



## wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 01:12 pm GMT

PDB ID : 5MLC  
EMDB ID : EMD-3525  
Title : Cryo-EM structure of the spinach chloroplast ribosome reveals the location of plastid-specific ribosomal proteins and extensions  
Authors : Graf, M.; Arenz, S.; Huter, P.; Doenhoefer, A.; Novacek, J.; Wilson, D.N.  
Deposited on : 2016-12-06  
Resolution : 3.90 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](mailto: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>.

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

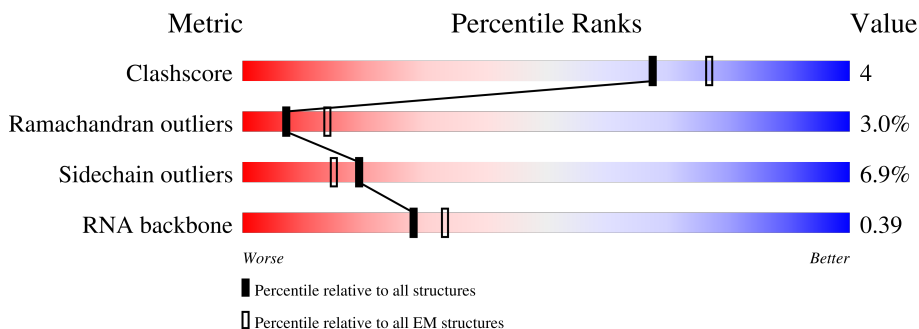
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP)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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 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  $\geq 3$ , 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  $\leq 5\%$ . 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	2811	16% (poor fit), 59% (0 outliers), 33% (1 outlier), 6% (2 outliers), 0% (3+ outliers)
2	B	121	57% (poor fit), 73% (0 outliers), 23% (1 outlier), 0% (2 outliers), 0% (3+ outliers)
3	C	103	6% (poor fit), 53% (0 outliers), 31% (1 outlier), 6% (2 outliers), 10% (3+ outliers)
4	D	272	19% (poor fit), 74% (0 outliers), 14% (1 outlier), 0% (2 outliers), 10% (3+ outliers)
5	E	305	8% (poor fit), 62% (0 outliers), 9% (1 outlier), 28% (2+ outliers)
6	F	293	8% (poor fit), 59% (0 outliers), 10% (1 outlier), 30% (2+ outliers)
7	G	220	80% (poor fit), 73% (0 outliers), 9% (1 outlier), 19% (2+ outliers)

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Mol	Chain	Length	Quality of chain
8	H	220	
9	I	196	
10	L	250	
11	M	121	
12	N	271	
13	O	135	
14	P	126	
15	Q	166	
16	R	233	
17	S	128	
18	T	256	
19	U	199	
20	V	198	
21	W	191	
22	X	194	
23	Y	148	
24	Z	168	
25	2	57	
26	3	66	
27	4	152	
28	5	159	
29	6	37	
30	9	271	
31	7	142	
32	8	116	

## 2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 90647 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2750	59074	26351	10944	19029	2750	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	120	2564	1145	464	835	120	0	0

- Molecule 3 is a RNA chain called 4.8S ribosomal RNA, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C	93	2001	893	374	641	93	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	246	1895	1175	388	326	6	0	0

- Molecule 5 is a protein called 50S ribosomal protein L3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	219	1669	1056	304	298	11	0	0

- Molecule 6 is a protein called 50S ribosomal protein L4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	205	1617	1024	303	287	3	0	0

- Molecule 7 is a protein called 50S ribosomal protein L5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	179	1387	883	241	255	8	0	0

- Molecule 8 is a protein called 50S ribosomal protein L6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	178	1386	874	255	253	4	0	0

- Molecule 9 is a protein called 50S ribosomal protein L9, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	I	45	359	237	65	57	0	0

- Molecule 10 is a protein called 50S ribosomal protein L13, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L	196	1489	942	280	264	3	0	0

- Molecule 11 is a protein called 50S ribosomal protein L14, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	M	120	934	582	178	169	5	0	0

- Molecule 12 is a protein called 50S ribosomal protein L15, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	N	182	1385	864	273	242	6	0	0

- Molecule 13 is a protein called 50S ribosomal protein L16, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	O	135	1075	677	218	174	6	0	0

- Molecule 14 is a protein called 50S ribosomal protein L17, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	116	Total	C	N	O	S	0	0
			945	592	193	156	4		

- Molecule 15 is a protein called 50S ribosomal protein L18, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	118	Total	C	N	O	S	0	0
			931	579	179	168	5		

- Molecule 16 is a protein called 50S ribosomal protein L19, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	114	Total	C	N	O	S	0	0
			915	586	178	150	1		

- Molecule 17 is a protein called 50S ribosomal protein L20, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	116	Total	C	N	O	S	0	0
			1003	637	209	155	2		

- Molecule 18 is a protein called 50S ribosomal protein L21, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	T	134	Total	C	N	O	0	0
			1017	653	183	181		

- Molecule 19 is a protein called 50S ribosomal protein L22, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	152	Total	C	N	O	S	0	0
			1165	738	212	208	7		

- Molecule 20 is a protein called 50S ribosomal protein L23, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	91	Total	C	N	O	S	0	0
			734	474	127	131	2		

- Molecule 21 is a protein called 50S ribosomal protein L24, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	129	Total	C	N	O	S	0	0
			1018	641	193	182	2		

- Molecule 22 is a protein called 50S ribosomal protein L27, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	108	Total	C	N	O	S	0	0
			866	545	172	149			

- Molecule 23 is a protein called 50S ribosomal protein L28, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	75	Total	C	N	O	S	0	0
			616	391	125	99	1		

- Molecule 24 is a protein called 50S ribosomal protein L29, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	94	Total	C	N	O	S	0	0
			788	492	156	137	3		

- Molecule 25 is a protein called 50S ribosomal protein L32, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	2	42	Total	C	N	O	0	0
			341	223	65	53		

- Molecule 26 is a protein called 50S ribosomal protein L33, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	3	60	Total	C	N	O	S	0	0
			489	304	98	83	4		

- Molecule 27 is a protein called 50S ribosomal protein L34, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4	61	Total	C	N	O	S	0	0
			471	284	108	76	3		

- Molecule 28 is a protein called 50S ribosomal protein L35, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	70	Total	C	N	O	S	0	0
			575	362	121	91	1		

- Molecule 29 is a protein called 50S ribosomal protein L36, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	6	37	Total	C	N	O	S	0	0
			305	186	70	45	4		

- Molecule 30 is a protein called Ribosome-recycling factor, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	9	107	Total	C	N	O	S	0	0
			881	545	158	175	3		

- Molecule 31 is a protein called PSRP5alpha, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	7	46	Total	C	N	O	S	0	0
			378	241	77	56	4		

- Molecule 32 is a protein called PSRP6, chloroplastic.

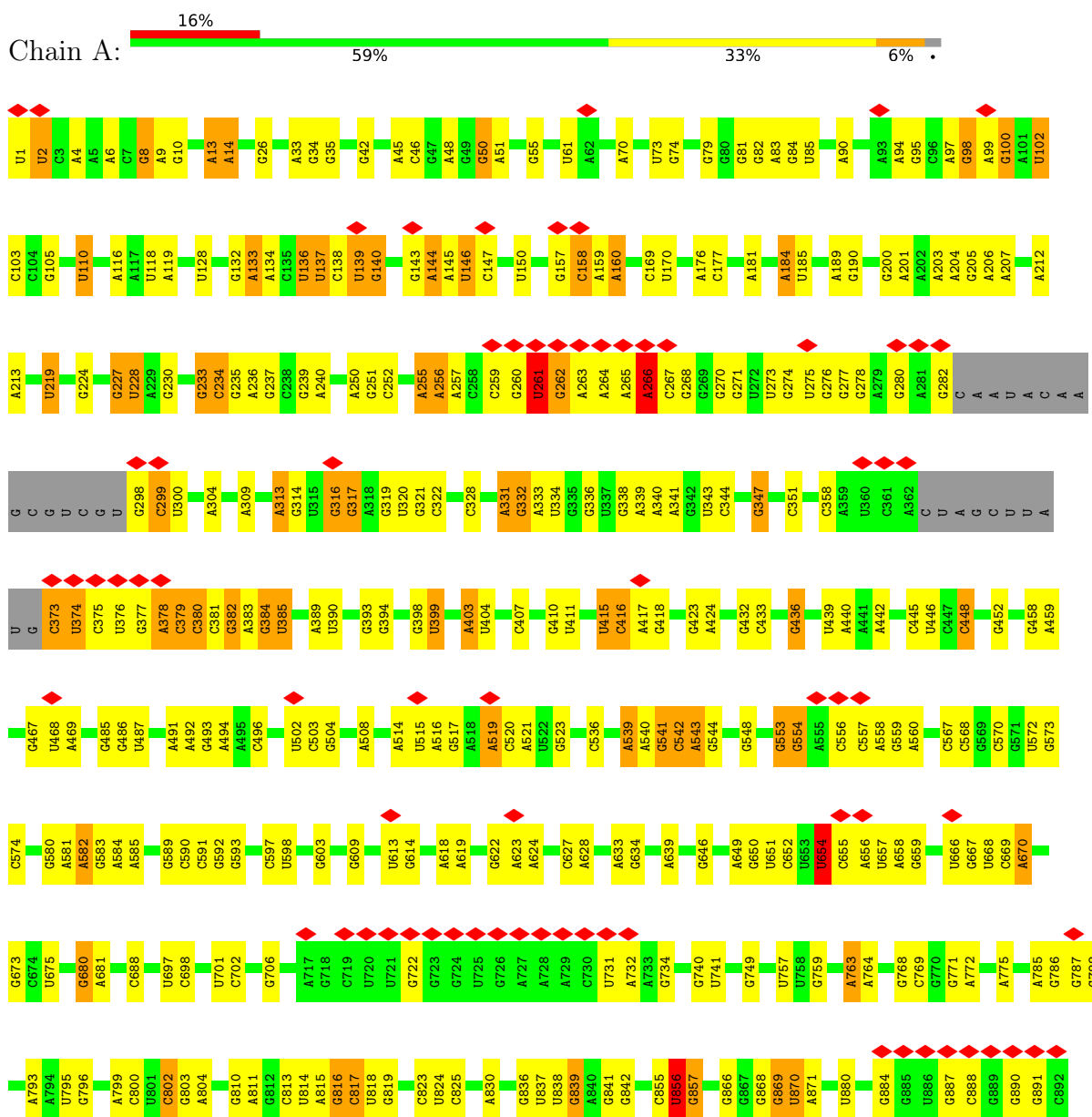
Mol	Chain	Residues	Atoms					AltConf	Trace
32	8	47	Total	C	N	O	S	0	0
			374	240	72	61	1		

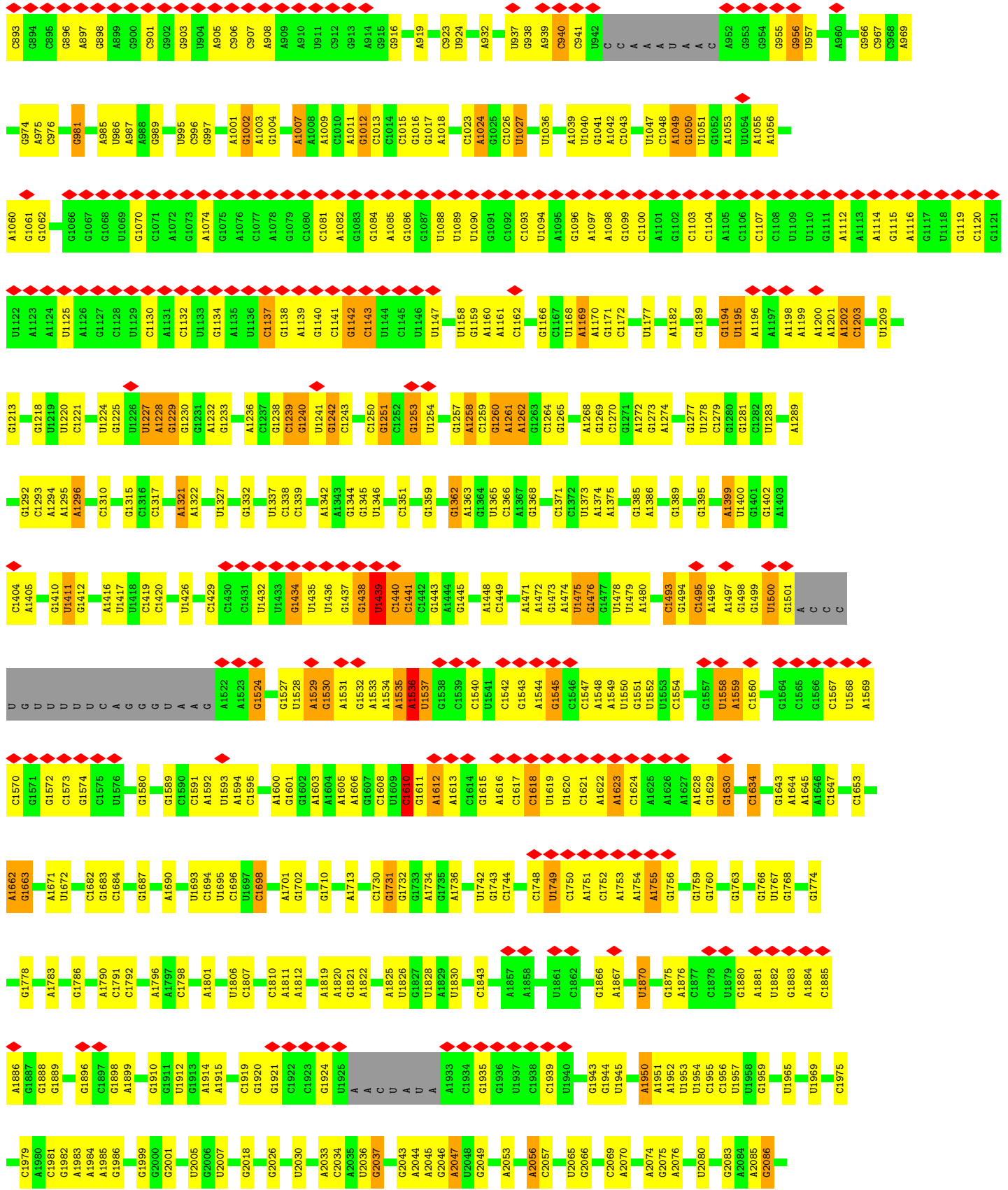


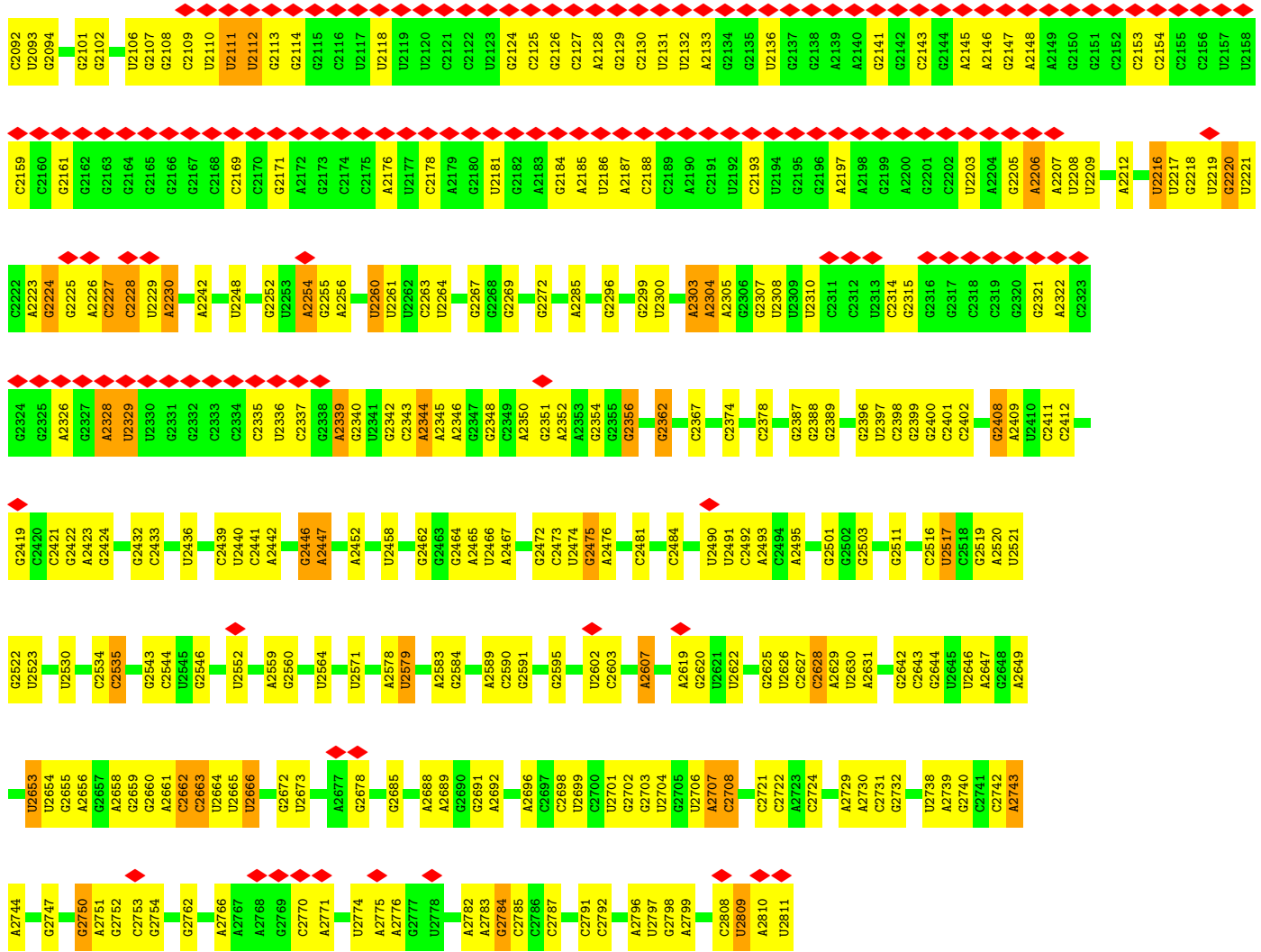
### 3 Residue-property plots

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.

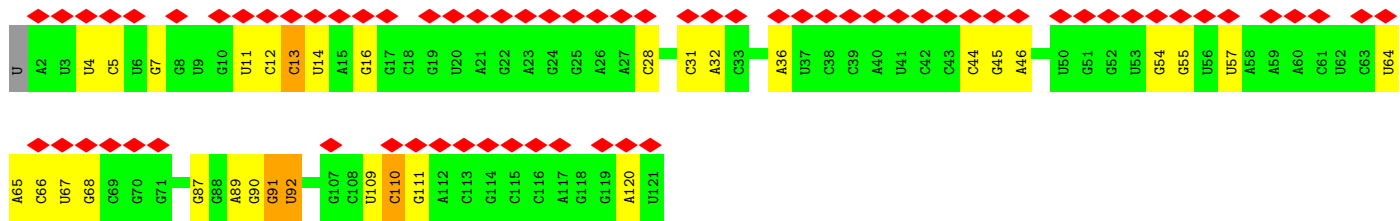
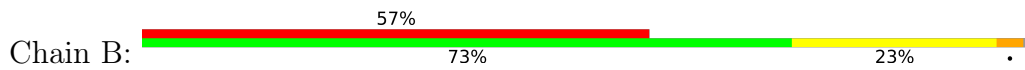
- Molecule 1: 23S ribosomal RNA, chloroplastic







• Molecule 2: 5S ribosomal RNA, chloroplastic

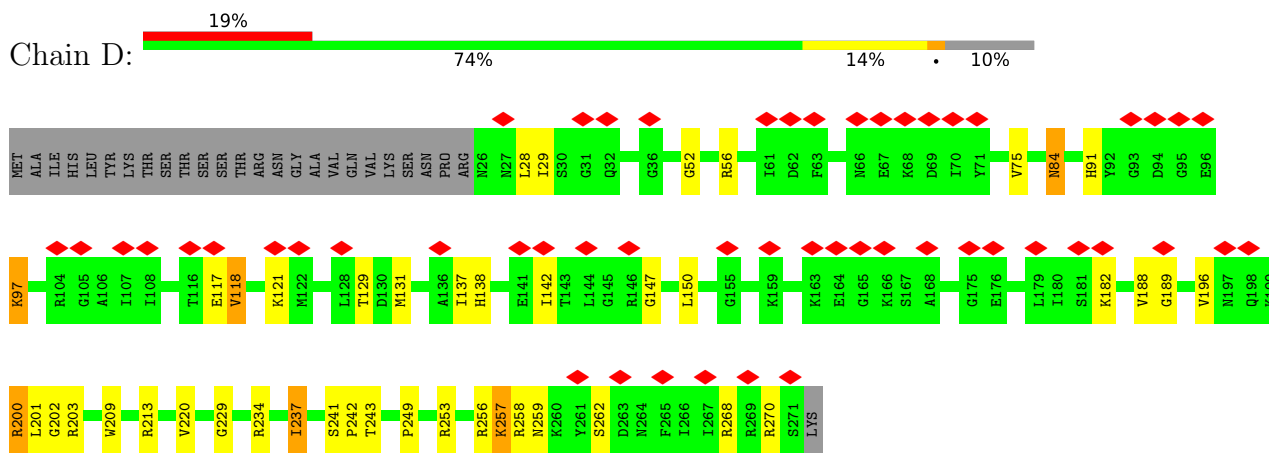


• Molecule 3: 4.8S ribosomal RNA, chloroplastic

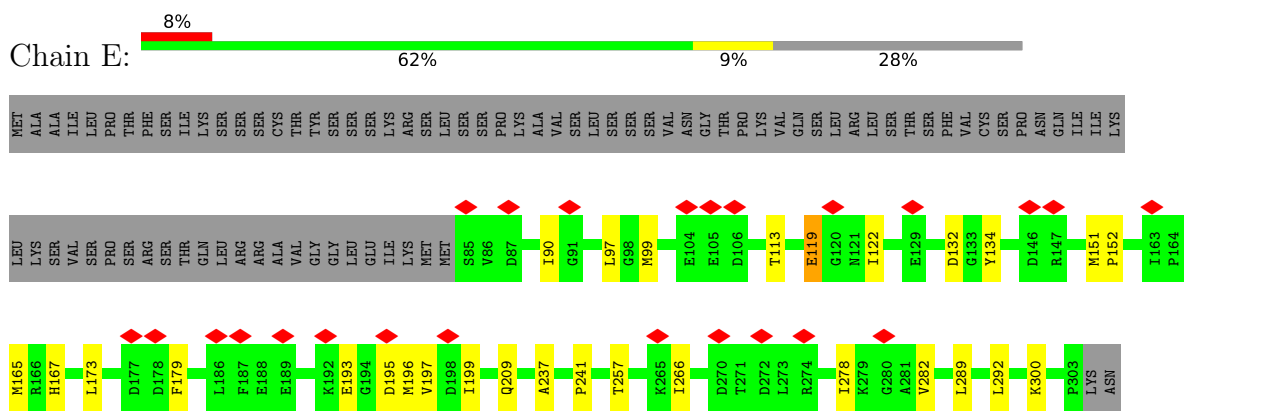




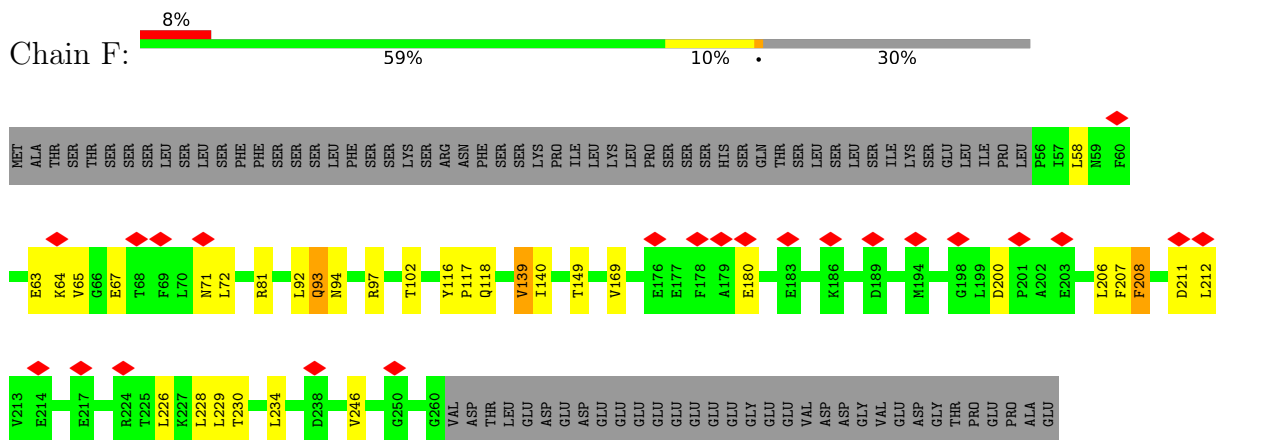
• Molecule 4: 50S ribosomal protein L2, chloroplastic



• Molecule 5: 50S ribosomal protein L3, chloroplastic

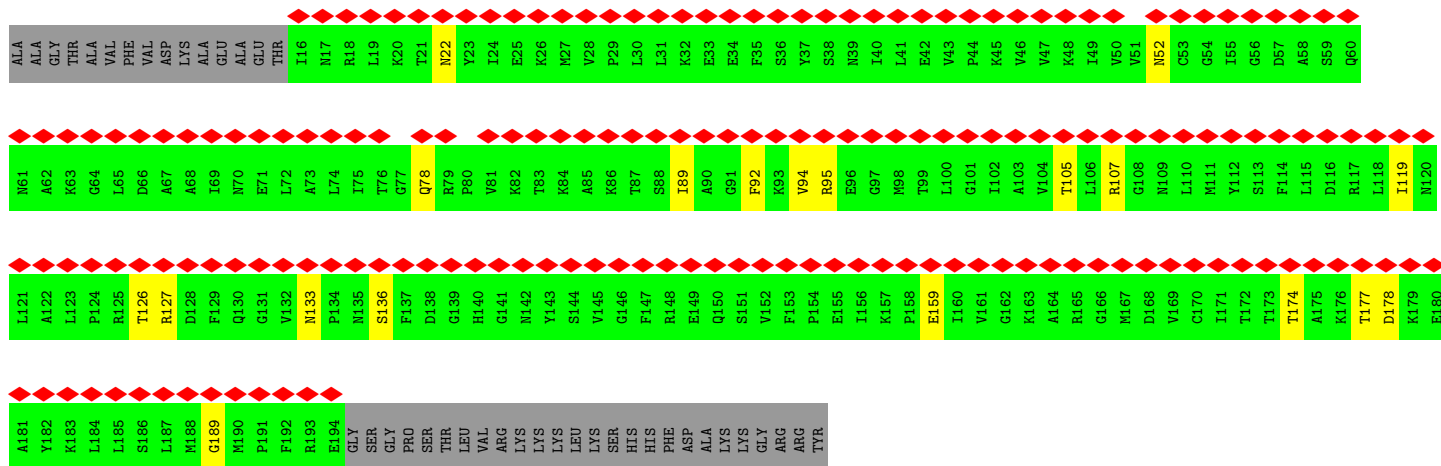


• Molecule 6: 50S ribosomal protein L4, chloroplastic

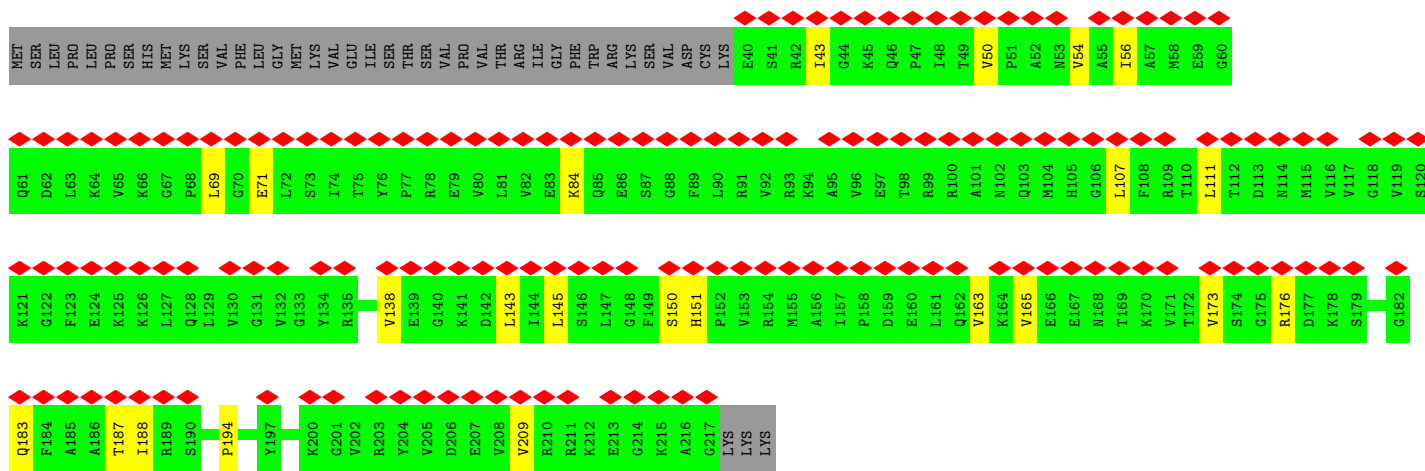


• Molecule 7: 50S ribosomal protein L5, chloroplastic

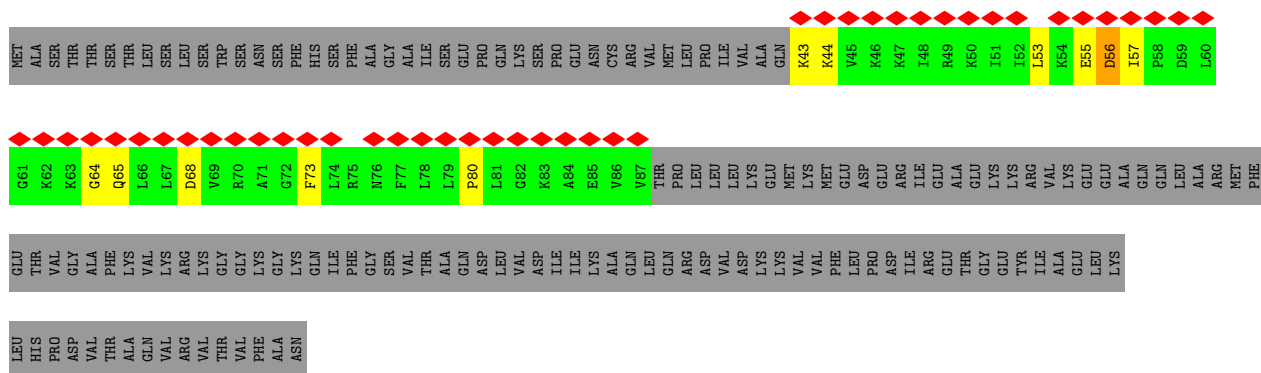




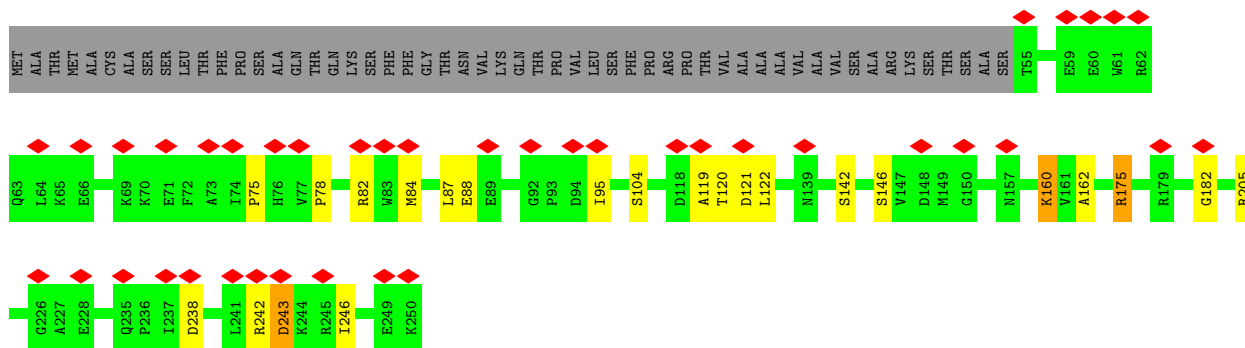
• Molecule 8: 50S ribosomal protein L6, chloroplastic



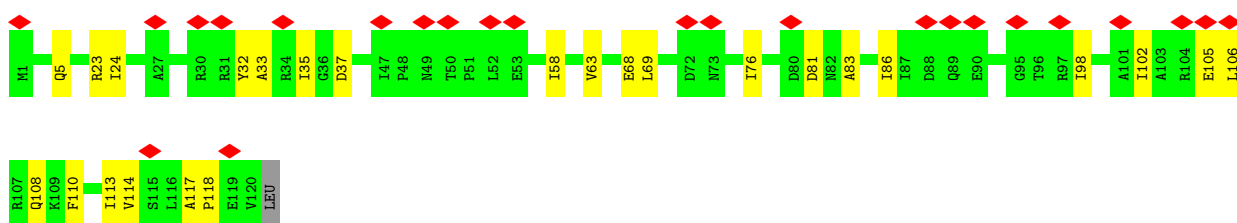
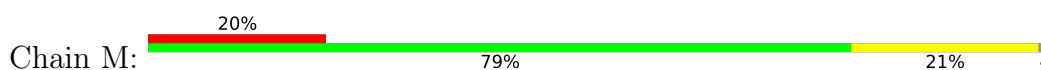
• Molecule 9: 50S ribosomal protein L9, chloroplastic



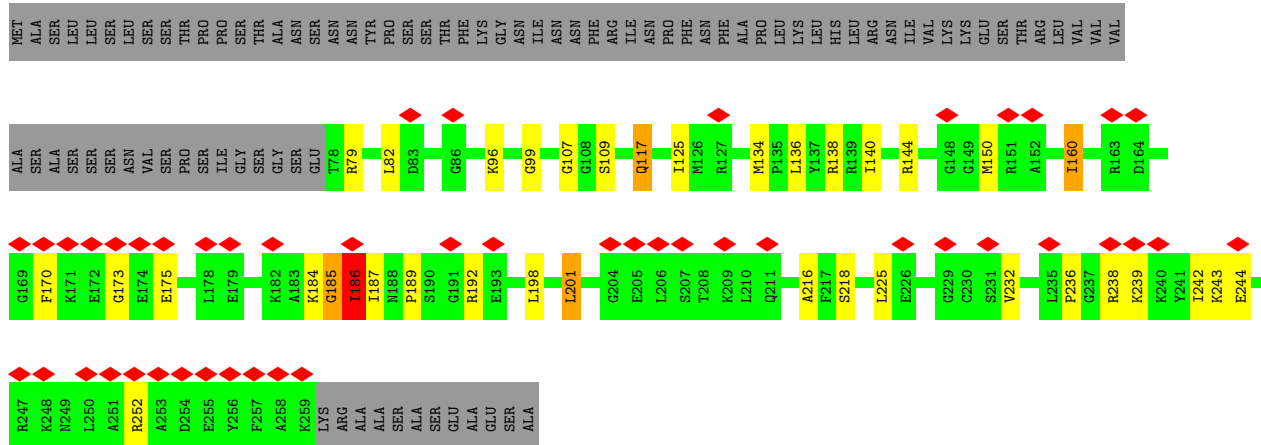
• Molecule 10: 50S ribosomal protein L13, chloroplastic



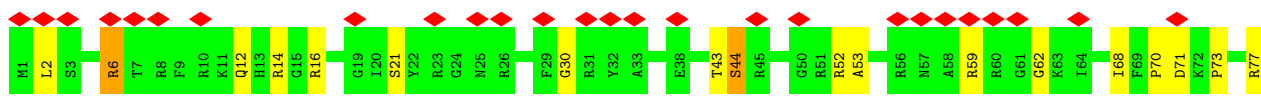
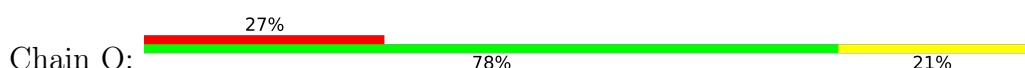
• Molecule 11: 50S ribosomal protein L14, chloroplastic



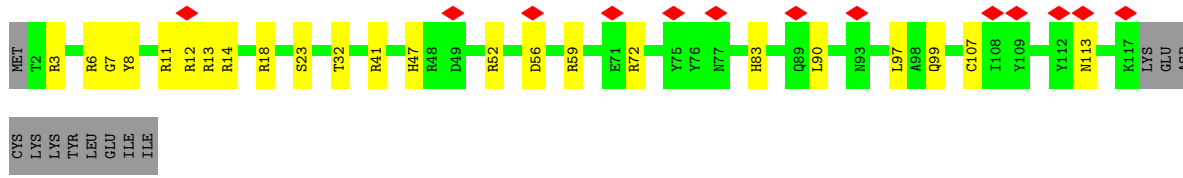
• Molecule 12: 50S ribosomal protein L15, chloroplastic



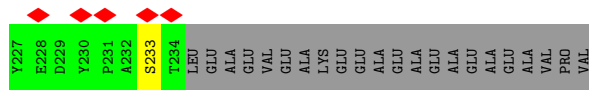
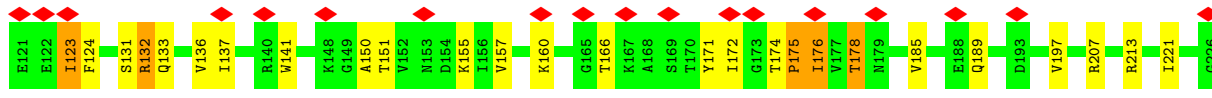
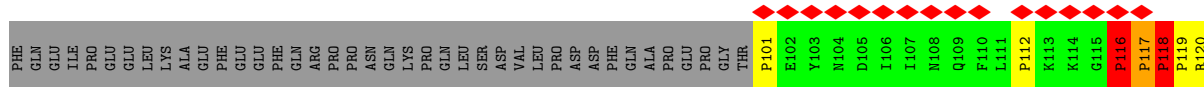
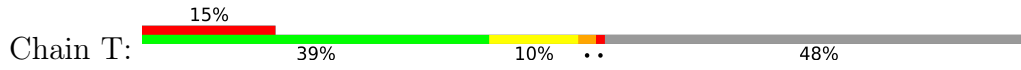
• Molecule 13: 50S ribosomal protein L16, chloroplastic



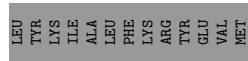
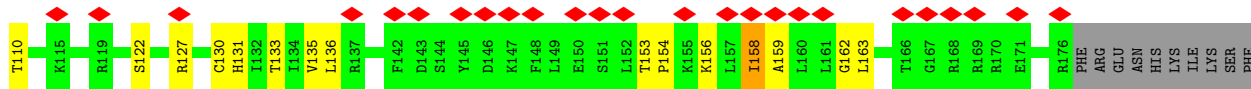




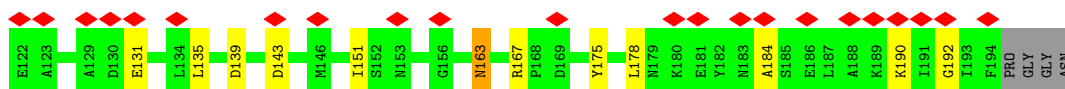
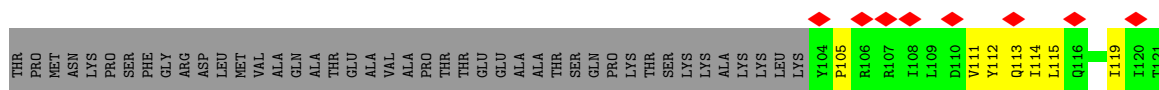
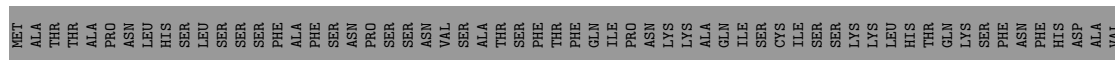
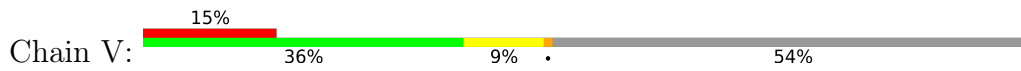
• Molecule 18: 50S ribosomal protein L21, chloroplastic



• Molecule 19: 50S ribosomal protein L22, chloroplastic



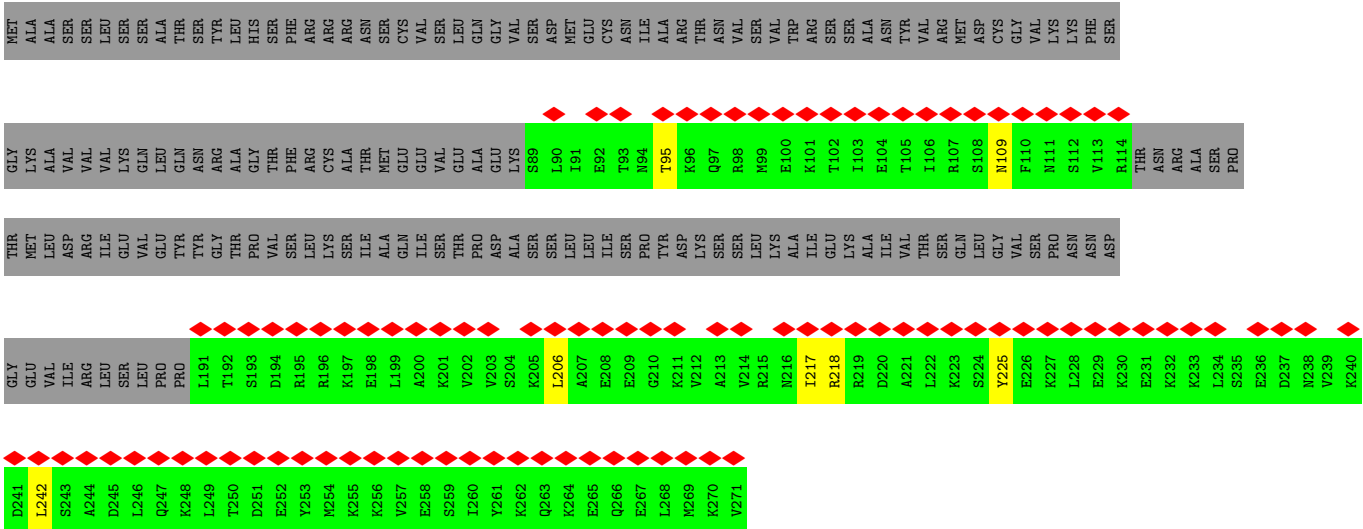
• Molecule 20: 50S ribosomal protein L23, chloroplastic



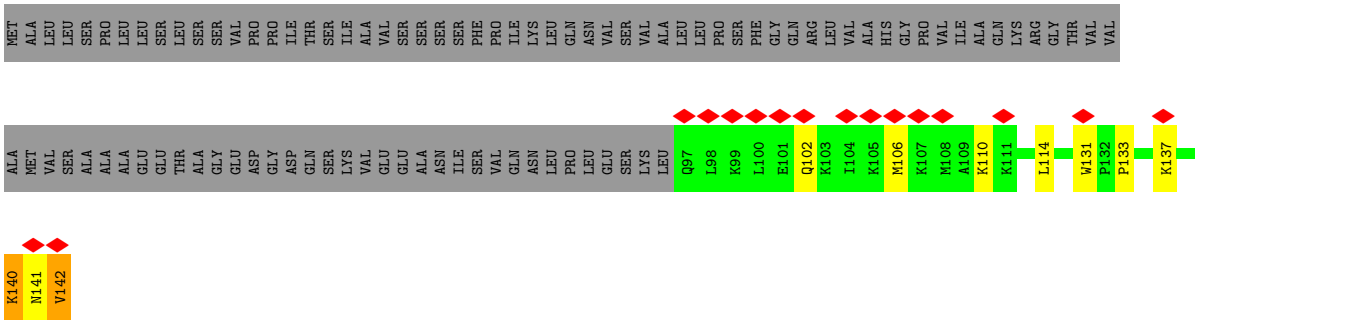




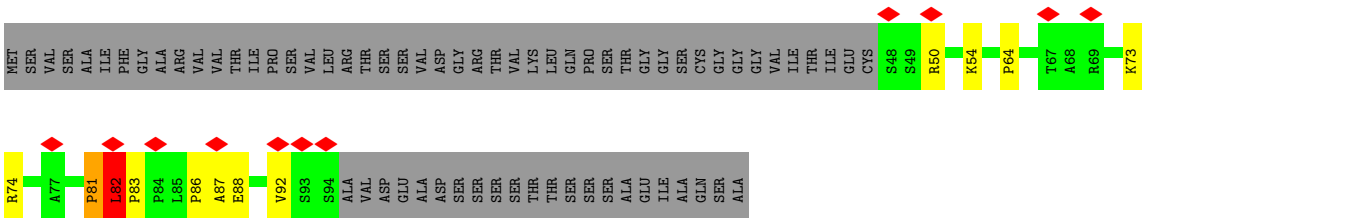




● Molecule 31: PSRP5alpha, chloroplatic



● Molecule 32: PSRP6, chloroplatic



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	37636	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	2.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	2.218	Depositor
Minimum map value	-1.456	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	390.448, 390.448, 390.448	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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	0.40	19/66169 (0.0%)	0.73	32/103225 (0.0%)
2	B	0.29	0/2868	0.71	0/4469
3	C	0.28	0/2241	0.69	0/3492
4	D	0.43	0/1928	0.74	0/2588
5	E	0.41	0/1696	0.71	0/2269
6	F	0.56	2/1648 (0.1%)	0.72	0/2215
7	G	0.46	0/1408	0.58	0/1896
8	H	0.57	2/1407 (0.1%)	0.61	0/1892
9	I	0.47	0/362	0.69	0/480
10	L	0.47	1/1521 (0.1%)	0.72	2/2062 (0.1%)
11	M	0.41	0/943	0.69	0/1271
12	N	0.44	0/1405	0.78	0/1864
13	O	0.43	0/1097	0.76	0/1471
14	P	0.47	0/960	0.82	0/1280
15	Q	0.43	0/946	0.69	0/1268
16	R	0.48	1/928 (0.1%)	0.71	0/1248
17	S	0.46	0/1020	0.82	0/1361
18	T	0.81	1/1034 (0.1%)	0.82	5/1405 (0.4%)
19	U	0.86	1/1184 (0.1%)	0.73	0/1593
20	V	0.50	1/744 (0.1%)	0.67	0/1000
21	W	0.55	1/1030 (0.1%)	0.71	1/1374 (0.1%)
22	X	0.41	0/882	0.64	1/1172 (0.1%)
23	Y	0.45	0/626	0.76	0/833
24	Z	0.42	0/796	0.77	0/1056
25	2	0.59	0/348	0.74	0/462
26	3	0.42	0/497	0.75	0/664
27	4	0.45	0/474	0.92	0/624
28	5	0.39	0/581	0.81	0/768
29	6	0.39	0/307	0.80	0/403
30	9	0.41	0/883	0.57	0/1169
31	7	0.45	0/381	0.75	0/498
32	8	0.45	0/388	0.73	0/528
All	All	0.43	29/98702 (0.0%)	0.73	41/147900 (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
18	T	0	1

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1554	C	O3'-P	-23.08	1.33	1.61
19	U	158	ILE	C-N	22.12	1.84	1.34
18	T	118	PRO	C-N	19.55	1.71	1.34
1	A	1435	U	O3'-P	-13.97	1.44	1.61
8	H	71	GLU	CD-OE2	12.96	1.40	1.25

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	U	N1-C1'-C2'	-11.30	99.31	114.00
1	A	1618	C	P-O3'-C3'	-10.44	107.17	119.70
1	A	763	A	C2'-C3'-O3'	8.73	128.71	109.50
1	A	50	G	C2'-C3'-O3'	7.76	126.57	109.50
1	A	261	U	C2'-C3'-O3'	7.38	125.74	109.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	T	116	PRO	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	59074	0	29746	384	0
2	B	2564	0	1295	7	0
3	C	2001	0	1008	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1895	0	1977	18	0
5	E	1669	0	1753	11	0
6	F	1617	0	1677	10	0
7	G	1387	0	1443	7	0
8	H	1386	0	1448	12	0
9	I	359	0	415	3	0
10	L	1489	0	1434	8	0
11	M	934	0	985	10	0
12	N	1385	0	1464	13	0
13	O	1075	0	1134	13	0
14	P	945	0	1004	11	0
15	Q	931	0	952	3	0
16	R	915	0	1008	8	0
17	S	1003	0	1069	6	0
18	T	1017	0	1017	15	0
19	U	1165	0	1175	11	0
20	V	734	0	780	9	0
21	W	1018	0	1072	7	0
22	X	866	0	909	7	0
23	Y	616	0	665	7	0
24	Z	788	0	849	23	0
25	2	341	0	379	5	0
26	3	489	0	511	5	0
27	4	471	0	529	2	0
28	5	575	0	642	3	0
29	6	305	0	344	0	0
30	9	881	0	932	4	0
31	7	378	0	445	6	0
32	8	374	0	391	5	0
All	All	90647	0	60452	575	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 4.

The worst 5 of 575 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:133:A:C6	24:Z:131:ARG:NH1	1.78	1.50
1:A:133:A:C2	24:Z:131:ARG:NH2	1.80	1.45
18:T:118:PRO:C	18:T:119:PRO:N	1.71	1.42
1:A:133:A:C5	24:Z:131:ARG:NH1	1.78	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:158:ILE:C	19:U:159:ALA:N	1.84	1.27

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	
4	D	244/272 (90%)	200 (82%)	34 (14%)	10 (4%)	3	27
5	E	217/305 (71%)	191 (88%)	24 (11%)	2 (1%)	17	54
6	F	203/293 (69%)	170 (84%)	28 (14%)	5 (2%)	5	36
7	G	177/220 (80%)	160 (90%)	15 (8%)	2 (1%)	14	51
8	H	176/220 (80%)	152 (86%)	23 (13%)	1 (1%)	25	63
9	I	43/196 (22%)	33 (77%)	7 (16%)	3 (7%)	1	17
10	L	194/250 (78%)	171 (88%)	19 (10%)	4 (2%)	7	39
11	M	118/121 (98%)	101 (86%)	15 (13%)	2 (2%)	9	43
12	N	180/271 (66%)	142 (79%)	26 (14%)	12 (7%)	1	18
13	O	133/135 (98%)	120 (90%)	10 (8%)	3 (2%)	6	38
14	P	114/126 (90%)	102 (90%)	10 (9%)	2 (2%)	8	42
15	Q	116/166 (70%)	103 (89%)	11 (10%)	2 (2%)	9	43
16	R	112/233 (48%)	95 (85%)	16 (14%)	1 (1%)	17	54
17	S	114/128 (89%)	105 (92%)	7 (6%)	2 (2%)	8	42
18	T	132/256 (52%)	99 (75%)	23 (17%)	10 (8%)	1	16
19	U	150/199 (75%)	119 (79%)	29 (19%)	2 (1%)	12	48
20	V	89/198 (45%)	77 (86%)	9 (10%)	3 (3%)	3	31
21	W	127/191 (66%)	102 (80%)	20 (16%)	5 (4%)	3	28
22	X	106/194 (55%)	99 (93%)	5 (5%)	2 (2%)	8	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	Y	73/148 (49%)	64 (88%)	6 (8%)	3 (4%)	3	27
24	Z	92/168 (55%)	73 (79%)	14 (15%)	5 (5%)	2	22
25	2	40/57 (70%)	36 (90%)	3 (8%)	1 (2%)	5	36
26	3	58/66 (88%)	43 (74%)	9 (16%)	6 (10%)	0	9
27	4	59/152 (39%)	55 (93%)	2 (3%)	2 (3%)	3	31
28	5	68/159 (43%)	60 (88%)	8 (12%)	0	100	100
29	6	35/37 (95%)	31 (89%)	3 (9%)	1 (3%)	4	33
30	9	103/271 (38%)	100 (97%)	3 (3%)	0	100	100
31	7	44/142 (31%)	39 (89%)	2 (4%)	3 (7%)	1	18
32	8	45/116 (39%)	32 (71%)	6 (13%)	7 (16%)	0	3
All	All	3362/5290 (64%)	2874 (86%)	387 (12%)	101 (3%)	7	33

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	118	VAL
4	D	201	LEU
4	D	253	ARG
4	D	257	LYS
12	N	201	LEU

### 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	
4	D	194/217 (89%)	181 (93%)	13 (7%)	16	46
5	E	180/259 (70%)	170 (94%)	10 (6%)	21	51
6	F	171/254 (67%)	160 (94%)	11 (6%)	17	47
7	G	152/183 (83%)	145 (95%)	7 (5%)	27	55
8	H	150/190 (79%)	147 (98%)	3 (2%)	55	74
9	I	39/170 (23%)	35 (90%)	4 (10%)	7	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	L	142/213 (67%)	134 (94%)	8 (6%)	21	51
11	M	100/101 (99%)	94 (94%)	6 (6%)	19	49
12	N	139/215 (65%)	125 (90%)	14 (10%)	7	30
13	O	108/108 (100%)	100 (93%)	8 (7%)	13	43
14	P	96/103 (93%)	83 (86%)	13 (14%)	4	22
15	Q	97/139 (70%)	93 (96%)	4 (4%)	30	58
16	R	100/207 (48%)	89 (89%)	11 (11%)	6	28
17	S	103/115 (90%)	90 (87%)	13 (13%)	4	23
18	T	101/223 (45%)	91 (90%)	10 (10%)	8	31
19	U	119/176 (68%)	107 (90%)	12 (10%)	7	30
20	V	80/171 (47%)	74 (92%)	6 (8%)	13	42
21	W	111/171 (65%)	101 (91%)	10 (9%)	9	36
22	X	90/163 (55%)	86 (96%)	4 (4%)	28	56
23	Y	65/130 (50%)	62 (95%)	3 (5%)	27	55
24	Z	87/153 (57%)	82 (94%)	5 (6%)	20	50
25	2	35/50 (70%)	31 (89%)	4 (11%)	5	26
26	3	56/60 (93%)	55 (98%)	1 (2%)	59	77
27	4	50/125 (40%)	45 (90%)	5 (10%)	7	30
28	5	61/140 (44%)	58 (95%)	3 (5%)	25	54
29	6	34/34 (100%)	33 (97%)	1 (3%)	42	65
30	9	101/244 (41%)	101 (100%)	0	100	100
31	7	41/121 (34%)	37 (90%)	4 (10%)	8	31
32	8	41/96 (43%)	38 (93%)	3 (7%)	14	43
All	All	2843/4531 (63%)	2647 (93%)	196 (7%)	19	45

5 of 196 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	S	13	ARG
19	U	110	THR
17	S	59	ARG
18	T	157	VAL
20	V	163	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
27	4	143	ASN
31	7	102	GLN
28	5	95	HIS
30	9	97	GLN
11	M	5	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2745/2811 (97%)	824 (30%)	128 (4%)
2	B	119/121 (98%)	29 (24%)	3 (2%)
3	C	92/103 (89%)	28 (30%)	2 (2%)
All	All	2956/3035 (97%)	881 (29%)	133 (4%)

5 of 881 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	4	A
1	A	8	G
1	A	9	A
1	A	10	G

5 of 133 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2408	G
1	A	2534	C
2	B	89	A
1	A	838	U
1	A	800	C

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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
19	U	1
18	T	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	158:ILE	C	159:ALA	N	1.84
1	T	118:PRO	C	119:PRO	N	1.71
1	A	1554:C	O3'	1555:G	P	1.33

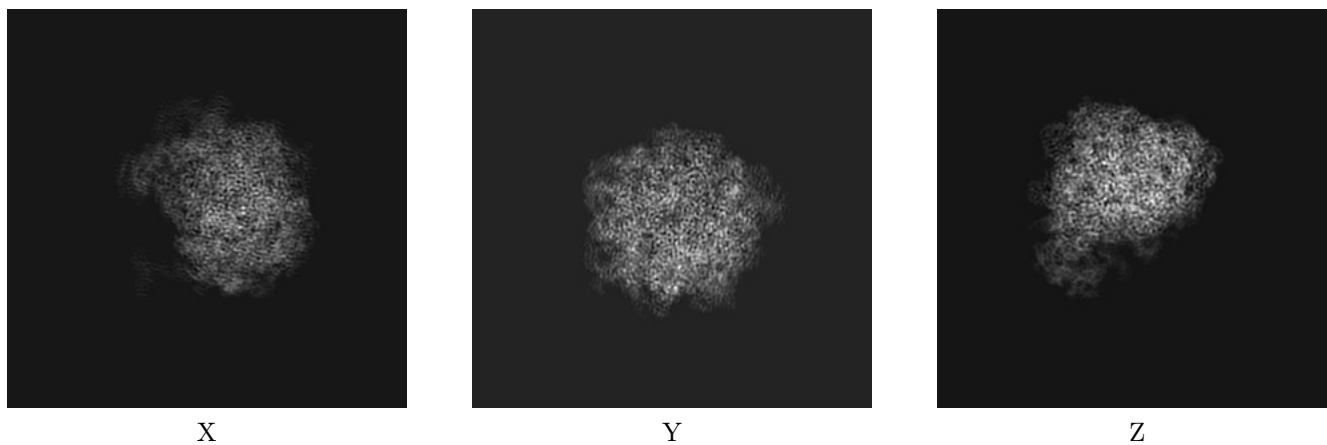
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3525. 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 [i](#)

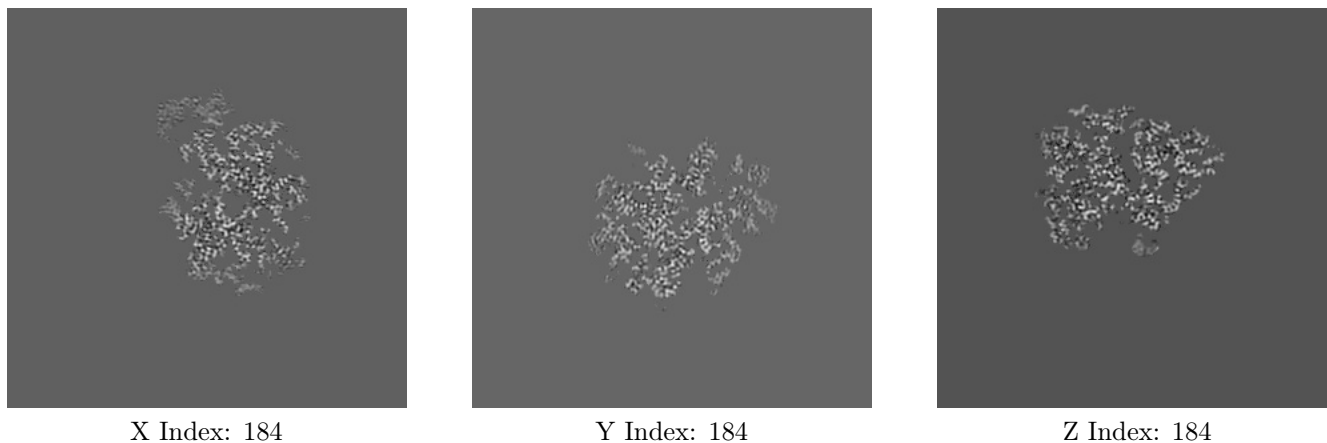
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

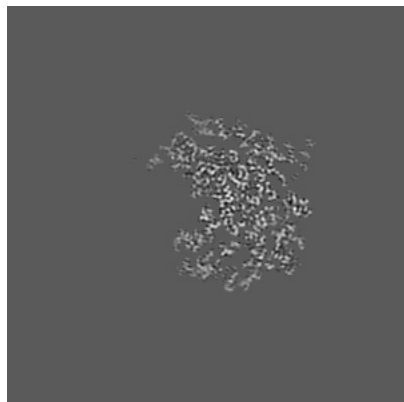
#### 6.2.1 Primary map



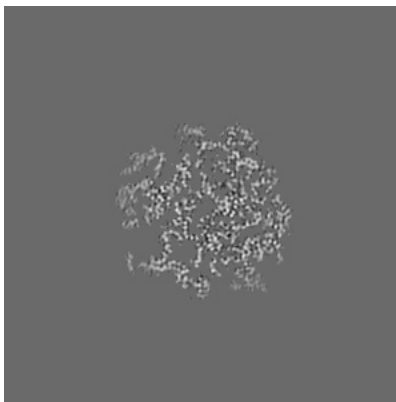
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 163



Y Index: 214

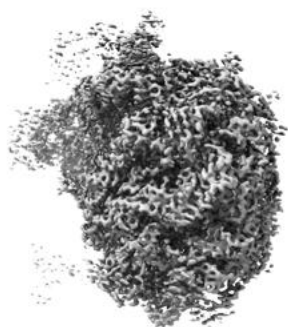


Z Index: 184

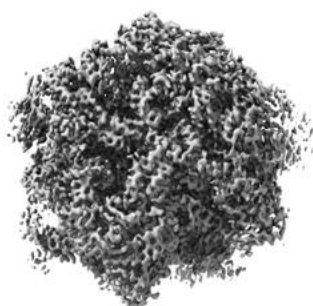
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

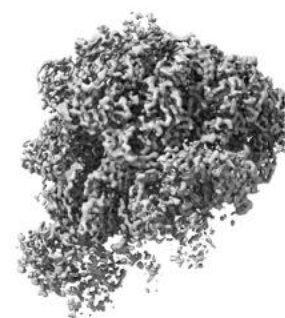
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

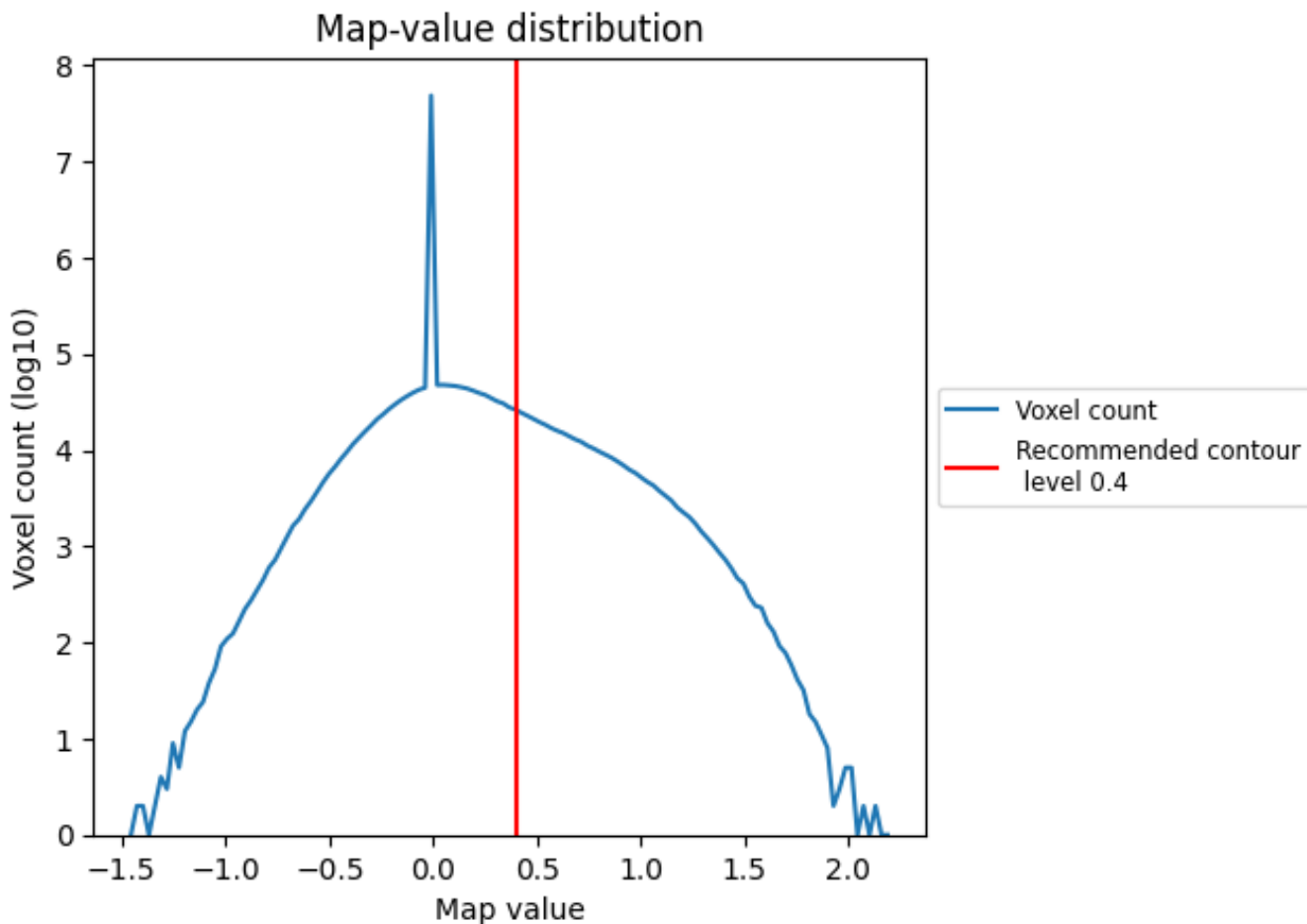
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

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

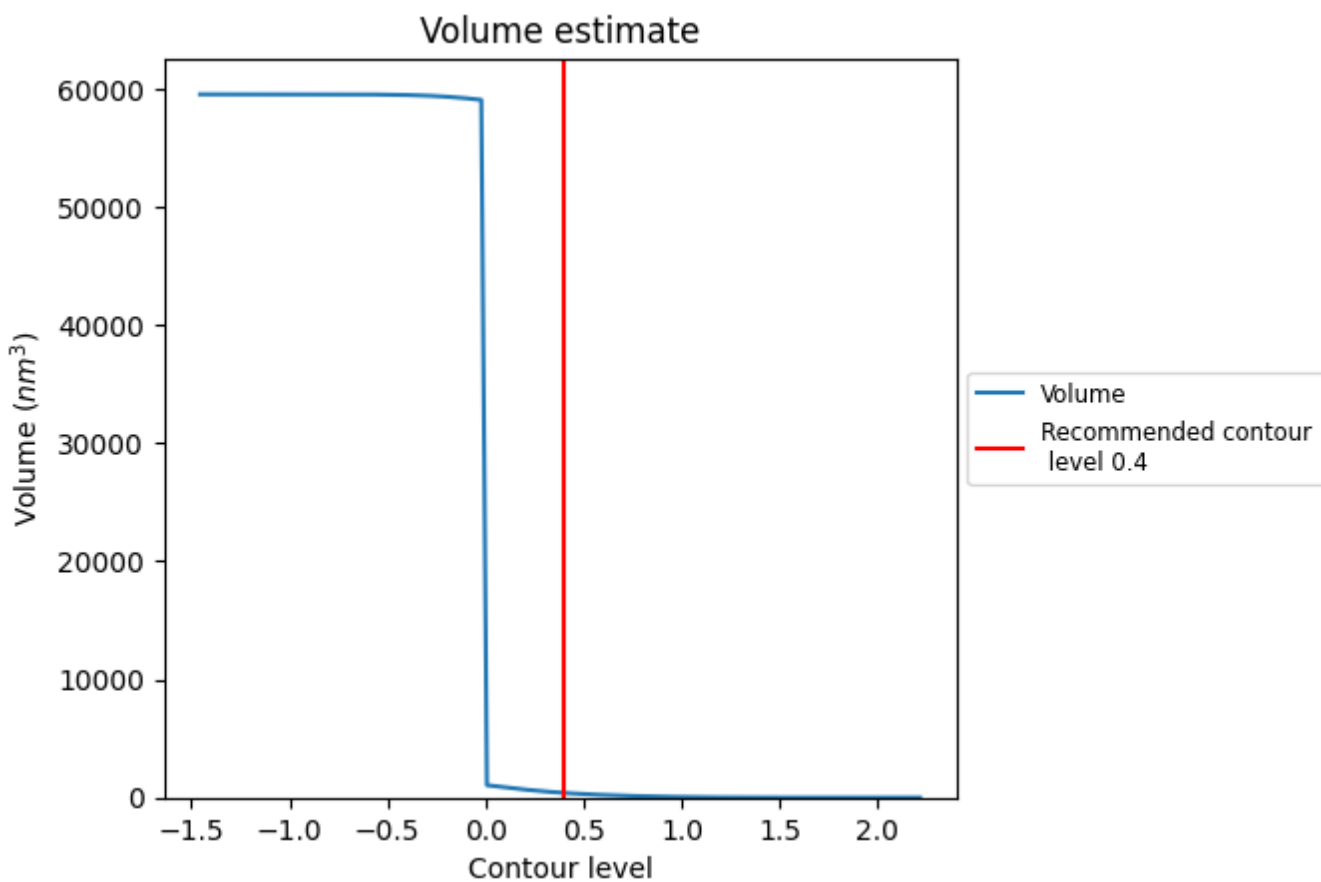
### 7.1 Map-value distribution [i](#)



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.



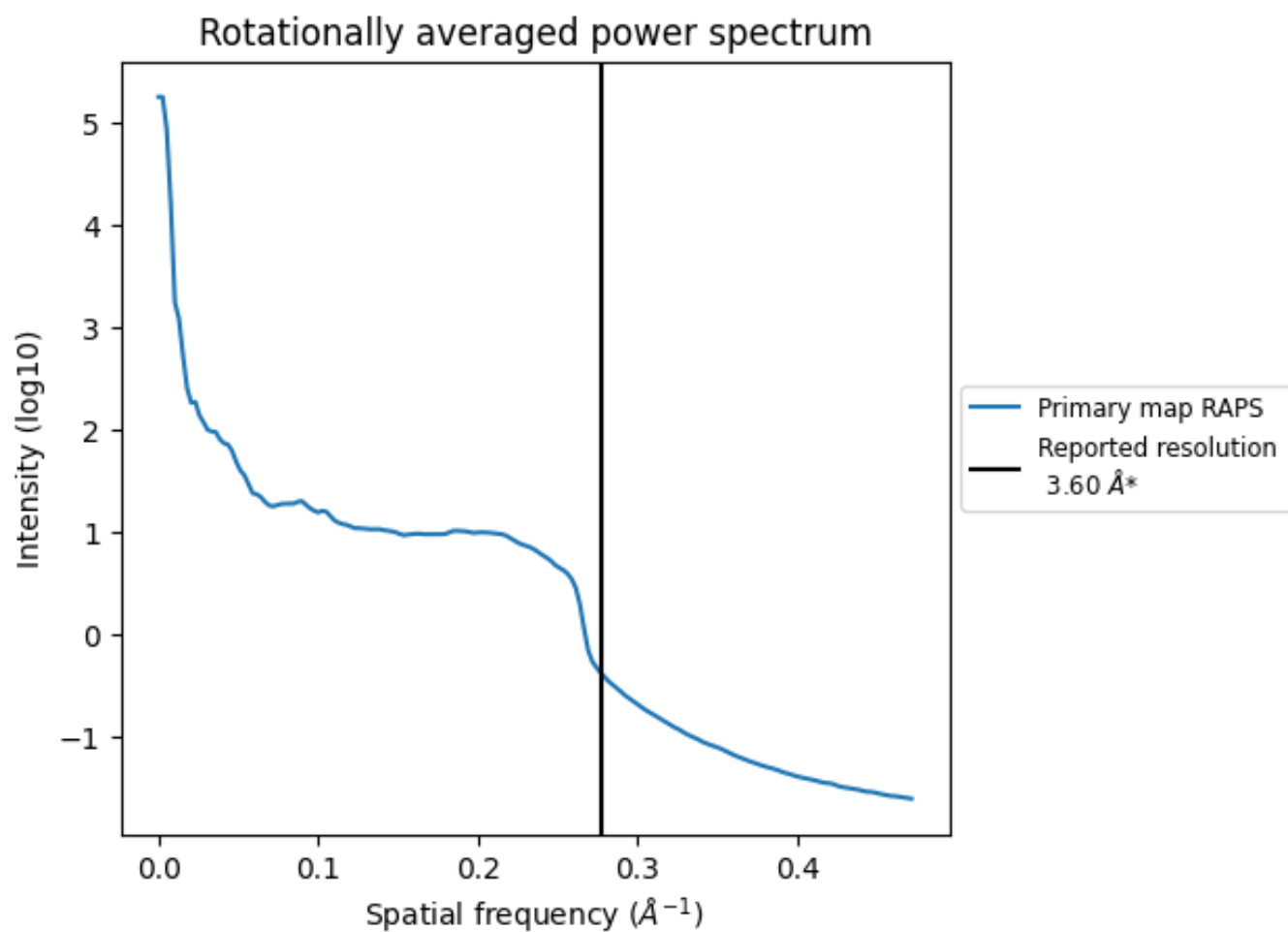
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 396 nm<sup>3</sup>; this corresponds to an approximate mass of 358 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.278 \text{\AA}^{-1}$

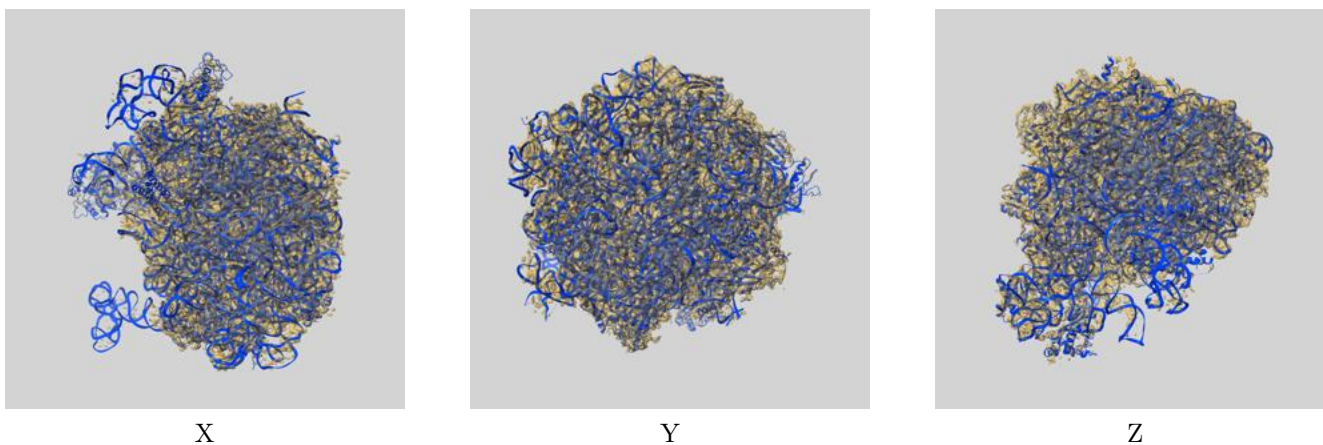
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

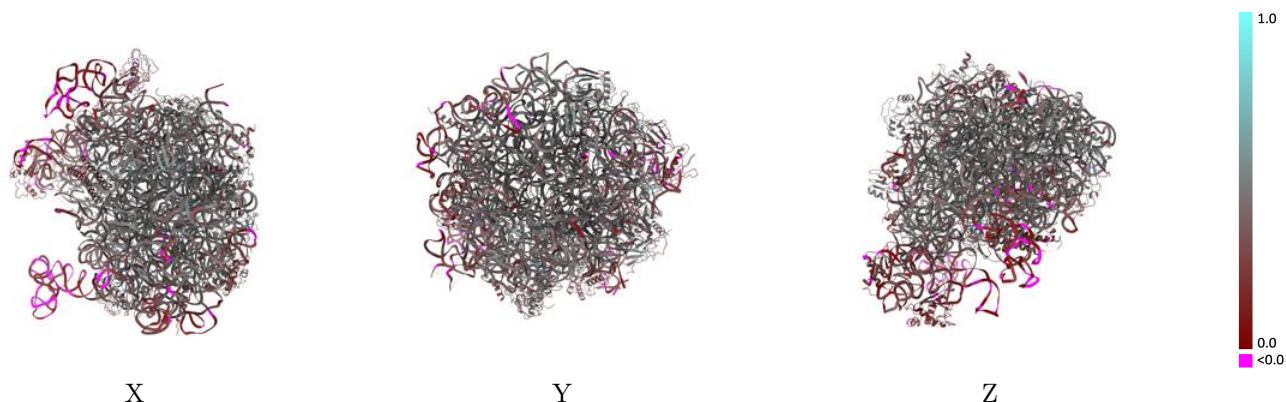
This section contains information regarding the fit between EMDB map EMD-3525 and PDB model 5MLC. Per-residue inclusion information can be found in section [3](#) on page [9](#).

### 9.1 Map-model overlay [i](#)



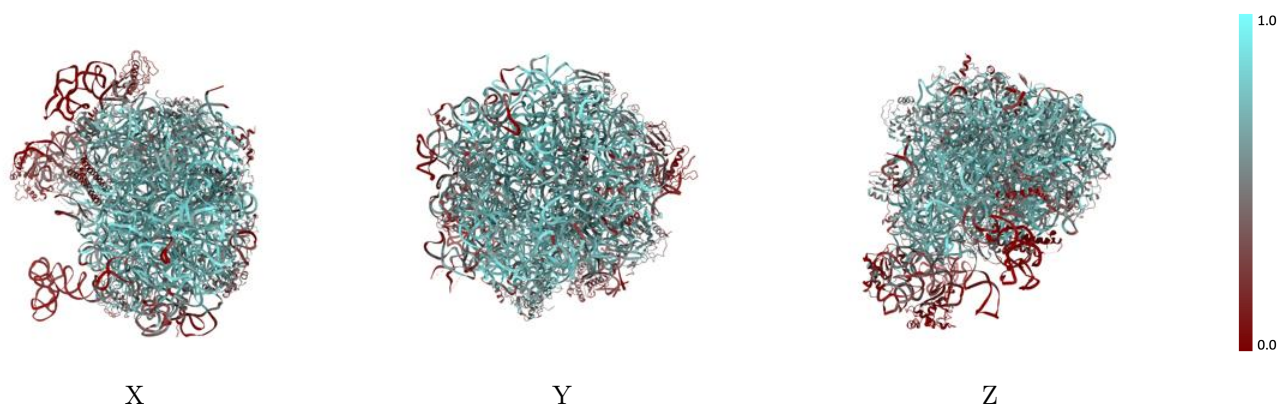
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



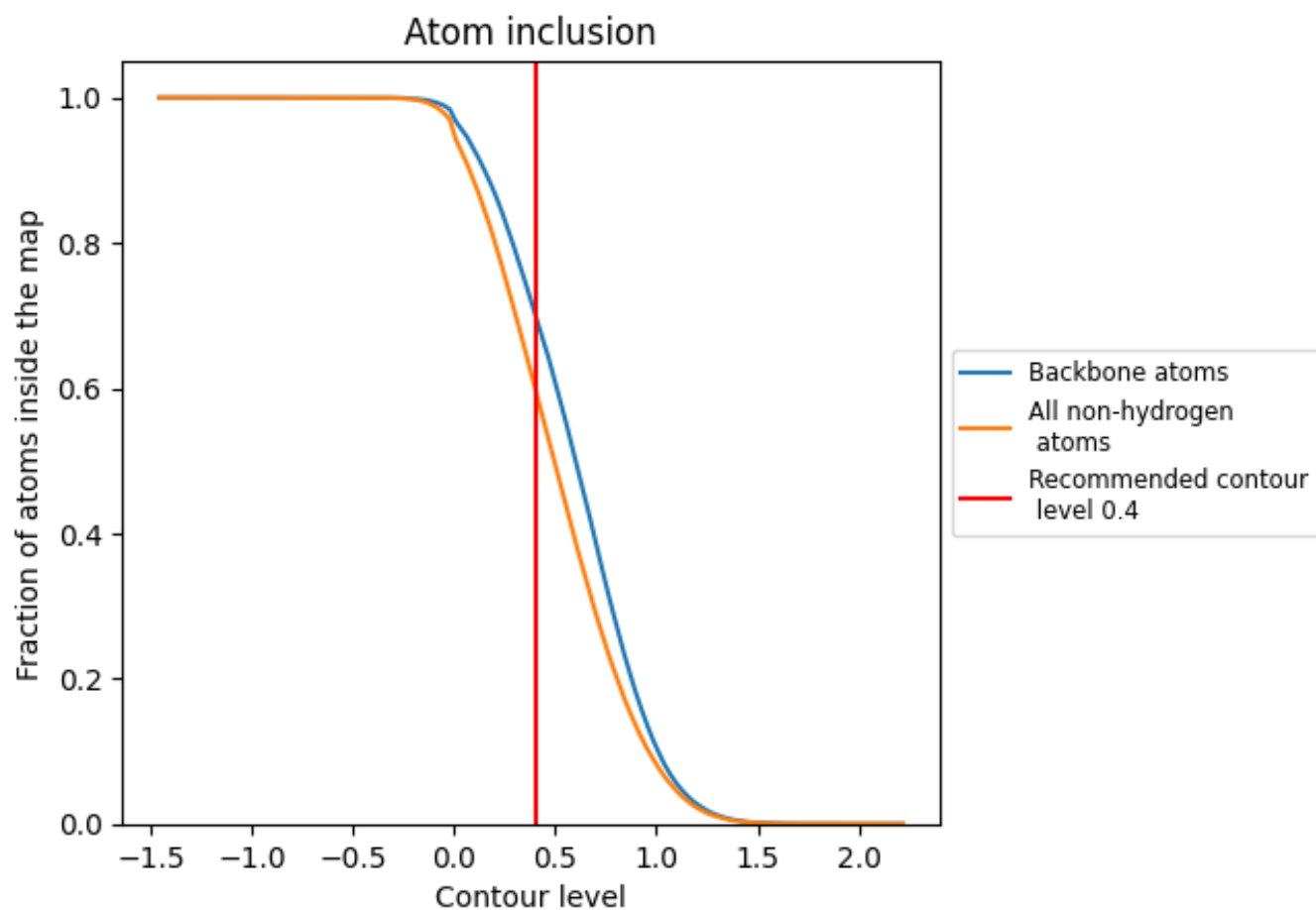
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.4).



































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 60% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6013	 0.3900
2	 0.5619	 0.3790
3	 0.5169	 0.4100
4	 0.6644	 0.4670
5	 0.6570	 0.4830
6	 0.5052	 0.4420
7	 0.4823	 0.3950
8	 0.5620	 0.4360
9	 0.1323	 0.3000
A	 0.6589	 0.3890
B	 0.3705	 0.2550
C	 0.7306	 0.4280
D	 0.5847	 0.4550
E	 0.6104	 0.4630
F	 0.6093	 0.4520
G	 0.0631	 0.2180
H	 0.1702	 0.2890
I	 0.1813	 0.2880
L	 0.5999	 0.4440
M	 0.5541	 0.4490
N	 0.5623	 0.4130
O	 0.5409	 0.4420
P	 0.6545	 0.4610
Q	 0.1705	 0.2770
R	 0.5651	 0.4460
S	 0.6204	 0.4510
T	 0.5327	 0.4180
U	 0.5458	 0.4420
V	 0.4889	 0.3990
W	 0.5020	 0.4220
X	 0.4715	 0.3950
Y	 0.5276	 0.4050
Z	 0.4190	 0.3330

