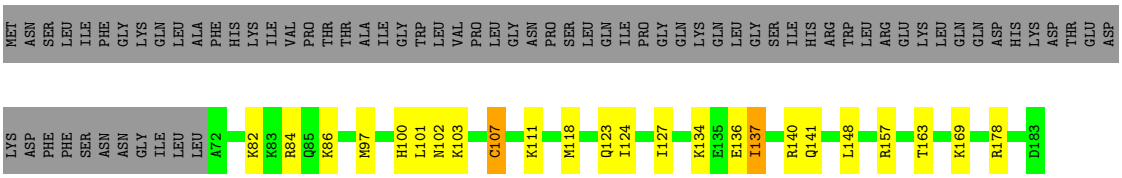
Chain V:



• Molecule 23: 54S ribosomal protein L32, mitochondrial

Chain W:



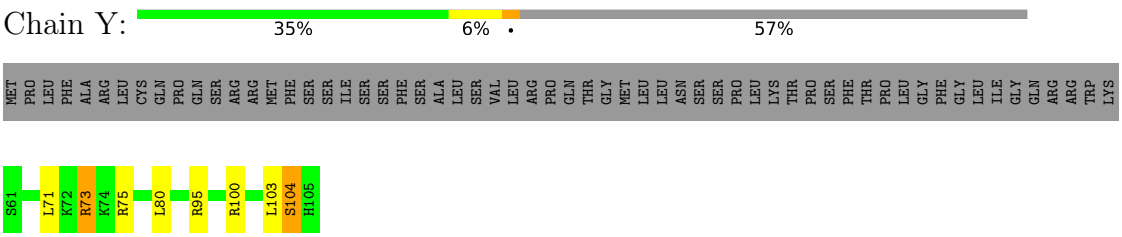


• Molecule 24: 54S ribosomal protein L39, mitochondrial

Chain X:

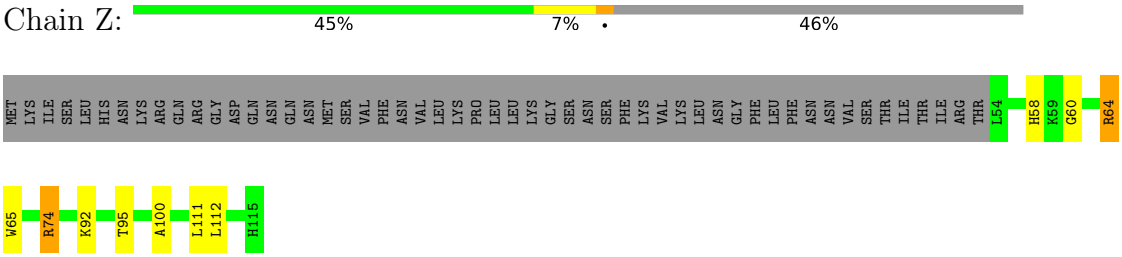
• Molecule 25: 54S ribosomal protein L34, mitochondrial

Chain Y:



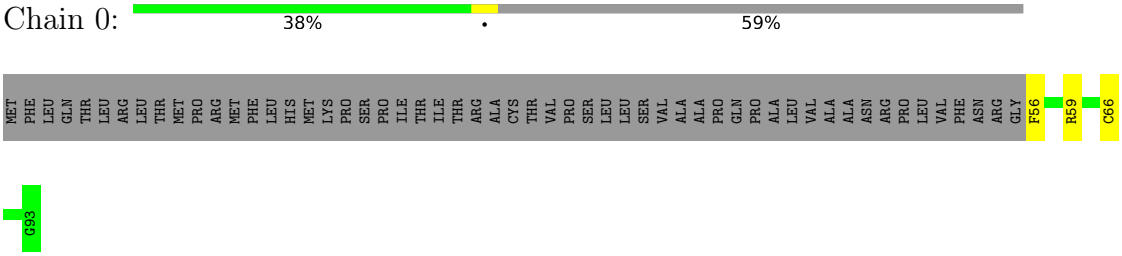
• Molecule 26: mitochondrial ribosomal protein YNL122C

Chain Z:



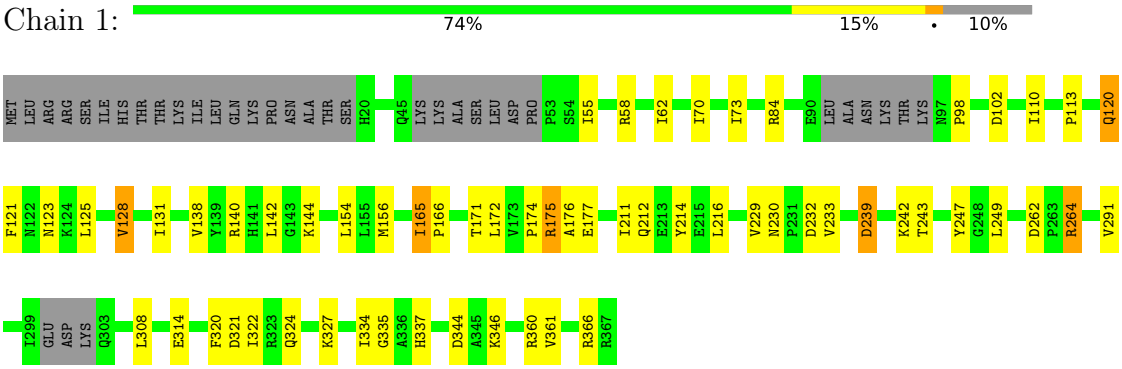
• Molecule 27: 54S ribosomal protein RTC6, mitochondrial

Chain 0:



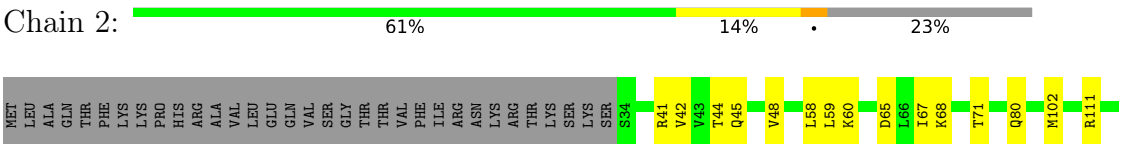
• Molecule 28: 54S ribosomal protein L35, mitochondrial

Chain 1:



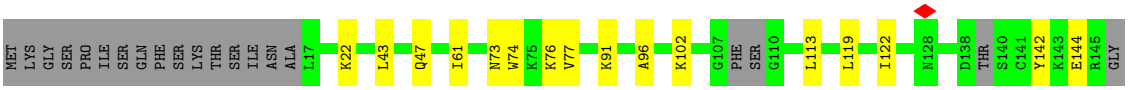
• Molecule 29: 54S ribosomal protein L28, mitochondrial

Chain 2:



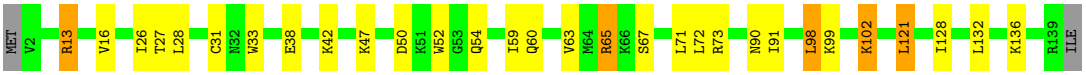
• Molecule 30: 54S ribosomal protein L27, mitochondrial

Chain 3:



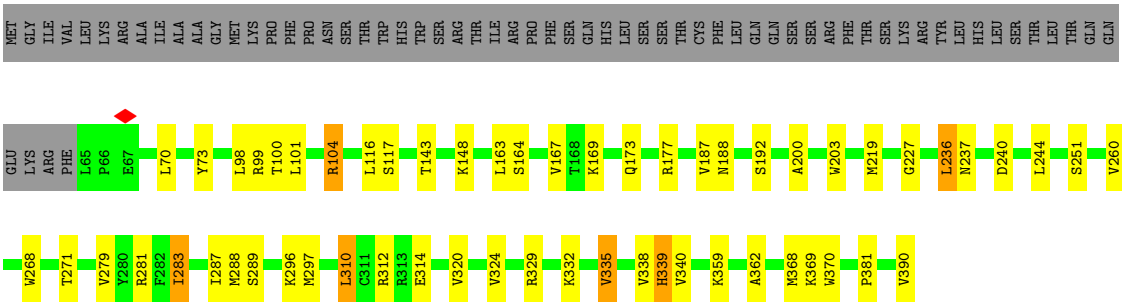
• Molecule 31: 54S ribosomal protein L51, mitochondrial

Chain 4:



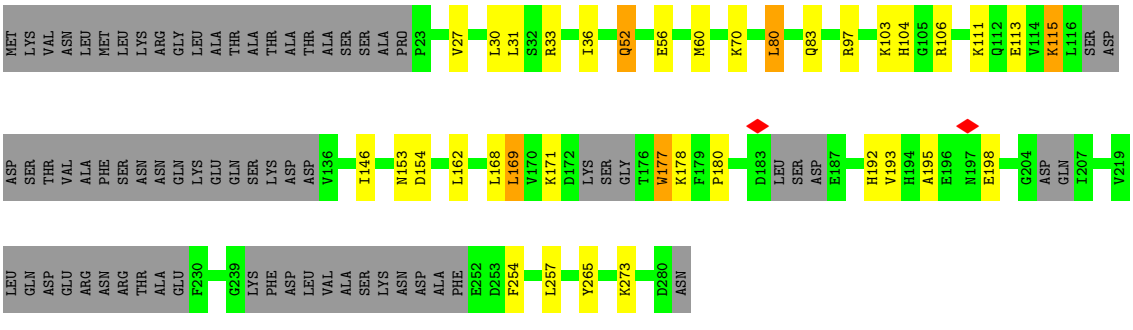
• Molecule 32: 54S ribosomal protein L3, mitochondrial

Chain 5:



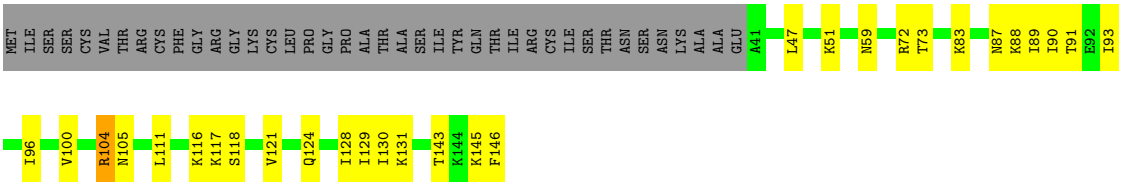
• Molecule 33: 54S ribosomal protein L17, mitochondrial

Chain 6:



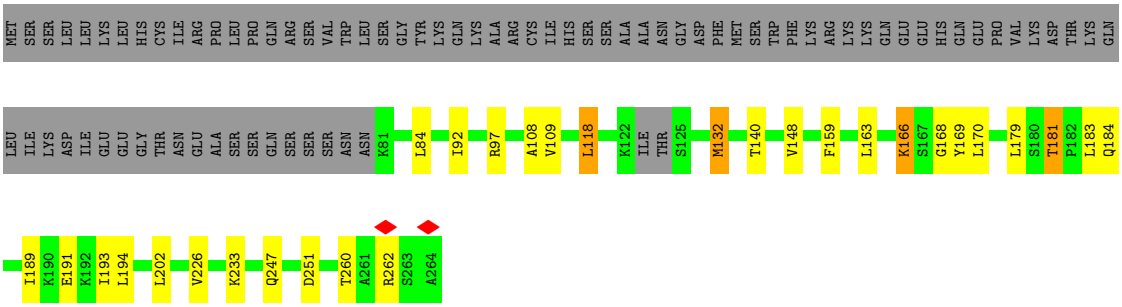
• Molecule 34: 54S ribosomal protein IMG2, mitochondrial

Chain 7:



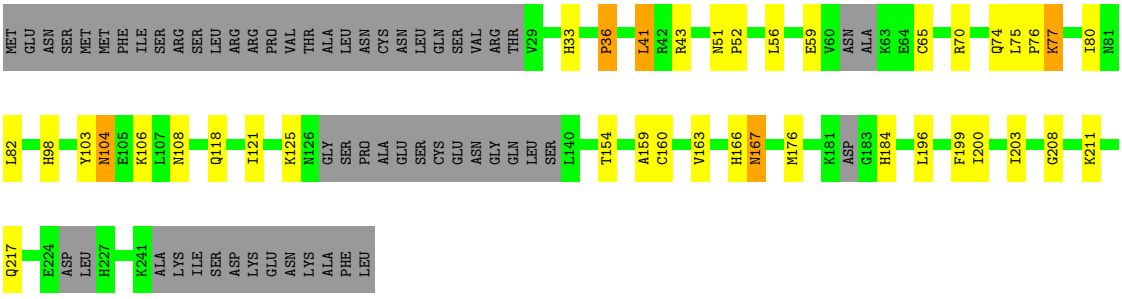
• Molecule 35: 54S ribosomal protein L13, mitochondrial

Chain 8:



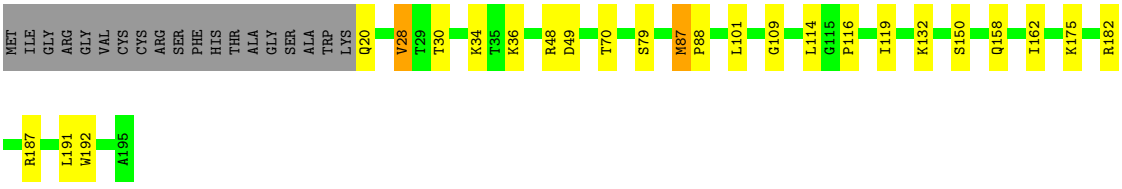
• Molecule 36: 54S ribosomal protein L15, mitochondrial

Chain 9:



• Molecule 37: 54S ribosomal protein L20, mitochondrial

Chain a:

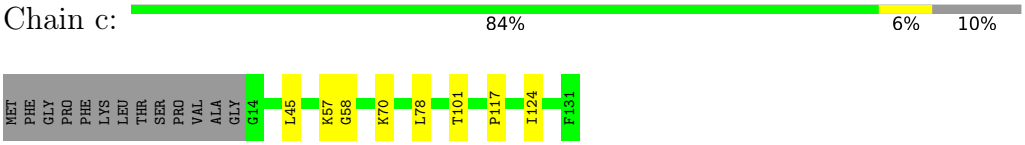


• Molecule 38: 54S ribosomal protein L25, mitochondrial

Chain b:

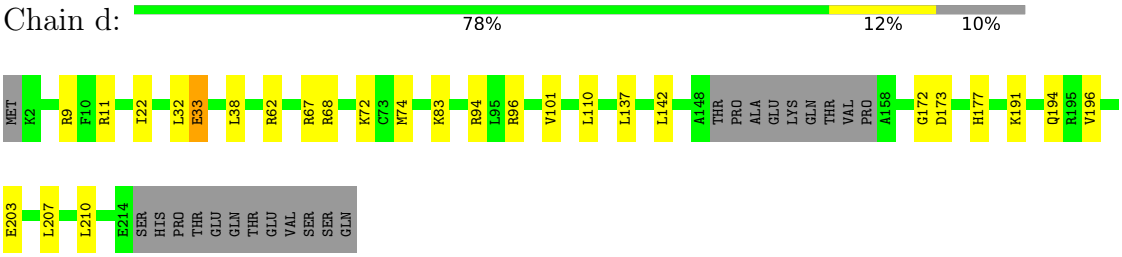
• Molecule 39: 54S ribosomal protein L31, mitochondrial

Chain c:



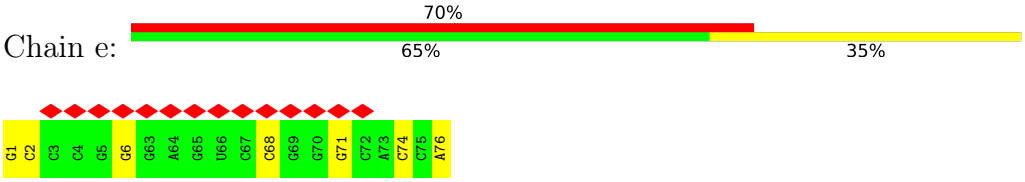
• Molecule 40: Mitochondrial homologous recombination protein 1

Chain d:



• Molecule 41: E-site tRNA

Chain e:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	47124	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4700	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.687	Depositor
Minimum map value	-0.940	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.0681	Depositor
Map size (Å)	482.40002, 482.40002, 482.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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: NA, ZN, MG

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	0.24	0/64599	0.70	13/100487 (0.0%)
2	B	0.32	0/2305	0.66	0/3102
3	C	0.32	0/1973	0.59	0/2654
4	D	0.33	0/1904	0.65	0/2579
5	E	0.31	0/2181	0.54	0/2955
6	F	0.31	0/1376	0.58	0/1869
7	G	0.32	0/468	0.57	0/628
8	H	0.36	0/1200	0.63	1/1610 (0.1%)
9	I	0.30	0/943	0.58	0/1260
10	J	0.33	0/1764	0.66	2/2360 (0.1%)
11	K	0.33	0/1606	0.65	0/2148
12	L	0.35	0/1843	0.64	0/2486
13	M	0.30	0/1224	0.64	0/1651
14	N	0.30	0/961	0.61	0/1295
15	O	0.35	0/1821	0.68	0/2444
16	P	0.34	0/1766	0.63	0/2381
17	Q	0.31	0/2174	0.57	0/2946
18	R	0.36	0/2522	0.68	0/3392
19	S	0.34	0/1216	0.58	0/1626
20	T	0.36	0/1689	0.69	0/2297
21	U	0.38	0/648	0.67	0/870
22	V	0.28	0/539	0.54	0/726
23	W	0.33	0/955	0.65	0/1273
24	X	0.33	0/520	0.62	0/696
25	Y	0.44	0/383	0.69	0/504
26	Z	0.38	0/522	0.71	0/695
27	0	0.32	0/329	0.56	0/432
28	1	0.32	0/2777	0.61	0/3772
29	2	0.37	0/938	0.70	0/1264
30	3	0.31	0/1018	0.57	0/1368
31	4	0.33	0/1138	0.65	0/1526
32	5	0.34	0/2538	0.66	1/3451 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	6	0.30	0/1631	0.54	0/2214
34	7	0.31	0/869	0.57	0/1166
35	8	0.35	0/1438	0.61	0/1945
36	9	0.34	0/1453	0.61	0/1969
37	a	0.33	0/1458	0.63	0/1961
38	b	0.34	0/1333	0.63	0/1783
39	c	0.35	0/1024	0.63	0/1367
40	d	0.34	0/1762	0.65	0/2381
41	e	0.21	0/476	0.73	2/739 (0.3%)
All	All	0.29	0/119284	0.67	19/174272 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
3	C	0	1
4	D	0	1
10	J	0	1
20	T	0	1
37	a	0	1
All	All	1	5

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2897	A	C2'-C3'-O3'	7.88	126.83	109.50
1	A	1892	G	C2'-C3'-O3'	7.84	126.75	109.50
1	A	733	A	C2'-C3'-O3'	7.69	126.42	109.50
10	J	76	ARG	NE-CZ-NH1	7.44	124.02	120.30
8	H	125	ARG	NE-CZ-NH1	7.28	123.94	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1665	G	C1'

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	210	ASP	Peptide
4	D	49	PHE	Peptide
10	J	93	GLN	Peptide
20	T	43	HIS	Peptide
37	a	87	MET	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	A	57671	28898	28934	625	0
2	B	2260	2343	2303	47	0
3	C	1930	1976	1964	21	0
4	D	1866	1914	1898	30	0
5	E	2125	2169	2125	23	0
6	F	1355	1392	1338	22	0
7	G	458	471	467	2	0
8	H	1176	1218	1210	19	0
9	I	937	1015	1013	10	0
10	J	1727	1828	1812	12	0
11	K	1573	1635	1629	9	0
12	L	1815	1883	1873	21	0
13	M	1206	1286	1283	13	0
14	N	948	1010	1006	2	0
15	O	1789	1895	1877	21	0
16	P	1722	1728	1718	22	0
17	Q	2126	2161	2092	19	0
18	R	2481	2500	2413	25	0
19	S	1191	1249	1234	16	0
20	T	1646	1618	1557	22	0
21	U	639	702	699	11	0
22	V	528	555	553	3	0
23	W	937	985	974	9	0
24	X	512	565	563	3	0
25	Y	376	412	410	4	0
26	Z	508	546	539	6	0
27	0	324	349	345	4	0
28	1	2707	2690	2661	24	0
29	2	919	939	923	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	3	995	1030	1012	10	0
31	4	1117	1146	1142	18	0
32	5	2485	2541	2488	26	0
33	6	1592	1595	1511	13	0
34	7	854	901	897	10	0
35	8	1413	1416	1381	14	0
36	9	1428	1437	1368	19	0
37	a	1427	1455	1449	0	0
38	b	1299	1372	1367	0	0
39	c	1000	1066	1062	0	0
40	d	1717	1706	1691	0	0
41	e	427	221	222	0	0
42	A	109	0	0	0	0
42	N	1	0	0	0	0
43	B	1	0	0	0	0
44	0	1	0	0	2	0
44	W	1	0	0	0	0
All	All	111319	83818	83003	1022	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 6.

The worst 5 of 1022 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)
1:A:45:U:O4	1:A:2895:A:N1	1.58	1.36
1:A:114:U:O4	1:A:118:A:N1	1.68	1.25
1:A:1913:A:N1	1:A:2880:U:O4	1.73	1.21
1:A:122:A:N6	1:A:139:U:N3	1.91	1.19
1:A:274:U:O4	1:A:367:A:N1	1.78	1.15

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	291/393 (74%)	272 (94%)	16 (6%)	3 (1%)	15 54
3	C	247/269 (92%)	226 (92%)	15 (6%)	6 (2%)	6 34
4	D	235/286 (82%)	211 (90%)	15 (6%)	9 (4%)	3 22
5	E	272/292 (93%)	246 (90%)	22 (8%)	4 (2%)	10 44
6	F	173/214 (81%)	163 (94%)	7 (4%)	3 (2%)	9 42
7	G	53/139 (38%)	50 (94%)	3 (6%)	0	100 100
8	H	146/163 (90%)	138 (94%)	8 (6%)	0	100 100
9	I	121/138 (88%)	110 (91%)	10 (8%)	1 (1%)	19 58
10	J	218/322 (68%)	202 (93%)	14 (6%)	2 (1%)	17 56
11	K	193/232 (83%)	182 (94%)	7 (4%)	4 (2%)	7 37
12	L	225/238 (94%)	208 (92%)	14 (6%)	3 (1%)	12 47
13	M	149/169 (88%)	138 (93%)	9 (6%)	2 (1%)	12 47
14	N	116/161 (72%)	109 (94%)	6 (5%)	1 (1%)	17 56
15	O	219/309 (71%)	199 (91%)	18 (8%)	2 (1%)	17 56
16	P	205/263 (78%)	189 (92%)	14 (7%)	2 (1%)	15 54
17	Q	269/297 (91%)	243 (90%)	22 (8%)	4 (2%)	10 44
18	R	310/371 (84%)	288 (93%)	17 (6%)	5 (2%)	9 43
19	S	142/258 (55%)	136 (96%)	6 (4%)	0	100 100
20	T	203/319 (64%)	184 (91%)	13 (6%)	6 (3%)	4 28
21	U	80/86 (93%)	77 (96%)	3 (4%)	0	100 100
22	V	62/177 (35%)	57 (92%)	5 (8%)	0	100 100
23	W	110/183 (60%)	100 (91%)	6 (6%)	4 (4%)	3 23
24	X	62/70 (89%)	55 (89%)	6 (10%)	1 (2%)	9 43
25	Y	43/105 (41%)	41 (95%)	1 (2%)	1 (2%)	6 34
26	Z	60/115 (52%)	57 (95%)	3 (5%)	0	100 100
27	0	36/93 (39%)	34 (94%)	2 (6%)	0	100 100
28	1	324/367 (88%)	293 (90%)	26 (8%)	5 (2%)	10 44
29	2	111/147 (76%)	103 (93%)	5 (4%)	3 (3%)	5 30
30	3	120/146 (82%)	103 (86%)	16 (13%)	1 (1%)	19 58
31	4	136/140 (97%)	128 (94%)	8 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
32	5	324/390 (83%)	299 (92%)	23 (7%)	2 (1%)	25 64
33	6	195/281 (69%)	179 (92%)	12 (6%)	4 (2%)	7 37
34	7	104/146 (71%)	99 (95%)	5 (5%)	0	100 100
35	8	178/264 (67%)	168 (94%)	10 (6%)	0	100 100
36	9	185/253 (73%)	163 (88%)	14 (8%)	8 (4%)	2 20
37	a	174/195 (89%)	161 (92%)	7 (4%)	6 (3%)	3 24
38	b	153/157 (98%)	139 (91%)	12 (8%)	2 (1%)	12 47
39	c	116/131 (88%)	108 (93%)	5 (4%)	3 (3%)	5 31
40	d	200/226 (88%)	179 (90%)	16 (8%)	5 (2%)	5 32
All	All	6560/8505 (77%)	6037 (92%)	421 (6%)	102 (2%)	13 43

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	382	VAL
3	C	211	PRO
4	D	49	PHE
4	D	50	PRO
4	D	135	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	233/337 (69%)	210 (90%)	23 (10%)	8 30
3	C	209/229 (91%)	190 (91%)	19 (9%)	9 34
4	D	200/248 (81%)	173 (86%)	27 (14%)	4 18
5	E	225/260 (86%)	201 (89%)	24 (11%)	6 27
6	F	141/190 (74%)	120 (85%)	21 (15%)	3 14
7	G	50/129 (39%)	47 (94%)	3 (6%)	19 54
8	H	126/141 (89%)	117 (93%)	9 (7%)	14 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	I	106/117 (91%)	101 (95%)	5 (5%)	26 62
10	J	175/274 (64%)	147 (84%)	28 (16%)	2 11
11	K	167/200 (84%)	138 (83%)	29 (17%)	2 10
12	L	202/212 (95%)	188 (93%)	14 (7%)	15 49
13	M	136/153 (89%)	124 (91%)	12 (9%)	10 36
14	N	107/147 (73%)	98 (92%)	9 (8%)	11 39
15	O	191/270 (71%)	169 (88%)	22 (12%)	5 24
16	P	183/236 (78%)	155 (85%)	28 (15%)	2 13
17	Q	219/268 (82%)	198 (90%)	21 (10%)	8 32
18	R	250/337 (74%)	218 (87%)	32 (13%)	4 20
19	S	126/231 (54%)	116 (92%)	10 (8%)	12 43
20	T	171/298 (57%)	156 (91%)	15 (9%)	10 36
21	U	73/77 (95%)	71 (97%)	2 (3%)	44 75
22	V	59/161 (37%)	58 (98%)	1 (2%)	60 83
23	W	104/167 (62%)	90 (86%)	14 (14%)	4 18
24	X	56/62 (90%)	52 (93%)	4 (7%)	14 47
25	Y	39/93 (42%)	37 (95%)	2 (5%)	24 60
26	Z	50/100 (50%)	45 (90%)	5 (10%)	7 30
27	0	36/84 (43%)	36 (100%)	0	100 100
28	1	299/341 (88%)	269 (90%)	30 (10%)	7 30
29	2	99/137 (72%)	90 (91%)	9 (9%)	9 34
30	3	102/126 (81%)	97 (95%)	5 (5%)	25 61
31	4	121/123 (98%)	107 (88%)	14 (12%)	5 24
32	5	263/345 (76%)	234 (89%)	29 (11%)	6 26
33	6	153/252 (61%)	134 (88%)	19 (12%)	4 21
34	7	94/128 (73%)	81 (86%)	13 (14%)	3 16
35	8	149/240 (62%)	134 (90%)	15 (10%)	7 29
36	9	140/221 (63%)	127 (91%)	13 (9%)	9 33
37	a	156/171 (91%)	136 (87%)	20 (13%)	4 20
38	b	144/146 (99%)	122 (85%)	22 (15%)	2 13
39	c	110/120 (92%)	105 (96%)	5 (4%)	27 63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	d	185/210 (88%)	162 (88%)	23 (12%)	4 21
All	All	5649/7581 (74%)	5053 (89%)	596 (11%)	10 27

5 of 596 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	5	368	MET
40	d	9	ARG
33	6	111	LYS
32	5	339	HIS
36	9	160	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
19	S	84	ASN
22	V	81	ASN
35	8	235	GLN
3	C	207	GLN
2	B	378	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2682/3296 (81%)	692 (25%)	132 (4%)
41	e	18/20 (90%)	6 (33%)	0
All	All	2700/3316 (81%)	698 (25%)	132 (4%)

5 of 698 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	22	U
1	A	26	A
1	A	27	A
1	A	28	U
1	A	29	A

5 of 132 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2906	U
1	A	3036	U
1	A	3252	U
1	A	840	C
1	A	781	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 113 ligands modelled in this entry, 113 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
1	A	5
41	e	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2226:A	O3'	2227:U	P	17.43
1	A	2197:A	O3'	2198:U	P	17.36
1	e	6:G	O3'	63:G	P	15.82
1	A	2344:A	O3'	2345:A	P	15.67
1	A	1374:U	O3'	1375:A	P	11.56

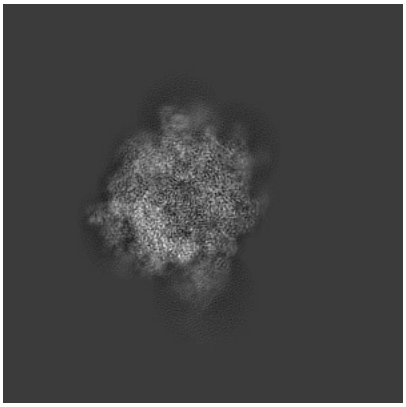
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2566. These allow visual inspection of the internal detail of the map and identification of artifacts.

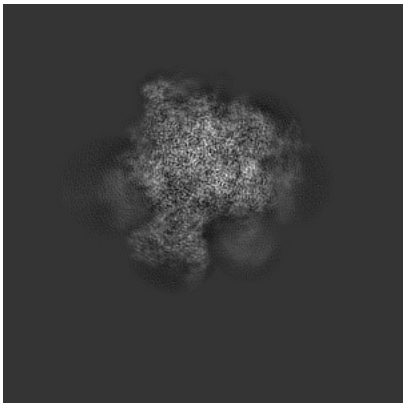
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

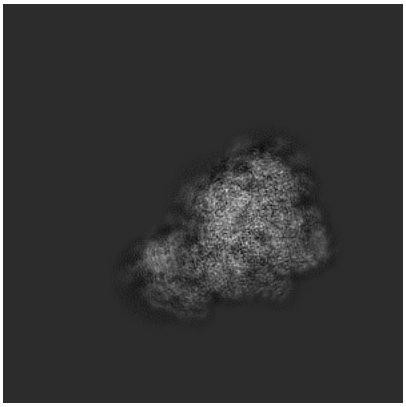
6.1.1 Primary map



X



Y

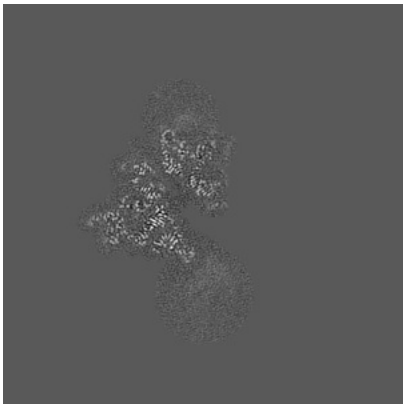


Z

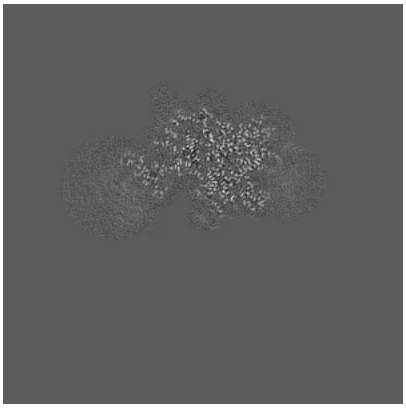
The images above show the map projected in three orthogonal directions.

6.2 Central slices

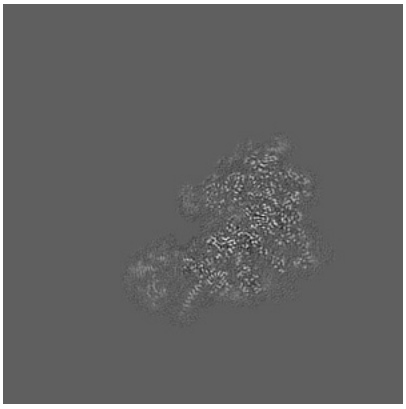
6.2.1 Primary map



X Index: 180



Y Index: 180

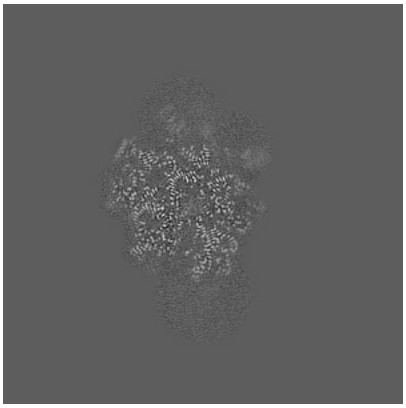


Z Index: 180

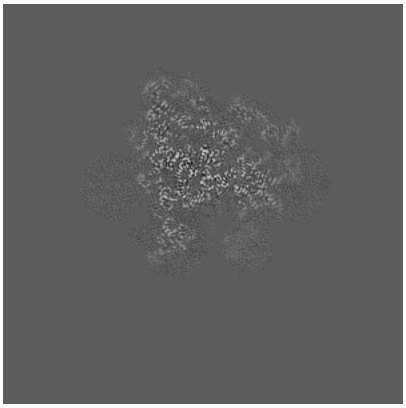
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

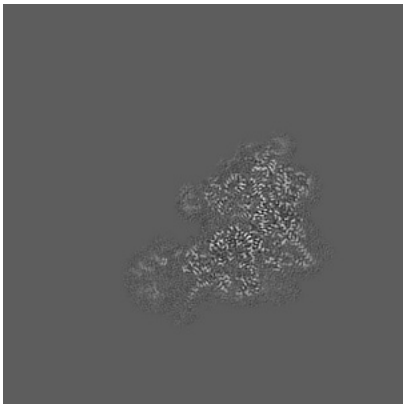
6.3.1 Primary map



X Index: 212



Y Index: 145

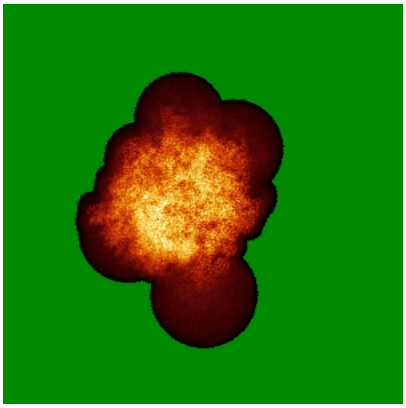


Z Index: 182

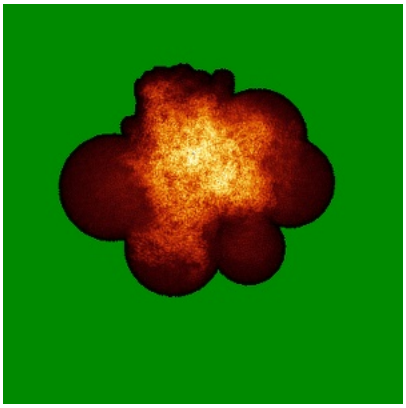
The images above show the largest variance slices of the map in three orthogonal directions.

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

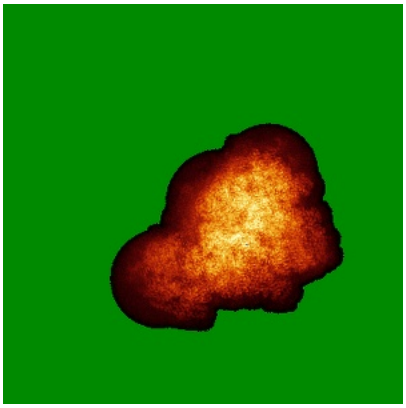
6.4.1 Primary map



X



Y

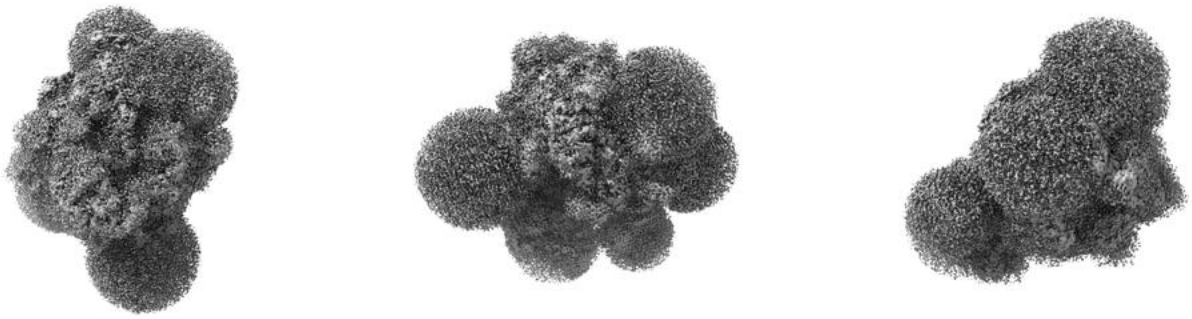


Z

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 0.0681. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

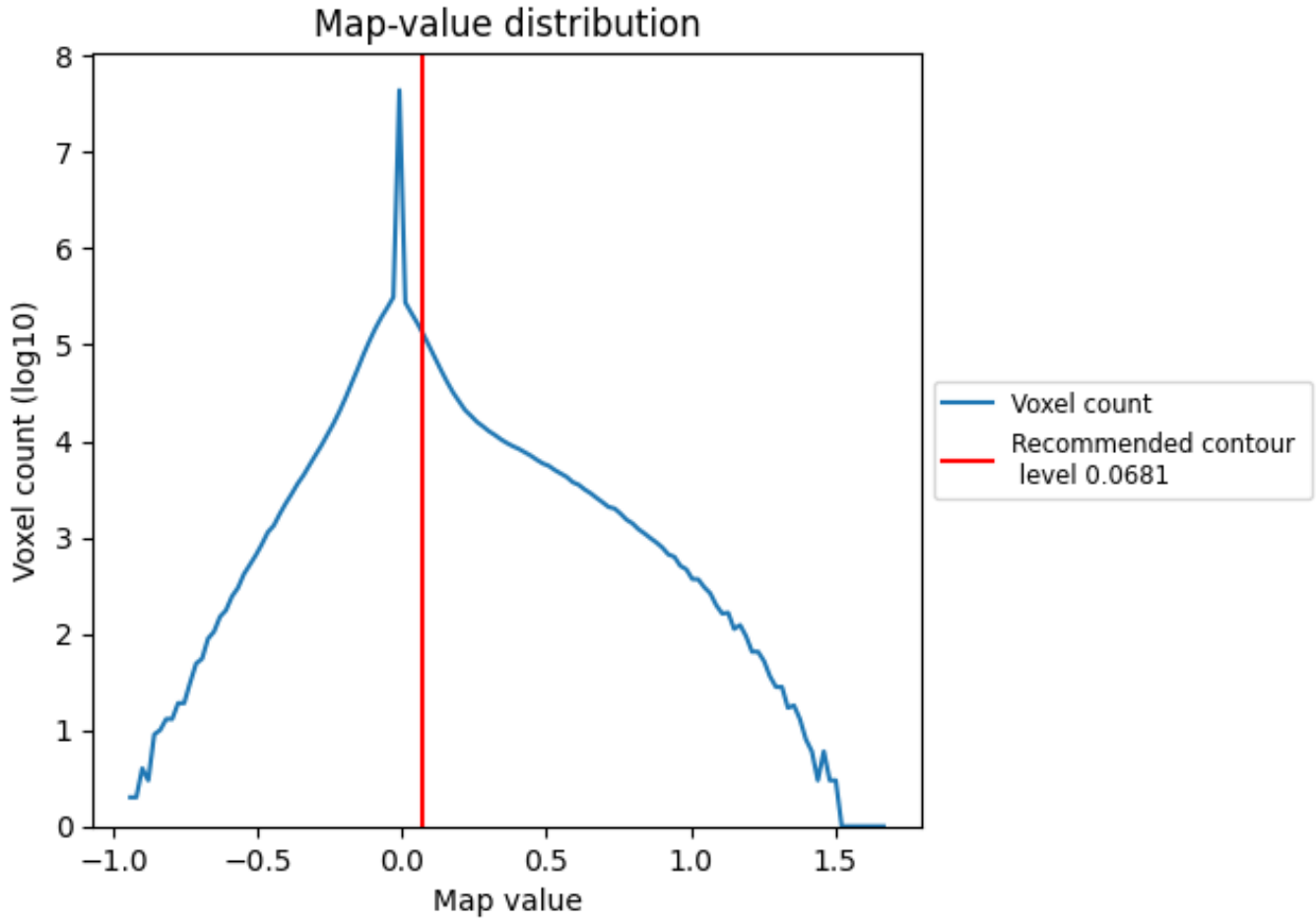
6.6 Mask visualisation (i)

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

7 Map analysis

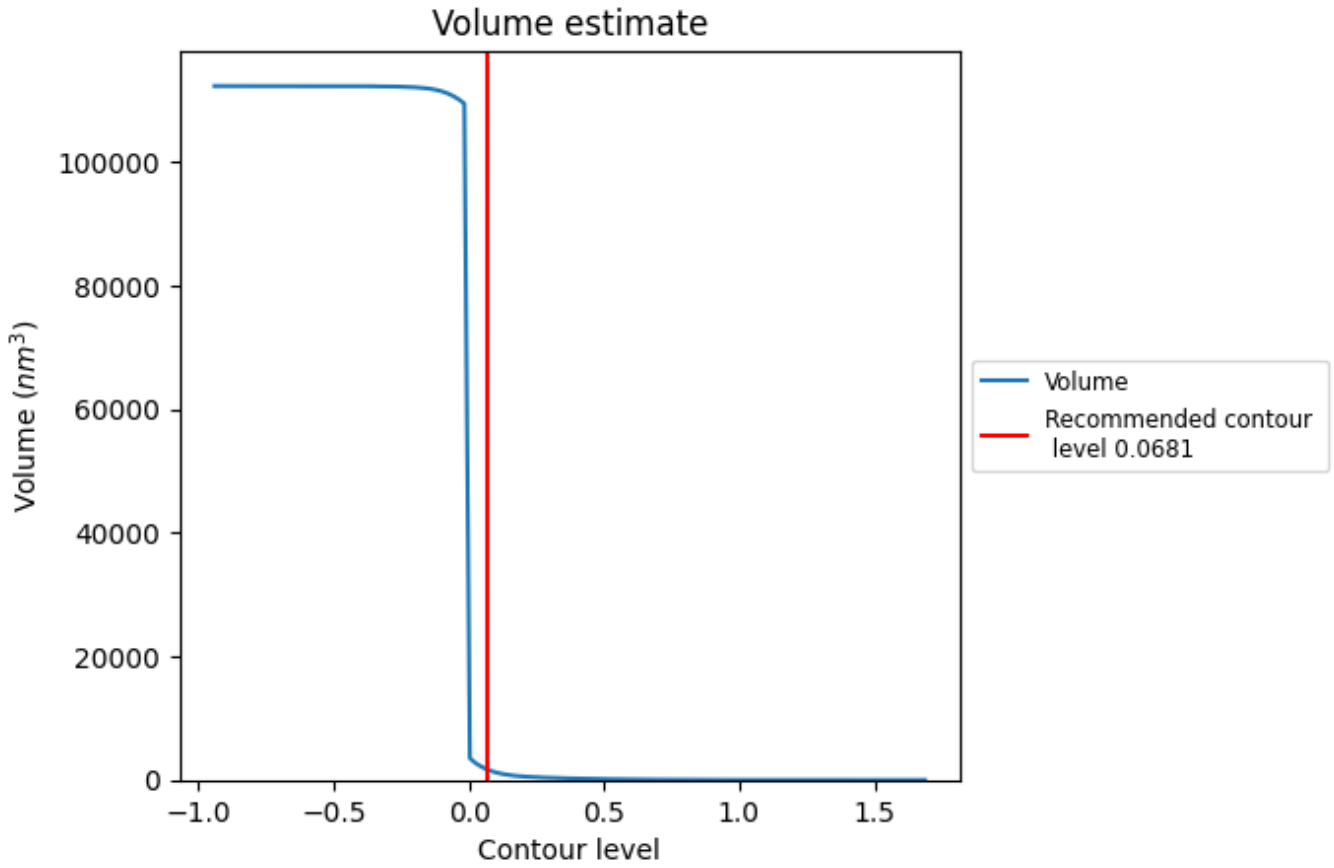
This section contains the results of statistical analysis of the map.

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.

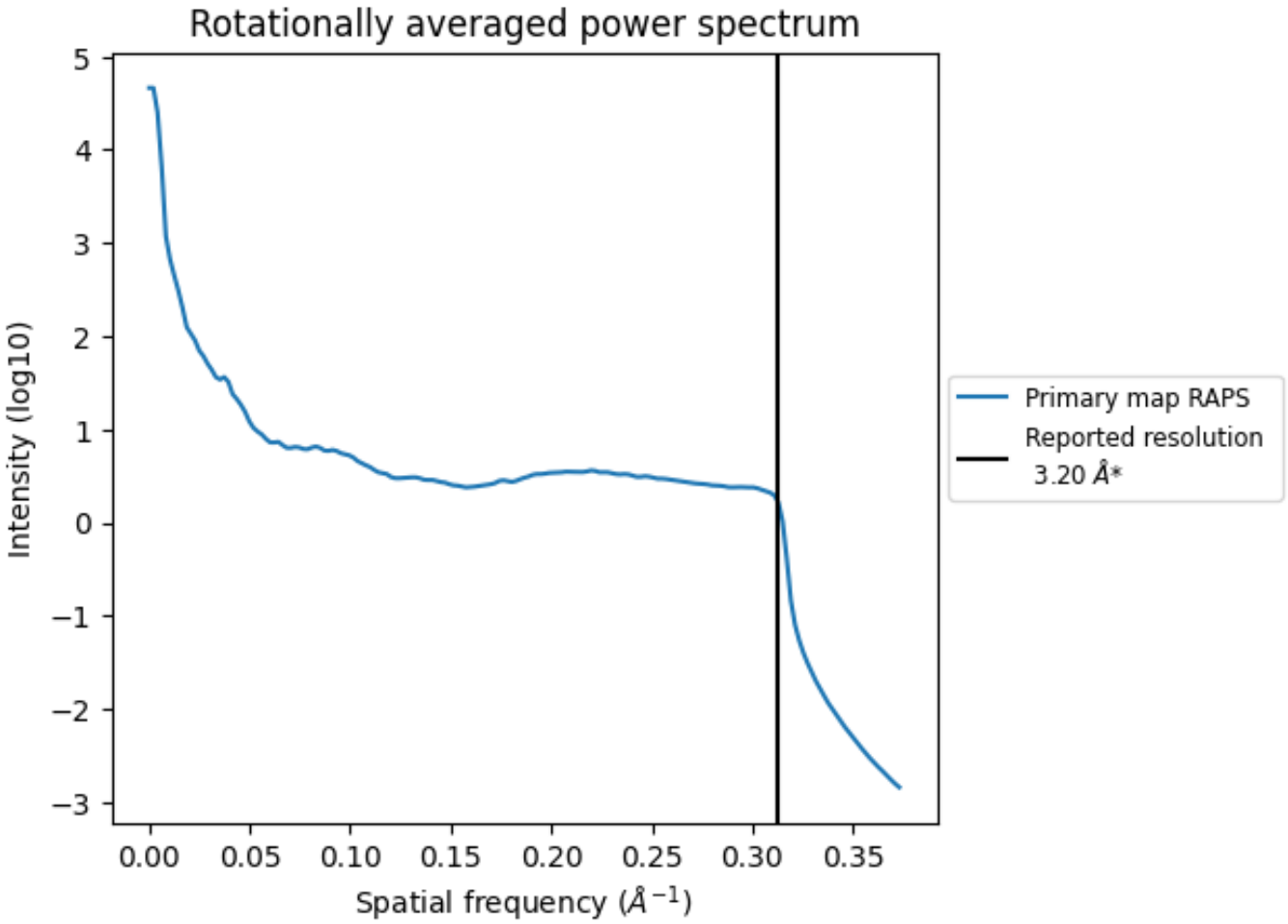
7.2 Volume estimate (i)



The volume at the recommended contour level is 1704 nm^3; this corresponds to an approximate mass of 1539 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)

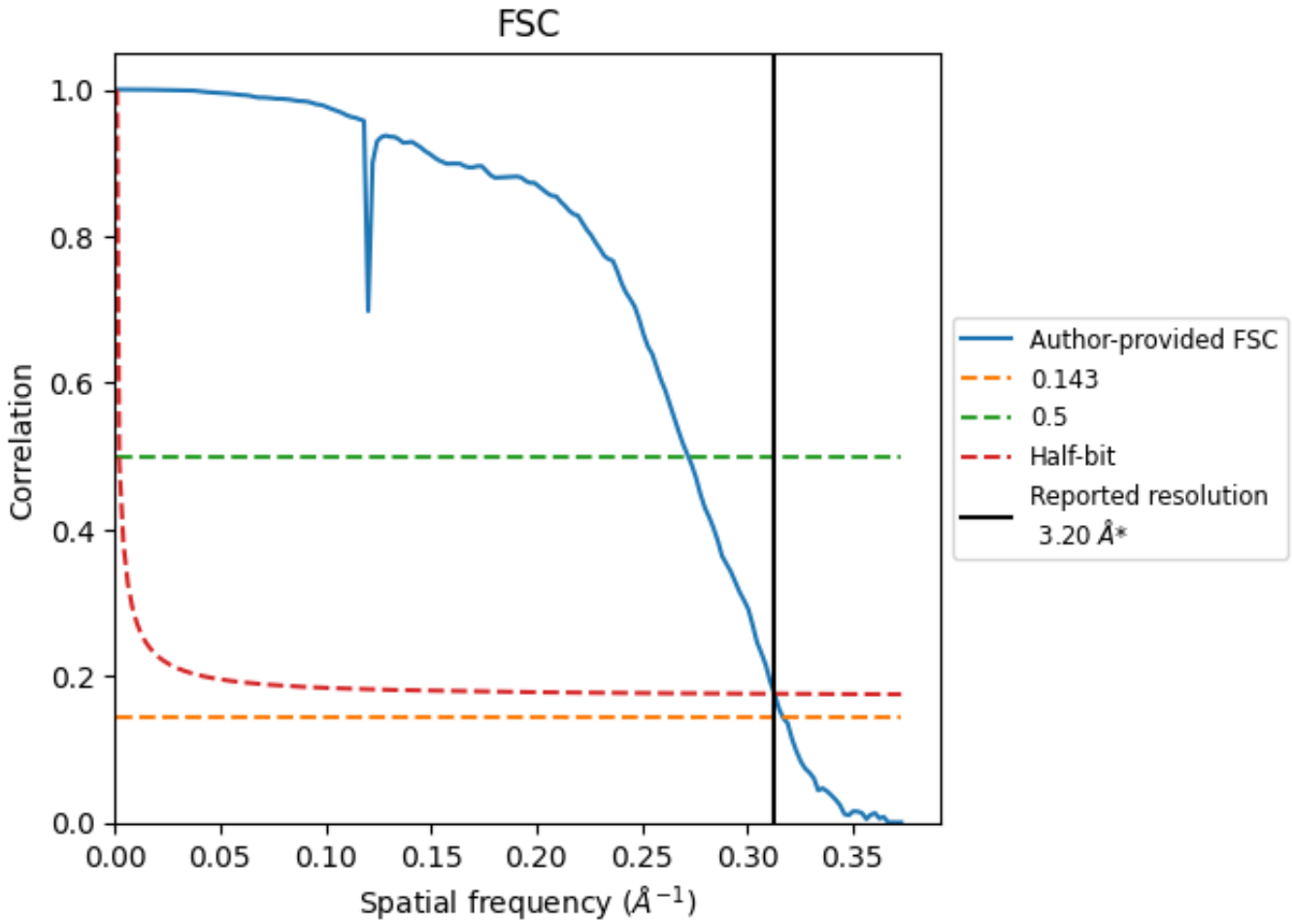


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

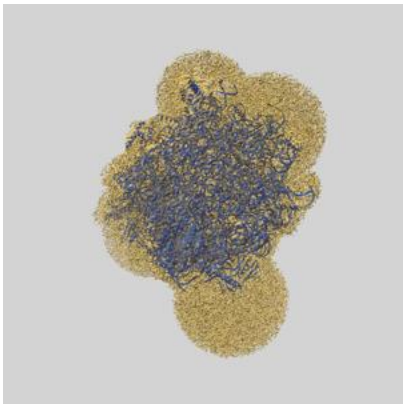
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.68	3.19
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

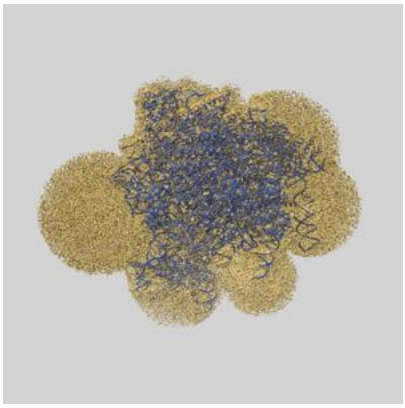
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2566 and PDB model 3J6B. Per-residue inclusion information can be found in section 3 on page 12.

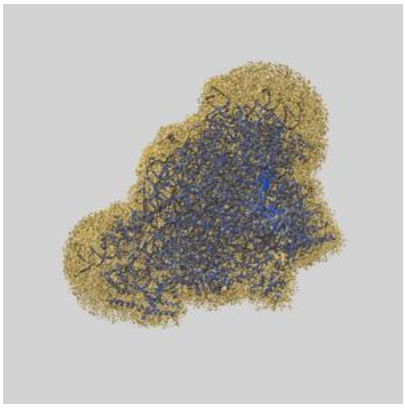
9.1 Map-model overlay



X



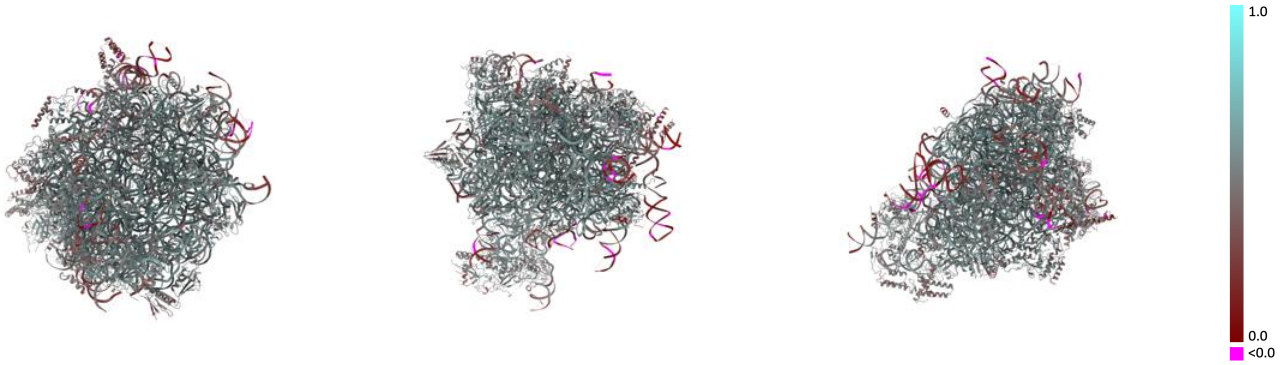
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0681 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.

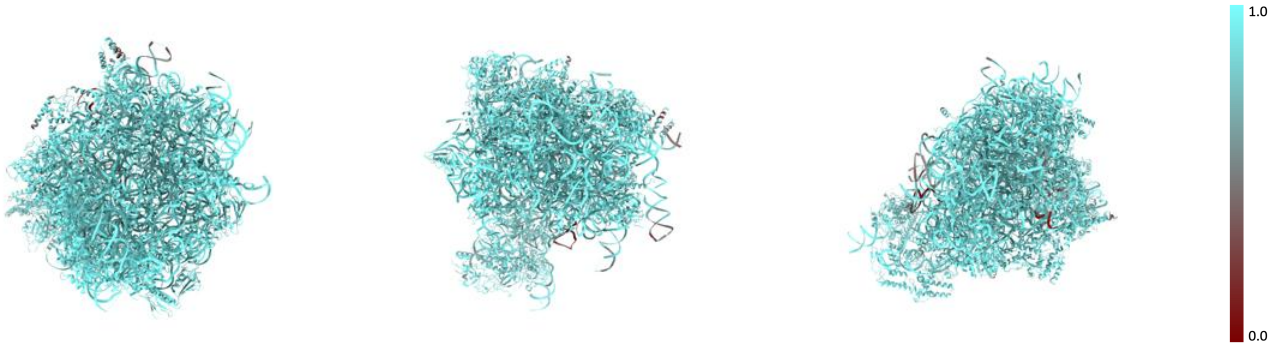
9.2 Q-score mapped to coordinate model



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.

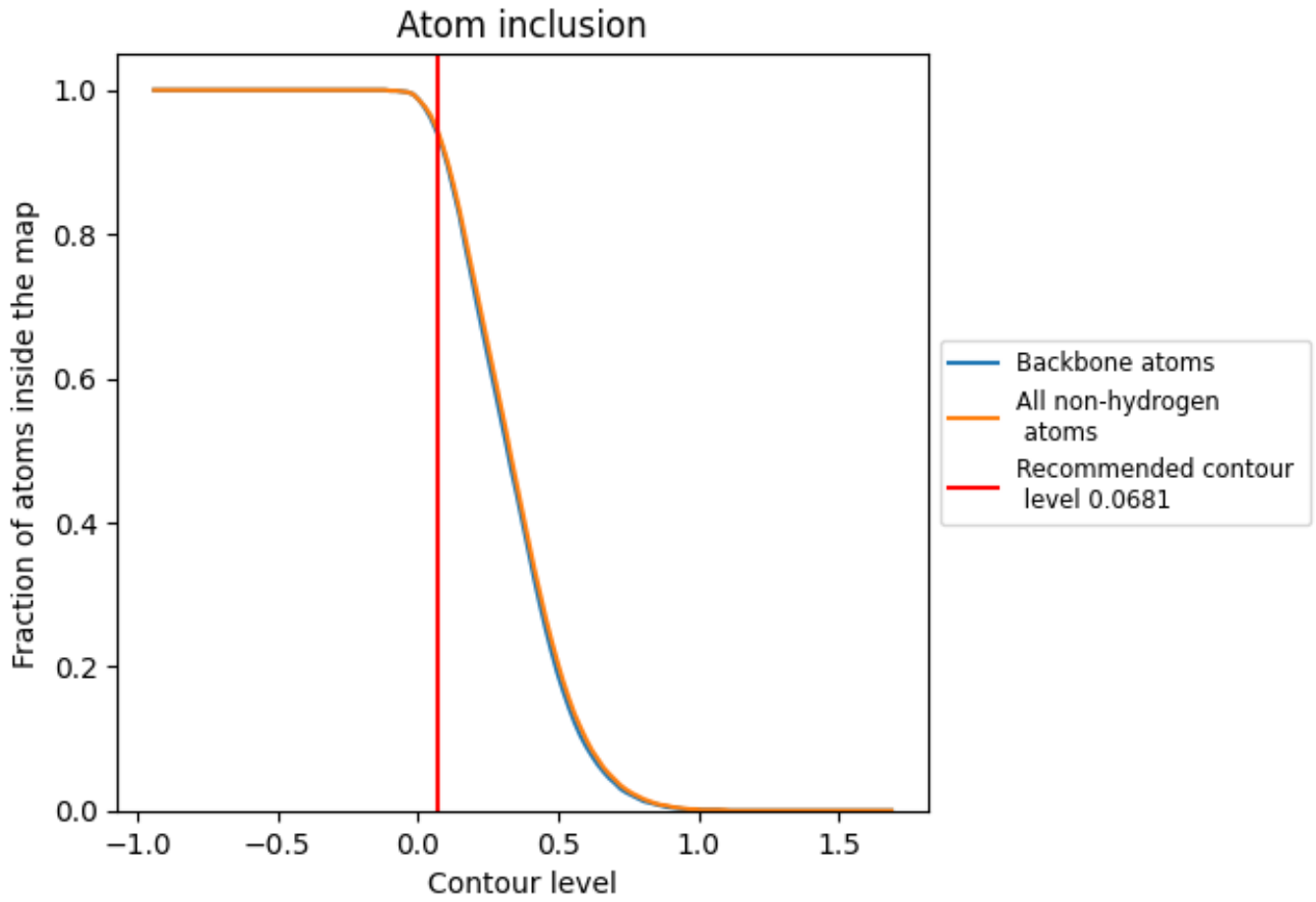
9.3 Atom inclusion mapped to coordinate model



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 (0.0681).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 95% 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 (0.0681) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9460	0.5070
0	0.9550	0.5600
1	0.9440	0.5060
2	0.9420	0.4870
3	0.9400	0.5180
4	0.9500	0.5420
5	0.9400	0.5190
6	0.9260	0.4600
7	0.9420	0.5170
8	0.8880	0.4180
9	0.9420	0.4650
A	0.9600	0.5070
B	0.9490	0.5350
C	0.9580	0.5580
D	0.9310	0.5210
E	0.9350	0.5150
F	0.9140	0.4500
G	0.9580	0.5080
H	0.9470	0.5580
I	0.9150	0.5150
J	0.9570	0.5360
K	0.9390	0.5240
L	0.9380	0.5230
M	0.9380	0.5120
N	0.9520	0.5500
O	0.9350	0.5230
P	0.9280	0.5110
Q	0.8950	0.4610
R	0.9300	0.4700
S	0.9430	0.5270
T	0.8780	0.4520
U	0.9490	0.5350
V	0.9330	0.5010
W	0.9440	0.5330
X	0.9260	0.5300

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Chain	Atom inclusion	Q-score
Y	0.9190	0.5590
Z	0.9610	0.5640
a	0.9390	0.5060
b	0.9180	0.4930
c	0.9370	0.5390
d	0.9390	0.5240
e	0.2880	0.1130