



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 12:39 am GMT

PDB ID : 6FYY
EMDB ID : EMD-4328
Title : Structure of a partial yeast 48S preinitiation complex with eIF5 N-terminal domain (model C2)
Authors : Llacer, J.L.; Hussain, T.; Gordiyenko, Y.; Ramakrishnan, V.
Deposited on : 2018-03-12
Resolution : 3.05 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:

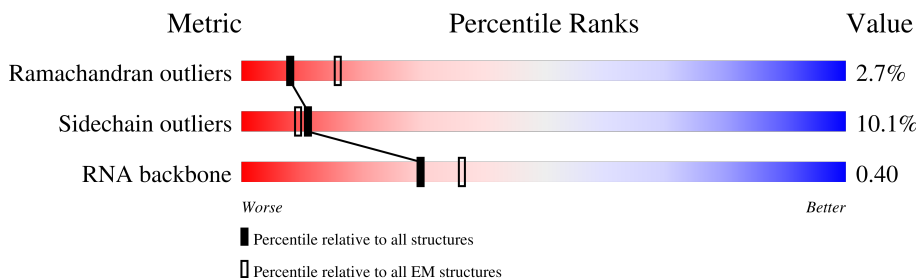
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1	76	
2	2	1798	
3	3	49	
4	A	254	
5	B	255	
6	C	259	
7	D	237	
8	E	261	

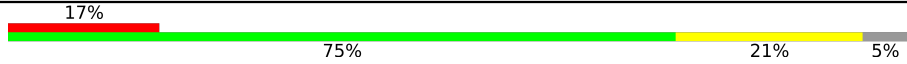
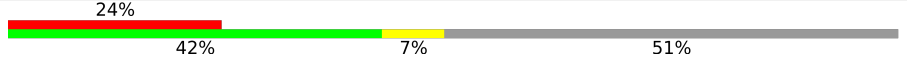
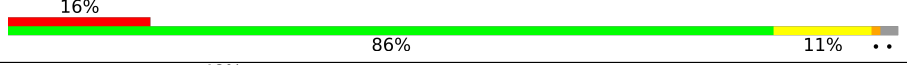
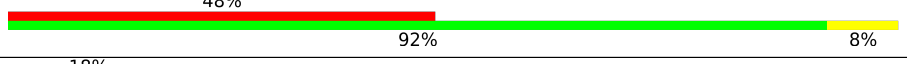

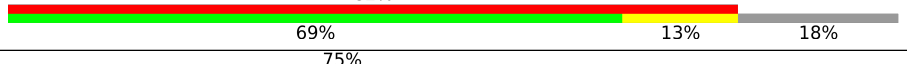






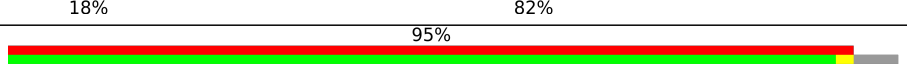
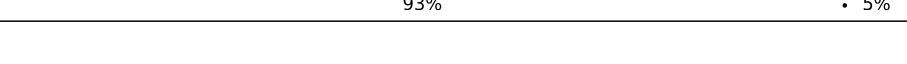
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Mol	Chain	Length	Quality of chain
9	F	227	10% 73% 18% 9%
10	G	236	17% 87% 11% 6%
11	H	190	23% 81% 15% 2%
12	I	201	10% 79% 13% 6%
13	J	188	1% 81% 15% 3%
14	K	106	8% 74% 17% 9%
15	L	156	15% 89% 10% 2%
16	M	134	56% 72% 15% 13%
17	N	151	7% 95% 5% 3%
18	O	137	1% 81% 12% 6%
19	P	142	7% 70% 12% 18%
20	Q	143	1% 85% 14% 2%
21	R	136	14% 83% 11% 3%
22	S	146	8% 85% 14% 3%
23	T	144	1% 86% 12% 3%
24	U	117	17% 78% 12% 9%
25	V	87	1% 94% 5% 2%
26	W	130	1% 89% 9% 3%
27	X	145	1% 88% 11% 3%
28	Y	135	5% 87% 11% 3%
29	Z	108	23% 64% 8% 28%
30	a	119	7% 76% 8% 13%
31	b	82	9% 87% 12% 3%
32	c	67	10% 79% 16% 3%
33	d	56	1% 86% 12% 3%

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Mol	Chain	Length	Quality of chain
34	e	63	
35	f	150	
36	g	326	
37	h	25	
38	i	153	
39	j	304	
40	k	527	
41	l	285	
42	m	405	
43	o	964	
44	p	763	
45	q	812	
46	r	274	
47	s	347	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	C4J	2	1190	X	-	-	-

2 Entry composition [i](#)

There are 51 unique types of molecules in this entry. The entry contains 104316 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called tRNAi.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	75	1639	734	298	531	76	0	0

- Molecule 2 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	1780	37812	16904	6659	12469	1780	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	676	G	U	conflict	GB 49642208
2	678	U	G	conflict	GB 49642208
2	1190	C4J	U	conflict	GB 49642208

- Molecule 3 is a RNA chain called mRNA (31-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	3	31	719	324	108	252	35	4	0

- Molecule 4 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	219	1702	1085	299	316	2	0	0

- Molecule 5 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	225	1797	1135	330	329	3	0	0

- Molecule 6 is a protein called KLLA0F09812p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	220	Total	C	N	O	S	0	0
			1648	1053	291	300	4		

- Molecule 7 is a protein called KLLA0D08305p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	227	Total	C	N	O	S	0	0
			1774	1126	320	323	5		

- Molecule 8 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 9 is a protein called KLLA0D10659p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 10 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	G	230	Total	C	N	O	S	0	0
			1832	1146	352	330	4		

- Molecule 11 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	H	184	Total	C	N	O	0	0
			1483	950	270	263		

- Molecule 12 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	I	188	Total	C	N	O	S	0	0
			1489	923	300	265	1		

- Molecule 13 is a protein called KLLA0E23673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 14 is a protein called KLLA0B08173p.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 15 is a protein called KLLA0A10483p.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 16 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	M	117	Total	C	N	O	0	0
			885	553	161	171		

- Molecule 17 is a protein called KLLA0F18040p.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	151	Total	C	N	O	S	0	0
			1195	761	224	207	3		

- Molecule 18 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	129	Total	C	N	O	S	0	0
			955	585	191	176	3		

- Molecule 19 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	117	Total	C	N	O	S	0	0
			923	592	165	161	5		

- Molecule 20 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Q	141	Total	C	N	O	0	0
			1105	709	204	192		

- Molecule 21 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	130	Total	C	N	O	S	0	0
			1033	643	194	193	3		

- Molecule 22 is a protein called KLLA0B01562p.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	145	Total	C	N	O	S	0	0
			1189	739	239	209	2		

- Molecule 23 is a protein called KLLA0A07194p.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	T	143	Total	C	N	O	0	0
			1110	693	210	207		

- Molecule 24 is a protein called KLLA0F25542p.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 25 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 26 is a protein called 40S ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 27 is a protein called KLLA0B11231p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	X	144	1119	708	218	191	2	0	0

- Molecule 28 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Y	134	1061	665	207	189		0	0

- Molecule 29 is a protein called KLLA0B06182p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Z	78	594	376	111	106	1	0	0

- Molecule 30 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	a	103	812	500	173	134	5	0	0

- Molecule 31 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	b	81	609	379	112	113	5	0	0

- Molecule 32 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	c	64	499	308	99	91	1	0	0

- Molecule 33 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	d	55	461	289	93	78	1	0	0

- Molecule 34 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	60	Total	C	N	O	S	0	0
			472	295	96	80	1		

- Molecule 35 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	74	Total	C	N	O	S	0	0
			584	374	111	95	4		

- Molecule 36 is a protein called KLLA0E12277p.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	320	Total	C	N	O	S	0	0
			2469	1561	432	471	5		

- Molecule 37 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 38 is a protein called Eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	121	Total	C	N	O	S	0	0
			958	587	183	183	5		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	249	Total	C	N	O	S	0	0
			2006	1283	333	382	8		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	396	Total	C	N	O	S	0	0
			3034	1932	542	544	16		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	l	128	1036	661	186	182	7	0	0

- Molecule 42 is a protein called Eukaryotic translation initiation factor 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	m	147	1140	724	201	208	7	0	0

- Molecule 43 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	o	529	4070	2597	697	769	7	0	0

- Molecule 44 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	p	647	5114	3274	880	942	18	0	0

- Molecule 45 is a protein called eIF3c, Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	q	621	4827	3076	813	926	12	0	0

- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
46	r	49	392	240	76	76	0	0

- Molecule 47 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	s	330	2606	1661	429	507	9	0	0

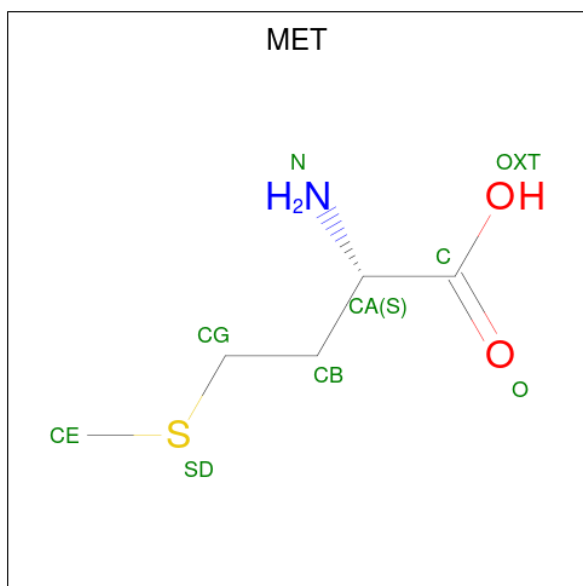
- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	2	116	Total	Mg	0
			116	116	
48	k	1	Total	Mg	0
			1	1	

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

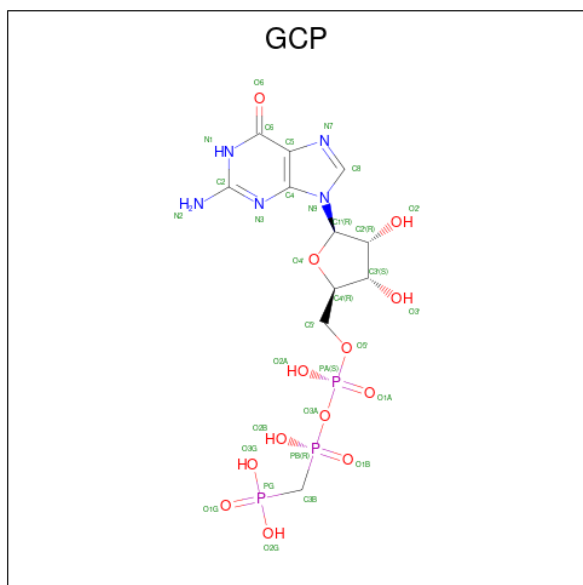
Mol	Chain	Residues	Atoms		AltConf
49	a	1	Total	Zn	0
			1	1	
49	b	1	Total	Zn	0
			1	1	
49	f	1	Total	Zn	0
			1	1	
49	l	1	Total	Zn	0
			1	1	
49	m	1	Total	Zn	0
			1	1	

- Molecule 50 is METHIONINE (three-letter code: MET) (formula: C₅H₁₁NO₂S).



Mol	Chain	Residues	Atoms					AltConf
50	k	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 51 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).

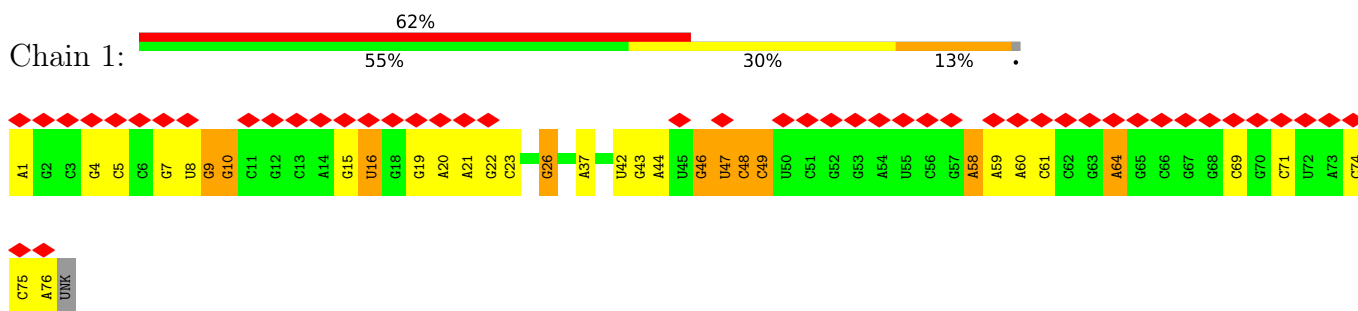


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
51	k	1	32	11	5	13	3	0

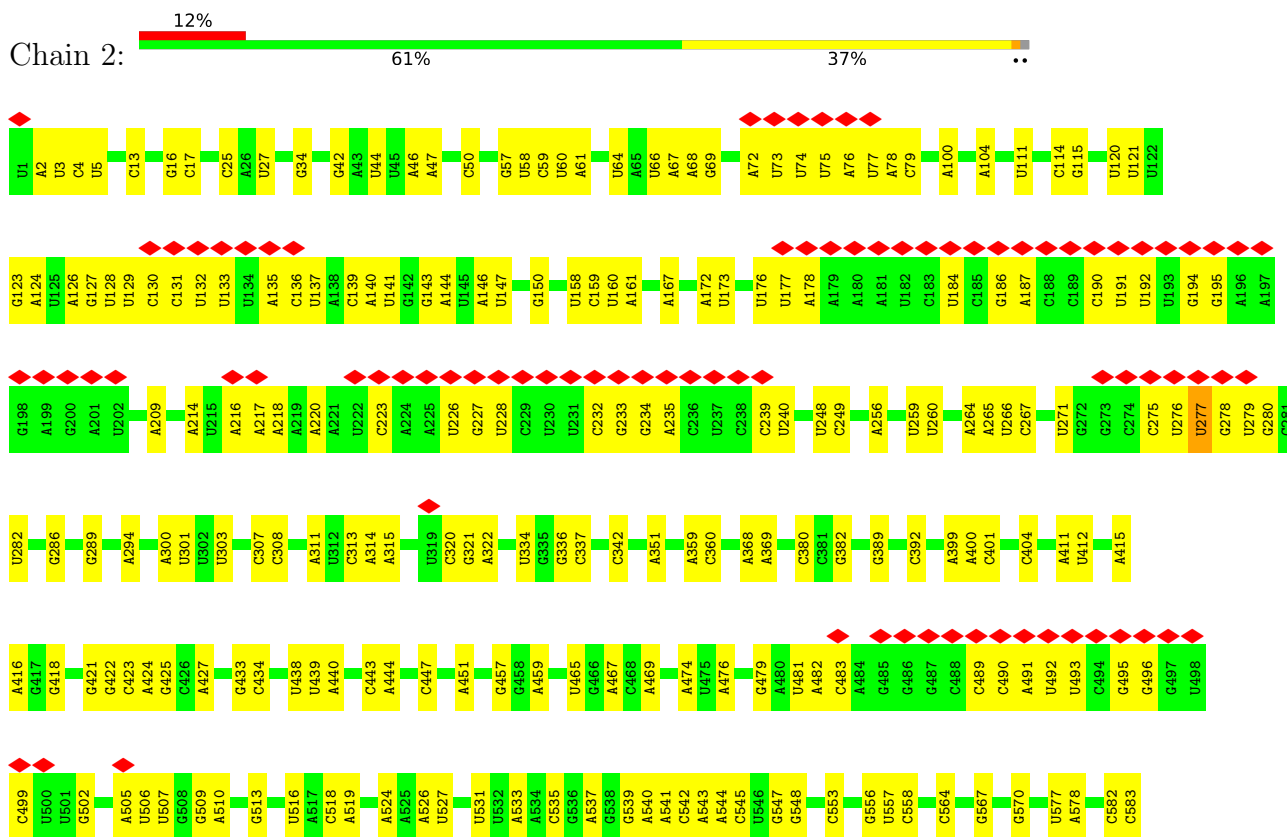
3 Residue-property plots

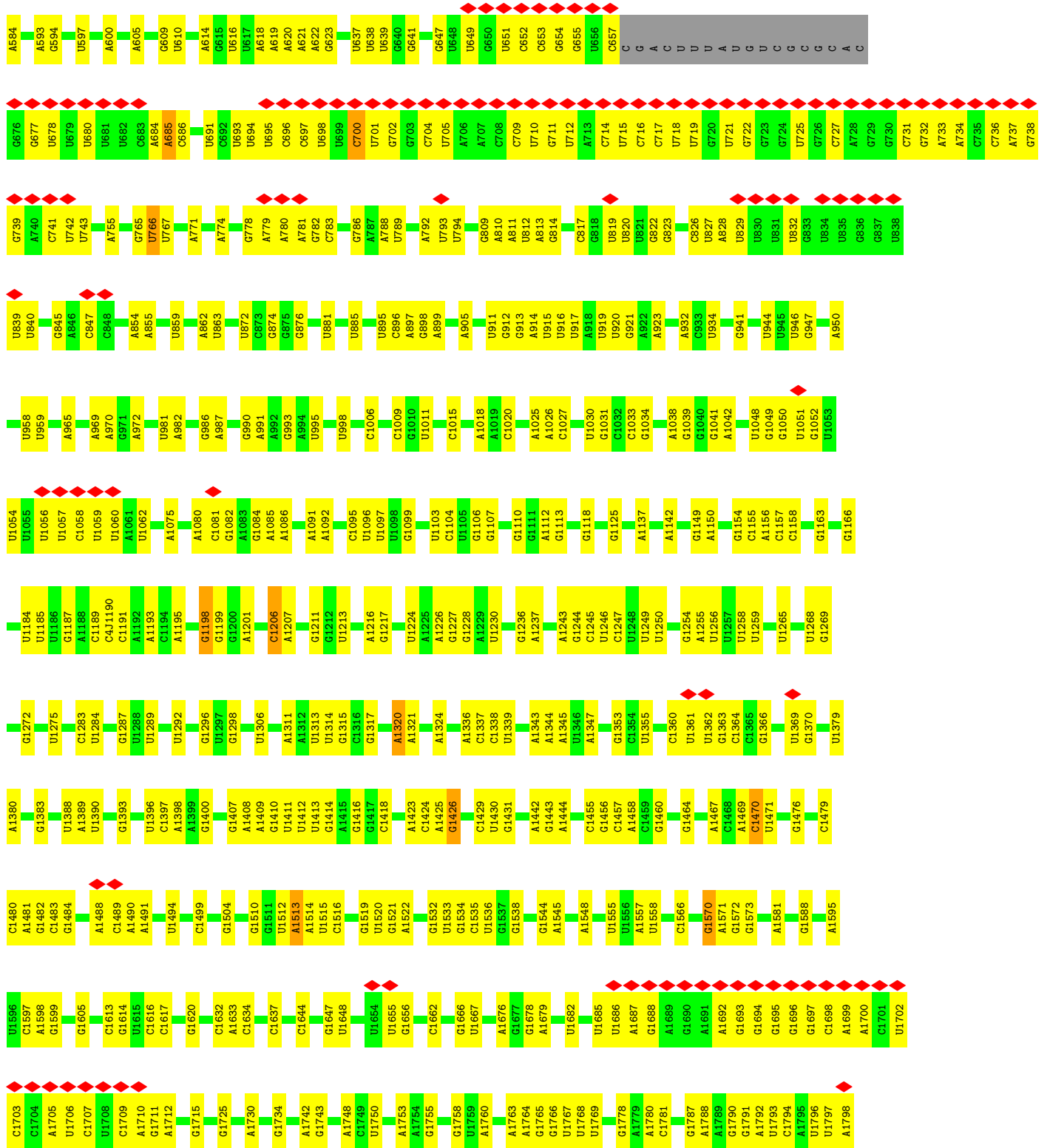
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

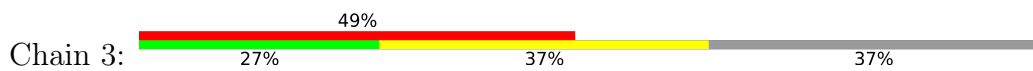


- Molecule 2: 18S ribosomal RNA



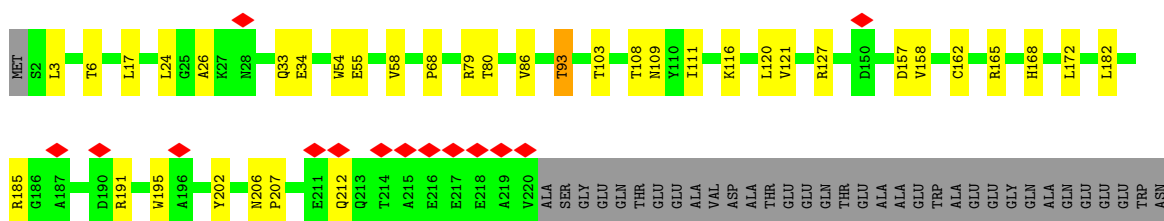
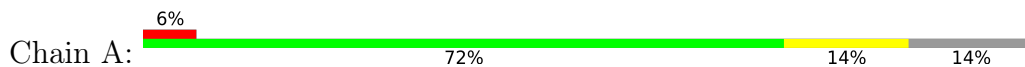


• Molecule 3: mRNA (31-MER)

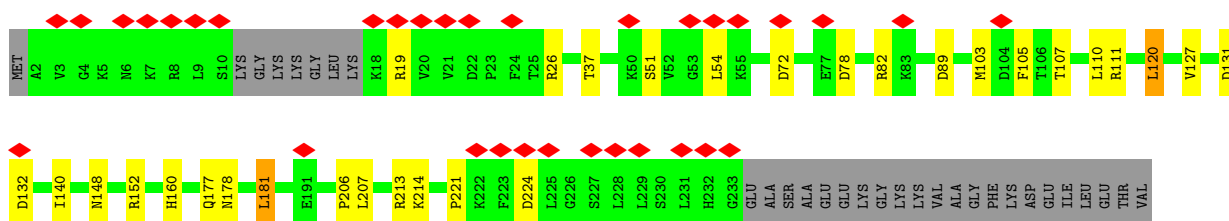
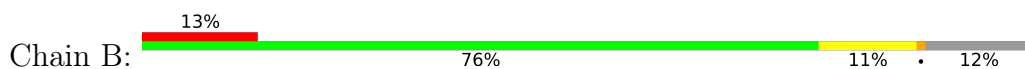




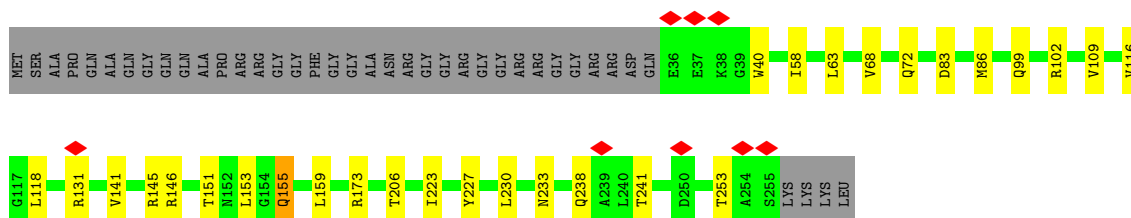
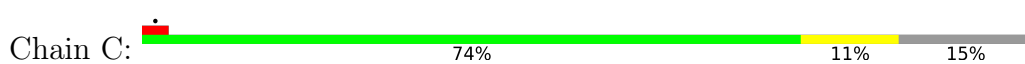
• Molecule 4: 40S ribosomal protein S0



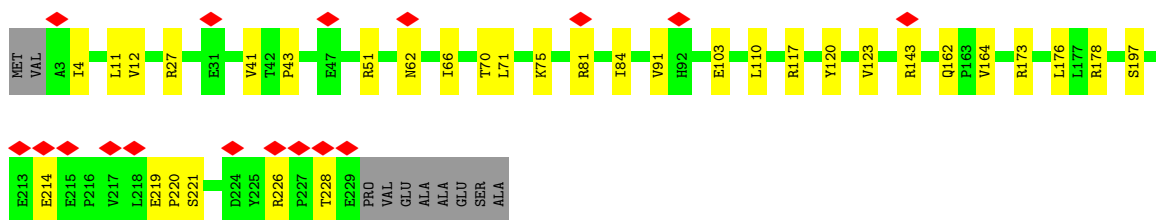
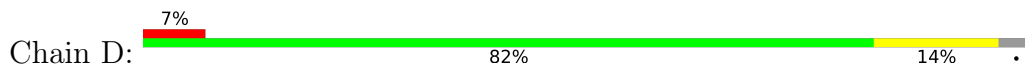
• Molecule 5: 40S ribosomal protein S1



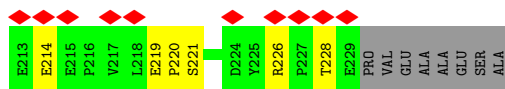
• Molecule 6: KLLA0F09812p

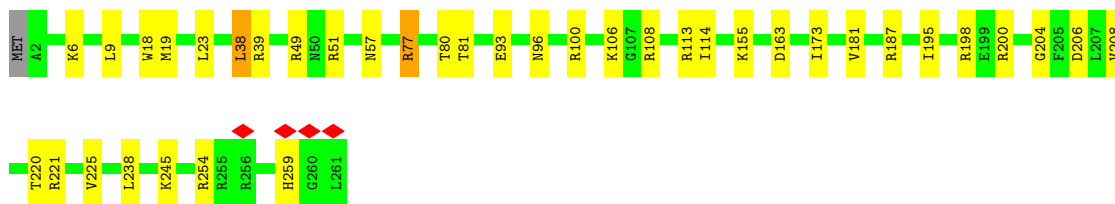
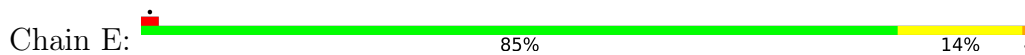


• Molecule 7: KLLA0D08305p

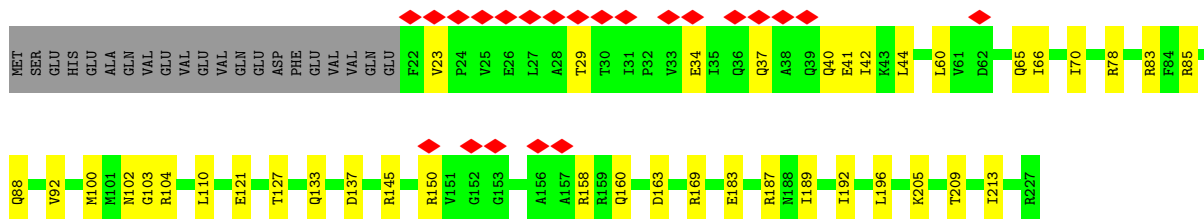
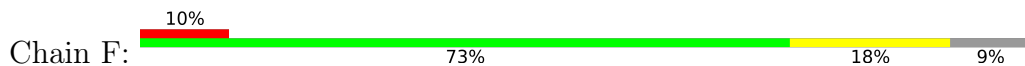


• Molecule 8: 40S ribosomal protein S4

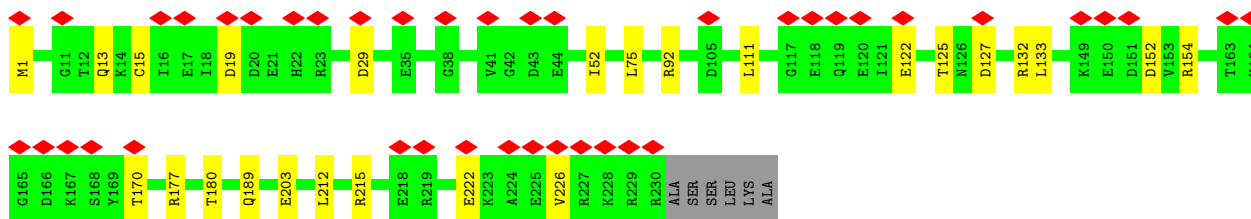
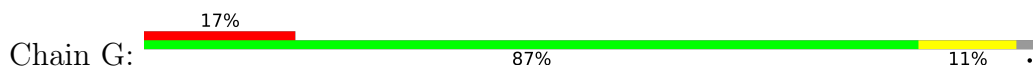




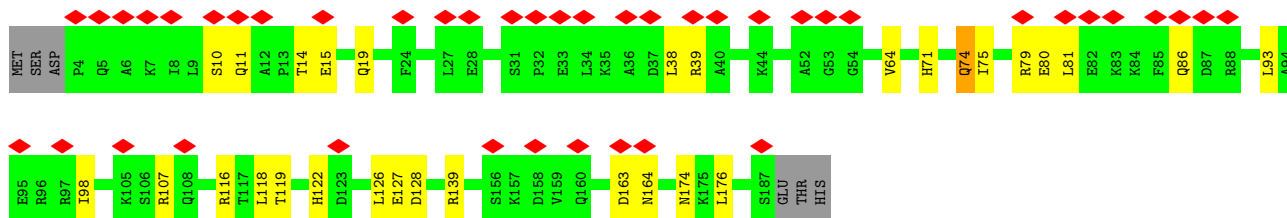
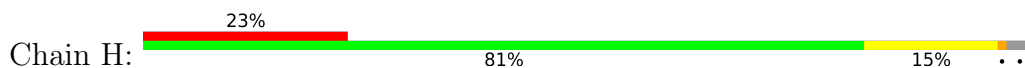
• Molecule 9: KLLA0D10659p



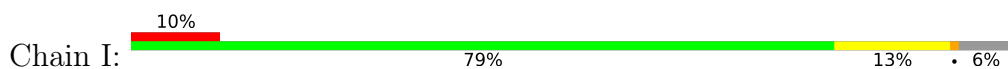
• Molecule 10: 40S ribosomal protein S6

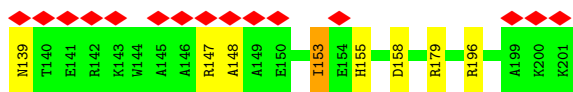


• Molecule 11: 40S ribosomal protein S7

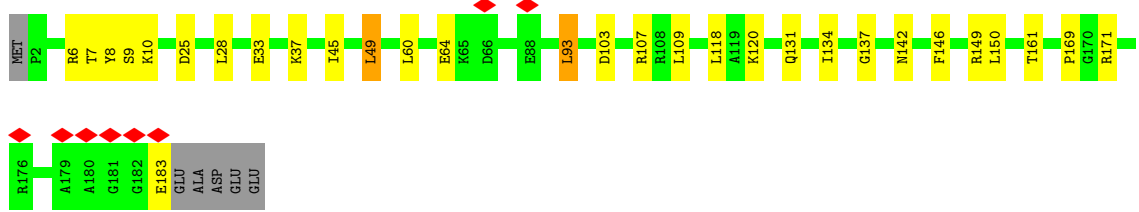
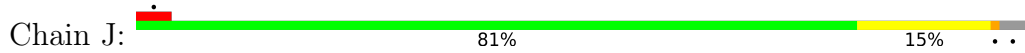


• Molecule 12: 40S ribosomal protein S8

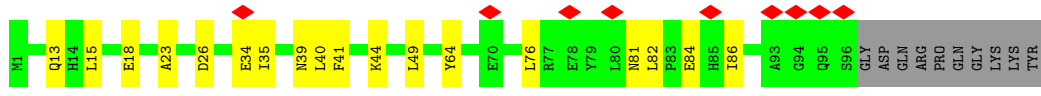
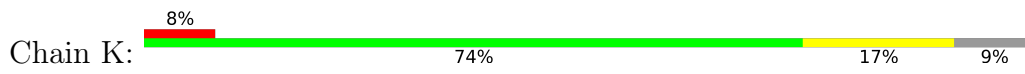




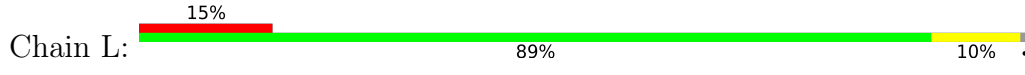
• Molecule 13: KLLA0E23673p



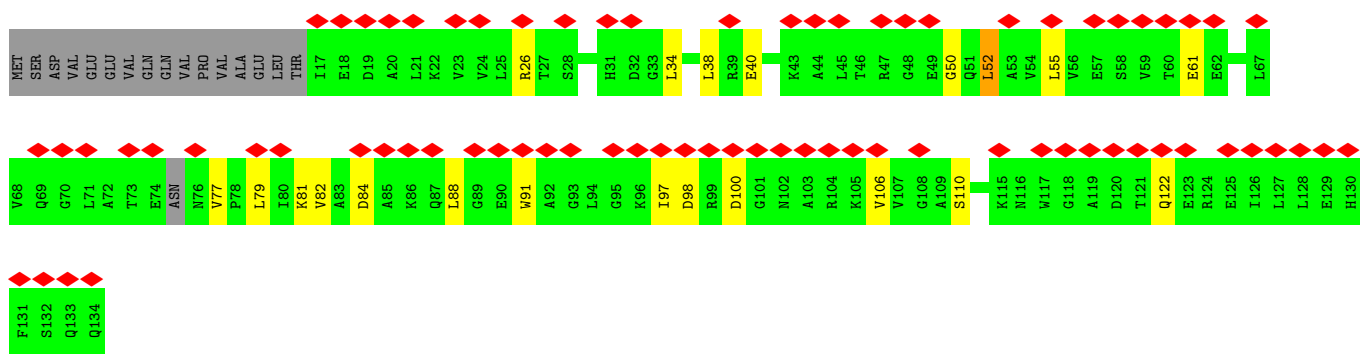
• Molecule 14: KLLA0B08173p



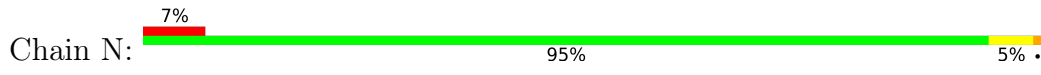
• Molecule 15: KLLA0A10483p



• Molecule 16: 40S ribosomal protein S12

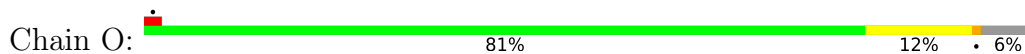


• Molecule 17: KLLA0F18040p

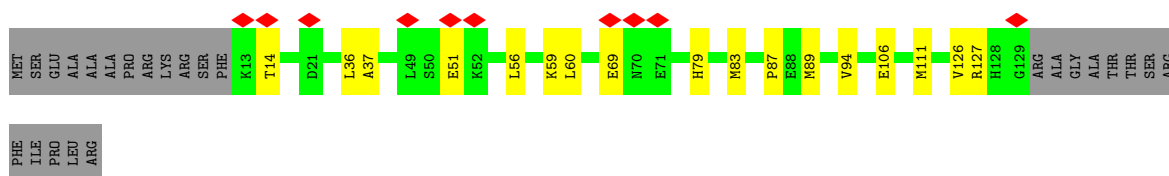




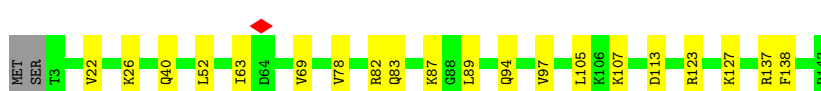
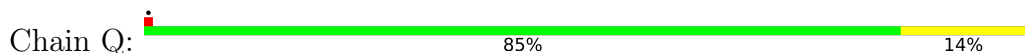
• Molecule 18: 40S ribosomal protein S14



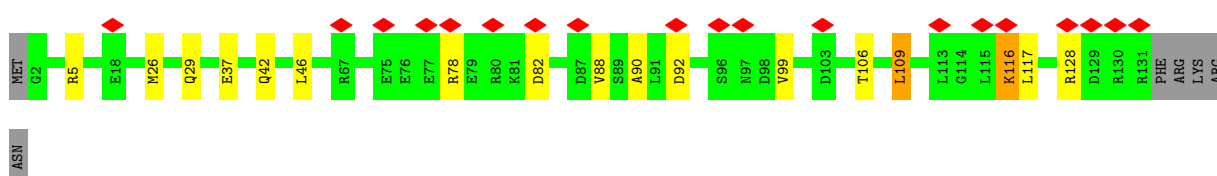
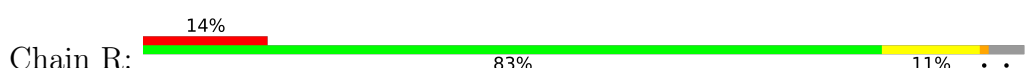
• Molecule 19: KLLA0F07843p



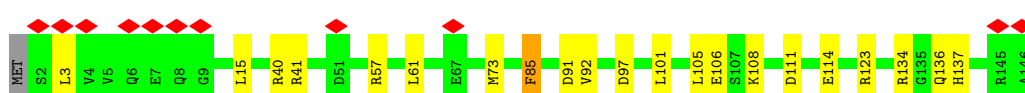
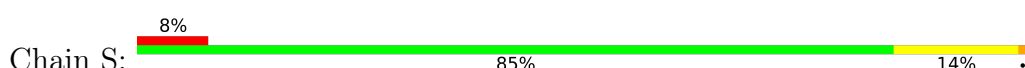
• Molecule 20: 40S ribosomal protein S16



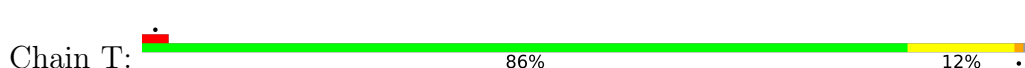
• Molecule 21: KLLA0B01474p



• Molecule 22: KLLA0B01562p

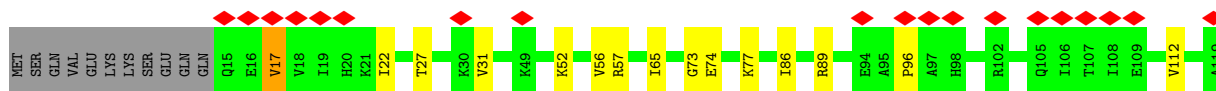
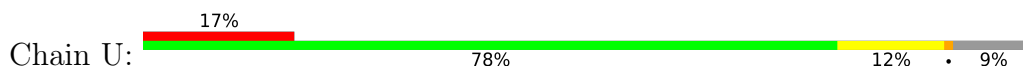


• Molecule 23: KLLA0A07194p





- Molecule 24: KLLA0F25542p



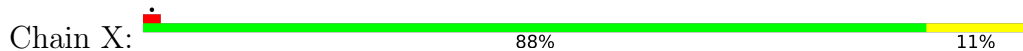
- Molecule 25: 40S ribosomal protein S21



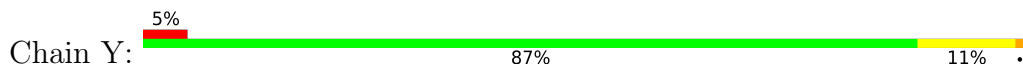
- Molecule 26: 40S ribosomal protein S22



- Molecule 27: KLLA0B11231p

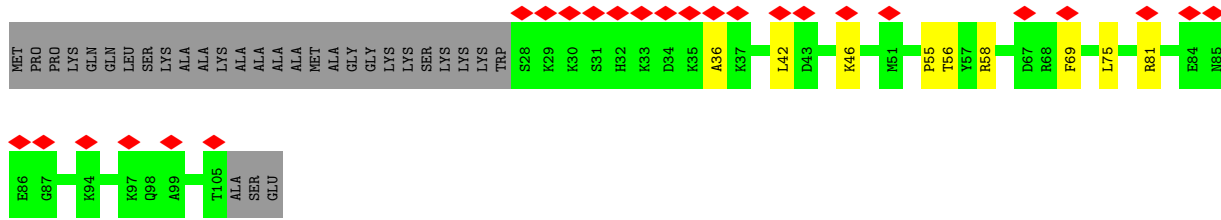


- Molecule 28: 40S ribosomal protein S24

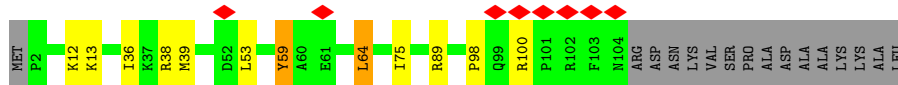
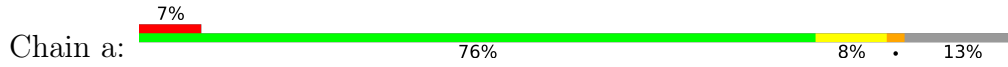


- Molecule 29: KLLA0B06182p

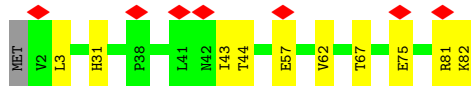
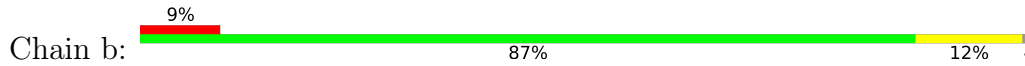




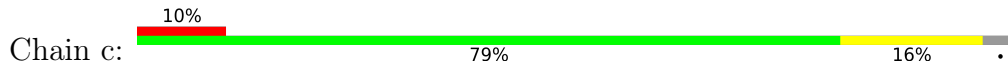
• Molecule 30: 40S ribosomal protein S26



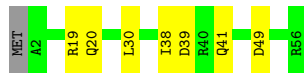
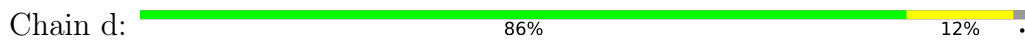
• Molecule 31: 40S ribosomal protein S27



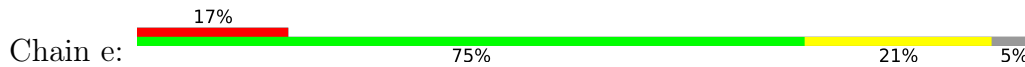
• Molecule 32: 40S ribosomal protein S28



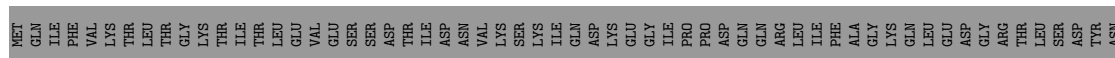
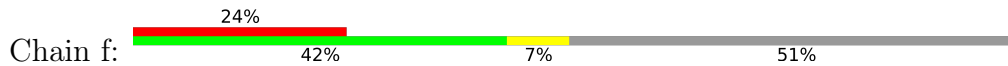
• Molecule 33: 40S ribosomal protein S29

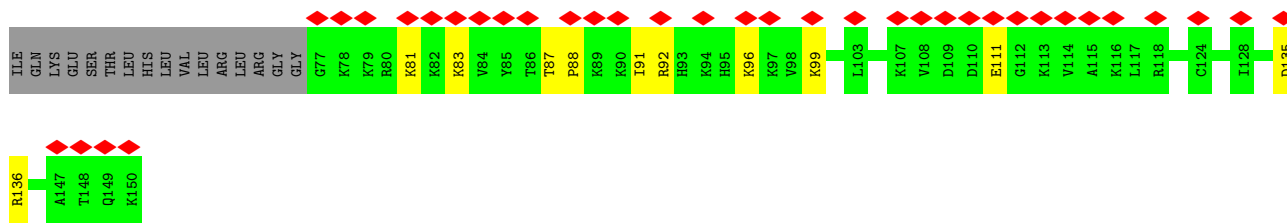


• Molecule 34: 40S ribosomal protein S30

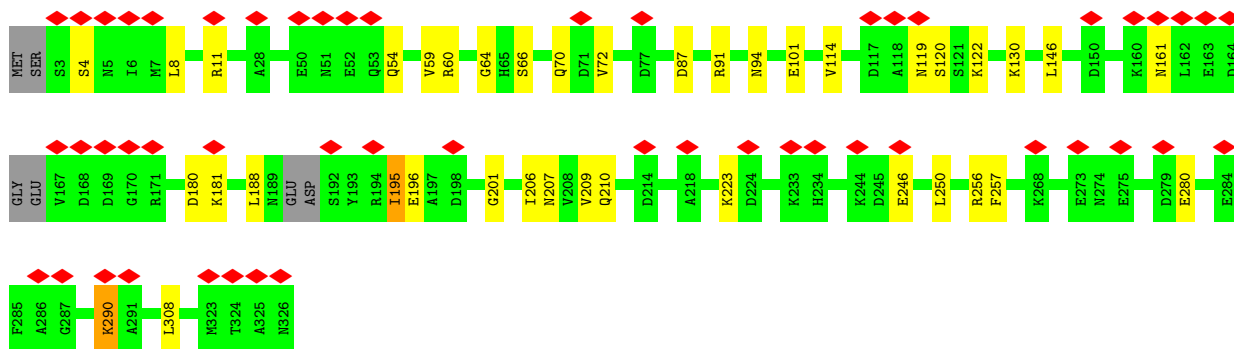
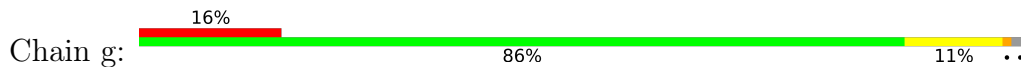


• Molecule 35: Ubiquitin-40S ribosomal protein S27a

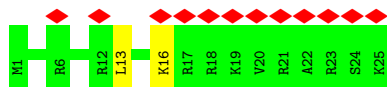
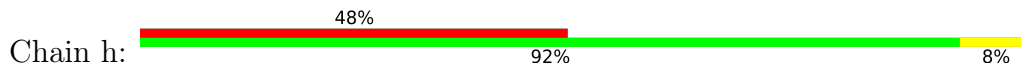




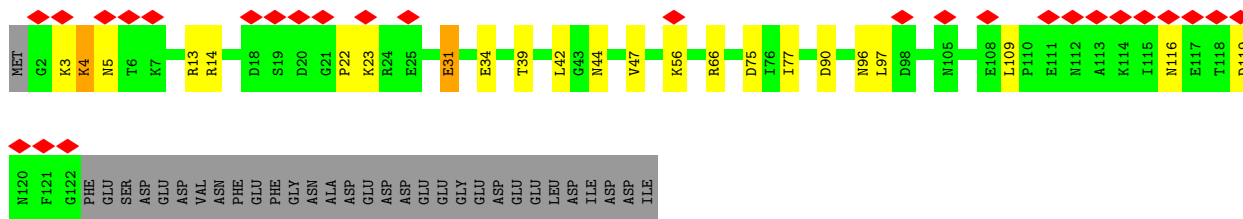
• Molecule 36: KLLA0E12277p



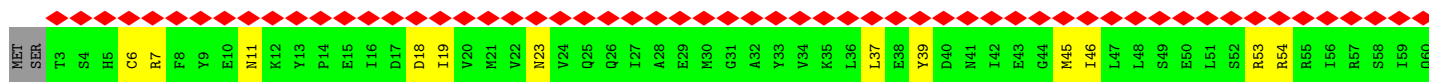
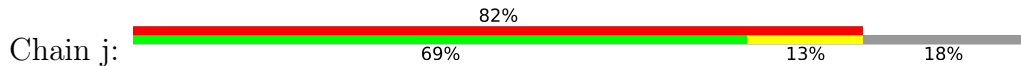
• Molecule 37: 60S ribosomal protein L41-A

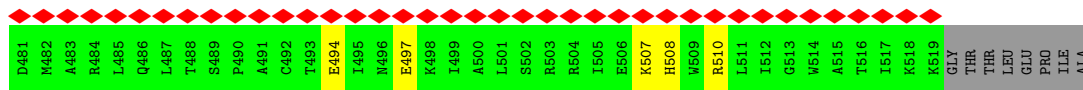


• Molecule 38: Eukaryotic translation initiation factor 1A

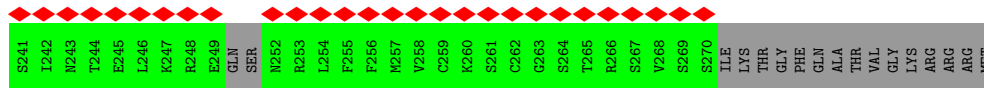
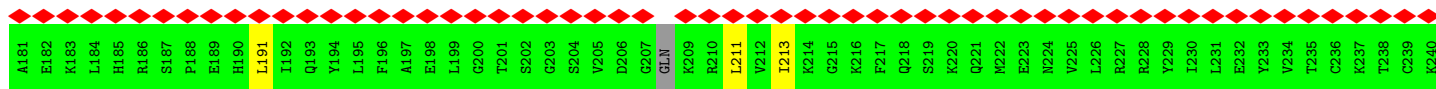
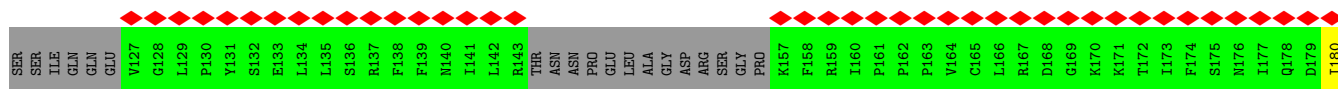
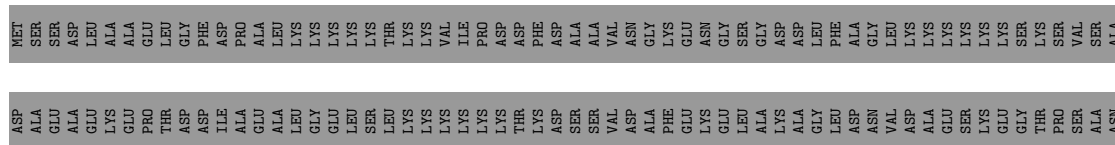
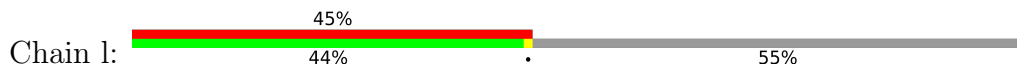


• Molecule 39: Eukaryotic translation initiation factor 2 subunit alpha

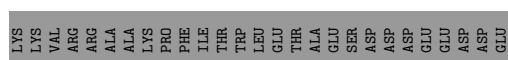
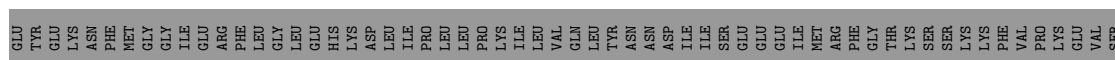
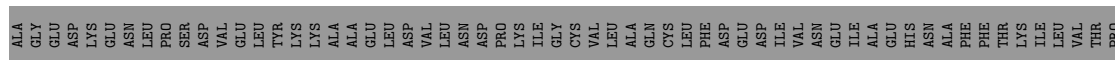
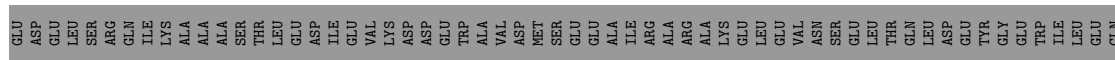
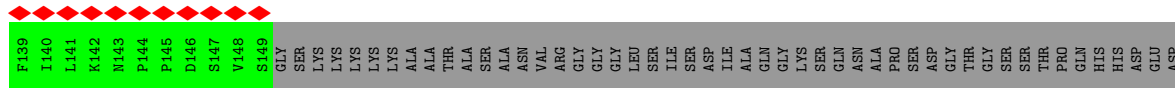
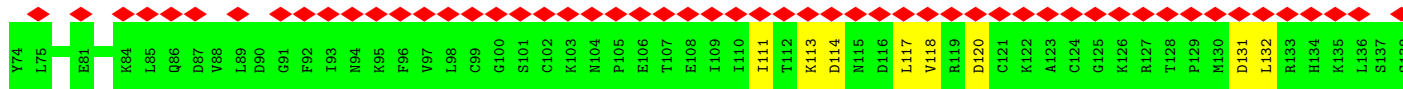
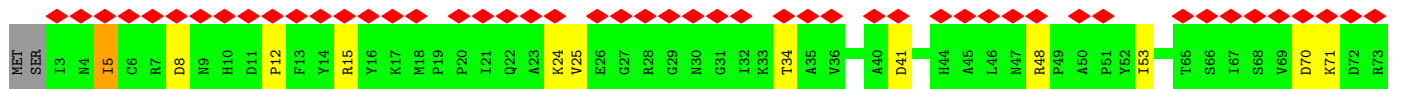




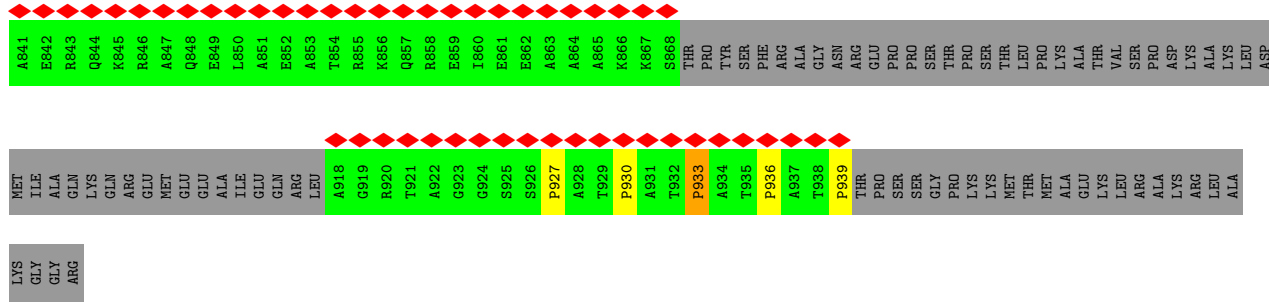
• Molecule 41: Eukaryotic translation initiation factor 2 subunit beta



• Molecule 42: Eukaryotic translation initiation factor 5

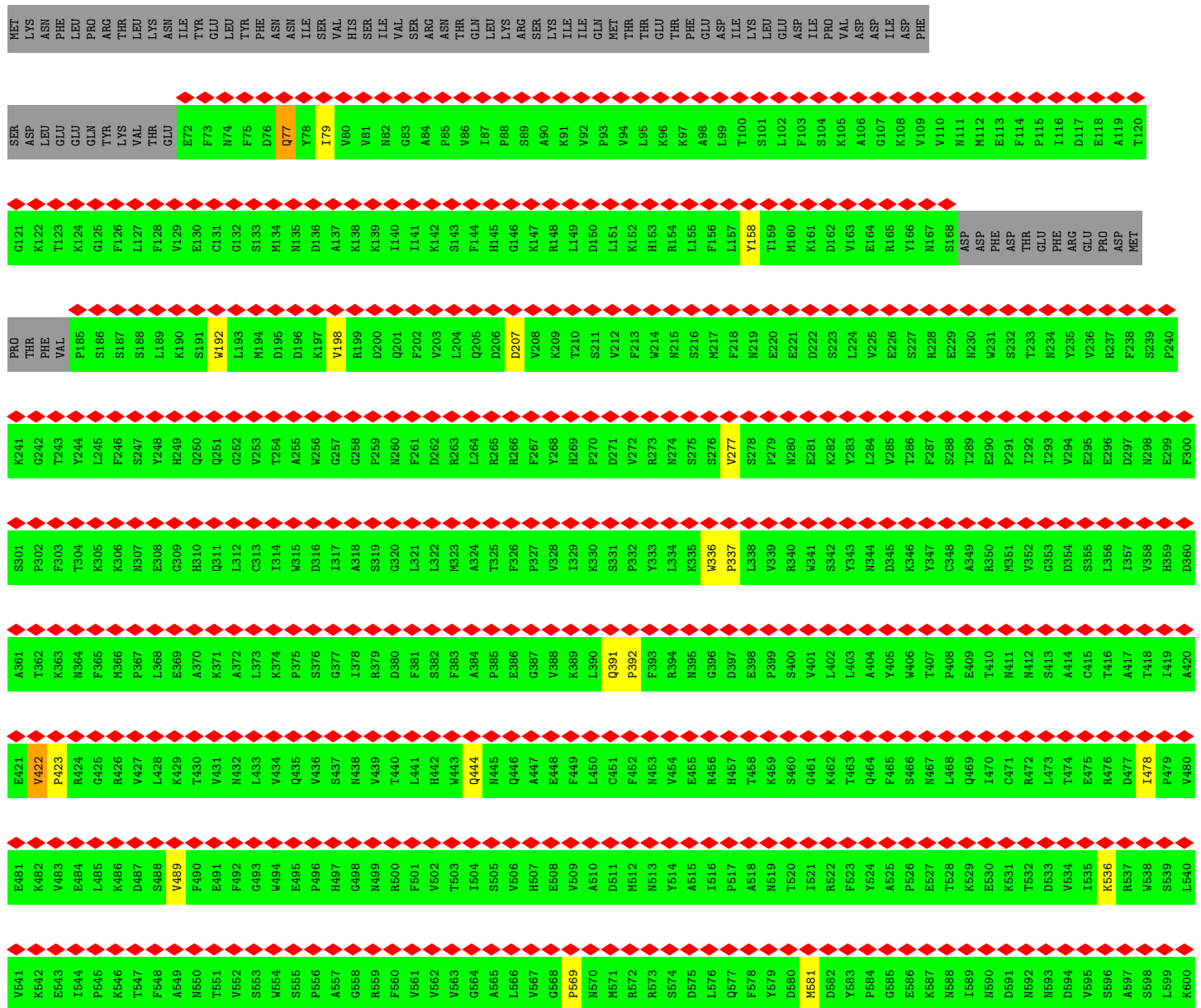


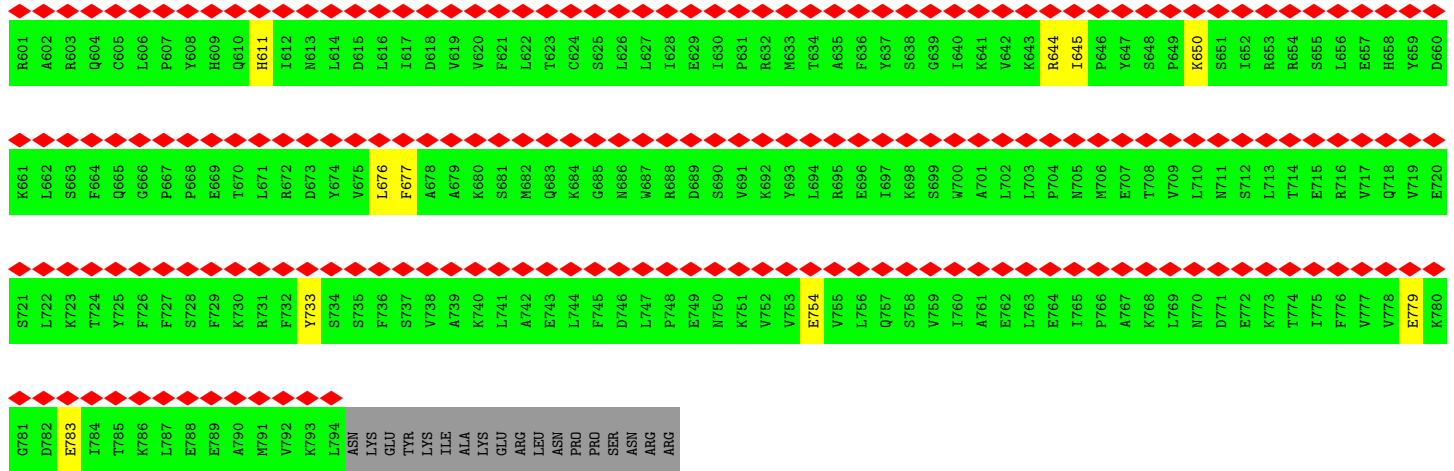
• Molecule 43: Eukaryotic translation initiation factor 3 subunit A



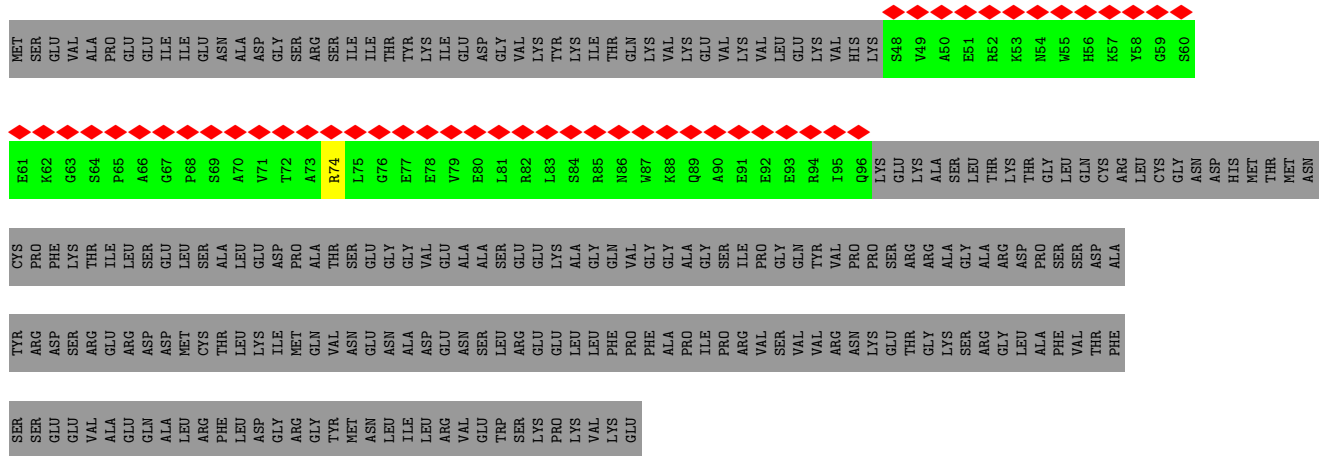
● Molecule 44: Eukaryotic translation initiation factor 3 subunit B

Chain p:

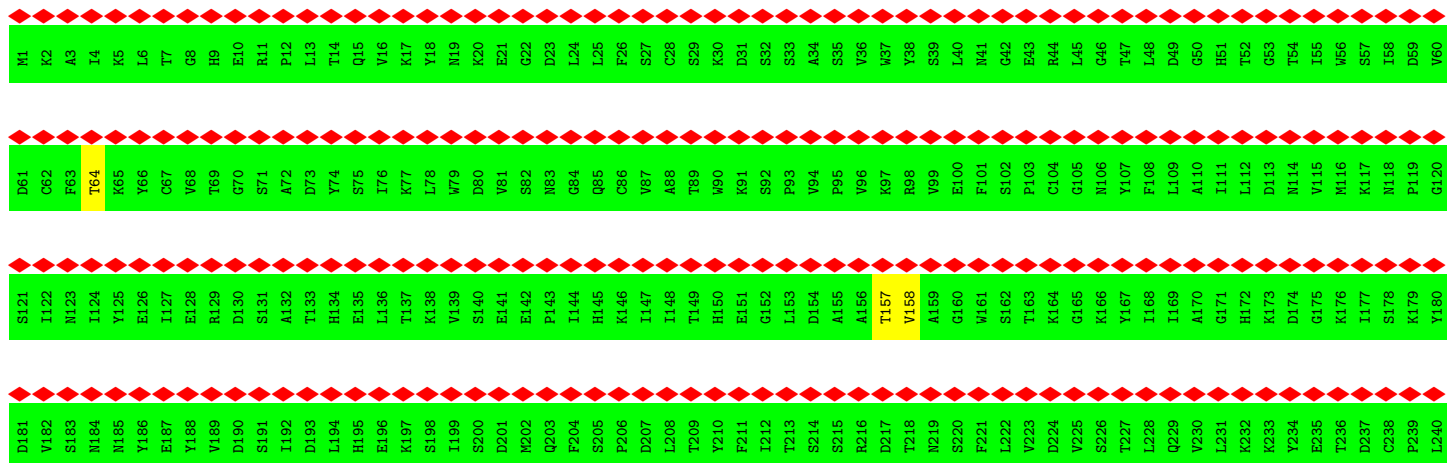
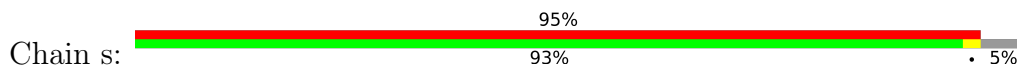




• Molecule 46: Eukaryotic translation initiation factor 3 subunit G



• Molecule 47: Eukaryotic translation initiation factor 3 subunit I



N241	T242	A243	V244	I245	T246	P247	L248	K249	E250	F251	I252	I253	L254	G255	G256	G257	Q258	GLU	ALA	LYS	ASP	VAL	THR	THR	THR	SER	ALA	ALA	ASN	GLU	G271	K272	F273	E274	A275	R276	F277	Y278	H279	K280	I281	F282	E283	E284	E285	I286	G287	R288	V289	Q290	G291	H292	F293	G294	P295	L296	N297	T298	V299	A300
I301	S302	P303	Q304	G305	T306	S307	Y308	A309	S310	G311	G312	E313	D314	G315	F316	I317	R318	L319	H320	H321	F322	E323	K324	S325	Y326	F327	D328	F329	K330	Y331	D332	V333	E334	K335	A336	A337	E338	A339	K340	E341	H342	MET	GLN	GLU	ALA	ASN														

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	157868	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.157	Depositor
Minimum map value	-0.645	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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: T6A, 1MA, C4J, 2MG, MG, MA6, M2G, PSU, 1MG, GCP, AYA, ZN, H2U, RIA, 5MC, 7MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.36	1/1529 (0.1%)	0.71	0/2376
2	2	0.29	0/41987	0.70	9/65416 (0.0%)
3	3	0.39	0/797	0.81	2/1233 (0.2%)
4	A	0.40	0/1742	0.72	1/2383 (0.0%)
5	B	0.37	0/1813	0.73	2/2438 (0.1%)
6	C	0.39	0/1678	0.71	0/2277
7	D	0.40	0/1800	0.73	0/2421
8	E	0.38	0/2122	0.71	1/2861 (0.0%)
9	F	0.39	0/1628	0.75	0/2198
10	G	0.38	0/1855	0.70	0/2479
11	H	0.40	0/1507	0.73	1/2028 (0.0%)
12	I	0.38	0/1515	0.72	0/2029
13	J	0.40	0/1495	0.78	1/2001 (0.0%)
14	K	0.46	0/831	0.76	1/1123 (0.1%)
15	L	0.40	0/1276	0.64	0/1718
16	M	0.42	0/891	0.75	1/1201 (0.1%)
17	N	0.40	0/1218	0.72	0/1638
18	O	0.39	0/966	0.74	0/1297
19	P	0.38	0/942	0.67	0/1269
20	Q	0.39	0/1125	0.73	0/1510
21	R	0.42	0/1044	0.78	1/1402 (0.1%)
22	S	0.39	0/1208	0.74	0/1624
23	T	0.39	0/1129	0.72	0/1520
24	U	0.38	0/857	0.72	0/1158
25	V	0.37	0/696	0.68	0/938
26	W	0.39	0/1039	0.74	0/1399
27	X	0.41	0/1137	0.71	0/1516
28	Y	0.38	0/1075	0.65	0/1433
29	Z	0.38	0/603	0.68	1/814 (0.1%)
30	a	0.37	0/825	0.68	0/1106
31	b	0.36	0/619	0.63	0/837
32	c	0.35	0/501	0.70	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.38	0/473	0.66	0/629
34	e	0.39	0/480	0.69	0/640
35	f	0.41	0/597	0.61	0/795
36	g	0.37	0/2523	0.65	0/3434
37	h	0.33	0/234	0.70	0/300
38	i	0.38	0/969	0.68	0/1287
39	j	0.42	0/2034	0.63	0/2737
40	k	0.39	0/3079	0.60	0/4157
41	l	0.42	0/1051	0.59	0/1402
42	m	0.40	0/1164	0.64	0/1575
43	o	0.42	0/4140	0.64	6/5608 (0.1%)
44	p	0.43	0/5245	0.59	0/7115
45	q	0.44	0/4523	0.61	0/6114
46	r	0.40	0/399	0.54	0/535
47	s	0.43	0/2669	0.59	0/3611
All	All	0.36	1/109030 (0.0%)	0.69	27/156255 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	1	0
20	Q	0	1
44	p	0	2
All	All	1	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1	A	OP3-P	-10.07	1.49	1.61

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	18[A]	U	P-O3'-C3'	8.96	130.45	119.70
3	3	18[B]	U	P-O3'-C3'	8.96	130.45	119.70
2	2	685	A	C2'-C3'-O3'	7.20	125.34	109.50
5	B	181	LEU	CA-CB-CG	6.82	130.97	115.30
2	2	616	U	N1-C1'-C2'	6.17	122.03	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	2	1190	C4J	C4'

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	Q	40	GLN	Peptide
44	p	336	TRP	Peptide
44	p	391	GLN	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	217/254 (85%)	192 (88%)	16 (7%)	9 (4%)	3	14
5	B	220/255 (86%)	191 (87%)	19 (9%)	10 (4%)	2	12
6	C	218/259 (84%)	197 (90%)	16 (7%)	5 (2%)	6	24
7	D	225/237 (95%)	211 (94%)	8 (4%)	6 (3%)	5	21
8	E	258/261 (99%)	233 (90%)	21 (8%)	4 (2%)	9	33
9	F	204/227 (90%)	173 (85%)	21 (10%)	10 (5%)	2	11
10	G	228/236 (97%)	211 (92%)	15 (7%)	2 (1%)	17	47
11	H	182/190 (96%)	161 (88%)	14 (8%)	7 (4%)	3	15
12	I	184/201 (92%)	162 (88%)	12 (6%)	10 (5%)	2	9
13	J	180/188 (96%)	152 (84%)	20 (11%)	8 (4%)	2	12
14	K	94/106 (89%)	83 (88%)	8 (8%)	3 (3%)	4	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	L	153/156 (98%)	132 (86%)	17 (11%)	4 (3%)	5	22
16	M	113/134 (84%)	85 (75%)	20 (18%)	8 (7%)	1	5
17	N	149/151 (99%)	139 (93%)	9 (6%)	1 (1%)	22	52
18	O	127/137 (93%)	107 (84%)	13 (10%)	7 (6%)	2	9
19	P	115/142 (81%)	98 (85%)	11 (10%)	6 (5%)	2	10
20	Q	139/143 (97%)	125 (90%)	11 (8%)	3 (2%)	6	25
21	R	128/136 (94%)	110 (86%)	11 (9%)	7 (6%)	2	9
22	S	143/146 (98%)	127 (89%)	13 (9%)	3 (2%)	7	26
23	T	141/144 (98%)	132 (94%)	7 (5%)	2 (1%)	11	36
24	U	104/117 (89%)	90 (86%)	9 (9%)	5 (5%)	2	11
25	V	85/87 (98%)	80 (94%)	2 (2%)	3 (4%)	3	17
26	W	127/130 (98%)	115 (91%)	7 (6%)	5 (4%)	3	15
27	X	142/145 (98%)	126 (89%)	12 (8%)	4 (3%)	5	21
28	Y	132/135 (98%)	123 (93%)	5 (4%)	4 (3%)	4	19
29	Z	76/108 (70%)	62 (82%)	10 (13%)	4 (5%)	2	10
30	a	101/119 (85%)	84 (83%)	11 (11%)	6 (6%)	1	8
31	b	79/82 (96%)	68 (86%)	9 (11%)	2 (2%)	5	22
32	c	62/67 (92%)	55 (89%)	5 (8%)	2 (3%)	4	18
33	d	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
34	e	58/63 (92%)	44 (76%)	9 (16%)	5 (9%)	1	3
35	f	72/150 (48%)	57 (79%)	13 (18%)	2 (3%)	5	21
36	g	314/326 (96%)	276 (88%)	29 (9%)	9 (3%)	4	20
37	h	23/25 (92%)	23 (100%)	0	0	100	100
38	i	119/153 (78%)	102 (86%)	11 (9%)	6 (5%)	2	11
39	j	243/304 (80%)	213 (88%)	25 (10%)	5 (2%)	7	26
40	k	388/527 (74%)	333 (86%)	47 (12%)	8 (2%)	7	26
41	l	120/285 (42%)	109 (91%)	11 (9%)	0	100	100
42	m	145/405 (36%)	126 (87%)	17 (12%)	2 (1%)	11	36
43	o	519/964 (54%)	483 (93%)	30 (6%)	6 (1%)	13	40
44	p	637/763 (84%)	583 (92%)	43 (7%)	11 (2%)	9	32
45	q	538/812 (66%)	490 (91%)	39 (7%)	9 (2%)	9	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	r	47/274 (17%)	43 (92%)	4 (8%)	0	100	100
47	s	326/347 (94%)	311 (95%)	15 (5%)	0	100	100
All	All	7928/10147 (78%)	7065 (89%)	650 (8%)	213 (3%)	8	21

5 of 213 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	C	141	VAL
7	D	220	PRO
9	F	104	ARG
11	H	64	VAL
11	H	74	GLN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	180/211 (85%)	152 (84%)	28 (16%)	2	10
5	B	201/228 (88%)	180 (90%)	21 (10%)	7	24
6	C	177/203 (87%)	152 (86%)	25 (14%)	3	13
7	D	188/196 (96%)	161 (86%)	27 (14%)	3	12
8	E	223/224 (100%)	188 (84%)	35 (16%)	2	10
9	F	174/194 (90%)	144 (83%)	30 (17%)	2	7
10	G	192/200 (96%)	169 (88%)	23 (12%)	5	18
11	H	164/170 (96%)	141 (86%)	23 (14%)	3	13
12	I	147/159 (92%)	124 (84%)	23 (16%)	2	10
13	J	153/158 (97%)	130 (85%)	23 (15%)	3	11
14	K	88/96 (92%)	74 (84%)	14 (16%)	2	9
15	L	136/137 (99%)	124 (91%)	12 (9%)	10	32
16	M	93/109 (85%)	80 (86%)	13 (14%)	3	13
17	N	128/128 (100%)	120 (94%)	8 (6%)	18	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	O	97/104 (93%)	84 (87%)	13 (13%)	4	14
19	P	99/119 (83%)	88 (89%)	11 (11%)	6	21
20	Q	117/119 (98%)	101 (86%)	16 (14%)	3	14
21	R	116/124 (94%)	105 (90%)	11 (10%)	8	28
22	S	127/129 (98%)	108 (85%)	19 (15%)	3	11
23	T	117/118 (99%)	99 (85%)	18 (15%)	2	10
24	U	96/107 (90%)	85 (88%)	11 (12%)	5	20
25	V	73/73 (100%)	70 (96%)	3 (4%)	30	61
26	W	110/111 (99%)	101 (92%)	9 (8%)	11	35
27	X	119/120 (99%)	107 (90%)	12 (10%)	7	25
28	Y	108/109 (99%)	95 (88%)	13 (12%)	5	18
29	Z	59/88 (67%)	55 (93%)	4 (7%)	16	42
30	a	85/100 (85%)	77 (91%)	8 (9%)	8	28
31	b	71/72 (99%)	63 (89%)	8 (11%)	6	21
32	c	55/59 (93%)	46 (84%)	9 (16%)	2	9
33	d	47/48 (98%)	40 (85%)	7 (15%)	3	11
34	e	51/55 (93%)	43 (84%)	8 (16%)	2	10
35	f	60/133 (45%)	51 (85%)	9 (15%)	3	11
36	g	264/272 (97%)	232 (88%)	32 (12%)	5	17
37	h	23/23 (100%)	21 (91%)	2 (9%)	10	33
38	i	100/130 (77%)	81 (81%)	19 (19%)	1	5
39	j	224/274 (82%)	189 (84%)	35 (16%)	2	10
40	k	332/449 (74%)	318 (96%)	14 (4%)	30	60
41	l	119/246 (48%)	115 (97%)	4 (3%)	37	67
42	m	125/352 (36%)	106 (85%)	19 (15%)	3	10
43	o	406/846 (48%)	379 (93%)	27 (7%)	16	43
44	p	544/693 (78%)	532 (98%)	12 (2%)	52	76
45	q	506/523 (97%)	485 (96%)	21 (4%)	30	60
46	r	40/232 (17%)	39 (98%)	1 (2%)	47	74
47	s	287/301 (95%)	281 (98%)	6 (2%)	53	77
All	All	6821/8542 (80%)	6135 (90%)	686 (10%)	11	25

5 of 686 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	c	38	ARG
39	j	195	TYR
33	d	49	ASP
32	c	26	THR
36	g	250	LEU

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

Mol	Chain	Res	Type
28	Y	29	HIS
38	i	5	ASN
47	s	145	HIS
30	a	80	HIS
34	e	46	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	72/76 (94%)	29 (40%)	8 (11%)
2	2	1775/1798 (98%)	654 (36%)	72 (4%)
3	3	27/49 (55%)	16 (59%)	4 (14%)
All	All	1874/1923 (97%)	699 (37%)	84 (4%)

5 of 699 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	4	G
1	1	5	C
1	1	8	U
1	1	9	1MG
1	1	10	2MG

5 of 84 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	1320	A
2	2	1599	G
2	2	1343	A
2	2	1513	A

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Mol	Chain	Res	Type
2	2	1678	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	7MG	1	46	1	22,26,27	1.44	4 (18%)	29,39,42	2.62	10 (34%)
5	AYA	B	2	-	6,7,8	0.65	0	5,8,10	0.72	0
2	5MC	2	1637	2	18,22,23	1.03	1 (5%)	26,32,35	1.36	6 (23%)
1	1MG	1	9	1	18,26,27	1.02	0	19,39,42	1.58	4 (21%)
2	PSU	2	120	2	18,21,22	1.40	2 (11%)	22,30,33	1.93	4 (18%)
1	M2G	1	26	1	20,27,28	1.74	3 (15%)	22,40,43	1.34	4 (18%)
2	5MC	2	1006	2	18,22,23	0.96	1 (5%)	26,32,35	1.66	6 (23%)
1	H2U	1	47	1	18,21,22	0.85	0	21,30,33	1.38	3 (14%)
2	MA6	2	1780	2	19,26,27	1.11	2 (10%)	18,38,41	1.77	4 (22%)
1	2MG	1	10	1	18,26,27	0.98	1 (5%)	16,38,41	1.08	2 (12%)
1	5MC	1	48	1	18,22,23	1.03	1 (5%)	26,32,35	1.26	3 (11%)
2	PSU	2	766	2	18,21,22	1.37	2 (11%)	22,30,33	2.12	5 (22%)
1	H2U	1	16	1	18,21,22	0.83	0	21,30,33	1.67	4 (19%)
2	2MG	2	1570	2	18,26,27	0.94	0	16,38,41	1.42	3 (18%)
2	PSU	2	465	2	18,21,22	1.51	3 (16%)	22,30,33	1.89	5 (22%)
1	RIA	1	64	1	31,38,39	0.51	0	39,57,60	0.71	1 (2%)
2	7MG	2	1573	1,2	22,26,27	1.55	7 (31%)	29,39,42	2.63	6 (20%)
2	2MG	2	1426	2,48	18,26,27	0.95	0	16,38,41	1.40	4 (25%)
2	PSU	2	1289	2	18,21,22	1.48	3 (16%)	22,30,33	1.89	3 (13%)
2	PSU	2	998	2	18,21,22	1.41	3 (16%)	22,30,33	1.92	4 (18%)
1	5MC	1	49	1	18,22,23	1.10	1 (5%)	26,32,35	1.34	4 (15%)
1	1MA	1	58	1	16,25,26	1.86	4 (25%)	18,37,40	1.48	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	T6A	1	37	1	27,34,35	1.04	2 (7%)	29,49,52	2.71	10 (34%)
2	C4J	2	1190	2	24,29,30	0.52	0	29,42,45	1.00	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	7MG	1	46	1	-	1/7/37/38	0/3/3/3
5	AYA	B	2	-	-	0/4/6/8	-
2	5MC	2	1637	2	-	1/7/25/26	0/2/2/2
1	1MG	1	9	1	-	3/3/25/26	0/3/3/3
2	PSU	2	120	2	-	0/7/25/26	0/2/2/2
1	M2G	1	26	1	-	2/7/29/30	0/3/3/3
2	5MC	2	1006	2	-	0/7/25/26	0/2/2/2
1	H2U	1	47	1	-	4/7/38/39	0/2/2/2
2	MA6	2	1780	2	-	5/7/29/30	0/3/3/3
1	2MG	1	10	1	-	2/5/27/28	0/3/3/3
1	5MC	1	48	1	-	3/7/25/26	0/2/2/2
2	PSU	2	766	2	-	1/7/25/26	0/2/2/2
1	H2U	1	16	1	-	2/7/38/39	0/2/2/2
2	2MG	2	1570	2	-	0/5/27/28	0/3/3/3
2	PSU	2	465	2	-	0/7/25/26	0/2/2/2
1	RIA	1	64	1	-	3/13/51/52	0/4/4/4
2	7MG	2	1573	1,2	-	2/7/37/38	0/3/3/3
2	2MG	2	1426	2,48	-	3/5/27/28	0/3/3/3
2	PSU	2	1289	2	-	0/7/25/26	0/2/2/2
2	PSU	2	998	2	-	0/7/25/26	0/2/2/2
1	5MC	1	49	1	-	2/7/25/26	0/2/2/2
1	1MA	1	58	1	-	0/3/25/26	0/3/3/3
1	T6A	1	37	1	-	5/19/41/42	0/3/3/3
2	C4J	2	1190	2	1/1/7/7	0/16/34/35	0/2/2/2

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	58	1MA	C2-N3	5.71	1.35	1.29
1	1	26	M2G	C2-N3	5.61	1.37	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	465	PSU	C6-C5	4.22	1.40	1.35
2	2	1289	PSU	C6-C5	4.21	1.40	1.35
2	2	120	PSU	C6-C5	3.89	1.39	1.35

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1573	7MG	N9-C4-N3	8.85	138.71	125.47
1	1	46	7MG	N9-C4-N3	8.73	138.53	125.47
1	1	37	T6A	C12-N11-C10	8.59	136.24	121.94
1	1	37	T6A	C2-N1-C6	7.43	122.96	116.59
2	2	1289	PSU	N1-C2-N3	6.10	122.04	115.13

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	2	1190	C4J	C4'

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	1780	MA6	O4'-C4'-C5'-O5'
2	2	1780	MA6	C5-C6-N6-C10
2	2	1780	MA6	N1-C6-N6-C10
1	1	9	1MG	O4'-C4'-C5'-O5'
1	1	9	1MG	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 124 ligands modelled in this entry, 122 are monoatomic - leaving 2 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
50	MET	k	601	-	6,7,8	0.47	0	2,7,9	0.12	0
51	GCP	k	603	-	27,34,34	1.91	7 (25%)	34,54,54	1.94	8 (23%)

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
50	MET	k	601	-	-	1/5/6/8	-
51	GCP	k	603	-	-	1/15/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	k	603	GCP	PG-O1G	5.35	1.61	1.50
51	k	603	GCP	C5-C6	4.61	1.49	1.41
51	k	603	GCP	PB-O3A	2.98	1.61	1.58
51	k	603	GCP	PG-O3G	-2.84	1.48	1.54
51	k	603	GCP	PG-O2G	2.83	1.61	1.54

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	k	603	GCP	C2-N3-C4	5.27	121.38	115.36
51	k	603	GCP	C2-N1-C6	4.05	122.36	115.93
51	k	603	GCP	C5-C6-N1	-3.83	118.19	123.43
51	k	603	GCP	C4-C5-C6	-3.77	117.20	120.80
51	k	603	GCP	N3-C2-N1	-3.51	122.55	127.22

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	k	601	MET	CA-CB-CG-SD

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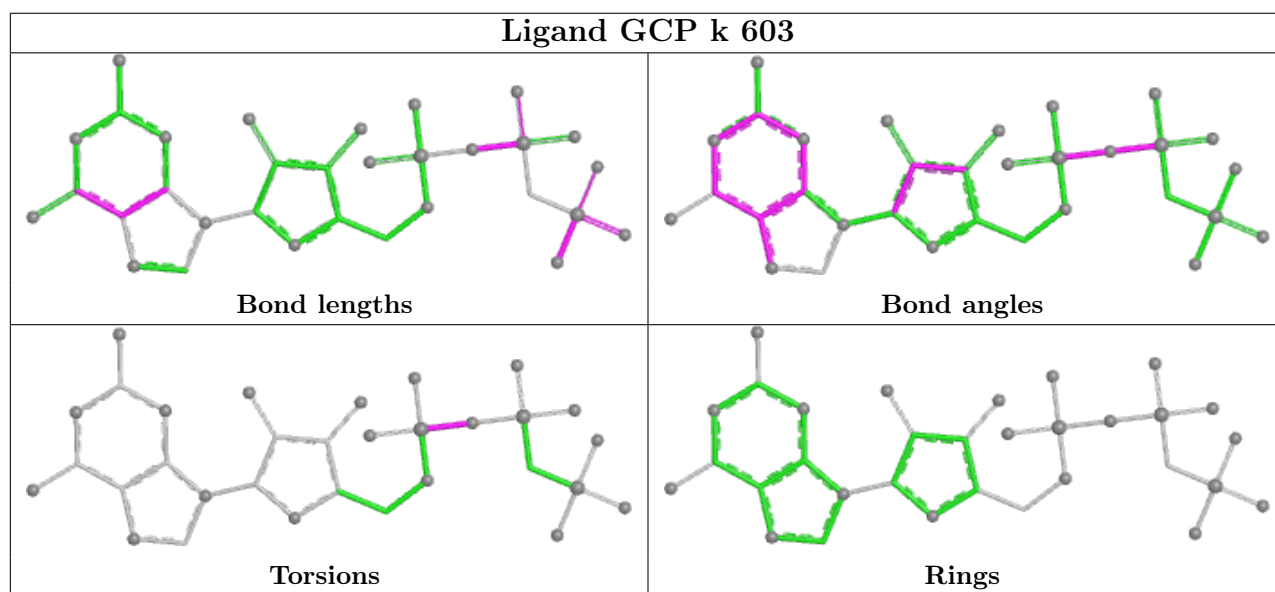
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Mol	Chain	Res	Type	Atoms
51	k	603	GCP	PB-O3A-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
45	q	8
2	2	1
1	1	1
44	p	1
5	B	1

The worst 5 of 12 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	q	214:UNK	C	251:GLN	N	50.55
1	q	158:UNK	C	166:UNK	N	17.71
1	q	181:UNK	C	190:UNK	N	14.31
1	q	135:UNK	C	139:UNK	N	7.79
1	q	203:UNK	C	207:UNK	N	6.84

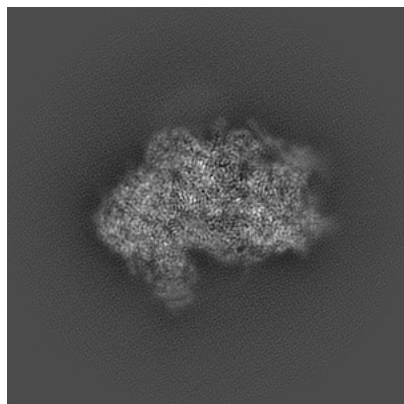
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4328. These allow visual inspection of the internal detail of the map and identification of artifacts.

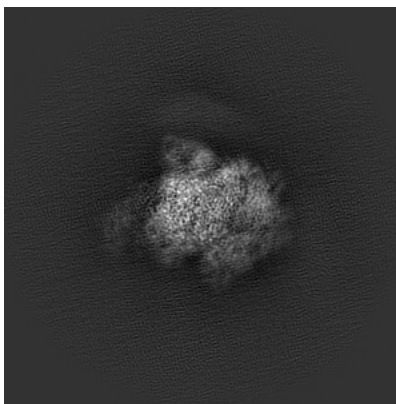
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

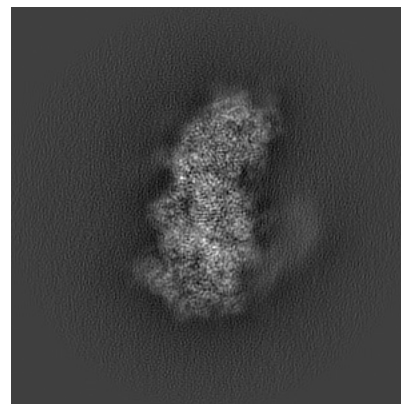
6.1.1 Primary map



X

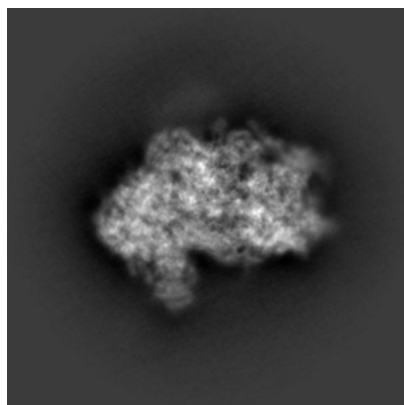


Y

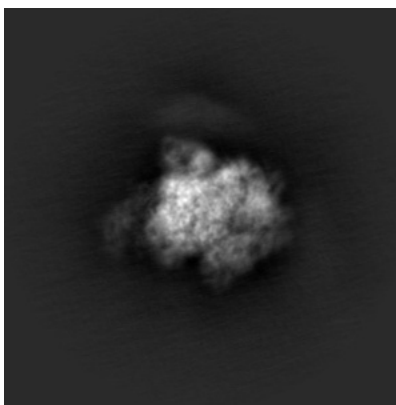


Z

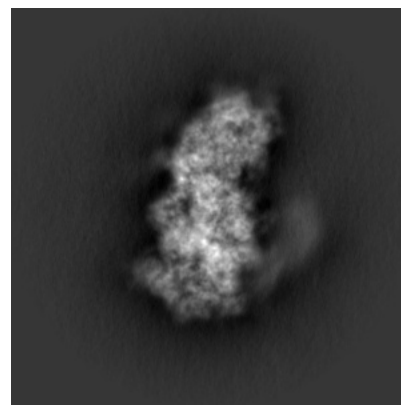
6.1.2 Raw map



X



Y

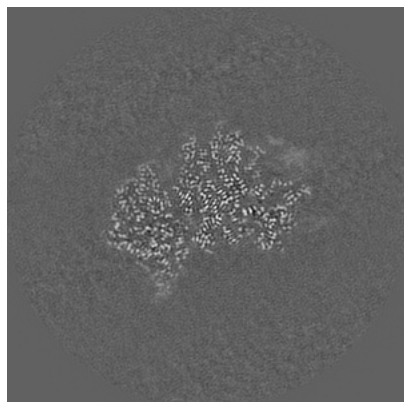


Z

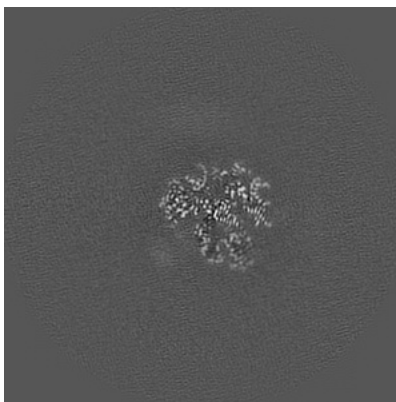
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

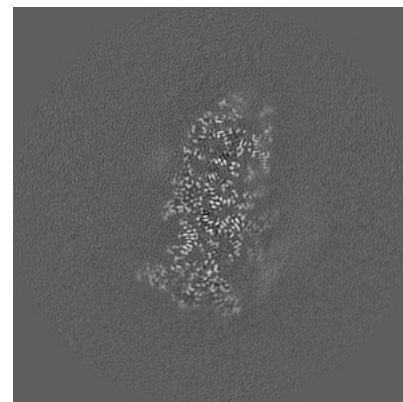
6.2.1 Primary map



X Index: 150

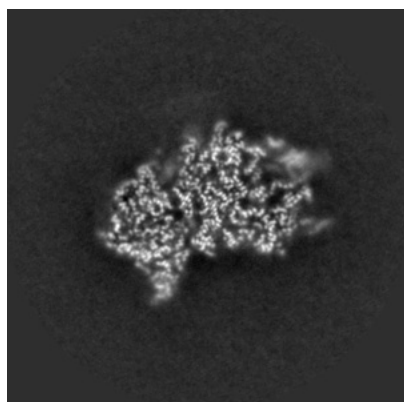


Y Index: 150

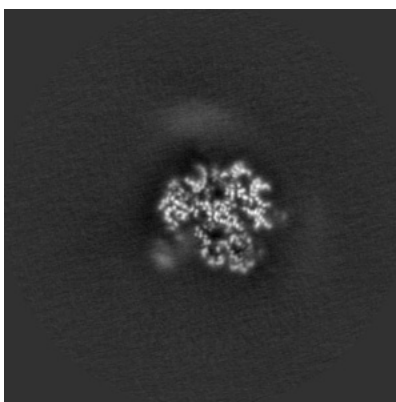


Z Index: 150

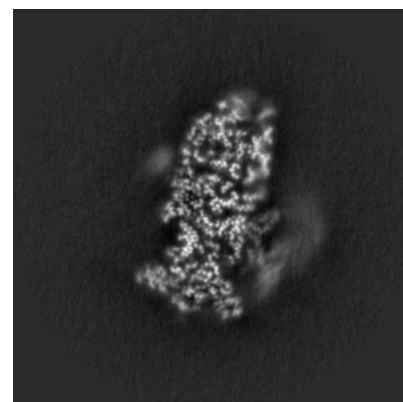
6.2.2 Raw map



X Index: 150



Y Index: 150

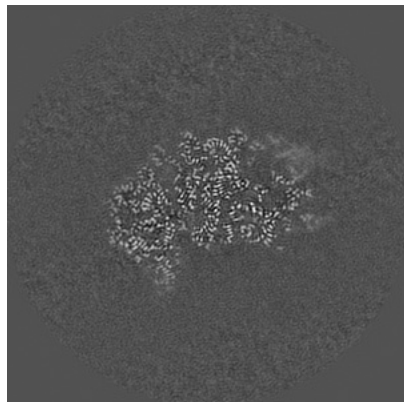


Z Index: 150

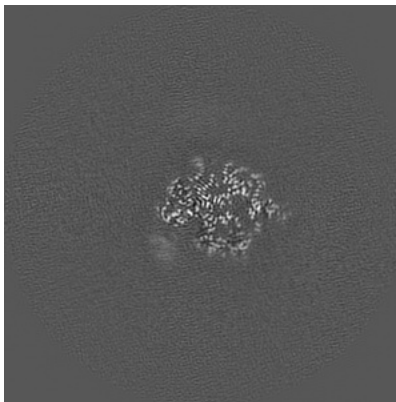
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

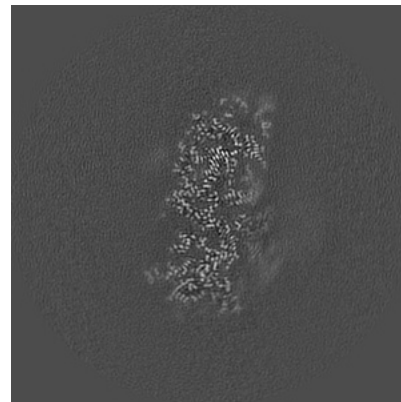
6.3.1 Primary map



X Index: 152

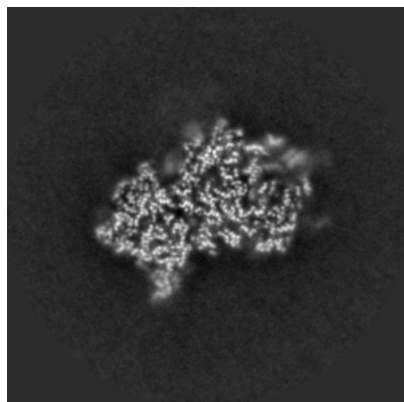


Y Index: 155

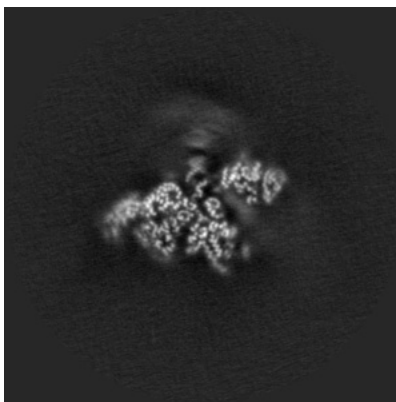


Z Index: 147

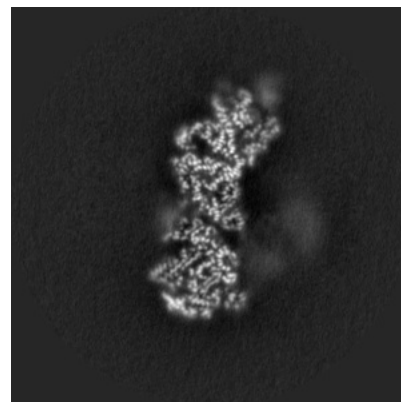
6.3.2 Raw map



X Index: 148



Y Index: 119

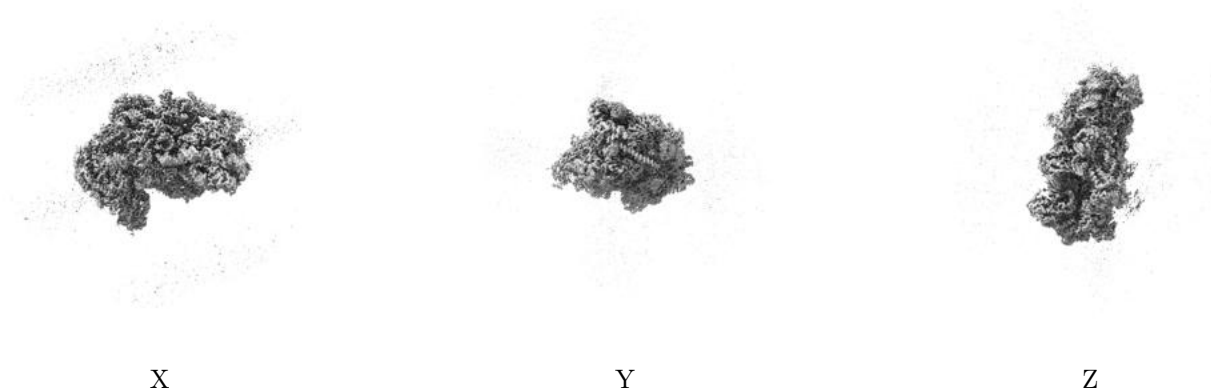


Z Index: 132

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

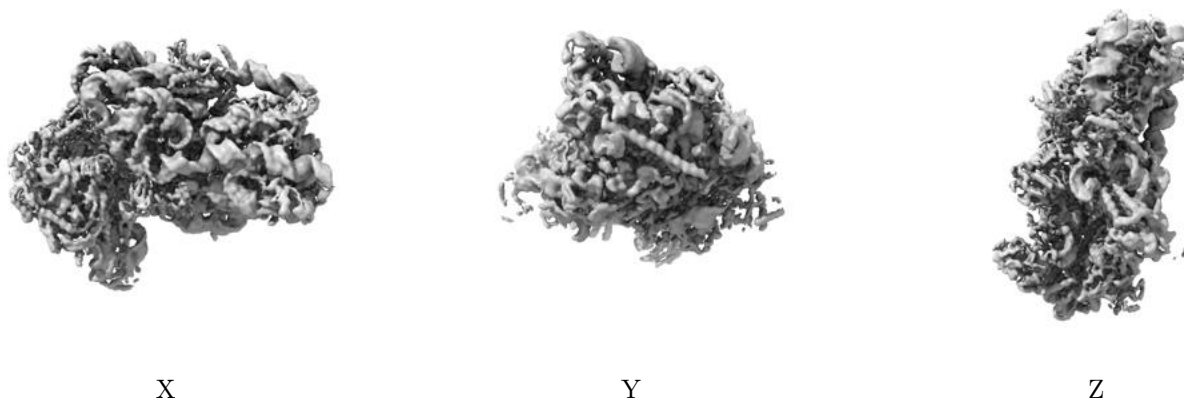
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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.

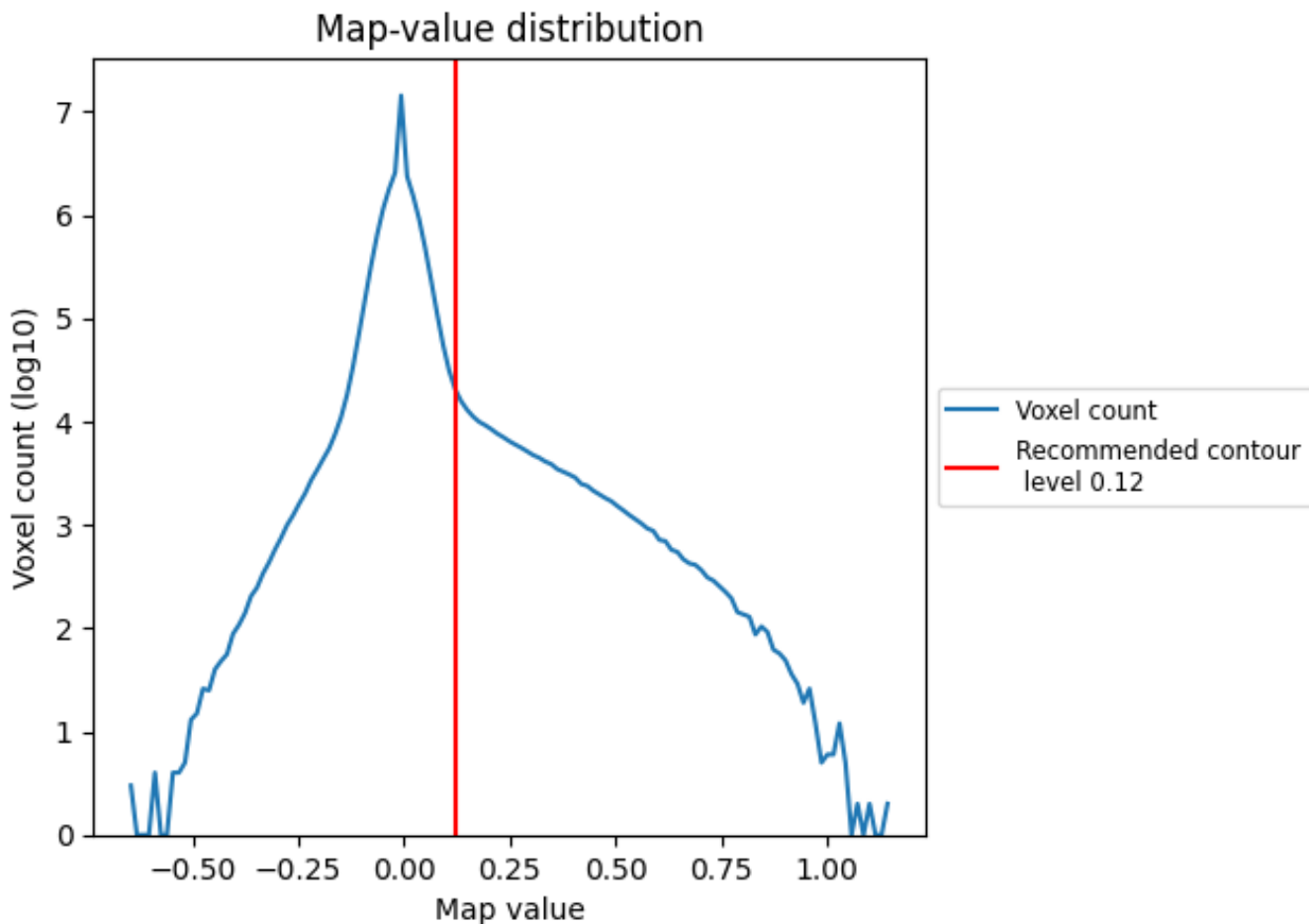
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

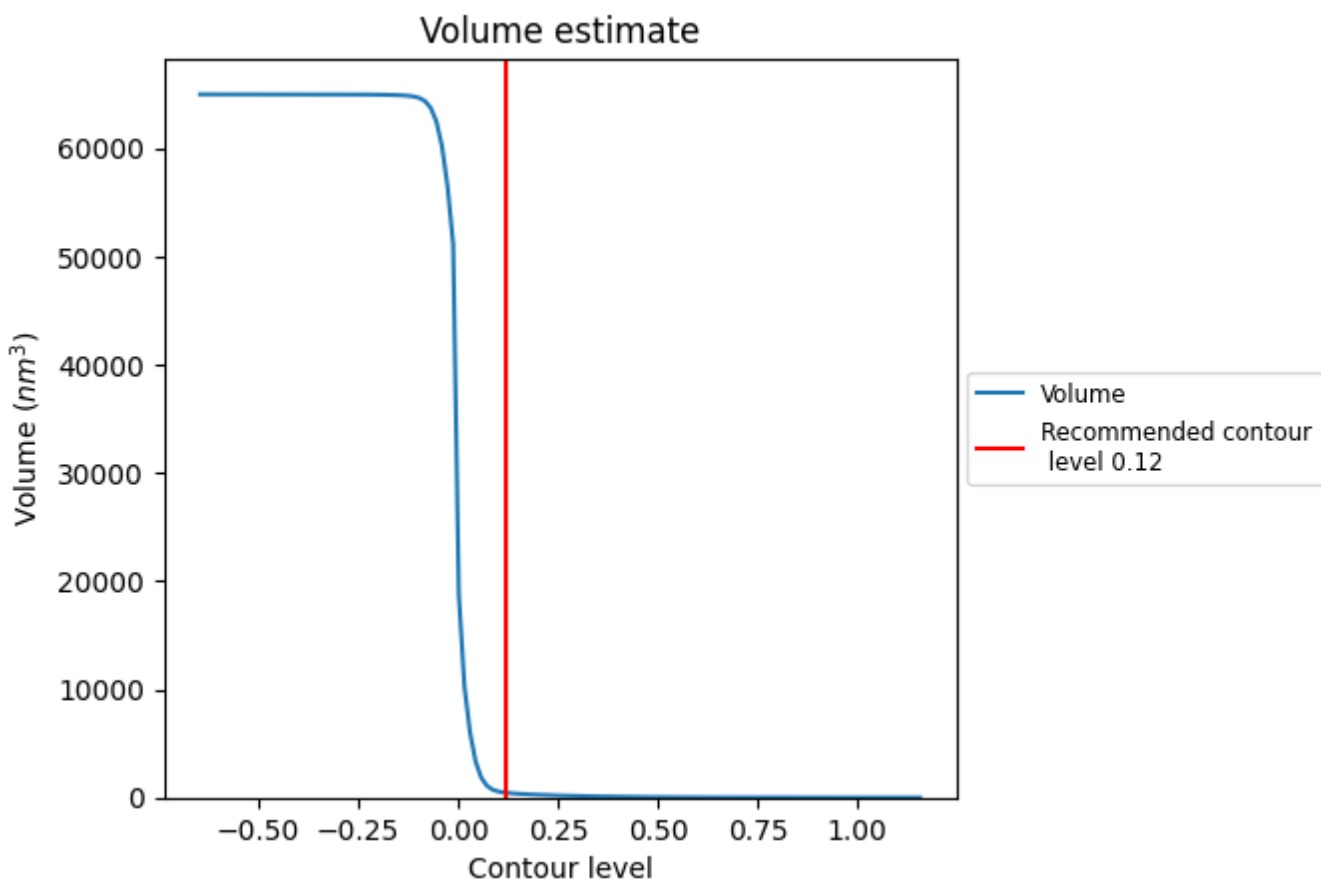
This section contains the results of statistical analysis of the map.

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.

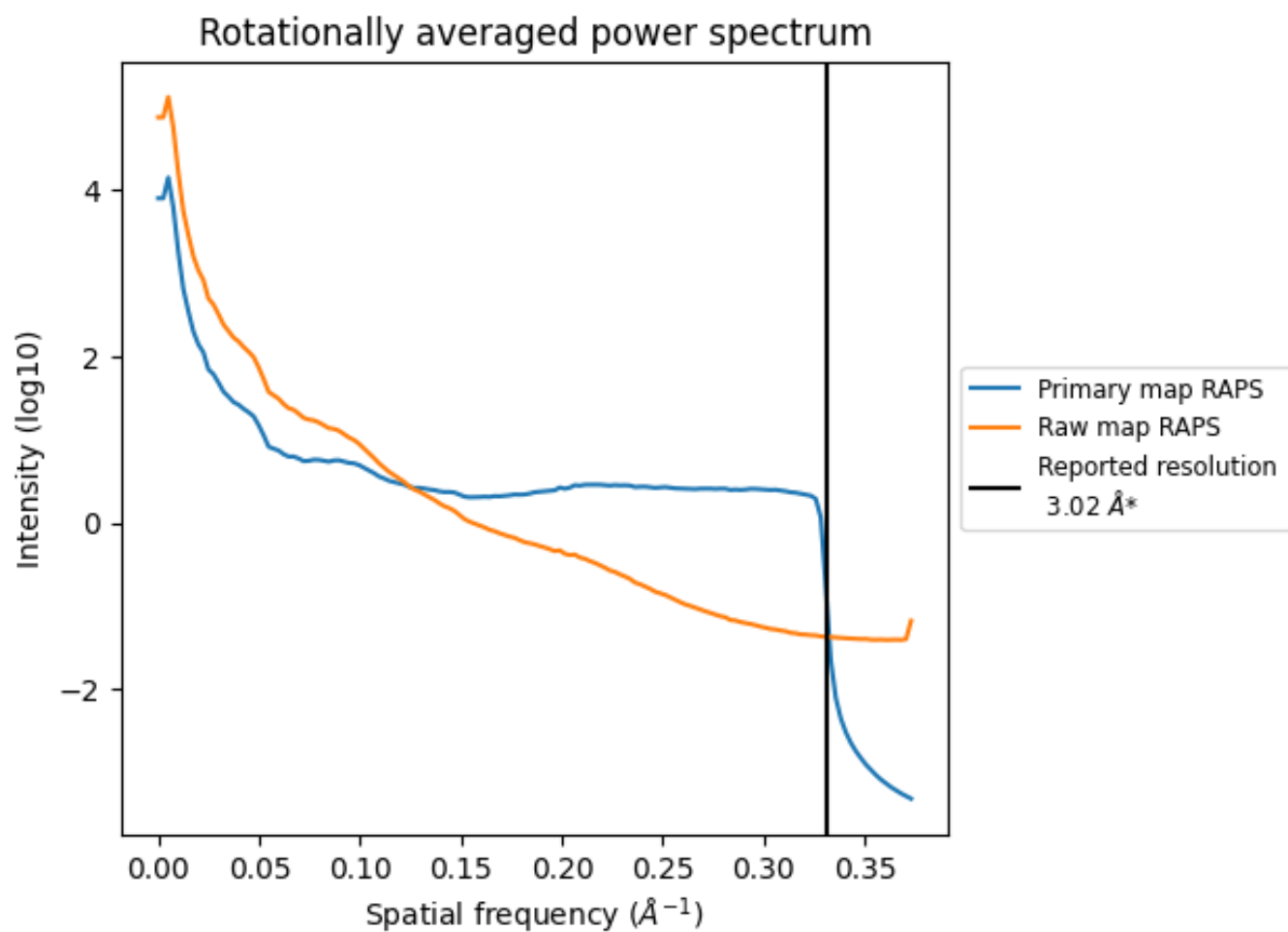
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 447 nm^3 ; this corresponds to an approximate mass of 404 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

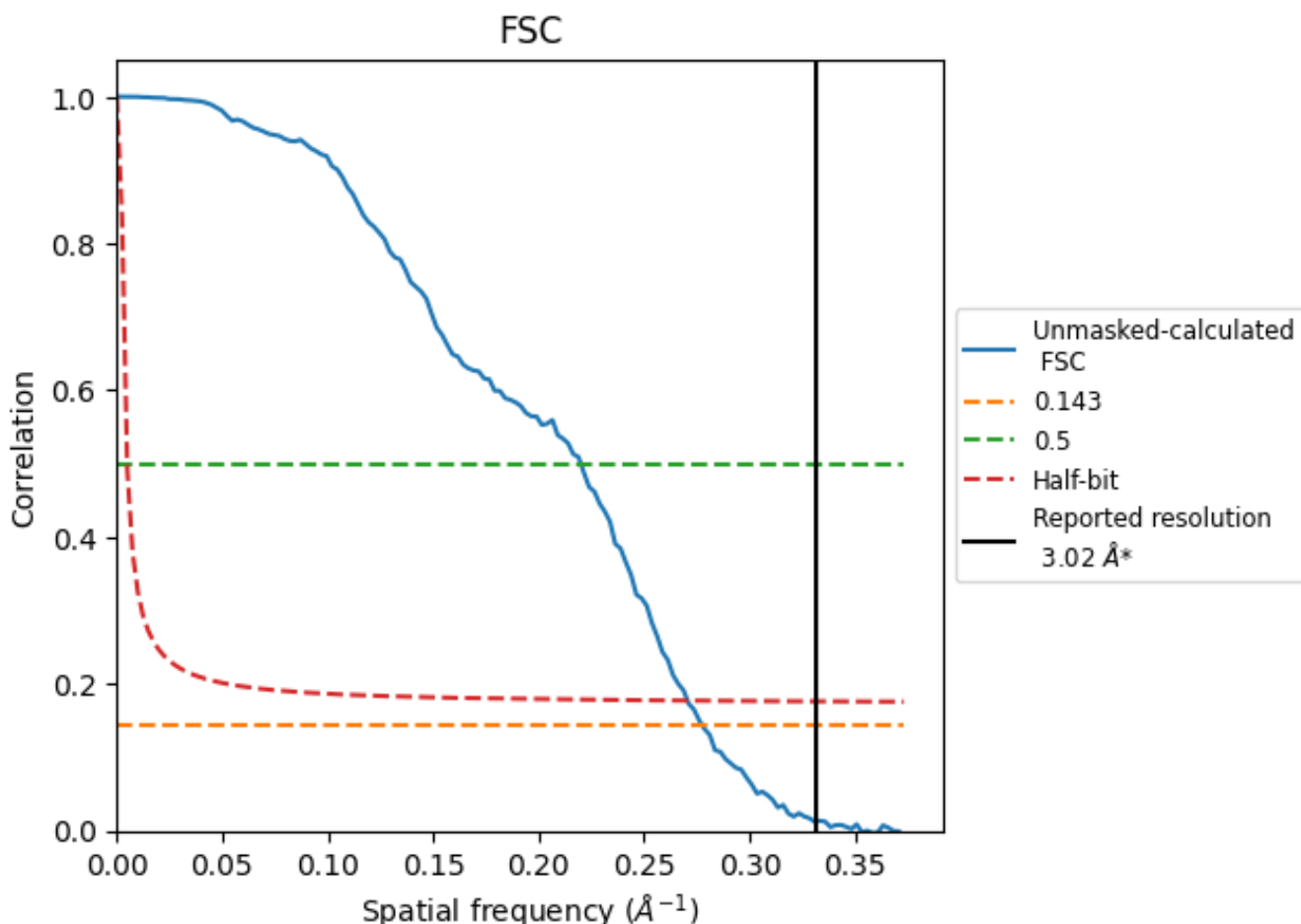


*Reported resolution corresponds to spatial frequency of 0.331 Å⁻¹

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 0.331 \AA^{-1}

8.2 Resolution estimates [i](#)

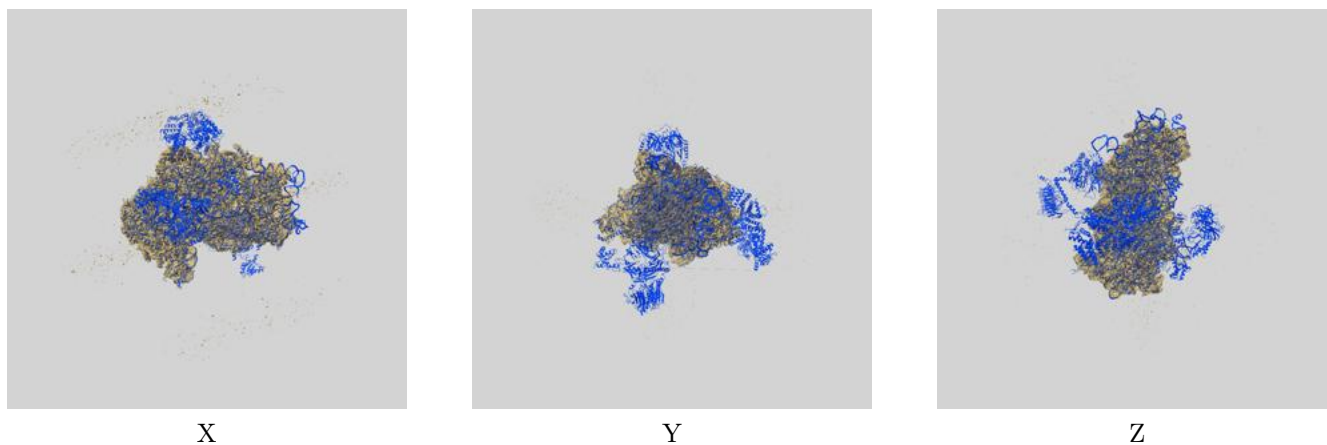
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.60	4.55	3.70

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.60 differs from the reported value 3.02 by more than 10 %

9 Map-model fit [i](#)

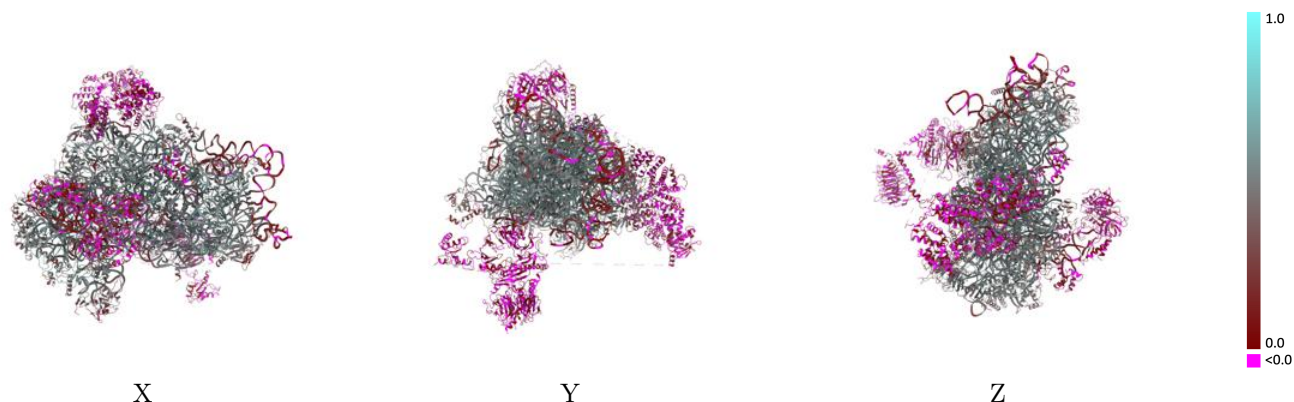
This section contains information regarding the fit between EMDB map EMD-4328 and PDB model 6FYY. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



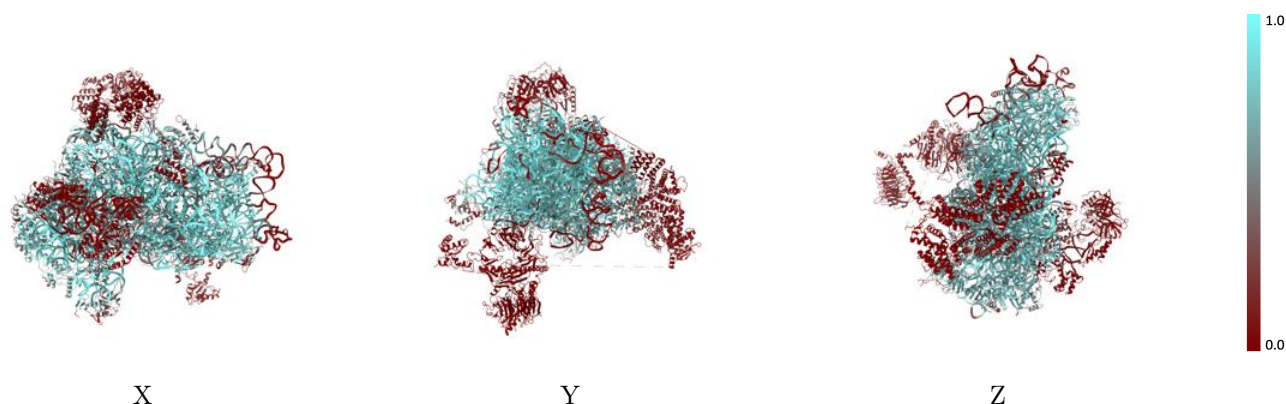
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



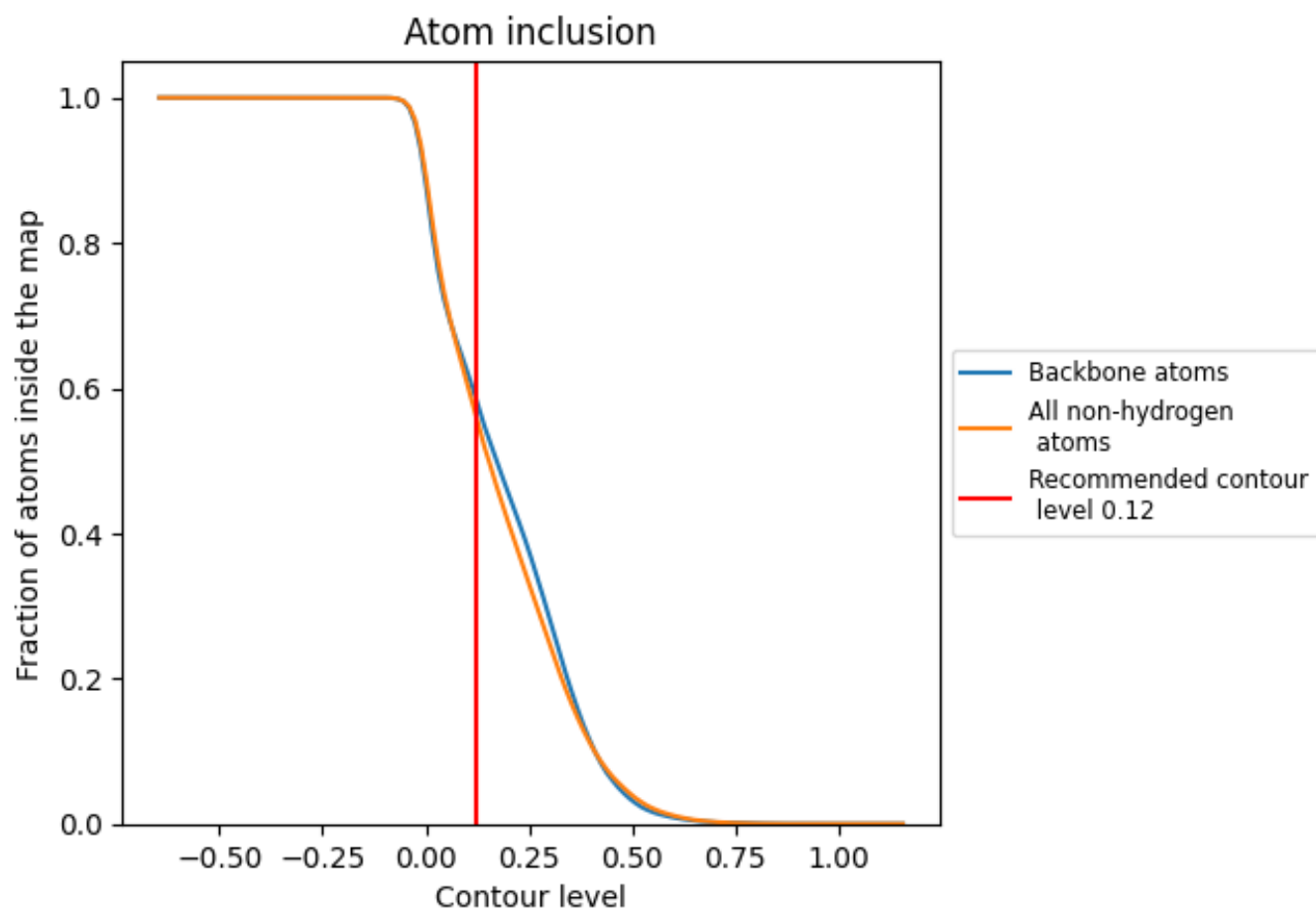
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 57% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5662	 0.3780
1	 0.3118	 0.2600
2	 0.8103	 0.4820
3	 0.2567	 0.2510
A	 0.7071	 0.4840
B	 0.6635	 0.4590
C	 0.7642	 0.5220
D	 0.6755	 0.4700
E	 0.7961	 0.5310
F	 0.6622	 0.4770
G	 0.6329	 0.4360
H	 0.5626	 0.4250
I	 0.7197	 0.4870
J	 0.7648	 0.5110
K	 0.6910	 0.4620
L	 0.6963	 0.4930
M	 0.2854	 0.2570
N	 0.7519	 0.5110
O	 0.7403	 0.5100
P	 0.7044	 0.4800
Q	 0.7481	 0.5120
R	 0.6328	 0.4600
S	 0.6997	 0.4680
T	 0.7694	 0.5010
U	 0.5916	 0.4170
V	 0.7361	 0.5000
W	 0.8000	 0.5420
X	 0.8049	 0.5470
Y	 0.7549	 0.5010
Z	 0.4991	 0.3820
a	 0.7568	 0.5150
b	 0.6894	 0.4940
c	 0.6618	 0.4980
d	 0.8575	 0.5620
e	 0.6790	 0.4730



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Chain	Atom inclusion	Q-score
f	 0.4188	 0.3750
g	 0.6164	 0.4590
h	 0.4717	 0.4180
i	 0.6143	 0.4750
j	 0.0031	 0.1410
k	 0.0007	 0.0430
l	 0.0010	 0.0530
m	 0.2219	 0.3860
o	 0.0003	 0.0240
p	 0.0000	 0.0450
q	 0.0008	 0.0430
r	 0.0000	 0.0090
s	 0.0004	 0.0250