



wwPDB EM Validation Summary Report ⓘ

Apr 12, 2026 – 12:43 PM UTC

PDB ID : 8SUP / pdb_00008sup
EMDB ID : EMD-40774
Title : Structure of the 48S translation initiation complex assembled on the encephalomyocarditis virus IRES
Authors : Bhattacharjee, S.; Abaeva, I.S.; Brown, Z.P.; Arhab, Y.; Fallah, H.; Jeevan, J.C.; Hellen, C.U.T.; Frank, J.; Pestova, T.V.
Deposited on : 2023-05-12
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:

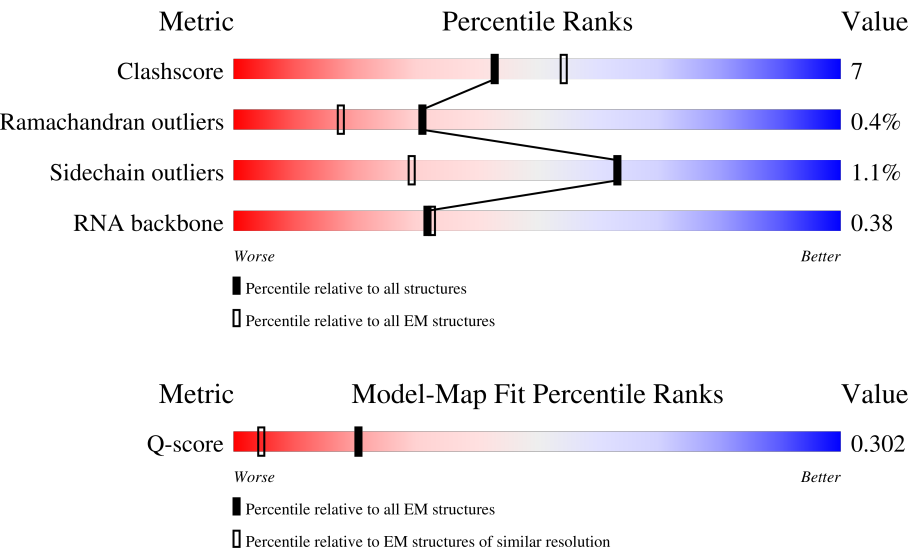
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	o	1362	<div><div>41%</div><div><div></div><div></div><div></div><div></div></div><div>33%10%•56%</div></div>
2	p	843	<div><div>56%</div><div><div></div><div></div><div></div><div></div></div><div>49%16%•34%</div></div>
3	q	445	<div><div>92%</div><div><div></div><div></div><div></div><div></div></div><div>68%24%•6%</div></div>

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Mol	Chain	Length	Quality of chain
4	r	364	
5	s	352	
6	t	218	
7	u	564	
8	v	374	
9	2	1870	
10	3	89	
11	A	144	
12	B	295	
13	C	264	
14	D	221	
15	E	281	
16	F	263	
17	G	204	
18	H	249	
19	I	432	
20	J	208	
21	K	194	
22	L	149	
23	M	158	
24	N	132	
25	O	151	
26	P	168	
27	Q	145	
28	R	172	

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Mol	Chain	Length	Quality of chain
29	S	135	
30	T	152	
31	U	145	
32	V	119	
33	W	83	
34	X	130	
35	Y	143	
36	Z	131	
37	a	124	
38	b	101	
39	c	84	
40	d	69	
41	e	56	
42	f	133	
43	g	188	
44	h	317	
45	i	75	
46	j	315	
47	n	25	

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 106317 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	o	600	Total	C	N	O	S	0	1
			4935	3107	893	914	21		

- Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	p	558	Total	C	N	O	S	0	1
			4529	2842	805	849	33		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p	577	TYR	ALA	conflict	UNP A0A5F9CMJ3

- Molecule 3 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	q	420	Total	C	N	O	S	0	1
			3466	2220	587	639	20		

- Molecule 4 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	r	272	Total	C	N	O	S	0	0
			2111	1330	359	410	12		

- Molecule 5 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	s	324	Total	C	N	O	S	0	0
			2624	1654	452	503	15		

- Molecule 6 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	t	216	Total	C	N	O	S	0	1
			1738	1109	286	330	13		

- Molecule 7 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	u	373	Total	C	N	O	S	0	1
			3110	2010	520	563	17		

- Molecule 8 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	v	366	Total	C	N	O	S	0	1
			2919	1850	494	558	17		

- Molecule 9 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2	1697	Total	C	N	O	P	0	0
			36227	16170	6504	11857	1696		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	197	U	C	conflict	GB 2488159015
2	1095	C	U	conflict	GB 2488159015
2	1203	U	-	insertion	GB 2488159015
2	1205	G	A	conflict	GB 2488159015
2	?	-	G	deletion	GB 2488159015

- Molecule 10 is a RNA chain called EMCV mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	3	89	Total	C	N	O	P	0	0
			1897	848	347	613	89		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	831	A	-	expression tag	GB 485965777
3	832	A	-	expression tag	GB 485965777
3	833	U	-	expression tag	GB 485965777

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Chain	Residue	Modelled	Actual	Comment	Reference
3	834	A	-	expression tag	GB 485965777
3	835	U	-	expression tag	GB 485965777
3	836	G	-	expression tag	GB 485965777

- Molecule 11 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	99	Total	C	N	O	S	0	0
			798	503	143	148	4		

- Molecule 12 is a protein called uS2 (SA).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	114	THR	ALA	conflict	UNP G1TLT8

- Molecule 13 is a protein called eS1.

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

- Molecule 14 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 15 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 16 is a protein called eS4 (S4 X isoform).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	25	GLY	SER	conflict	UNP G1TK17
F	51	ARG	LYS	conflict	UNP G1TK17
F	78	THR	ALA	conflict	UNP G1TK17
F	156	VAL	MET	conflict	UNP G1TK17

- Molecule 17 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 18 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	H	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 19 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	I	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 20 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	206	Total	C	N	O	S	1	0
			1691	1061	333	292	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 21 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	K	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 22 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 23 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	151	Total	C	N	O	S	0	0
			1233	785	231	211	6		

- Molecule 24 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 25 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 26 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	P	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 27 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 28 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	R	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 29 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	S	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 30 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	T	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 31 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	U	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

- Molecule 32 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	V	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 33 is a protein called eS21.

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	3	ASN	SER	conflict	UNP G1TM82
W	4	ASP	ASN	conflict	UNP G1TM82
W	33	GLN	PRO	conflict	UNP G1TM82
W	50	PHE	SER	conflict	UNP G1TM82
W	75	ALA	SER	conflict	UNP G1TM82
W	76	ASP	HIS	conflict	UNP G1TM82

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Chain	Residue	Modelled	Actual	Comment	Reference
W	81	LYS	GLN	conflict	UNP G1TM82

- Molecule 34 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	X	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 35 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Y	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 36 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Z	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 37 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	a	77	Total	C	N	O	S	0	0
			614	393	114	106	1		

- Molecule 38 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	b	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	28	ARG	CYS	conflict	UNP G1TFE8
b	56	ALA	VAL	conflict	UNP G1TFE8

- Molecule 39 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	c	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 40 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	d	67	Total	C	N	O	S	0	0
			530	321	108	99	2		

- Molecule 41 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	e	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 42 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	f	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 43 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	g	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 44 is a protein called Receptor for Activated C Kinase 1 (RACK1).

Mol	Chain	Residues	Atoms					AltConf	Trace
44	h	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 45 is a RNA chain called Met-tRNAiMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	i	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	j	182	Total	C	N	O	S	0	0
			1245	795	234	213	3		

- Molecule 47 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

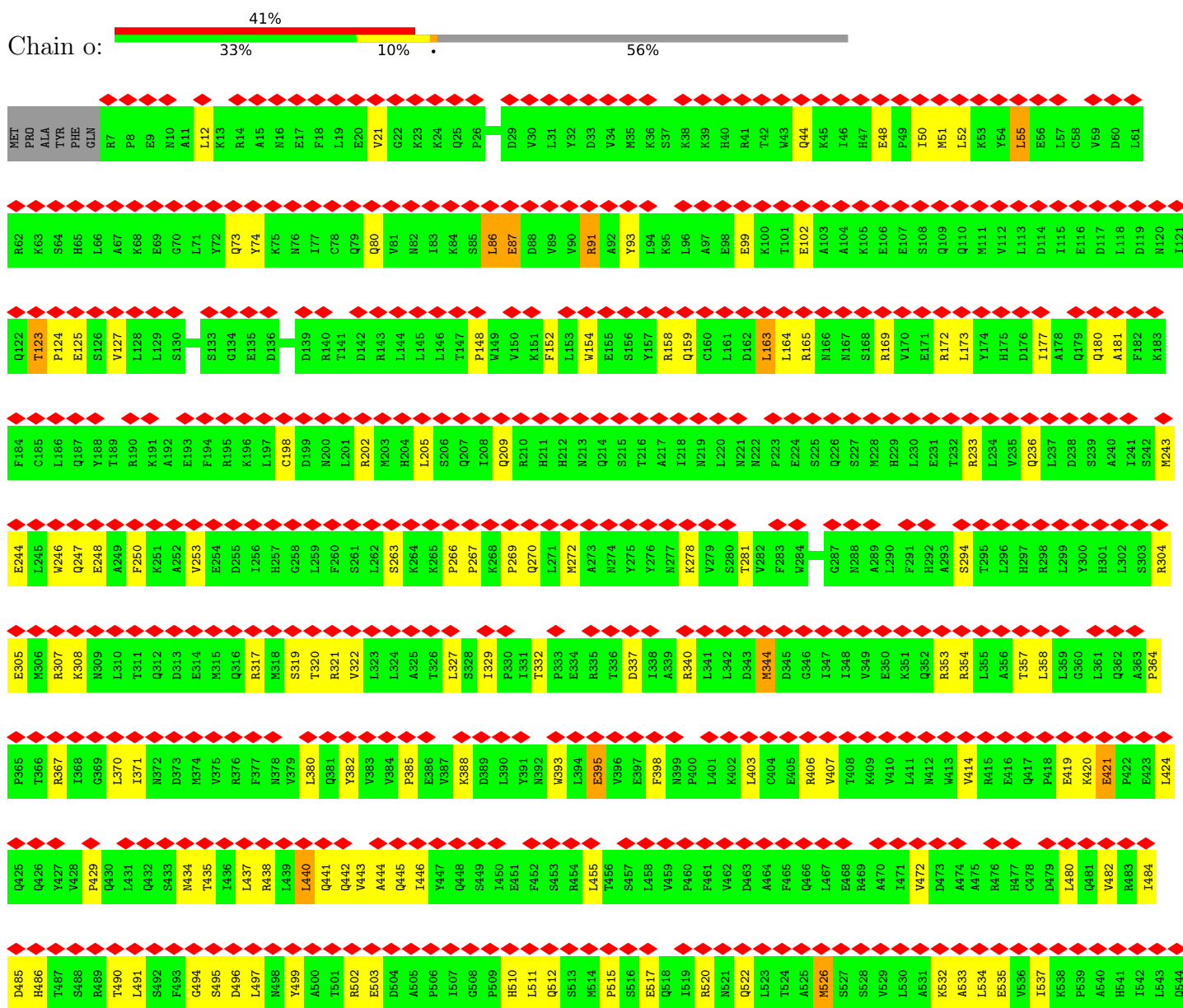
- Molecule 48 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
48	b	1	Total	Zn	0
			1	1	

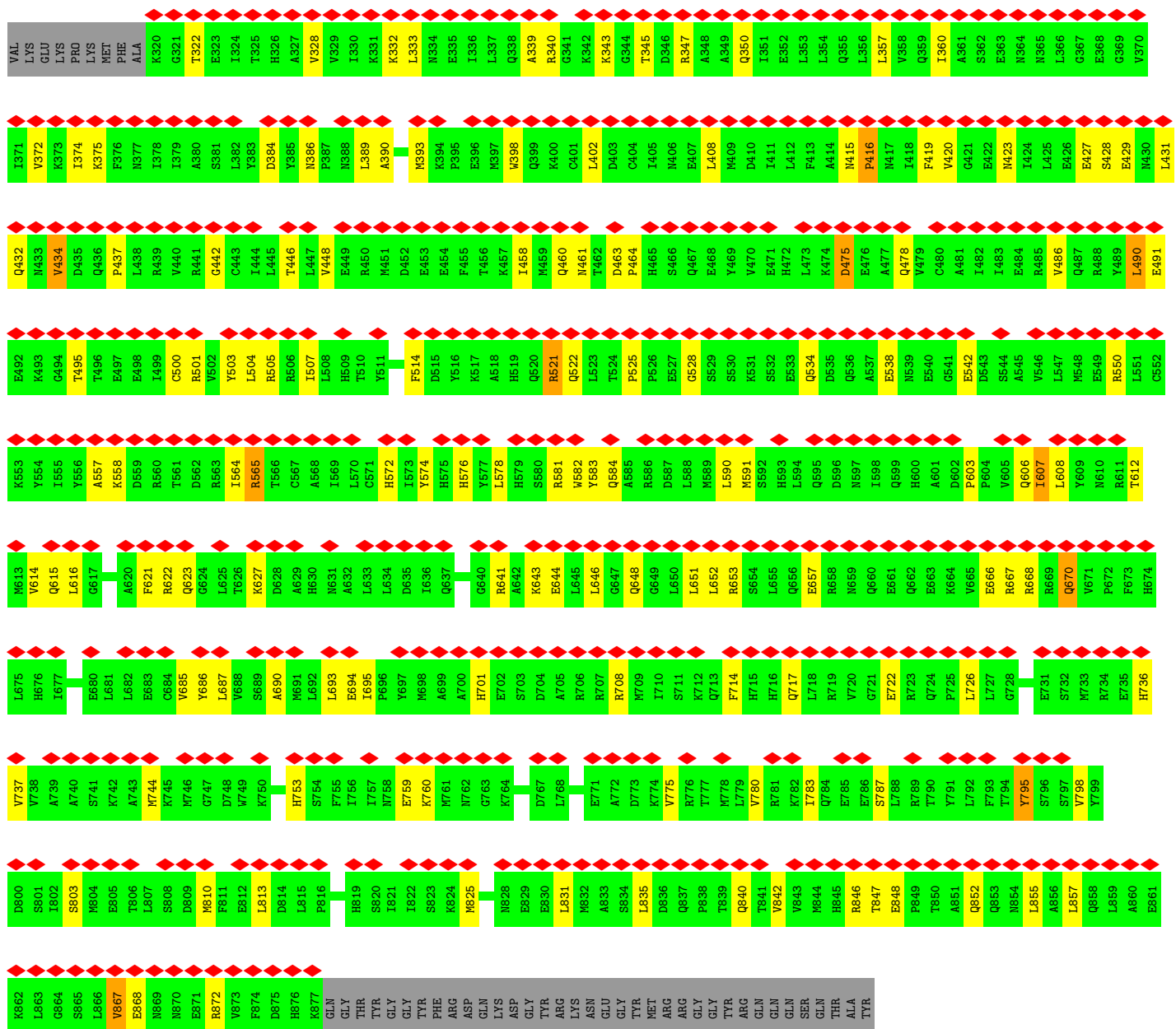
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

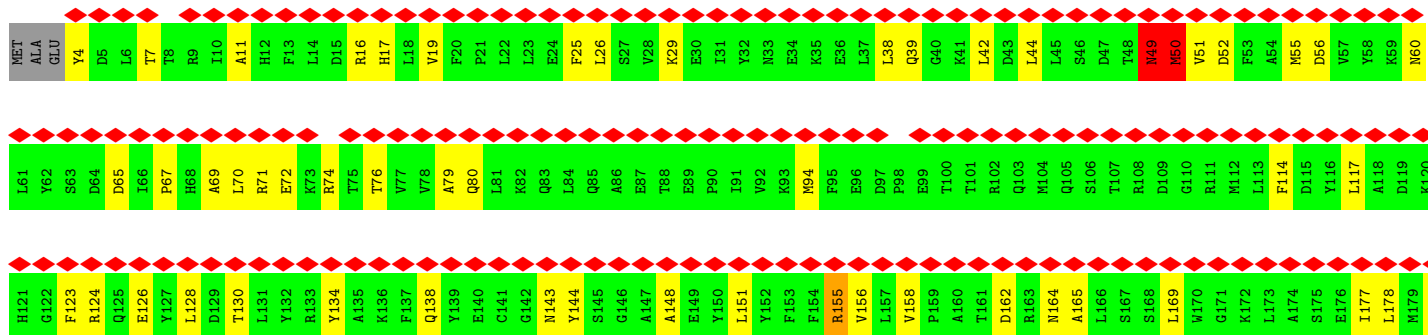
- Molecule 1: Eukaryotic translation initiation factor 3 subunit A

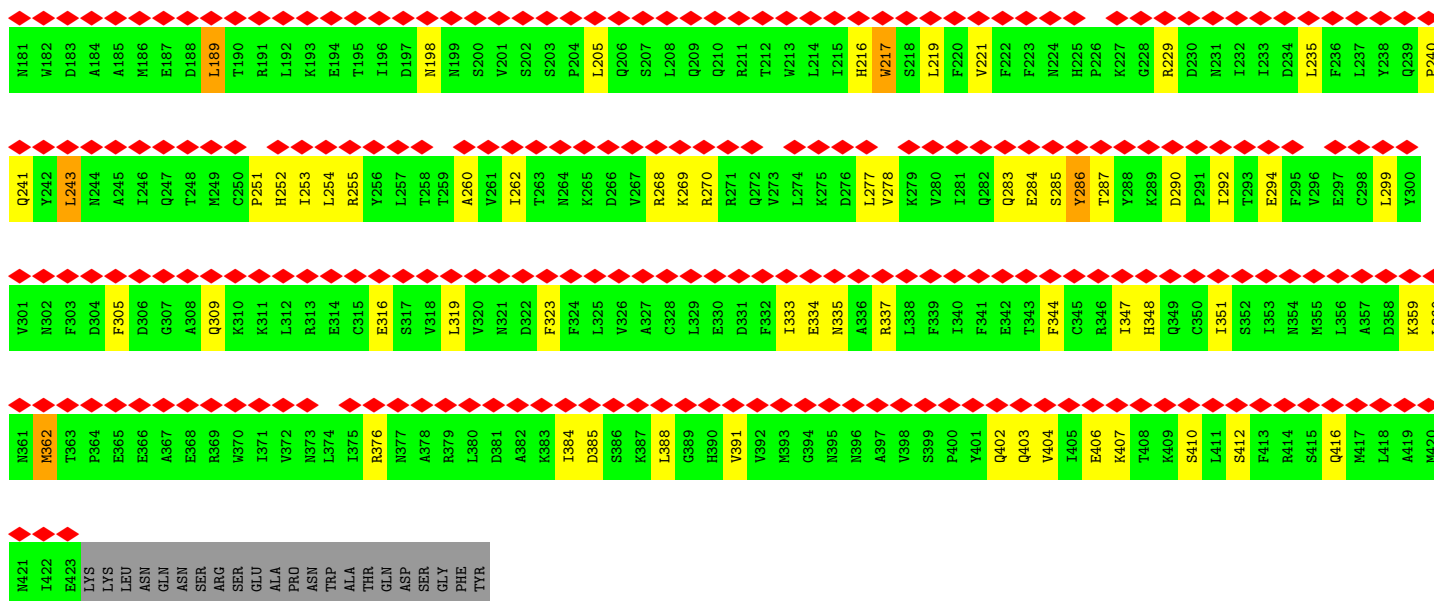




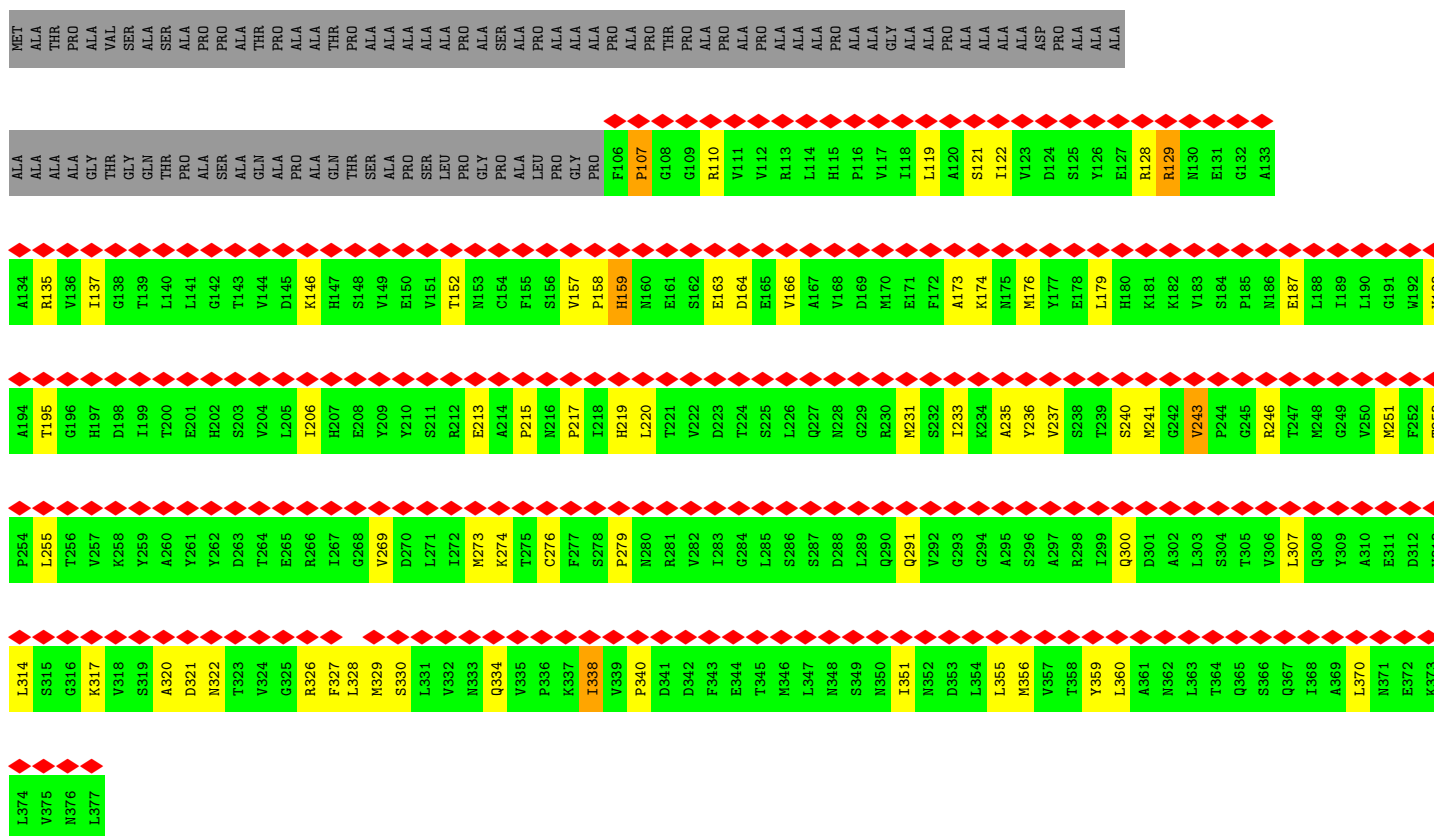
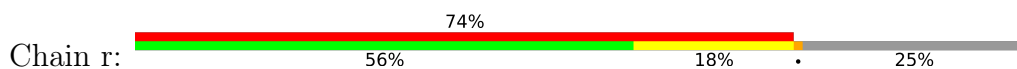


• Molecule 3: Eukaryotic translation initiation factor 3 subunit E



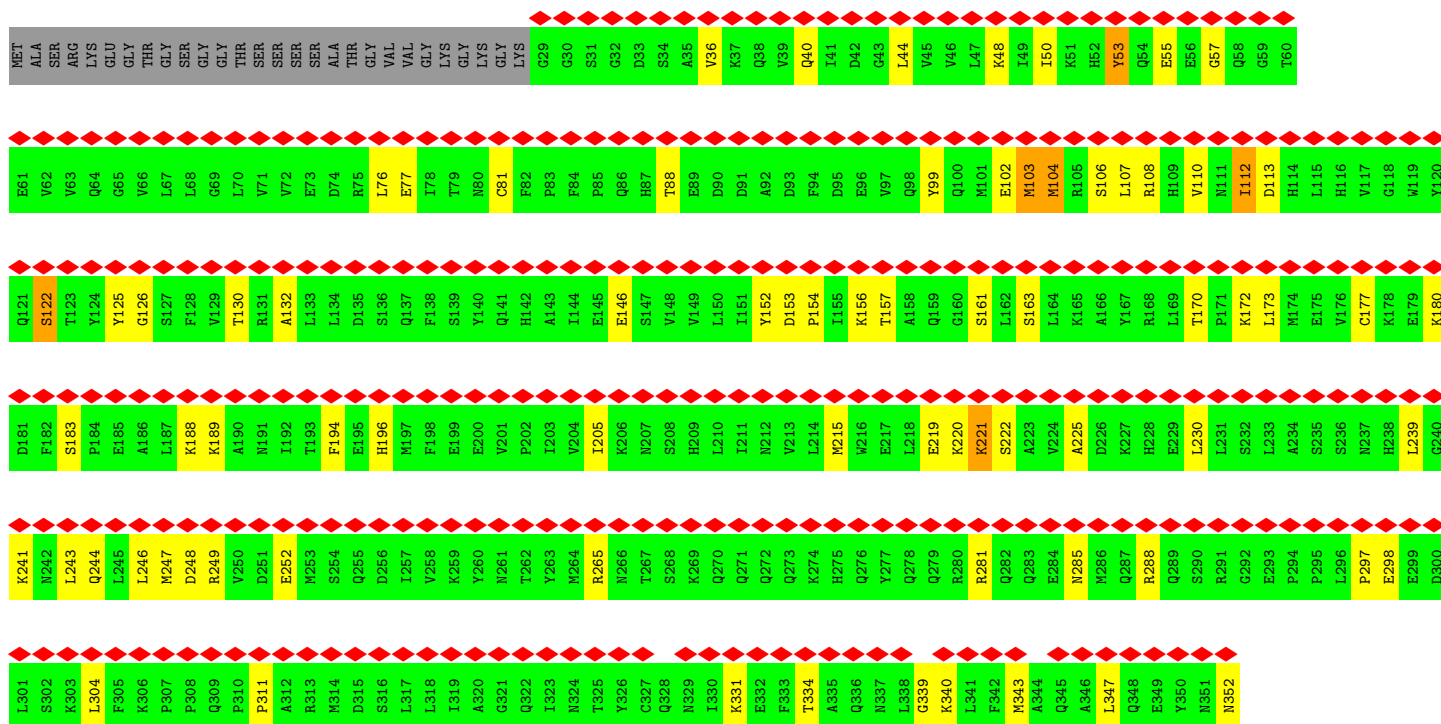


- Molecule 4: Eukaryotic translation initiation factor 3 subunit F

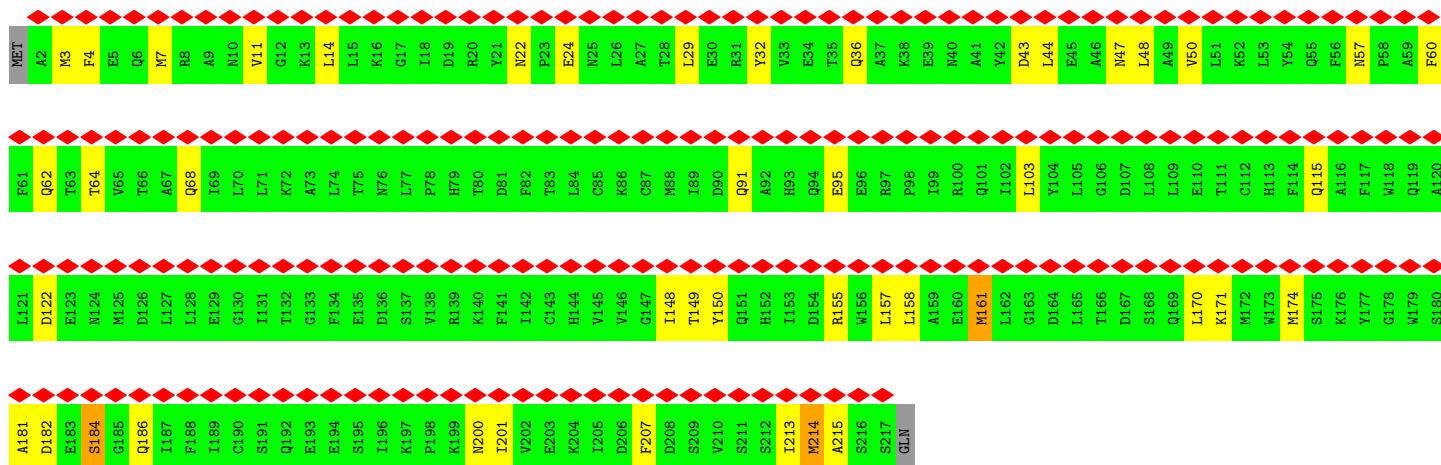
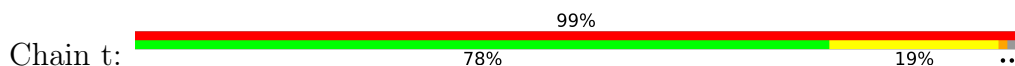


- Molecule 5: Eukaryotic translation initiation factor 3 subunit H

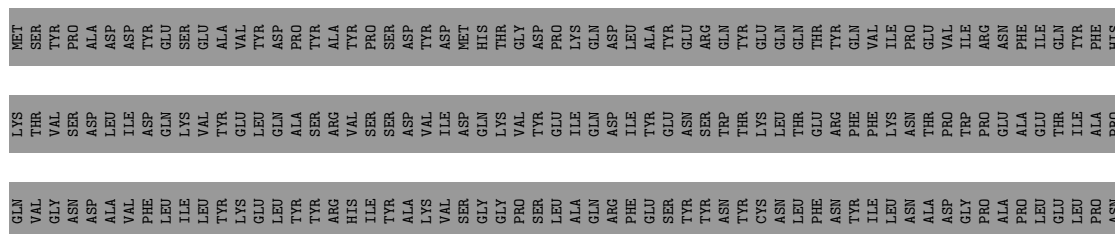


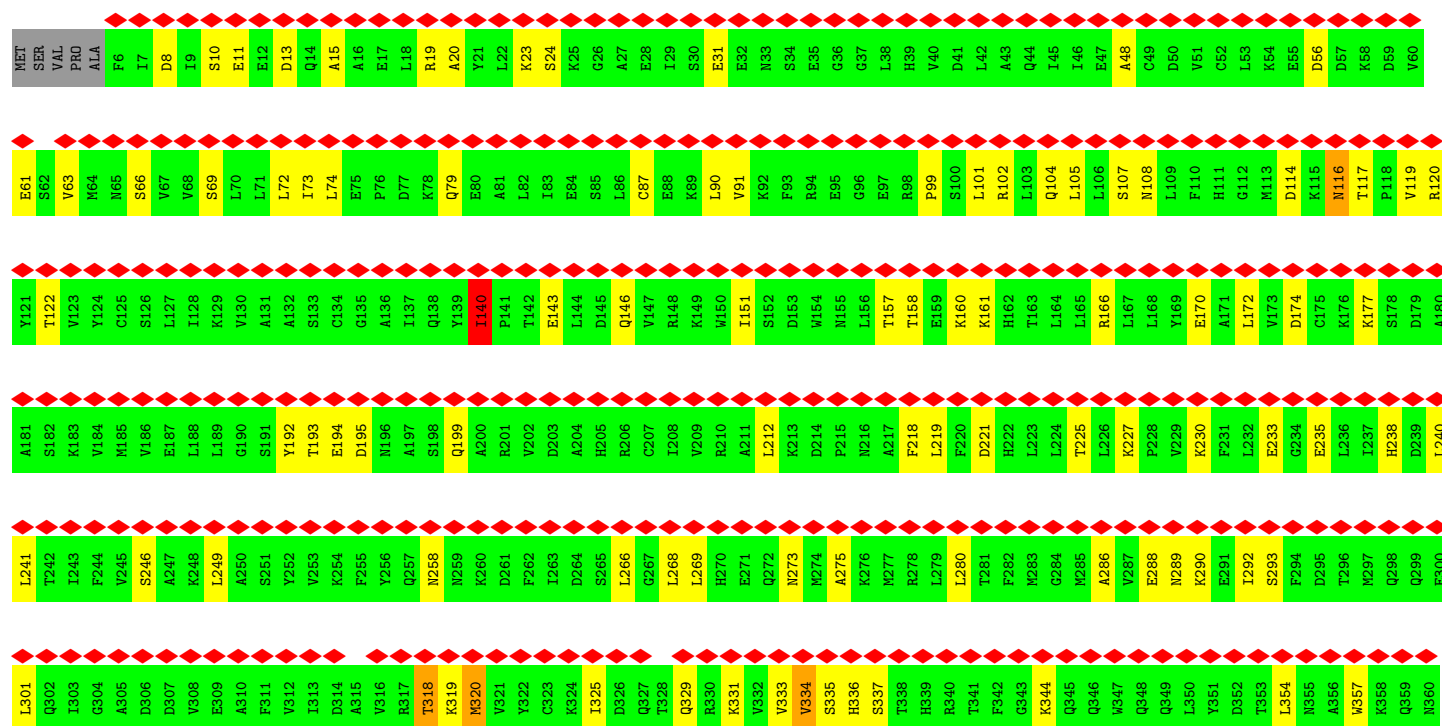


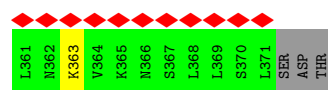
- Molecule 6: Eukaryotic translation initiation factor 3 subunit K



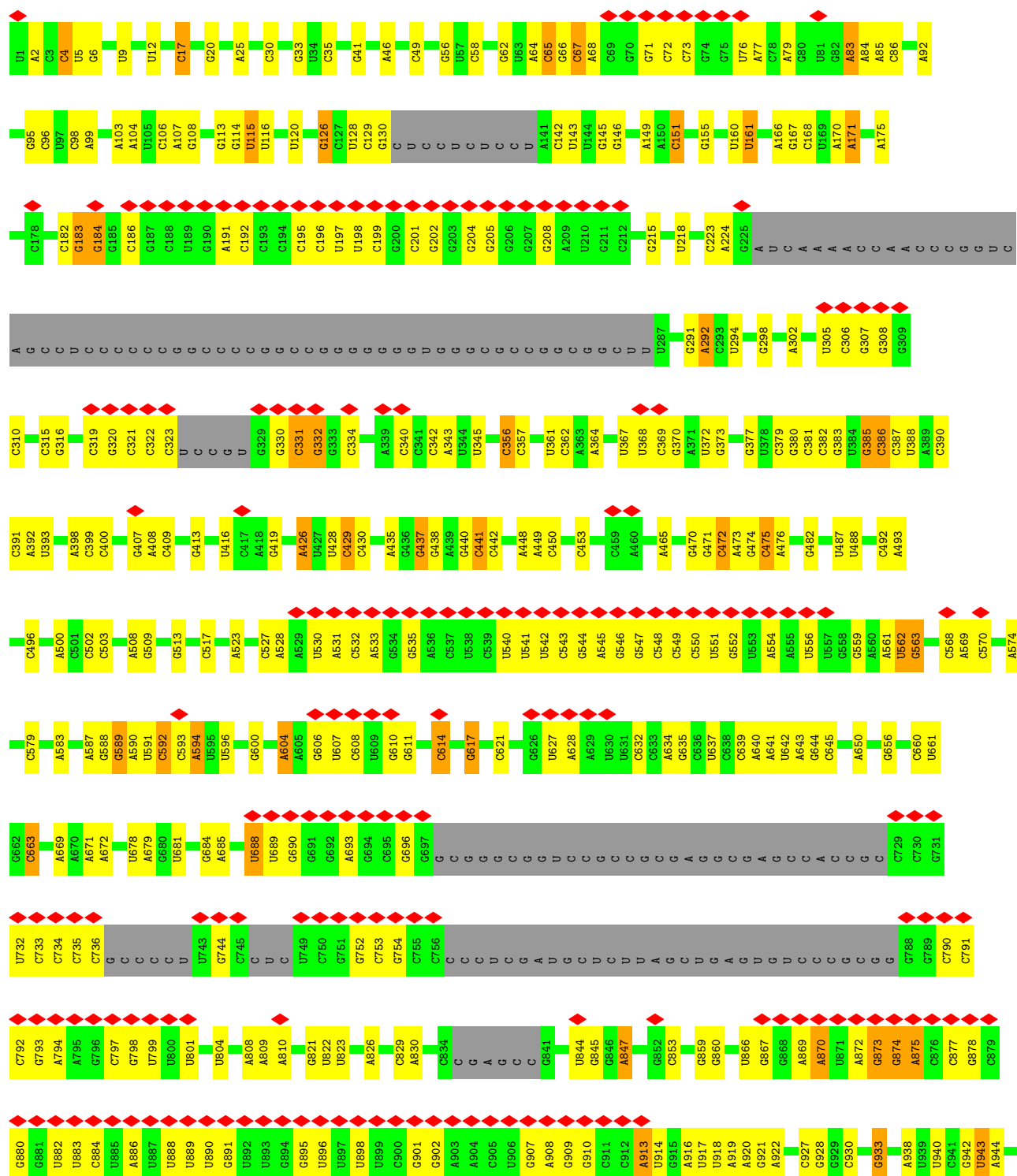
- Molecule 7: Eukaryotic translation initiation factor 3 subunit L

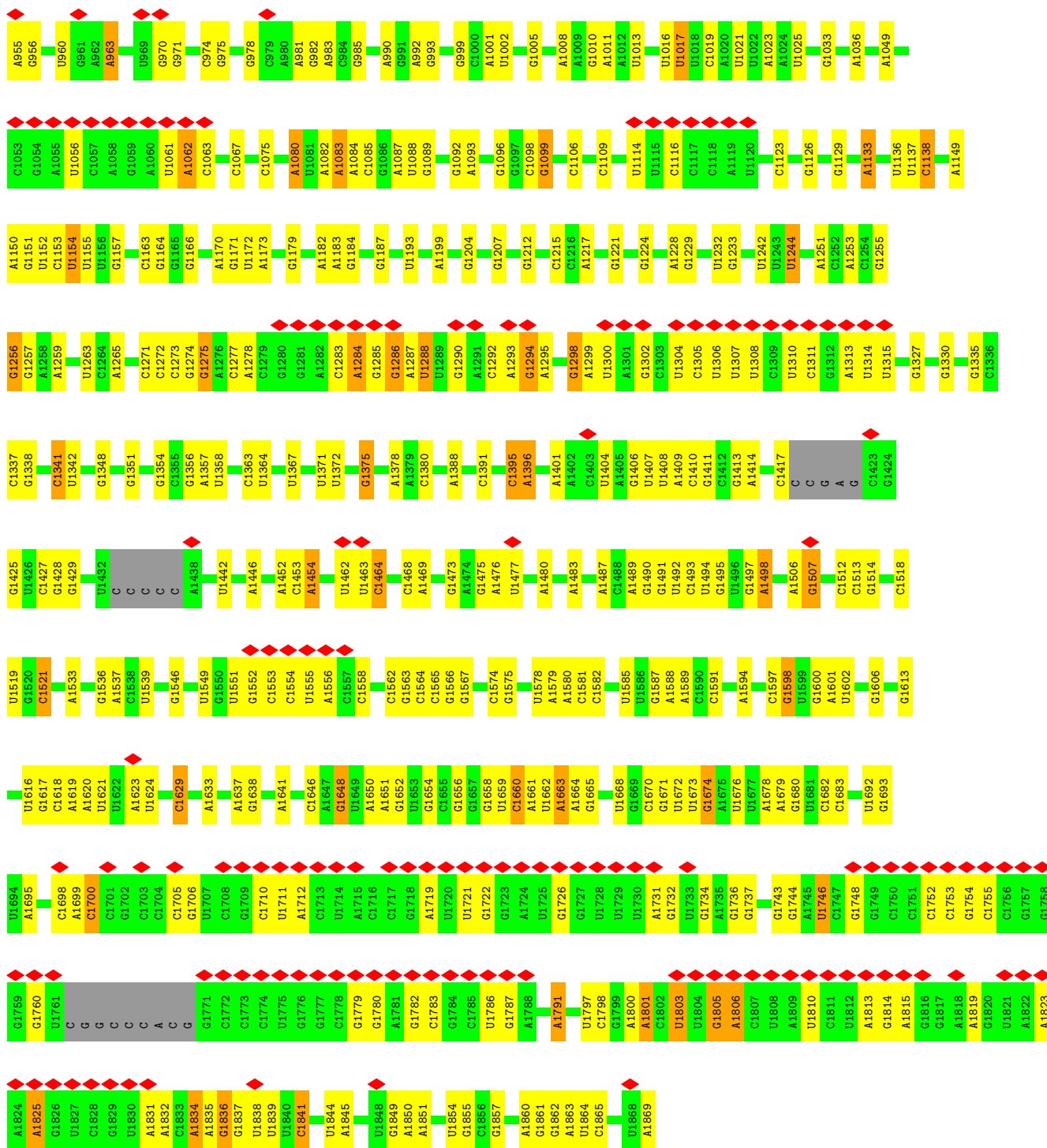


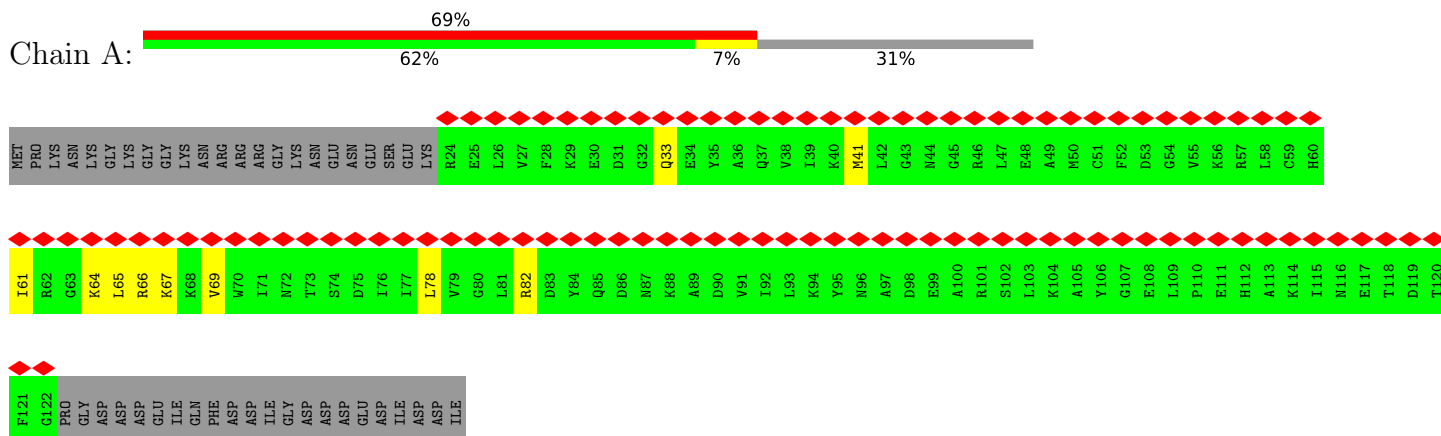




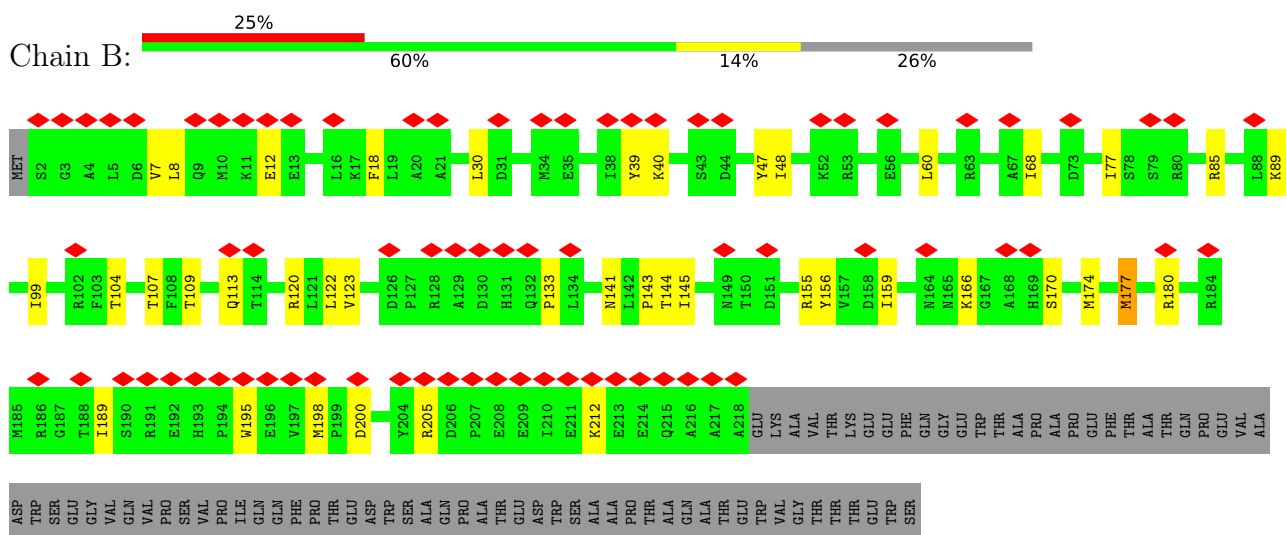
• Molecule 9: 18S rRNA



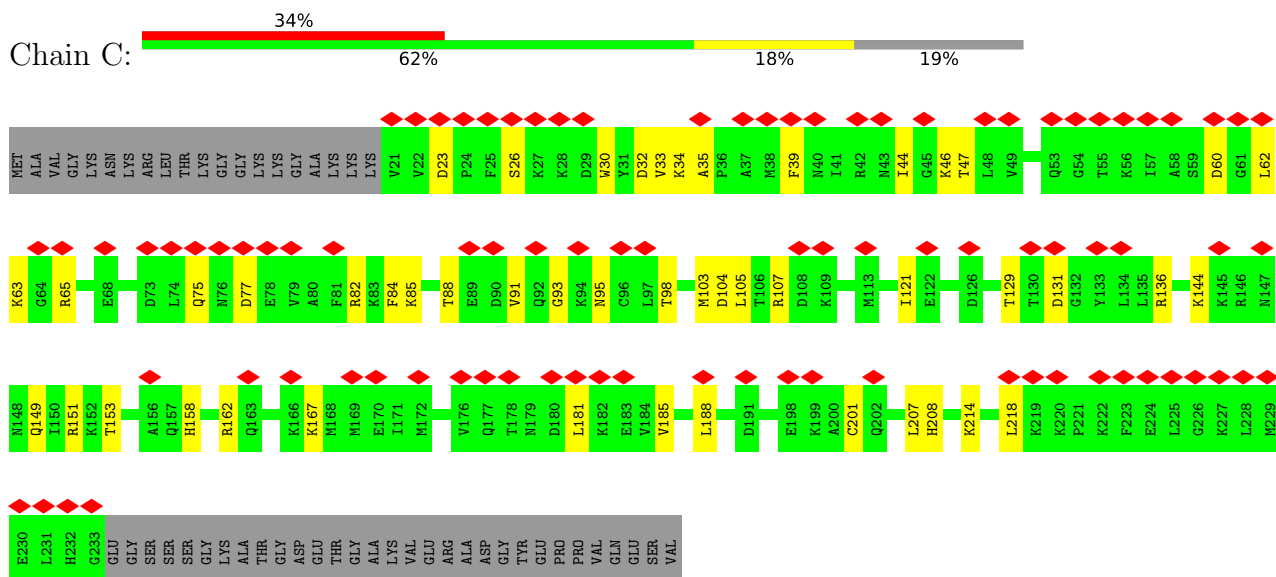




- Molecule 12: uS2 (SA)

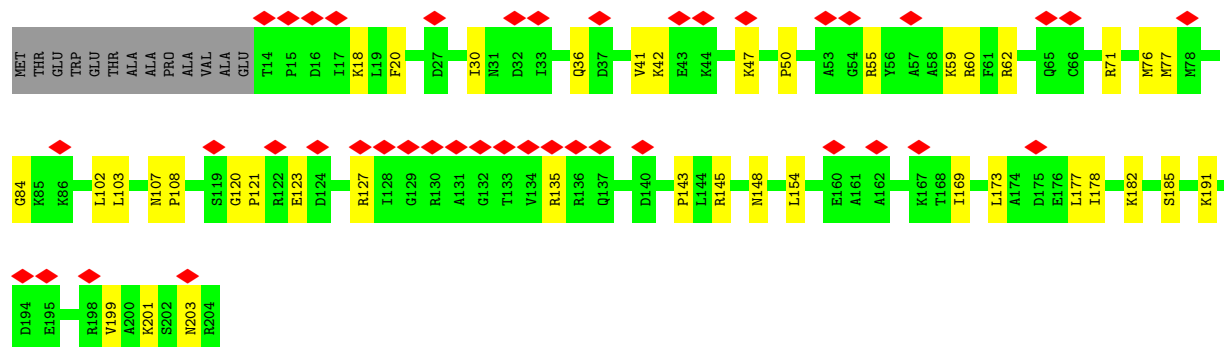
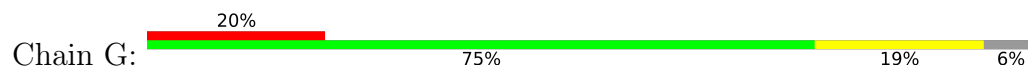


- Molecule 13: eS1

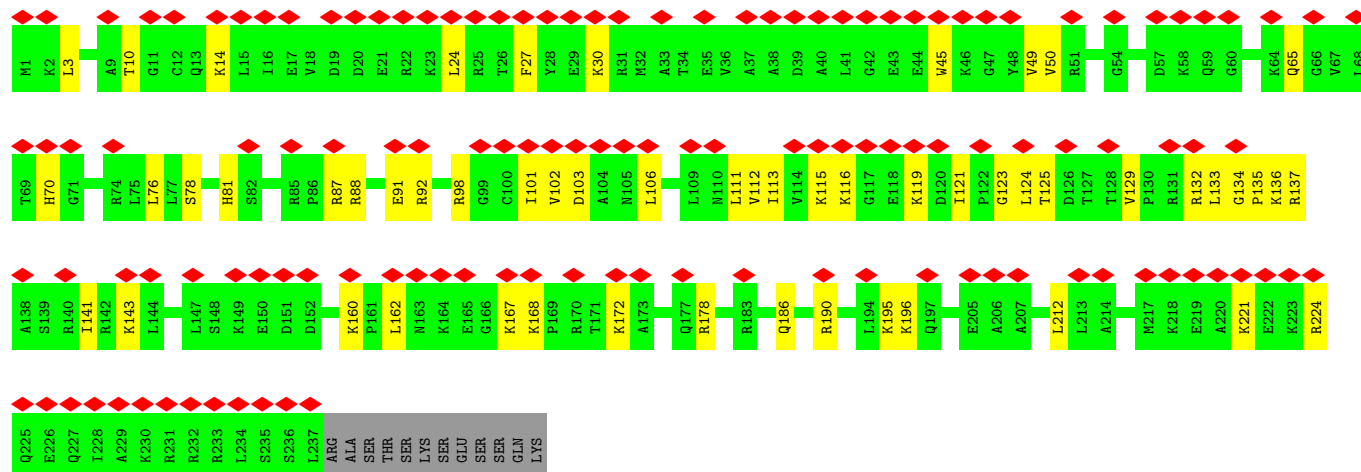
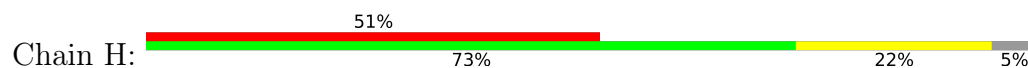


- Molecule 14: 40S ribosomal protein S2

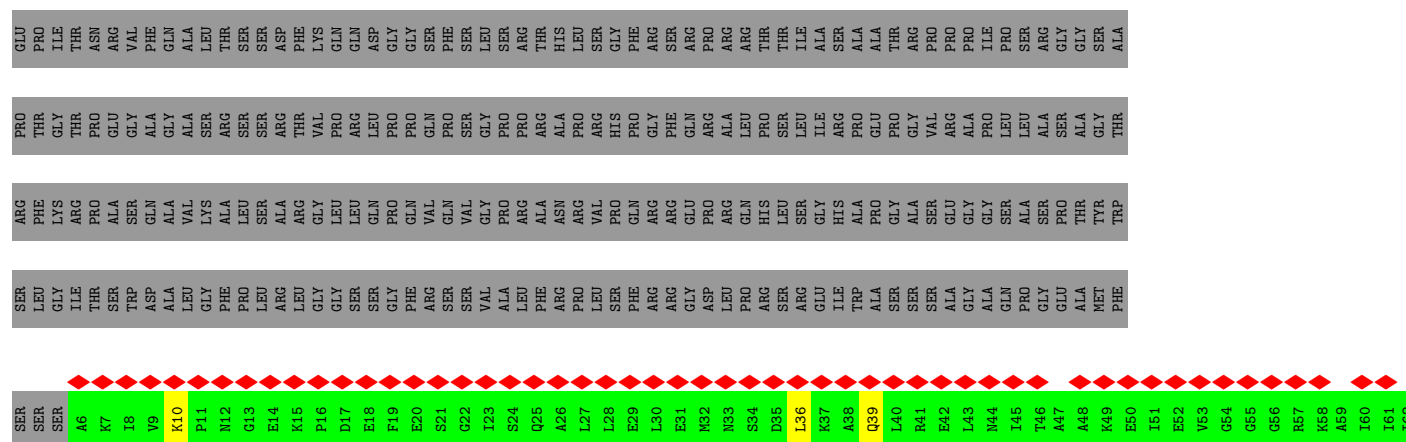
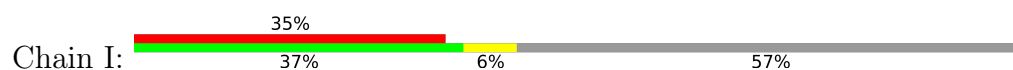
• Molecule 17: uS7

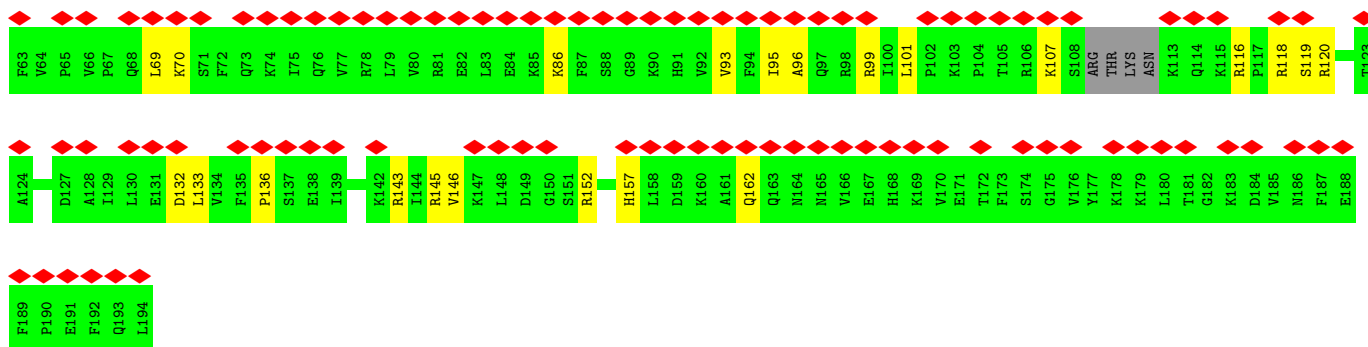


• Molecule 18: eS6

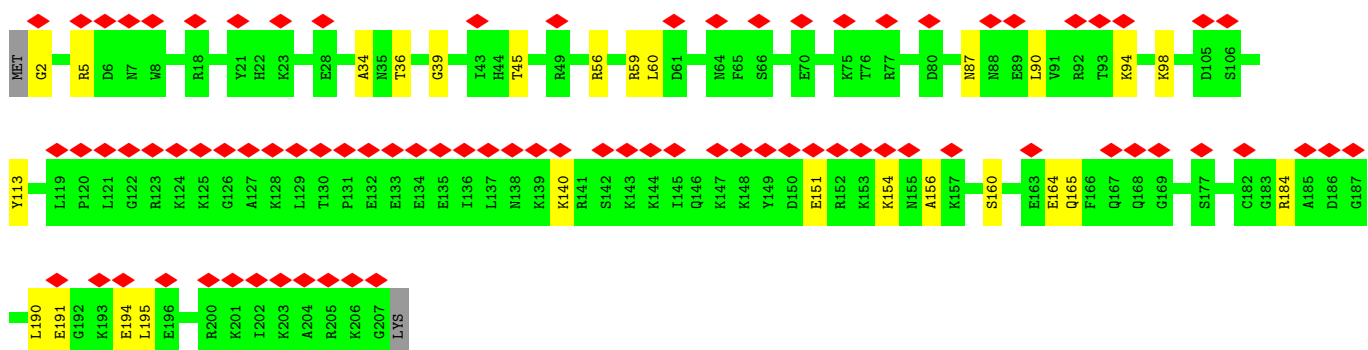
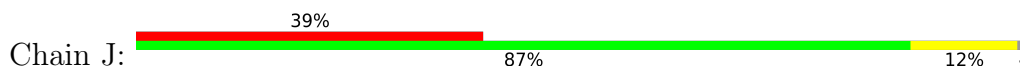


• Molecule 19: eS7

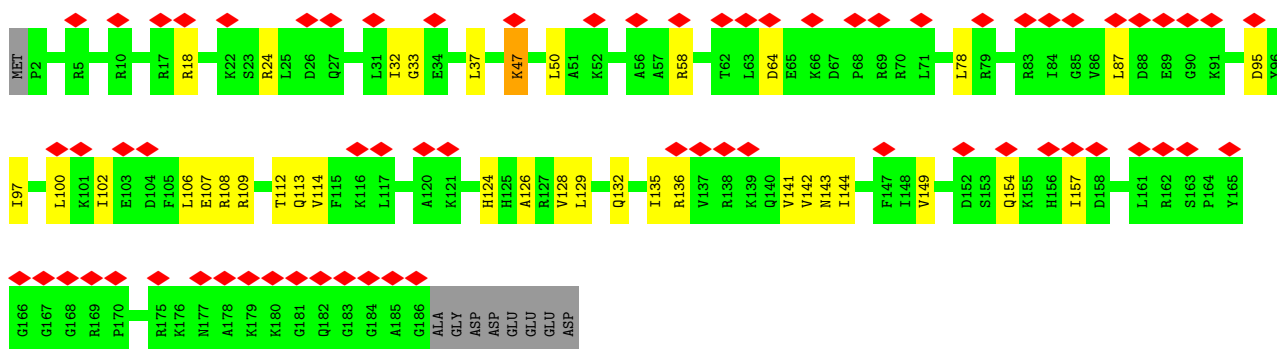
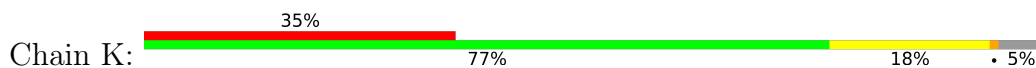




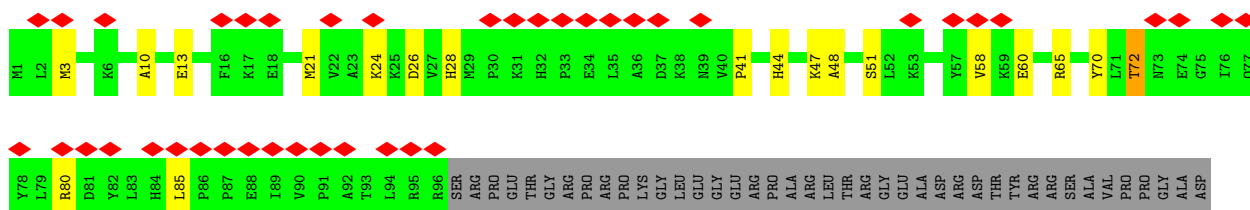
• Molecule 20: eS8



• Molecule 21: uS4



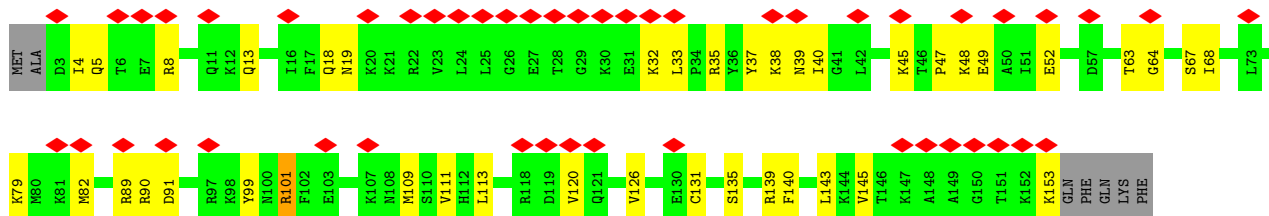
• Molecule 22: eS10




LYS
LYS
ALA
GLU
ALA
GLY
ALA
GLY
SER
ALA
THR
GLU

• Molecule 23: uS17

Chain M: 




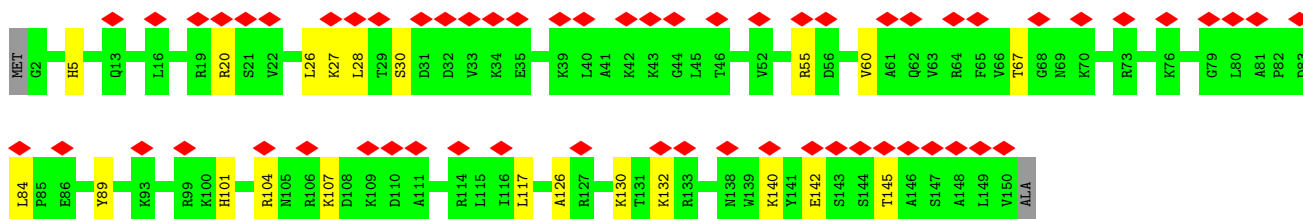
• Molecule 24: eS12

Chain N: 



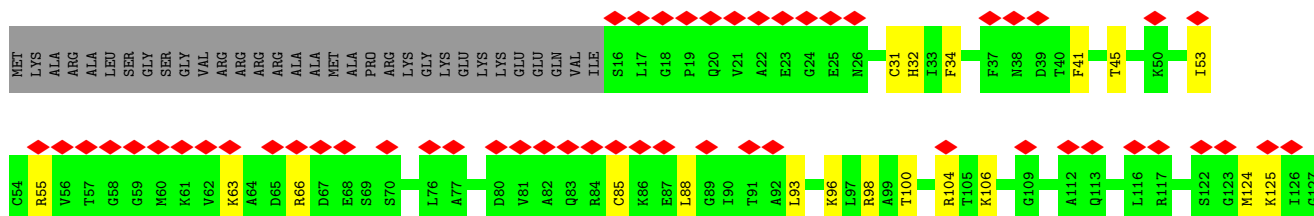
• Molecule 25: uS15

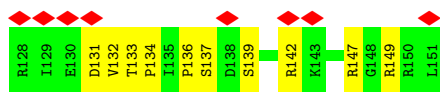
Chain O: 



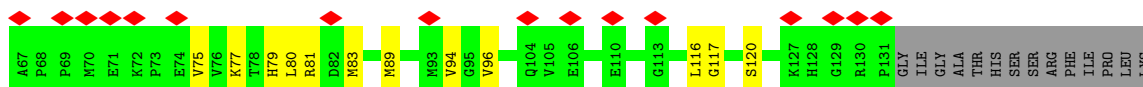
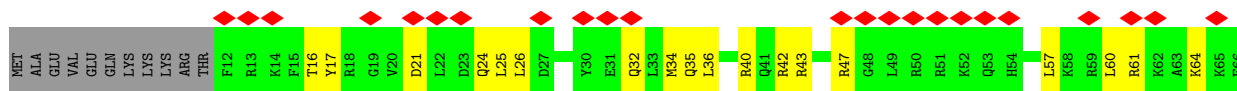
• Molecule 26: Small ribosomal subunit protein uS11

Chain P: 

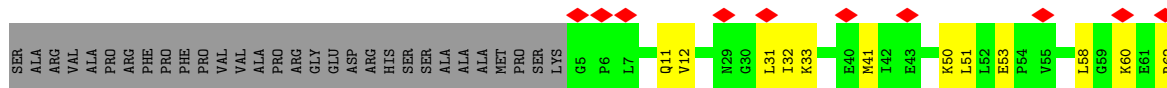




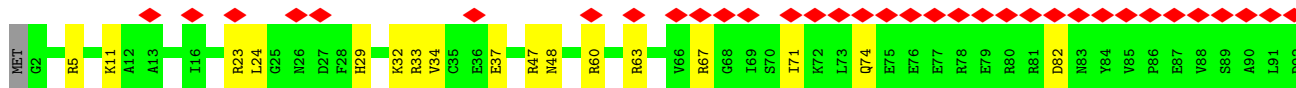
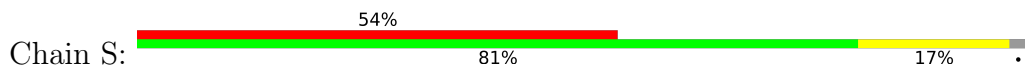
• Molecule 27: uS19



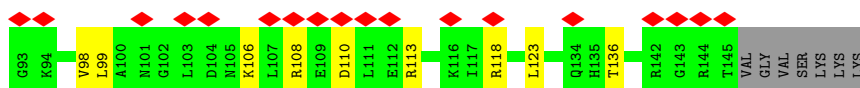
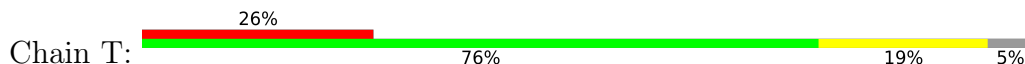
• Molecule 28: uS9



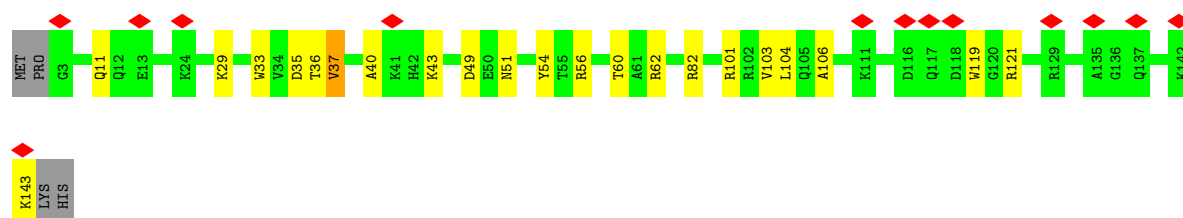
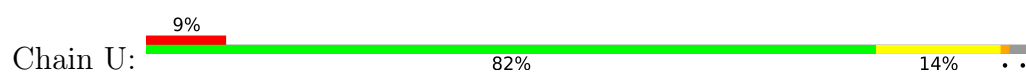
• Molecule 29: eS17



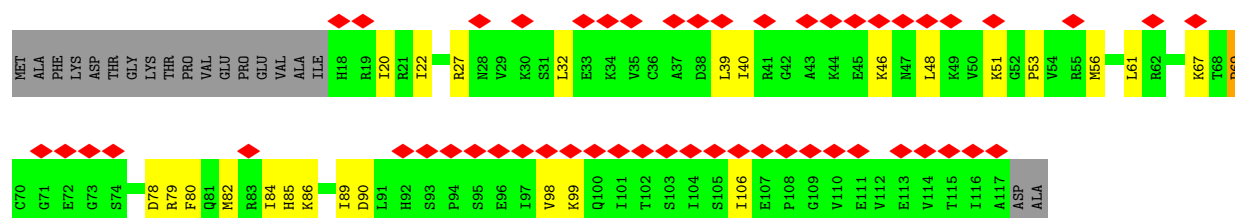
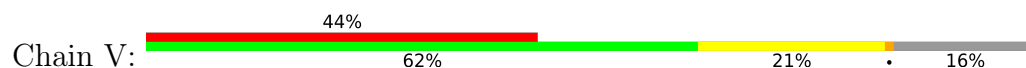
• Molecule 30: uS13



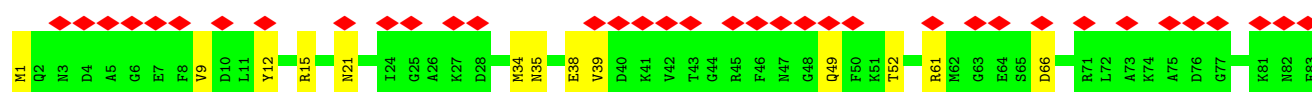
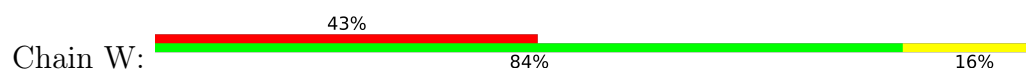
• Molecule 31: eS19



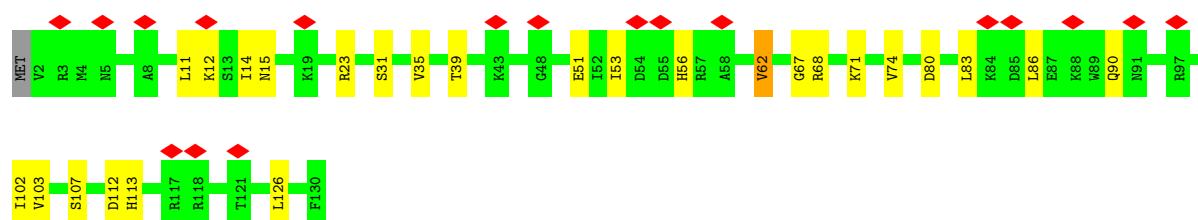
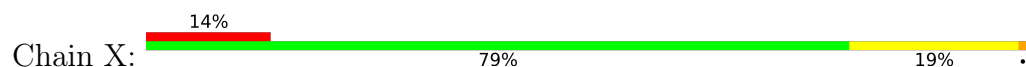
• Molecule 32: uS10



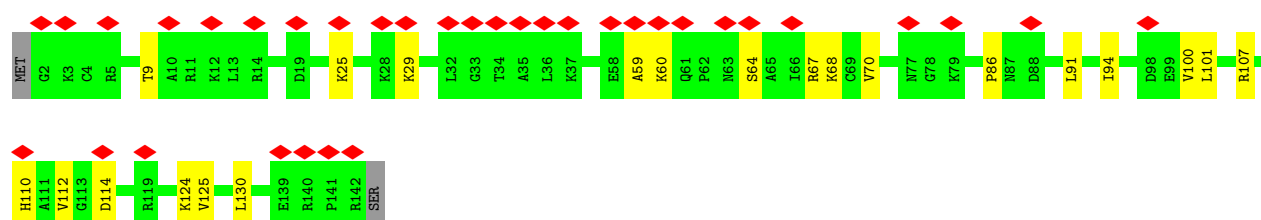
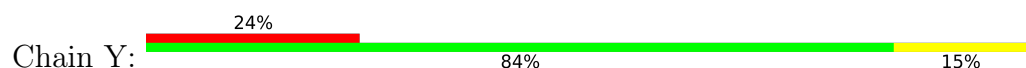
• Molecule 33: eS21



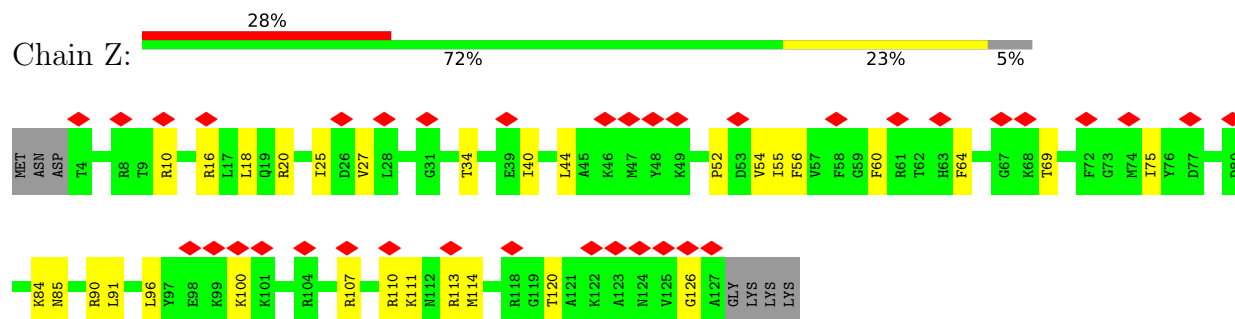
• Molecule 34: uS8



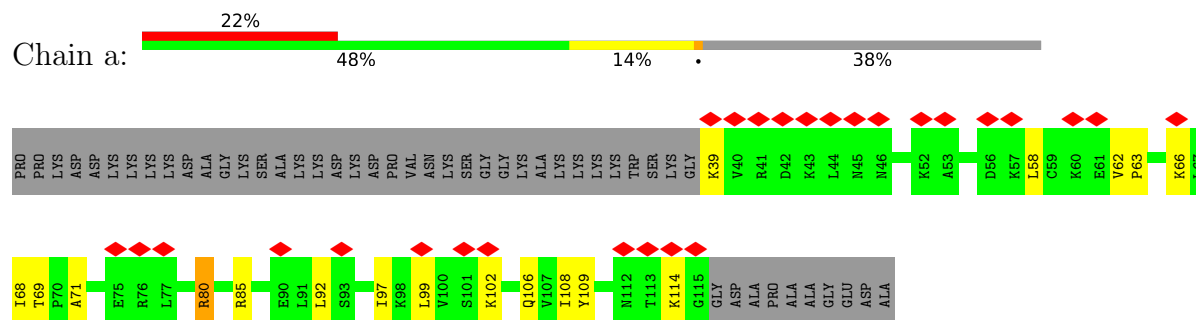
• Molecule 35: uS12



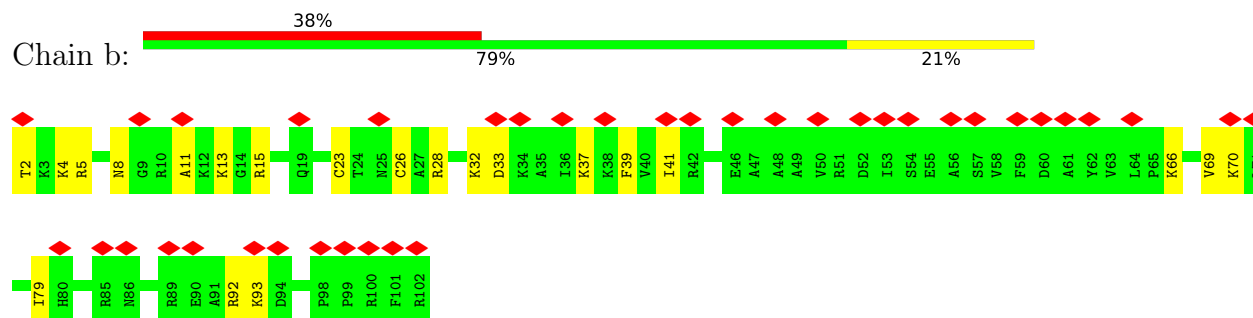
- Molecule 36: eS24



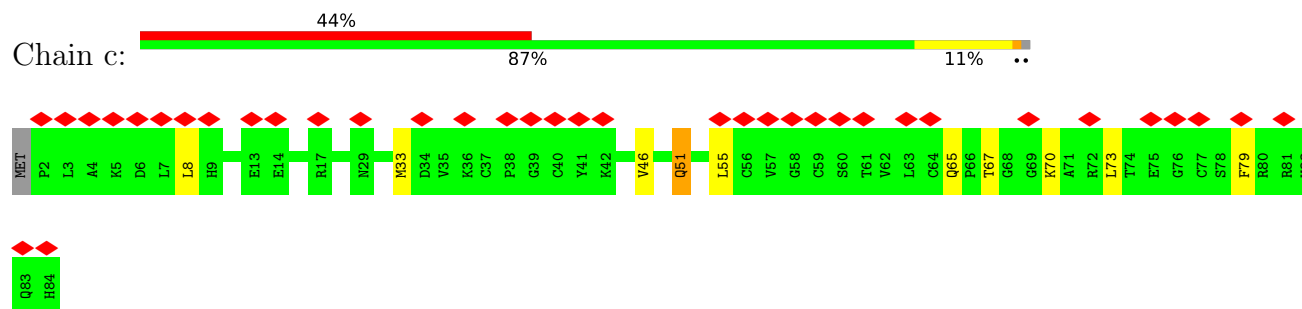
- Molecule 37: eS25



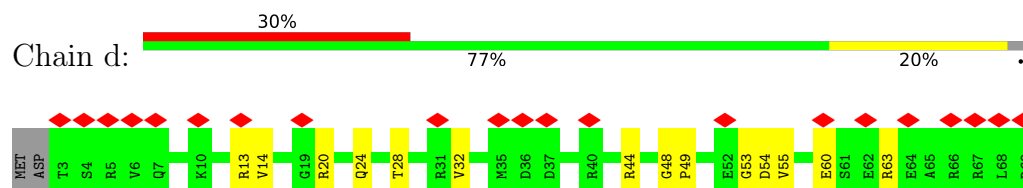
- Molecule 38: eS26



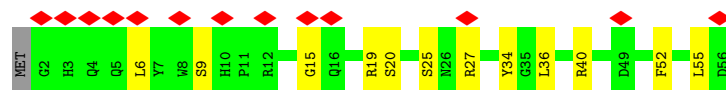
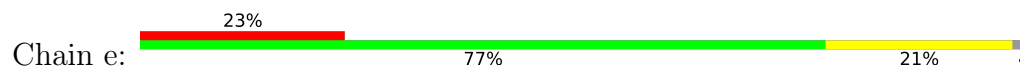
- Molecule 39: eS27



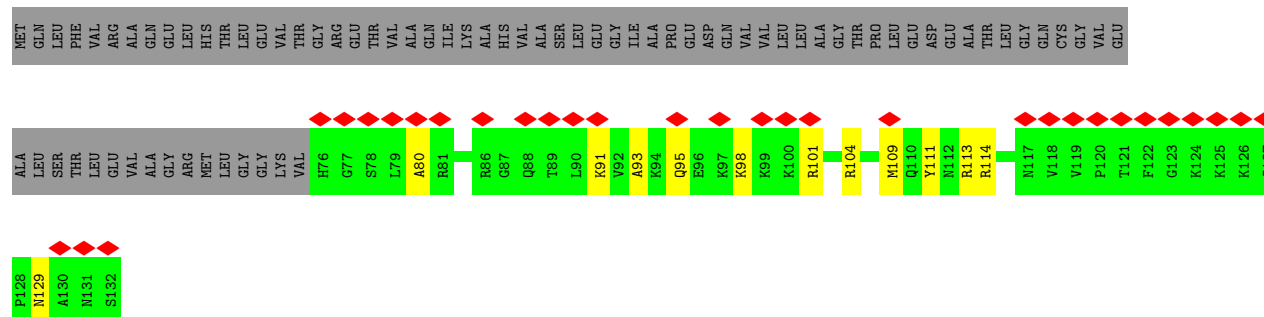
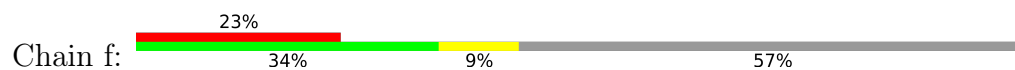
- Molecule 40: eS28



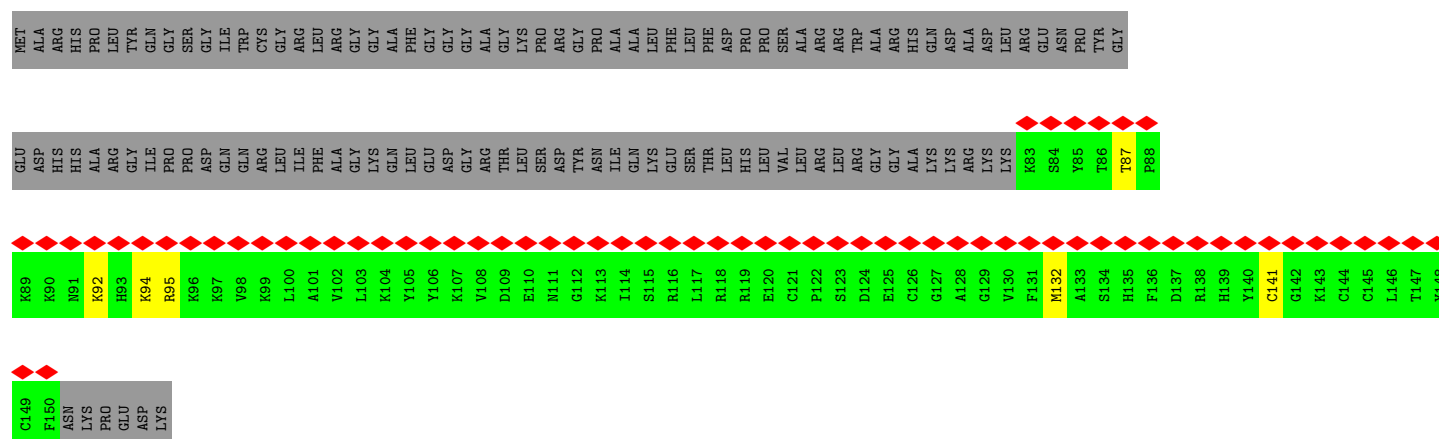
- Molecule 41: uS14



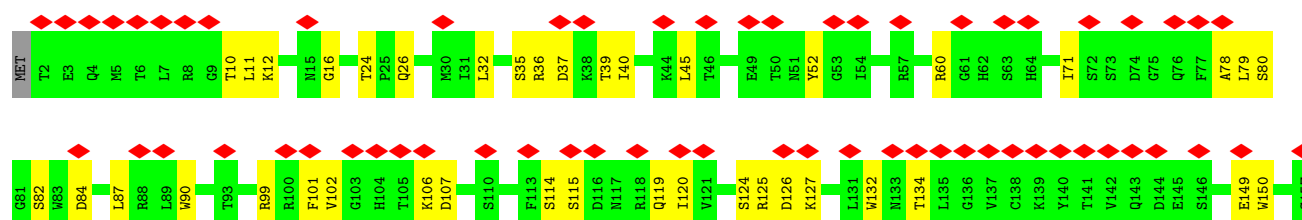
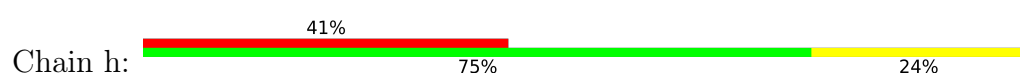
- Molecule 42: eS30

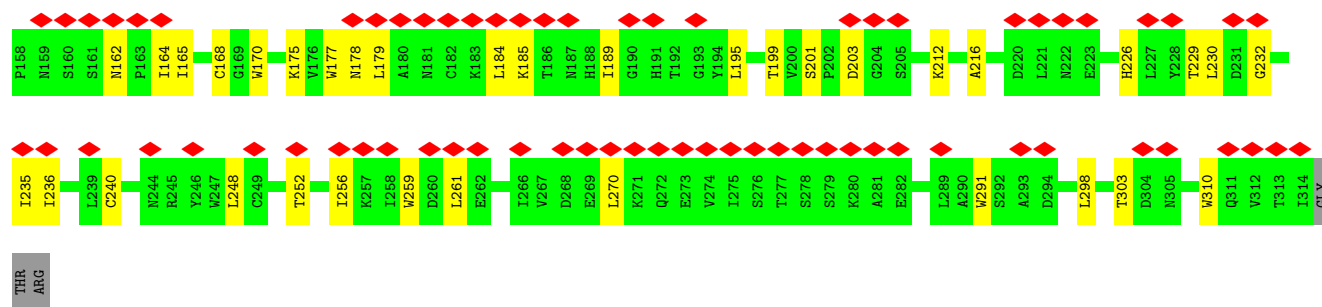


- Molecule 43: eS31

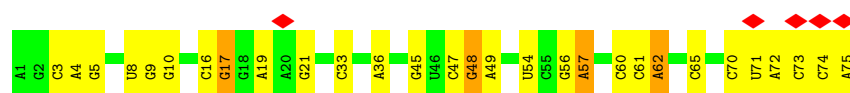


- Molecule 44: Receptor for Activated C Kinase 1 (RACK1)

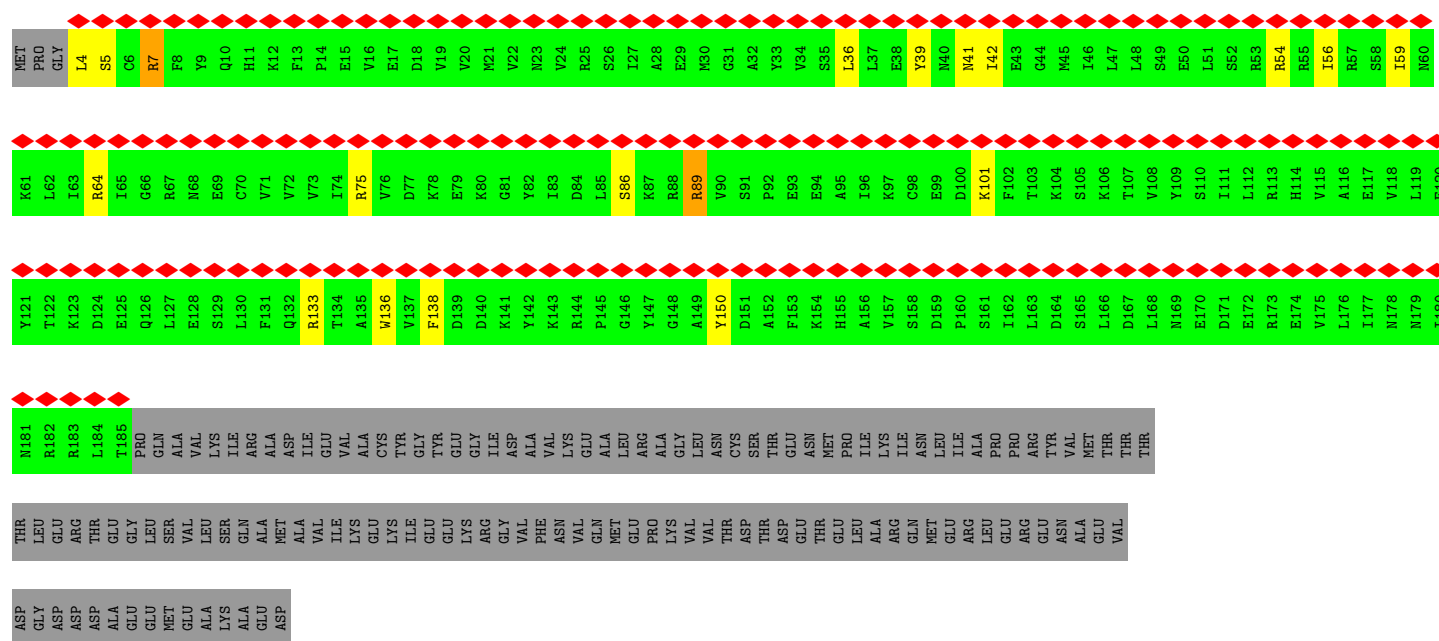




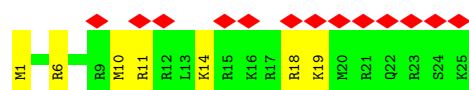
• Molecule 45: Met-tRNA_iMet



• Molecule 46: Eukaryotic translation initiation factor 2 subunit 1



• Molecule 47: eL41



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	262752	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.730	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.198	Depositor
Map size (Å)	396.8, 396.8, 396.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	o	0.64	5/5021 (0.1%)	0.97	21/6781 (0.3%)
2	p	0.42	1/4608 (0.0%)	0.85	8/6219 (0.1%)
3	q	2.35	8/3539 (0.2%)	0.97	22/4788 (0.5%)
4	r	0.59	3/2149 (0.1%)	0.93	10/2920 (0.3%)
5	s	0.40	0/2675	0.82	3/3609 (0.1%)
6	t	0.35	0/1773	0.78	6/2398 (0.3%)
7	u	0.46	2/3186 (0.1%)	0.96	10/4298 (0.2%)
8	v	0.44	1/2964 (0.0%)	0.94	22/4000 (0.6%)
9	2	0.21	0/40506	0.39	1/63123 (0.0%)
10	3	0.22	0/2120	0.41	0/3299
11	A	0.14	0/809	0.36	0/1083
12	B	0.27	0/1747	0.61	1/2374 (0.0%)
13	C	0.27	0/1756	0.60	0/2350
14	D	0.26	0/1753	0.57	0/2369
15	E	0.31	0/1796	0.66	2/2417 (0.1%)
16	F	0.26	0/2118	0.57	1/2849 (0.0%)
17	G	0.30	0/1531	0.60	1/2059 (0.0%)
18	H	0.24	0/1946	0.53	0/2590
19	I	0.21	0/1510	0.50	0/2022
20	J	0.24	0/1723	0.54	0/2298
21	K	0.24	0/1550	0.55	0/2069
22	L	0.28	0/834	0.61	0/1125
23	M	0.22	0/1254	0.51	0/1677
24	N	0.21	0/918	0.51	0/1233
25	O	0.23	0/1226	0.46	0/1649
26	P	0.24	0/1029	0.51	1/1380 (0.1%)
27	Q	0.27	0/1017	0.65	1/1358 (0.1%)
28	R	0.27	0/1146	0.58	0/1534
29	S	0.23	0/1082	0.51	0/1452
30	T	0.27	0/1208	0.59	0/1618
31	U	0.25	0/1115	0.53	1/1493 (0.1%)
32	V	0.23	0/805	0.58	1/1081 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	W	0.21	0/643	0.59	1/860 (0.1%)
34	X	0.25	0/1051	0.55	0/1406
35	Y	0.21	0/1116	0.46	0/1490
36	Z	0.24	0/1028	0.54	0/1366
37	a	0.26	0/620	0.60	0/831
38	b	0.23	0/828	0.53	0/1109
39	c	0.24	0/665	0.55	1/891 (0.1%)
40	d	0.29	0/532	0.61	0/712
41	e	0.19	0/470	0.46	0/623
42	f	0.23	0/462	0.59	0/607
43	g	0.13	0/567	0.32	0/753
44	h	0.24	0/2493	0.57	0/3394
45	i	0.21	0/1795	0.39	0/2798
46	j	0.31	0/1263	0.52	2/1708 (0.1%)
47	n	0.25	0/240	0.70	0/305
All	All	0.52	20/112187 (0.0%)	0.60	116/160368 (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
1	o	0	1
2	p	0	6
3	q	0	3
4	r	0	5
5	s	0	3
6	t	0	1
7	u	0	5
8	v	0	1
14	D	0	1
16	F	0	1
23	M	0	1
29	S	0	1
37	a	0	1
All	All	0	30

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	q	189	LEU	CB-CG	83.09	3.19	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	q	217	TRP	CE3-CZ3	78.94	3.75	1.38
3	q	217	TRP	CE2-CZ2	40.20	2.24	1.39
3	q	217	TRP	CZ3-CH2	40.04	2.40	1.40
3	q	217	TRP	CZ2-CH2	32.13	1.98	1.37

The worst 5 of 116 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	u	439	PRO	CB-CG-CD	23.07	179.93	106.10
1	o	148	PRO	N-CD-CG	-21.46	71.01	103.20
3	q	217	TRP	CE3-CZ3-CH2	-16.22	100.02	121.10
4	r	107	PRO	N-CD-CG	-15.61	79.78	103.20
7	u	439	PRO	N-CD-CG	-14.80	80.99	103.20

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	o	91	ARG	Sidechain
2	p	390	ALA	Peptide
2	p	415	ASN	Peptide
2	p	434	VAL	Peptide
2	p	490	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	o	4935	0	5017	97	0
2	p	4529	0	4533	84	0
3	q	3466	0	3446	91	0
4	r	2111	0	2105	47	0
5	s	2624	0	2592	55	0
6	t	1738	0	1706	27	0
7	u	3110	0	3084	61	0
8	v	2919	0	2950	54	0
9	2	36227	0	18299	237	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	3	1897	0	967	13	0
11	A	798	0	807	7	0
12	B	1710	0	1708	30	0
13	C	1729	0	1803	38	0
14	D	1716	0	1806	26	0
15	E	1768	0	1866	26	0
16	F	2076	0	2177	48	0
17	G	1509	0	1563	25	0
18	H	1923	0	2089	44	0
19	I	1488	0	1582	20	0
20	J	1691	0	1778	19	0
21	K	1525	0	1640	22	0
22	L	810	0	836	13	0
23	M	1233	0	1310	28	0
24	N	908	0	939	10	0
25	O	1202	0	1289	15	0
26	P	1016	0	1039	23	0
27	Q	997	0	1045	22	0
28	R	1128	0	1195	19	0
29	S	1068	0	1121	16	0
30	T	1190	0	1249	19	0
31	U	1097	0	1130	17	0
32	V	795	0	862	17	0
33	W	636	0	637	10	0
34	X	1034	0	1080	21	0
35	Y	1098	0	1167	15	0
36	Z	1011	0	1083	20	0
37	a	614	0	678	13	0
38	b	814	0	863	18	0
39	c	651	0	672	10	0
40	d	530	0	561	12	0
41	e	459	0	452	10	0
42	f	457	0	502	10	0
43	g	555	0	565	6	0
44	h	2436	0	2393	43	0
45	i	1604	0	816	5	0
46	j	1245	0	1024	9	0
47	n	239	0	289	7	0
48	b	1	0	0	0	0
All	All	106317	0	88315	1265	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 1265 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:q:217:TRP:CE3	3:q:217:TRP:CD2	1.85	1.61
3:q:217:TRP:CH2	3:q:217:TRP:CZ2	1.98	1.52
3:q:217:TRP:CD2	3:q:217:TRP:CE2	1.92	1.44
3:q:217:TRP:CZ2	3:q:217:TRP:CE2	2.24	1.25
3:q:217:TRP:CH2	3:q:217:TRP:CZ3	2.40	1.10

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	o	598/1362 (44%)	561 (94%)	35 (6%)	2 (0%)	36	67
2	p	556/843 (66%)	533 (96%)	20 (4%)	3 (0%)	24	57
3	q	418/445 (94%)	387 (93%)	26 (6%)	5 (1%)	10	37
4	r	270/364 (74%)	253 (94%)	13 (5%)	4 (2%)	8	32
5	s	322/352 (92%)	299 (93%)	19 (6%)	4 (1%)	10	37
6	t	214/218 (98%)	206 (96%)	7 (3%)	1 (0%)	24	57
7	u	371/564 (66%)	348 (94%)	18 (5%)	5 (1%)	9	35
8	v	364/374 (97%)	344 (94%)	16 (4%)	4 (1%)	11	39
11	A	97/144 (67%)	96 (99%)	1 (1%)	0	100	100
12	B	215/295 (73%)	204 (95%)	10 (5%)	1 (0%)	24	57
13	C	211/264 (80%)	202 (96%)	9 (4%)	0	100	100
14	D	219/221 (99%)	214 (98%)	5 (2%)	0	100	100
15	E	226/281 (80%)	224 (99%)	2 (1%)	0	100	100
16	F	260/263 (99%)	254 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	G	189/204 (93%)	182 (96%)	7 (4%)	0	100	100
18	H	235/249 (94%)	231 (98%)	4 (2%)	0	100	100
19	I	181/432 (42%)	179 (99%)	2 (1%)	0	100	100
20	J	205/208 (99%)	194 (95%)	11 (5%)	0	100	100
21	K	183/194 (94%)	180 (98%)	3 (2%)	0	100	100
22	L	94/149 (63%)	86 (92%)	8 (8%)	0	100	100
23	M	149/158 (94%)	142 (95%)	7 (5%)	0	100	100
24	N	115/132 (87%)	112 (97%)	3 (3%)	0	100	100
25	O	147/151 (97%)	144 (98%)	3 (2%)	0	100	100
26	P	134/168 (80%)	126 (94%)	8 (6%)	0	100	100
27	Q	118/145 (81%)	111 (94%)	7 (6%)	0	100	100
28	R	140/172 (81%)	135 (96%)	5 (4%)	0	100	100
29	S	130/135 (96%)	130 (100%)	0	0	100	100
30	T	142/152 (93%)	138 (97%)	4 (3%)	0	100	100
31	U	139/145 (96%)	134 (96%)	4 (3%)	1 (1%)	18	49
32	V	98/119 (82%)	97 (99%)	1 (1%)	0	100	100
33	W	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
34	X	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
35	Y	139/143 (97%)	136 (98%)	3 (2%)	0	100	100
36	Z	122/131 (93%)	120 (98%)	2 (2%)	0	100	100
37	a	75/124 (60%)	74 (99%)	1 (1%)	0	100	100
38	b	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
39	c	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
40	d	65/69 (94%)	64 (98%)	1 (2%)	0	100	100
41	e	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
42	f	55/133 (41%)	54 (98%)	1 (2%)	0	100	100
43	g	66/188 (35%)	66 (100%)	0	0	100	100
44	h	311/317 (98%)	298 (96%)	13 (4%)	0	100	100
46	j	180/315 (57%)	178 (99%)	1 (1%)	1 (1%)	21	52
47	n	23/25 (92%)	23 (100%)	0	0	100	100
All	All	8217/10802 (76%)	7888 (96%)	298 (4%)	31 (0%)	31	61

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	o	21	VAL
2	p	416	PRO
3	q	51	VAL
3	q	269	LYS
4	r	129	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	o	551/1245 (44%)	543 (98%)	8 (2%)	57	75
2	p	503/750 (67%)	491 (98%)	12 (2%)	43	69
3	q	384/406 (95%)	379 (99%)	5 (1%)	61	77
4	r	239/282 (85%)	238 (100%)	1 (0%)	84	86
5	s	293/311 (94%)	291 (99%)	2 (1%)	76	82
6	t	190/193 (98%)	186 (98%)	4 (2%)	47	71
7	u	342/516 (66%)	340 (99%)	2 (1%)	78	83
8	v	327/335 (98%)	323 (99%)	4 (1%)	63	78
11	A	84/123 (68%)	84 (100%)	0	100	100
12	B	180/245 (74%)	179 (99%)	1 (1%)	78	83
13	C	194/231 (84%)	194 (100%)	0	100	100
14	D	187/187 (100%)	185 (99%)	2 (1%)	65	78
15	E	190/232 (82%)	187 (98%)	3 (2%)	55	75
16	F	224/225 (100%)	224 (100%)	0	100	100
17	G	161/170 (95%)	159 (99%)	2 (1%)	63	78
18	H	207/218 (95%)	206 (100%)	1 (0%)	81	85
19	I	165/360 (46%)	165 (100%)	0	100	100
20	J	179/180 (99%)	178 (99%)	1 (1%)	78	83
21	K	161/168 (96%)	159 (99%)	2 (1%)	63	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	L	87/125 (70%)	85 (98%)	2 (2%)	44	70
23	M	136/142 (96%)	134 (98%)	2 (2%)	57	75
24	N	99/108 (92%)	99 (100%)	0	100	100
25	O	130/131 (99%)	130 (100%)	0	100	100
26	P	106/130 (82%)	106 (100%)	0	100	100
27	Q	109/130 (84%)	108 (99%)	1 (1%)	70	80
28	R	117/140 (84%)	114 (97%)	3 (3%)	40	68
29	S	119/121 (98%)	118 (99%)	1 (1%)	73	81
30	T	125/132 (95%)	123 (98%)	2 (2%)	55	75
31	U	111/116 (96%)	111 (100%)	0	100	100
32	V	92/107 (86%)	92 (100%)	0	100	100
33	W	67/67 (100%)	67 (100%)	0	100	100
34	X	112/113 (99%)	111 (99%)	1 (1%)	70	80
35	Y	113/115 (98%)	113 (100%)	0	100	100
36	Z	107/113 (95%)	104 (97%)	3 (3%)	38	66
37	a	68/102 (67%)	68 (100%)	0	100	100
38	b	88/88 (100%)	88 (100%)	0	100	100
39	c	75/76 (99%)	75 (100%)	0	100	100
40	d	60/62 (97%)	60 (100%)	0	100	100
41	e	48/49 (98%)	48 (100%)	0	100	100
42	f	47/106 (44%)	47 (100%)	0	100	100
43	g	61/154 (40%)	61 (100%)	0	100	100
44	h	272/275 (99%)	268 (98%)	4 (2%)	57	75
46	j	90/280 (32%)	83 (92%)	7 (8%)	11	38
47	n	24/24 (100%)	24 (100%)	0	100	100
All	All	7224/9383 (77%)	7148 (99%)	76 (1%)	63	78

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	R	41	MET
46	j	75	ARG
30	T	45	LEU

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Mol	Chain	Res	Type
44	h	45	LEU
46	j	150	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 183 such sidechains are listed below:

Mol	Chain	Res	Type
16	F	157	ASN
25	O	69	ASN
16	F	216	ASN
20	J	35	ASN
28	R	80	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	3	87/89 (97%)	31 (35%)	0
45	i	74/75 (98%)	25 (33%)	0
9	2	1685/1870 (90%)	490 (29%)	6 (0%)
All	All	1846/2034 (90%)	546 (29%)	6 (0%)

5 of 546 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	2	2	A
9	2	4	C
9	2	9	U
9	2	17	C
9	2	20	G

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	2	874	G
9	2	1137	U
9	2	1637	A
9	2	561	A
9	2	65	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	3	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3	600:G	O3'	831:A	P	118.16

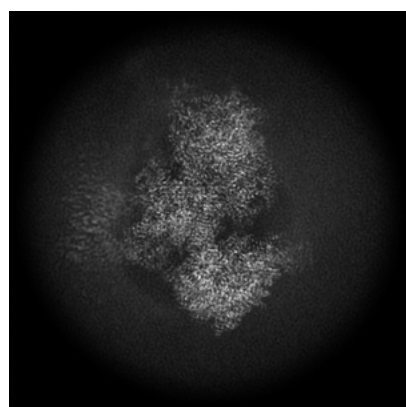
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40774. These allow visual inspection of the internal detail of the map and identification of artifacts.

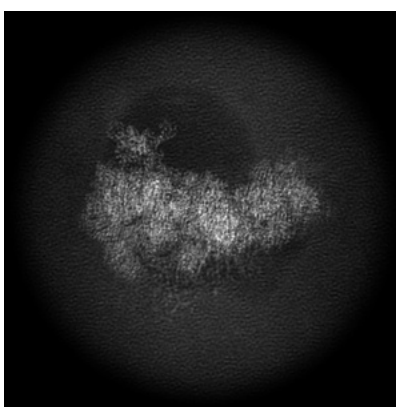
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

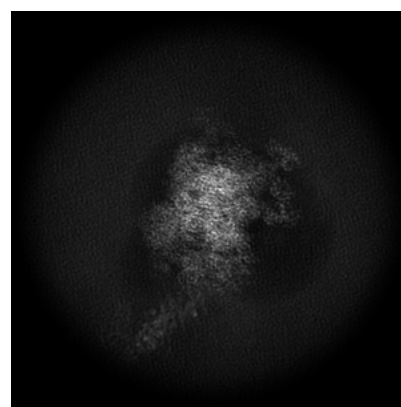
6.1.1 Primary map



X



Y

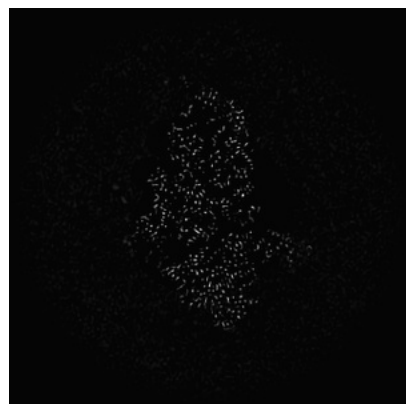


Z

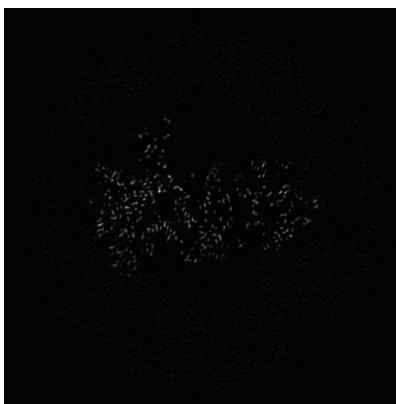
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

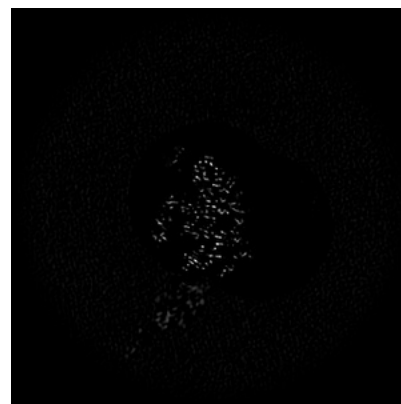
6.2.1 Primary map



X Index: 160



Y Index: 160

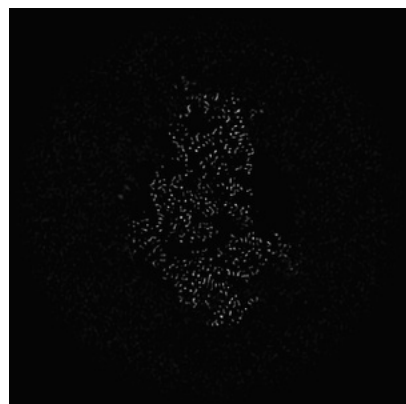


Z Index: 160

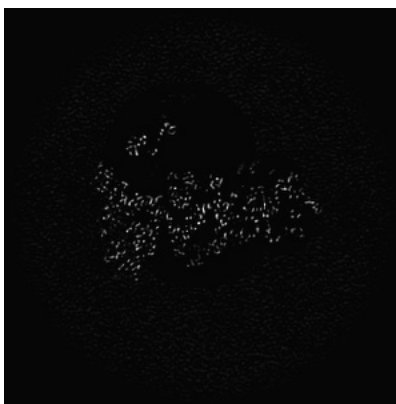
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

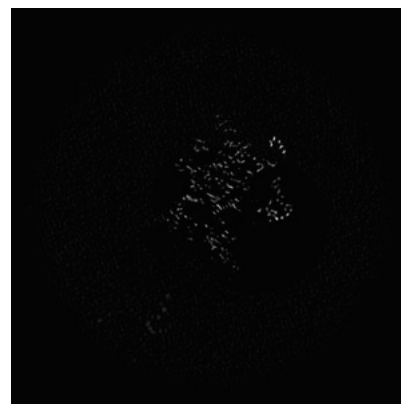
6.3.1 Primary map



X Index: 163



Y Index: 152

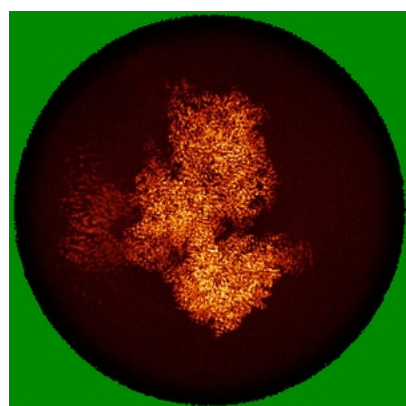


Z Index: 112

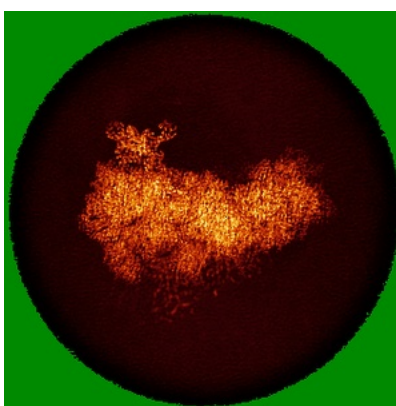
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

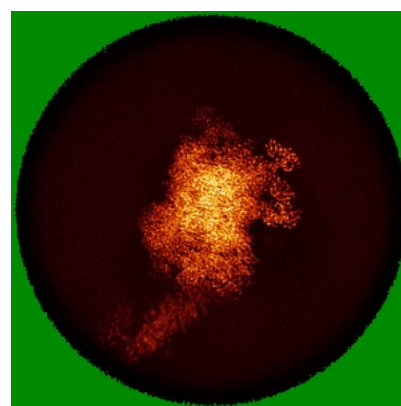
6.4.1 Primary map



X



Y

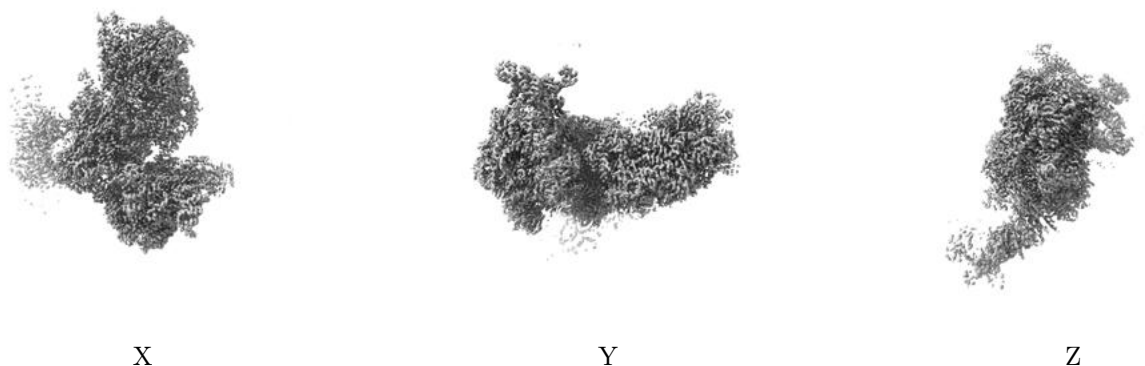


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.198. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

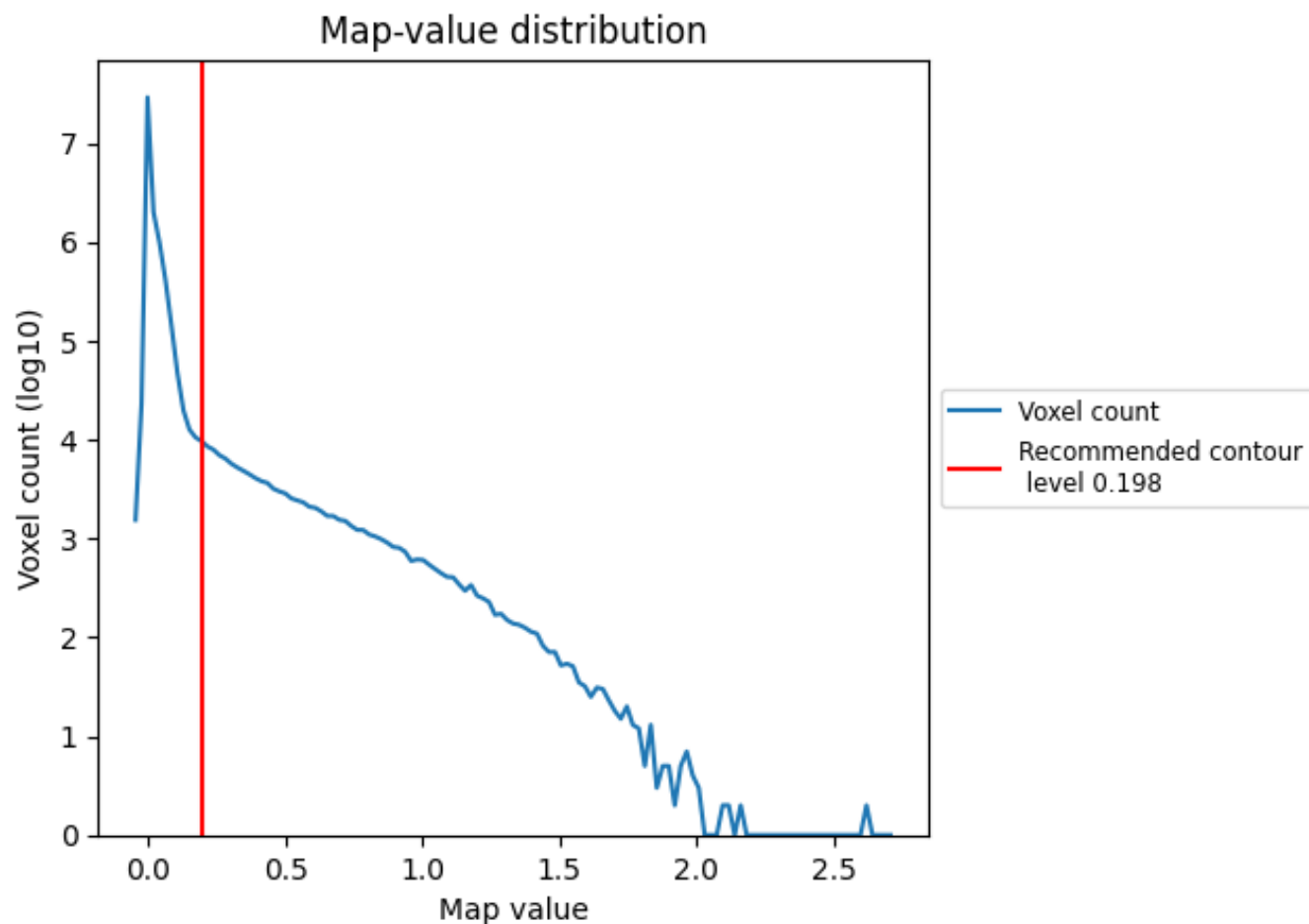
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

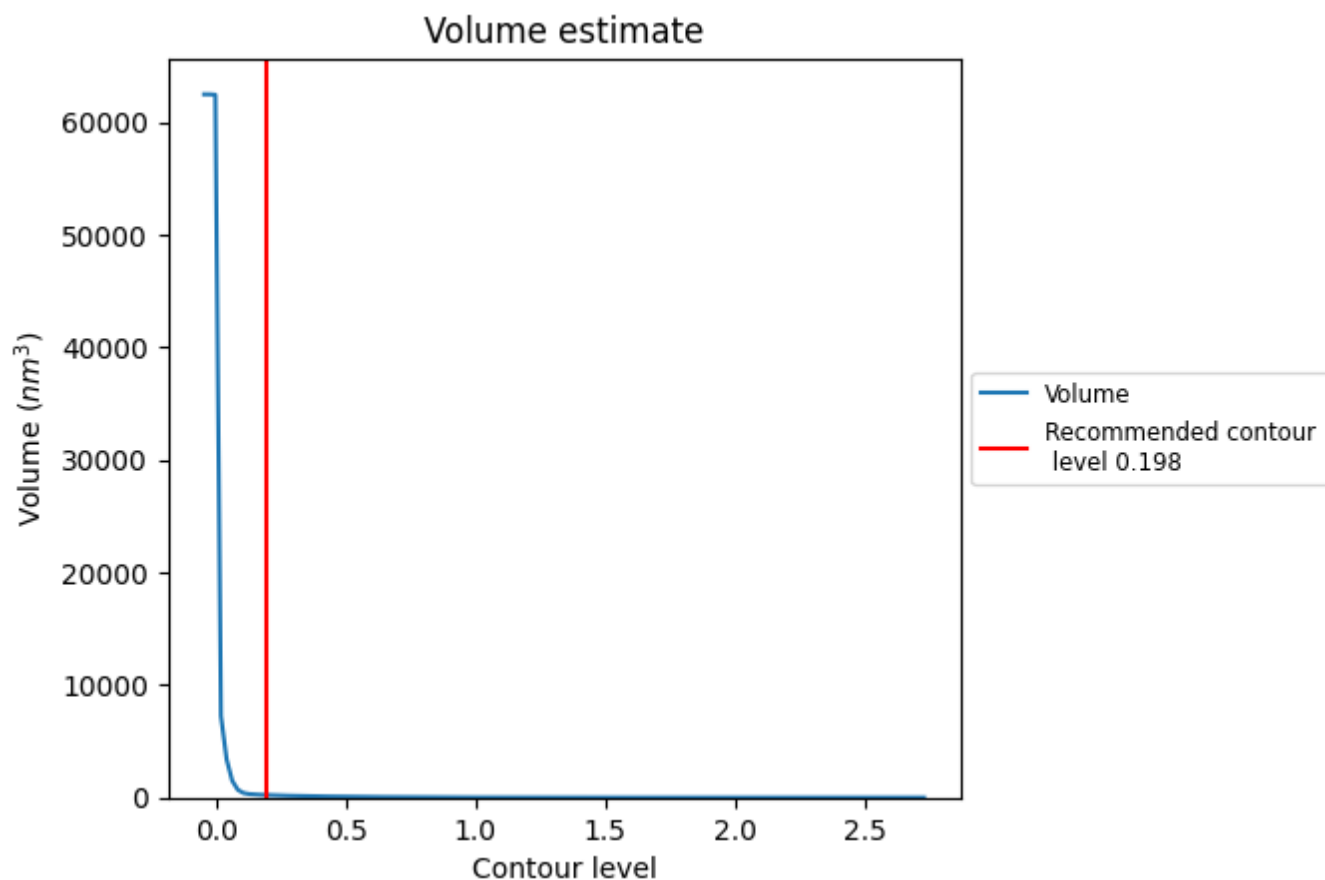
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

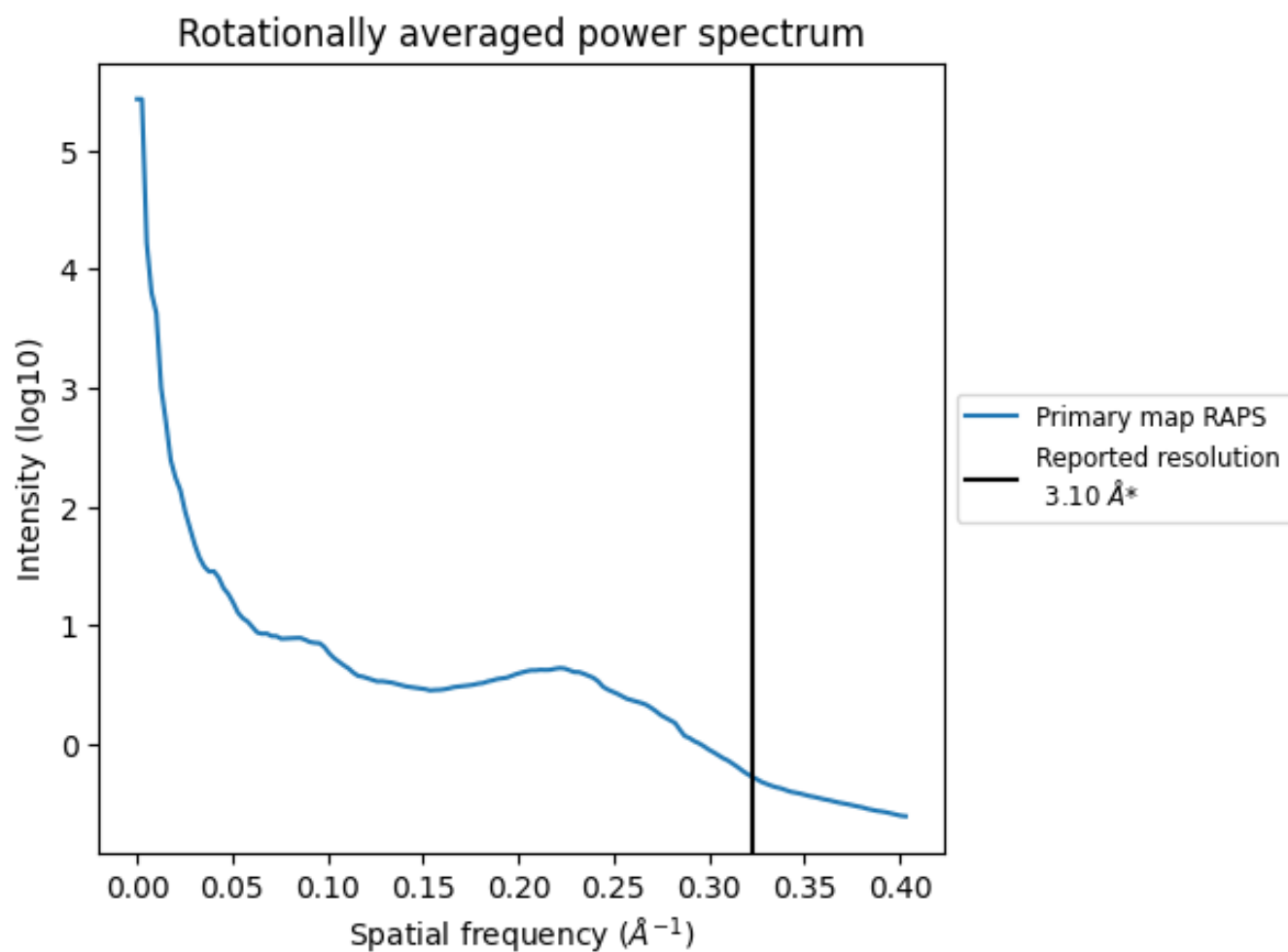
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 222 nm³; this corresponds to an approximate mass of 201 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

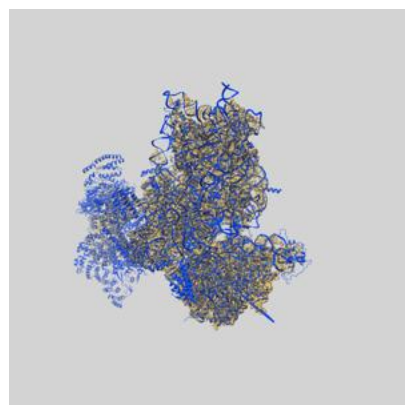
8 Fourier-Shell correlation ⓘ

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

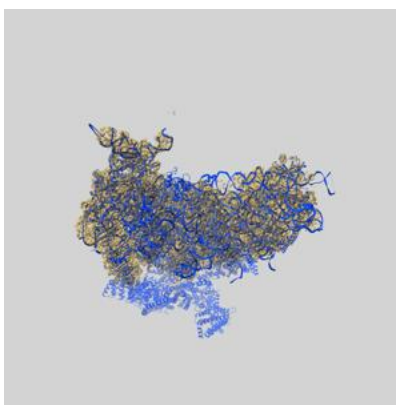
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40774 and PDB model 8SUP. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

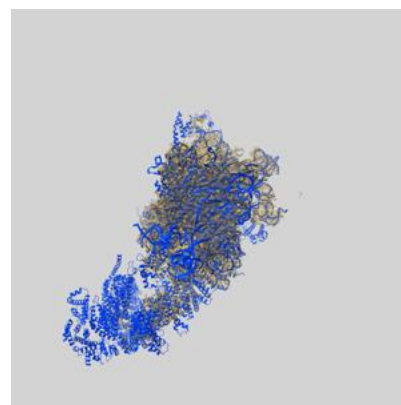
9.1 Map-model overlay [i](#)



X



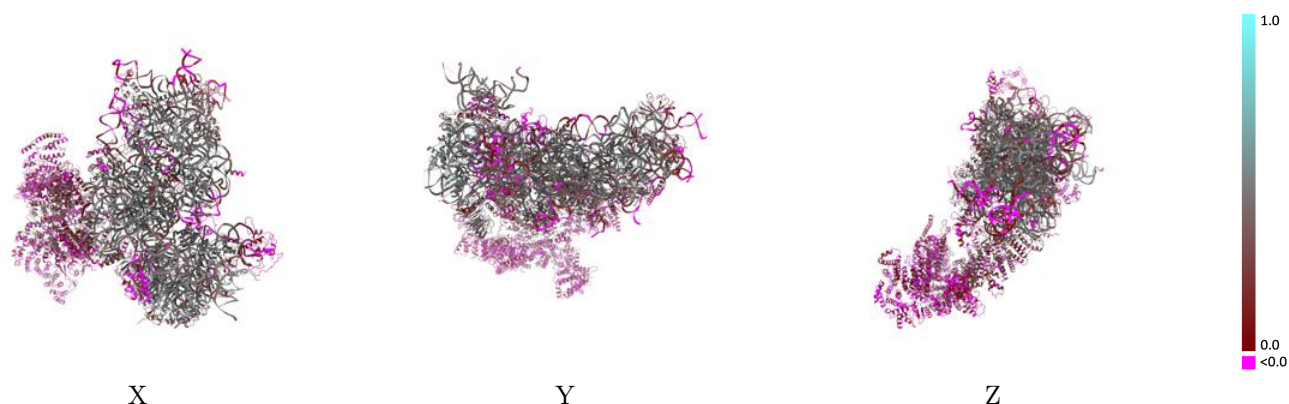
Y



Z

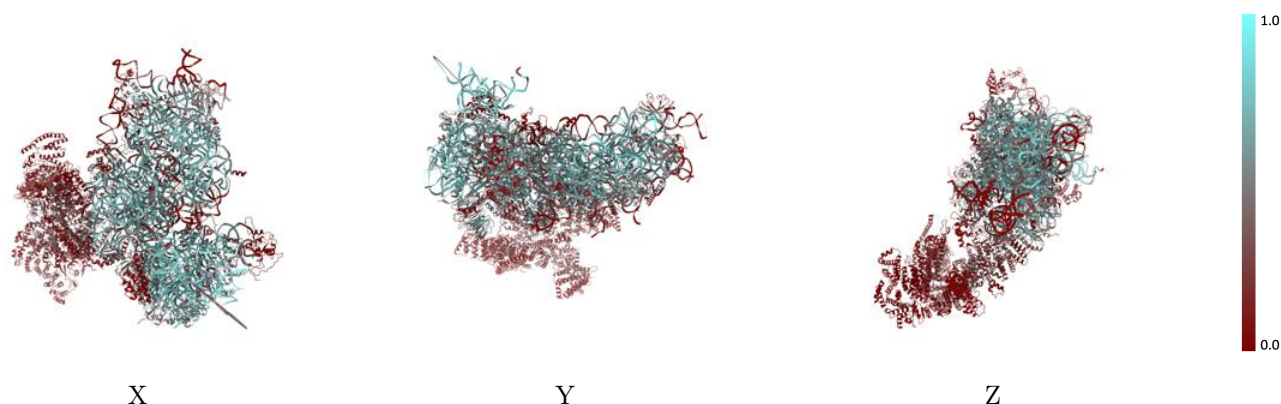
The images above show the 3D surface view of the map at the recommended contour level 0.198 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



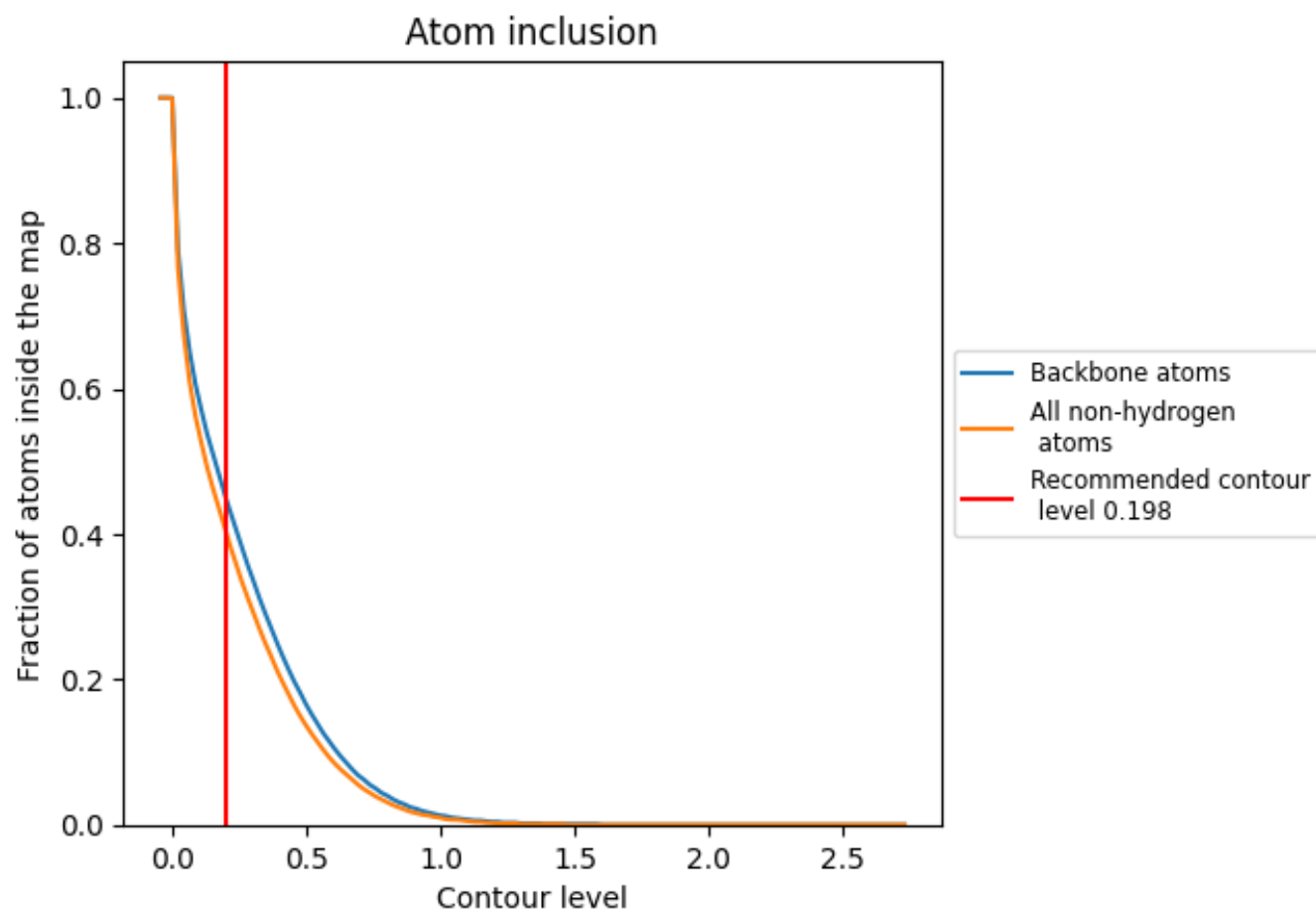
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.198).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 45% of all backbone atoms, 40% 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 (0.198) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4030	 0.3020
2	 0.5750	 0.3870
3	 0.6870	 0.4240
A	 0.0000	 -0.0500
B	 0.4750	 0.3730
C	 0.4440	 0.3530
D	 0.4830	 0.4120
E	 0.4760	 0.3750
F	 0.5270	 0.4260
G	 0.5740	 0.4360
H	 0.3560	 0.2900
I	 0.2150	 0.2060
J	 0.4550	 0.3650
K	 0.4880	 0.3810
L	 0.4410	 0.2980
M	 0.4870	 0.3910
N	 0.0430	 0.0150
O	 0.4720	 0.3750
P	 0.4190	 0.3610
Q	 0.5130	 0.3790
R	 0.6130	 0.4630
S	 0.3430	 0.2650
T	 0.5330	 0.4190
U	 0.6620	 0.4760
V	 0.3760	 0.3350
W	 0.4530	 0.3830
X	 0.5750	 0.4560
Y	 0.5490	 0.4400
Z	 0.4960	 0.3920
a	 0.4640	 0.3600
b	 0.4940	 0.4240
c	 0.4460	 0.3490
d	 0.4800	 0.3740
e	 0.5400	 0.4080
f	 0.3410	 0.2910



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Chain	Atom inclusion	Q-score
g	 0.0180	 -0.0310
h	 0.4440	 0.3470
i	 0.6570	 0.4160
j	 0.0020	 -0.0240
n	 0.4220	 0.3240
o	 0.1290	 0.1530
p	 0.1910	 0.2180
q	 0.0510	 0.0770
r	 0.0130	 0.0520
s	 0.0140	 0.0670
t	 0.0010	 -0.0000
u	 0.0000	 0.0580
v	 0.0130	 0.0520