wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 06:55 pm GMT

PDB ID	:	4CE4
EMDB ID	:	EMD-2490
Title	:	39S large subunit of the porcine mitochondrial ribosome
Authors	:	Greber, B.J.; Boehringer, D.; Leitner, A.; Bieri, P.; Voigts-Hoffmann, F.; Erzberger, J.P.; Leibundgut, M.; Aebersold, R.; Ban, N.
Deposited on	:	2013-11-08
Resolution	:	4.90 Å(reported)
Based on initial models	:	1J26, 1S3A, 2CW9, 1O0W, 1R73, 2QYQ, 2XZN, 1QF6, 3V2D

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:

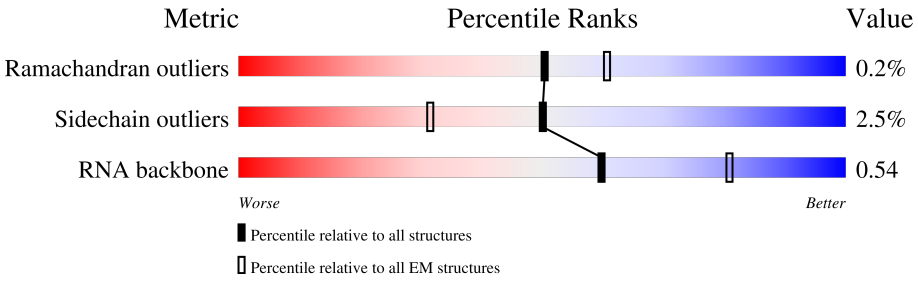
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.90 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.



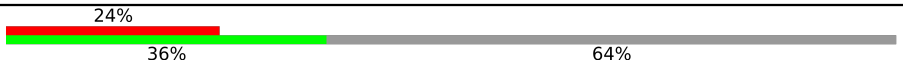
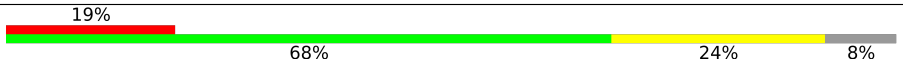
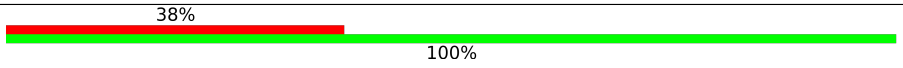
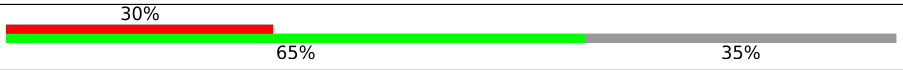
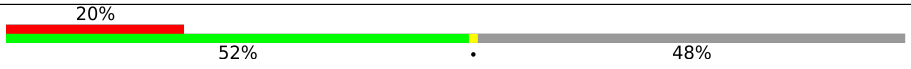
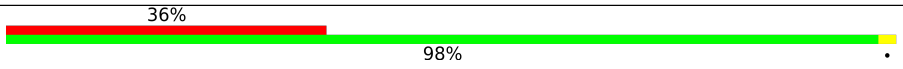
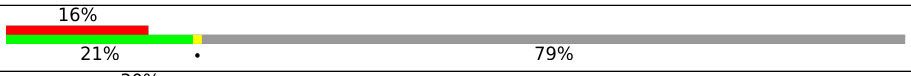
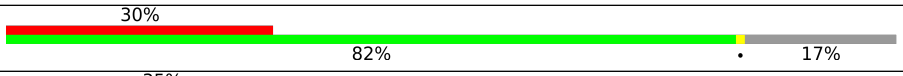
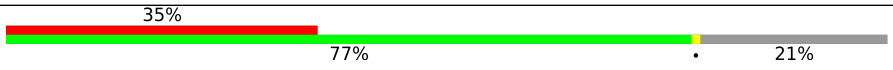
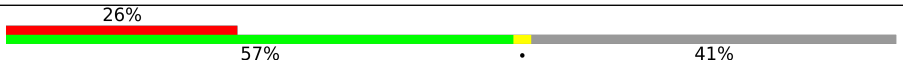
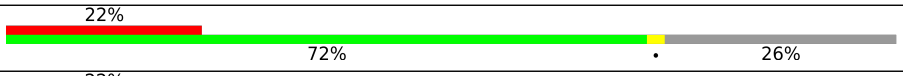
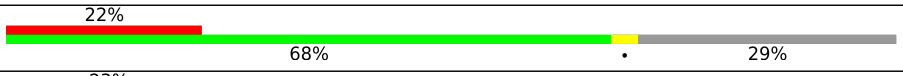
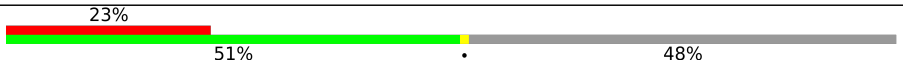
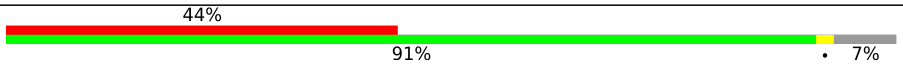
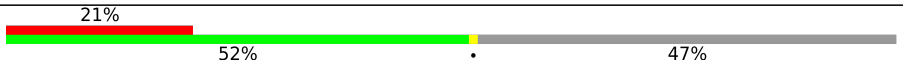
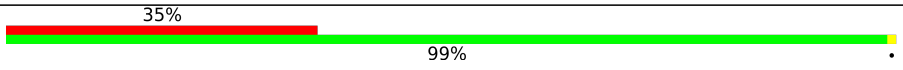
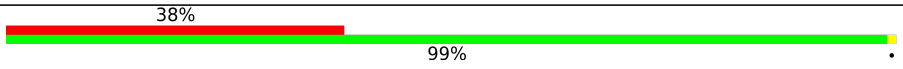
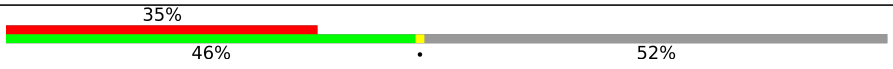
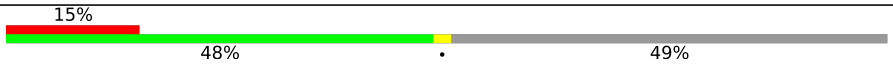
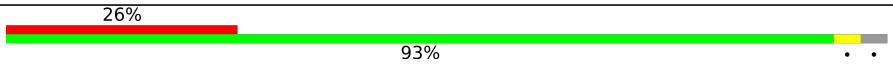
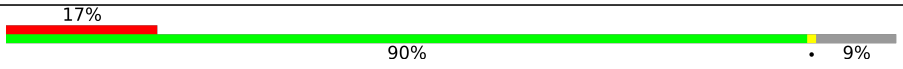
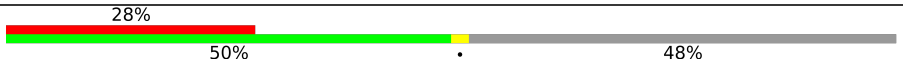
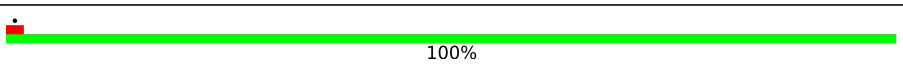
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	148	25% 50% · 49%
2	1	256	11% 21% · 77%
3	2	252	7% 30% 70%
4	3	161	16% 37% 63%
5	5	146	16% 46% · 53%
6	6	65	63% 74% 26%
7	7	95	19% 45% 55%
8	8	188	20% 31% · 68%

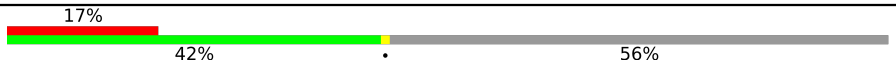
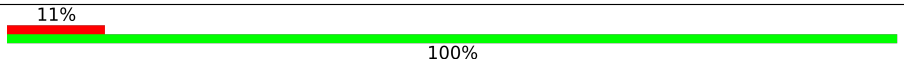
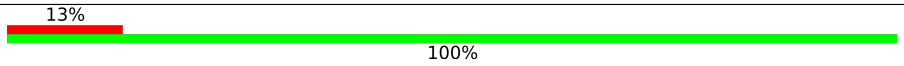
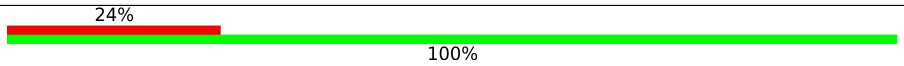
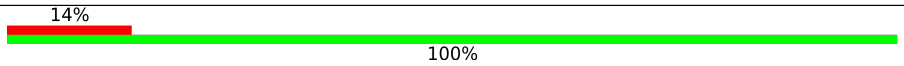
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	9	100	
10	A	1570	
11	B	29	
12	D	306	
13	E	399	
14	F	224	
15	I	268	
16	N	178	
17	O	145	
18	P	288	
19	Q	208	
20	R	169	
21	S	180	
22	T	292	
23	U	132	
24	V	207	
25	W	134	
26	X	87	
27	Y	216	
28	b	380	
29	c	301	
30	h	298	
31	i	312	
32	l	166	
33	o	56	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	u	205	
35	v	91	
35	w	91	
36	x	85	
37	z	426	

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 65473 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 MRPL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	76	607	392	114	99	2	0	0

- Molecule 2 is a protein called MRPL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	58	489	312	90	85	2	0	0

- Molecule 3 is a protein called MRPL47.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	76	633	394	116	119	4	0	0

- Molecule 4 is a protein called MRPL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	59	491	321	95	74	1	0	0

- Molecule 5 is a protein called MRPL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	68	508	317	103	83	5	0	0

- Molecule 6 is a protein called MRPL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	48	391	253	70	66	2	0	0

- Molecule 7 is a protein called MRPL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	43	Total	C	N	O	S	0	0
			362	224	82	55	1		

- Molecule 8 is a protein called MRPL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	60	Total	C	N	O	S	0	0
			520	338	106	74	2		

- Molecule 9 is a protein called MRPL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	36	Total	C	N	O	S	0	0
			316	200	68	45	3		

- Molecule 10 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	1444	Total	C	N	O	P	0	0
			30656	13760	5548	9904	1444		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127A	G	-	insertion	GB AJ002189

- Molecule 11 is a RNA chain called UNASSIGNED RNA.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	B	29	Total	C	O	P	0	0
			348	145	174	29		

- Molecule 12 is a protein called MRPL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	200	Total	C	N	O	S	0	0
			1531	944	309	269	9		

- Molecule 13 is a protein called MRPL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	208	Total	C	N	O	S	0	0
			1621	1040	300	274	7		

- Molecule 14 is a protein called MRPL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	224	Total	C	N	O	S	0	0
			1713	1101	310	298	4		

- Molecule 15 is a protein called MRPL9.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	I	57	Total	C	N	O	0	0
			447	282	79	86		

- Molecule 16 is a protein called MRPL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	147	Total	C	N	O	S	0	0
			1178	756	210	204	8		

- Molecule 17 is a protein called MRPL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	114	Total	C	N	O	S	0	0
			891	559	175	153	4		

- Molecule 18 is a protein called MRPL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	169	Total	C	N	O	S	0	0
			1309	816	258	233	2		

- Molecule 19 is a protein called MRPL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	154	Total	C	N	O	S	0	0
			1179	758	218	195	8		

- Molecule 20 is a protein called MRPL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	120	Total	C	N	O	S	0	0
			982	619	187	172	4		

- Molecule 21 is a protein called MRPL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	94	Total	C	N	O	S	0	0
			748	467	146	131	4		

- Molecule 22 is a protein called MRPL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	119	Total	C	N	O	S	0	0
			962	615	166	177	4		

- Molecule 23 is a protein called MRPL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	123	Total	C	N	O	S	0	0
			1018	647	212	156	3		

- Molecule 24 is a protein called MRPL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	109	Total	C	N	O	S	0	0
			877	565	156	154	2		

- Molecule 25 is a protein called MRPL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	134	Total	C	N	O	S	0	0
			1058	679	191	182	6		

- Molecule 26 is a protein called MRPL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	87	Total	C	N	O	S	0	0
			689	436	133	118	2		

- Molecule 27 is a protein called MRPL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	103	Total	C	N	O	S	0	0
			835	526	156	151	2		

- Molecule 28 is a protein called MRPL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	192	Total	C	N	O	S	0	0
			1562	1006	266	284	6		

- Molecule 29 is a protein called MRPL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	292	Total	C	N	O	S	0	0
			2310	1489	391	415	15		

- Molecule 30 is a protein called MRPL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	272	Total	C	N	O	S	0	0
			2075	1333	344	391	7		

- Molecule 31 is a protein called MRPL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	161	Total	C	N	O	S	0	0
			1335	845	243	239	8		

- Molecule 32 is a protein called MRPL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	l	76	Total	C	N	O	S	0	0
			619	398	108	111	2		

- Molecule 33 is a protein called MRPL52.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	o	56	Total	C	N	O	0	0
			336	224	56	56		

- Molecule 34 is a protein called ICT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	u	90	Total	C	N	O	S	0	0
			717	444	137	132	4		

- Molecule 35 is a protein called UNASSIGNED HELICES.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	v	91	Total	C	N	O	0	0
			546	364	91	91		
35	w	91	Total	C	N	O	0	0
			546	364	91	91		

- Molecule 36 is a protein called THIOREDOXIN FOLD.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	x	85	Total	C	N	O	0	0
			510	340	85	85		

- Molecule 37 is a protein called UNASSIGNED HELICES.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	z	426	Total	C	N	O	0	0
			2556	1704	426	426		

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

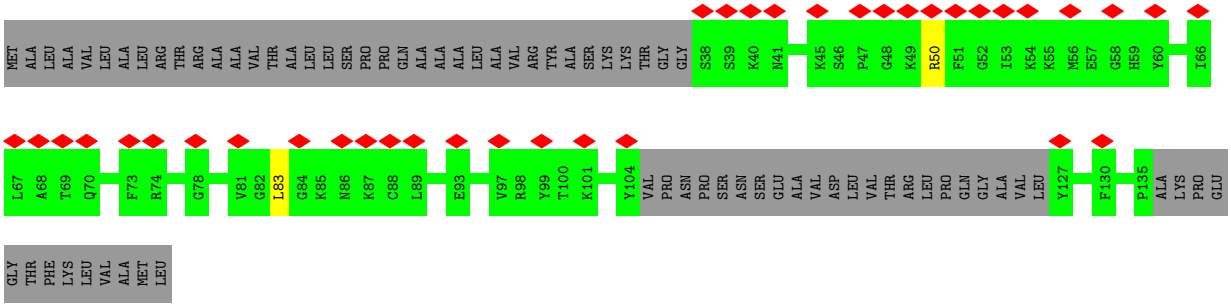
Mol	Chain	Residues	Atoms		AltConf
38	5	1	Total	Zn	0
			1	1	
38	9	1	Total	Zn	0
			1	1	

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.

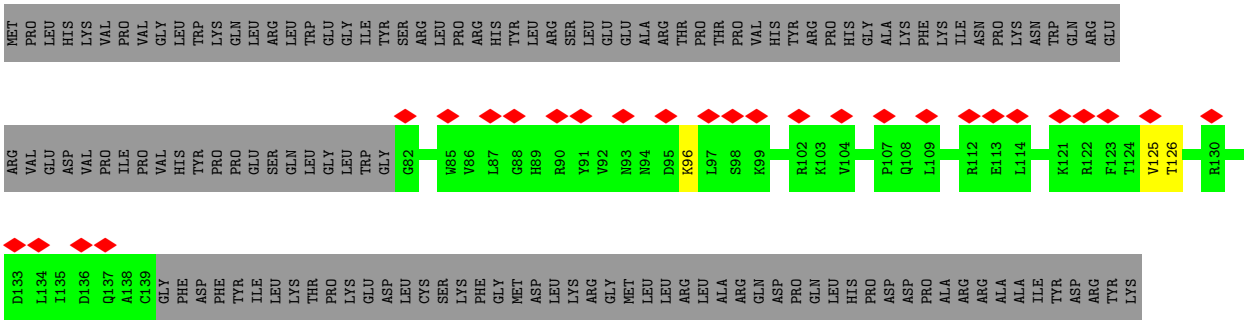
• Molecule 1: MRPL27

Chain 0:



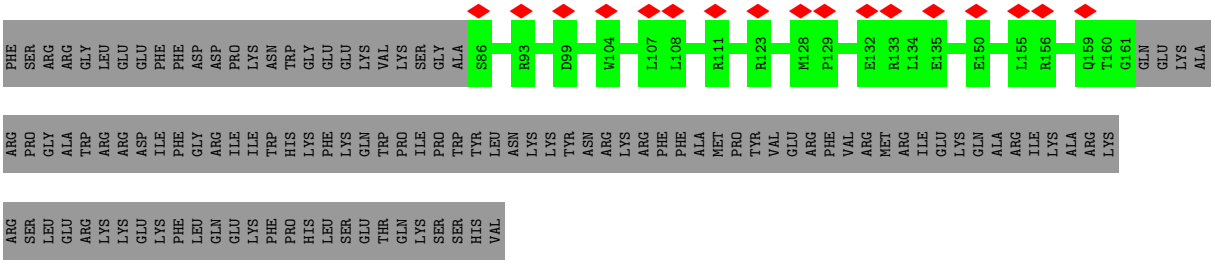
• Molecule 2: MRPL28

Chain 1:



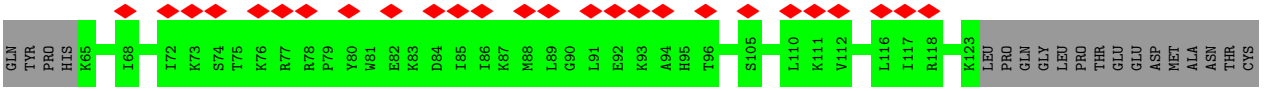
• Molecule 3: MRPL47

Chain 2:



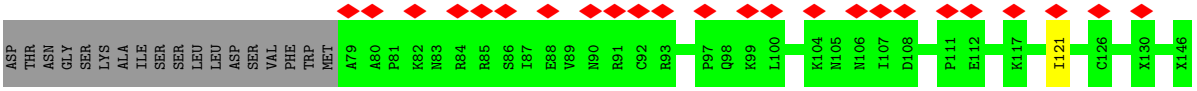
• Molecule 4: MRPL30

Chain 3:



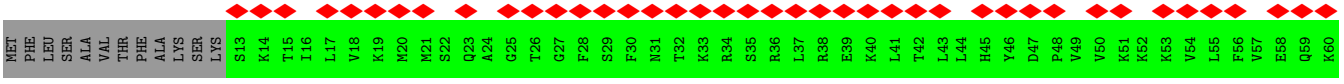
• Molecule 5: MRPL32

Chain 5:



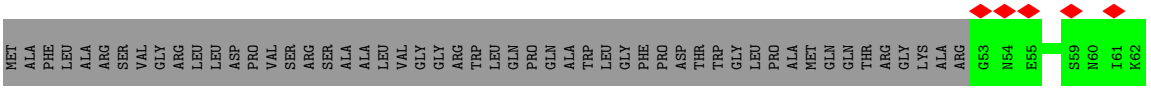
• Molecule 6: MRPL33

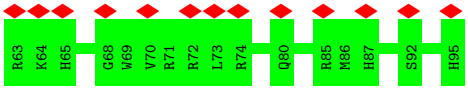
Chain 6:



• Molecule 7: MRPL34

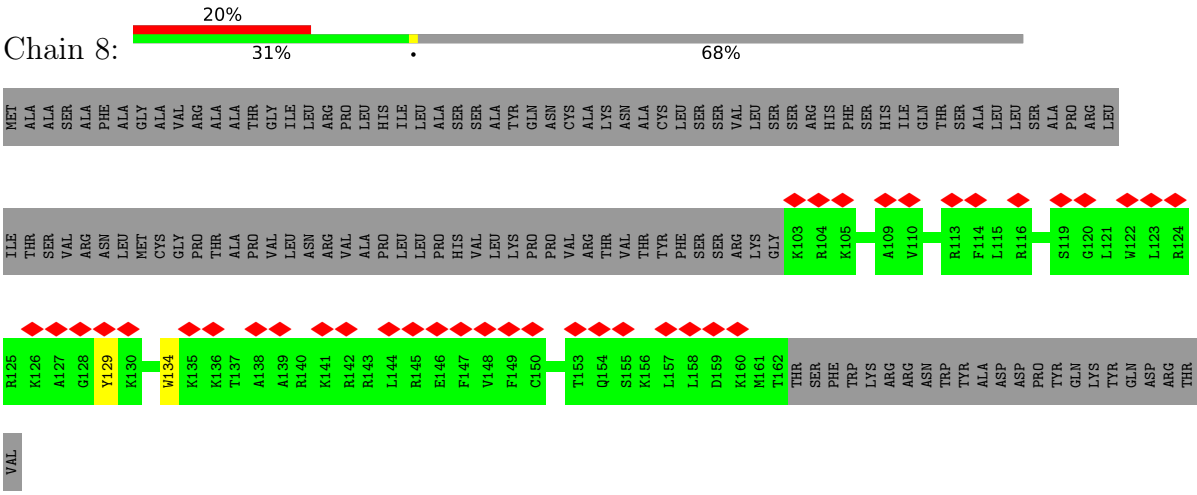
Chain 7:





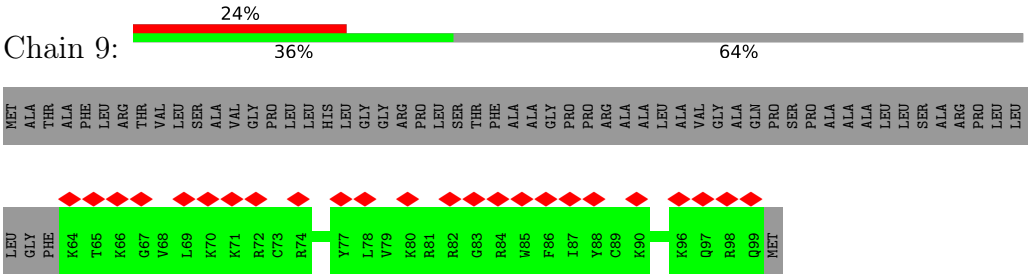
• Molecule 8: MRPL35

Chain 8:



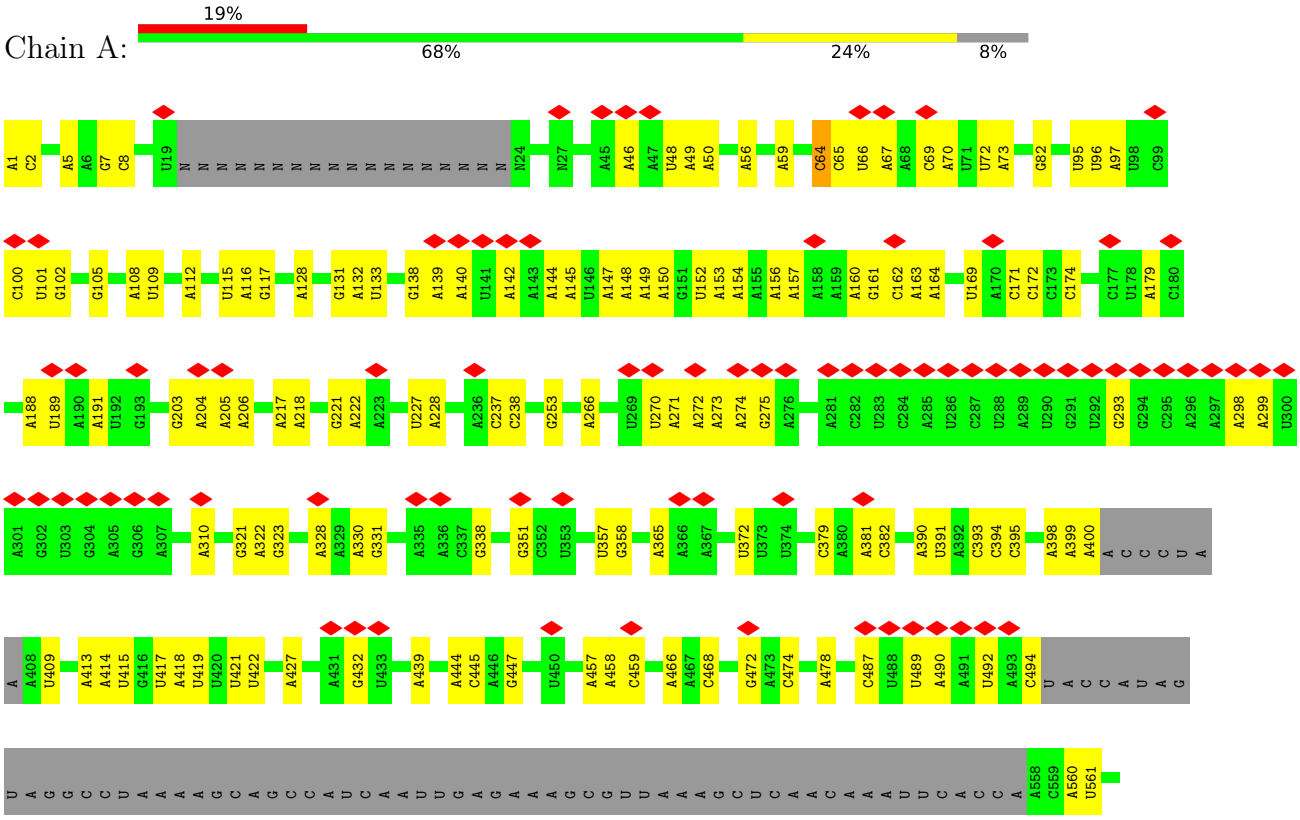
• Molecule 9: MRPL36

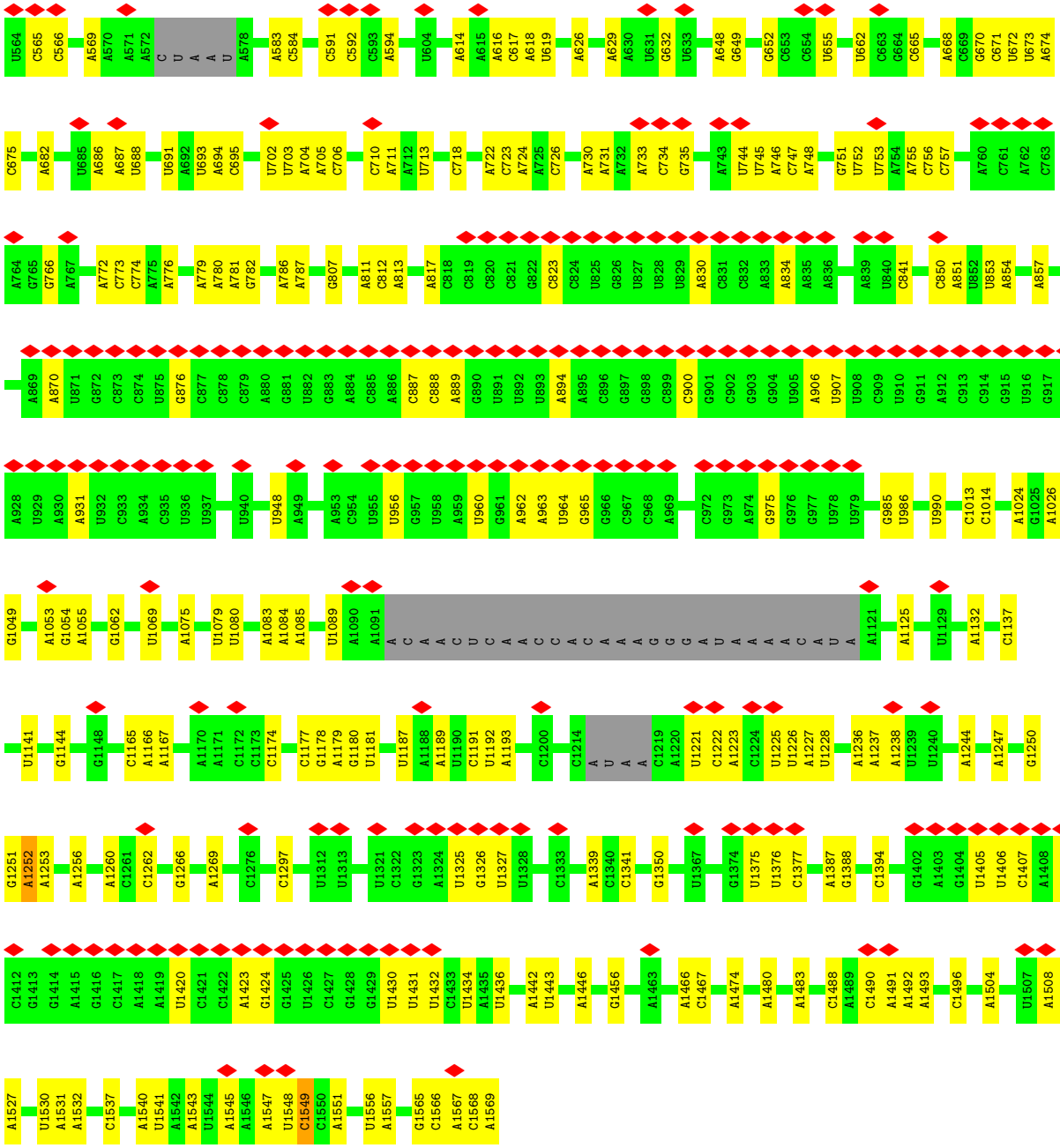
Chain 9:



• Molecule 10: 16S Ribosomal RNA

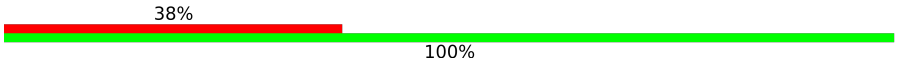
Chain A:

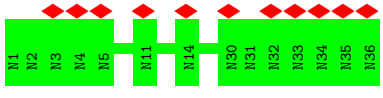




• Molecule 11: UNASSIGNED RNA

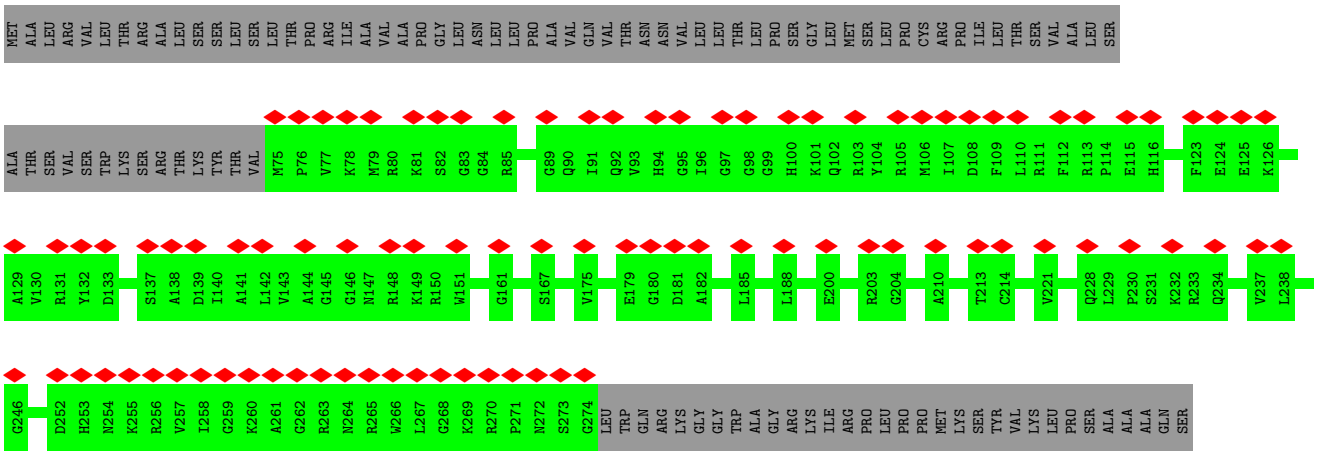
Chain B:





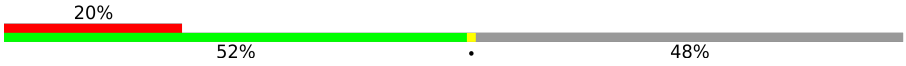
• Molecule 12: MRPL2

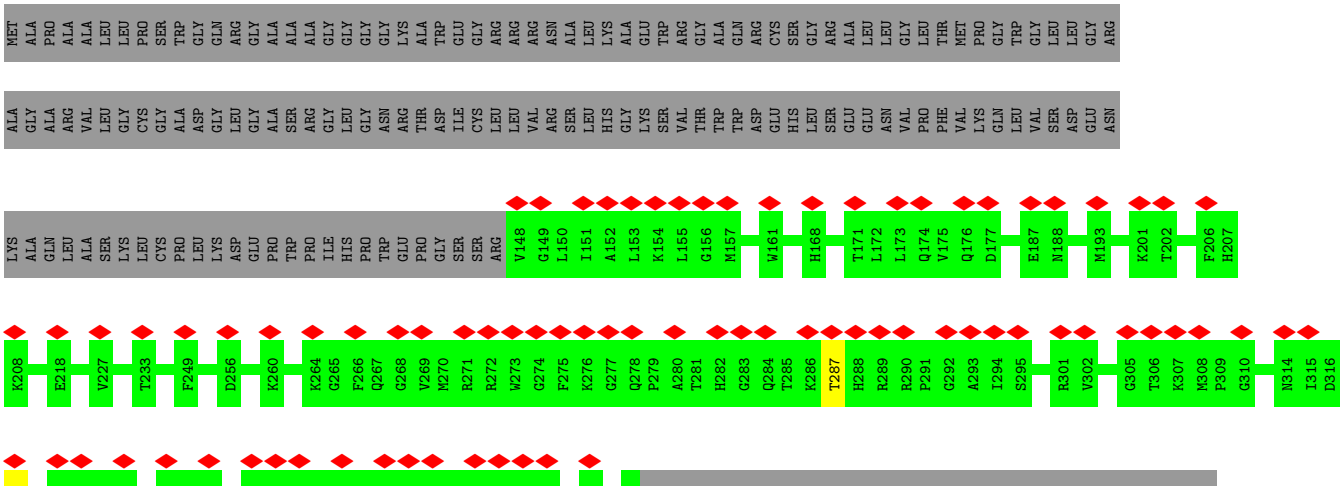
Chain D:



• Molecule 13: MRPL3

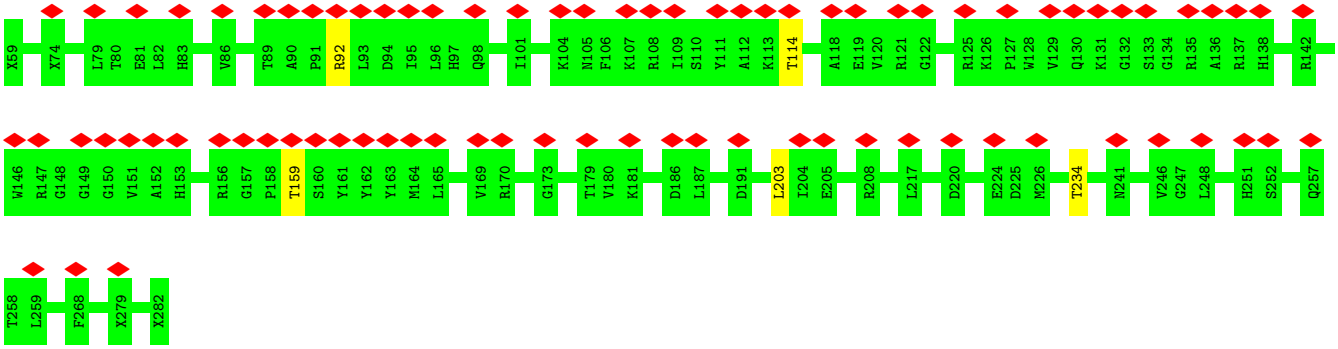
Chain E:





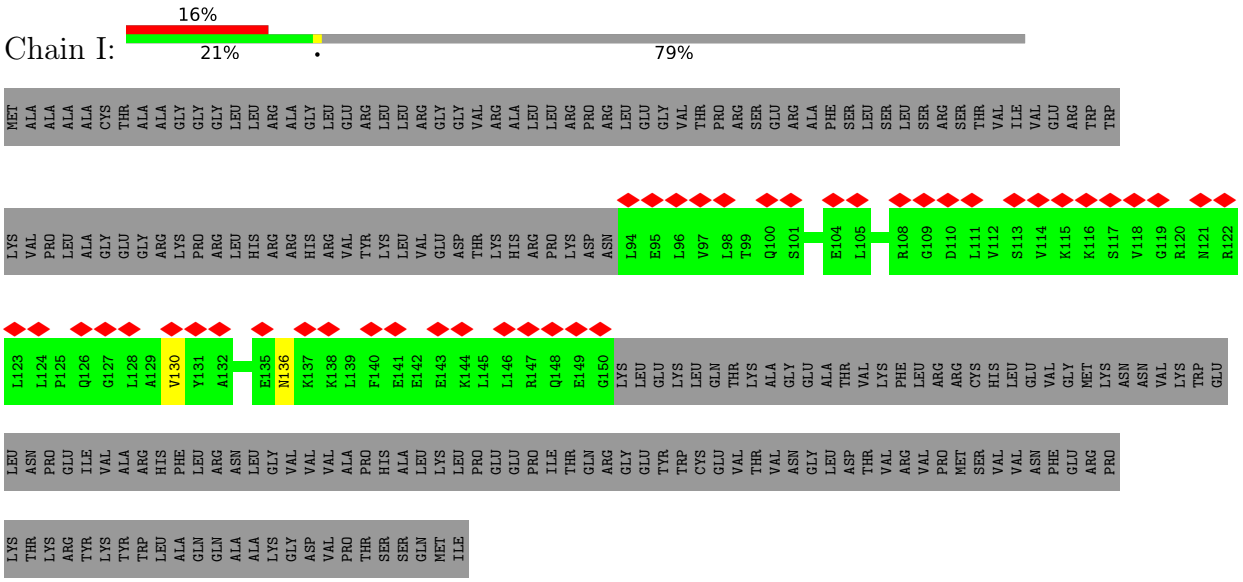
• Molecule 14: MRPL4

Chain F:



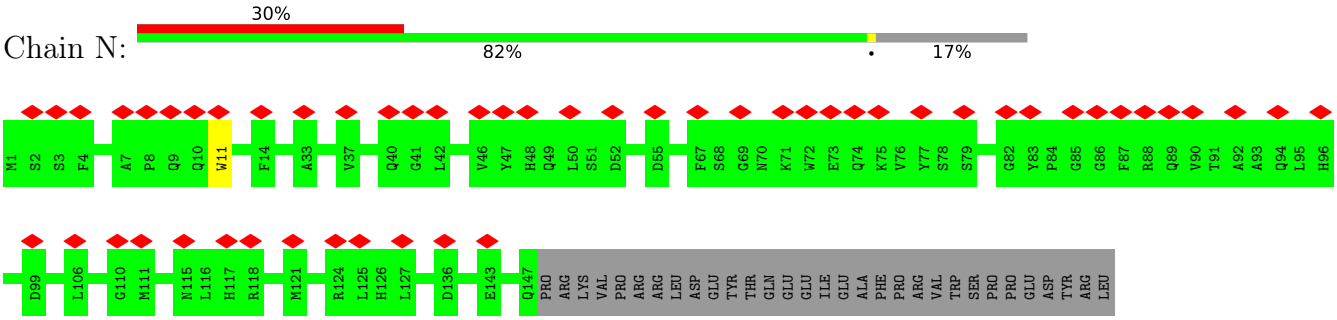
• Molecule 15: MRPL9

Chain I:



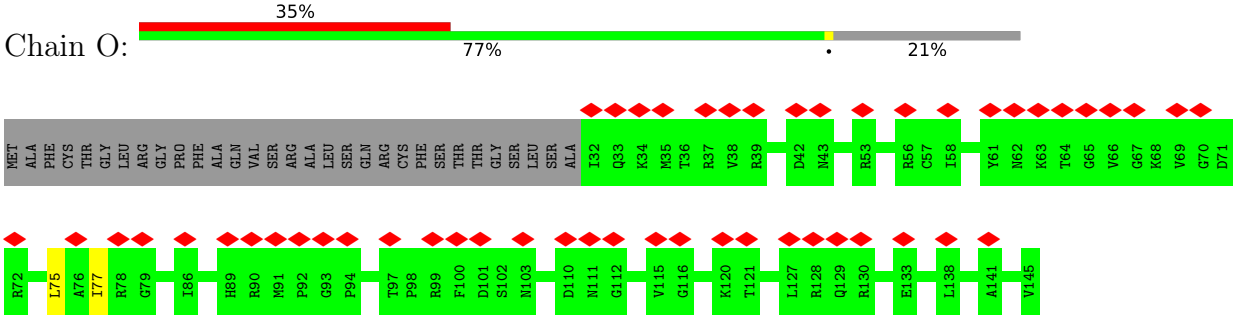
• Molecule 16: MRPL13

Chain N:



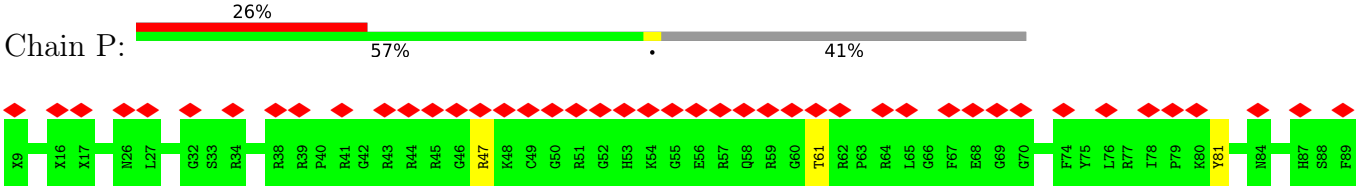
• Molecule 17: MRPL14

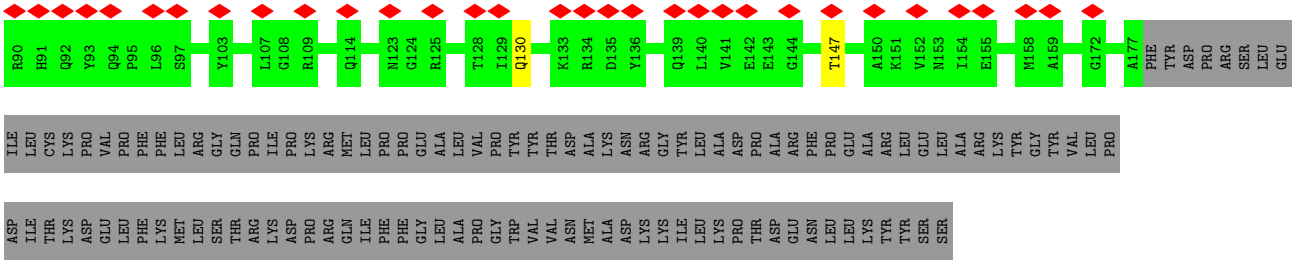
Chain O:



• Molecule 18: MRPL15

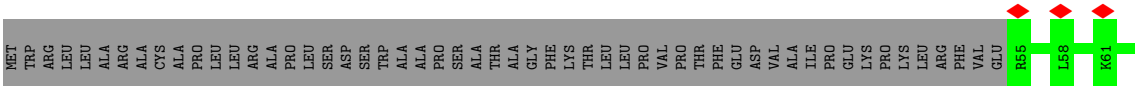
Chain P:

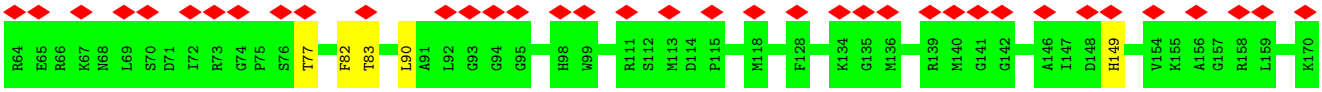




• Molecule 19: MRPL16

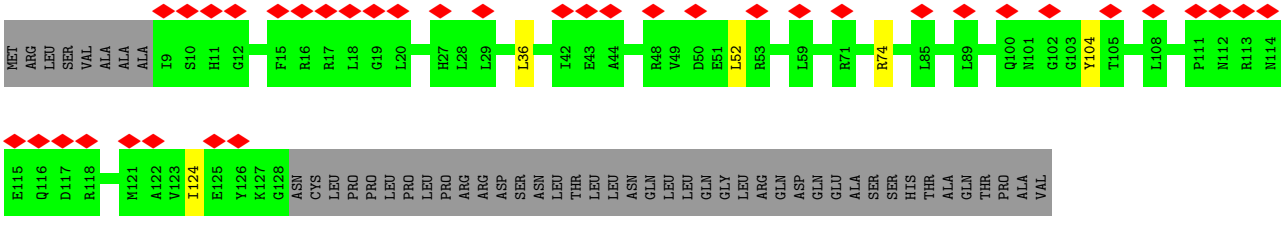
Chain Q:





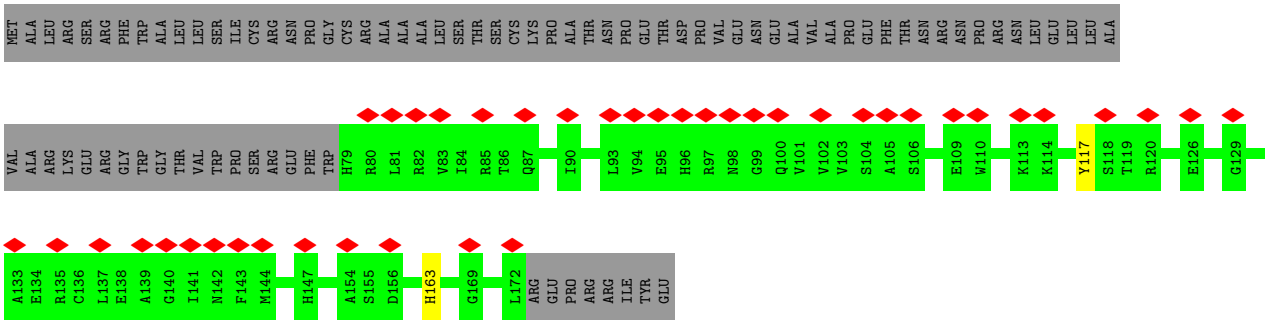
• Molecule 20: MRPL17

Chain R:



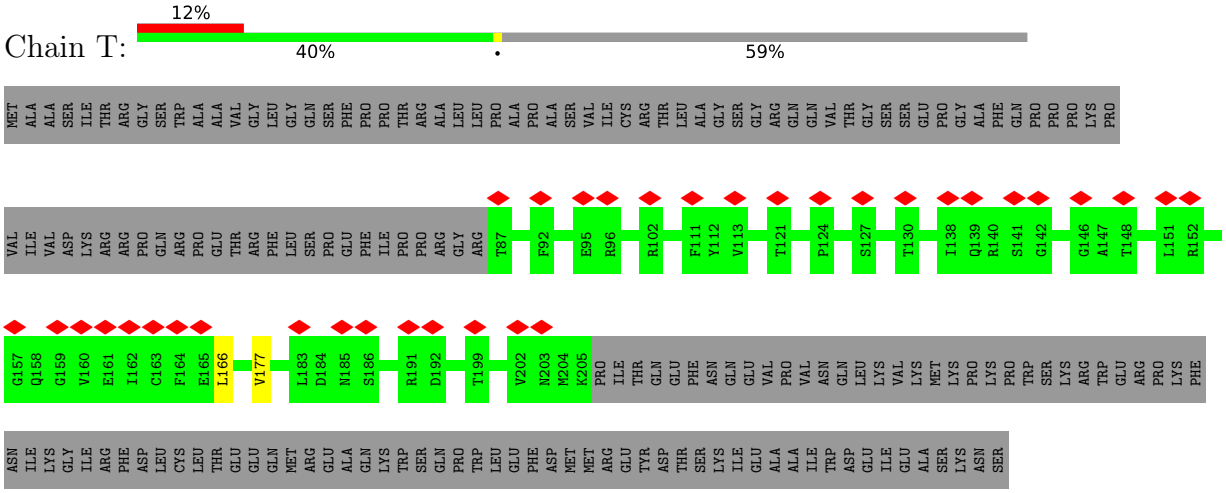
• Molecule 21: MRPL18

Chain S:



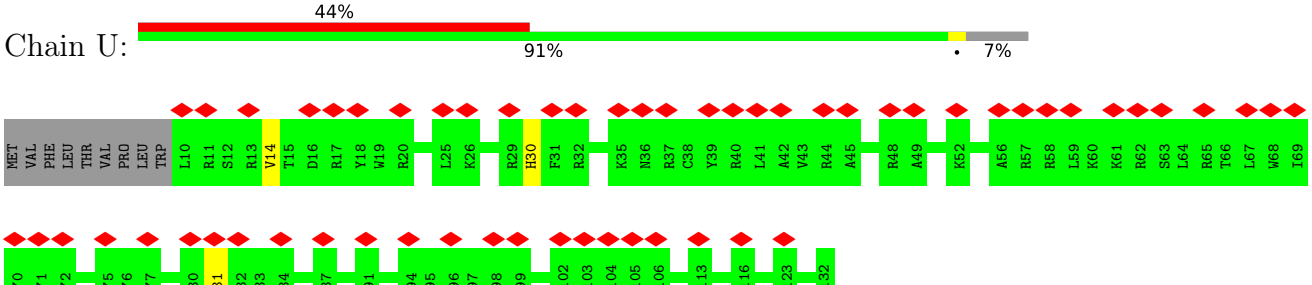
• Molecule 22: MRPL19

Chain T:



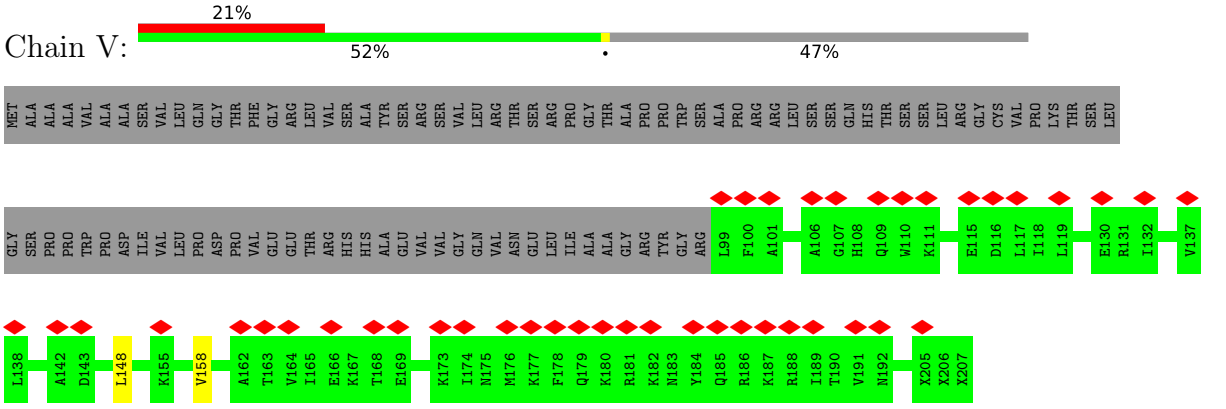
• Molecule 23: MRPL20

Chain U:



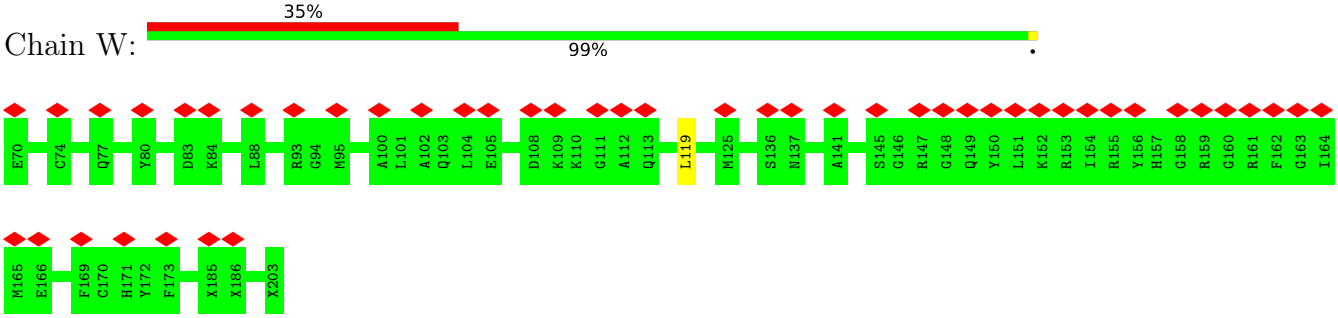
• Molecule 24: MRPL21

Chain V:



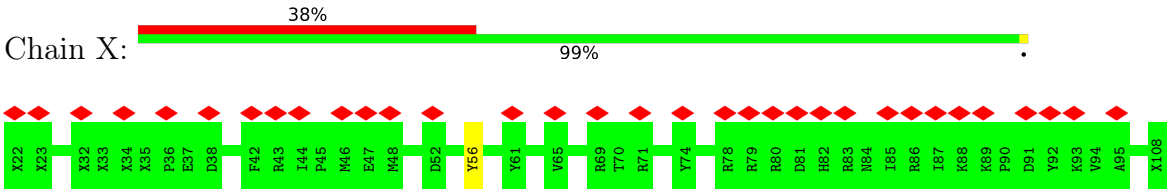
• Molecule 25: MRPL22

Chain W:



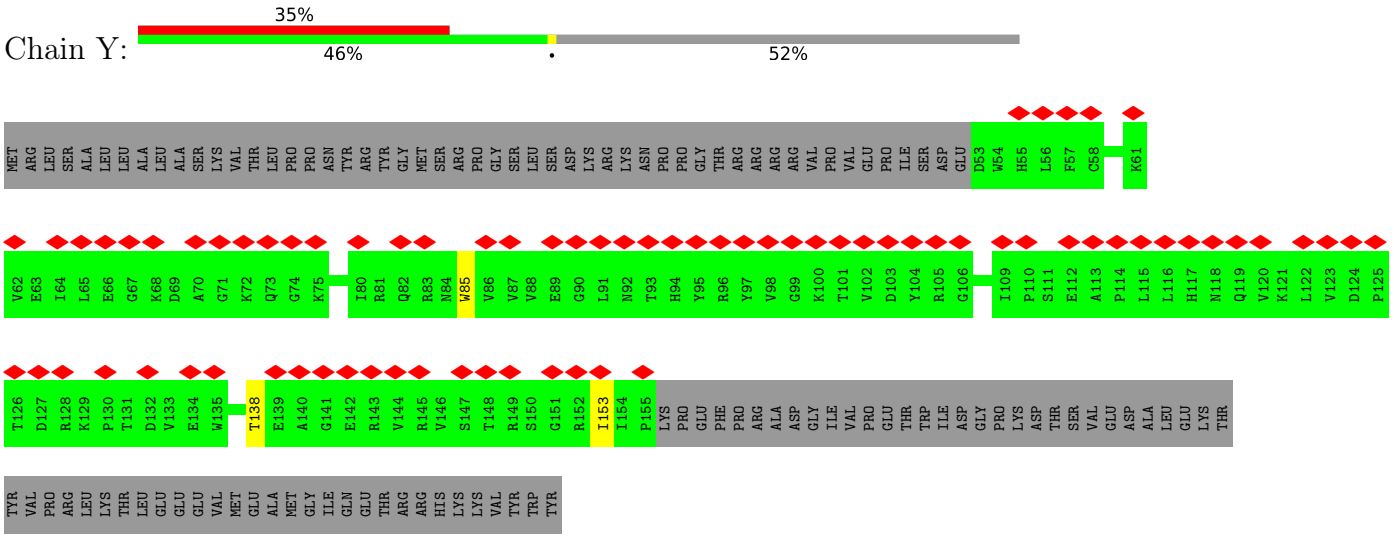
• Molecule 26: MRPL23

Chain X:



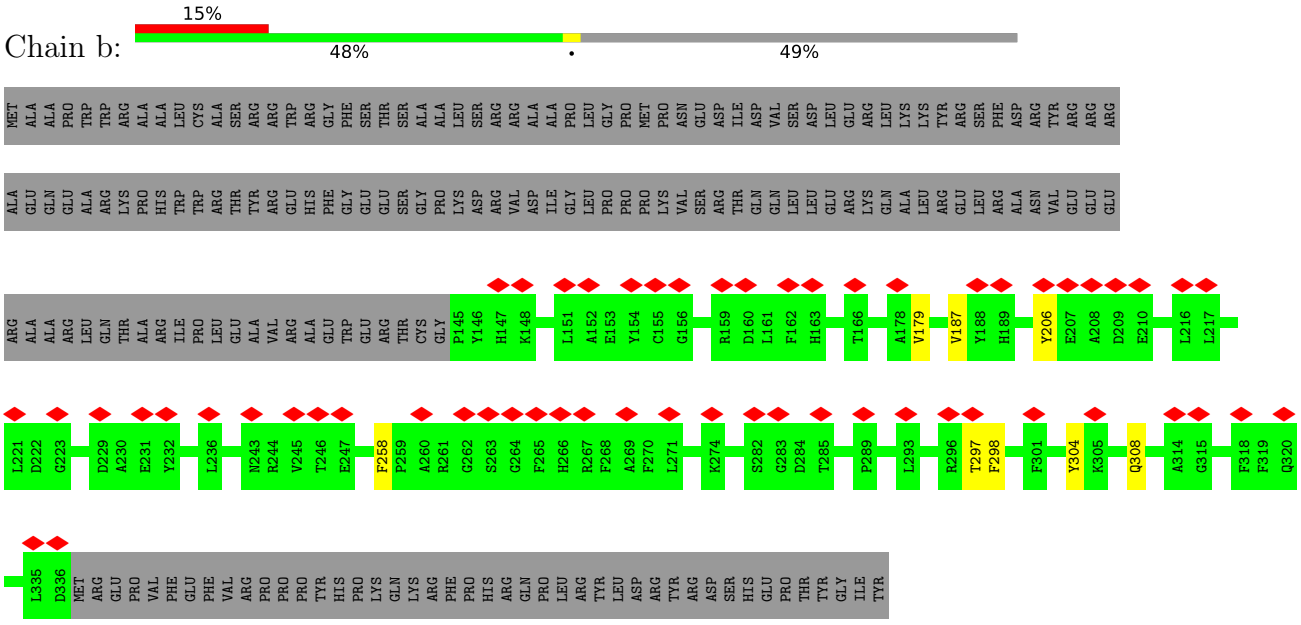
• Molecule 27: MRPL24

Chain Y:



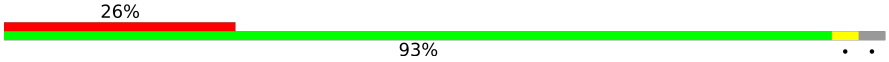
• Molecule 28: MRPL38

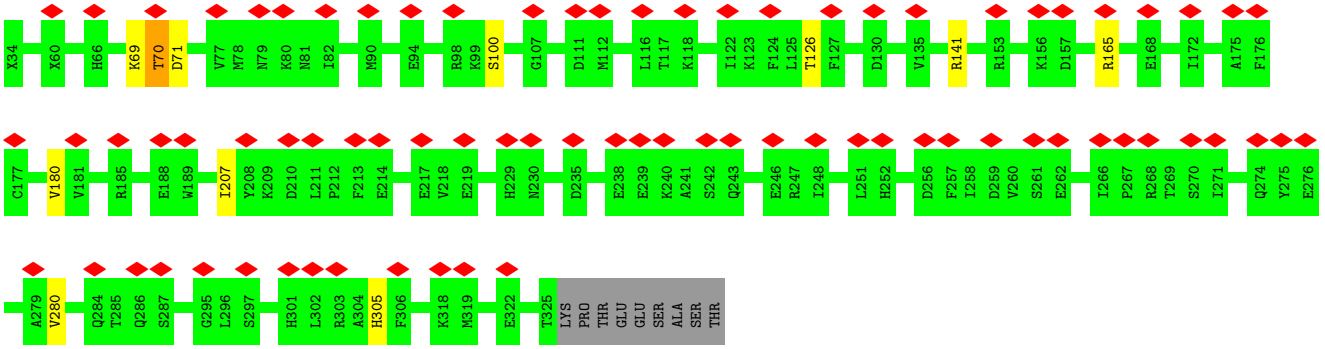
Chain b:



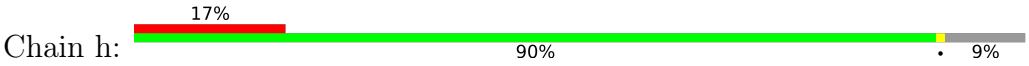
• Molecule 29: MRPL39

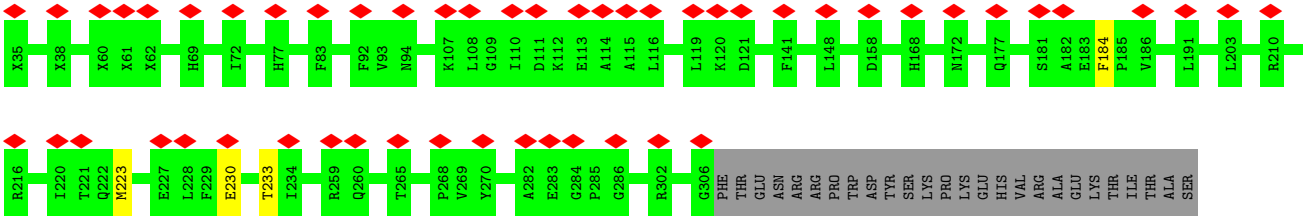
Chain c:



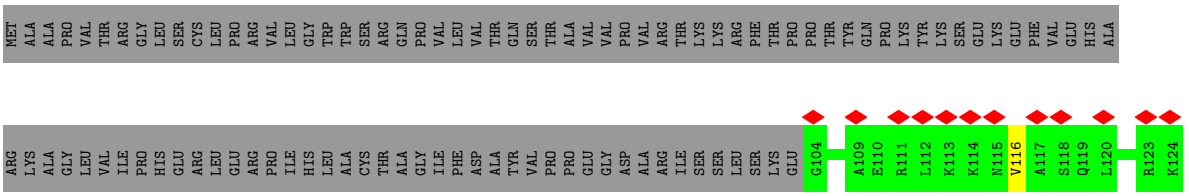


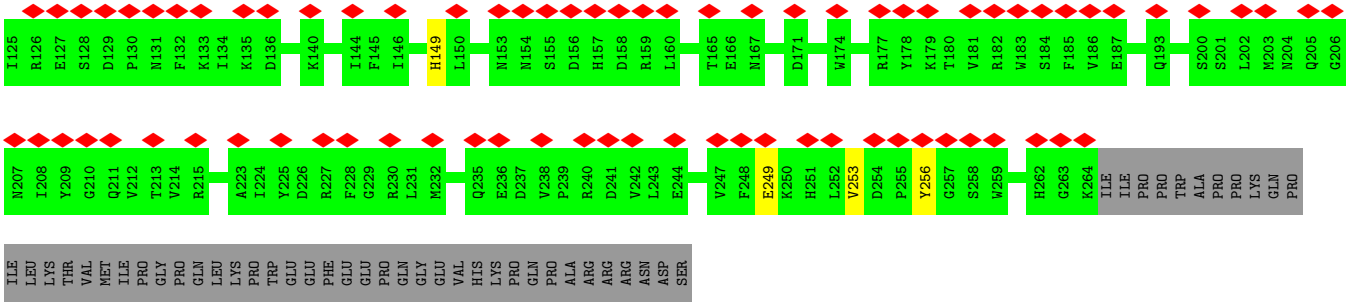
• Molecule 30: MRPL44



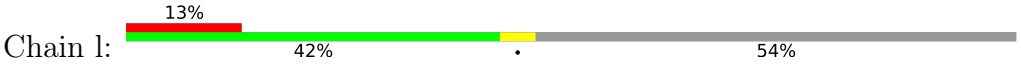


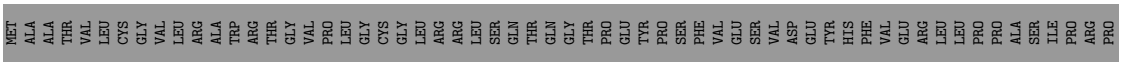
• Molecule 31: MRPL45

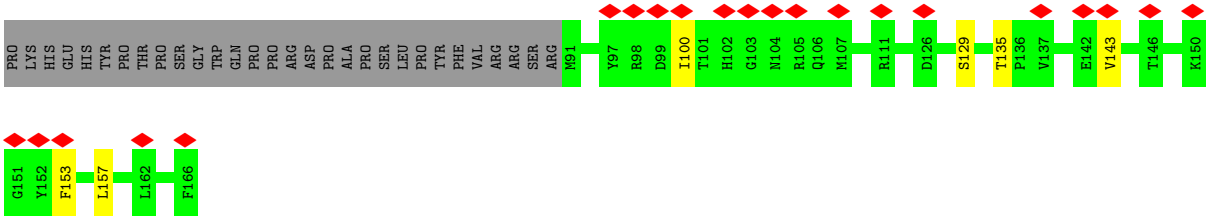




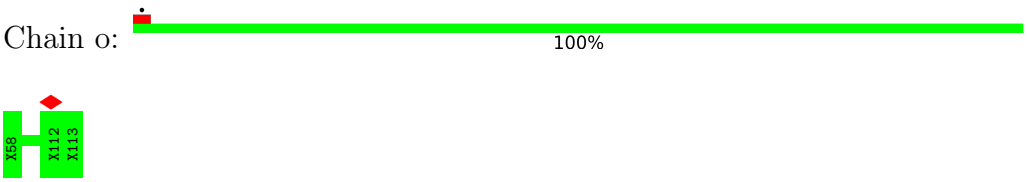
• Molecule 32: MRPL49



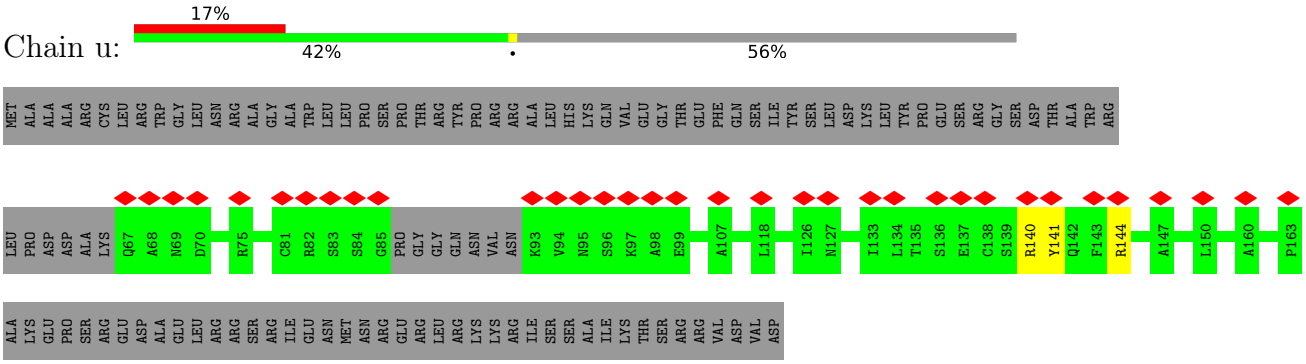




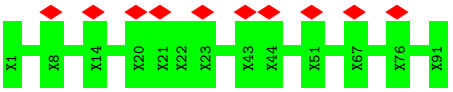
• Molecule 33: MRPL52



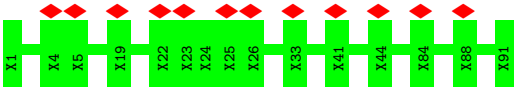
• Molecule 34: ICT1



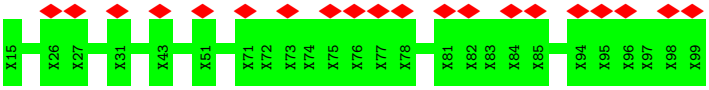
• Molecule 35: UNASSIGNED HELICES



• Molecule 35: UNASSIGNED HELICES



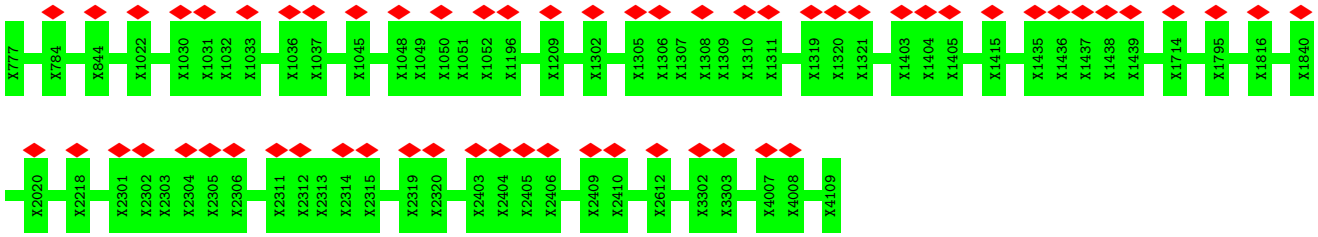
• Molecule 36: THIOREDOXIN FOLD



• Molecule 37: UNASSIGNED HELICES

Chain z:


14%
100%


X777
X784
X844
X1022
X1030
X1031
X1032
X1033
X1036
X1037
X1045
X1048
X1049
X1050
X1051
X1052
X1196
X1209
X1302
X1305
X1306
X1307
X1308
X1309
X1310
X1311
X1319
X1320
X1321
X1403
X1404
X1405
X1415
X1435
X1436
X1437
X1438
X1439
X1714
X1795
X1816
X1840
X2020
X2218
X2301
X2302
X2303
X2304
X2305
X2306
X2311
X2312
X2313
X2314
X2315
X2319
X2320
X2403
X2404
X2405
X2406
X2409
X2410
X2612
X3302
X3303
X4007
X4008
X4109

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	232181	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PER DETECTOR FRAME	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	48.929	Depositor
Minimum map value	-45.891	Depositor
Average map value	-0.047	Depositor
Map value standard deviation	3.830	Depositor
Recommended contour level	11.0	Depositor
Map size (Å)	360.96, 360.96, 360.96	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.41, 1.41, 1.41	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.20	0/624	0.34	0/836
2	1	0.20	0/498	0.41	0/670
3	2	0.19	0/641	0.32	0/862
4	3	0.19	0/501	0.40	0/671
5	5	0.19	0/393	0.37	0/524
6	6	0.21	0/396	0.36	0/526
7	7	0.19	0/370	0.35	0/492
8	8	0.21	0/529	0.33	0/698
9	9	0.20	0/322	0.32	0/424
10	A	0.16	0/34230	0.72	8/53284 (0.0%)
12	D	0.19	0/1557	0.36	0/2093
13	E	0.21	0/1662	0.37	0/2246
14	F	0.20	0/1582	0.38	0/2148
15	I	0.20	0/450	0.37	0/603
16	N	0.21	0/1211	0.40	0/1639
17	O	0.21	0/907	0.40	0/1224
18	P	0.21	0/1254	0.40	0/1686
19	Q	0.21	0/1104	0.36	0/1483
20	R	0.21	0/1000	0.38	0/1342
21	S	0.18	0/763	0.36	0/1033
22	T	0.22	0/978	0.39	0/1318
23	U	0.21	0/986	0.36	0/1319
24	V	0.21	0/866	0.41	0/1168
25	W	0.20	0/931	0.33	0/1241
26	X	0.20	0/585	0.37	0/788
27	Y	0.20	0/853	0.40	0/1155
28	b	0.21	0/1616	0.39	0/2205
29	c	0.29	1/2171 (0.0%)	0.43	1/2937 (0.0%)
30	h	0.23	0/1918	0.38	0/2597
31	i	0.21	0/1366	0.41	0/1844
32	l	0.22	0/632	0.42	0/855
34	u	0.20	0/726	0.38	0/975

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	0.19	1/63622 (0.0%)	0.60	9/92886 (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
29	c	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	141	ARG	C-N	6.05	1.48	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	753	U	C2-N1-C1'	7.69	126.93	117.70
10	A	1549	C	N3-C2-O2	-7.49	116.66	121.90
10	A	753	U	N1-C2-O2	7.31	127.92	122.80
10	A	753	U	N3-C2-O2	-6.98	117.31	122.20
10	A	1549	C	C6-N1-C2	-6.66	117.64	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	c	70	THR	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	72/148 (49%)	69 (96%)	3 (4%)	0	100	100
2	1	56/256 (22%)	51 (91%)	5 (9%)	0	100	100
3	2	74/252 (29%)	73 (99%)	1 (1%)	0	100	100
4	3	57/161 (35%)	56 (98%)	1 (2%)	0	100	100
5	5	47/146 (32%)	44 (94%)	3 (6%)	0	100	100
6	6	46/65 (71%)	43 (94%)	3 (6%)	0	100	100
7	7	41/95 (43%)	41 (100%)	0	0	100	100
8	8	58/188 (31%)	58 (100%)	0	0	100	100
9	9	34/100 (34%)	34 (100%)	0	0	100	100
12	D	198/306 (65%)	188 (95%)	10 (5%)	0	100	100
13	E	206/399 (52%)	194 (94%)	12 (6%)	0	100	100
14	F	196/224 (88%)	188 (96%)	8 (4%)	0	100	100
15	I	55/268 (20%)	47 (86%)	8 (14%)	0	100	100
16	N	145/178 (82%)	132 (91%)	13 (9%)	0	100	100
17	O	112/145 (77%)	109 (97%)	3 (3%)	0	100	100
18	P	155/288 (54%)	144 (93%)	10 (6%)	1 (1%)	25	65
19	Q	136/208 (65%)	131 (96%)	5 (4%)	0	100	100
20	R	118/169 (70%)	107 (91%)	11 (9%)	0	100	100
21	S	92/180 (51%)	87 (95%)	5 (5%)	0	100	100
22	T	117/292 (40%)	113 (97%)	4 (3%)	0	100	100
23	U	114/132 (86%)	110 (96%)	3 (3%)	1 (1%)	17	56
24	V	104/207 (50%)	97 (93%)	7 (7%)	0	100	100
25	W	109/134 (81%)	106 (97%)	3 (3%)	0	100	100
26	X	68/87 (78%)	68 (100%)	0	0	100	100
27	Y	101/216 (47%)	95 (94%)	6 (6%)	0	100	100
28	b	190/380 (50%)	179 (94%)	10 (5%)	1 (0%)	29	68
29	c	259/301 (86%)	246 (95%)	12 (5%)	1 (0%)	34	72
30	h	239/298 (80%)	220 (92%)	18 (8%)	1 (0%)	34	72
31	i	159/312 (51%)	148 (93%)	11 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
32	l	74/166 (45%)	70 (95%)	3 (4%)	1 (1%)	11 46
34	u	86/205 (42%)	77 (90%)	9 (10%)	0	100 100
All	All	3518/6506 (54%)	3325 (94%)	187 (5%)	6 (0%)	50 81

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	l	143	VAL
23	U	14	VAL
28	b	187	VAL
18	P	47	ARG
30	h	223	MET

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	62/115 (54%)	60 (97%)	2 (3%)	39 61
2	1	54/229 (24%)	51 (94%)	3 (6%)	21 48
3	2	72/228 (32%)	72 (100%)	0	100 100
4	3	56/147 (38%)	56 (100%)	0	100 100
5	5	44/108 (41%)	43 (98%)	1 (2%)	50 70
6	6	45/60 (75%)	45 (100%)	0	100 100
7	7	39/78 (50%)	39 (100%)	0	100 100
8	8	54/162 (33%)	52 (96%)	2 (4%)	34 58
9	9	34/77 (44%)	34 (100%)	0	100 100
12	D	158/248 (64%)	158 (100%)	0	100 100
13	E	173/320 (54%)	171 (99%)	2 (1%)	71 84
14	F	166/166 (100%)	161 (97%)	5 (3%)	41 63
15	I	50/228 (22%)	48 (96%)	2 (4%)	31 56
16	N	127/157 (81%)	126 (99%)	1 (1%)	81 89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	O	99/123 (80%)	97 (98%)	2 (2%)	55 73
18	P	129/235 (55%)	125 (97%)	4 (3%)	40 62
19	Q	111/155 (72%)	106 (96%)	5 (4%)	27 53
20	R	101/143 (71%)	96 (95%)	5 (5%)	24 50
21	S	80/153 (52%)	78 (98%)	2 (2%)	47 68
22	T	107/258 (42%)	105 (98%)	2 (2%)	57 75
23	U	100/109 (92%)	98 (98%)	2 (2%)	55 73
24	V	94/173 (54%)	92 (98%)	2 (2%)	53 72
25	W	95/95 (100%)	94 (99%)	1 (1%)	73 85
26	X	62/62 (100%)	61 (98%)	1 (2%)	62 79
27	Y	91/192 (47%)	88 (97%)	3 (3%)	38 61
28	b	165/328 (50%)	158 (96%)	7 (4%)	30 54
29	c	236/244 (97%)	228 (97%)	8 (3%)	37 60
30	h	206/230 (90%)	203 (98%)	3 (2%)	65 80
31	i	148/281 (53%)	143 (97%)	5 (3%)	37 60
32	l	68/147 (46%)	63 (93%)	5 (7%)	13 40
34	u	79/177 (45%)	76 (96%)	3 (4%)	33 57
All	All	3105/5428 (57%)	3027 (98%)	78 (2%)	50 68

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	c	165	ARG
32	l	129	SER
29	c	207	ILE
31	i	116	VAL
34	u	140	ARG

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

Mol	Chain	Res	Type
28	b	147	HIS
34	u	122	HIS
28	b	191	ASN
32	l	92	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	P	26	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	1431/1570 (91%)	368 (25%)	25 (1%)
11	B	0/29	-	-
All	All	1431/1599 (89%)	368 (25%)	25 (1%)

5 of 368 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	2	C
10	A	5	A
10	A	7	G
10	A	8	C
10	A	46	A

5 of 25 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	786	A
10	A	1013	C
10	A	1568	C
10	A	985	G
10	A	1079	U

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 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
37	z	20
35	v	4
35	w	4
10	A	2
11	B	1

The worst 5 of 31 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	z	3019:UNK	C	3301:UNK	N	179.35
1	z	1718:UNK	C	1795:UNK	N	178.65
1	z	1325:UNK	C	1403:UNK	N	151.39
1	z	844:UNK	C	1001:UNK	N	141.39
1	z	2220:UNK	C	2301:UNK	N	132.08

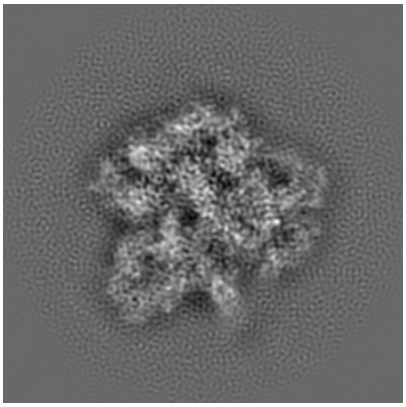
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2490. These allow visual inspection of the internal detail of the map and identification of artifacts.

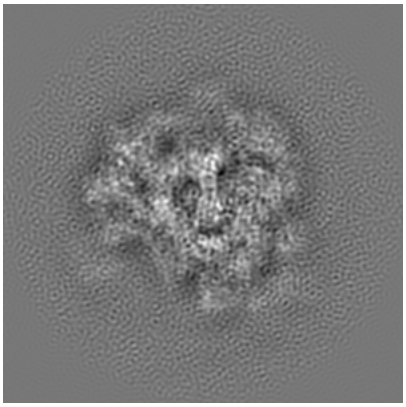
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

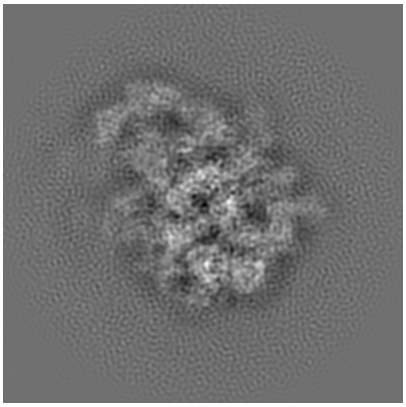
6.1.1 Primary map



X



Y

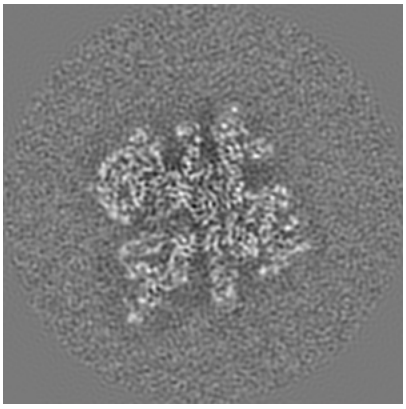


Z

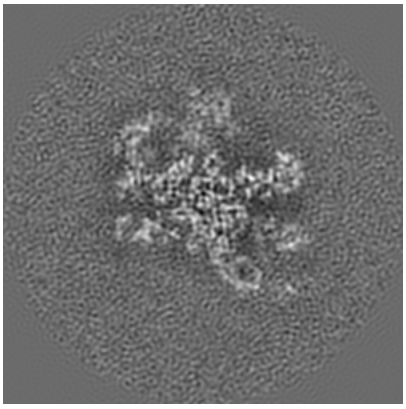
The images above show the map projected in three orthogonal directions.

6.2 Central slices

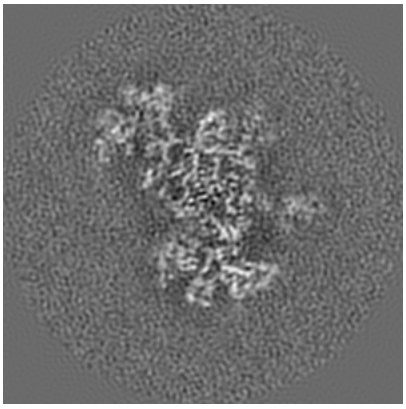
6.2.1 Primary map



X Index: 128



Y Index: 128

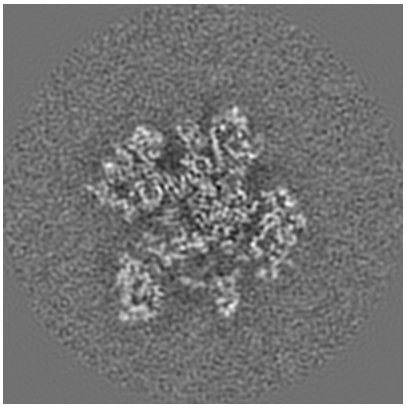


Z Index: 128

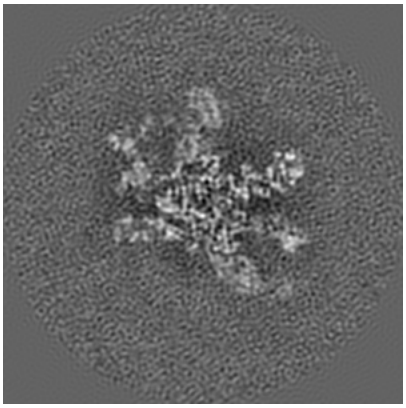
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

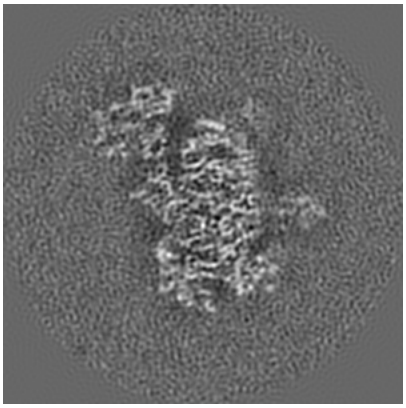
6.3.1 Primary map



X Index: 132



Y Index: 130

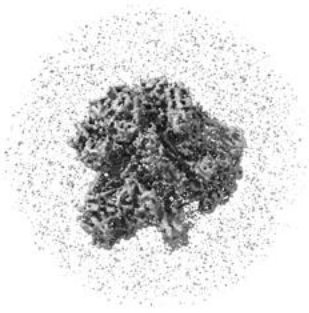


Z Index: 134

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

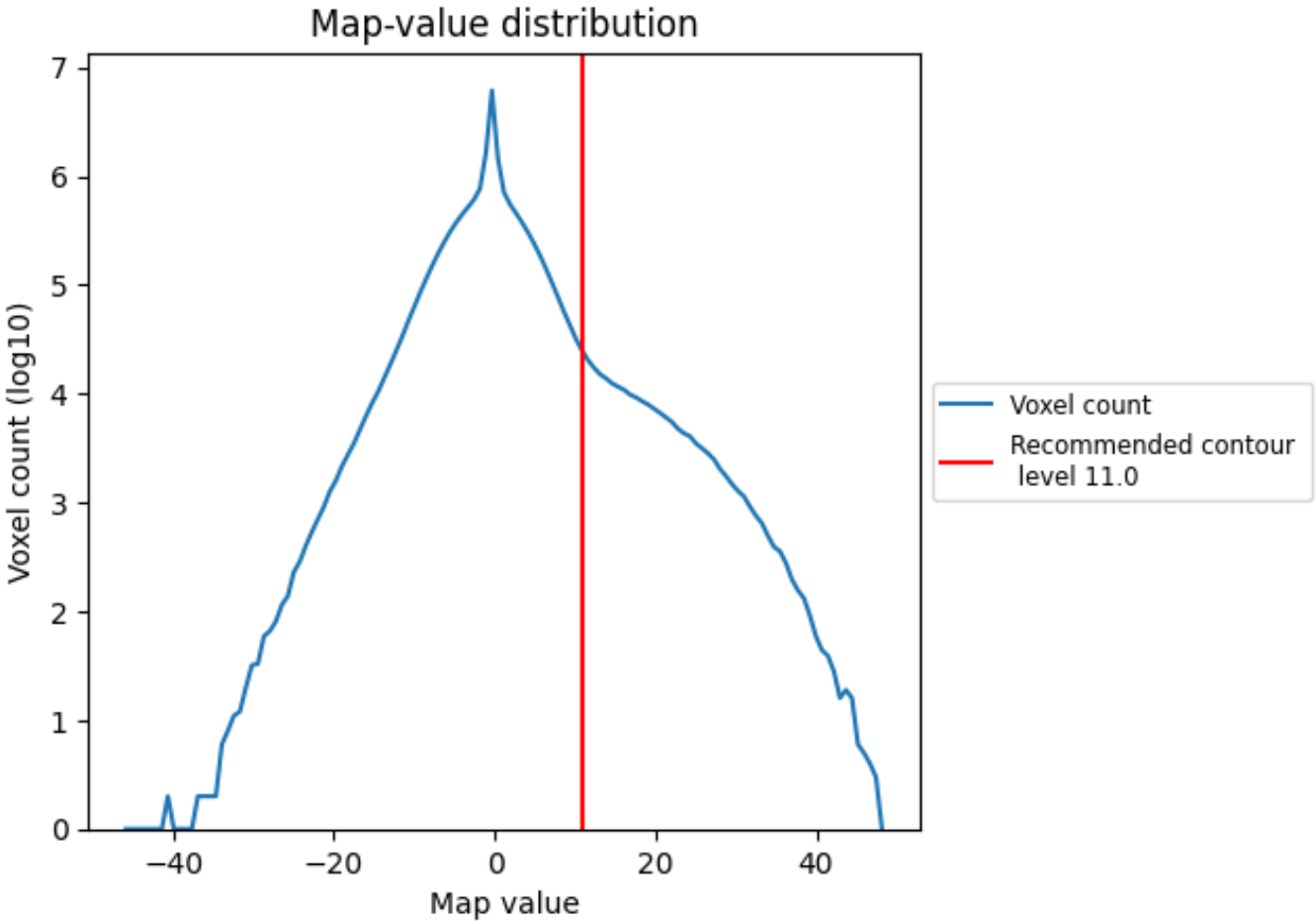
6.5 Mask visualisation (i)

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

7 Map analysis

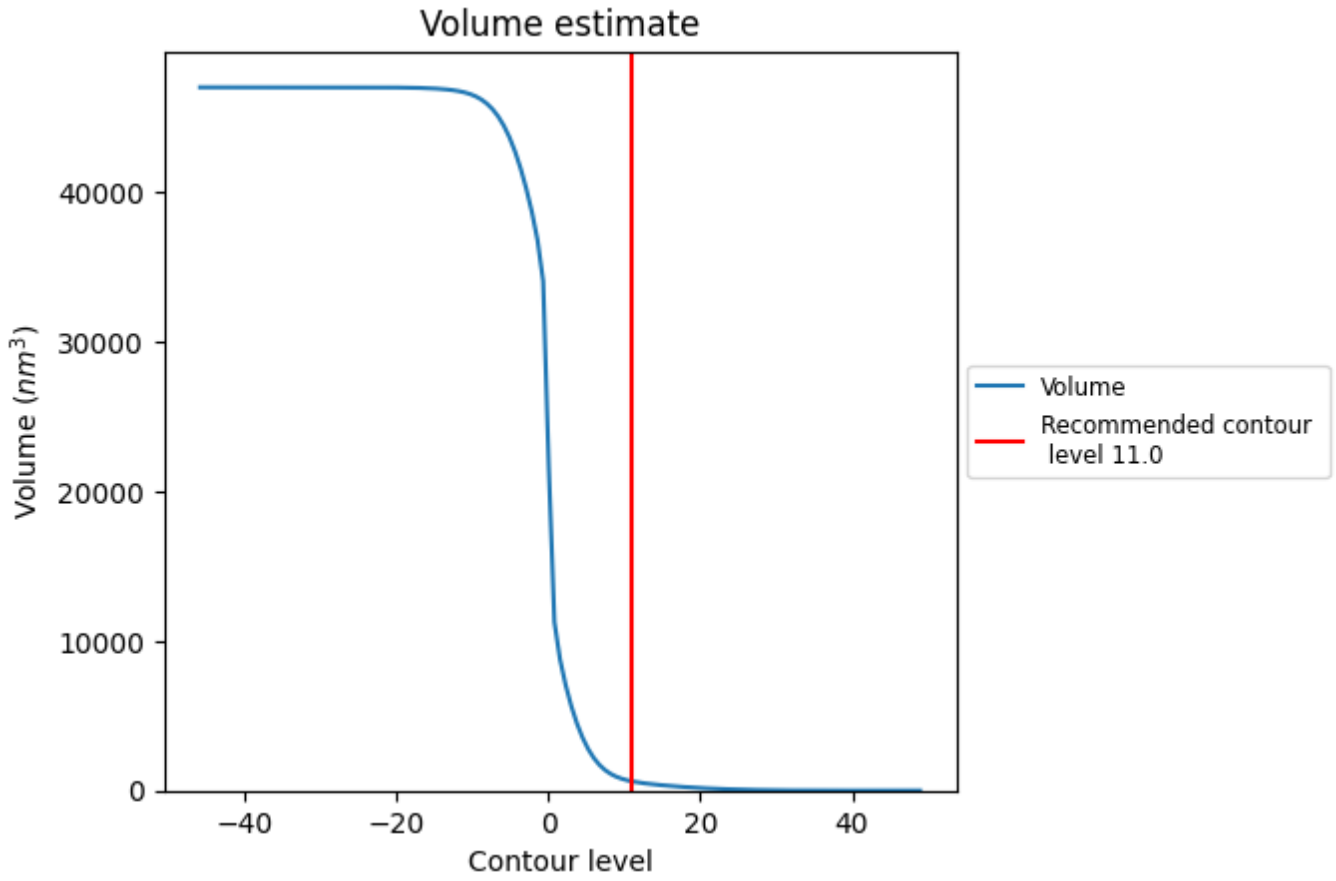
This section contains the results of statistical analysis of the map.

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.

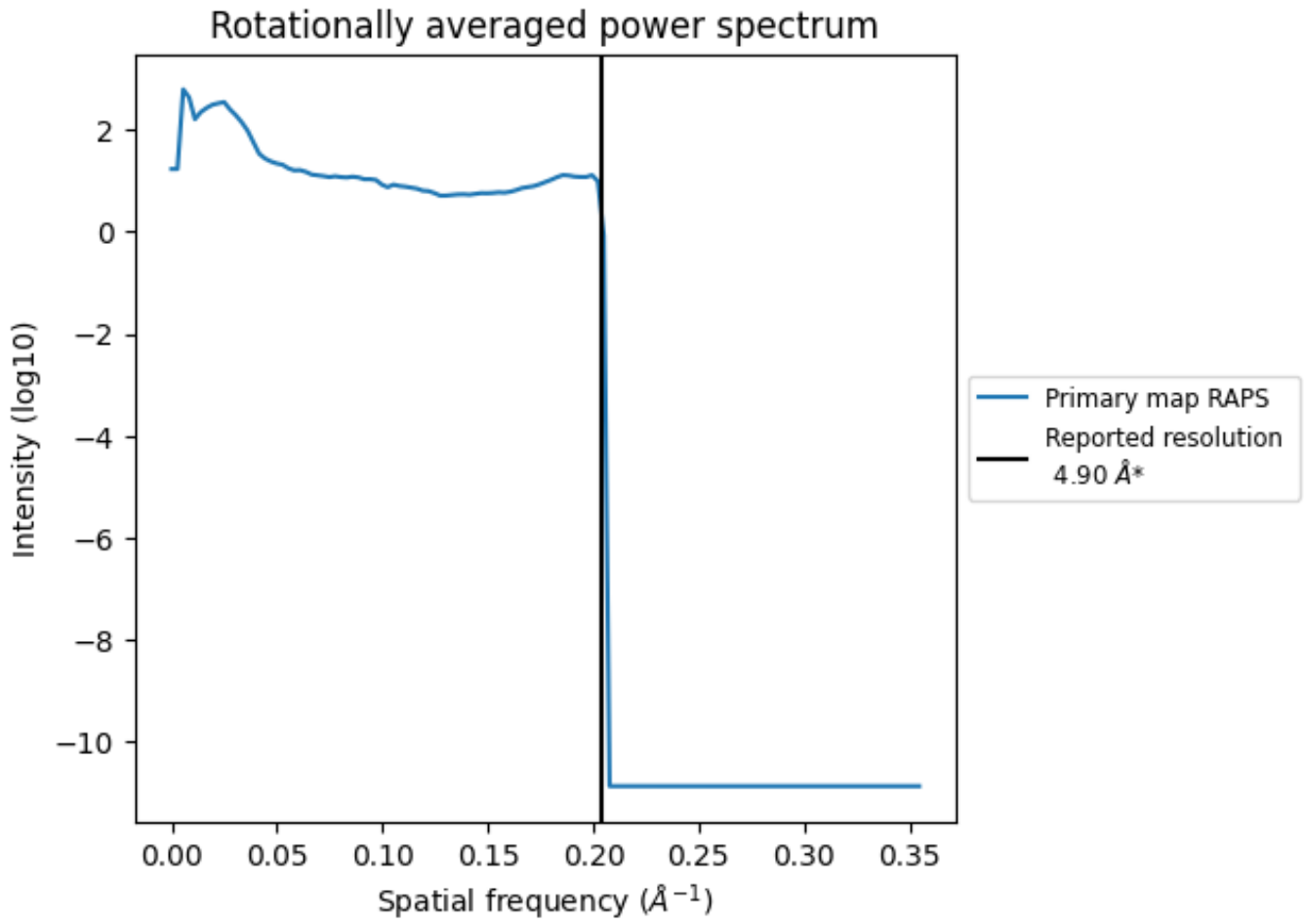
7.2 Volume estimate (i)



The volume at the recommended contour level is 619 nm^3; this corresponds to an approximate mass of 559 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 0.204 Å^{-1}

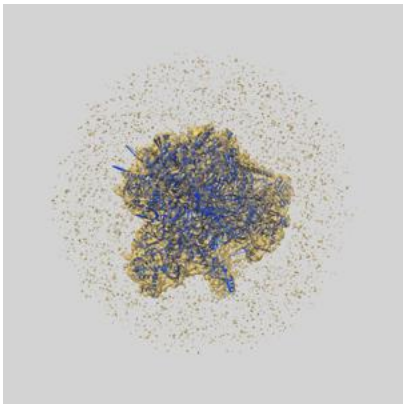
8 Fourier-Shell correlation (i)

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

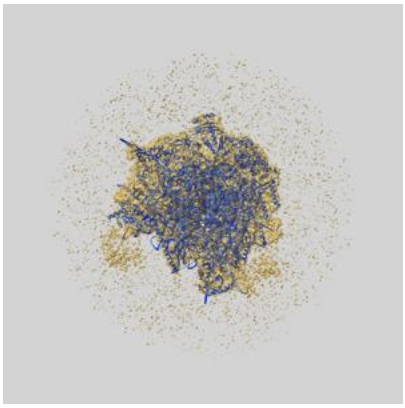
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2490 and PDB model 4CE4. Per-residue inclusion information can be found in section 3 on page 11.

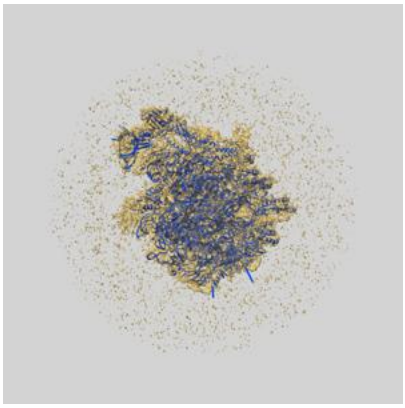
9.1 Map-model overlay



X



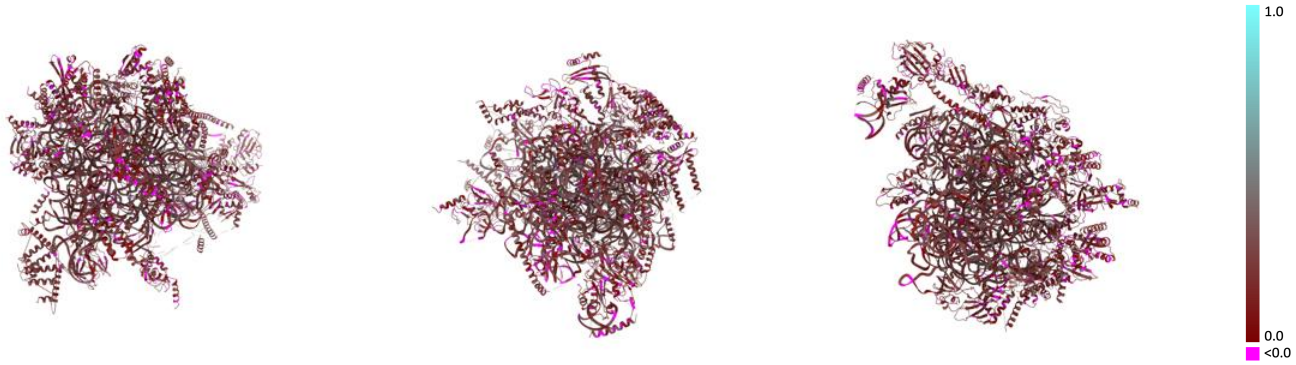
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 11.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

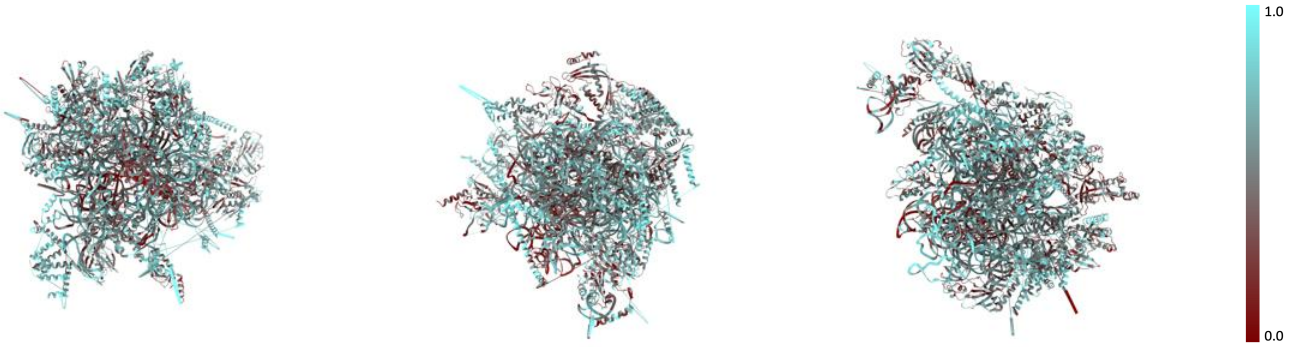
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

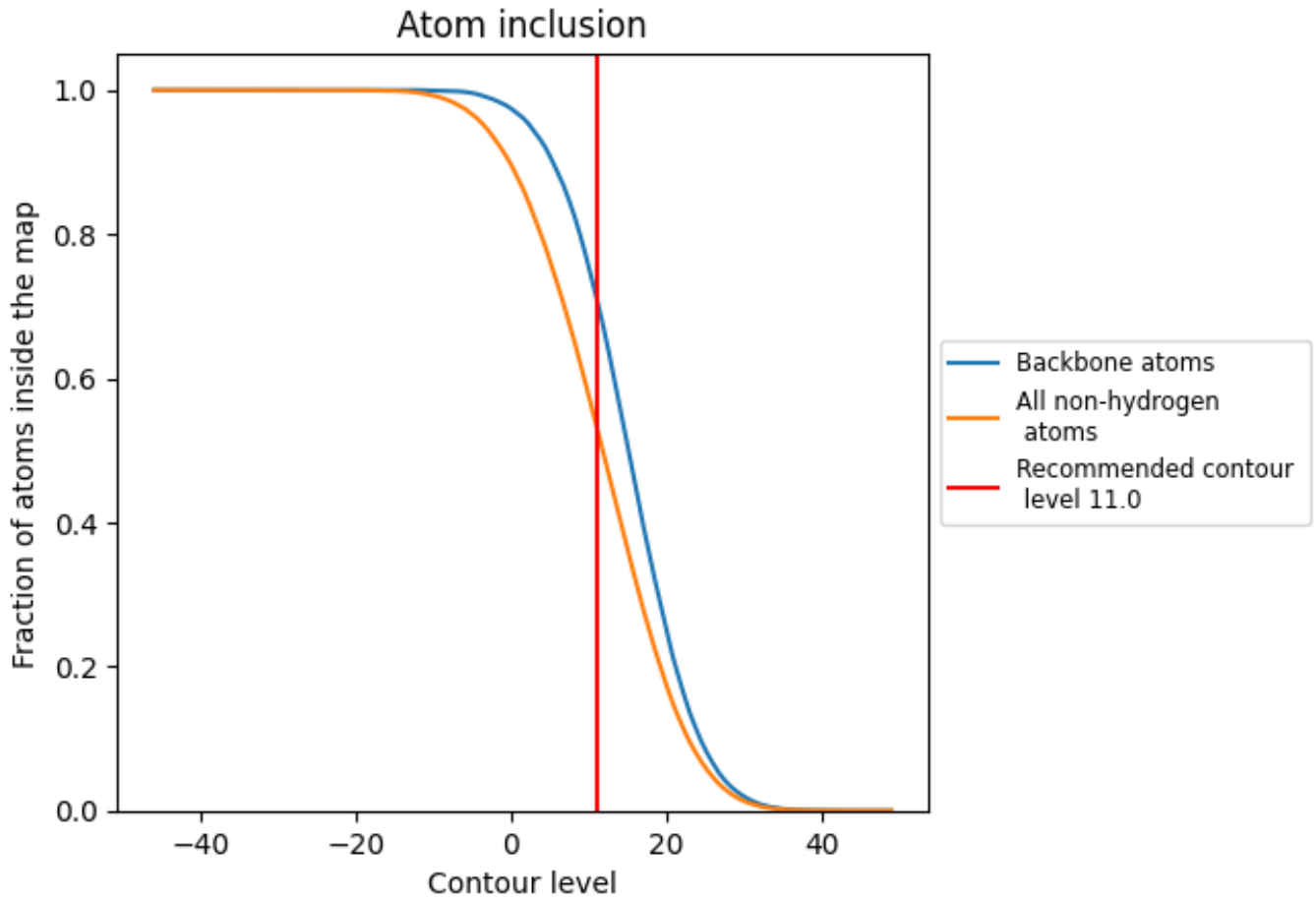
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (11.0).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 53% 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 (11.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5338	0.2120
0	0.4132	0.2170
1	0.4630	0.1570
2	0.5698	0.1350
3	0.4595	0.2120
5	0.5343	0.2220
6	0.1927	0.0790
7	0.4277	0.2160
8	0.3735	0.2070
9	0.3477	0.2100
A	0.5763	0.2430
B	0.5086	0.1790
D	0.4178	0.1520
E	0.4686	0.1920
F	0.4794	0.1970
I	0.2420	0.1430
N	0.4870	0.2170
O	0.4277	0.2010
P	0.4139	0.1780
Q	0.5091	0.2000
R	0.5105	0.1860
S	0.4601	0.1730
T	0.5335	0.1820
U	0.4227	0.2040
V	0.4547	0.2230
W	0.4689	0.2180
X	0.4562	0.2160
Y	0.2769	0.1180
b	0.5409	0.1730
c	0.5256	0.1590
h	0.5850	0.1590
i	0.3652	0.1510
l	0.5354	0.1460
o	0.7619	0.1880
u	0.4641	0.1450

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
v	0.7161	0.2320
w	0.6832	0.2250
x	0.6431	0.2130
z	0.6839	0.2170