wwPDB EM Validation Summary Report

Nov 19, 2022 – 01:13 pm GMT

PDB ID	:	5MMI
EMDB ID	:	EMD-3531
Title	:	Structure of the large subunit of the chloroplast ribosome
Authors	:	Bieri, P.; Leibundgut, M.; Saurer, M.; Boehringer, D.; Ban, N.
Deposited on	:	2016-12-10
Resolution	:	3.25 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:

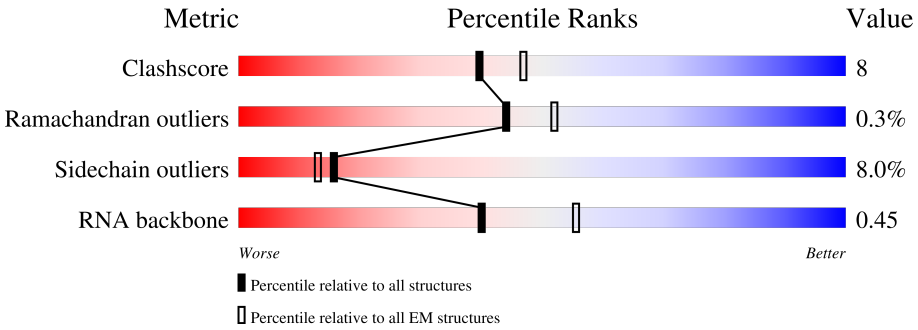
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.25 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	130	15%, 13%, 18%, •, 66%
2	1	57	•, 54%, 30%, 16%
3	2	66	11%, 67%, 23%, •, 9%
4	3	152	•, 24%, 15%, •, 61%
5	4	159	•, 32%, 12%, •, 55%
6	5	37	5%, 62%, 35%, •
7	6	142	•, 24%, 8%, ••, 65%

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Mol	Chain	Length	Quality of chain
8	7	116	32% 60%
9	A	2810	6% 57% 33% 9%
10	B	121	59% 33% 6%
11	C	272	61% 29% 7%
12	D	305	50% 19% 28%
13	E	293	51% 20% 28%
14	F	258	19% 50% 21% 25%
15	G	220	15% 55% 25% 19%
16	H	196	9% 20% 76%
17	I	232	59% 38% 20% 41%
18	J	224	58% 45% 14% 41%
19	K	250	59% 21% 19%
20	L	121	7% 67% 31%
21	M	271	46% 19% 32%
22	N	135	27% 73% 27%
23	O	126	59% 29% 5% 8%
24	P	166	49% 22% 27%
25	Q	233	33% 16% 49%
26	R	128	58% 34% 7%
27	S	256	8% 46% 19% 34%
28	T	199	54% 30% 14%
29	U	198	30% 15% 52%
30	V	192	7% 53% 17% 30%
31	W	106	54% 30% 16%
32	X	194	42% 13% 44%

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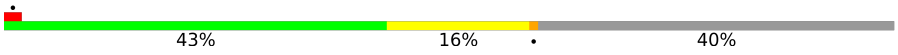
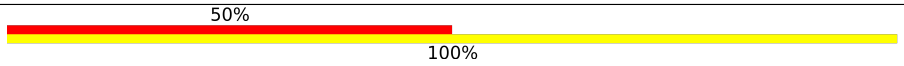
Mol	Chain	Length	Quality of chain
33	Y	148	
34	Z	168	
35	z	2	

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 95397 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	44	359	226	61	70	2	0	0

- Molecule 2 is a protein called 50S ribosomal protein L32, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	48	396	261	75	60	0	0

- Molecule 3 is a protein called 50S ribosomal protein L33, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	60	489	304	98	83	4	0	0

- Molecule 4 is a protein called 50S ribosomal protein L34, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	60	467	282	107	75	3	0	0

- Molecule 5 is a protein called 50S ribosomal protein L35, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	72	588	370	124	93	1	0	0

- Molecule 6 is a protein called 50S ribosomal protein L36, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	37	305	186	70	45	4	0	0

- Molecule 7 is a protein called plastid ribosomal protein cL37, PSRP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	49	Total	C	N	O	S	0	0
			422	268	92	57	5		

- Molecule 8 is a protein called 50S ribosomal protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	46	Total	C	N	O	S	0	0
			368	237	71	59	1		

- Molecule 9 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	2798	Total	C	N	O	P	0	0
			60083	26804	11116	19365	2798		

- Molecule 10 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	121	Total	C	N	O	P	0	0
			2584	1154	466	843	121		

- Molecule 11 is a protein called 50S ribosomal protein L2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	253	Total	C	N	O	S	0	0
			1952	1209	401	336	6		

- Molecule 12 is a protein called plastid ribosomal protein uL3c.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	221	Total	C	N	O	S	0	0
			1686	1066	308	301	11		

- Molecule 13 is a protein called plastid ribosomal protein uL4c.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	212	Total	C	N	O	S	0	0
			1676	1061	312	300	3		

- Molecule 14 is a protein called plastid ribosomal protein uL5c.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	193	Total	C	N	O	S	0	0
			1454	923	255	268	8		

- Molecule 15 is a protein called plastid ribosomal protein uL6c.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	178	Total	C	N	O	S	0	0
			1391	878	256	253	4		

- Molecule 16 is a protein called plastid ribosomal protein bL9c.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	H	48	Total	C	N	O	0	0
			382	251	69	62		

- Molecule 17 is a protein called plastid ribosomal protein uL10c.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	137	Total	C	N	O	S	0	0
			1106	711	186	203	6		

- Molecule 18 is a protein called 50S ribosomal protein L11, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	133	Total	C	N	O	S	0	0
			977	624	161	186	6		

- Molecule 19 is a protein called 50S ribosomal protein L13, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	203	Total	C	N	O	S	0	0
			1648	1047	307	289	5		

- Molecule 20 is a protein called 50S ribosomal protein L14, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	121	Total	C	N	O	S	0	0
			942	588	179	170	5		

- Molecule 21 is a protein called plastid ribosomal protein uL15c.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	185	Total	C	N	O	S	0	0
			1410	879	280	245	6		

- Molecule 22 is a protein called 50S ribosomal protein L16, chloroplastic.

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

- Molecule 23 is a protein called plastid ribosomal protein bL17c.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	116	Total	C	N	O	S	0	0
			944	592	193	155	4		

- Molecule 24 is a protein called plastid ribosomal protein uL18c.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	122	Total	C	N	O	S	0	0
			962	598	186	173	5		

- Molecule 25 is a protein called 50S ribosomal protein L19, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	118	Total	C	N	O	S	0	0
			953	611	186	155	1		

- Molecule 26 is a protein called 50S ribosomal protein L20, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	119	Total	C	N	O	S	0	0
			1029	652	213	162	2		

- Molecule 27 is a protein called 50S ribosomal protein L21, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	S	170	Total	C	N	O	0	0
			1310	844	227	239		

- Molecule 28 is a protein called 50S ribosomal protein L22, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	172	Total	C	N	O	S	0	0
			1395	892	257	237	9		

- Molecule 29 is a protein called 50S ribosomal protein L23, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	96	Total	C	N	O	S	0	0
			776	503	135	136	2		

- Molecule 30 is a protein called plastid ribosomal protein uL24c.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	134	Total	C	N	O	S	0	0
			1078	677	203	195	3		

- Molecule 31 is a RNA chain called 4.5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	106	Total	C	N	O	P	0	0
			2277	1017	423	731	106		

- Molecule 32 is a protein called plastid ribosomal protein bL27c.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	X	109	Total	C	N	O	0	0
			888	560	175	153		

- Molecule 33 is a protein called plastid ribosomal protein bL28c.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y	77	Total	C	N	O	S	0	0
			634	402	128	103	1		

- Molecule 34 is a protein called plastid ribosomal protein uL29c.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Z	101	Total	C	N	O	S	0	0
			846	529	167	147	3		

- Molecule 35 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	z	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

- Molecule 36 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
36	2	1	Total	Zn	0
			1	1	
36	5	1	Total	Zn	0
			1	1	

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

Mol	Chain	Residues	Atoms		AltConf
37	4	1	Total	Mg	0
			1	1	
37	6	1	Total	Mg	0
			1	1	
37	7	1	Total	Mg	0
			1	1	
37	A	453	Total	Mg	0
			453	453	
37	B	15	Total	Mg	0
			15	15	
37	C	1	Total	Mg	0
			1	1	
37	D	2	Total	Mg	0
			2	2	
37	E	1	Total	Mg	0
			1	1	
37	H	1	Total	Mg	0
			1	1	
37	M	2	Total	Mg	0
			2	2	
37	N	1	Total	Mg	0
			1	1	
37	P	1	Total	Mg	0
			1	1	
37	R	1	Total	Mg	0
			1	1	
37	T	1	Total	Mg	0
			1	1	
37	U	1	Total	Mg	0
			1	1	

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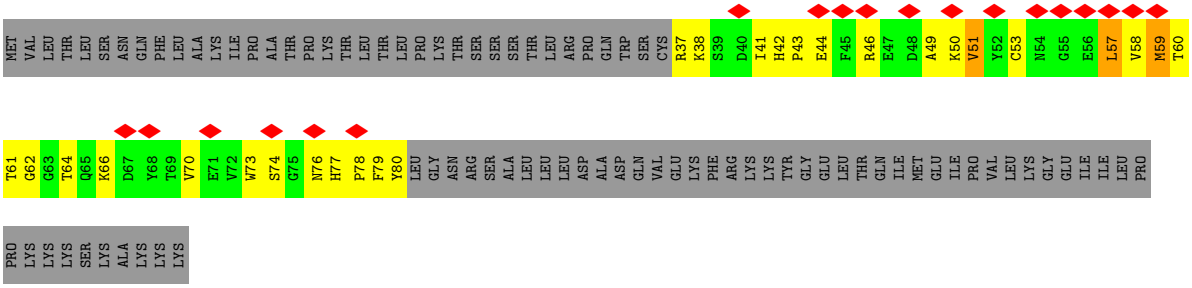
Mol	Chain	Residues	Atoms	AltConf
37	V	2	Total Mg 2 2	0
37	W	14	Total Mg 14 14	0
37	X	1	Total Mg 1 1	0
37	Y	1	Total Mg 1 1	0

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.

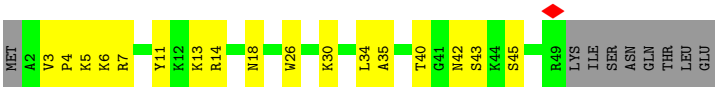
• Molecule 1: 50S ribosomal protein L31

Chain 0:



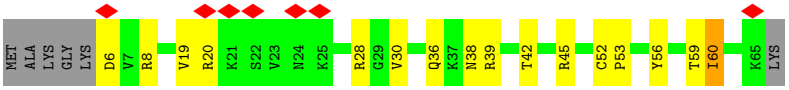
• Molecule 2: 50S ribosomal protein L32, chloroplastic

Chain 1:



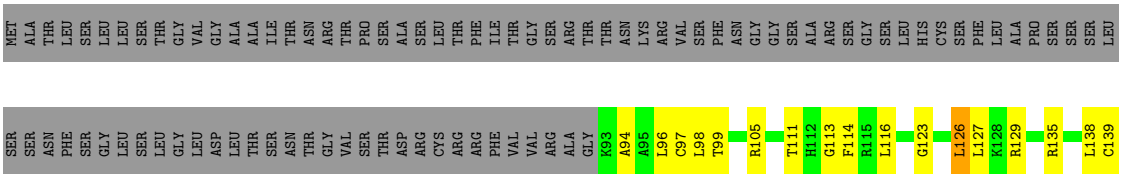
• Molecule 3: 50S ribosomal protein L33, chloroplastic

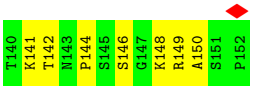
Chain 2:



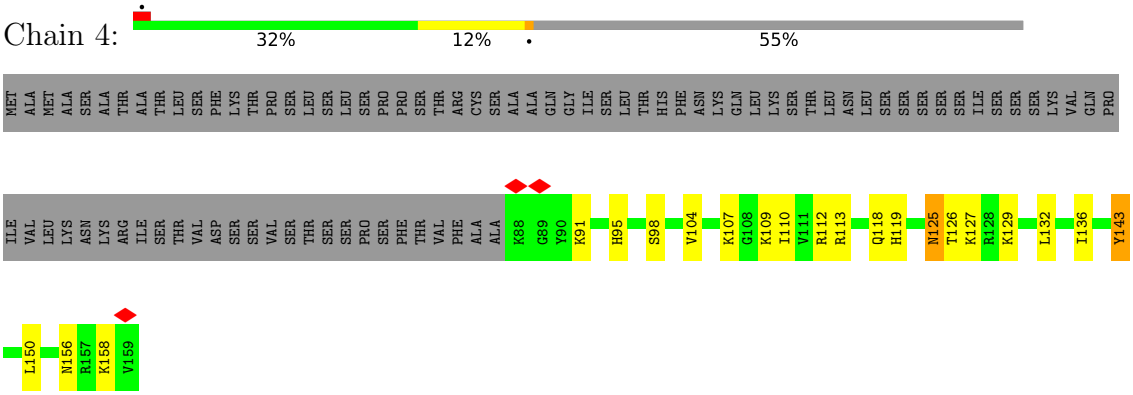
• Molecule 4: 50S ribosomal protein L34, chloroplastic

Chain 3:

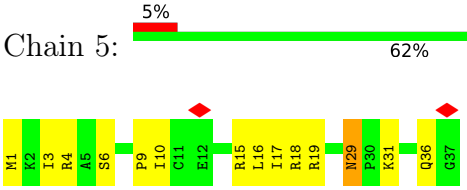




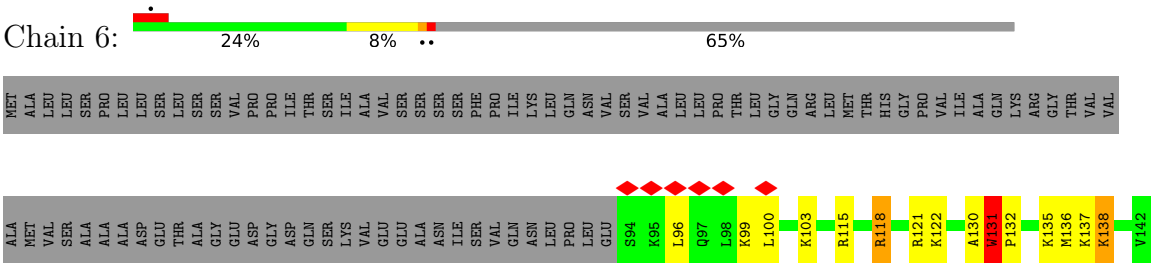
• Molecule 5: 50S ribosomal protein L35, chloroplastic



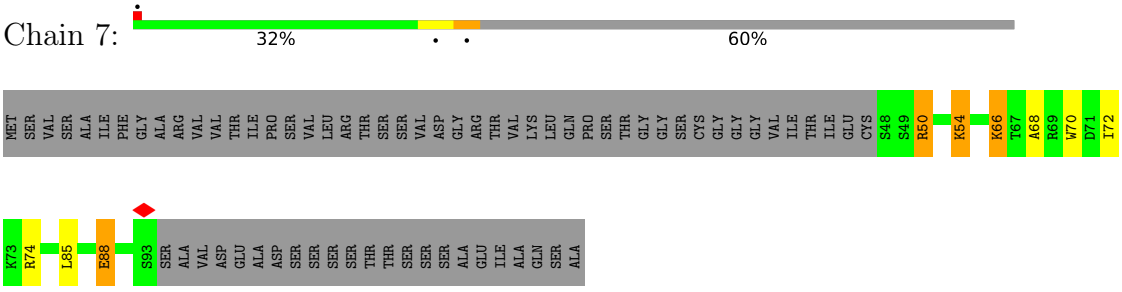
• Molecule 6: 50S ribosomal protein L36, chloroplastic



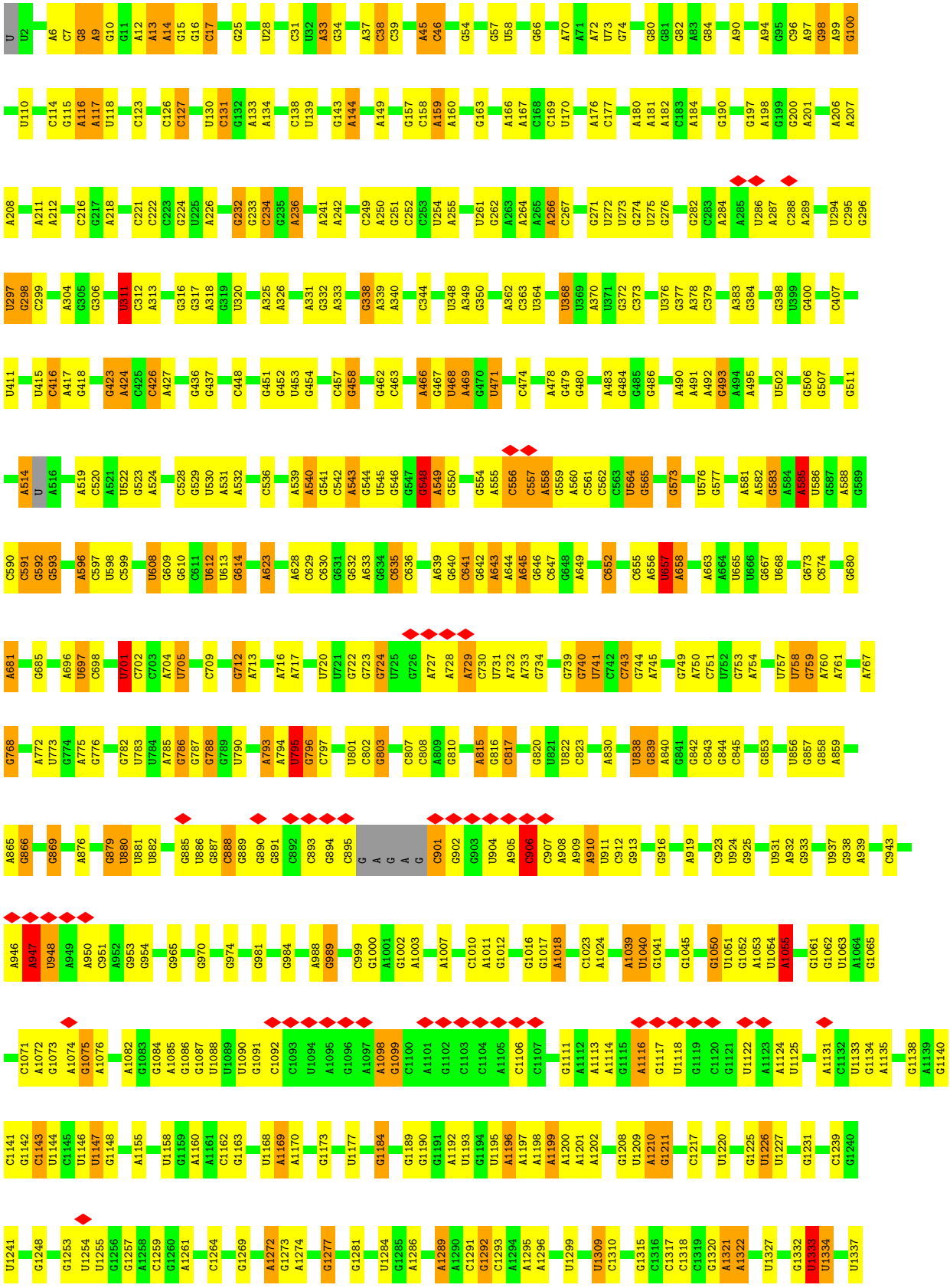
• Molecule 7: plastid ribosomal protein cL37, PSRP5

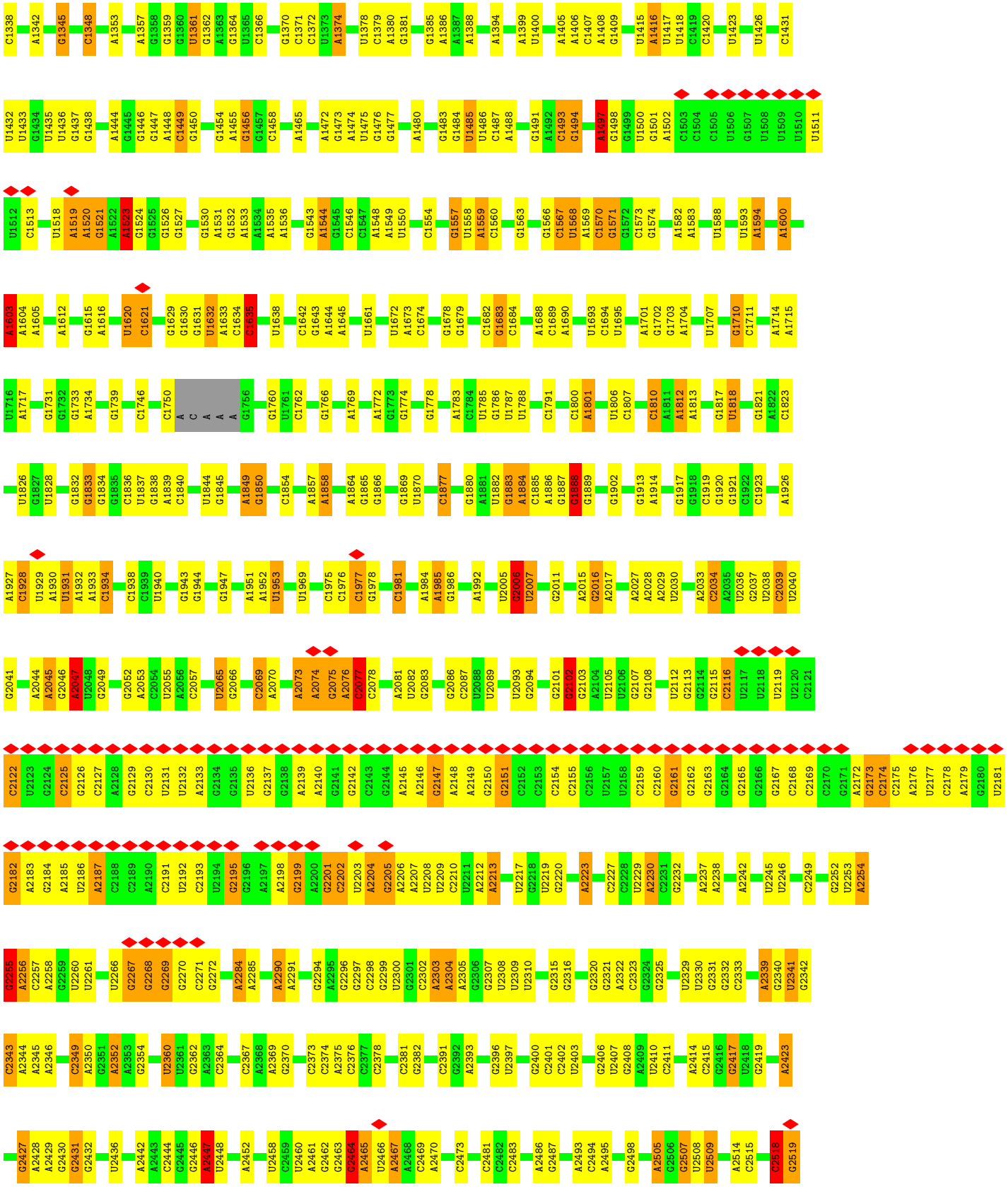


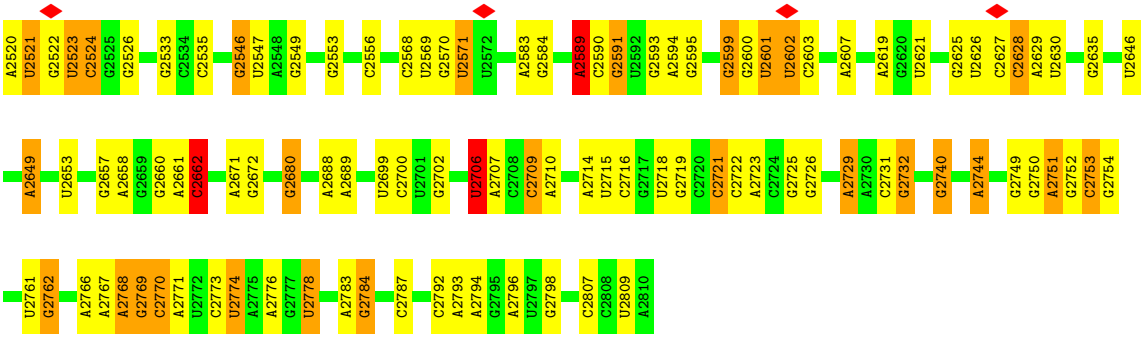
• Molecule 8: 50S ribosomal protein 6, chloroplastic



• Molecule 9: 23S ribosomal RNA

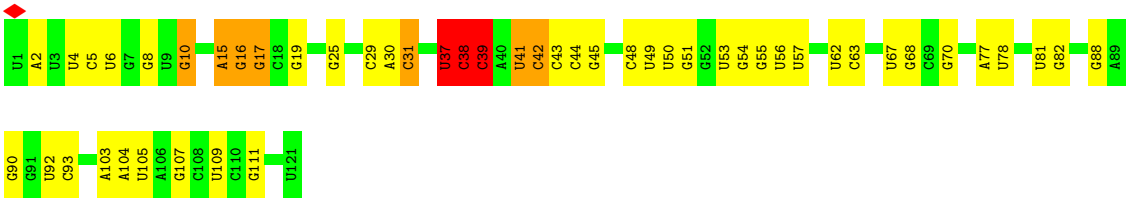






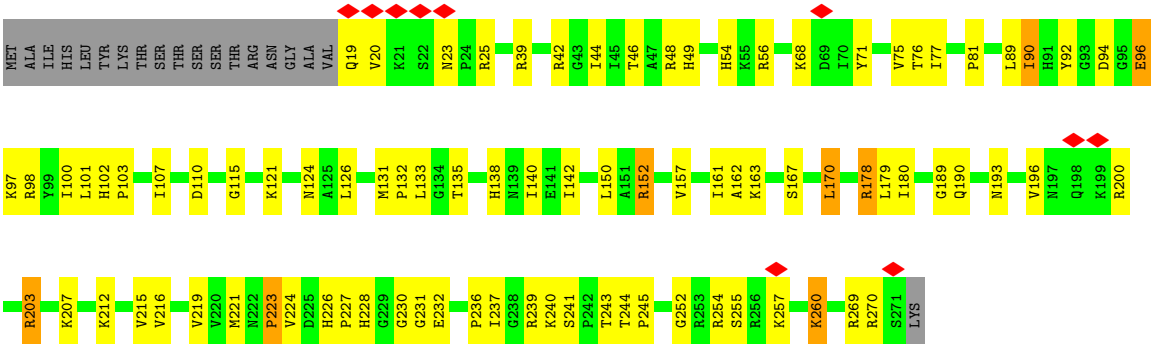
• Molecule 10: 5S ribosomal RNA

Chain B:



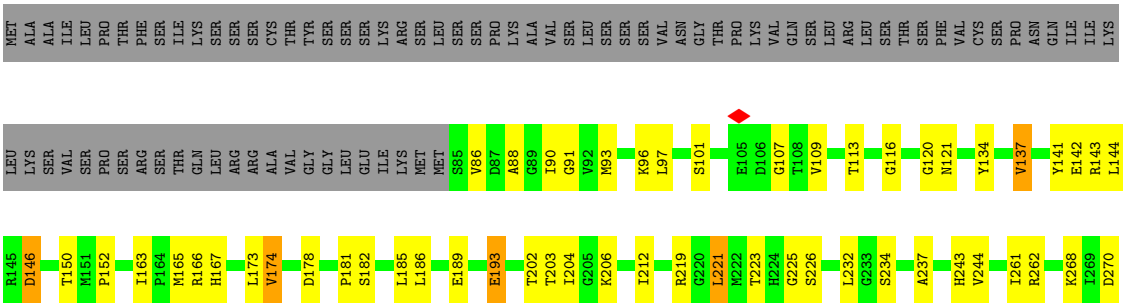
• Molecule 11: 50S ribosomal protein L2, chloroplastic

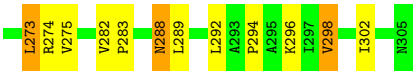
Chain C:



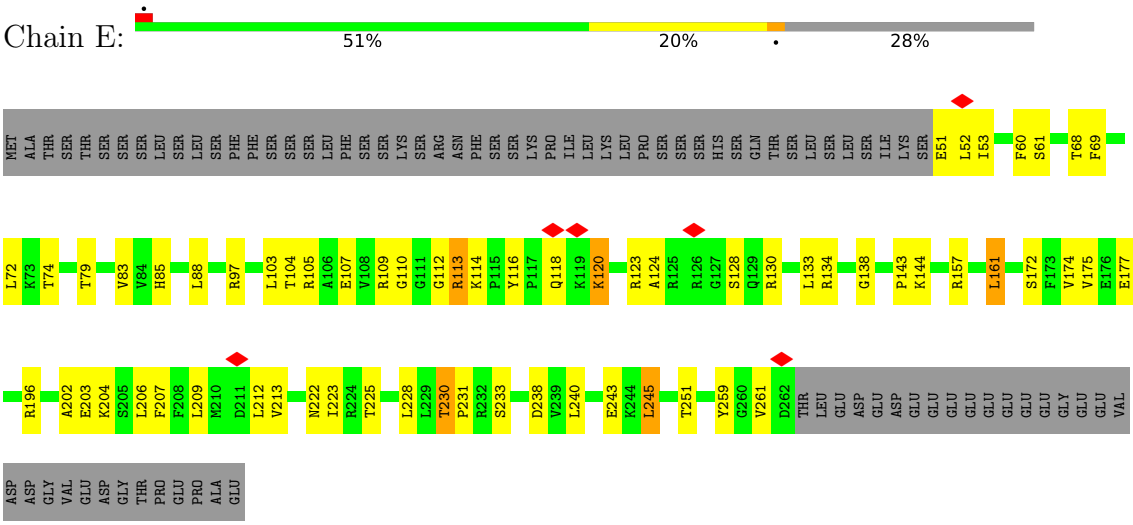
• Molecule 12: plastid ribosomal protein uL3c

Chain D:

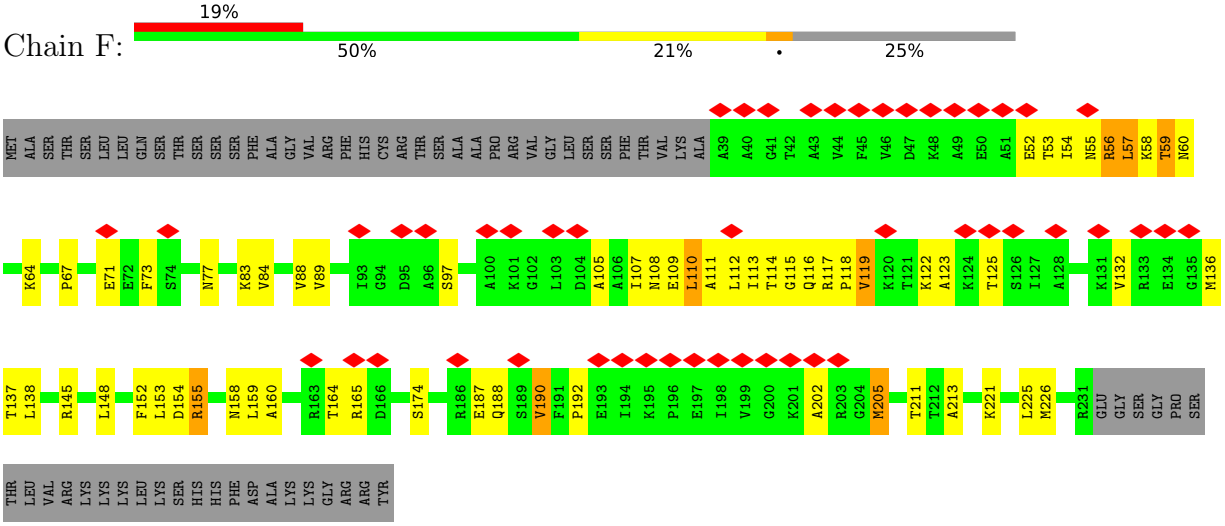




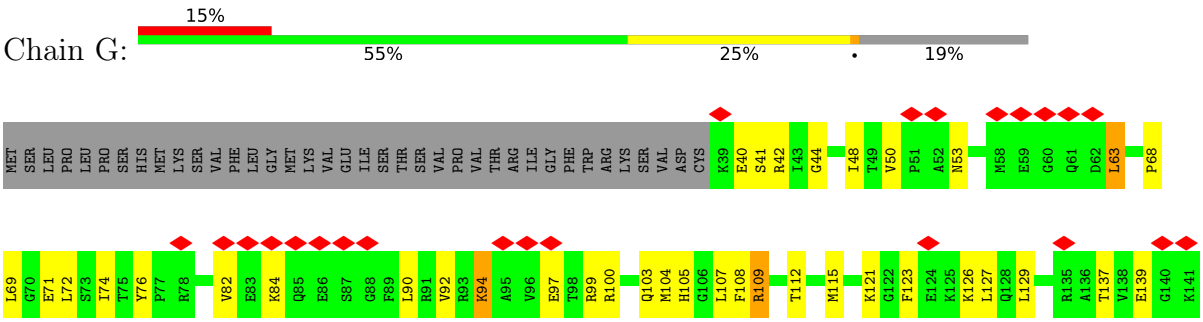
• Molecule 13: plastid ribosomal protein uL4c

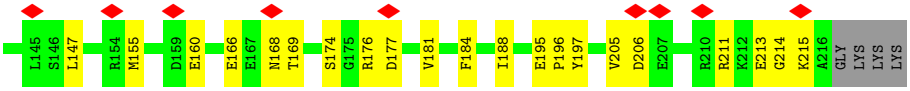


• Molecule 14: plastid ribosomal protein uL5c

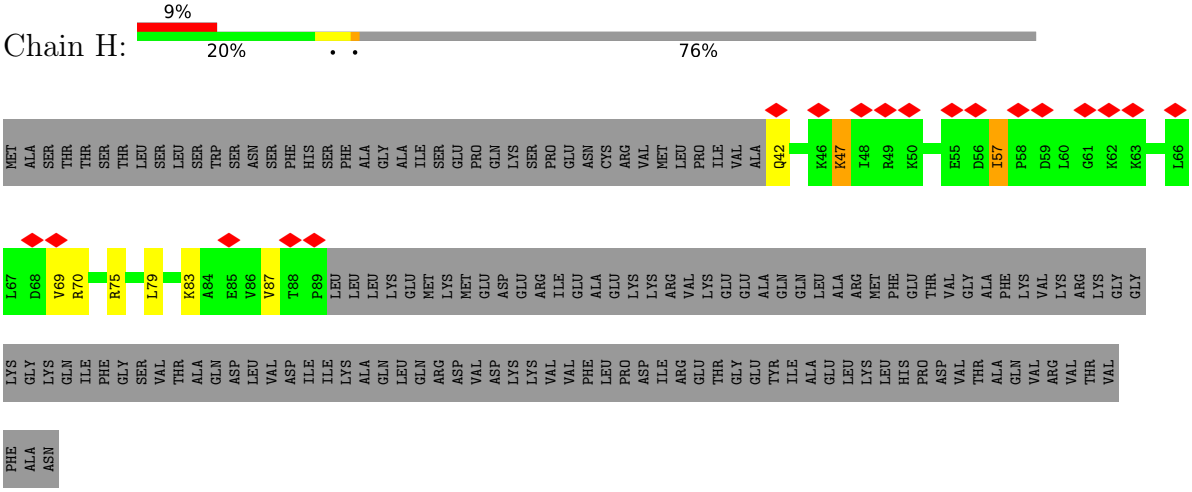


• Molecule 15: plastid ribosomal protein uL6c

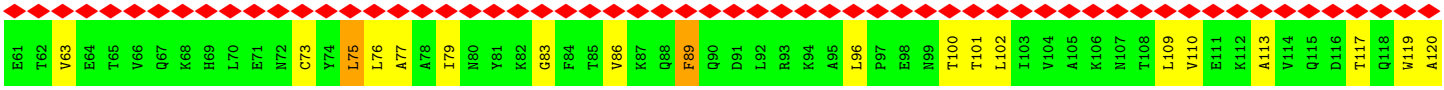


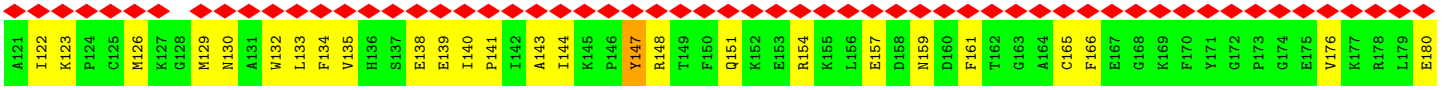


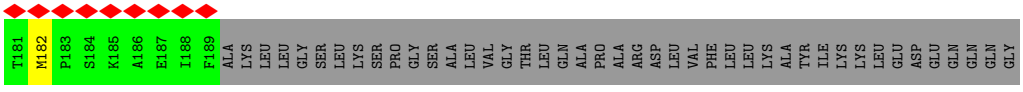
• Molecule 16: plastid ribosomal protein bL9c



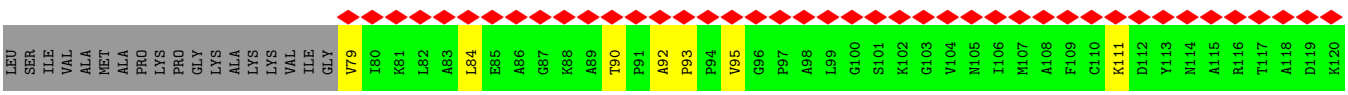
• Molecule 17: plastid ribosomal protein uL10c

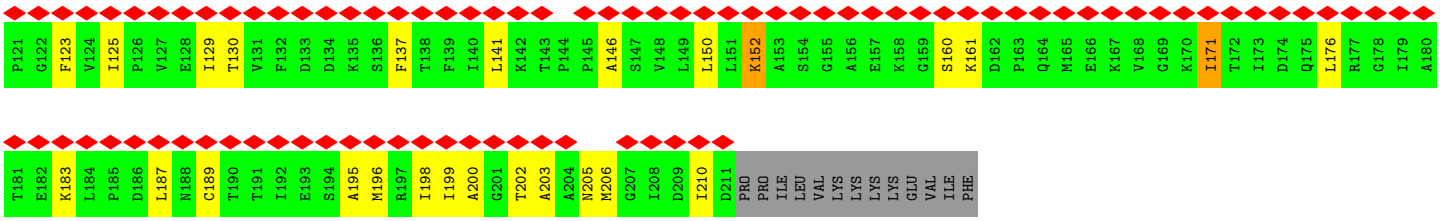






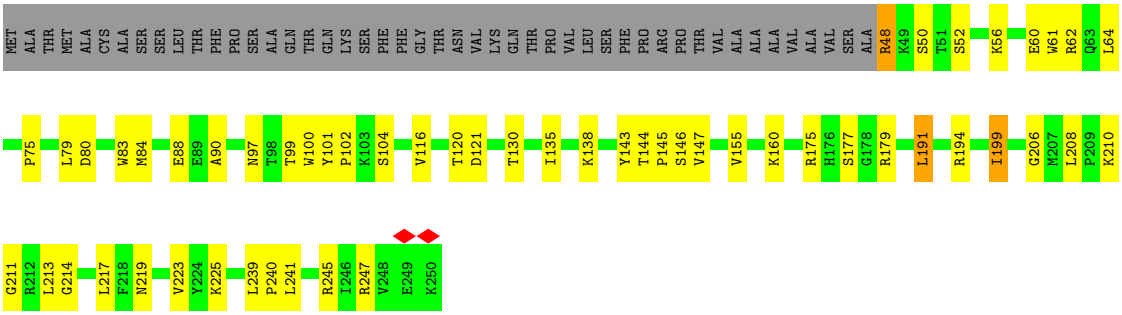
• Molecule 18: 50S ribosomal protein L11, chloroplastic





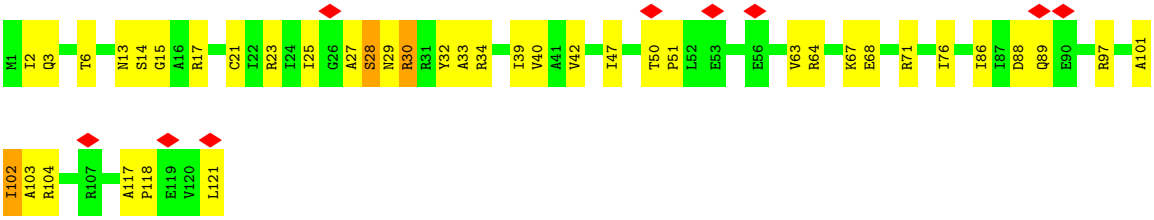
• Molecule 19: 50S ribosomal protein L13, chloroplastic

Chain K:



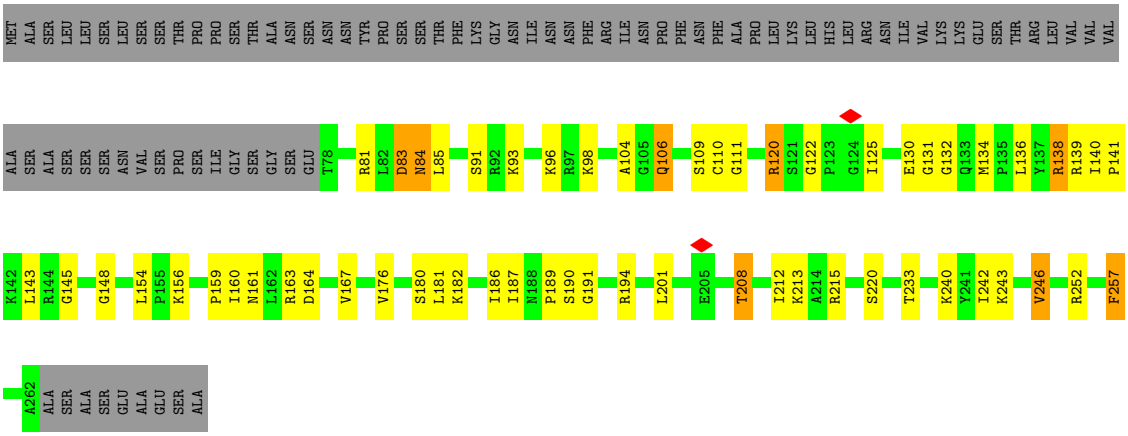
• Molecule 20: 50S ribosomal protein L14, chloroplastic

Chain L:

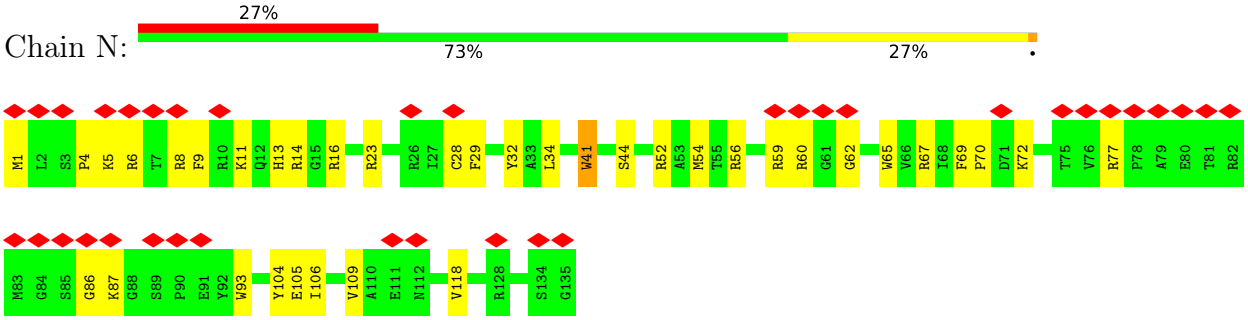


• Molecule 21: plastid ribosomal protein uL15c

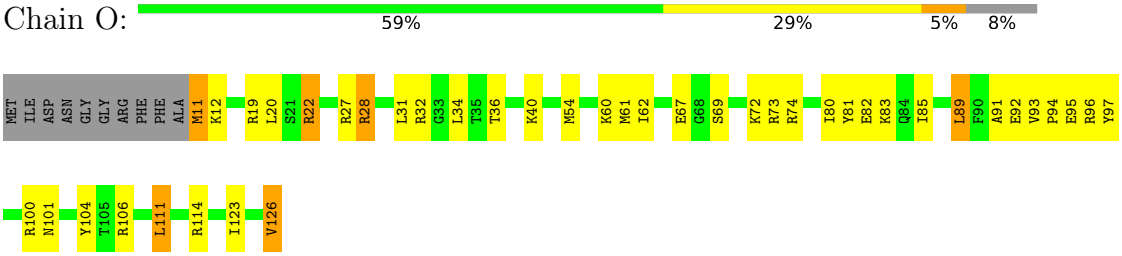
Chain M:



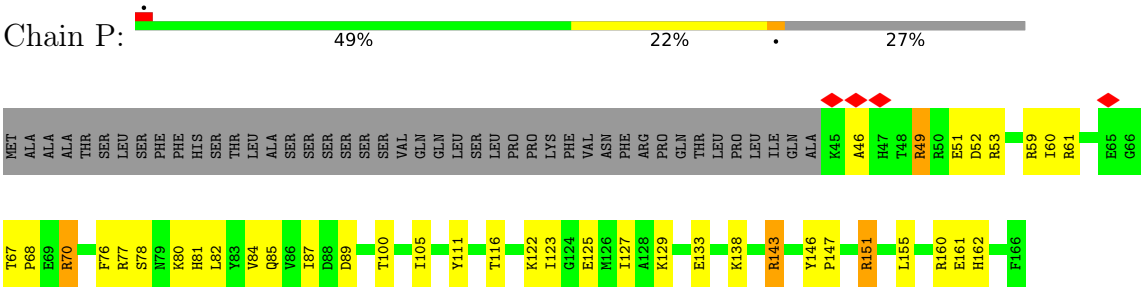
• Molecule 22: 50S ribosomal protein L16, chloroplastic



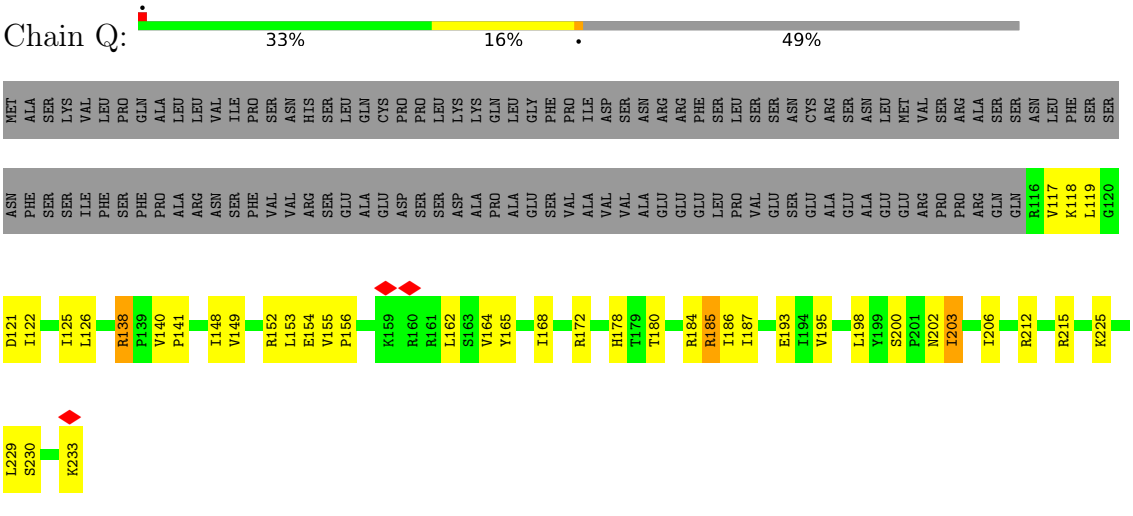
• Molecule 23: plastid ribosomal protein bL17c



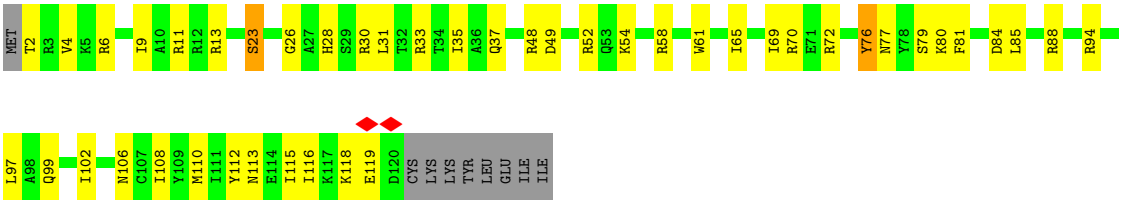
• Molecule 24: plastid ribosomal protein uL18c



• Molecule 25: 50S ribosomal protein L19, chloroplastic

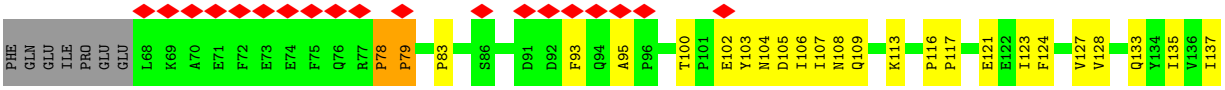


• Molecule 26: 50S ribosomal protein L20, chloroplastic



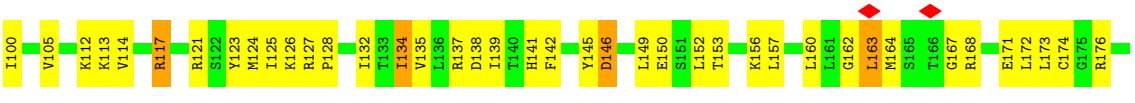
• Molecule 27: 50S ribosomal protein L21, chloroplastic

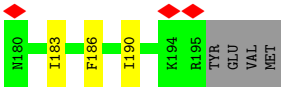
Chain S:



• Molecule 28: 50S ribosomal protein L22, chloroplastic

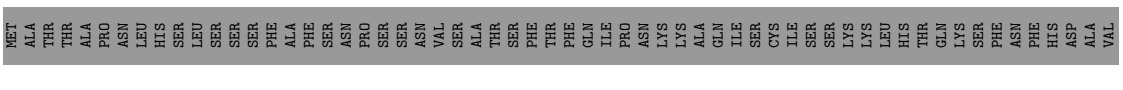
Chain T:

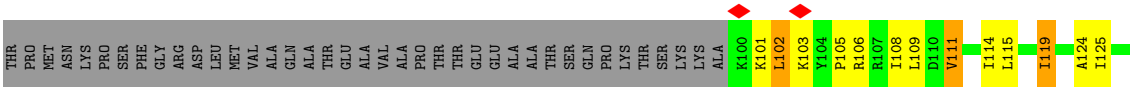


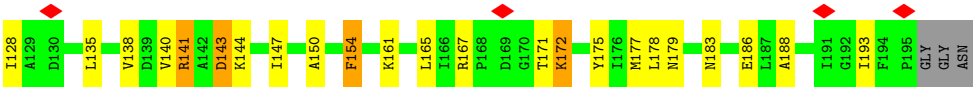


• Molecule 29: 50S ribosomal protein L23, chloroplastic

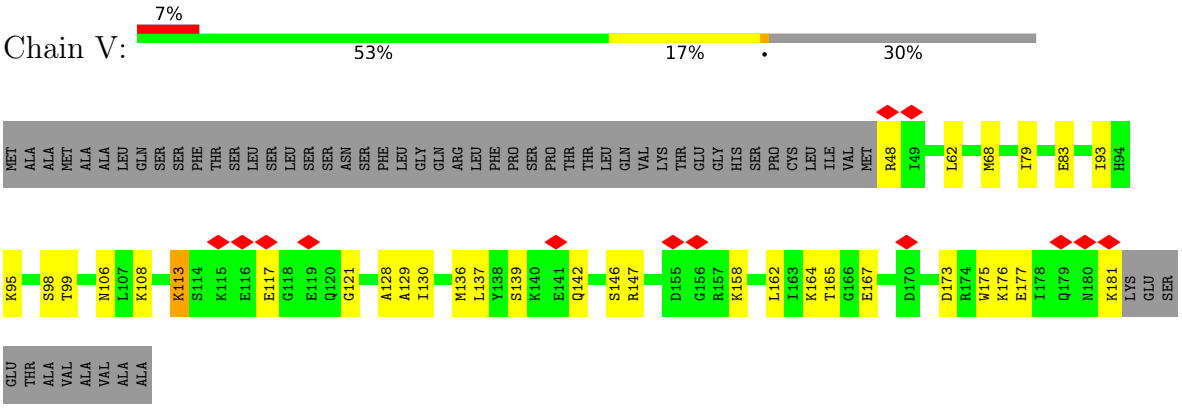
Chain U:



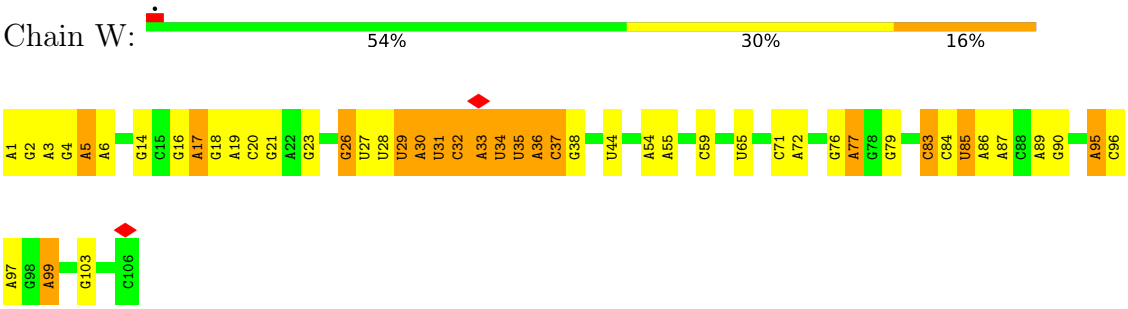




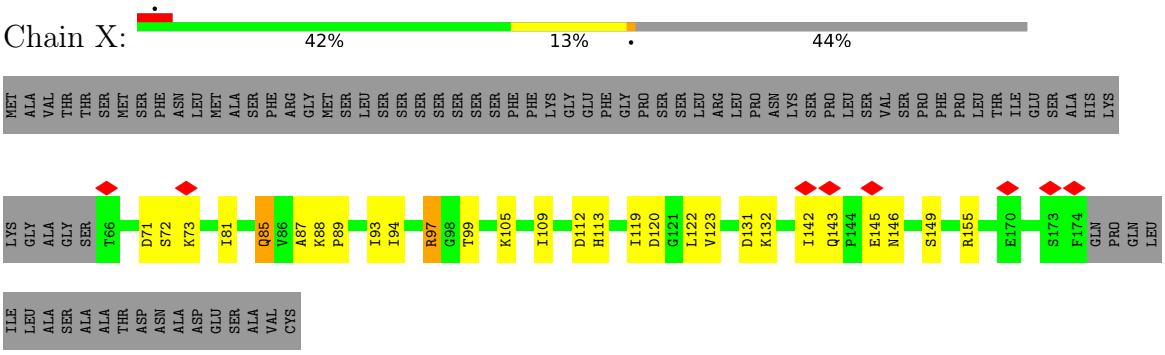
• Molecule 30: plastid ribosomal protein uL24c



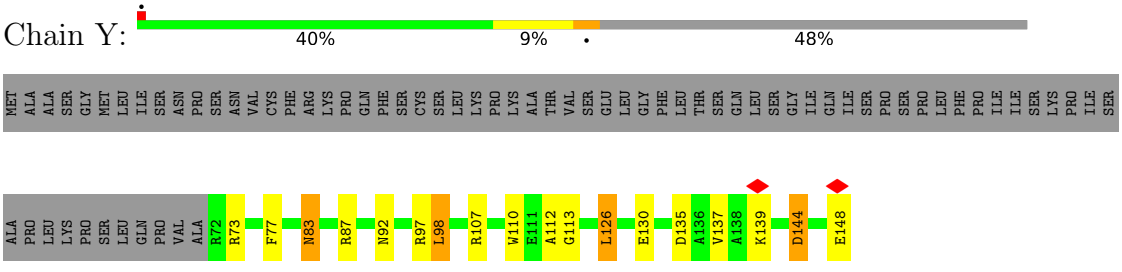
• Molecule 31: 4.5S ribosomal RNA



• Molecule 32: plastid ribosomal protein bL27c

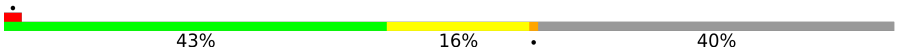


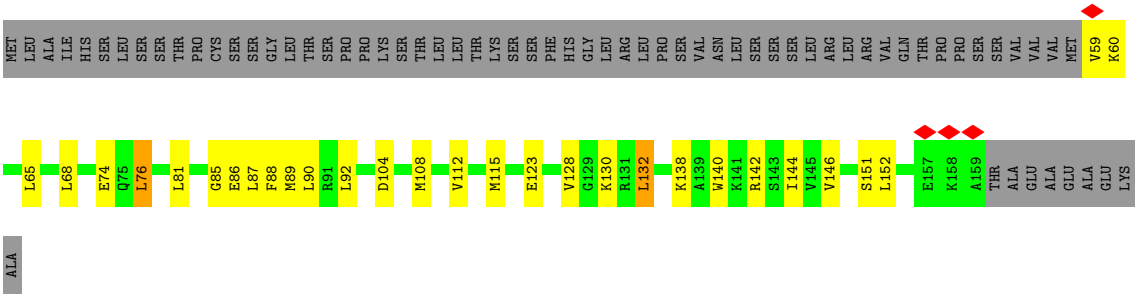
• Molecule 33: plastid ribosomal protein bL28c



• Molecule 34: plastid ribosomal protein uL29c

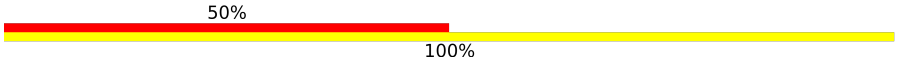
Chain Z:





• Molecule 35: E-site tRNA

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	154332	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.616	Depositor
Minimum map value	-0.270	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	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: MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.46	0/369	0.67	0/499
2	1	0.62	0/405	0.69	0/537
3	2	0.49	0/497	0.66	0/664
4	3	0.62	0/470	0.80	0/619
5	4	0.61	0/594	0.75	0/784
6	5	0.39	0/307	0.53	0/403
7	6	0.53	0/425	0.84	1/551 (0.2%)
8	7	0.53	0/382	0.58	0/520
9	A	0.85	39/67297 (0.1%)	1.19	236/104984 (0.2%)
10	B	0.45	1/2890 (0.0%)	1.00	5/4503 (0.1%)
11	C	0.52	0/1986	0.73	1/2666 (0.0%)
12	D	0.56	0/1713	0.72	0/2291
13	E	0.56	0/1707	0.80	1/2298 (0.0%)
14	F	0.42	0/1475	0.61	1/1990 (0.1%)
15	G	0.39	0/1412	0.60	0/1898
16	H	0.41	0/386	0.62	0/514
17	I	0.49	0/1129	0.53	0/1521
18	J	0.50	0/992	0.55	0/1343
19	K	0.51	0/1688	0.64	0/2279
20	L	0.48	0/951	0.66	0/1282
21	M	0.52	0/1430	0.71	0/1896
22	N	0.48	0/1097	0.64	1/1471 (0.1%)
23	O	0.57	0/959	0.77	0/1280
24	P	0.38	0/978	0.56	0/1311
25	Q	0.52	0/967	0.67	0/1299
26	R	0.61	0/1046	0.74	0/1395
27	S	0.51	0/1339	0.72	3/1826 (0.2%)
28	T	0.50	0/1420	0.64	0/1900
29	U	0.50	0/787	0.68	0/1056
30	V	0.43	0/1093	0.63	0/1457
31	W	0.74	0/2551	1.15	3/3977 (0.1%)
32	X	0.47	0/905	0.61	0/1204

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Y	0.51	0/644	0.64	0/856
34	Z	0.41	0/854	0.58	0/1131
35	z	0.89	0/46	1.88	2/69 (2.9%)
All	All	0.75	40/103191 (0.0%)	1.07	254/154274 (0.2%)

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
21	M	0	1

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	591	C	N1-C6	-7.28	1.32	1.37
9	A	1272	A	N9-C4	-7.03	1.33	1.37
9	A	1272	A	N3-C4	-6.93	1.30	1.34
9	A	1272	A	N7-C5	-6.68	1.35	1.39
9	A	810	G	C6-N1	-6.13	1.35	1.39

The worst 5 of 254 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1272	A	C2-N3-C4	-11.16	105.02	110.60
9	A	1272	A	N1-C2-N3	9.97	134.28	129.30
9	A	1272	A	C6-C5-N7	-9.58	125.60	132.30
9	A	2464	G	C8-N9-C4	9.23	110.09	106.40
9	A	2464	G	N9-C4-C5	-9.22	101.71	105.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	M	104	ALA	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	359	0	330	26	0
2	1	396	0	437	15	0
3	2	489	0	507	10	0
4	3	467	0	526	13	0
5	4	588	0	658	12	0
6	5	305	0	344	9	0
7	6	422	0	508	16	0
8	7	368	0	386	5	0
9	A	60083	0	30260	539	0
10	B	2584	0	1305	37	0
11	C	1952	0	2038	56	0
12	D	1686	0	1772	49	0
13	E	1676	0	1737	38	0
14	F	1454	0	1488	50	0
15	G	1391	0	1458	34	0
16	H	382	0	437	5	0
17	I	1106	0	1122	40	0
18	J	977	0	1027	28	0
19	K	1648	0	1684	41	0
20	L	942	0	996	25	0
21	M	1410	0	1495	45	0
22	N	1075	0	1134	27	0
23	O	944	0	1004	31	0
24	P	962	0	984	28	0
25	Q	953	0	1050	26	0
26	R	1029	0	1092	34	0
27	S	1310	0	1315	37	0
28	T	1395	0	1482	41	0
29	U	776	0	837	23	0
30	V	1078	0	1144	23	0
31	W	2277	0	1146	27	0
32	X	888	0	923	13	0
33	Y	634	0	684	12	0
34	Z	846	0	918	17	0
35	z	42	0	23	0	0
36	2	1	0	0	0	0
36	5	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	4	1	0	0	0	0
37	6	1	0	0	0	0
37	7	1	0	0	0	0
37	A	453	0	0	0	0
37	B	15	0	0	0	0
37	C	1	0	0	0	0
37	D	2	0	0	0	0
37	E	1	0	0	0	0
37	H	1	0	0	0	0
37	M	2	0	0	0	0
37	N	1	0	0	0	0
37	P	1	0	0	0	0
37	R	1	0	0	0	0
37	T	1	0	0	0	0
37	U	1	0	0	0	0
37	V	2	0	0	0	0
37	W	14	0	0	0	0
37	X	1	0	0	0	0
37	Y	1	0	0	0	0
All	All	95397	0	64251	1207	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 8.

The worst 5 of 1207 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)
9:A:652:C:N4	9:A:657:U:O4	1.86	1.08
9:A:2077:C:H42	9:A:2464:G:H1	1.10	0.98
20:L:15:GLY:HA3	20:L:50:THR:HG21	1.51	0.90
9:A:817:C:OP2	21:M:120:ARG:NH1	2.06	0.89
9:A:540:A:H62	9:A:2055:U:H3	1.18	0.88

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	42/130 (32%)	39 (93%)	3 (7%)	0	100	100
2	1	46/57 (81%)	44 (96%)	2 (4%)	0	100	100
3	2	58/66 (88%)	53 (91%)	5 (9%)	0	100	100
4	3	58/152 (38%)	54 (93%)	4 (7%)	0	100	100
5	4	70/159 (44%)	66 (94%)	4 (6%)	0	100	100
6	5	35/37 (95%)	35 (100%)	0	0	100	100
7	6	47/142 (33%)	46 (98%)	0	1 (2%)	7	32
8	7	44/116 (38%)	40 (91%)	3 (7%)	1 (2%)	6	29
11	C	251/272 (92%)	238 (95%)	12 (5%)	1 (0%)	34	67
12	D	219/305 (72%)	205 (94%)	13 (6%)	1 (0%)	29	62
13	E	210/293 (72%)	193 (92%)	17 (8%)	0	100	100
14	F	191/258 (74%)	178 (93%)	13 (7%)	0	100	100
15	G	176/220 (80%)	167 (95%)	9 (5%)	0	100	100
16	H	46/196 (24%)	43 (94%)	3 (6%)	0	100	100
17	I	135/232 (58%)	132 (98%)	3 (2%)	0	100	100
18	J	131/224 (58%)	126 (96%)	5 (4%)	0	100	100
19	K	201/250 (80%)	194 (96%)	7 (4%)	0	100	100
20	L	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
21	M	183/271 (68%)	169 (92%)	12 (7%)	2 (1%)	14	46
22	N	133/135 (98%)	122 (92%)	11 (8%)	0	100	100
23	O	114/126 (90%)	110 (96%)	4 (4%)	0	100	100
24	P	120/166 (72%)	114 (95%)	6 (5%)	0	100	100
25	Q	116/233 (50%)	114 (98%)	2 (2%)	0	100	100
26	R	117/128 (91%)	110 (94%)	7 (6%)	0	100	100
27	S	168/256 (66%)	157 (94%)	9 (5%)	2 (1%)	13	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
28	T	170/199 (85%)	161 (95%)	8 (5%)	1 (1%)	25 59
29	U	94/198 (48%)	89 (95%)	5 (5%)	0	100 100
30	V	132/192 (69%)	121 (92%)	10 (8%)	1 (1%)	19 52
32	X	107/194 (55%)	95 (89%)	12 (11%)	0	100 100
33	Y	75/148 (51%)	74 (99%)	1 (1%)	0	100 100
34	Z	99/168 (59%)	95 (96%)	3 (3%)	1 (1%)	15 47
All	All	3707/5644 (66%)	3499 (94%)	197 (5%)	11 (0%)	44 72

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	C	232	GLU
21	M	131	GLY
27	S	78	PRO
34	Z	151	SER
7	6	131	TRP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	39/117 (33%)	36 (92%)	3 (8%)	13 38
2	1	41/50 (82%)	39 (95%)	2 (5%)	25 55
3	2	56/60 (93%)	51 (91%)	5 (9%)	9 32
4	3	50/125 (40%)	45 (90%)	5 (10%)	7 27
5	4	62/140 (44%)	55 (89%)	7 (11%)	6 22
6	5	34/34 (100%)	30 (88%)	4 (12%)	5 21
7	6	46/124 (37%)	44 (96%)	2 (4%)	29 59
8	7	40/96 (42%)	35 (88%)	5 (12%)	4 19
11	C	201/217 (93%)	181 (90%)	20 (10%)	7 27
12	D	182/259 (70%)	167 (92%)	15 (8%)	11 36

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	E	179/255 (70%)	160 (89%)	19 (11%)	6 25
14	F	152/214 (71%)	141 (93%)	11 (7%)	14 41
15	G	151/190 (80%)	141 (93%)	10 (7%)	16 45
16	H	42/170 (25%)	37 (88%)	5 (12%)	5 20
17	I	119/204 (58%)	113 (95%)	6 (5%)	24 55
18	J	106/189 (56%)	103 (97%)	3 (3%)	43 69
19	K	176/213 (83%)	168 (96%)	8 (4%)	27 58
20	L	101/101 (100%)	94 (93%)	7 (7%)	15 43
21	M	141/215 (66%)	126 (89%)	15 (11%)	6 25
22	N	108/108 (100%)	101 (94%)	7 (6%)	17 46
23	O	96/103 (93%)	84 (88%)	12 (12%)	4 19
24	P	100/139 (72%)	90 (90%)	10 (10%)	7 27
25	Q	104/207 (50%)	94 (90%)	10 (10%)	8 29
26	R	106/115 (92%)	98 (92%)	8 (8%)	13 39
27	S	137/223 (61%)	134 (98%)	3 (2%)	52 74
28	T	152/176 (86%)	138 (91%)	14 (9%)	9 31
29	U	85/171 (50%)	74 (87%)	11 (13%)	4 18
30	V	121/169 (72%)	116 (96%)	5 (4%)	30 60
32	X	92/163 (56%)	83 (90%)	9 (10%)	8 29
33	Y	67/130 (52%)	60 (90%)	7 (10%)	7 25
34	Z	93/153 (61%)	87 (94%)	6 (6%)	17 46
All	All	3179/4830 (66%)	2925 (92%)	254 (8%)	16 37

5 of 254 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	I	101	THR
29	U	143	ASP
21	M	154	LEU
29	U	119	ILE
32	X	105	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
24	P	108	ASN
26	R	113	ASN
24	P	162	HIS
26	R	37	GLN
27	S	189	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B	120/121 (99%)	19 (15%)	0
31	W	105/106 (99%)	38 (36%)	0
35	z	1/2 (50%)	1 (100%)	0
9	A	2794/2810 (99%)	642 (22%)	8 (0%)
All	All	3020/3039 (99%)	700 (23%)	8 (0%)

5 of 700 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A	9	A
9	A	10	G
9	A	12	A
9	A	13	A
9	A	14	A

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	2753	C
9	A	2518	C
9	A	1520	A
9	A	795	U
9	A	2447	A

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 503 ligands modelled in this entry, 503 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)

There are no chain breaks in this entry.

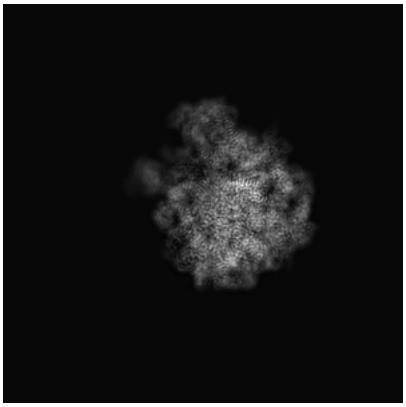
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3531. These allow visual inspection of the internal detail of the map and identification of artifacts.

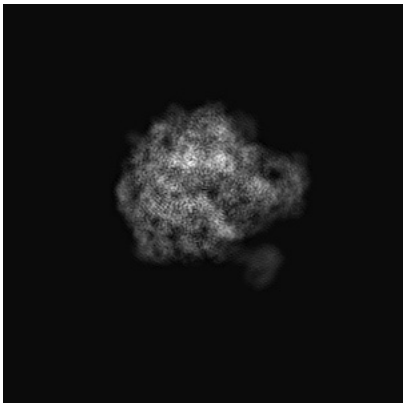
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

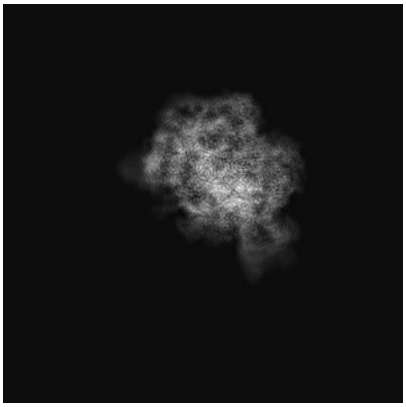
6.1.1 Primary map



X



Y

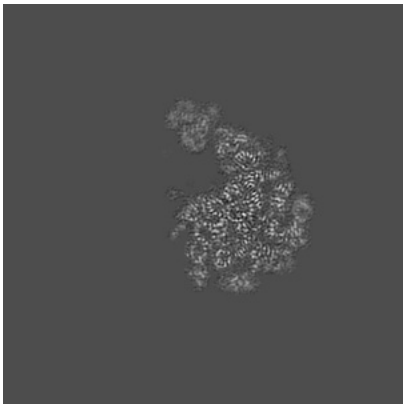


Z

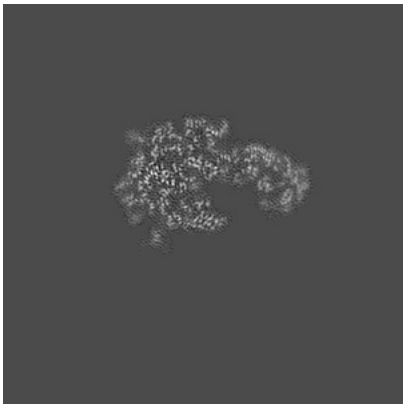
The images above show the map projected in three orthogonal directions.

6.2 Central slices

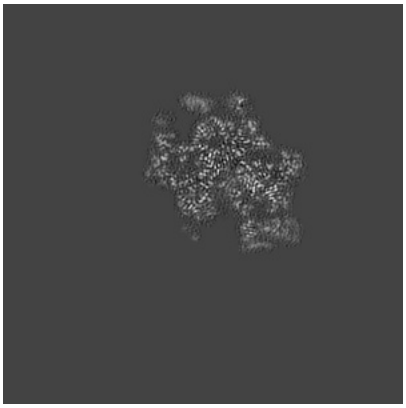
6.2.1 Primary map



X Index: 160



Y Index: 160

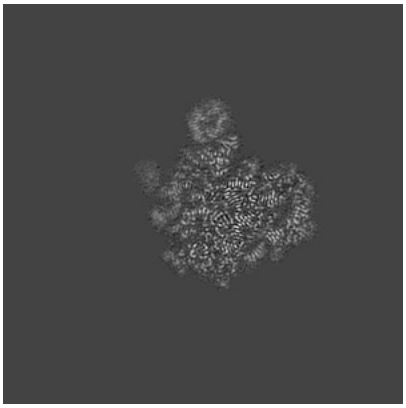


Z Index: 160

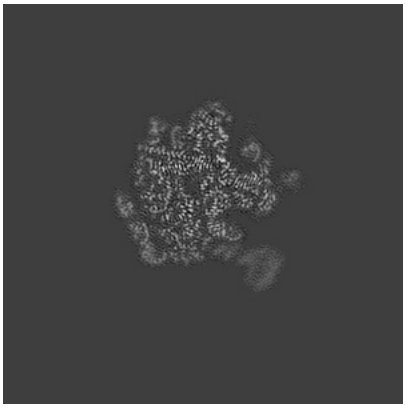
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 190



Y Index: 187

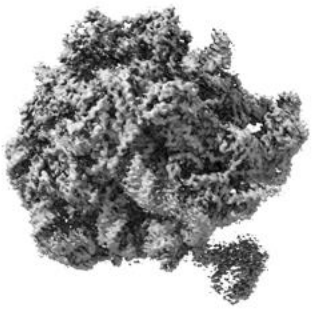
Z Index: 149

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

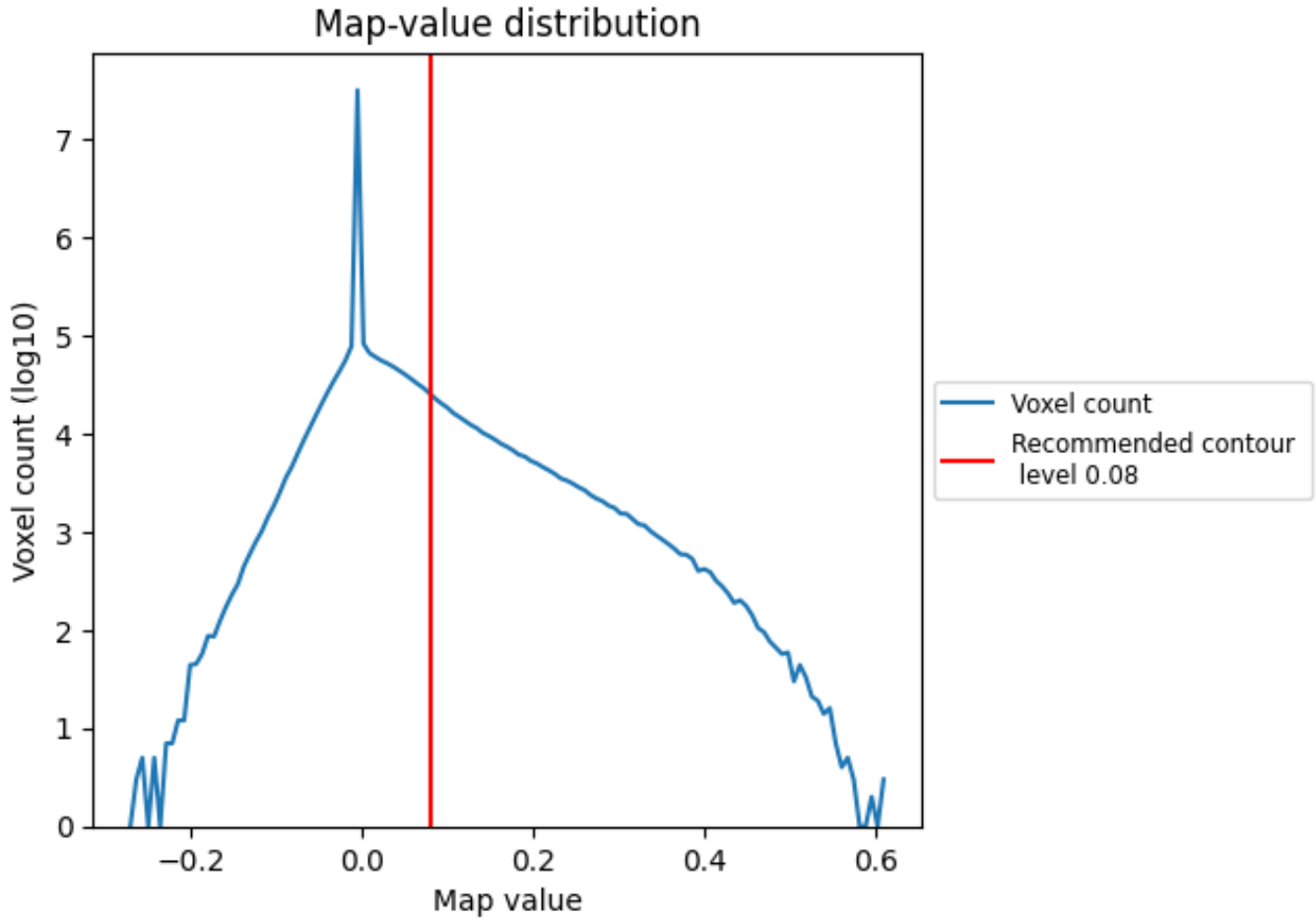
6.5 Mask visualisation (i)

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

7 Map analysis

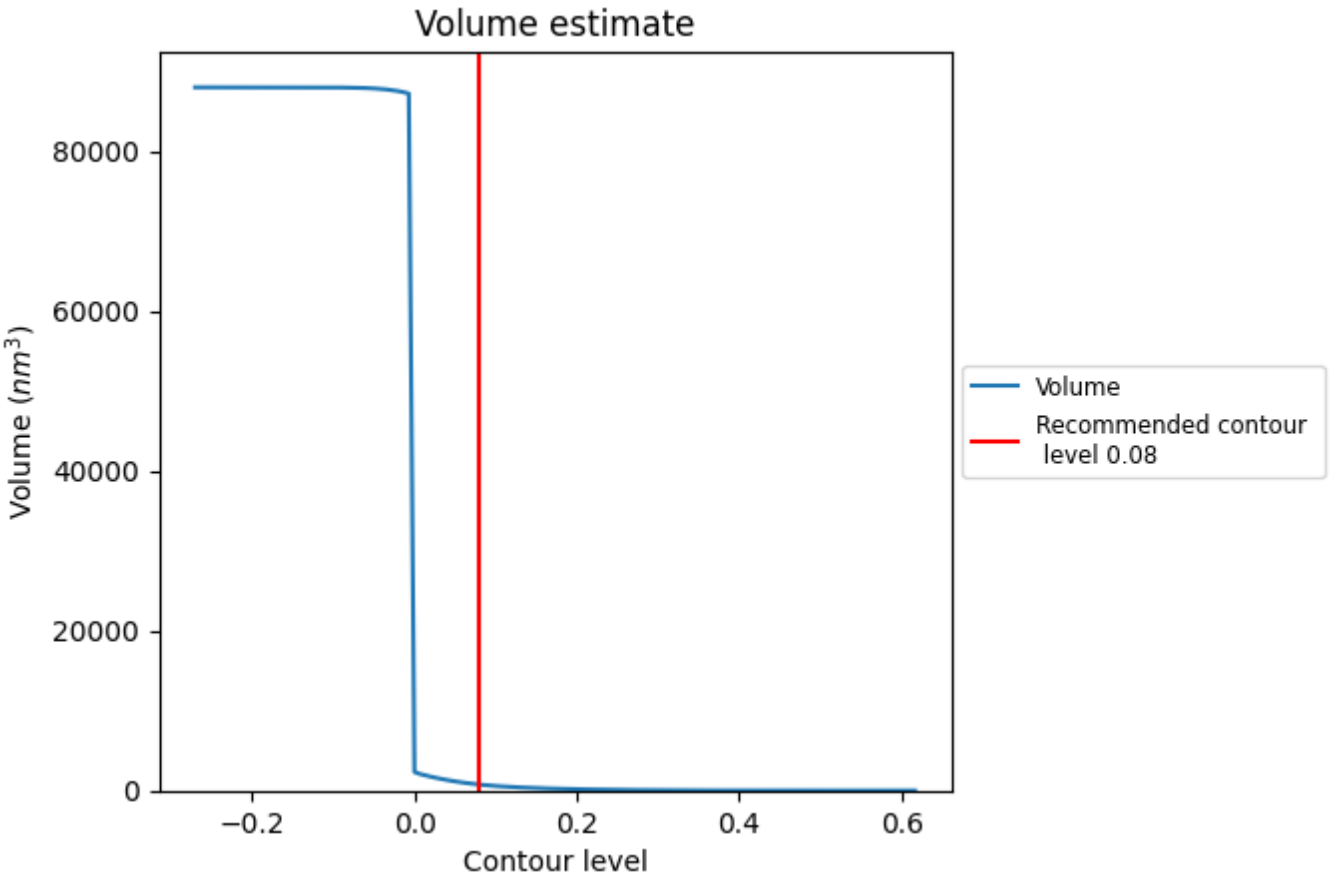
This section contains the results of statistical analysis of the map.

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.

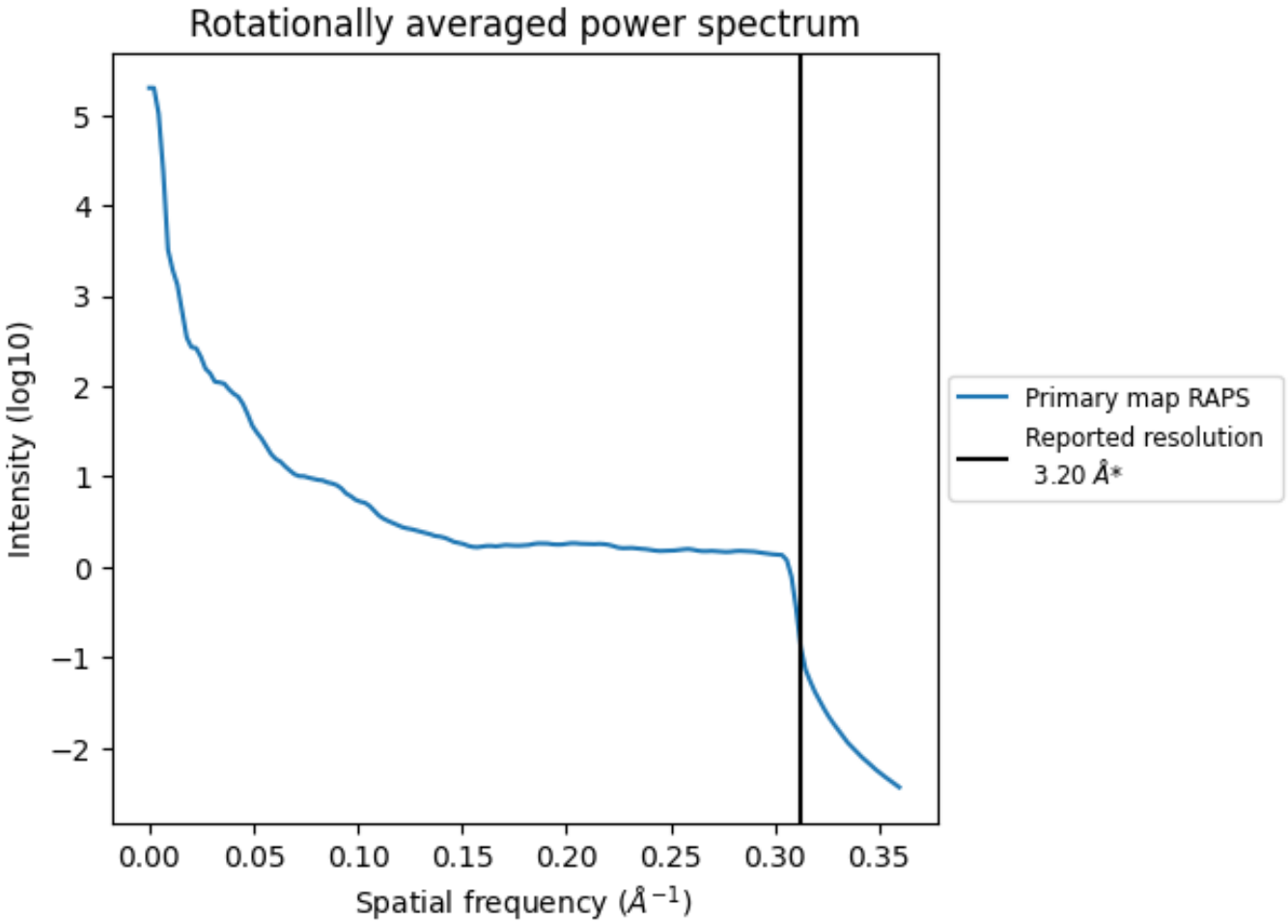
7.2 Volume estimate (i)



The volume at the recommended contour level is 750 nm^3; this corresponds to an approximate mass of 678 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)

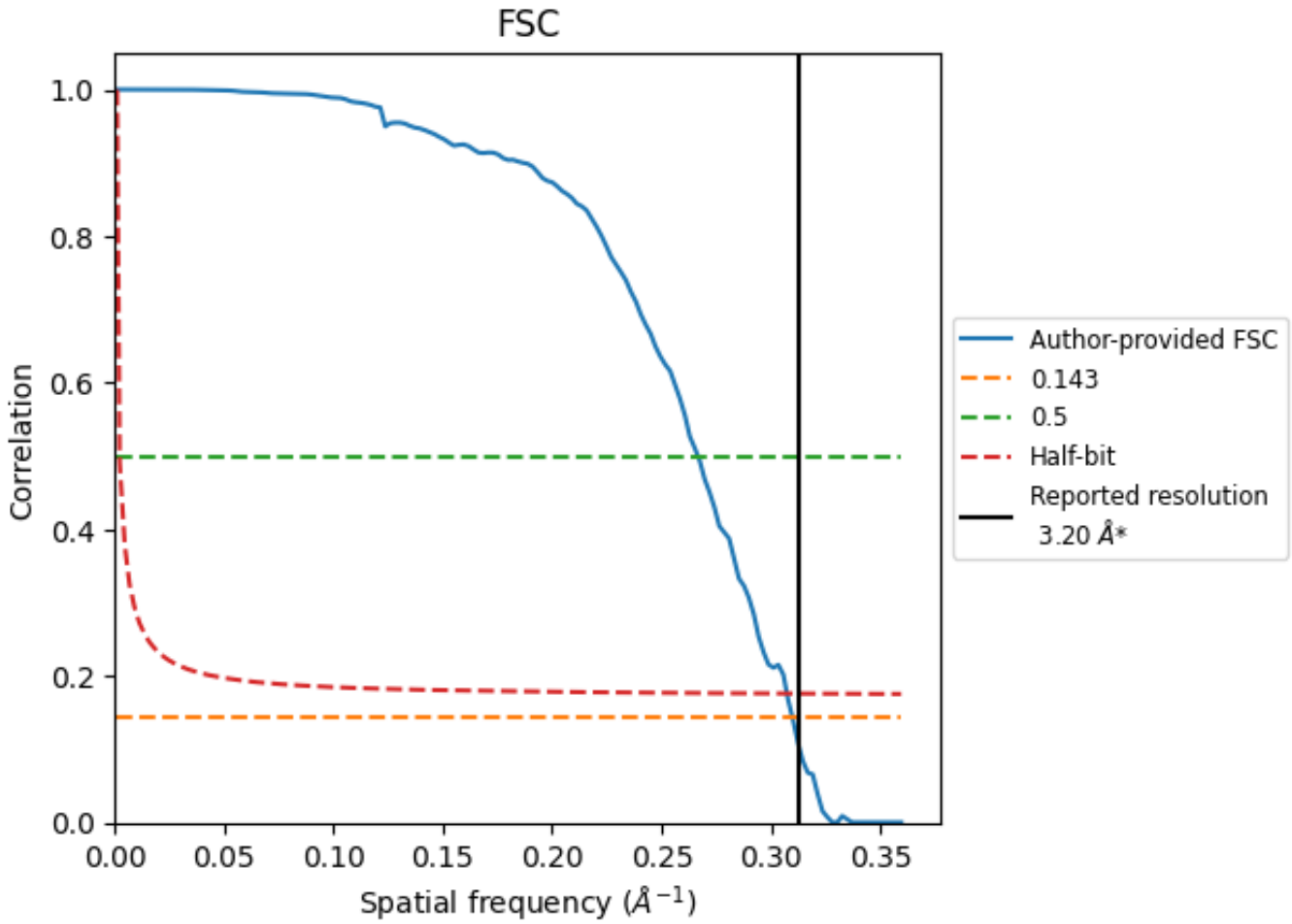


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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)

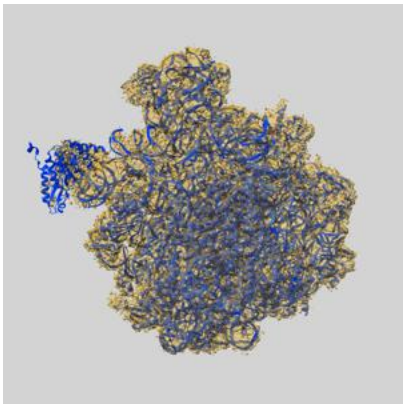
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.23	3.75	3.25
Unmasked-calculated*	-	-	-

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

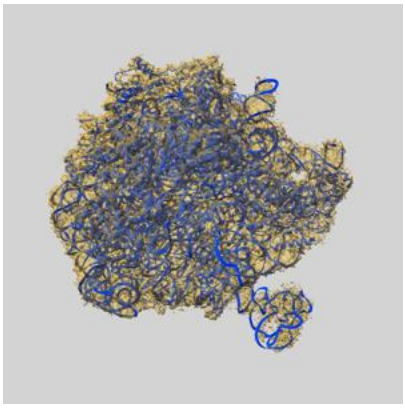
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3531 and PDB model 5MMI. Per-residue inclusion information can be found in section 3 on page 12.

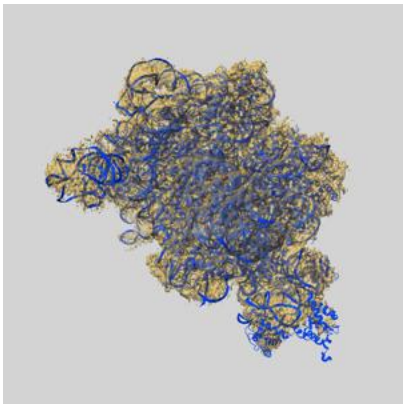
9.1 Map-model overlay



X



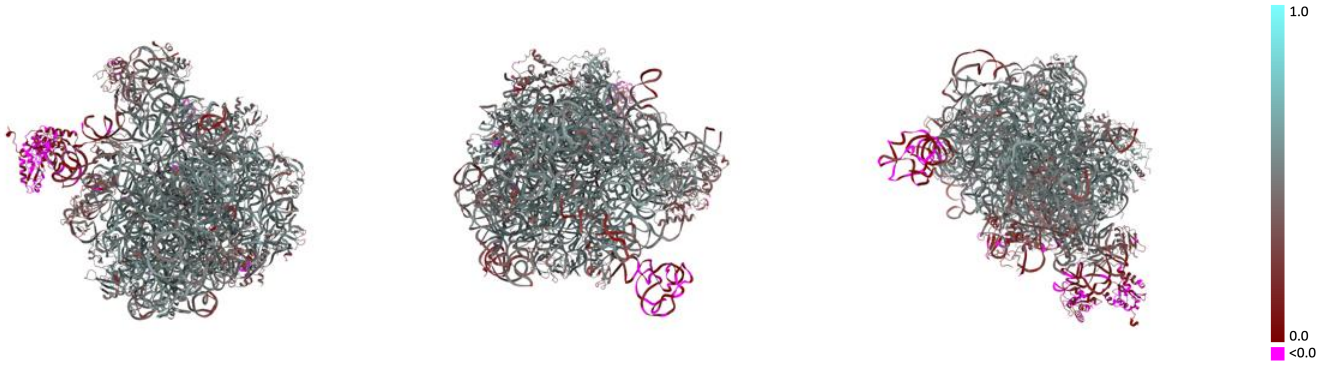
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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.

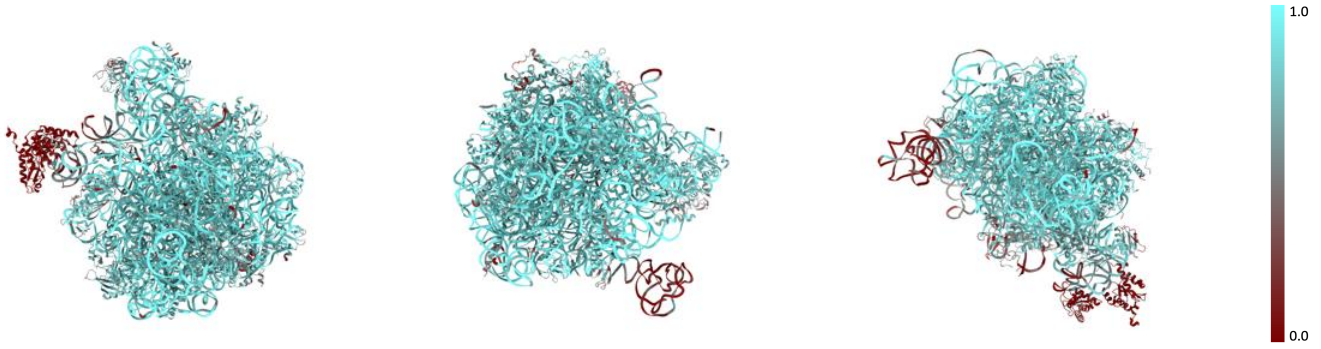
9.2 Q-score mapped to coordinate model



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.

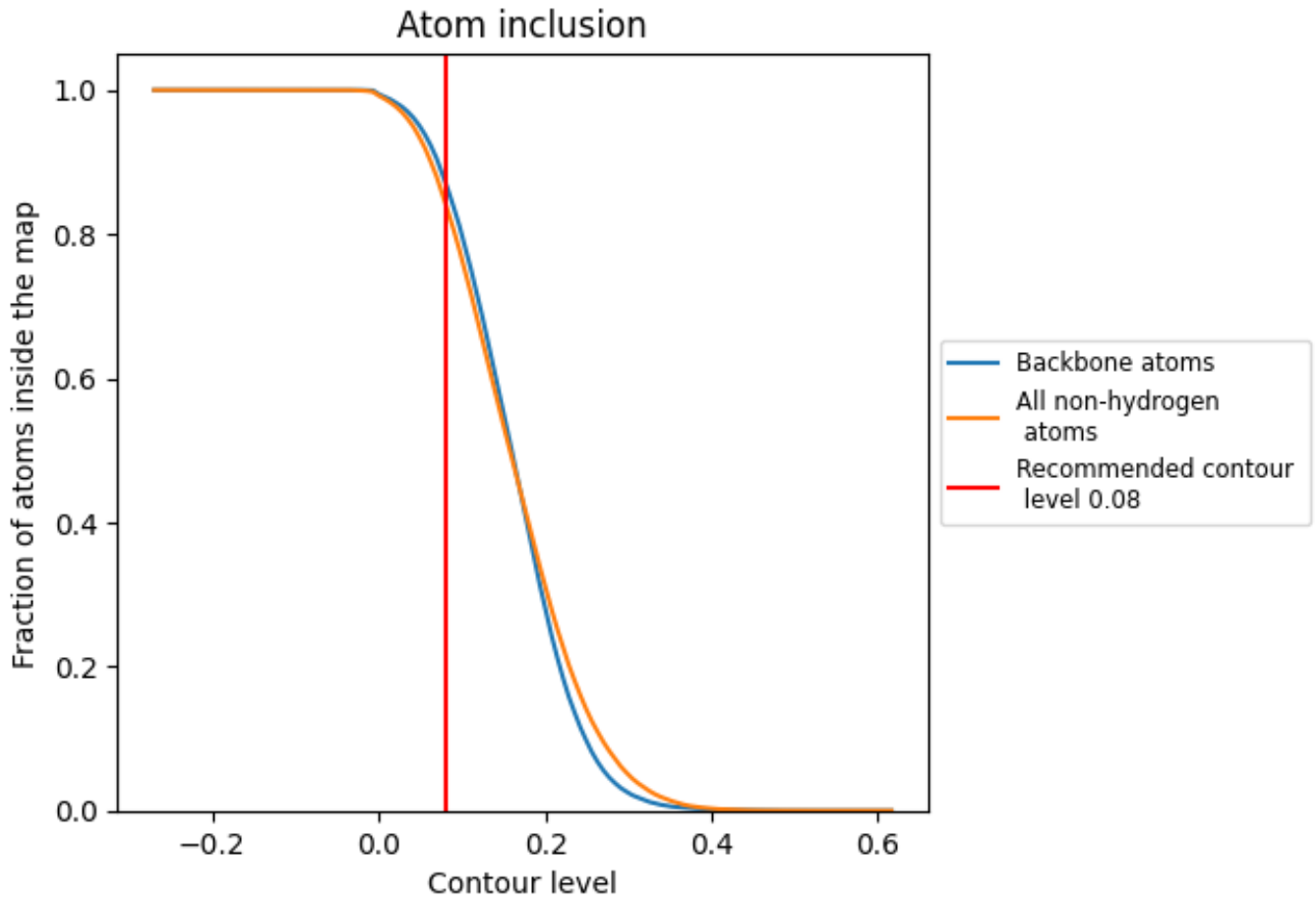
9.3 Atom inclusion mapped to coordinate model



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 (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 84% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8434	0.4690
0	0.4416	0.2120
1	0.8359	0.5280
2	0.7611	0.4720
3	0.8600	0.5580
4	0.8310	0.5360
5	0.7552	0.4690
6	0.7266	0.4260
7	0.8268	0.4900
A	0.8993	0.4880
B	0.9396	0.4510
C	0.7868	0.4900
D	0.8463	0.5130
E	0.8082	0.4880
F	0.5710	0.3020
G	0.6578	0.3450
H	0.4828	0.3860
I	0.0376	0.0180
J	0.0701	0.0320
K	0.8322	0.4980
L	0.7309	0.4880
M	0.8287	0.4810
N	0.5414	0.4030
O	0.8497	0.5190
P	0.8053	0.4350
Q	0.7780	0.4790
R	0.8712	0.5220
S	0.7603	0.4590
T	0.7688	0.4630
U	0.7464	0.4570
V	0.7458	0.4450
W	0.9459	0.5100
X	0.8174	0.4850
Y	0.8068	0.5030
Z	0.7466	0.4290
z	0.4048	0.4000