wwPDB EM Validation Summary Report (i)

Apr 23, 2024 – 04:30 am BST

PDB ID	:	6ZP4
EMDB ID	:	EMD-11335
Title	:	SARS-CoV-2 Nsp1 bound to a human 43S preinitiation ribosome complex - state 2
Authors	:	Thoms, M.; Buschauer, R.; Ameismeier, M.; Denk, T.; Kratzat, H.; Mackens-Kiani, T.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on	:	2020-07-08
Resolution	:	2.90 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 (i) symbol.

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

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

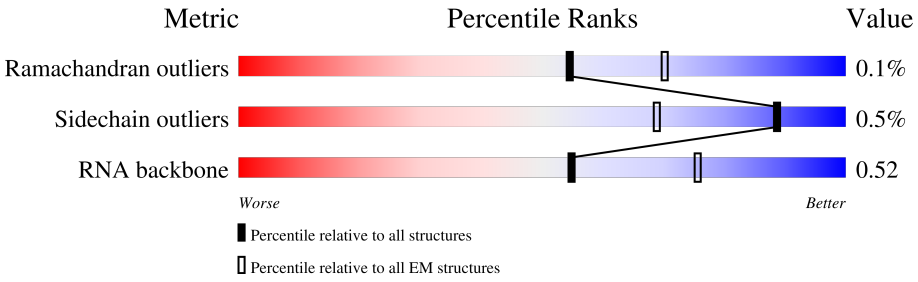
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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 <=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	73% 27%
2	p	264	80% 20%
3	d	293	74% 26%
4	Q	115	86% 12%
5	q	263	97%
6	W	25	96%
7	r	249	89% 11%
8	s	194	89% 11%

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Mol	Chain	Length	Quality of chain
9	t	208	96%
10	c	194	93% 7%
11	n	158	84% 15%
12	m	151	98%
13	y	83	99%
14	D	130	98%
15	z	133	92% 8%
16	R	84	96%
17	T	59	75% 25%
18	2	1868	67% 23% 8%
19	w	135	93% 5%
20	b	243	92% 8%
21	e	204	92% 7%
22	u	165	58% 42%
23	v	132	12% 84% 16%
24	o	145	82% 18%
25	g	146	94% 5%
26	k	152	91% 8%
27	x	145	97%
28	h	119	82% 18%
29	P	125	56% 44%
30	S	69	88% 12%
31	l	56	96%
32	U	156	37% 63%
33	V	317	93% 7%

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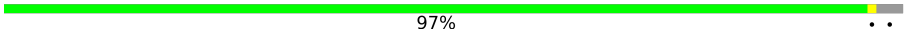
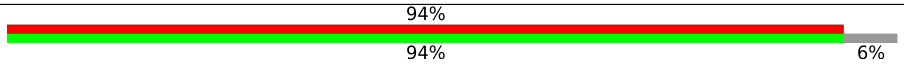
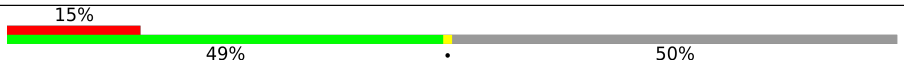
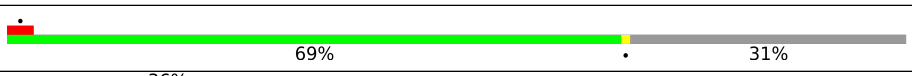
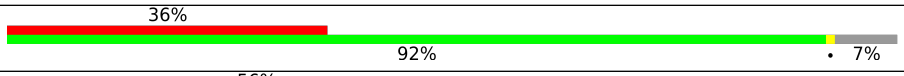
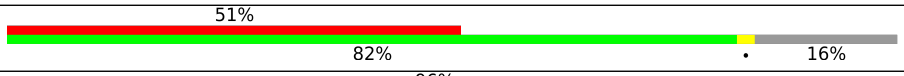
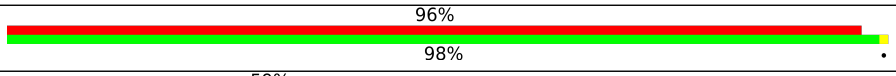
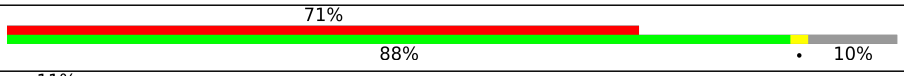
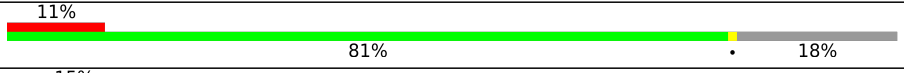
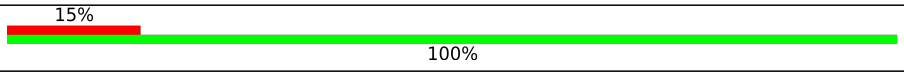
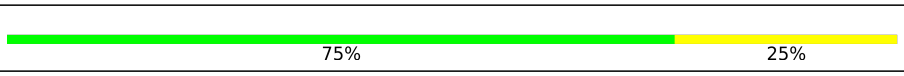
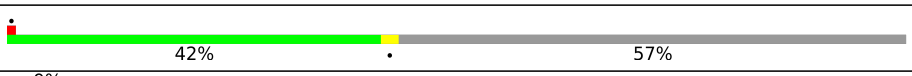
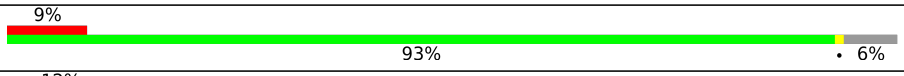
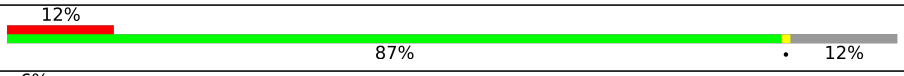
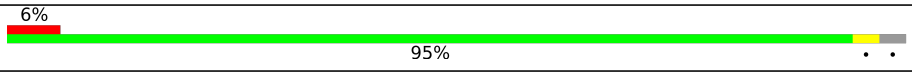
Mol	Chain	Length	Quality of chain
34	i	151	
35	j	143	
36	G	144	
37	I	325	
38	B	814	
39	A	1382	
40	C	913	
41	E	445	
42	F	357	
43	H	352	
44	K	218	
45	L	564	
46	M	374	
47	N	548	
48	X	78	
49	1	75	
50	4	333	
51	O	315	
52	Y	472	
53	Z	113	
54	J	180	

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 117784 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
7	r	222	Total	C	N	O	S	0	0
			1794	1123	357	308	6		

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

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

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

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

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

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

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

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

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

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

- Molecule 13 is a protein called 40S ribosomal protein S21.

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

- Molecule 14 is a protein called 40S ribosomal protein S15a.

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

- Molecule 15 is a protein called 40S ribosomal protein S24.

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

- Molecule 16 is a protein called 40S ribosomal protein S27.

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

- Molecule 17 is a protein called 40S ribosomal protein S30.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	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 19 is a protein called 40S ribosomal protein S17.

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

- Molecule 20 is a protein called 40S ribosomal protein S3.

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

- Molecule 21 is a protein called 40S ribosomal protein S5.

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

- Molecule 22 is a protein called 40S ribosomal protein S10.

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

- Molecule 23 is a protein called 40S ribosomal protein S12.

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

- Molecule 24 is a protein called 40S ribosomal protein S15.

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

- Molecule 25 is a protein called 40S ribosomal protein S16.

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

- Molecule 26 is a protein called 40S ribosomal protein S18.

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

- Molecule 27 is a protein called 40S ribosomal protein S19.

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

- Molecule 28 is a protein called 40S ribosomal protein S20.

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

- Molecule 29 is a protein called 40S ribosomal protein S25.

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

- Molecule 30 is a protein called 40S ribosomal protein S28.

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

- Molecule 31 is a protein called 40S ribosomal protein S29.

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

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 33 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 34 is a protein called 40S ribosomal protein S14.

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

- Molecule 35 is a protein called 40S ribosomal protein S23.

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

- Molecule 36 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	G	88	Total	C	N	O	S	0	0
			712	451	129	128	4		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	A	692	Total	C	N	O	S	0	0
			5380	3375	980	1003	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	C	633	Total	C	N	O	S	0	0
			5110	3228	906	941	35		

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	M	338	Total 2705	C 1727	N 457	O 504	S 17	0	0

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

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

- Molecule 48 is a protein called Unknown factor.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	X	78	Total	C	N	O	0	0
			390	234	78	78		

- Molecule 49 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	75	Total	C	N	O	P	0	0
			1603	717	298	514	74		

- Molecule 50 is a protein called Eukaryotic translation initiation factor 2 subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	4	144	Total	C	N	O	S	0	0
			1080	679	202	192	7		

- Molecule 51 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

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

- Molecule 52 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	Y	414	Total	C	N	O	0	0
			2156	1296	433	427		

- Molecule 53 is a protein called Eukaryotic translation initiation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Z	110	Total	C	N	O	S	0	0
			830	524	150	154	2		

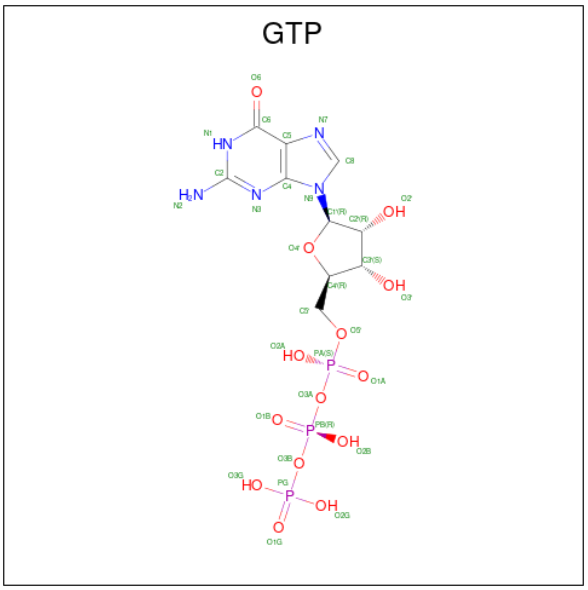
- Molecule 54 is a protein called Non-structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	J	33	Total	C	N	O	S	0	0
			261	159	47	54	1		

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
55	Q	1	Total Zn 1 1	0
55	l	1	Total Zn 1 1	0
55	U	1	Total Zn 1 1	0
55	4	1	Total Zn 1 1	0

- Molecule 56 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

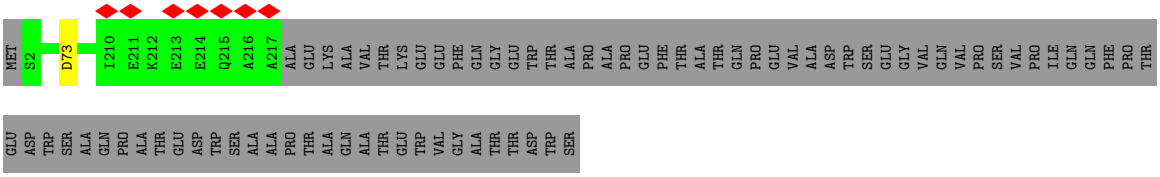
Mol	Chain	Residues	Atoms	AltConf
57	Y	1	Total Mg 1 1	0

3 Residue-property plots (i)

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

• Molecule 1: 40S ribosomal protein SA

Chain a:

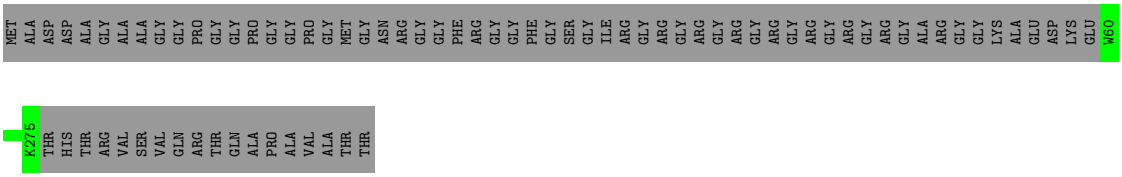


• Molecule 2: 40S ribosomal protein S3a

Chain p:

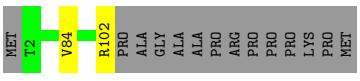
• Molecule 3: 40S ribosomal protein S2

Chain d:



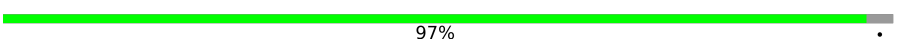
• Molecule 4: 40S ribosomal protein S26

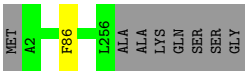
Chain Q:



• Molecule 5: 40S ribosomal protein S4, X isoform

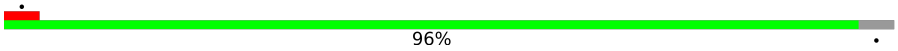
Chain q:

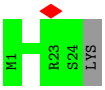




• Molecule 6: 60S ribosomal protein L41

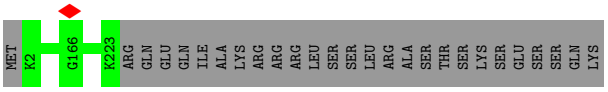
Chain W:





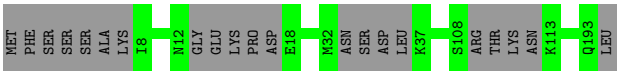
• Molecule 7: 40S ribosomal protein S6

Chain r:



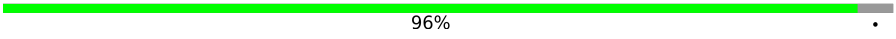
• Molecule 8: 40S ribosomal protein S7

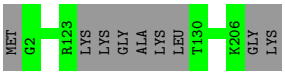
Chain s:



• Molecule 9: 40S ribosomal protein S8

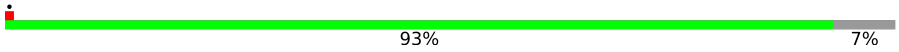
Chain t:

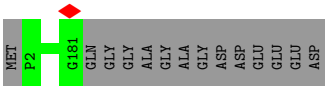




• Molecule 10: 40S ribosomal protein S9

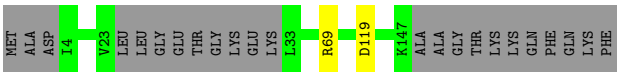
Chain c:





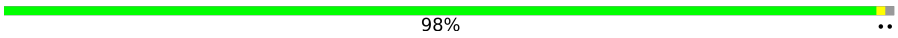
• Molecule 11: 40S ribosomal protein S11

Chain n:



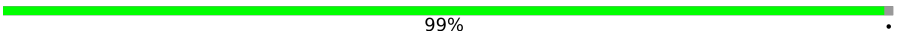
• Molecule 12: 40S ribosomal protein S13

Chain m:



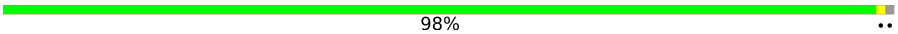
• Molecule 13: 40S ribosomal protein S21

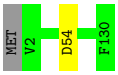
Chain y:



• Molecule 14: 40S ribosomal protein S15a

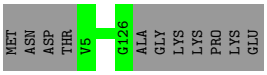
Chain D:





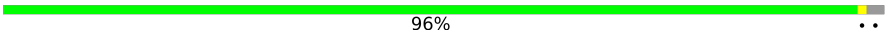
• Molecule 15: 40S ribosomal protein S24

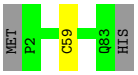
Chain z:



• Molecule 16: 40S ribosomal protein S27

Chain R:



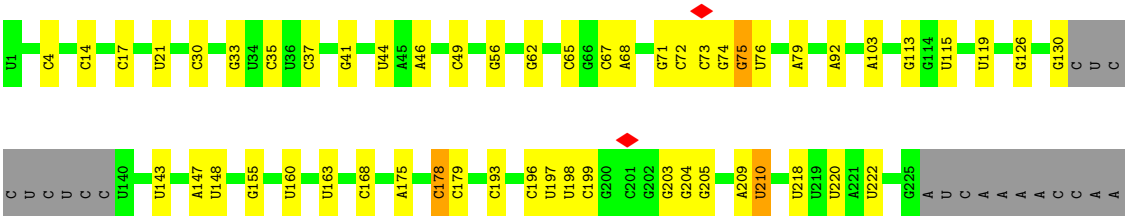


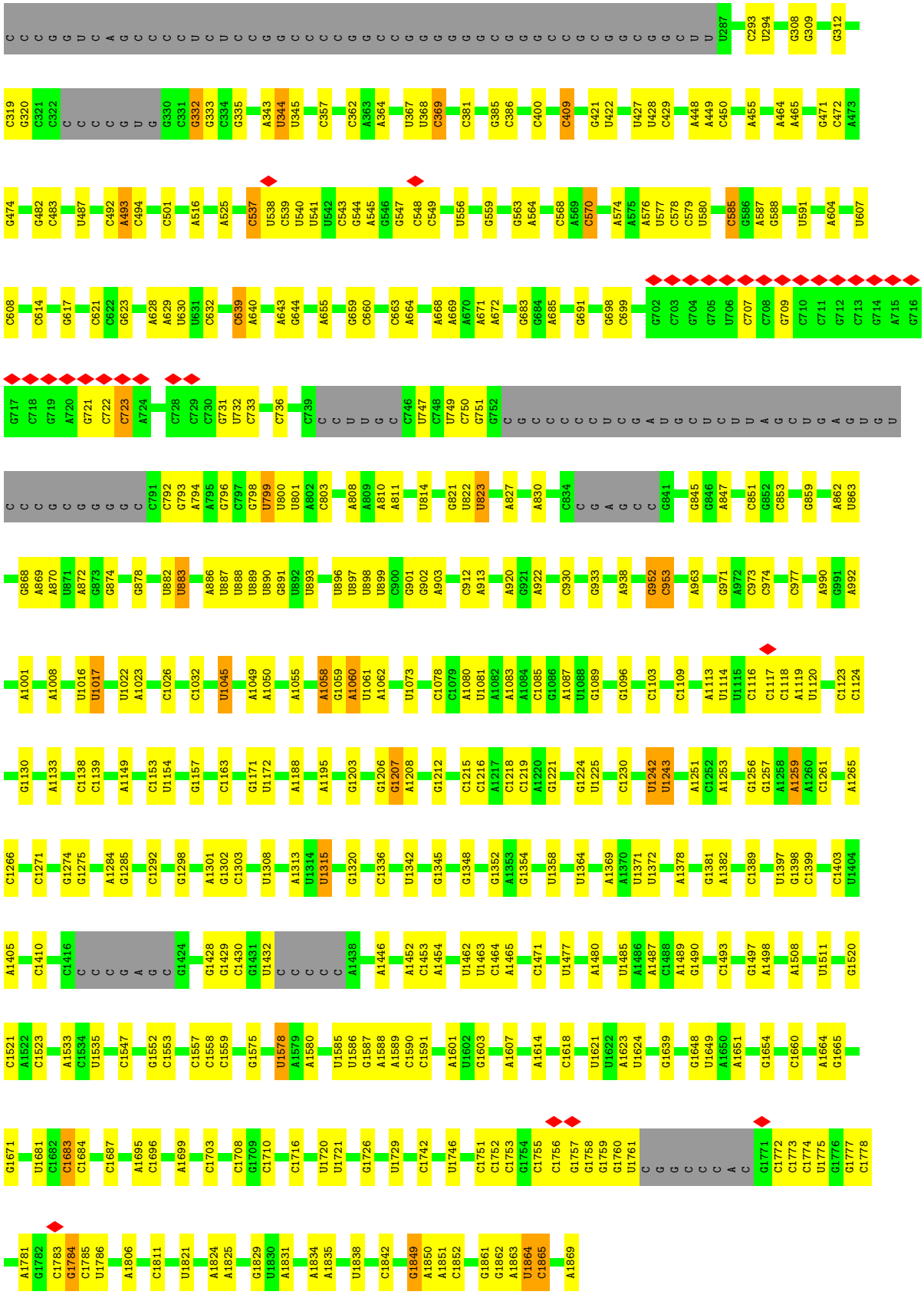
• Molecule 17: 40S ribosomal protein S30

Chain T:

• Molecule 18: 18S ribosomal RNA

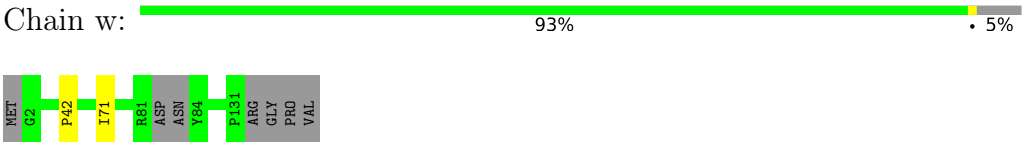
Chain 2:





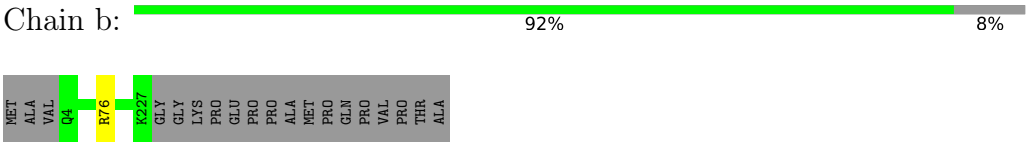
• Molecule 19: 40S ribosomal protein S17

Chain w:



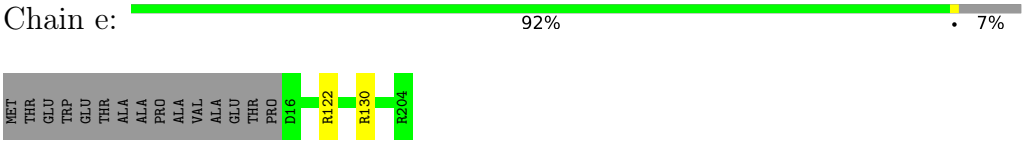
• Molecule 20: 40S ribosomal protein S3

Chain b:



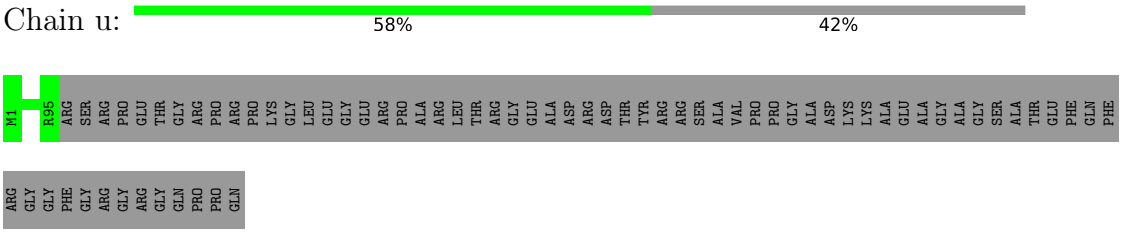
• Molecule 21: 40S ribosomal protein S5

Chain e:



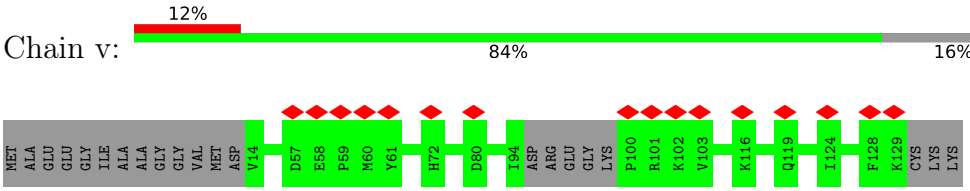
• Molecule 22: 40S ribosomal protein S10

Chain u:



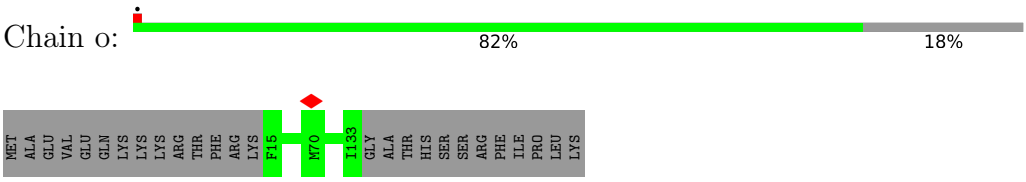
• Molecule 23: 40S ribosomal protein S12

Chain v:



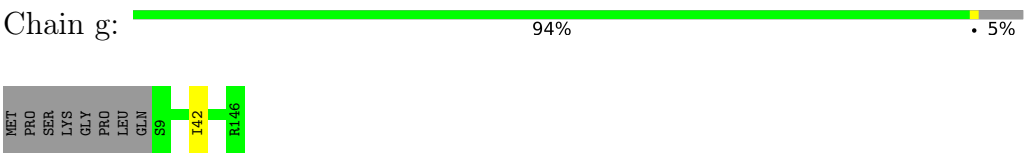
• Molecule 24: 40S ribosomal protein S15

Chain o:



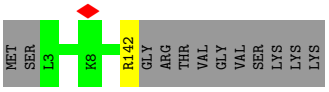
• Molecule 25: 40S ribosomal protein S16

Chain g:



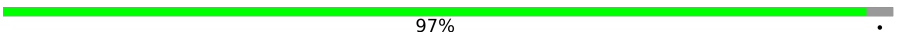
• Molecule 26: 40S ribosomal protein S18

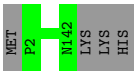
Chain k:



• Molecule 27: 40S ribosomal protein S19

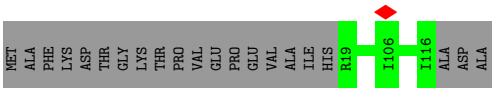
Chain x:





• Molecule 28: 40S ribosomal protein S20

Chain h:

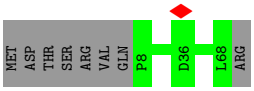


• Molecule 29: 40S ribosomal protein S25

Chain P:

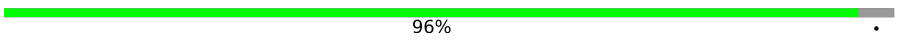
• Molecule 30: 40S ribosomal protein S28

Chain S:



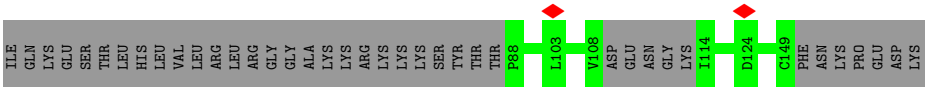
• Molecule 31: 40S ribosomal protein S29

Chain l:



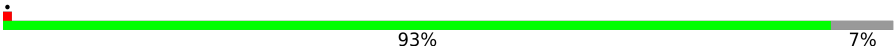
• Molecule 32: Ubiquitin-40S ribosomal protein S27a

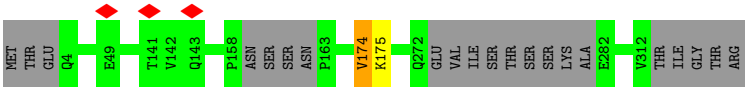
Chain U:



• Molecule 33: Receptor of activated protein C kinase 1

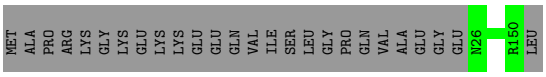
Chain V:





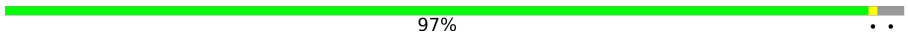
• Molecule 34: 40S ribosomal protein S14

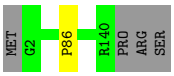
Chain i:



• Molecule 35: 40S ribosomal protein S23

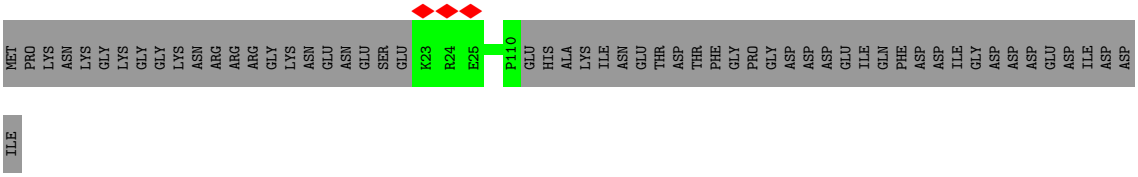
Chain j:





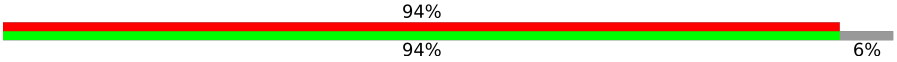
• Molecule 36: Eukaryotic translation initiation factor 1A, X-chromosomal

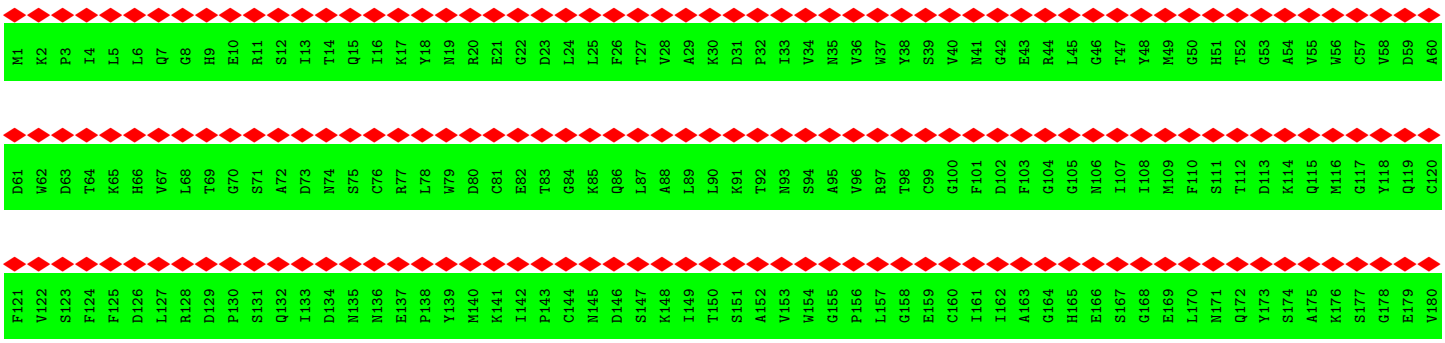
Chain G:

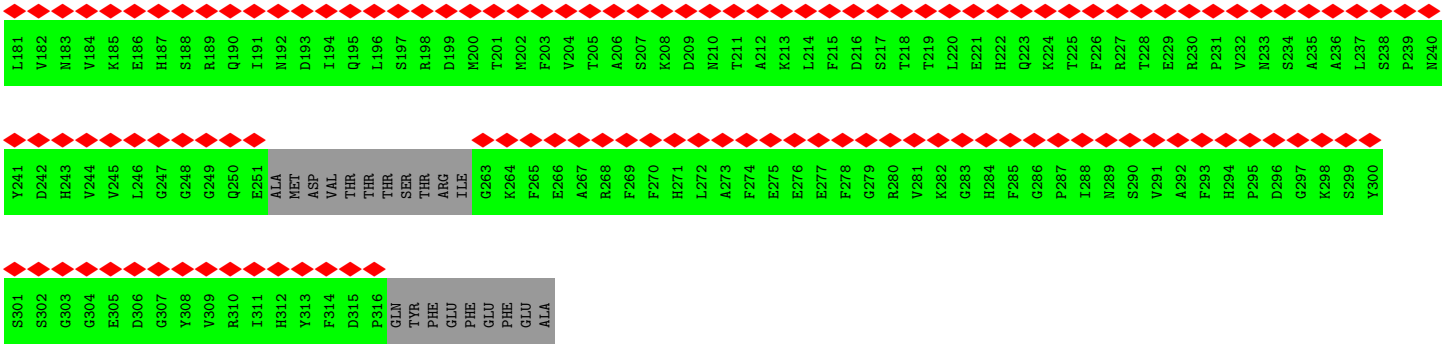


• Molecule 37: Eukaryotic translation initiation factor 3 subunit I

Chain I:

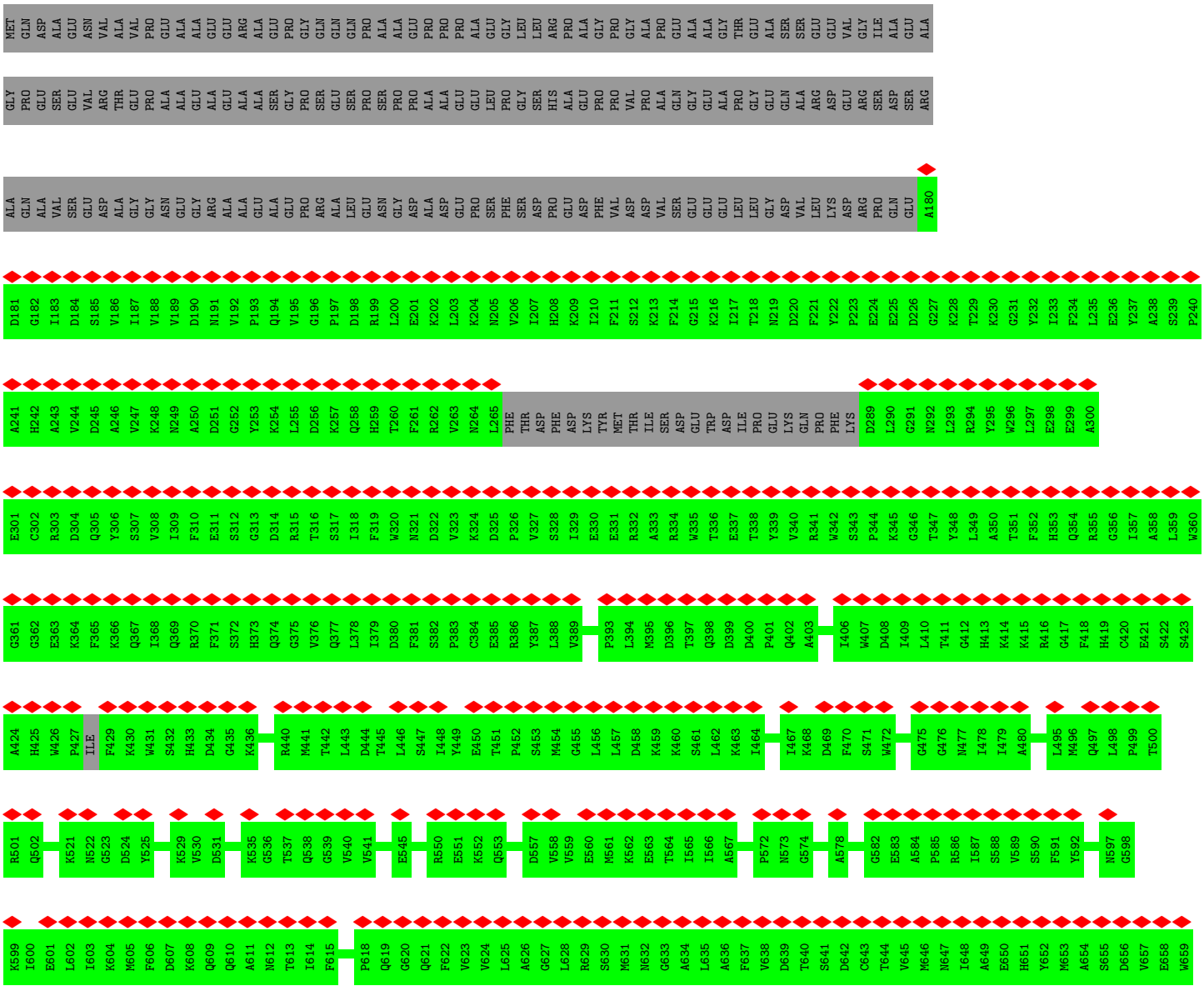


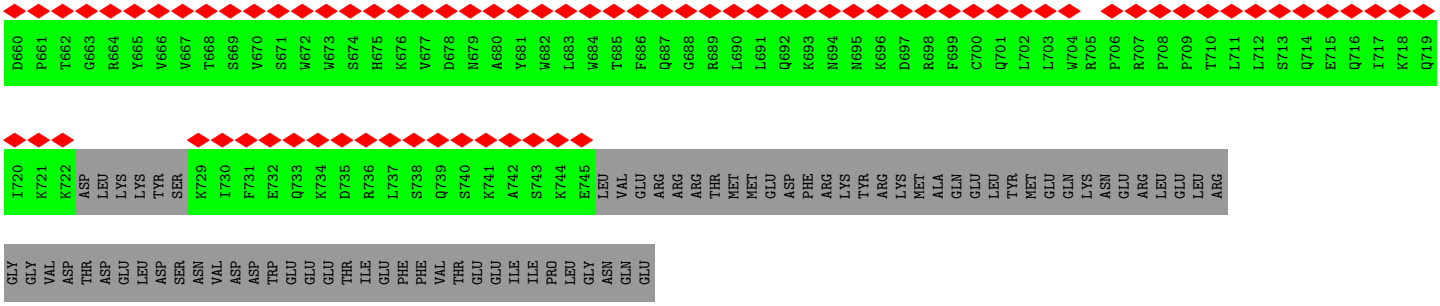




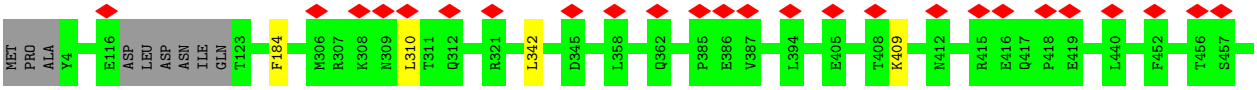
• Molecule 38: Eukaryotic translation initiation factor 3 subunit B

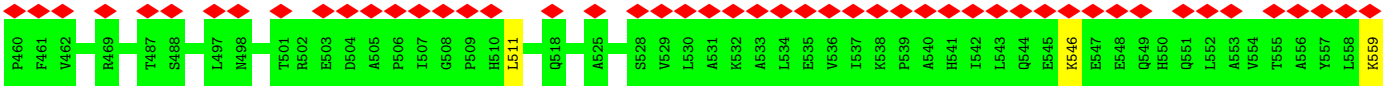
Chain B:

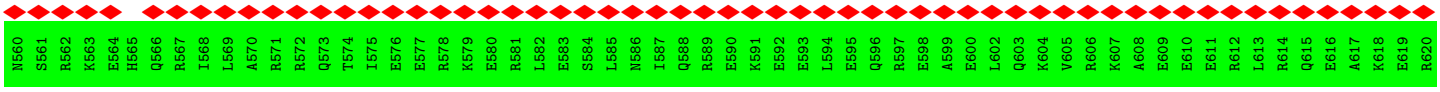


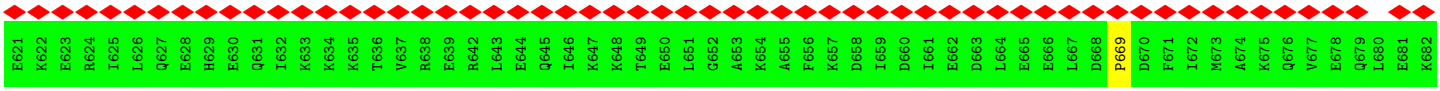


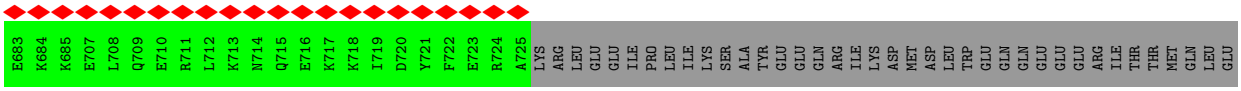
• Molecule 39: Eukaryotic translation initiation factor 3 subunit A

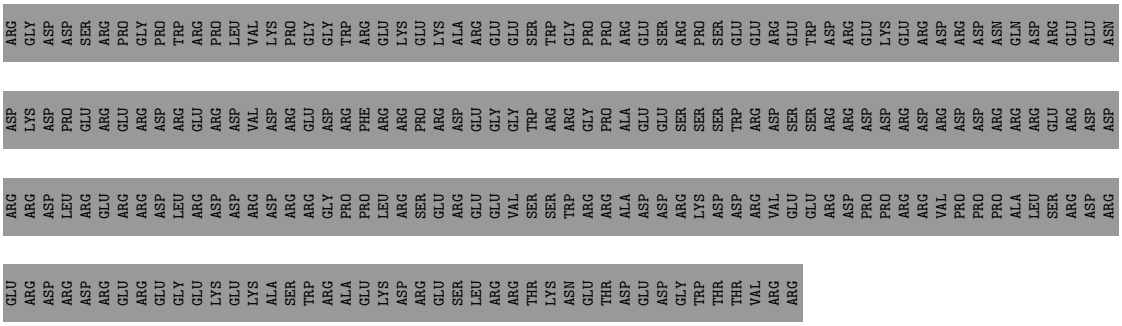






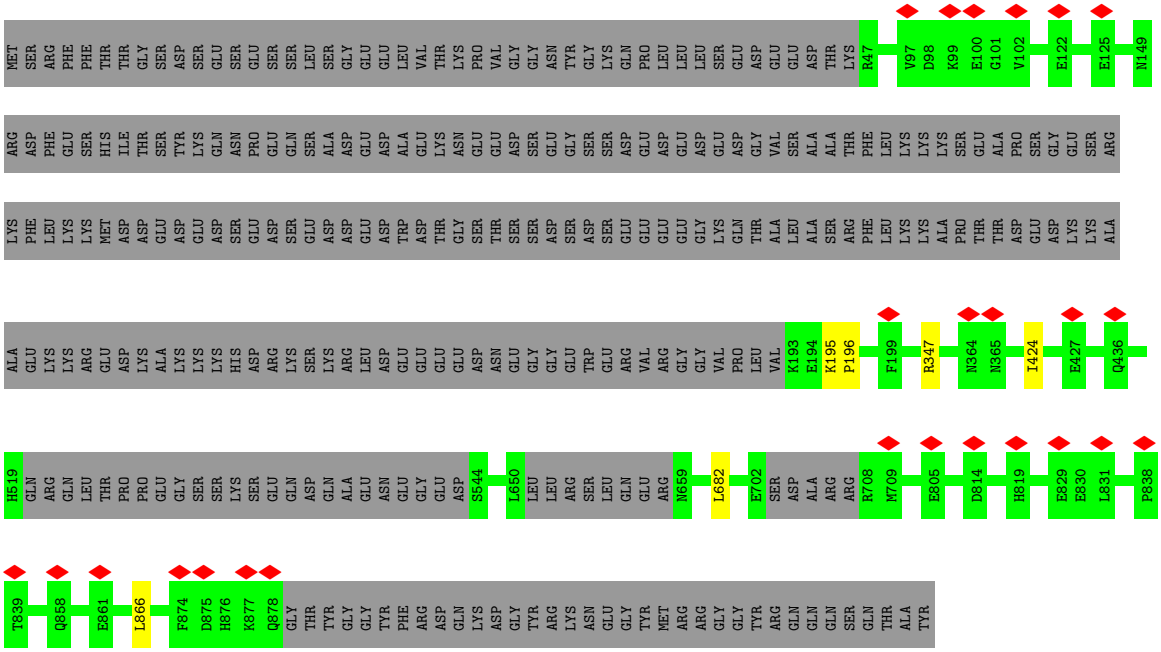






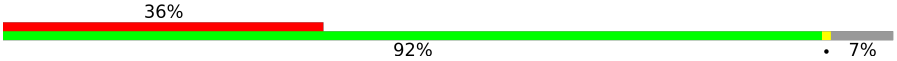
• Molecule 40: Eukaryotic translation initiation factor 3 subunit C

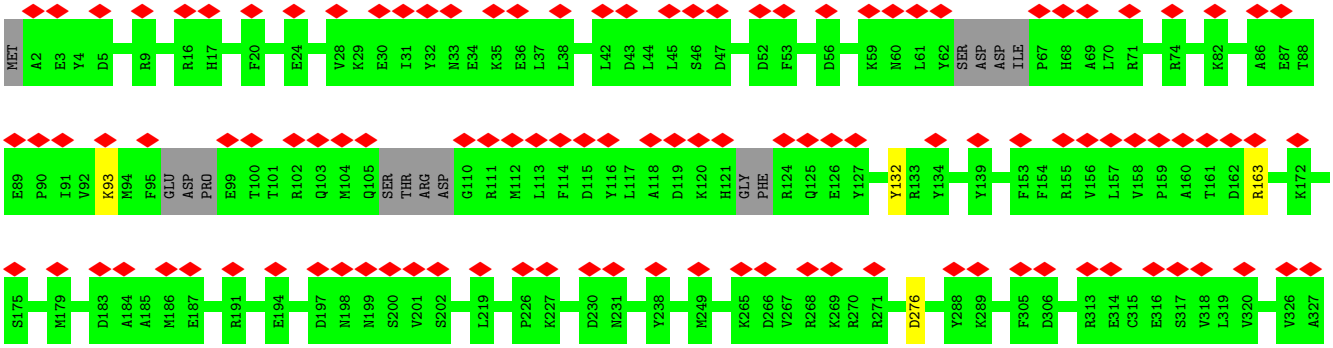
Chain C:



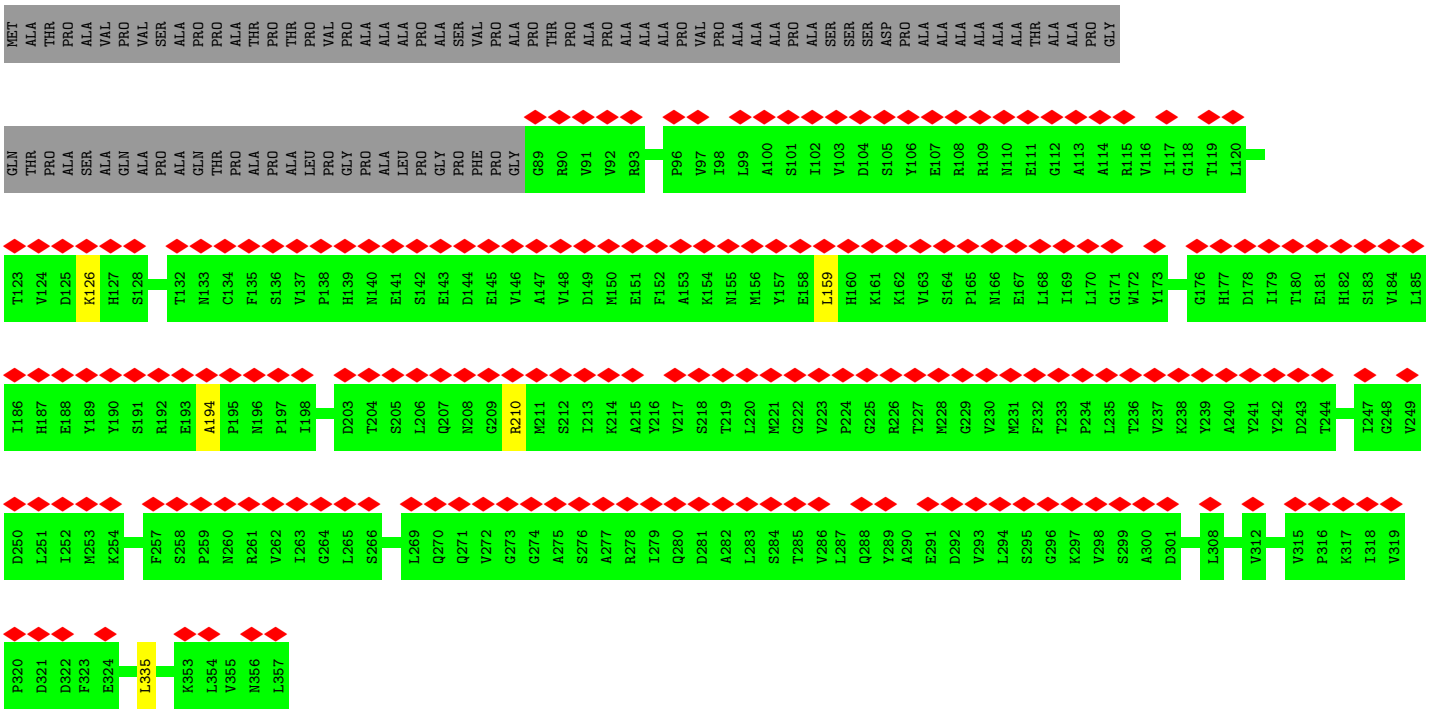
• Molecule 41: Eukaryotic translation initiation factor 3 subunit E

Chain E:

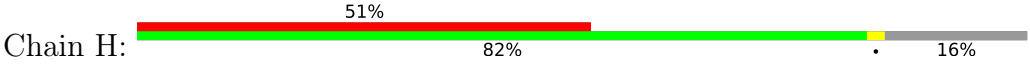


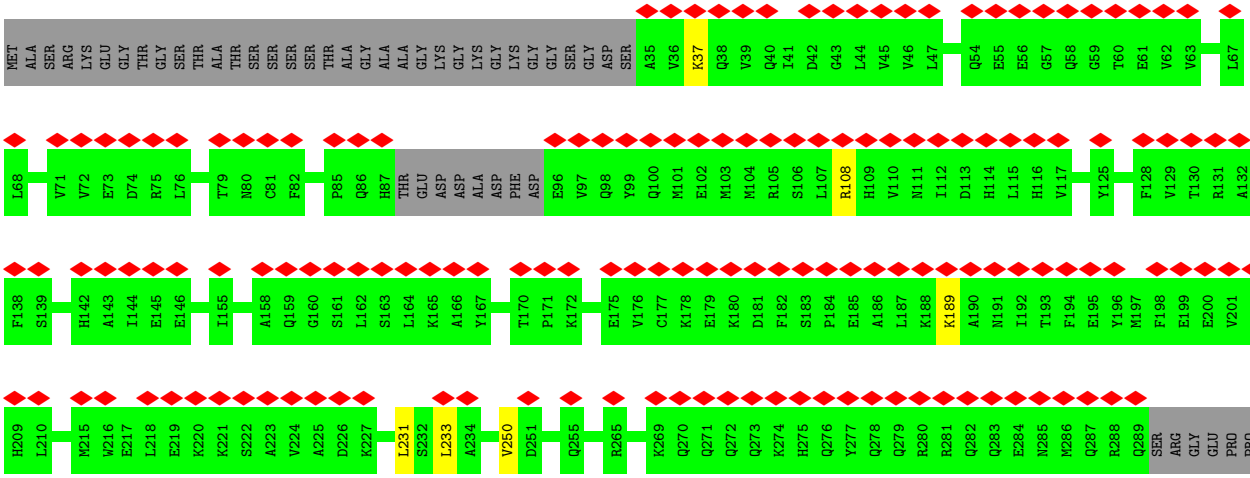


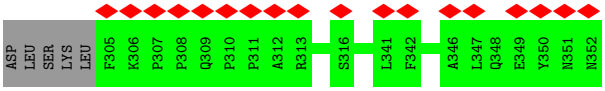
• Molecule 42: Eukaryotic translation initiation factor 3 subunit F



• Molecule 43: Eukaryotic translation initiation factor 3 subunit H

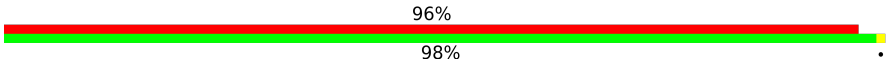


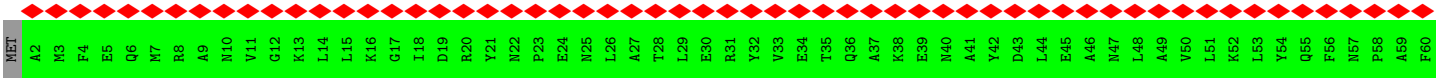


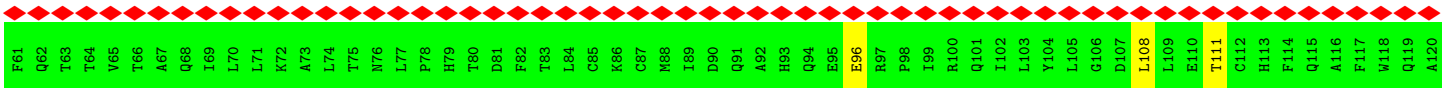


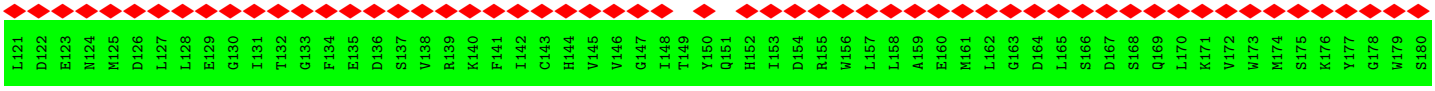
• Molecule 44: Eukaryotic translation initiation factor 3 subunit K

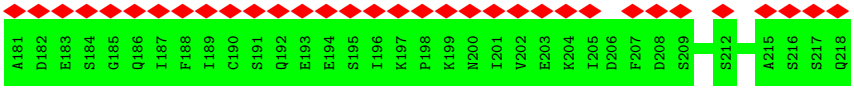
Chain K:





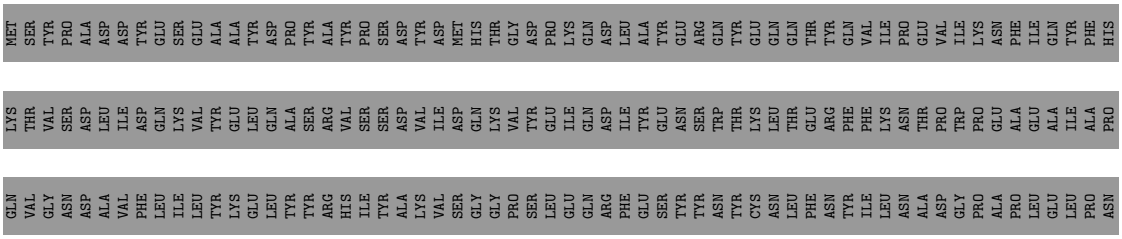


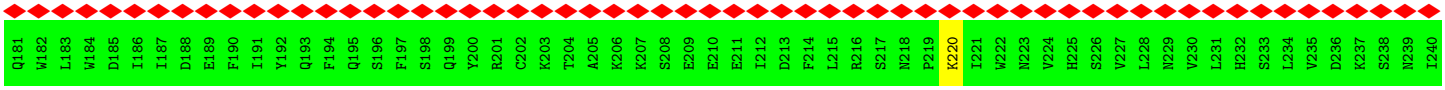


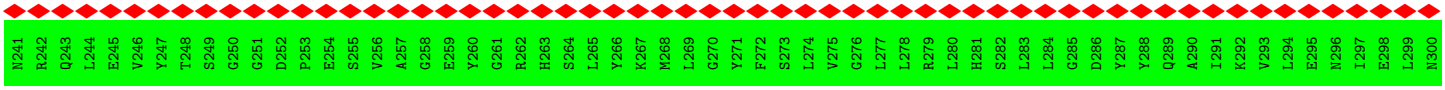


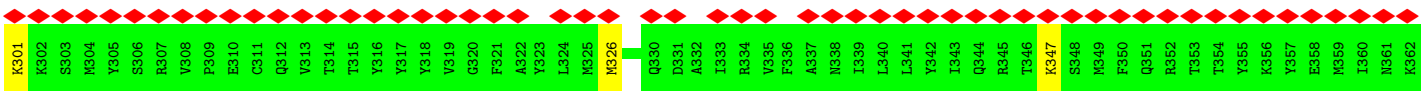
• Molecule 45: Eukaryotic translation initiation factor 3 subunit L

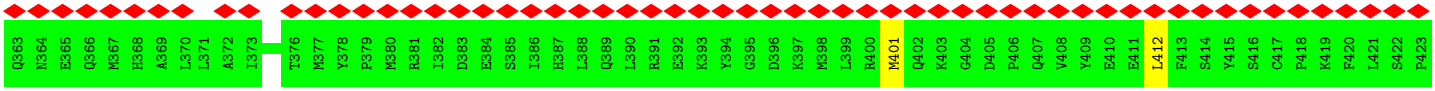
Chain L:

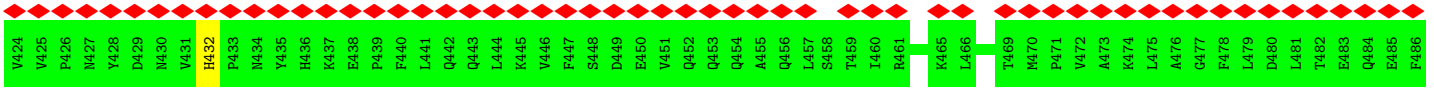


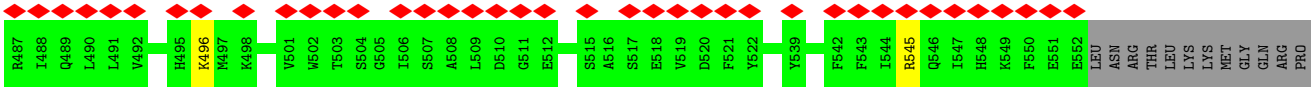




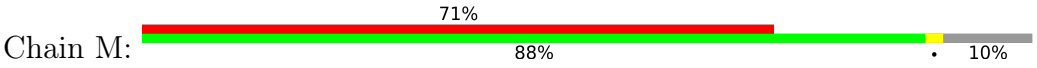


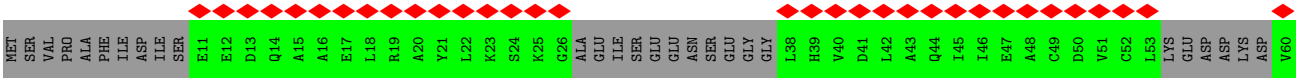


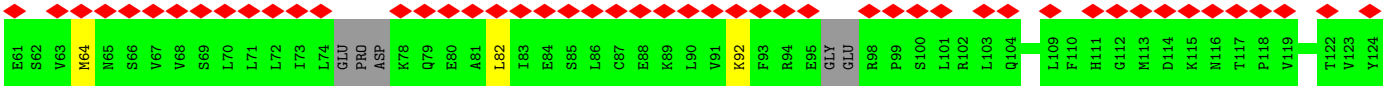


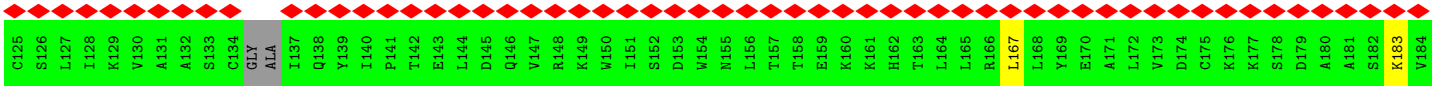


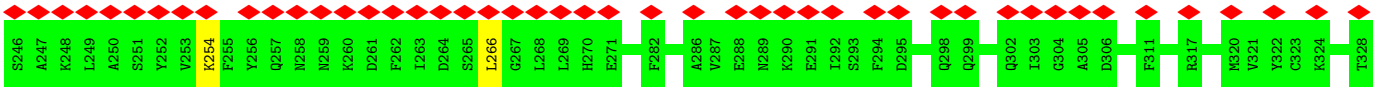
• Molecule 46: Eukaryotic translation initiation factor 3 subunit M

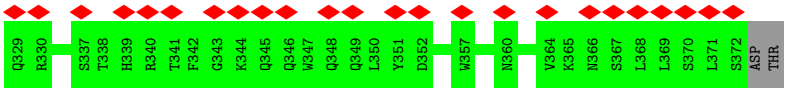




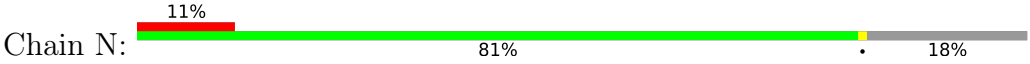


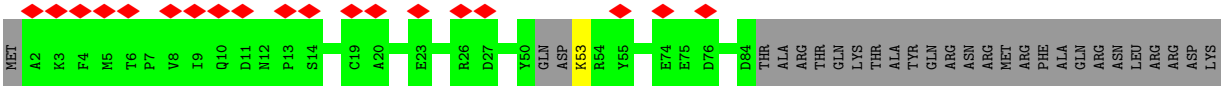


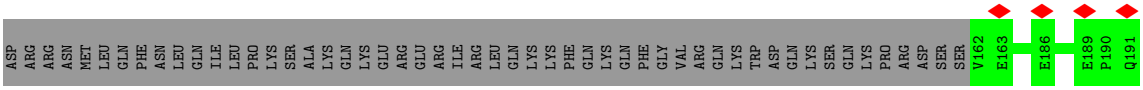


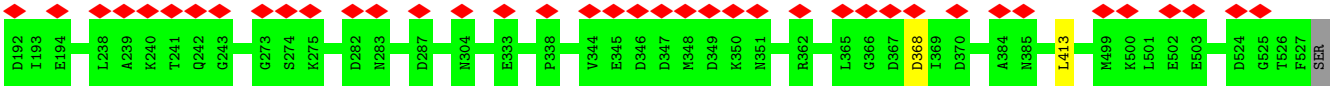


• Molecule 47: Eukaryotic translation initiation factor 3 subunit D

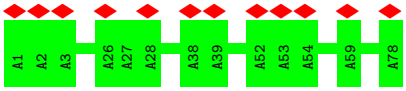






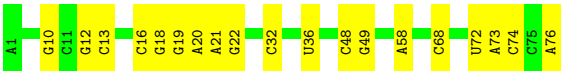


• Molecule 48: Unknown factor



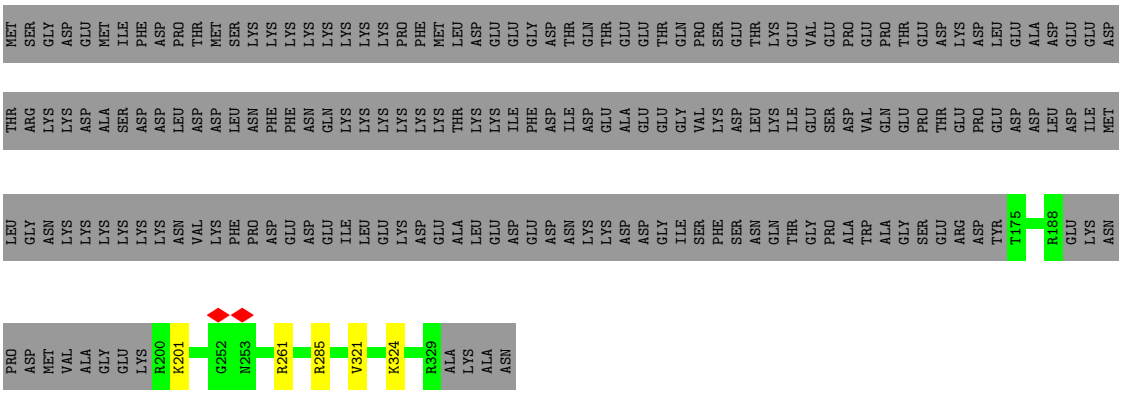
• Molecule 49: tRNA

Chain 1:



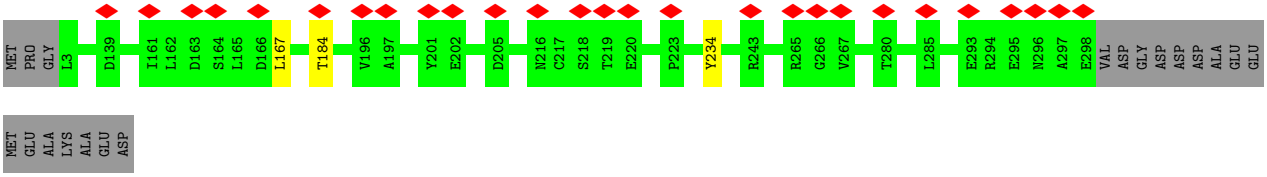
• Molecule 50: Eukaryotic translation initiation factor 2 subunit 2

Chain 4:



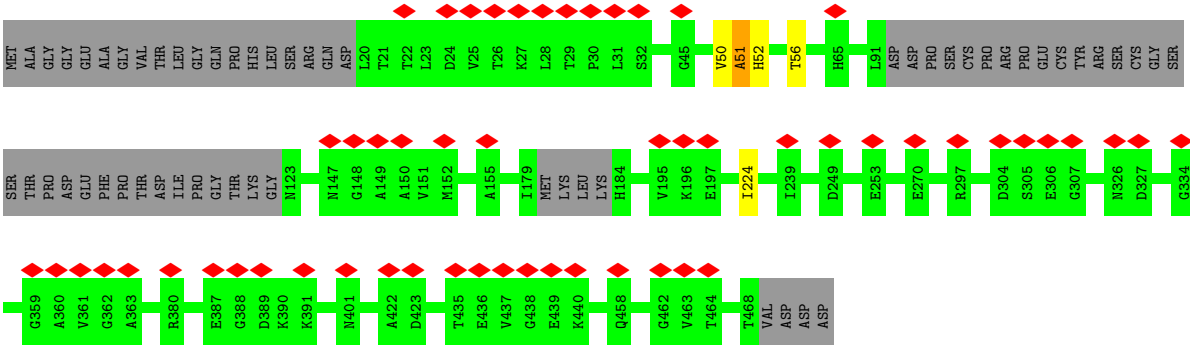
• Molecule 51: Eukaryotic translation initiation factor 2 subunit 1

Chain O:



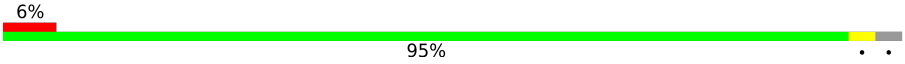
• Molecule 52: Eukaryotic translation initiation factor 2 subunit 3

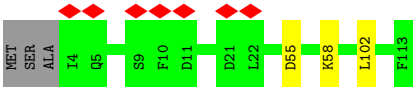
Chain Y:



• Molecule 53: Eukaryotic translation initiation factor 1

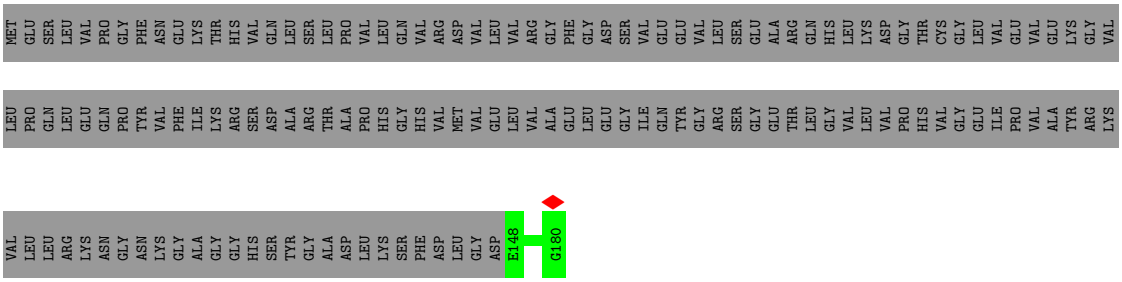
Chain Z:





• Molecule 54: Non-structural protein 1

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53769	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 ($e^-/Å^2$)	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	0.332	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: GTP, 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	0.41	0/1742	0.51	0/2367
2	p	0.38	0/1742	0.54	1/2330 (0.0%)
3	d	0.44	0/1710	0.55	0/2310
4	Q	0.41	0/828	0.54	0/1109
5	q	0.38	0/2073	0.54	0/2791
6	W	0.38	0/231	0.56	0/294
7	r	0.32	0/1817	0.50	0/2421
8	s	0.33	0/1418	0.52	0/1895
9	t	0.38	0/1666	0.51	0/2223
10	c	0.37	0/1524	0.50	0/2035
11	n	0.43	0/1139	0.54	1/1524 (0.1%)
12	m	0.39	0/1226	0.51	0/1649
13	y	0.38	0/631	0.49	0/844
14	D	0.41	0/1051	0.54	0/1406
15	z	0.36	0/1016	0.53	0/1349
16	R	0.40	0/653	0.55	1/876 (0.1%)
17	T	0.38	0/356	0.48	0/466
18	2	0.82	4/41061 (0.0%)	1.14	317/64001 (0.5%)
19	w	0.38	0/1024	0.57	0/1377
20	b	0.38	0/1773	0.52	0/2387
21	e	0.37	0/1516	0.52	0/2037
22	u	0.36	0/823	0.50	0/1111
23	v	0.29	0/870	0.62	0/1168
24	o	0.38	0/999	0.49	0/1336
25	g	0.43	0/1117	0.54	0/1494
26	k	0.38	0/1180	0.53	0/1581
27	x	0.39	0/1113	0.50	0/1493
28	h	0.37	0/789	0.57	0/1059
29	P	0.35	0/563	0.50	0/758
30	S	0.37	0/481	0.54	0/643
31	l	0.45	0/461	0.59	0/612
32	U	0.29	0/474	0.52	0/626

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	V	0.34	0/2369	0.58	0/3221
34	i	0.38	0/951	0.55	0/1275
35	j	0.41	0/1097	0.53	0/1464
36	G	0.29	0/721	0.50	0/963
37	I	0.25	0/1495	0.48	0/2073
38	B	0.26	0/2981	0.50	0/4115
39	A	0.28	0/5464	0.57	4/7396 (0.1%)
40	C	0.29	0/5193	0.56	3/6995 (0.0%)
41	E	0.29	0/3503	0.64	1/4728 (0.0%)
42	F	0.29	0/2126	0.65	2/2890 (0.1%)
43	H	0.28	0/2458	0.63	2/3313 (0.1%)
44	K	0.30	0/1785	0.62	2/2414 (0.1%)
45	L	0.30	0/3187	0.64	2/4299 (0.0%)
46	M	0.31	0/2743	0.69	4/3697 (0.1%)
47	N	0.29	0/3699	0.52	2/5001 (0.0%)
48	X	0.29	0/389	0.52	0/543
49	1	0.57	0/1794	1.05	7/2796 (0.3%)
50	4	0.31	0/1095	0.55	0/1477
51	O	0.30	0/2167	0.51	1/2943 (0.0%)
52	Y	0.26	0/2161	0.50	0/2985
53	Z	0.34	0/843	0.57	1/1134 (0.1%)
54	J	0.40	0/266	0.48	0/358
All	All	0.55	4/123554 (0.0%)	0.83	351/175652 (0.2%)

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
14	D	0	1
19	w	0	2
21	e	0	1
25	g	0	1
33	V	0	1
40	C	0	1
42	F	0	1
45	L	0	2
50	4	0	2
51	O	0	1
52	Y	0	3

Continued on next page...

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Mol	Chain	#Chirality outliers	#Planarity outliers
53	Z	0	2
All	All	0	19

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	367	U	O3'-P	-7.75	1.51	1.61
18	2	1206	G	O3'-P	-5.62	1.54	1.61
18	2	1681	U	O3'-P	-5.41	1.54	1.61
18	2	1850	A	O3'-P	-5.36	1.54	1.61

The worst 5 of 351 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	2	501	C	N1-C2-O2	14.65	127.69	118.90
18	2	501	C	C2-N1-C1'	13.15	133.26	118.80
18	2	293	C	N1-C2-O2	12.41	126.35	118.90
18	2	501	C	N3-C2-O2	-11.69	113.71	121.90
18	2	119	U	N3-C2-O2	-11.46	114.18	122.20

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	D	54	ASP	Peptide
1	a	73	ASP	Peptide
21	e	130	ARG	Peptide
19	w	42	PRO	Peptide
19	w	71	ILE	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%)	212 (99%)	2 (1%)	0	100	100
2	p	209/264 (79%)	199 (95%)	10 (5%)	0	100	100
3	d	214/293 (73%)	202 (94%)	12 (6%)	0	100	100
4	Q	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
5	q	253/263 (96%)	243 (96%)	9 (4%)	1 (0%)	34	66
6	W	22/25 (88%)	22 (100%)	0	0	100	100
7	r	220/249 (88%)	215 (98%)	5 (2%)	0	100	100
8	s	165/194 (85%)	162 (98%)	3 (2%)	0	100	100
9	t	195/208 (94%)	187 (96%)	8 (4%)	0	100	100
10	c	178/194 (92%)	172 (97%)	6 (3%)	0	100	100
11	n	131/158 (83%)	129 (98%)	2 (2%)	0	100	100
12	m	147/151 (97%)	146 (99%)	1 (1%)	0	100	100
13	y	80/83 (96%)	80 (100%)	0	0	100	100
14	D	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
15	z	120/133 (90%)	111 (92%)	9 (8%)	0	100	100
16	R	80/84 (95%)	74 (92%)	6 (8%)	0	100	100
17	T	40/59 (68%)	40 (100%)	0	0	100	100
19	w	124/135 (92%)	115 (93%)	9 (7%)	0	100	100
20	b	222/243 (91%)	217 (98%)	5 (2%)	0	100	100
21	e	187/204 (92%)	175 (94%)	12 (6%)	0	100	100
22	u	93/165 (56%)	87 (94%)	6 (6%)	0	100	100
23	v	107/132 (81%)	104 (97%)	3 (3%)	0	100	100
24	o	117/145 (81%)	115 (98%)	2 (2%)	0	100	100
25	g	136/146 (93%)	130 (96%)	6 (4%)	0	100	100
26	k	138/152 (91%)	131 (95%)	7 (5%)	0	100	100
27	x	139/145 (96%)	136 (98%)	3 (2%)	0	100	100
28	h	96/119 (81%)	92 (96%)	4 (4%)	0	100	100
29	P	68/125 (54%)	67 (98%)	1 (2%)	0	100	100
30	S	59/69 (86%)	54 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	l	52/56 (93%)	48 (92%)	4 (8%)	0	100	100
32	U	53/156 (34%)	47 (89%)	6 (11%)	0	100	100
33	V	290/317 (92%)	260 (90%)	28 (10%)	2 (1%)	22	54
34	i	123/151 (82%)	115 (94%)	8 (6%)	0	100	100
35	j	137/143 (96%)	133 (97%)	3 (2%)	1 (1%)	22	54
36	G	86/144 (60%)	84 (98%)	2 (2%)	0	100	100
37	I	301/325 (93%)	293 (97%)	8 (3%)	0	100	100
38	B	528/814 (65%)	503 (95%)	25 (5%)	0	100	100
39	A	682/1382 (49%)	665 (98%)	17 (2%)	0	100	100
40	C	621/913 (68%)	586 (94%)	34 (6%)	1 (0%)	47	78
41	E	406/445 (91%)	394 (97%)	12 (3%)	0	100	100
42	F	267/357 (75%)	251 (94%)	16 (6%)	0	100	100
43	H	289/352 (82%)	275 (95%)	14 (5%)	0	100	100
44	K	215/218 (99%)	197 (92%)	18 (8%)	0	100	100
45	L	370/564 (66%)	336 (91%)	34 (9%)	0	100	100
46	M	326/374 (87%)	315 (97%)	11 (3%)	0	100	100
47	N	441/548 (80%)	412 (93%)	29 (7%)	0	100	100
48	X	76/78 (97%)	75 (99%)	1 (1%)	0	100	100
50	4	140/333 (42%)	115 (82%)	25 (18%)	0	100	100
51	O	294/315 (93%)	278 (95%)	16 (5%)	0	100	100
52	Y	408/472 (86%)	334 (82%)	71 (17%)	3 (1%)	22	54
53	Z	108/113 (96%)	95 (88%)	13 (12%)	0	100	100
54	J	31/180 (17%)	29 (94%)	2 (6%)	0	100	100
All	All	10224/13428 (76%)	9679 (95%)	537 (5%)	8 (0%)	54	82

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	V	175	LYS
52	Y	56	THR
5	q	86	PHE
52	Y	51	ALA
33	V	174	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	a	180/243 (74%)	180 (100%)	0	100 100
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%)	86 (98%)	2 (2%)	50 80
5	q	220/225 (98%)	220 (100%)	0	100 100
6	W	23/24 (96%)	23 (100%)	0	100 100
7	r	193/218 (88%)	193 (100%)	0	100 100
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
11	n	125/142 (88%)	124 (99%)	1 (1%)	81 94
12	m	130/131 (99%)	129 (99%)	1 (1%)	81 94
13	y	66/67 (98%)	66 (100%)	0	100 100
14	D	112/113 (99%)	112 (100%)	0	100 100
15	z	106/115 (92%)	106 (100%)	0	100 100
16	R	74/76 (97%)	74 (100%)	0	100 100
17	T	35/48 (73%)	35 (100%)	0	100 100
19	w	111/122 (91%)	111 (100%)	0	100 100
20	b	188/202 (93%)	187 (100%)	1 (0%)	88 96
21	e	159/170 (94%)	158 (99%)	1 (1%)	86 96
22	u	86/136 (63%)	86 (100%)	0	100 100
23	v	94/108 (87%)	94 (100%)	0	100 100
24	o	107/130 (82%)	107 (100%)	0	100 100
25	g	114/121 (94%)	114 (100%)	0	100 100
26	k	122/132 (92%)	121 (99%)	1 (1%)	81 94
27	x	111/115 (96%)	111 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
28	h	91/107 (85%)	91 (100%)	0	100 100
29	P	62/103 (60%)	62 (100%)	0	100 100
30	S	54/62 (87%)	54 (100%)	0	100 100
31	l	47/49 (96%)	47 (100%)	0	100 100
32	U	51/140 (36%)	51 (100%)	0	100 100
33	V	256/275 (93%)	256 (100%)	0	100 100
34	i	98/119 (82%)	98 (100%)	0	100 100
35	j	111/115 (96%)	111 (100%)	0	100 100
36	G	75/123 (61%)	75 (100%)	0	100 100
38	B	90/702 (13%)	90 (100%)	0	100 100
39	A	544/1259 (43%)	540 (99%)	4 (1%)	84 95
40	C	553/811 (68%)	552 (100%)	1 (0%)	93 98
41	E	380/406 (94%)	375 (99%)	5 (1%)	69 90
42	F	237/289 (82%)	235 (99%)	2 (1%)	81 94
43	H	269/310 (87%)	265 (98%)	4 (2%)	65 87
44	K	192/193 (100%)	191 (100%)	1 (0%)	88 96
45	L	342/515 (66%)	337 (98%)	5 (2%)	65 87
46	M	304/335 (91%)	300 (99%)	4 (1%)	69 90
47	N	398/494 (81%)	397 (100%)	1 (0%)	92 98
50	4	109/304 (36%)	106 (97%)	3 (3%)	43 76
51	O	190/280 (68%)	189 (100%)	1 (0%)	88 96
52	Y	33/397 (8%)	33 (100%)	0	100 100
53	Z	79/96 (82%)	79 (100%)	0	100 100
54	J	27/151 (18%)	27 (100%)	0	100 100
All	All	7899/11349 (70%)	7861 (100%)	38 (0%)	89 96

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	L	545	ARG
50	4	261	ARG
46	M	64	MET
46	M	254	LYS
51	O	234	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 146 such sidechains are listed below:

Mol	Chain	Res	Type
45	L	281	HIS
51	O	180	ASN
45	L	364	ASN
46	M	302	GLN
27	x	128	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	2	1711/1868 (91%)	362 (21%)	8 (0%)
49	1	74/75 (98%)	15 (20%)	0
All	All	1785/1943 (91%)	377 (21%)	8 (0%)

5 of 377 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	2	17	C
18	2	33	G
18	2	41	G
18	2	44	U
18	2	46	A

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	2	1060	A
18	2	1058	A
18	2	868	G
18	2	369	C
18	2	912	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 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	GTP	Y	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.66	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	GTP	Y	501	57	-	6/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Y	501	GTP	C5-C6	-4.14	1.39	1.47
56	Y	501	GTP	C2-N3	2.20	1.38	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	Y	501	GTP	PA-O3A-PB	-4.44	117.60	132.83
56	Y	501	GTP	PB-O3B-PG	-3.61	120.45	132.83
56	Y	501	GTP	C5-C6-N1	3.45	120.04	113.95
56	Y	501	GTP	C2-N1-C6	-3.19	119.23	125.10
56	Y	501	GTP	C8-N7-C5	2.91	108.53	102.99

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	Y	501	GTP	C5'-O5'-PA-O1A

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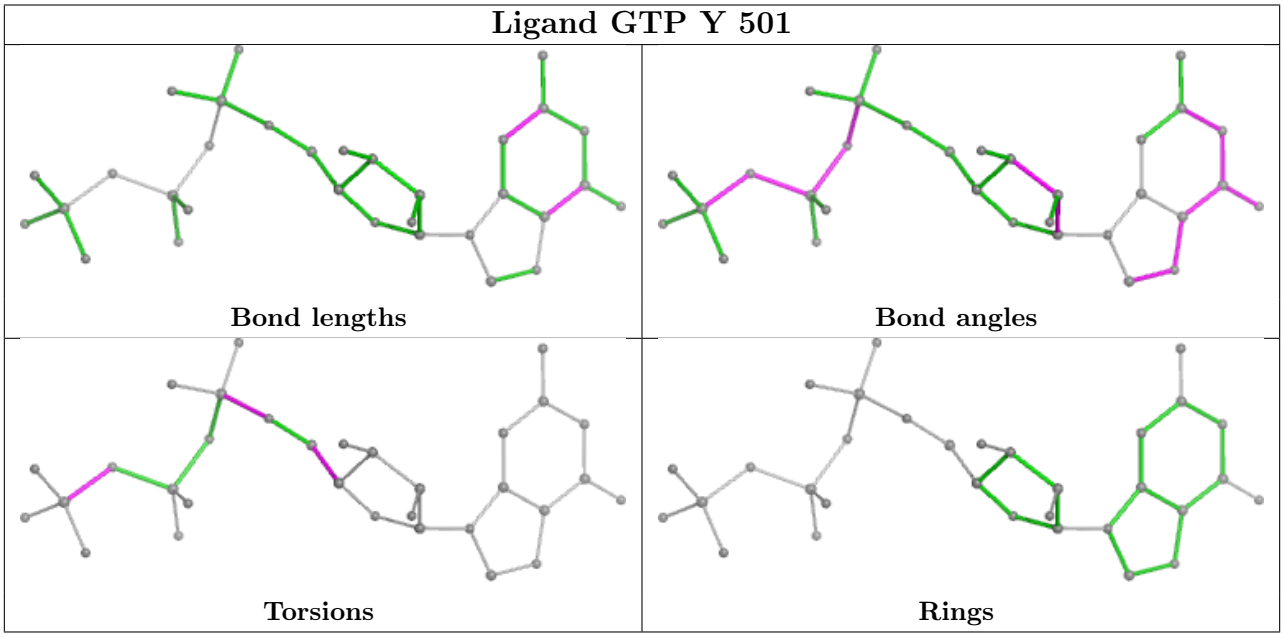
Mol	Chain	Res	Type	Atoms
56	Y	501	GTP	PB-O3B-PG-O1G
56	Y	501	GTP	PB-O3B-PG-O2G
56	Y	501	GTP	PB-O3B-PG-O3G
56	Y	501	GTP	C5'-O5'-PA-O3A

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
39	A	3
40	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	200:ALA	C	320:LYS	N	76.80
1	A	685:LYS	C	707:GLU	N	37.30
1	A	639:GLU	C	642:ARG	N	9.91
1	A	600:GLU	C	602:LEU	N	9.04

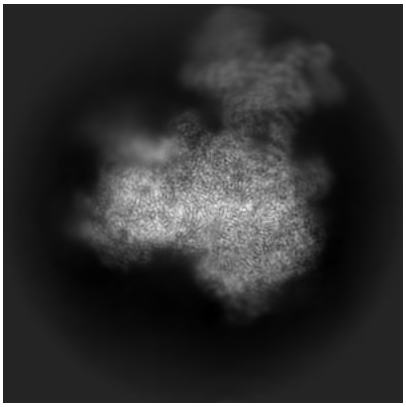
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11335. These allow visual inspection of the internal detail of the map and identification of artifacts.

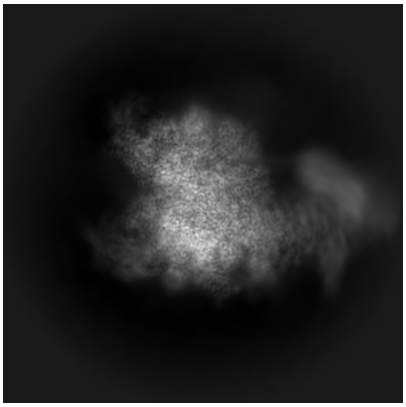
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

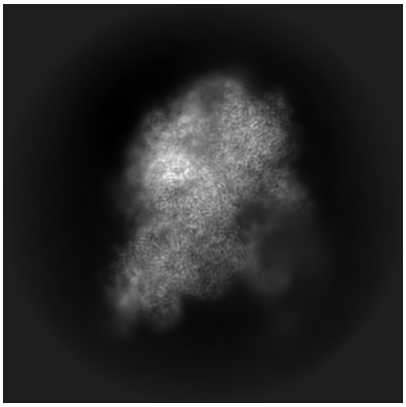
6.1.1 Primary map



X



Y

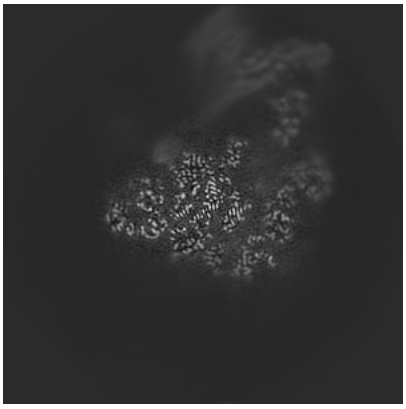


Z

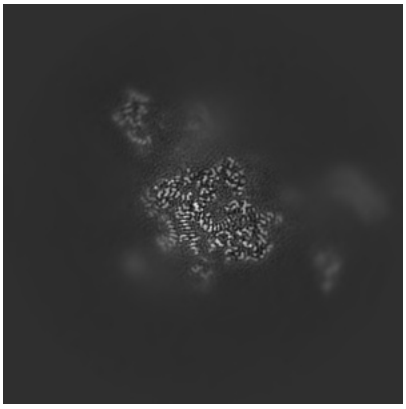
The images above show the map projected in three orthogonal directions.

6.2 Central slices

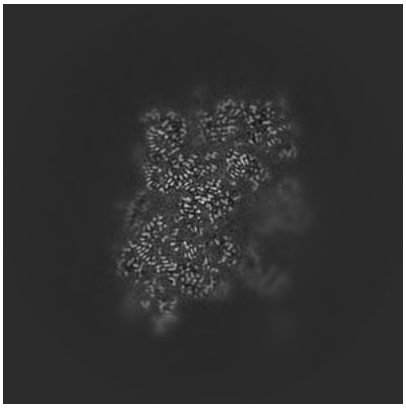
6.2.1 Primary map



X Index: 180



Y Index: 180

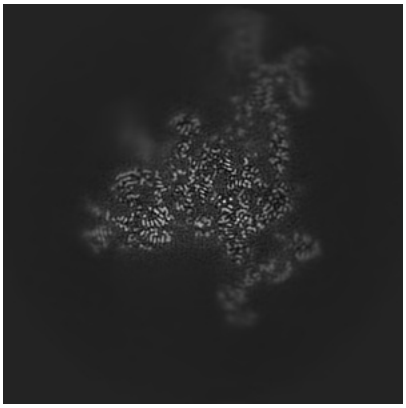


Z Index: 180

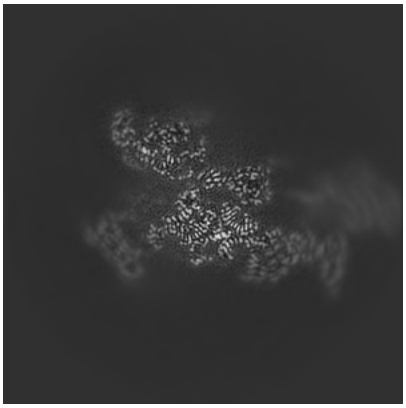
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

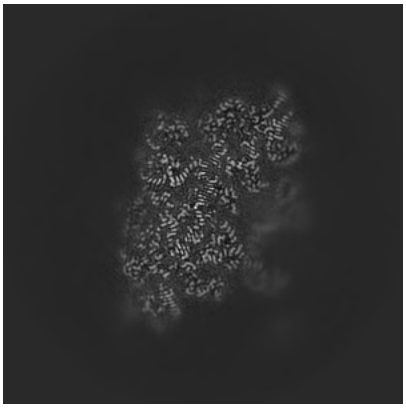
6.3.1 Primary map



X Index: 157



Y Index: 203

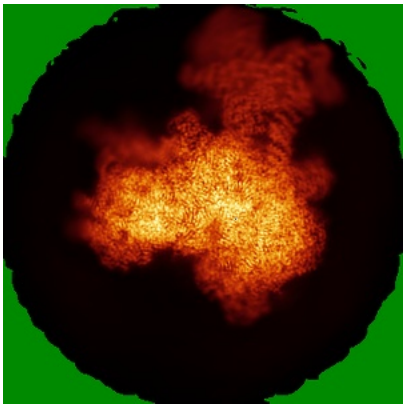


Z Index: 174

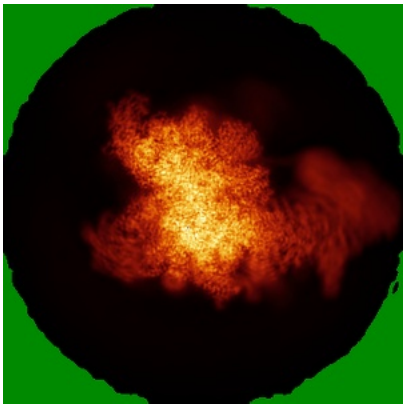
The images above show the largest variance slices of the map in three orthogonal directions.

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

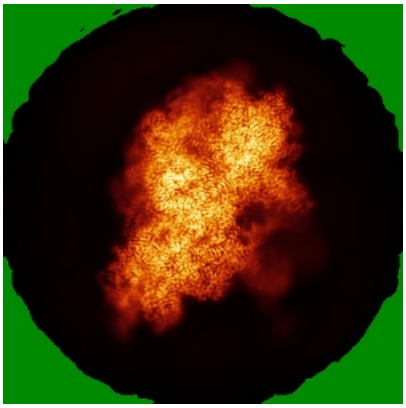
6.4.1 Primary map



X



Y

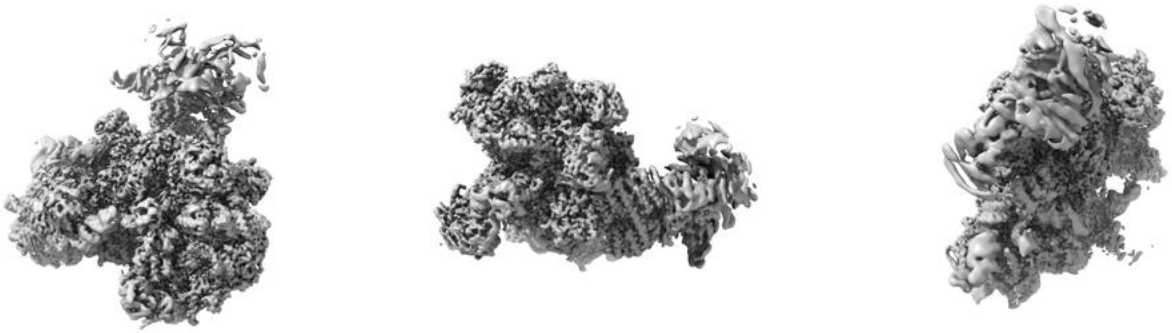


Z

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



X Y Z

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.

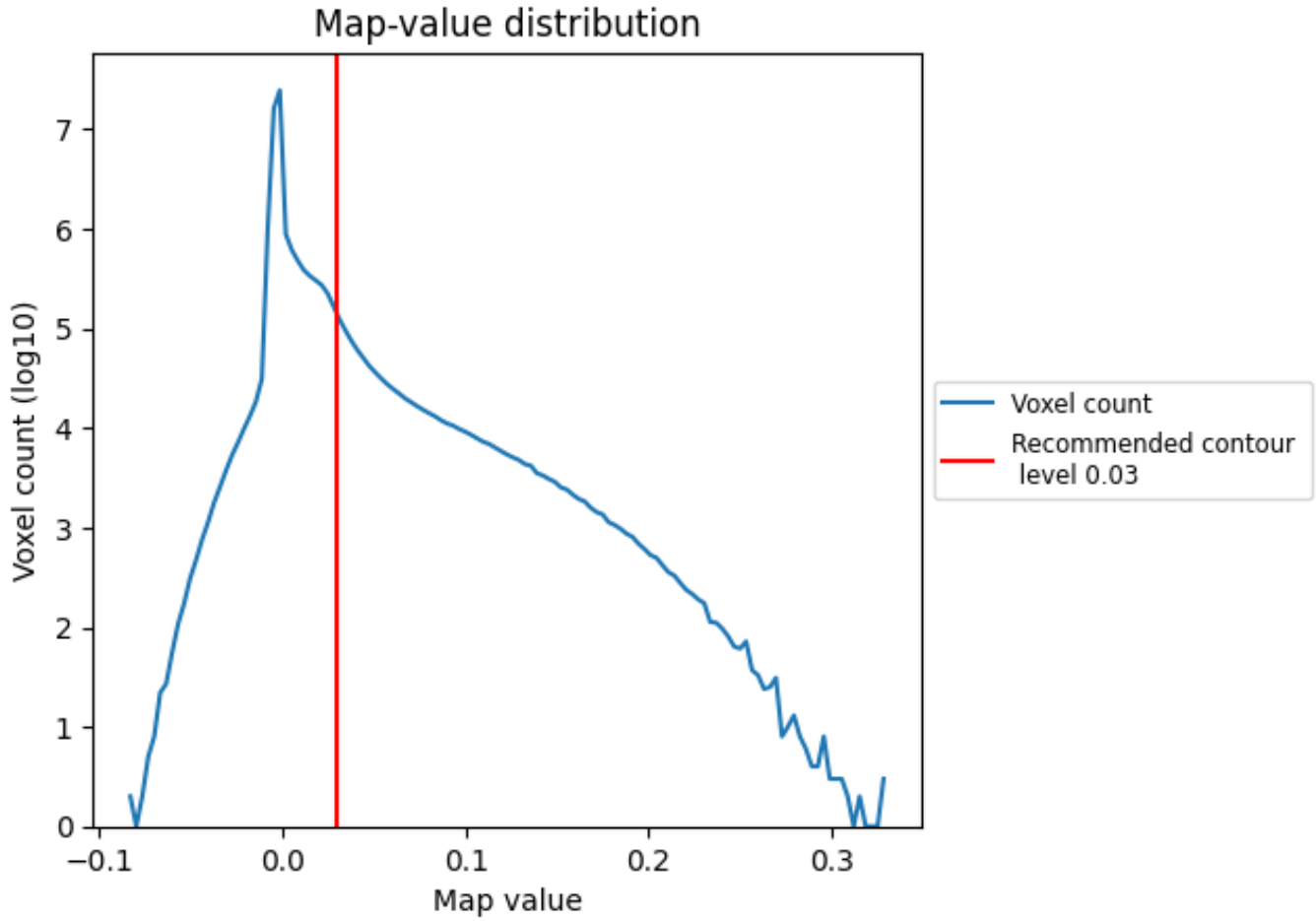
6.6 Mask visualisation (i)

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

7 Map analysis

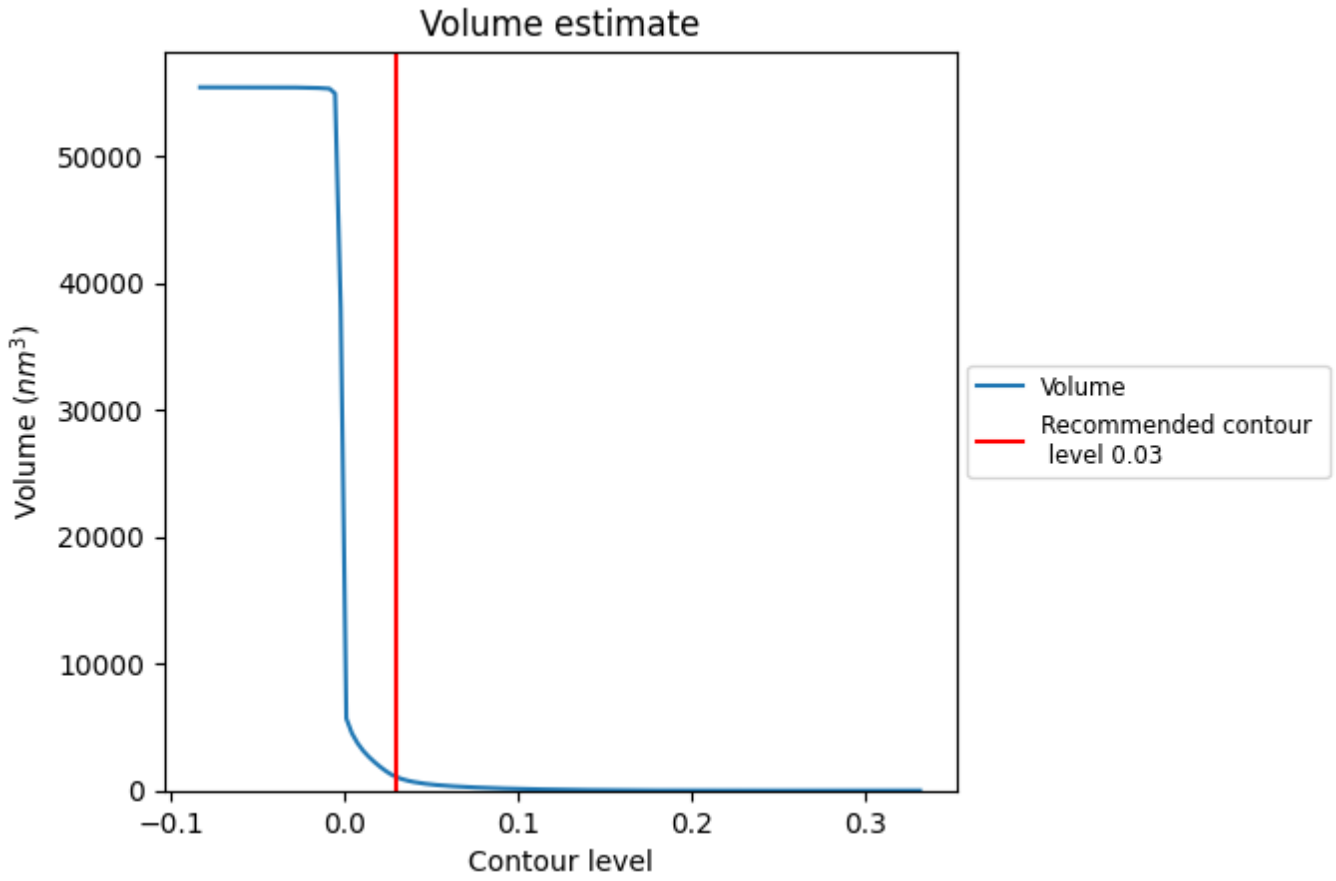
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

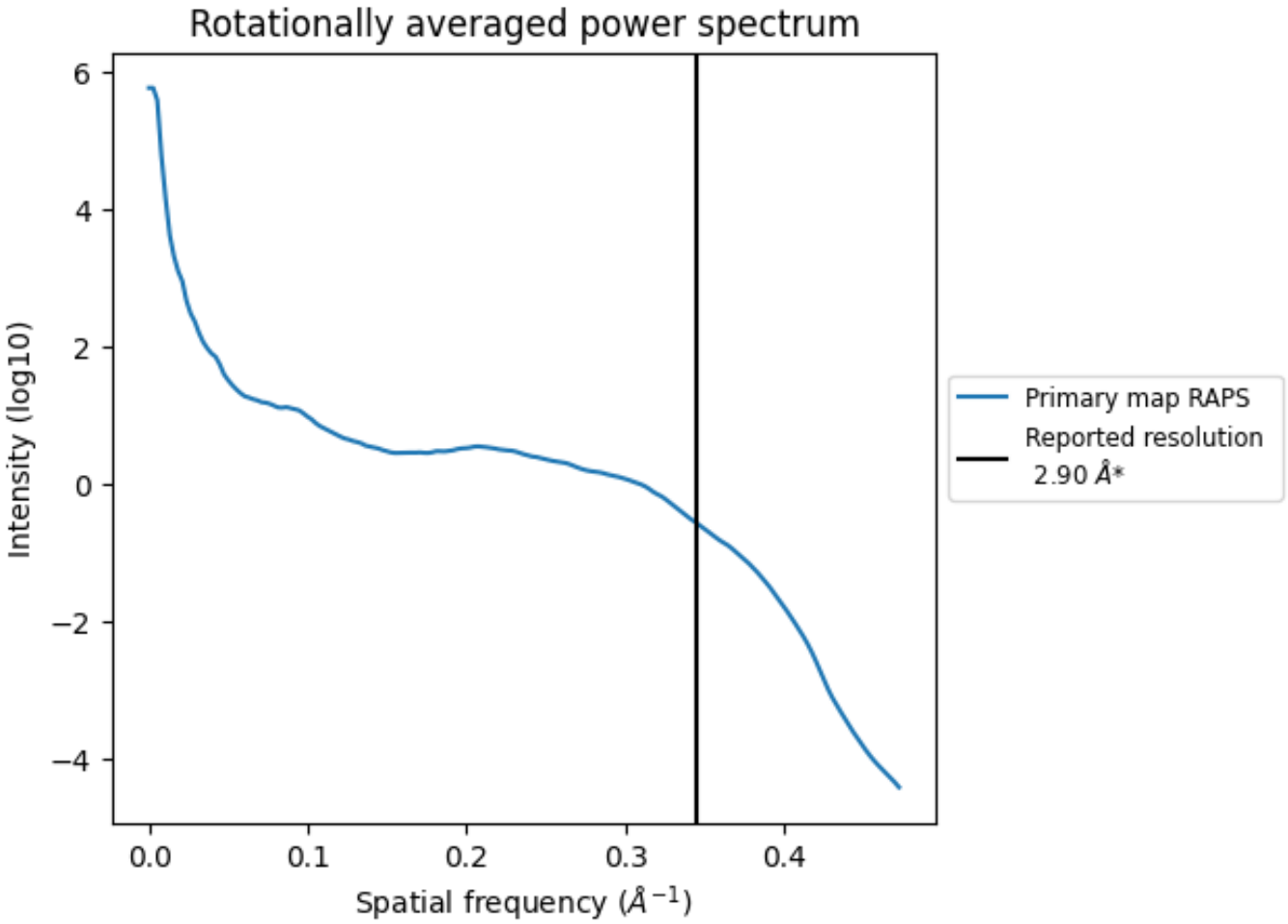
7.2 Volume estimate (i)



The volume at the recommended contour level is 1065 nm^3; this corresponds to an approximate mass of 962 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)

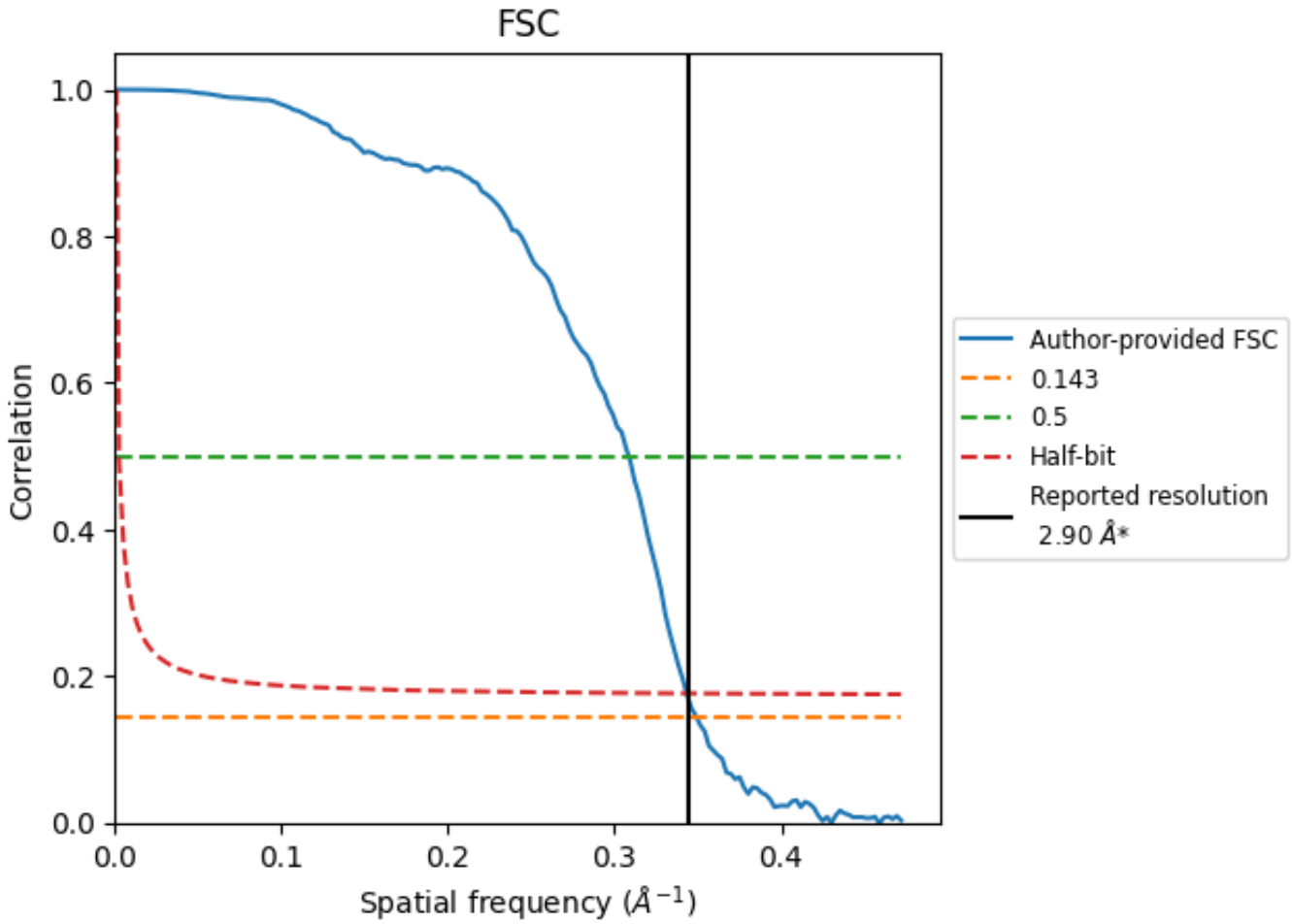


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

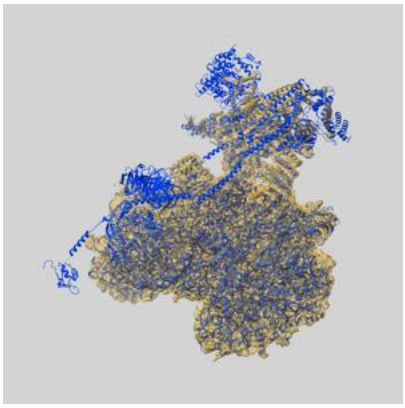
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.86	3.24	2.91
Unmasked-calculated*	-	-	-

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

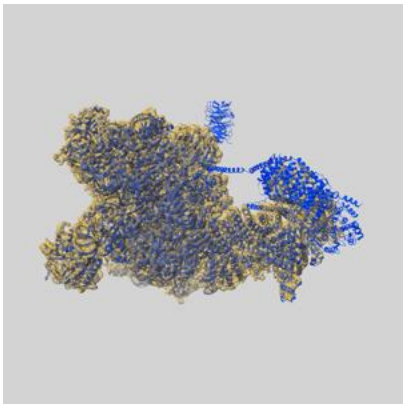
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11335 and PDB model 6ZP4. Per-residue inclusion information can be found in section 3 on page 14.

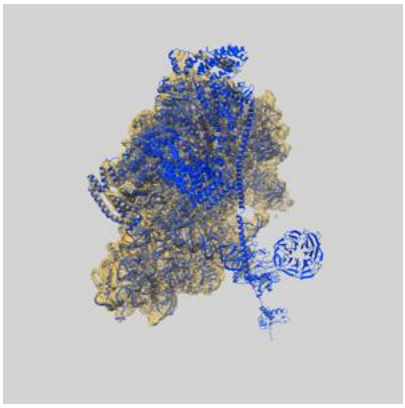
9.1 Map-model overlay



X



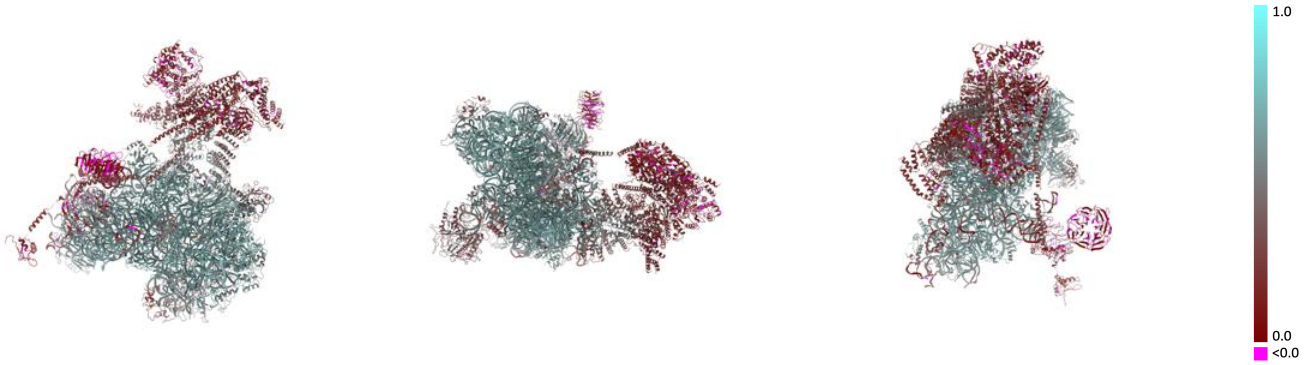
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

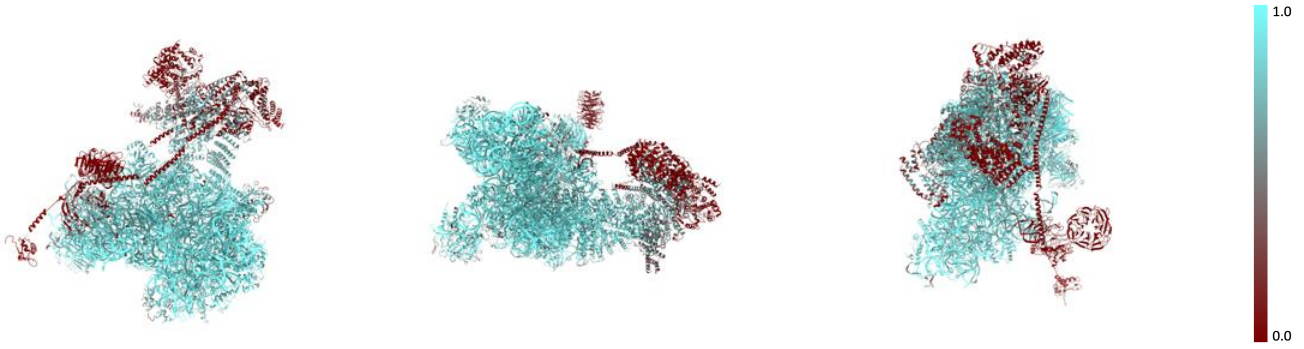
9.2 Q-score mapped to coordinate model



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.

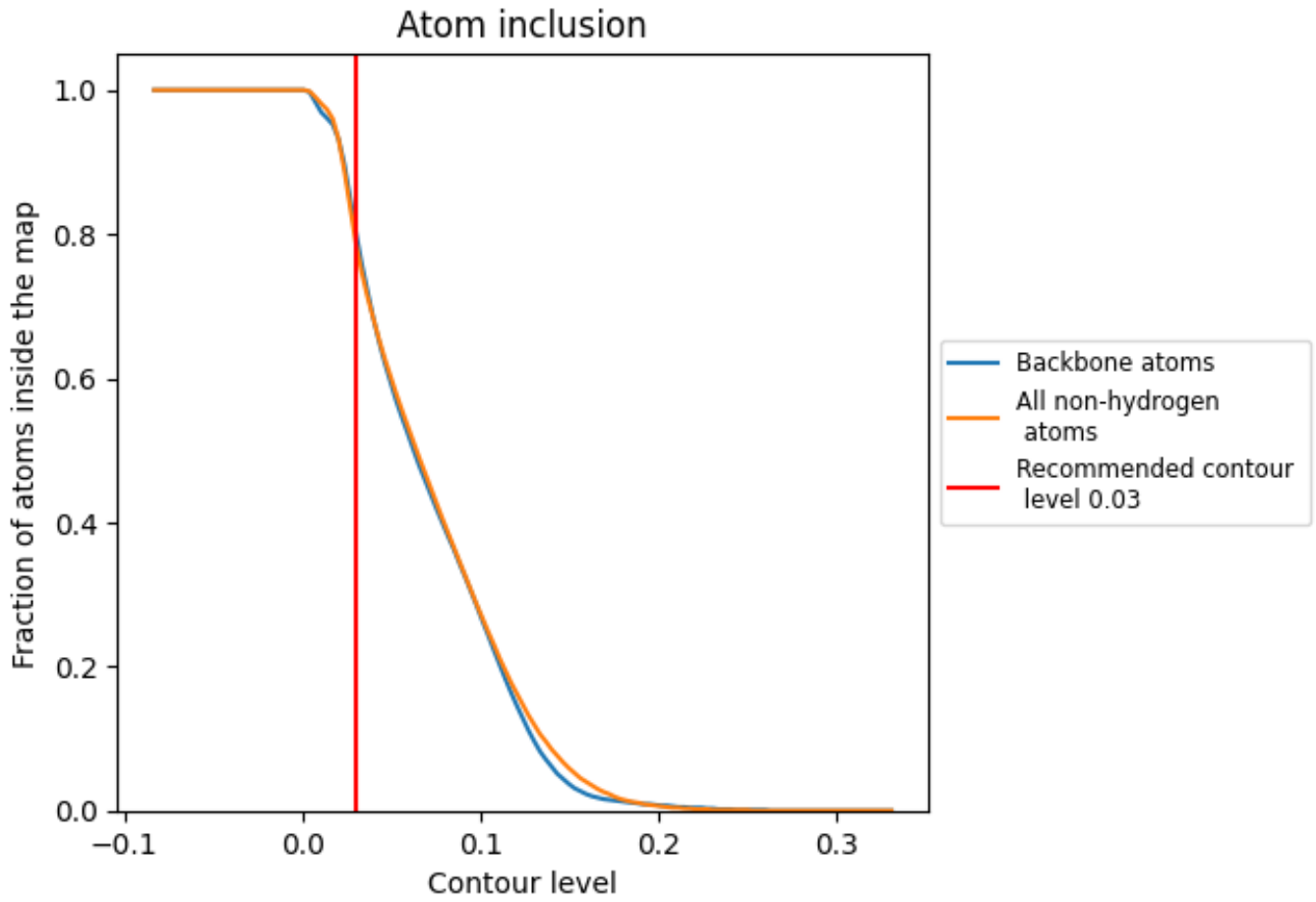
9.3 Atom inclusion mapped to coordinate model



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 79% 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	0.7920	0.4760
1	0.9840	0.5230
2	0.9730	0.5860
4	0.9070	0.4890
A	0.5830	0.3170
B	0.1780	0.2080
C	0.8010	0.4020
D	0.9900	0.6430
E	0.4520	0.1970
F	0.2080	0.1340
G	0.8440	0.5510
H	0.2990	0.1580
I	0.0000	0.0540
J	0.9770	0.6310
K	0.0280	0.1220
L	0.0980	0.1200
M	0.1770	0.1630
N	0.7380	0.4130
O	0.7960	0.4200
P	0.9280	0.5630
Q	0.9730	0.6160
R	0.9700	0.5950
S	0.9310	0.5630
T	0.9790	0.6060
U	0.8250	0.4630
V	0.9330	0.5490
W	0.9470	0.5850
X	0.7820	0.3710
Y	0.7850	0.3630
Z	0.8820	0.5170
a	0.9510	0.6040
b	0.9580	0.5890
c	0.9740	0.6160
d	0.9820	0.6360
e	0.9750	0.6060

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Chain	Atom inclusion	Q-score
g	0.9680	0.6230
h	0.9100	0.5670
i	0.9800	0.6130
j	0.9820	0.6300
k	0.9060	0.5710
l	0.9890	0.6450
m	0.9670	0.6060
n	0.9780	0.6160
o	0.9100	0.5770
p	0.9560	0.6050
q	0.9750	0.6100
r	0.9040	0.5250
s	0.9220	0.5360
t	0.9410	0.5660
u	0.9480	0.5760
v	0.6000	0.3280
w	0.9440	0.5850
x	0.9610	0.6170
y	0.9710	0.6220
z	0.9580	0.5790