wwPDB EM Validation Summary Report (i)

Dec 11, 2022 – 07:03 am GMT

PDB ID	:	4D61
EMDB ID	:	EMD-2813
Title	:	Cryo-EM structures of ribosomal 80S complexes with termination factors and cricket paralysis virus IRES reveal the IRES in the translocated state
Authors	:	Muhs, M.; Hilal, T.; Mielke, T.; Skabkin, M.A.; Sanbonmatsu, K.Y.; Pestova, T.V.; Spahn, C.M.T.
Deposited on	:	2014-11-07
Resolution	:	9.00 Å(reported)

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

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

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

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

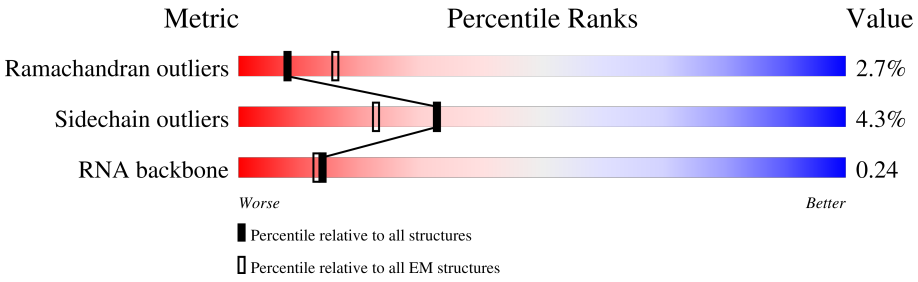
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 9.00 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	1	1869	36% 55% 7%
2	A	295	30% 72% 26%
3	B	264	12% 71% 8% 19%
4	C	293	14% 72% 24%
5	D	243	21% 81% 6% 13%
6	E	263	16% 92% 6%
7	F	204	20% 84% 8% 8%
8	G	249	16% 87% 6% 7%

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Mol	Chain	Length	Quality of chain
9	H	194	54% 94%
10	I	208	22% 91% 8%
11	J	194	9% 86% 7% 8%
12	K	165	12% 52% 5% 43%
13	L	158	26% 87% 5% 8%
14	M	132	54% 83% 7% 9%
15	N	151	17% 95%
16	O	151	17% 85% 5% 9%
17	P	145	23% 75% 6% 19%
18	Q	146	17% 91% 5%
19	R	135	29% 76% 5% 19%
20	S	152	18% 82% 11% 7%
21	T	145	26% 92% 6%
22	U	119	29% 81% 15%
23	V	83	43% 96%
24	W	130	21% 94% 5%
25	X	143	14% 85% 8% 6%
26	Y	133	17% 84% 8% 8%
27	Z	125	11% 55% 6% 39%
28	a	115	20% 74% 9% 17%
29	b	84	25% 90% 5% 5%
30	c	69	26% 83% 7% 10%
31	d	56	9% 88% 7% 5%
32	e	59	32% 81% 5% 14%
33	f	156	24% 37% 61%

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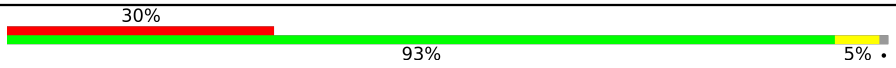
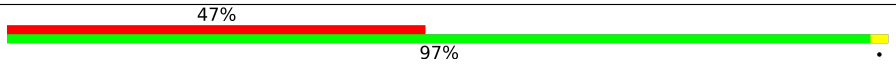
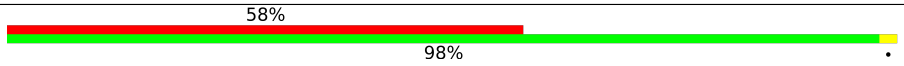
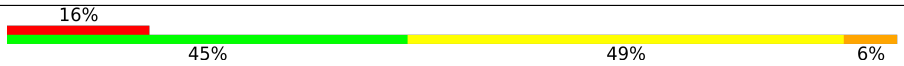
Mol	Chain	Length	Quality of chain
34	g	317	
35	h	436	
36	i	426	
37	j	201	

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 86384 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 18S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	1742	37159	16589	6665	12164	1741	0	0

- Molecule 2 is a protein called 40S RIBOSOMAL PROTEIN SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	218	1719	1091	301	319	8	0	0

- Molecule 3 is a protein called 40S RIBOSOMAL PROTEIN S3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	213	1729	1098	309	308	14	0	0

- Molecule 4 is a protein called 40S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	222	1724	1114	296	304	10	0	0

- Molecule 5 is a protein called 40S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	212	1646	1050	299	290	7	0	0

- Molecule 6 is a protein called 40S RIBOSOMAL PROTEIN S4, Y ISOFORM 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	257	2031	1298	381	344	8	0	0

- Molecule 7 is a protein called 40S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	188	Total	C	N	O	S	0	0
			1486	930	283	266	7		

- Molecule 8 is a protein called 40S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	232	Total	C	N	O	S	0	0
			1884	1176	379	322	7		

- Molecule 9 is a protein called 40S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	191	Total	C	N	O	S	0	0
			1535	978	282	274	1		

- Molecule 10 is a protein called 40S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	207	Total	C	N	O	S	0	0
			1695	1064	334	292	5		

- Molecule 11 is a protein called 40S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	179	Total	C	N	O	S	0	0
			1495	953	299	241	2		

- Molecule 12 is a protein called 40S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	94	Total	C	N	O	S	0	0
			791	519	138	129	5		

- Molecule 13 is a protein called 40S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	146	Total	C	N	O	S	0	0
			1199	764	224	205	6		

- Molecule 14 is a protein called 40S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	120	Total	C	N	O	S	0	0
			931	584	164	174	9		

- Molecule 15 is a protein called 40S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	150	Total	C	N	O	S	0	0
			1207	773	229	204	1		

- Molecule 16 is a protein called 40S RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	137	Total	C	N	O	S	0	0
			1023	627	200	190	6		

- Molecule 17 is a protein called 40S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	118	Total	C	N	O	S	0	0
			981	625	183	166	7		

- Molecule 18 is a protein called 40S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	139	Total	C	N	O	S	0	0
			1108	704	210	191	3		

- Molecule 19 is a protein called 40S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	109	Total	C	N	O	S	0	0
			893	561	170	159	3		

- Molecule 20 is a protein called 40S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	142	Total	C	N	O	S	0	0
			1172	736	236	199	1		

- Molecule 21 is a protein called 40S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 22 is a protein called 40S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	101	Total	C	N	O	S	0	0
			803	502	153	144	4		

- Molecule 23 is a protein called 40S RIBOSOMAL PROTEIN S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 24 is a protein called 40S RIBOSOMAL PROTEIN S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	129	Total	C	N	O	S	0	0
			1033	659	193	175	6		

- Molecule 25 is a protein called 40S RIBOSOMAL PROTEIN S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	134	Total	C	N	O	S	0	0
			1046	663	205	176	2		

- Molecule 26 is a protein called 40S RIBOSOMAL PROTEIN S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	122	Total	C	N	O	S	0	0
			1002	635	196	166	5		

- Molecule 27 is a protein called 40S RIBOSOMAL PROTEIN S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	76	Total	C	N	O	S	0	0
			605	387	112	105	1		

- Molecule 28 is a protein called 40S RIBOSOMAL PROTEIN S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	96	Total	C	N	O	S	0	0
			767	476	159	127	5		

- Molecule 29 is a protein called 40S RIBOSOMAL PROTEIN S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	80	Total	C	N	O	S	0	0
			625	391	116	111	7		

- Molecule 30 is a protein called 40S RIBOSOMAL PROTEIN S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	62	Total	C	N	O	S	0	0
			490	298	99	91	2		

- Molecule 31 is a protein called 40S RIBOSOMAL PROTEIN S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	53	Total	C	N	O	S	0	0
			444	278	90	71	5		

- Molecule 32 is a protein called 40S RIBOSOMAL PROTEIN S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	51	Total	C	N	O	S	0	0
			412	258	90	63	1		

- Molecule 33 is a protein called UBIQUITIN-40S RIBOSOMAL PROTEIN S27A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	61	Total	C	N	O	S	0	0
			497	312	94	84	7		

- Molecule 34 is a protein called GUANINE NUCLEOTIDE-BINDING PROTEIN SUBUNIT BETA-2-LIKE 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	g	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 35 is a protein called EUKARYOTIC PEPTIDE CHAIN RELEASE FACTOR SUBUNIT 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	h	436	Total	C	N	O	S	0	0
			3450	2193	582	663	12		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	438	LEU	-	expression tag	UNP P62495
h	439	GLU	-	expression tag	UNP P62495
h	440	HIS	-	expression tag	UNP P62495

- Molecule 36 is a protein called EUKARYOTIC PEPTIDE CHAIN RELEASE FACTOR GTP-BINDING SUBUNIT ERF3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	426	Total	C	N	O	S	0	0
			3357	2135	577	624	21		

- Molecule 37 is a RNA chain called CRICKET PARALYSIS VIRUS IRES RNA.

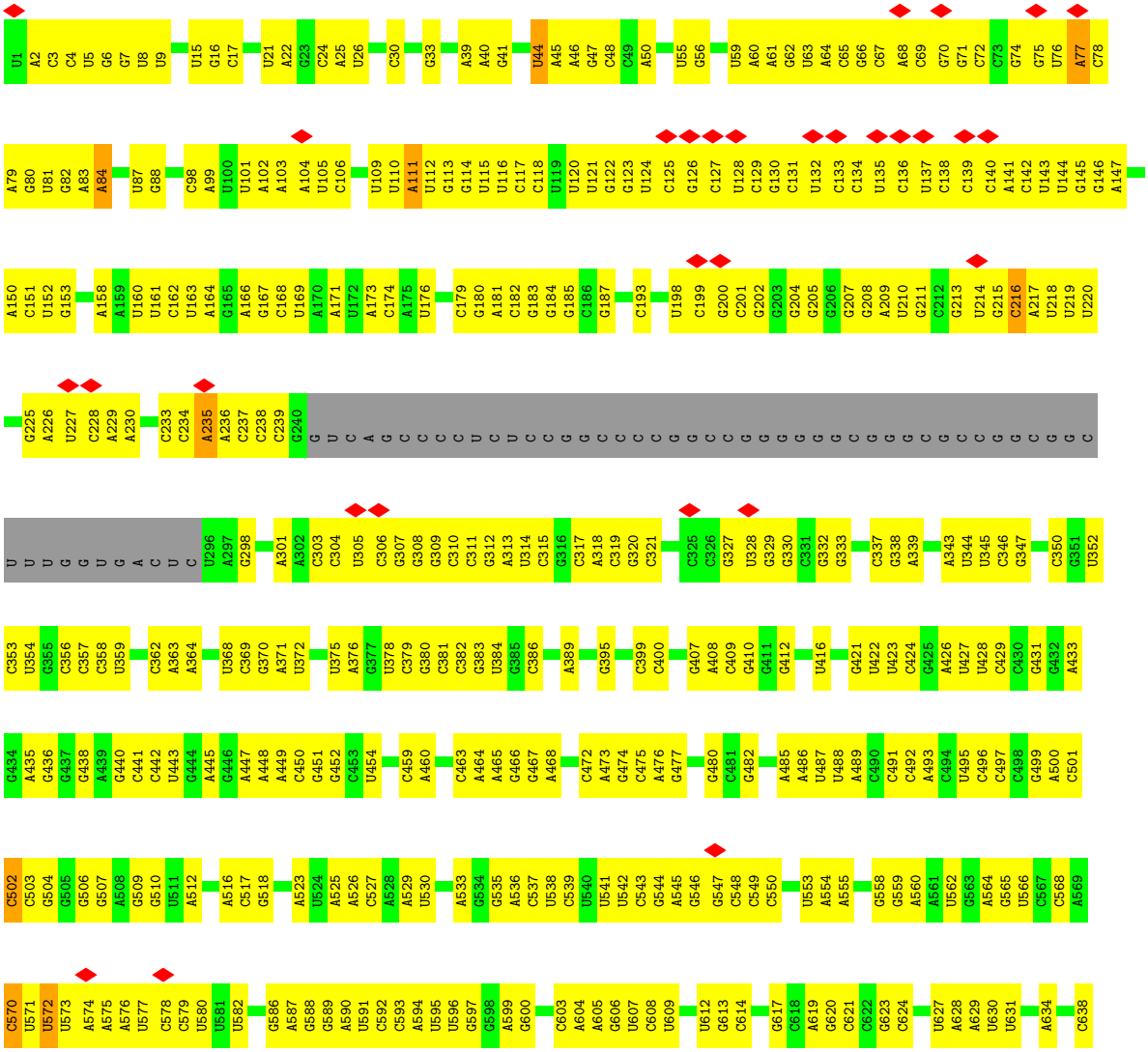
Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	201	Total	C	N	O	P	0	0
			4257	1908	735	1413	201		

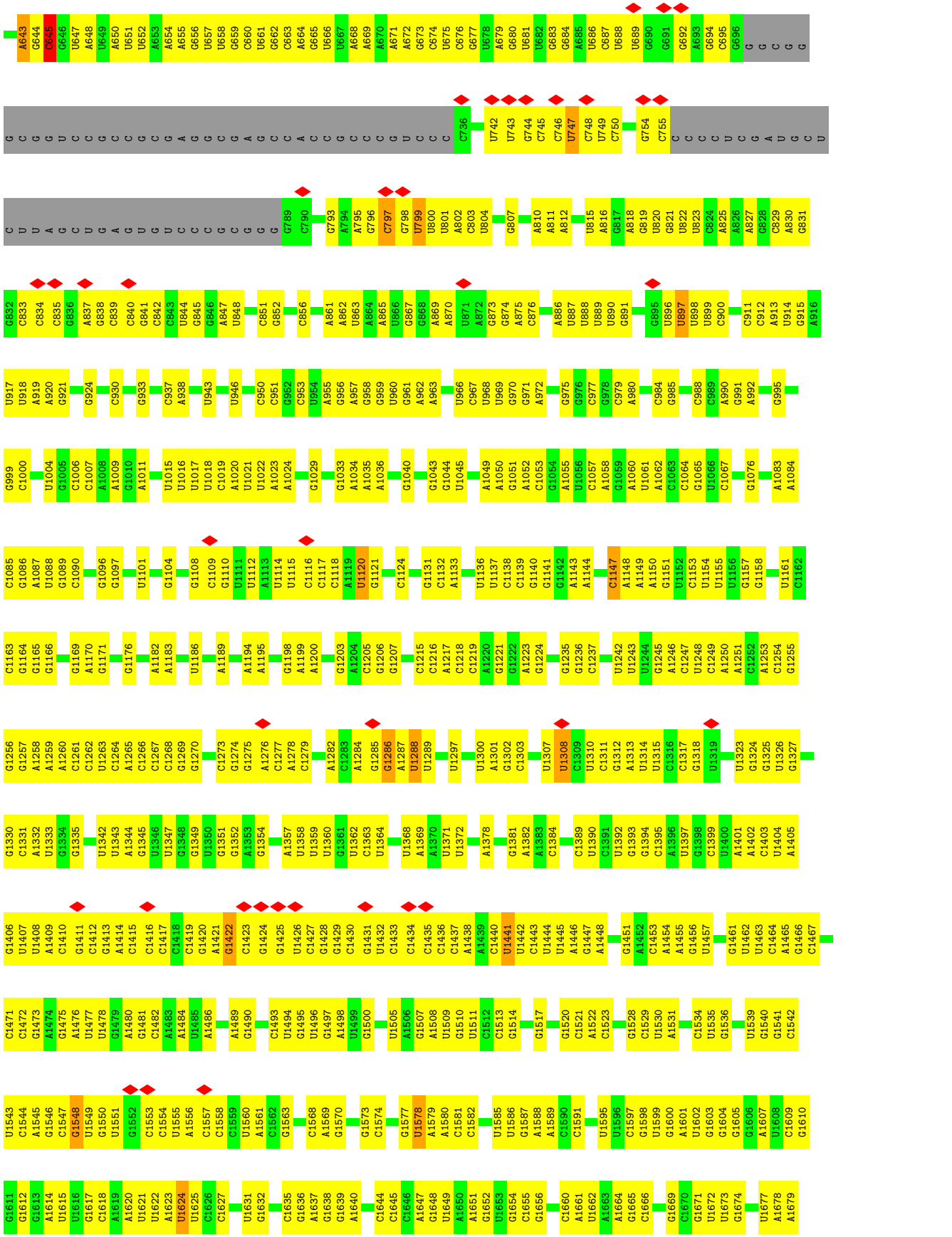
3 Residue-property plots (i)

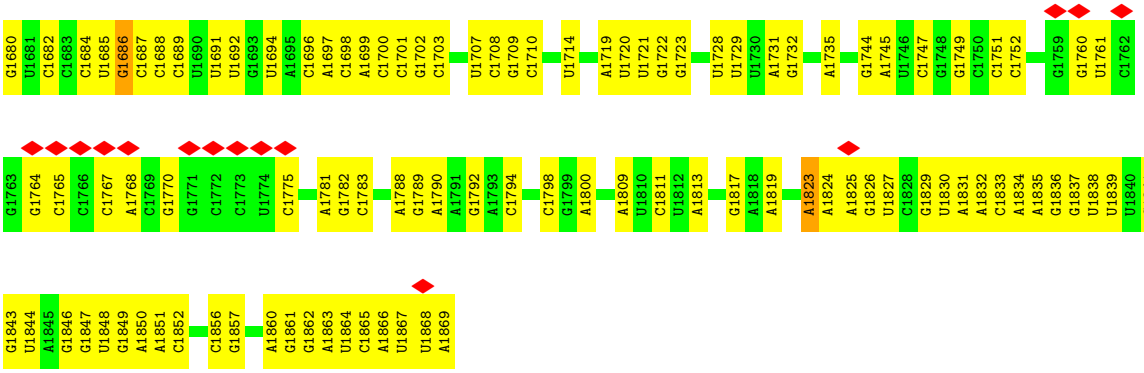
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 18S RRNA

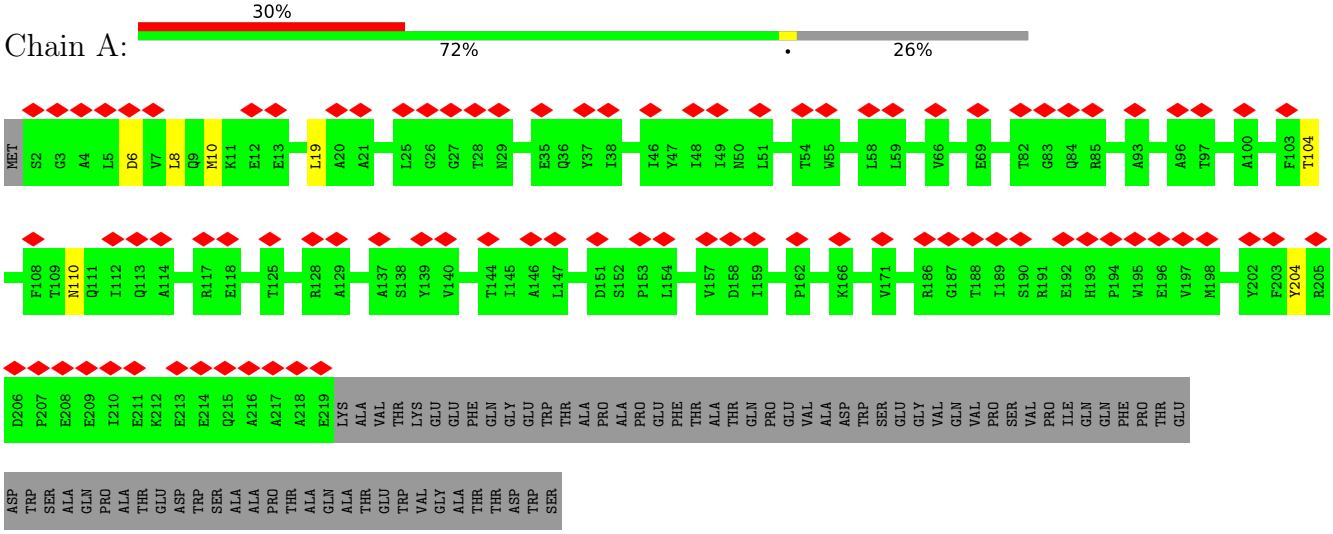
Chain 1:



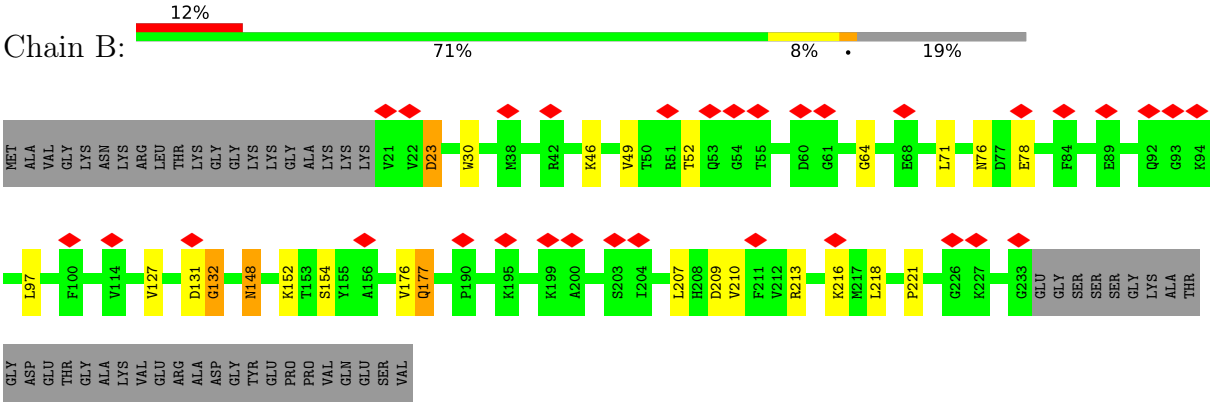




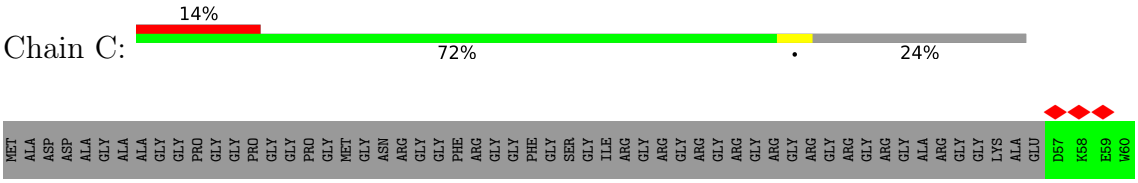
• Molecule 2: 40S RIBOSOMAL PROTEIN SA

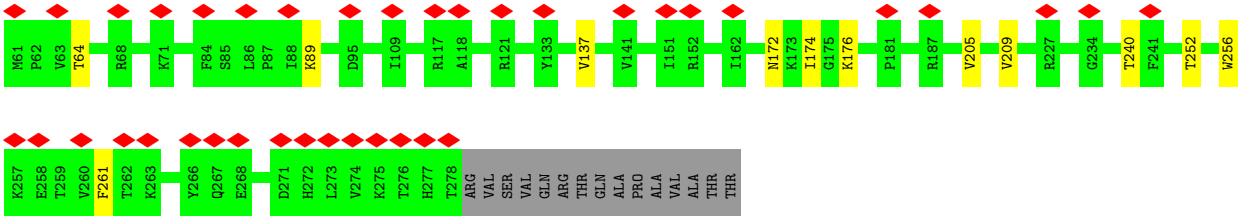


• Molecule 3: 40S RIBOSOMAL PROTEIN S3A

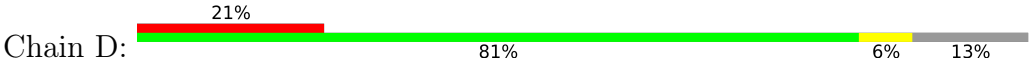


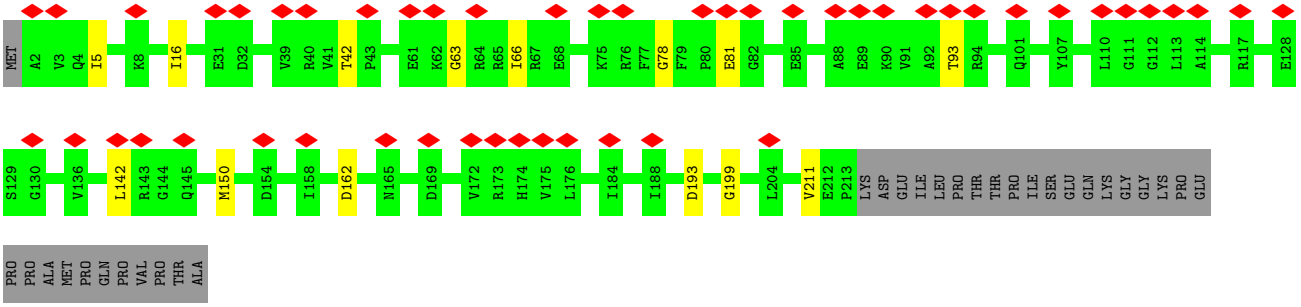
• Molecule 4: 40S RIBOSOMAL PROTEIN S2



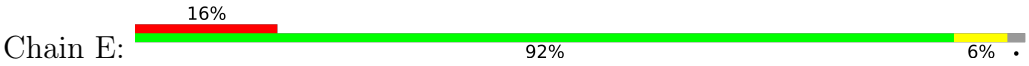


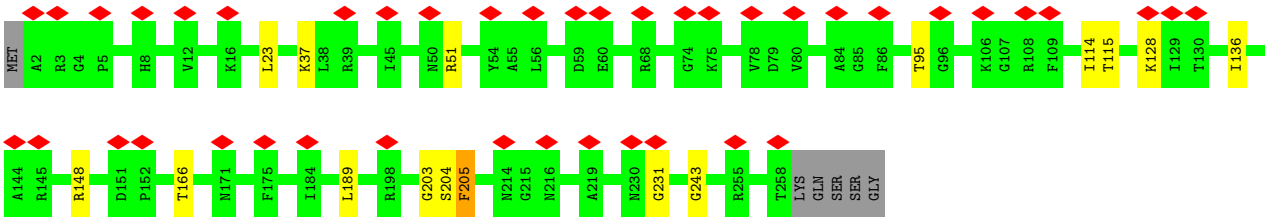
• Molecule 5: 40S RIBOSOMAL PROTEIN S3



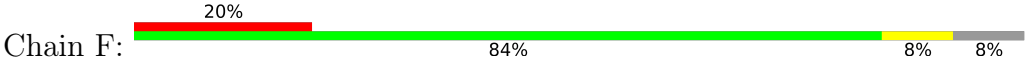


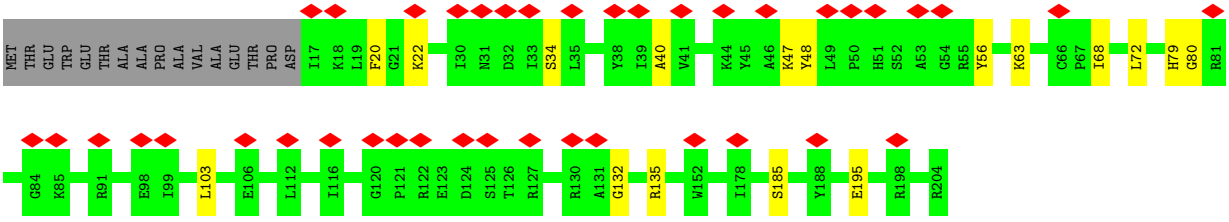
• Molecule 6: 40S RIBOSOMAL PROTEIN S4, Y ISOFORM 1



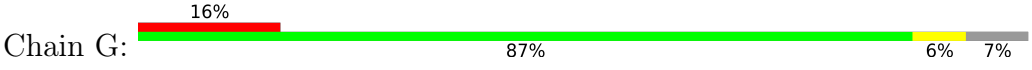


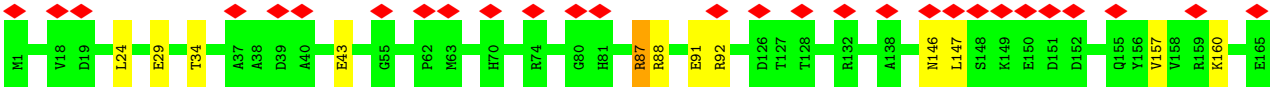
• Molecule 7: 40S RIBOSOMAL PROTEIN S5

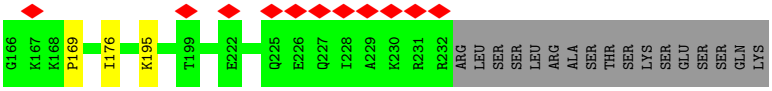




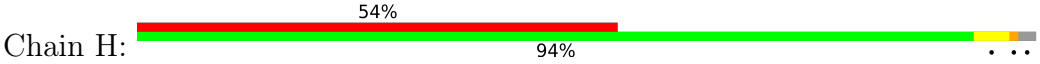
• Molecule 8: 40S RIBOSOMAL PROTEIN S6

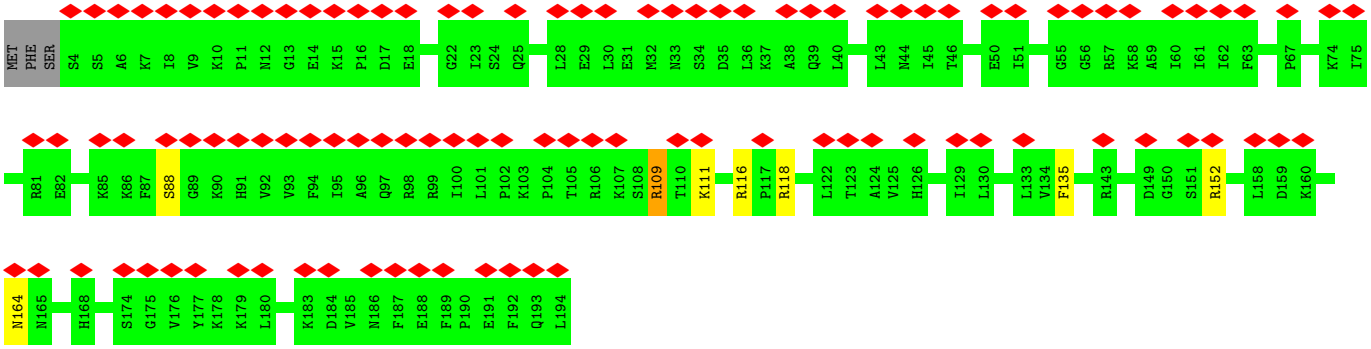




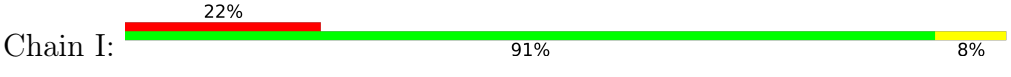


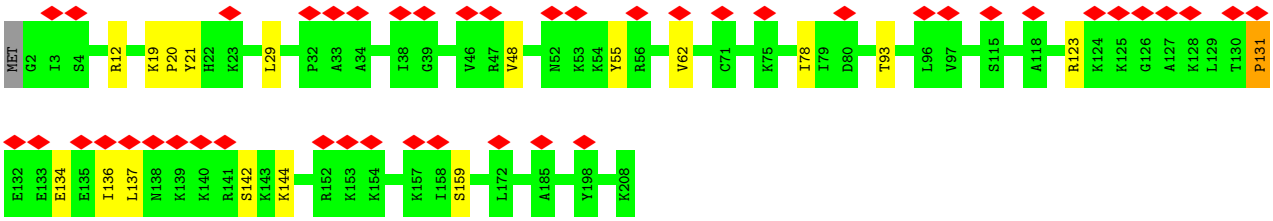
• Molecule 9: 40S RIBOSOMAL PROTEIN S7



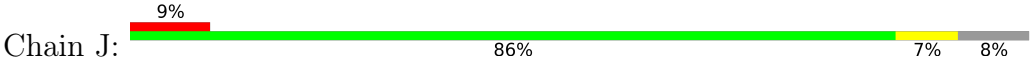


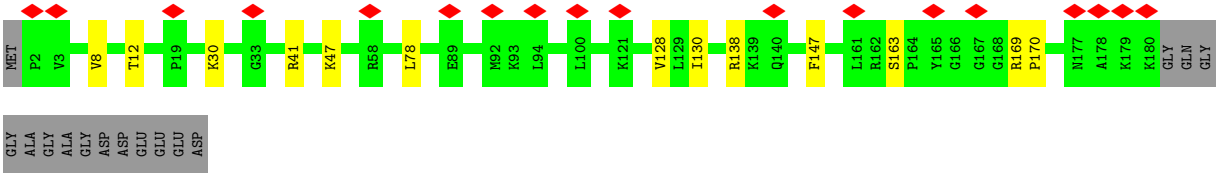
• Molecule 10: 40S RIBOSOMAL PROTEIN S8



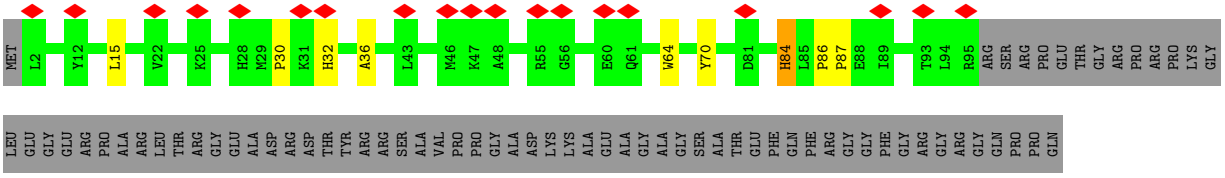


• Molecule 11: 40S RIBOSOMAL PROTEIN S9



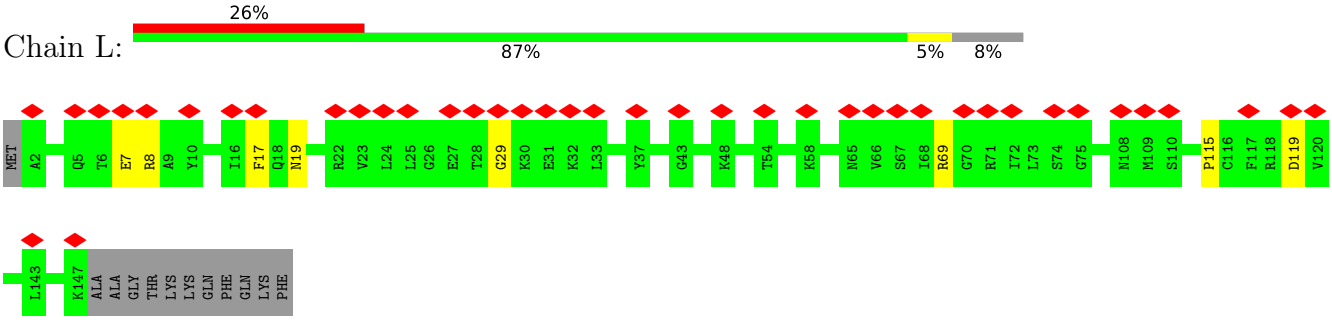


• Molecule 12: 40S RIBOSOMAL PROTEIN S10



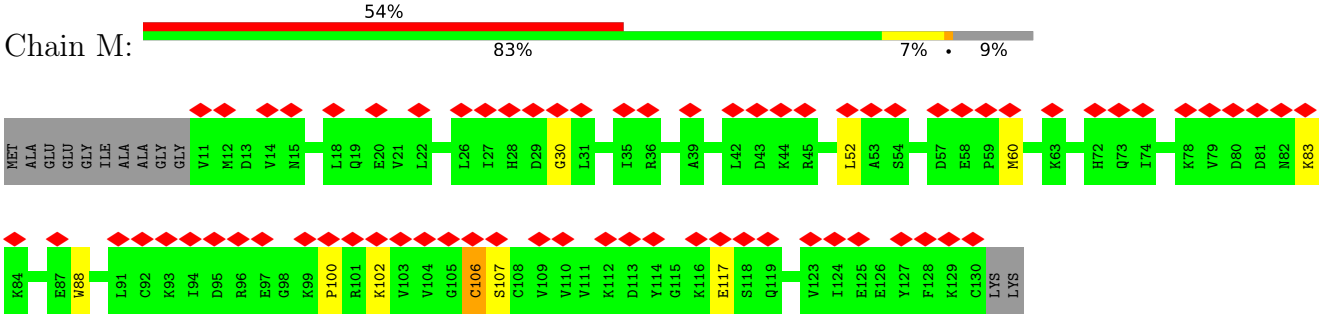
• Molecule 13: 40S RIBOSOMAL PROTEIN S11

Chain L:



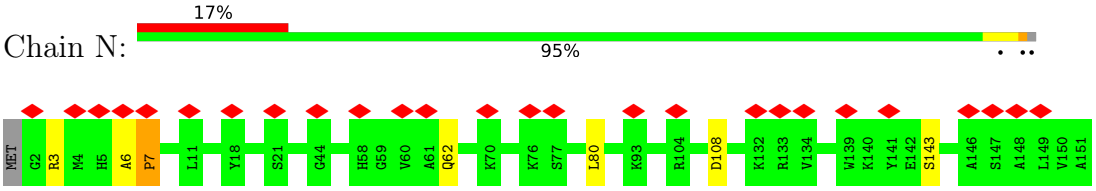
• Molecule 14: 40S RIBOSOMAL PROTEIN S12

Chain M:



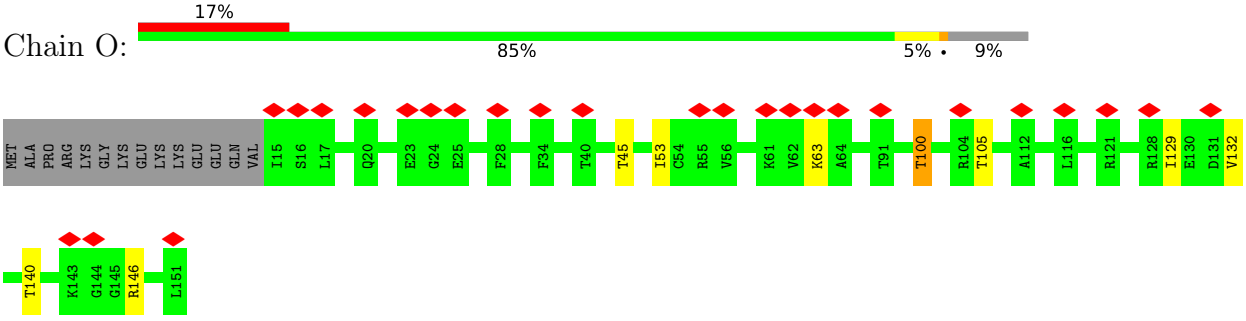
• Molecule 15: 40S RIBOSOMAL PROTEIN S13

Chain N:



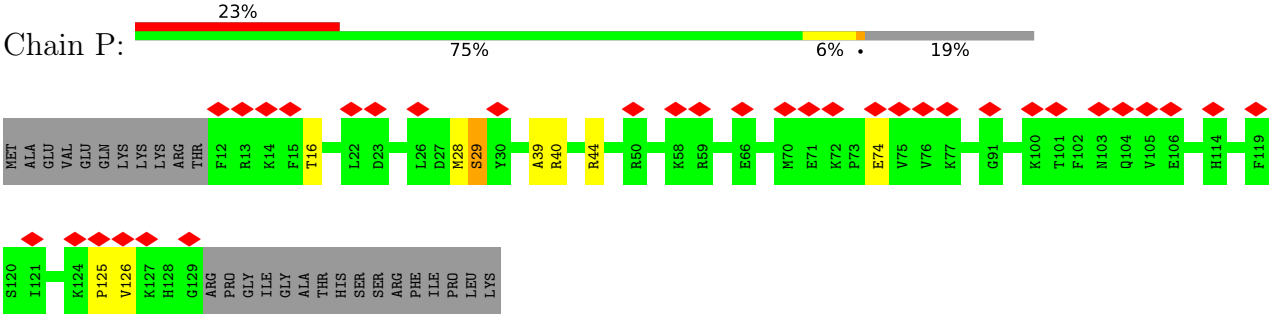
• Molecule 16: 40S RIBOSOMAL PROTEIN S14

Chain O:



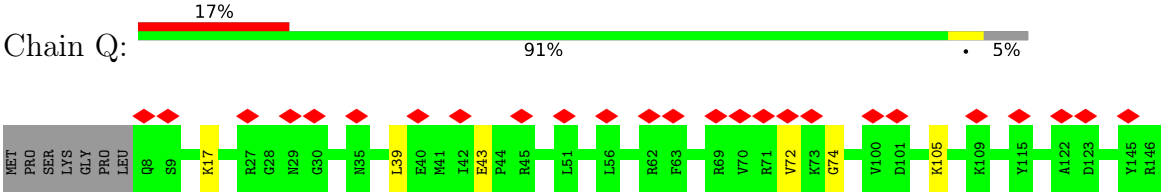
• Molecule 17: 40S RIBOSOMAL PROTEIN S15

Chain P:



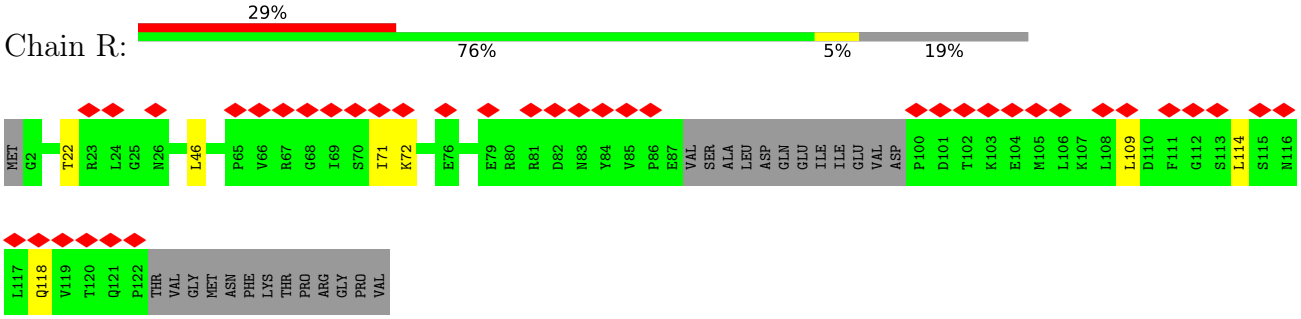
• Molecule 18: 40S RIBOSOMAL PROTEIN S16

Chain Q:



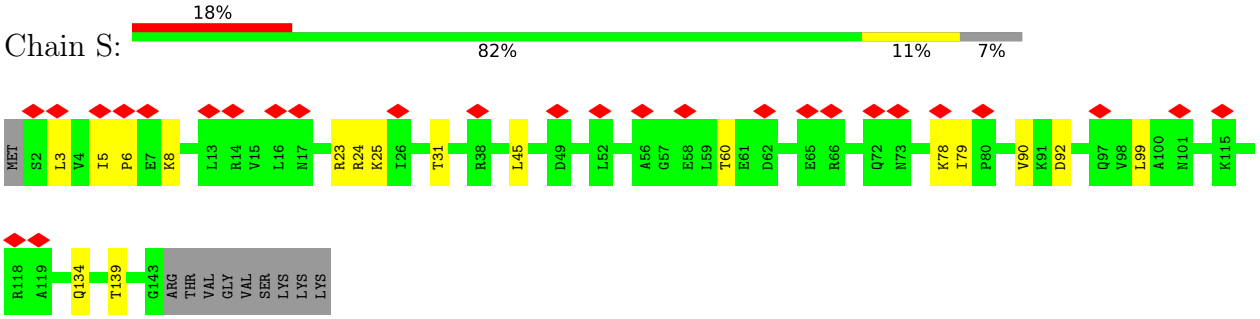
• Molecule 19: 40S RIBOSOMAL PROTEIN S17

Chain R:



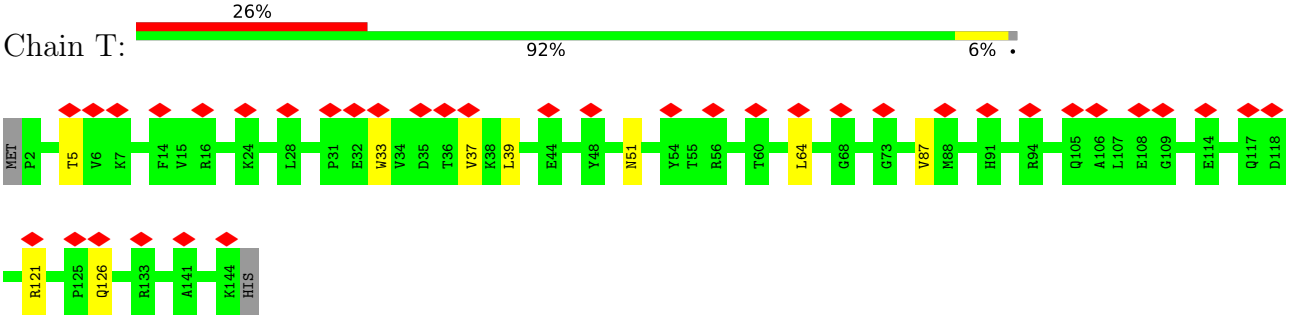
• Molecule 20: 40S RIBOSOMAL PROTEIN S18

Chain S:



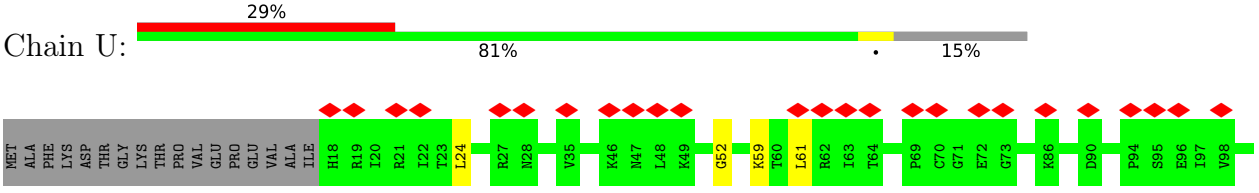
• Molecule 21: 40S RIBOSOMAL PROTEIN S19

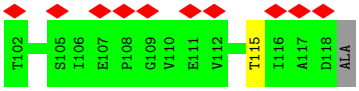
Chain T:



• Molecule 22: 40S RIBOSOMAL PROTEIN S20

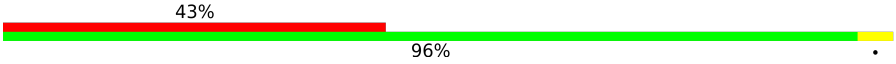
Chain U:

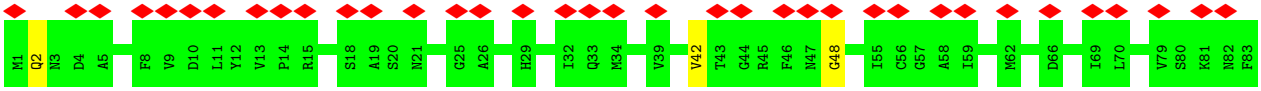




• Molecule 23: 40S RIBOSOMAL PROTEIN S21

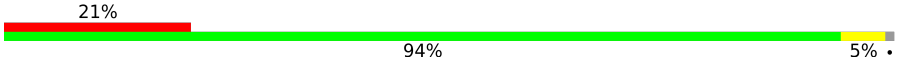
Chain V:

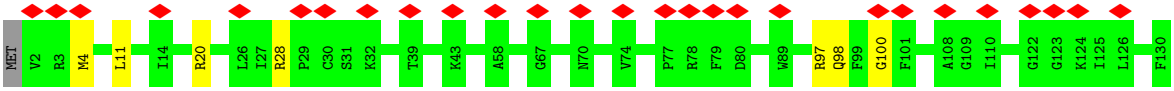




• Molecule 24: 40S RIBOSOMAL PROTEIN S15A

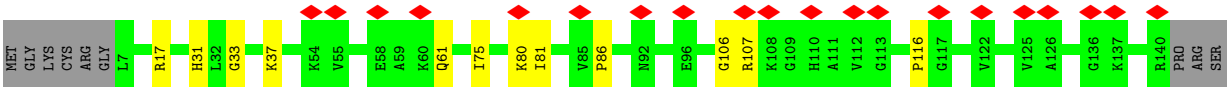
Chain W:





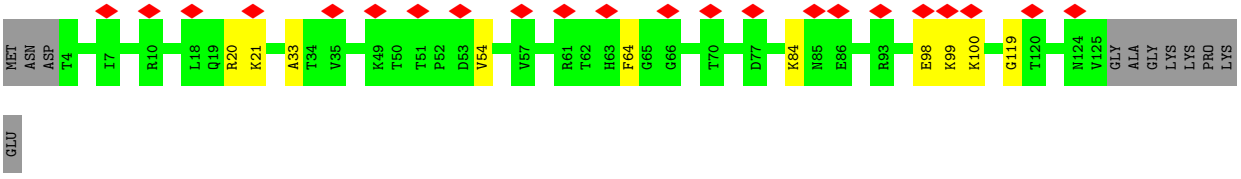
• Molecule 25: 40S RIBOSOMAL PROTEIN S23

Chain X:



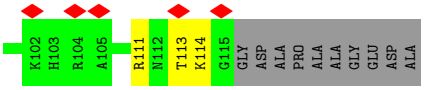
• Molecule 26: 40S RIBOSOMAL PROTEIN S24

Chain Y:



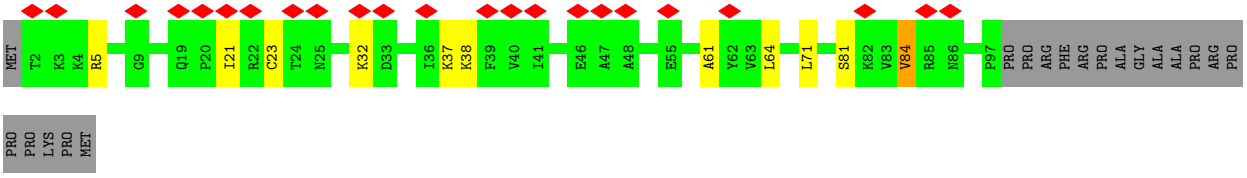
• Molecule 27: 40S RIBOSOMAL PROTEIN S25

Chain Z:

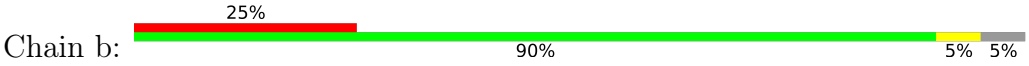


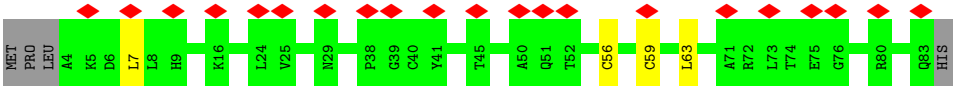
• Molecule 28: 40S RIBOSOMAL PROTEIN S26

Chain a:

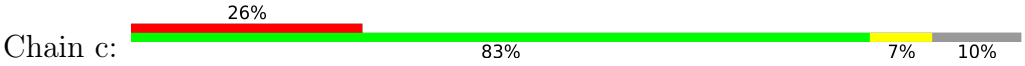


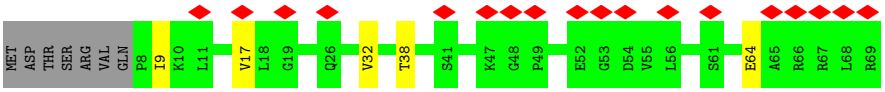
• Molecule 29: 40S RIBOSOMAL PROTEIN S27



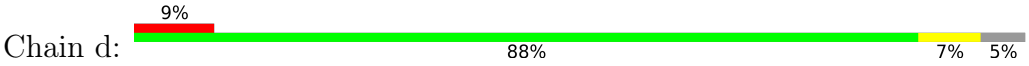


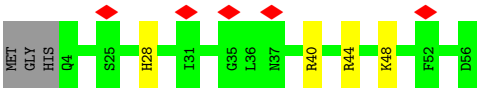
• Molecule 30: 40S RIBOSOMAL PROTEIN S28



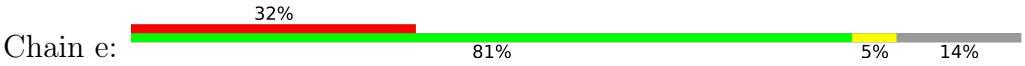


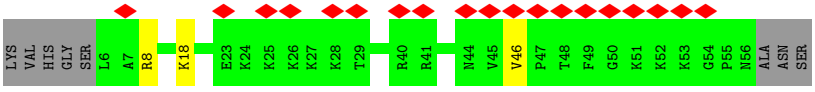
• Molecule 31: 40S RIBOSOMAL PROTEIN S29



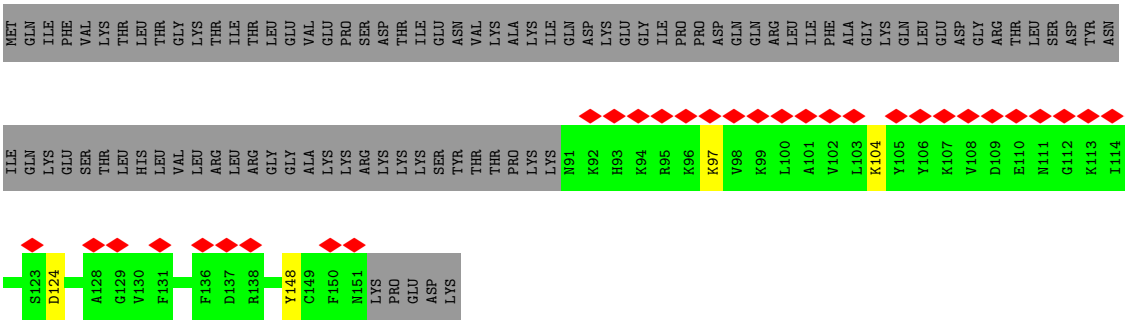


• Molecule 32: 40S RIBOSOMAL PROTEIN S30



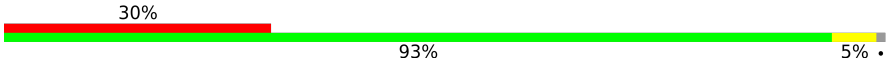


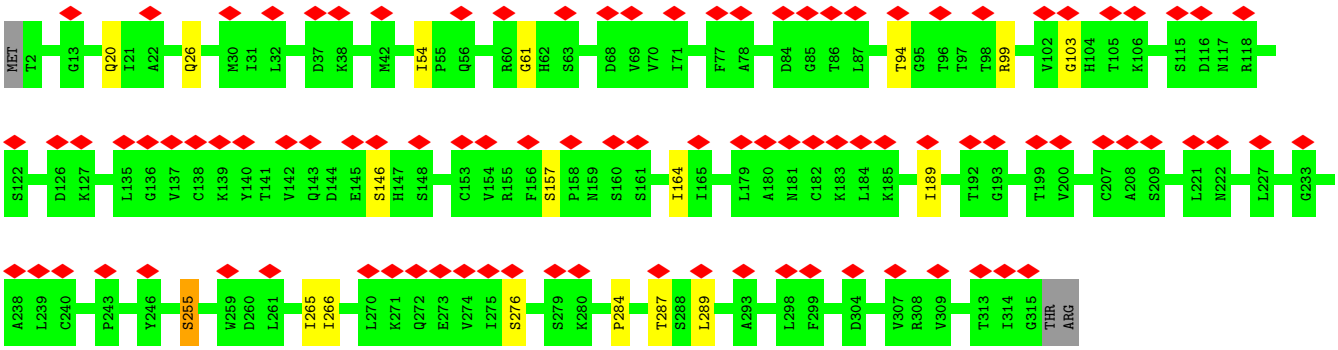
• Molecule 33: UBIQUITIN-40S RIBOSOMAL PROTEIN S27A



• Molecule 34: GUANINE NUCLEOTIDE-BINDING PROTEIN SUBUNIT BETA-2-LIKE 1

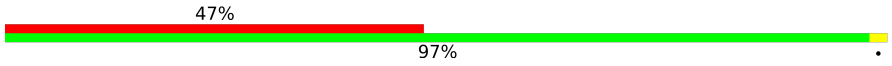
Chain g:

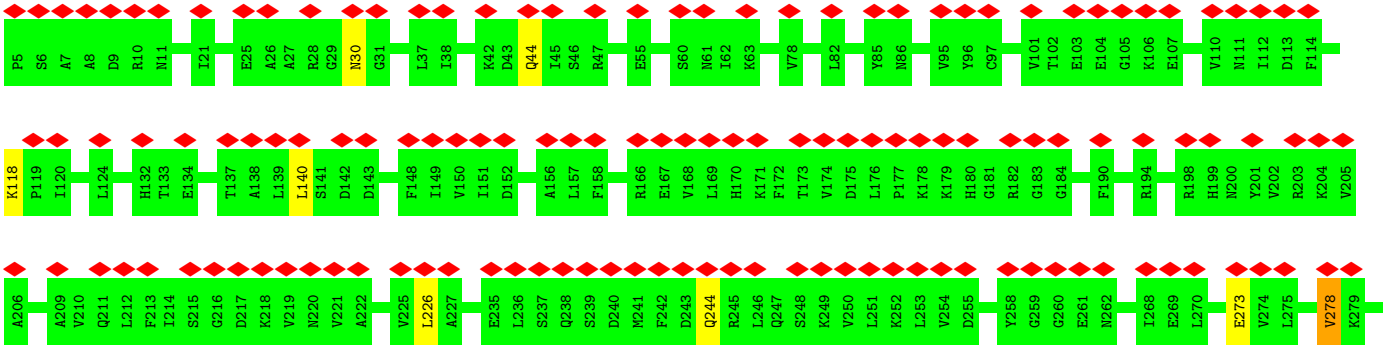




• Molecule 35: EUKARYOTIC PEPTIDE CHAIN RELEASE FACTOR SUBUNIT 1

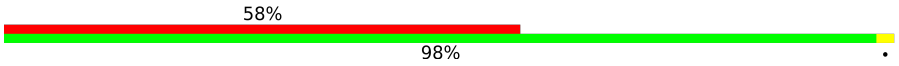
Chain h:

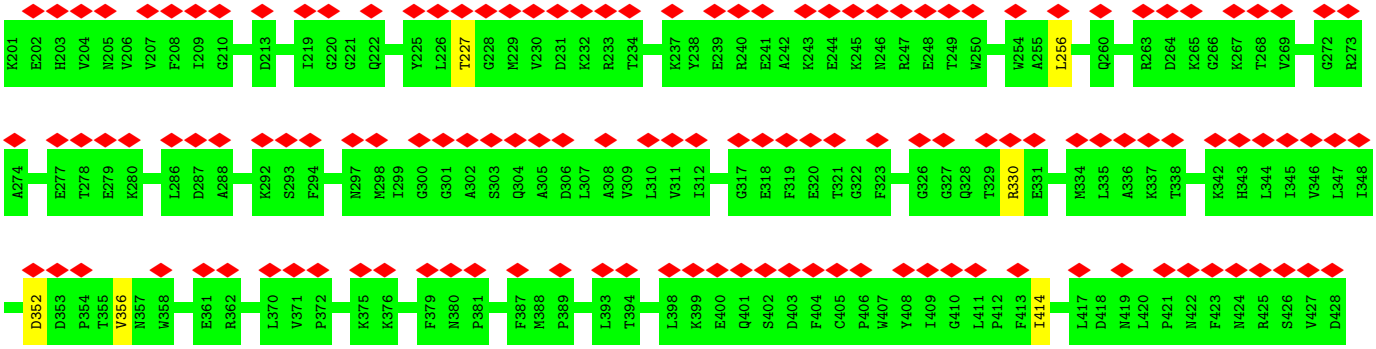


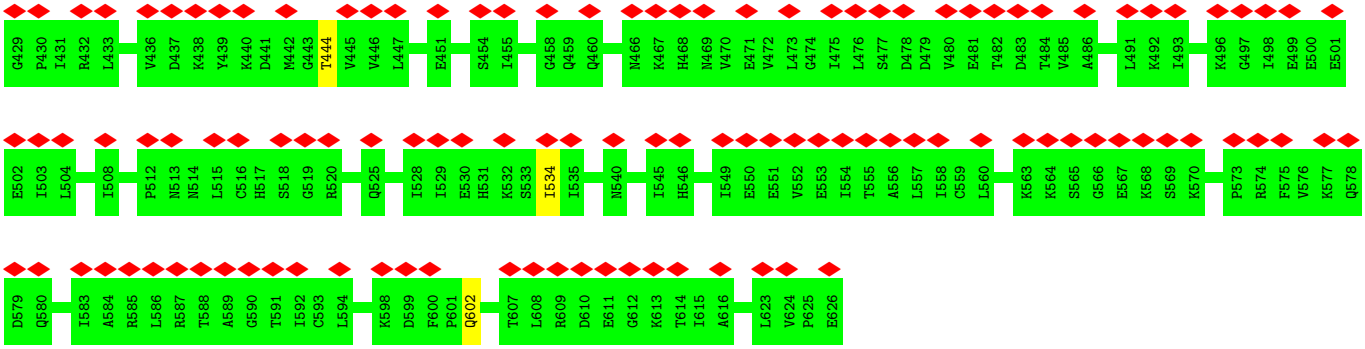


• Molecule 36: EUKARYOTIC PEPTIDE CHAIN RELEASE FACTOR GTP-BINDING SUBUNIT ERF3A

Chain i:

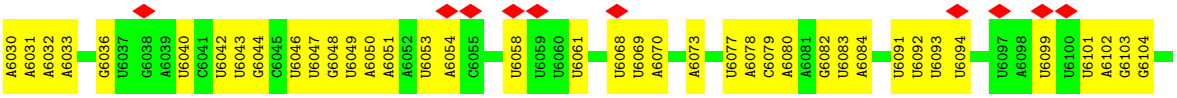


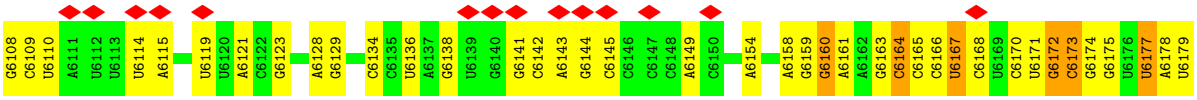


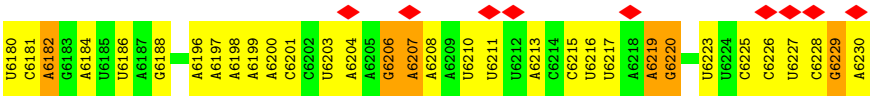


• Molecule 37: CRICKET PARALYSIS VIRUS IRES RNA

Chain j:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	64902	Depositor
Resolution determination method	Not provided	
CTF correction method	DEFOCUS GROUPS	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	194805	Depositor
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor
Maximum map value	12.165	Depositor
Minimum map value	-4.363	Depositor
Average map value	0.164	Depositor
Map value standard deviation	0.954	Depositor
Recommended contour level	3.0	Depositor
Map size (Å)	467.99997, 467.99997, 467.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.56, 1.56, 1.56	Depositor

5 Model quality

5.1 Standard geometry

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	1	0.37	2/41550 (0.0%)	0.80	6/64763 (0.0%)
2	A	0.51	0/1756	0.68	0/2386
3	B	0.51	0/1756	0.75	1/2350 (0.0%)
4	C	0.42	0/1761	0.65	0/2379
5	D	0.41	0/1672	0.66	0/2250
6	E	0.47	0/2072	0.70	0/2793
7	F	0.43	0/1507	0.74	0/2026
8	G	0.48	0/1907	0.74	0/2538
9	H	0.46	0/1558	0.74	1/2087 (0.0%)
10	I	0.48	0/1724	0.72	0/2298
11	J	0.45	0/1520	0.77	0/2030
12	K	0.48	0/815	0.68	0/1101
13	L	0.45	0/1220	0.72	0/1633
14	M	0.48	0/941	0.72	0/1264
15	N	0.43	0/1231	0.73	1/1656 (0.1%)
16	O	0.46	0/1036	0.71	0/1391
17	P	0.43	0/1000	0.67	0/1335
18	Q	0.43	0/1125	0.66	0/1506
19	R	0.42	0/904	0.67	0/1208
20	S	0.42	0/1190	0.68	0/1594
21	T	0.44	0/1131	0.69	0/1515
22	U	0.50	0/813	0.70	0/1092
23	V	0.47	0/643	0.71	0/860
24	W	0.44	0/1050	0.69	0/1406
25	X	0.46	0/1063	0.70	0/1421
26	Y	0.45	0/1019	0.70	0/1354
27	Z	0.46	0/611	0.71	0/820
28	a	0.48	0/778	0.75	1/1041 (0.1%)
29	b	0.48	0/637	0.68	0/854
30	c	0.46	0/492	0.74	0/657
31	d	0.51	0/454	0.77	0/603
32	e	0.45	0/417	0.69	0/548
33	f	0.53	0/507	0.84	1/673 (0.1%)
34	g	0.45	0/2497	0.67	0/3399

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	h	0.35	0/3506	0.56	0/4709
36	i	0.37	0/3418	0.55	0/4600
37	j	1.42	85/4752 (1.8%)	1.74	207/7383 (2.8%)
All	All	0.52	87/92033 (0.1%)	0.83	218/133523 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	24
37	j	0	1
All	All	0	25

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	j	6173	C	O3'-P	-20.14	1.36	1.61
37	j	6229	G	O3'-P	19.64	1.84	1.61
37	j	6079	C	N3-C4	19.19	1.47	1.33
37	j	6177	U	O3'-P	-18.39	1.39	1.61
37	j	6219	A	O3'-P	-15.97	1.42	1.61

The worst 5 of 218 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	j	6079	C	C5-C6-N1	19.25	130.62	121.00
37	j	6114	U	C4-C5-C6	-18.58	108.55	119.70
37	j	6114	U	N3-C4-C5	17.39	125.03	114.60
37	j	6077	U	C2-N3-C4	-15.00	118.00	127.00
37	j	6161	A	N1-C2-N3	-15.00	121.80	129.30

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	111	A	Sidechain
1	1	44	U	Sidechain
1	1	77	A	Sidechain
1	1	84	A	Sidechain

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Mol	Chain	Res	Type	Group
1	1	88	G	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
2	A	216/295 (73%)	209 (97%)	5 (2%)	2 (1%)	17 57
3	B	211/264 (80%)	176 (83%)	18 (8%)	17 (8%)	1 12
4	C	220/293 (75%)	213 (97%)	2 (1%)	5 (2%)	6 34
5	D	210/243 (86%)	201 (96%)	4 (2%)	5 (2%)	6 33
6	E	255/263 (97%)	237 (93%)	13 (5%)	5 (2%)	7 38
7	F	186/204 (91%)	163 (88%)	13 (7%)	10 (5%)	2 19
8	G	230/249 (92%)	216 (94%)	5 (2%)	9 (4%)	3 23
9	H	189/194 (97%)	178 (94%)	7 (4%)	4 (2%)	7 36
10	I	205/208 (99%)	184 (90%)	14 (7%)	7 (3%)	3 26
11	J	177/194 (91%)	168 (95%)	6 (3%)	3 (2%)	9 42
12	K	92/165 (56%)	84 (91%)	1 (1%)	7 (8%)	1 13
13	L	144/158 (91%)	133 (92%)	5 (4%)	6 (4%)	3 22
14	M	118/132 (89%)	111 (94%)	1 (1%)	6 (5%)	2 19
15	N	148/151 (98%)	138 (93%)	5 (3%)	5 (3%)	3 26
16	O	135/151 (89%)	129 (96%)	3 (2%)	3 (2%)	6 35
17	P	116/145 (80%)	106 (91%)	5 (4%)	5 (4%)	2 22
18	Q	137/146 (94%)	129 (94%)	6 (4%)	2 (2%)	10 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	R	105/135 (78%)	99 (94%)	4 (4%)	2 (2%)	8 38
20	S	140/152 (92%)	125 (89%)	7 (5%)	8 (6%)	1 18
21	T	141/145 (97%)	135 (96%)	4 (3%)	2 (1%)	11 46
22	U	99/119 (83%)	95 (96%)	3 (3%)	1 (1%)	15 55
23	V	81/83 (98%)	78 (96%)	1 (1%)	2 (2%)	5 32
24	W	127/130 (98%)	118 (93%)	7 (6%)	2 (2%)	9 44
25	X	132/143 (92%)	120 (91%)	5 (4%)	7 (5%)	2 19
26	Y	120/133 (90%)	114 (95%)	2 (2%)	4 (3%)	4 26
27	Z	74/125 (59%)	71 (96%)	0	3 (4%)	3 23
28	a	94/115 (82%)	85 (90%)	5 (5%)	4 (4%)	2 22
29	b	78/84 (93%)	70 (90%)	8 (10%)	0	100 100
30	c	60/69 (87%)	57 (95%)	1 (2%)	2 (3%)	4 26
31	d	51/56 (91%)	44 (86%)	7 (14%)	0	100 100
32	e	49/59 (83%)	43 (88%)	5 (10%)	1 (2%)	7 38
33	f	59/156 (38%)	53 (90%)	6 (10%)	0	100 100
34	g	312/317 (98%)	291 (93%)	14 (4%)	7 (2%)	6 35
35	h	428/436 (98%)	410 (96%)	14 (3%)	4 (1%)	17 57
36	i	414/426 (97%)	403 (97%)	9 (2%)	2 (0%)	29 69
All	All	5553/6338 (88%)	5186 (93%)	215 (4%)	152 (3%)	8 31

5 of 152 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	76	ASN
3	B	132	GLY
3	B	148	ASN
3	B	154	SER
3	B	176	VAL

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	181/243 (74%)	176 (97%)	5 (3%)	43	65
3	B	194/231 (84%)	183 (94%)	11 (6%)	20	45
4	C	188/225 (84%)	181 (96%)	7 (4%)	34	58
5	D	175/202 (87%)	166 (95%)	9 (5%)	24	48
6	E	220/225 (98%)	208 (94%)	12 (6%)	21	47
7	F	158/170 (93%)	151 (96%)	7 (4%)	28	53
8	G	202/218 (93%)	195 (96%)	7 (4%)	36	59
9	H	171/174 (98%)	167 (98%)	4 (2%)	50	70
10	I	179/180 (99%)	167 (93%)	12 (7%)	16	41
11	J	160/168 (95%)	150 (94%)	10 (6%)	18	43
12	K	85/136 (62%)	82 (96%)	3 (4%)	36	59
13	L	133/142 (94%)	131 (98%)	2 (2%)	65	80
14	M	102/108 (94%)	97 (95%)	5 (5%)	25	50
15	N	130/131 (99%)	128 (98%)	2 (2%)	65	80
16	O	107/119 (90%)	100 (94%)	7 (6%)	17	42
17	P	107/130 (82%)	102 (95%)	5 (5%)	26	51
18	Q	115/121 (95%)	111 (96%)	4 (4%)	36	59
19	R	99/122 (81%)	94 (95%)	5 (5%)	24	48
20	S	123/132 (93%)	114 (93%)	9 (7%)	14	39
21	T	113/115 (98%)	106 (94%)	7 (6%)	18	43
22	U	93/107 (87%)	89 (96%)	4 (4%)	29	53
23	V	67/67 (100%)	66 (98%)	1 (2%)	65	80
24	W	112/113 (99%)	107 (96%)	5 (4%)	27	52
25	X	108/115 (94%)	103 (95%)	5 (5%)	27	52
26	Y	107/115 (93%)	101 (94%)	6 (6%)	21	46
27	Z	67/103 (65%)	63 (94%)	4 (6%)	19	44
28	a	83/98 (85%)	76 (92%)	7 (8%)	11	33
29	b	72/76 (95%)	68 (94%)	4 (6%)	21	46
30	c	55/62 (89%)	52 (94%)	3 (6%)	21	47
31	d	47/49 (96%)	43 (92%)	4 (8%)	10	33
32	e	42/48 (88%)	40 (95%)	2 (5%)	25	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
33	f	54/140 (39%)	51 (94%)	3 (6%)	21 46
34	g	272/275 (99%)	260 (96%)	12 (4%)	28 53
35	h	376/376 (100%)	368 (98%)	8 (2%)	53 72
36	i	371/371 (100%)	364 (98%)	7 (2%)	57 75
All	All	4868/5407 (90%)	4660 (96%)	208 (4%)	33 53

5 of 208 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	R	109	LEU
25	X	17	ARG
35	h	333	LEU
20	S	8	LYS
21	T	87	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
21	T	63	HIS
28	a	19	GLN
36	i	578	GLN
22	U	100	GLN
25	X	73	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1738/1869 (92%)	1037 (59%)	152 (8%)
37	j	195/201 (97%)	50 (25%)	0
All	All	1933/2070 (93%)	1087 (56%)	152 (7%)

5 of 1087 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	A
1	1	3	C
1	1	4	C
1	1	5	U
1	1	6	G

5 of 152 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	1494	U
1	1	1824	A
1	1	1534	C
1	1	1637	A
1	1	1862	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
37	j	10
36	i	5
35	h	3

The worst 5 of 18 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	j	6150:C	O3'	6151:A	P	11.37
1	j	6065:A	O3'	6066:G	P	10.23
1	j	6106:U	O3'	6107:A	P	9.31
1	j	6136:U	O3'	6137:A	P	8.47

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	i	325:LYS	C	326:GLY	N	5.91

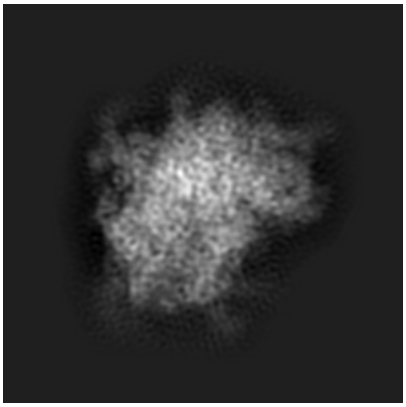
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2813. These allow visual inspection of the internal detail of the map and identification of artifacts.

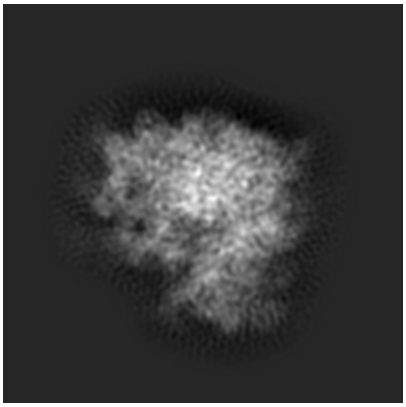
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

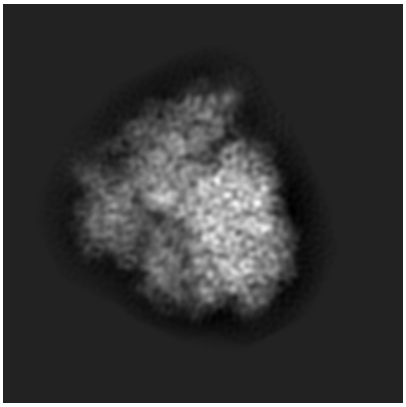
6.1.1 Primary map



X



Y

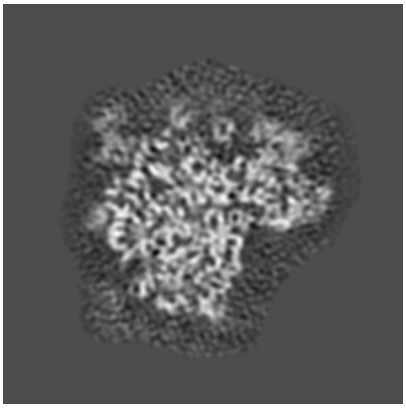


Z

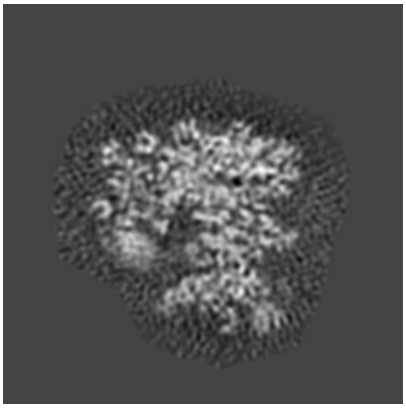
The images above show the map projected in three orthogonal directions.

6.2 Central slices

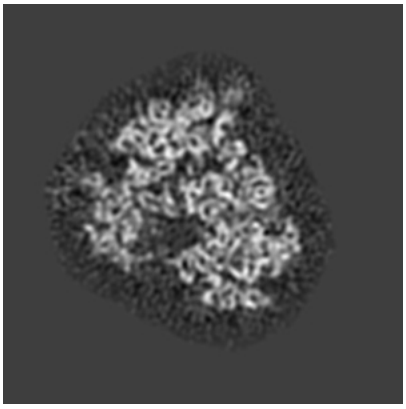
6.2.1 Primary map



X Index: 150



Y Index: 150

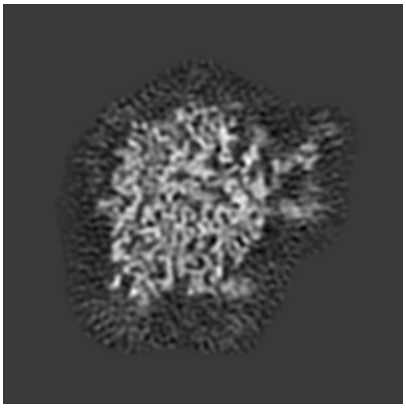


Z Index: 150

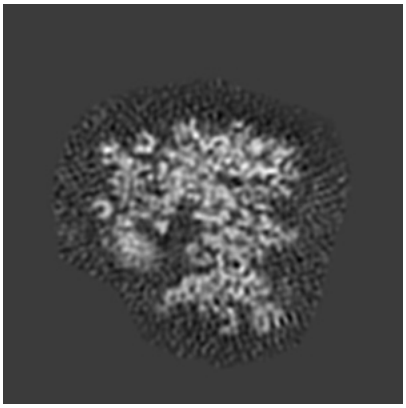
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

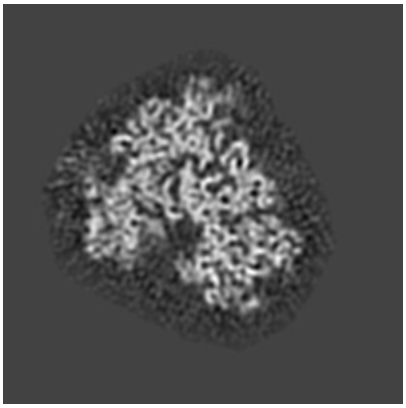
6.3.1 Primary map



X Index: 172



Y Index: 149



Z Index: 154

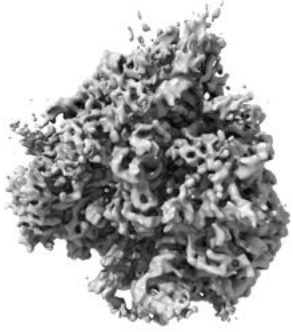
The images above show the largest variance slices of the map in three orthogonal directions.

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

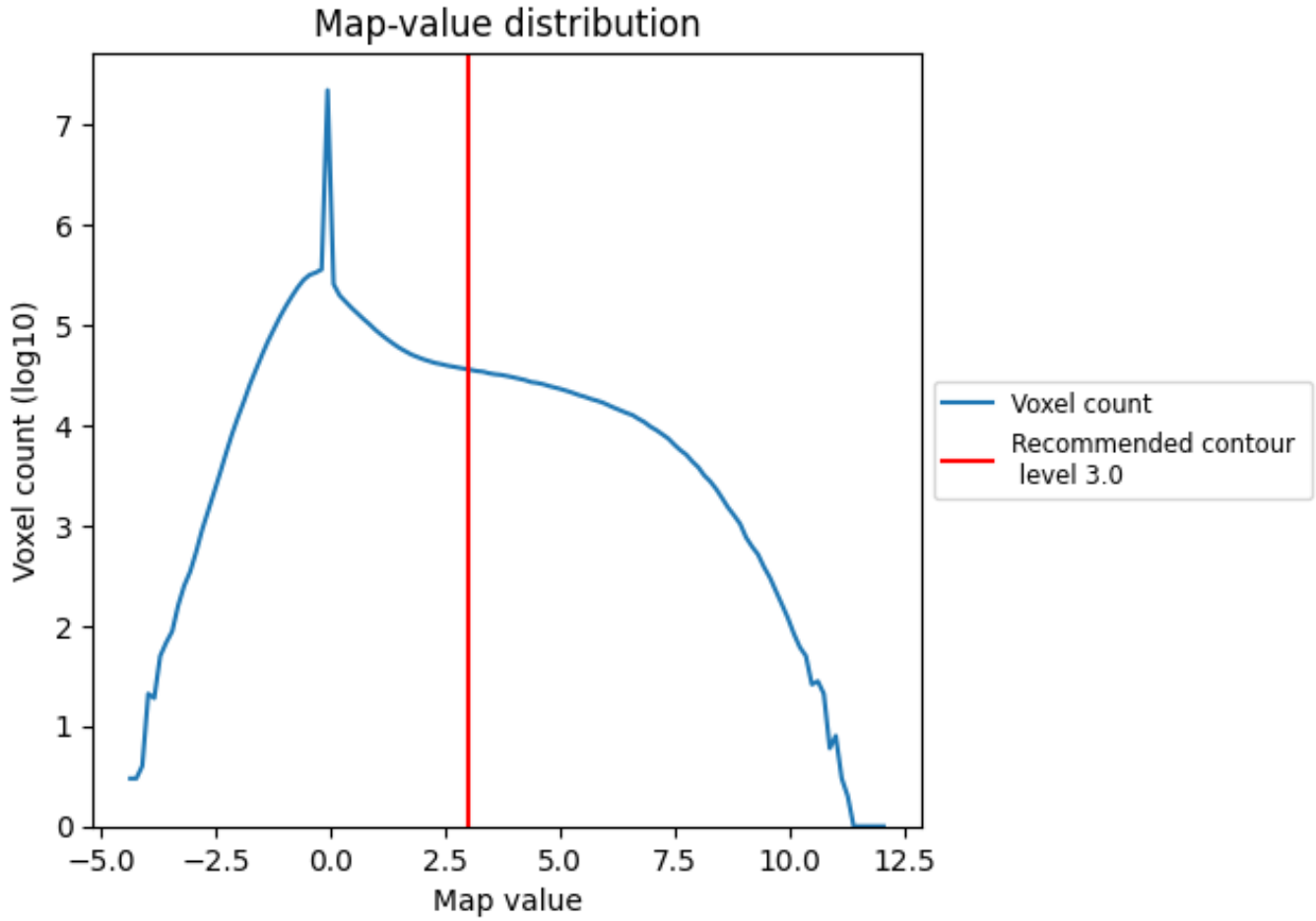
6.5 Mask visualisation (i)

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

7 Map analysis

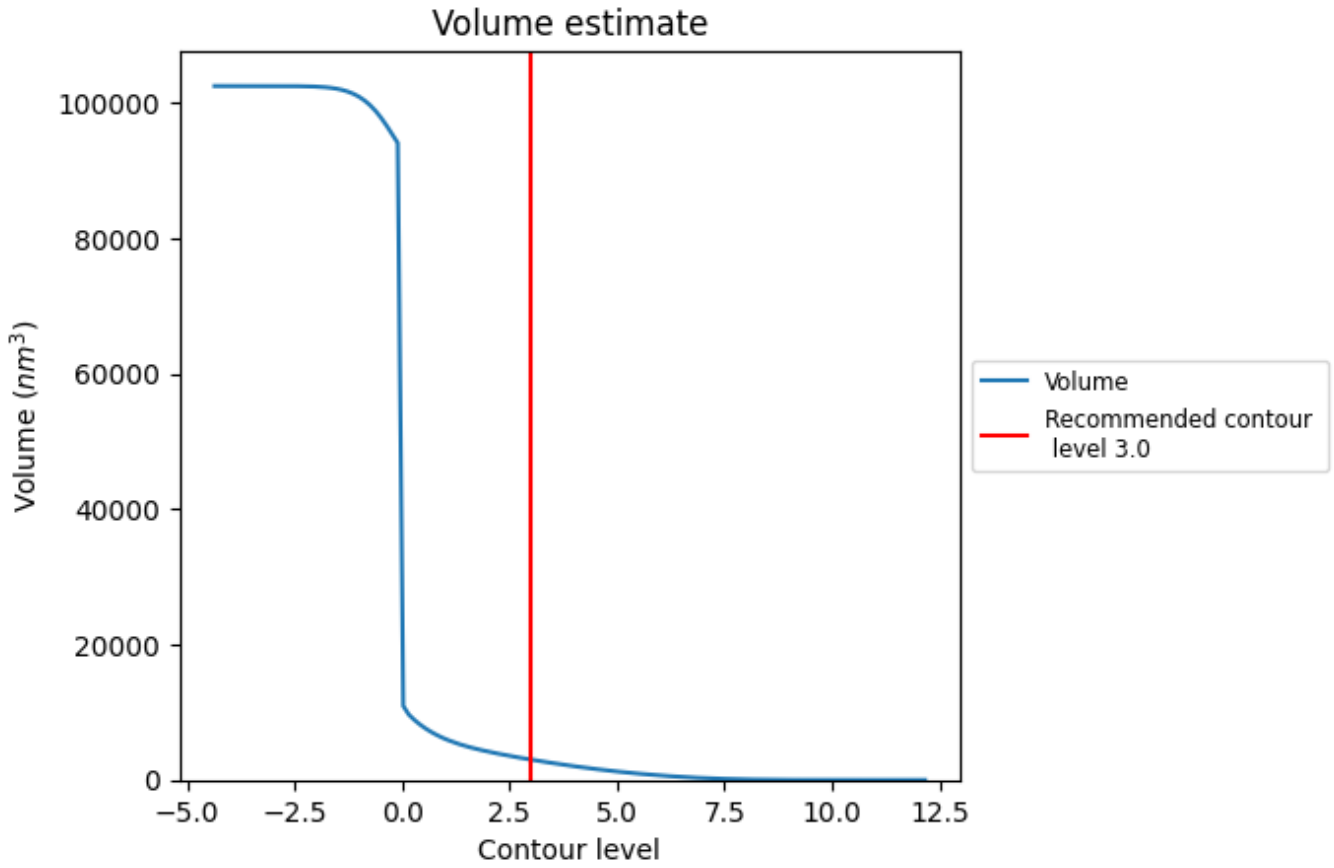
This section contains the results of statistical analysis of the map.

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.

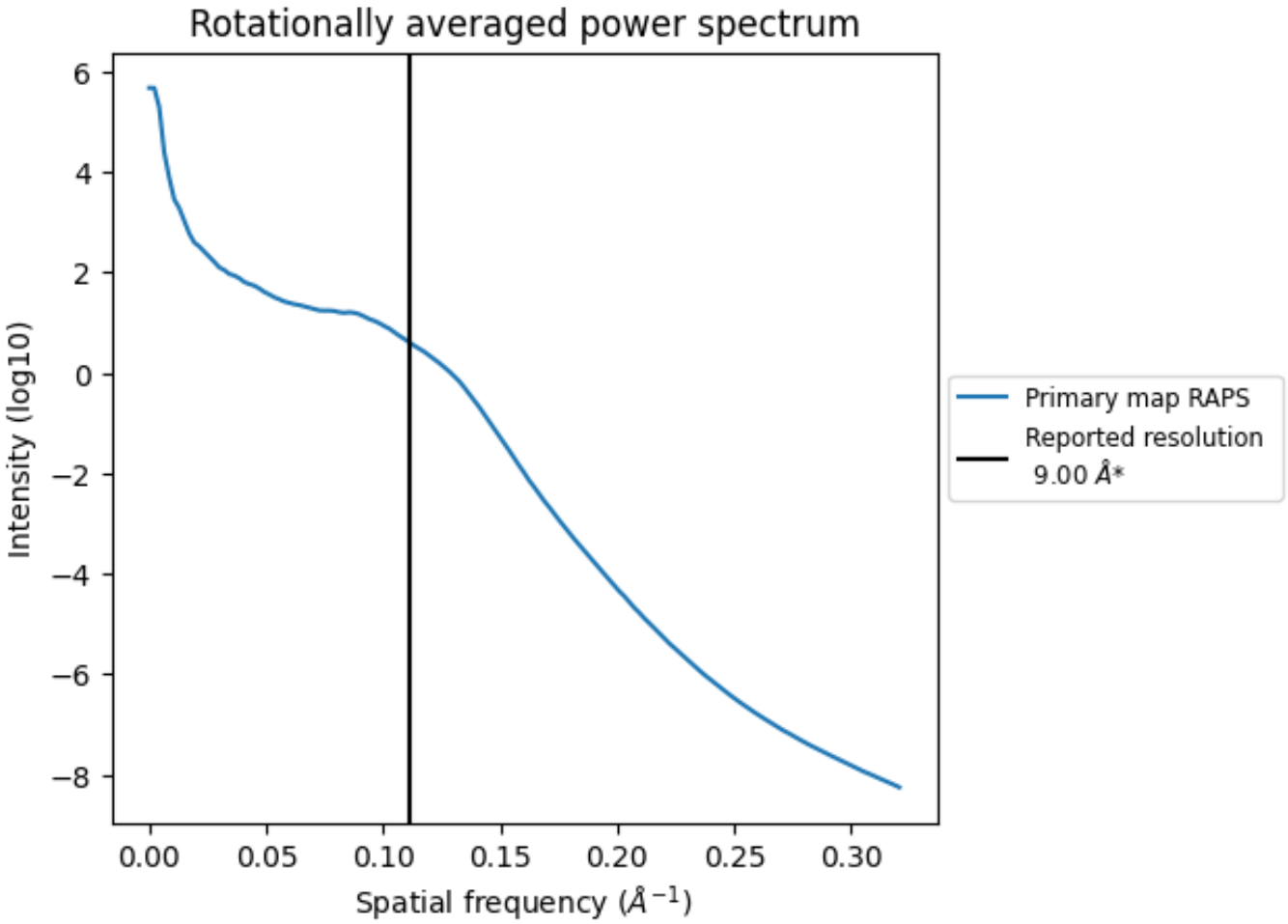
7.2 Volume estimate (i)



The volume at the recommended contour level is 3001 nm^3; this corresponds to an approximate mass of 2711 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 0.111 Å^{-1}

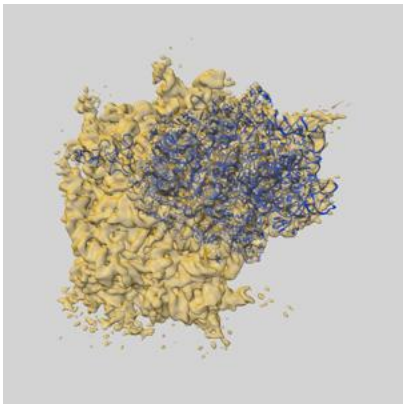
8 Fourier-Shell correlation (i)

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

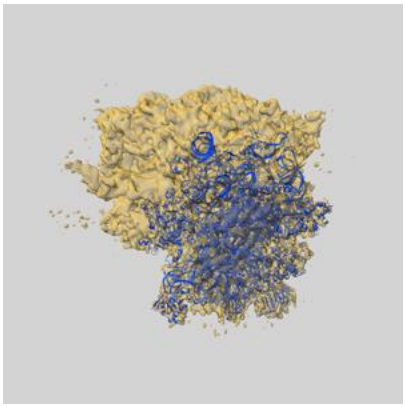
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2813 and PDB model 4D61. Per-residue inclusion information can be found in section 3 on page 11.

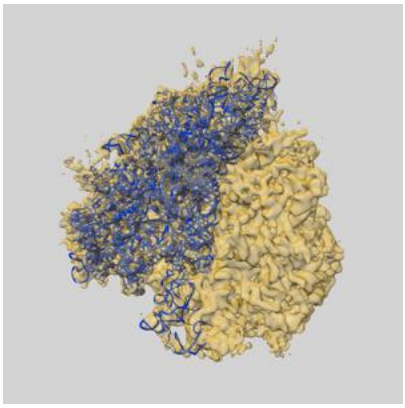
9.1 Map-model overlay



X



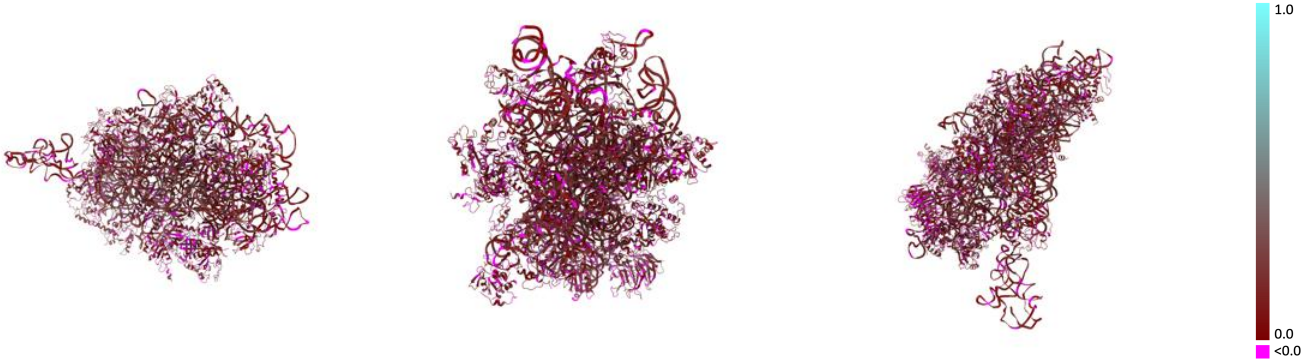
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 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.

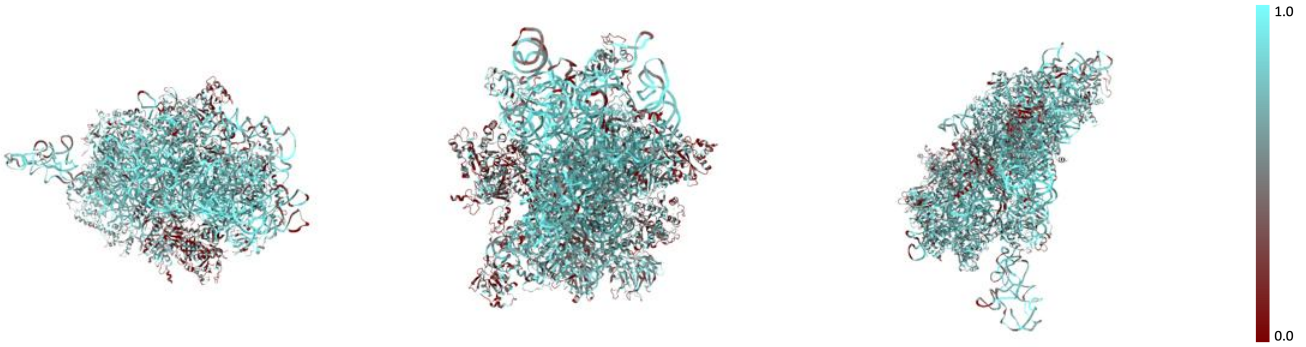
9.2 Q-score mapped to coordinate model (i)



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.

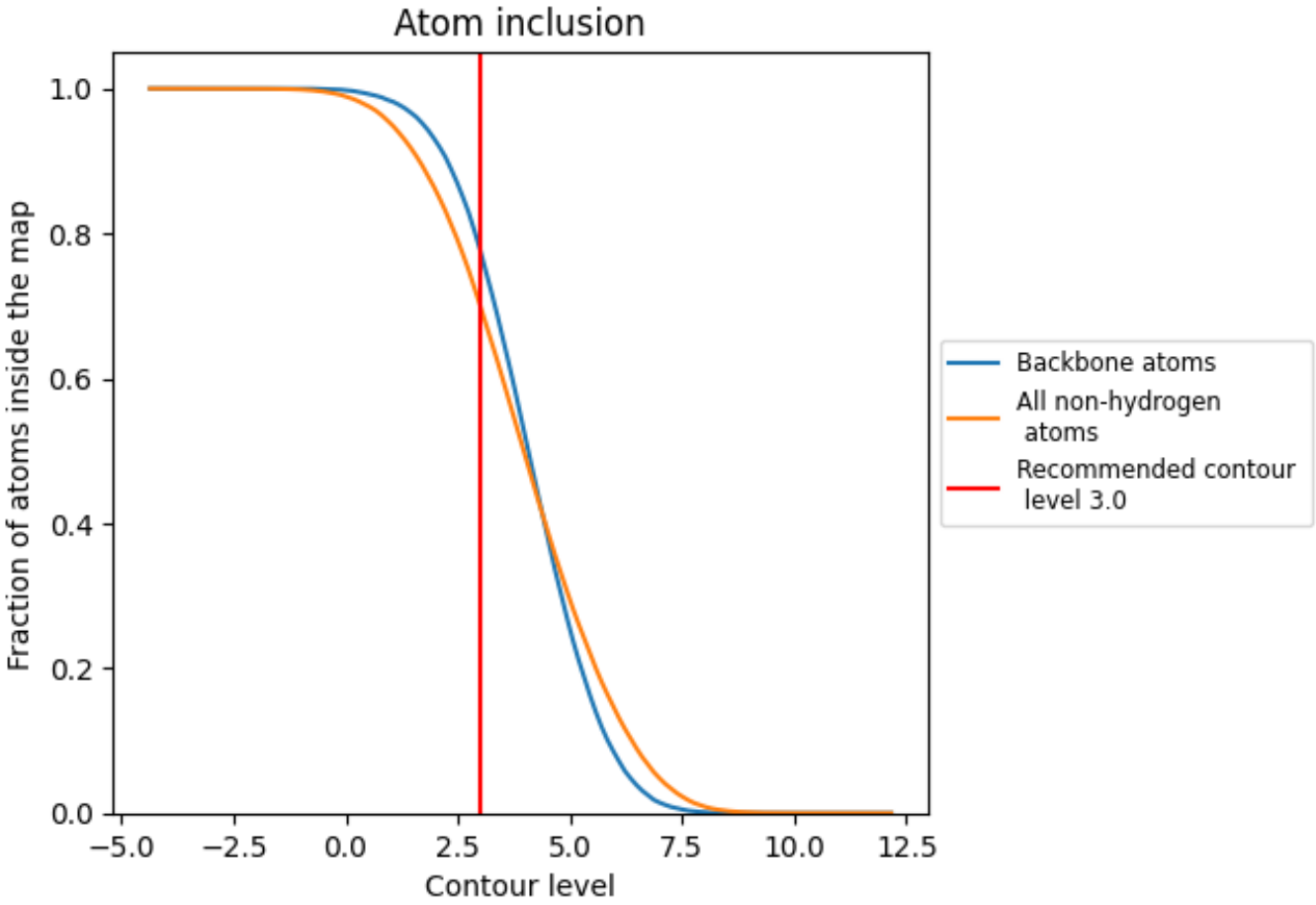
9.3 Atom inclusion mapped to coordinate model (i)



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 (3.0).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 70% 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 (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7002	0.1270
1	0.8652	0.1580
A	0.4654	0.1120
B	0.6698	0.1340
C	0.6099	0.1280
D	0.5852	0.1170
E	0.6687	0.1090
F	0.6284	0.0970
G	0.6601	0.0980
H	0.3619	0.1000
I	0.6253	0.0930
J	0.6794	0.1080
K	0.6365	0.0860
L	0.6040	0.1150
M	0.3293	0.0670
N	0.6080	0.1130
O	0.6439	0.1060
P	0.5920	0.0850
Q	0.6791	0.0870
R	0.4925	0.0900
S	0.6546	0.1070
T	0.6322	0.0850
U	0.5371	0.0690
V	0.4855	0.1050
W	0.6244	0.1050
X	0.6256	0.1140
Y	0.6204	0.1000
Z	0.6559	0.1180
a	0.6206	0.0910
b	0.6020	0.1140
c	0.5681	0.1030
d	0.7160	0.0630
e	0.5214	0.1160
f	0.3706	0.0750
g	0.5858	0.0860

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Chain	Atom inclusion	Q-score
h	0.4202	0.0970
i	0.3540	0.0920
j	0.6869	0.1270