wwPDB EM Validation Summary Report (i)

Dec 10, 2022 – 09:53 am GMT

PDB ID	:	5FLX
EMDB ID	:	EMD-3221
Title	:	Mammalian 40S HCV-IRES complex
Authors	:	Yamamoto, H.; Collier, M.; Loerke, J.; Ismer, J.; Schmidt, A.; Hilal, T.; Sprink, T.; Yamamoto, K.; Mielke, T.; Burger, J.; Shaikh, T.R.; Dabrowski, M.; Hildebrand, P.W.; Scheerer, P.; Spahn, C.M.T.
Deposited on	:	2015-10-28
Resolution	:	3.90 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:

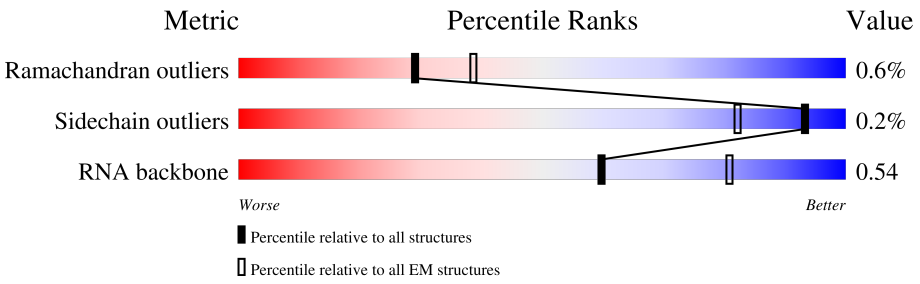
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.90 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	1	1869	9% 75% 16% 9%
2	A	295	20% 73% 27%
3	B	264	17% 80% 20%
4	C	293	12% 75% • 24%
5	D	243	51% 90% • 9%
6	E	263	11% 97% •
7	F	204	24% 92% • 7%
8	G	249	20% 93% 7%

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Mol	Chain	Length	Quality of chain
9	H	194	53% 94% 6%
10	I	208	16% 100%
11	J	194	14% 92% • 8%
12	K	165	45% 58% • 41%
13	L	158	22% 96% • •
14	M	132	90% 91% 9%
15	N	151	19% 99% •
16	O	151	19% 88% • • 10%
17	P	145	72% 81% • 17%
18	Q	146	42% 95% • 5%
19	R	135	60% 88% • 10%
20	S	152	63% 91% 9%
21	T	145	50% 99% •
22	U	119	50% 82% 18%
23	V	83	19% 96% • •
24	W	130	13% 99% •
25	X	143	14% 97% •
26	Y	133	21% 94% 6%
27	Z	125	25% 58% • 42%
28	a	115	14% 75% 8% • 16%
29	b	84	30% 90% • • 5%
30	c	69	22% 84% • • 12%
31	d	56	41% 91% 9%
32	e	59	29% 92% • 7%
33	f	156	46% 47% 53%

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Mol	Chain	Length	Quality of chain
34	g	317	81% 99%
35	z	504	12% 42% 10% 48%

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 80592 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	1708	36456	16274	6546	11928	1708	0	0

- Molecule 2 is a protein called 40S RIBOSOMAL PROTEIN SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	215	1704	1083	298	315	8	0	0

- Molecule 3 is a protein called 40S RIBOSOMAL PROTEIN S3A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	212	1722	1093	308	307	14	0	0

- Molecule 4 is a protein called 40S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	222	1724	1114	296	304	10	0	0

- Molecule 5 is a protein called 40S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	220	1709	1090	308	304	7	0	0

- Molecule 6 is a protein called 40S RIBOSOMAL PROTEIN S4, Y ISOFORM 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	257	2031	1298	381	344	8	0	0

- Molecule 7 is a protein called 40S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	F	190	1502	939	285	271	7	0	0

- Molecule 8 is a protein called 40S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	G	232	1884	1176	379	322	7	0	0

- Molecule 9 is a protein called 40S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	H	183	1479	941	272	265	1	0	0

- Molecule 10 is a protein called 40S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	I	207	1696	1064	334	293	5	0	0

- Molecule 11 is a protein called 40S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	J	179	1495	953	299	241	2	0	0

- Molecule 12 is a protein called 40S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	K	98	827	539	148	134	6	0	0

- Molecule 13 is a protein called 40S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	L	153	1258	804	235	213	6	0	0

- Molecule 14 is a protein called 40S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	M	120	931	584	164	174	9	0	0

- Molecule 15 is a protein called 40S RIBOSOMAL PROTEIN S13.

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

- Molecule 16 is a protein called 40S RIBOSOMAL PROTEIN S14.

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

- Molecule 17 is a protein called 40S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	P	120	999	636	188	168	7	0	0

- Molecule 18 is a protein called 40S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Q	139	1109	704	210	192	3	0	0

- Molecule 19 is a protein called 40S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	R	121	985	618	183	181	3	0	0

- Molecule 20 is a protein called 40S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	S	139	1154	725	233	195	1	0	0

- Molecule 21 is a protein called 40S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	T	143	1112	697	214	198	3	0	0

- Molecule 22 is a protein called 40S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	U	97	769	483	144	138	4	0	0

- Molecule 23 is a protein called 40S RIBOSOMAL PROTEIN S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	V	81	617	380	114	118	5	0	0

- Molecule 24 is a protein called 40S RIBOSOMAL PROTEIN S15A.

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

- Molecule 25 is a protein called 40S RIBOSOMAL PROTEIN S23.

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

- Molecule 26 is a protein called 40S RIBOSOMAL PROTEIN S24.

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

- Molecule 27 is a protein called 40S RIBOSOMAL PROTEIN S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Z	73	585	374	108	102	1	0	0

- Molecule 28 is a protein called 40S RIBOSOMAL PROTEIN S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	a	97	774	481	160	128	5	0	0

- Molecule 29 is a protein called 40S RIBOSOMAL PROTEIN S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	b	80	625	391	116	111	7	0	0

- Molecule 30 is a protein called 40S RIBOSOMAL PROTEIN S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	c	61	480	291	96	91	2	0	0

- Molecule 31 is a protein called 40S RIBOSOMAL PROTEIN S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	d	51	427	269	87	66	5	0	0

- Molecule 32 is a protein called 40S RIBOSOMAL PROTEIN S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	e	55	437	272	96	68	1	0	0

- Molecule 33 is a protein called UBIQUITIN-40S RIBOSOMAL PROTEIN S27A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	f	73	601	379	115	100	7	0	0

- Molecule 34 is a protein called GUANINE NUCLEOTIDE-BINDING PROTEIN SUBUNIT BETA-2-LIKE 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	g	314	2440	1537	425	466	12	0	0

- Molecule 35 is a RNA chain called HCV-IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
35	z	264	5637	2512	1009	1852	264	0	0

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
36	1	72	72	72	0
36	D	1	1	1	0
36	X	1	1	1	0

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

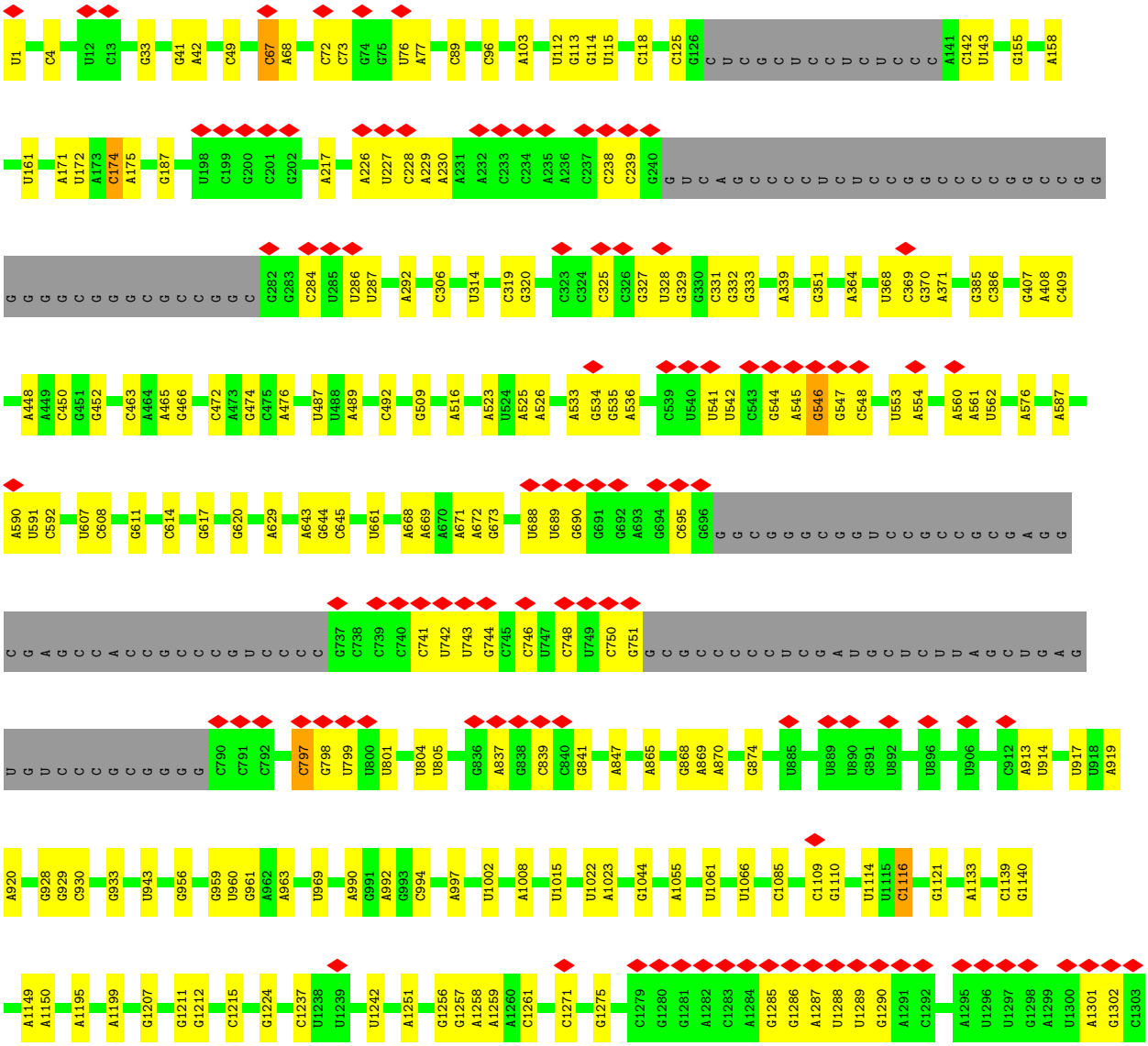
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
37	a	1	1	1	0
37	d	1	1	1	0

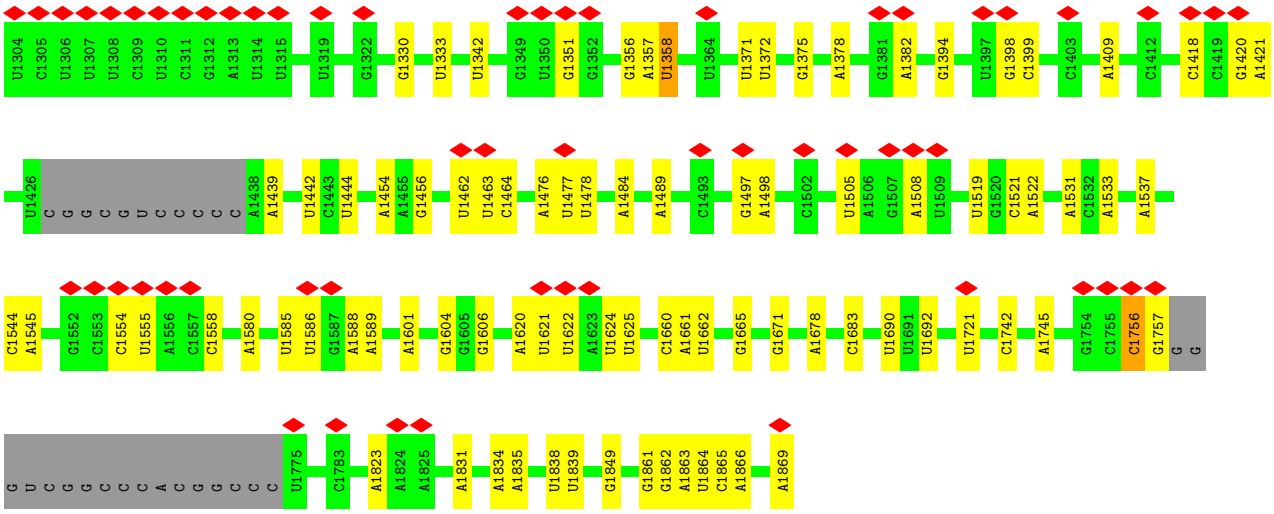
3 Residue-property plots (i)

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: 18S RRNA

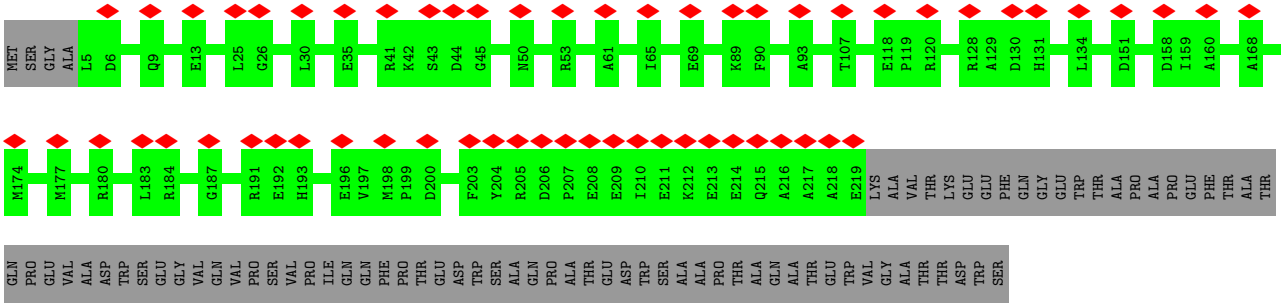
Chain 1:





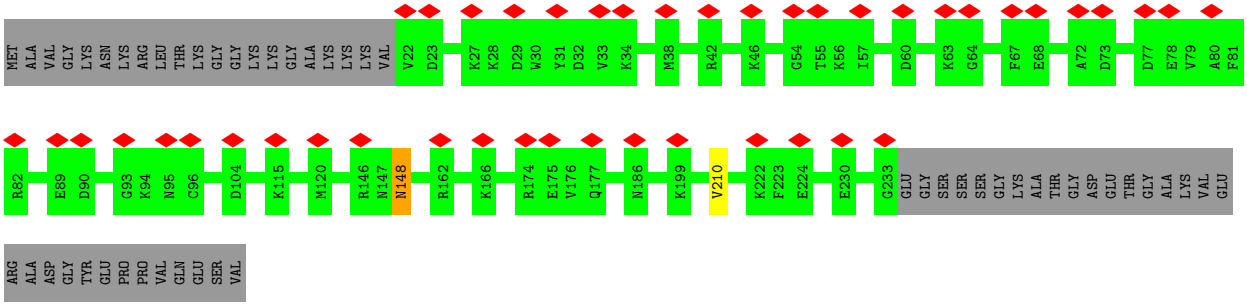
- Molecule 2: 40S RIBOSOMAL PROTEIN SA

Chain A:



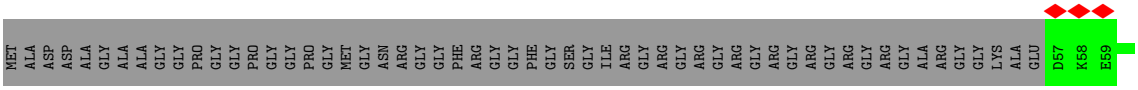
- Molecule 3: 40S RIBOSOMAL PROTEIN S3A

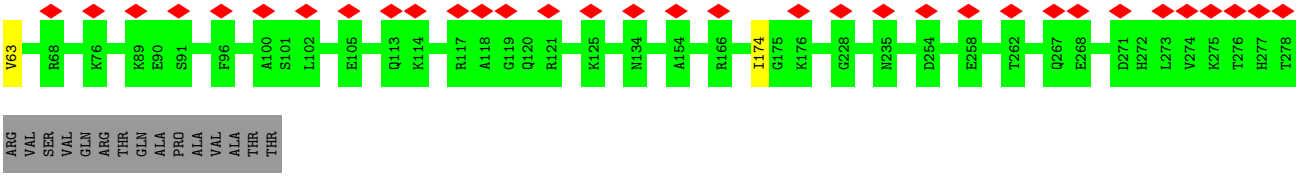
Chain B:



- Molecule 4: 40S RIBOSOMAL PROTEIN S2

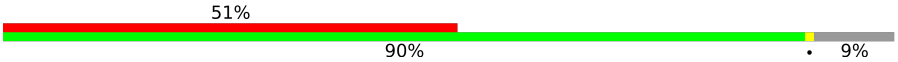
Chain C:

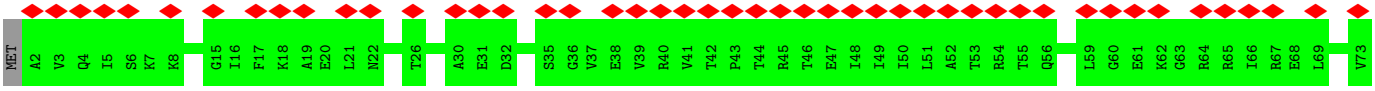


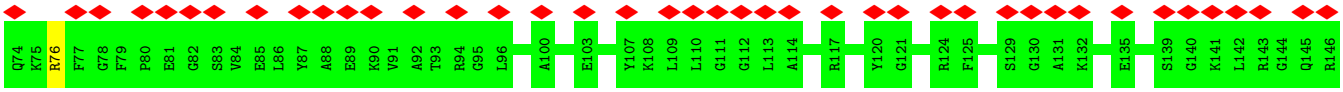


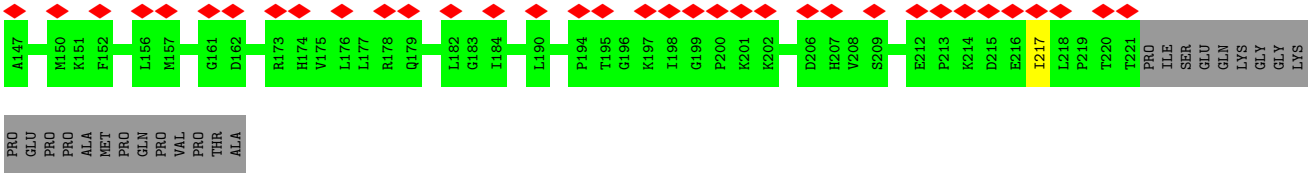
- Molecule 5: 40S RIBOSOMAL PROTEIN S3

Chain D:



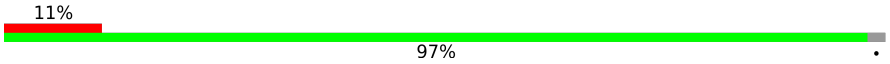


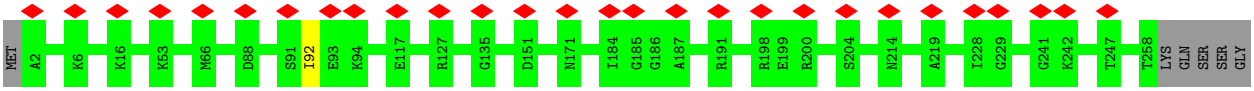




- Molecule 6: 40S RIBOSOMAL PROTEIN S4, Y ISOFORM 1

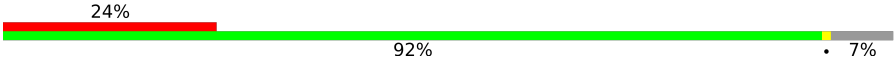
Chain E:

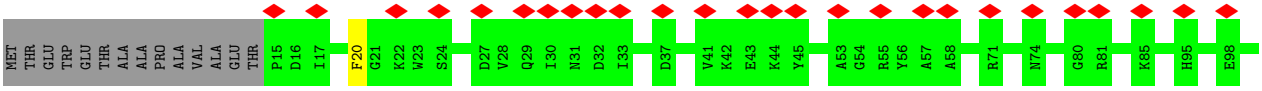


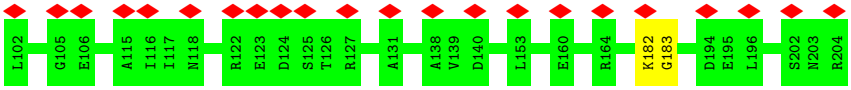


- Molecule 7: 40S RIBOSOMAL PROTEIN S5

Chain F:

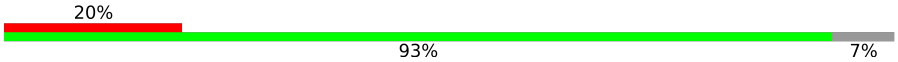


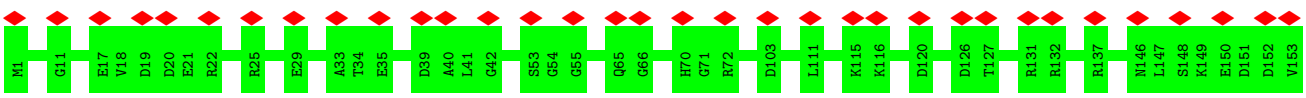


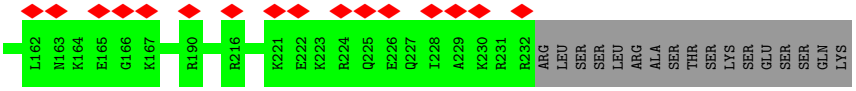


- Molecule 8: 40S RIBOSOMAL PROTEIN S6

Chain G:

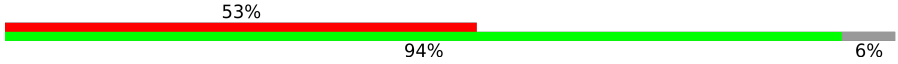


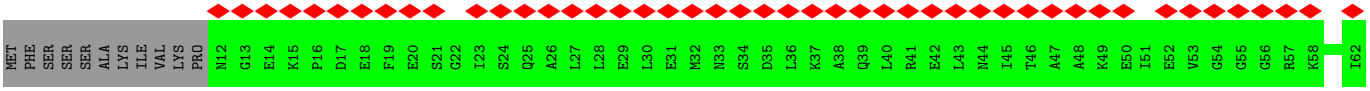


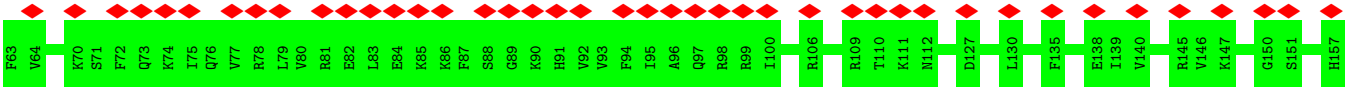


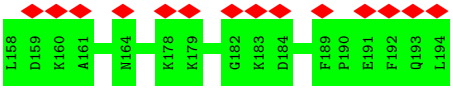
- Molecule 9: 40S RIBOSOMAL PROTEIN S7

Chain H:



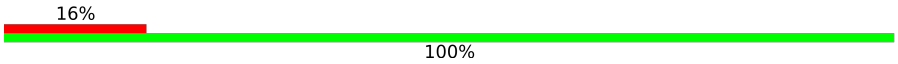


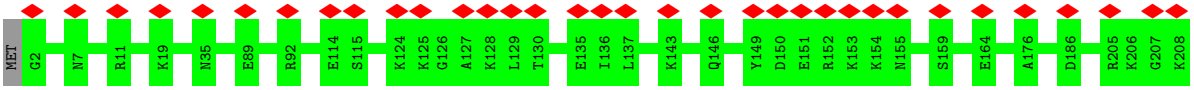




- Molecule 10: 40S RIBOSOMAL PROTEIN S8

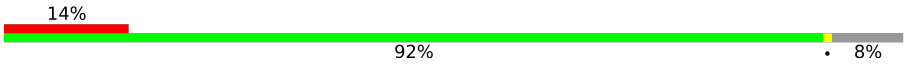
Chain I:

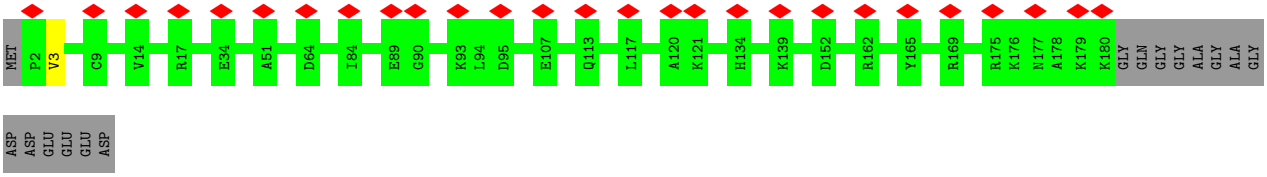




- Molecule 11: 40S RIBOSOMAL PROTEIN S9

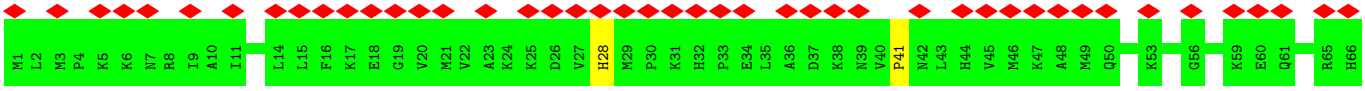
Chain J:

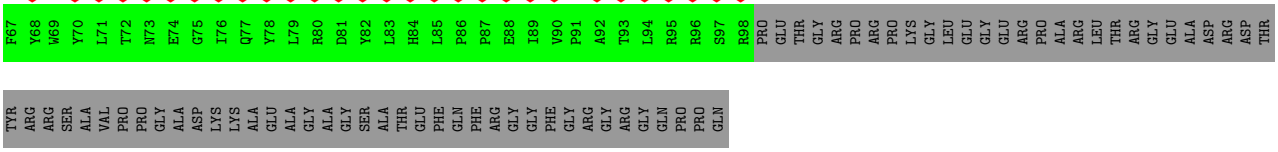




- Molecule 12: 40S RIBOSOMAL PROTEIN S10

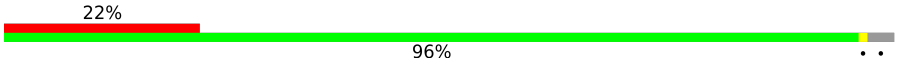
Chain K:

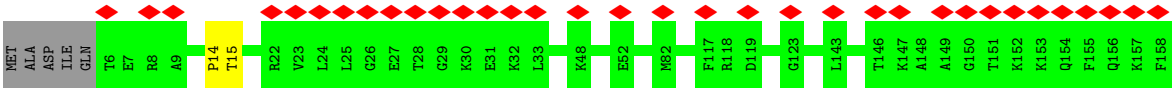




- Molecule 13: 40S RIBOSOMAL PROTEIN S11

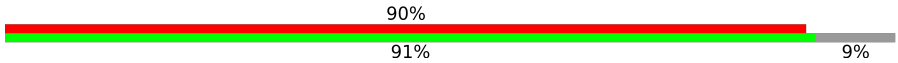
Chain L:

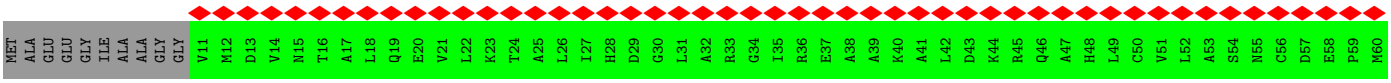


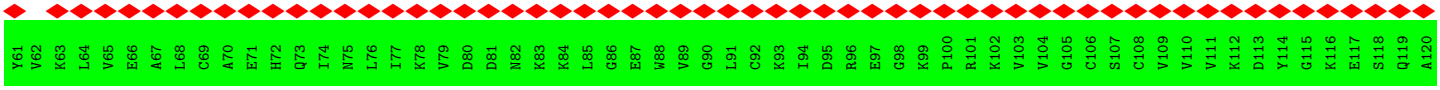


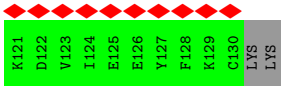
- Molecule 14: 40S RIBOSOMAL PROTEIN S12

Chain M:



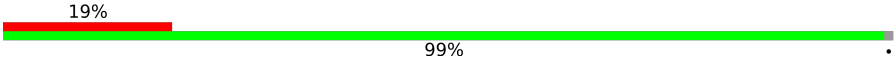


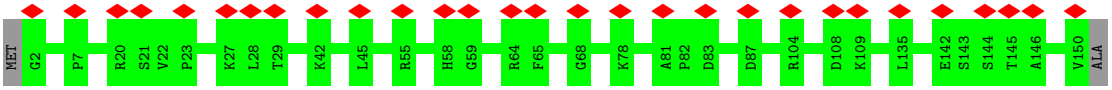




- Molecule 15: 40S RIBOSOMAL PROTEIN S13

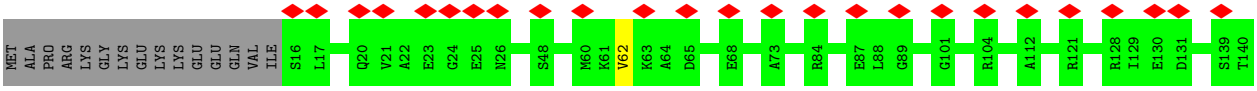
Chain N:

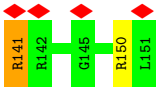




- Molecule 16: 40S RIBOSOMAL PROTEIN S14

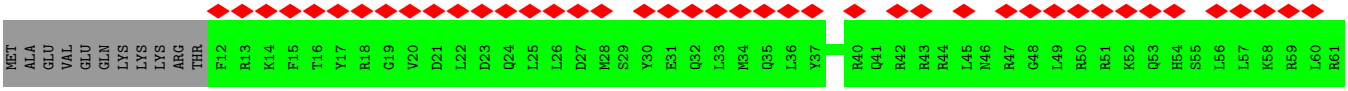
Chain O:

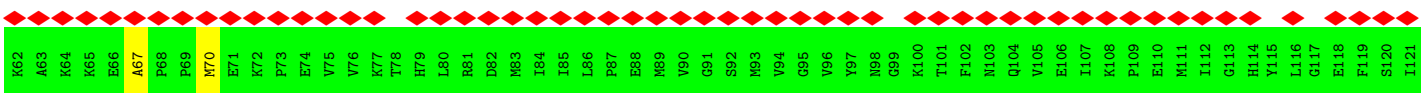


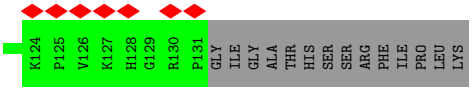


- Molecule 17: 40S RIBOSOMAL PROTEIN S15

Chain P:

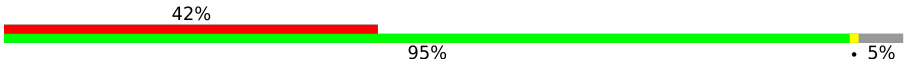


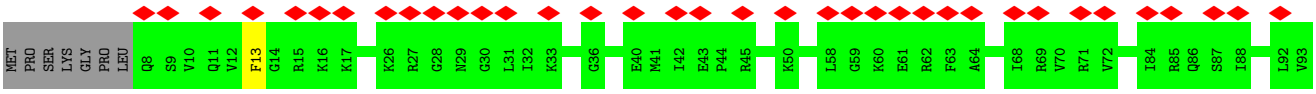


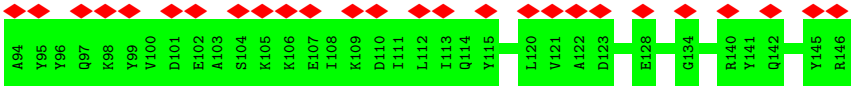


- Molecule 18: 40S RIBOSOMAL PROTEIN S16

Chain Q:

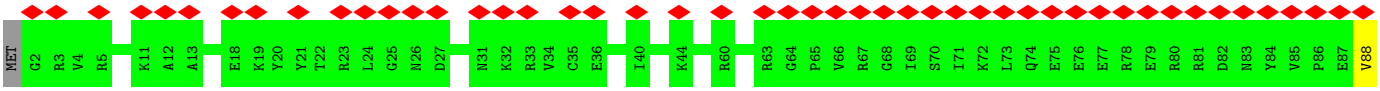


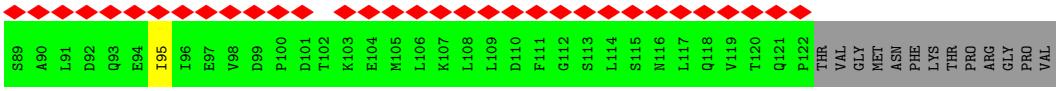




- Molecule 19: 40S RIBOSOMAL PROTEIN S17

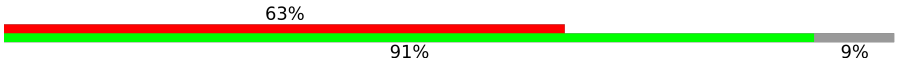
Chain R:

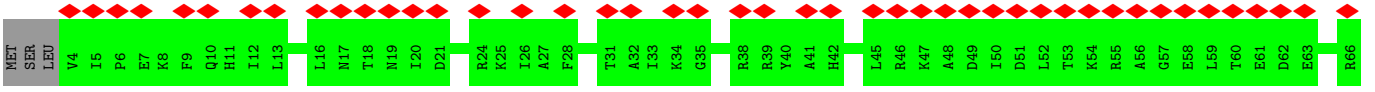


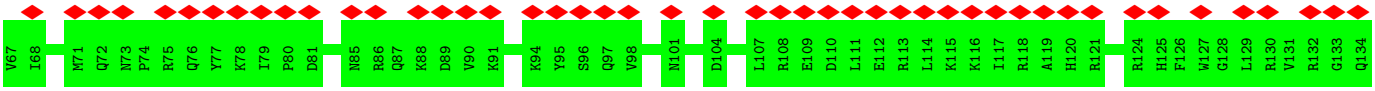


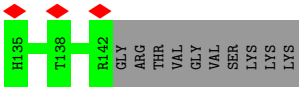
- Molecule 20: 40S RIBOSOMAL PROTEIN S18

Chain S:



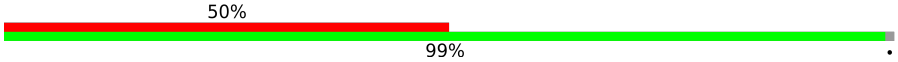


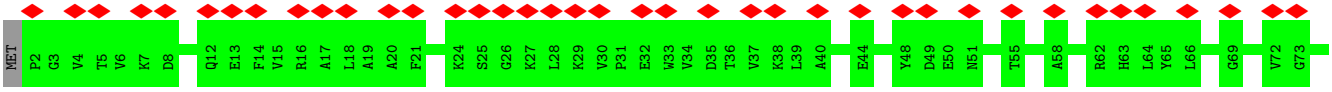


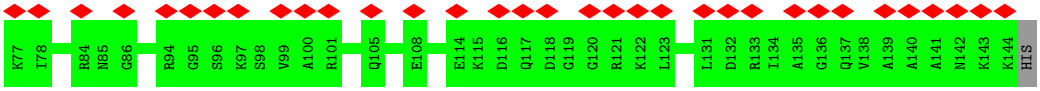


- Molecule 21: 40S RIBOSOMAL PROTEIN S19

Chain T:

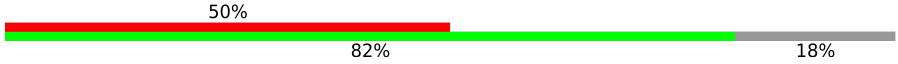


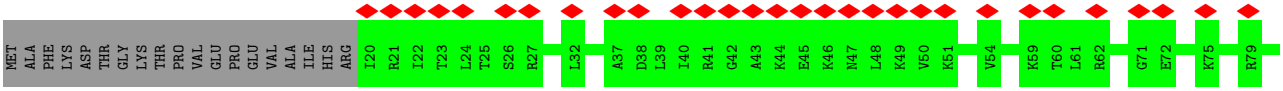


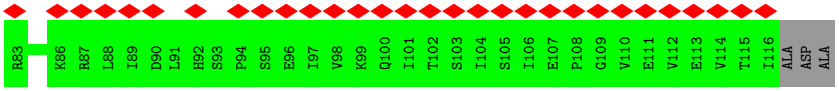


• Molecule 22: 40S RIBOSOMAL PROTEIN S20

Chain U:

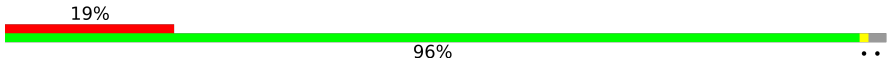


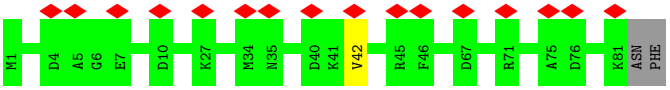




• Molecule 23: 40S RIBOSOMAL PROTEIN S21

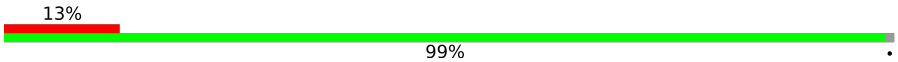
Chain V:

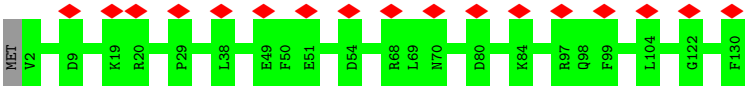




• Molecule 24: 40S RIBOSOMAL PROTEIN S15A

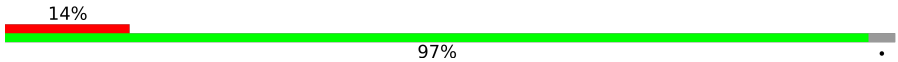
Chain W:

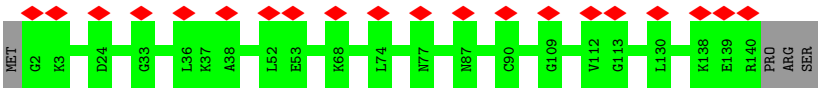




• Molecule 25: 40S RIBOSOMAL PROTEIN S23

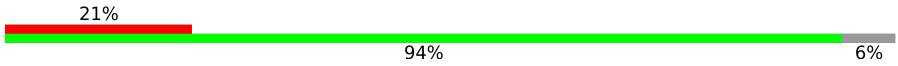
Chain X:

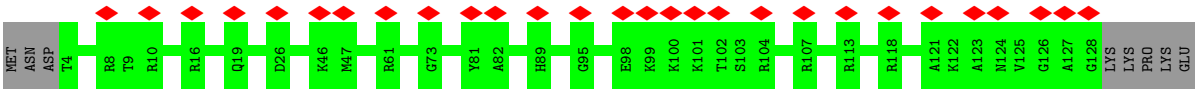




• Molecule 26: 40S RIBOSOMAL PROTEIN S24

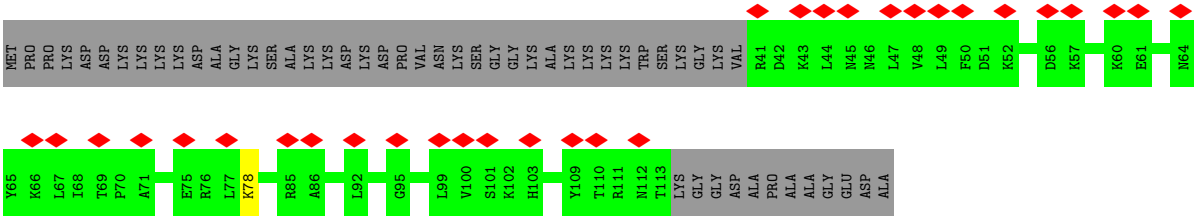
Chain Y:





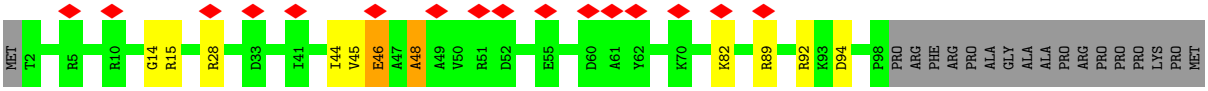
• Molecule 27: 40S RIBOSOMAL PROTEIN S25

Chain Z:



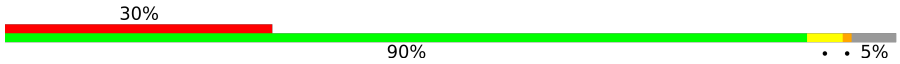
• Molecule 28: 40S RIBOSOMAL PROTEIN S26

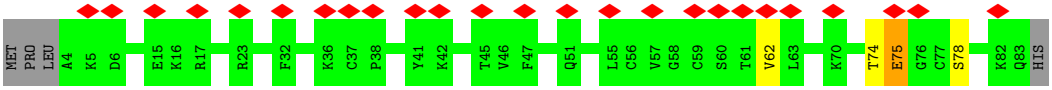
Chain a:



• Molecule 29: 40S RIBOSOMAL PROTEIN S27

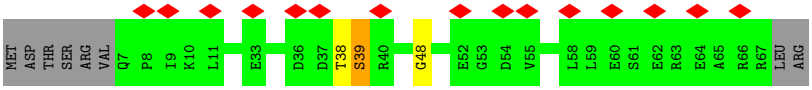
Chain b:





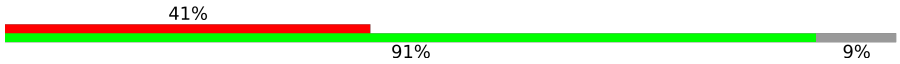
• Molecule 30: 40S RIBOSOMAL PROTEIN S28

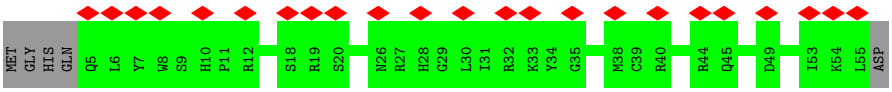
Chain c:



• Molecule 31: 40S RIBOSOMAL PROTEIN S29

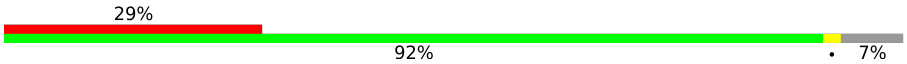
Chain d:

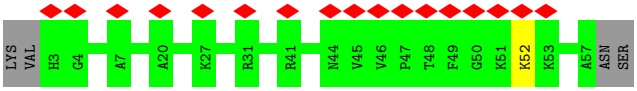




• Molecule 32: 40S RIBOSOMAL PROTEIN S30

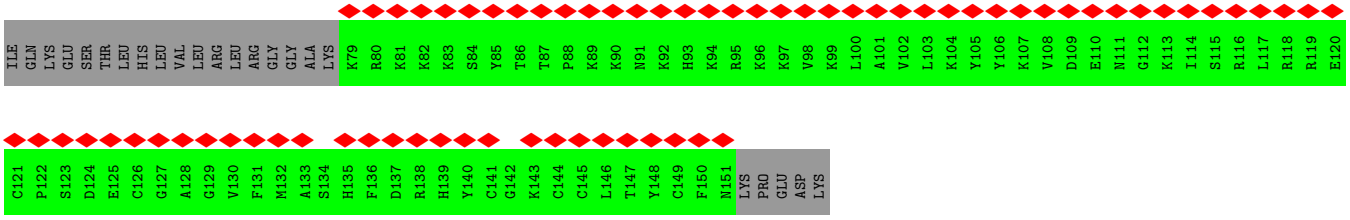
Chain e:





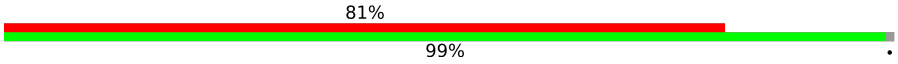
• Molecule 33: UBIQUITIN-40S RIBOSOMAL PROTEIN S27A

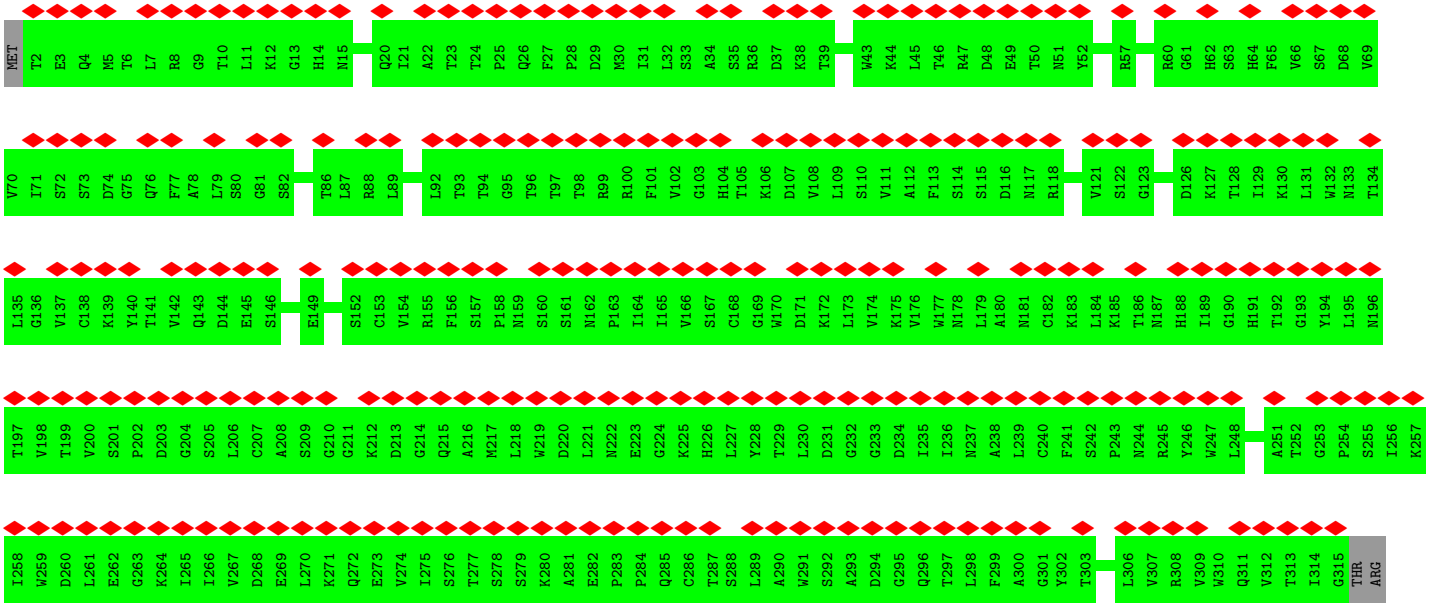
Chain f:



• Molecule 34: GUANINE NUCLEOTIDE-BINDING PROTEIN SUBUNIT BETA-2-LIKE 1

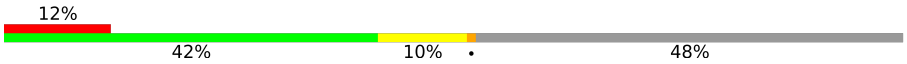
Chain g:

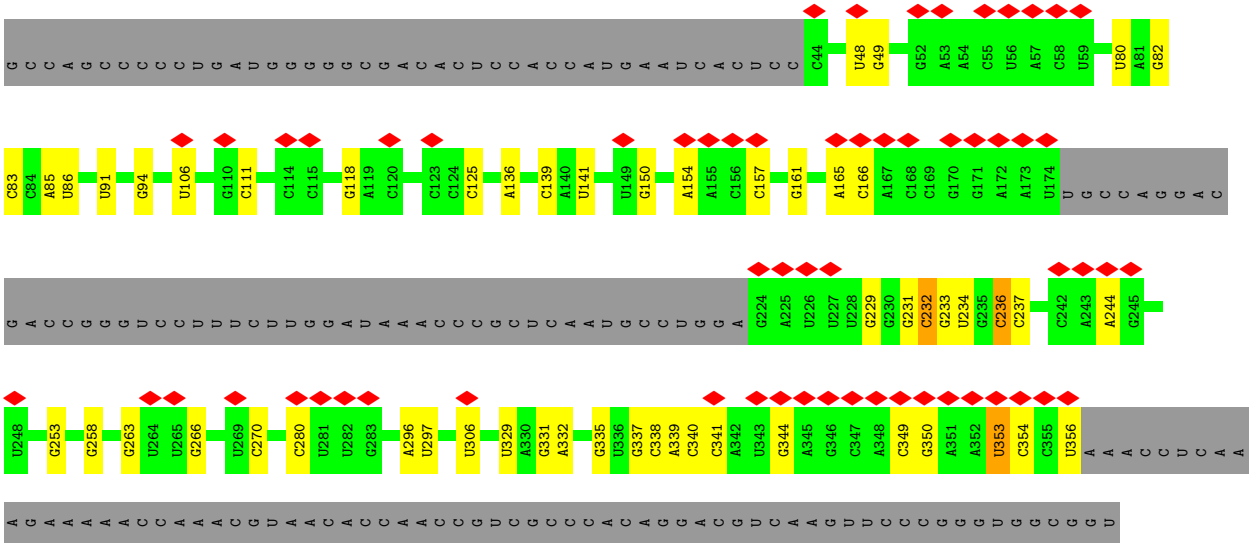




• Molecule 35: HCV-IRES

Chain z:





C U A G A C G G C C G A A G A U C A G G A A A A U C C C C U C U C U C U C G G A U C G G C A U U U G G G A C U U U C U G G C C U U U C G G G G C A

C C A C G G G U C C G G A A U C C C G A A A U U

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	171820	Depositor
Resolution determination method	Not provided	
CTF correction method	CTFFIND3	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	130293	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	17.786	Depositor
Minimum map value	-10.561	Depositor
Average map value	-0.008	Depositor
Map value standard deviation	0.997	Depositor
Recommended contour level	3.0	Depositor
Map size (Å)	406.6, 406.6, 406.6	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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: 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	1	0.19	1/40766 (0.0%)	0.78	23/63532 (0.0%)
2	A	0.25	0/1741	0.46	0/2366
3	B	0.23	0/1749	0.48	0/2340
4	C	0.25	0/1761	0.43	0/2379
5	D	0.25	0/1736	0.44	0/2338
6	E	0.24	0/2072	0.45	0/2793
7	F	0.24	0/1524	0.45	0/2048
8	G	0.24	0/1907	0.43	0/2538
9	H	0.28	0/1501	0.49	0/2009
10	I	0.24	0/1725	0.44	0/2298
11	J	0.23	0/1520	0.40	0/2030
12	K	0.25	0/851	0.48	0/1147
13	L	0.24	0/1281	0.49	0/1710
14	M	0.24	0/941	0.42	0/1264
15	N	0.23	0/1226	0.44	0/1649
16	O	0.25	0/1029	0.50	0/1380
17	P	0.24	0/1019	0.49	0/1361
18	Q	0.24	0/1126	0.49	0/1506
19	R	0.25	0/997	0.48	0/1338
20	S	0.24	0/1172	0.44	0/1570
21	T	0.25	0/1131	0.44	0/1515
22	U	0.22	0/778	0.43	0/1045
23	V	0.24	0/623	0.41	0/833
24	W	0.24	0/1051	0.44	0/1406
25	X	0.24	0/1097	0.44	0/1464
26	Y	0.24	0/1032	0.43	0/1371
27	Z	0.24	0/591	0.49	0/794
28	a	0.71	4/786 (0.5%)	1.26	6/1053 (0.6%)
29	b	0.25	0/637	0.54	0/854
30	c	1.01	1/482 (0.2%)	1.07	5/645 (0.8%)
31	d	0.27	0/437	0.50	0/580
32	e	0.65	3/443 (0.7%)	0.83	2/583 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	f	0.24	0/613	0.48	0/811
34	g	0.24	0/2497	0.44	0/3399
35	z	0.34	4/6299 (0.1%)	0.92	24/9818 (0.2%)
All	All	0.25	13/86141 (0.0%)	0.69	60/125767 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	D	0	1
6	E	0	1
7	F	0	1
13	L	0	1
16	O	0	1
17	P	0	1
18	Q	0	1
28	a	2	1
30	c	1	0
All	All	3	8

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	39	SER	CA-CB	-20.82	1.21	1.52
35	z	353	U	N1-C2	-12.82	1.27	1.38
28	a	48	ALA	CA-CB	-11.41	1.28	1.52
1	1	1	U	OP3-P	-10.53	1.48	1.61
28	a	44	ILE	CA-CB	-9.59	1.32	1.54

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	48	ALA	CB-CA-C	29.24	153.96	110.10
30	c	39	SER	CB-CA-C	18.56	145.36	110.10
35	z	234	U	O5'-P-OP1	-16.34	90.99	105.70
35	z	353	U	N3-C4-O4	-16.19	108.06	119.40
35	z	234	U	P-O5'-C5'	15.32	145.42	120.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	a	44	ILE	CA
28	a	48	ALA	CA
30	c	39	SER	CA

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	D	76	ARG	Peptide
6	E	92	ILE	Peptide
7	F	20	PHE	Peptide
13	L	15	THR	Peptide
16	O	141	ARG	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	
2	A	213/295 (72%)	202 (95%)	11 (5%)	0	100	100
3	B	210/264 (80%)	182 (87%)	26 (12%)	2 (1%)	15	52
4	C	220/293 (75%)	209 (95%)	9 (4%)	2 (1%)	17	54
5	D	218/243 (90%)	206 (94%)	11 (5%)	1 (0%)	29	67
6	E	255/263 (97%)	244 (96%)	11 (4%)	0	100	100
7	F	188/204 (92%)	165 (88%)	22 (12%)	1 (0%)	29	67
8	G	230/249 (92%)	221 (96%)	9 (4%)	0	100	100
9	H	181/194 (93%)	165 (91%)	16 (9%)	0	100	100
10	I	205/208 (99%)	186 (91%)	19 (9%)	0	100	100
11	J	177/194 (91%)	163 (92%)	13 (7%)	1 (1%)	25	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	K	96/165 (58%)	90 (94%)	4 (4%)	2 (2%)	7	39
13	L	151/158 (96%)	142 (94%)	8 (5%)	1 (1%)	22	60
14	M	118/132 (89%)	111 (94%)	7 (6%)	0	100	100
15	N	147/151 (97%)	131 (89%)	16 (11%)	0	100	100
16	O	134/151 (89%)	119 (89%)	13 (10%)	2 (2%)	10	45
17	P	118/145 (81%)	107 (91%)	10 (8%)	1 (1%)	19	57
18	Q	137/146 (94%)	132 (96%)	5 (4%)	0	100	100
19	R	119/135 (88%)	108 (91%)	9 (8%)	2 (2%)	9	43
20	S	137/152 (90%)	125 (91%)	12 (9%)	0	100	100
21	T	141/145 (97%)	135 (96%)	6 (4%)	0	100	100
22	U	95/119 (80%)	94 (99%)	1 (1%)	0	100	100
23	V	79/83 (95%)	77 (98%)	1 (1%)	1 (1%)	12	48
24	W	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
25	X	137/143 (96%)	128 (93%)	9 (7%)	0	100	100
26	Y	123/133 (92%)	118 (96%)	5 (4%)	0	100	100
27	Z	71/125 (57%)	64 (90%)	7 (10%)	0	100	100
28	a	95/115 (83%)	78 (82%)	10 (10%)	7 (7%)	1	16
29	b	78/84 (93%)	67 (86%)	7 (9%)	4 (5%)	2	23
30	c	59/69 (86%)	48 (81%)	10 (17%)	1 (2%)	9	43
31	d	49/56 (88%)	43 (88%)	6 (12%)	0	100	100
32	e	53/59 (90%)	49 (92%)	4 (8%)	0	100	100
33	f	71/156 (46%)	66 (93%)	5 (7%)	0	100	100
34	g	312/317 (98%)	298 (96%)	14 (4%)	0	100	100
All	All	4744/5476 (87%)	4395 (93%)	321 (7%)	28 (1%)	29	63

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	O	62	VAL
23	V	42	VAL
28	a	92	ARG
28	a	94	ASP
29	b	74	THR

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	
2	A	180/243 (74%)	180 (100%)	0	100	100
3	B	193/231 (84%)	192 (100%)	1 (0%)	88	93
4	C	188/225 (84%)	188 (100%)	0	100	100
5	D	183/202 (91%)	183 (100%)	0	100	100
6	E	220/225 (98%)	220 (100%)	0	100	100
7	F	160/170 (94%)	159 (99%)	1 (1%)	86	91
8	G	202/218 (93%)	202 (100%)	0	100	100
9	H	164/174 (94%)	164 (100%)	0	100	100
10	I	179/180 (99%)	179 (100%)	0	100	100
11	J	160/168 (95%)	160 (100%)	0	100	100
12	K	89/136 (65%)	89 (100%)	0	100	100
13	L	138/142 (97%)	138 (100%)	0	100	100
14	M	102/108 (94%)	102 (100%)	0	100	100
15	N	130/131 (99%)	130 (100%)	0	100	100
16	O	106/119 (89%)	105 (99%)	1 (1%)	78	87
17	P	109/130 (84%)	109 (100%)	0	100	100
18	Q	115/121 (95%)	115 (100%)	0	100	100
19	R	110/122 (90%)	110 (100%)	0	100	100
20	S	121/132 (92%)	121 (100%)	0	100	100
21	T	113/115 (98%)	113 (100%)	0	100	100
22	U	90/107 (84%)	90 (100%)	0	100	100
23	V	65/67 (97%)	65 (100%)	0	100	100
24	W	112/113 (99%)	112 (100%)	0	100	100
25	X	111/115 (96%)	111 (100%)	0	100	100
26	Y	107/115 (93%)	107 (100%)	0	100	100
27	Z	65/103 (63%)	64 (98%)	1 (2%)	65	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	a	84/98 (86%)	81 (96%)	3 (4%)	35	61
29	b	72/76 (95%)	71 (99%)	1 (1%)	67	81
30	c	54/62 (87%)	53 (98%)	1 (2%)	57	75
31	d	45/49 (92%)	45 (100%)	0	100	100
32	e	44/48 (92%)	44 (100%)	0	100	100
33	f	66/140 (47%)	66 (100%)	0	100	100
34	g	272/275 (99%)	272 (100%)	0	100	100
All	All	4149/4660 (89%)	4140 (100%)	9 (0%)	93	96

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	b	75	GLU
30	c	39	SER
27	Z	78	LYS
28	a	15	ARG
28	a	46	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
12	K	42	ASN
27	Z	89	GLN
17	P	41	GLN
26	Y	19	GLN
34	g	143	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1700/1869 (90%)	286 (16%)	9 (0%)
35	z	262/504 (51%)	52 (19%)	0
All	All	1962/2373 (82%)	338 (17%)	9 (0%)

5 of 338 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	4	C
1	1	33	G
1	1	41	G
1	1	42	A
1	1	49	C

5 of 9 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	1554	C
1	1	1756	C
1	1	546	G
1	1	797	C
1	1	869	A

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 76 ligands modelled in this entry, 76 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
1	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	1112:U	O3'	1113:A	P	5.18

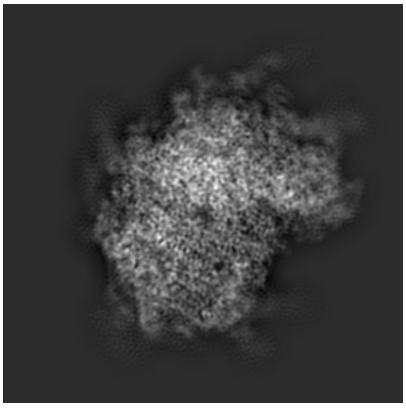
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3221. These allow visual inspection of the internal detail of the map and identification of artifacts.

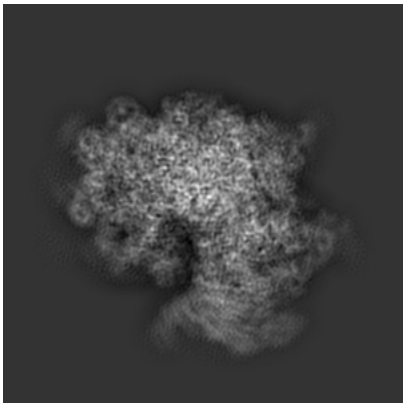
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

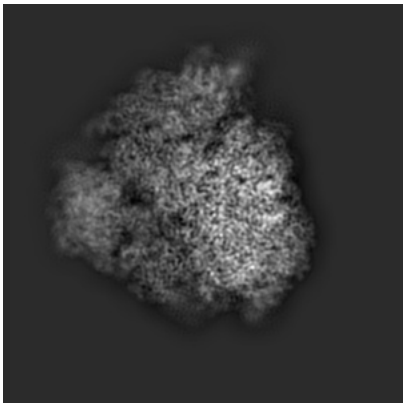
6.1.1 Primary map



X



Y

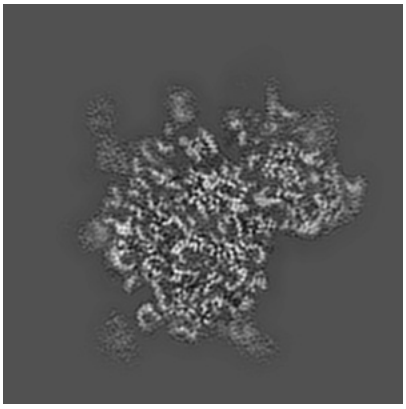


Z

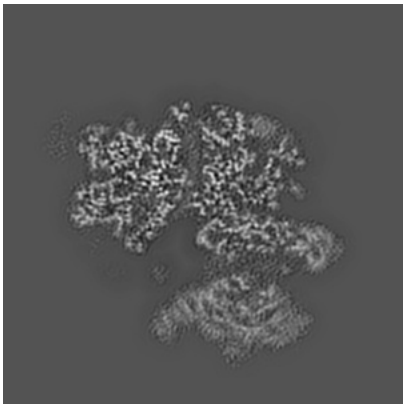
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

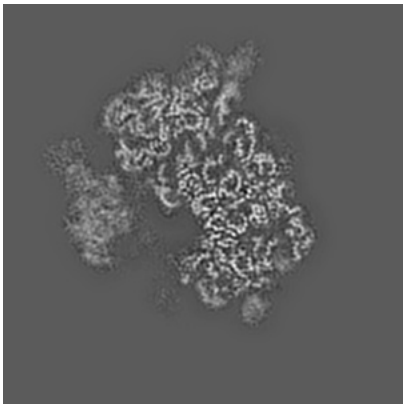
6.2.1 Primary map



X Index: 190



Y Index: 190

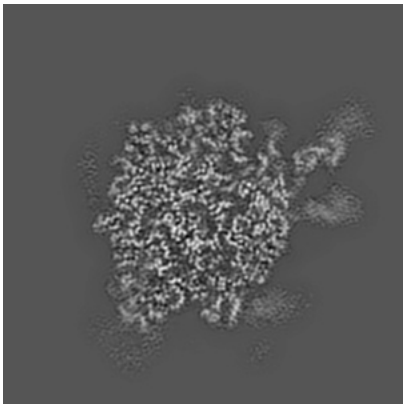


Z Index: 190

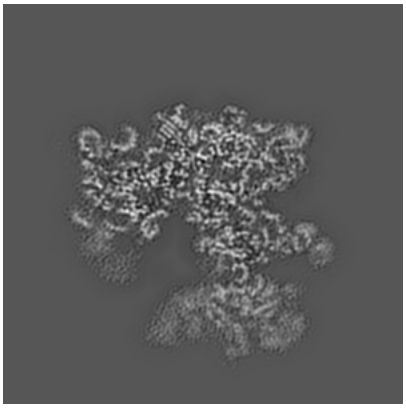
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

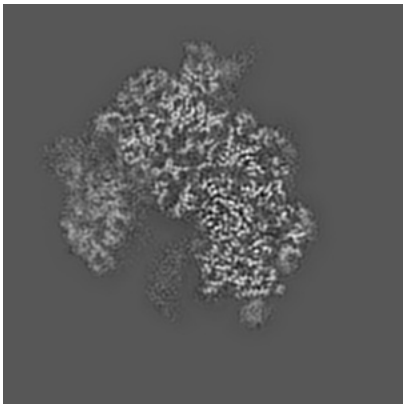
6.3.1 Primary map



X Index: 224



Y Index: 201



Z Index: 198

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

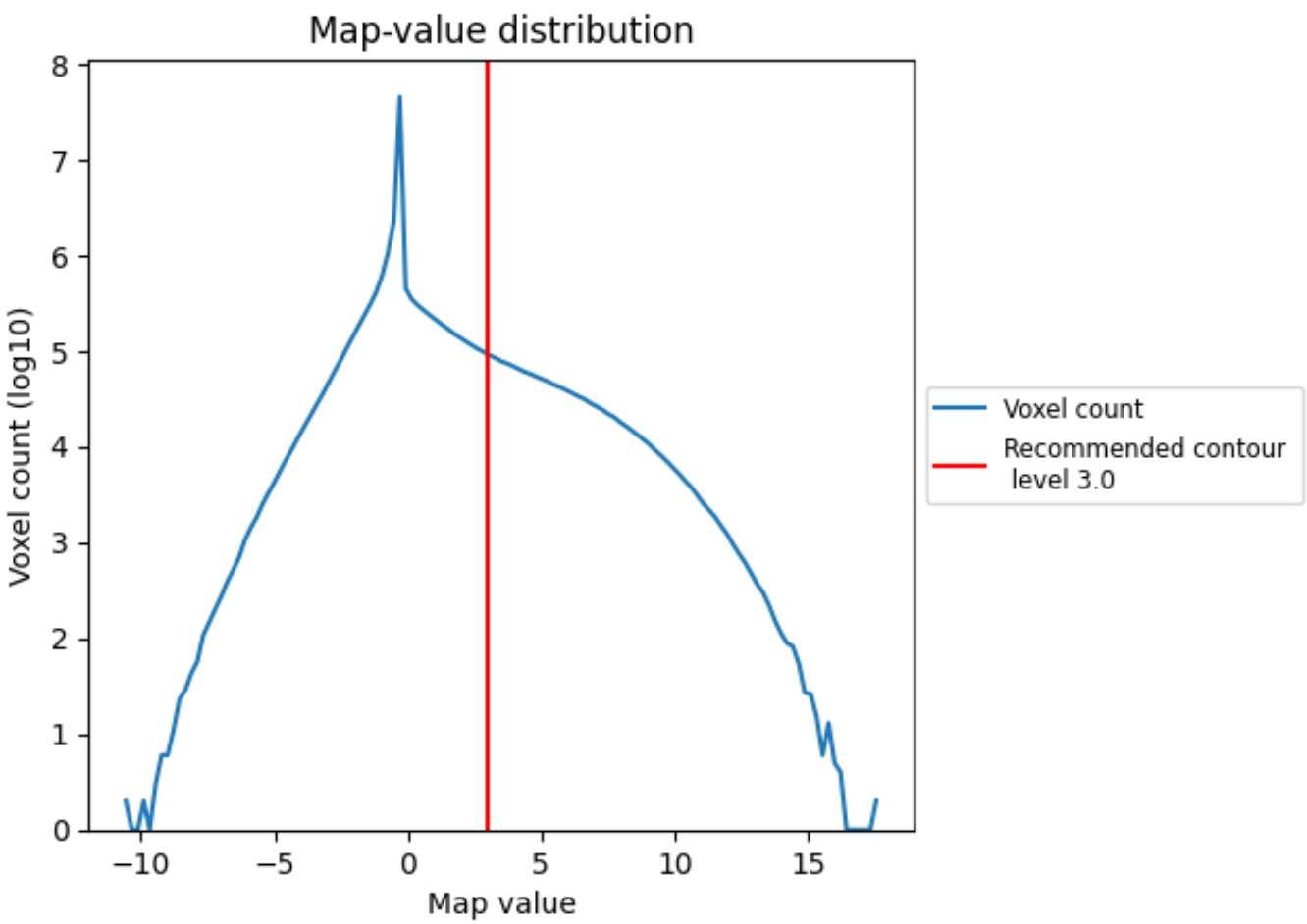
6.5 Mask visualisation (i)

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

7 Map analysis (i)

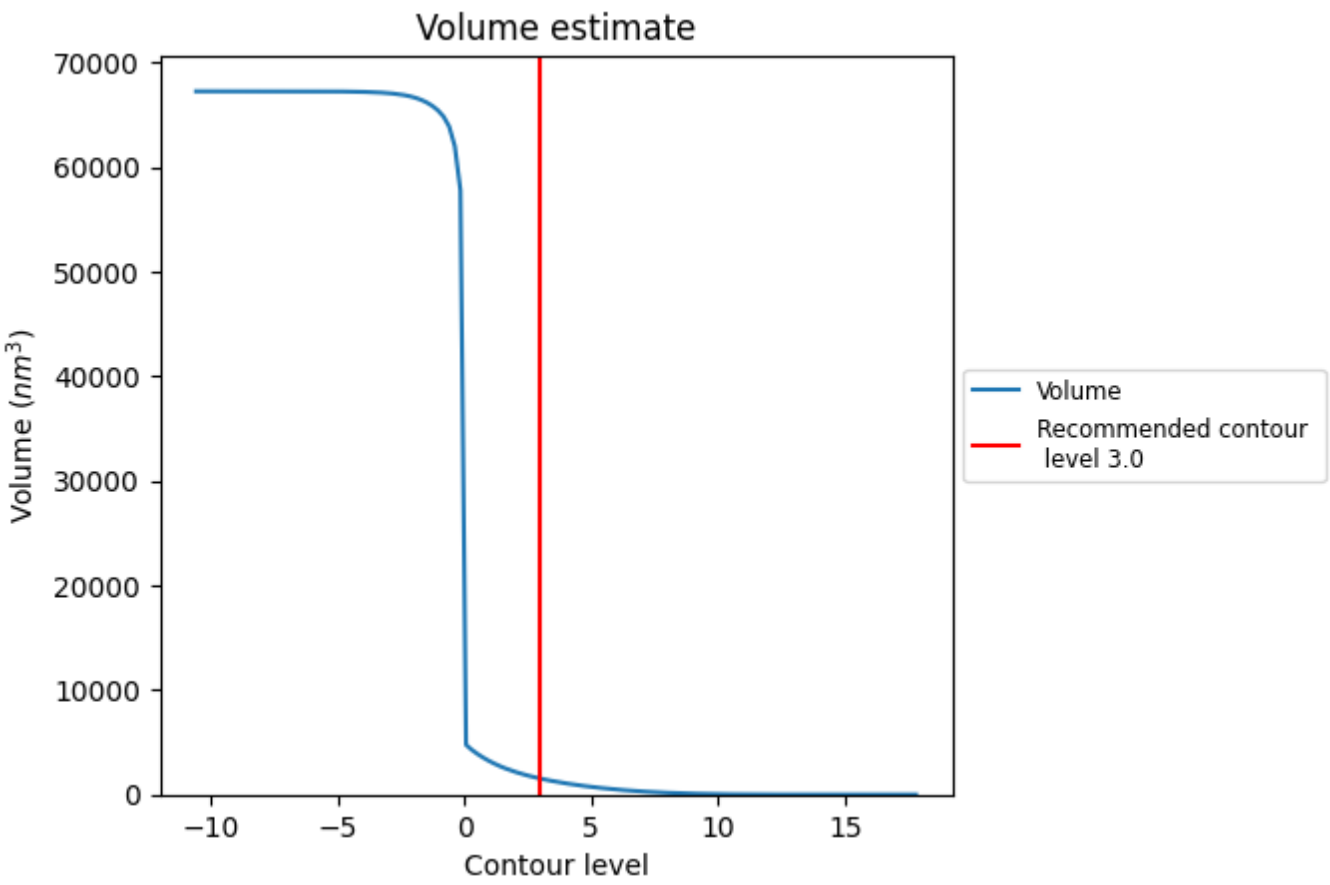
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

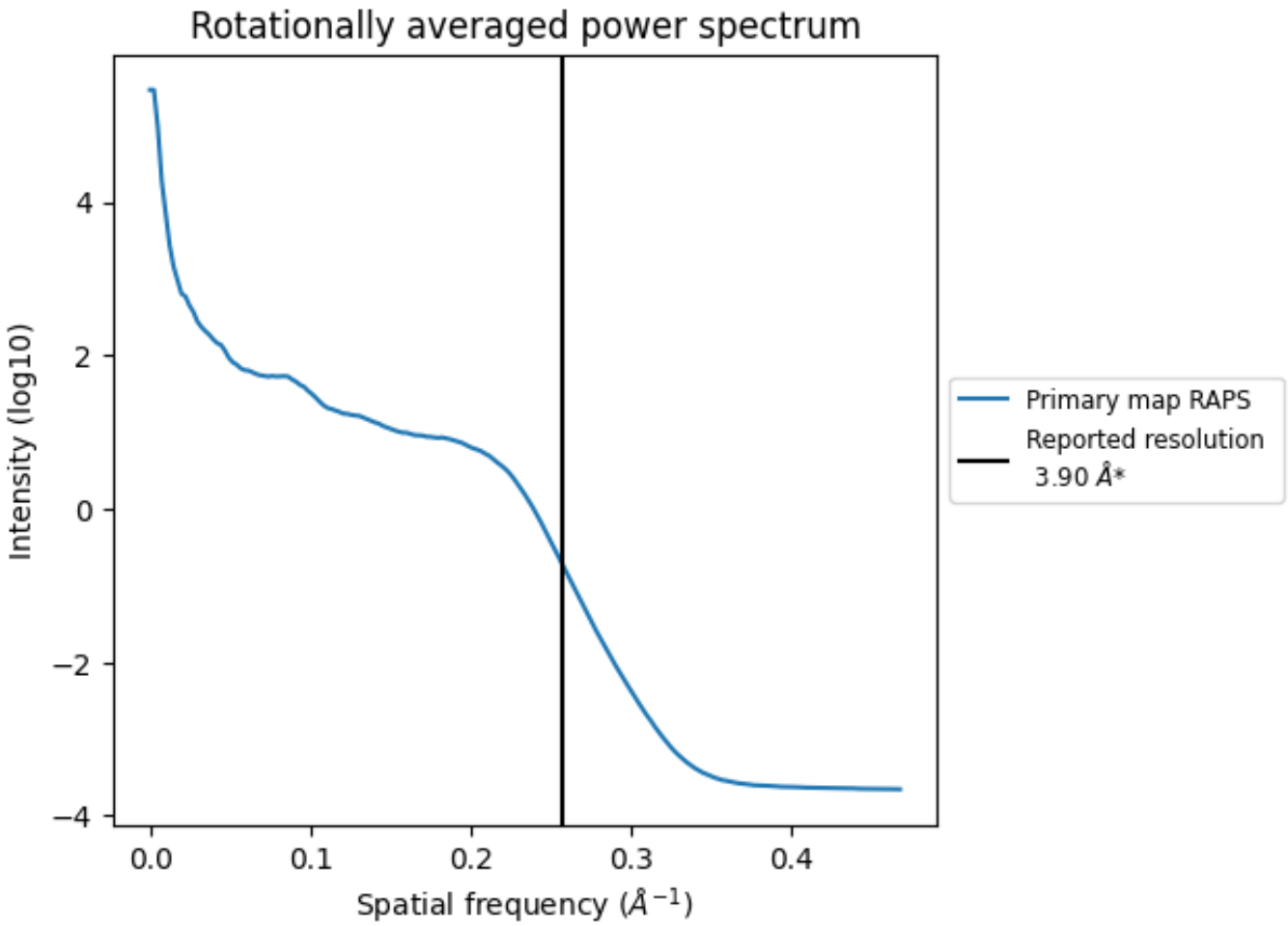
7.2 Volume estimate (i)



The volume at the recommended contour level is 1526 nm^3; this corresponds to an approximate mass of 1379 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 0.256 Å^{-1}

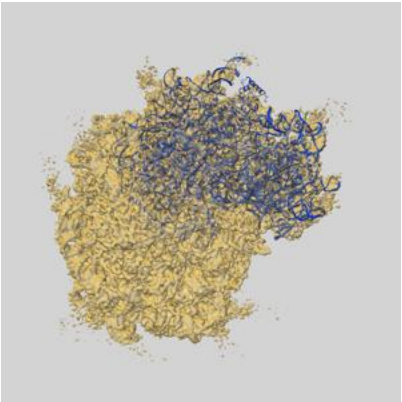
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

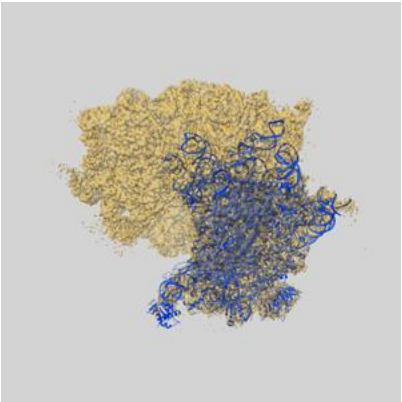
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3221 and PDB model 5FLX. Per-residue inclusion information can be found in section 3 on page 11.

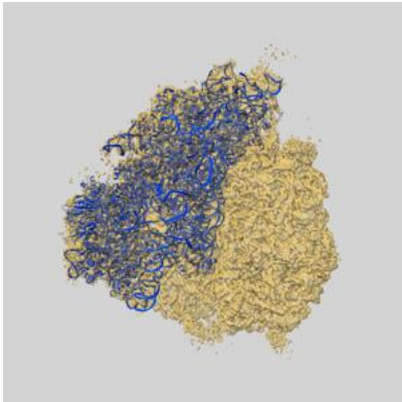
9.1 Map-model overlay (i)



X



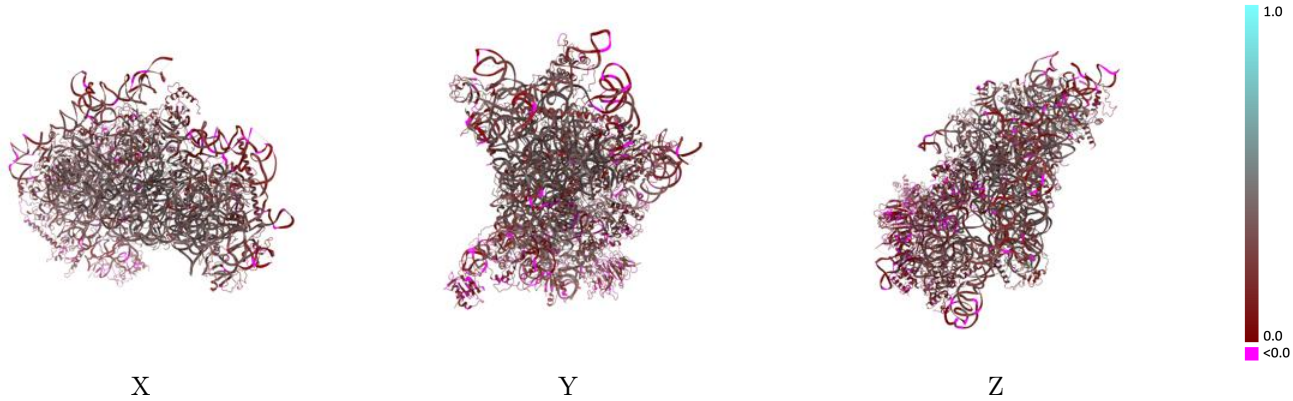
Y



Z

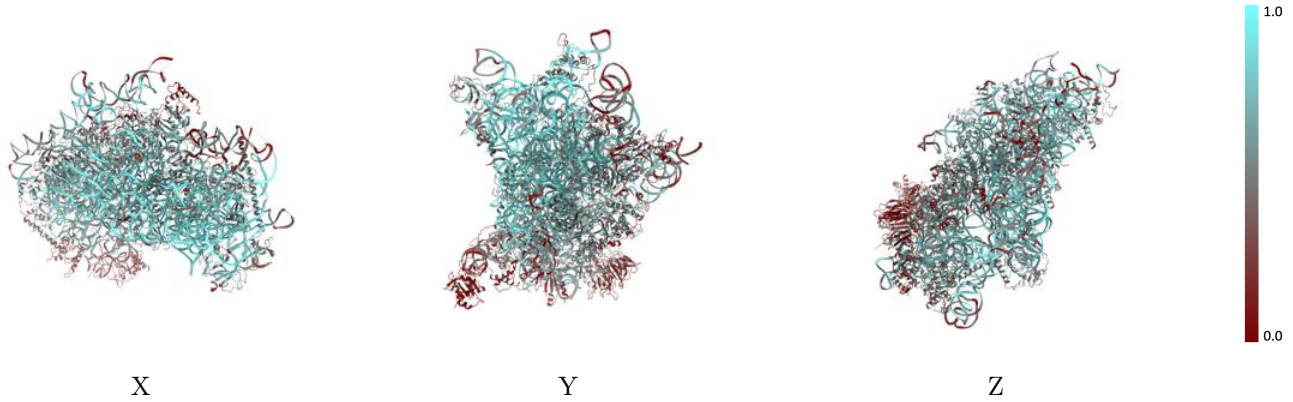
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



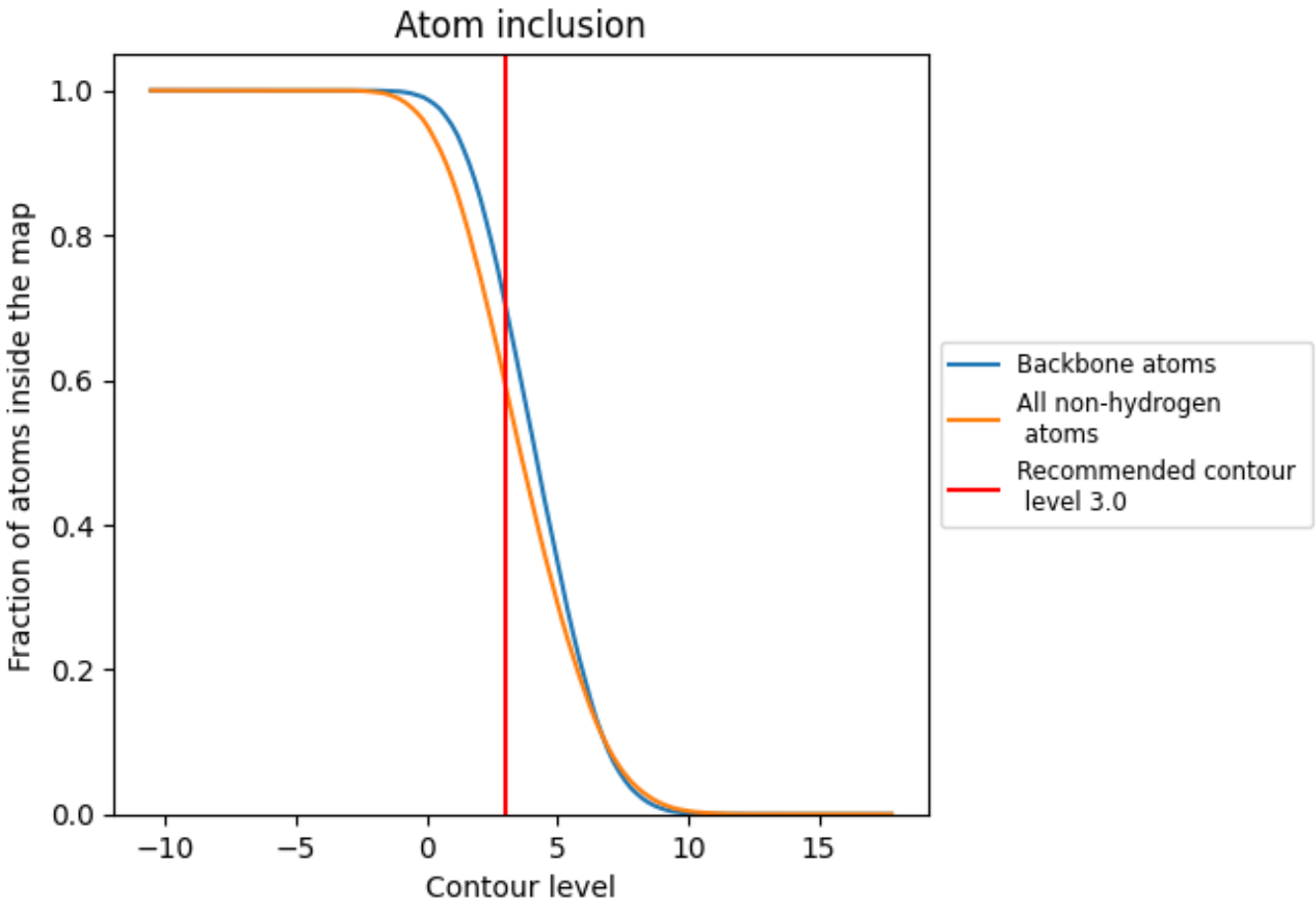
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.0).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5934	0.2610
1	0.7409	0.2940
A	0.5015	0.2580
B	0.5496	0.3100
C	0.5621	0.2970
D	0.3641	0.1720
E	0.6152	0.3160
F	0.5188	0.2720
G	0.5363	0.2410
H	0.3524	0.2290
I	0.5828	0.2920
J	0.5854	0.2750
K	0.2398	0.1520
L	0.5503	0.2980
M	0.0305	0.0950
N	0.5643	0.2890
O	0.5481	0.3110
P	0.1934	0.1100
Q	0.4418	0.1720
R	0.2654	0.1450
S	0.3141	0.1500
T	0.4057	0.1610
U	0.3200	0.1810
V	0.5373	0.2780
W	0.5723	0.3120
X	0.5843	0.3420
Y	0.5543	0.2600
Z	0.4386	0.1860
a	0.5898	0.3130
b	0.5057	0.2880
c	0.5368	0.3330
d	0.4390	0.1510
e	0.4905	0.2560
f	0.0548	0.0510
g	0.2150	0.1310
z	0.5820	0.2210