wwPDB EM Validation Summary Report

Jul 12, 2023 – 01:07 PM JST

PDB ID	:	8I9R
EMDB ID	:	EMD-35281
Title	:	Cryo-EM structure of a Chaetomium thermophilum pre-60S ribosomal subunit - State 5S RNP
Authors	:	Lau, B.; Huang, Z.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on	:	2023-02-07
Resolution	:	3.10 Å(reported)

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

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

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

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

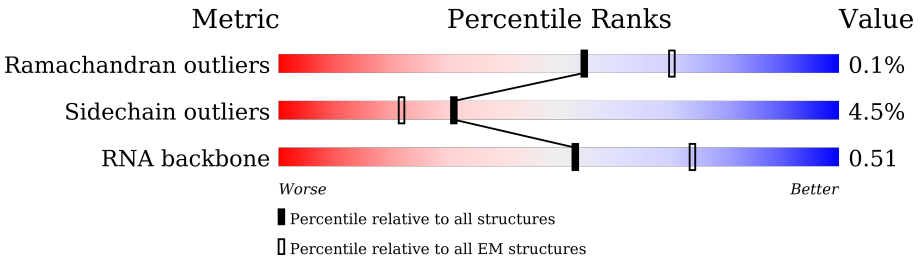
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 3.10 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	C1	3341	8% 45% 15% 39%
2	C2	256	63% 25% 11%
3	CA	316	78% 18%
4	CB	391	62% 5% 34%
5	CC	801	9% 32% 66%
6	CE	598	75% 23%
7	CH	661	9% 15% 84%
8	CI	414	34% 65%

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Mol	Chain	Length	Quality of chain
9	CJ	679	24% 54% 44%
10	CM	249	11% 68% 7% 25%
10	LF	249	94%
11	CN	246	59% 97%
12	CQ	225	11% 48% 50%
13	CR	237	67% 30%
14	CU	451	25% 73%
15	Ch	354	19% 80%
16	LB	392	6% 80% 7% 13%
17	LC	365	97%
18	LE	200	82% 15%
19	LG	262	66% 30%
20	LL	213	54% 45%
21	LM	142	5% 92%
22	LN	203	87% 10%
23	LO	204	98%
24	LP	187	6% 81% 18%
25	LQ	213	60% 39%
26	LS	174	97%
27	LT	160	8% 74% 5% 21%
28	LV	139	53% 93%
29	LY	138	93%
30	Le	131	97%
31	Lf	109	95%
32	Lh	935	13% 87%

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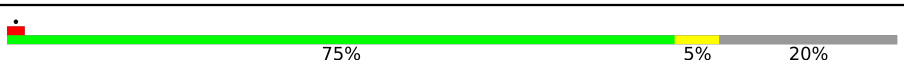
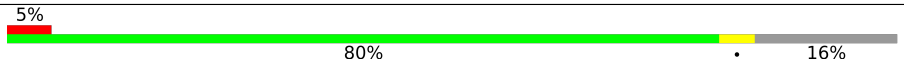
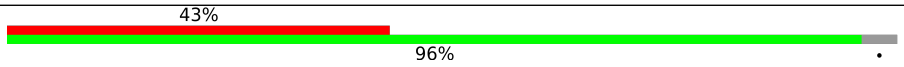
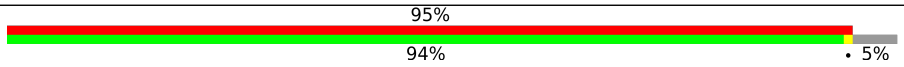
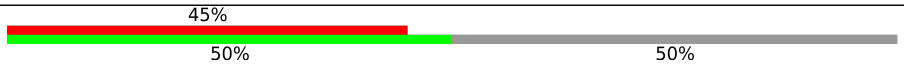
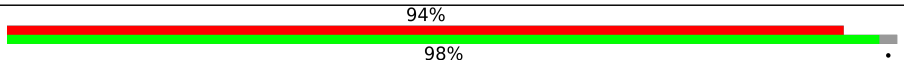
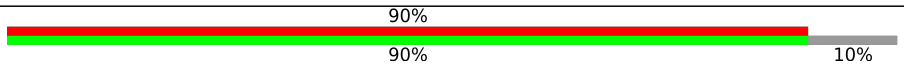
Mol	Chain	Length	Quality of chain
33	Li	110	
34	Lj	95	
35	Cc	282	
36	Cd	436	
37	Ce	336	
38	Cf	570	
39	Cy	350	
40	Cg	478	
41	CP	751	
42	CG	184	
43	Lq	217	
44	Cx	202	
45	LJ	173	
46	LD	304	
47	C4	119	
48	CX	203	

2 Entry composition (i)

There are 49 unique types of molecules in this entry. The entry contains 117417 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called RNA (3341-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	C1	2048	43814	19561	7931	14274	2048	0	0

- Molecule 2 is a RNA chain called RNA (256-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	C2	228	4846	2162	864	1592	228	0	0

- Molecule 3 is a protein called Brix domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	CA	260	2144	1371	393	373	7	0	0

- Molecule 4 is a protein called Ribosome biogenesis protein C8F11.04.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	CB	260	2063	1322	367	371	3	0	0

- Molecule 5 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	CC	272	2258	1438	379	434	7	0	0

- Molecule 6 is a protein called RNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	CE	463	3673	2352	643	667	11	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CE	543	LYS	-	insertion	UNP G0RYU9
CE	544	SER	-	insertion	UNP G0RYU9
CE	545	PHE	-	insertion	UNP G0RYU9
CE	546	GLY	-	insertion	UNP G0RYU9
CE	547	PHE	-	insertion	UNP G0RYU9
CE	548	SER	-	insertion	UNP G0RYU9
CE	549	THR	-	insertion	UNP G0RYU9
CE	550	PRO	-	insertion	UNP G0RYU9
CE	551	PRO	-	insertion	UNP G0RYU9
CE	552	ARG	-	insertion	UNP G0RYU9
CE	553	VAL	-	insertion	UNP G0RYU9
CE	554	ASP	-	insertion	UNP G0RYU9
CE	555	ILE	-	insertion	UNP G0RYU9
CE	556	THR	-	insertion	UNP G0RYU9
CE	557	LEU	-	insertion	UNP G0RYU9
CE	558	SER	-	insertion	UNP G0RYU9
CE	559	ALA	-	insertion	UNP G0RYU9
CE	560	SER	-	insertion	UNP G0RYU9
CE	561	LEU	-	insertion	UNP G0RYU9
CE	562	SER	-	insertion	UNP G0RYU9
CE	563	ARG	-	insertion	UNP G0RYU9
CE	564	ASP	-	insertion	UNP G0RYU9
CE	565	LYS	-	insertion	UNP G0RYU9
CE	566	LYS	-	insertion	UNP G0RYU9
CE	567	PRO	-	insertion	UNP G0RYU9
CE	568	GLN	-	insertion	UNP G0RYU9
CE	569	GLY	-	insertion	UNP G0RYU9
CE	570	ARG	-	insertion	UNP G0RYU9
CE	571	ARG	-	insertion	UNP G0RYU9
CE	572	ALA	-	insertion	UNP G0RYU9
CE	573	TYR	-	insertion	UNP G0RYU9
CE	574	GLY	-	insertion	UNP G0RYU9
CE	575	SER	-	insertion	UNP G0RYU9
CE	576	GLN	-	insertion	UNP G0RYU9
CE	577	PRO	-	insertion	UNP G0RYU9
CE	578	ARG	-	insertion	UNP G0RYU9
CE	579	GLN	-	insertion	UNP G0RYU9
CE	580	GLY	-	insertion	UNP G0RYU9
CE	581	GLY	-	insertion	UNP G0RYU9
CE	582	ARG	-	insertion	UNP G0RYU9
CE	583	TYR	-	insertion	UNP G0RYU9
CE	584	LYS	-	insertion	UNP G0RYU9

- Molecule 7 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CH	108	Total	C	N	O	S	0	0
			891	561	146	183	1		

- Molecule 8 is a protein called Putative RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CI	146	Total	C	N	O	S	0	0
			1196	763	224	204	5		

- Molecule 9 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CJ	380	Total	C	N	O	S	0	0
			3109	2003	547	549	10		

- Molecule 10 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	CM	187	Total	C	N	O	S	0	0
			1525	987	278	257	3		
10	LF	240	Total	C	N	O	S	0	0
			1967	1264	368	332	3		

- Molecule 11 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	CN	246	Total	C	N	O	S	0	0
			1856	1158	322	369	7		

- Molecule 12 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	CQ	112	Total	C	N	O	S	0	0
			960	607	195	148	10		

- Molecule 13 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	CR	167	Total	C	N	O	S	0	0
			1354	827	278	247	2		

- Molecule 14 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	CU	121	Total	C	N	O	S	0	0
			969	604	179	183	3		

- Molecule 15 is a protein called Ribosomal RNA-processing protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ch	71	Total	C	N	O	S	0	0
			562	350	109	102	1		

- Molecule 16 is a protein called 60S ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LB	341	Total	C	N	O	S	0	0
			2708	1721	493	482	12		

- Molecule 17 is a protein called 60S ribosomal protein L4-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LC	362	Total	C	N	O	S	0	0
			2752	1738	526	479	9		

- Molecule 18 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LE	170	Total	C	N	O	S	0	0
			1338	861	241	233	3		

- Molecule 19 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LG	183	Total	C	N	O	S	0	0
			1470	951	263	252	4		

- Molecule 20 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LL	117	Total	C	N	O	S	0	0
			964	608	206	148	2		

- Molecule 21 is a protein called 60S ribosomal protein L14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LM	137	Total	C	N	O	S	0	0
			1101	699	211	190	1		

- Molecule 22 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LN	183	Total	C	N	O	S	0	0
			1563	974	332	253	4		

- Molecule 23 is a protein called 60S ribosomal protein L16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LO	204	Total	C	N	O	S	0	0
			1618	1039	306	267	6		

- Molecule 24 is a protein called 60S ribosomal protein l17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LP	154	Total	C	N	O	S	0	0
			1212	758	233	218	3		

- Molecule 25 is a protein called Ribosomal protein L18-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LQ	129	Total	C	N	O	S	0	0
			1021	646	200	173	2		

- Molecule 26 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LS	174	Total	C	N	O	S	0	0
			1433	922	267	239	5		

- Molecule 27 is a protein called 60S ribosomal protein l21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LT	126	Total	C	N	O	S	0	0
			1014	643	196	173	2		

- Molecule 28 is a protein called 60S ribosomal protein l23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LV	135	Total	C	N	O	S	0	0
			995	633	185	170	7		

- Molecule 29 is a protein called 60S ribosomal protein L26-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LY	134	Total	C	N	O	S	0	0
			1065	664	215	184	2		

- Molecule 30 is a protein called 60S ribosomal protein L32-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Le	131	Total	C	N	O	S	0	0
			1055	663	213	172	7		

- Molecule 31 is a protein called 60S ribosomal protein l33-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Lf	108	Total	C	N	O	S	0	0
			862	546	171	144	1		

- Molecule 32 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Lh	121	Total	C	N	O	0	0
			995	633	196	166		

- Molecule 33 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Li	88	Total	C	N	O	S	0	0
			731	449	162	119	1		

- Molecule 34 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lj	74	Total	C	N	O	S	0	0
			595	365	132	93	5		

- Molecule 35 is a protein called Ribosomal RNA-processing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Cc	236	Total	C	N	O	S	0	0
			1898	1208	337	343	10		

- Molecule 36 is a protein called Brix domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Cd	347	Total	C	N	O	S	0	0
			2800	1764	538	494	4		

- Molecule 37 is a protein called Protein MAK16.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ce	194	Total	C	N	O	S	0	0
			1609	1020	304	276	9		

- Molecule 38 is a protein called 60S ribosome biogenesis protein Rrp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Cf	147	Total	C	N	O	S	0	0
			1225	755	245	224	1		

- Molecule 39 is a protein called Ribosome production factor 2 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	Cy	244	Total	C	N	O	0	0
			1210	722	244	244		

- Molecule 40 is a protein called Brix domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Cg	233	Total	C	N	O	S	0	0
			1850	1168	348	324	10		

- Molecule 41 is a protein called RNA methyltransferase nop2-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	CP	324	Total	C	N	O	0	0
			1596	948	324	324		

- Molecule 42 is a protein called 60S ribosome subunit biogenesis protein NIP7.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	CG	177	Total 873	C 519	N 177	O 177	0	0

- Molecule 43 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	Lq	207	Total 1021	C 607	N 207	O 207	0	0

- Molecule 44 is a protein called Ribosome biogenesis regulatory protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	Cx	102	Total 565	C 340	N 114	O 111	0	0

- Molecule 45 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	LJ	169	Total 831	C 492	N 169	O 170	0	0

- Molecule 46 is a protein called 60S ribosomal protein l5-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	LD	273	Total 1346	C 801	N 273	O 272	0	0

- Molecule 47 is a RNA chain called RNA (119-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
47	C4	119	Total 2536	C 1131	N 453	O 833	P 119	0	0

- Molecule 48 is a protein called 60S ribosomal subunit-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	CX	63	Total 375	C 233	N 68	O 74	0	0

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

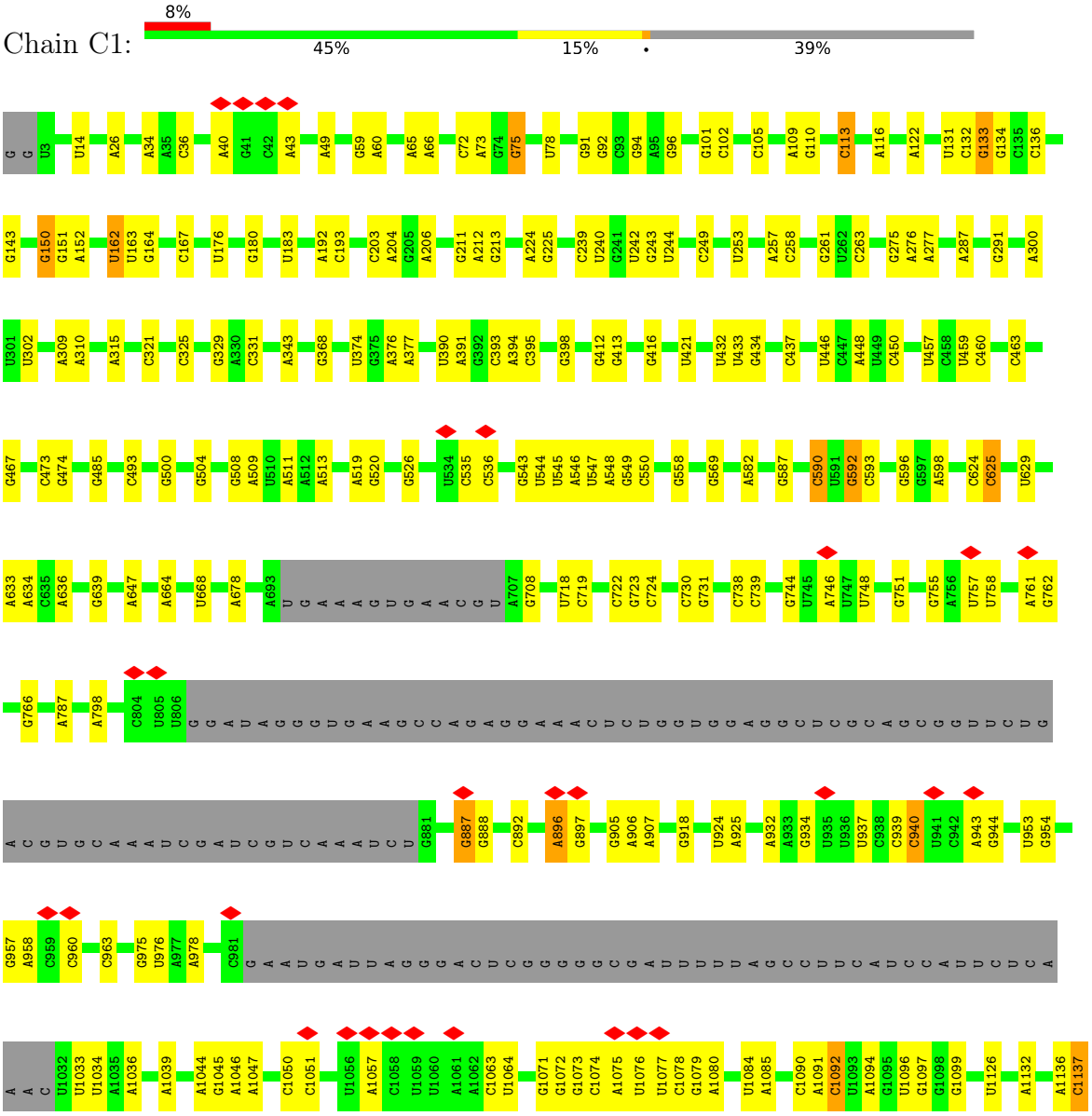
Mol	Chain	Residues	Atoms	AltConf
49	C1	1	Total Zn 1 1	0
49	Lj	1	Total Zn 1 1	0
49	Ce	1	Total Zn 1 1	0

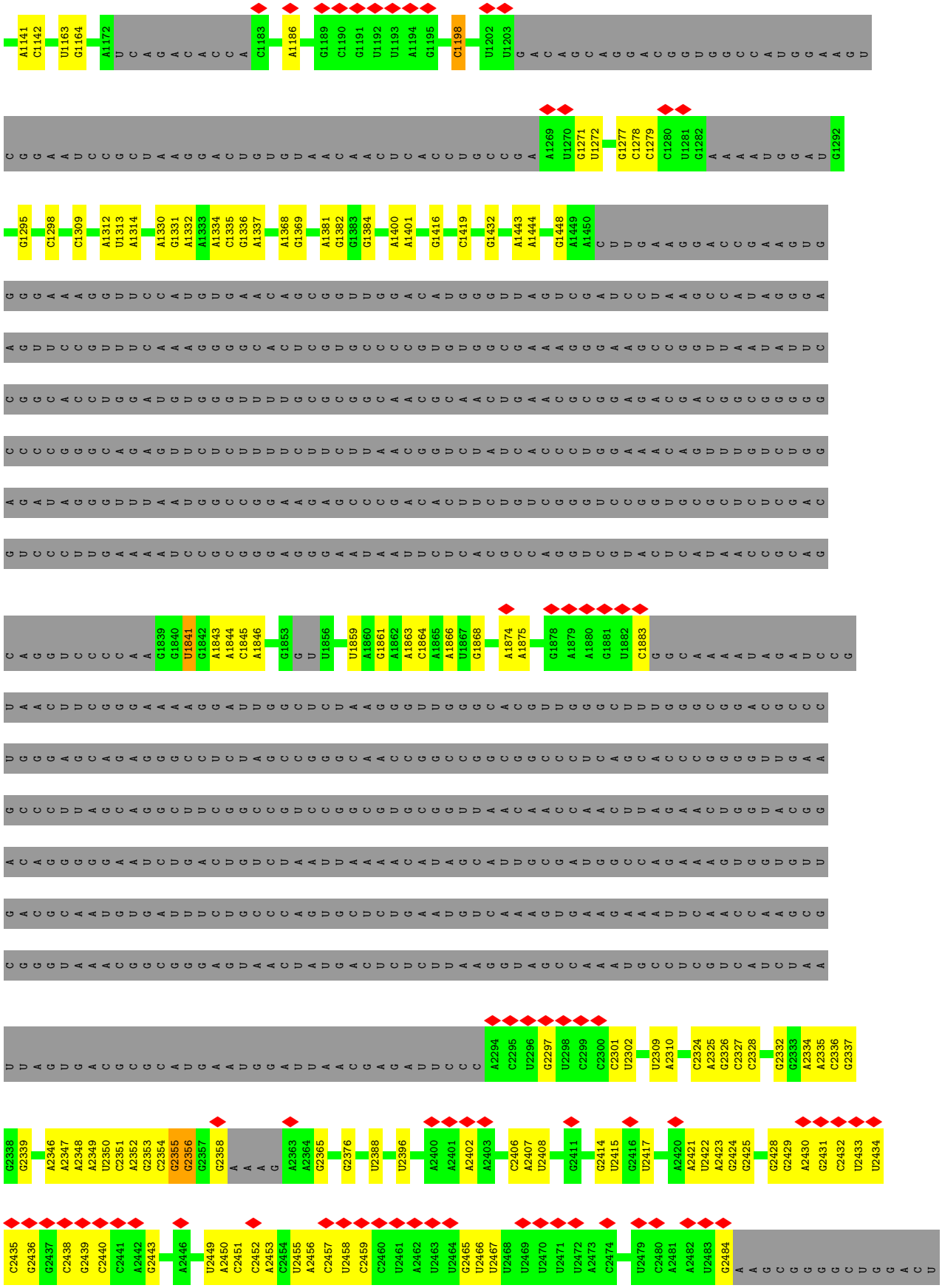
3 Residue-property plots (i)

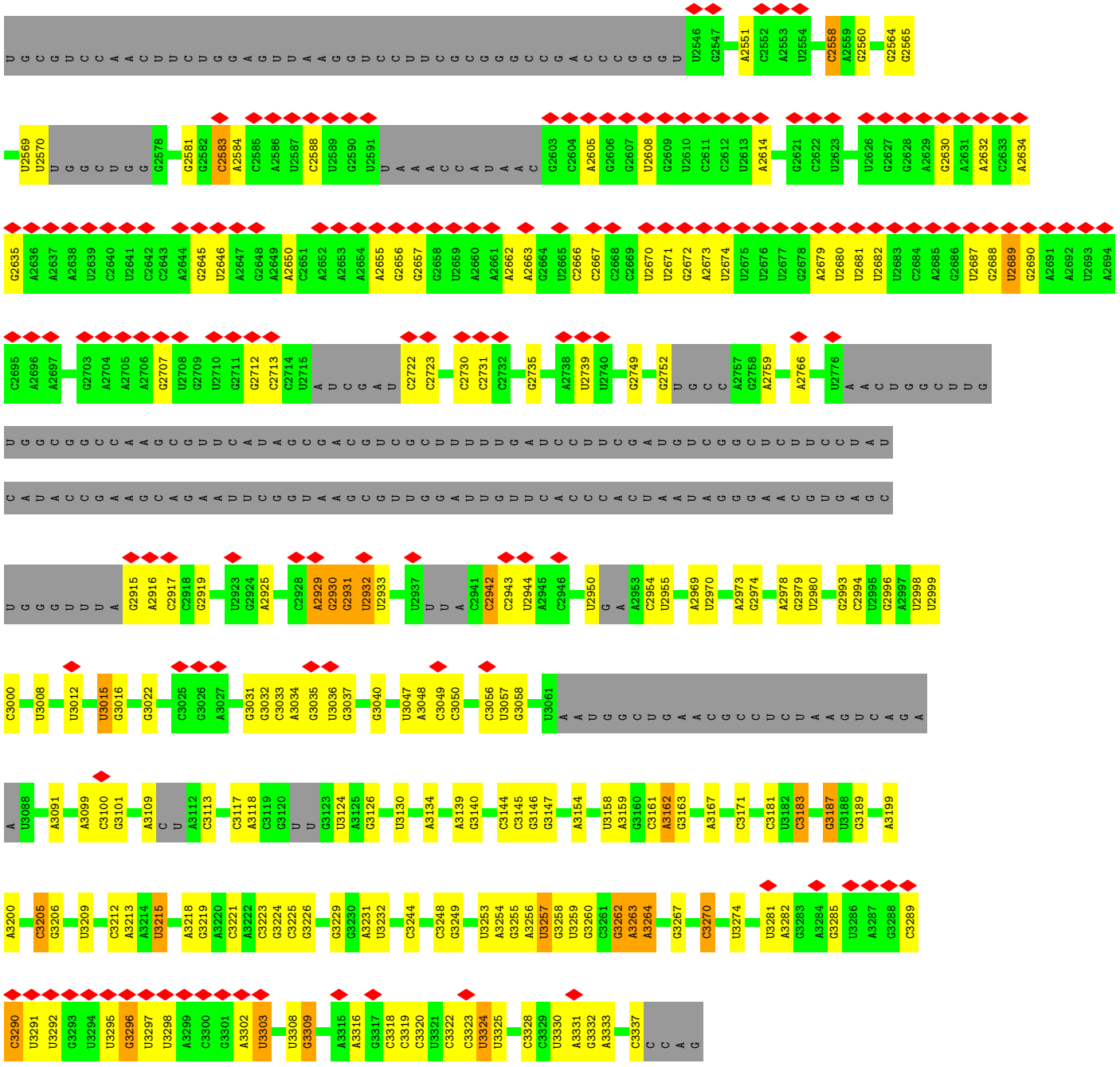
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: RNA (3341-MER)

Chain C1:

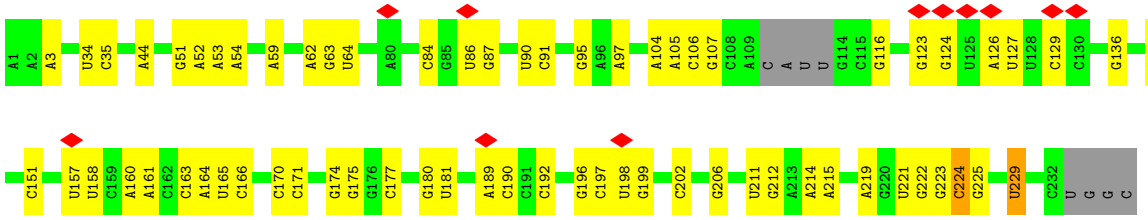






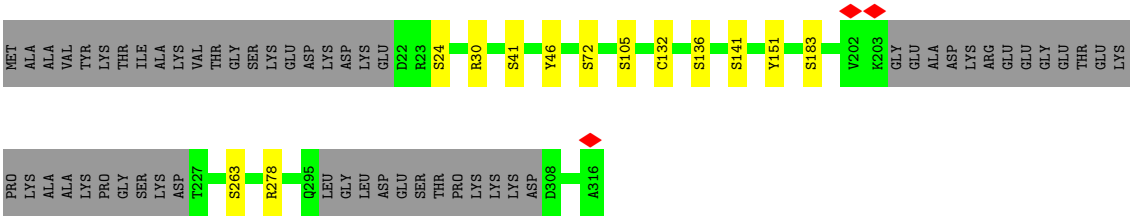
• Molecule 2: RNA (256-MER)

Chain C2:



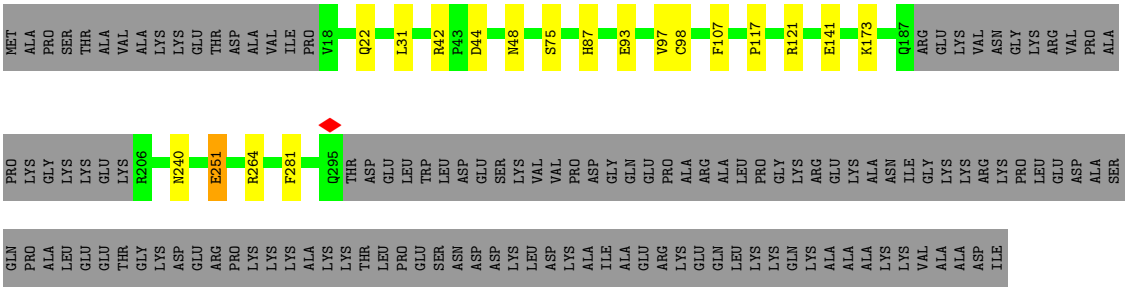
• Molecule 3: Brix domain-containing protein

Chain CA:



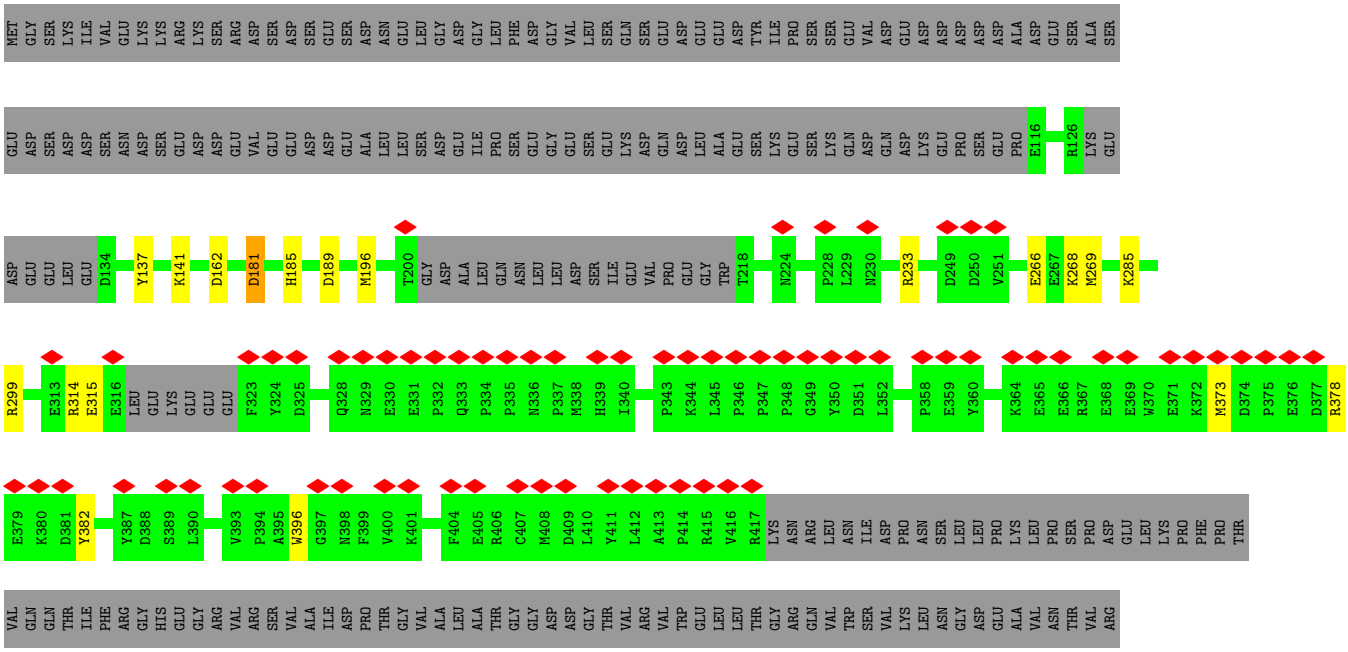
• Molecule 4: Ribosome biogenesis protein C8F11.04

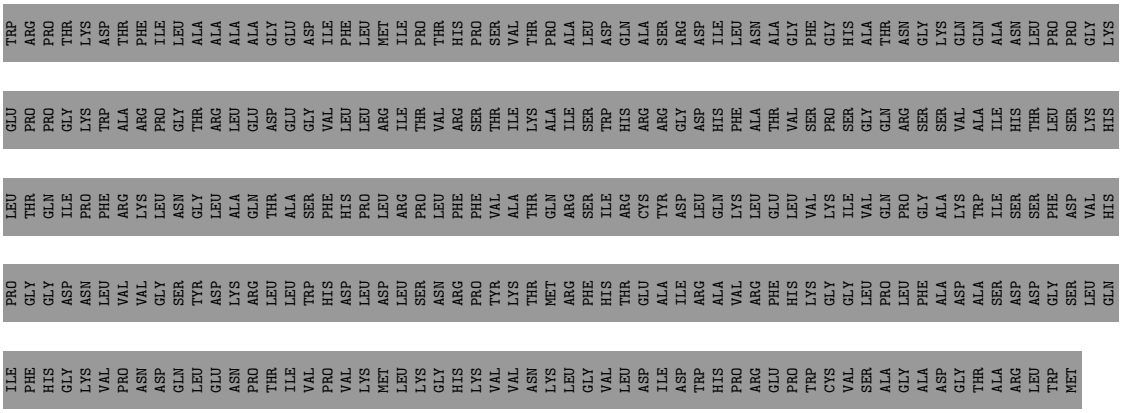
Chain CB:



• Molecule 5: Ribosome biogenesis protein ERB1

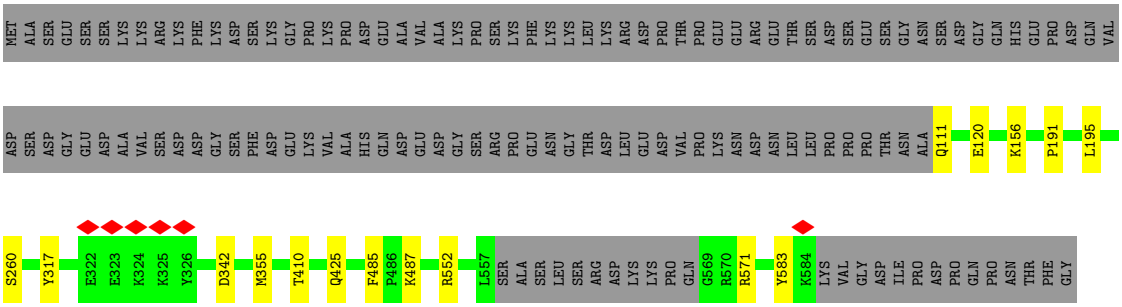
Chain CC:





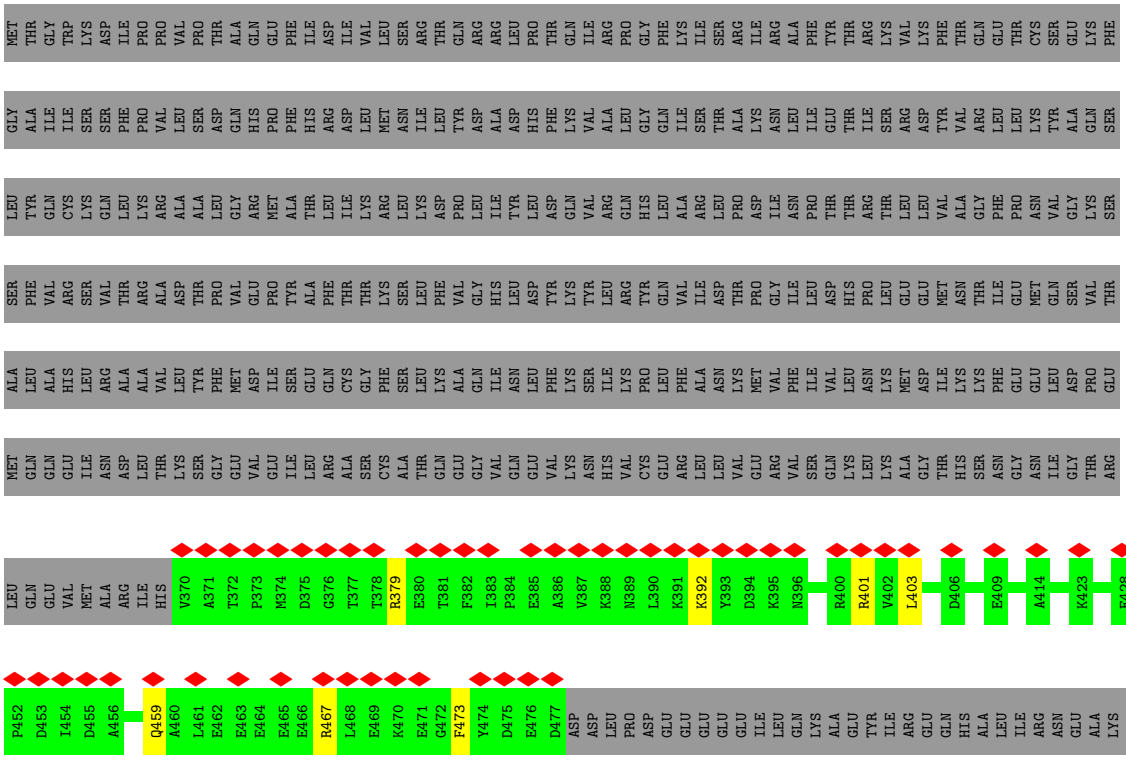
• Molecule 6: RNA helicase

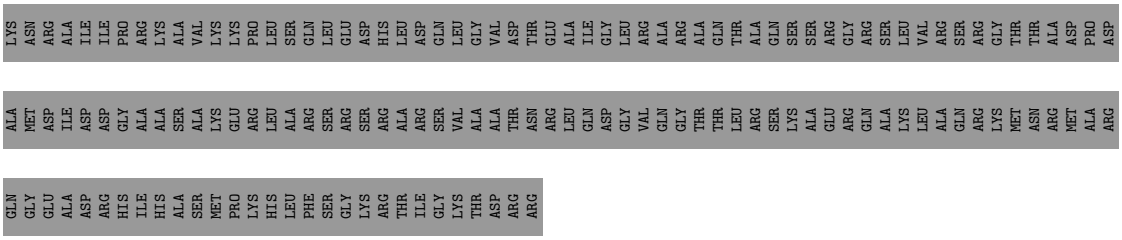
Chain CE:



• Molecule 7: Nucleolar GTP-binding protein 1

Chain CH:



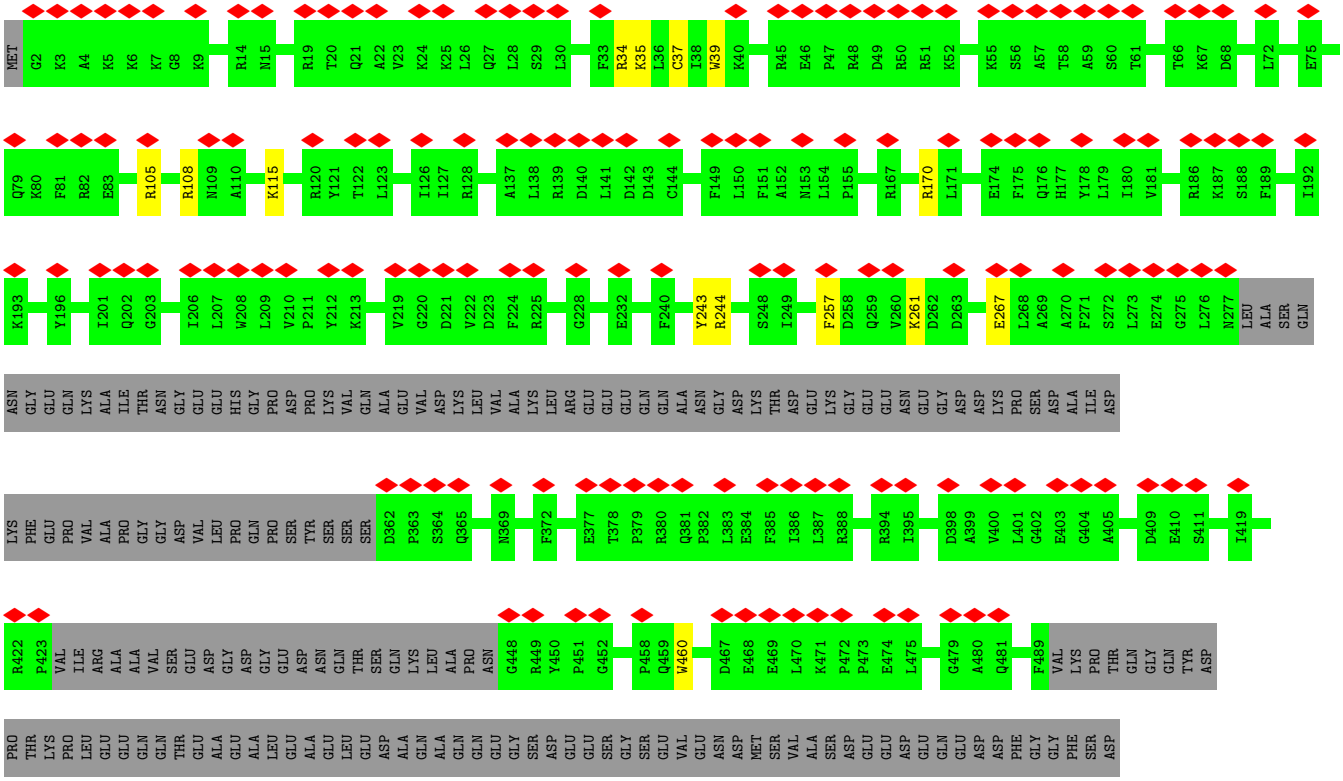


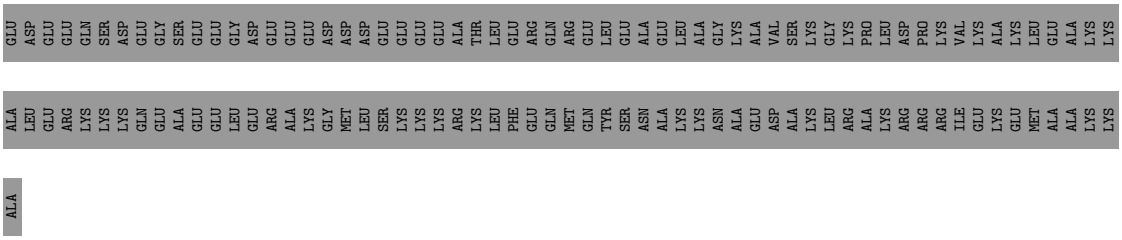
• Molecule 8: Putative RNA-binding protein

Chain CI:

• Molecule 9: Pescadillo homolog

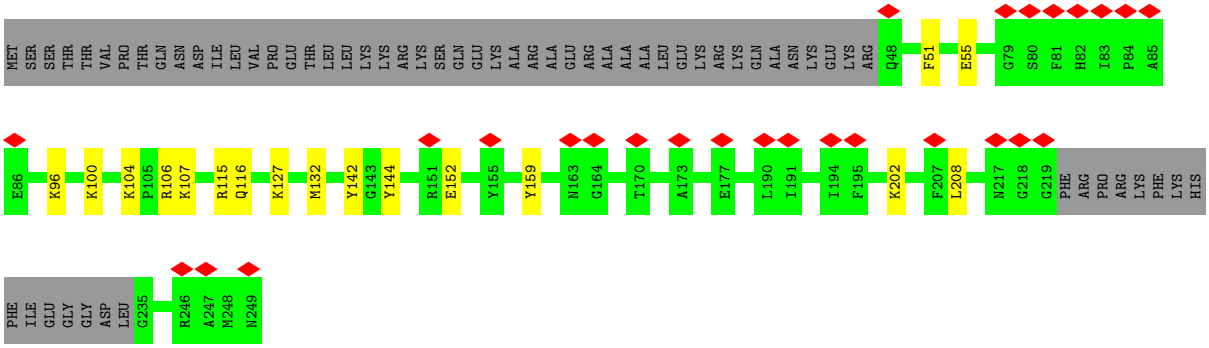
Chain CJ:





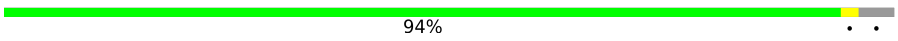
• Molecule 10: 60S ribosomal protein l7-like protein

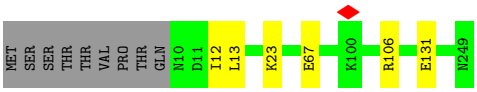
Chain CM:



• Molecule 10: 60S ribosomal protein l7-like protein

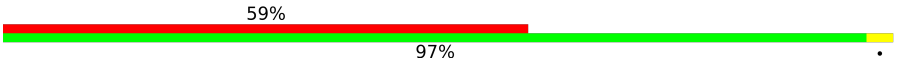
Chain LF:

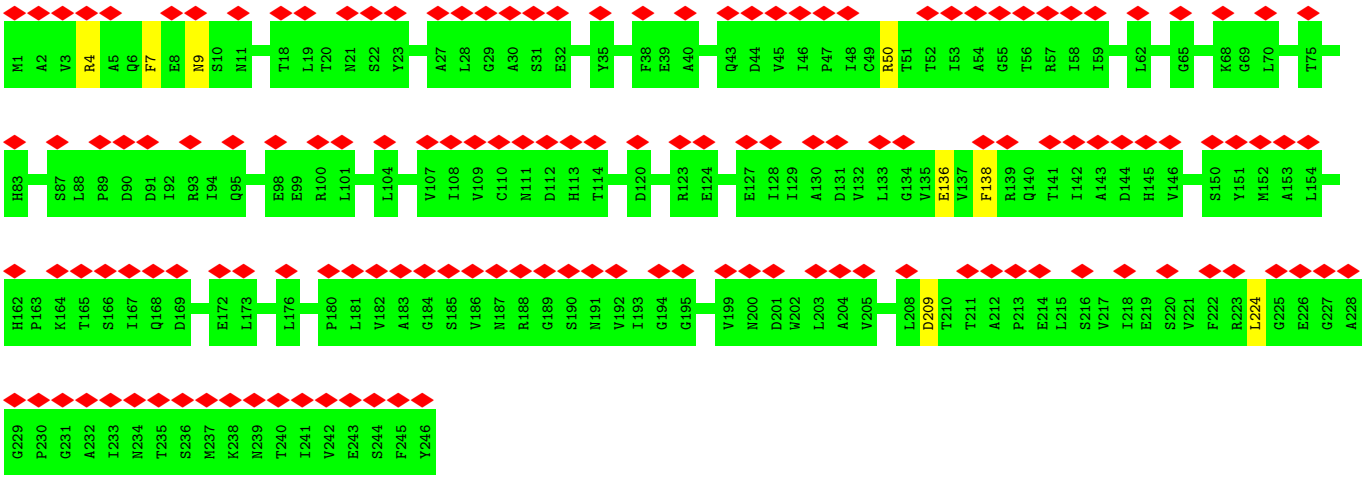




• Molecule 11: Eukaryotic translation initiation factor 6

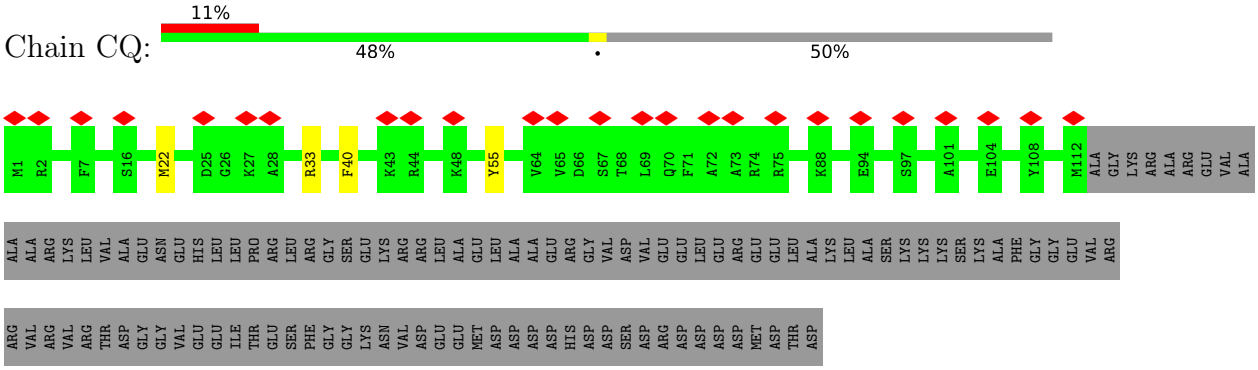
Chain CN:





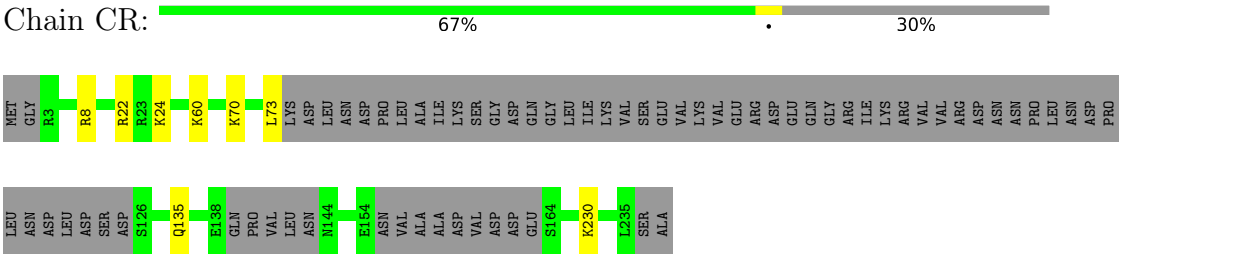
• Molecule 12: Ribosome biogenesis protein RLP24

Chain CQ:



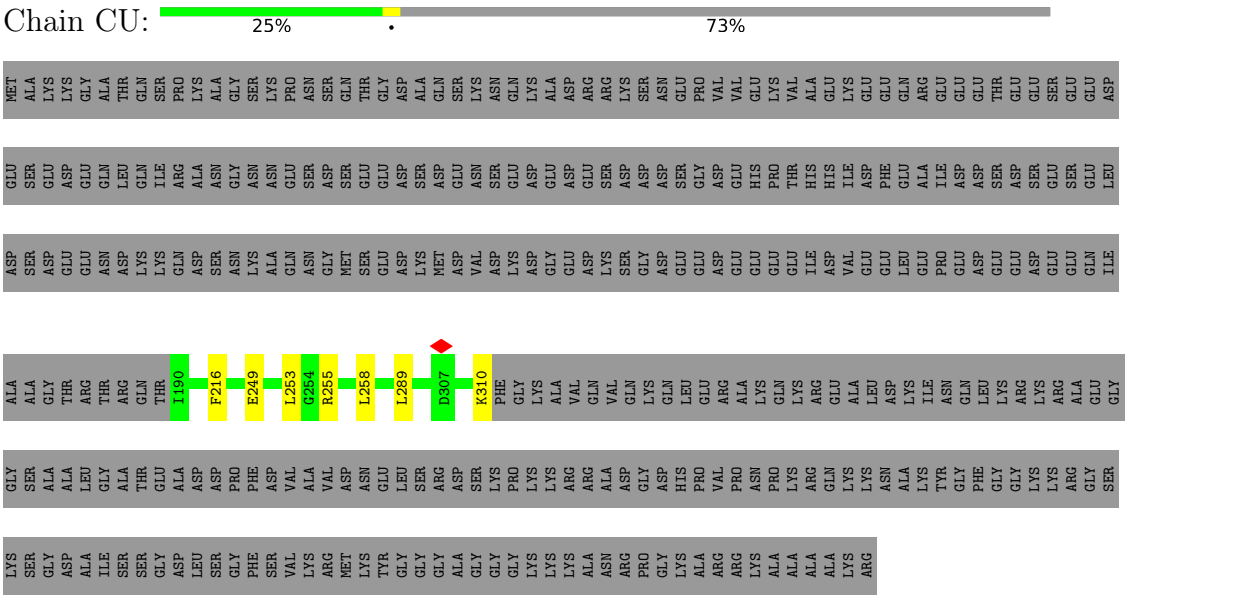
• Molecule 13: Nucleolar protein 16

Chain CR:



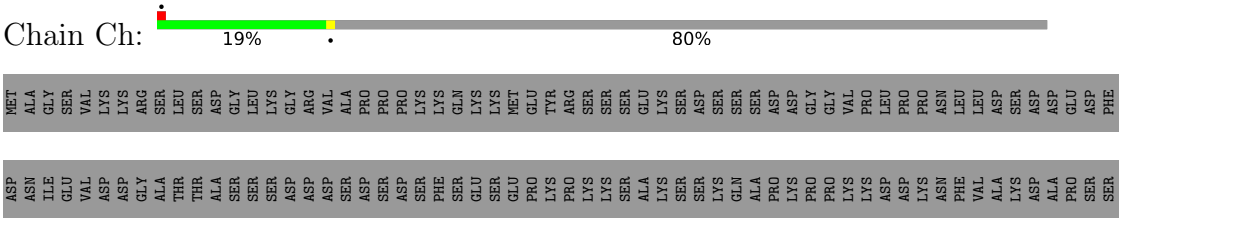
• Molecule 14: rRNA-processing protein EBP2

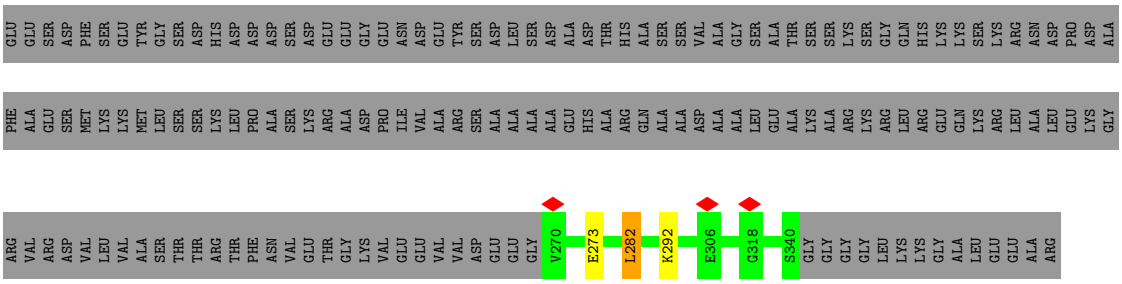
Chain CU:



• Molecule 15: Ribosomal RNA-processing protein 15

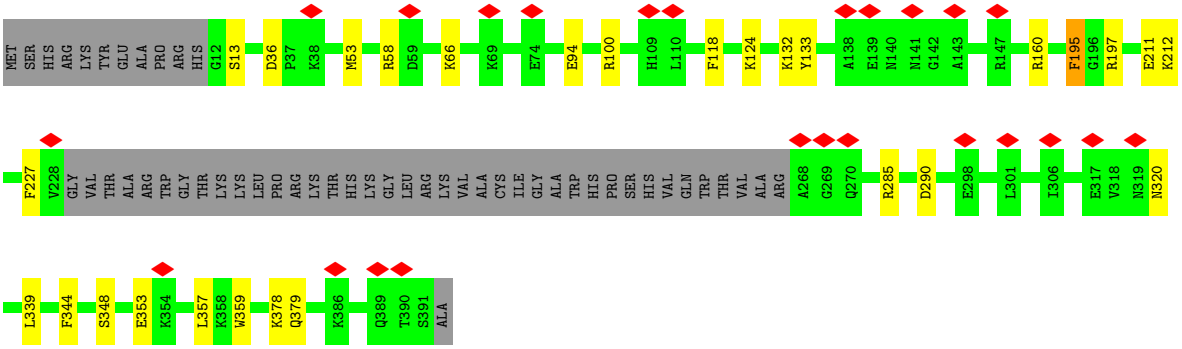
Chain Ch:





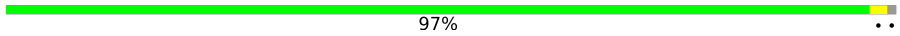
• Molecule 16: 60S ribosomal protein L3-like protein

Chain LB:



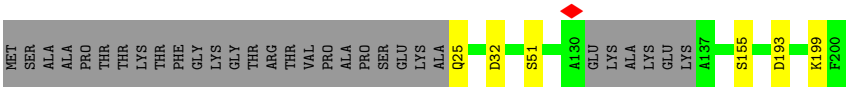
• Molecule 17: 60S ribosomal protein L4-like protein

Chain LC:



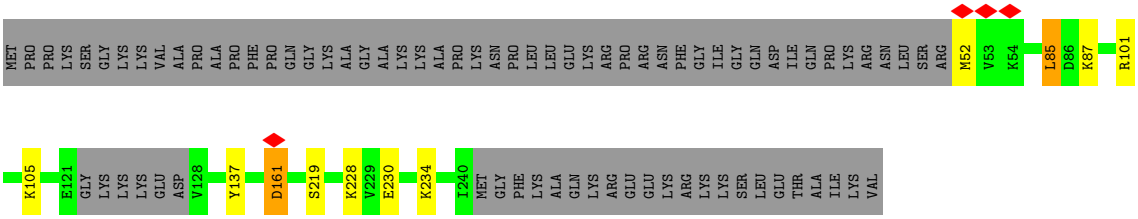
• Molecule 18: 60S ribosomal protein L6

Chain LE:



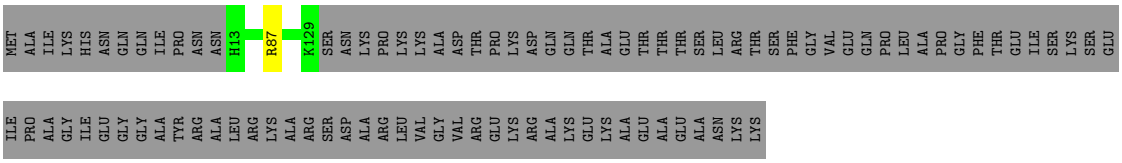
• Molecule 19: 60S ribosomal protein L8

Chain LG:



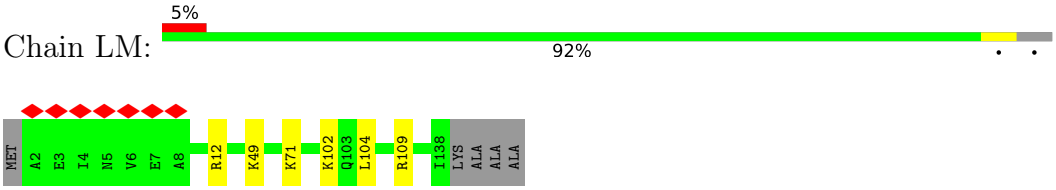
• Molecule 20: 60S ribosomal protein L13

Chain LL:



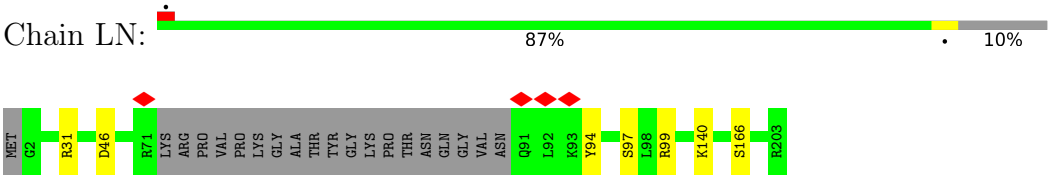
• Molecule 21: 60S ribosomal protein L14-like protein

Chain LM:



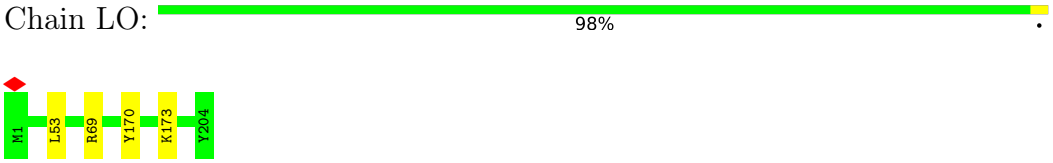
• Molecule 22: Ribosomal protein L15

Chain LN:



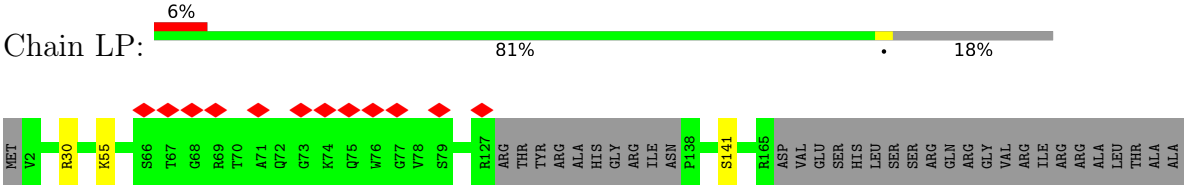
• Molecule 23: 60S ribosomal protein L16-like protein

Chain LO:



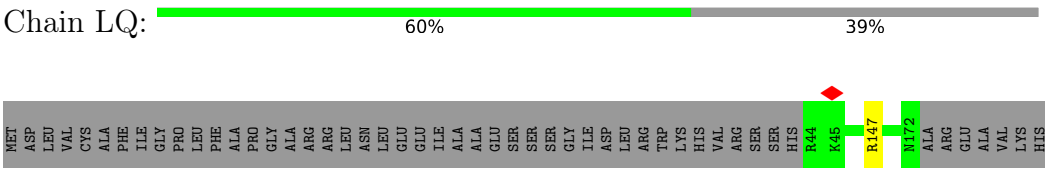
• Molecule 24: 60S ribosomal protein l17-like protein

Chain LP:



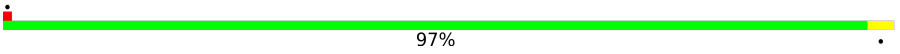
• Molecule 25: Ribosomal protein L18-like protein

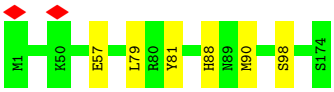
Chain LQ:



• Molecule 26: 60S ribosomal protein L20

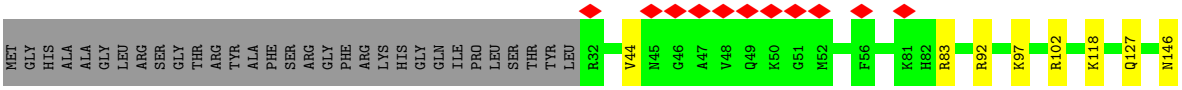
Chain LS:

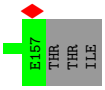




• Molecule 27: 60S ribosomal protein l21-like protein

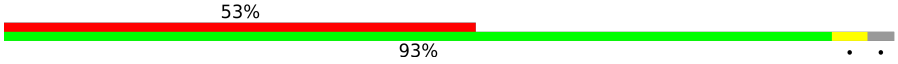
Chain LT:

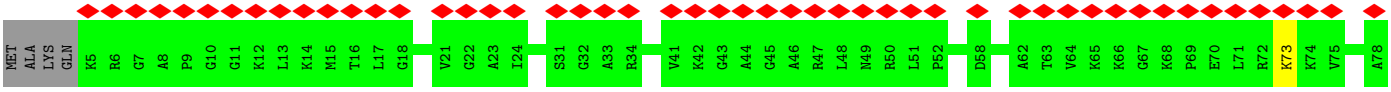


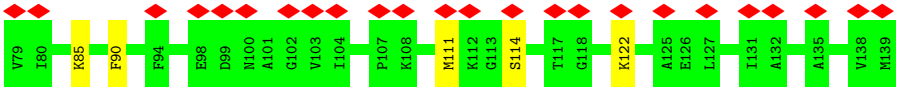


• Molecule 28: 60S ribosomal protein l23-like protein

Chain LV:

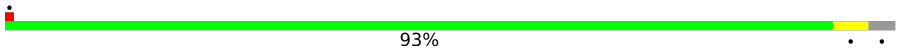


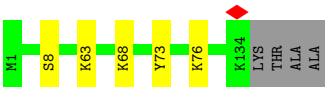




• Molecule 29: 60S ribosomal protein L26-like protein

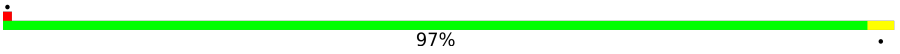
Chain LY:





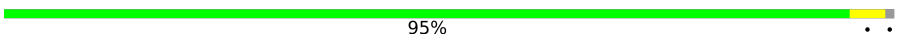
• Molecule 30: 60S ribosomal protein L32-like protein

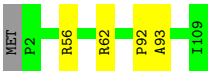
Chain Le:



• Molecule 31: 60S ribosomal protein l33-like protein

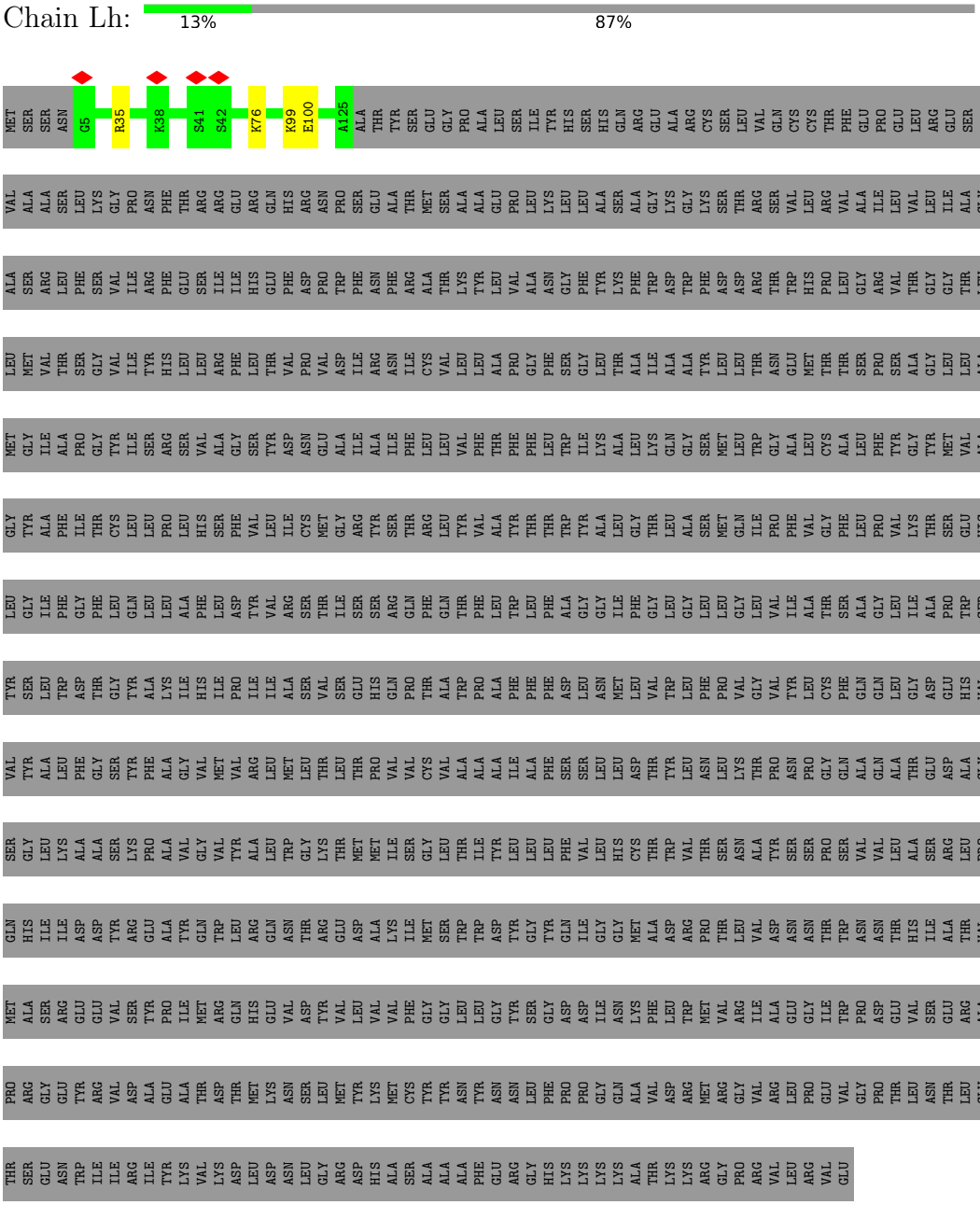
Chain Lf:





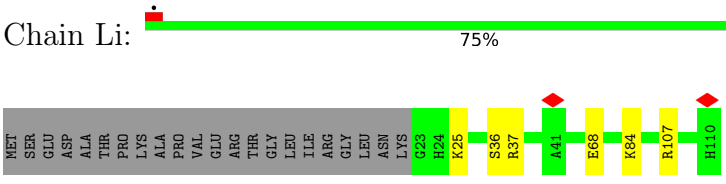
• Molecule 32: dolichyl-diphosphooligosaccharide--protein glycotransferase

Chain Lh:



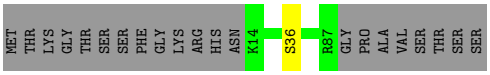
• Molecule 33: 60S ribosomal protein L36

Chain Li:



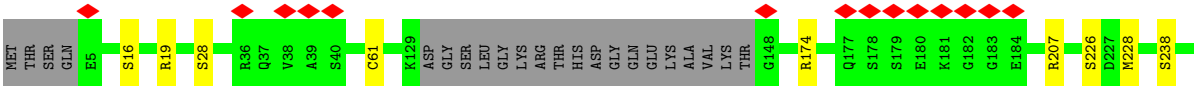
• Molecule 34: Ribosomal protein L37

Chain Lj:



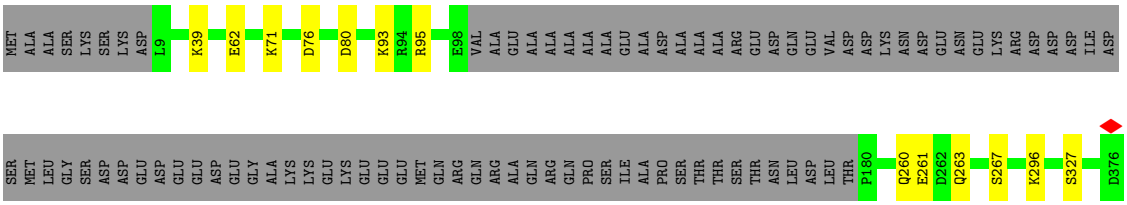
• Molecule 35: Ribosomal RNA-processing protein 1

Chain Cc:



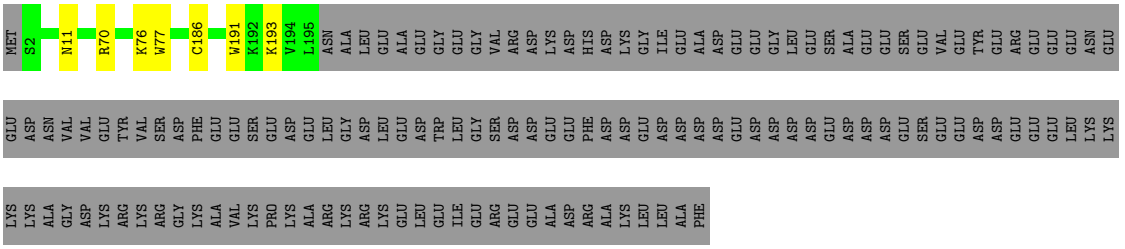
• Molecule 36: Brix domain-containing protein

Chain Cd:



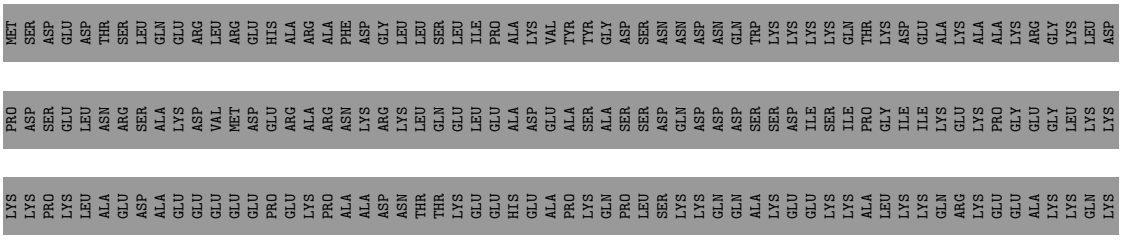
• Molecule 37: Protein MAK16

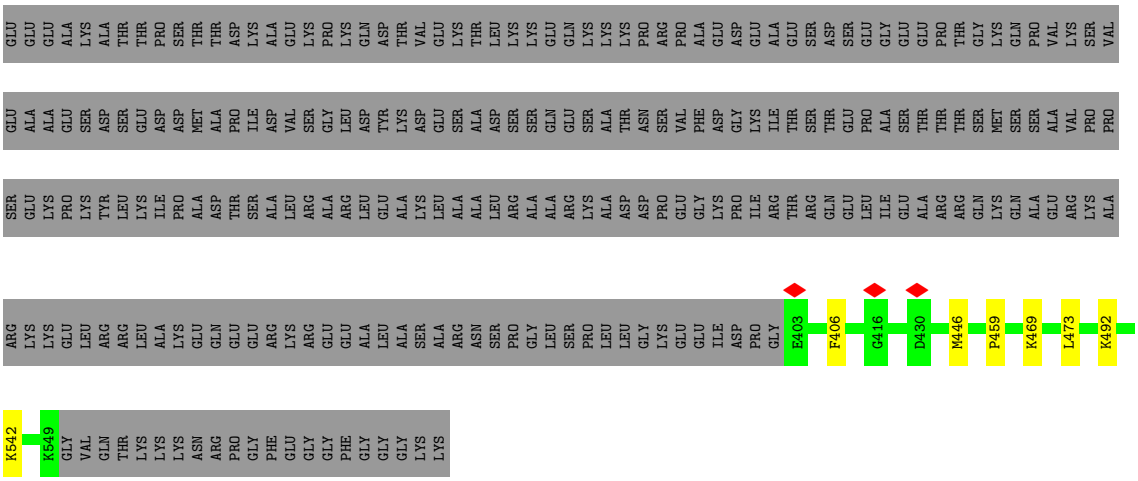
Chain Ce:



• Molecule 38: 60S ribosome biogenesis protein Rrp14

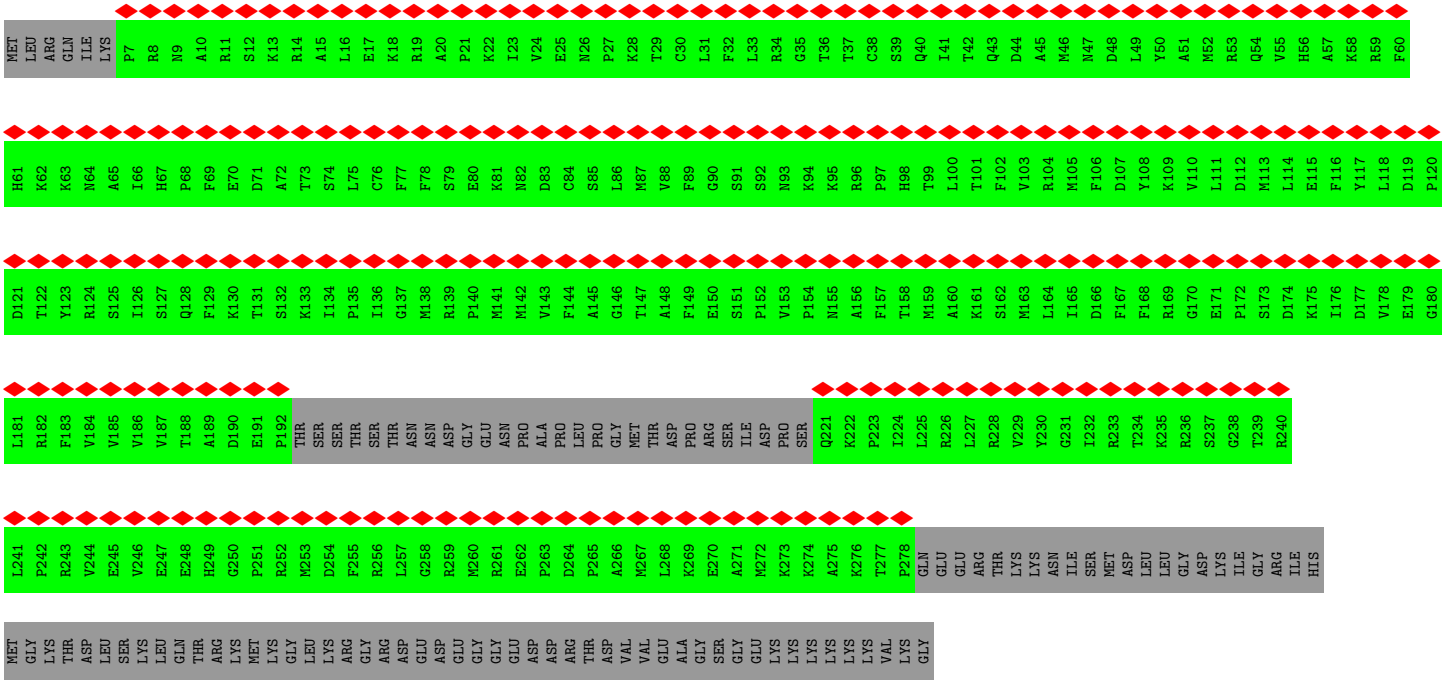
Chain Cf:





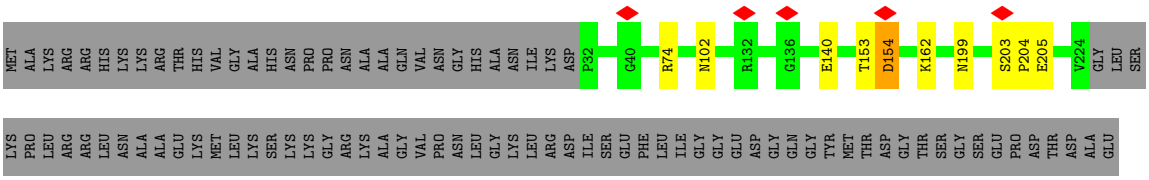
• Molecule 39: Ribosome production factor 2 homolog

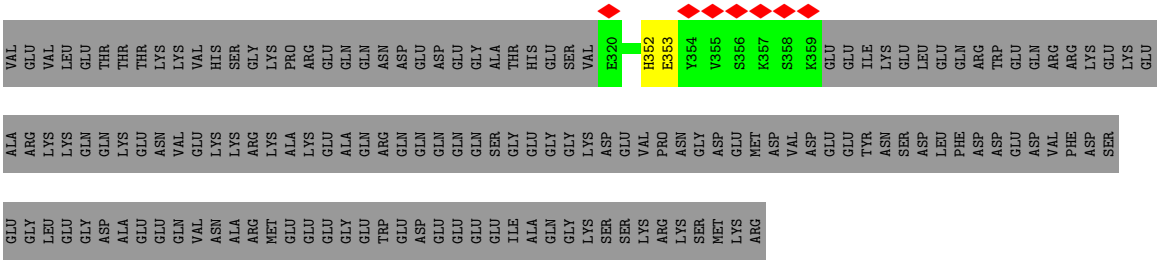
Chain Cy:



• Molecule 40: Brix domain-containing protein

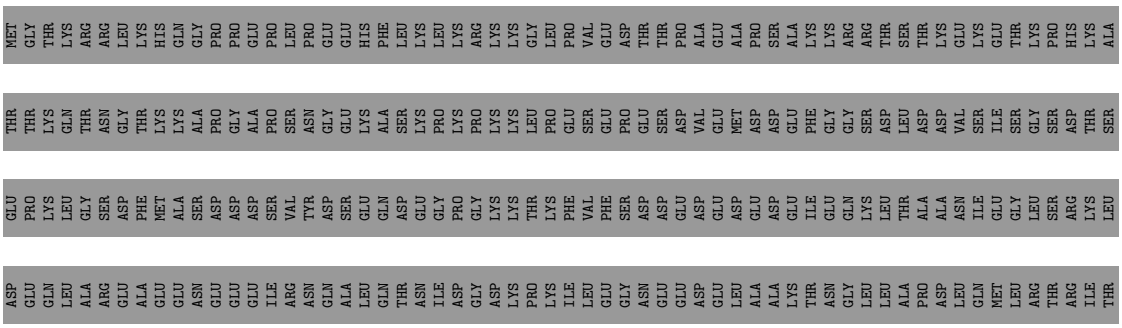
Chain Cg:

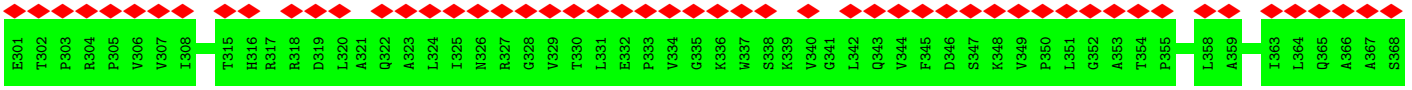


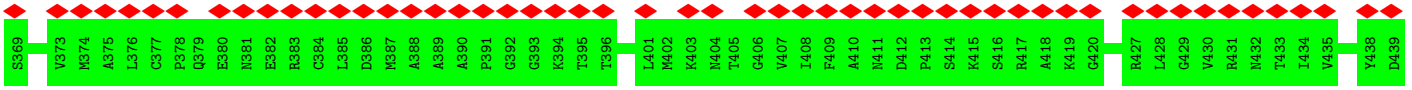


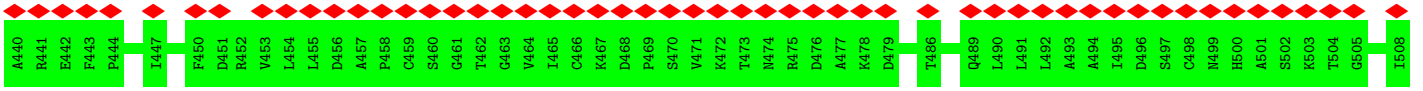
• Molecule 41: RNA methyltransferase nop2-like protein

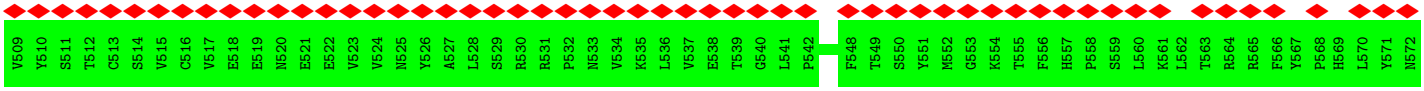
Chain CP:

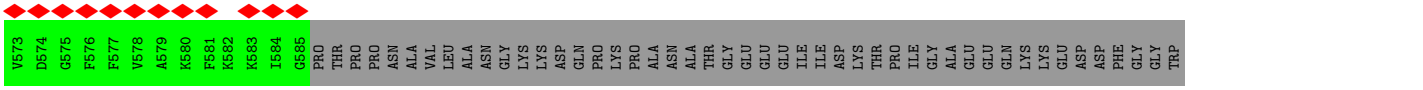


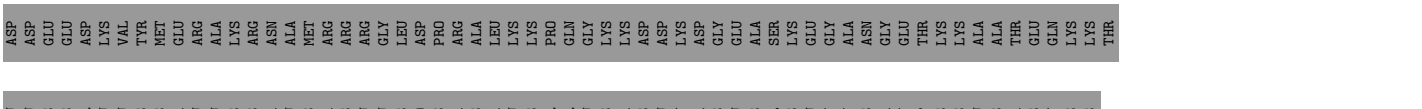






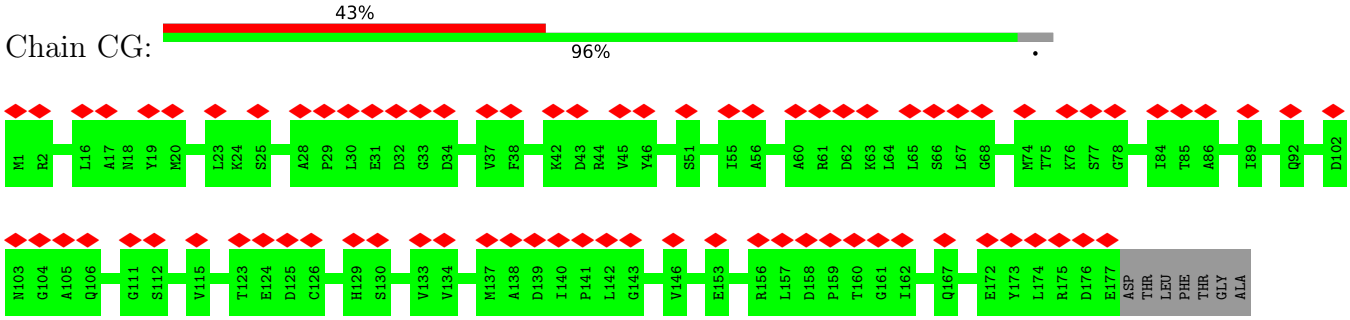






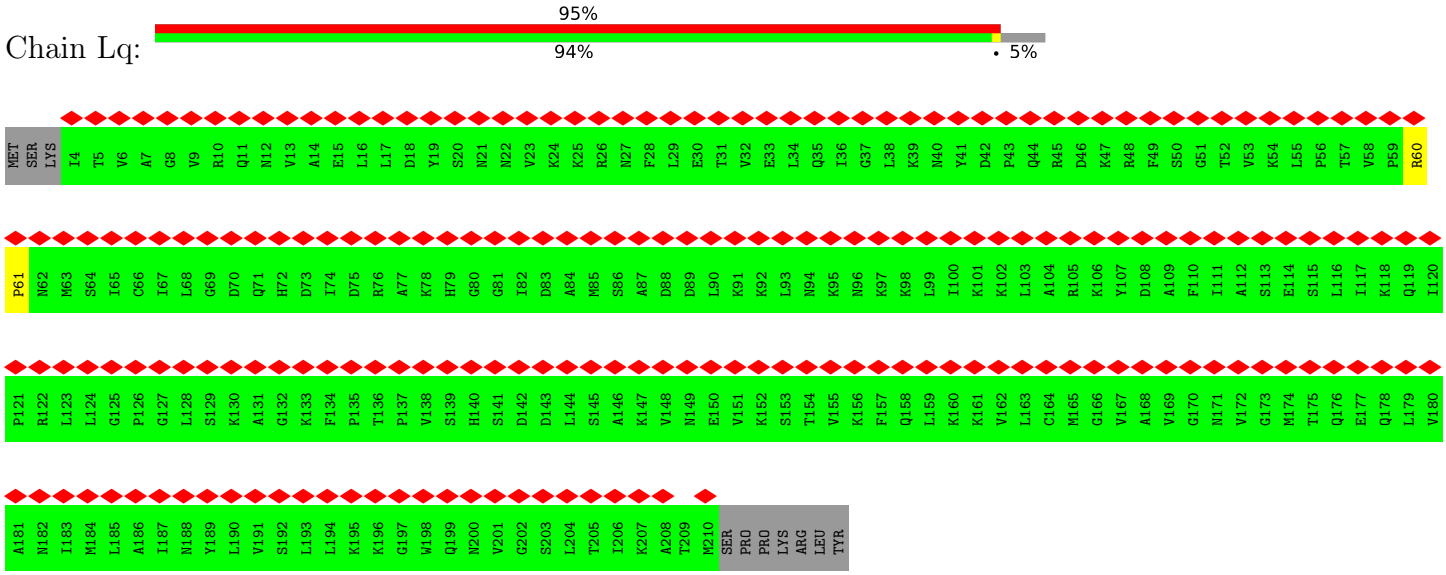
• Molecule 42: 60S ribosome subunit biogenesis protein NIP7

Chain CG:



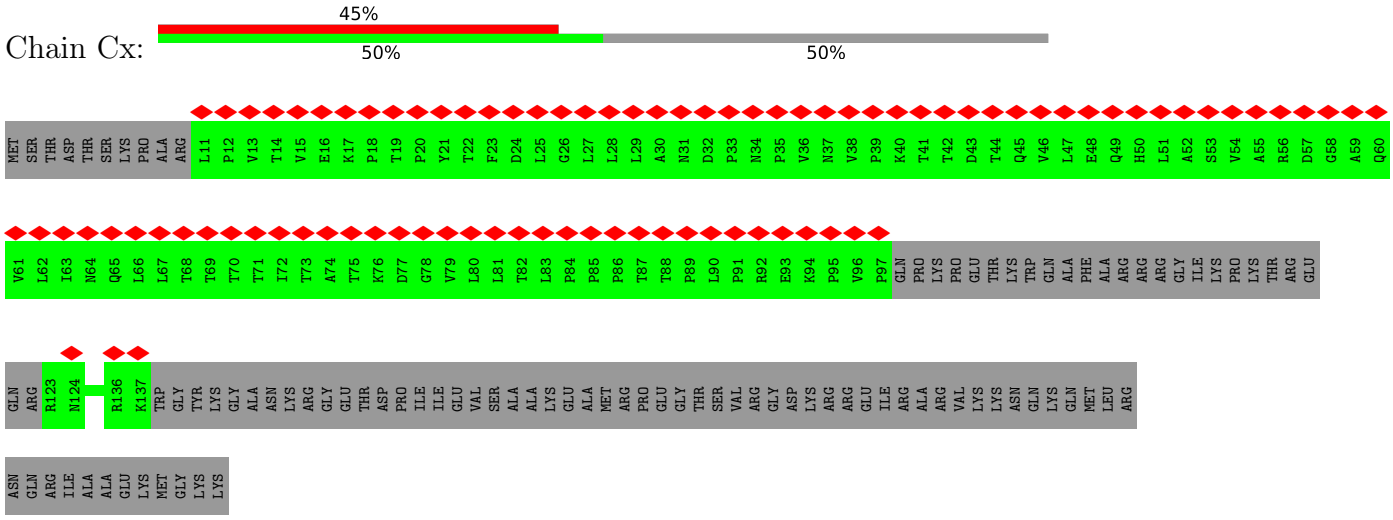
• Molecule 43: Ribosomal protein

Chain Lq:



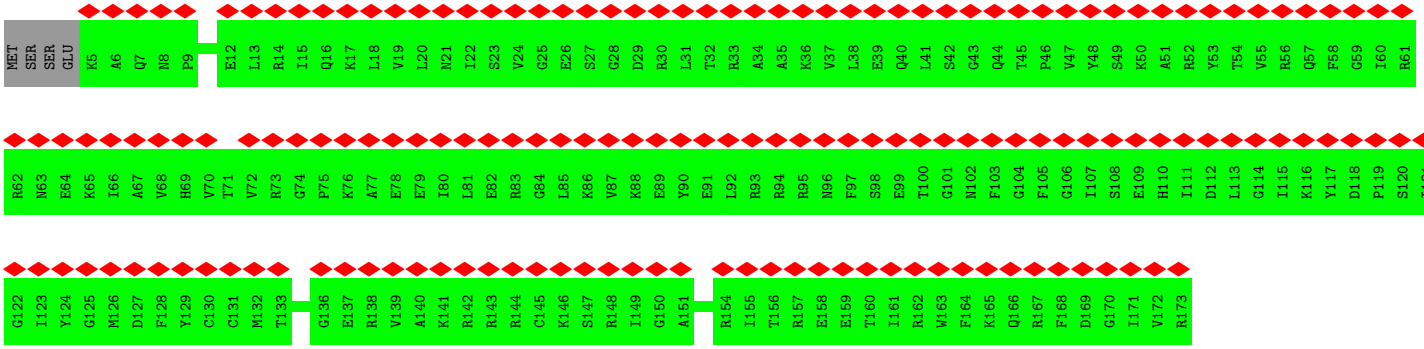
• Molecule 44: Ribosome biogenesis regulatory protein

Chain Cx:

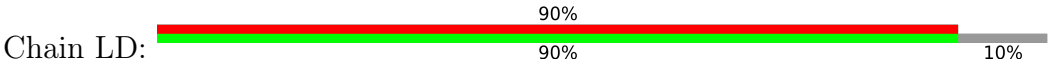


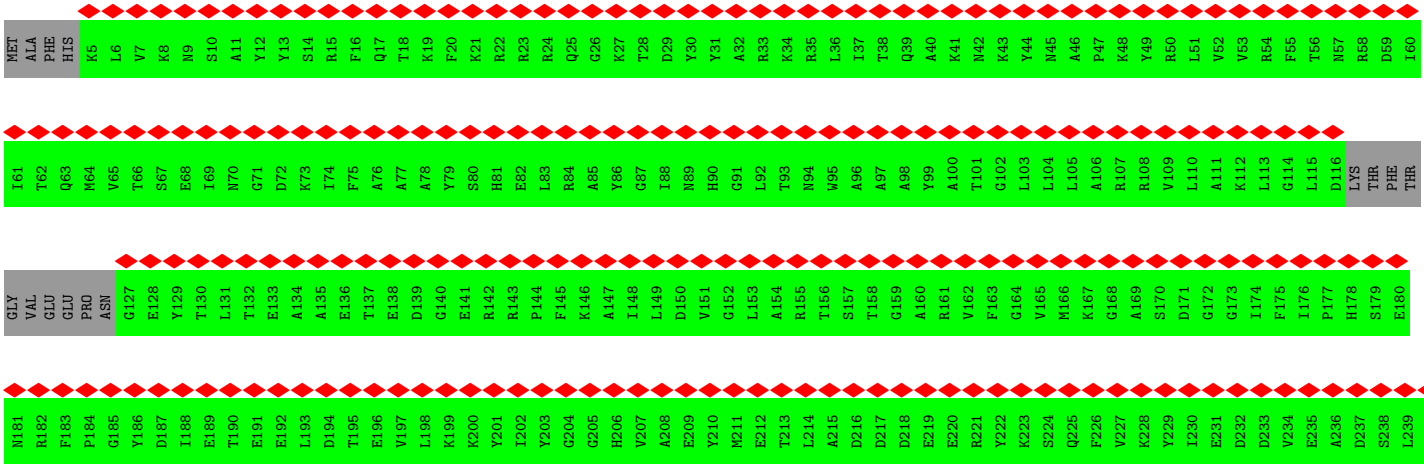
• Molecule 45: Putative ribosomal protein

Chain LJ:

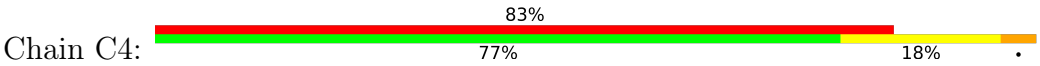


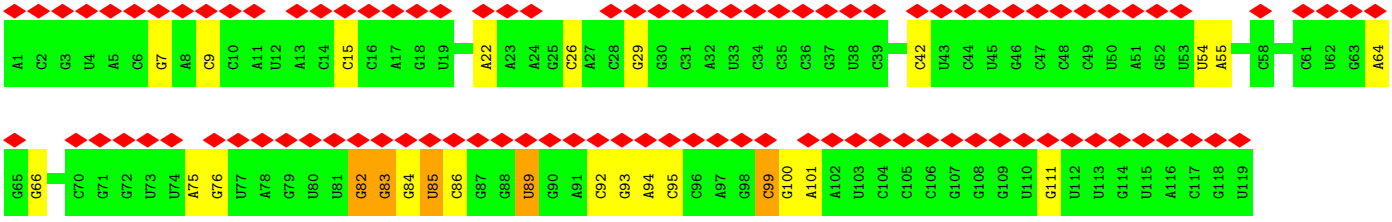
• Molecule 46: 60S ribosomal protein l5-like protein



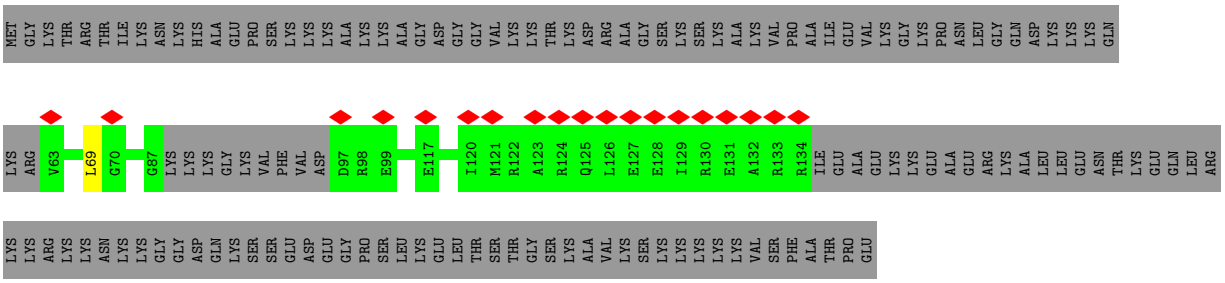


• Molecule 47: RNA (119-MER)





• Molecule 48: 60S ribosomal subunit-like protein


MET GLY LYS THR ARG THR ILE LYS ASN LYS HIS ALA GLU PRO SER LYS LYS LYS ALA LYS LYS ALA GLY ASP GLY GLY VAL LYS LYS THR LYS ASP ARG ALA GLY SER LYS SER LYS ALA LYS VAL PRO ALA ILE GLU VAL LYS GLY LYS PRO ASN LEU GLY GLN ASP LYS LYS GLN
LYS ARG V63 L69 G70 G87 LYS LYS LYS GLY LYS VAL PHE VAL ASP D97 R98 E99 E117 I120 M121 R122 A123 R124 Q125 L126 E127 E128 I129 R130 E131 A132 R133 R134 ILE GLU ALA GLU LYS LYS GLU ALA GLU ARG LYS ALA LEU LEU GLU ASN THR LYS GLU GLN LEU ARG
LYS LYS ARG LYS LYS ASN LYS LYS GLY GLY ASP GLN LYS SER SER GLU ASP GLU GLY PRO SER LEU LYS GLU LEU THR SER THR GLY SER LYS ALA VAL LYS SER LYS LYS LYS LYS LYS VAL SER PHE ALA THR PRO GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41599	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 ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.491	Depositor
Minimum map value	-0.237	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	438.9, 438.9, 438.9	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	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: OMU, 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	C1	0.55	1/48945 (0.0%)	1.02	181/76270 (0.2%)
2	C2	0.57	0/5415	0.96	11/8436 (0.1%)
3	CA	0.34	0/2190	0.68	0/2940
4	CB	0.34	0/2109	0.65	2/2866 (0.1%)
5	CC	0.33	0/2325	0.67	4/3164 (0.1%)
6	CE	0.35	0/3743	0.61	1/5045 (0.0%)
7	CH	0.31	0/909	0.68	0/1229
8	CI	0.34	0/1225	0.64	0/1645
9	CJ	0.28	0/3189	0.58	2/4309 (0.0%)
10	CM	0.31	0/1555	0.65	1/2091 (0.0%)
10	LF	0.37	0/2004	0.60	1/2686 (0.0%)
11	CN	0.30	0/1881	0.66	1/2560 (0.0%)
12	CQ	0.34	0/981	0.70	0/1301
13	CR	0.33	0/1369	0.62	0/1828
14	CU	0.28	0/980	0.64	1/1314 (0.1%)
15	Ch	0.26	0/563	0.68	1/746 (0.1%)
16	LB	0.35	0/2760	0.72	5/3701 (0.1%)
17	LC	0.36	0/2809	0.58	0/3787
18	LE	0.34	0/1363	0.57	0/1833
19	LG	0.36	0/1492	0.59	1/2003 (0.0%)
20	LL	0.36	0/983	0.66	0/1318
21	LM	0.34	0/1120	0.64	1/1507 (0.1%)
22	LN	0.37	0/1595	0.63	1/2132 (0.0%)
23	LO	0.36	0/1652	0.64	1/2215 (0.0%)
24	LP	0.29	0/1231	0.56	0/1658
25	LQ	0.35	0/1033	0.61	0/1391
26	LS	0.35	0/1468	0.63	0/1975
27	LT	0.31	0/1033	0.62	0/1389
28	LV	0.32	0/1013	0.66	2/1361 (0.1%)
29	LY	0.34	0/1079	0.59	0/1443
30	Le	0.34	0/1073	0.57	0/1431
31	Lf	0.38	0/883	0.62	0/1187

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Lh	0.30	0/1006	0.56	0/1338
33	Li	0.32	0/738	0.63	0/971
34	Lj	0.37	0/606	0.64	0/803
35	Cc	0.33	0/1934	0.58	1/2614 (0.0%)
36	Cd	0.33	0/2857	0.59	0/3843
37	Ce	0.38	0/1638	0.63	1/2196 (0.0%)
38	Cf	0.31	0/1238	0.67	2/1631 (0.1%)
39	Cy	0.24	0/1208	0.43	0/1682
40	Cg	0.51	2/1887 (0.1%)	0.85	4/2544 (0.2%)
41	CP	0.24	0/1595	0.46	0/2217
42	CG	0.26	0/872	0.50	0/1212
43	Lq	0.26	0/1020	0.49	0/1418
44	Cx	0.25	0/567	0.49	0/783
45	LJ	0.24	0/830	0.44	0/1150
46	LD	0.23	0/1344	0.41	0/1868
47	C4	0.30	0/2833	1.08	19/4414 (0.4%)
48	CX	0.58	0/377	0.66	0/518
All	All	0.44	3/124520 (0.0%)	0.84	244/179963 (0.1%)

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
4	CB	0	1
15	Ch	0	1
16	LB	0	1
19	LG	0	1
25	LQ	0	1
40	Cg	0	1
43	Lq	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	Cg	204	PRO	CG-CD	-15.22	1.00	1.50
40	Cg	204	PRO	N-CD	6.92	1.57	1.47
1	C1	3215	U	C1'-N1	6.65	1.58	1.48

The worst 5 of 244 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	Cg	204	PRO	N-CD-CG	-16.54	78.39	103.20
1	C1	1050	C	N3-C2-O2	-12.57	113.10	121.90
1	C1	1050	C	N1-C2-O2	10.13	124.98	118.90
37	Ce	186	CYS	C-N-CA	10.04	146.80	121.70
1	C1	625	C	C6-N1-C2	-10.02	116.29	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	CB	42	ARG	Peptide
15	Ch	282	LEU	Peptide
16	LB	58	ARG	Sidechain
19	LG	161	ASP	Peptide
25	LQ	147	ARG	Sidechain

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	
3	CA	254/316 (80%)	236 (93%)	18 (7%)	0	100	100
4	CB	256/391 (66%)	235 (92%)	20 (8%)	1 (0%)	34	69
5	CC	264/801 (33%)	250 (95%)	14 (5%)	0	100	100
6	CE	459/598 (77%)	440 (96%)	19 (4%)	0	100	100
7	CH	106/661 (16%)	101 (95%)	4 (4%)	1 (1%)	17	52
8	CI	144/414 (35%)	133 (92%)	10 (7%)	1 (1%)	22	57
9	CJ	374/679 (55%)	357 (96%)	16 (4%)	1 (0%)	41	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	CM	183/249 (74%)	171 (93%)	12 (7%)	0	100	100
10	LF	238/249 (96%)	230 (97%)	7 (3%)	1 (0%)	34	69
11	CN	244/246 (99%)	228 (93%)	16 (7%)	0	100	100
12	CQ	110/225 (49%)	107 (97%)	3 (3%)	0	100	100
13	CR	159/237 (67%)	153 (96%)	6 (4%)	0	100	100
14	CU	119/451 (26%)	113 (95%)	6 (5%)	0	100	100
15	Ch	69/354 (20%)	66 (96%)	3 (4%)	0	100	100
16	LB	337/392 (86%)	319 (95%)	18 (5%)	0	100	100
17	LC	360/365 (99%)	349 (97%)	11 (3%)	0	100	100
18	LE	166/200 (83%)	161 (97%)	5 (3%)	0	100	100
19	LG	179/262 (68%)	174 (97%)	5 (3%)	0	100	100
20	LL	115/213 (54%)	111 (96%)	4 (4%)	0	100	100
21	LM	135/142 (95%)	131 (97%)	4 (3%)	0	100	100
22	LN	179/203 (88%)	175 (98%)	4 (2%)	0	100	100
23	LO	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
24	LP	150/187 (80%)	148 (99%)	2 (1%)	0	100	100
25	LQ	127/213 (60%)	123 (97%)	4 (3%)	0	100	100
26	LS	172/174 (99%)	164 (95%)	8 (5%)	0	100	100
27	LT	124/160 (78%)	115 (93%)	8 (6%)	1 (1%)	19	54
28	LV	133/139 (96%)	127 (96%)	6 (4%)	0	100	100
29	LY	132/138 (96%)	128 (97%)	4 (3%)	0	100	100
30	Le	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
31	Lf	106/109 (97%)	102 (96%)	2 (2%)	2 (2%)	8	33
32	Lh	119/935 (13%)	117 (98%)	2 (2%)	0	100	100
33	Li	86/110 (78%)	84 (98%)	2 (2%)	0	100	100
34	Lj	72/95 (76%)	71 (99%)	1 (1%)	0	100	100
35	Cc	232/282 (82%)	222 (96%)	10 (4%)	0	100	100
36	Cd	343/436 (79%)	321 (94%)	22 (6%)	0	100	100
37	Ce	192/336 (57%)	188 (98%)	4 (2%)	0	100	100
38	Cf	145/570 (25%)	136 (94%)	9 (6%)	0	100	100
39	Cy	240/350 (69%)	238 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
40	Cg	229/478 (48%)	215 (94%)	12 (5%)	2 (1%)	17 52
41	CP	322/751 (43%)	314 (98%)	8 (2%)	0	100 100
42	CG	175/184 (95%)	171 (98%)	4 (2%)	0	100 100
43	Lq	205/217 (94%)	183 (89%)	21 (10%)	1 (0%)	29 64
44	Cx	98/202 (48%)	98 (100%)	0	0	100 100
45	LJ	167/173 (96%)	167 (100%)	0	0	100 100
46	LD	269/304 (88%)	266 (99%)	3 (1%)	0	100 100
48	CX	59/203 (29%)	56 (95%)	3 (5%)	0	100 100
All	All	8678/14729 (59%)	8315 (96%)	352 (4%)	11 (0%)	54 83

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	CB	117	PRO
8	CI	268	VAL
40	Cg	154	ASP
31	Lf	93	ALA
7	CH	403	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	CA	231/276 (84%)	218 (94%)	13 (6%)	21 52
4	CB	222/329 (68%)	206 (93%)	16 (7%)	14 44
5	CC	252/710 (36%)	236 (94%)	16 (6%)	18 48
6	CE	398/517 (77%)	383 (96%)	15 (4%)	33 66
7	CH	95/575 (16%)	88 (93%)	7 (7%)	13 42
8	CI	121/336 (36%)	117 (97%)	4 (3%)	38 69
9	CJ	332/579 (57%)	321 (97%)	11 (3%)	38 69
10	CM	161/215 (75%)	145 (90%)	16 (10%)	8 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	LF	206/215 (96%)	202 (98%)	4 (2%)	57 81
11	CN	206/206 (100%)	199 (97%)	7 (3%)	37 69
12	CQ	100/192 (52%)	96 (96%)	4 (4%)	31 65
13	CR	144/206 (70%)	136 (94%)	8 (6%)	21 52
14	CU	104/376 (28%)	98 (94%)	6 (6%)	20 51
15	Ch	58/291 (20%)	56 (97%)	2 (3%)	37 69
16	LB	290/331 (88%)	267 (92%)	23 (8%)	12 40
17	LC	283/285 (99%)	274 (97%)	9 (3%)	39 69
18	LE	143/166 (86%)	137 (96%)	6 (4%)	30 62
19	LG	157/222 (71%)	146 (93%)	11 (7%)	15 45
20	LL	99/176 (56%)	98 (99%)	1 (1%)	76 90
21	LM	115/117 (98%)	110 (96%)	5 (4%)	29 62
22	LN	164/180 (91%)	158 (96%)	6 (4%)	34 66
23	LO	163/163 (100%)	160 (98%)	3 (2%)	59 82
24	LP	125/152 (82%)	122 (98%)	3 (2%)	49 76
25	LQ	110/178 (62%)	110 (100%)	0	100 100
26	LS	154/154 (100%)	148 (96%)	6 (4%)	32 65
27	LT	109/135 (81%)	102 (94%)	7 (6%)	17 48
28	LV	99/102 (97%)	95 (96%)	4 (4%)	31 65
29	LY	117/119 (98%)	112 (96%)	5 (4%)	29 62
30	Le	114/114 (100%)	110 (96%)	4 (4%)	36 68
31	Lf	89/90 (99%)	87 (98%)	2 (2%)	52 78
32	Lh	108/781 (14%)	104 (96%)	4 (4%)	34 66
33	Li	75/93 (81%)	69 (92%)	6 (8%)	12 40
34	Lj	61/78 (78%)	60 (98%)	1 (2%)	62 84
35	Cc	204/244 (84%)	194 (95%)	10 (5%)	25 57
36	Cd	295/367 (80%)	279 (95%)	16 (5%)	22 53
37	Ce	173/297 (58%)	167 (96%)	6 (4%)	36 68
38	Cf	127/482 (26%)	121 (95%)	6 (5%)	26 59
40	Cg	210/417 (50%)	202 (96%)	8 (4%)	33 66
44	Cx	14/176 (8%)	14 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
48	CX	22/172 (13%)	21 (96%)	1 (4%)	27 60
All	All	6250/10814 (58%)	5968 (96%)	282 (4%)	31 60

5 of 282 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	Li	68	GLU
35	Cc	61	CYS
36	Cd	436	LEU
10	CM	202	LYS
10	CM	144	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
40	Cg	100	ASN
32	Lh	47	ASN
12	CQ	45	ASN
10	CM	242	ASN
15	Ch	321	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	2026/3341 (60%)	482 (23%)	17 (0%)
2	C2	225/256 (87%)	61 (27%)	1 (0%)
47	C4	118/119 (99%)	23 (19%)	0
All	All	2369/3716 (63%)	566 (23%)	18 (0%)

5 of 566 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	14	U
1	C1	26	A
1	C1	40	A
1	C1	43	A
1	C1	49	A

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	3257	U
2	C2	123	G
1	C1	3297	U
1	C1	2569	U
1	C1	3255	G

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OMU	C1	2689	1	19,22,23	2.98	8 (42%)	26,31,34	1.68	4 (15%)
1	OMU	C1	2687	1	19,22,23	2.96	8 (42%)	26,31,34	1.67	4 (15%)
1	OMU	C1	2682	1	19,22,23	2.97	8 (42%)	26,31,34	1.64	4 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	C1	2689	1	-	2/9/27/28	0/2/2/2
1	OMU	C1	2687	1	-	0/9/27/28	0/2/2/2
1	OMU	C1	2682	1	-	1/9/27/28	0/2/2/2

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	2682	OMU	C2-N1	7.20	1.50	1.38
1	C1	2689	OMU	C2-N1	7.20	1.50	1.38
1	C1	2687	OMU	C2-N1	7.15	1.49	1.38
1	C1	2689	OMU	C2-N3	6.72	1.49	1.38
1	C1	2682	OMU	C2-N3	6.71	1.49	1.38

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	2689	OMU	C4-N3-C2	-5.14	119.80	126.58
1	C1	2687	OMU	C4-N3-C2	-5.12	119.83	126.58
1	C1	2682	OMU	C4-N3-C2	-4.98	120.01	126.58
1	C1	2689	OMU	N3-C2-N1	3.71	119.82	114.89
1	C1	2687	OMU	N3-C2-N1	3.67	119.77	114.89

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C1	2682	OMU	C1'-C2'-O2'-CM2
1	C1	2689	OMU	C3'-C4'-C5'-O5'
1	C1	2689	OMU	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 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.

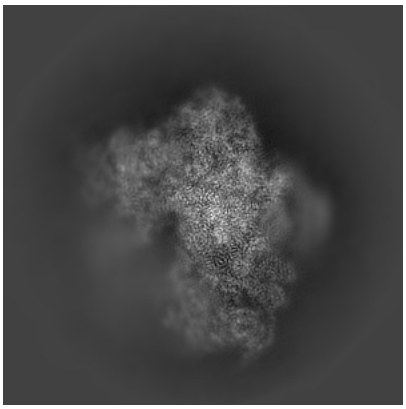
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35281. These allow visual inspection of the internal detail of the map and identification of artifacts.

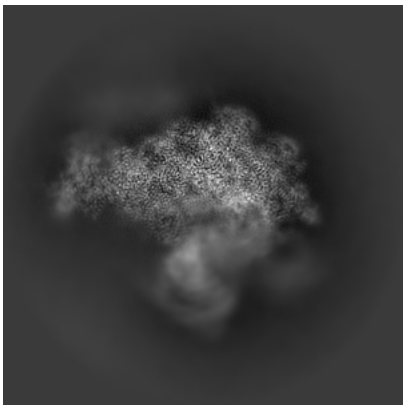
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

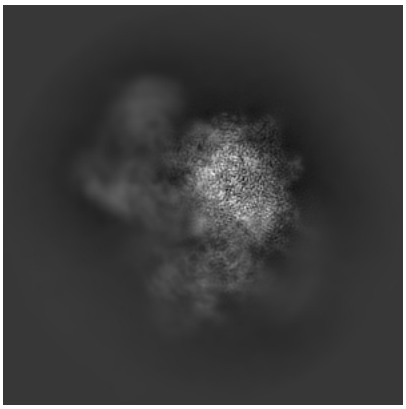
6.1.1 Primary map



X

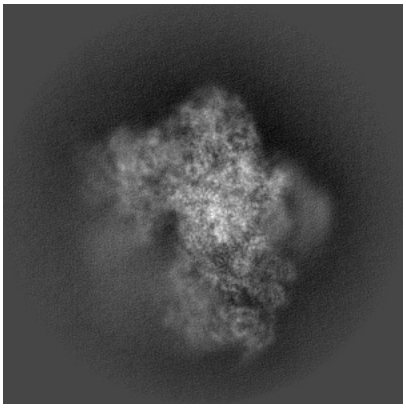


Y

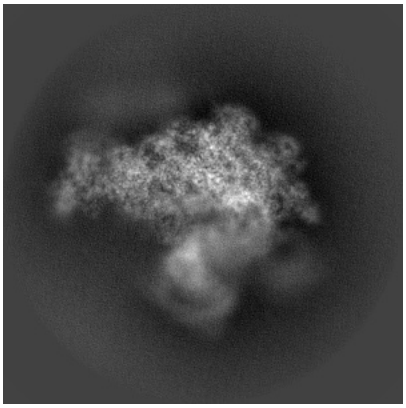


Z

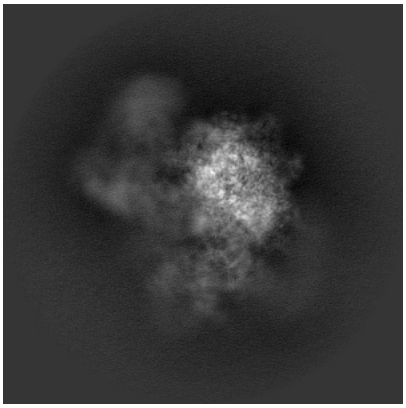
6.1.2 Raw map



X



Y

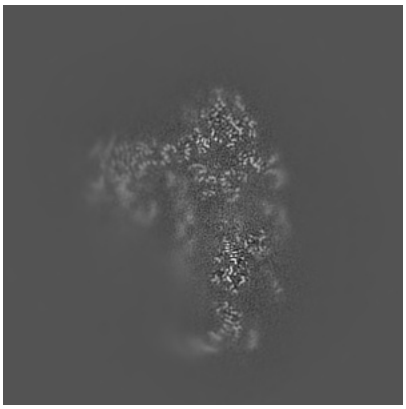


Z

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

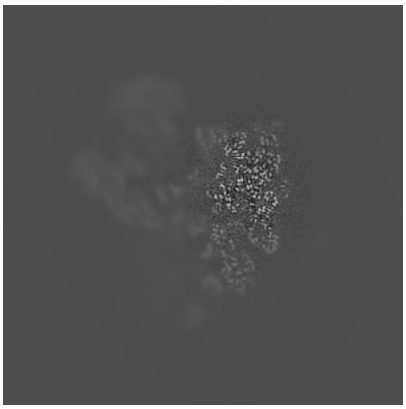
6.2 Central slices (i)

6.2.1 Primary map



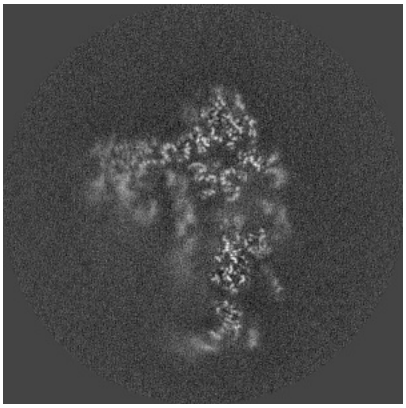
X Index: 210

Y Index: 210

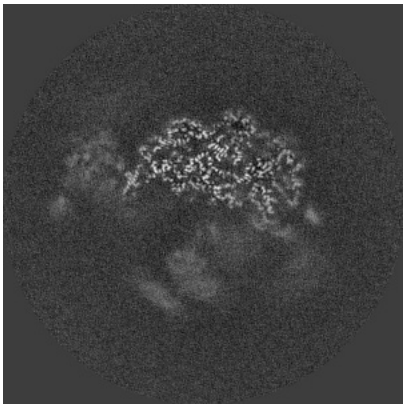


Z Index: 210

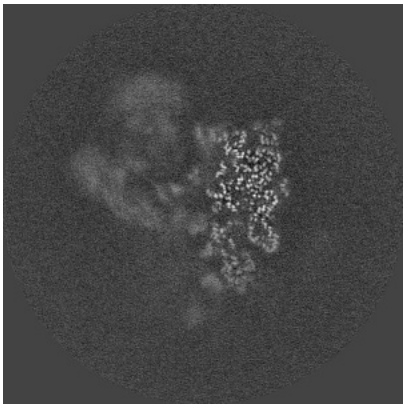
6.2.2 Raw map



X Index: 210



Y Index: 210

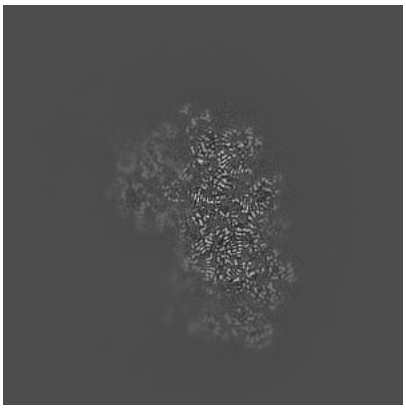


Z Index: 210

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

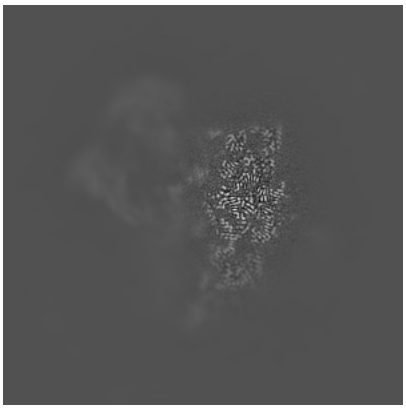
6.3 Largest variance slices (i)

6.3.1 Primary map



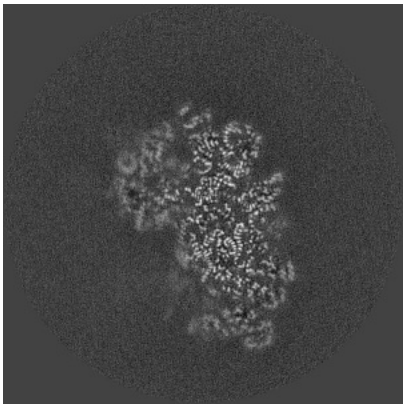
X Index: 243

Y Index: 229

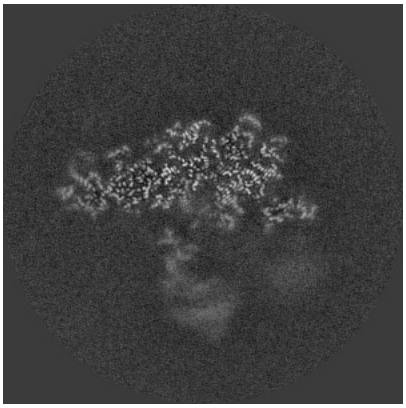


Z Index: 216

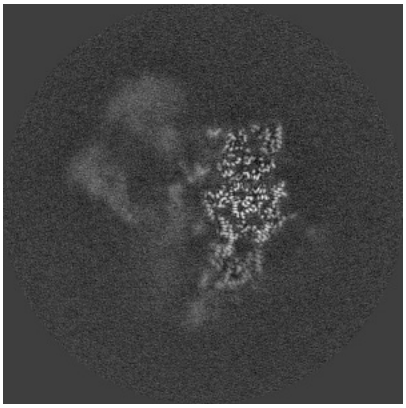
6.3.2 Raw map



X Index: 241



Y Index: 233

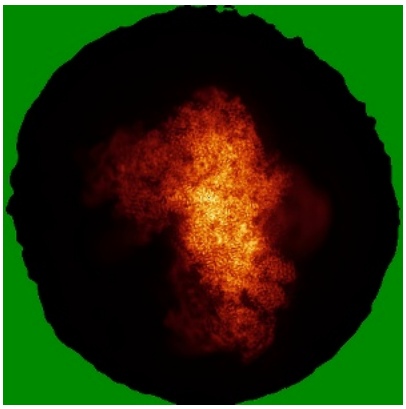


Z Index: 217

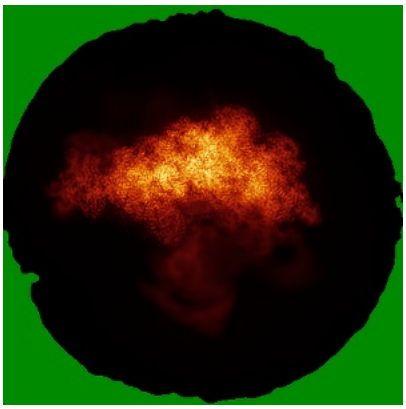
The images above show the largest variance slices of the map in three orthogonal directions.

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

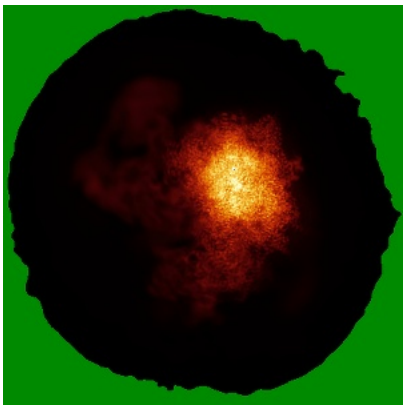
6.4.1 Primary map



X

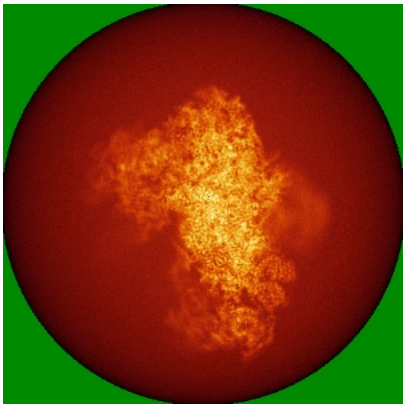


Y

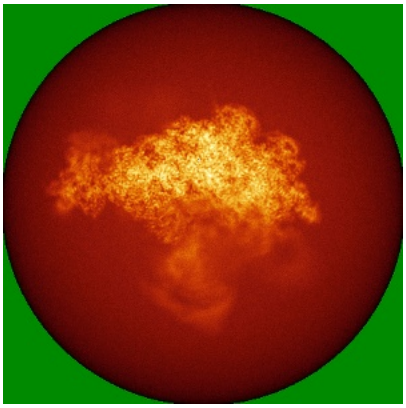


Z

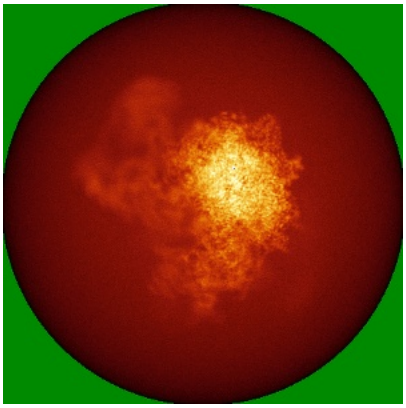
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

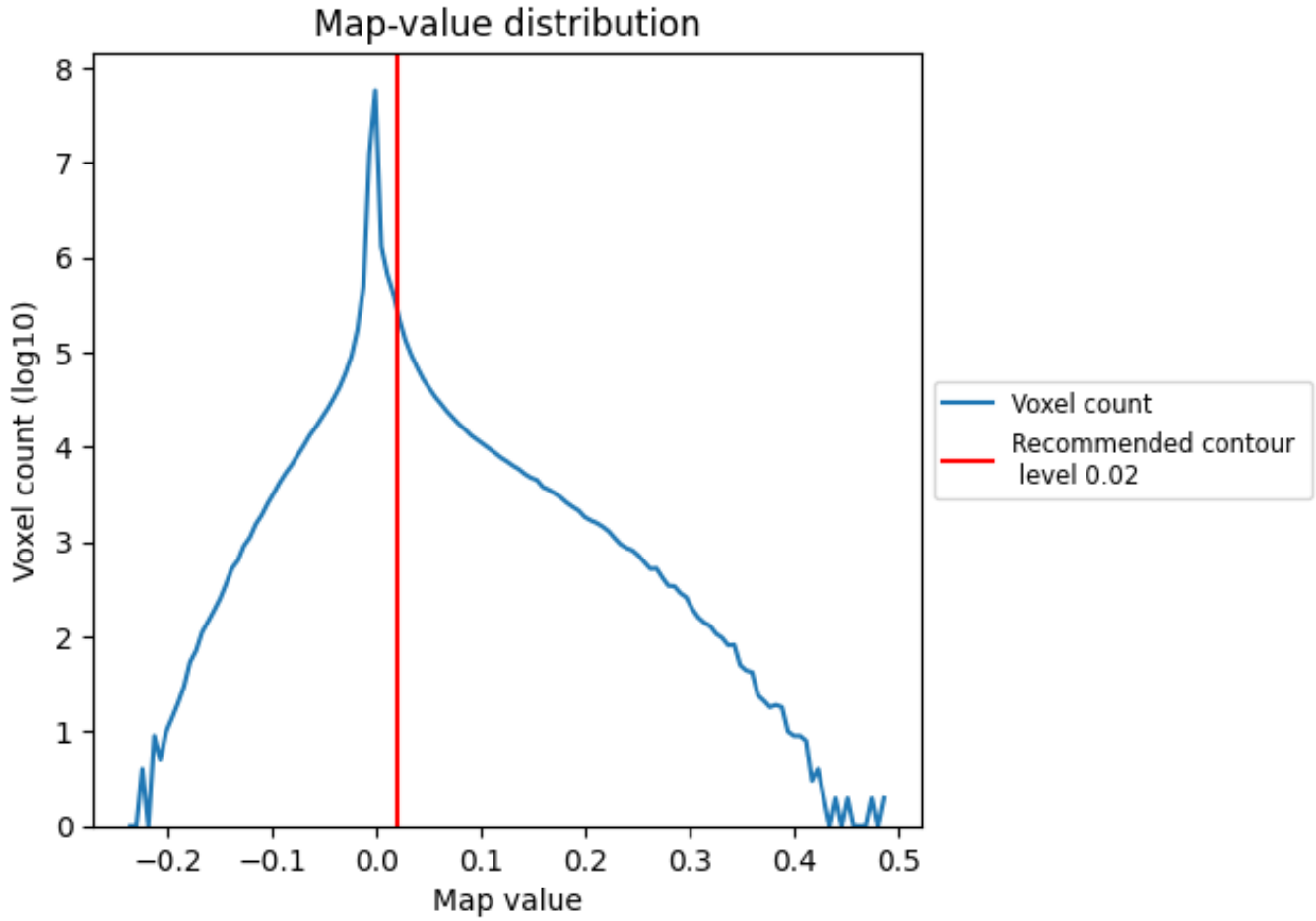
6.6 Mask visualisation (i)

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

7 Map analysis

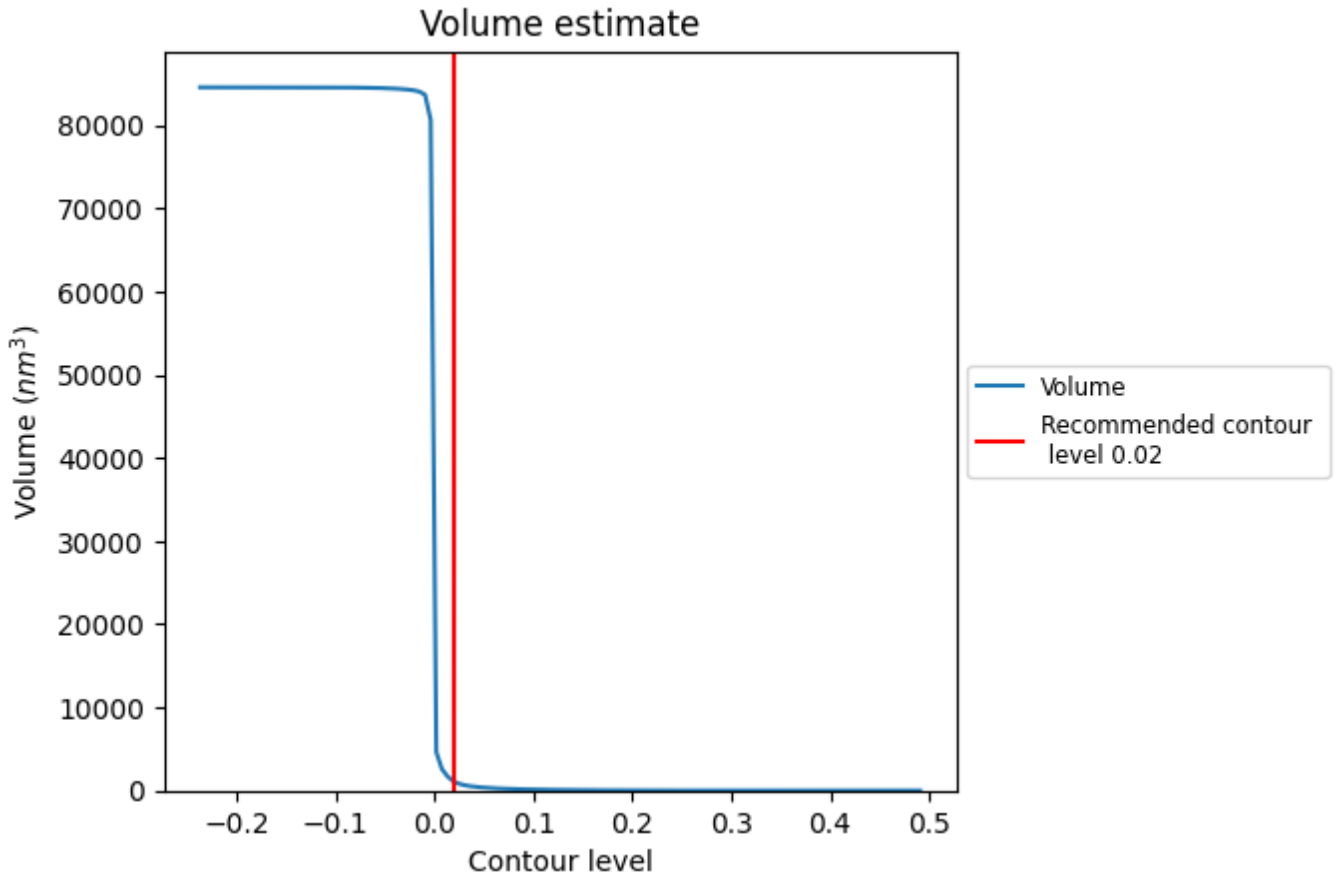
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

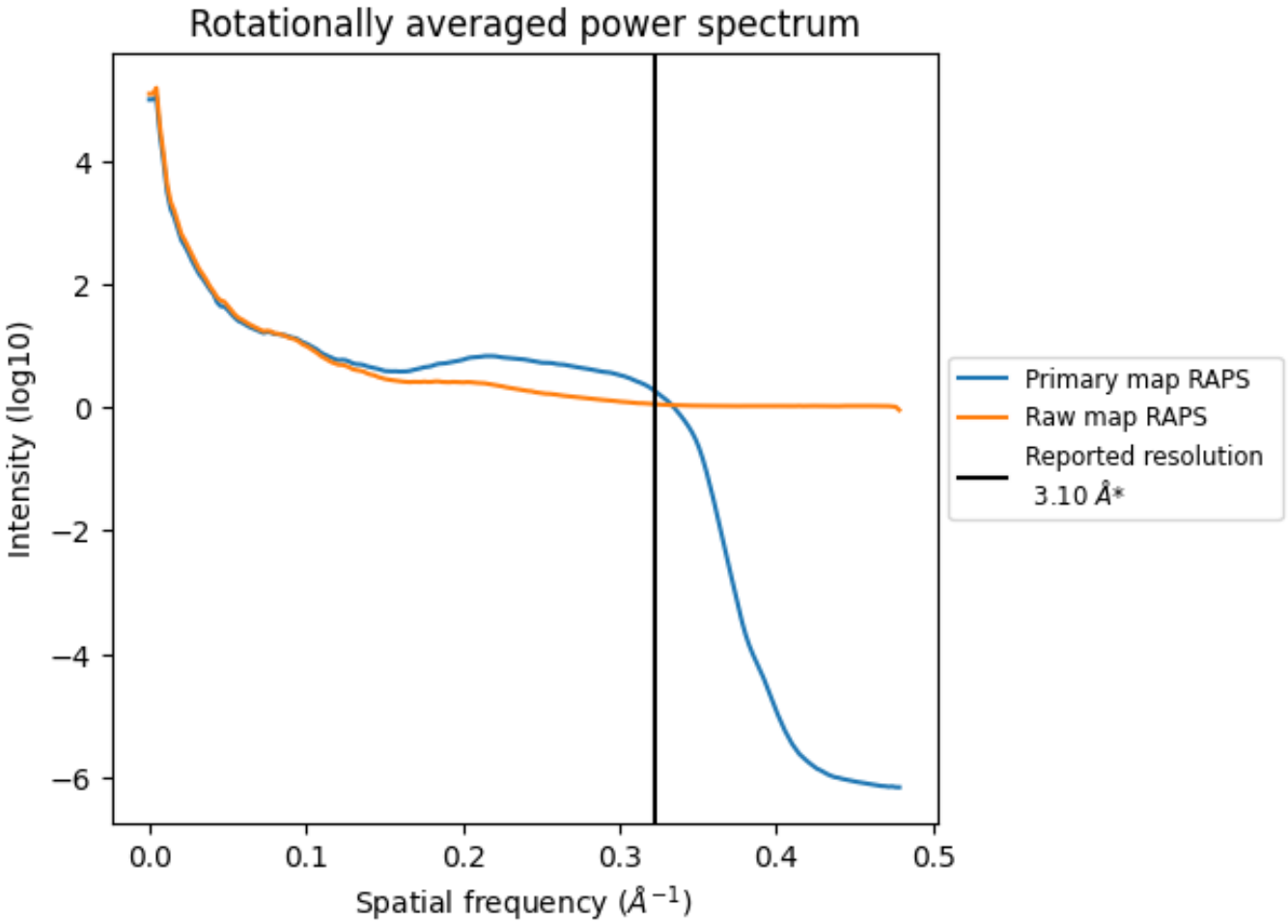
7.2 Volume estimate (i)



The volume at the recommended contour level is 1087 nm^3; this corresponds to an approximate mass of 982 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)

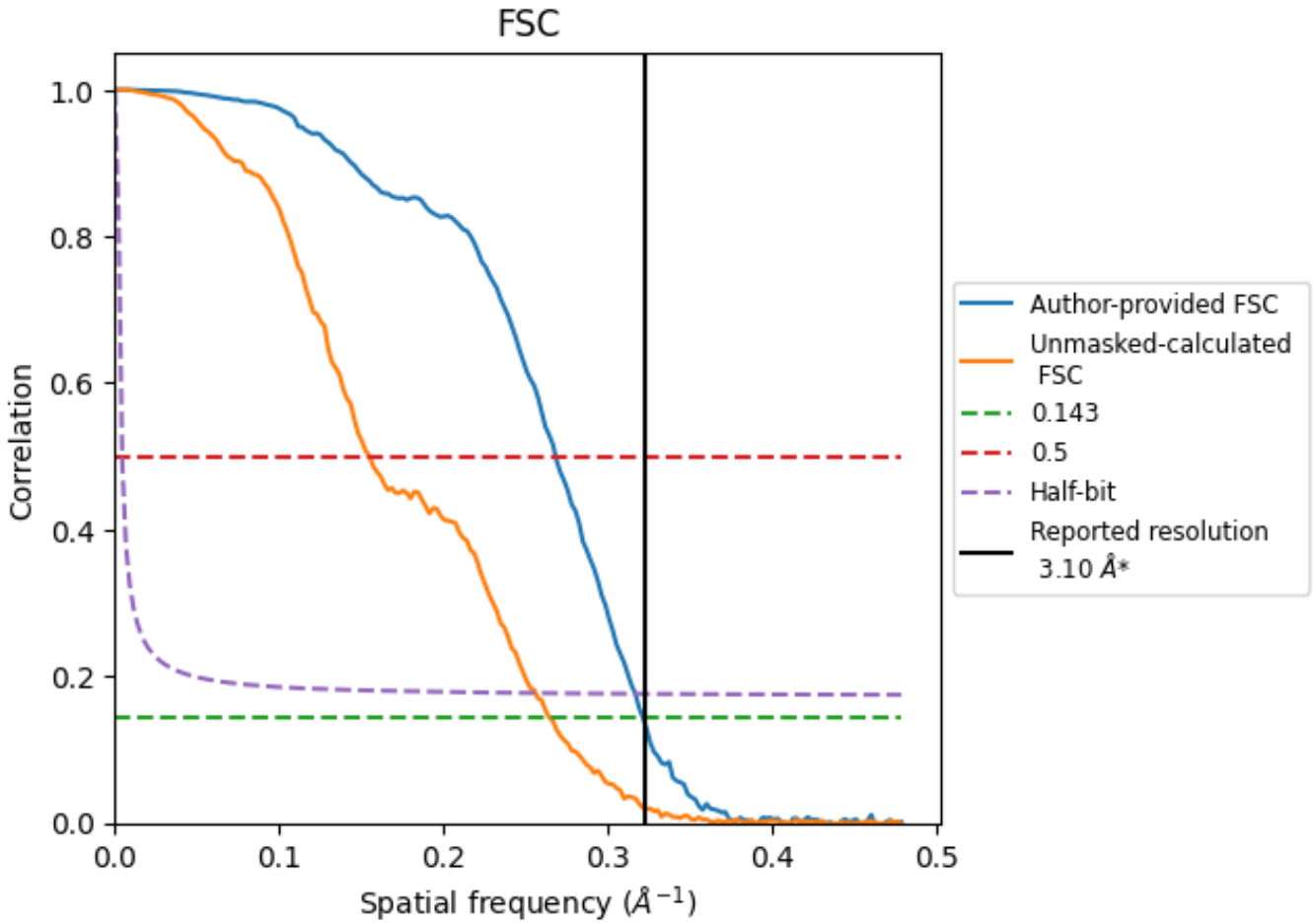


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

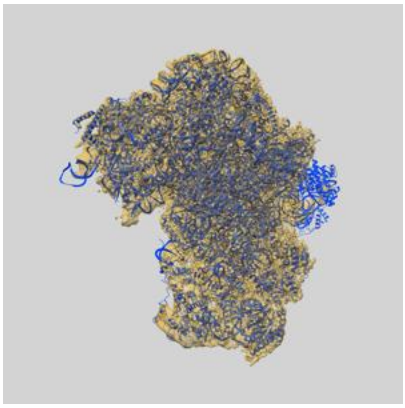
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.11	3.73	3.16
Unmasked-calculated*	3.78	6.45	3.91

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.78 differs from the reported value 3.1 by more than 10 %

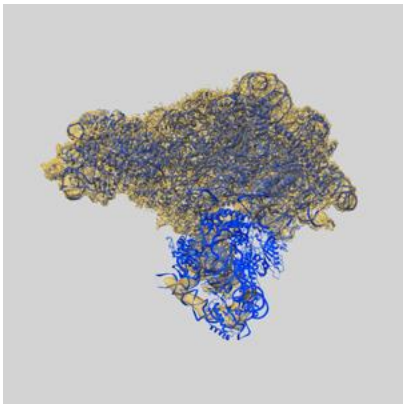
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35281 and PDB model 8I9R. Per-residue inclusion information can be found in section 3 on page 14.

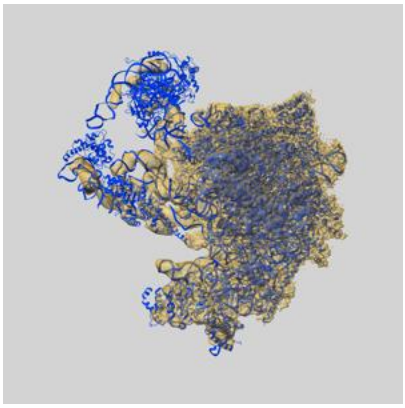
9.1 Map-model overlay



X



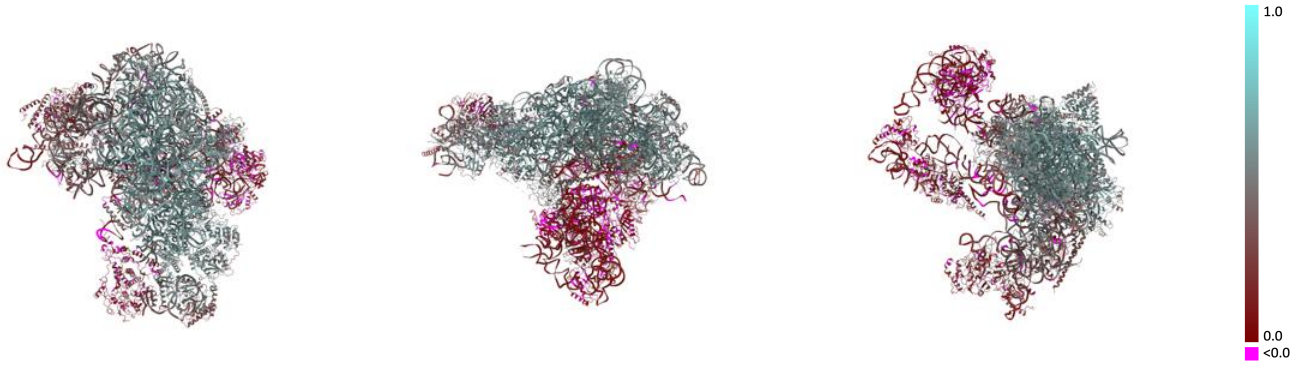
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

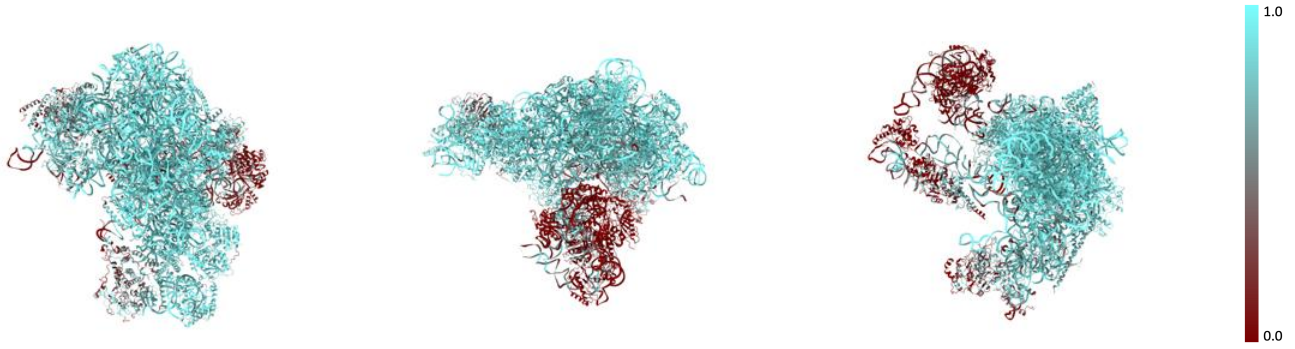
9.2 Q-score mapped to coordinate model



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.

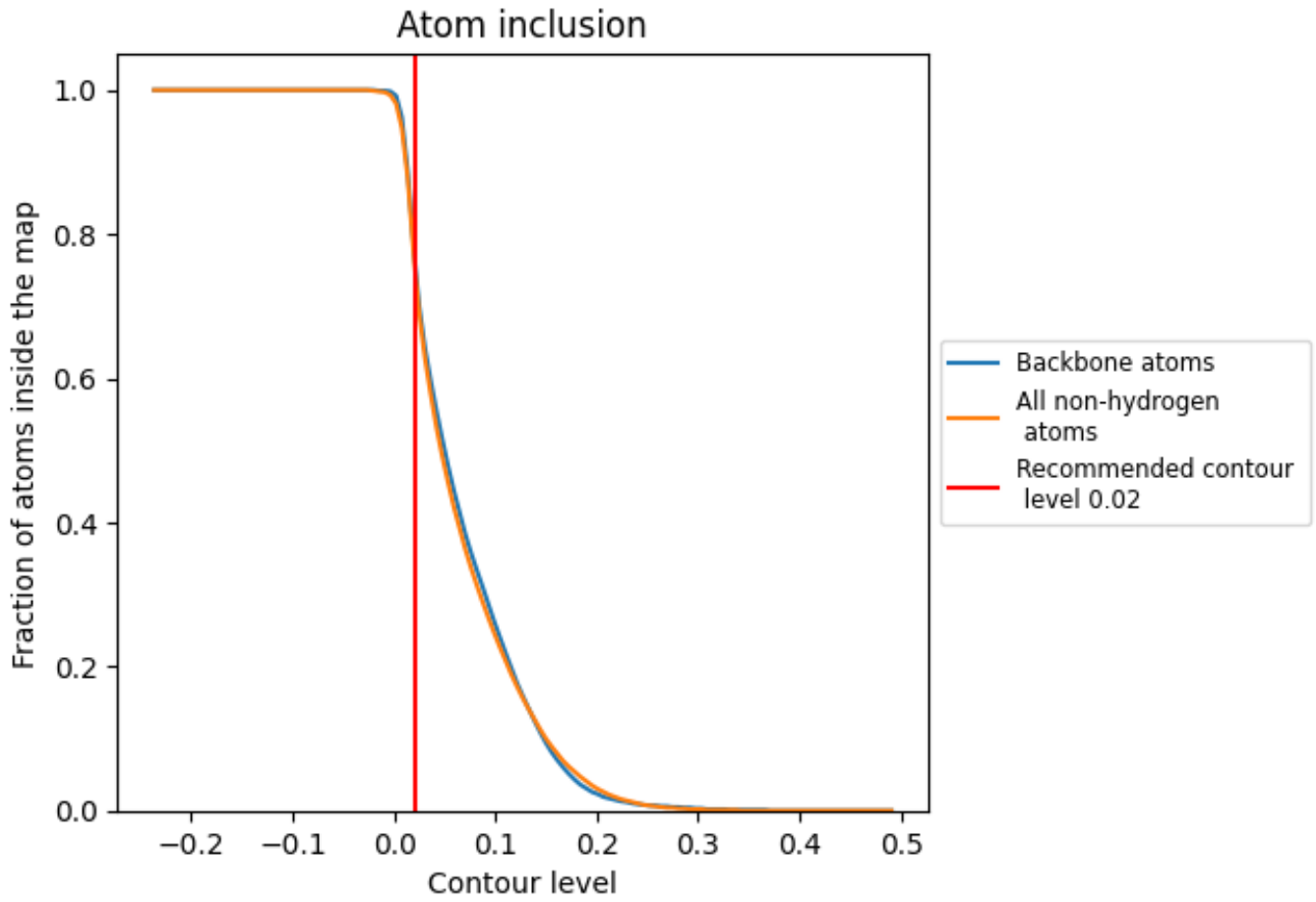
9.3 Atom inclusion mapped to coordinate model



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 76% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7610	0.4050
C1	0.8260	0.4090
C2	0.9150	0.4740
C4	0.1690	0.1000
CA	0.8840	0.4900
CB	0.8480	0.4450
CC	0.6290	0.3320
CE	0.9000	0.5130
CG	0.5290	0.1640
CH	0.3820	0.2080
CI	0.8720	0.4490
CJ	0.4900	0.1550
CM	0.6900	0.3100
CN	0.3660	0.1790
CP	0.1970	0.1380
CQ	0.6160	0.2450
CR	0.9140	0.5420
CU	0.8040	0.4050
CX	0.6150	0.3430
Cc	0.8530	0.5030
Cd	0.9130	0.5400
Ce	0.9410	0.5680
Cf	0.7690	0.4040
Cg	0.7650	0.3980
Ch	0.7200	0.3060
Cx	0.1520	0.1030
Cy	0.0000	0.0720
LB	0.7710	0.3770
LC	0.9510	0.5860
LD	0.0010	0.0380
LE	0.9140	0.5320
LF	0.9320	0.5550
LG	0.9050	0.5470
LJ	0.0380	0.0310
LL	0.9420	0.5770

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
LM	0.8660	0.4960
LN	0.9470	0.5970
LO	0.9350	0.5440
LP	0.8320	0.4810
LQ	0.9480	0.5760
LS	0.9110	0.5070
LT	0.7370	0.3560
LV	0.3700	0.1870
LY	0.9300	0.5690
Le	0.9430	0.5900
Lf	0.9470	0.5880
Lh	0.8670	0.4900
Li	0.8930	0.5270
Lj	0.9590	0.6060
Lq	0.0080	0.0760