



wwPDB EM Validation Summary Report ⓘ

Apr 23, 2024 – 08:42 am BST

PDB ID : 6ZON
EMDB ID : EMD-11325
Title : SARS-CoV-2 Nsp1 bound to a human 43S preinitiation ribosome complex - state 1
Authors : Thoms, M.; Buschauer, R.; Ameismeier, M.; Denk, T.; Kratzat, H.; Mackens-Kiani, T.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on : 2020-07-07
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

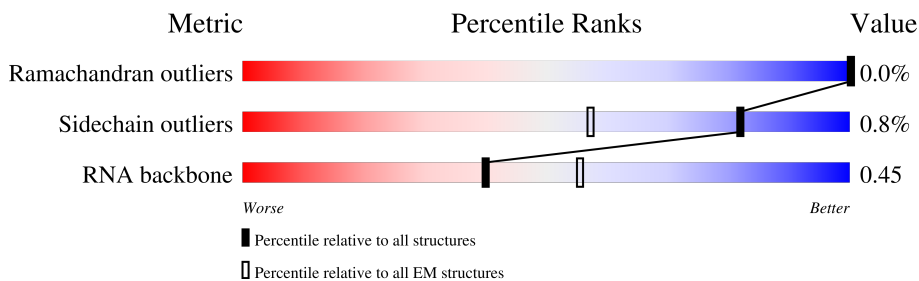
EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	a	295	
2	p	264	
3	d	293	
4	Q	115	
5	q	263	
6	W	25	
7	r	249	
8	s	194	


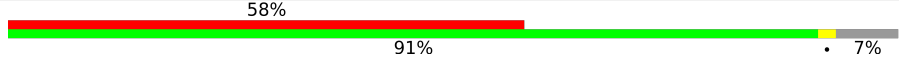
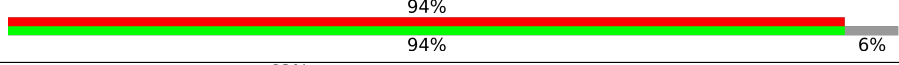
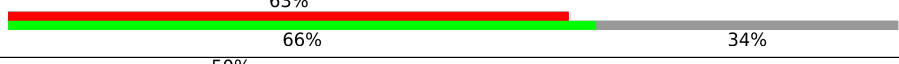
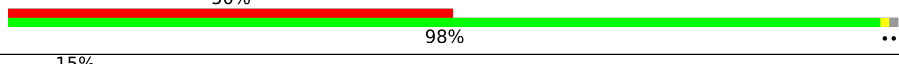

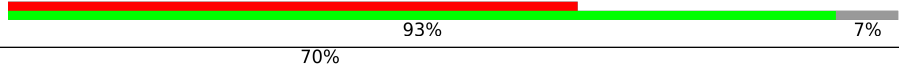

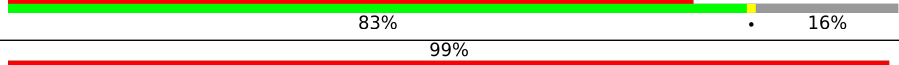
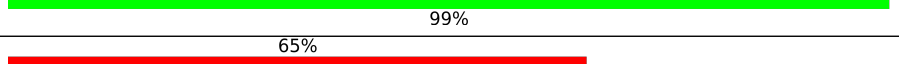



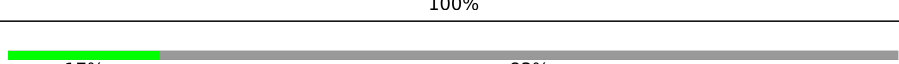
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Mol	Chain	Length	Quality of chain
9	t	208	96%
10	c	194	92% 7%
11	n	158	85% 15%
12	m	151	98%
13	i	151	82% 17%
14	y	83	99%
15	f	130	98%
16	j	143	97%
17	z	133	92% 8%
18	R	84	96%
19	T	59	75% 25%
20	2	1868	58% 29% 8%
21	w	135	95% 5%
22	g	146	21% 94% 5%
23	b	243	23% 91% 8%
24	e	204	28% 91% 7%
25	u	165	29% 58% 42%
26	v	132	75% 83% 16%
27	o	145	64% 82% 18%
28	k	152	74% 89% 8%
29	x	145	34% 95%
30	h	119	30% 82% 18%
31	P	125	44% 55% 44%
32	S	69	19% 83% 6% 12%
33	l	56	91% 5%

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Mol	Chain	Length	Quality of chain
34	U	156	
35	V	317	
36	I	325	
37	B	814	
38	A	703	
39	C	913	
40	E	445	
41	F	357	
42	H	352	
43	K	218	
44	L	564	
45	M	374	
46	D	548	
47	Y	78	
48	J	180	

2 Entry composition [i](#)

There are 49 unique types of molecules in this entry. The entry contains 109201 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 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	216	1705	1083	299	315	8	0	0

- Molecule 2 is a protein called 40S ribosomal protein S3a.

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

- Molecule 3 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	d	216	1674	1085	287	292	10	0	0

- Molecule 4 is a protein called 40S ribosomal protein S26.

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

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	q	255	2031	1299	377	347	8	0	0

- Molecule 6 is a protein called 60S ribosomal protein L41.

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

- Molecule 7 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	r	222	1794	1123	357	308	6	0	0

- Molecule 8 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	s	173	1399	898	256	244	1	0	0

- Molecule 9 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	t	199	1638	1027	322	284	5	0	0

- Molecule 10 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	c	180	1499	955	300	242	2	0	0

- Molecule 11 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	n	135	1119	715	211	187	6	0	0

- Molecule 12 is a protein called 40S ribosomal protein S13.

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

- Molecule 13 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	i	125	939	574	187	172	6	0	0

- Molecule 14 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	y	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 15 is a protein called 40S ribosomal protein S15a.

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

- Molecule 16 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	j	139	Total	C	N	O	S	0	0
			1080	682	214	181	3		

- Molecule 17 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	z	122	Total	C	N	O	S	0	0
			999	633	196	165	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 19 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	44	Total	C	N	O	S	0	0
			354	216	81	56	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2	1721	Total	C	N	O	P	0	0
			36718	16400	6603	12004	1711		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	1772	C	G	conflict	GB 337376

- Molecule 21 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	w	128	1011	641	182	184	4	0	0

- Molecule 22 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	g	138	1100	699	208	190	3	0	0

- Molecule 23 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	b	224	1745	1112	314	312	7	0	0

- Molecule 24 is a protein called 40S ribosomal protein S5.

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

- Molecule 25 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	u	95	799	524	139	130	6	0	0

- Molecule 26 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	v	111	861	544	151	159	7	0	0

- Molecule 27 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	o	119	Total	C	N	O	S	0	0
			980	623	183	167	7		

- Molecule 28 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	k	140	Total	C	N	O	S	0	0
			1162	731	234	196	1		

- Molecule 29 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	x	141	Total	C	N	O	S	0	0
			1094	685	210	196	3		

- Molecule 30 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	98	Total	C	N	O	S	0	0
			780	489	148	139	4		

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	P	70	Total	C	N	O	S	0	0
			557	358	101	97	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S	61	Total	C	N	O	S	0	0
			479	292	95	90	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	l	54	Total	C	N	O	S	0	0
			450	282	93	70	5		

- Molecule 34 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	U	57	Total	C	N	O	S	0	0
			465	295	89	74	7		

- Molecule 35 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	V	296	Total	C	N	O	S	0	0
			2314	1464	404	434	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
36	I	305	Total	C	N	O	0	0
			1497	887	305	305		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	B	536	Total	C	N	O	S	0	0
			2966	1801	580	580	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A	694	Total	C	N	O	S	0	0
			5394	3385	982	1005	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	C	625	Total	C	N	O	S	0	0
			5070	3204	898	933	35		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	E	416	Total	C	N	O	S	0	0
			3437	2202	585	630	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	F	269	2090	1317	356	405	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	H	295	2413	1532	417	449	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	K	217	1750	1116	288	334	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	L	372	3111	2011	520	563	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	M	340	2718	1734	459	508	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	D	447	3617	2279	625	691	22	0	0

- Molecule 47 is a protein called Unknown factor.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	Y	78	390	234	78	78	0	0

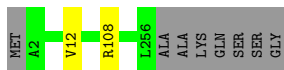
- Molecule 48 is a protein called Host translation inhibitor Nsp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	J	30	244	148	44	51	1	0	0

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

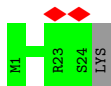
Mol	Chain	Residues	Atoms		AltConf
49	Q	1	Total	Zn	0
			1	1	
49	l	1	Total	Zn	0
			1	1	
49	U	1	Total	Zn	0
			1	1	

Chain q:  96%




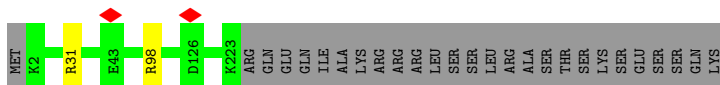
- Molecule 6: 60S ribosomal protein L41

Chain W:  96%




- Molecule 7: 40S ribosomal protein S6

Chain r:  88%



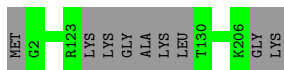
- Molecule 8: 40S ribosomal protein S7

Chain s:  89%



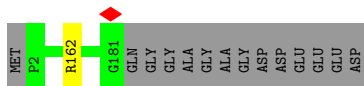
- Molecule 9: 40S ribosomal protein S8

Chain t:  96%




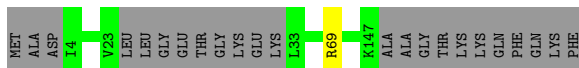
- Molecule 10: 40S ribosomal protein S9

Chain c:  92%



- Molecule 11: 40S ribosomal protein S11

Chain n:  85%




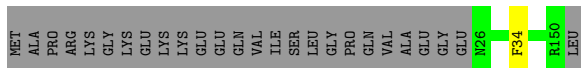
- Molecule 12: 40S ribosomal protein S13

Chain m:  98%



- Molecule 13: 40S ribosomal protein S14

Chain i:  82%



- Molecule 14: 40S ribosomal protein S21

Chain y:  99%



- Molecule 15: 40S ribosomal protein S15a

Chain f:  98%



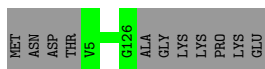
- Molecule 16: 40S ribosomal protein S23

Chain j:  97%



- Molecule 17: 40S ribosomal protein S24

Chain z:  92%



- Molecule 18: 40S ribosomal protein S27

Chain R:  96%

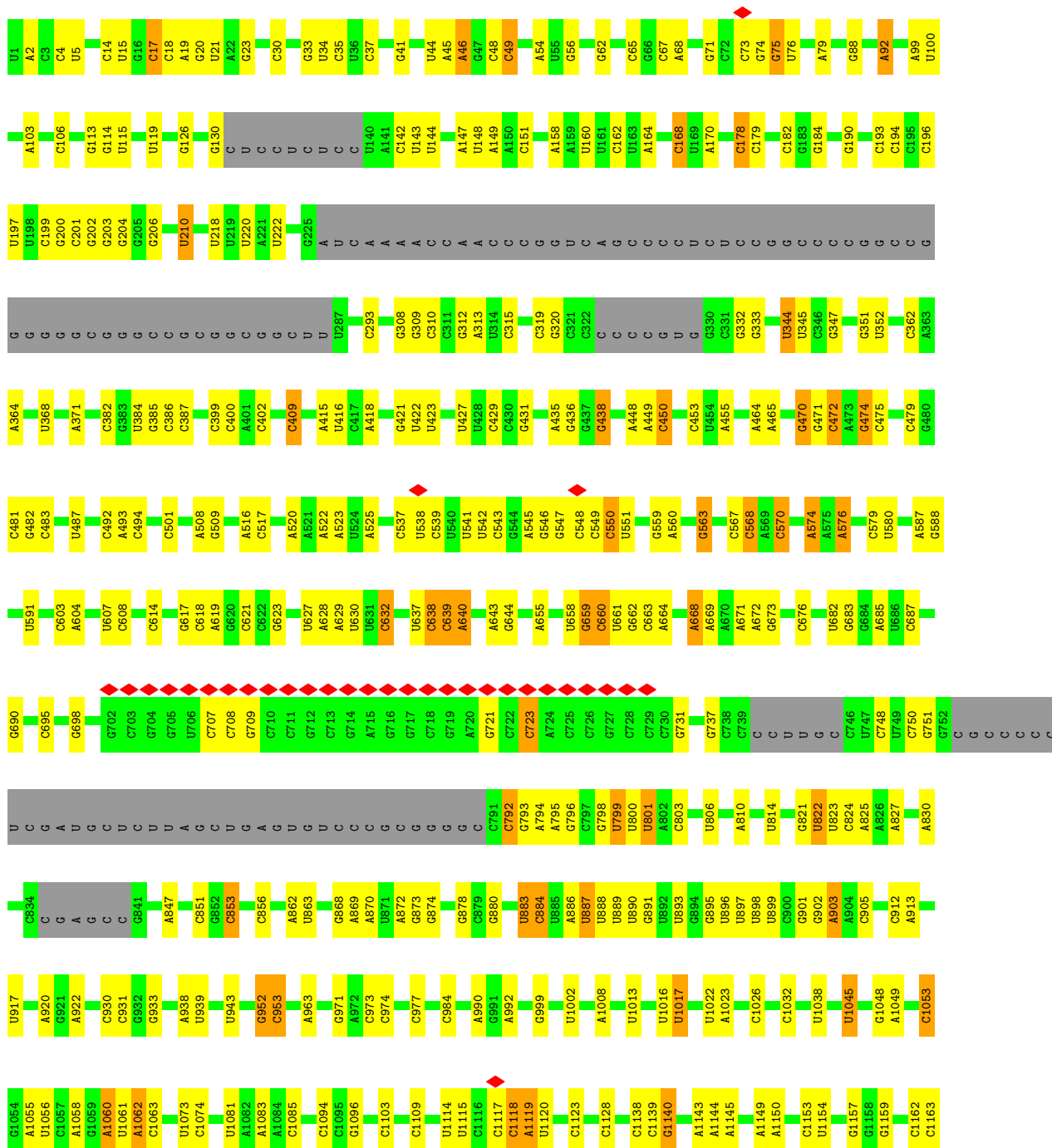


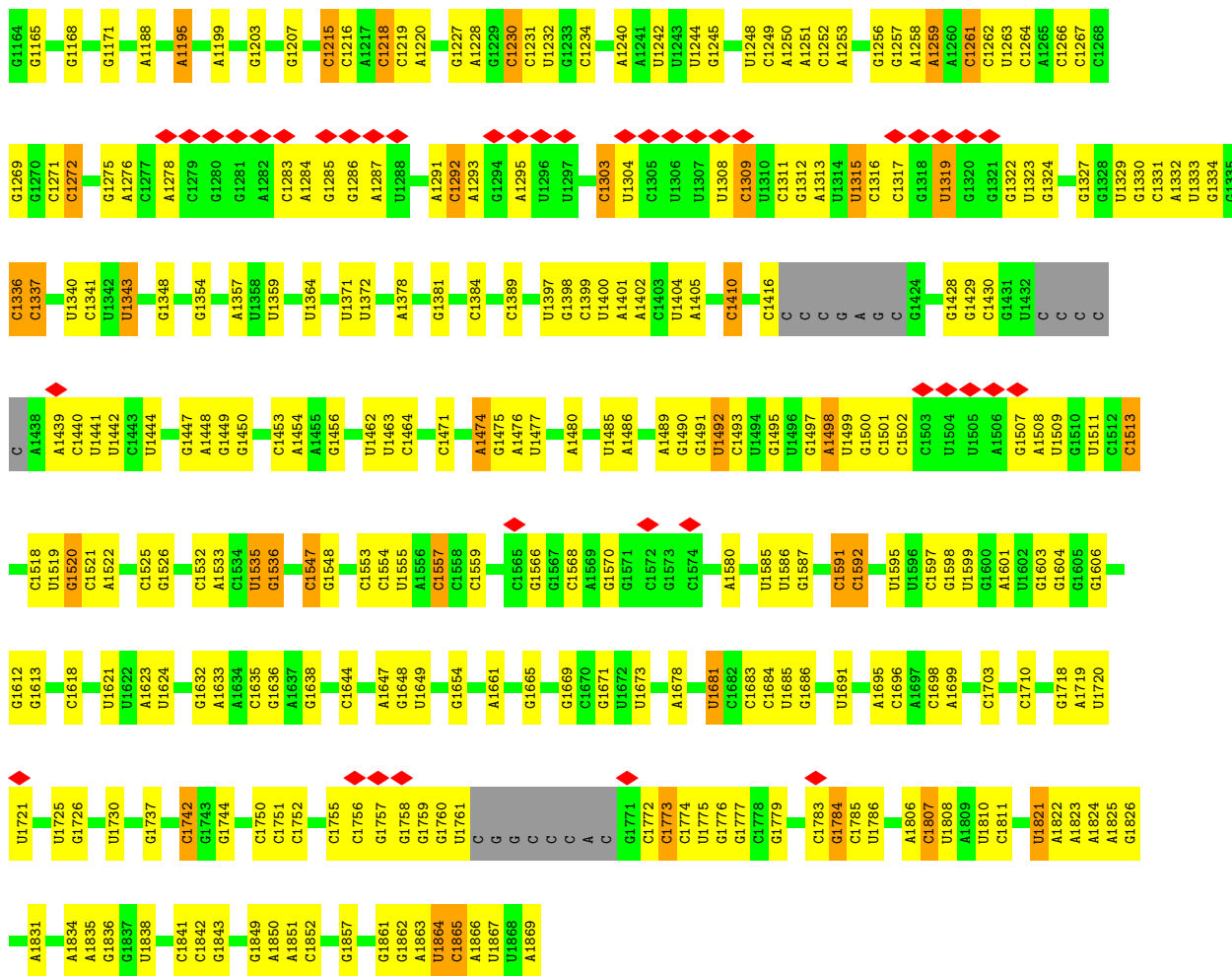
- Molecule 19: 40S ribosomal protein S30



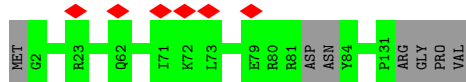
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● Molecule 20: 18S ribosomal RNA

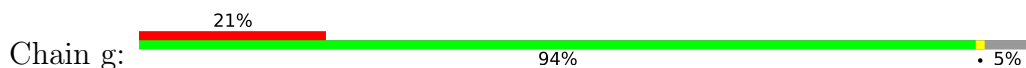




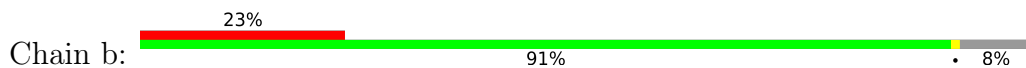
• Molecule 21: 40S ribosomal protein S17

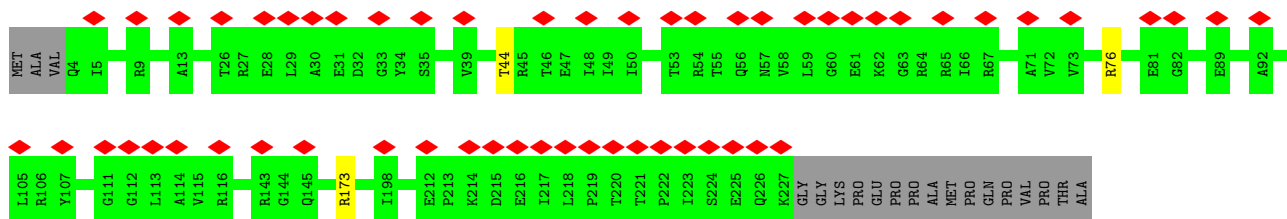


• Molecule 22: 40S ribosomal protein S16

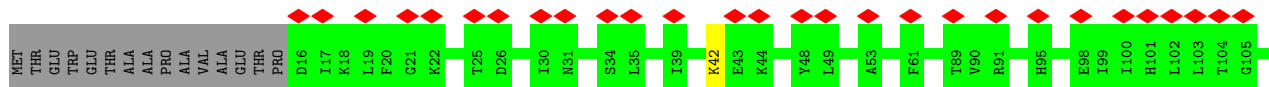
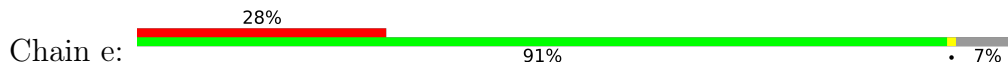


• Molecule 23: 40S ribosomal protein S3

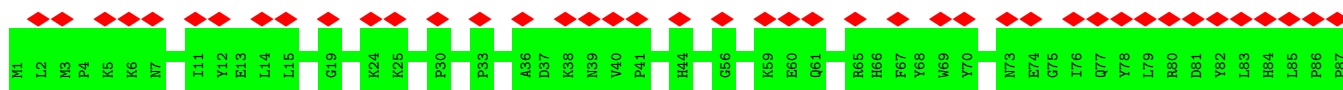




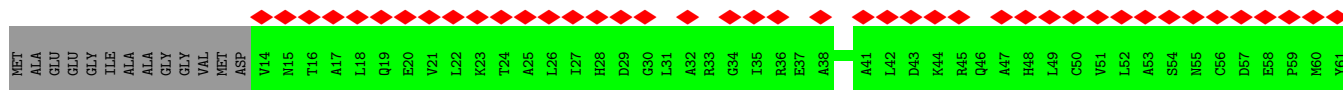
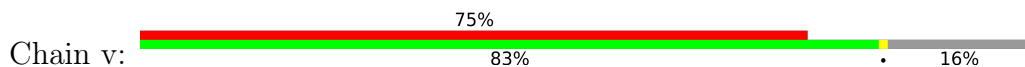
• Molecule 24: 40S ribosomal protein S5



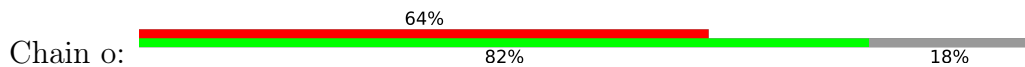
• Molecule 25: 40S ribosomal protein S10

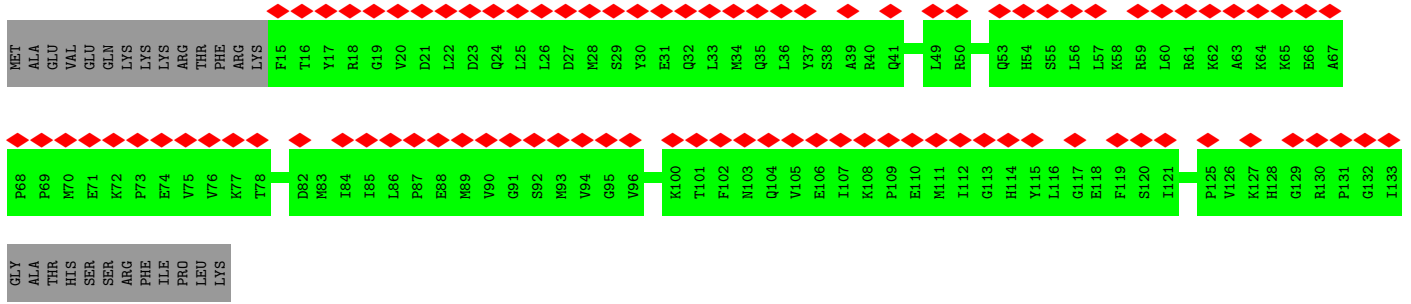


• Molecule 26: 40S ribosomal protein S12

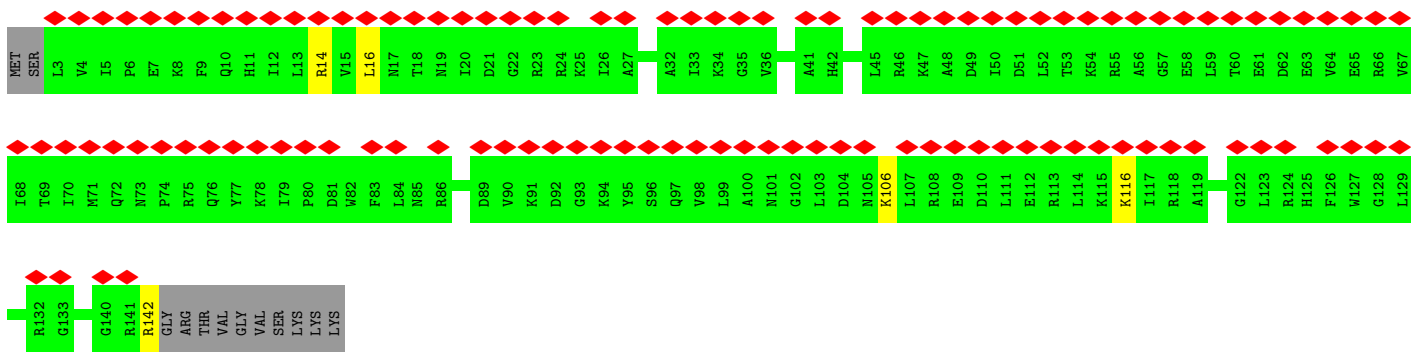
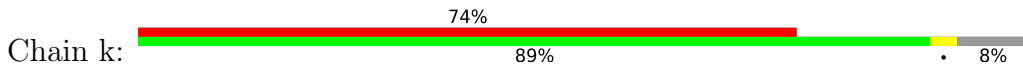


• Molecule 27: 40S ribosomal protein S15

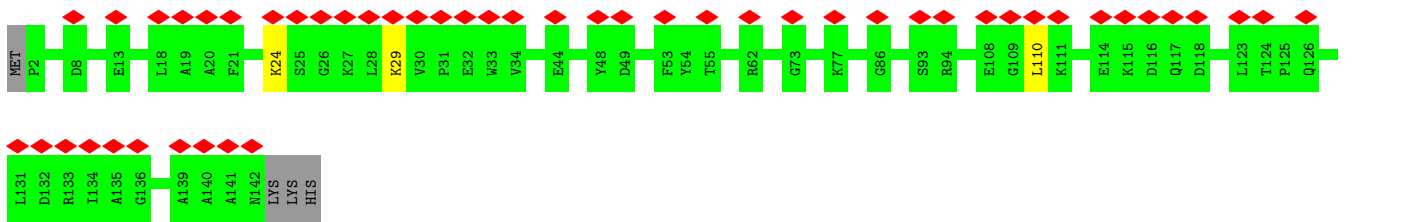
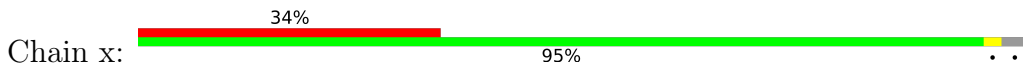




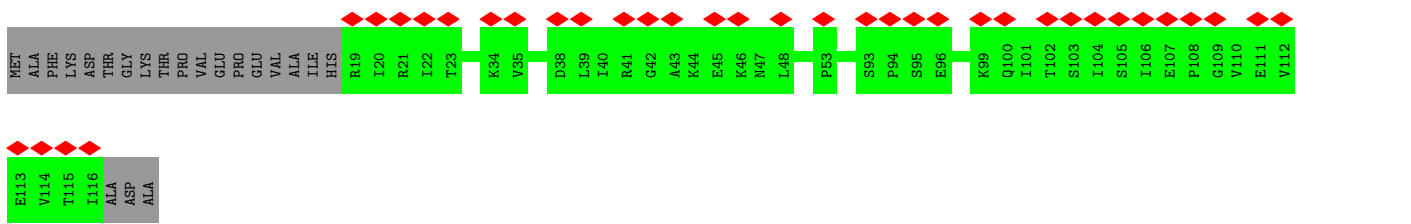
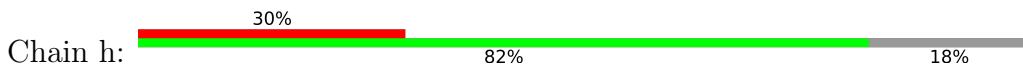
• Molecule 28: 40S ribosomal protein S18



• Molecule 29: 40S ribosomal protein S19

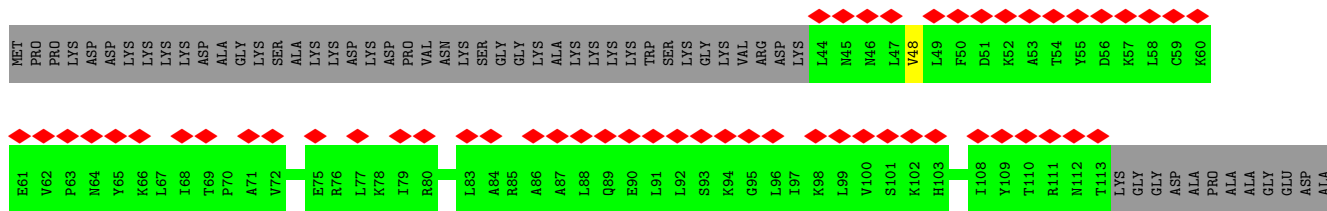


• Molecule 30: 40S ribosomal protein S20

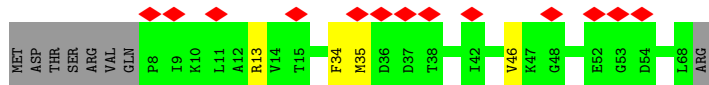
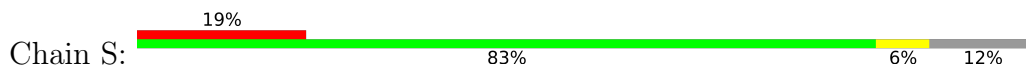


• Molecule 31: 40S ribosomal protein S25

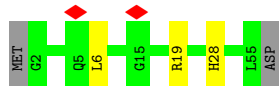
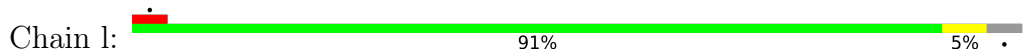




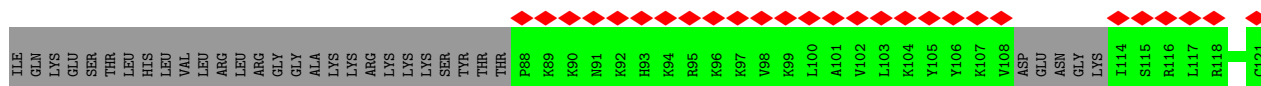
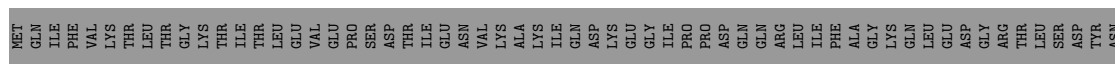
● Molecule 32: 40S ribosomal protein S28



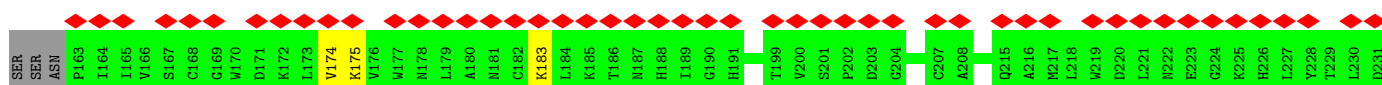
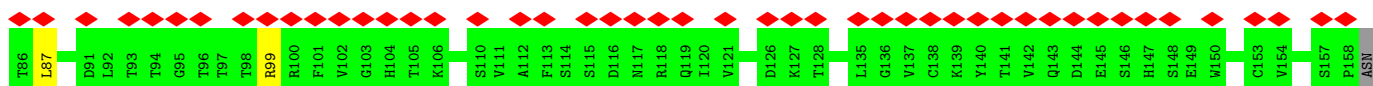
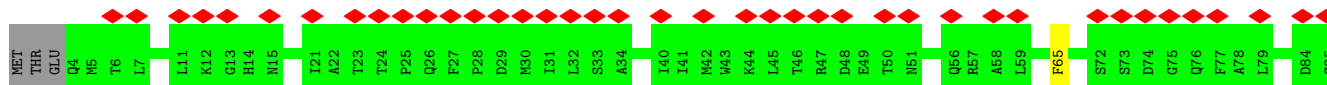
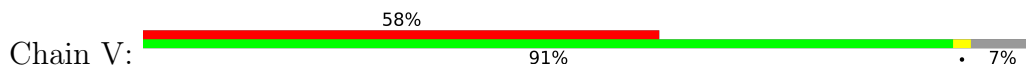
● Molecule 33: 40S ribosomal protein S29



● Molecule 34: Ubiquitin-40S ribosomal protein S27a



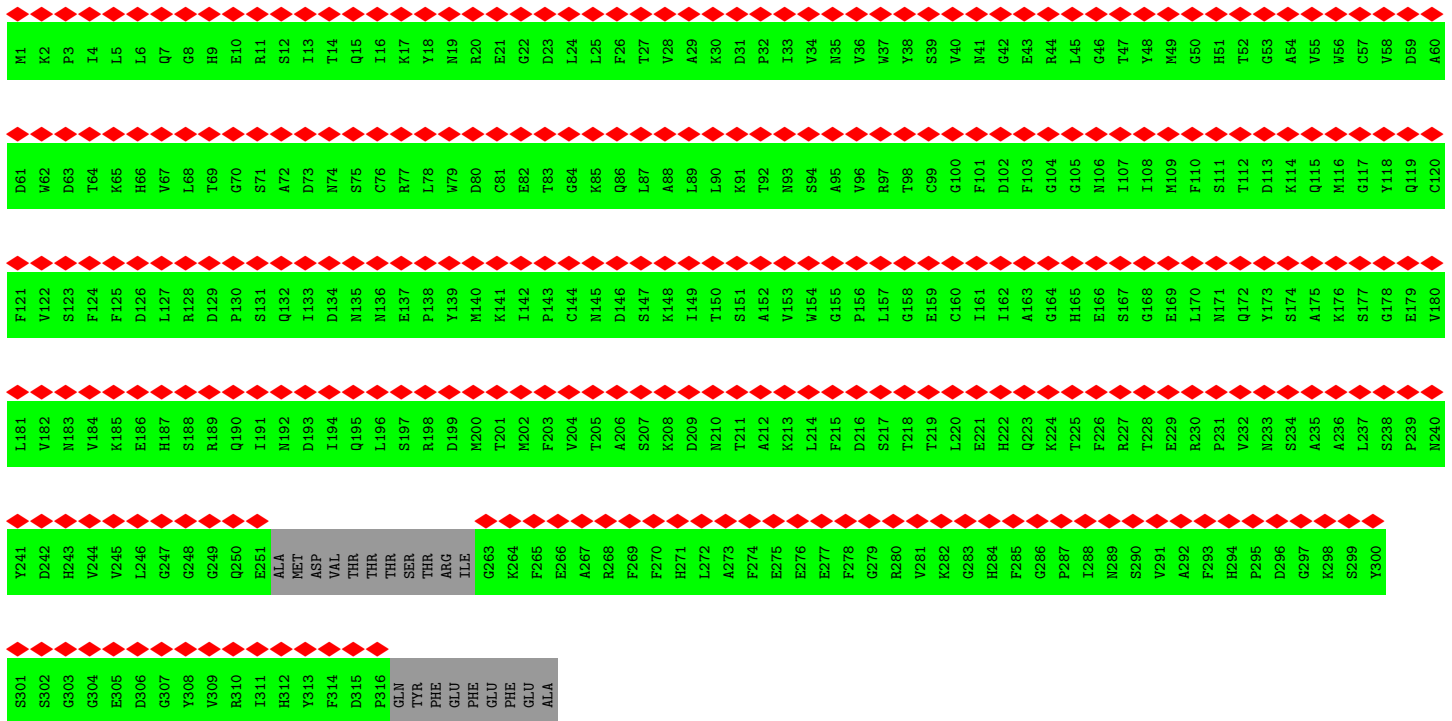
● Molecule 35: Receptor of activated protein C kinase 1





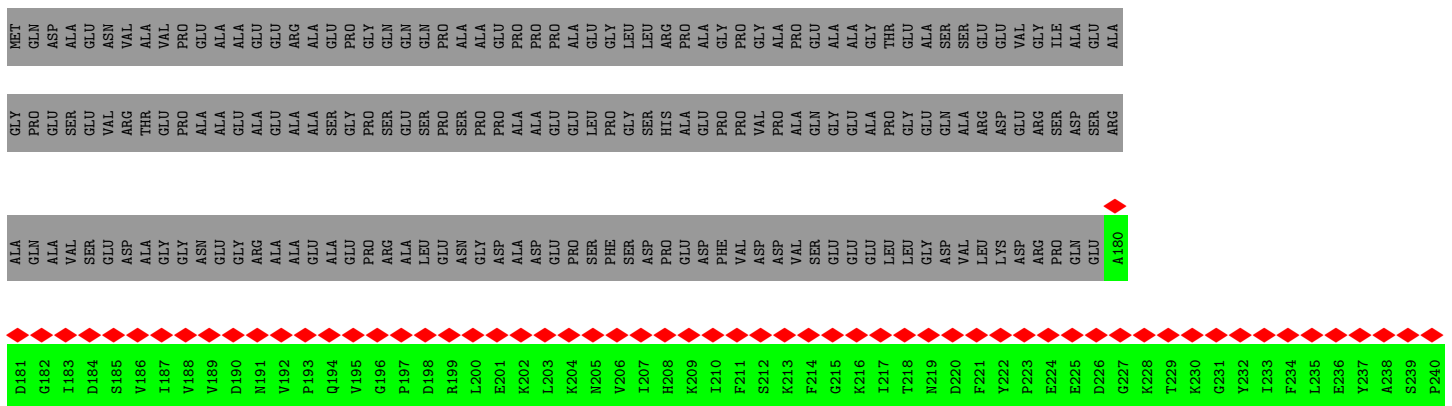
• Molecule 36: Eukaryotic translation initiation factor 3 subunit I

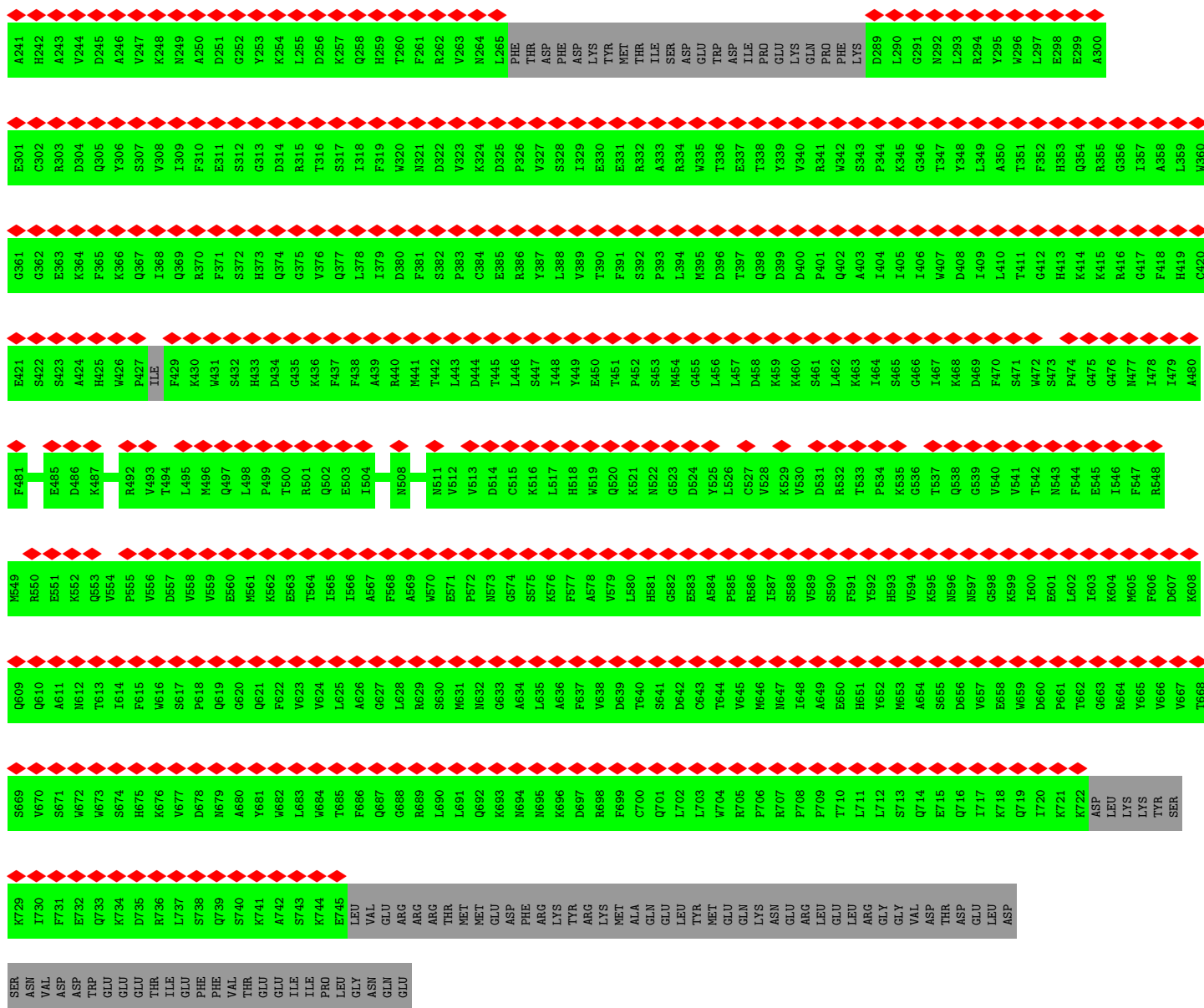
Chain I: 94%
94% 6%



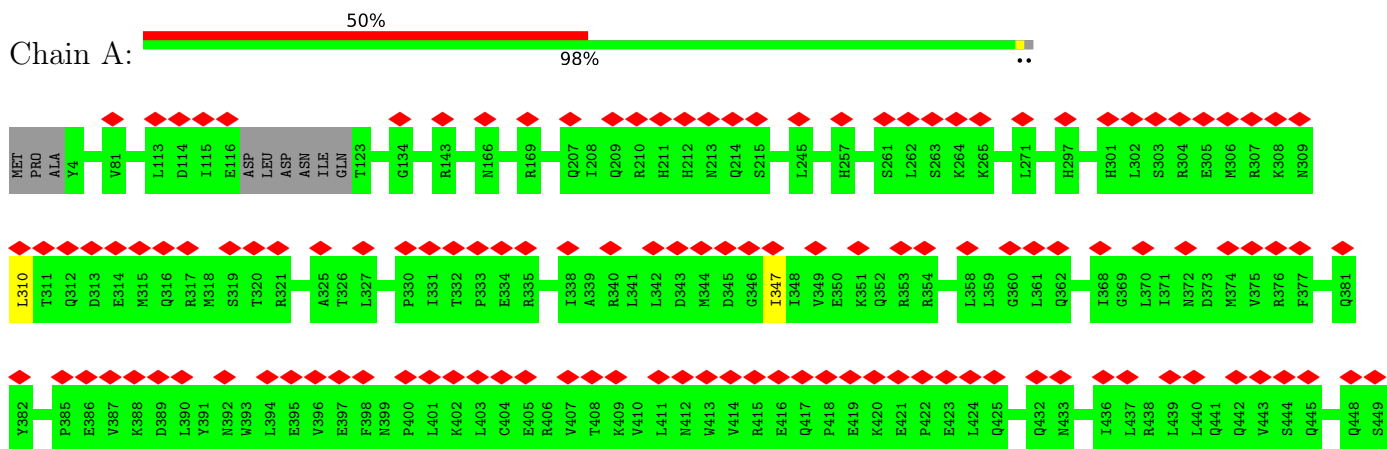
• Molecule 37: Eukaryotic translation initiation factor 3 subunit B

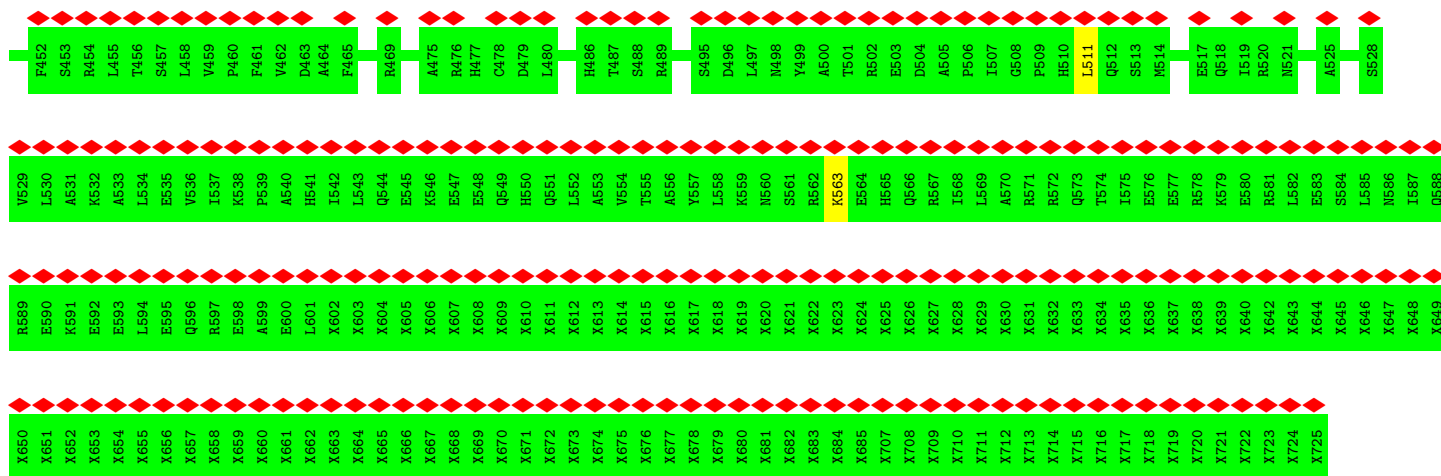
Chain B: 63%
66% 34%



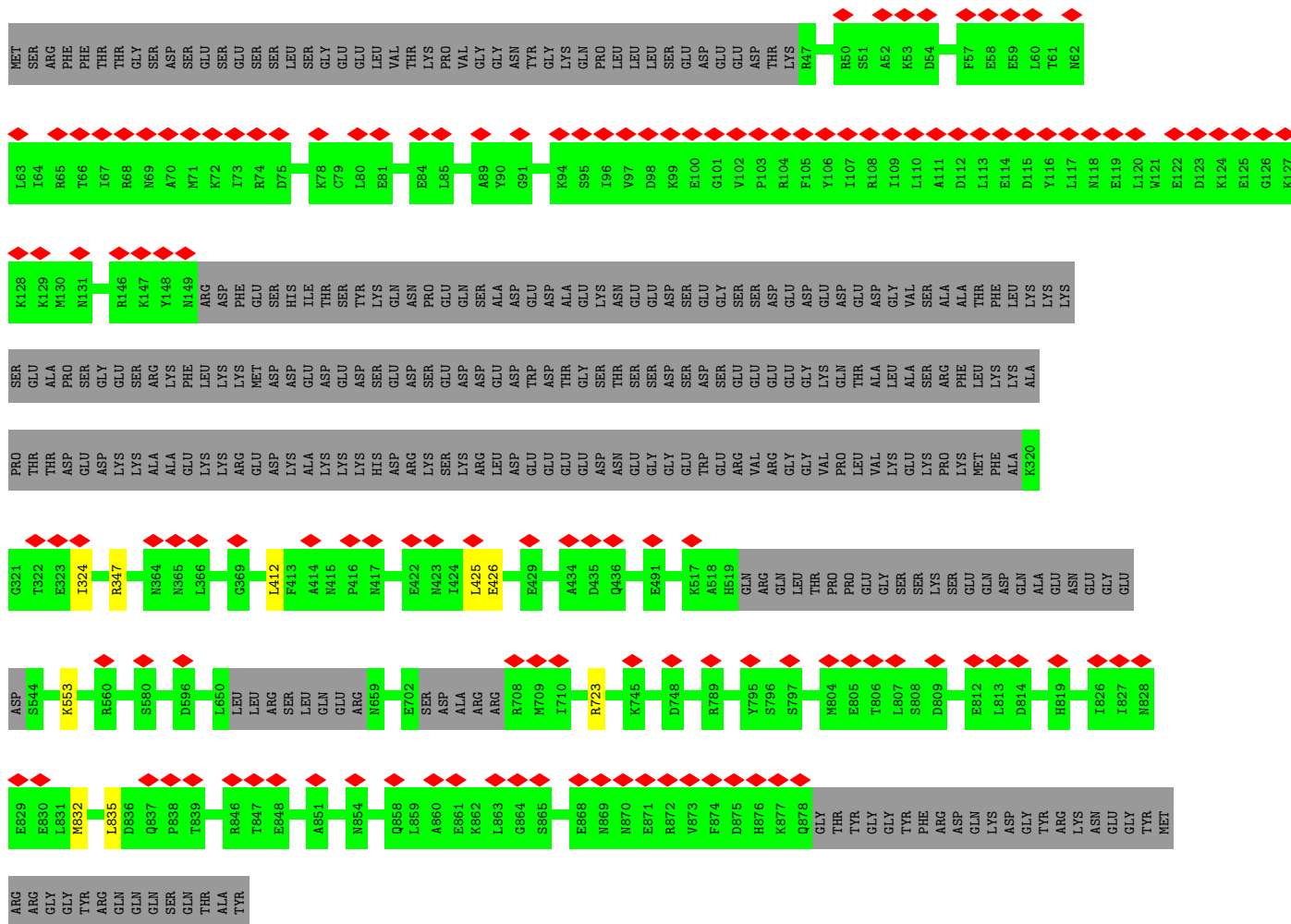


● Molecule 38: Eukaryotic translation initiation factor 3 subunit A, Eukaryotic translation initiation factor 3 subunit A

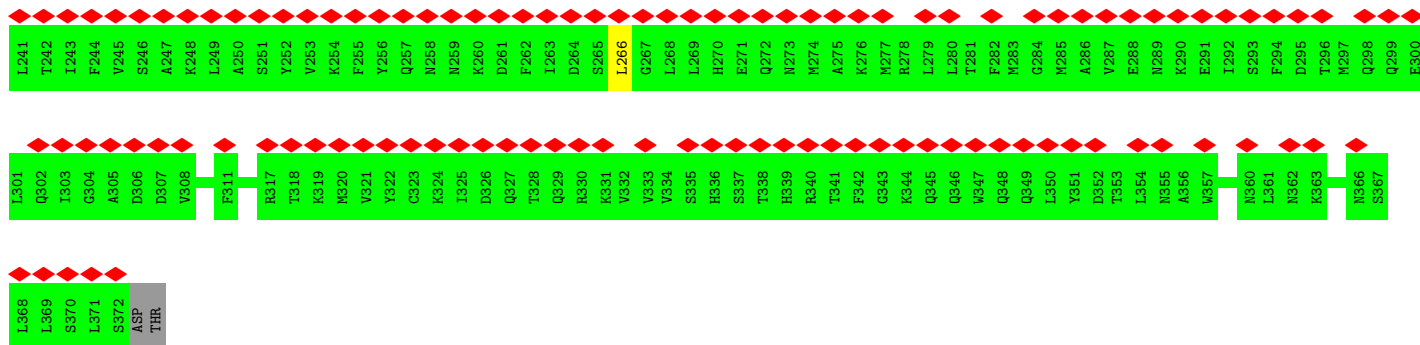




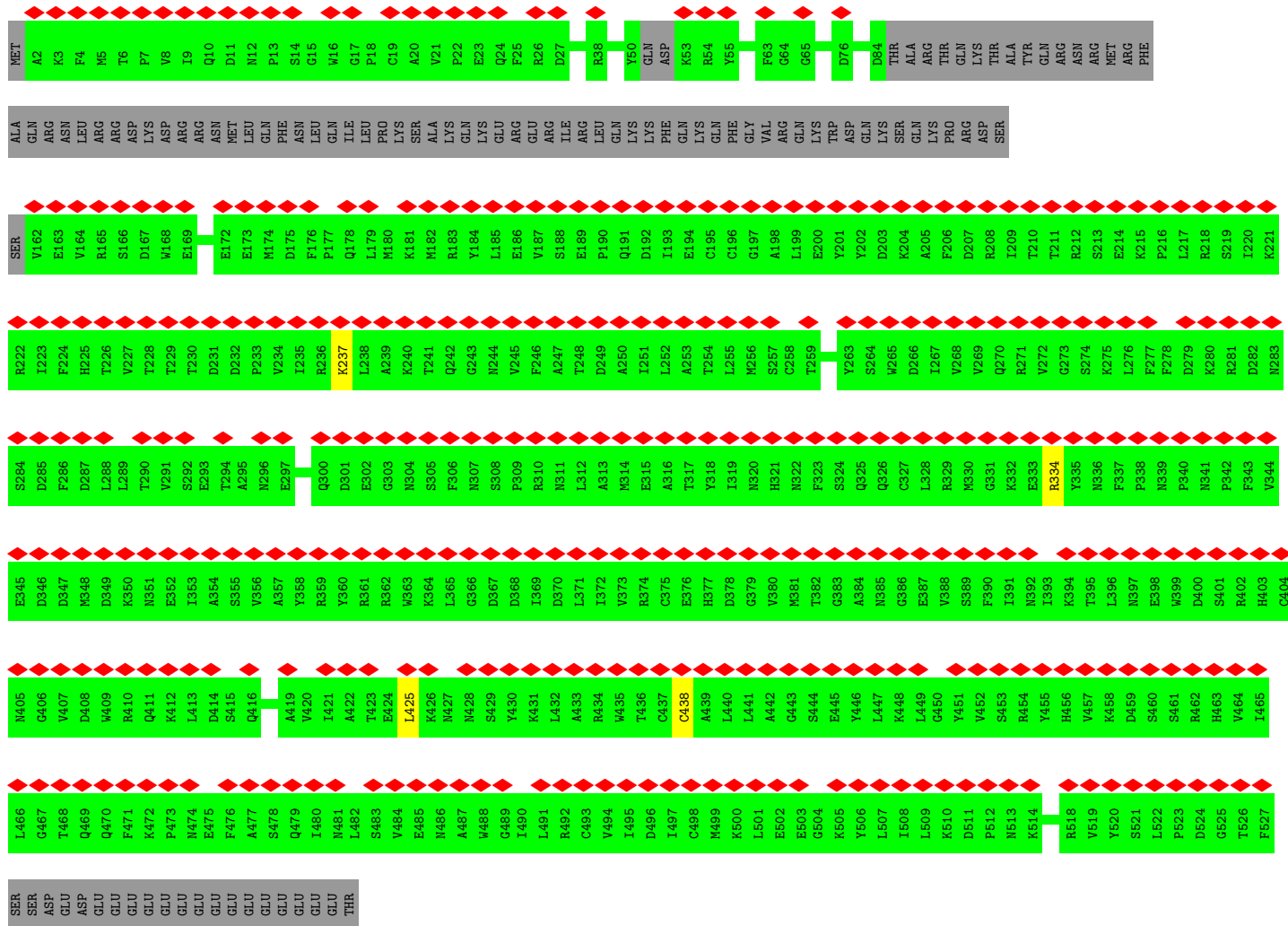
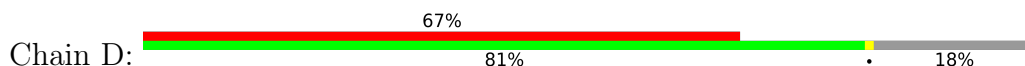
• Molecule 39: Eukaryotic translation initiation factor 3 subunit C



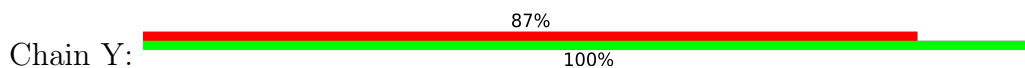
• Molecule 40: Eukaryotic translation initiation factor 3 subunit E

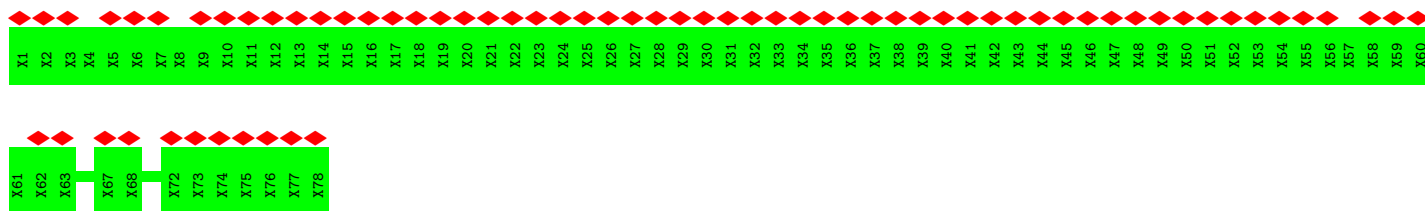


• Molecule 46: Eukaryotic translation initiation factor 3 subunit D



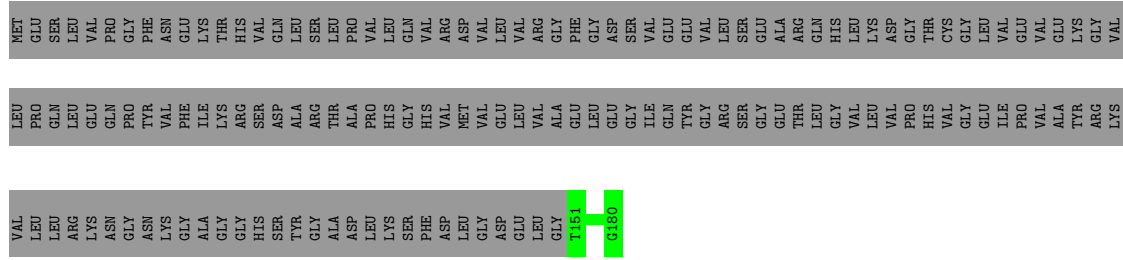
• Molecule 47: Unknown factor





● Molecule 48: Host translation inhibitor Nsp1

Chain J: 17% 83%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13928	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44.8	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	0.299	Depositor
Minimum map value	-0.075	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.059, 1.059, 1.059	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:
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	0.64	0/1742	0.58	0/2367
2	p	0.59	0/1742	0.60	1/2330 (0.0%)
3	d	0.71	0/1710	0.65	0/2310
4	Q	0.73	1/828 (0.1%)	0.65	1/1109 (0.1%)
5	q	0.65	0/2073	0.65	0/2791
6	W	0.48	0/231	0.62	0/294
7	r	0.51	0/1817	0.57	0/2421
8	s	0.51	0/1418	0.58	0/1895
9	t	0.65	0/1666	0.60	0/2223
10	c	0.72	1/1524 (0.1%)	0.63	0/2035
11	n	0.76	0/1139	0.61	0/1524
12	m	0.65	1/1226 (0.1%)	0.60	0/1649
13	i	0.58	0/951	0.64	0/1275
14	y	0.63	0/631	0.59	0/844
15	f	0.73	1/1051 (0.1%)	0.68	0/1406
16	j	0.67	0/1097	0.63	0/1464
17	z	0.64	0/1016	0.62	0/1349
18	R	0.63	0/653	0.61	0/876
19	T	0.59	0/356	0.55	0/466
20	2	1.34	58/41057 (0.1%)	1.30	491/63985 (0.8%)
21	w	0.37	0/1024	0.58	0/1377
22	g	0.32	0/1117	0.57	0/1494
23	b	0.35	0/1773	0.65	0/2387
24	e	0.31	0/1516	0.58	1/2037 (0.0%)
25	u	0.28	0/823	0.55	0/1111
26	v	0.30	0/870	0.56	0/1168
27	o	0.29	0/999	0.58	0/1336
28	k	0.29	0/1180	0.61	1/1581 (0.1%)
29	x	0.27	0/1113	0.53	1/1493 (0.1%)
30	h	0.29	0/789	0.56	0/1059
31	P	0.29	0/563	0.62	0/758
32	S	0.35	0/481	0.63	0/643

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	I	0.34	0/461	0.70	2/612 (0.3%)
34	U	0.31	0/474	0.63	0/626
35	V	0.29	0/2369	0.63	2/3221 (0.1%)
36	I	0.25	0/1495	0.48	0/2073
37	B	0.27	0/2981	0.51	0/4115
38	A	0.31	0/4971	0.55	2/6711 (0.0%)
39	C	0.33	0/5154	0.55	3/6942 (0.0%)
40	E	0.28	0/3503	0.54	0/4728
41	F	0.27	0/2126	0.56	0/2890
42	H	0.27	0/2458	0.57	2/3313 (0.1%)
43	K	0.28	0/1785	0.58	0/2414
44	L	0.30	0/3187	0.61	0/4299
45	M	0.27	0/2756	0.58	2/3714 (0.1%)
46	D	0.30	0/3699	0.58	1/5001 (0.0%)
48	J	0.66	0/249	0.52	0/335
All	All	0.88	62/113844 (0.1%)	0.94	510/162051 (0.3%)

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
8	s	0	1
32	S	0	3
33	I	0	1
35	V	0	1
44	L	0	1
All	All	0	8

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	1139	C	N3-C4	-7.08	1.28	1.33
10	c	162	ARG	C-N	-6.99	1.18	1.34
20	2	501	C	N3-C4	-6.50	1.29	1.33
20	2	422	U	N3-C4	-6.45	1.32	1.38
20	2	422	U	C2-O2	-6.40	1.16	1.22

The worst 5 of 510 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	501	C	N1-C2-O2	15.01	127.91	118.90
20	2	422	U	N3-C2-O2	-14.66	111.94	122.20
20	2	501	C	C2-N1-C1'	13.96	134.16	118.80
20	2	119	U	N3-C2-O2	-13.69	112.62	122.20
20	2	293	C	N1-C2-O2	13.10	126.76	118.90

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	S	34	PHE	Peptide
32	S	35	MET	Peptide
32	S	46	VAL	Peptide
1	a	73	ASP	Peptide
8	s	134	VAL	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	214/295 (72%)	209 (98%)	5 (2%)	0	100	100
2	p	209/264 (79%)	196 (94%)	13 (6%)	0	100	100
3	d	214/293 (73%)	199 (93%)	15 (7%)	0	100	100
4	Q	99/115 (86%)	95 (96%)	4 (4%)	0	100	100
5	q	253/263 (96%)	241 (95%)	12 (5%)	0	100	100
6	W	22/25 (88%)	22 (100%)	0	0	100	100
7	r	220/249 (88%)	209 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	s	165/194 (85%)	160 (97%)	5 (3%)	0	100	100
9	t	195/208 (94%)	182 (93%)	13 (7%)	0	100	100
10	c	178/194 (92%)	172 (97%)	6 (3%)	0	100	100
11	n	131/158 (83%)	126 (96%)	5 (4%)	0	100	100
12	m	147/151 (97%)	147 (100%)	0	0	100	100
13	i	123/151 (82%)	114 (93%)	9 (7%)	0	100	100
14	y	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
15	f	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
16	j	137/143 (96%)	133 (97%)	4 (3%)	0	100	100
17	z	120/133 (90%)	115 (96%)	5 (4%)	0	100	100
18	R	80/84 (95%)	75 (94%)	5 (6%)	0	100	100
19	T	40/59 (68%)	39 (98%)	1 (2%)	0	100	100
21	w	124/135 (92%)	112 (90%)	12 (10%)	0	100	100
22	g	136/146 (93%)	125 (92%)	11 (8%)	0	100	100
23	b	222/243 (91%)	196 (88%)	26 (12%)	0	100	100
24	e	187/204 (92%)	167 (89%)	20 (11%)	0	100	100
25	u	93/165 (56%)	83 (89%)	10 (11%)	0	100	100
26	v	107/132 (81%)	97 (91%)	10 (9%)	0	100	100
27	o	117/145 (81%)	112 (96%)	5 (4%)	0	100	100
28	k	138/152 (91%)	126 (91%)	12 (9%)	0	100	100
29	x	139/145 (96%)	131 (94%)	8 (6%)	0	100	100
30	h	96/119 (81%)	87 (91%)	9 (9%)	0	100	100
31	P	68/125 (54%)	61 (90%)	7 (10%)	0	100	100
32	S	59/69 (86%)	51 (86%)	8 (14%)	0	100	100
33	l	52/56 (93%)	45 (86%)	7 (14%)	0	100	100
34	U	53/156 (34%)	51 (96%)	2 (4%)	0	100	100
35	V	290/317 (92%)	258 (89%)	31 (11%)	1 (0%)	41	76
36	I	301/325 (93%)	293 (97%)	8 (3%)	0	100	100
37	B	528/814 (65%)	491 (93%)	37 (7%)	0	100	100
38	A	588/703 (84%)	562 (96%)	26 (4%)	0	100	100
39	C	615/913 (67%)	575 (94%)	40 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	E	406/445 (91%)	394 (97%)	12 (3%)	0	100	100
41	F	267/357 (75%)	244 (91%)	23 (9%)	0	100	100
42	H	289/352 (82%)	270 (93%)	19 (7%)	0	100	100
43	K	215/218 (99%)	202 (94%)	13 (6%)	0	100	100
44	L	370/564 (66%)	332 (90%)	38 (10%)	0	100	100
45	M	328/374 (88%)	314 (96%)	14 (4%)	0	100	100
46	D	441/548 (80%)	402 (91%)	39 (9%)	0	100	100
48	J	28/180 (16%)	25 (89%)	3 (11%)	0	100	100
All	All	9011/11294 (80%)	8443 (94%)	567 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	V	175	LYS

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	180/243 (74%)	179 (99%)	1 (1%)	86	95
2	p	192/231 (83%)	192 (100%)	0	100	100
3	d	182/225 (81%)	182 (100%)	0	100	100
4	Q	88/98 (90%)	88 (100%)	0	100	100
5	q	220/225 (98%)	218 (99%)	2 (1%)	78	92
6	W	23/24 (96%)	23 (100%)	0	100	100
7	r	193/218 (88%)	191 (99%)	2 (1%)	76	91
8	s	155/174 (89%)	155 (100%)	0	100	100
9	t	174/180 (97%)	174 (100%)	0	100	100
10	c	160/168 (95%)	160 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	n	125/142 (88%)	124 (99%)	1 (1%)	81	93
12	m	130/131 (99%)	130 (100%)	0	100	100
13	i	98/119 (82%)	97 (99%)	1 (1%)	76	91
14	y	66/67 (98%)	66 (100%)	0	100	100
15	f	112/113 (99%)	111 (99%)	1 (1%)	78	92
16	j	111/115 (96%)	110 (99%)	1 (1%)	78	92
17	z	106/115 (92%)	106 (100%)	0	100	100
18	R	74/76 (97%)	73 (99%)	1 (1%)	67	88
19	T	35/48 (73%)	35 (100%)	0	100	100
21	w	111/122 (91%)	111 (100%)	0	100	100
22	g	114/121 (94%)	113 (99%)	1 (1%)	78	92
23	b	188/202 (93%)	185 (98%)	3 (2%)	62	86
24	e	159/170 (94%)	157 (99%)	2 (1%)	69	89
25	u	86/136 (63%)	86 (100%)	0	100	100
26	v	94/108 (87%)	93 (99%)	1 (1%)	73	90
27	o	107/130 (82%)	107 (100%)	0	100	100
28	k	122/132 (92%)	118 (97%)	4 (3%)	38	73
29	x	111/115 (96%)	109 (98%)	2 (2%)	59	85
30	h	91/107 (85%)	91 (100%)	0	100	100
31	P	62/103 (60%)	61 (98%)	1 (2%)	62	86
32	S	54/62 (87%)	53 (98%)	1 (2%)	57	84
33	l	47/49 (96%)	46 (98%)	1 (2%)	53	82
34	U	51/140 (36%)	50 (98%)	1 (2%)	55	83
35	V	256/275 (93%)	253 (99%)	3 (1%)	71	90
37	B	90/702 (13%)	90 (100%)	0	100	100
38	A	545/553 (99%)	543 (100%)	2 (0%)	91	97
39	C	553/811 (68%)	547 (99%)	6 (1%)	73	90
40	E	380/406 (94%)	378 (100%)	2 (0%)	88	96
41	F	237/289 (82%)	234 (99%)	3 (1%)	69	89
42	H	269/310 (87%)	267 (99%)	2 (1%)	84	94
43	K	192/193 (100%)	191 (100%)	1 (0%)	88	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	L	342/515 (66%)	336 (98%)	6 (2%)	59	85
45	M	305/335 (91%)	304 (100%)	1 (0%)	92	97
46	D	398/494 (81%)	395 (99%)	3 (1%)	81	93
48	J	26/151 (17%)	26 (100%)	0	100	100
All	All	7414/9443 (78%)	7358 (99%)	56 (1%)	82	93

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	V	183	LYS
46	D	438	CYS
39	C	553	LYS
46	D	334	ARG
44	L	468	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 140 such sidechains are listed below:

Mol	Chain	Res	Type
42	H	336	GLN
43	K	186	GLN
46	D	62	GLN
25	u	73	ASN
24	e	179	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	2	1707/1868 (91%)	457 (26%)	9 (0%)

5 of 457 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	2	2	A
20	2	17	C
20	2	23	G
20	2	33	G
20	2	41	G

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	2	1474	A
20	2	1807	C
20	2	912	C
20	2	1060	A
20	2	1292	C

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
20	2	4
38	A	3

Continued on next page...

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Mol	Chain	Number of breaks
45	M	1
10	c	1

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	685:UNK	C	707:UNK	N	30.94
1	A	640:UNK	C	642:UNK	N	11.63
1	M	96:GLY	C	97:GLU	N	9.05
1	2	746:C	O3'	747:U	P	4.59
1	2	1207:G	O3'	1208:A	P	4.33

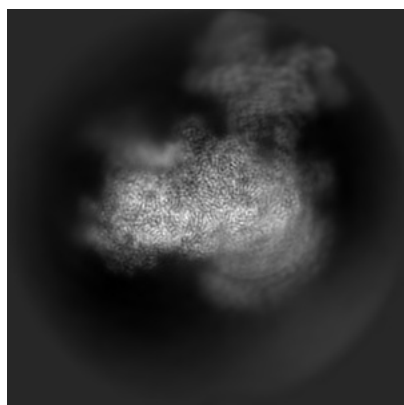
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11325. These allow visual inspection of the internal detail of the map and identification of artifacts.

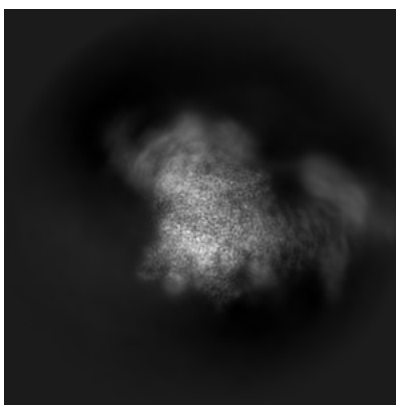
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

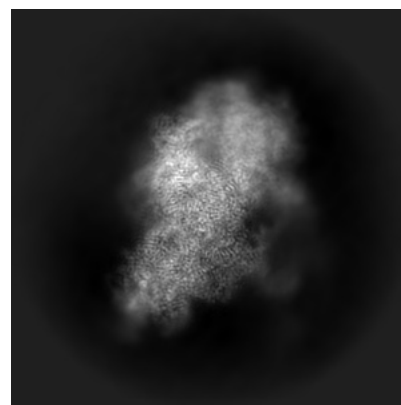
6.1.1 Primary map



X



Y

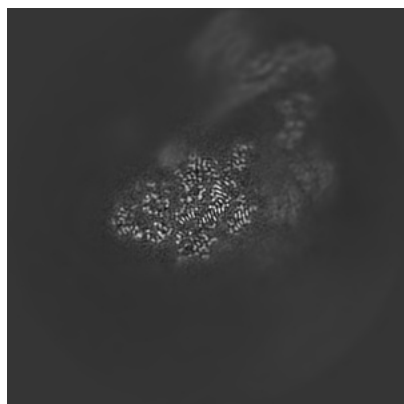


Z

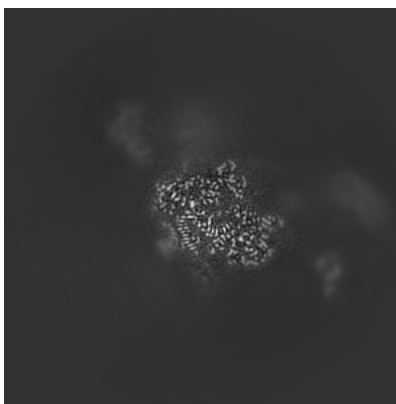
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

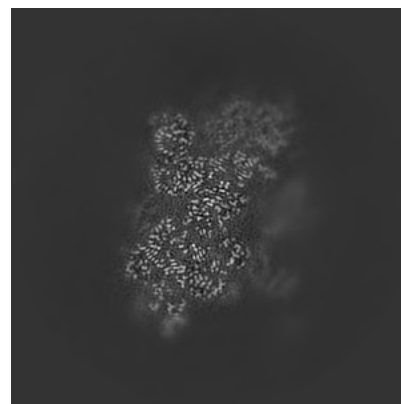
6.2.1 Primary map



X Index: 180



Y Index: 180

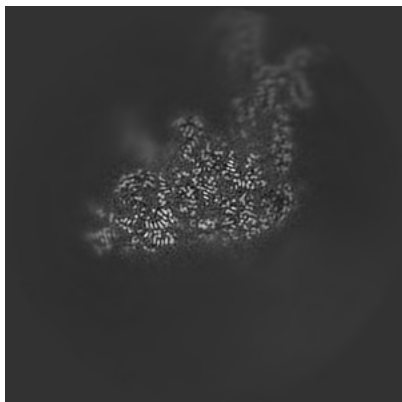


Z Index: 180

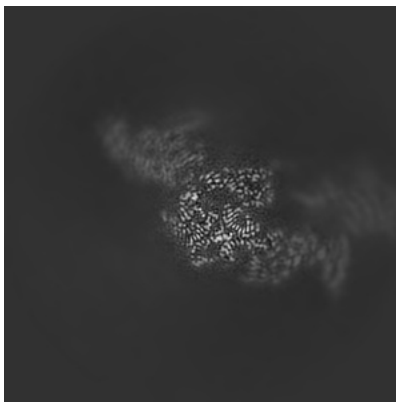
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

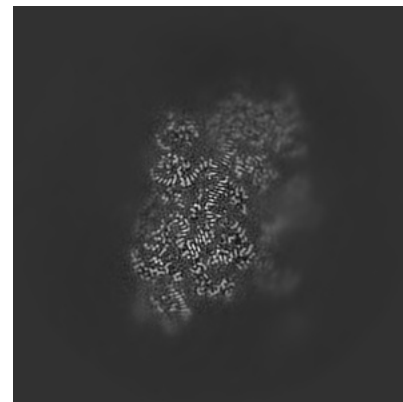
6.3.1 Primary map



X Index: 158



Y Index: 204

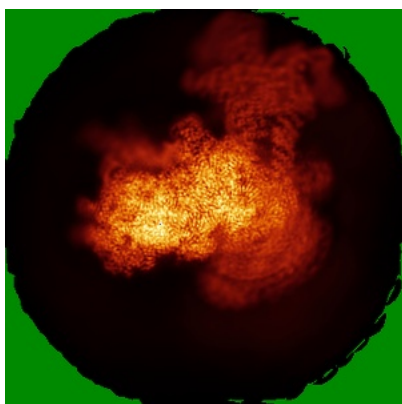


Z Index: 175

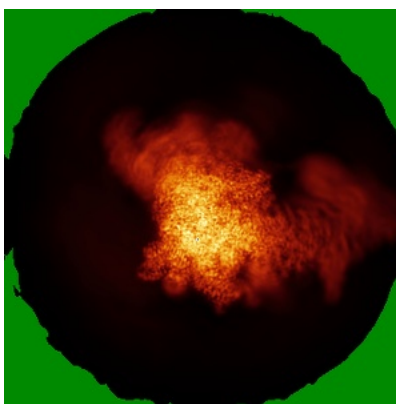
The images above show the largest variance slices of the map in three orthogonal directions.

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

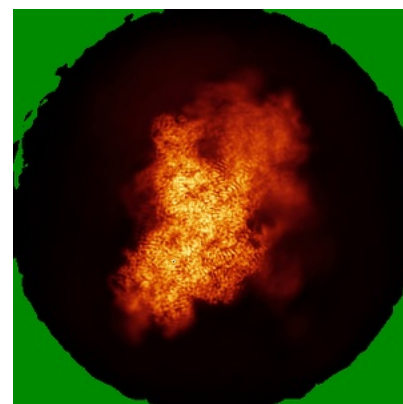
6.4.1 Primary map



X



Y

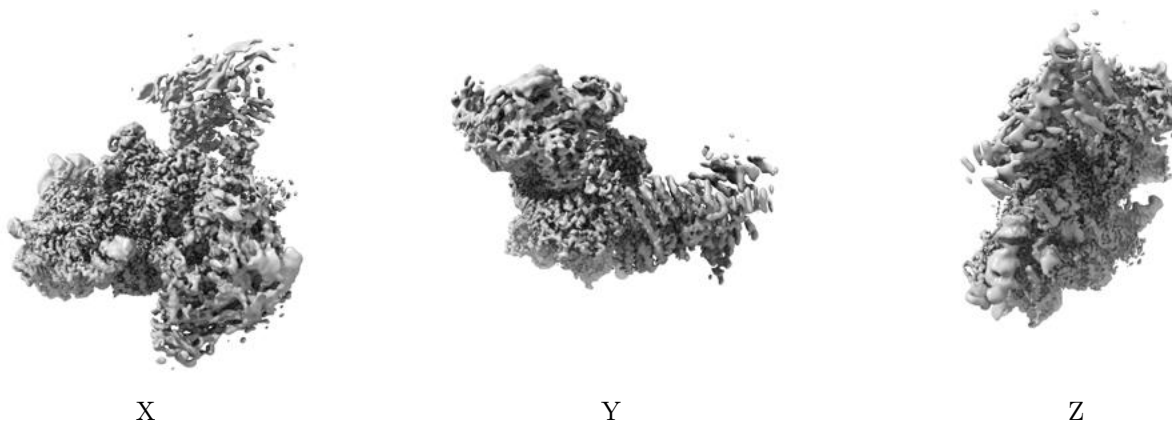


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

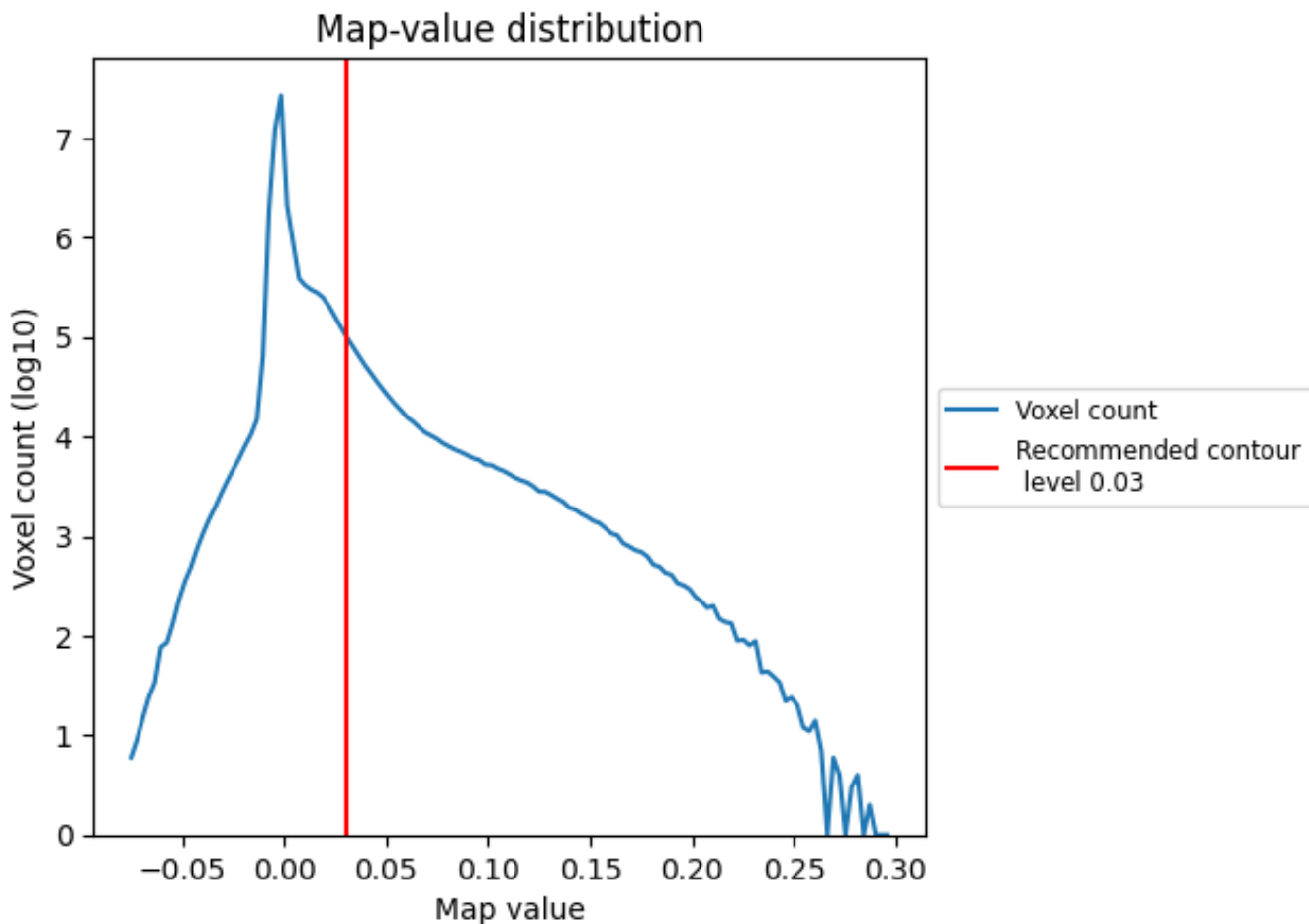
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

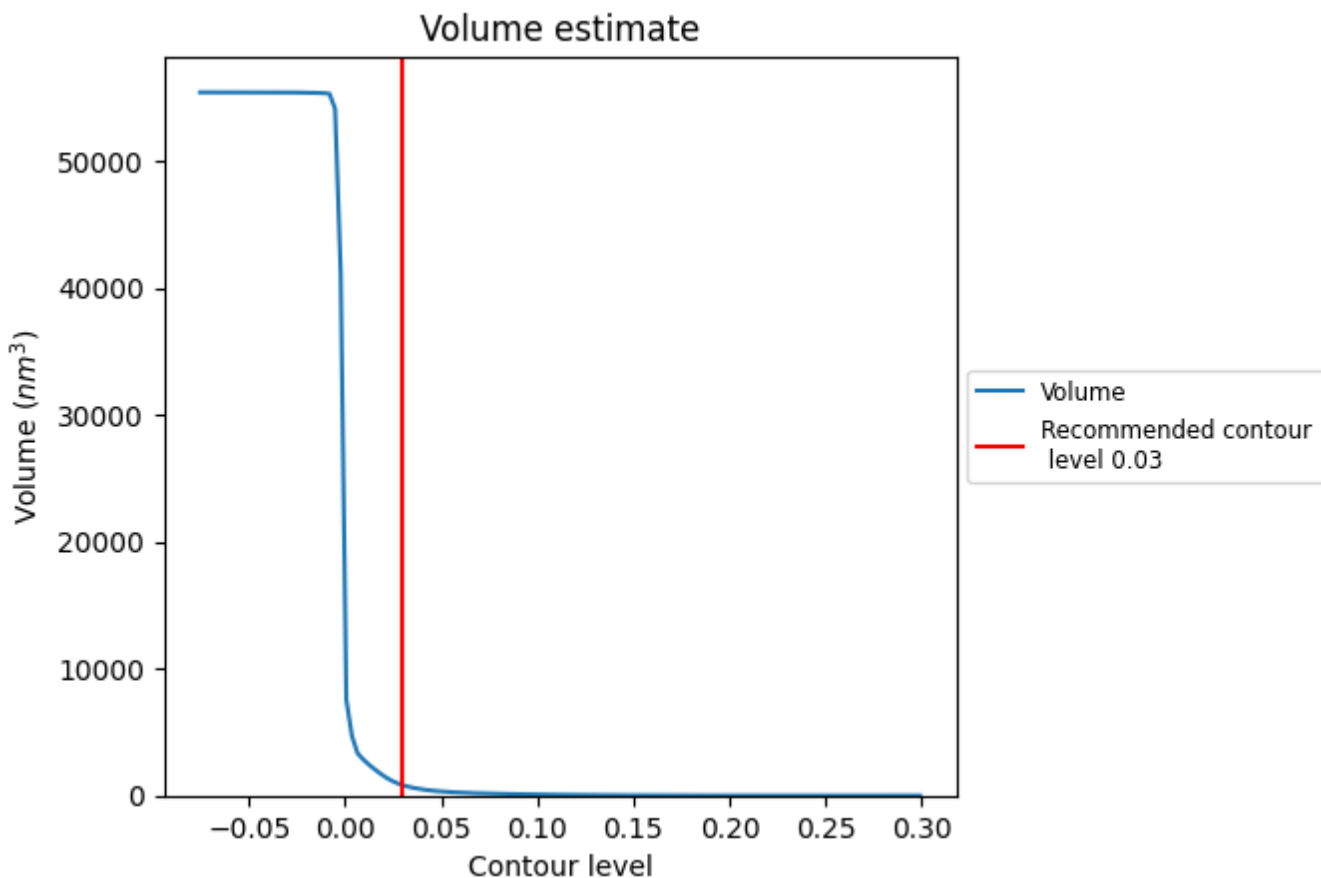
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

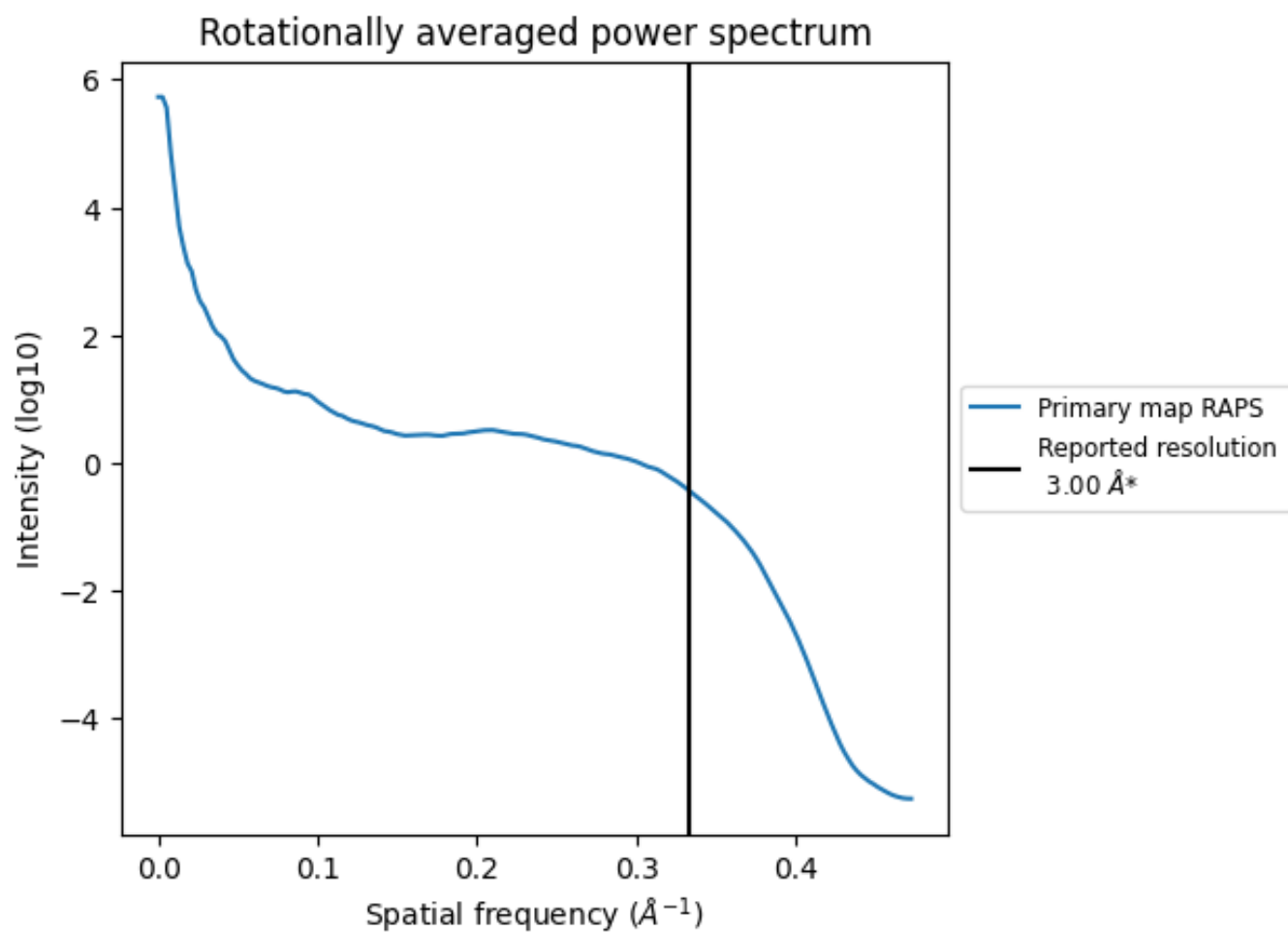
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 823 nm^3 ; this corresponds to an approximate mass of 744 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](#)

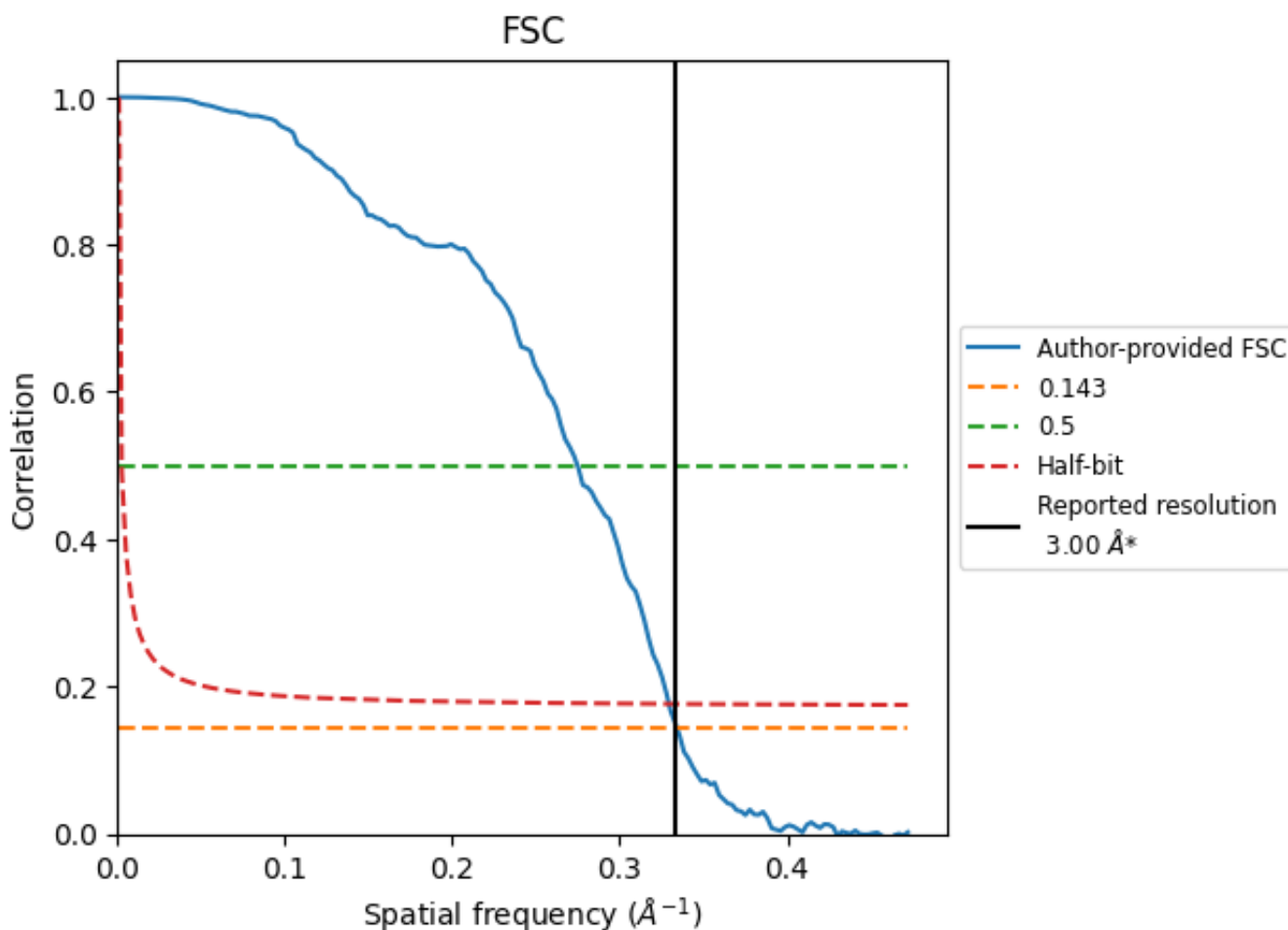


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

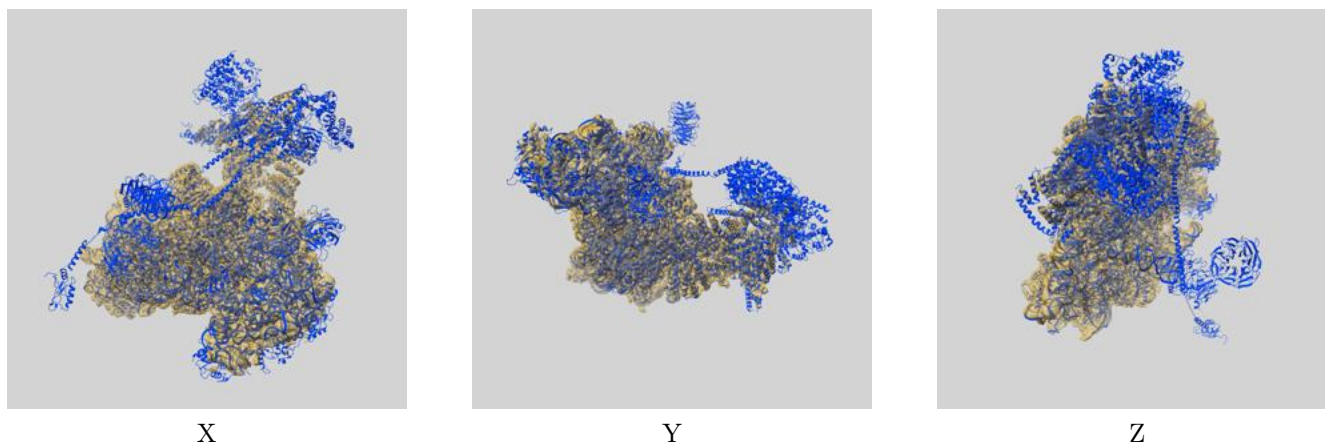
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.99	3.64	3.04
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

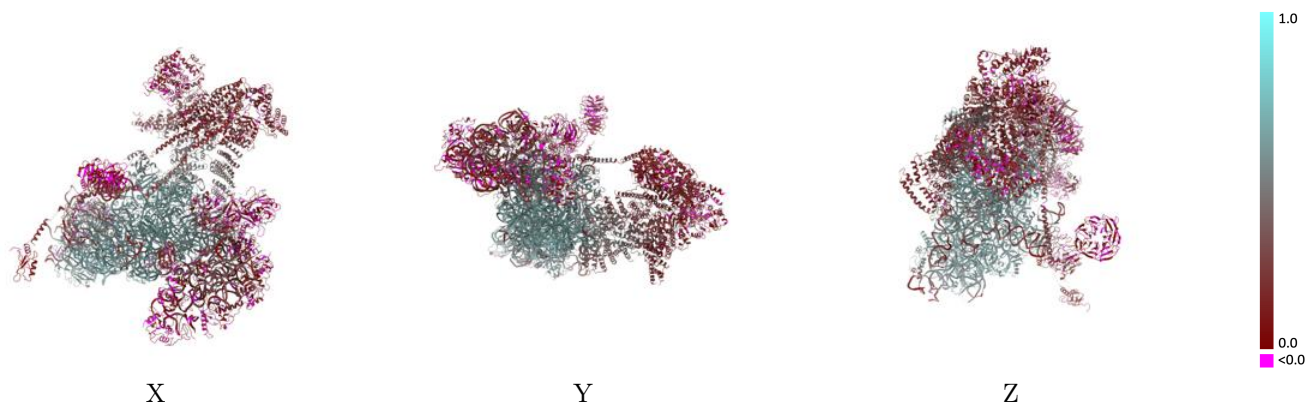
This section contains information regarding the fit between EMDB map EMD-11325 and PDB model 6ZON. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



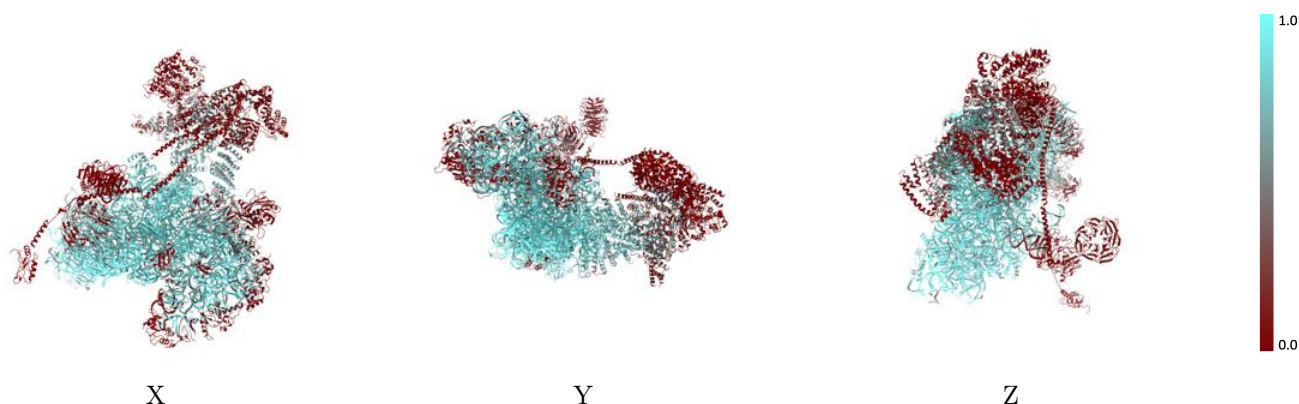
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



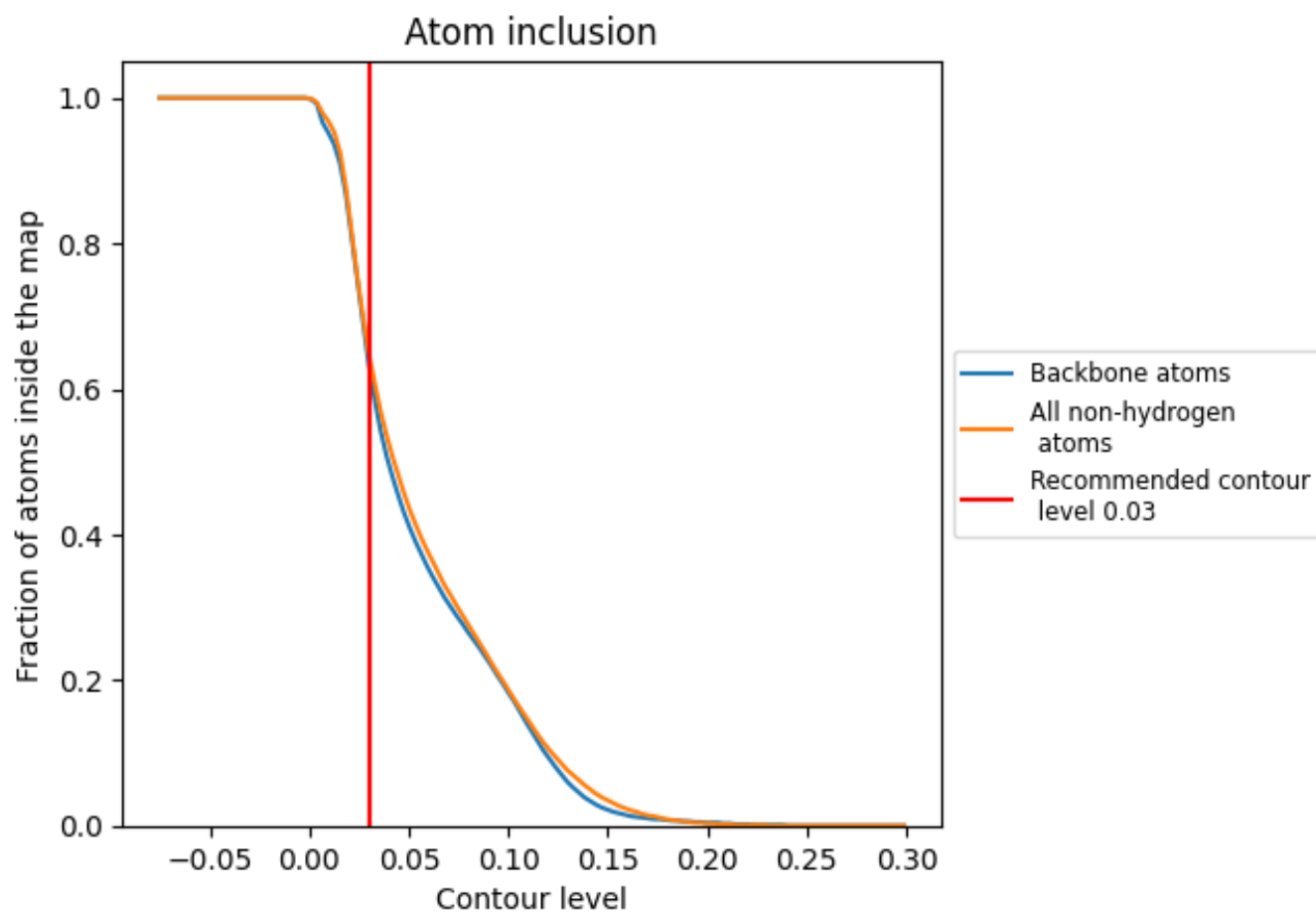
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 65% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6460	 0.3830
2	 0.9280	 0.4900
A	 0.4200	 0.3060
B	 0.0590	 0.2170
C	 0.6080	 0.3870
D	 0.1590	 0.1600
E	 0.2590	 0.1990
F	 0.0650	 0.1380
H	 0.0940	 0.1550
I	 0.0000	 0.0460
J	 0.9620	 0.6020
K	 0.0070	 0.1210
L	 0.0170	 0.1190
M	 0.0650	 0.1540
P	 0.1760	 0.1100
Q	 0.9510	 0.6040
R	 0.9630	 0.5890
S	 0.6750	 0.2810
T	 0.9760	 0.6080
U	 0.1950	 0.0920
V	 0.3440	 0.1140
W	 0.8660	 0.5620
Y	 0.1640	 0.1650
a	 0.9430	 0.5910
b	 0.6390	 0.2680
c	 0.9650	 0.6150
d	 0.9740	 0.6240
e	 0.5740	 0.2270
f	 0.9860	 0.6390
g	 0.6710	 0.2320
h	 0.5470	 0.2410
i	 0.9560	 0.5900
j	 0.9810	 0.6290
k	 0.1890	 0.1370
l	 0.8410	 0.2370



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Chain	Atom inclusion	Q-score
m	 0.9590	 0.5960
n	 0.9780	 0.6220
o	 0.1850	 0.0840
p	 0.9320	 0.5880
q	 0.9810	 0.6190
r	 0.9160	 0.5420
s	 0.9030	 0.5270
t	 0.9350	 0.5730
u	 0.4370	 0.1460
v	 0.1080	 0.0660
w	 0.8130	 0.4160
x	 0.5410	 0.2130
y	 0.9640	 0.6080
z	 0.9580	 0.5970