wwPDB EM Validation Summary Report ⓘ

Feb 26, 2024 – 06:21 AM EST

PDB ID	:	6W2S
EMDB ID	:	EMD-21529
Title	:	Structure of the Cricket Paralysis Virus 5-UTR IRES (CrPV 5-UTR-IRES) bound to the small ribosomal subunit in the open state (Class 1)
Authors	:	Neupane, R.; Pisareva, V.; Rodriguez, C.F.; Pisarev, A.; Fernandez, I.S.
Deposited on	:	2020-03-08
Resolution	:	3.47 Å(reported)

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

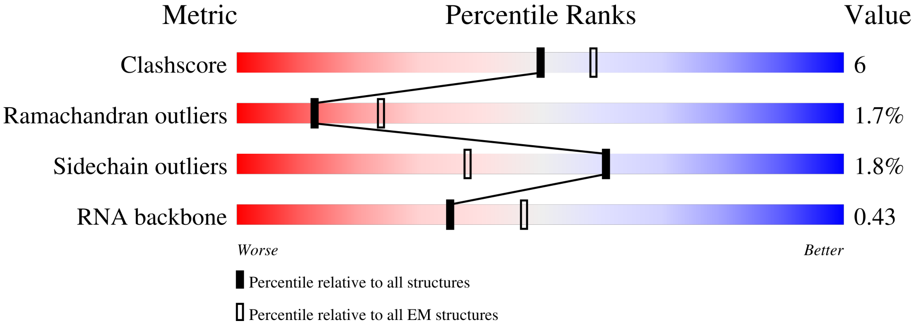
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

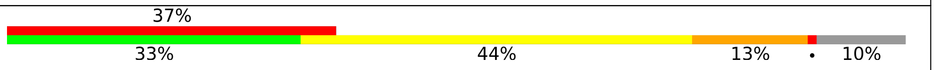
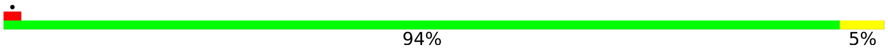
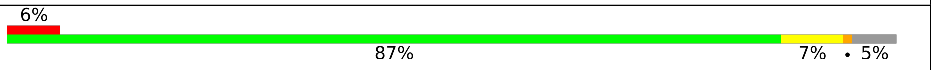
The reported resolution of this entry is 3.47 Å.

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	1697	
2	0	377	
3	B	295	
4	C	264	
5	D	255	
6	F	263	
7	H	249	

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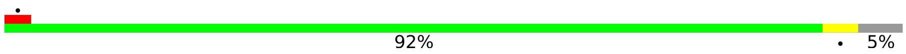
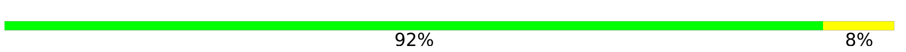
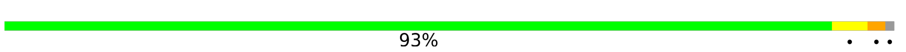
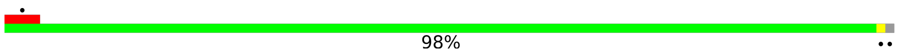
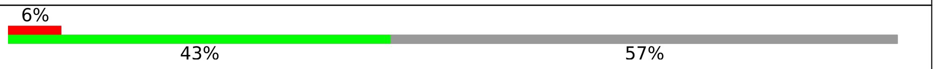
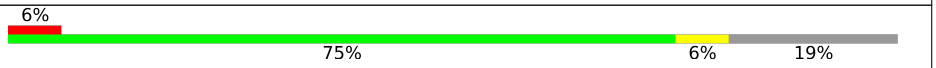
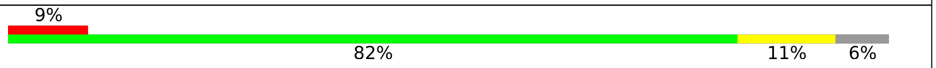
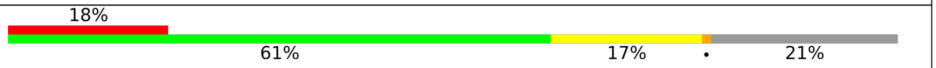
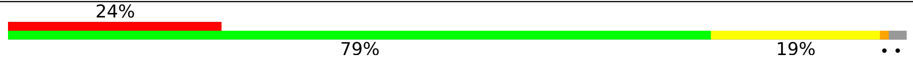
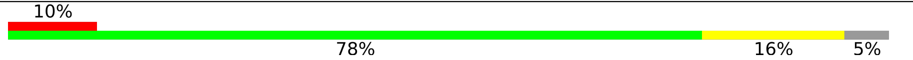
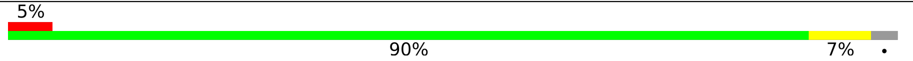
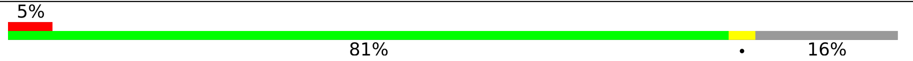
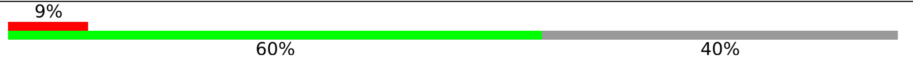
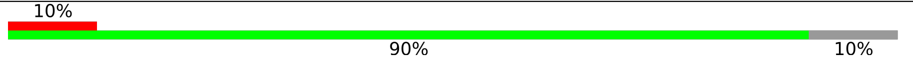
Mol	Chain	Length	Quality of chain
8	I	194	
9	J	208	
10	K	194	
11	M	158	
12	O	151	
13	P	151	
14	W	83	
15	X	130	
16	Y	143	
17	Z	134	
18	b	115	
19	c	84	
20	f	133	
21	E	281	
22	G	204	
23	L	149	
24	N	132	
25	Q	145	
26	R	172	
27	S	135	
28	T	152	
29	U	145	
30	V	119	
31	a	125	
32	d	69	

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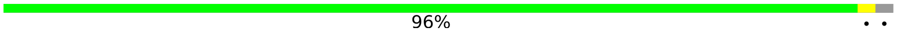
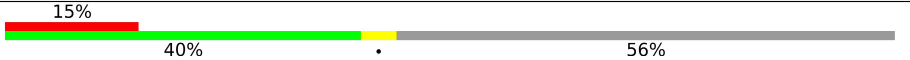
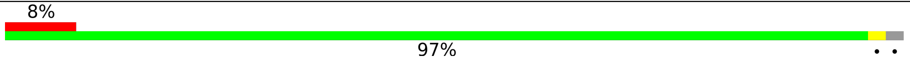
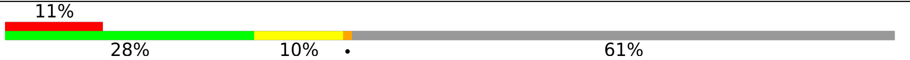
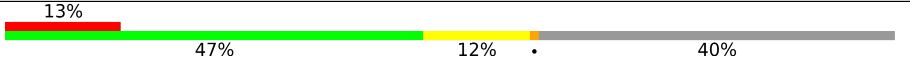
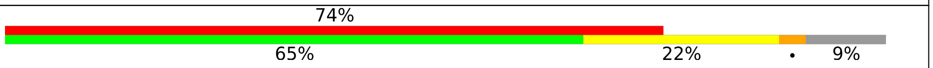
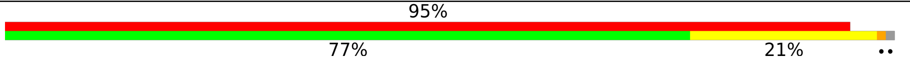
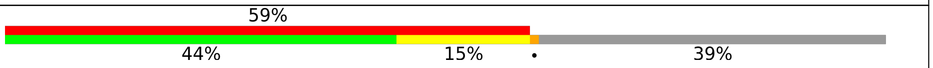
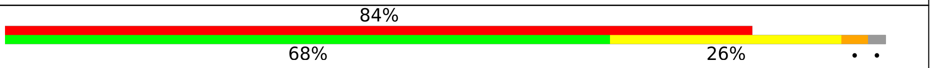
Mol	Chain	Length	Quality of chain
33	e	56	
34	g	156	
35	h	317	
36	1	1362	
37	2	913	
38	3	462	
39	4	364	
40	5	363	
41	6	218	
42	7	607	
43	8	374	

2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 106911 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1697	36229	16171	6507	11855	1696	0	0

- Molecule 2 is a RNA chain called CrPV 5'-UTR IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	0	339	7205	3222	1255	2389	339	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	569	U	C	conflict	GB 8895506
0	570	U	C	conflict	GB 8895506
0	571	U	A	conflict	GB 8895506
0	572	U	C	conflict	GB 8895506
0	574	U	C	conflict	GB 8895506
0	575	U	G	conflict	GB 8895506
0	729	G	-	expression tag	GB 8895506
0	730	G	-	expression tag	GB 8895506
0	731	A	-	expression tag	GB 8895506
0	732	U	-	expression tag	GB 8895506
0	733	C	-	expression tag	GB 8895506

- Molecule 3 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	217	1706	1084	296	318	8	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	114	THR	ALA	conflict	UNP G1TWL4
B	135	THR	MET	conflict	UNP G1TWL4
B	155	ARG	HIS	conflict	UNP G1TWL4
B	162	PRO	LEU	conflict	UNP G1TWL4

- Molecule 4 is a protein called eS1.

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

- Molecule 5 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	221	1717	1113	296	299	9	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	57	ASN	ASP	conflict	UNP G1SWM1
D	97	PHE	CYS	conflict	UNP G1SWM1
D	181	PRO	LEU	conflict	UNP G1SWM1
D	191	VAL	-	insertion	UNP G1SWM1

- Molecule 6 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	262	2072	1323	384	357	8	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	25	GLY	SER	conflict	UNP G1TK17
F	156	VAL	MET	conflict	UNP G1TK17

- Molecule 7 is a protein called eS6.

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

- Molecule 8 is a protein called eS7.

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

- Molecule 9 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	206	1686	1058	332	291	5	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 10 is a protein called uS4.

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

- Molecule 11 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	M	143	1175	749	222	198	6	0	0

- Molecule 12 is a protein called uS15.

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

- Molecule 13 is a protein called uS11.

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

- Molecule 14 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	83	Total 634	C 390	N 116	O 123	S 5	0	0

- Molecule 15 is a protein called uS8.

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

- Molecule 16 is a protein called uS12.

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

- Molecule 17 is a protein called eS24.

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

- Molecule 18 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	101	Total 816	C 509	N 170	O 132	S 5	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 19 is a protein called eS27.

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

- Molecule 20 is a protein called eS30.

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

- Molecule 21 is a protein called uS3.

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

- Molecule 22 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	G	191	1499	937	283	272	7	0	0

- Molecule 23 is a protein called eS10.

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

- Molecule 24 is a protein called eS12.

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

- Molecule 25 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Q	115	956	610	176	163	7	0	0

- Molecule 26 is a protein called uS9.

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

- Molecule 27 is a protein called eS17.

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

- Molecule 28 is a protein called uS13.

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

- Molecule 29 is a protein called eS19.

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

- Molecule 30 is a protein called uS10.

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

- Molecule 31 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 32 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 33 is a protein called eS29.

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

- Molecule 34 is a protein called eS31.

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

- Molecule 35 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	h	312	2429	1531	423	463	12	0	0

- Molecule 36 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	1	534	4377	2770	778	808	21	0	0

- Molecule 37 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	2	547	4446	2791	785	837	33	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	671	GLU	VAL	conflict	UNP G1U971

- Molecule 38 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	3	419	3465	2220	586	639	20	0	0

- Molecule 39 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	4	272	2111	1330	359	410	12	0	0

- Molecule 40 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	5	324	Total	C	N	O	S	0	0
			2624	1654	452	503	15		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	6	215	Total	C	N	O	S	0	0
			1737	1109	285	330	13		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	7	372	Total	C	N	O	S	0	0
			3109	2010	519	563	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	8	365	Total	C	N	O	S	0	0
			2918	1850	493	558	17		

- Molecule 44 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
44	A	1	Total	Mg	0
			1	1	

- Molecule 45 is ZINC ION (three-letter code: ZN) (formula: Zn).

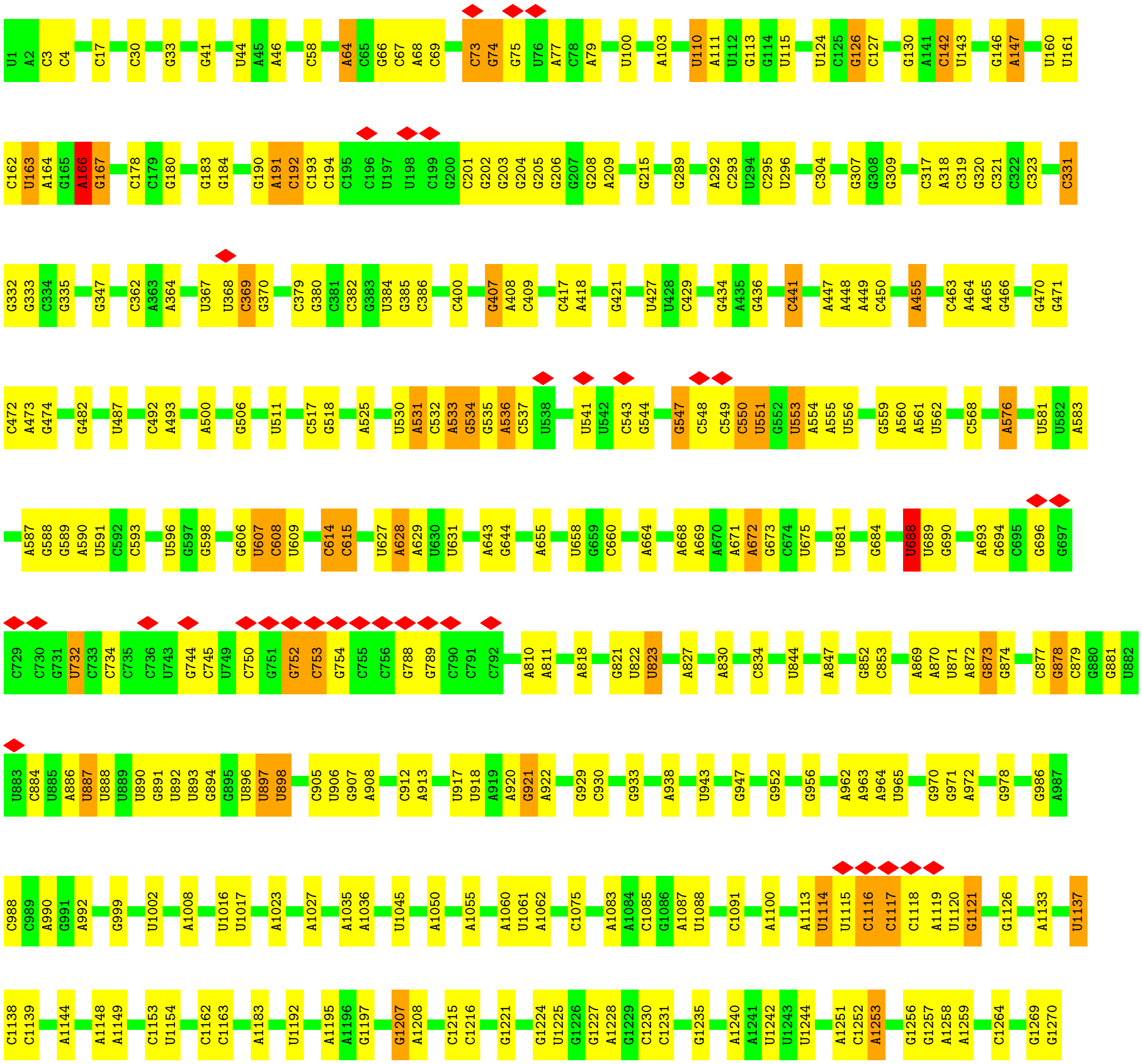
Mol	Chain	Residues	Atoms		AltConf
45	b	1	Total	Zn	0
			1	1	

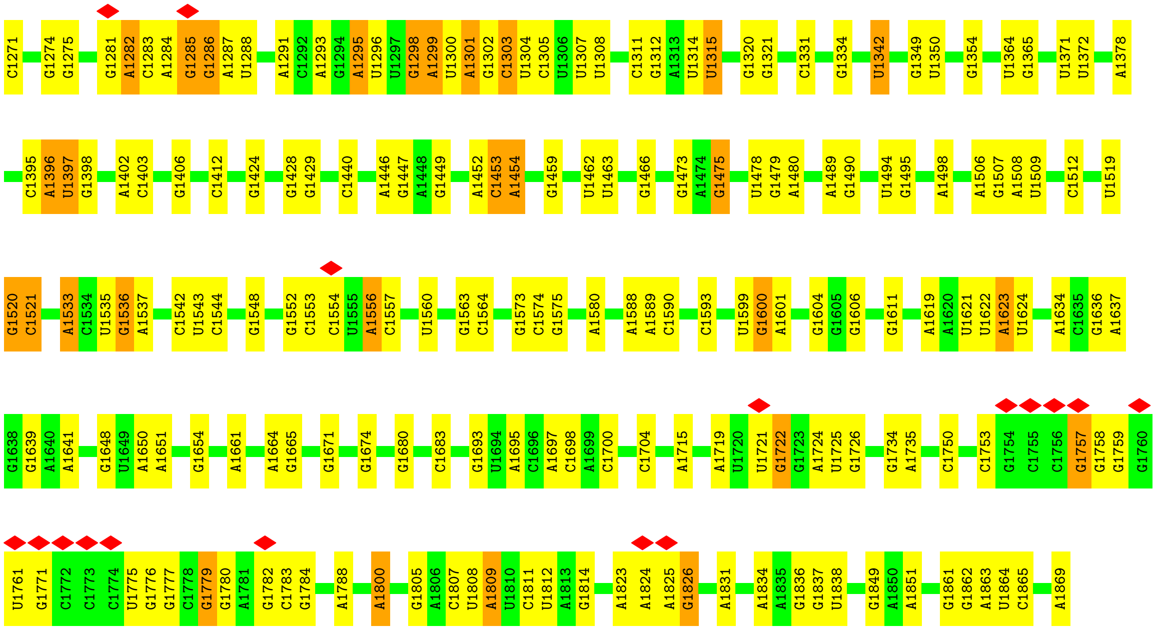
3 Residue-property plots

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

- Molecule 1: 18S rRNA

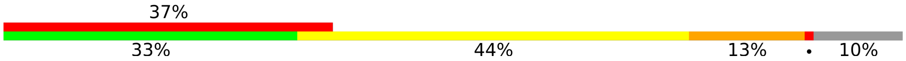
Chain A:

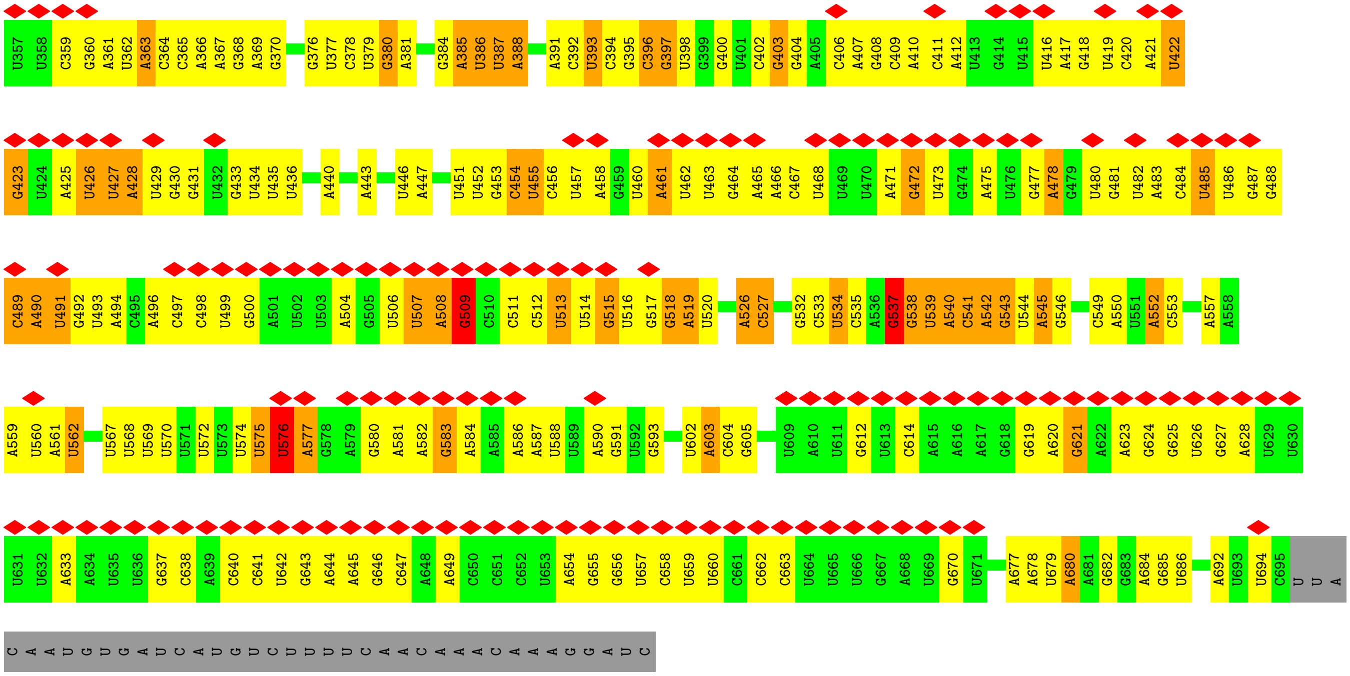




- Molecule 2: CrPV 5'-UTR IRES

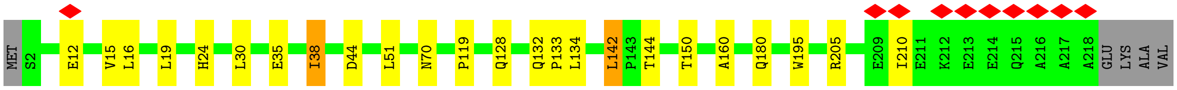
Chain 0:

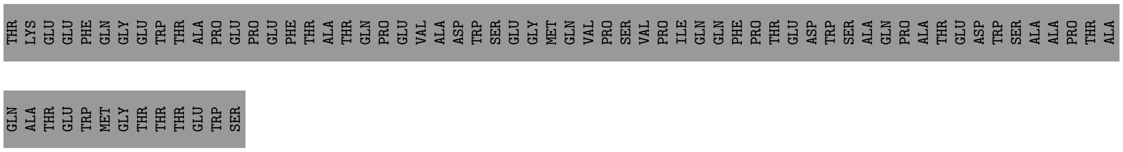




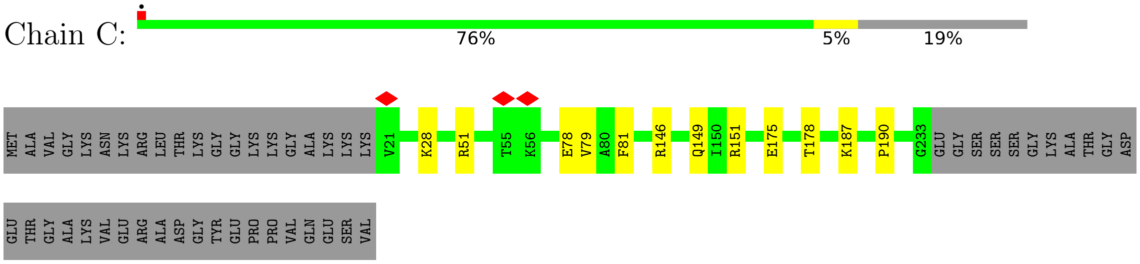
- Molecule 3: uS2

Chain B:

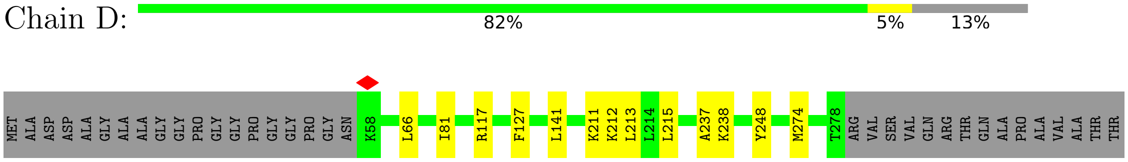




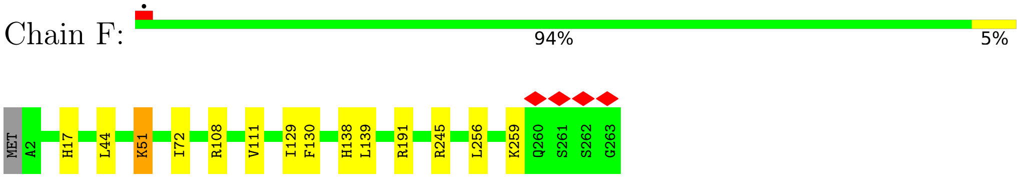
- Molecule 4: eS1



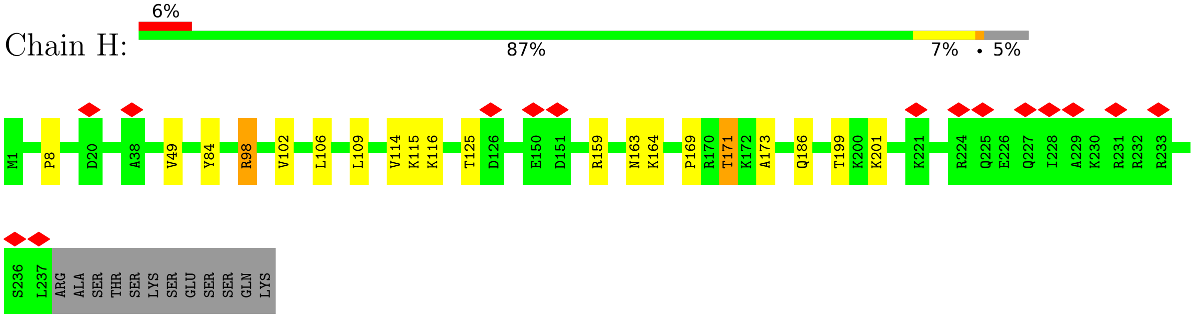
- Molecule 5: uS5



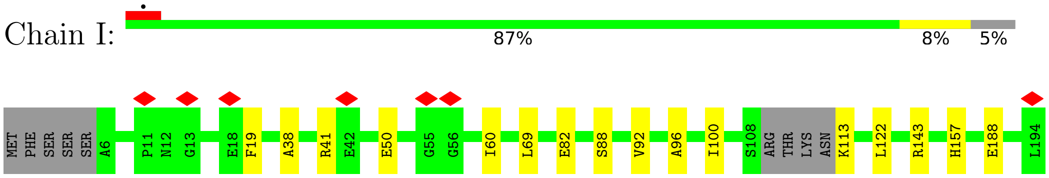
- Molecule 6: eS4



- Molecule 7: eS6

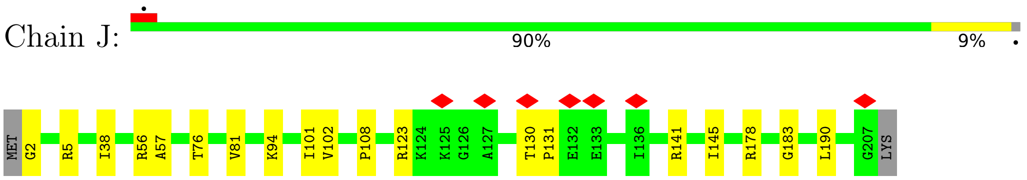


- Molecule 8: eS7



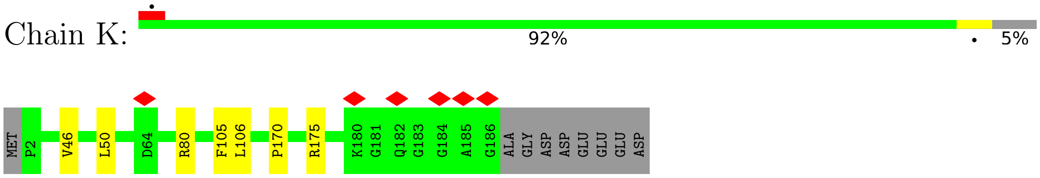
- Molecule 9: eS8

Chain J:



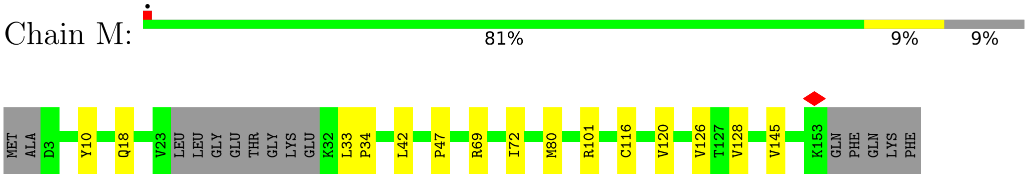
- Molecule 10: uS4

Chain K:



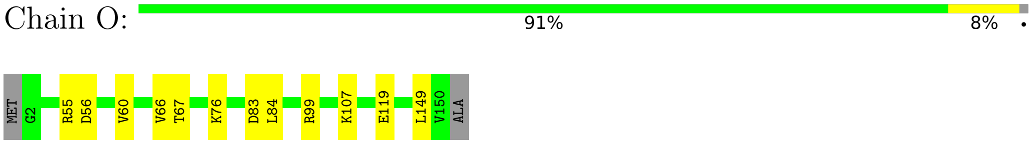
- Molecule 11: uS17

Chain M:



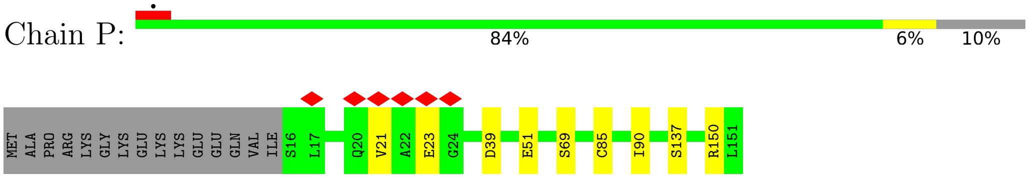
- Molecule 12: uS15

Chain O:



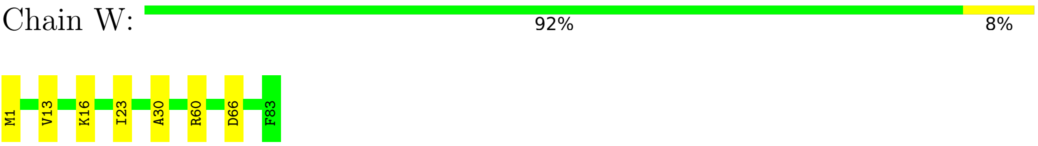
- Molecule 13: uS11

Chain P:



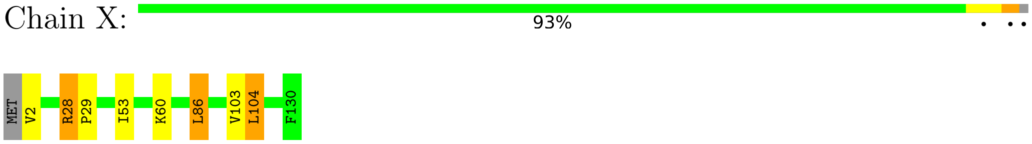
- Molecule 14: eS21

Chain W:



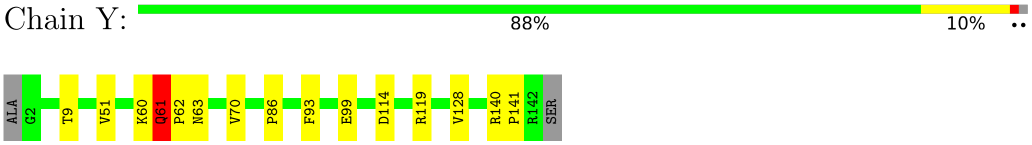
- Molecule 15: uS8

Chain X:



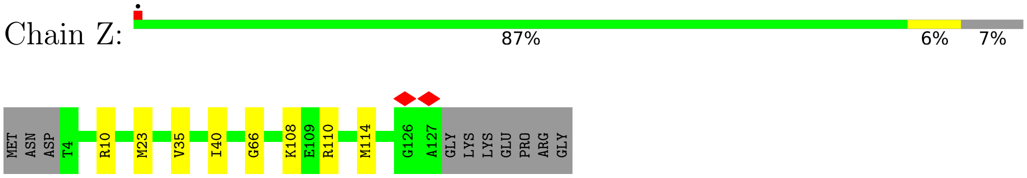
- Molecule 16: uS12

Chain Y:



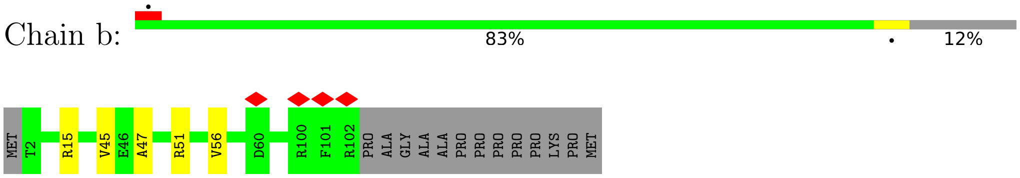
- Molecule 17: eS24

Chain Z:



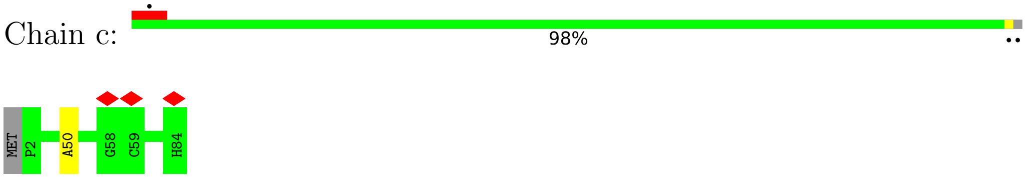
- Molecule 18: eS26

Chain b:



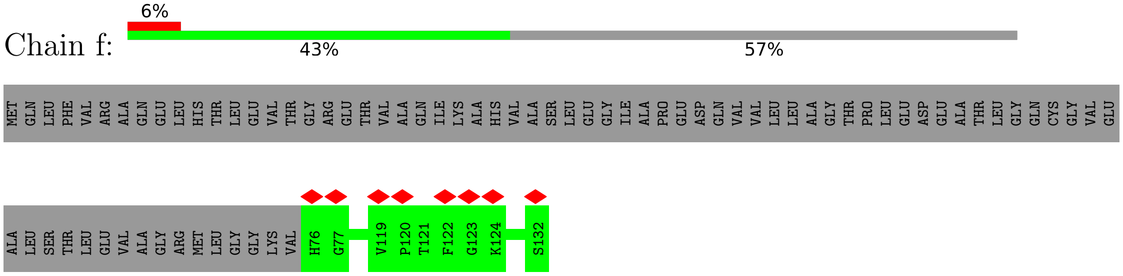
- Molecule 19: eS27

Chain c:



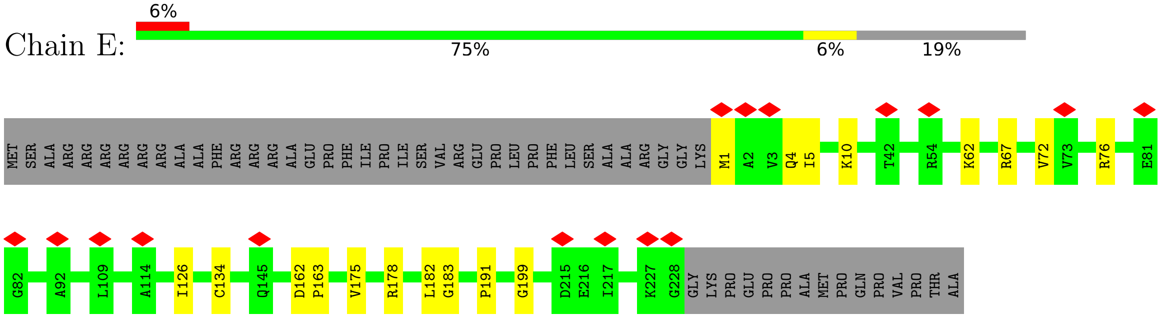
- Molecule 20: eS30

Chain f:



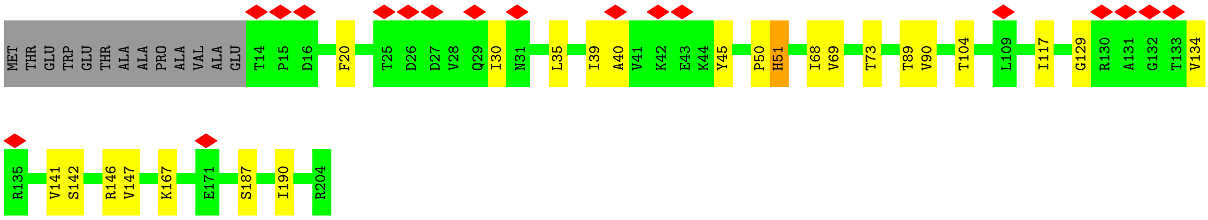
- Molecule 21: uS3

Chain E:



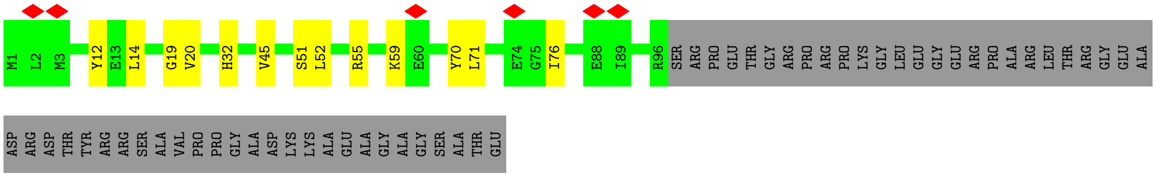
- Molecule 22: uS7

Chain G:



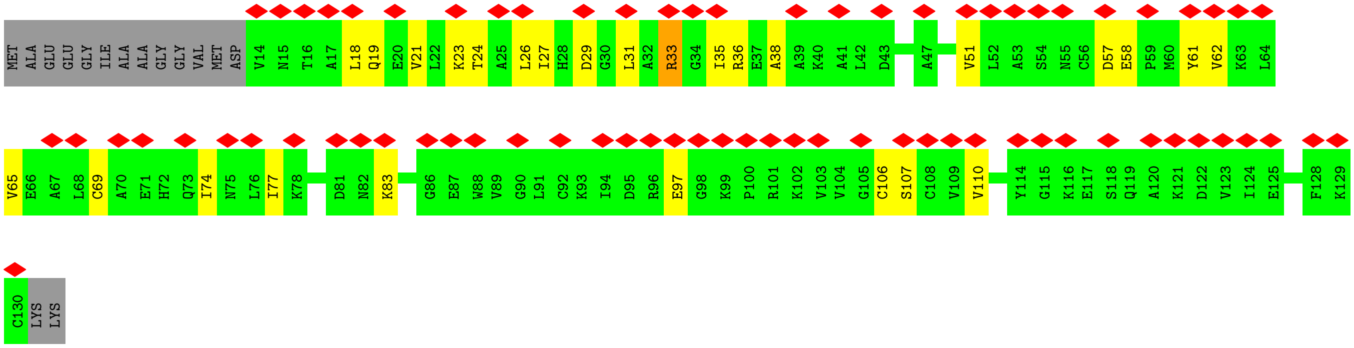
- Molecule 23: eS10

Chain L:



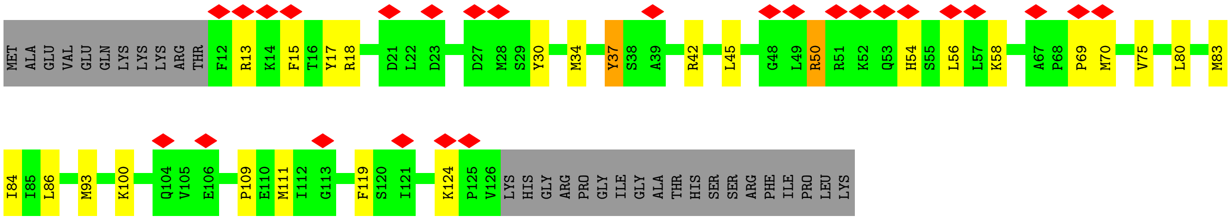
- Molecule 24: eS12

Chain N:



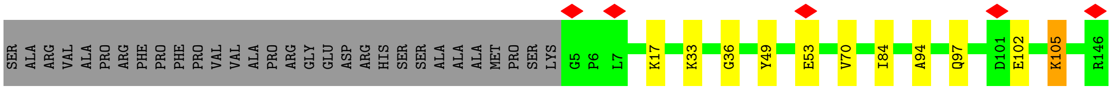
- Molecule 25: uS19

Chain Q:



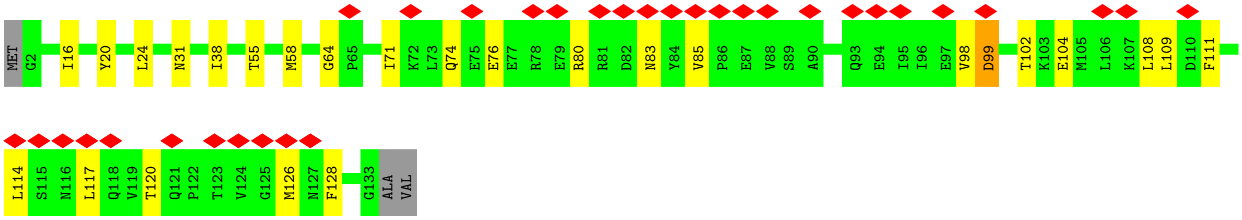
- Molecule 26: uS9

Chain R:



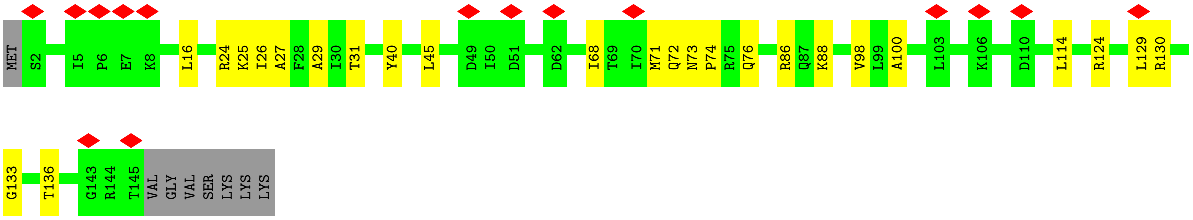
- Molecule 27: eS17

Chain S:



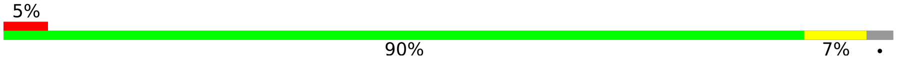
- Molecule 28: uS13

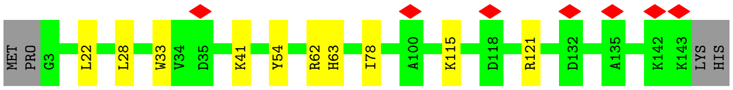
Chain T:



- Molecule 29: eS19

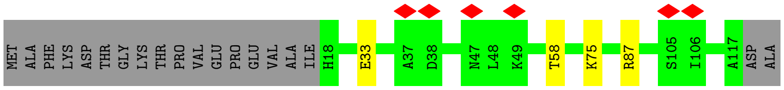
Chain U:





- Molecule 30: uS10

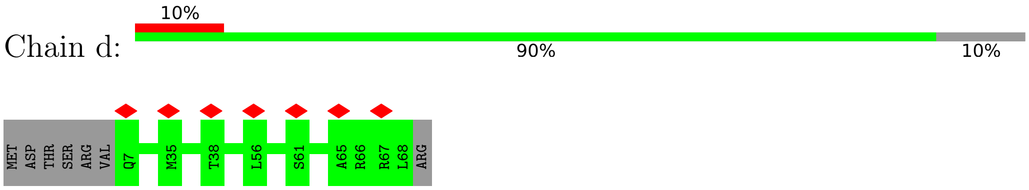
Chain V:



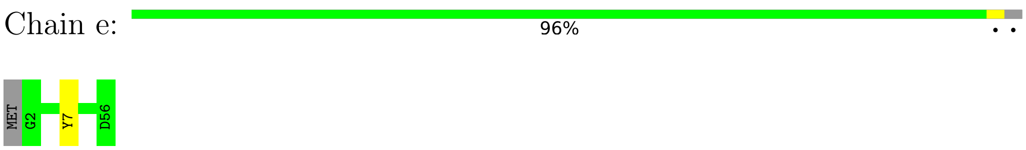
- Molecule 31: eS25

Chain a:

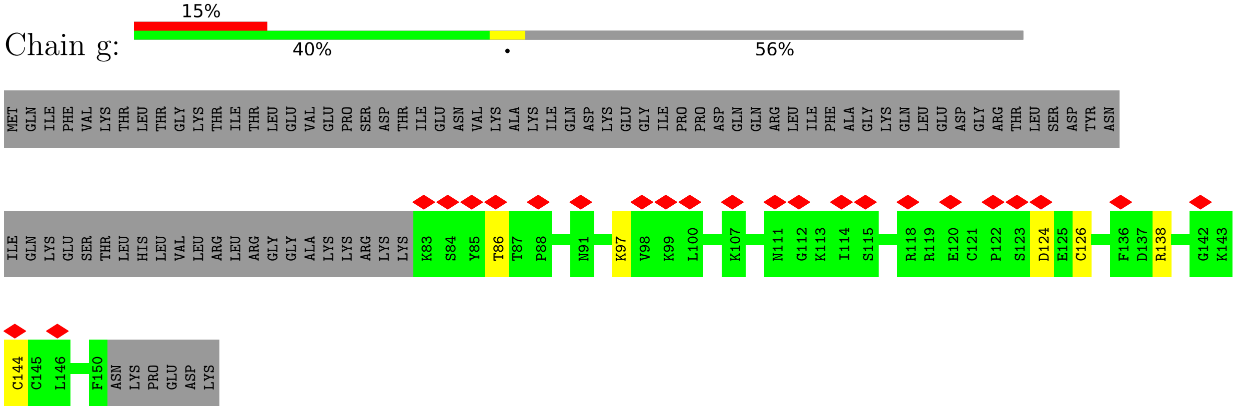
- Molecule 32: eS28



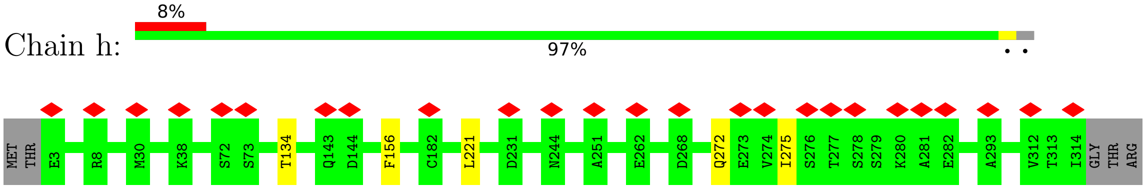
- Molecule 33: eS29



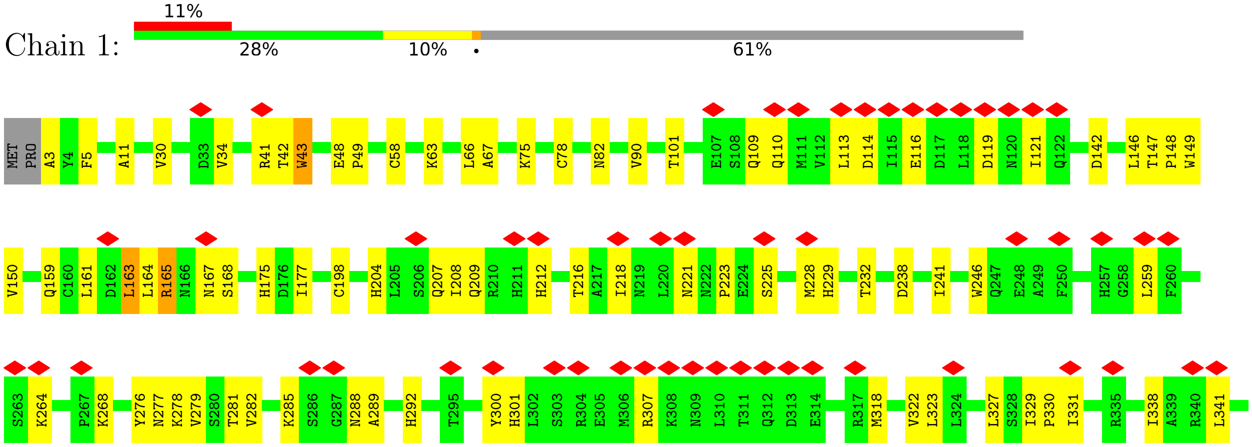
- Molecule 34: eS31

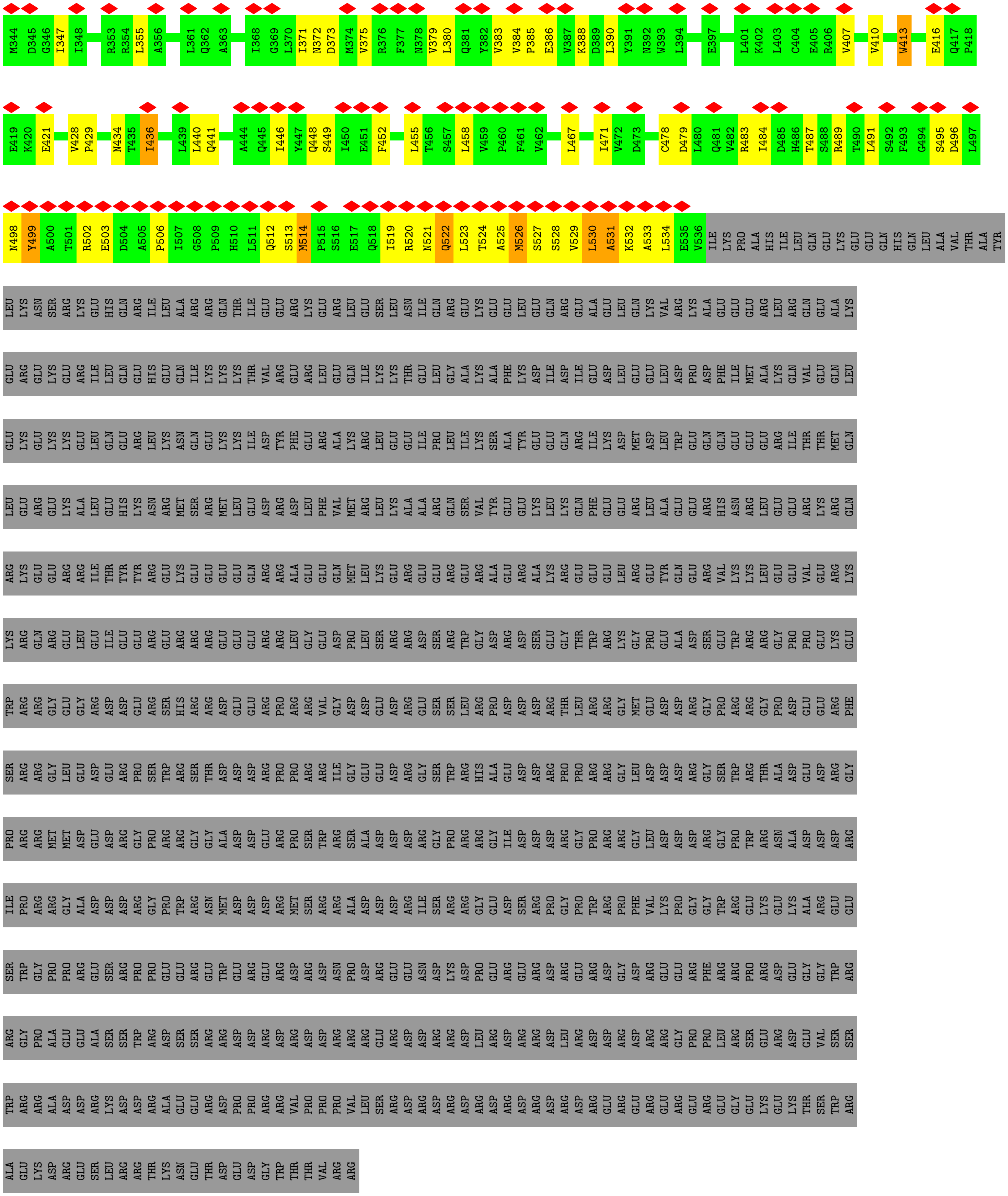


- Molecule 35: RACK1



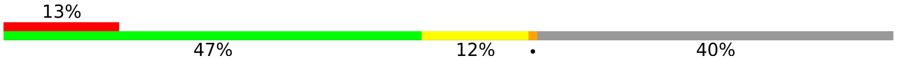
- Molecule 36: Eukaryotic translation initiation factor 3 subunit A

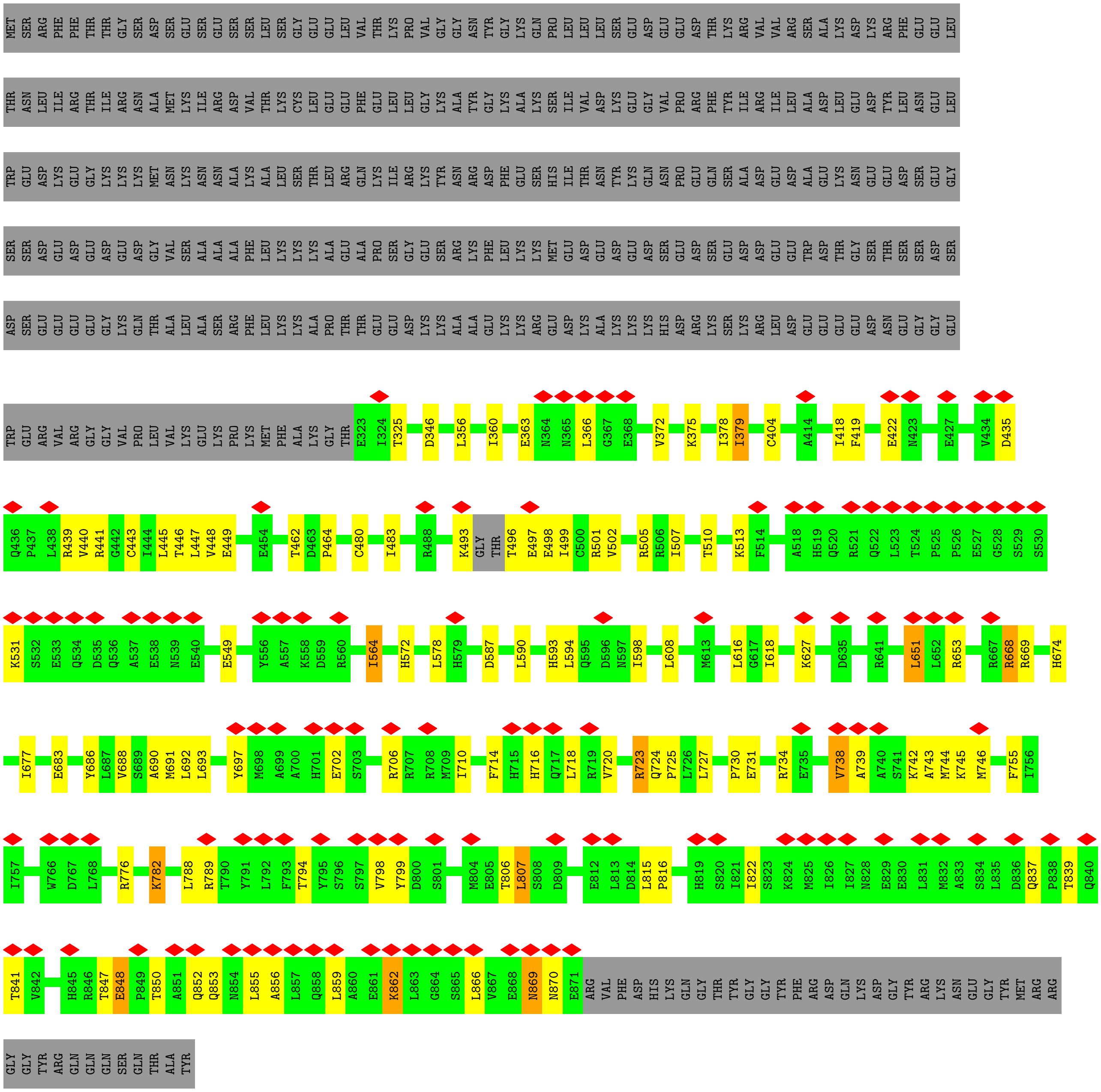




- Molecule 37: Eukaryotic translation initiation factor 3 subunit C

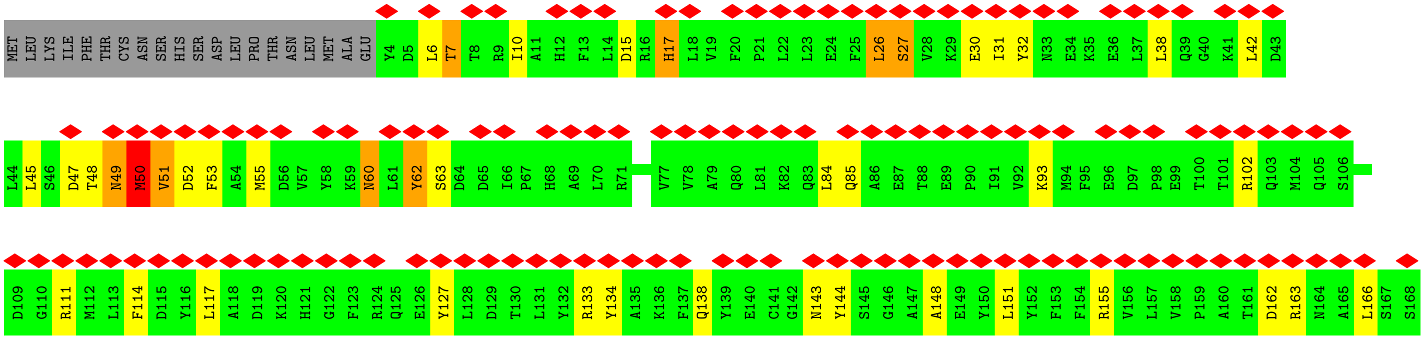
Chain 2:

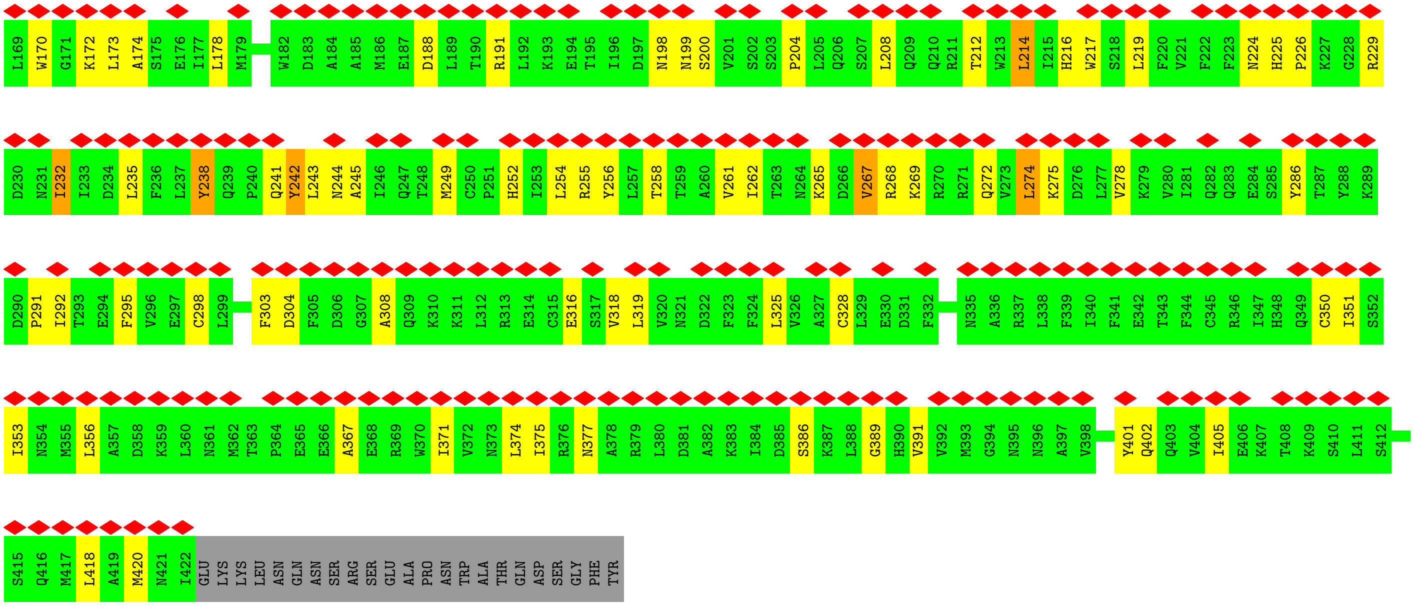




- Molecule 38: Eukaryotic translation initiation factor 3 subunit E

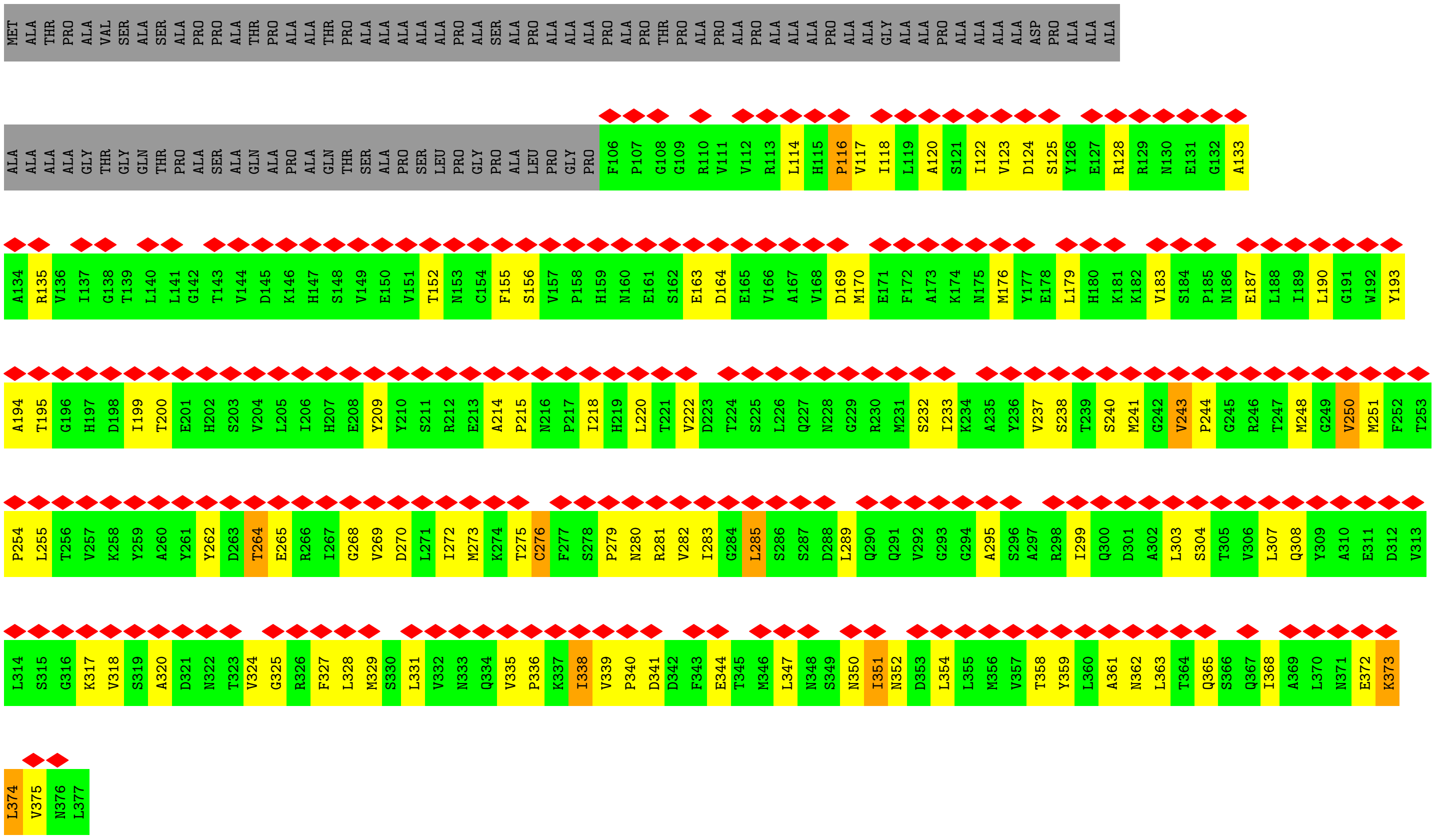
Chain 3:





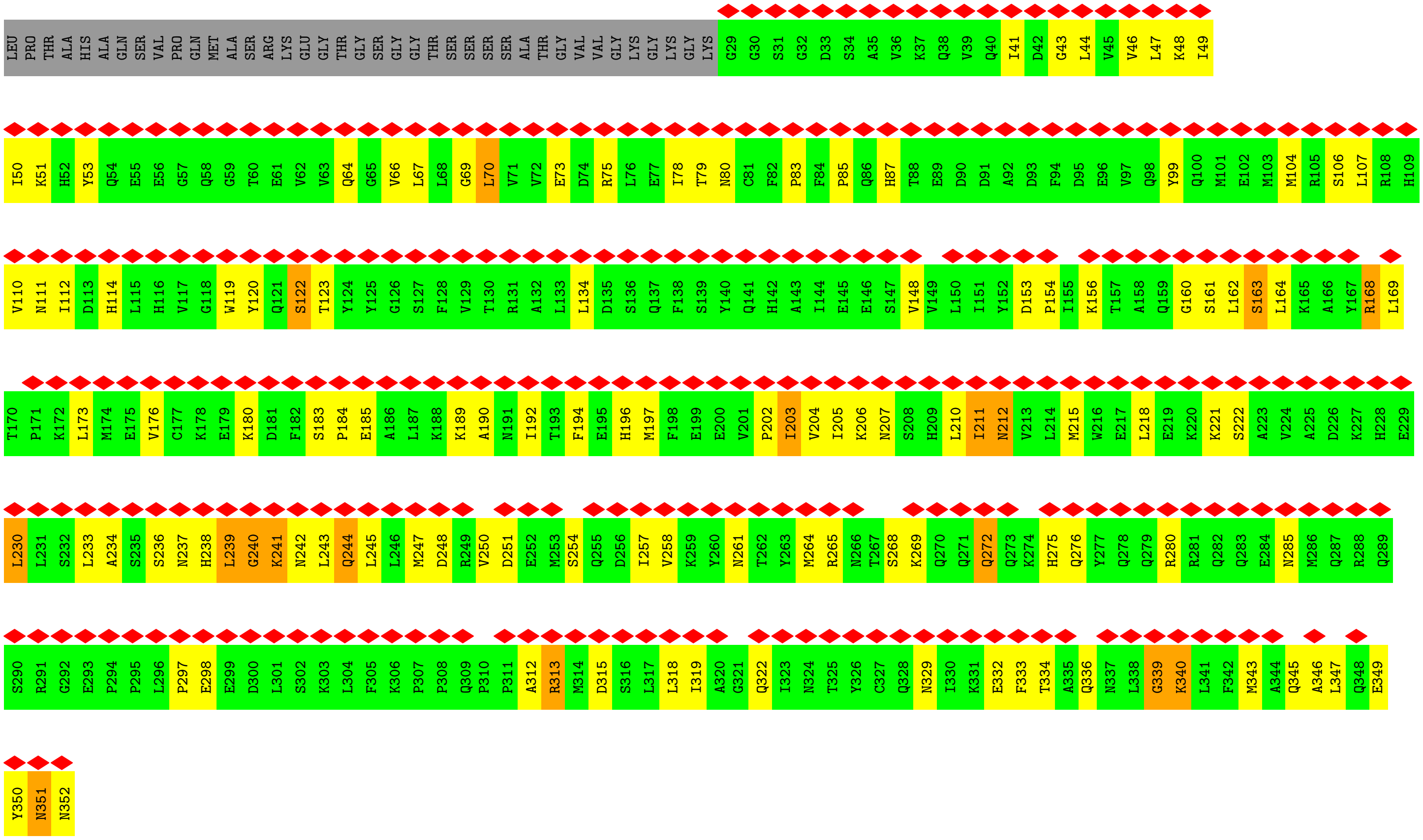
- Molecule 39: Eukaryotic translation initiation factor 3 subunit F

Chain 4:



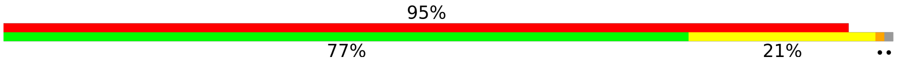
- Molecule 40: Eukaryotic translation initiation factor 3 subunit H

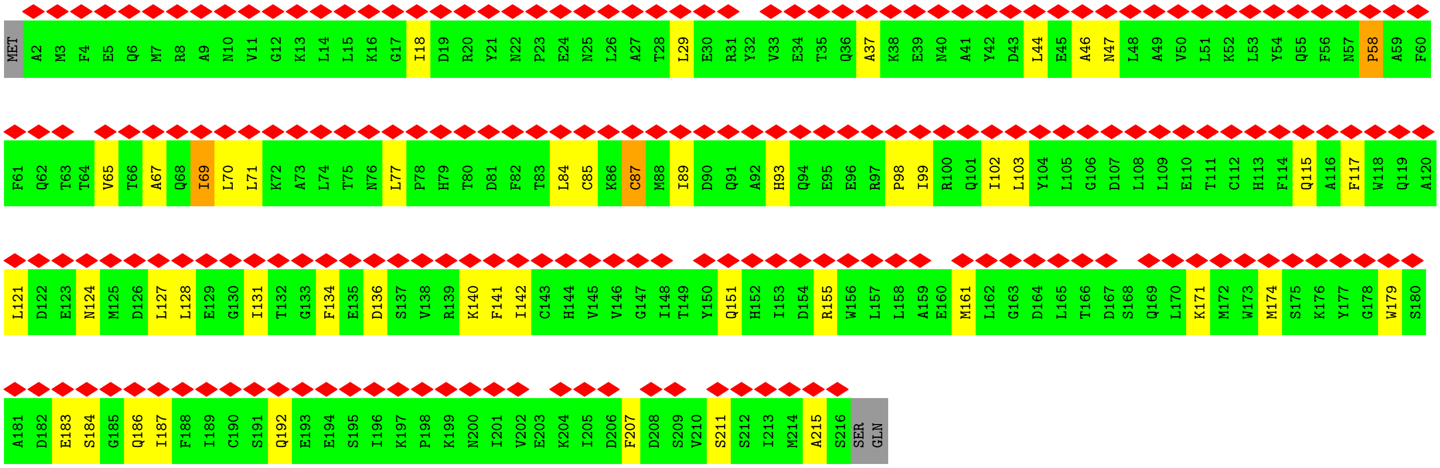
Chain 5:



• Molecule 41: Eukaryotic translation initiation factor 3 subunit K

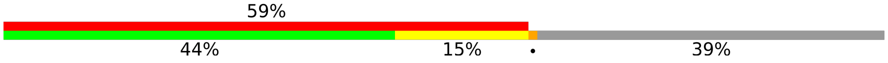
Chain 6:

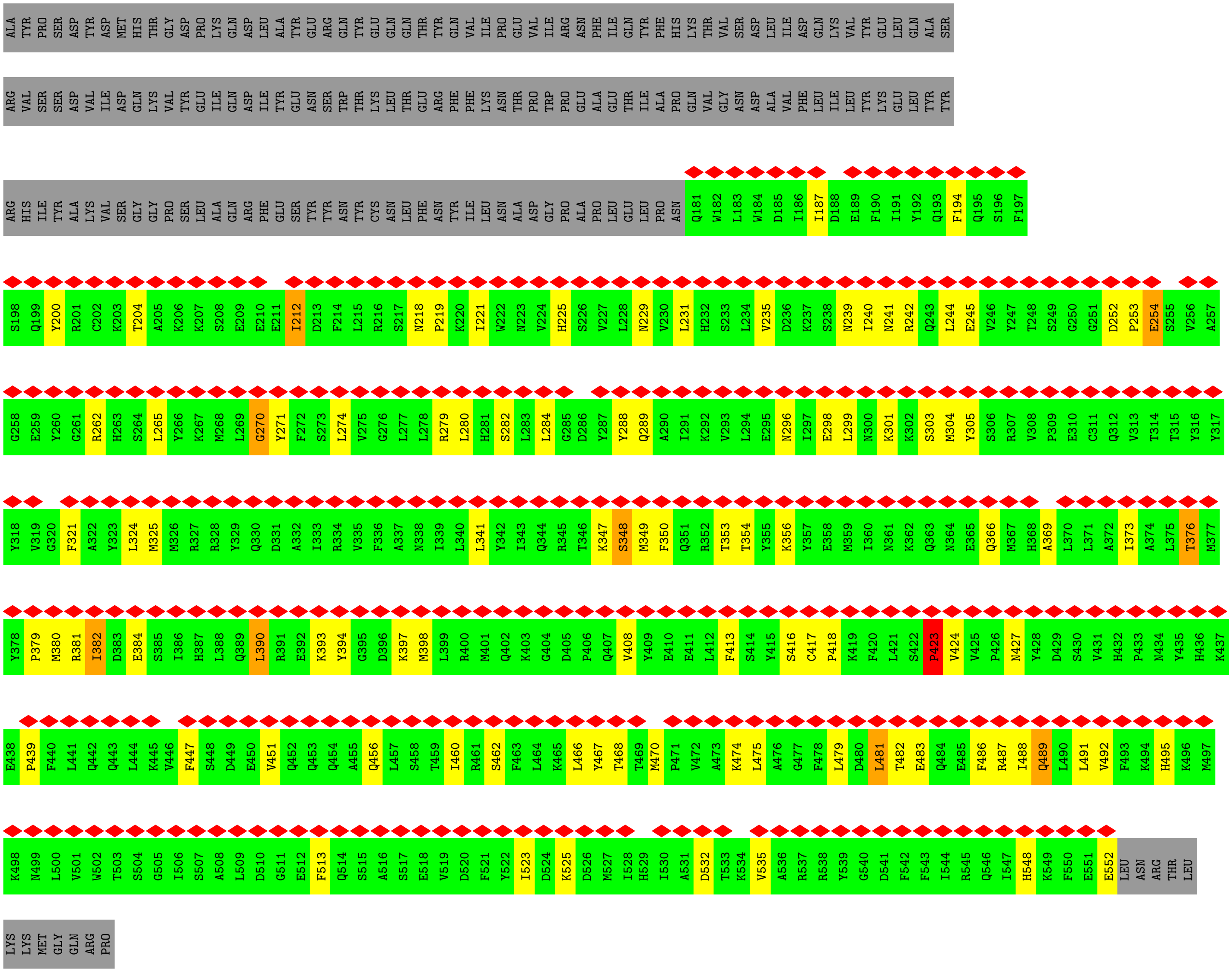




• Molecule 42: Eukaryotic translation initiation factor 3 subunit L

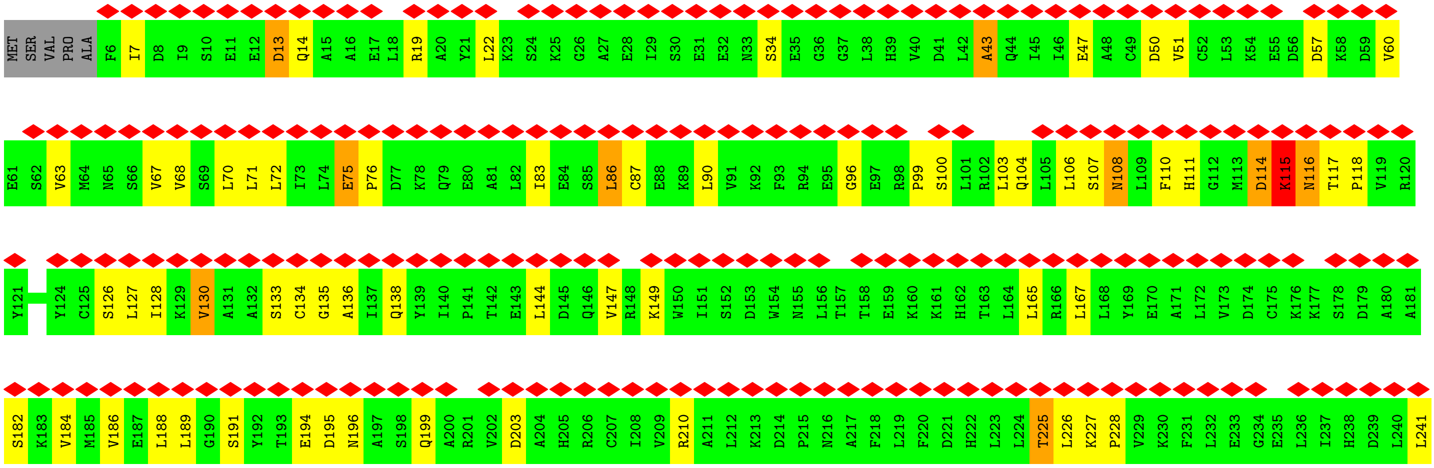
Chain 7:

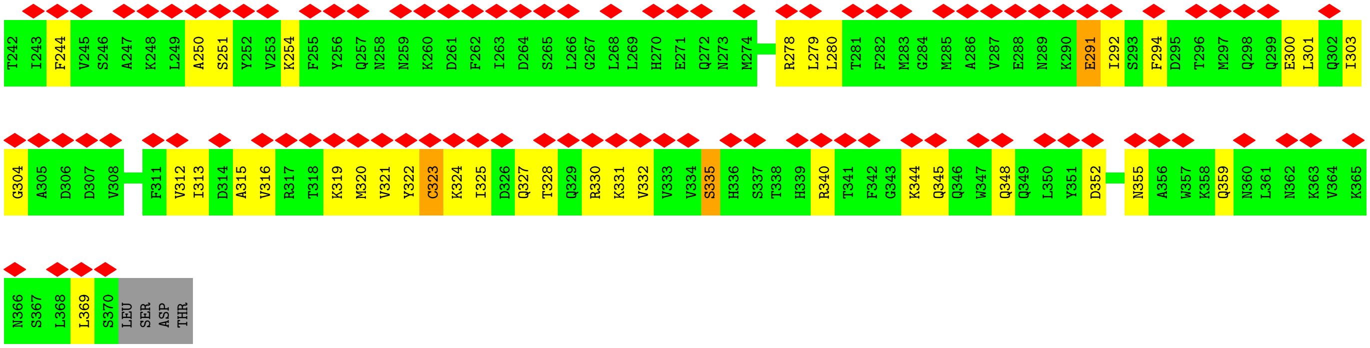




- Molecule 43: Eukaryotic translation initiation factor 3 subunit M

Chain 8:




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
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
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
N355
A356
W357
K358
Q359
N360
L361
N362
K363
V364
K365
N366
S367
L368
L369
S370
LEU
SER
ASP
THR

4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	36100	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	56.90	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.154	Depositor
Minimum map value	-0.093	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	424.2, 424.2, 424.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0605, 1.0605, 1.0605	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.21	0/40505	0.69	5/63112 (0.0%)
2	0	0.30	2/8053 (0.0%)	0.77	2/12543 (0.0%)
3	B	0.67	0/1743	0.78	0/2370
4	C	0.67	0/1756	0.78	0/2350
5	D	0.67	0/1754	0.78	0/2370
6	F	0.67	0/2114	0.79	0/2843
7	H	0.68	0/1946	0.83	0/2590
8	I	0.68	0/1510	0.79	0/2022
9	J	0.67	0/1715	0.82	0/2287
10	K	0.67	0/1550	0.80	0/2069
11	M	0.66	0/1195	0.80	0/1597
12	O	0.67	0/1226	0.79	0/1649
13	P	0.69	0/1029	0.82	0/1380
14	W	0.70	0/641	0.82	0/858
15	X	0.67	0/1051	0.79	0/1406
16	Y	0.68	0/1116	0.81	0/1490
17	Z	0.67	0/1028	0.80	0/1366
18	b	0.66	0/830	0.82	0/1112
19	c	0.67	0/665	0.81	0/891
20	f	0.68	0/462	0.86	0/607
21	E	0.69	0/1796	0.81	0/2417
22	G	0.70	0/1521	0.81	0/2046
23	L	0.65	0/834	0.77	0/1125
24	N	0.70	0/918	0.81	0/1233
25	Q	0.67	0/974	0.85	0/1301
26	R	0.69	0/1146	0.81	0/1534
27	S	0.69	0/1082	0.83	0/1452
28	T	0.68	0/1208	0.82	0/1618
29	U	0.69	0/1115	0.79	0/1493
30	V	0.69	0/805	0.81	0/1081
31	a	0.69	0/604	0.81	0/810
32	d	0.70	0/490	0.85	0/656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	e	0.67	0/470	0.79	0/623
34	g	0.68	0/567	0.84	0/753
35	h	0.69	0/2486	0.80	0/3384
36	1	0.68	0/4460	0.81	0/6034
37	2	0.69	0/4522	0.82	1/6102 (0.0%)
38	3	0.69	0/3538	0.83	0/4786
39	4	0.71	1/2149 (0.0%)	0.89	0/2920
40	5	0.67	0/2674	0.88	1/3606 (0.0%)
41	6	0.73	1/1772 (0.1%)	0.79	1/2396 (0.0%)
42	7	0.71	2/3185 (0.1%)	0.86	3/4296 (0.1%)
43	8	0.71	0/2963	0.85	1/3998 (0.0%)
All	All	0.54	6/113168 (0.0%)	0.77	14/162576 (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
16	Y	0	1
18	b	0	1
22	G	0	1
25	Q	0	1
27	S	0	1
36	1	0	4
37	2	0	4
38	3	0	6
39	4	0	3
40	5	0	6
42	7	0	3
43	8	0	4
All	All	0	35

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	6	69	ILE	CG1-CD1	-7.53	0.98	1.50
42	7	187	ILE	CG1-CD1	-6.45	1.05	1.50
39	4	351	ILE	CG1-CD1	6.23	1.93	1.50
2	0	509	G	C1'-N9	-5.98	1.38	1.46
2	0	576	U	C1'-N1	5.62	1.57	1.48

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	7	382	ILE	CB-CG1-CD1	9.61	140.82	113.90
42	7	240	ILE	CB-CG1-CD1	8.06	136.47	113.90
42	7	187	ILE	CB-CG1-CD1	7.27	134.25	113.90
1	A	688	U	C2'-C3'-O3'	6.76	124.51	113.70
1	A	166	A	C2'-C3'-O3'	6.62	124.30	113.70

There are no chirality outliers.

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	G	129	GLY	Peptide
25	Q	54	HIS	Peptide
27	S	64	GLY	Peptide
16	Y	61	GLN	Peptide
18	b	45	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	36229	0	18304	152	0
2	0	7205	0	3626	54	0
3	B	1706	0	1698	18	0
4	C	1729	0	1803	5	0
5	D	1717	0	1812	17	0
6	F	2072	0	2175	9	0
7	H	1923	0	2089	13	0
8	I	1488	0	1582	7	0
9	J	1686	0	1772	12	0
10	K	1525	0	1640	4	0
11	M	1175	0	1249	7	0
12	O	1202	0	1289	5	0
13	P	1016	0	1039	5	0
14	W	634	0	629	4	0
15	X	1034	0	1080	5	0
16	Y	1098	0	1167	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Z	1011	0	1083	5	0
18	b	816	0	867	0	0
19	c	651	0	672	0	0
20	f	457	0	502	0	0
21	E	1768	0	1866	11	0
22	G	1499	0	1540	10	0
23	L	810	0	836	6	0
24	N	908	0	939	13	0
25	Q	956	0	1002	13	0
26	R	1128	0	1195	6	0
27	S	1068	0	1121	17	0
28	T	1190	0	1249	16	0
29	U	1097	0	1130	5	0
30	V	795	0	862	3	0
31	a	598	0	656	0	0
32	d	488	0	514	0	0
33	e	459	0	452	0	0
34	g	555	0	567	0	0
35	h	2429	0	2386	0	0
36	1	4377	0	4433	151	0
37	2	4446	0	4444	118	0
38	3	3465	0	3446	69	0
39	4	2111	0	2105	169	0
40	5	2624	0	2591	249	0
41	6	1737	0	1706	33	0
42	7	3109	0	3084	65	0
43	8	2918	0	2950	66	0
44	A	1	0	0	0	0
45	b	1	0	0	0	0
All	All	106911	0	87152	1080	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 6.

The worst 5 of 1080 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)
5:D:127:PHE:CD1	5:D:141:LEU:HD21	1.26	1.61
5:D:127:PHE:CD1	5:D:141:LEU:CD2	1.95	1.50
36:1:523:LEU:HA	36:1:526:MET:SD	1.71	1.30
37:2:710:ILE:O	37:2:714:PHE:HD2	1.09	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1:526:MET:HG2	40:5:236:SER:O	1.26	1.28

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
3	B	215/295 (73%)	201 (94%)	13 (6%)	1 (0%)	29	66
4	C	211/264 (80%)	189 (90%)	21 (10%)	1 (0%)	29	66
5	D	219/255 (86%)	201 (92%)	17 (8%)	1 (0%)	29	66
6	F	260/263 (99%)	248 (95%)	12 (5%)	0	100	100
7	H	235/249 (94%)	216 (92%)	18 (8%)	1 (0%)	34	70
8	I	181/194 (93%)	160 (88%)	20 (11%)	1 (1%)	25	63
9	J	204/208 (98%)	188 (92%)	14 (7%)	2 (1%)	15	52
10	K	183/194 (94%)	170 (93%)	13 (7%)	0	100	100
11	M	139/158 (88%)	130 (94%)	9 (6%)	0	100	100
12	O	147/151 (97%)	137 (93%)	9 (6%)	1 (1%)	22	60
13	P	134/151 (89%)	120 (90%)	14 (10%)	0	100	100
14	W	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
15	X	127/130 (98%)	119 (94%)	7 (6%)	1 (1%)	19	57
16	Y	139/143 (97%)	128 (92%)	7 (5%)	4 (3%)	4	29
17	Z	122/134 (91%)	115 (94%)	7 (6%)	0	100	100
18	b	99/115 (86%)	87 (88%)	10 (10%)	2 (2%)	7	37
19	c	81/84 (96%)	75 (93%)	5 (6%)	1 (1%)	13	47
20	f	55/133 (41%)	51 (93%)	4 (7%)	0	100	100
21	E	226/281 (80%)	209 (92%)	17 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	G	189/204 (93%)	165 (87%)	21 (11%)	3 (2%)	9	41
23	L	94/149 (63%)	83 (88%)	10 (11%)	1 (1%)	14	50
24	N	115/132 (87%)	96 (84%)	16 (14%)	3 (3%)	5	31
25	Q	113/145 (78%)	92 (81%)	17 (15%)	4 (4%)	3	26
26	R	140/172 (81%)	130 (93%)	9 (6%)	1 (1%)	22	60
27	S	130/135 (96%)	111 (85%)	17 (13%)	2 (2%)	10	42
28	T	142/152 (93%)	132 (93%)	8 (6%)	2 (1%)	11	43
29	U	139/145 (96%)	126 (91%)	12 (9%)	1 (1%)	22	60
30	V	98/119 (82%)	92 (94%)	6 (6%)	0	100	100
31	a	73/125 (58%)	67 (92%)	6 (8%)	0	100	100
32	d	60/69 (87%)	59 (98%)	1 (2%)	0	100	100
33	e	53/56 (95%)	49 (92%)	3 (6%)	1 (2%)	8	37
34	g	66/156 (42%)	54 (82%)	9 (14%)	3 (4%)	2	20
35	h	310/317 (98%)	274 (88%)	34 (11%)	2 (1%)	25	63
36	1	532/1362 (39%)	430 (81%)	85 (16%)	17 (3%)	4	27
37	2	543/913 (60%)	428 (79%)	105 (19%)	10 (2%)	8	38
38	3	417/462 (90%)	333 (80%)	67 (16%)	17 (4%)	3	22
39	4	270/364 (74%)	217 (80%)	45 (17%)	8 (3%)	4	28
40	5	320/363 (88%)	255 (80%)	54 (17%)	11 (3%)	3	26
41	6	213/218 (98%)	179 (84%)	31 (15%)	3 (1%)	11	43
42	7	370/607 (61%)	301 (81%)	57 (15%)	12 (3%)	4	27
43	8	363/374 (97%)	290 (80%)	61 (17%)	12 (3%)	4	27
All	All	7808/10224 (76%)	6786 (87%)	893 (11%)	129 (2%)	13	40

5 of 129 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	94	LYS
15	X	28	ARG
16	Y	61	GLN
22	G	134	VAL
24	N	57	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	180/246 (73%)	177 (98%)	3 (2%)	60	82
4	C	194/231 (84%)	191 (98%)	3 (2%)	65	84
5	D	186/205 (91%)	183 (98%)	3 (2%)	62	82
6	F	223/224 (100%)	222 (100%)	1 (0%)	91	96
7	H	207/218 (95%)	203 (98%)	4 (2%)	57	80
8	I	165/174 (95%)	162 (98%)	3 (2%)	59	81
9	J	178/180 (99%)	178 (100%)	0	100	100
10	K	161/168 (96%)	161 (100%)	0	100	100
11	M	130/142 (92%)	128 (98%)	2 (2%)	65	84
12	O	130/131 (99%)	128 (98%)	2 (2%)	65	84
13	P	106/119 (89%)	105 (99%)	1 (1%)	78	91
14	W	68/68 (100%)	67 (98%)	1 (2%)	65	84
15	X	112/113 (99%)	109 (97%)	3 (3%)	44	72
16	Y	113/114 (99%)	112 (99%)	1 (1%)	78	91
17	Z	107/115 (93%)	106 (99%)	1 (1%)	78	91
18	b	89/99 (90%)	87 (98%)	2 (2%)	52	77
19	c	75/76 (99%)	75 (100%)	0	100	100
20	f	47/106 (44%)	47 (100%)	0	100	100
21	E	190/232 (82%)	189 (100%)	1 (0%)	88	95
22	G	158/170 (93%)	156 (99%)	2 (1%)	69	86
23	L	87/125 (70%)	86 (99%)	1 (1%)	73	88
24	N	99/108 (92%)	96 (97%)	3 (3%)	41	70
25	Q	105/130 (81%)	101 (96%)	4 (4%)	33	64
26	R	117/140 (84%)	116 (99%)	1 (1%)	78	91
27	S	119/121 (98%)	119 (100%)	0	100	100
28	T	125/132 (95%)	123 (98%)	2 (2%)	62	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	U	111/116 (96%)	109 (98%)	2 (2%)	59	81
30	V	92/107 (86%)	92 (100%)	0	100	100
31	a	66/103 (64%)	66 (100%)	0	100	100
32	d	55/62 (89%)	55 (100%)	0	100	100
33	e	48/49 (98%)	48 (100%)	0	100	100
34	g	61/140 (44%)	58 (95%)	3 (5%)	25	57
35	h	271/275 (98%)	268 (99%)	3 (1%)	73	88
36	1	490/1245 (39%)	476 (97%)	14 (3%)	42	71
37	2	494/812 (61%)	477 (97%)	17 (3%)	37	67
38	3	384/423 (91%)	375 (98%)	9 (2%)	50	76
39	4	239/282 (85%)	233 (98%)	6 (2%)	47	74
40	5	293/320 (92%)	283 (97%)	10 (3%)	37	67
41	6	190/193 (98%)	188 (99%)	2 (1%)	73	88
42	7	342/544 (63%)	335 (98%)	7 (2%)	55	79
43	8	327/335 (98%)	319 (98%)	8 (2%)	49	75
All	All	6934/8893 (78%)	6809 (98%)	125 (2%)	61	81

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	1	264	LYS
42	7	254	GLU
37	2	578	LEU
41	6	183	GLU
43	8	75	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
38	3	244	ASN
40	5	345	GLN
38	3	302	ASN
40	5	261	ASN
42	7	239	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1682/1697 (99%)	406 (24%)	26 (1%)
2	0	338/377 (89%)	186 (55%)	20 (5%)
All	All	2020/2074 (97%)	592 (29%)	46 (2%)

5 of 592 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	3	C
1	A	4	C
1	A	17	C
1	A	33	G
1	A	41	G

5 of 46 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	0	406	C
2	0	485	U
2	0	416	U
2	0	456	C
2	0	508	A

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	15
40	5	1

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	697:G	O3'	729:C	P	18.10
1	A	834:C	O3'	841:G	P	17.97
1	A	130:G	O3'	141:A	P	17.73
1	A	756:C	O3'	788:G	P	15.69
1	A	323:C	O3'	329:G	P	15.54

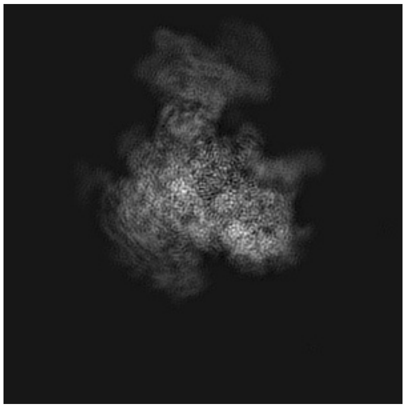
6 Map visualisation

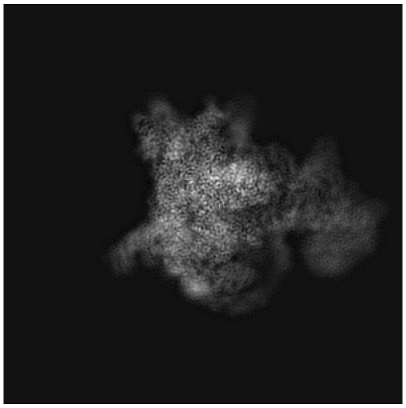
This section contains visualisations of the EMDB entry EMD-21529. These allow visual inspection of the internal detail of the map and identification of artifacts.

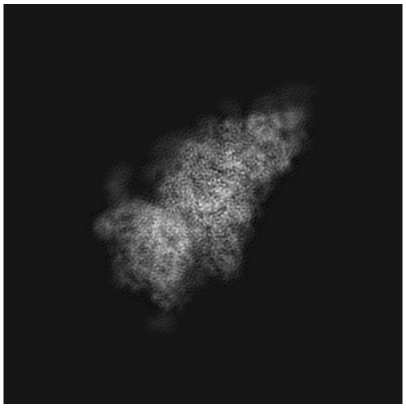
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

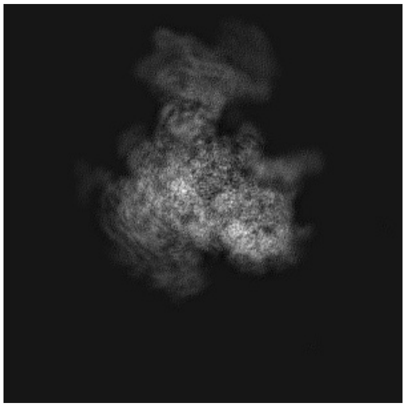
6.1.1 Primary map

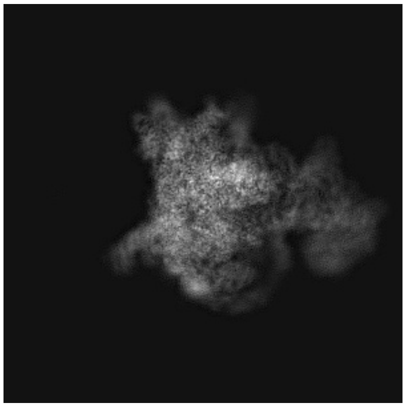

X

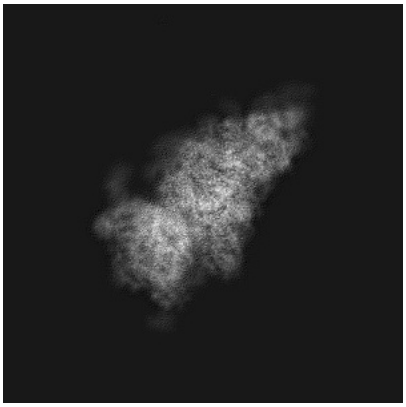

Y


Z

6.1.2 Raw map


X

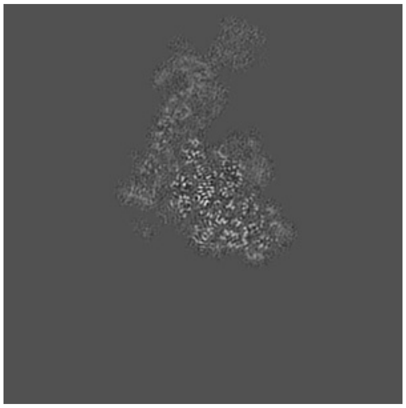

Y


Z

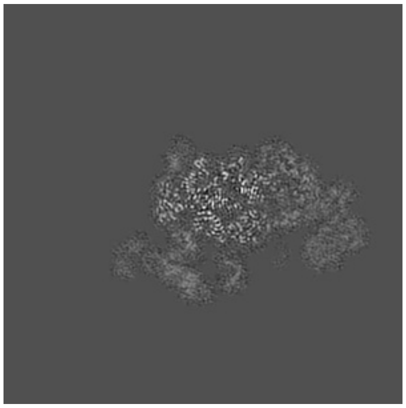
The images above show the map projected in three orthogonal directions.

6.2 Central slices

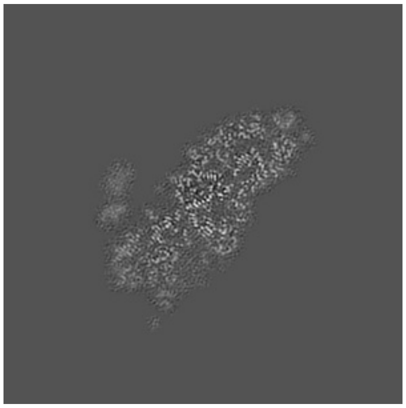
6.2.1 Primary map



X Index: 200

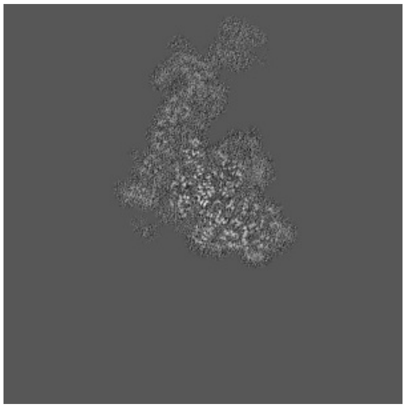


Y Index: 200

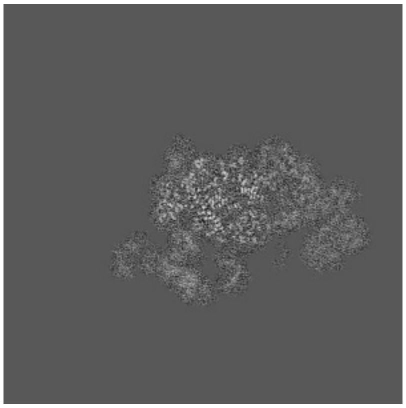


Z Index: 200

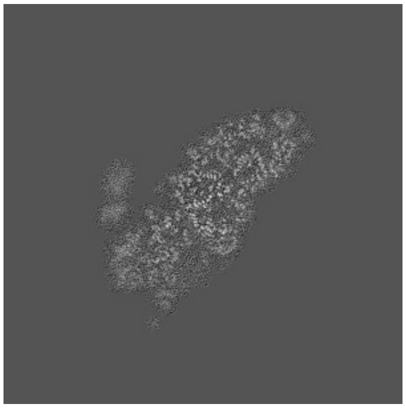
6.2.2 Raw map



X Index: 200



Y Index: 200

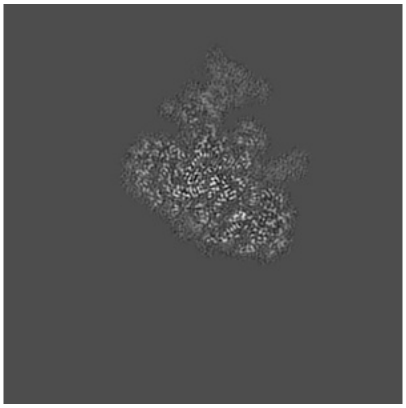


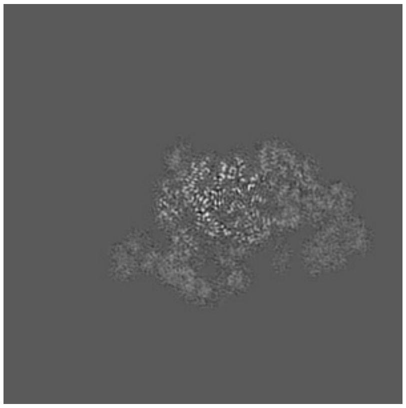
Z Index: 200

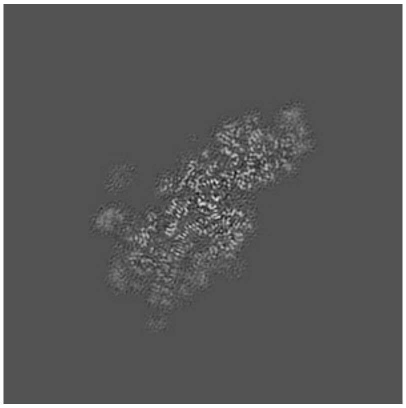
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

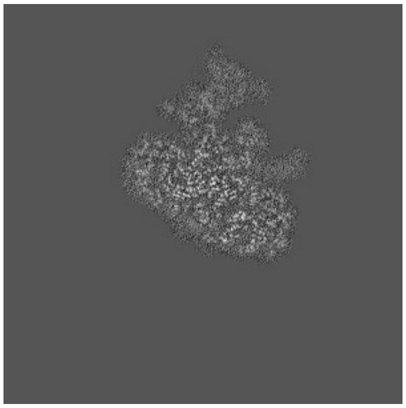
6.3.1 Primary map

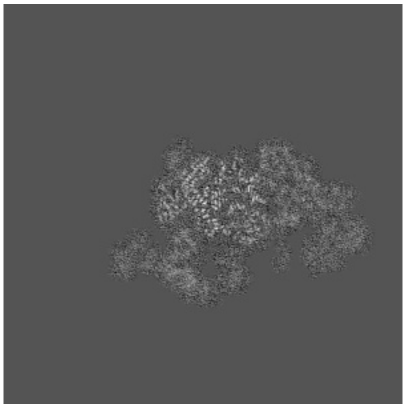

X Index: 225

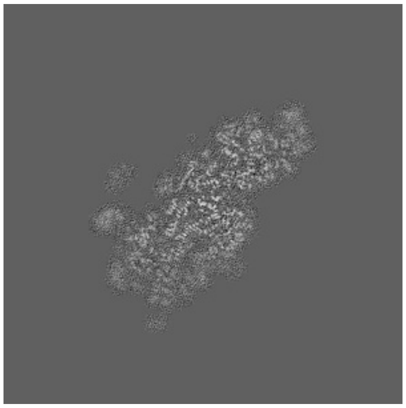

Y Index: 197


Z Index: 209

6.3.2 Raw map


X Index: 225

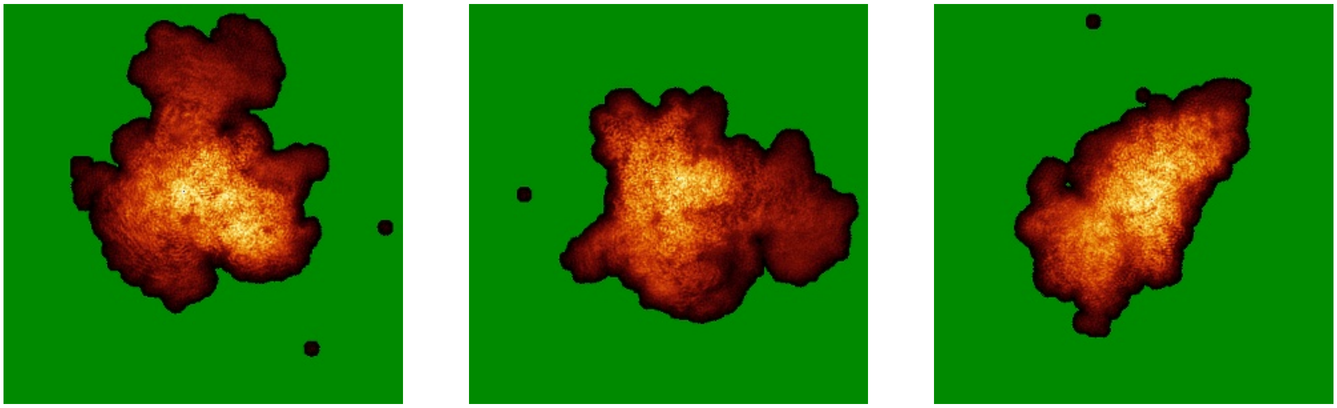

Y Index: 198


Z Index: 209

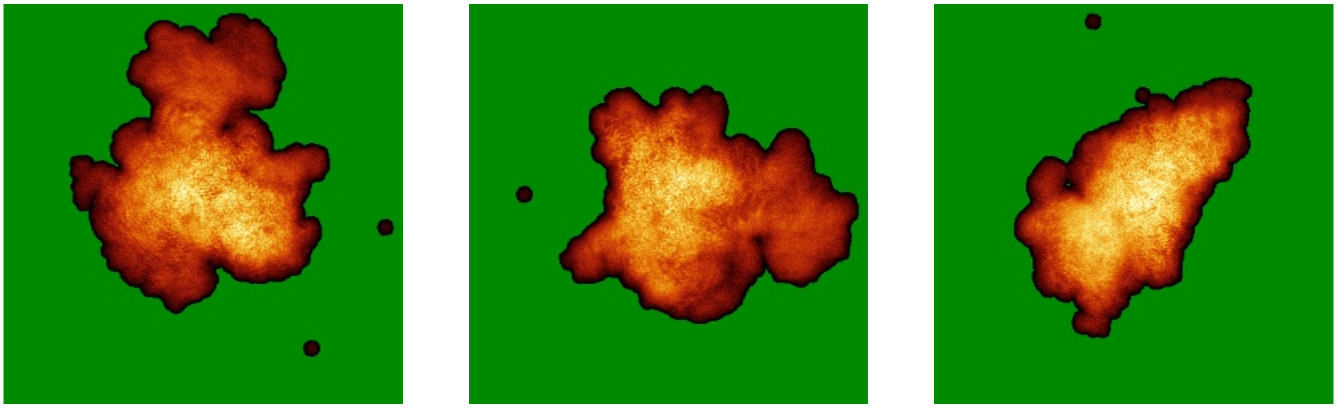
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X Y Z

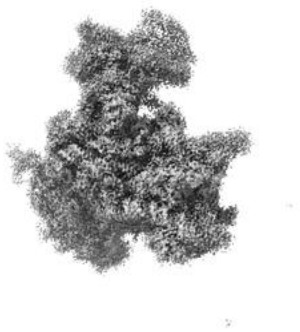
6.4.2 Raw map


X Y Z

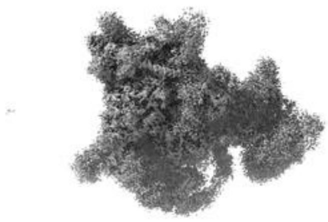
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

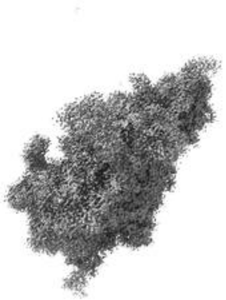
6.5.1 Primary map



X



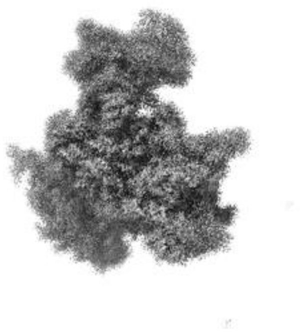
Y



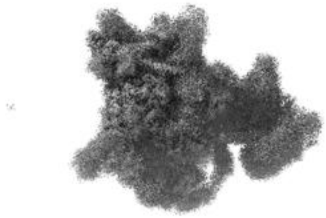
Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. 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.

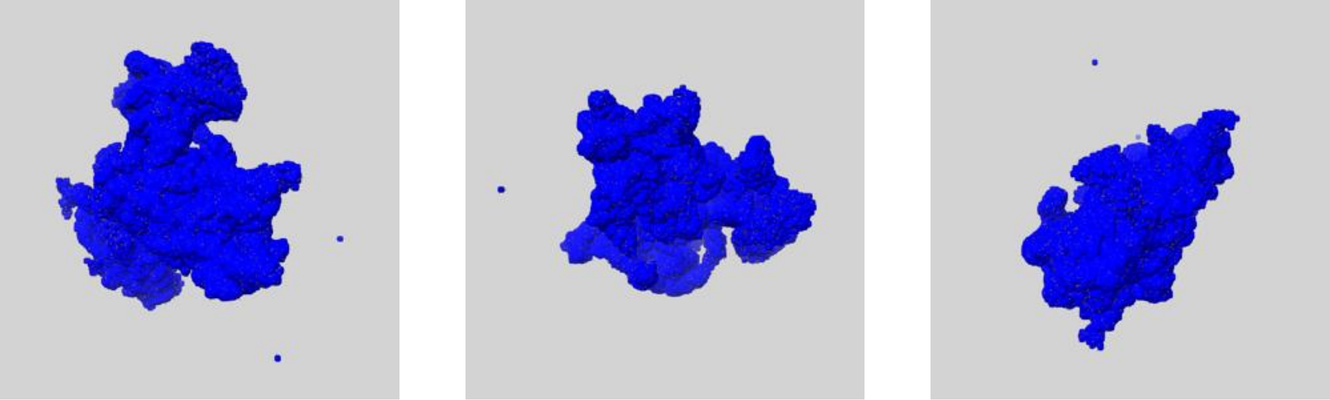
6.6 Mask visualisation ⓘ

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_21529_msk_1.map ⓘ

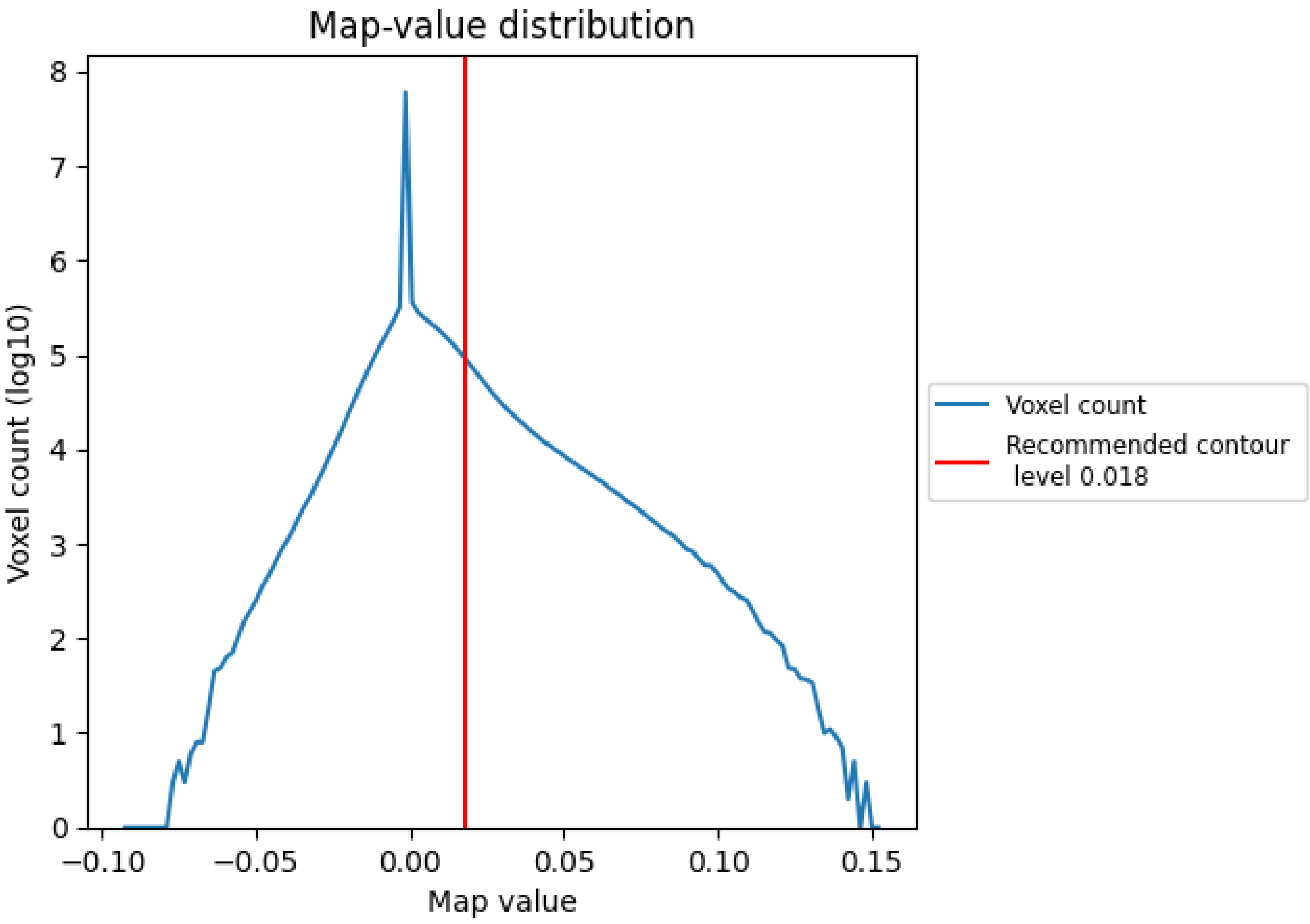


X Y Z

7 Map analysis ⓘ

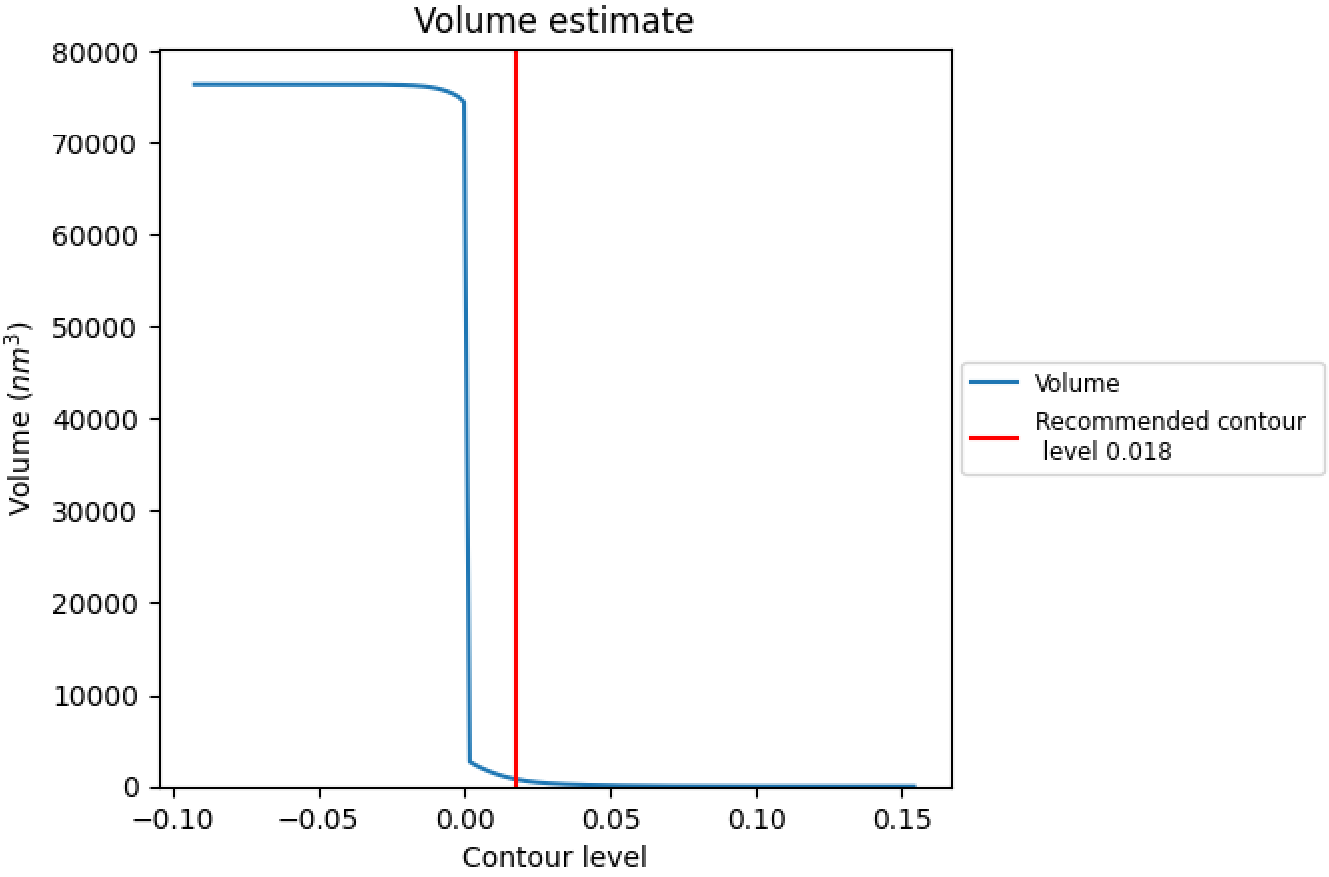
This section contains the results of statistical analysis of the map.

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.

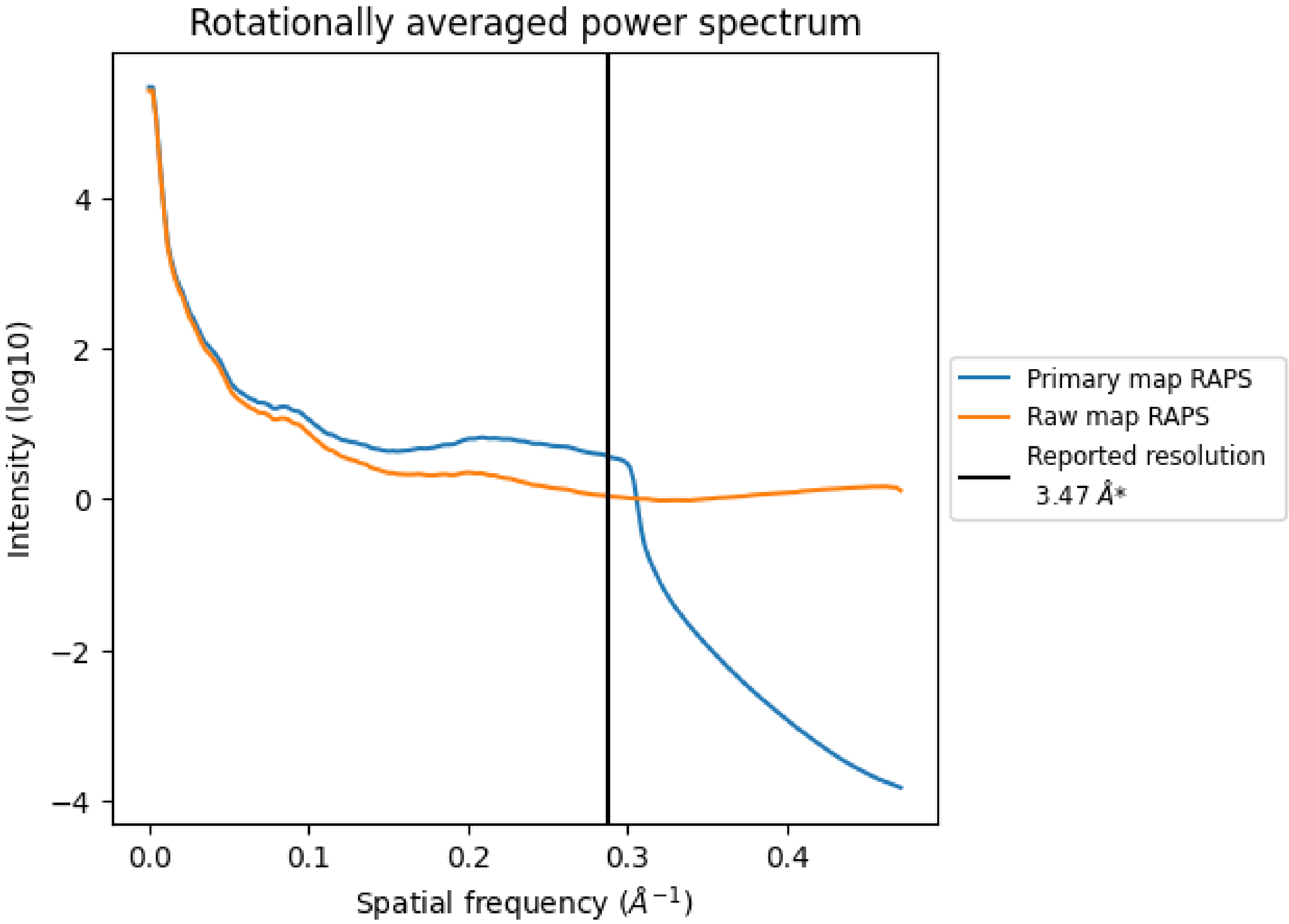
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 758 nm^3; this corresponds to an approximate mass of 685 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

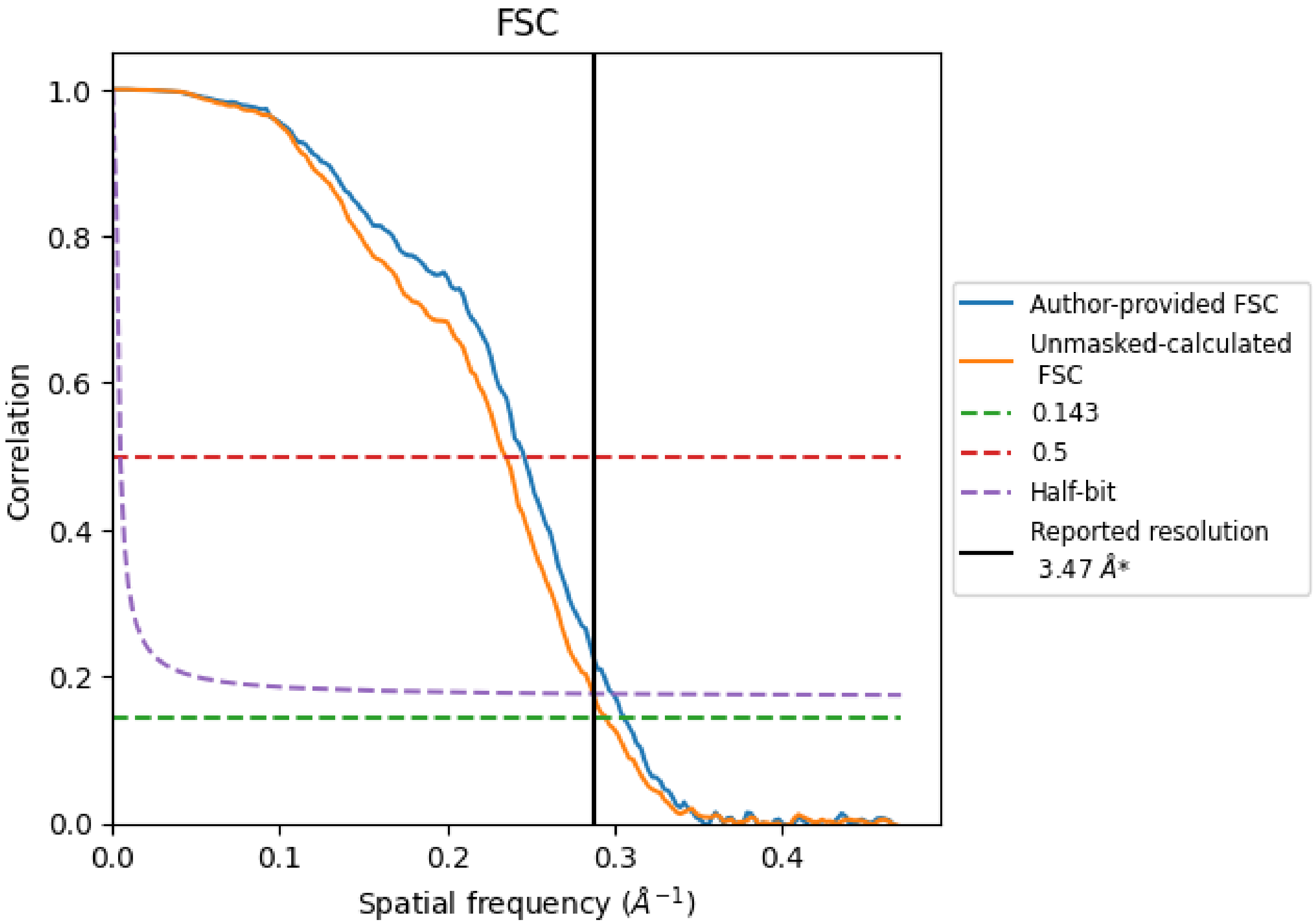


*Reported resolution corresponds to spatial frequency of 0.288 Å^{-1}

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 0.288 Å^{-1}

8.2 Resolution estimates ⓘ

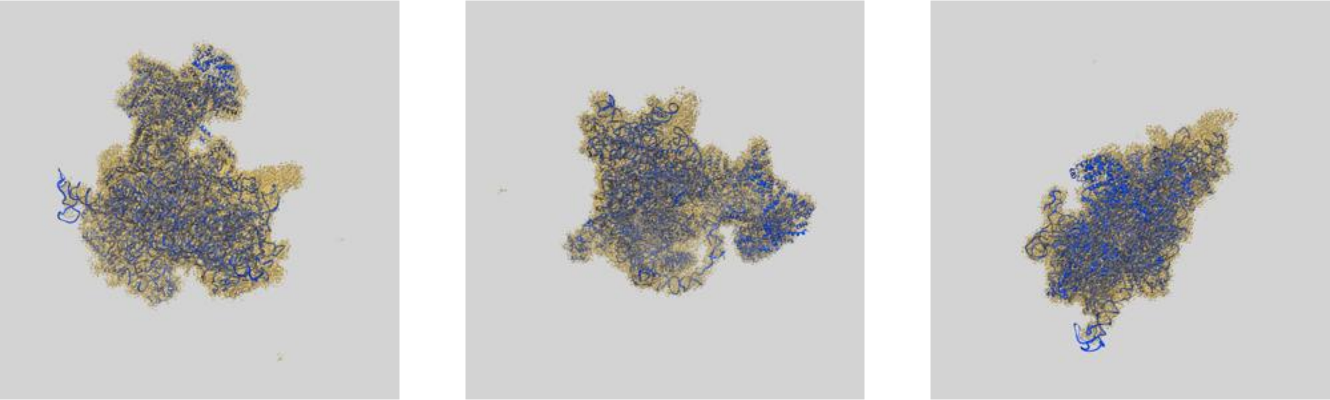
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.47	-	-
Author-provided FSC curve	3.27	4.06	3.34
Unmasked-calculated*	3.39	4.26	3.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21529 and PDB model 6W2S. Per-residue inclusion information can be found in section 3 on page 13.

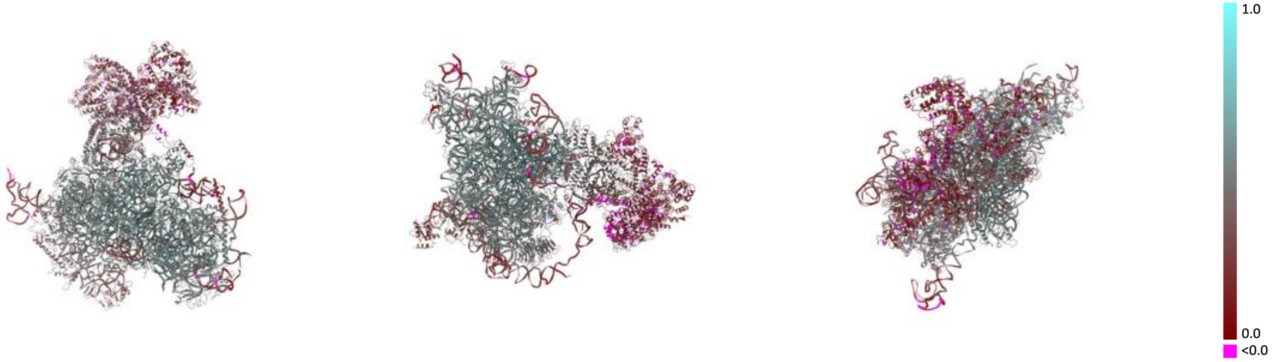
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 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.

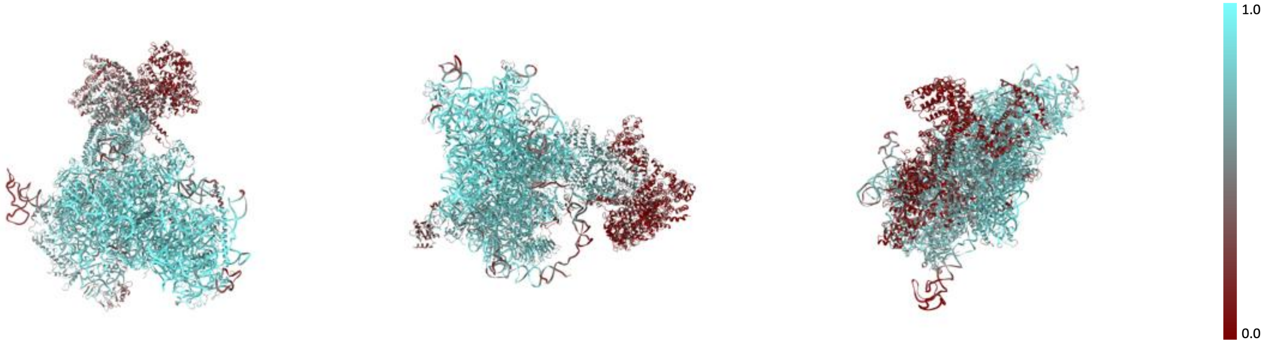
9.2 Q-score mapped to coordinate model ⓘ



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.

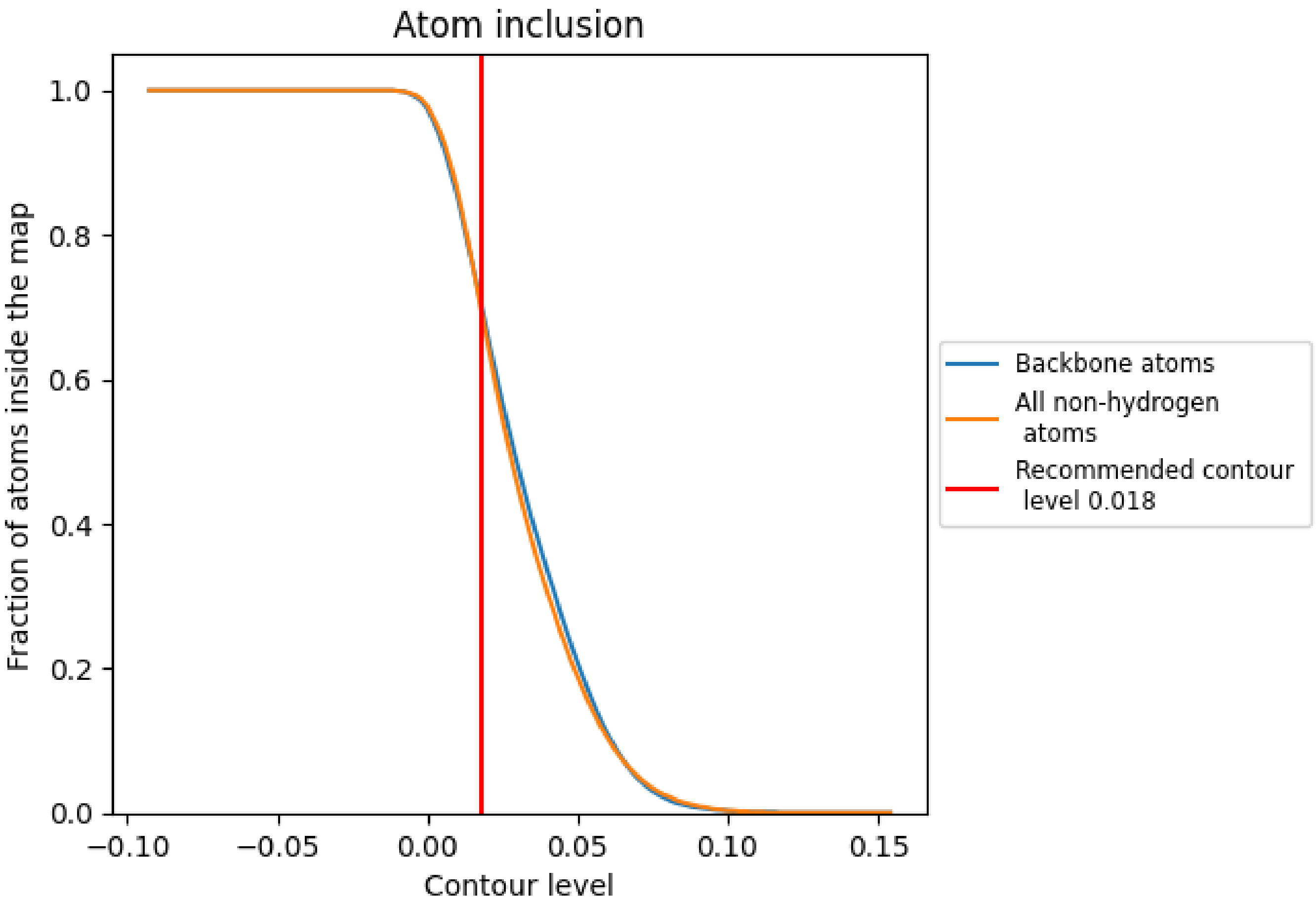
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.018).

9.4 Atom inclusion ⓘ



At the recommended contour level, 70% of all backbone atoms, 69% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6930	0.4150
0	0.5050	0.2600
1	0.5660	0.3510
2	0.5910	0.3680
3	0.2170	0.2080
4	0.1820	0.2000
5	0.1130	0.0170
6	0.1010	0.2130
7	0.0900	0.1990
8	0.1990	0.2230
A	0.9030	0.4920
B	0.8470	0.5350
C	0.8270	0.5230
D	0.8700	0.5460
E	0.7560	0.4730
F	0.8630	0.5440
G	0.7100	0.4560
H	0.7680	0.4610
I	0.7800	0.4770
J	0.8420	0.5090
K	0.8560	0.5340
L	0.6890	0.3860
M	0.8800	0.5510
N	0.3510	0.2660
O	0.8660	0.5370
P	0.8220	0.5250
Q	0.5890	0.3520
R	0.7800	0.4900
S	0.6170	0.4090
T	0.6500	0.3970
U	0.7770	0.4520
V	0.7730	0.4750
W	0.8820	0.5410
X	0.9030	0.5660
Y	0.8870	0.5530

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Chain	Atom inclusion	Q-score
Z	0.8530	0.5190
a	0.6230	0.4040
b	0.8300	0.5350
c	0.8310	0.5280
d	0.6790	0.4590
e	0.8460	0.4960
f	0.7770	0.4890
g	0.4560	0.3000
h	0.7320	0.4350