wwPDB EM Validation Summary Report

Oct 28, 2026 – 05:33 pm GMT

PDB ID	:	9SJ3 / pdb_00009sj3
EMDB ID	:	EMD-54936
Title	:	Structure of a circMbl 48S translation initiation complex in the AUG recognition state
Authors	:	Zuber, P.K.; Li, X.; Du, Y.; Gordiyenko, Y.; Haddad, T.F.M.; Ramakrishnan, V.
Deposited on	:	2025-08-29
Resolution	:	4.00 Å(reported)
Based on initial models	:	1YFG, 6ZMW

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

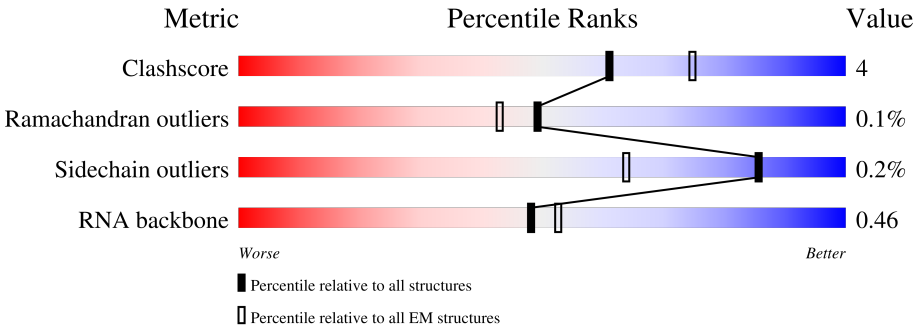
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

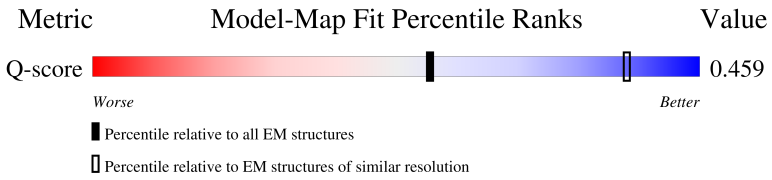
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	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	7587 (3.50 - 4.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1382	39% 45% 8% 47%
2	B	445	84% 76% 10% 14%
3	D	315	44% 77% 11% 12%

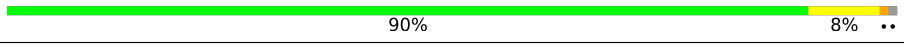
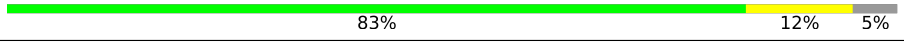
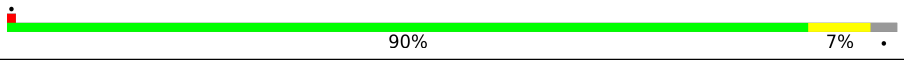
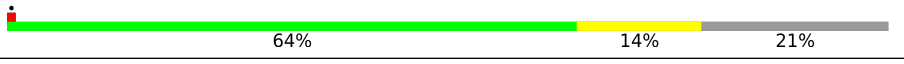
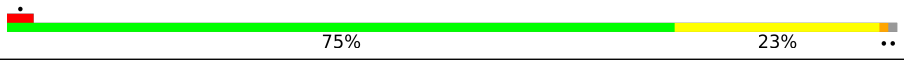
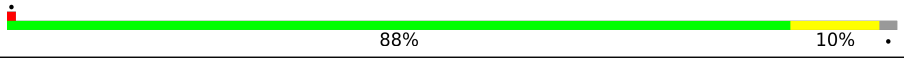
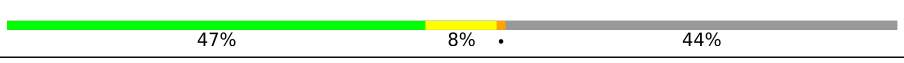
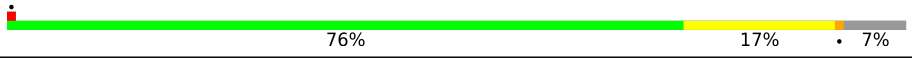
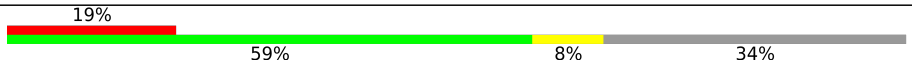
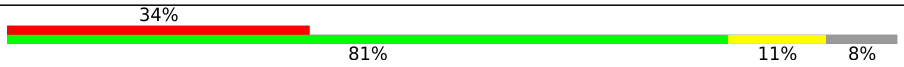
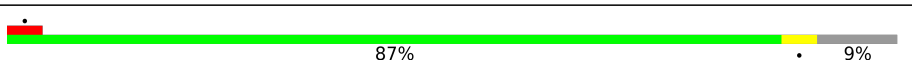
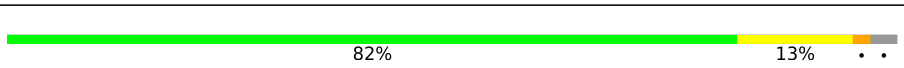
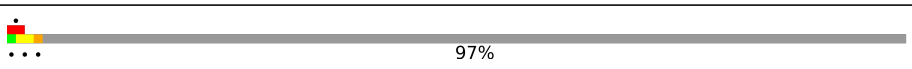
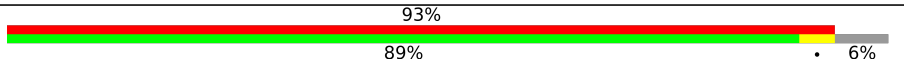
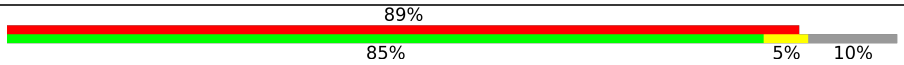
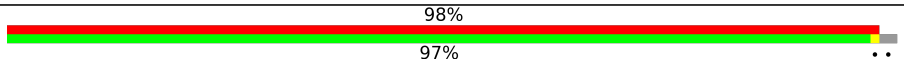
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Mol	Chain	Length	Quality of chain
4	E	472	98% 85% 13%
5	F	325	100% 97%
6	G	147	26% 56% 10% 34%
7	H	116	67% 60% 13% 27%
8	I	814	71% 63% 8% 29%
9	J	913	45% 60% 10% 29%
10	L	194	76% 15% 8%
11	M	84	74% 21%
12	N	83	90% 7%
13	O	293	68% 7% 25%
14	P	264	67% 12% 20%
15	Q	295	62% 11% 28%
16	R	115	80% 6% 14%
17	S	249	79% 14% 8%
18	T	151	75% 13% 12%
19	V	151	95% 5%
20	W	1869	59% 26% 5% 8%
21	X	158	81% 9% 10%
22	Y	263	90% 7%
23	Z	194	82% 9% 9%
24	y	75	24% 55% 32% 11%
25	7	320	22% 21% 76%
26	9	25	8% 80% 16%
27	a	143	90% 8%
28	b	59	14% 90% 7%

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Mol	Chain	Length	Quality of chain
29	c	130	
30	d	208	
31	e	133	
32	f	204	
33	g	146	
34	h	243	
35	i	165	
36	j	145	
37	k	317	
38	l	145	
39	m	125	
40	n	152	
41	o	56	
42	p	80	
43	q	132	
44	s	69	
45	v	135	
46	w	119	
47	z	774	
48	x	548	
49	6	374	
50	4	357	
51	8	352	
52	3	218	
53	5	564	

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 114857 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	733	5504	3452	1005	1024	23	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	384	2635	1657	477	489	12	0	0

- Molecule 3 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	278	2234	1410	390	421	13	0	0

- Molecule 4 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	464	3540	2245	620	658	17	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	F	325	1598	947	325	326	0	0

- Molecule 6 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	97	789	492	147	146	4	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	GLY	-	expression tag	UNP P47813
G	-1	ALA	-	expression tag	UNP P47813
G	0	HIS	-	expression tag	UNP P47813

- Molecule 7 is a protein called Eukaryotic translation initiation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	85	Total	C	N	O	S	0	0
			691	438	125	126	2		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	GLY	-	expression tag	UNP P41567
H	-1	ALA	-	expression tag	UNP P41567
H	0	HIS	-	expression tag	UNP P41567

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	575	Total	C	N	O	S	0	0
			4569	2935	788	828	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	645	Total	C	N	O	S	0	0
			4940	3096	888	923	33		

- Molecule 10 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	178	Total	C	N	O	S	0	0
			1439	923	262	253	1		

- Molecule 11 is a protein called 40S ribosomal protein S27.

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

- Molecule 12 is a protein called 40S ribosomal protein S21.

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

- Molecule 13 is a protein called 40S ribosomal protein S2.

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

- Molecule 14 is a protein called 40S ribosomal protein S3a.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	213	Total	C	N	O	S	0	0
			1686	1072	295	311	8		

- Molecule 16 is a protein called 40S ribosomal protein S26.

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

- Molecule 17 is a protein called 40S ribosomal protein S6.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	133	Total	C	N	O	S	0	0
			998	610	196	186	6		

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

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

- Molecule 20 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	1717	Total	C	N	O	P	0	0
			36695	16405	6575	11998	1717		

- Molecule 21 is a protein called 40S ribosomal protein S11.

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

- Molecule 22 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	257	Total	C	N	O	S	0	0
			2041	1305	379	349	8		

- Molecule 23 is a protein called 40S ribosomal protein S9.

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

- Molecule 24 is a RNA chain called tRNAi-Met.

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

- Molecule 25 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	7	77	Total	C	N	O	0	0
			616	389	111	116		

- Molecule 26 is a protein called 60S ribosomal protein L41.

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

- Molecule 27 is a protein called 40S ribosomal protein S23.

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

- Molecule 28 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	57	Total	C	N	O	S	0	0
			452	279	99	73	1		

- Molecule 29 is a protein called 40S ribosomal protein S15a.

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

- Molecule 30 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	198	Total	C	N	O	S	0	0
			1628	1021	322	280	5		

- Molecule 31 is a protein called 40S ribosomal protein S24.

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

- Molecule 32 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	184	Total	C	N	O	S	0	0
			1461	914	276	264	7		

- Molecule 33 is a protein called 40S ribosomal protein S16.

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

- Molecule 34 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	225	Total	C	N	O	S	0	0
			1752	1117	315	313	7		

- Molecule 35 is a protein called 40S ribosomal protein S10.

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

- Molecule 36 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	114	Total	C	N	O	S	0	0
			946	602	175	162	7		

- Molecule 37 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 38 is a protein called 40S ribosomal protein S19.

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

- Molecule 39 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	70	Total	C	N	O	S	0	0
			559	360	102	96	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	142	Total	C	N	O	S	0	0
			1176	737	239	199	1		

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

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

- Molecule 42 is a protein called Ubiquitin-ribosomal protein eS31 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	p	53	Total	C	N	O	S	0	0
			435	276	82	70	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	q	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	s	63	Total	C	N	O	S	0	0
			498	302	101	93	2		

- Molecule 45 is a protein called 40S ribosomal protein S17.

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

- Molecule 46 is a protein called 40S ribosomal protein S20.

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

- Molecule 47 is a RNA chain called circMbl-FLAG.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	z	27	Total	C	N	O	P	0	0
			575	258	106	184	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	x	440	Total	C	N	O	S	0	0
			2920	1798	539	574	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	6	350	Total	C	N	O	S	0	0
			1917	1159	376	380	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
50	4	257	Total	C	N	O	0	0
			1272	757	257	258		

- Molecule 51 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	8	317	Total	C	N	O	0	0
			1571	936	317	318		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
52	3	213	Total	C	N	O	0	0
			1057	631	213	213		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
53	5	319	Total	C	N	O	0	0
			1581	943	319	319		

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
54	R	1	Total Zn 1 1	0
54	o	1	Total Zn 1 1	0
54	p	1	Total Zn 1 1	0

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
55	S	1	Total Mg 1 1	0
55	T	1	Total Mg 1 1	0
55	W	85	Total Mg 85 85	0
55	f	1	Total Mg 1 1	0

- Molecule 56 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
56	W	3	Total K 3 3	0

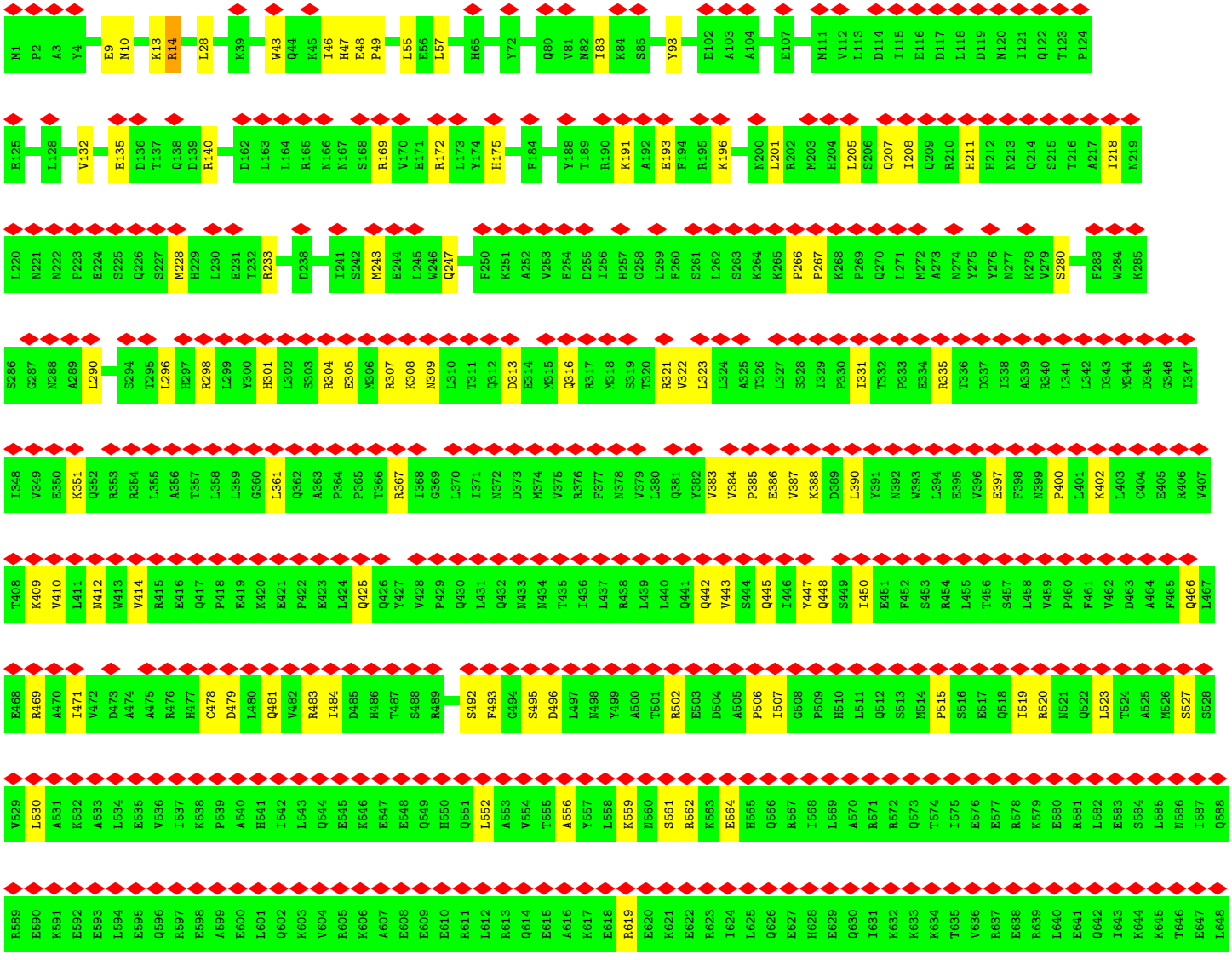
3 Residue-property plots (i)

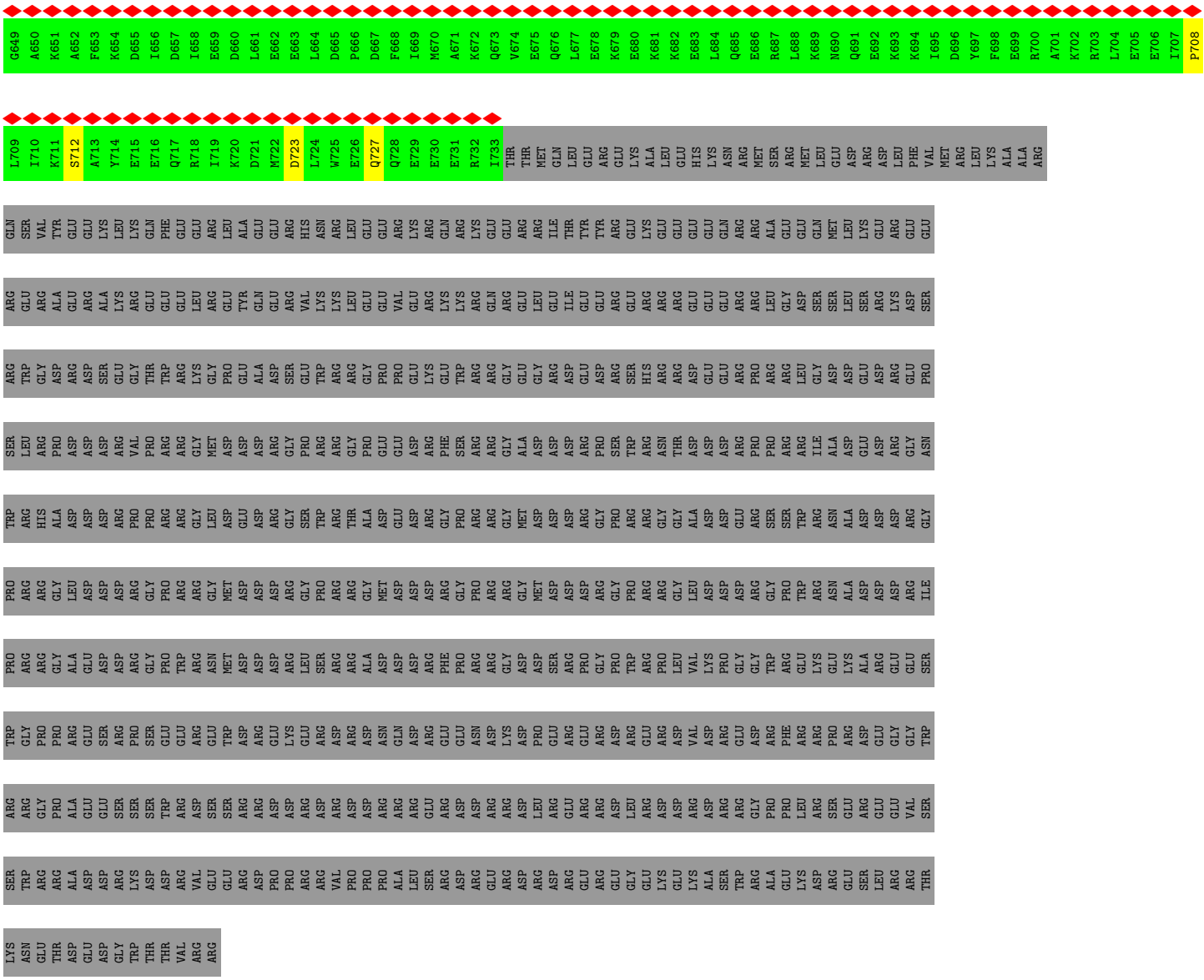
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Eukaryotic translation initiation factor 3 subunit A

Chain A:



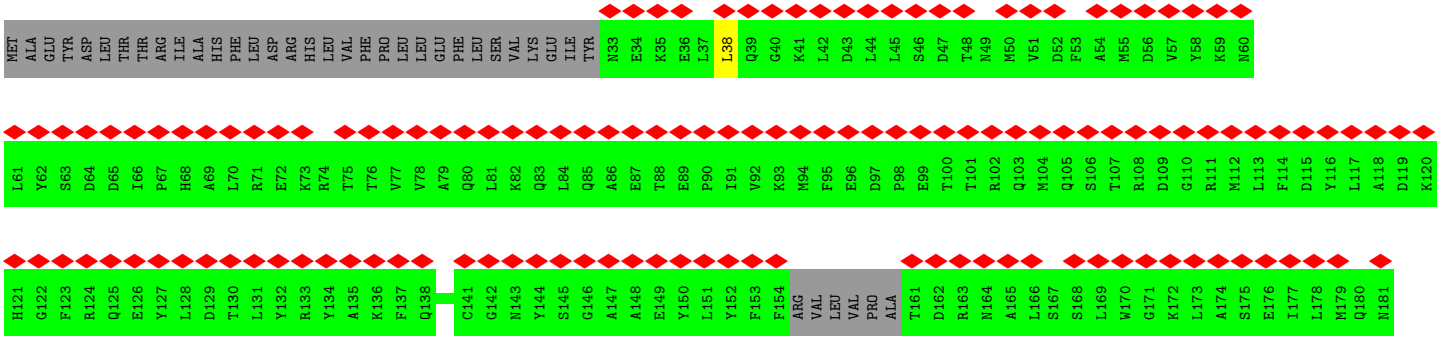


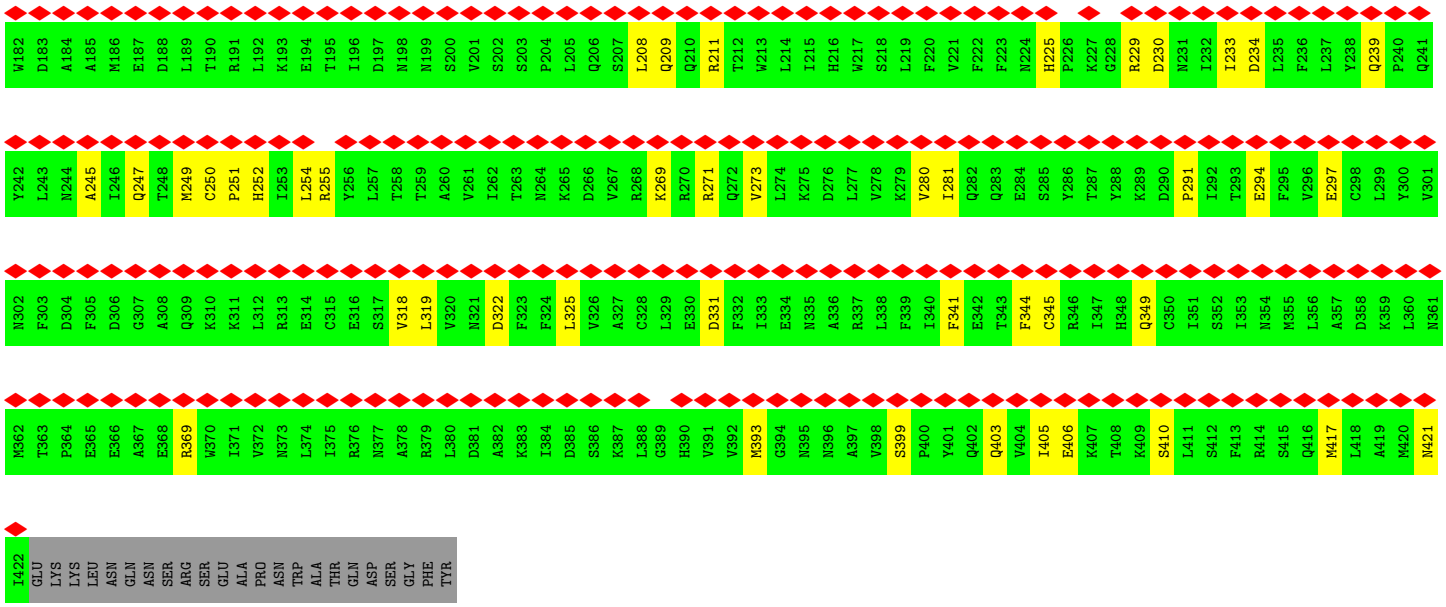


• Molecule 2: Eukaryotic translation initiation factor 3 subunit E

Chain B:



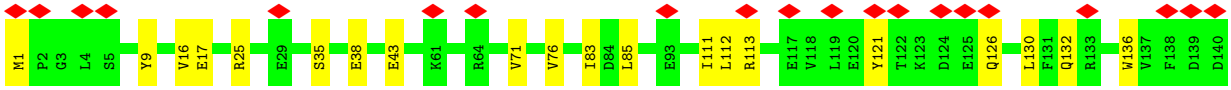




• Molecule 3: Eukaryotic translation initiation factor 2 subunit 1

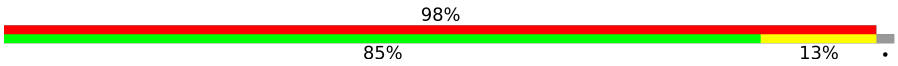
Chain D:

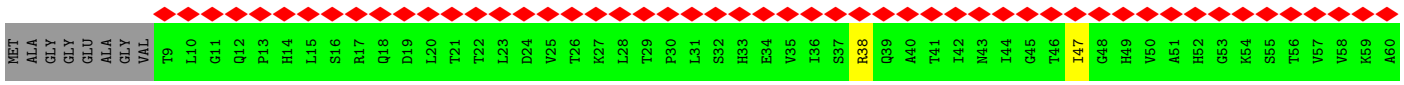


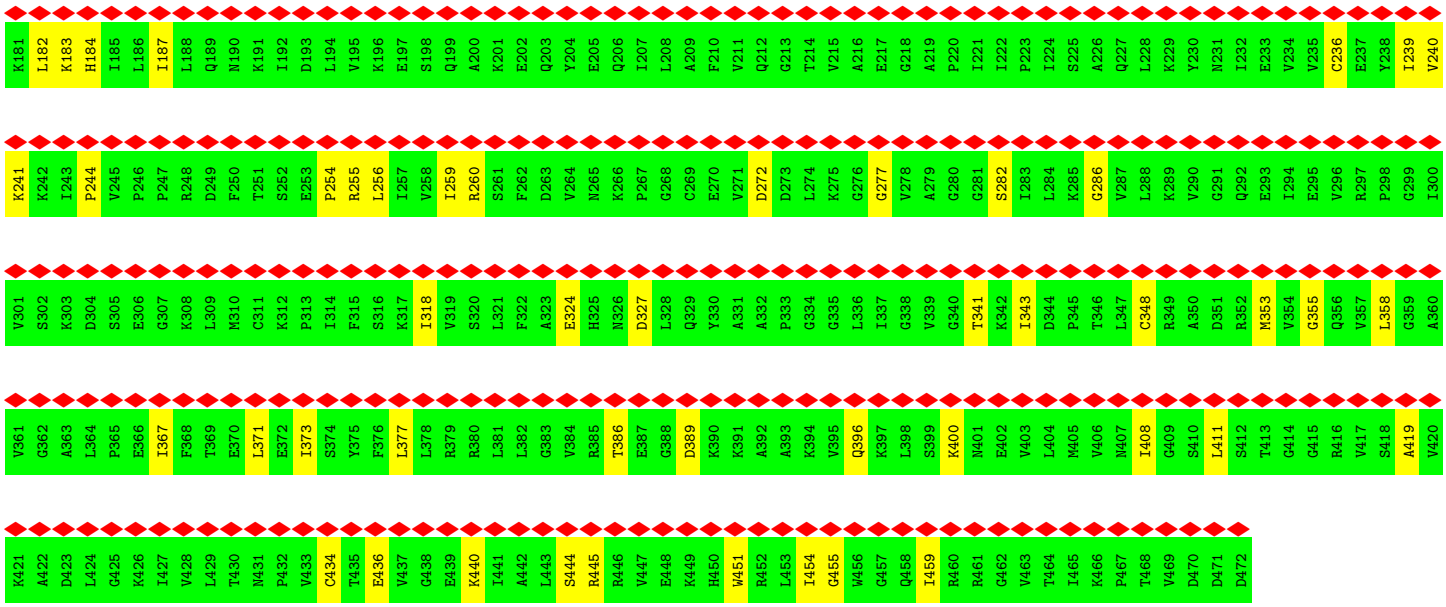


• Molecule 4: Eukaryotic translation initiation factor 2 subunit 3

Chain E:



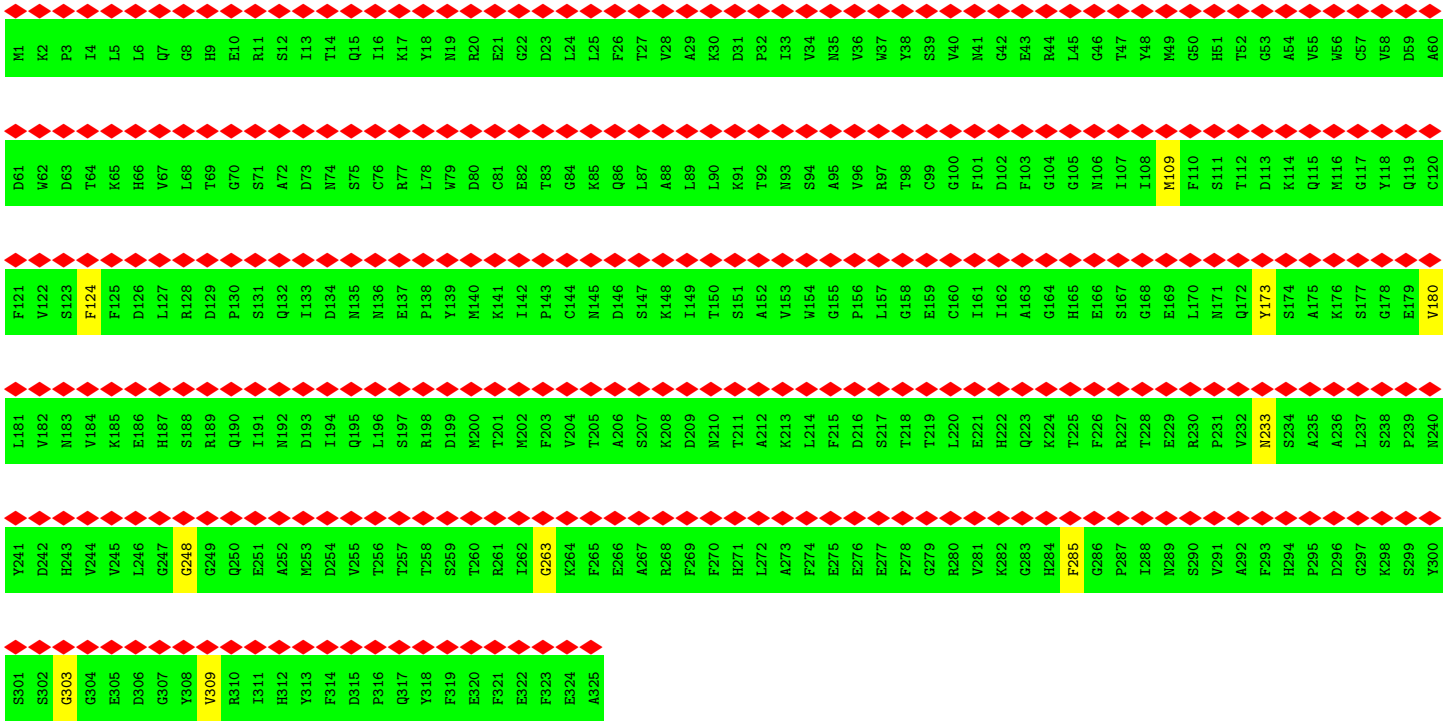




• Molecule 5: Eukaryotic translation initiation factor 3 subunit I

Chain F:

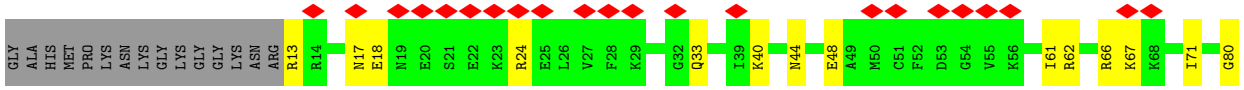


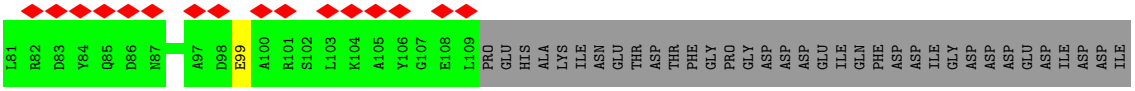


• Molecule 6: Eukaryotic translation initiation factor 1A, X-chromosomal

Chain G:



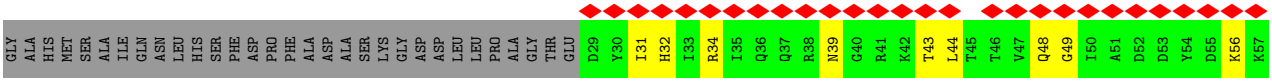


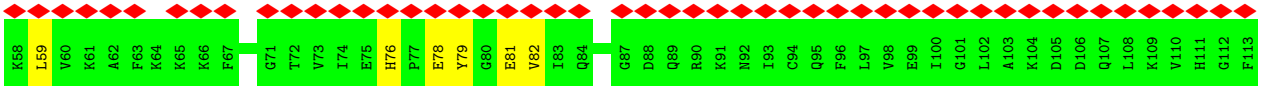


• Molecule 7: Eukaryotic translation initiation factor 1

Chain H:



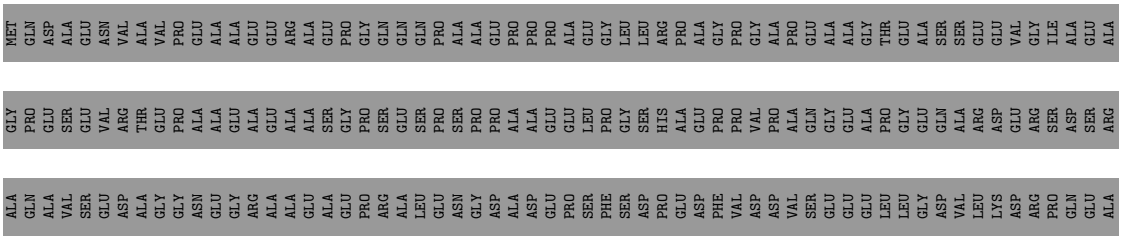


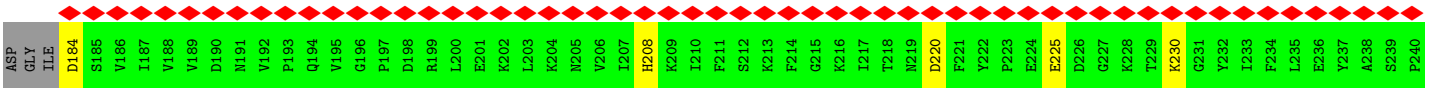


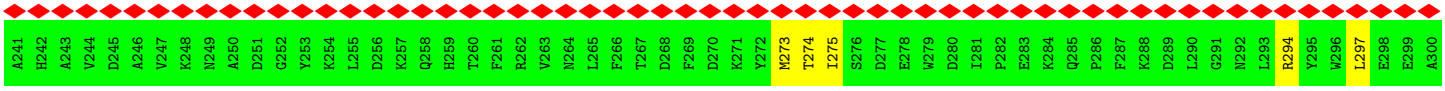
• Molecule 8: Eukaryotic translation initiation factor 3 subunit B

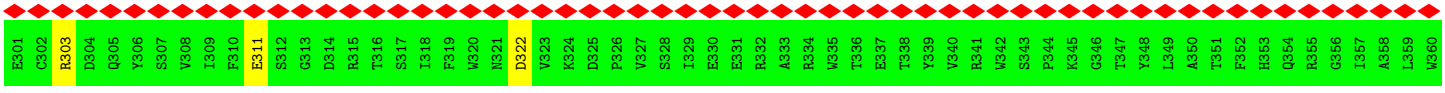
Chain I:

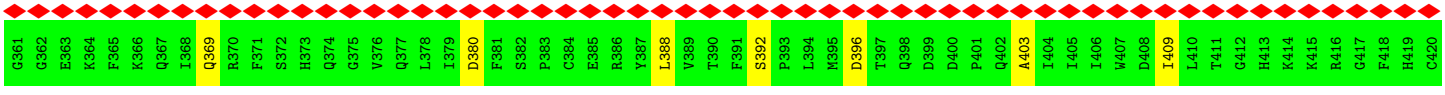






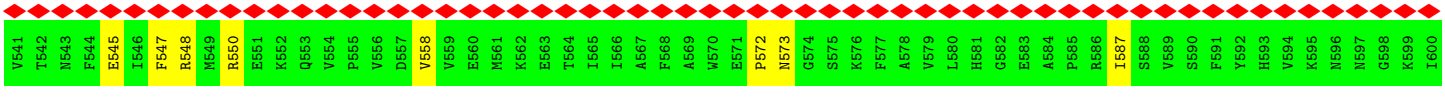


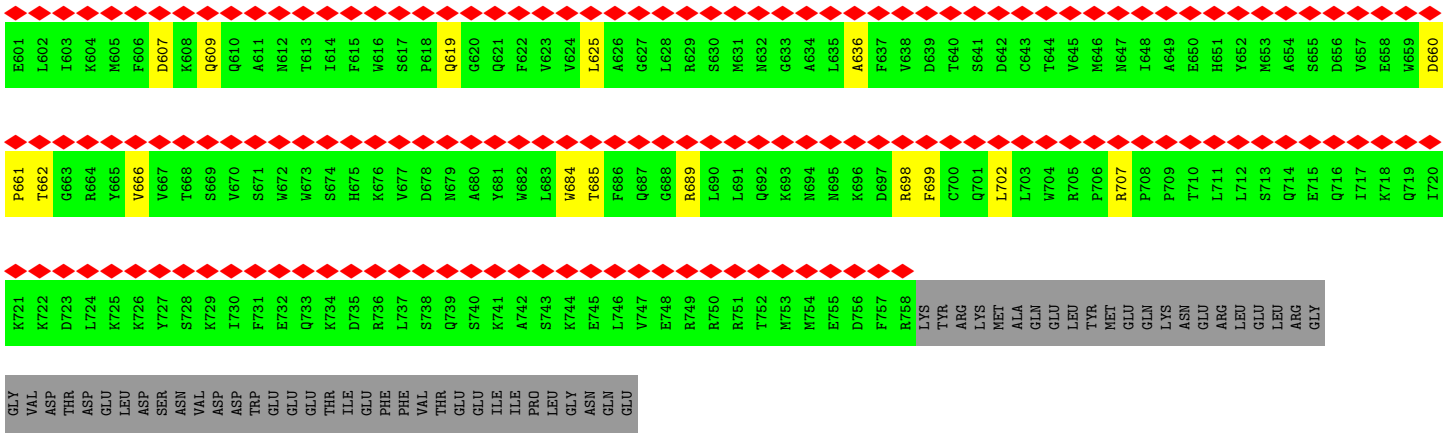








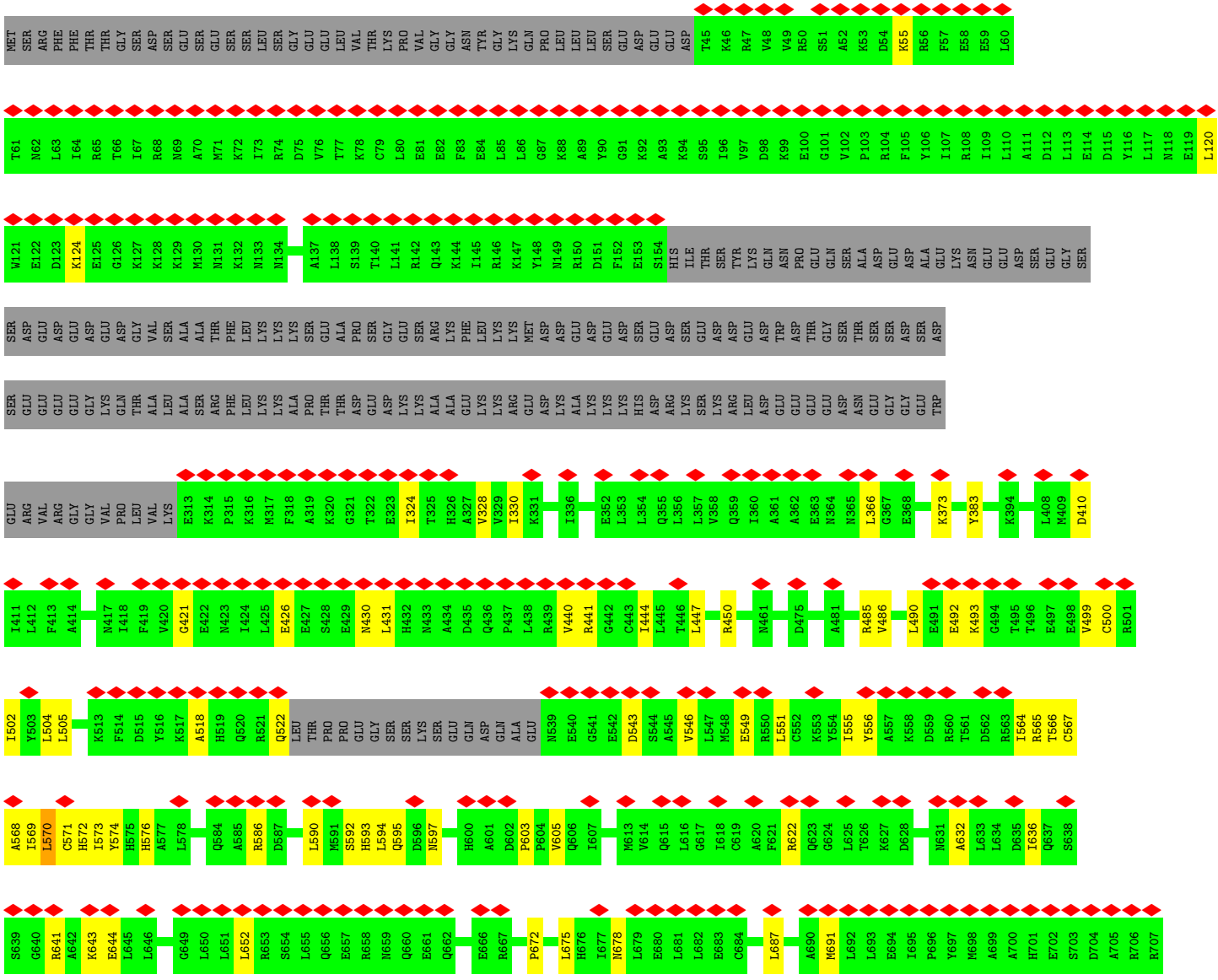


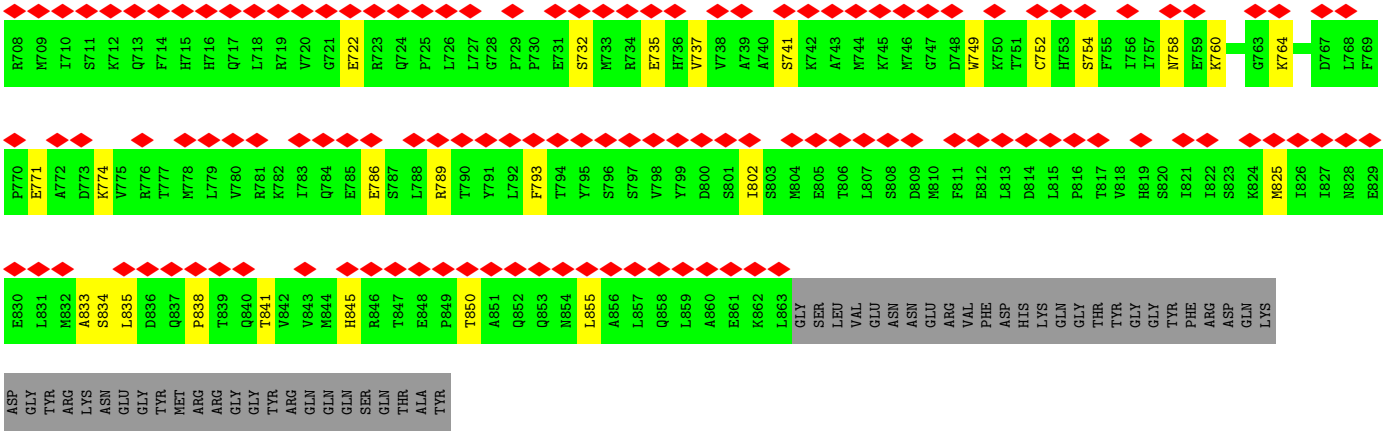


• Molecule 9: Eukaryotic translation initiation factor 3 subunit C

Chain J:



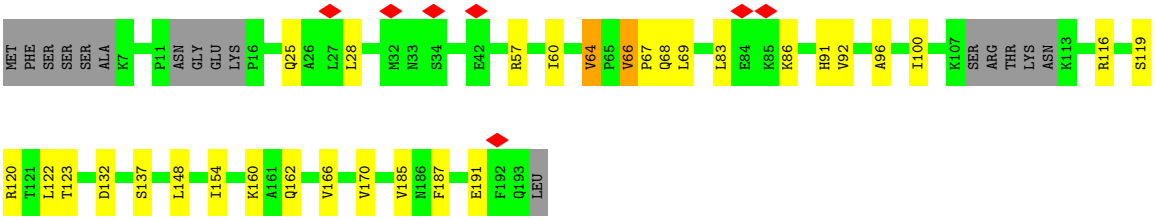




• Molecule 10: 40S ribosomal protein S7

Chain L:

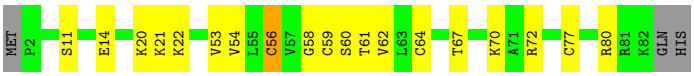




• Molecule 11: 40S ribosomal protein S27

Chain M:

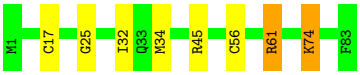




• Molecule 12: 40S ribosomal protein S21

Chain N:

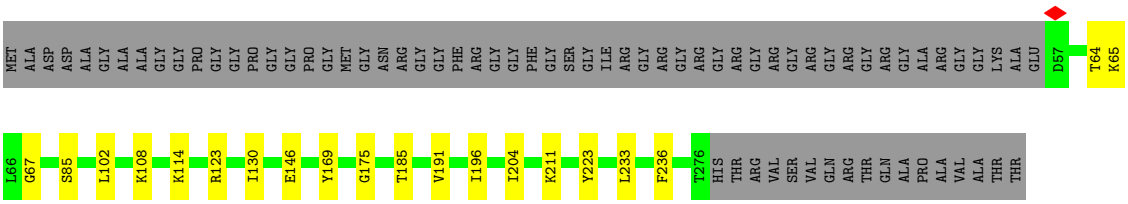




• Molecule 13: 40S ribosomal protein S2

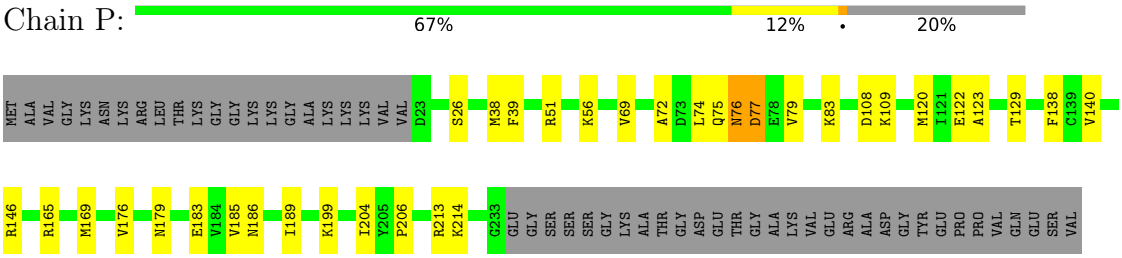
Chain O:





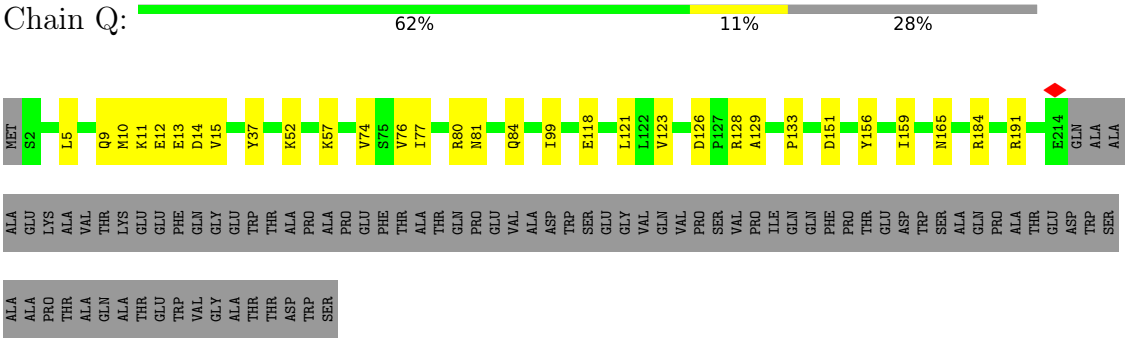
• Molecule 14: 40S ribosomal protein S3a

Chain P:



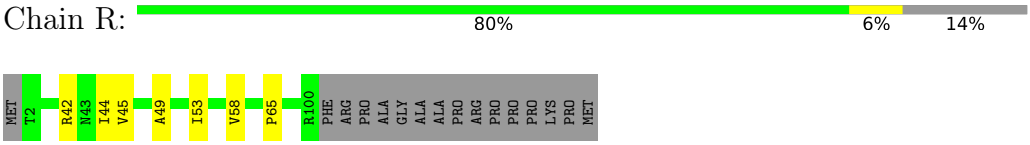
• Molecule 15: 40S ribosomal protein SA

Chain Q:



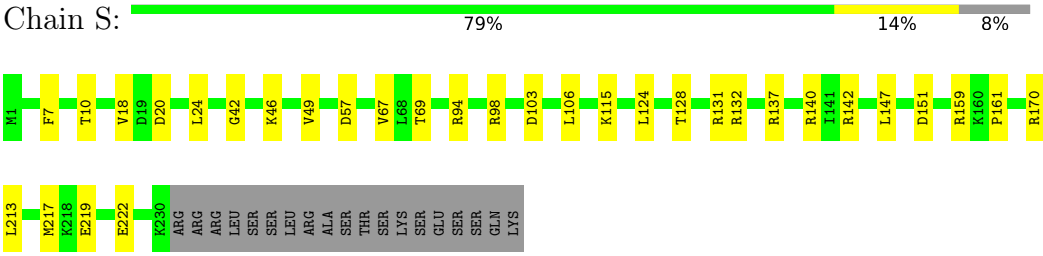
• Molecule 16: 40S ribosomal protein S26

Chain R:



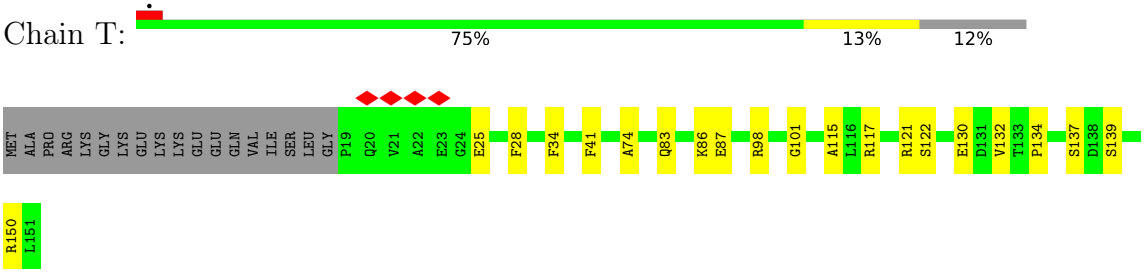
• Molecule 17: 40S ribosomal protein S6

Chain S:



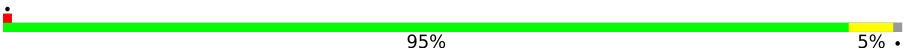
• Molecule 18: 40S ribosomal protein S14

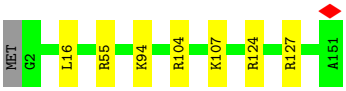
Chain T:



• Molecule 19: 40S ribosomal protein S13

Chain V:

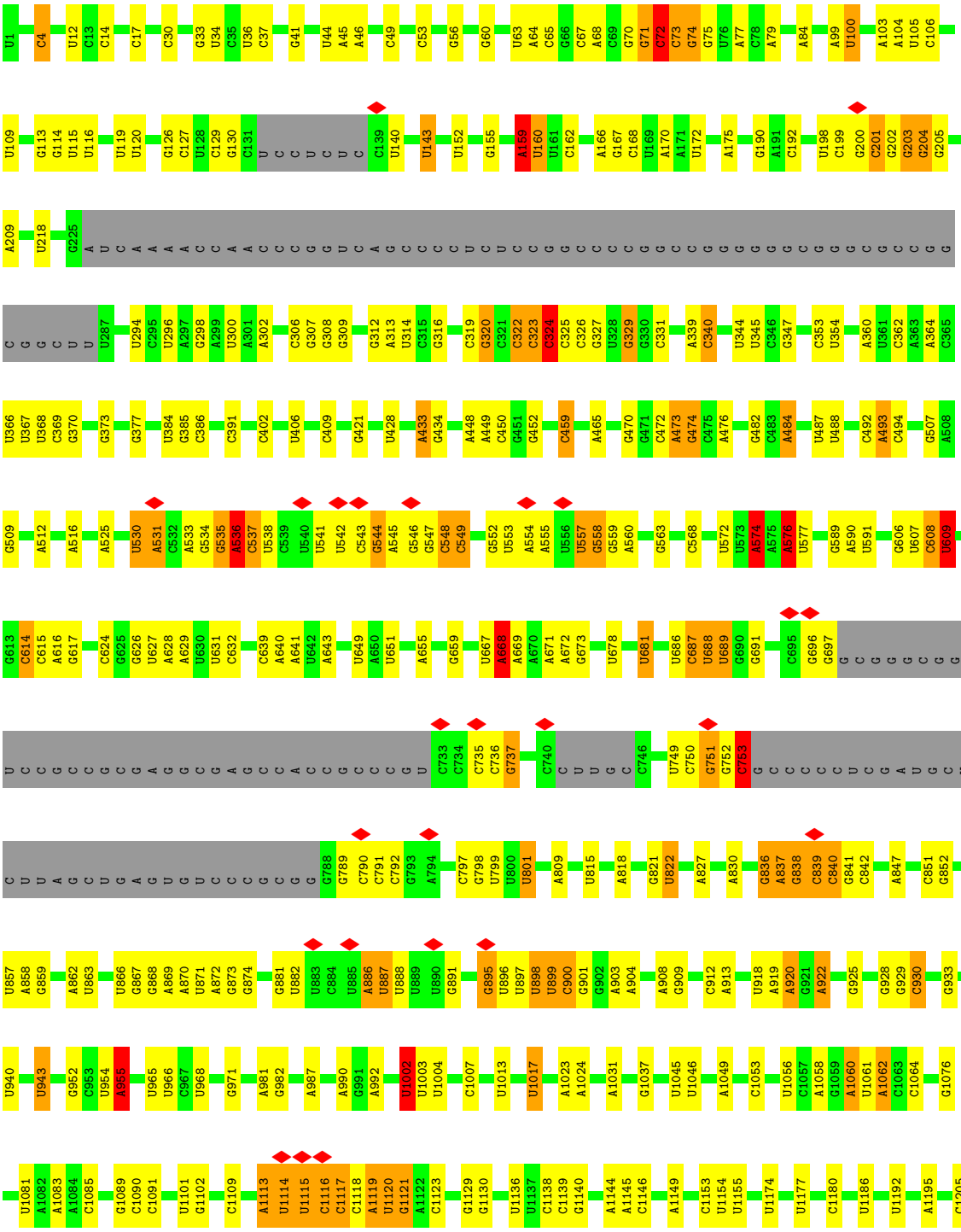


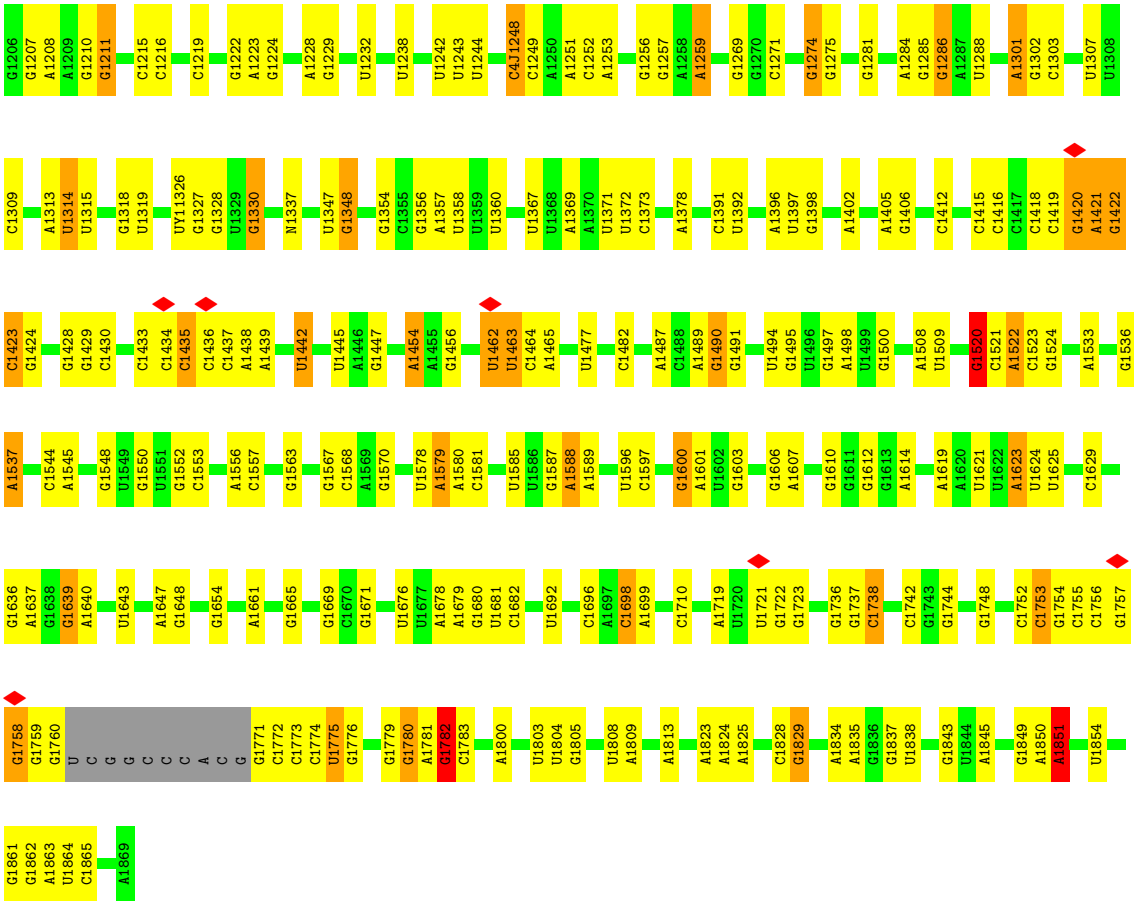


• Molecule 20: 18S rRNA

Chain W:







• Molecule 21: 40S ribosomal protein S11

Chain X:





• Molecule 22: Small ribosomal subunit protein eS4, X isoform

Chain Y:





• Molecule 23: 40S ribosomal protein S9

Chain Z:

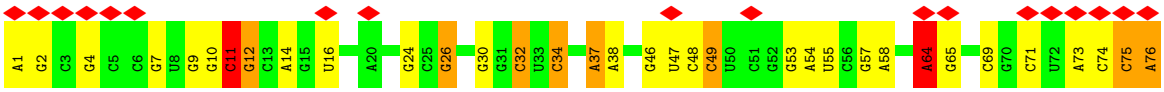




• Molecule 24: tRNAi-Met

Chain y:

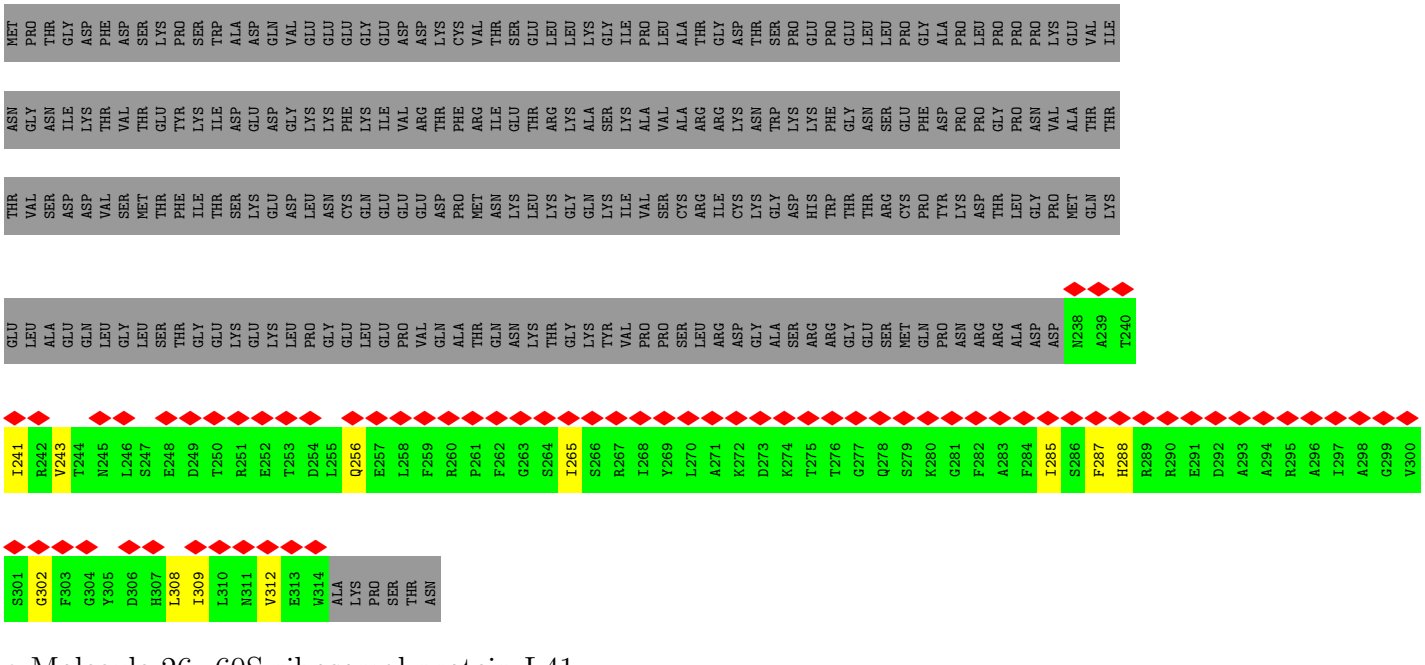




• Molecule 25: Eukaryotic translation initiation factor 3 subunit G

Chain 7:

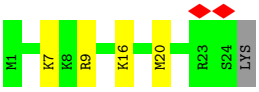




• Molecule 26: 60S ribosomal protein L41

Chain 9:

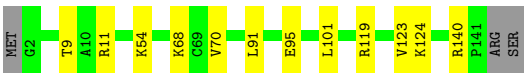




• Molecule 27: 40S ribosomal protein S23

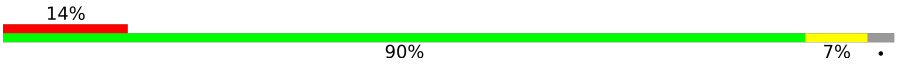
Chain a:

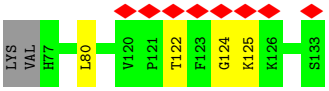




• Molecule 28: 40S ribosomal protein S30

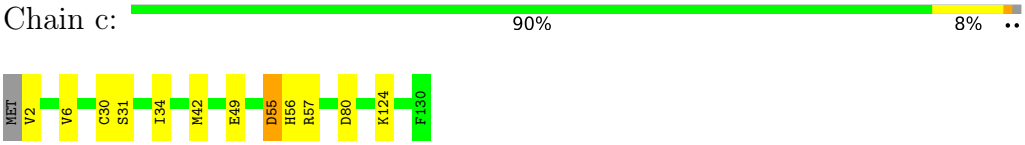
Chain b:





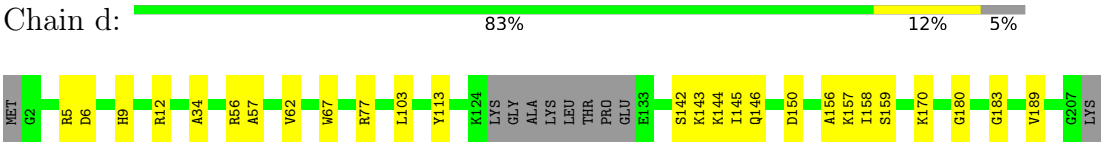
• Molecule 29: 40S ribosomal protein S15a

Chain c:



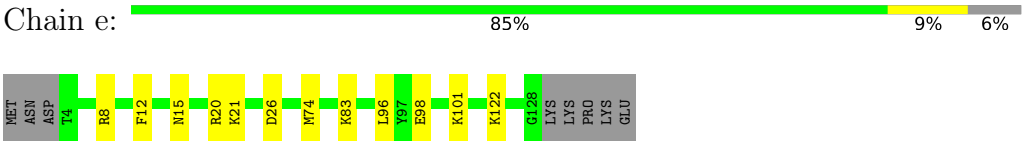
• Molecule 30: 40S ribosomal protein S8

Chain d:



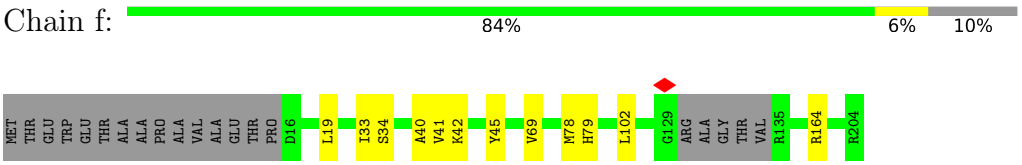
• Molecule 31: 40S ribosomal protein S24

Chain e:



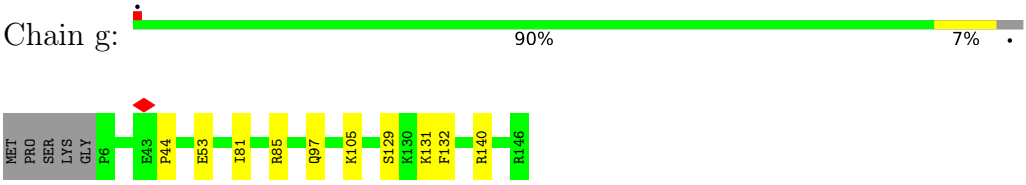
• Molecule 32: 40S ribosomal protein S5

Chain f:



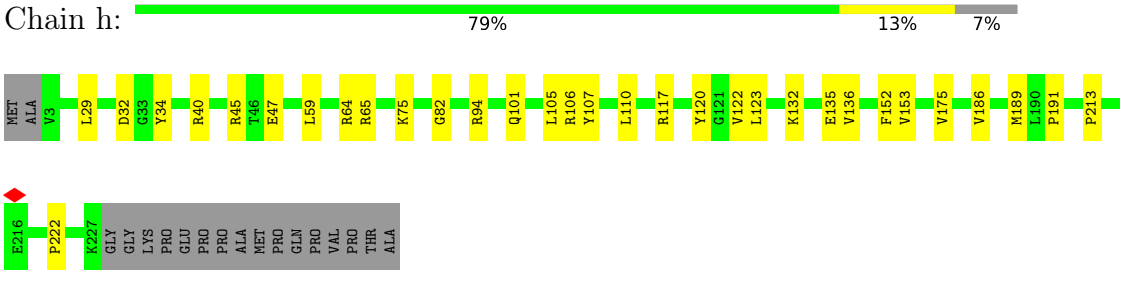
• Molecule 33: 40S ribosomal protein S16

Chain g:



• Molecule 34: 40S ribosomal protein S3

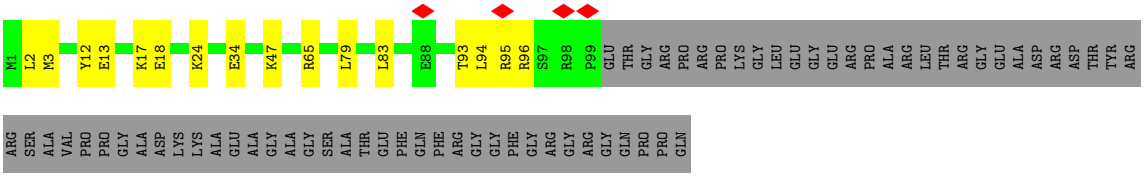
Chain h:



• Molecule 35: 40S ribosomal protein S10

Chain i:

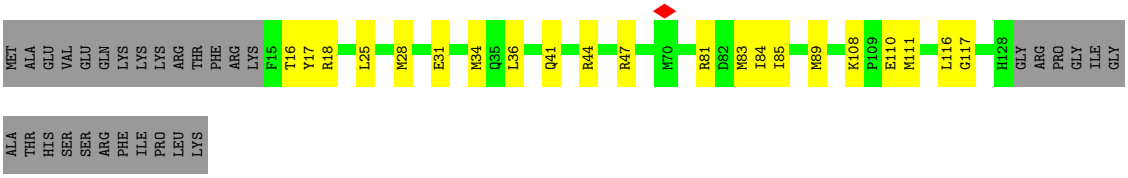




• Molecule 36: 40S ribosomal protein S15

Chain j:

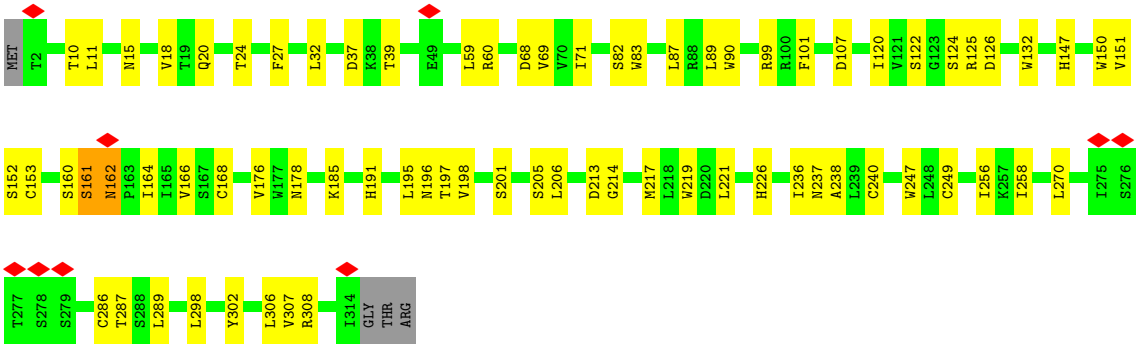




• Molecule 37: Receptor of activated protein C kinase 1

Chain k:

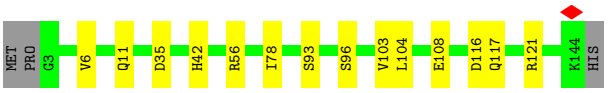




• Molecule 38: 40S ribosomal protein S19

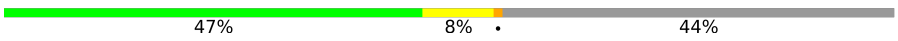
Chain l:

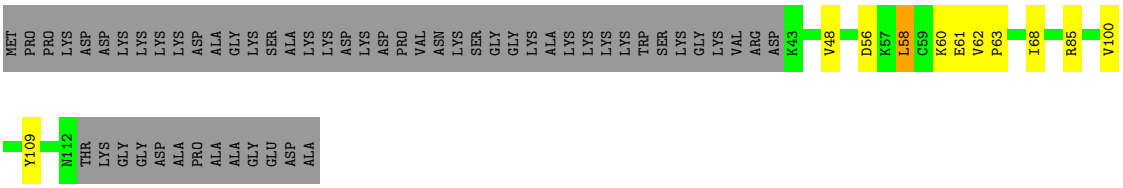




• Molecule 39: 40S ribosomal protein S25

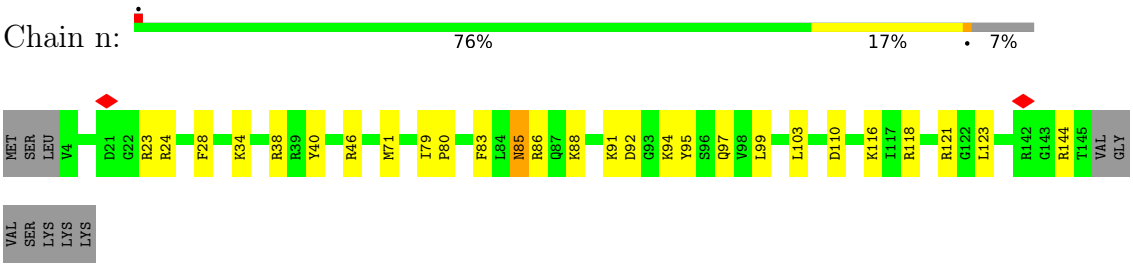
Chain m:





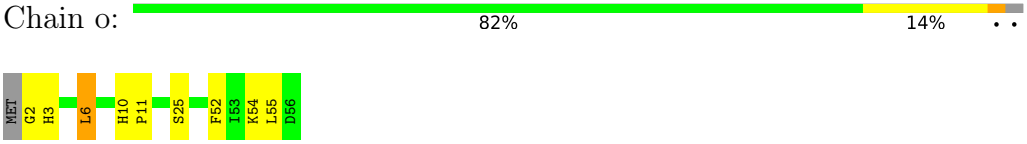
• Molecule 40: 40S ribosomal protein S18

Chain n:



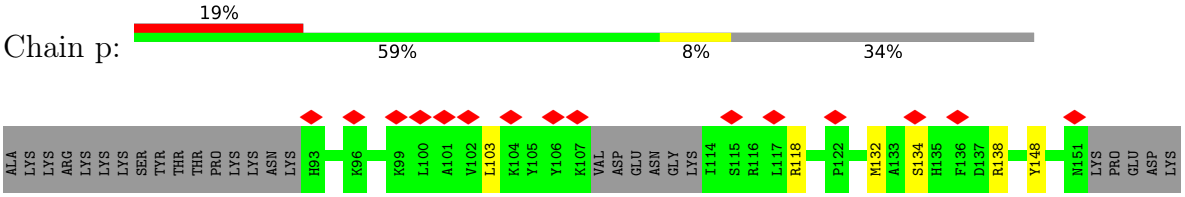
• Molecule 41: 40S ribosomal protein S29

Chain o:



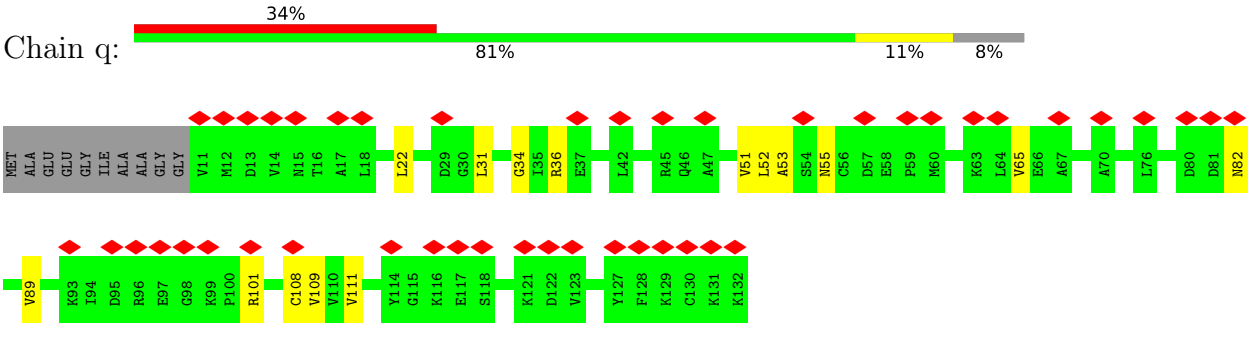
• Molecule 42: Ubiquitin-ribosomal protein eS31 fusion protein

Chain p:



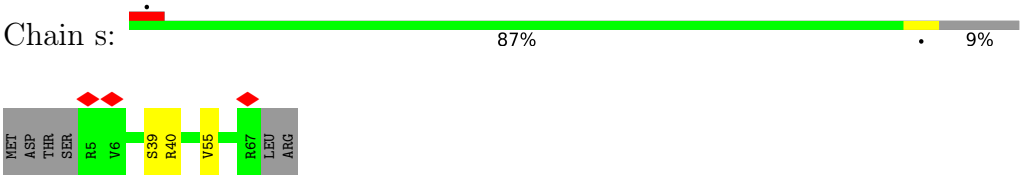
• Molecule 43: 40S ribosomal protein S12

Chain q:



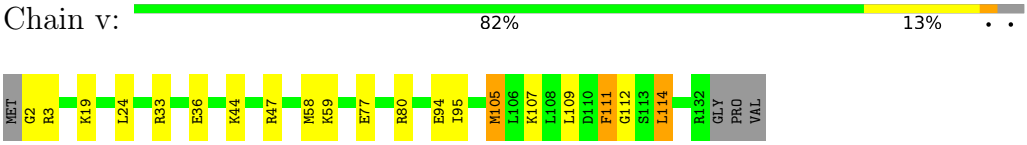
• Molecule 44: 40S ribosomal protein S28

Chain s:



• Molecule 45: 40S ribosomal protein S17

Chain v:



• Molecule 46: 40S ribosomal protein S20

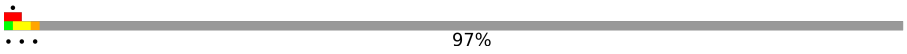
Chain w:

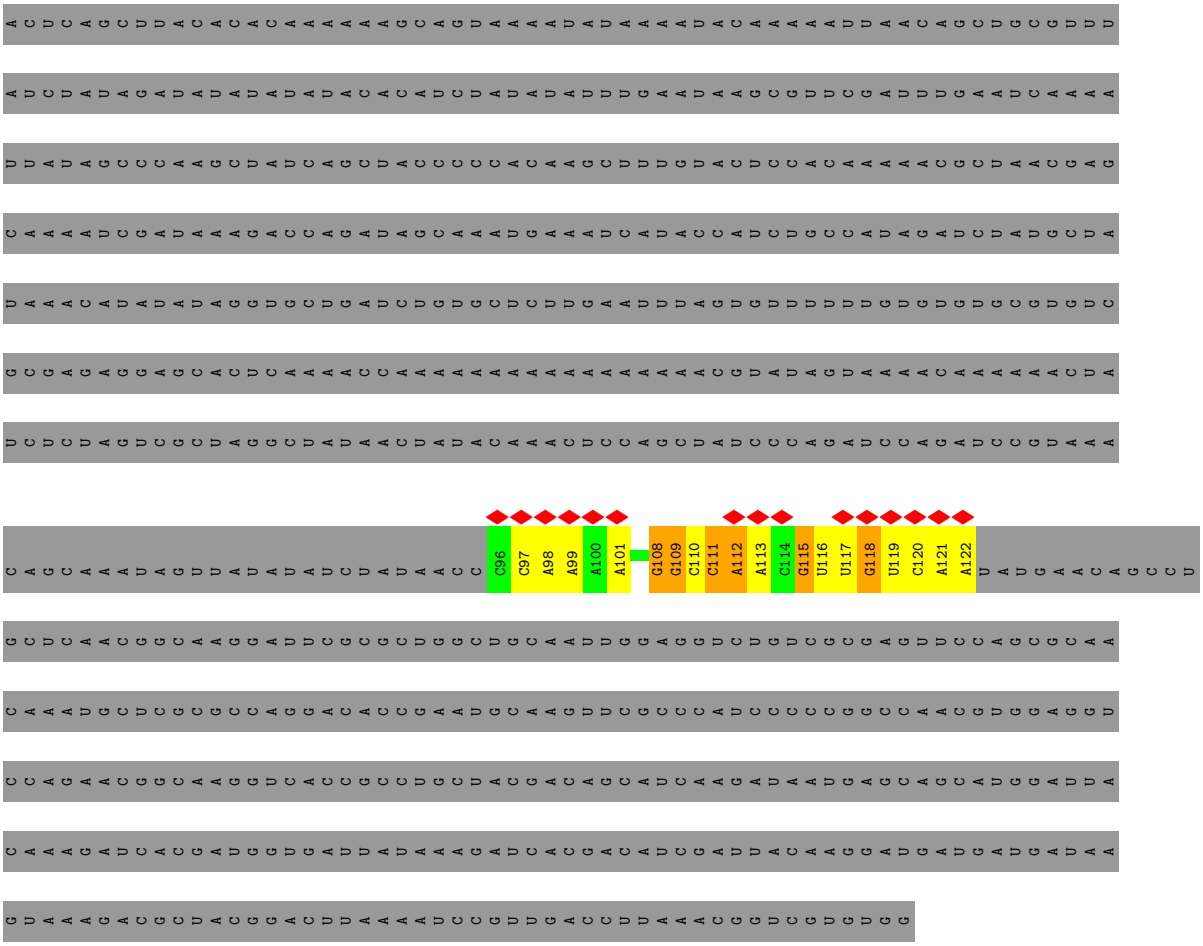




• Molecule 47: circMbl-FLAG

Chain z:

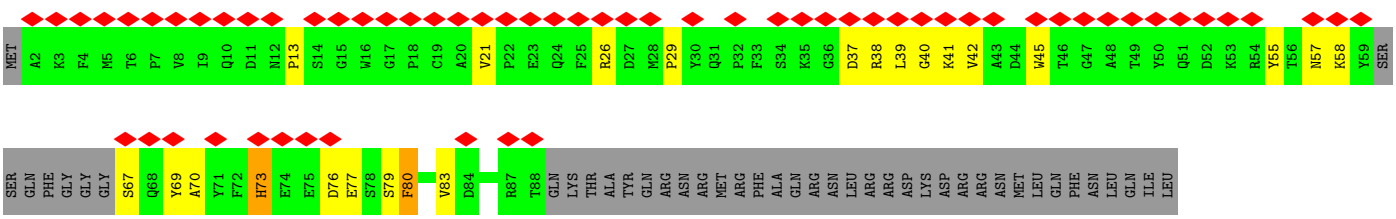




• Molecule 48: Eukaryotic translation initiation factor 3 subunit D

Chain x:





PRO LYS SER ALA LYS GLN LYS GLU ARG GLU ARG ILE ARG LEU GLN LYS LYS PHE GLN LYS GLN PHE GLY VAL ARG GLN LYS TRP ASP GLN LYS SER GLN LYS PRO ARG ASP SER SER VAL GLU VAL ARG SER ASP W168 E169 V170 K171 E172 E173 M174 D175 F176 P177 Q178 L179 M180 K181 M182

R183 Y184 L185 E186 V187 S188 E189 P190 Q191 D192 I193 E194 C195 C196 G197 A198 L199 E200 Y201 Y202 D203 K204 A205 F206 D207 T210 T211 R212 S213 E214 L217 R218 S219 I220 K221 R222 I223 F224 H225 T226 V227 T228 T229 T230 D231 D232 P233 V234 I235 R236 K237 L238 A239 K240 T241 Q242 G243 N244

V245 F246 A247 T248 D249 A250 I251 L252 A253 T254 L255 M256 S257 C258 T259 R260 S261 V262 Y263 S264 W265 D266 I267 V268 V269 Q270 R271 V272 G273 S274 K275 L276 F277 F278 D279 K280 R281 D282 N283 S284 D285 F286 D287 L288 L289 T290 E293 T294 A295 N296 E297 P298 P299 Q300 D301 E302 G303 N304 S305

F306 N307 S308 P309 R310 N311 L312 A313 M314 Y318 I319 N320 H321 N322 F323 S324 Q325 Q326 C327 L328 R329 M330 G331 K332 E333 R334 Y335 N336 F337 P338 N339 P340 N341 P342 F343 V344 E345 D346 D347 M348 D349 K350 N351 E352 I353 A354 S355 V356 A357 Y358 R359 Y360 R361 R362 W363 K364 L365 G366 D367

D368 I369 D370 L371 I372 V373 R374 C375 E376 H377 D378 G379 V380 M381 T382 G383 A384 N385 G386 E387 V388 S389 F390 I391 N392 I393 K394 T395 L396 N397 E398 W399 D400 S401 R402 H403 C404 N405 G406 V407 D408 W409 R410 Q411 D414 T423 E424 L425 K426 N427 N428 S429 Y430 K431 L432 A433 R434 W435

A439 L440 L441 A442 G443 S444 E445 Y446 L447 K448 L449 R454 Y455 H456 V457 K458 D459 S460 S461 R462 H463 V464 I465 L466 Q469 Q470 F471 K472 P473 N474 E475 F476 A477 S478 Q479 I480 N481 L482 S483 V484 E485 N486 A487 W488 G489 I490 L491 R492 C493 V494 I495 D496 I497 C498 M499 K500 L501

E502 E503 G504 K505 Y506 L507 I508 L509 K510 D511 P512 N513 K514 Q515 V516 I517 R518 V519 Y520 S521 L522 P523 D524 G525 T526 F527 SER SER ASP GLU ASP GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU THR

• Molecule 49: Eukaryotic translation initiation factor 3 subunit M

Chain 6: 93% 89% • 6%

MET SER VAL PRO ALA PHE ILE D8 I9 S10 E11 E12 D13 Q14 A15 A16 E17 L18 R19 A20 Y21 L22 K23 S24 K25 G26 A27 E28 I29 S30 E31 E32 N33 S34 E35 G36 G37 L38 H39 V40 D41 L42 A43 Q44 I45 I46 E47 A48 C49 D50 V51 C52 L53 K54 E55 D56 D57 K58 D59 V60

E61 S62 V63 M64 N65 S66 V67 V68 S69 L70 L71 L72 I73 L74 E75 P76 D77 K78 Q79 E80 A81 L82 I83 E84 S85 L86 C87 E88 K89 L90 V91 K92 F93 R94 E95 G96 E97 R98 P99 S100 L101 R102 L103 Q104 L105 L106 S107 N108 L109 F110 H111 G112 M113 D114 K115 N116 T117 P118 V119 R120

Y121 T122 V123 Y124 C125 S126 L127 I128 K129 V130 A131 A132 S133 C134 G135 A136 I137 Q138 Y139 I140 P141 T142 E143 L144 D145 Q146 V147 R148 K149 W150 I151 S152 D153 W154 N155 L156 T157 T158 E159 K160 K161 H162 T163 L164 L165 R166 L167 L168 Y169 E170 A171 L172 V173 D174 C175 K176 K177 S178 D179 A180

A181 S182 K183 V184 M185 V186 E187 L188 L189 G190 S191 Y192 T193 E194 D195 N196 A197 S198 Q199 A200 R201 V202 D203 A204 H205 R206 C207 I208 V209 R210 A211 L212 K213 D214 P215 N216 A217 F218 L219 F220 D221 H222 L223 L224 T225 L226 K227 P228 V229 K230 F231 L232 E233 G234 E235 L236 I237 H238 D239 L240

L241 T242 I243 F244 V245 S246 A247 K248 L249 A250 S251 Y252 V253 K254 F255 Y256 Q257 N258 N259 K260 D261 F262 I263 D264 S265 L266 G267 L268 L269 H270 E271 Q272 N273 M274 A275 K276 M277 R278 L279 L280 T281 F282 M283 G284 M285 A286 V287 E288 N289 K290 E291 I292 S293 F294 D295 T296 M297 Q298 Q299 E300

L301 Q302 I303 G304 A305 D306 D307 V308 E309 A310 F311 V312 I313 D314 A315 V316 R317 T318 K319 M320 V321 Y322 C323 K324 I325 D326 Q327 T328 Q329 R330 K331 V332 V333 V334 S335 H336 S337 T338 H339 R340 T341 F342 G343 K344 Q345 Q346 W347 Q348 Q349 L350 Y351 D352 T353 L354 N355 A356 W357 LYS GLN ASN

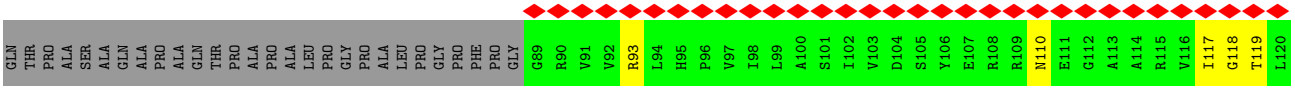


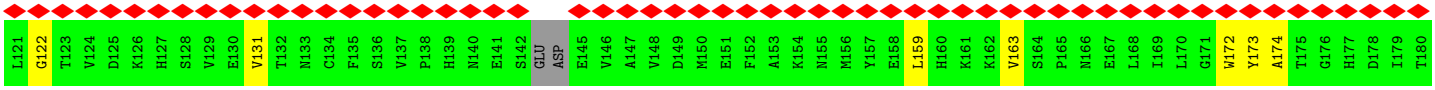
• Molecule 50: Eukaryotic translation initiation factor 3 subunit F

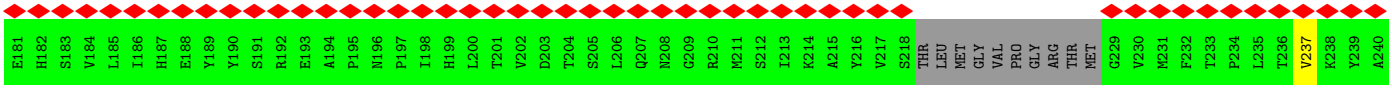
Chain 4:

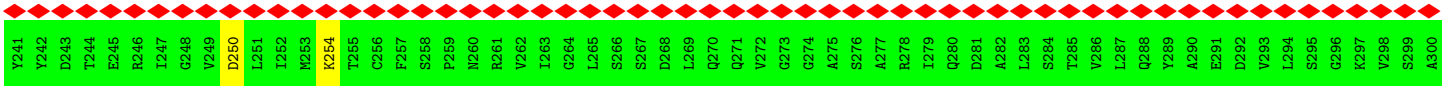


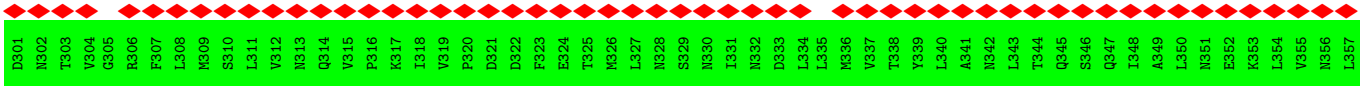








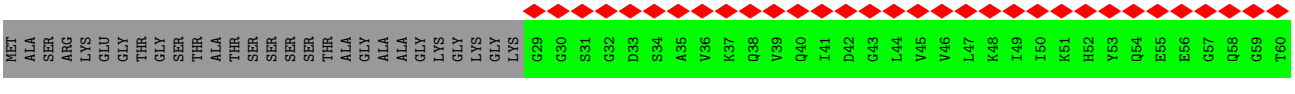


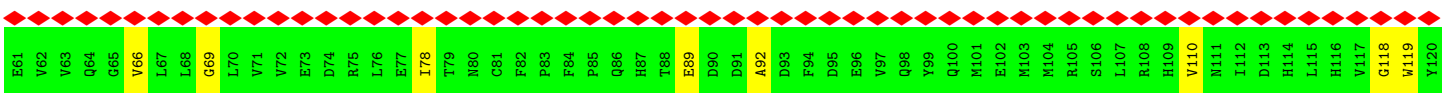


• Molecule 51: Eukaryotic translation initiation factor 3 subunit H

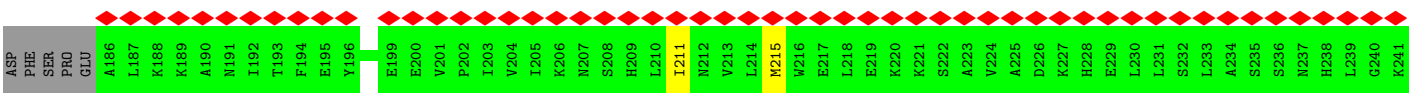
Chain 8:













S302 K303 L304 F305 K306 P307 P308 Q309 P310 P311 A312 R313 M314 D315 S316 L317 L318 I319 A320 G321 Q322 I323 N324 T325 Y326 C327 Q328 N329 I330 K331 E332 F333 T334 A335 Q336 N337 L338 G339 K340 L341 F342 M343 A344 Q345 A346 L347 Q348 E349 Y350 N351 N352

• Molecule 52: Eukaryotic translation initiation factor 3 subunit K

Chain 3: 98% 97%

MET A2 M3 F4 E5 Q6 M7 R8 A9 N10 V11 G12 K13 L14 L15 K16 G17 I18 D19 R20 Y21 N22 P23 E24 N25 L26 A27 T28 L29 E30 R31 Y32 V33 E34 T35 Q36 A37 K38 E39 N40 A41 Y42 D43 L44 E45 A46 N47 L48 A49 V50 L51 K52 L53 Y54 Q55 F56 N57 P58 A59 F60

F61 Q62 T63 T64 V65 T66 A67 Q68 I69 L70 L71 K72 A73 L74 T75 N76 L77 P78 H79 T80 D81 F82 T83 L84 C85 K86 C87 M88 I89 D90 Q91 A92 H93 Q94 E95 E96 R97 P98 I99 R100 Q101 I102 L103 Y104 L105 G106 D107 L108 L109 E110 T111 C112 H113 F114 Q115 A116 F117 W118 Q119 A120

L121 D122 E123 N124 M125 D126 L127 L128 E129 G130 I131 T132 G133 F134 E135 D136 S137 V138 R139 K140 F141 I142 C143 H144 V145 V146 G147 I148 T149 Y150 Q151 H152 I153 D154 R155 W156 L157 L158 A159 E160 M161 L162 G163 D164 L165 S166 D167 S168 Q169 L170 K171 V172 W173 M174 S175 K176 Y177 G178 W179 S180

A181 D182 E183 SER GLY Q186 I187 F188 I189 C190 S191 Q192 E193 E194 S195 I196 K197 P198 K199 N200 I201 V202 E203 K204 I205 D206 F207 D208 S209 V210 S211 S212 I213 M214 A215 S216 SER GLN

• Molecule 53: Eukaryotic translation initiation factor 3 subunit L

Chain 5: 56% 55% 43%

MET SER TYR PRO ALA ASP ASP TYR GLU SER GLU ALA ALA TYR ASP PRO TYR ALA TYR PRO SER ASP TYR ASP MET HIS THR GLY ASP PRO LYS GLN ASP LEU ALA TYR GLU ARG GLN TYR GLU GLN GLN THR TYR GLN VAL ILE PRO GLU VAL ILE LYS ASN PHE ILE GLN TYR PHE HIS

LYS THR VAL SER ASP LEU ILE ASP GLN LYS VAL TYR GLU LEU GLN ALA SER ARG VAL SER SER ASP VAL ILE ASP GLN LYS VAL TYR GLU ILE GLN ASP ILE TYR GLU ASN SER TRP THR LYS LEU THR GLU ARG PHE PHE LYS ASN THR PRO TRP PRO GLU ALA GLU ALA ILE ALA PRO

GLN VAL GLY ASN ASP ALA VAL PHE LEU ILE LEU LEU TYR LYS GLU LEU TYR TYR ARG HIS ILE TYR ALA LYS VAL SER GLY GLY PRO SER LEU GLU GLN ARG PHE GLU SER TYR TYR ASN TYR CYS ASN LEU PHE ASN TYR ILE LEU ASN ALA ASP GLY PRO ALA PRO LEU GLU LEU PRO ASN

GLN TRP L183 W184 D185 I186 I187 D188 E189 F190 I191 Y192 Q193 F194 Q195 S196 F197 S198 Q199 Y200 R201 C202 K203 T204 A205 K206 K207 S208 E209 E210 E211 I212 D213 F214 L215 R216 S217 N218 P219 K220 I221 W222 N223 V224 H225 S226 V227 L228 N229 V230 L231 H232 S233 L234 V235 D236 K237 S238 N239 I240

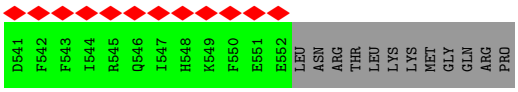
N241 R242 Q243 L244 E245 V246 Y247 T248 S249 G250 G251 D252 P253 E254 S255 V256 A257 G258 E259 Y260 G261 R262 H263 S264 L265 Y266 K267 M268 L269 G270 Y271 F272 S273 L274 V275 G276 L277 L278 R279 L280 H281 S282 L283 L284 G285 D286 Y287 Y288 Q289 A290 I291 K292 V293 L294 E295 N296 I297 E298 L299 N300

K301 K302 S303 M304 TYR SER ARG VAL PRO GLU C311 Q312 V313 T314 T315 Y316 Y317 Y318 V319 G320 F321 A322 Y323 L324 M325 M326 R327 R328 Y329 Q330 D331 A332 I333 R334 V335 F336 A337 N338 I339 L340 L341 Y342 I343 GLN ARG THR LYS SER MET PHE GLN ARG THR THR TYR LYS Y357 E358 M359 I360

N361 K362 Q363 N364 E365 Q366 M367 H368 A369 L370 L371 A372 I373 A374 L375 THR MET TYR PRO MET ARG I382 D383 E384 S385 I386 H387 L388 Q389 L390 R391 E392 K393 Y394 G395 D396 K397 M398 L399 R400 M401 Q402 K403 G404 D405 P406 Q407 V408 Y409 E410 E411 L412 F413 S414 Y415 S416 C417 PRO LYS PHE

LEU SER PRO VAL VAL PRO ASN TYR ASP ASN VAL HIS PRO ASN TYR H436 K437 E438 P439 F440 L441 Q442 Q443 L444 K445 V446 F447 S448 D449 E450 V451 Q452 Q453 Q454 A455 Q456 L457 S458 T459 I460 R461 S462 F463 L464 K465 L466 Y467 T468 T469 M470 P471 V472 A473 K474 L475 A476 G477 F478 L479 D480


L481 THR GLU GLN GLU PHE ARG ILE GLN L490 L491 V492 F493 K494 H495 K496 M497 K498 N499 L500 V501 W502 T503 S504 G505 I506 S507 A508 L509 D510 G511 E512 F513 Q514 S515 A516 S517 E518 V519 D520 F521 Y522 I523 D524 K525 D526 M527 I528 H529 I530 A531 D532 T533 K534 V535 A536 R537 R538 Y539 G540


D541 F542 F543 I544 R545 Q546 I547 H548 K549 F550 E551 E552 LEU ASN ARG THR LEU LYS LYS MET GLY GLN ARG PRO

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21721	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.0	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.048	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0045	Depositor
Map size (Å)	494.4, 494.4, 494.4	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	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, OMC, M2G, MG, 5MC, PSU, 1MG, A2M, UY1, MA6, H2U, 1MA, OMG, 2MG, OMU, 4AC, ZN, 5MU, K, RIA, 7MG, G7M, C4J, 6MZ, JMH

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	A	0.25	0/5593	0.59	0/7599
2	B	0.23	0/2672	0.55	0/3647
3	D	0.24	0/2267	0.57	0/3056
4	E	0.22	0/3598	0.54	0/4868
5	F	0.11	0/1597	0.30	0/2216
6	G	0.26	0/797	0.65	0/1061
7	H	0.29	0/701	0.73	0/936
8	I	0.21	0/4696	0.49	0/6379
9	J	0.28	0/5018	0.60	0/6791
10	L	0.40	0/1460	0.69	3/1953 (0.2%)
11	M	0.58	0/644	0.84	0/864
12	N	0.48	0/643	0.72	1/860 (0.1%)
13	O	0.42	0/1743	0.52	0/2354
14	P	0.41	0/1742	0.63	2/2330 (0.1%)
15	Q	0.44	0/1723	0.68	0/2341
16	R	0.43	0/805	0.57	0/1079
17	S	0.30	0/1885	0.53	0/2510
18	T	0.54	0/1011	0.81	1/1355 (0.1%)
19	V	0.38	0/1232	0.45	0/1656
20	W	0.93	3/38778 (0.0%)	1.00	76/60434 (0.1%)
21	X	0.43	0/1186	0.47	0/1585
22	Y	0.45	0/2083	0.60	2/2805 (0.1%)
23	Z	0.40	0/1502	0.57	0/2008
24	y	0.61	2/1531 (0.1%)	1.01	5/2384 (0.2%)
25	7	0.26	0/628	0.61	0/846
26	9	0.45	0/231	0.72	0/294
27	a	0.44	0/1105	0.54	0/1476
28	b	0.46	0/458	0.73	1/602 (0.2%)
29	c	0.54	0/1051	0.85	4/1406 (0.3%)
30	d	0.44	0/1655	0.65	0/2205
31	e	0.35	0/1032	0.48	0/1371

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	f	0.39	0/1481	0.58	0/1988
33	g	0.38	0/1142	0.59	0/1528
34	h	0.35	0/1780	0.51	0/2397
35	i	0.42	0/859	0.68	0/1159
36	j	0.31	0/964	0.54	0/1289
37	k	0.35	0/2493	0.59	0/3394
38	l	0.38	0/1123	0.58	0/1504
39	m	0.43	0/565	0.67	0/759
40	n	0.36	0/1194	0.68	1/1599 (0.1%)
41	o	0.47	0/470	0.73	1/623 (0.2%)
42	p	0.23	0/444	0.59	0/588
43	q	0.32	0/960	0.73	0/1286
44	s	0.40	0/500	0.55	0/669
45	v	0.44	0/1078	0.81	1/1447 (0.1%)
46	w	0.36	0/827	0.56	0/1110
47	z	0.71	0/643	0.99	1/999 (0.1%)
48	x	0.29	0/2963	0.58	1/4050 (0.0%)
49	6	0.17	0/1926	0.47	0/2669
50	4	0.12	0/1269	0.33	0/1762
51	8	0.14	0/1569	0.42	0/2183
52	3	0.11	0/1055	0.32	0/1469
53	5	0.12	0/1575	0.36	0/2187
All	All	0.60	5/117947 (0.0%)	0.77	100/167930 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
18	T	0	1
22	Y	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	W	159	A2M	O3'-P	5.31	1.61	1.56
20	W	576	A2M	O3'-P	5.26	1.61	1.56
20	W	512	A2M	O3'-P	5.17	1.61	1.56
24	y	64	RIA	O3'-P	5.03	1.61	1.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	76	A	N9-C4	5.02	1.40	1.37

The worst 5 of 100 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	55	ASP	N-CA-C	-7.76	98.46	110.17
22	Y	30	ARG	N-CA-CB	7.32	119.47	110.17
18	T	139	SER	N-CA-C	7.30	122.15	108.65
20	W	1782	G	P-O3'-C3'	7.06	128.17	119.70
40	n	85	ASN	CB-CA-C	-6.71	98.43	110.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	ARG	Sidechain
18	T	137	SER	Peptide
22	Y	30	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5504	0	5117	69	0
2	B	2635	0	2207	27	0
3	D	2234	0	2288	22	0
4	E	3540	0	3690	37	0
5	F	1598	0	723	5	0
6	G	789	0	806	10	0
7	H	691	0	706	13	0
8	I	4569	0	4317	38	0
9	J	4940	0	4682	67	0
10	L	1439	0	1533	17	0
11	M	631	0	655	14	0
12	N	636	0	637	6	0
13	O	1707	0	1794	13	0
14	P	1715	0	1785	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	Q	1686	0	1688	22	0
16	R	792	0	841	5	0
17	S	1862	0	2018	23	0
18	T	998	0	1021	13	0
19	V	1208	0	1294	8	0
20	W	36695	0	18566	204	0
21	X	1166	0	1233	9	0
22	Y	2041	0	2143	11	0
23	Z	1477	0	1589	12	0
24	y	1639	0	850	21	0
25	7	616	0	600	6	0
26	9	230	0	276	3	0
27	a	1087	0	1154	11	0
28	b	452	0	494	1	0
29	c	1034	0	1080	7	0
30	d	1628	0	1706	16	0
31	e	1015	0	1086	7	0
32	f	1461	0	1511	9	0
33	g	1124	0	1193	5	0
34	h	1752	0	1848	22	0
35	i	834	0	861	14	0
36	j	946	0	988	16	0
37	k	2436	0	2391	45	0
38	l	1105	0	1138	10	0
39	m	559	0	616	8	0
40	n	1176	0	1233	20	0
41	o	459	0	448	8	0
42	p	435	0	434	5	0
43	q	950	0	985	9	0
44	s	498	0	525	4	0
45	v	1064	0	1118	17	0
46	w	817	0	882	7	0
47	z	575	0	293	7	0
48	x	2920	0	2231	42	0
49	6	1917	0	1096	8	0
50	4	1272	0	564	8	0
51	8	1571	0	683	10	0
52	3	1057	0	475	1	0
53	5	1581	0	689	4	0
54	R	1	0	0	0	0
54	o	1	0	0	0	0
54	p	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	S	1	0	0	0	0
55	T	1	0	0	0	0
55	W	85	0	0	0	0
55	f	1	0	0	0	0
56	W	3	0	0	0	0
All	All	114857	0	90781	873	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 4.

The worst 5 of 873 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)
11:M:72:ARG:HH12	20:W:1120:U:H1'	1.39	0.86
20:W:928:G:H1	20:W:1013:U:H3	1.23	0.86
20:W:1301:A:HO2'	41:o:2:GLY:N	1.74	0.85
20:W:925:G:H1	20:W:1017:U:H3	1.36	0.73
11:M:72:ARG:NH1	20:W:1120:U:H1'	2.03	0.73

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	A	731/1382 (53%)	687 (94%)	44 (6%)	0	100	100
2	B	380/445 (85%)	344 (90%)	36 (10%)	0	100	100
3	D	276/315 (88%)	260 (94%)	15 (5%)	1 (0%)	30	65
4	E	462/472 (98%)	435 (94%)	26 (6%)	1 (0%)	43	75
5	F	323/325 (99%)	305 (94%)	18 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	G	95/147 (65%)	89 (94%)	6 (6%)	0	100	100
7	H	83/116 (72%)	65 (78%)	18 (22%)	0	100	100
8	I	573/814 (70%)	538 (94%)	35 (6%)	0	100	100
9	J	639/913 (70%)	601 (94%)	38 (6%)	0	100	100
10	L	172/194 (89%)	161 (94%)	11 (6%)	0	100	100
11	M	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
12	N	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
13	O	218/293 (74%)	214 (98%)	4 (2%)	0	100	100
14	P	209/264 (79%)	201 (96%)	6 (3%)	2 (1%)	12	45
15	Q	211/295 (72%)	203 (96%)	8 (4%)	0	100	100
16	R	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
17	S	228/249 (92%)	213 (93%)	15 (7%)	0	100	100
18	T	131/151 (87%)	120 (92%)	11 (8%)	0	100	100
19	V	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
21	X	138/158 (87%)	135 (98%)	3 (2%)	0	100	100
22	Y	255/263 (97%)	251 (98%)	4 (2%)	0	100	100
23	Z	175/194 (90%)	173 (99%)	2 (1%)	0	100	100
25	7	75/320 (23%)	68 (91%)	7 (9%)	0	100	100
26	9	22/25 (88%)	22 (100%)	0	0	100	100
27	a	138/143 (96%)	136 (99%)	2 (1%)	0	100	100
28	b	55/59 (93%)	50 (91%)	5 (9%)	0	100	100
29	c	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
30	d	194/208 (93%)	184 (95%)	10 (5%)	0	100	100
31	e	123/133 (92%)	122 (99%)	1 (1%)	0	100	100
32	f	180/204 (88%)	173 (96%)	7 (4%)	0	100	100
33	g	139/146 (95%)	133 (96%)	6 (4%)	0	100	100
34	h	223/243 (92%)	220 (99%)	3 (1%)	0	100	100
35	i	97/165 (59%)	92 (95%)	5 (5%)	0	100	100
36	j	112/145 (77%)	111 (99%)	1 (1%)	0	100	100
37	k	311/317 (98%)	282 (91%)	29 (9%)	0	100	100
38	l	140/145 (97%)	131 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	m	68/125 (54%)	67 (98%)	1 (2%)	0	100	100
40	n	140/152 (92%)	137 (98%)	3 (2%)	0	100	100
41	o	53/56 (95%)	53 (100%)	0	0	100	100
42	p	49/80 (61%)	46 (94%)	3 (6%)	0	100	100
43	q	120/132 (91%)	105 (88%)	15 (12%)	0	100	100
44	s	61/69 (88%)	57 (93%)	4 (7%)	0	100	100
45	v	129/135 (96%)	126 (98%)	3 (2%)	0	100	100
46	w	101/119 (85%)	95 (94%)	6 (6%)	0	100	100
48	x	434/548 (79%)	384 (88%)	48 (11%)	2 (0%)	24	60
49	6	348/374 (93%)	315 (90%)	33 (10%)	0	100	100
50	4	251/357 (70%)	233 (93%)	18 (7%)	0	100	100
51	8	313/352 (89%)	281 (90%)	32 (10%)	0	100	100
52	3	209/218 (96%)	200 (96%)	9 (4%)	0	100	100
53	5	307/564 (54%)	290 (94%)	17 (6%)	0	100	100
All	All	10223/13087 (78%)	9627 (94%)	590 (6%)	6 (0%)	49	81

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
48	x	13	PRO
4	E	324	GLU
48	x	80	PHE
14	P	77	ASP
14	P	79	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	525/1259 (42%)	525 (100%)	0	100	100
2	B	206/406 (51%)	206 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	249/280 (89%)	249 (100%)	0	100	100
4	E	394/397 (99%)	394 (100%)	0	100	100
6	G	83/124 (67%)	83 (100%)	0	100	100
7	H	74/97 (76%)	74 (100%)	0	100	100
8	I	470/702 (67%)	470 (100%)	0	100	100
9	J	489/811 (60%)	488 (100%)	1 (0%)	87	87
10	L	160/174 (92%)	159 (99%)	1 (1%)	78	81
11	M	73/76 (96%)	72 (99%)	1 (1%)	59	71
12	N	67/67 (100%)	66 (98%)	1 (2%)	57	70
13	O	186/225 (83%)	186 (100%)	0	100	100
14	P	192/231 (83%)	191 (100%)	1 (0%)	81	82
15	Q	179/243 (74%)	179 (100%)	0	100	100
16	R	86/98 (88%)	86 (100%)	0	100	100
17	S	200/218 (92%)	200 (100%)	0	100	100
18	T	104/119 (87%)	104 (100%)	0	100	100
19	V	130/131 (99%)	130 (100%)	0	100	100
21	X	129/142 (91%)	129 (100%)	0	100	100
22	Y	220/225 (98%)	219 (100%)	1 (0%)	81	82
23	Z	158/168 (94%)	158 (100%)	0	100	100
25	7	64/277 (23%)	64 (100%)	0	100	100
26	9	23/24 (96%)	23 (100%)	0	100	100
27	a	112/115 (97%)	112 (100%)	0	100	100
28	b	46/48 (96%)	44 (96%)	2 (4%)	26	48
29	c	112/113 (99%)	112 (100%)	0	100	100
30	d	172/180 (96%)	172 (100%)	0	100	100
31	e	107/115 (93%)	107 (100%)	0	100	100
32	f	156/170 (92%)	156 (100%)	0	100	100
33	g	117/121 (97%)	117 (100%)	0	100	100
34	h	189/202 (94%)	189 (100%)	0	100	100
35	i	90/136 (66%)	90 (100%)	0	100	100
36	j	104/130 (80%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
37	k	272/275 (99%)	269 (99%)	3 (1%)	65 74
38	l	112/115 (97%)	112 (100%)	0	100 100
39	m	62/103 (60%)	61 (98%)	1 (2%)	55 70
40	n	123/132 (93%)	123 (100%)	0	100 100
41	o	48/49 (98%)	47 (98%)	1 (2%)	47 65
42	p	47/72 (65%)	47 (100%)	0	100 100
43	q	104/108 (96%)	104 (100%)	0	100 100
44	s	56/62 (90%)	56 (100%)	0	100 100
45	v	119/122 (98%)	117 (98%)	2 (2%)	53 68
46	w	94/107 (88%)	94 (100%)	0	100 100
48	x	205/494 (42%)	204 (100%)	1 (0%)	81 82
49	6	49/335 (15%)	49 (100%)	0	100 100
All	All	6957/9798 (71%)	6941 (100%)	16 (0%)	85 87

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	v	114	LEU
45	v	105	MET
37	k	160	SER
41	o	6	LEU
28	b	125	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
37	k	272	GLN
48	x	416	GLN
38	l	10	ASN
40	n	97	GLN
9	J	472	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	W	1709/1869 (91%)	375 (21%)	24 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	y	74/75 (98%)	17 (22%)	0
47	z	26/774 (3%)	15 (57%)	0
All	All	1809/2718 (66%)	407 (22%)	24 (1%)

5 of 407 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	W	4	C
20	W	17	C
20	W	33	G
20	W	41	G
20	W	44	U

5 of 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	W	1420	G
20	W	1429	G
20	W	1428	G
20	W	1463	U
20	W	837	A

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

106 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	$\#\|Z\| > 2$
20	PSU	W	1643	55,20	18,21,22	1.08	1 (5%)	22,30,33	0.69	0
20	PSU	W	1596	20	18,21,22	1.04	1 (5%)	22,30,33	0.76	0
24	5MC	y	48	24	18,22,23	0.35	0	26,32,35	0.54	0
20	A2M	W	668	55,20	22,25,26	0.22	0	31,36,39	1.22	1 (3%)
20	PSU	W	651	20	18,21,22	1.04	1 (5%)	22,30,33	0.75	0
24	T6A	y	37	24	31,34,35	0.52	0	44,49,52	1.36	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	PSU	W	572	20	18,21,22	1.03	1 (5%)	22,30,33	0.71	0
20	PSU	W	1081	20	18,21,22	1.06	2 (11%)	22,30,33	0.80	0
20	PSU	W	1445	20	18,21,22	0.88	1 (5%)	22,30,33	0.69	0
20	OMG	W	436	20	23,26,27	0.44	0	33,38,41	0.49	0
20	OMU	W	172	20	19,22,23	0.31	0	26,31,34	1.11	1 (3%)
24	M2G	y	26	24	24,27,28	0.45	0	35,40,43	0.47	0
20	JMH	W	1219	55,20	18,22,23	0.70	1 (5%)	21,32,35	0.68	0
20	5MU	W	814	20	19,22,23	0.46	0	28,32,35	0.51	0
20	OMU	W	121	20	19,22,23	0.46	0	26,31,34	0.57	0
20	PSU	W	966	20	18,21,22	1.01	1 (5%)	22,30,33	0.75	0
20	PSU	W	1045	20	18,21,22	0.96	1 (5%)	22,30,33	0.84	0
20	OMU	W	1442	20	19,22,23	0.49	0	26,31,34	0.56	0
20	A2M	W	590	20	22,25,26	0.20	0	31,36,39	0.50	0
20	PSU	W	34	20	18,21,22	0.99	1 (5%)	22,30,33	0.72	0
20	PSU	W	612	20	18,21,22	1.03	2 (11%)	22,30,33	0.74	0
24	H2U	y	47	24	18,21,22	0.57	0	21,30,33	0.54	0
20	PSU	W	105	20	18,21,22	1.02	1 (5%)	22,30,33	0.74	0
20	OMU	W	1288	20	19,22,23	0.50	0	26,31,34	0.69	0
24	RIA	y	64	24	35,38,39	0.30	0	53,57,60	0.73	1 (1%)
20	A2M	W	576	20	22,25,26	0.22	0	31,36,39	1.51	4 (12%)
20	PSU	W	296	20	18,21,22	1.03	1 (5%)	22,30,33	0.80	0
20	A2M	W	484	20	22,25,26	0.22	0	31,36,39	1.36	3 (9%)
20	A2M	W	99	55,20	22,25,26	0.25	0	31,36,39	0.44	0
20	PSU	W	109	20	18,21,22	1.02	1 (5%)	22,30,33	0.71	0
20	PSU	W	1625	20	18,21,22	1.04	1 (5%)	22,30,33	0.73	0
20	PSU	W	863	20	18,21,22	1.03	1 (5%)	22,30,33	0.70	0
20	PSU	W	1186	20	18,21,22	1.03	1 (5%)	22,30,33	0.79	0
20	OMG	W	867	20	23,26,27	0.39	0	33,38,41	0.38	0
20	PSU	W	119	20	18,21,22	0.99	1 (5%)	22,30,33	0.68	0
24	H2U	y	16	24	18,21,22	0.52	0	21,30,33	0.73	0
20	C4J	W	1248	20	24,29,30	0.87	1 (4%)	29,42,45	0.81	0
20	OMG	W	1490	55,20	23,26,27	0.35	0	33,38,41	0.40	0
20	PSU	W	649	20	18,21,22	1.02	1 (5%)	22,30,33	0.84	0
20	A2M	W	1678	20	22,25,26	0.24	0	31,36,39	0.48	0
20	OMC	W	1703	20	19,22,23	0.48	0	26,31,34	0.60	0
20	A2M	W	1383	20	22,25,26	0.25	0	31,36,39	0.59	0
20	PSU	W	918	20	18,21,22	1.07	2 (11%)	22,30,33	0.79	1 (4%)
20	PSU	W	815	20	18,21,22	1.03	1 (5%)	22,30,33	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	OMC	W	174	55,20	19,22,23	0.47	0	26,31,34	0.57	0
20	4AC	W	1842	20	21,24,25	0.49	0	29,34,37	0.66	0
20	4AC	W	1337	20	21,24,25	0.54	0	29,34,37	0.83	1 (3%)
20	PSU	W	801	20	18,21,22	1.05	1 (5%)	22,30,33	0.64	0
20	OMC	W	462	20	19,22,23	0.46	0	26,31,34	0.63	0
20	PSU	W	1004	20	18,21,22	1.05	1 (5%)	22,30,33	0.72	0
20	PSU	W	1046	20	18,21,22	1.05	2 (11%)	22,30,33	0.62	0
20	PSU	W	1238	20	18,21,22	0.89	1 (5%)	22,30,33	0.75	1 (4%)
20	MA6	W	1851	20	23,26,27	0.36	0	34,38,41	0.79	1 (2%)
20	A2M	W	159	20	22,25,26	0.24	0	31,36,39	1.21	3 (9%)
20	PSU	W	1056	20	18,21,22	1.04	1 (5%)	22,30,33	0.73	0
24	1MA	y	58	24	21,25,26	0.40	0	31,37,40	0.68	0
20	OMG	W	601	20	23,26,27	0.40	0	33,38,41	0.39	0
20	PSU	W	406	20	18,21,22	0.87	1 (5%)	22,30,33	0.67	0
20	OMC	W	517	20	19,22,23	0.50	0	26,31,34	0.59	0
20	OMG	W	644	20	23,26,27	0.44	0	33,38,41	0.46	0
20	A2M	W	512	20	22,25,26	0.22	0	31,36,39	1.64	5 (16%)
20	PSU	W	1003	20	18,21,22	1.04	1 (5%)	22,30,33	0.70	0
20	OMU	W	428	20	19,22,23	0.36	0	26,31,34	0.50	0
20	PSU	W	1692	20	18,21,22	1.04	1 (5%)	22,30,33	0.70	0
20	PSU	W	686	20	18,21,22	0.88	1 (5%)	22,30,33	0.74	0
20	PSU	W	681	20	18,21,22	1.07	1 (5%)	22,30,33	0.77	0
20	OMG	W	1328	20	23,26,27	0.28	0	33,38,41	0.33	0
20	OMU	W	116	20	19,22,23	0.42	0	26,31,34	0.60	0
20	PSU	W	1360	56,55,20	18,21,22	1.08	2 (11%)	22,30,33	0.76	0
20	PSU	W	822	20	18,21,22	0.85	1 (5%)	22,30,33	0.77	1 (4%)
20	OMU	W	354	20	19,22,23	0.49	0	26,31,34	0.79	1 (3%)
24	7MG	y	46	24	22,26,27	1.12	1 (4%)	29,39,42	0.72	0
20	A2M	W	27	55,20	22,25,26	0.26	0	31,36,39	0.42	0
20	OMG	W	683	20	23,26,27	0.49	0	33,38,41	0.49	0
20	PSU	W	1174	20	18,21,22	1.04	1 (5%)	22,30,33	0.77	0
20	PSU	W	63	20	18,21,22	1.04	1 (5%)	22,30,33	0.87	0
24	2MG	y	10	24	23,26,27	0.40	0	32,38,41	0.50	0
20	PSU	W	36	20	18,21,22	1.03	1 (5%)	22,30,33	0.73	0
20	A2M	W	166	20	22,25,26	0.20	0	31,36,39	0.45	0
20	OMG	W	1447	20	23,26,27	0.30	0	33,38,41	0.39	0
20	PSU	W	218	20	18,21,22	1.00	1 (5%)	22,30,33	0.72	0
20	A2M	W	468	20	22,25,26	0.23	0	31,36,39	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	OMG	W	509	55,20	23,26,27	0.42	0	33,38,41	0.51	0
24	5MC	y	49	24	18,22,23	0.37	0	26,32,35	0.55	0
20	PSU	W	1244	20	18,21,22	0.84	1 (5%)	22,30,33	0.64	0
20	PSU	W	1136	20	18,21,22	1.02	1 (5%)	22,30,33	0.74	0
20	PSU	W	866	20	18,21,22	1.05	1 (5%)	22,30,33	0.65	0
20	PSU	W	100	55,20	18,21,22	0.92	1 (5%)	22,30,33	0.81	0
20	6MZ	W	1832	55,20	22,25,26	0.40	0	30,36,39	0.67	0
24	1MG	y	9	24	22,26,27	0.53	0	33,39,42	0.66	0
20	PSU	W	1177	20	18,21,22	1.02	1 (5%)	22,30,33	0.73	0
20	A2M	W	1031	20	22,25,26	0.25	0	31,36,39	0.40	0
20	G7M	W	1639	20,24	23,26,27	0.66	0	35,39,42	0.55	0
20	PSU	W	300	20	18,21,22	1.01	1 (5%)	22,30,33	0.77	0
20	PSU	W	667	20	18,21,22	1.11	2 (11%)	22,30,33	0.70	0
20	UY1	W	1326	55,20	19,22,23	0.84	1 (5%)	22,31,34	0.70	0
20	PSU	W	1232	20	18,21,22	1.06	1 (5%)	22,30,33	0.78	0
20	OMC	W	1272	20	19,22,23	0.50	0	26,31,34	0.61	0
20	5MC	W	1374	20	18,22,23	0.46	0	26,32,35	0.52	0
20	MA6	W	1850	20	23,26,27	0.35	0	34,38,41	0.65	1 (2%)
20	OMU	W	1804	20	19,22,23	0.46	0	26,31,34	0.74	0
20	PSU	W	366	20	18,21,22	1.04	1 (5%)	22,30,33	0.72	0
20	PSU	W	1347	20	18,21,22	1.03	1 (5%)	22,30,33	0.73	0
20	PSU	W	609	20	18,21,22	0.87	1 (5%)	22,30,33	0.71	0
20	OMC	W	1391	20	19,22,23	0.50	0	26,31,34	0.69	0
20	PSU	W	1367	20	18,21,22	1.01	1 (5%)	22,30,33	0.78	0

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
20	PSU	W	1643	55,20	-	0/7/25/26	0/2/2/2
20	PSU	W	1596	20	-	0/7/25/26	0/2/2/2
24	5MC	y	48	24	-	0/7/25/26	0/2/2/2
20	A2M	W	668	55,20	-	4/9/27/28	0/3/3/3
20	PSU	W	651	20	-	0/7/25/26	0/2/2/2
24	T6A	y	37	24	-	3/23/41/42	0/3/3/3
20	PSU	W	572	20	-	0/7/25/26	0/2/2/2
20	PSU	W	1081	20	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PSU	W	1445	20	-	0/7/25/26	0/2/2/2
20	OMG	W	436	20	-	0/9/27/28	0/3/3/3
20	OMU	W	172	20	-	1/9/27/28	0/2/2/2
24	M2G	y	26	24	-	2/11/29/30	0/3/3/3
20	JMH	W	1219	55,20	-	0/7/25/26	0/2/2/2
20	5MU	W	814	20	-	0/7/25/26	0/2/2/2
20	OMU	W	121	20	-	0/9/27/28	0/2/2/2
20	PSU	W	966	20	-	0/7/25/26	0/2/2/2
20	PSU	W	1045	20	-	0/7/25/26	0/2/2/2
20	OMU	W	1442	20	-	2/9/27/28	0/2/2/2
20	A2M	W	590	20	-	1/9/27/28	0/3/3/3
20	PSU	W	34	20	-	0/7/25/26	0/2/2/2
20	PSU	W	612	20	-	0/7/25/26	0/2/2/2
24	H2U	y	47	24	-	5/7/38/39	0/2/2/2
20	PSU	W	105	20	-	0/7/25/26	0/2/2/2
20	OMU	W	1288	20	-	2/9/27/28	0/2/2/2
24	RIA	y	64	24	-	2/17/51/52	0/4/4/4
20	A2M	W	576	20	-	2/9/27/28	0/3/3/3
20	PSU	W	296	20	-	2/7/25/26	0/2/2/2
20	A2M	W	484	20	-	1/9/27/28	0/3/3/3
20	A2M	W	99	55,20	-	0/9/27/28	0/3/3/3
20	PSU	W	109	20	-	0/7/25/26	0/2/2/2
20	PSU	W	1625	20	-	0/7/25/26	0/2/2/2
20	PSU	W	863	20	-	0/7/25/26	0/2/2/2
20	PSU	W	1186	20	-	0/7/25/26	0/2/2/2
20	OMG	W	867	20	-	0/9/27/28	0/3/3/3
20	PSU	W	119	20	-	0/7/25/26	0/2/2/2
24	H2U	y	16	24	-	5/7/38/39	0/2/2/2
20	C4J	W	1248	20	-	2/16/34/35	0/2/2/2
20	OMG	W	1490	55,20	-	3/9/27/28	0/3/3/3
20	PSU	W	649	20	-	0/7/25/26	0/2/2/2
20	A2M	W	1678	20	-	0/9/27/28	0/3/3/3
20	OMC	W	1703	20	-	0/9/27/28	0/2/2/2
20	A2M	W	1383	20	-	0/9/27/28	0/3/3/3
20	PSU	W	918	20	-	0/7/25/26	0/2/2/2
20	PSU	W	815	20	-	0/7/25/26	0/2/2/2
20	OMC	W	174	55,20	-	0/9/27/28	0/2/2/2
20	4AC	W	1842	20	-	0/11/29/30	0/2/2/2
20	4AC	W	1337	20	-	0/11/29/30	0/2/2/2
20	PSU	W	801	20	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	OMC	W	462	20	-	0/9/27/28	0/2/2/2
20	PSU	W	1004	20	-	0/7/25/26	0/2/2/2
20	PSU	W	1046	20	-	0/7/25/26	0/2/2/2
20	PSU	W	1238	20	-	0/7/25/26	0/2/2/2
20	MA6	W	1851	20	-	2/11/29/30	0/3/3/3
20	A2M	W	159	20	-	3/9/27/28	0/3/3/3
20	PSU	W	1056	20	-	0/7/25/26	0/2/2/2
24	1MA	y	58	24	-	1/7/25/26	0/3/3/3
20	OMG	W	601	20	-	0/9/27/28	0/3/3/3
20	PSU	W	406	20	-	0/7/25/26	0/2/2/2
20	OMC	W	517	20	-	0/9/27/28	0/2/2/2
20	OMG	W	644	20	-	1/9/27/28	0/3/3/3
20	A2M	W	512	20	-	3/9/27/28	0/3/3/3
20	PSU	W	1003	20	-	0/7/25/26	0/2/2/2
20	OMU	W	428	20	-	6/9/27/28	0/2/2/2
20	PSU	W	1692	20	-	0/7/25/26	0/2/2/2
20	PSU	W	686	20	-	2/7/25/26	0/2/2/2
20	PSU	W	681	20	-	0/7/25/26	0/2/2/2
20	OMG	W	1328	20	-	1/9/27/28	0/3/3/3
20	OMU	W	116	20	-	0/9/27/28	0/2/2/2
20	PSU	W	1360	56,55,20	-	0/7/25/26	0/2/2/2
20	PSU	W	822	20	-	0/7/25/26	0/2/2/2
20	OMU	W	354	20	-	0/9/27/28	0/2/2/2
24	7MG	y	46	24	-	1/7/37/38	0/3/3/3
20	A2M	W	27	55,20	-	0/9/27/28	0/3/3/3
20	OMG	W	683	20	-	0/9/27/28	0/3/3/3
20	PSU	W	1174	20	-	0/7/25/26	0/2/2/2
20	PSU	W	63	20	-	0/7/25/26	0/2/2/2
24	2MG	y	10	24	-	0/9/27/28	0/3/3/3
20	PSU	W	36	20	-	0/7/25/26	0/2/2/2
20	A2M	W	166	20	-	1/9/27/28	0/3/3/3
20	OMG	W	1447	20	-	3/9/27/28	0/3/3/3
20	PSU	W	218	20	-	0/7/25/26	0/2/2/2
20	A2M	W	468	20	-	0/9/27/28	0/3/3/3
20	OMG	W	509	55,20	-	1/9/27/28	0/3/3/3
24	5MC	y	49	24	-	2/7/25/26	0/2/2/2
20	PSU	W	1244	20	-	0/7/25/26	0/2/2/2
20	PSU	W	1136	20	-	0/7/25/26	0/2/2/2
20	PSU	W	866	20	-	0/7/25/26	0/2/2/2
20	PSU	W	100	55,20	-	0/7/25/26	0/2/2/2
20	6MZ	W	1832	55,20	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	1MG	y	9	24	-	2/7/25/26	0/3/3/3
20	PSU	W	1177	20	-	0/7/25/26	0/2/2/2
20	A2M	W	1031	20	-	0/9/27/28	0/3/3/3
20	G7M	W	1639	20,24	-	2/7/25/26	0/3/3/3
20	PSU	W	300	20	-	0/7/25/26	0/2/2/2
20	PSU	W	667	20	-	1/7/25/26	0/2/2/2
20	UY1	W	1326	55,20	-	1/9/27/28	0/2/2/2
20	PSU	W	1232	20	-	0/7/25/26	0/2/2/2
20	OMC	W	1272	20	-	0/9/27/28	0/2/2/2
20	5MC	W	1374	20	-	0/7/25/26	0/2/2/2
20	MA6	W	1850	20	-	0/11/29/30	0/3/3/3
20	OMU	W	1804	20	-	0/9/27/28	0/2/2/2
20	PSU	W	366	20	-	0/7/25/26	0/2/2/2
20	PSU	W	1347	20	-	0/7/25/26	0/2/2/2
20	PSU	W	609	20	-	2/7/25/26	0/2/2/2
20	OMC	W	1391	20	-	1/9/27/28	0/2/2/2
20	PSU	W	1367	20	-	0/7/25/26	0/2/2/2

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	46	7MG	C5-N7	4.69	1.41	1.35
20	W	1625	PSU	C6-C5	3.41	1.39	1.35
20	W	866	PSU	C6-C5	3.40	1.39	1.35
20	W	801	PSU	C6-C5	3.36	1.39	1.35
20	W	1232	PSU	C6-C5	3.34	1.39	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	37	T6A	C12-N11-C10	7.74	134.83	121.94
20	W	576	A2M	C2'-C1'-N9	-5.46	104.34	113.53
20	W	512	A2M	O3'-C3'-C4'	5.16	125.97	111.05
20	W	668	A2M	O3'-C3'-C2'	5.00	125.36	111.17
20	W	512	A2M	C2'-C1'-N9	-4.74	105.55	113.53

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	W	159	A2M	C1'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
20	W	166	A2M	C1'-C2'-O2'-CM'
20	W	172	OMU	C1'-C2'-O2'-CM2
20	W	296	PSU	C3'-C4'-C5'-O5'
20	W	484	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

29 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	W	668	A2M	1	0
24	y	37	T6A	2	0
24	y	26	M2G	1	0
20	W	1442	OMU	1	0
24	y	64	RIA	1	0
20	W	576	A2M	1	0
20	W	484	A2M	2	0
20	W	99	A2M	2	0
20	W	867	OMG	1	0
20	W	1490	OMG	2	0
20	W	1678	A2M	1	0
20	W	1851	MA6	1	0
20	W	159	A2M	1	0
20	W	428	OMU	1	0
20	W	681	PSU	1	0
20	W	1328	OMG	1	0
20	W	116	OMU	1	0
24	y	10	2MG	1	0
20	W	166	A2M	2	0
20	W	1447	OMG	1	0
20	W	509	OMG	1	0
24	y	49	5MC	1	0
20	W	100	PSU	1	0
24	y	9	1MG	2	0
20	W	1031	A2M	1	0
20	W	1639	G7M	1	0
20	W	1804	OMU	1	0
20	W	609	PSU	1	0
20	W	1391	OMC	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 94 ligands modelled in this entry, 94 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

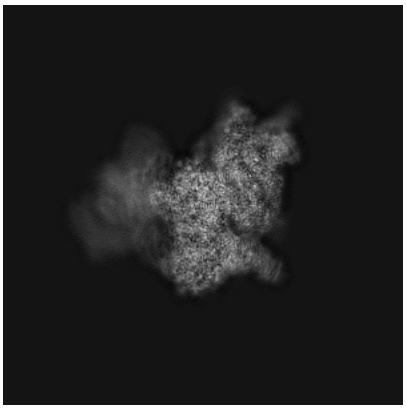
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-54936. These allow visual inspection of the internal detail of the map and identification of artifacts.

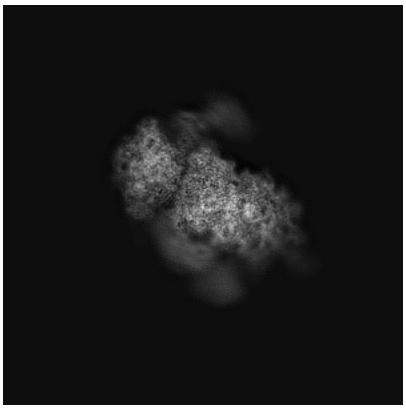
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

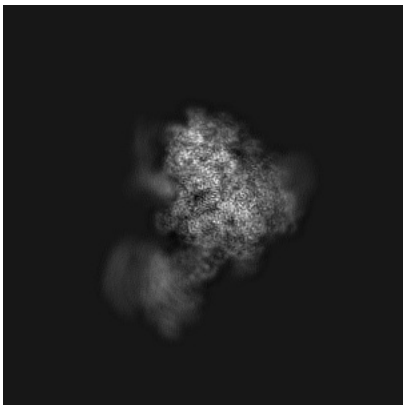
6.1.1 Primary map



X

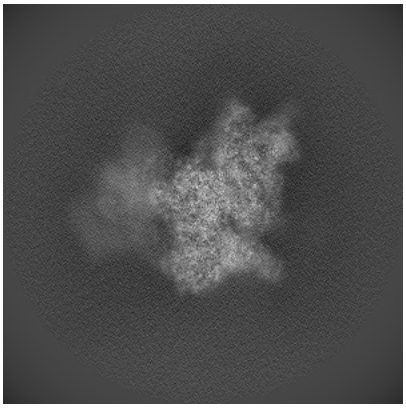


Y

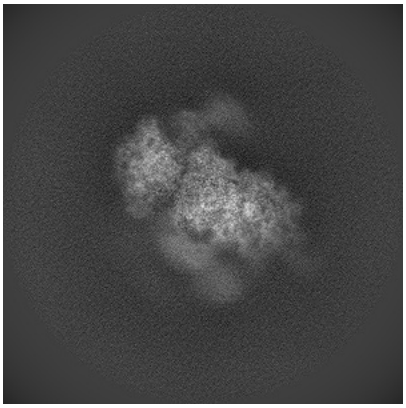


Z

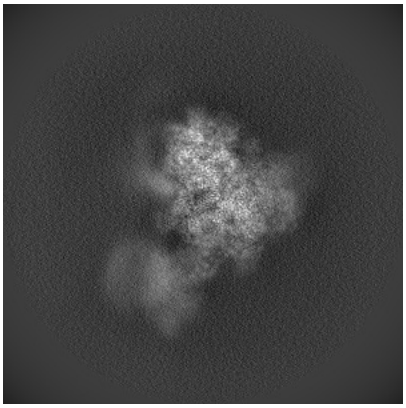
6.1.2 Raw map



X



Y



Z

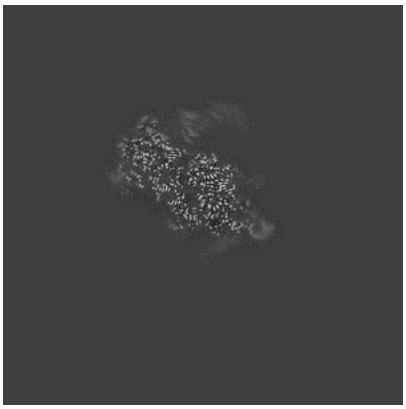
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 300

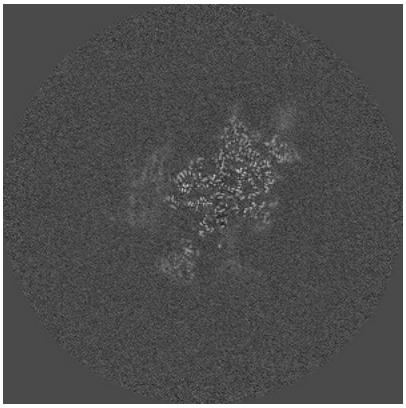


Y Index: 300

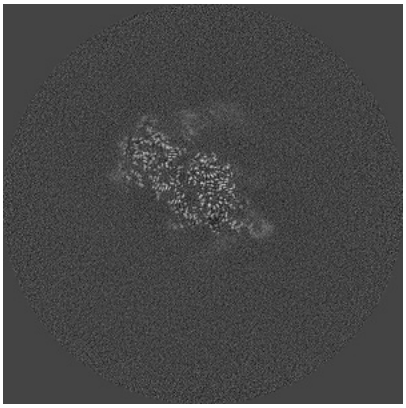


Z Index: 300

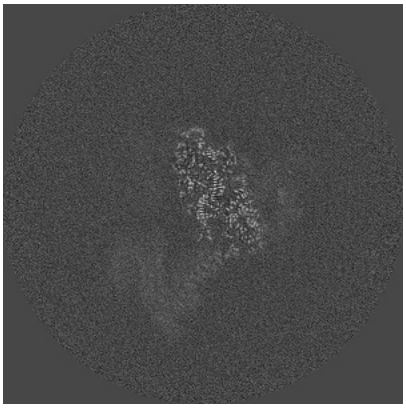
6.2.2 Raw map



X Index: 300



Y Index: 300

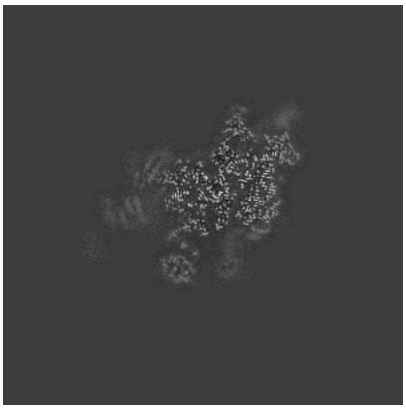


Z Index: 300

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

6.3 Largest variance slices (i)

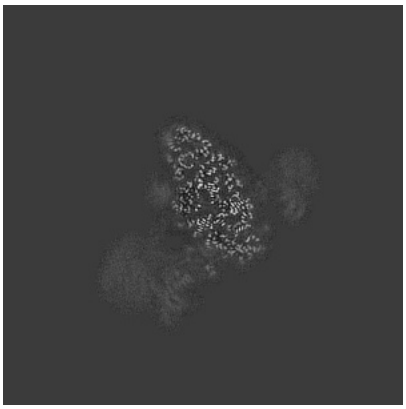
6.3.1 Primary map



X Index: 293

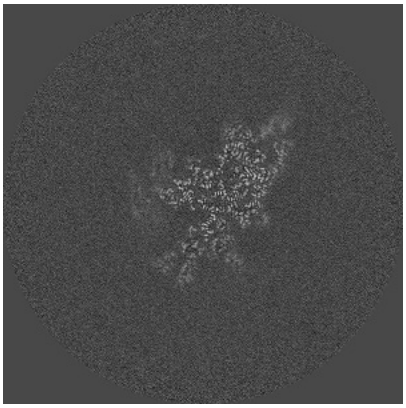


Y Index: 296

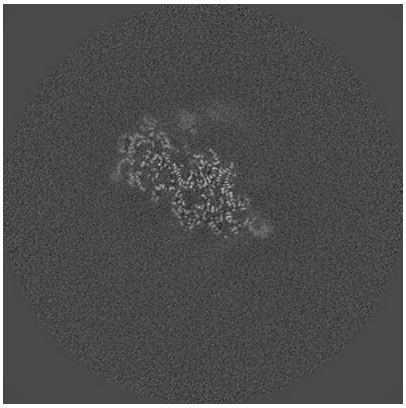


Z Index: 318

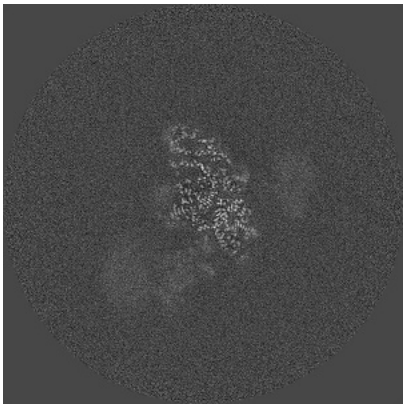
6.3.2 Raw map



X Index: 309



Y Index: 296

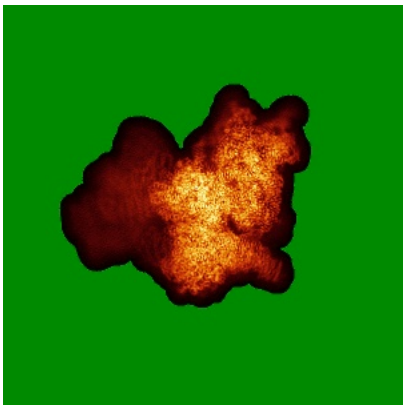


Z Index: 325

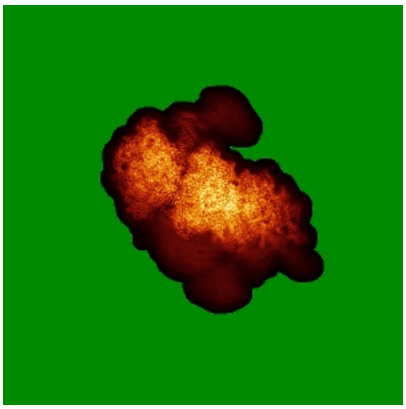
The images above show the largest variance slices of the map in three orthogonal directions.

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

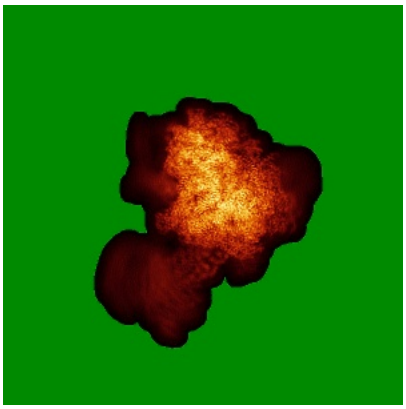
6.4.1 Primary map



X

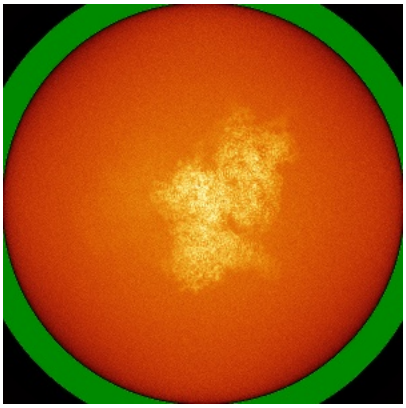


Y

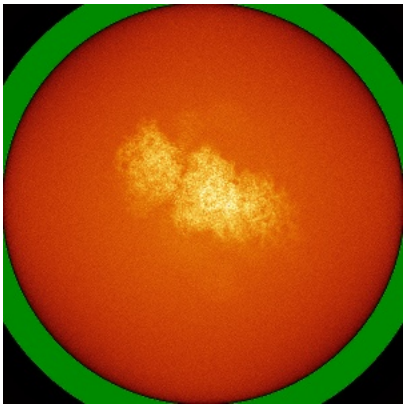


Z

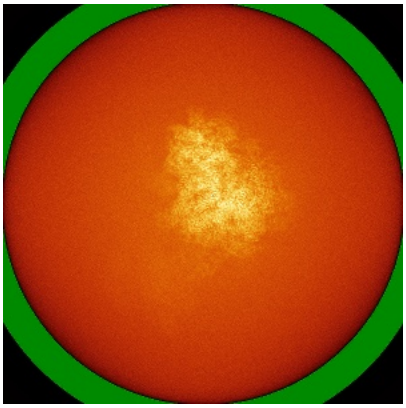
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

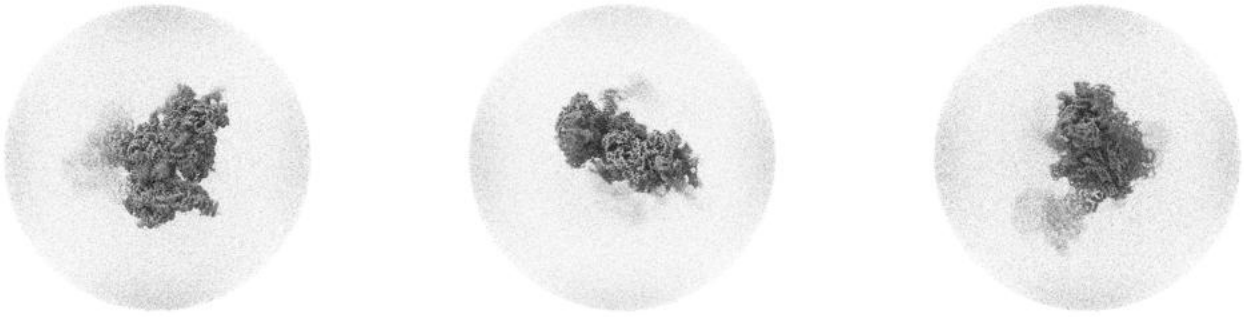
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0045. 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.

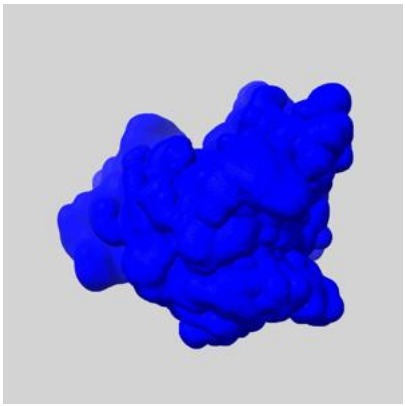
6.6 Mask visualisation

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

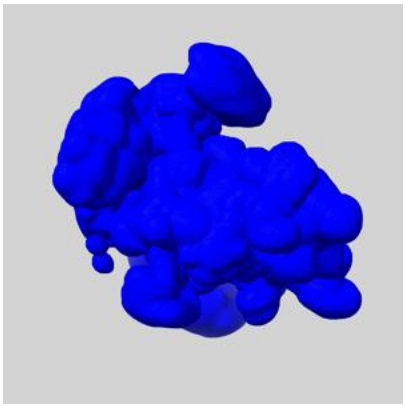
A mask typically either:

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

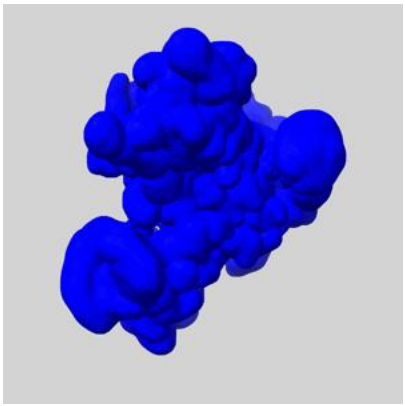
6.6.1 emd_54936_msk_1.map



X



Y

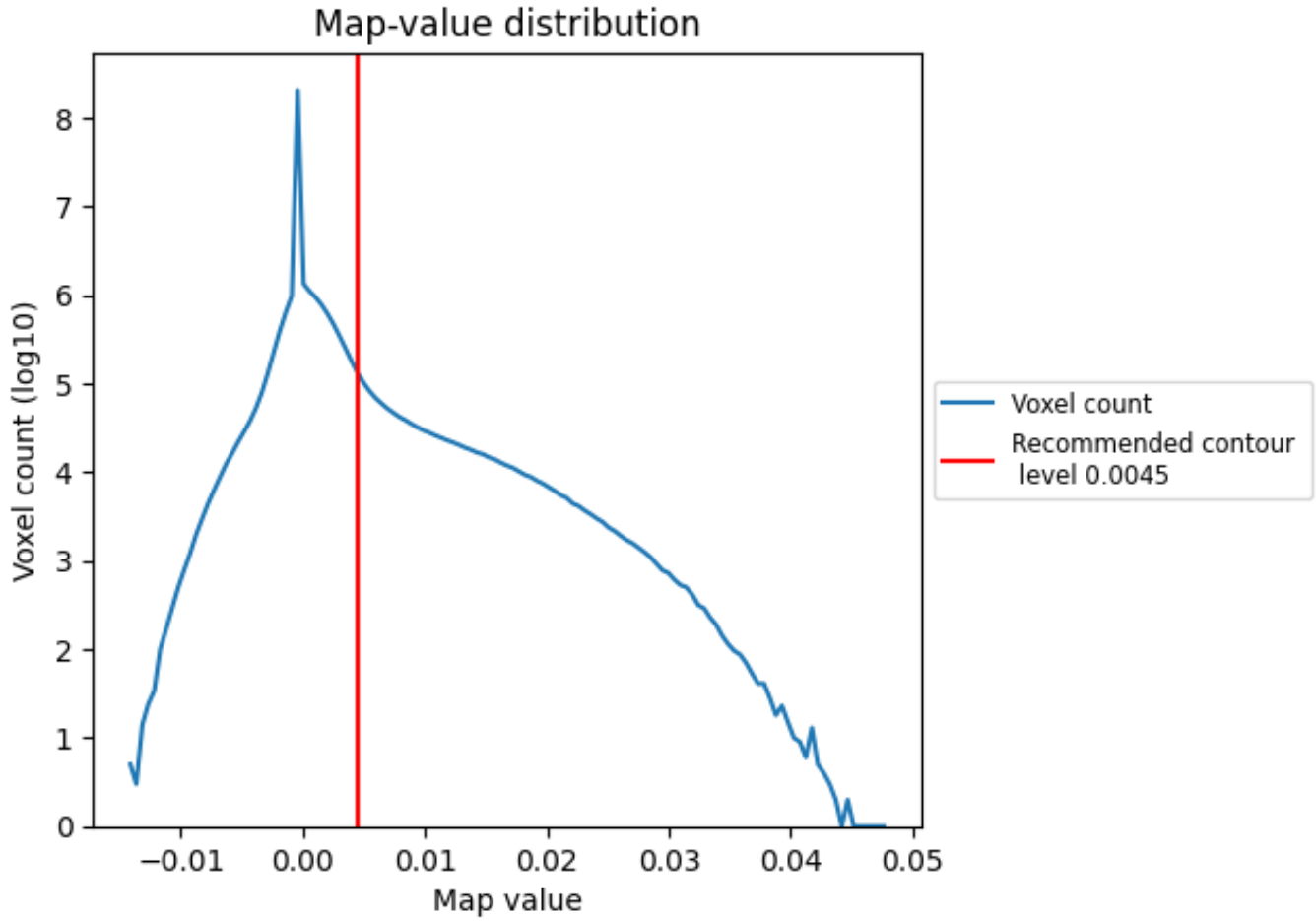


Z

7 Map analysis

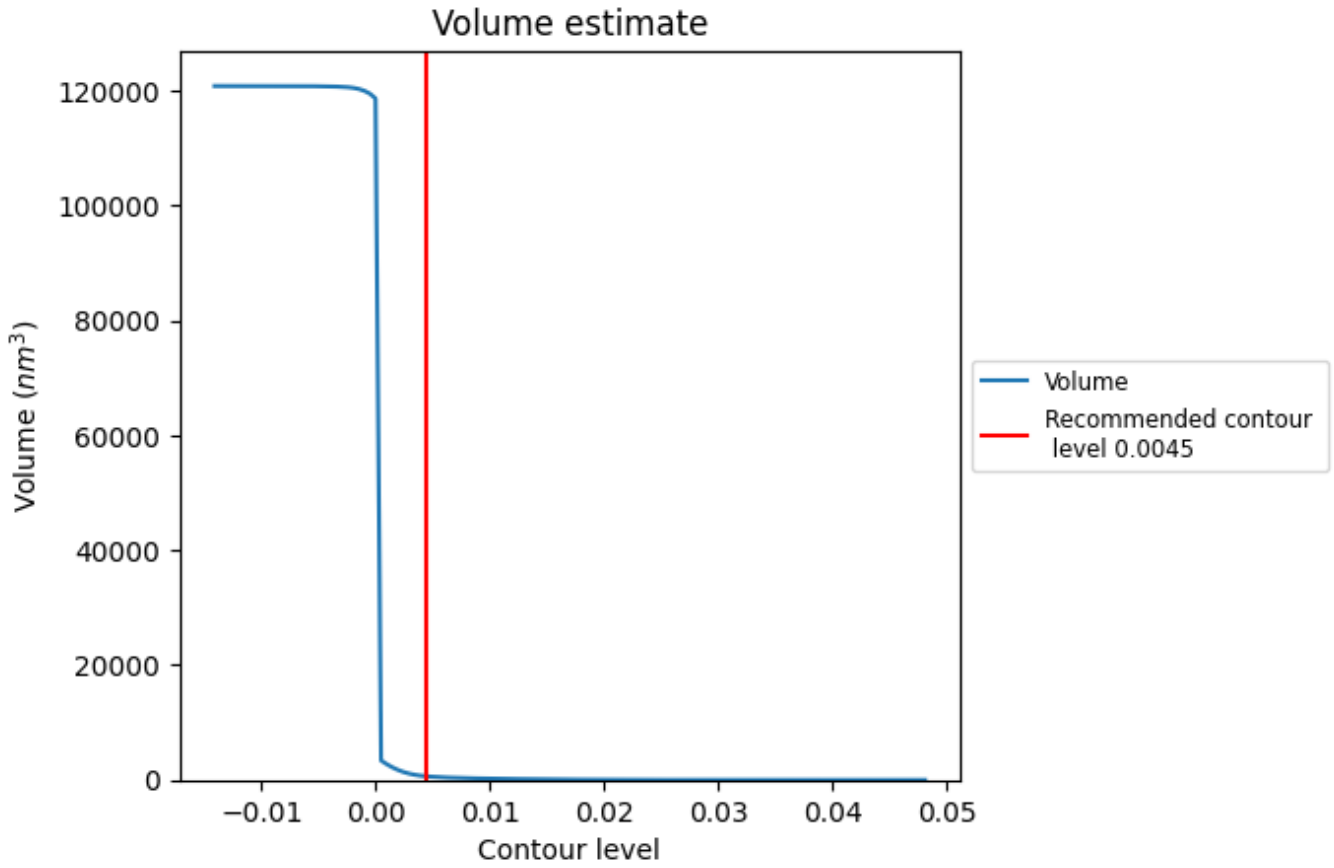
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

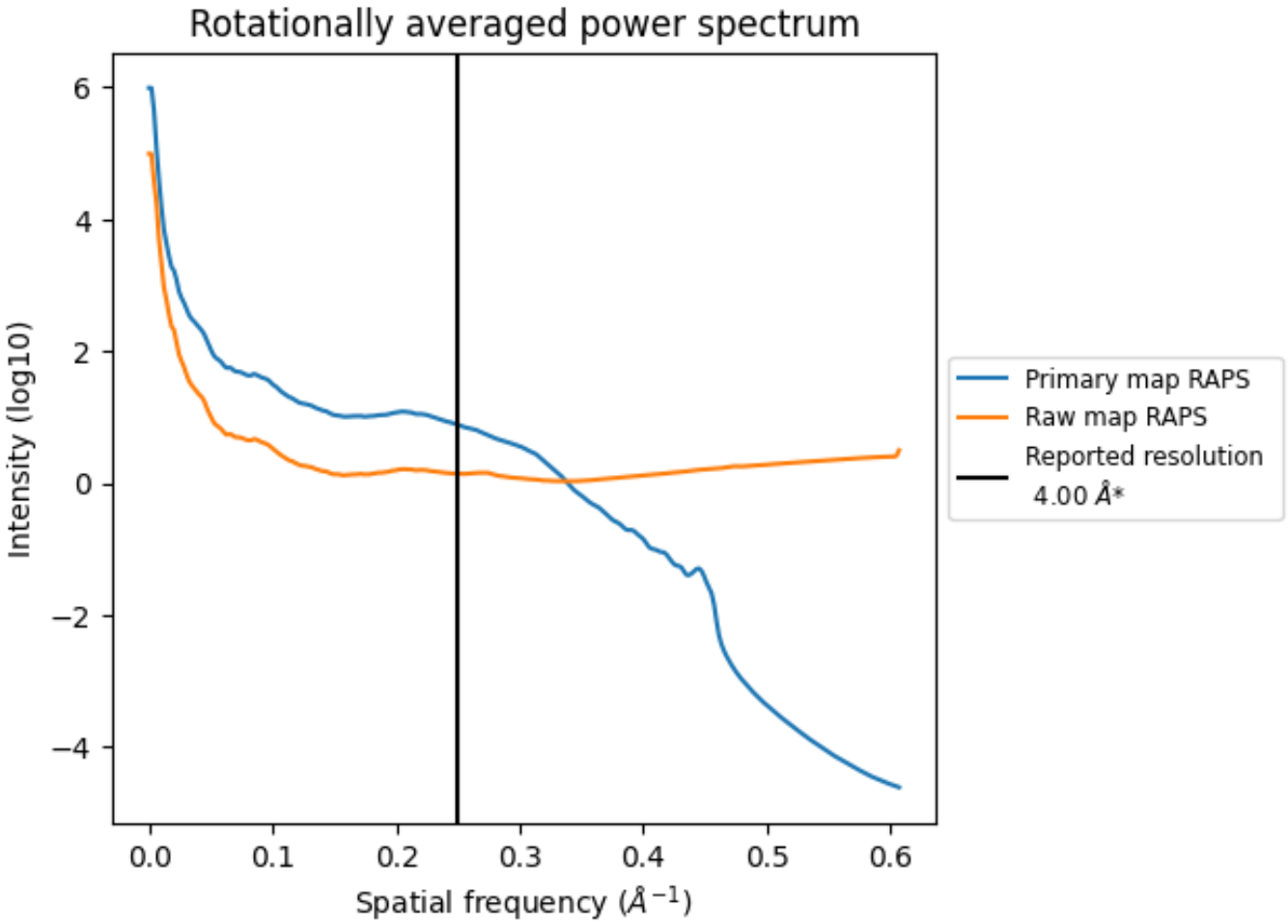
7.2 Volume estimate (i)



The volume at the recommended contour level is 623 nm^3; this corresponds to an approximate mass of 563 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)

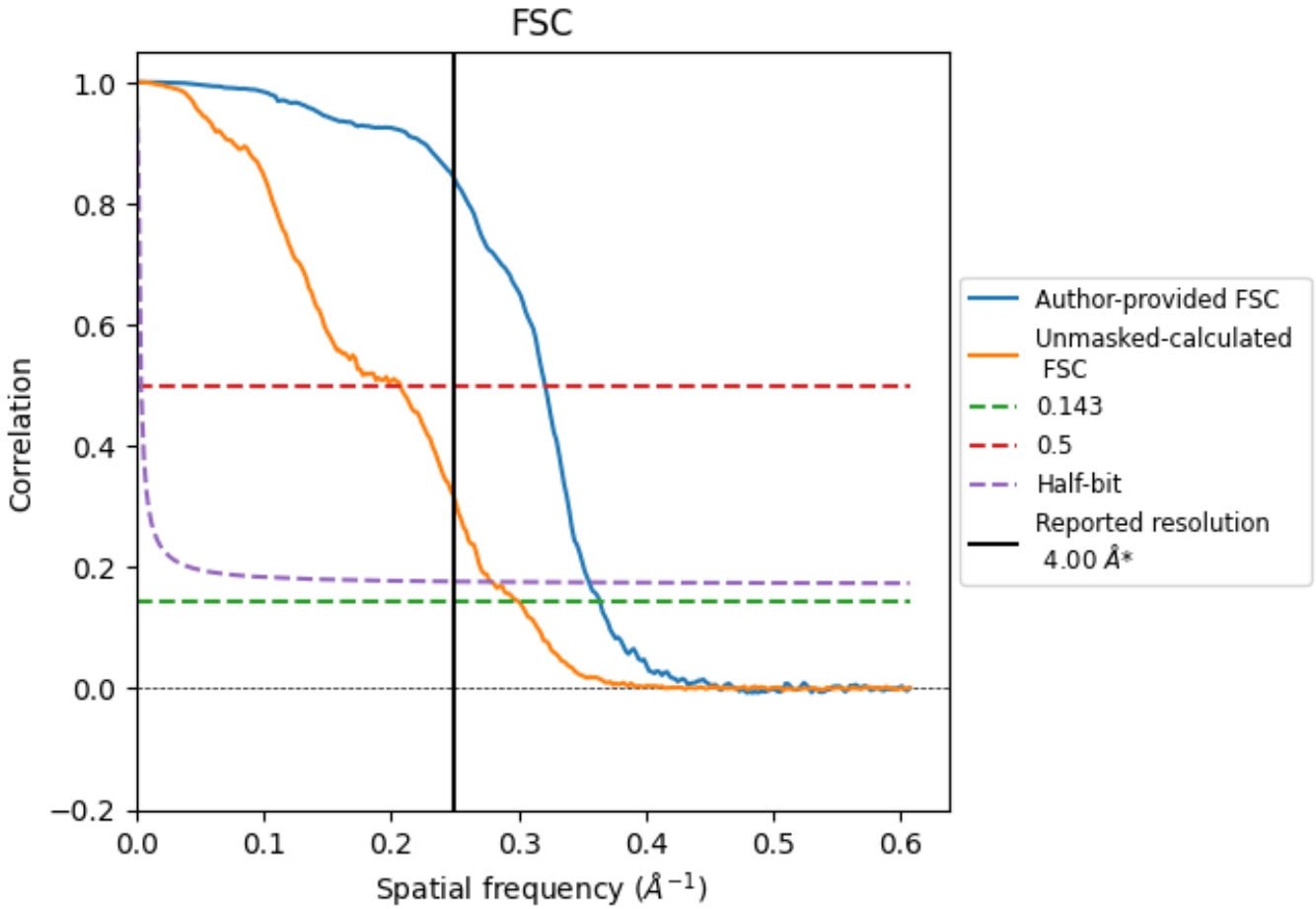


*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	2.75	3.12	2.81
Unmasked-calculated*	3.33	4.83	3.58

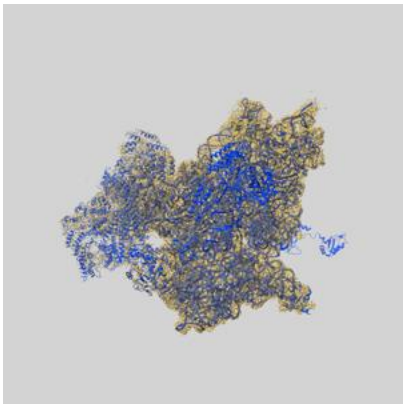
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.75 differs from the reported value 4.0 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.33 differs from the reported value 4.0 by more than 10 %

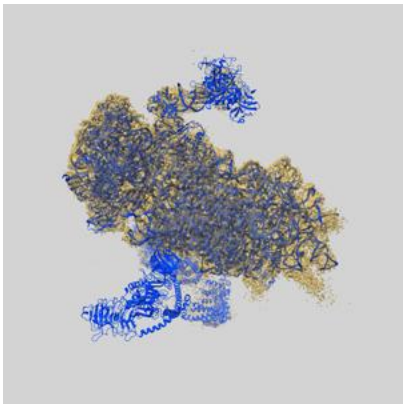
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-54936 and PDB model 9SJ3. Per-residue inclusion information can be found in section 3 on page 14.

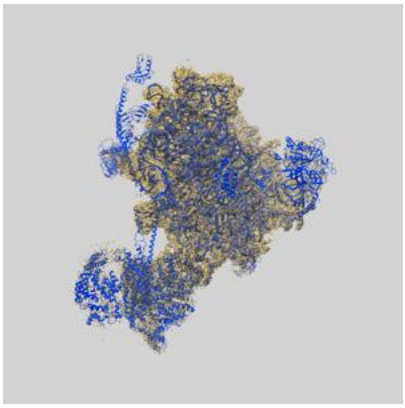
9.1 Map-model overlay



X



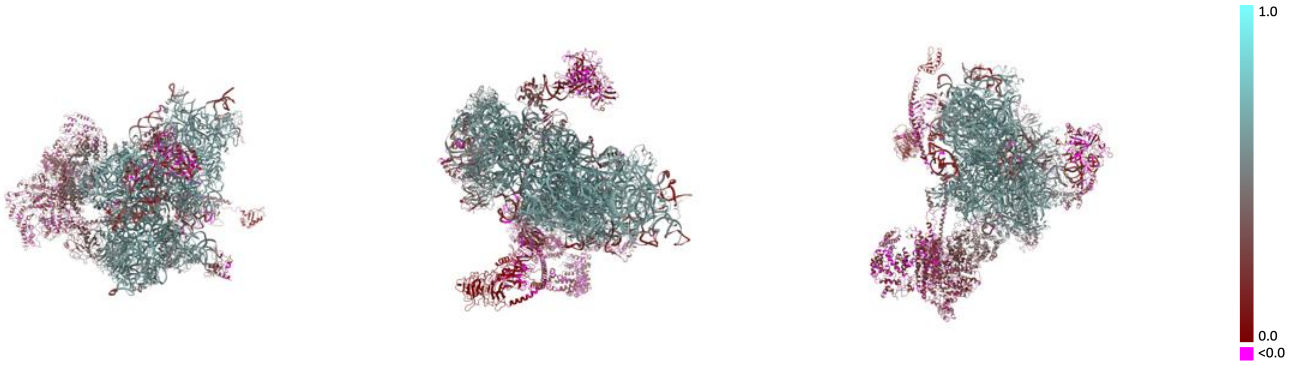
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

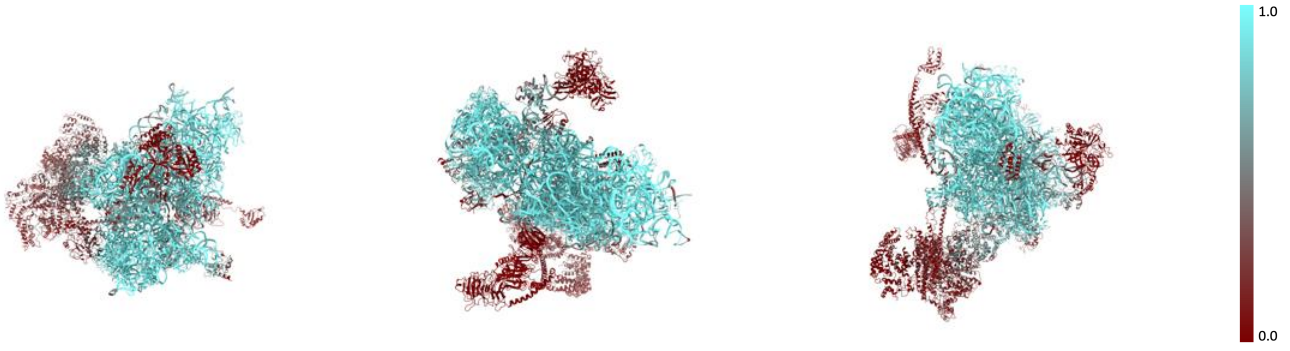
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

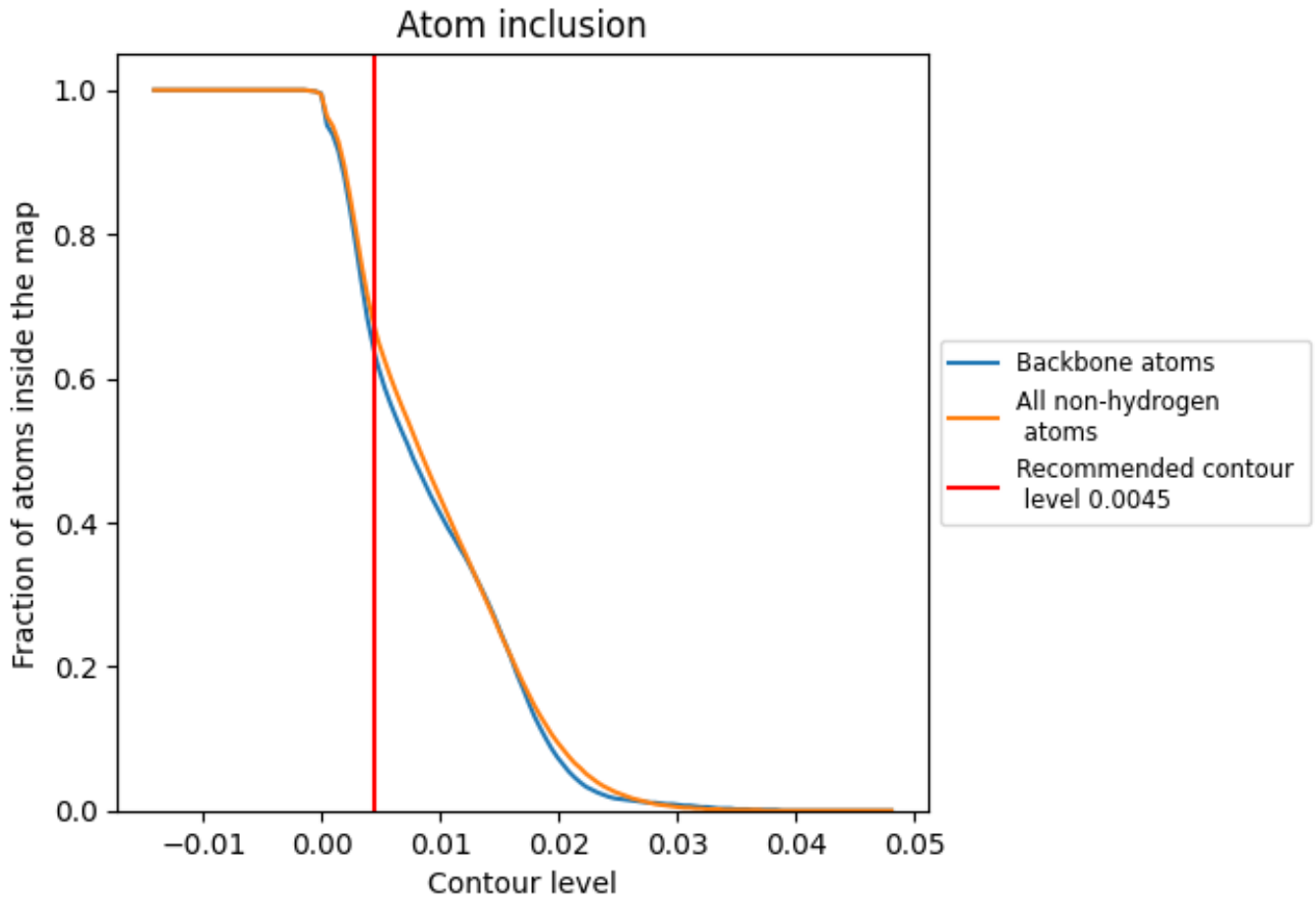
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0045).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 67% 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 (0.0045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6690	0.4590
3	0.0290	0.1560
4	0.0730	0.1770
5	0.0410	0.1320
6	0.0740	0.1630
7	0.1400	0.2640
8	0.0450	0.1390
9	0.8610	0.5980
A	0.2570	0.2620
B	0.1000	0.1740
D	0.4000	0.3380
E	0.0140	0.1030
F	0.0000	-0.0010
G	0.5030	0.4110
H	0.1130	0.2860
I	0.0040	0.1130
J	0.3320	0.3200
L	0.8020	0.5260
M	0.9080	0.6040
N	0.9340	0.6140
O	0.9430	0.6390
P	0.9330	0.6090
Q	0.9420	0.6200
R	0.9420	0.6240
S	0.9000	0.5410
T	0.9290	0.6140
V	0.9300	0.6100
W	0.9560	0.5880
X	0.9370	0.6290
Y	0.9600	0.6330
Z	0.9370	0.6280
a	0.9620	0.6380
b	0.8080	0.5750
c	0.9620	0.6480
d	0.9270	0.5910



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	0.9350	0.6100
f	0.9290	0.6080
g	0.9390	0.6170
h	0.8810	0.5820
i	0.8530	0.5450
j	0.8960	0.5660
k	0.8570	0.5320
l	0.9270	0.5920
m	0.8940	0.5680
n	0.8850	0.5560
o	0.9410	0.6310
p	0.5780	0.2630
q	0.4690	0.2730
s	0.8600	0.5770
v	0.8690	0.5730
w	0.8370	0.5430
x	0.2380	0.3250
y	0.6500	0.3620
z	0.4350	0.3690