



wwPDB EM Validation Summary Report ⓘ

Jun 21, 2026 – 07:59 am BST

PDB ID : 8PJ3 / pdb_00008pj3
EMDB ID : EMD-17698
Title : Structure of human 48S translation initiation complex upon transfer of initiator tRNA to eIF5B (48S-3)
Authors : Petrychenko, V.; Yi, S.-H.; Liedtke, D.; Peng, B.Z.; Rodnina, M.V.; Fischer, N.
Deposited on : 2023-06-22
Resolution : 3.70 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:

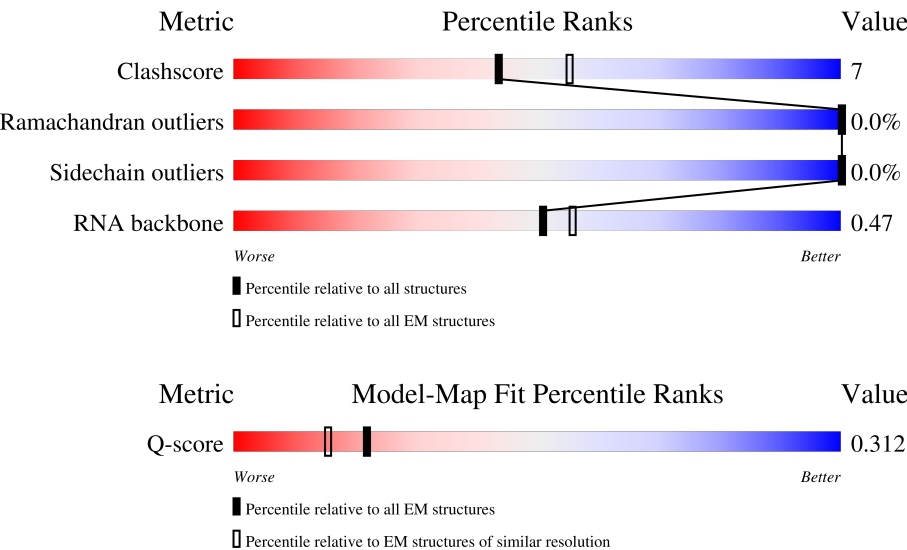
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.70 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	11569 (3.20 - 4.20)

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	0	1220	11% 39% 12% 49%
2	1	814	66% 67% 5% 28%
3	2	325	94% 94% 6%

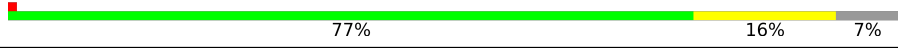
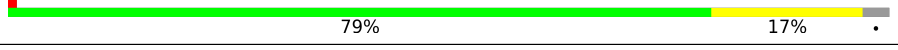
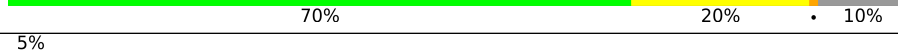
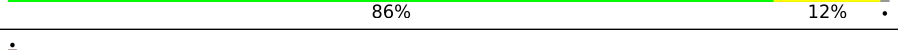
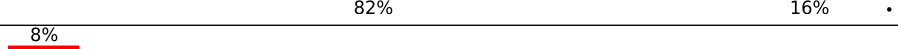
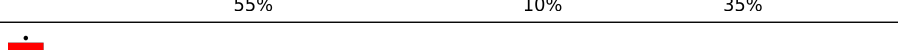
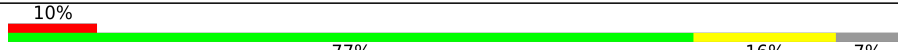
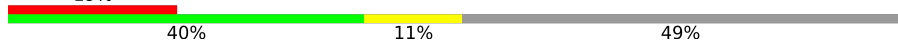
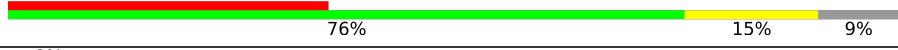
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Mol	Chain	Length	Quality of chain
4	3	218	
5	4	357	
6	5	564	
7	6	374	
8	7	255	
9	8	352	
10	9	25	
11	A	1869	
12	B	158	
13	C	263	
14	D	194	
15	E	143	
16	F	133	
17	G	194	
18	H	84	
19	I	151	
20	J	130	
21	K	83	
22	L	293	
23	M	135	
24	N	295	
25	O	264	
26	P	151	
27	Q	115	
28	R	208	

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Mol	Chain	Length	Quality of chain
29	S	249	
30	T	133	
31	V	204	
32	Y	146	
33	Z	243	
34	a	165	
35	b	145	
36	c	317	
37	d	145	
38	e	125	
39	f	152	
40	h	119	
41	i	56	
42	k	156	
43	m	132	
44	n	69	
45	o	320	
46	q	144	
47	r	315	
48	t	472	
49	u	1382	
50	v	445	
51	w	75	
52	x	548	
53	y	913	

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Mol	Chain	Length	Quality of chain
54	z	430	12% 22% 8% 69%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 123641 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 5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	621	Total	C	N	O	S	0	0
			4920	3135	850	913	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	588	Total	C	N	O	S	0	0
			3258	1986	633	634	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	2	304	Total	C	N	O	0	0
			1493	885	304	304		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	3	213	Total	C	N	O	0	0
			1057	631	213	213		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	4	257	Total	C	N	O	0	0
			1272	757	257	258		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	520	Total	C	N	O	S	0	0
			4347	2814	721	793	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	362	Total	C	N	O	S	0	0
			2196	1348	414	427	7		

- Molecule 8 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	57	Total	C	N	O	P	0	0
			1218	547	231	383	57		

- Molecule 9 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	8	317	Total	C	N	O	0	0
			1574	937	318	319		

- Molecule 10 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	9	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 11 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A	1754	Total	C	N	O	P	0	0
			37429	16718	6714	12244	1753		

- Molecule 12 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	B	142	Total	C	N	O	S	0	0
			1166	743	218	199	6		

- Molecule 13 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	256	Total	C	N	O	S	0	0
			2035	1302	378	347	8		

- Molecule 14 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	D	177	Total	C	N	O	S	0	0
			1477	941	295	239	2		

- Molecule 15 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	140	Total	C	N	O	S	0	0
			1087	687	215	182	3		

- Molecule 16 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	59	Total	C	N	O	S	0	0
			461	285	100	75	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	125	PRO	LYS	conflict	UNP P62861

- Molecule 17 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	G	177	Total	C	N	O	S	0	0
			1430	917	260	252	1		

- Molecule 18 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	H	81	Total	C	N	O	S	0	0
			631	397	116	111	7		

- Molecule 19 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	I	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 20 is a protein called 40S ribosomal protein S15a.

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

- Molecule 21 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	K	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

- Molecule 22 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L	220	Total	C	N	O	S	0	0
			1707	1104	292	301	10		

- Molecule 23 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	M	131	Total	C	N	O	S	0	0
			1064	668	198	194	4		

- Molecule 24 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	N	207	Total	C	N	O	S	0	0
			1633	1040	288	297	8		

- Molecule 25 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	O	211	Total	C	N	O	S	0	0
			1715	1088	307	306	14		

- Molecule 26 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	P	133	Total	C	N	O	S	0	0
			997	610	196	185	6		

- Molecule 27 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 28 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	R	198	Total	C	N	O	S	0	0
			1627	1021	322	279	5		

- Molecule 29 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	S	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 30 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	T	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 31 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	V	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 32 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 33 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 34 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	99	Total	C	N	O	S	0	0
			834	544	149	135	6		

- Molecule 35 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	131	Total	C	N	O	S	0	0
			1072	682	201	182	7		

- Molecule 36 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 37 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	142	Total	C	N	O	S	0	0
			1105	692	213	197	3		

- Molecule 38 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	81	Total	C	N	O	S	0	0
			649	420	119	109	1		

- Molecule 39 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	149	Total	C	N	O	S	0	0
			1227	770	249	207	1		

- Molecule 40 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	103	Total	C	N	O	S	0	0
			817	511	155	147	4		

- Molecule 41 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	50	Total	C	N	O	S	0	0
			419	262	85	67	5		

- Molecule 42 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	68	Total	C	N	O	S	0	0
			554	349	103	95	7		

- Molecule 43 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	122	Total	C	N	O	S	0	0
			950	596	168	177	9		

- Molecule 44 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	o	77	Total	C	N	O	0	0
			616	389	111	116		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	q	117	Total	C	N	O	S	0	0
			943	585	180	174	4		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	296	Total	C	N	O	S	0	0
			2138	1342	384	404	8		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	t	455	Total	C	N	O	S	0	0
			3439	2179	599	643	18		

- Molecule 49 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	u	706	Total	C	N	O	S	1	0
			5383	3379	982	999	23		

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	v	405	Total	C	N	O	S	0	0
			2740	1720	498	510	12		

- Molecule 51 is a RNA chain called Initiator Met-tRNA-i.

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

- Molecule 52 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	x	423	Total	C	N	O	S	0	0
			2842	1752	523	557	10		

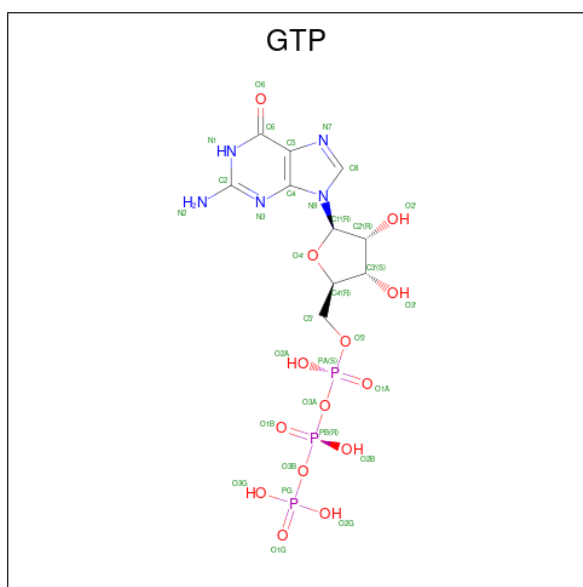
- Molecule 53 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	y	656	Total	C	N	O	S	0	0
			5263	3312	939	977	35		

- Molecule 54 is a protein called Eukaryotic translation initiation factor 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	z	132	Total	C	N	O	S	0	0
			1044	662	184	188	10		

- Molecule 55 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
55	0	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 56 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
56	0	1	Total	Na	0
			1	1	

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	0	1	Total	Mg	0
			1	1	
57	A	87	Total	Mg	0
			87	87	
57	f	1	Total	Mg	0
			1	1	

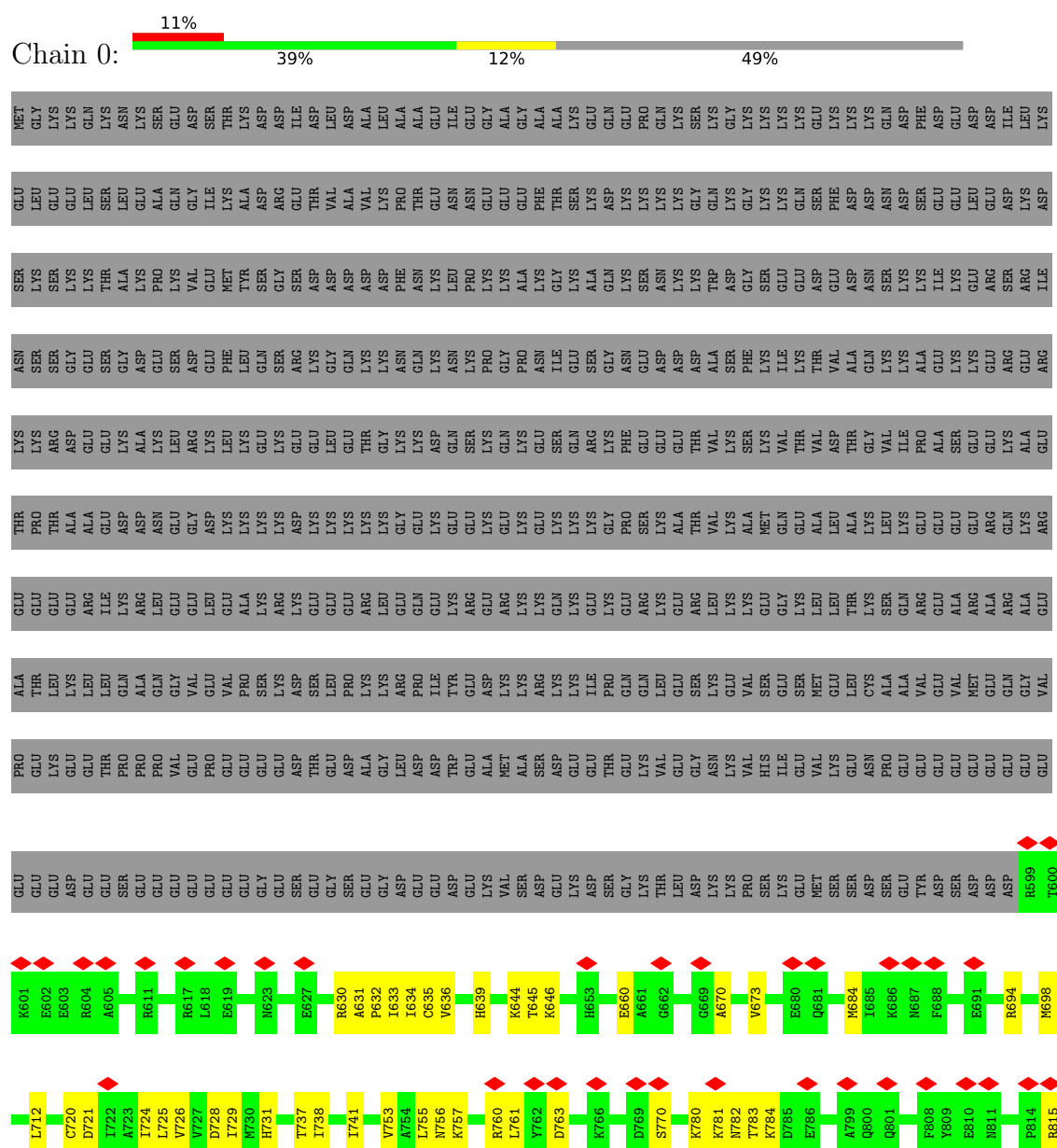
- Molecule 58 is ZINC ION (CCD ID: ZN) (formula: Zn).

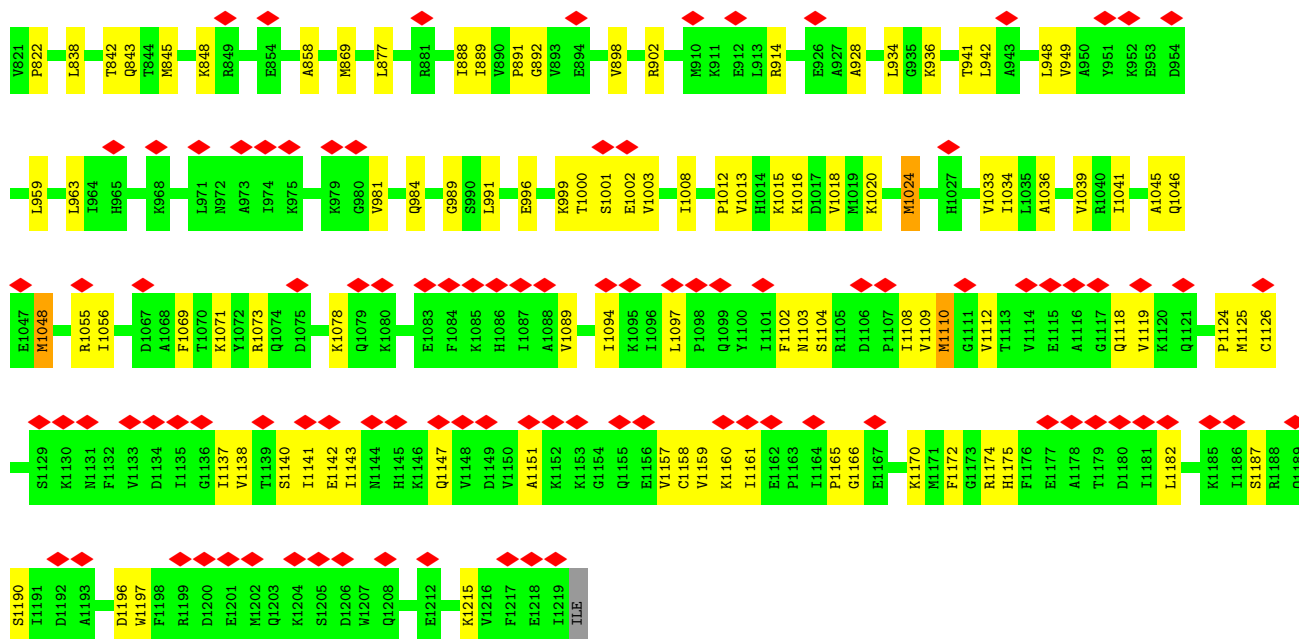
Mol	Chain	Residues	Atoms		AltConf
58	Q	1	Total	Zn	0
			1	1	
58	k	1	Total	Zn	0
			1	1	

3 Residue-property plots

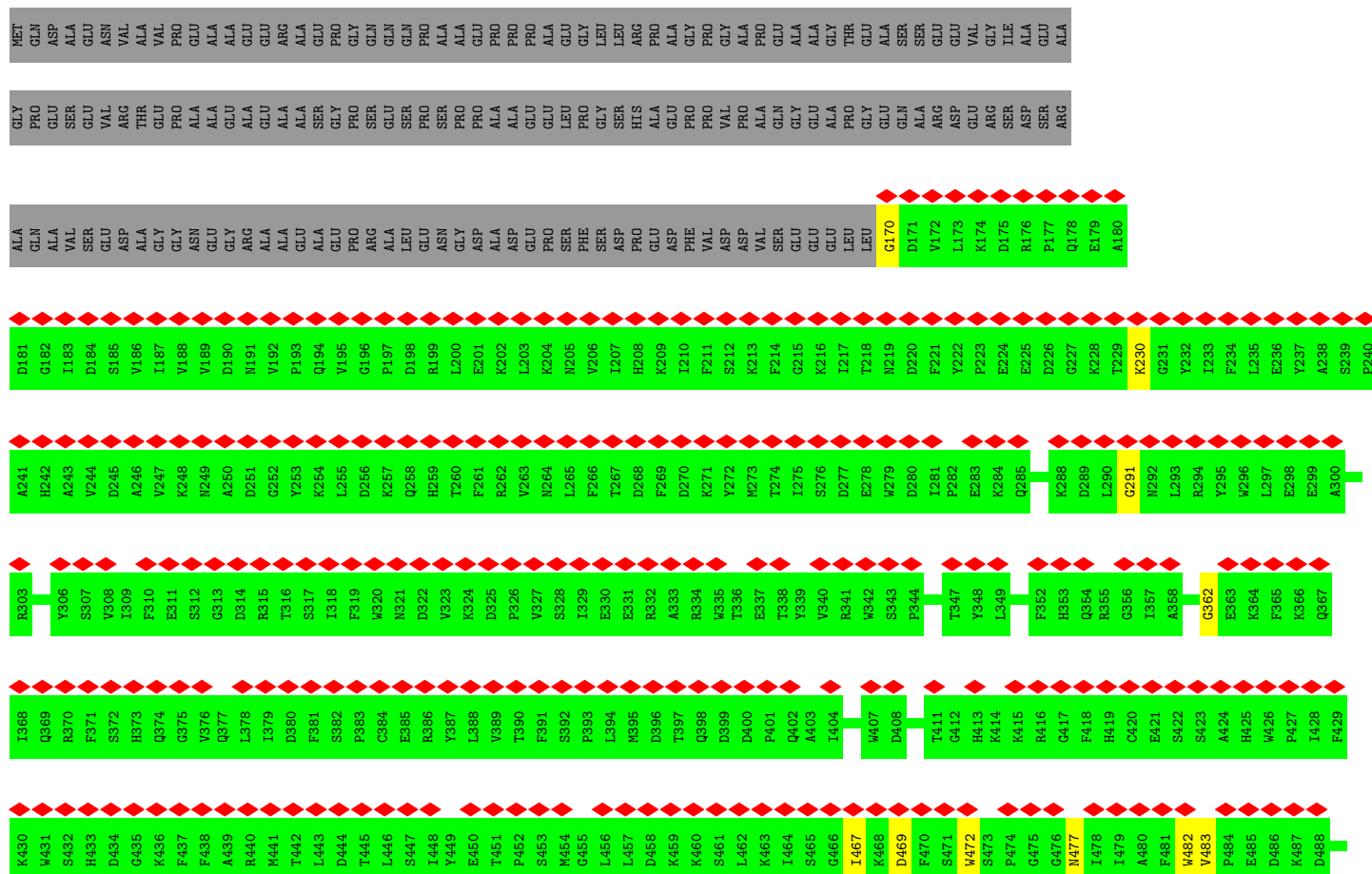
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

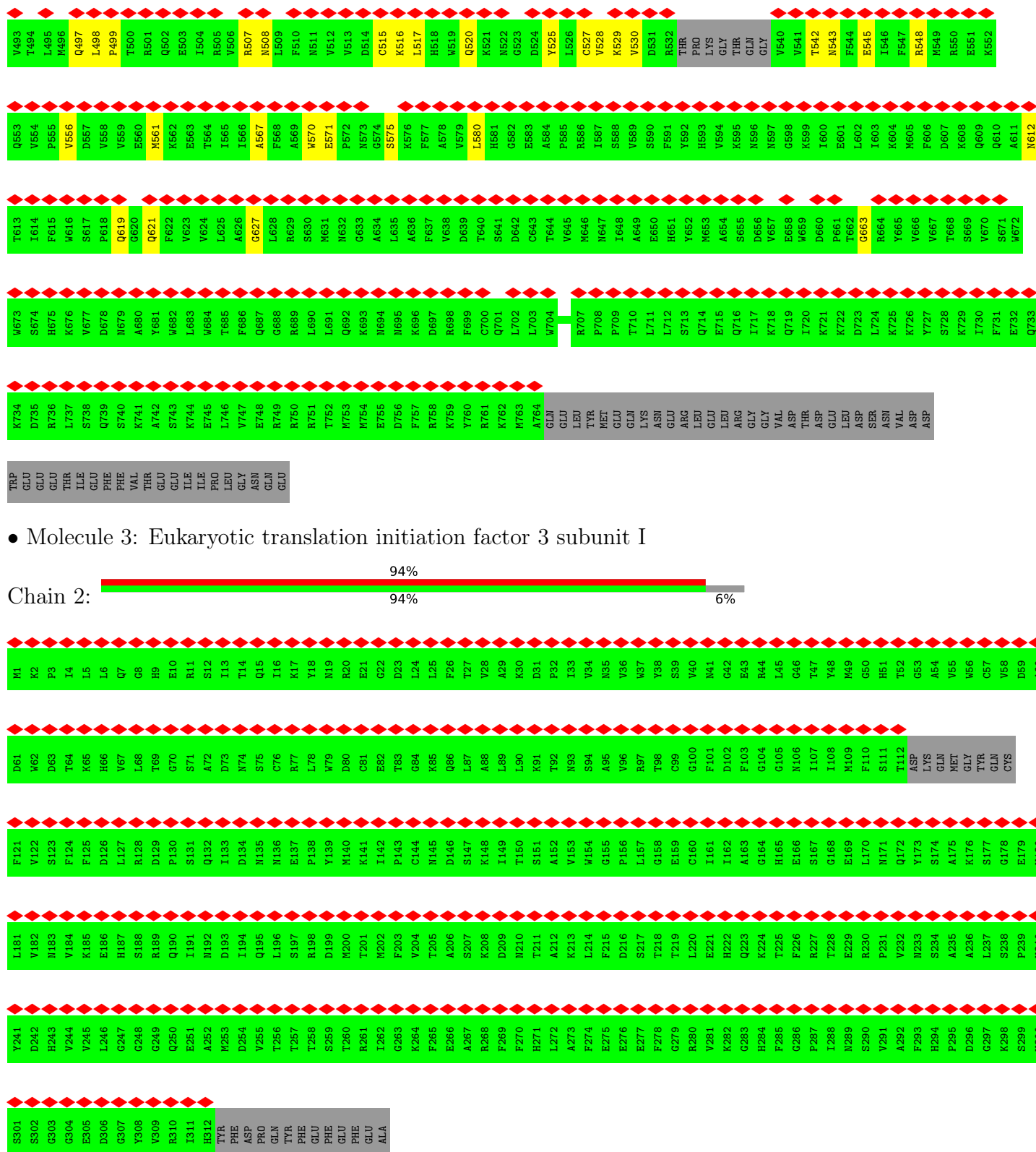
- Molecule 1: Eukaryotic translation initiation factor 5B

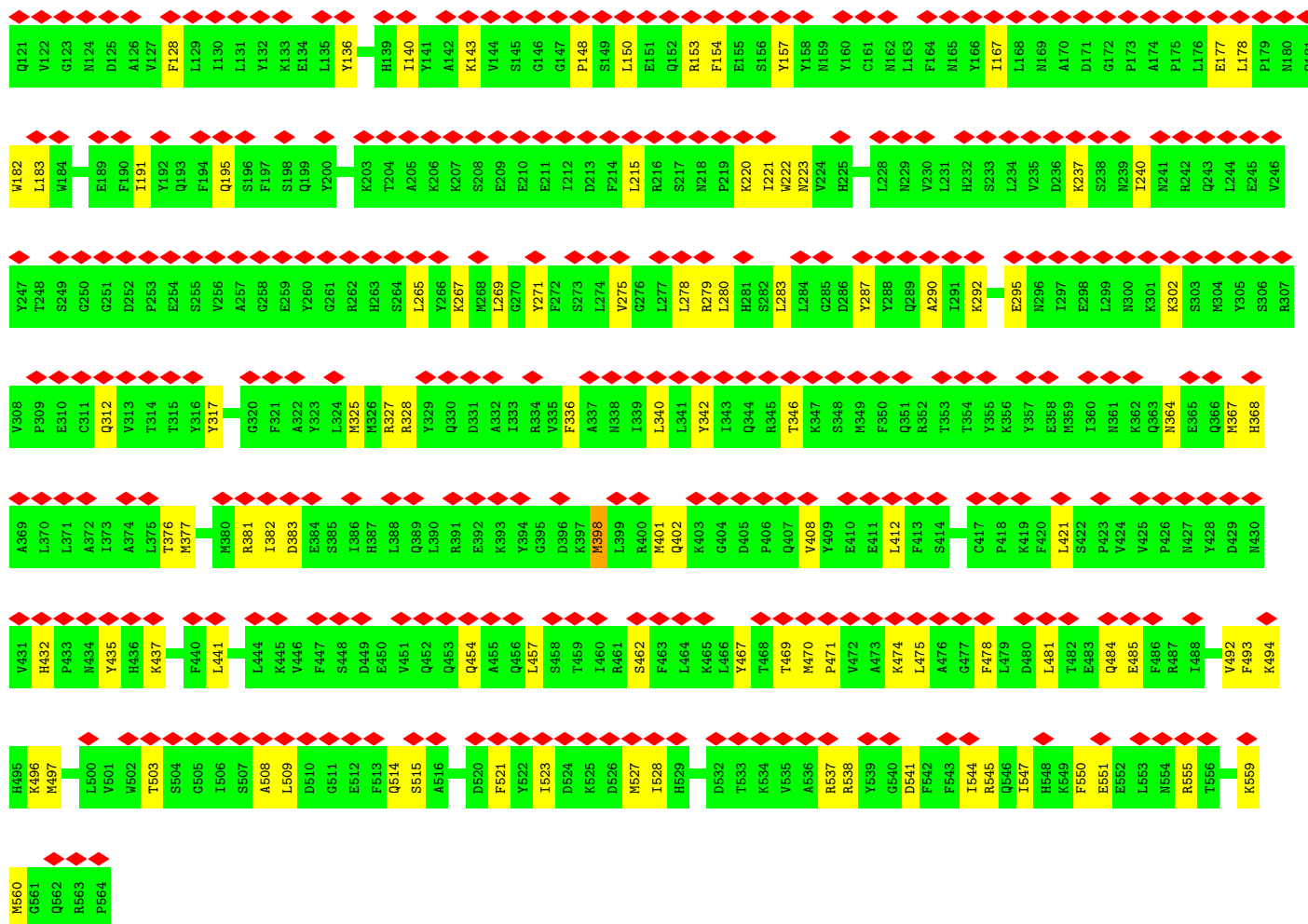




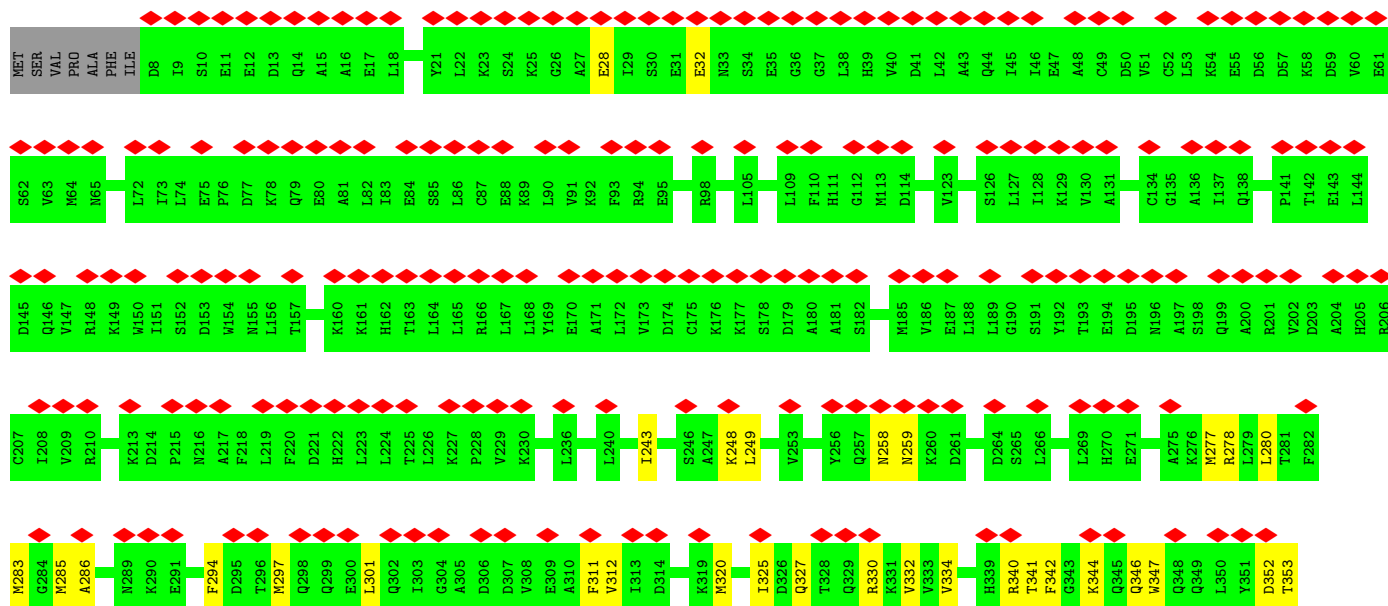
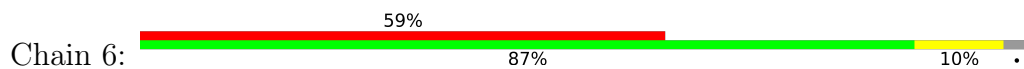
• Molecule 2: Eukaryotic translation initiation factor 3 subunit B







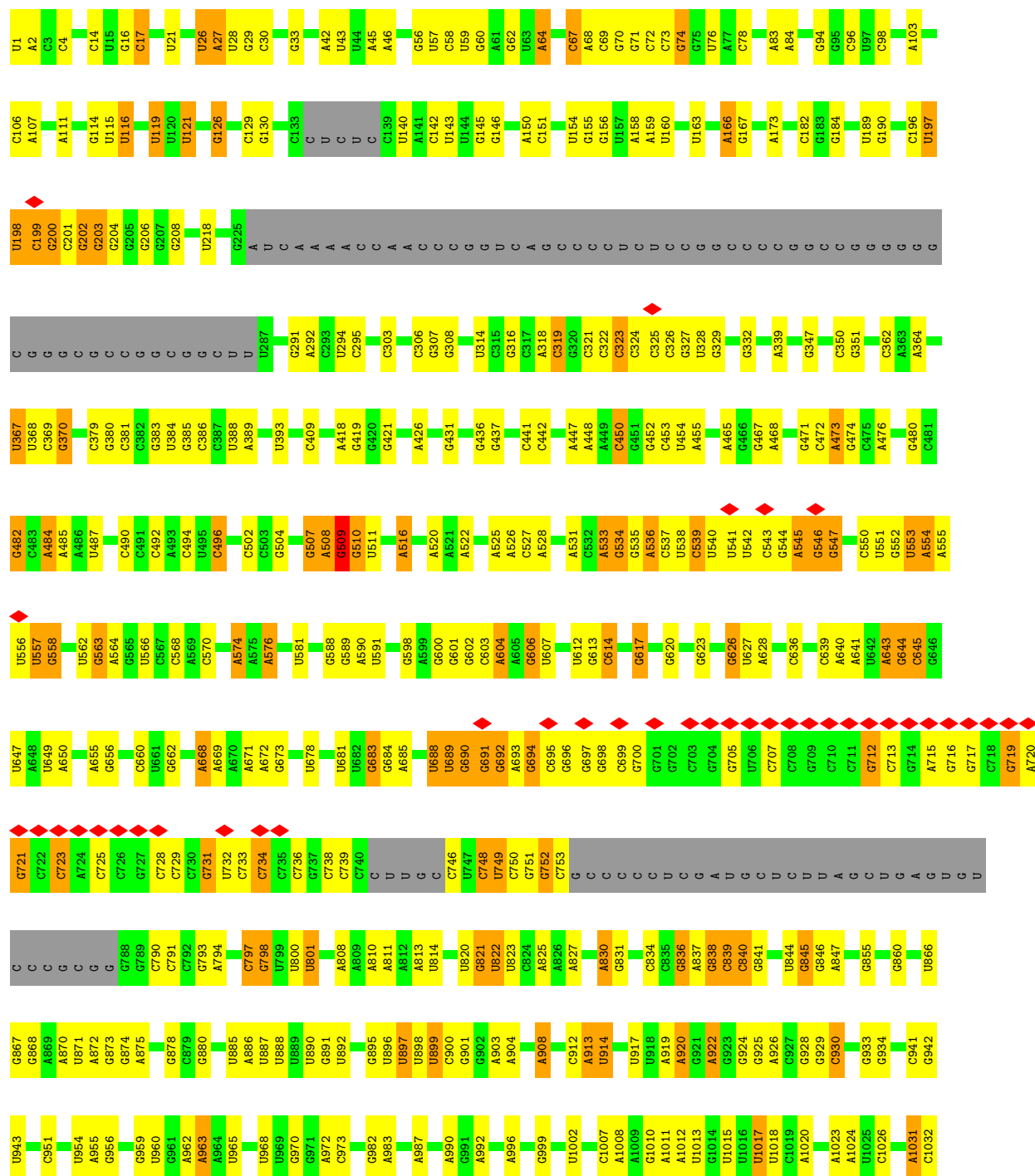
• Molecule 7: Eukaryotic translation initiation factor 3 subunit M

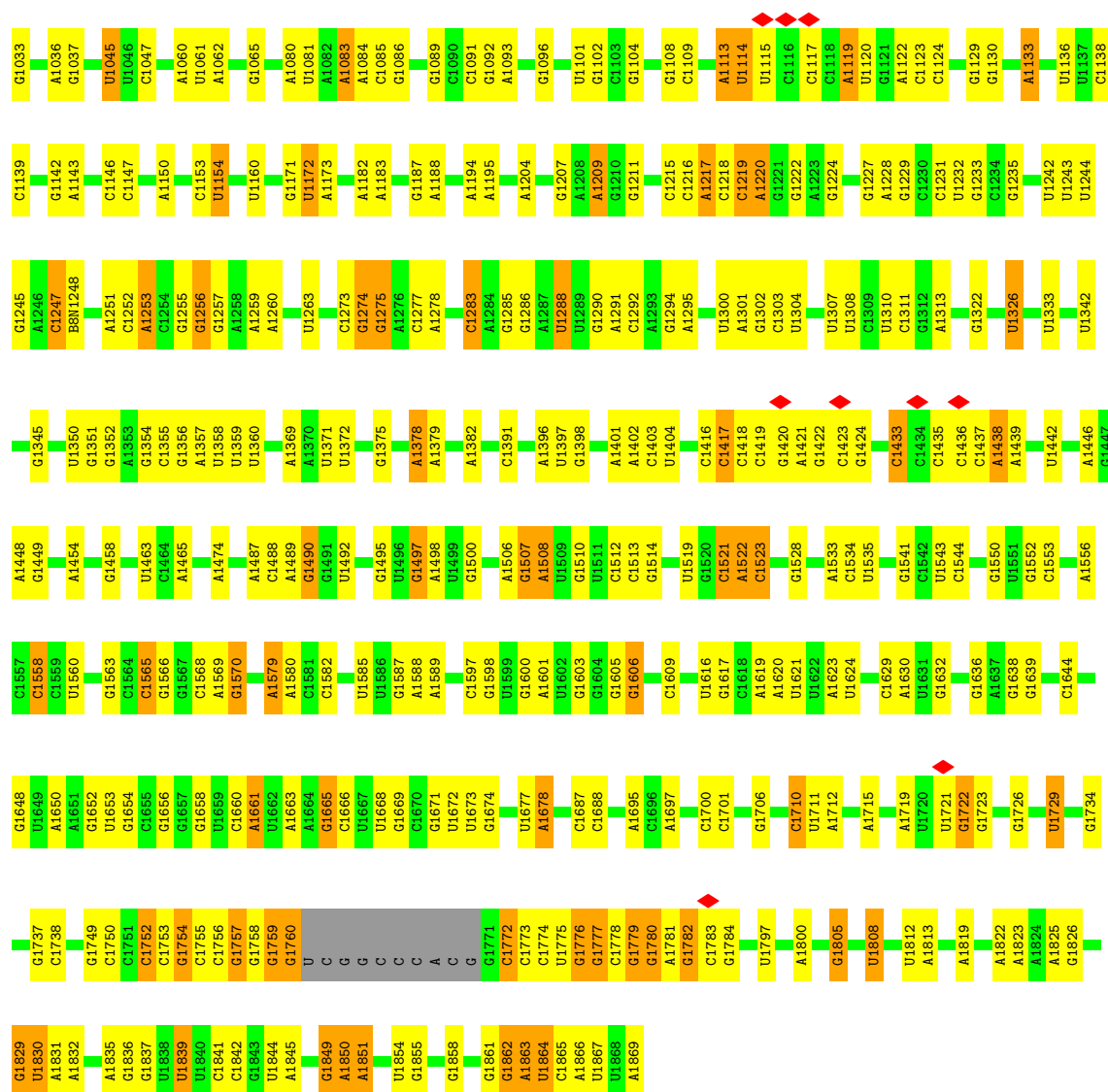




• Molecule 11: 18S rRNA

Chain A: 54% 32% 8% 6%





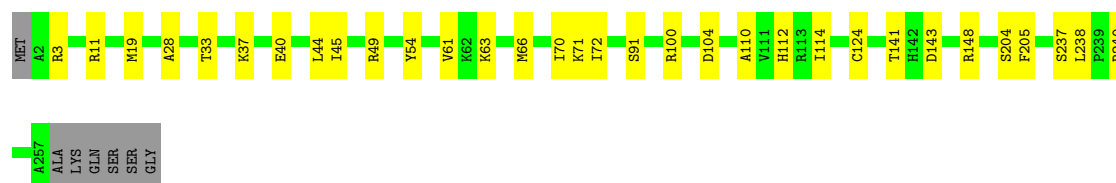
• Molecule 12: 40S ribosomal protein S11

Chain B: 78% 11% 10%

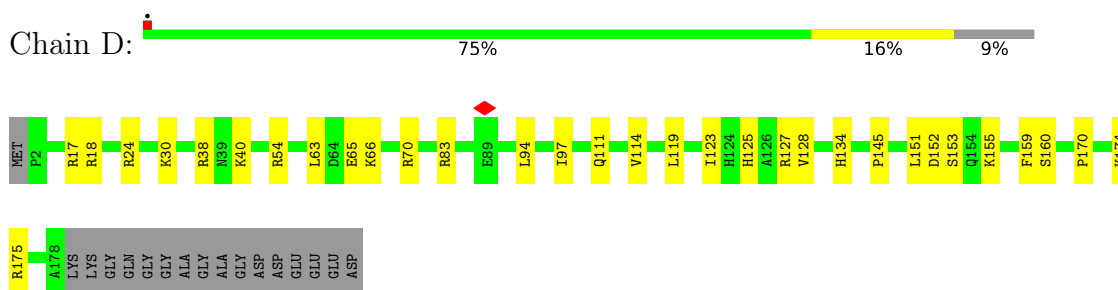


• Molecule 13: 40S ribosomal protein S4, X isoform

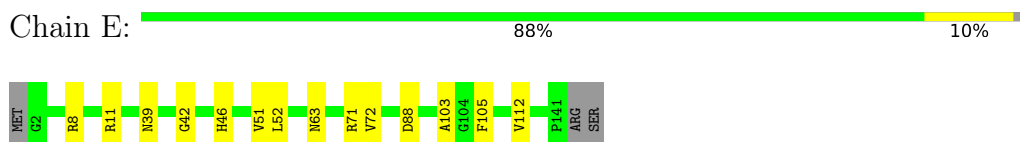
Chain C: 85% 12% 3%



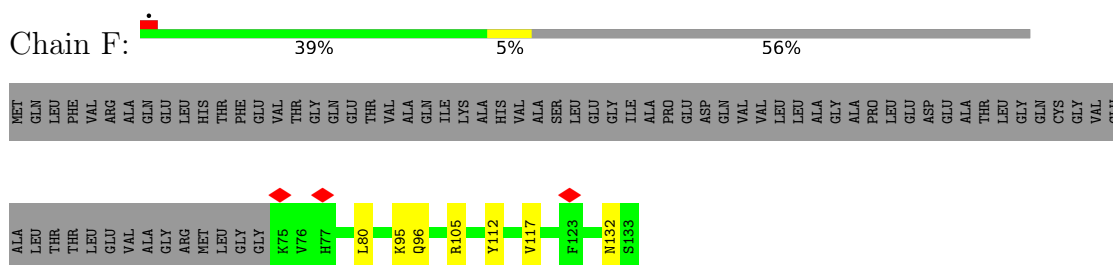
- Molecule 14: 40S ribosomal protein S9



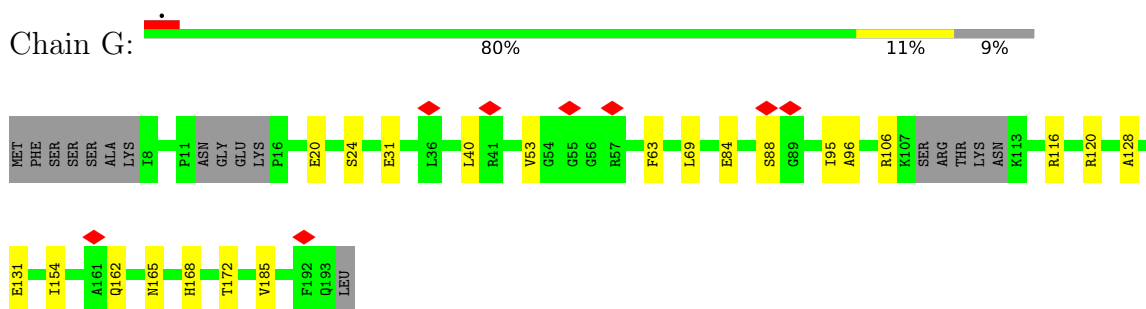
- Molecule 15: 40S ribosomal protein S23



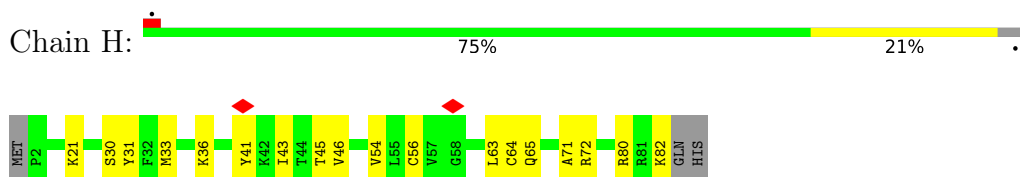
- Molecule 16: Small ribosomal subunit protein eS30



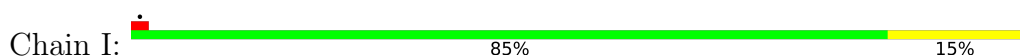
- Molecule 17: 40S ribosomal protein S7



- Molecule 18: 40S ribosomal protein S27

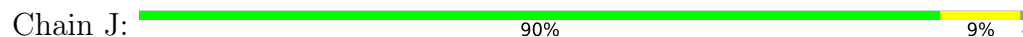


- Molecule 19: 40S ribosomal protein S13

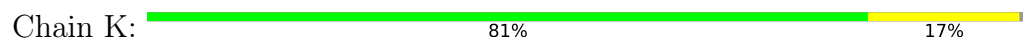




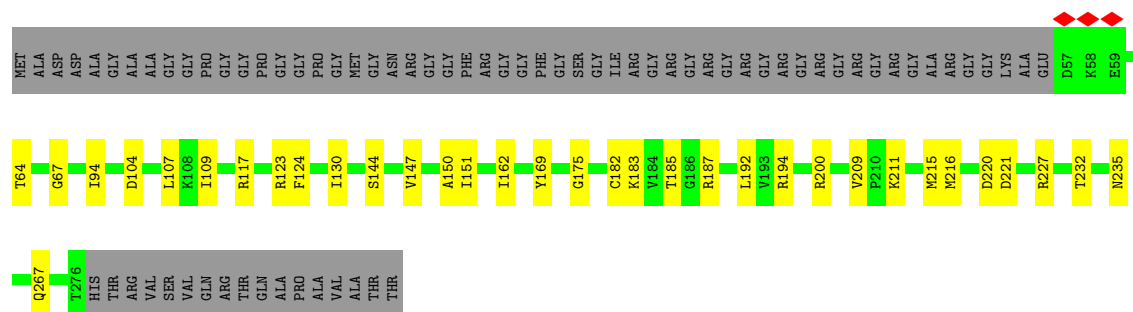
- Molecule 20: 40S ribosomal protein S15a



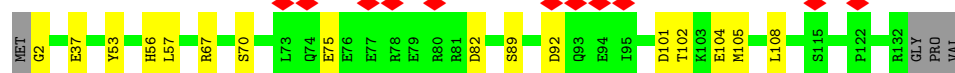
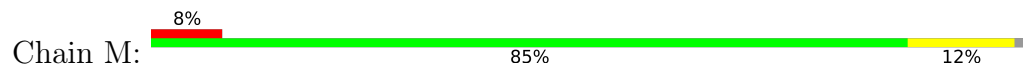
- Molecule 21: 40S ribosomal protein S21



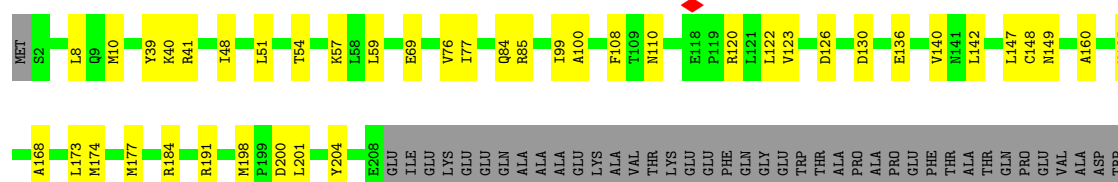
- Molecule 22: 40S ribosomal protein S2

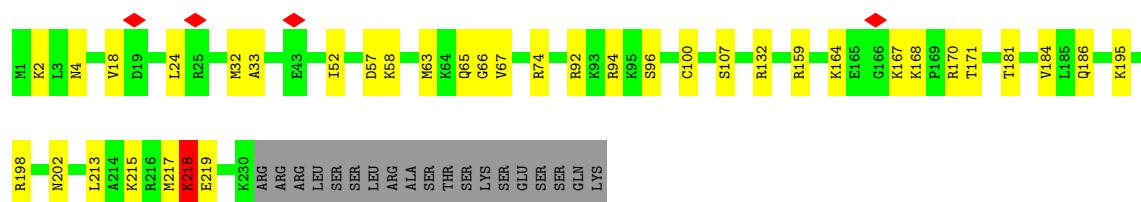


- Molecule 23: 40S ribosomal protein S17

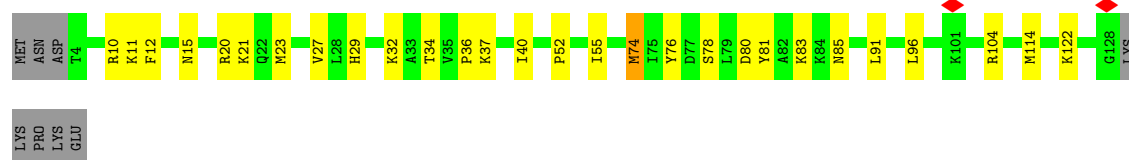


- Molecule 24: 40S ribosomal protein SA

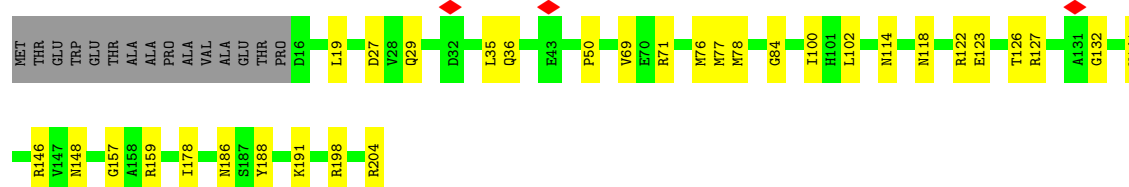
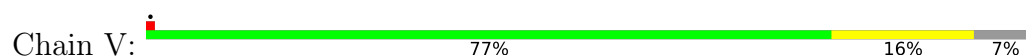




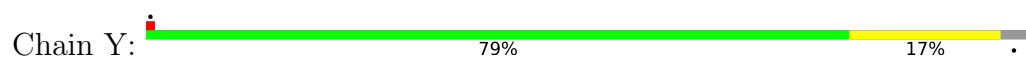
- Molecule 30: 40S ribosomal protein S24



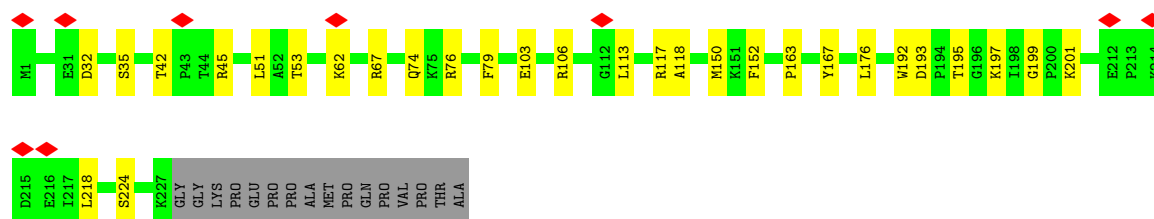
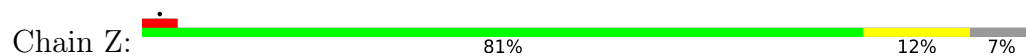
- Molecule 31: 40S ribosomal protein S5



- Molecule 32: 40S ribosomal protein S16

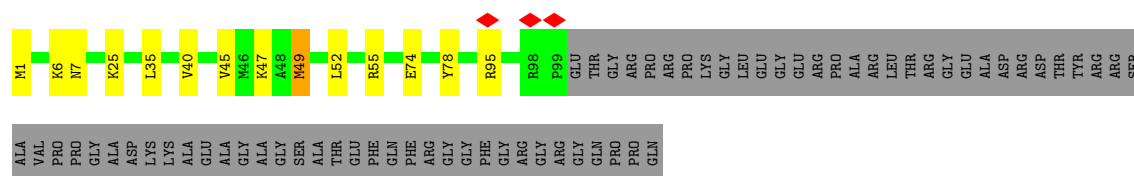


- Molecule 33: 40S ribosomal protein S3

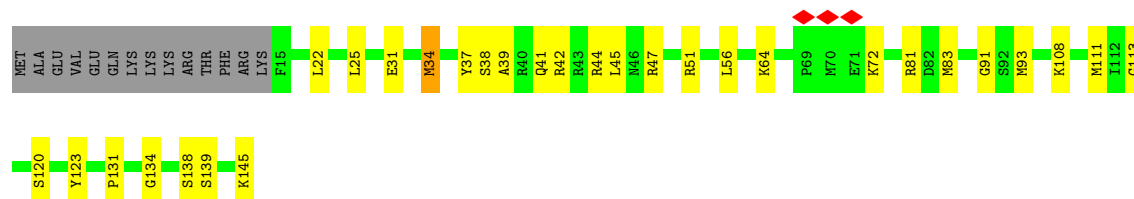


- Molecule 34: 40S ribosomal protein S10

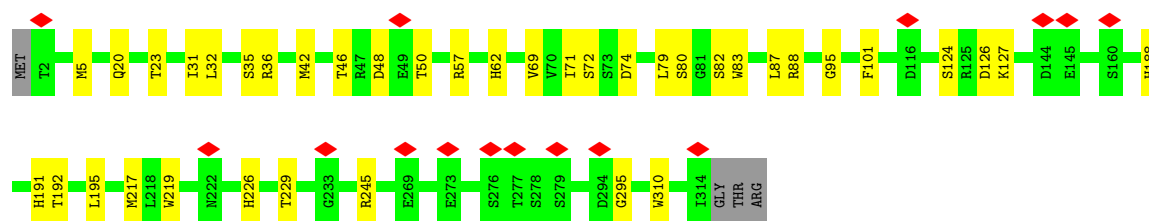
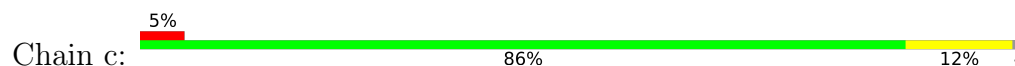




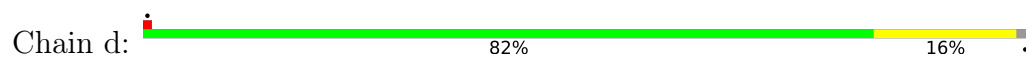
- Molecule 35: 40S ribosomal protein S15



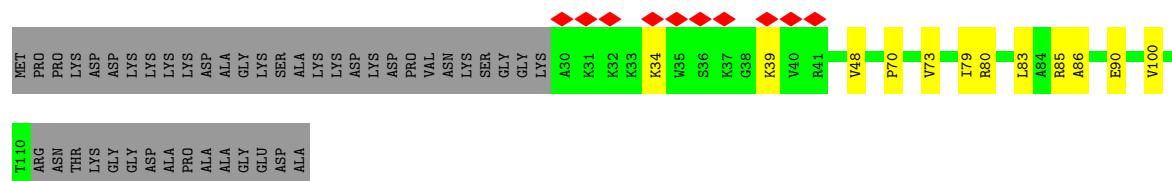
- Molecule 36: Receptor of activated protein C kinase 1



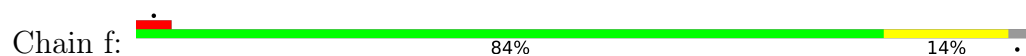
- Molecule 37: 40S ribosomal protein S19



- Molecule 38: 40S ribosomal protein S25

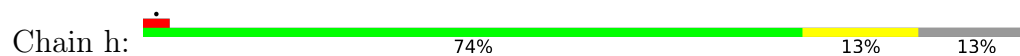


- Molecule 39: 40S ribosomal protein S18

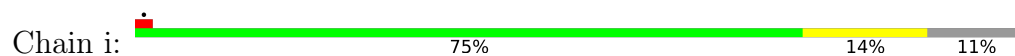




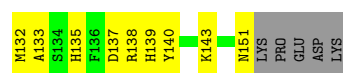
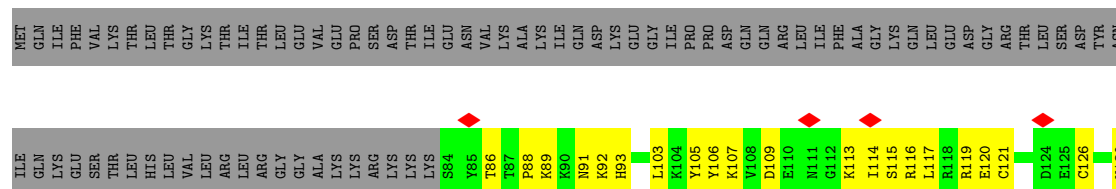
- Molecule 40: 40S ribosomal protein S20



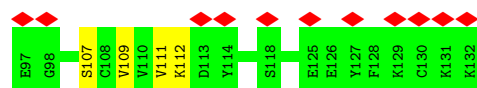
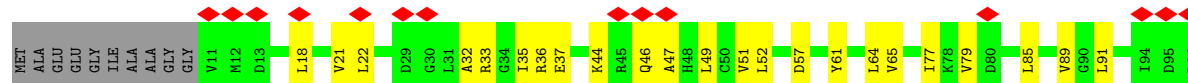
- Molecule 41: 40S ribosomal protein S29



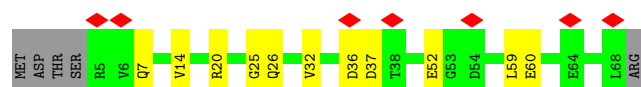
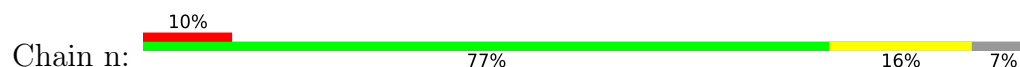
- Molecule 42: Ubiquitin

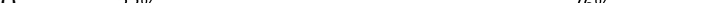


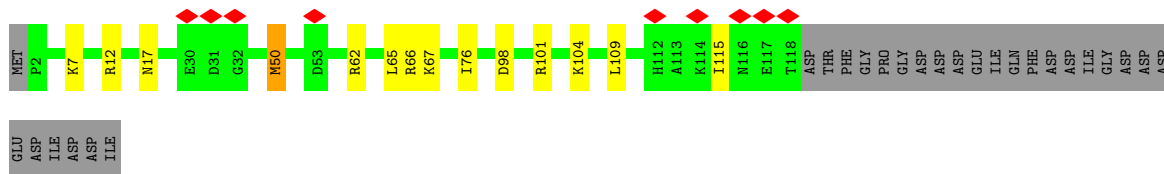
- Molecule 43: 40S ribosomal protein S12

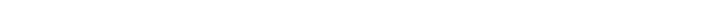


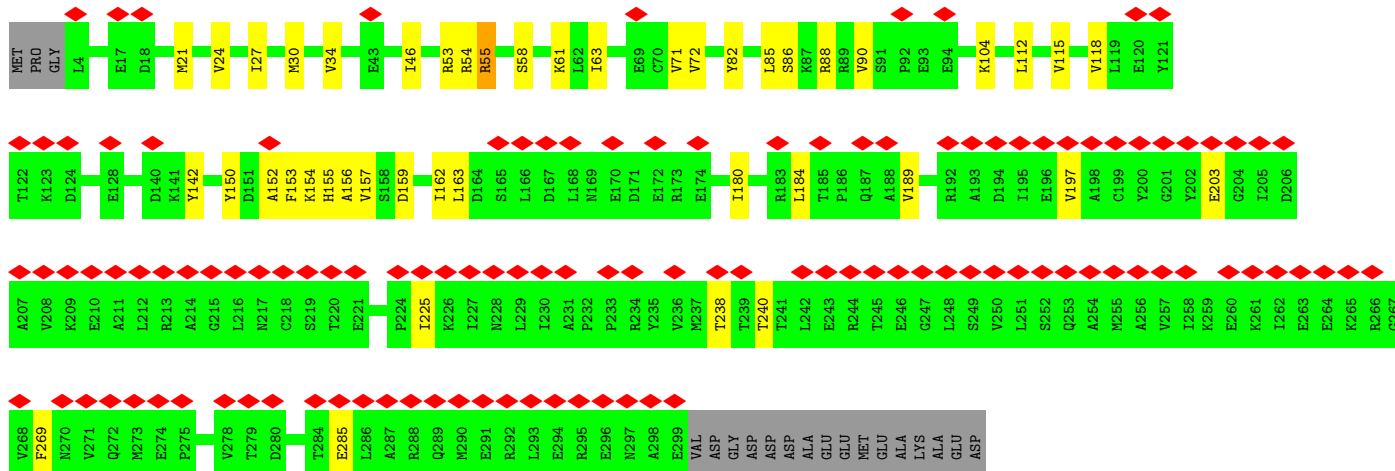
- Molecule 44: 40S ribosomal protein S28



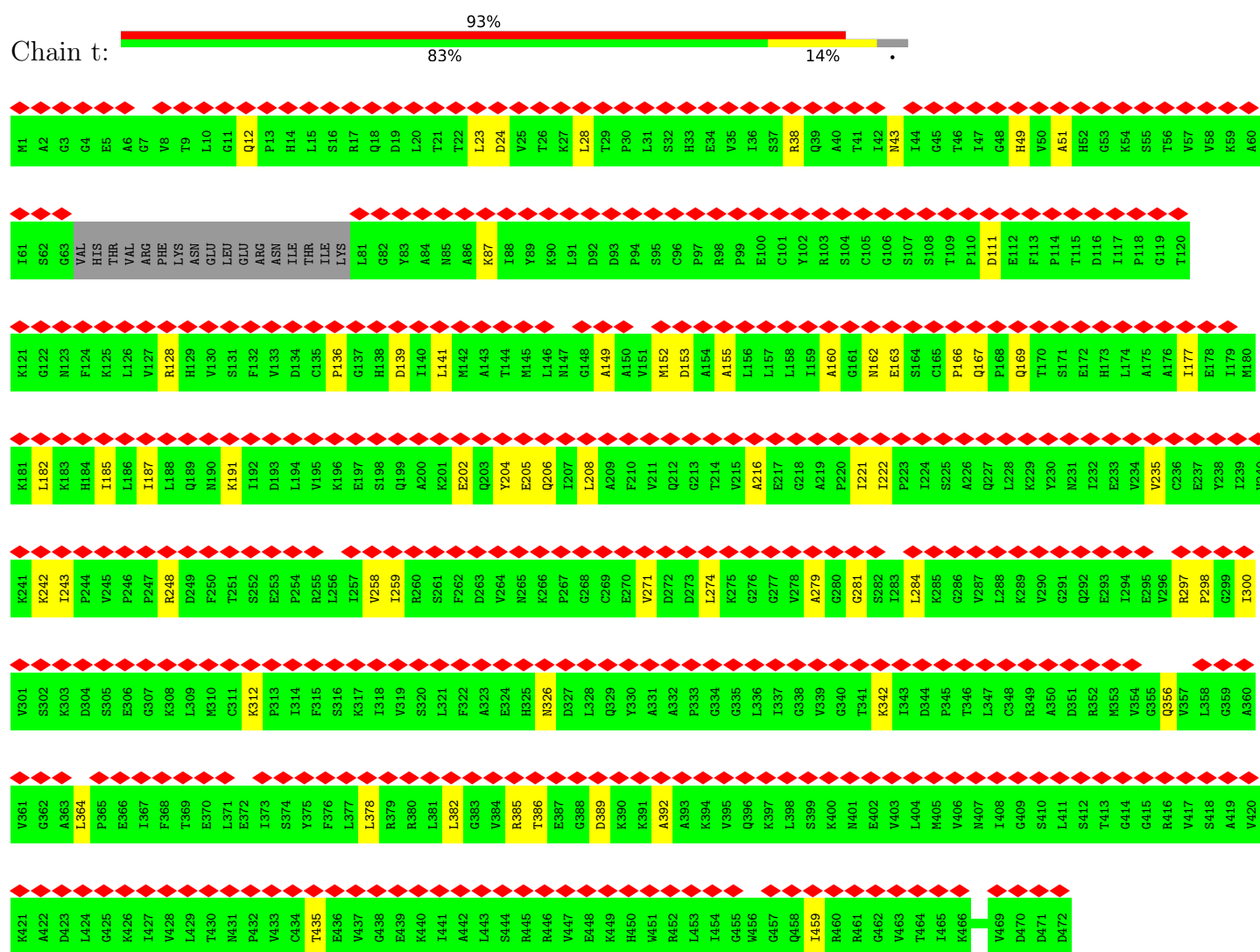
- Chain o:  12% 22% 76%



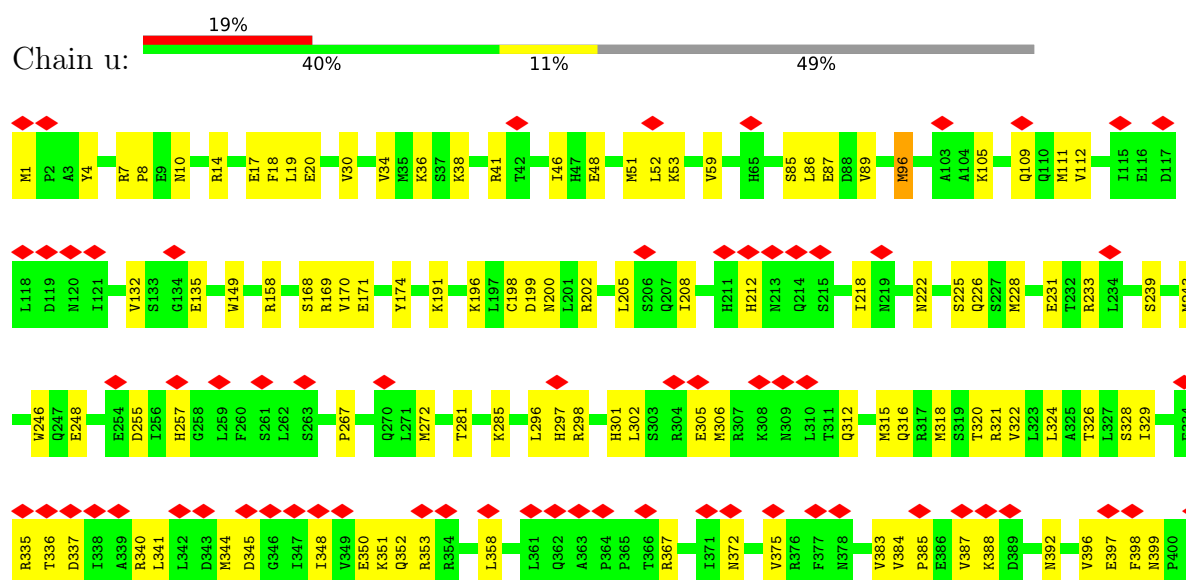
- Chain r:  38% 80% 14% 6%



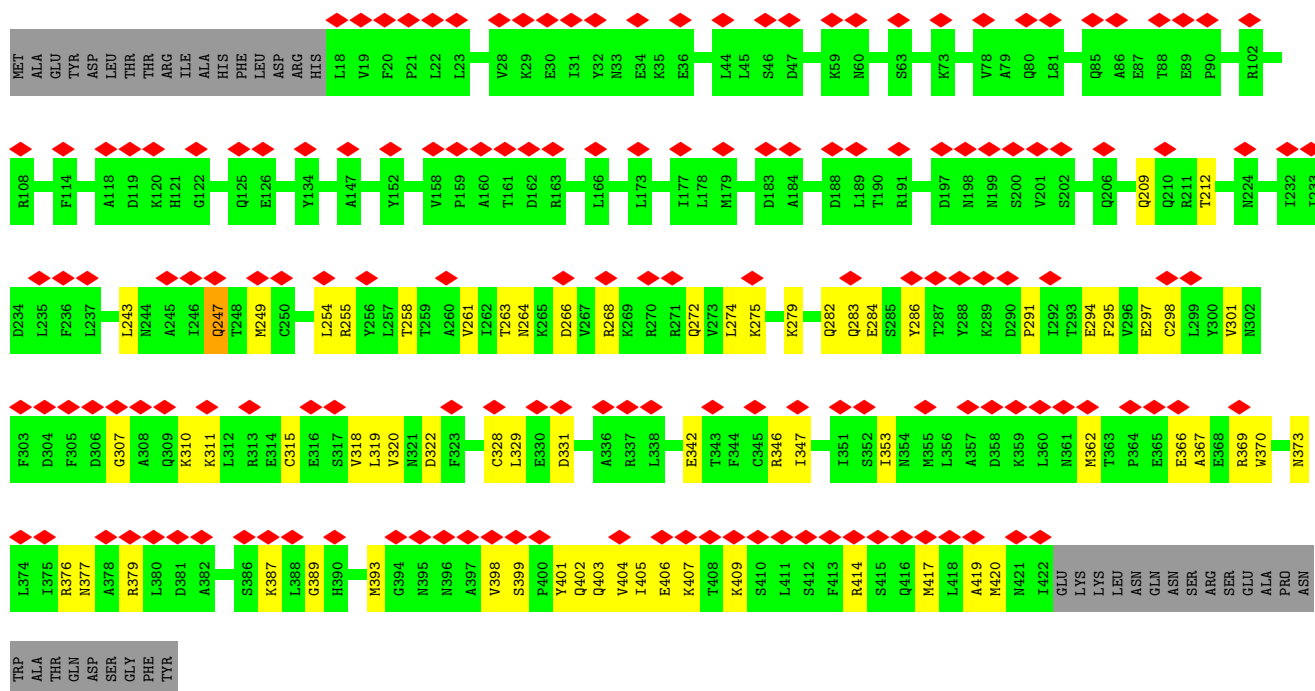
- 



• Molecule 49: Eukaryotic translation initiation factor 3 subunit A



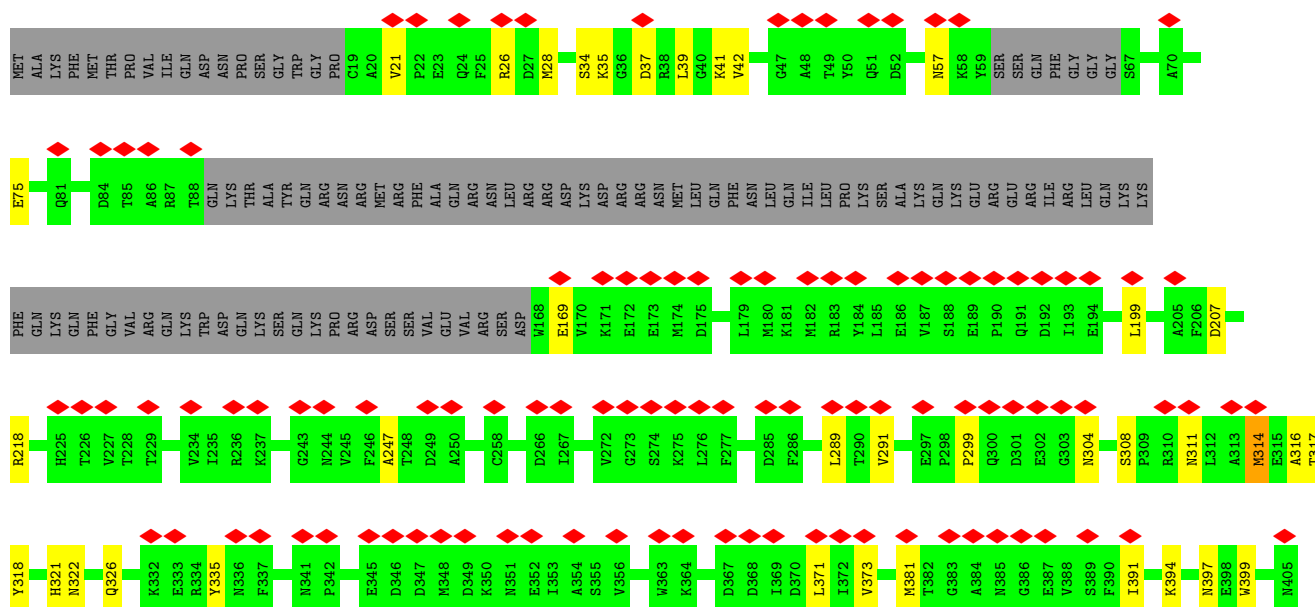


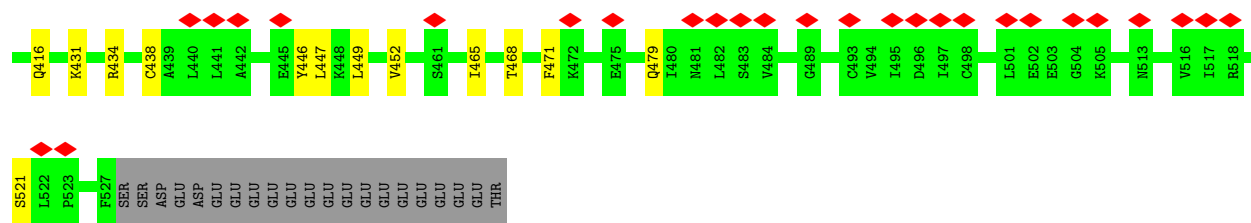


• Molecule 51: Initiator Met-tRNA-i

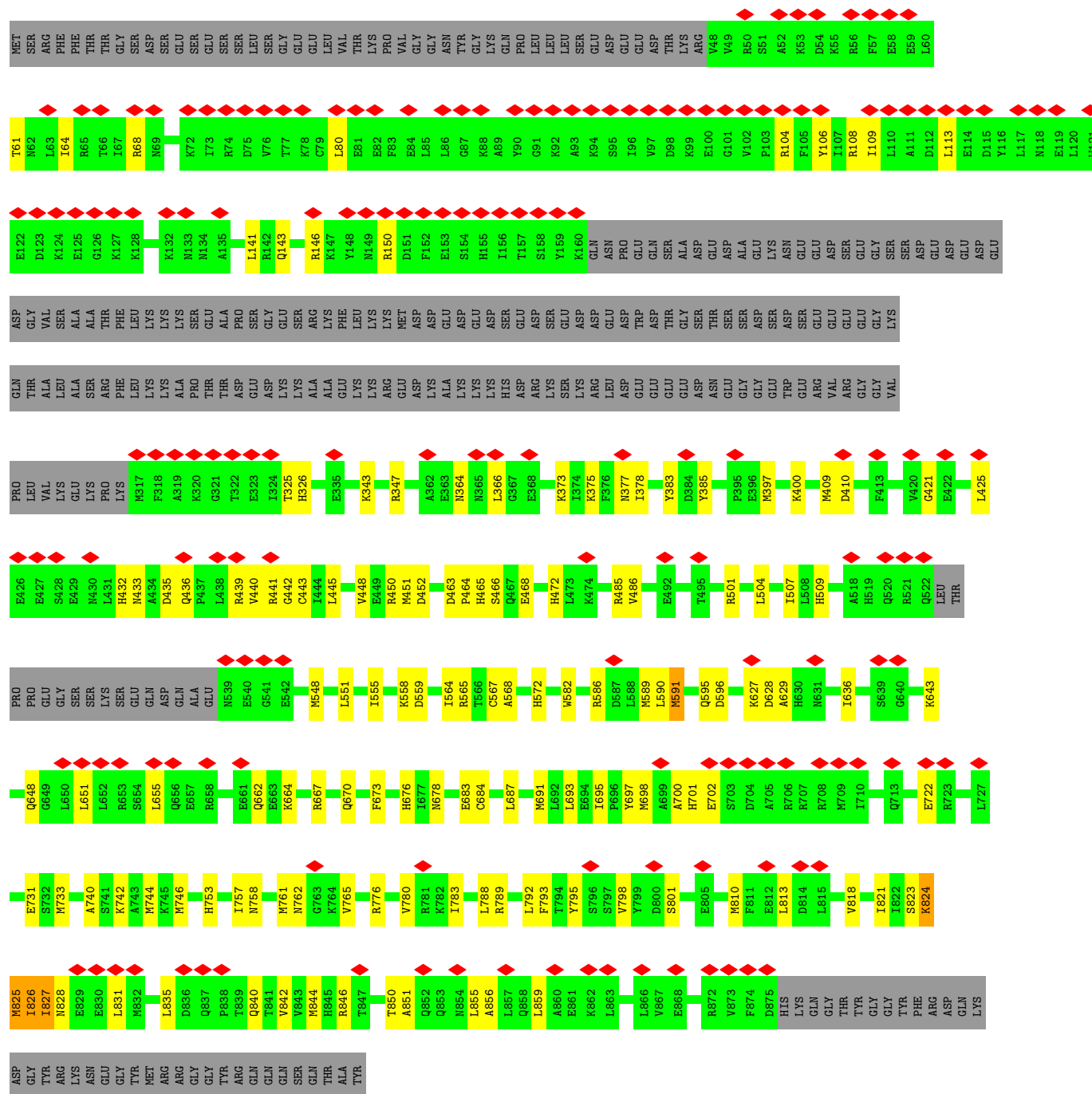


• Molecule 52: Eukaryotic translation initiation factor 3 subunit D

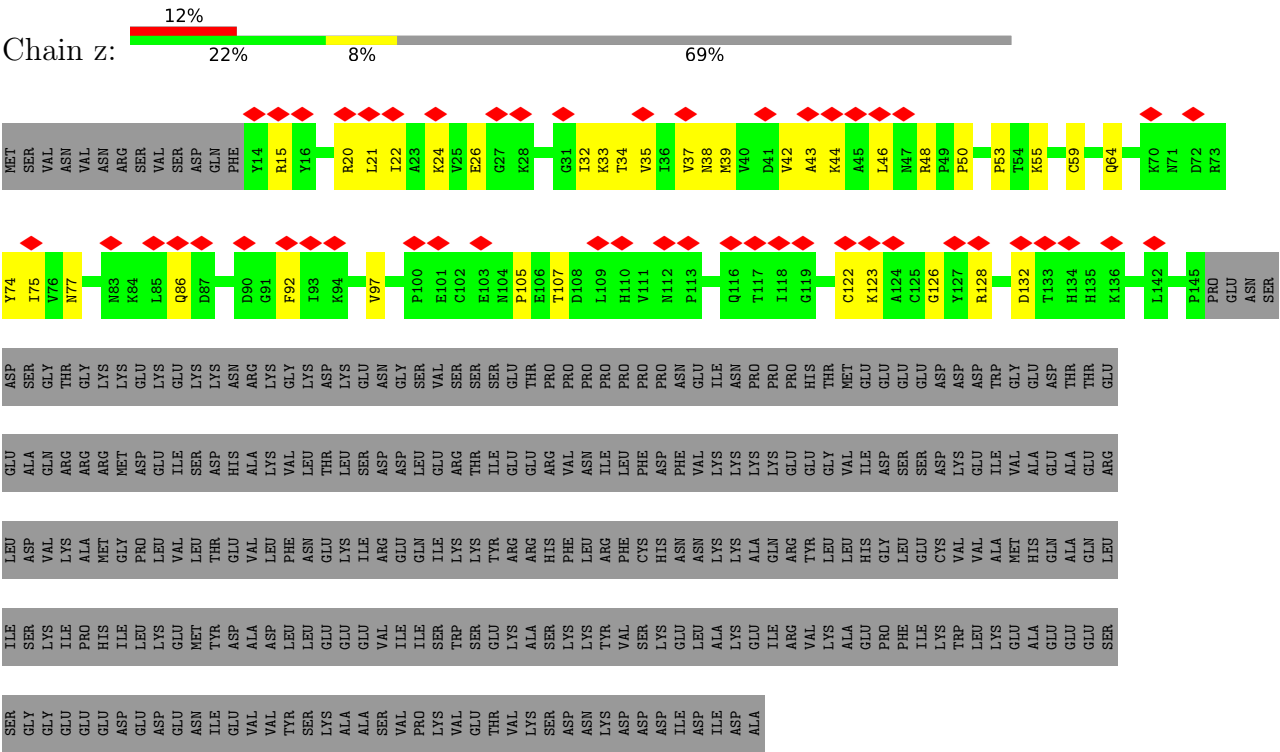




• Molecule 53: Eukaryotic translation initiation factor 3 subunit C



● Molecule 54: Eukaryotic translation initiation factor 5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25632	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	20.786	Depositor
Minimum map value	-9.149	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3	Depositor
Map size ($\text{\AA}$)	417.59998, 417.59998, 417.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.16, 1.16, 1.16	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 6MZ, OMC, 5MC, NA, PSU, UR3, JMH, B8N, OMG, ZN, GTP, MG, A2M, MA6, 5MU, OMU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.23	0/5002	0.63	5/6743 (0.1%)
2	1	0.19	0/3279	0.55	0/4534
3	2	0.11	0/1491	0.38	0/2068
4	3	0.14	0/1055	0.41	0/1469
5	4	0.14	0/1269	0.42	0/1762
6	5	0.21	0/4458	0.53	2/6027 (0.0%)
7	6	0.21	0/2212	0.57	0/3034
8	7	0.20	0/1365	0.51	1/2124 (0.0%)
9	8	0.16	0/1572	0.47	0/2187
10	9	0.28	0/231	0.57	0/294
11	A	0.22	0/41130	0.41	3/64100 (0.0%)
12	B	0.18	0/1186	0.39	0/1585
13	C	0.20	0/2077	0.49	1/2796 (0.0%)
14	D	0.22	0/1502	0.52	0/2008
15	E	0.20	0/1105	0.48	0/1476
16	F	0.19	0/468	0.58	0/618
17	G	0.21	0/1451	0.53	0/1942
18	H	0.19	0/644	0.47	0/864
19	I	0.34	2/1232 (0.2%)	0.56	0/1656
20	J	0.25	0/1051	0.63	4/1406 (0.3%)
21	K	0.21	0/623	0.48	0/833
22	L	0.23	0/1743	0.53	0/2354
23	M	0.24	0/1078	0.64	0/1447
24	N	0.21	0/1670	0.51	0/2271
25	O	0.23	0/1742	0.58	0/2330
26	P	0.24	0/1010	0.64	1/1353 (0.1%)
27	Q	0.21	0/805	0.50	0/1079
28	R	0.16	0/1654	0.36	0/2203
29	S	0.21	0/1885	0.46	1/2510 (0.0%)
30	T	0.22	0/1032	0.56	1/1371 (0.1%)
31	V	0.22	0/1516	0.54	1/2037 (0.0%)
32	Y	0.23	0/1142	0.56	0/1528

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Z	0.21	0/1793	0.50	0/2414
34	a	0.26	0/859	0.65	1/1159 (0.1%)
35	b	0.25	0/1094	0.67	1/1464 (0.1%)
36	c	0.19	0/2493	0.52	1/3394 (0.0%)
37	d	0.19	0/1123	0.47	0/1504
38	e	0.23	0/657	0.57	0/878
39	f	0.21	0/1245	0.52	0/1665
40	h	0.24	0/827	0.56	0/1110
41	i	0.21	0/429	0.43	0/568
42	k	0.42	0/566	0.80	0/753
43	m	0.21	0/960	0.56	0/1286
44	n	0.24	0/508	0.58	0/680
45	o	0.20	0/628	0.52	0/846
46	q	0.19	0/954	0.52	1/1268 (0.1%)
47	r	0.27	1/2167 (0.0%)	0.57	0/2943
48	t	0.20	0/3494	0.47	0/4726
49	u	0.26	0/5475	0.67	1/7432 (0.0%)
50	v	0.26	0/2778	0.68	1/3797 (0.0%)
51	w	0.29	0/1795	0.55	0/2798
52	x	0.19	0/2885	0.54	2/3940 (0.1%)
53	y	0.38	4/5350 (0.1%)	0.70	8/7215 (0.1%)
54	z	0.23	0/1066	0.58	0/1436
All	All	0.23	7/128826 (0.0%)	0.51	36/183285 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	y	824	LYS	C-N	13.64	1.50	1.33
53	y	825	MET	C-N	-9.93	1.21	1.33
53	y	826	ILE	C-N	-8.13	1.23	1.33
53	y	827	ILE	C-N	6.95	1.44	1.33
19	I	34	LYS	C-N	-6.91	1.25	1.33

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	y	824	LYS	O-C-N	9.57	131.93	122.07
53	y	826	ILE	O-C-N	-8.03	114.09	121.87
49	u	96	MET	CA-CB-CG	7.59	129.29	114.10
53	y	827	ILE	CA-C-N	-7.37	110.79	122.73
53	y	827	ILE	C-N-CA	-7.37	110.79	122.73

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	4920	0	5102	96	0
2	1	3258	0	1917	25	0
3	2	1493	0	677	0	0
4	3	1057	0	475	2	0
5	4	1272	0	564	3	0
6	5	4347	0	4294	69	0
7	6	2196	0	1547	28	0
8	7	1218	0	620	6	0
9	8	1574	0	687	7	0
10	9	230	0	276	6	0
11	A	37429	0	18903	397	0
12	B	1166	0	1233	12	0
13	C	2035	0	2138	19	0
14	D	1477	0	1589	23	0
15	E	1087	0	1154	10	0
16	F	461	0	498	7	0
17	G	1430	0	1520	13	0
18	H	631	0	657	13	0
19	I	1208	0	1294	18	0
20	J	1034	0	1080	10	0
21	K	617	0	622	9	0
22	L	1707	0	1794	23	0
23	M	1064	0	1118	15	0
24	N	1633	0	1640	31	0
25	O	1715	0	1785	42	0
26	P	997	0	1021	43	0
27	Q	792	0	843	22	0
28	R	1627	0	1706	13	0
29	S	1862	0	2018	33	0
30	T	1015	0	1086	22	0
31	V	1495	0	1549	24	0
32	Y	1124	0	1193	18	0
33	Z	1765	0	1865	18	0

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Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	a	834	0	861	10	0
35	b	1072	0	1121	21	0
36	c	2436	0	2393	25	0
37	d	1105	0	1138	19	0
38	e	649	0	724	9	0
39	f	1227	0	1298	17	0
40	h	817	0	882	13	0
41	i	419	0	415	8	0
42	k	554	0	556	28	0
43	m	950	0	987	20	0
44	n	506	0	536	10	0
45	o	616	0	600	3	0
46	q	943	0	968	12	0
47	r	2138	0	1930	37	0
48	t	3439	0	3578	39	0
49	u	5383	0	5085	105	0
50	v	2740	0	2251	50	0
51	w	1604	0	816	4	0
52	x	2842	0	2209	32	0
53	y	5263	0	5219	116	0
54	z	1044	0	1058	26	0
55	0	32	0	12	2	0
56	0	1	0	0	0	0
57	0	1	0	0	0	0
57	A	87	0	0	0	0
57	f	1	0	0	0	0
58	Q	1	0	0	0	0
58	k	1	0	0	0	0
All	All	123641	0	99102	1401	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 1401 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)
50:v:347:ILE:HD11	53:y:827:ILE:HG22	1.38	1.04
11:A:1656:G:H1	11:A:1668:U:H3	1.02	1.01
53:y:823:SER:O	53:y:827:ILE:HG23	1.74	0.88
47:r:54:ARG:HG3	47:r:55:ARG:H	1.39	0.85
11:A:1304:U:H4'	42:k:92:LYS:HZ1	1.42	0.84

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	619/1220 (51%)	593 (96%)	26 (4%)	0	100	100
2	1	584/814 (72%)	544 (93%)	40 (7%)	0	100	100
3	2	300/325 (92%)	291 (97%)	9 (3%)	0	100	100
4	3	209/218 (96%)	203 (97%)	6 (3%)	0	100	100
5	4	251/357 (70%)	237 (94%)	14 (6%)	0	100	100
6	5	518/564 (92%)	500 (96%)	18 (4%)	0	100	100
7	6	360/374 (96%)	342 (95%)	18 (5%)	0	100	100
9	8	313/352 (89%)	289 (92%)	24 (8%)	0	100	100
10	9	22/25 (88%)	22 (100%)	0	0	100	100
12	B	138/158 (87%)	133 (96%)	5 (4%)	0	100	100
13	C	254/263 (97%)	249 (98%)	5 (2%)	0	100	100
14	D	175/194 (90%)	170 (97%)	5 (3%)	0	100	100
15	E	138/143 (96%)	137 (99%)	1 (1%)	0	100	100
16	F	57/133 (43%)	51 (90%)	6 (10%)	0	100	100
17	G	171/194 (88%)	163 (95%)	8 (5%)	0	100	100
18	H	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
19	I	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
20	J	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
21	K	79/83 (95%)	75 (95%)	4 (5%)	0	100	100
22	L	218/293 (74%)	211 (97%)	7 (3%)	0	100	100
23	M	129/135 (96%)	120 (93%)	9 (7%)	0	100	100
24	N	205/295 (70%)	198 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	O	209/264 (79%)	202 (97%)	7 (3%)	0	100	100
26	P	131/151 (87%)	121 (92%)	10 (8%)	0	100	100
27	Q	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
28	R	194/208 (93%)	190 (98%)	4 (2%)	0	100	100
29	S	228/249 (92%)	222 (97%)	6 (3%)	0	100	100
30	T	123/133 (92%)	123 (100%)	0	0	100	100
31	V	187/204 (92%)	178 (95%)	9 (5%)	0	100	100
32	Y	139/146 (95%)	135 (97%)	4 (3%)	0	100	100
33	Z	225/243 (93%)	221 (98%)	4 (2%)	0	100	100
34	a	97/165 (59%)	91 (94%)	6 (6%)	0	100	100
35	b	129/145 (89%)	122 (95%)	7 (5%)	0	100	100
36	c	311/317 (98%)	290 (93%)	21 (7%)	0	100	100
37	d	140/145 (97%)	134 (96%)	6 (4%)	0	100	100
38	e	79/125 (63%)	76 (96%)	3 (4%)	0	100	100
39	f	147/152 (97%)	139 (95%)	8 (5%)	0	100	100
40	h	101/119 (85%)	95 (94%)	6 (6%)	0	100	100
41	i	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
42	k	66/156 (42%)	59 (89%)	6 (9%)	1 (2%)	8	36
43	m	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
44	n	62/69 (90%)	60 (97%)	2 (3%)	0	100	100
45	o	75/320 (23%)	72 (96%)	3 (4%)	0	100	100
46	q	115/144 (80%)	108 (94%)	7 (6%)	0	100	100
47	r	294/315 (93%)	276 (94%)	18 (6%)	0	100	100
48	t	451/472 (96%)	443 (98%)	8 (2%)	0	100	100
49	u	705/1382 (51%)	659 (94%)	46 (6%)	0	100	100
50	v	403/445 (91%)	371 (92%)	32 (8%)	0	100	100
52	x	417/548 (76%)	390 (94%)	27 (6%)	0	100	100
53	y	650/913 (71%)	621 (96%)	29 (4%)	0	100	100
54	z	130/430 (30%)	123 (95%)	7 (5%)	0	100	100
All	All	11167/14768 (76%)	10648 (95%)	518 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
42	k	93	HIS

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	0	546/1081 (50%)	546 (100%)	0	100	100
2	1	97/702 (14%)	97 (100%)	0	100	100
6	5	477/515 (93%)	477 (100%)	0	100	100
7	6	112/335 (33%)	112 (100%)	0	100	100
9	8	1/310 (0%)	1 (100%)	0	100	100
10	9	23/24 (96%)	23 (100%)	0	100	100
12	B	129/142 (91%)	129 (100%)	0	100	100
13	C	220/225 (98%)	220 (100%)	0	100	100
14	D	158/168 (94%)	158 (100%)	0	100	100
15	E	112/115 (97%)	112 (100%)	0	100	100
16	F	47/104 (45%)	47 (100%)	0	100	100
17	G	159/174 (91%)	159 (100%)	0	100	100
18	H	73/76 (96%)	73 (100%)	0	100	100
19	I	130/131 (99%)	130 (100%)	0	100	100
20	J	112/113 (99%)	112 (100%)	0	100	100
21	K	65/67 (97%)	65 (100%)	0	100	100
22	L	186/225 (83%)	186 (100%)	0	100	100
23	M	119/122 (98%)	119 (100%)	0	100	100
24	N	173/243 (71%)	173 (100%)	0	100	100
25	O	192/231 (83%)	192 (100%)	0	100	100
26	P	104/119 (87%)	104 (100%)	0	100	100
27	Q	86/98 (88%)	86 (100%)	0	100	100
28	R	172/180 (96%)	172 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	S	200/218 (92%)	199 (100%)	1 (0%)	81	80
30	T	107/115 (93%)	107 (100%)	0	100	100
31	V	159/170 (94%)	159 (100%)	0	100	100
32	Y	117/121 (97%)	117 (100%)	0	100	100
33	Z	190/202 (94%)	190 (100%)	0	100	100
34	a	90/136 (66%)	90 (100%)	0	100	100
35	b	117/130 (90%)	117 (100%)	0	100	100
36	c	272/275 (99%)	272 (100%)	0	100	100
37	d	112/115 (97%)	112 (100%)	0	100	100
38	e	71/103 (69%)	71 (100%)	0	100	100
39	f	129/132 (98%)	129 (100%)	0	100	100
40	h	94/107 (88%)	94 (100%)	0	100	100
41	i	44/49 (90%)	44 (100%)	0	100	100
42	k	61/140 (44%)	61 (100%)	0	100	100
43	m	104/108 (96%)	104 (100%)	0	100	100
44	n	57/62 (92%)	57 (100%)	0	100	100
45	o	64/277 (23%)	64 (100%)	0	100	100
46	q	99/123 (80%)	99 (100%)	0	100	100
47	r	190/280 (68%)	190 (100%)	0	100	100
48	t	380/397 (96%)	380 (100%)	0	100	100
49	u	528/1259 (42%)	528 (100%)	0	100	100
50	v	206/406 (51%)	206 (100%)	0	100	100
52	x	207/494 (42%)	207 (100%)	0	100	100
53	y	562/811 (69%)	562 (100%)	0	100	100
54	z	116/388 (30%)	116 (100%)	0	100	100
All	All	7769/12118 (64%)	7768 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	S	218	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67

such sidechains are listed below:

Mol	Chain	Res	Type
52	x	392	ASN
53	y	149	ASN
53	y	670	GLN
27	Q	72	HIS
25	O	118	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	A	1746/1869 (93%)	423 (24%)	15 (0%)
51	w	74/75 (98%)	33 (44%)	0
8	7	56/255 (21%)	40 (71%)	3 (5%)
All	All	1876/2199 (85%)	496 (26%)	18 (0%)

5 of 496 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	-34	C
8	7	-32	A
8	7	-31	C
8	7	-30	A
8	7	-29	A

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	A	731	G
11	A	1836	G
11	A	1600	G
11	A	626	G
11	A	716	G

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	B8N	A	1248	11	24,29,30	3.06	6 (25%)	29,42,45	1.72	6 (20%)
11	MA6	A	1850	11	23,26,27	1.56	3 (13%)	34,38,41	3.10	11 (32%)
11	PSU	A	1243	11	18,21,22	1.04	1 (5%)	22,30,33	1.84	5 (22%)
11	OMG	A	644	11	23,26,27	2.38	7 (30%)	33,38,41	3.13	16 (48%)
11	PSU	A	612	11	18,21,22	1.03	1 (5%)	22,30,33	1.81	5 (22%)
11	OMC	A	517	11	19,22,23	0.58	0	26,31,34	0.80	0
11	MA6	A	1851	11	23,26,27	1.56	3 (13%)	34,38,41	3.24	12 (35%)
11	JMH	A	1219	11,57	18,22,23	2.93	5 (27%)	21,32,35	1.76	5 (23%)
11	OMC	A	174	11,57	19,22,23	0.55	0	26,31,34	0.68	0
11	A2M	A	484	11	22,25,26	3.86	11 (50%)	31,36,39	3.30	11 (35%)
11	OMU	A	121	11	19,22,23	3.01	6 (31%)	26,31,34	1.67	5 (19%)
11	A2M	A	27	11,57	22,25,26	3.91	11 (50%)	31,36,39	3.32	13 (41%)
11	OMG	A	509	11,57	23,26,27	2.50	8 (34%)	33,38,41	3.44	13 (39%)
11	A2M	A	159	11	22,25,26	3.90	10 (45%)	31,36,39	3.32	13 (41%)
11	PSU	A	823	11	18,21,22	1.09	1 (5%)	22,30,33	1.77	4 (18%)
11	OMC	A	1703	11	19,22,23	0.58	0	26,31,34	0.65	0
11	PSU	A	822	11	18,21,22	1.03	1 (5%)	22,30,33	1.78	5 (22%)
11	OMU	A	116	11	19,22,23	3.00	6 (31%)	26,31,34	1.58	4 (15%)
11	UR3	A	1830	11	19,22,23	2.82	7 (36%)	26,32,35	1.47	4 (15%)
11	OMG	A	683	11	23,26,27	2.43	8 (34%)	33,38,41	3.35	17 (51%)
11	A2M	A	166	11	22,25,26	3.92	11 (50%)	31,36,39	3.28	12 (38%)
11	A2M	A	668	11,57	22,25,26	3.89	11 (50%)	31,36,39	3.24	15 (48%)
11	A2M	A	1678	11	22,25,26	3.94	12 (54%)	31,36,39	3.39	13 (41%)
11	PSU	A	1081	11	18,21,22	1.01	1 (5%)	22,30,33	1.82	3 (13%)
11	5MU	A	814	11	19,22,23	0.23	0	28,32,35	0.32	0
11	6MZ	A	1832	11,57	22,25,26	2.32	5 (22%)	30,36,39	2.30	12 (40%)
11	A2M	A	1031	11	22,25,26	3.94	10 (45%)	31,36,39	3.23	12 (38%)
11	5MC	A	1374	11	18,22,23	0.59	0	26,32,35	0.64	0
11	PSU	A	119	11	18,21,22	1.01	1 (5%)	22,30,33	1.61	4 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	B8N	A	1248	11	-	3/16/34/35	0/2/2/2
11	MA6	A	1850	11	-	3/11/29/30	0/3/3/3
11	PSU	A	1243	11	-	0/7/25/26	0/2/2/2
11	OMG	A	644	11	-	4/9/27/28	0/3/3/3
11	PSU	A	612	11	-	0/7/25/26	0/2/2/2
11	OMC	A	517	11	-	0/9/27/28	0/2/2/2
11	MA6	A	1851	11	-	6/11/29/30	0/3/3/3
11	JMH	A	1219	11,57	-	1/7/25/26	0/2/2/2
11	OMC	A	174	11,57	-	0/9/27/28	0/2/2/2
11	A2M	A	484	11	-	1/9/27/28	0/3/3/3
11	OMU	A	121	11	-	0/9/27/28	0/2/2/2
11	A2M	A	27	11,57	-	1/9/27/28	0/3/3/3
11	OMG	A	509	11,57	-	3/9/27/28	0/3/3/3
11	A2M	A	159	11	-	1/9/27/28	0/3/3/3
11	PSU	A	823	11	-	0/7/25/26	0/2/2/2
11	OMC	A	1703	11	-	0/9/27/28	0/2/2/2
11	PSU	A	822	11	-	2/7/25/26	0/2/2/2
11	OMU	A	116	11	-	1/9/27/28	0/2/2/2
11	UR3	A	1830	11	-	2/7/25/26	0/2/2/2
11	OMG	A	683	11	-	2/9/27/28	0/3/3/3
11	A2M	A	166	11	-	1/9/27/28	0/3/3/3
11	A2M	A	668	11,57	-	3/9/27/28	0/3/3/3
11	A2M	A	1678	11	-	1/9/27/28	0/3/3/3
11	PSU	A	1081	11	-	1/7/25/26	0/2/2/2
11	5MU	A	814	11	-	0/7/25/26	0/2/2/2
11	6MZ	A	1832	11,57	-	2/9/27/28	0/3/3/3
11	A2M	A	1031	11	-	1/9/27/28	0/3/3/3
11	5MC	A	1374	11	-	0/7/25/26	0/2/2/2
11	PSU	A	119	11	-	2/7/25/26	0/2/2/2

The worst 5 of 146 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	1031	A2M	C3'-C2'	-12.96	1.24	1.52
11	A	27	A2M	C3'-C2'	-12.90	1.24	1.52
11	A	1678	A2M	C3'-C2'	-12.77	1.24	1.52
11	A	166	A2M	C3'-C2'	-12.76	1.24	1.52
11	A	159	A2M	C3'-C2'	-12.66	1.24	1.52

The worst 5 of 220 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1851	MA6	N1-C6-N6	-12.73	103.17	117.08
11	A	1850	MA6	N1-C6-N6	-11.98	103.99	117.08
11	A	1678	A2M	C1'-N9-C8	-9.26	106.22	127.14
11	A	27	A2M	C1'-N9-C8	-8.73	107.43	127.14
11	A	159	A2M	C1'-N9-C8	-8.61	107.68	127.14

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	27	A2M	C1'-C2'-O2'-CM'
11	A	116	OMU	C1'-C2'-O2'-CM2
11	A	166	A2M	C1'-C2'-O2'-CM'
11	A	484	A2M	C1'-C2'-O2'-CM'
11	A	509	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

13 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	1850	MA6	1	0
11	A	1219	JMH	1	0
11	A	484	A2M	1	0
11	A	121	OMU	1	0
11	A	27	A2M	1	0
11	A	509	OMG	5	0
11	A	116	OMU	1	0
11	A	1830	UR3	1	0
11	A	166	A2M	2	0
11	A	1678	A2M	2	0
11	A	814	5MU	1	0
11	A	1031	A2M	1	0
11	A	119	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 93 ligands modelled in this entry, 92 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
55	GTP	0	2001	56,57	30,34,34	0.82	1 (3%)	46,54,54	1.87	10 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	GTP	0	2001	56,57	-	1/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	0	2001	GTP	C2-N3	2.11	1.38	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	0	2001	GTP	PA-O3A-PB	-5.04	115.52	132.83
55	0	2001	GTP	C5-C4-N3	-4.88	120.54	128.46
55	0	2001	GTP	C2-N3-C4	4.46	120.25	112.30
55	0	2001	GTP	PB-O3B-PG	-3.25	121.67	132.83
55	0	2001	GTP	N9-C4-N3	2.93	131.83	125.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

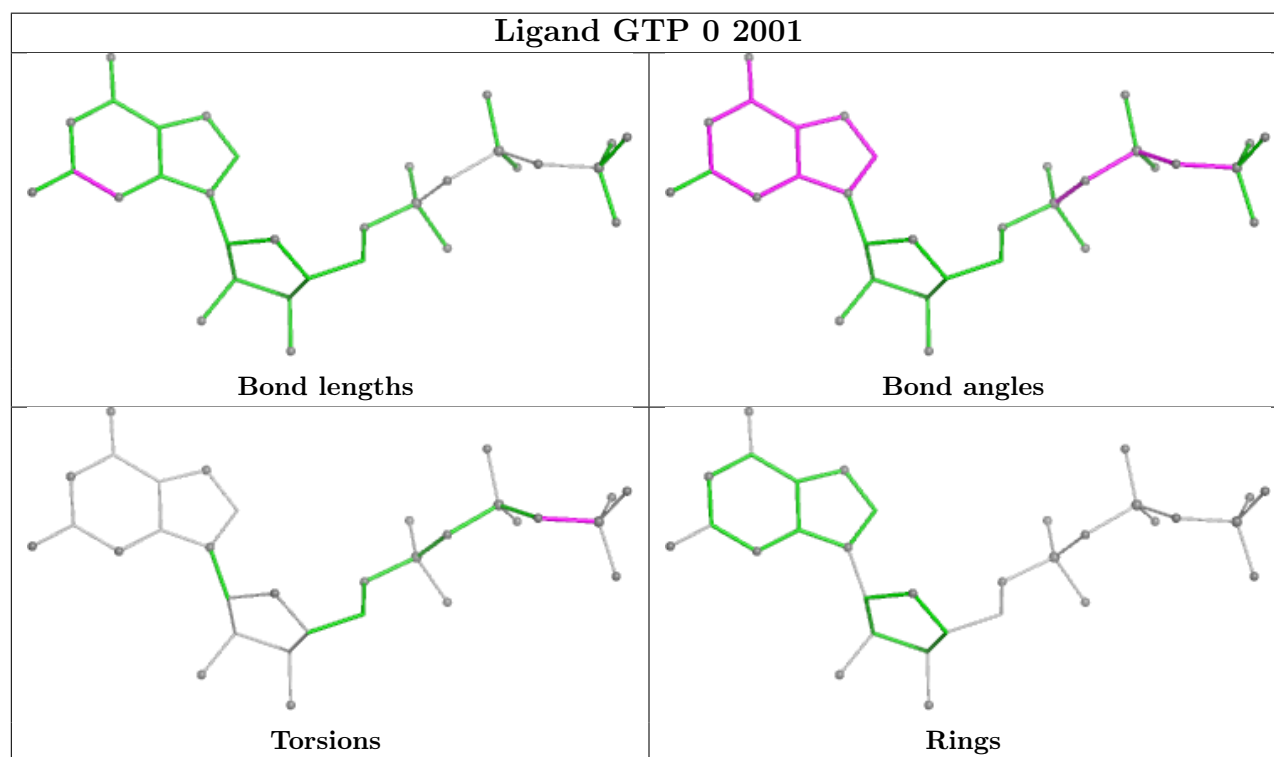
Mol	Chain	Res	Type	Atoms
55	0	2001	GTP	PB-O3B-PG-O2G

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	0	2001	GTP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

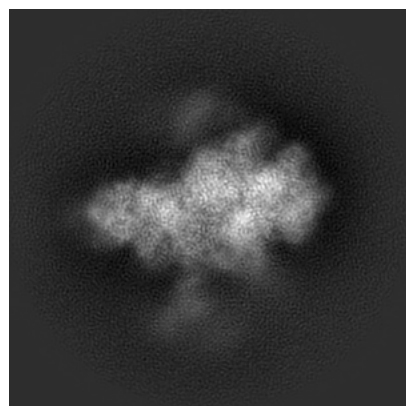
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17698. These allow visual inspection of the internal detail of the map and identification of artifacts.

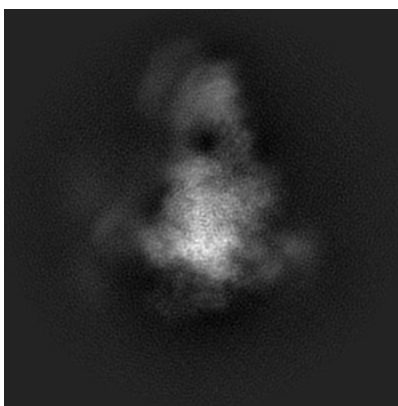
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

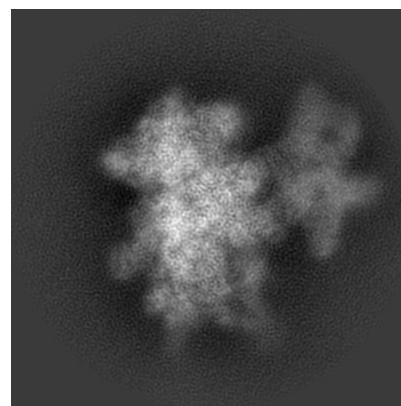
6.1.1 Primary map



X

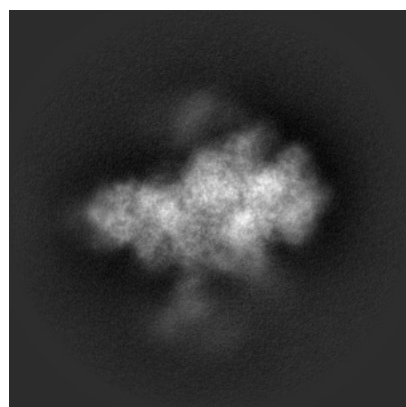


Y

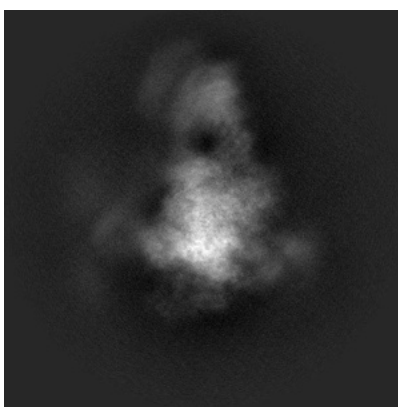


Z

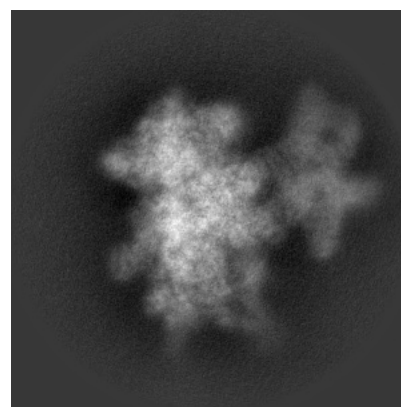
6.1.2 Raw map



X



Y

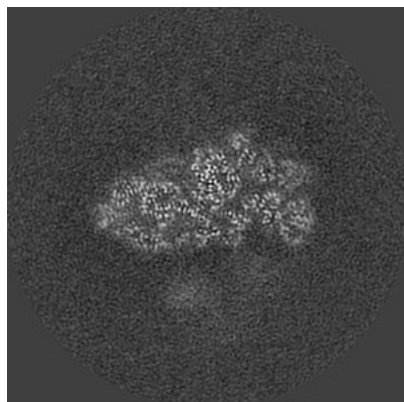


Z

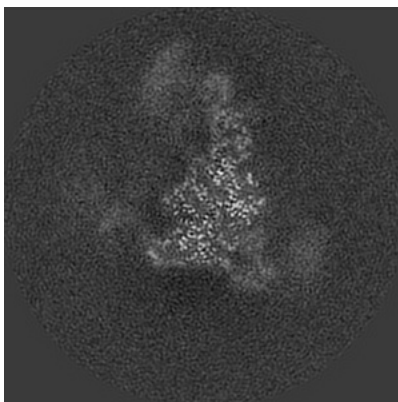
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

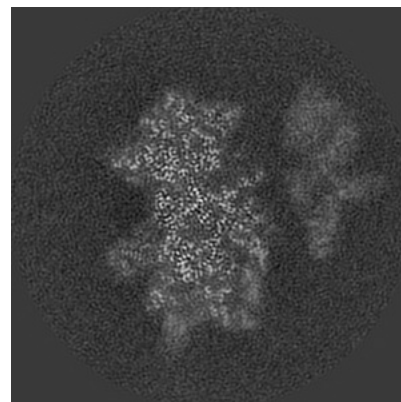
6.2.1 Primary map



X Index: 180

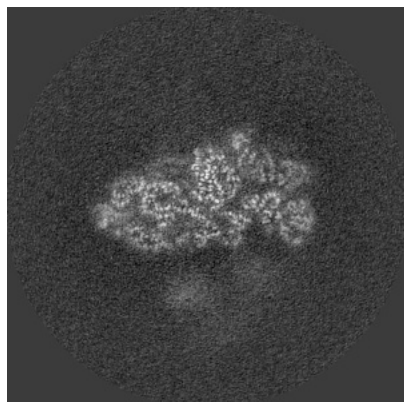


Y Index: 180

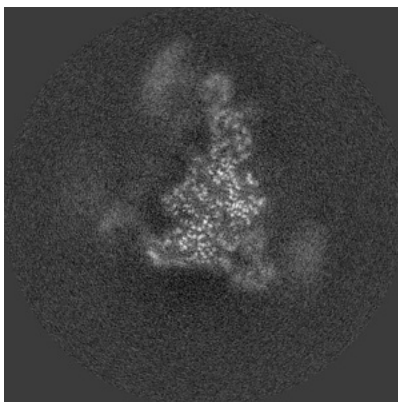


Z Index: 180

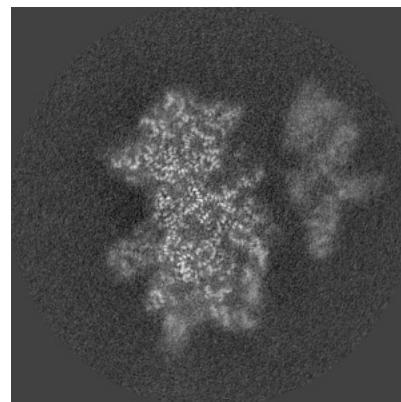
6.2.2 Raw map



X Index: 180



Y Index: 180

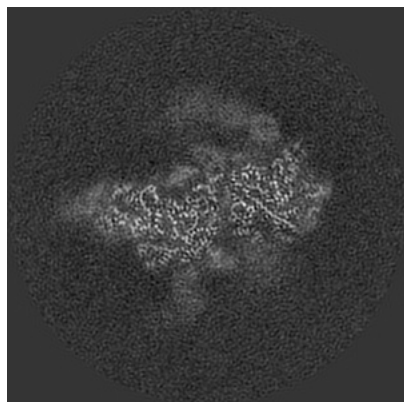


Z Index: 180

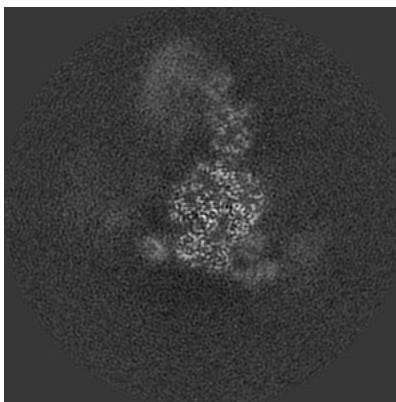
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

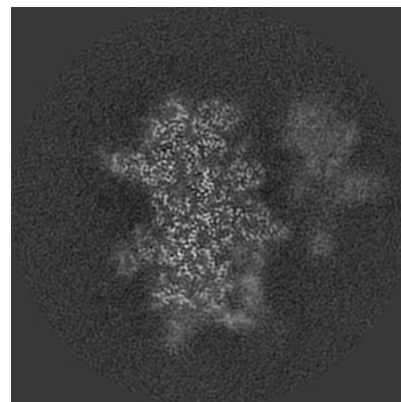
6.3.1 Primary map



X Index: 147

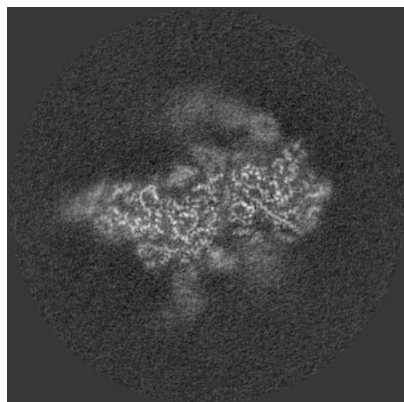


Y Index: 185

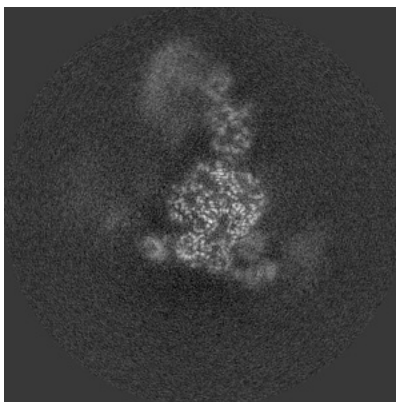


Z Index: 174

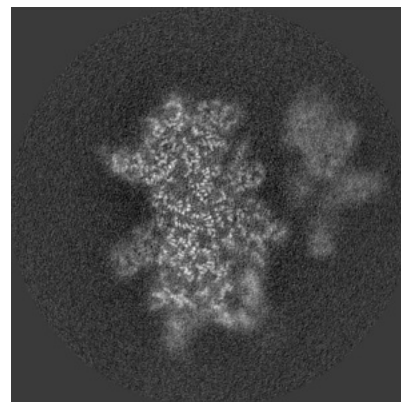
6.3.2 Raw map



X Index: 147



Y Index: 185

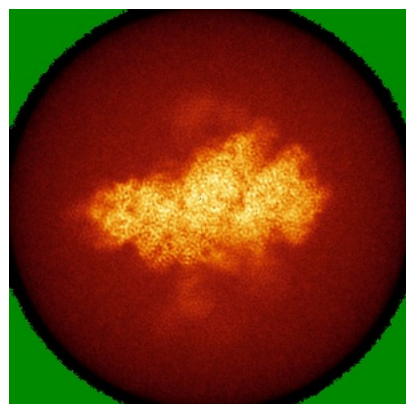


Z Index: 175

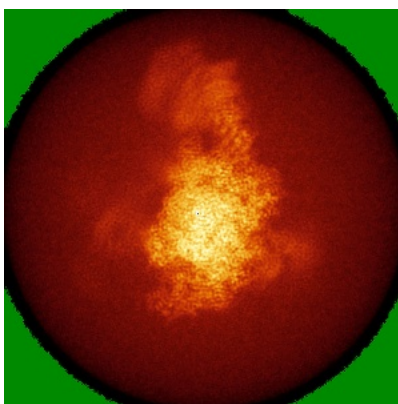
The images above show the largest variance slices of the map in three orthogonal directions.

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

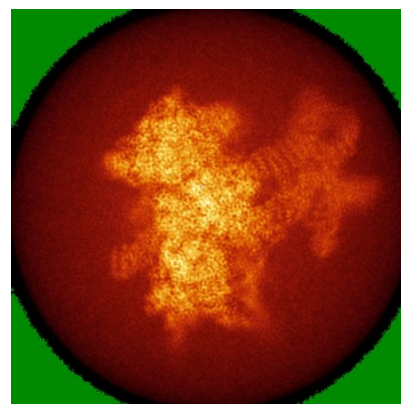
6.4.1 Primary map



X

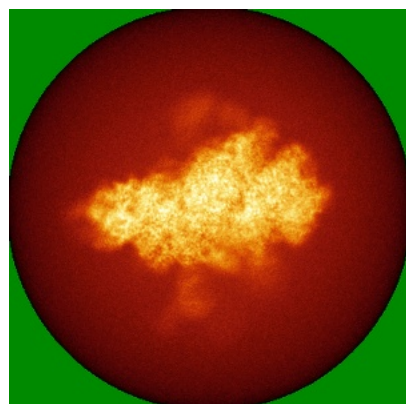


Y

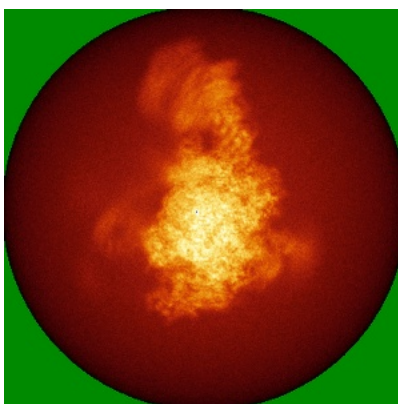


Z

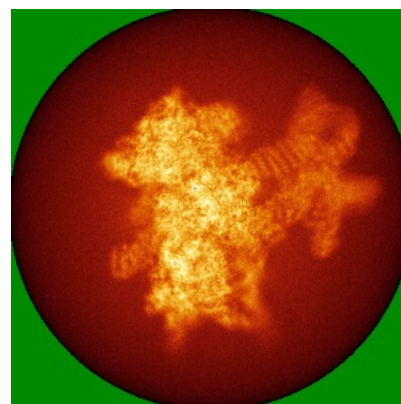
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

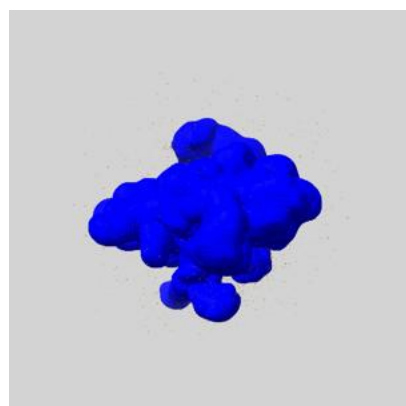
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

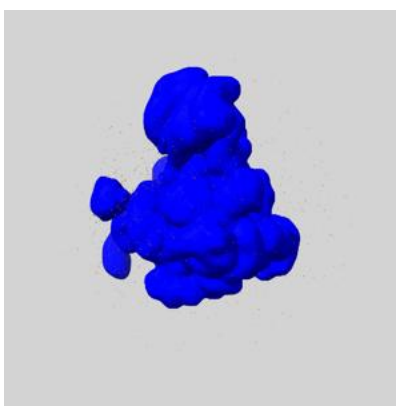
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

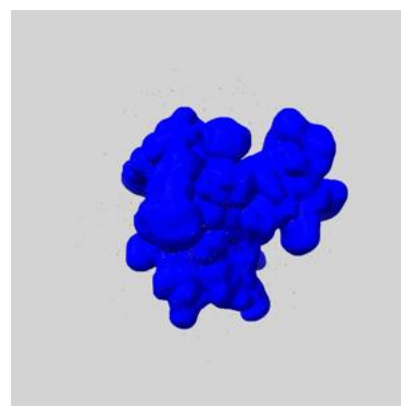
6.6.1 emd_17698_msk_1.map [i](#)



X



Y

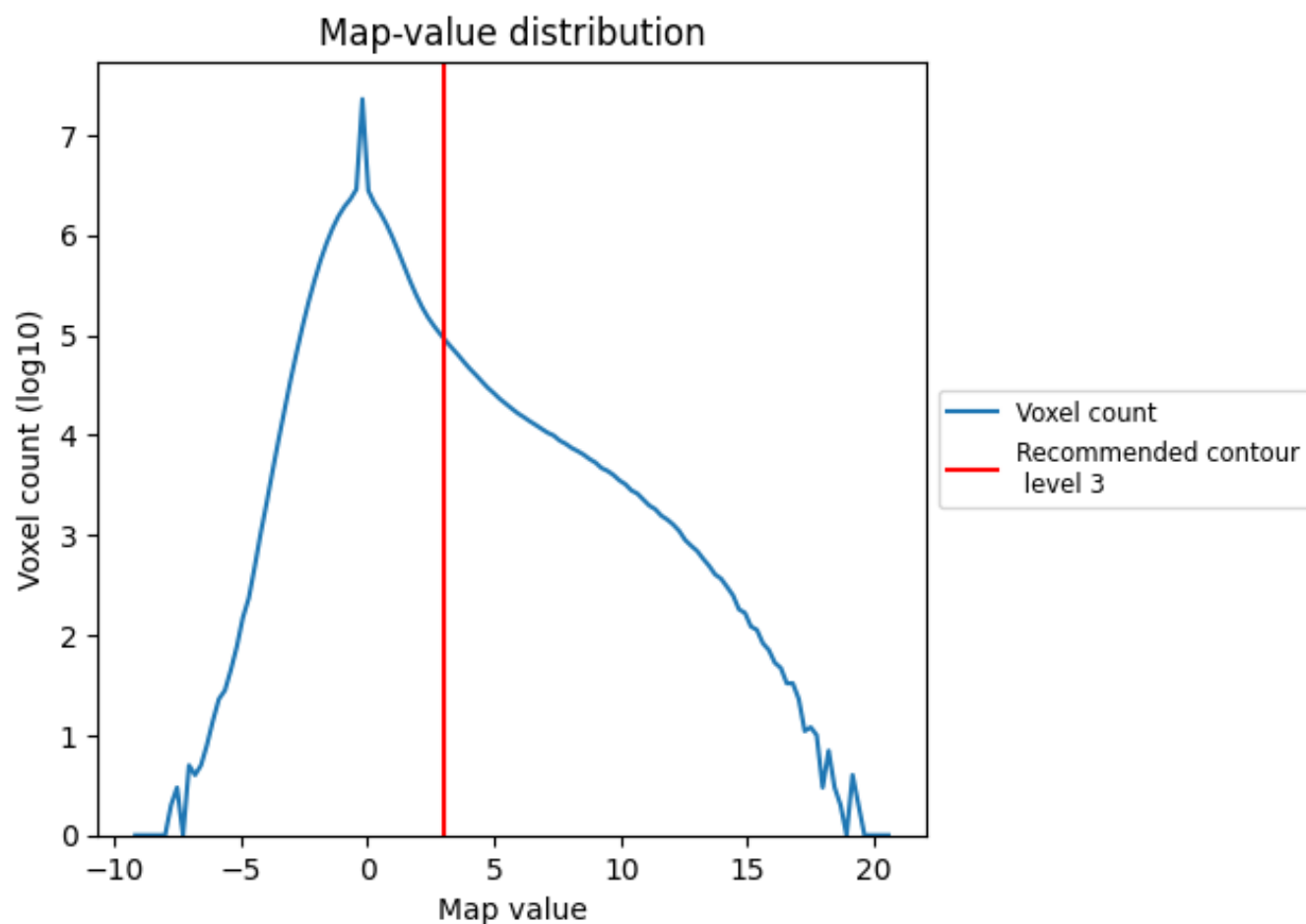


Z

7 Map analysis [i](#)

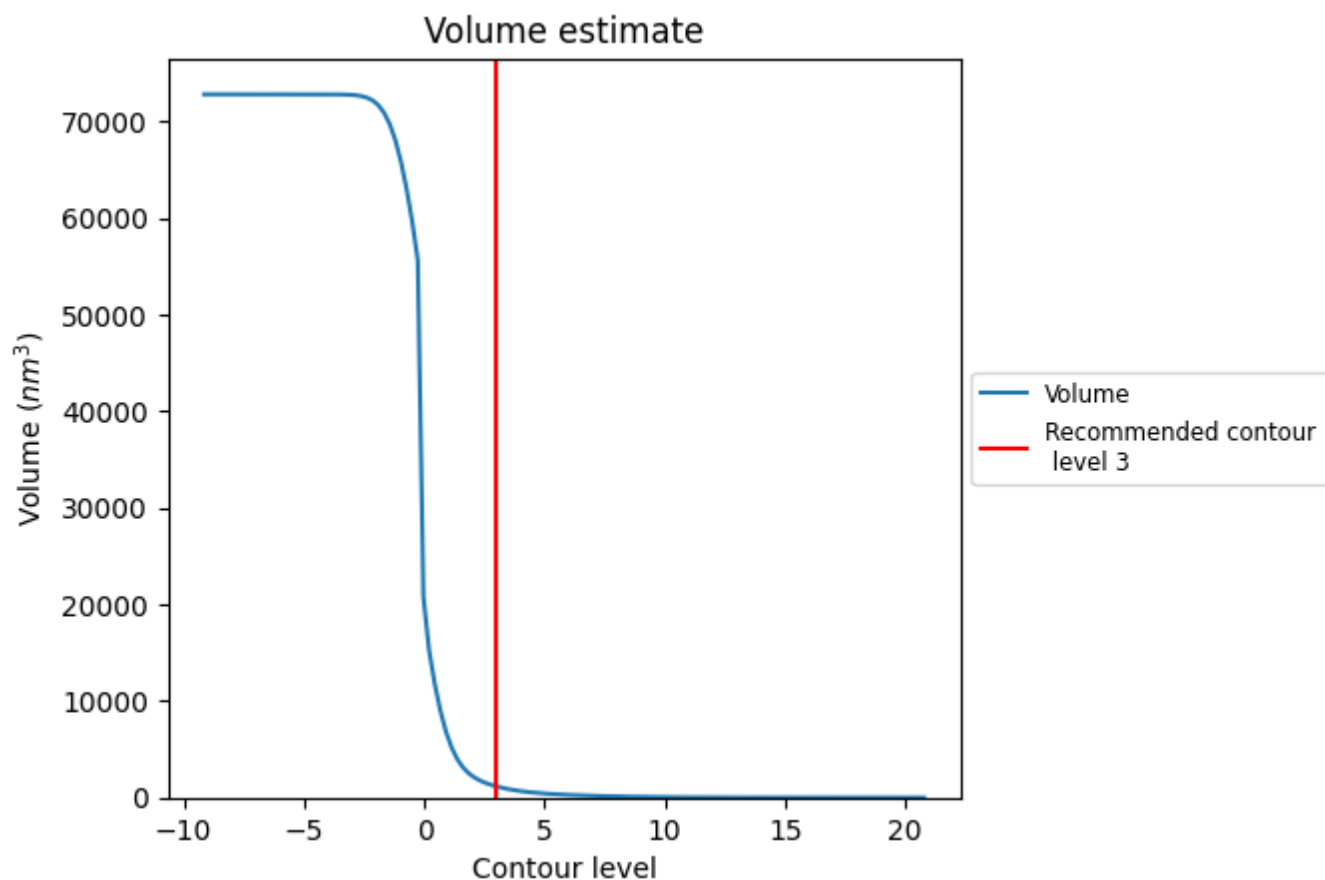
This section contains the results of statistical analysis of the map.

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.

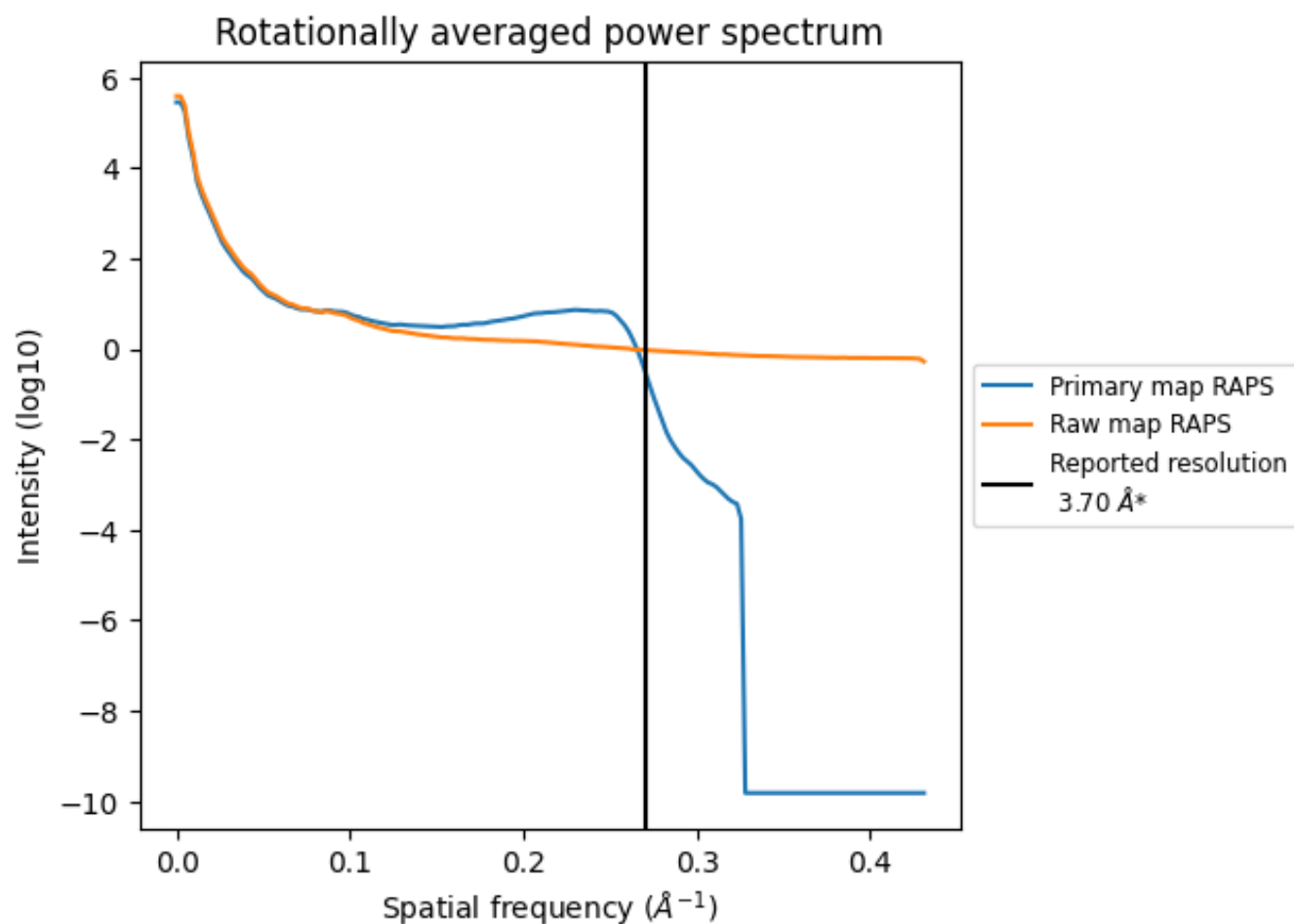
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1159 nm³; this corresponds to an approximate mass of 1047 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 ⓘ

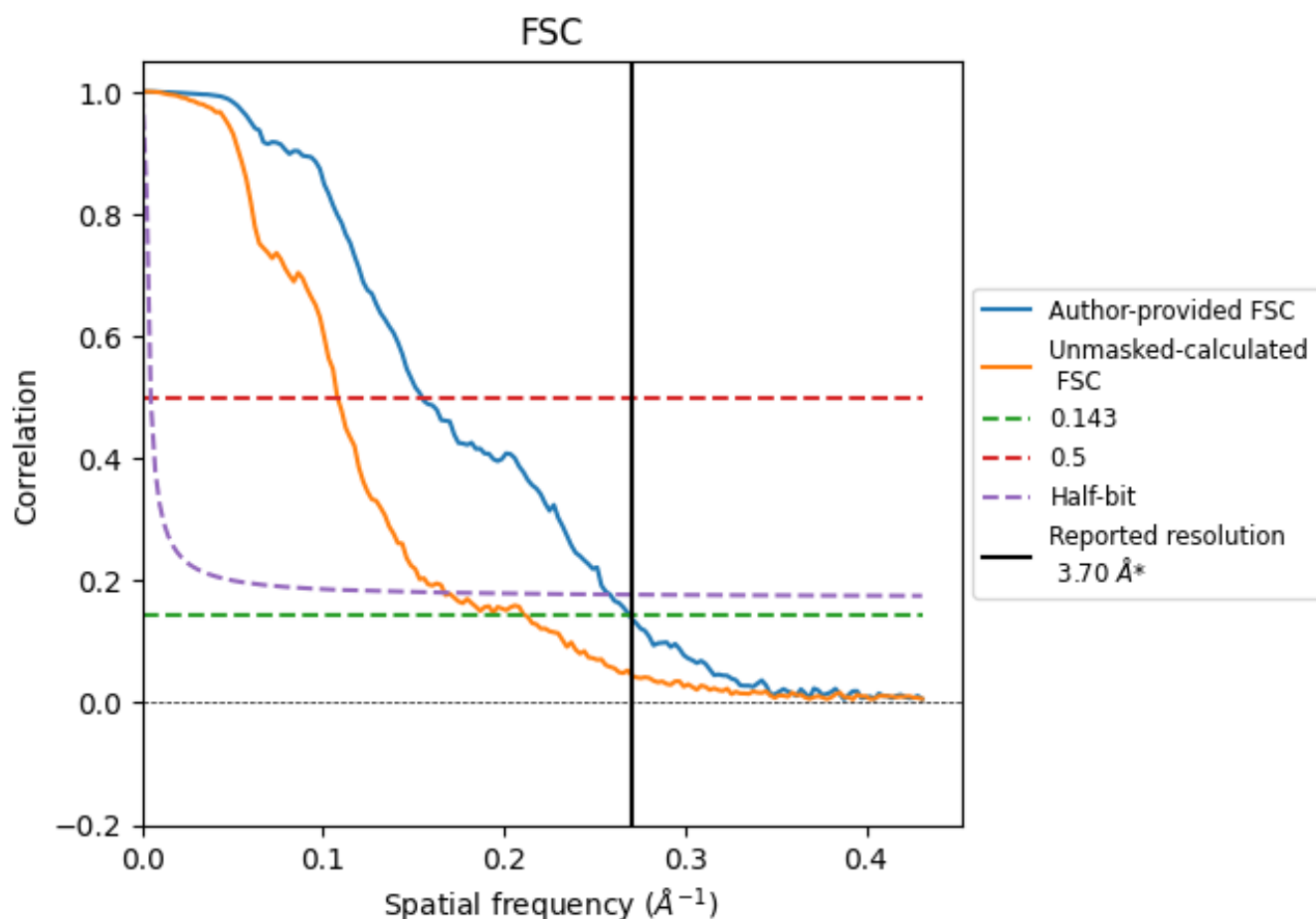


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

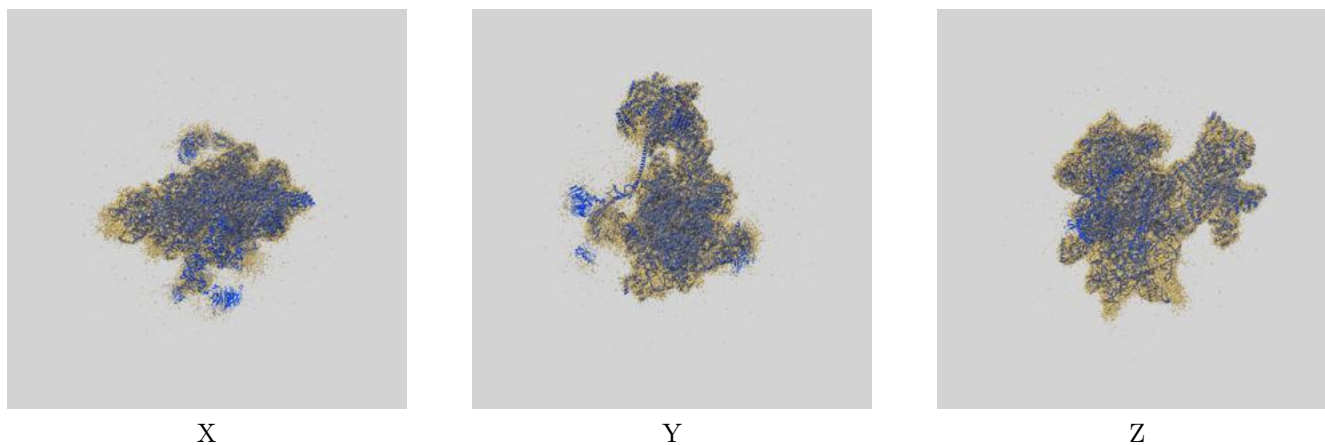
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.71	6.47	3.87
Unmasked-calculated*	4.73	9.28	5.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.73 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

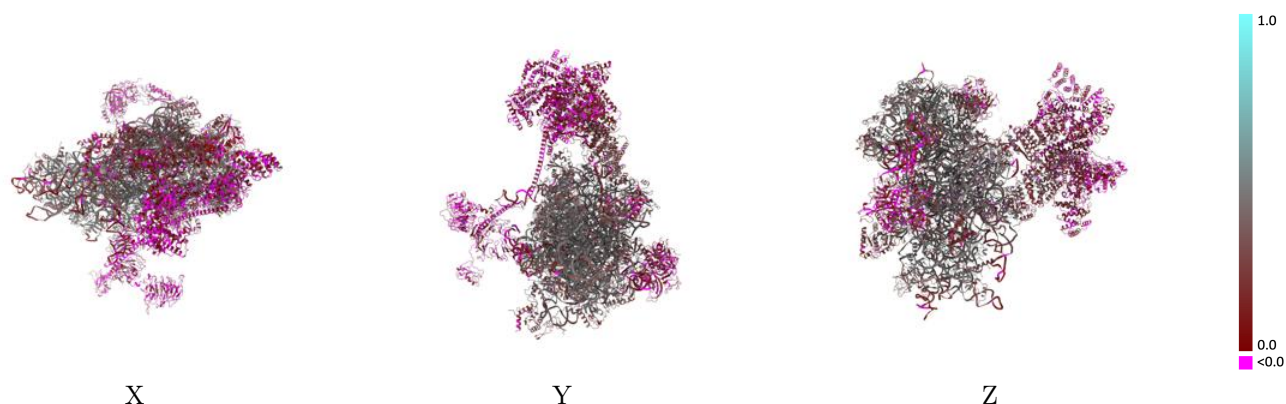
This section contains information regarding the fit between EMDB map EMD-17698 and PDB model 8PJ3. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



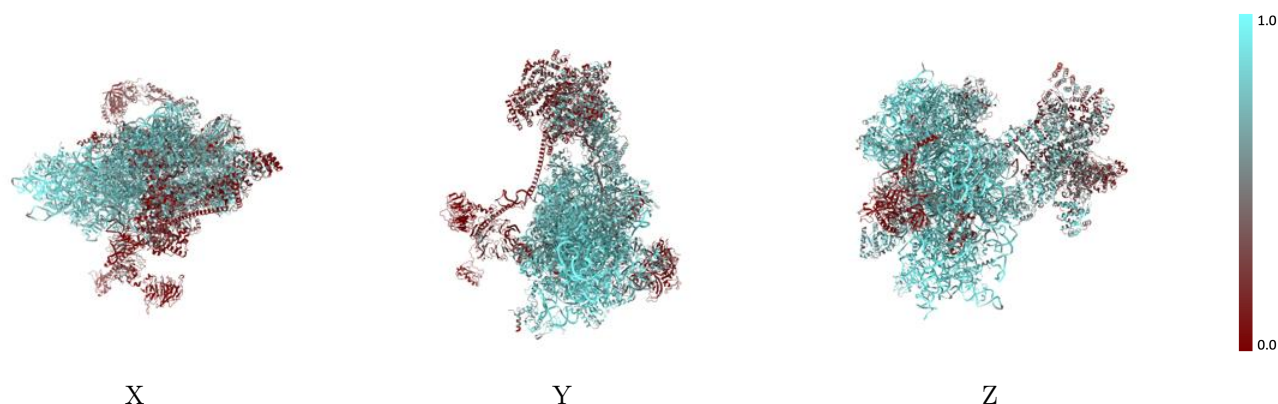
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



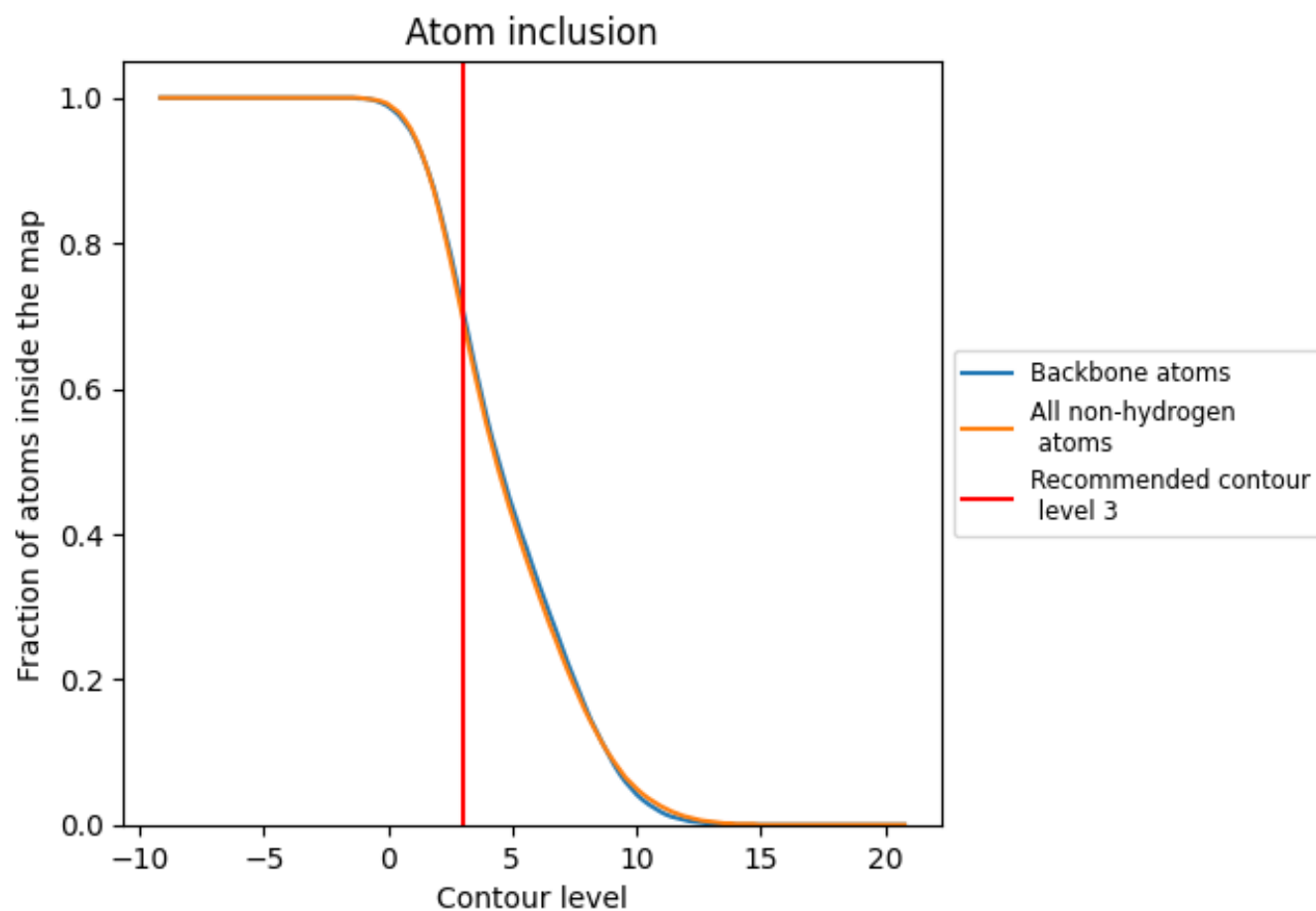
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3).

9.4 Atom inclusion ⓘ



At the recommended contour level, 71% 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) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6980	 0.3120
0	 0.5780	 0.2760
1	 0.1450	 0.0790
2	 0.0030	 0.0290
3	 0.2580	 0.0400
4	 0.4140	 0.0820
5	 0.2490	 0.0460
6	 0.3860	 0.0960
7	 0.4730	 0.1680
8	 0.3820	 0.0720
9	 0.7270	 0.3710
A	 0.9310	 0.3970
B	 0.8420	 0.4530
C	 0.8670	 0.4520
D	 0.8370	 0.4350
E	 0.8560	 0.4640
F	 0.7600	 0.4010
G	 0.7550	 0.3780
H	 0.7950	 0.4370
I	 0.8260	 0.4360
J	 0.8550	 0.4620
K	 0.8080	 0.4430
L	 0.7980	 0.4370
M	 0.7350	 0.3970
N	 0.8300	 0.4350
O	 0.7990	 0.4200
P	 0.8050	 0.4220
Q	 0.8710	 0.4590
R	 0.8690	 0.4210
S	 0.8370	 0.3790
T	 0.8720	 0.4300
V	 0.8130	 0.4360
Y	 0.8710	 0.4420
Z	 0.7560	 0.4070
a	 0.8200	 0.4240



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Chain	Atom inclusion	Q-score
b	 0.8100	 0.4010
c	 0.8010	 0.3880
d	 0.8800	 0.4330
e	 0.7170	 0.3790
f	 0.8050	 0.3940
h	 0.7810	 0.3970
i	 0.9080	 0.4610
k	 0.6870	 0.2650
m	 0.6080	 0.2420
n	 0.7160	 0.4150
o	 0.3860	 0.1630
q	 0.7190	 0.4110
r	 0.5270	 0.2080
t	 0.0800	 0.0790
u	 0.5210	 0.2010
v	 0.4960	 0.1120
w	 0.7200	 0.1600
x	 0.5450	 0.2260
y	 0.5770	 0.2550
z	 0.4810	 0.2130