wwPDB EM Validation Summary Report

Oct 6, 2024 – 09:11 am BST

PDB ID	:	6S12
EMDB ID	:	EMD-10078
Title	:	Erythromycin Resistant Staphylococcus aureus 50S ribosome (delta R88 A89 uL22).
Authors	:	Halfon, Y.; Matozv, D.; Eyal, Z.; Bashan, A.; Zimmerman, E.; Kjeldgaard, J.; Ingmer, H.; Yonath, A.
Deposited on	:	2019-06-18
Resolution	:	3.20 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:

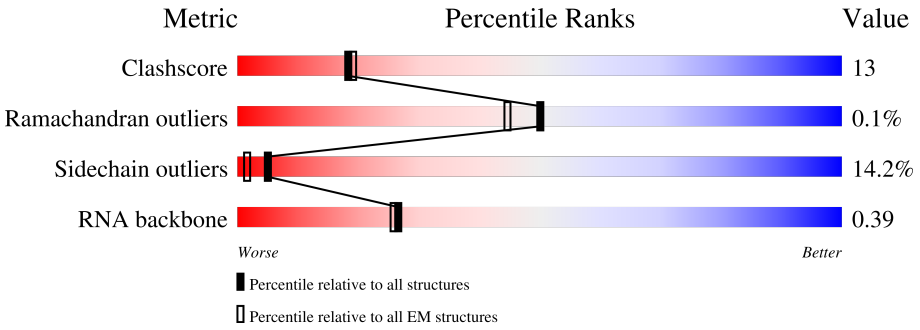
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	2905	7%, 35%, 40%, 21%, .
2	B	115	34%, 40%, 21%, 5%
3	C	274	., 63%, 28%, 9%
4	D	215	67%, 28%, .
5	E	206	57%, 39%, .
6	F	175	19%, 58%, 37%, 6%
7	G	175	68%, 70%, 23%, 6%

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Mol	Chain	Length	Quality of chain
8	H	145	65% 32%
9	I	122	54% 42%
10	J	146	75% 21%
11	K	137	63% 32% 5%
12	L	120	63% 32% 5%
13	M	119	58% 37% 5%
14	N	114	70% 27%
15	O	116	61% 38%
16	P	102	65% 33%
17	Q	110	64% 27% 9%
18	R	89	63% 33%
19	S	103	6% 62% 33% 5%
20	T	94	6% 71% 24%
21	U	82	51% 41% 7%
22	V	58	10% 66% 29% 5%
23	W	67	55% 39% 6%
24	X	58	67% 29%
25	Y	59	83% 83% 15%
26	Z	48	60% 29% 8%
27	1	47	34% 47% 47% 6%
28	2	43	53% 40% 7%
29	3	64	53% 41% 6%
30	4	37	35% 62% 30% 5%

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 146017 atoms, of which 57352 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	A	2905	93573	27803	31296	11387	20182	2905	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	B	115	3685	1094	1240	436	801	114	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	C	274	4291	1301	2201	415	369	5	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	D	215	3294	1018	1667	299	305	5	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	E	206	3192	986	1620	288	296	2	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	175	2667	837	1342	227	255	6	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	175	Total	C	H	N	O	S	0	0
			2488	790	1225	239	231	3		

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	145	Total	C	H	N	O	S	0	0
			2277	714	1134	208	218	3		

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	122	Total	C	H	N	O	S	0	0
			1899	572	981	174	168	4		

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	146	Total	C	H	N	O	S	0	0
			2211	674	1125	214	197	1		

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	137	Total	C	H	N	O	S	0	0
			2194	689	1123	203	175	4		

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	120	Total	C	H	N	O	S	0	0
			1915	576	983	182	173	1		

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	119	Total	C	H	N	O	S	0	0
			1816	557	925	174	159	1		

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	114	Total	C	H	N	O	0	0
			1826	563	937	175	151		

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	116	Total	C	H	N	O	S	0	0
			1956	593	1014	189	156	4		

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	102	Total	C	H	N	O	S	0	0
			1620	503	830	142	144	1		

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	110	Total	C	H	N	O	S	0	0
			1724	523	887	158	153	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	?	-	ARG	deletion	UNP A0A077UKF9
Q	?	-	ALA	deletion	UNP A0A077UKF9

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	89	Total	C	H	N	O	S	0	0
			1463	453	748	127	131	4		

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	103	Total	C	H	N	O	S	0	0
			1579	486	809	142	141	1		

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	94	Total	C	H	N	O	0	0
			1488	463	766	130	129		

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	82	Total	C	H	N	O	0	0
			1265	385	643	122	115		

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	58	Total	C	H	N	O	0	0
			911	277	466	96	72		

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	67	Total	C	H	N	O	0	0
			1104	333	563	102	106		

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	58	Total	C	H	N	O	0	0
			940	280	491	85	84		

- Molecule 25 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Y	59	Total	C	H	N	O	S	0	0
			613	225	243	68	76	1		

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	Z	48	Total	C	H	N	O	S	0	0
			718	222	358	77	59	2		

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	1	47	Total	C	H	N	O	S	0	0
			784	238	394	78	70	4		

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	2	43	Total	C	H	N	O	S	0	0
			782	225	415	89	52	1		

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	3	64	Total	C	H	N	O	S	0	0
			1107	324	586	113	82	2		

- Molecule 30 is a protein called 50S ribosomal protein L36.

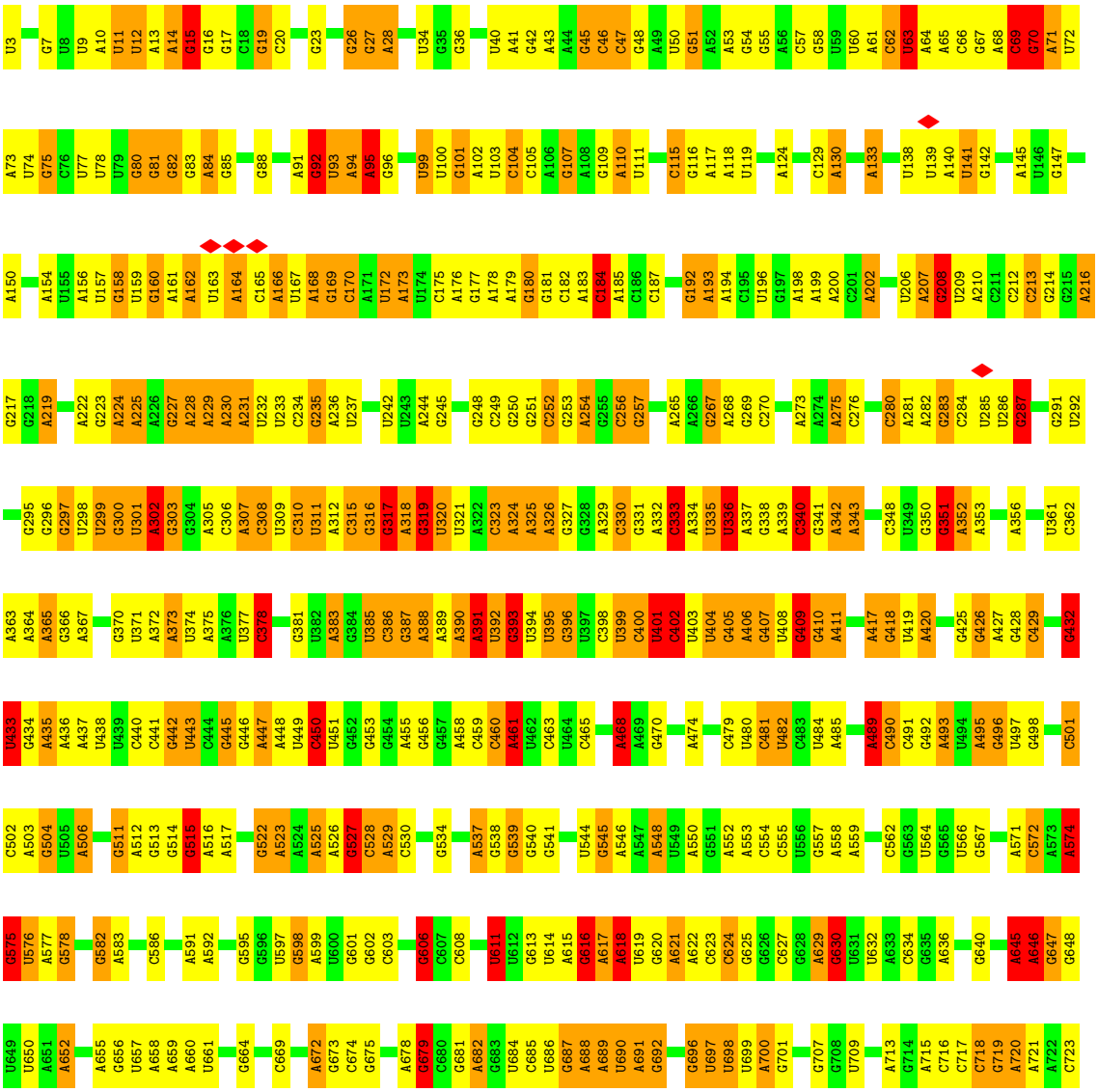
Mol	Chain	Residues	Atoms						AltConf	Trace
30	4	37	Total	C	H	N	O	S	0	0
			635	186	340	60	44	5		

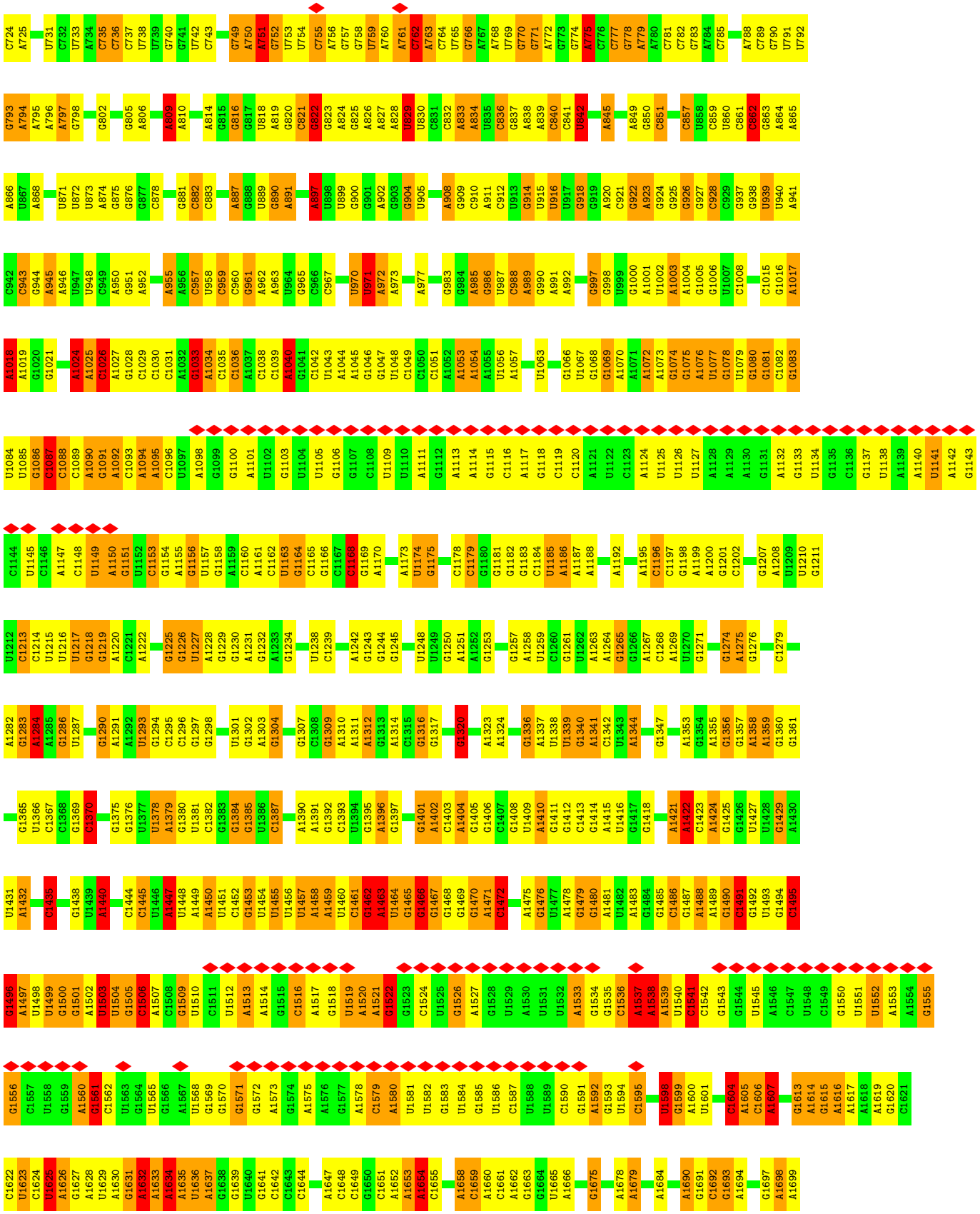
3 Residue-property plots (i)

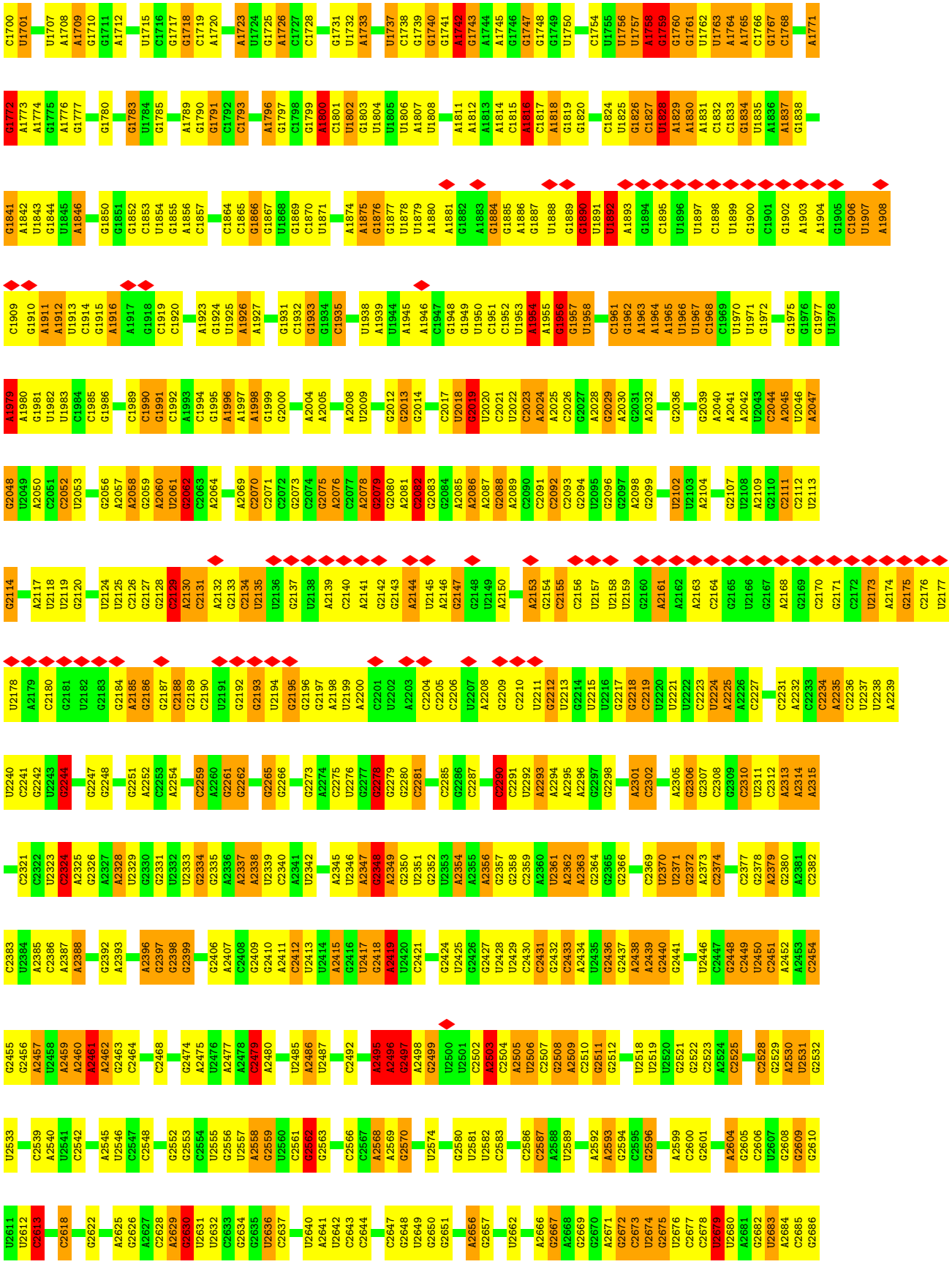
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

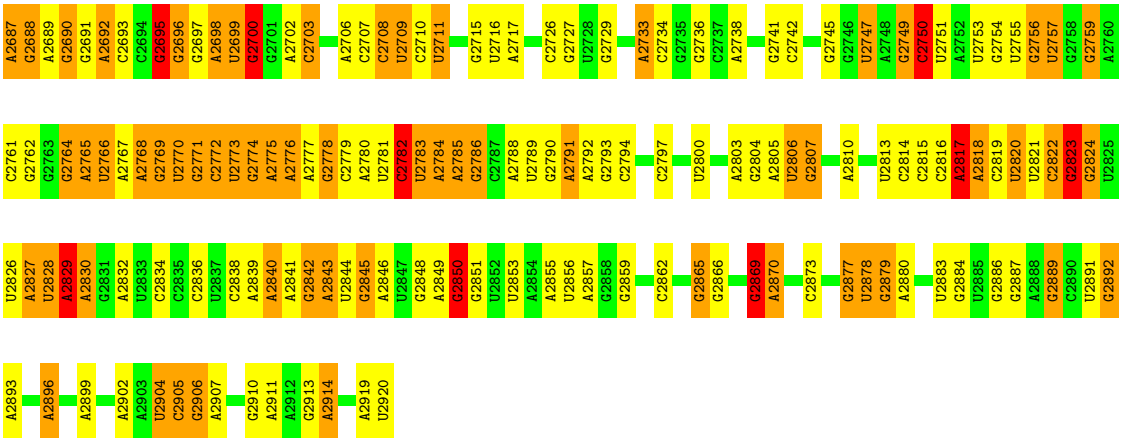
- Molecule 1: 23S ribosomal RNA

Chain A:



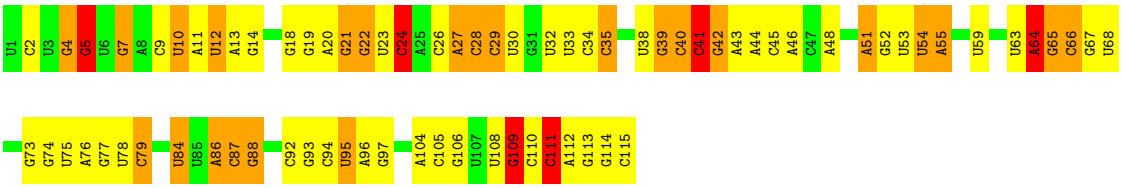






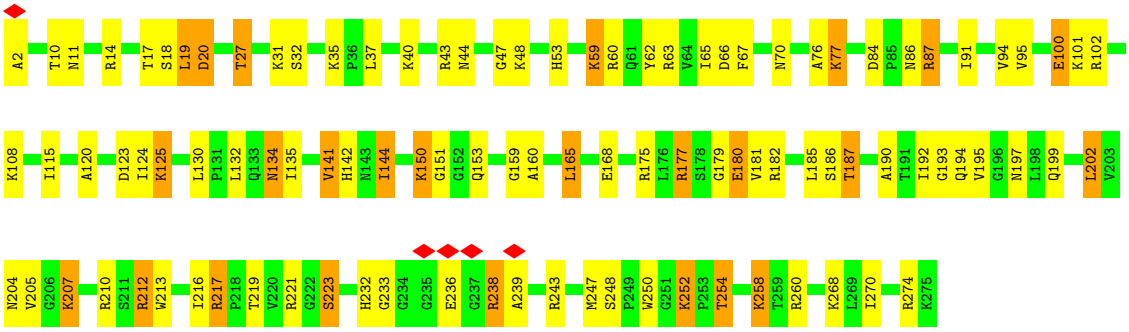
• Molecule 2: 5S ribosomal RNA

Chain B:



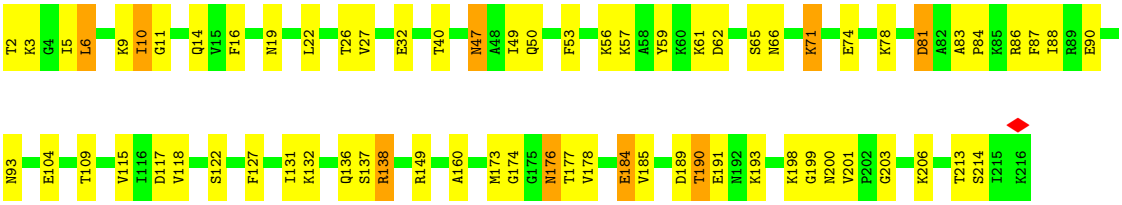
• Molecule 3: 50S ribosomal protein L2

Chain C:



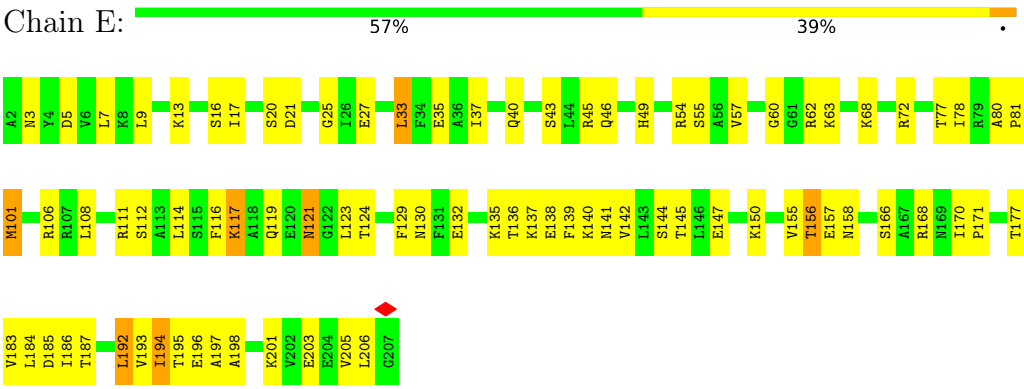
• Molecule 4: 50S ribosomal protein L3

Chain D:



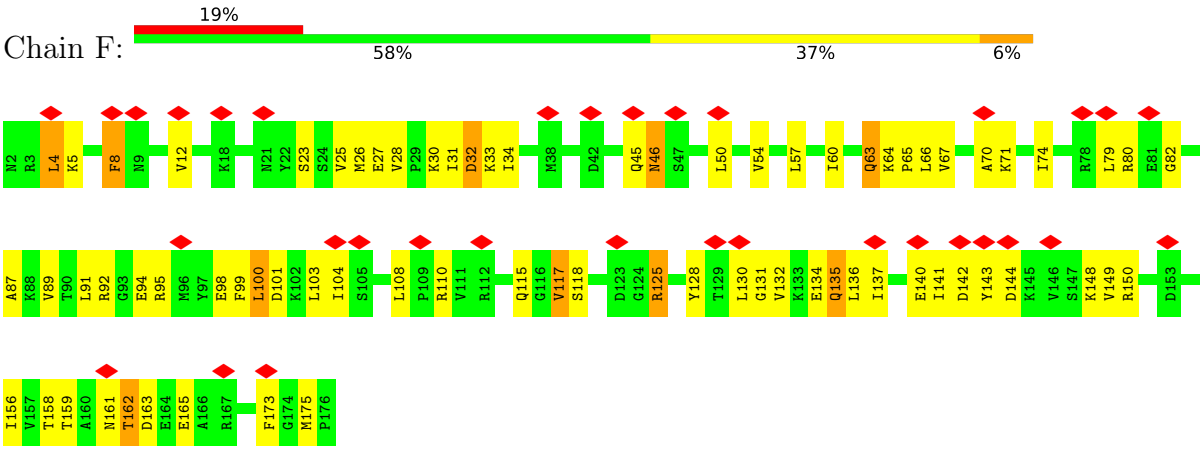
• Molecule 5: 50S ribosomal protein L4

Chain E:



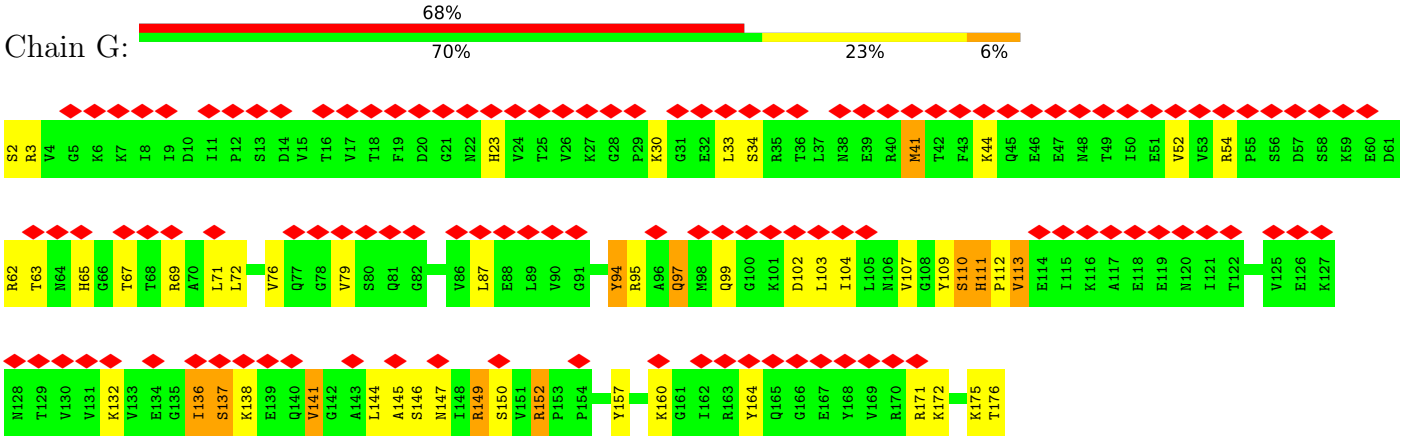
• Molecule 6: 50S ribosomal protein L5

Chain F:



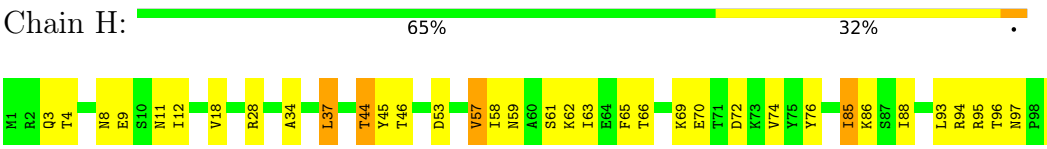
• Molecule 7: 50S ribosomal protein L6

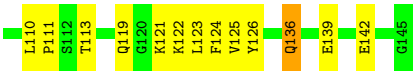
Chain G:



• Molecule 8: 50S ribosomal protein L13

Chain H:



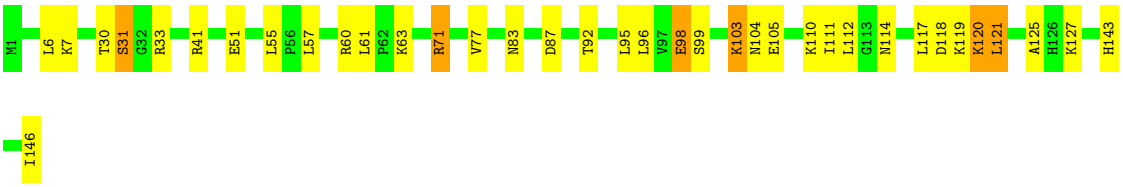


• Molecule 9: 50S ribosomal protein L14

Chain I:

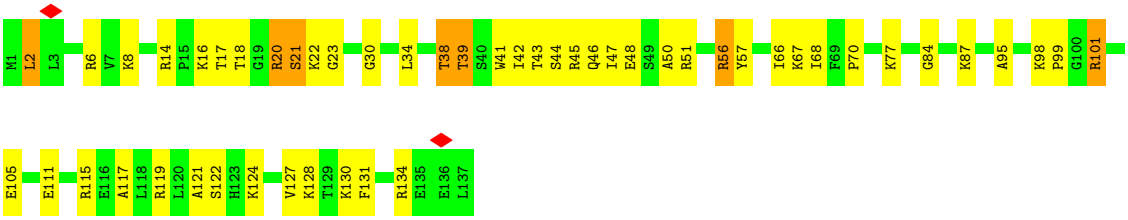
• Molecule 10: 50S ribosomal protein L15

Chain J:



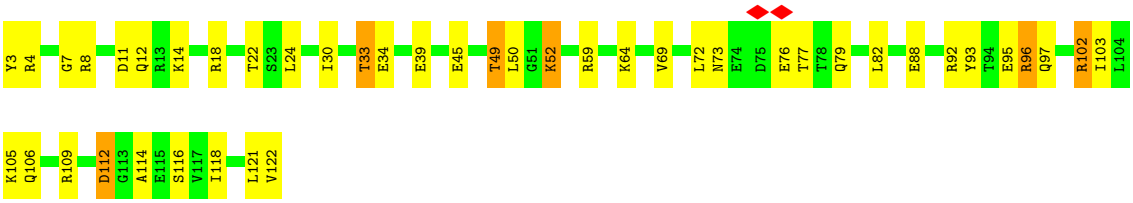
• Molecule 11: 50S ribosomal protein L16

Chain K:



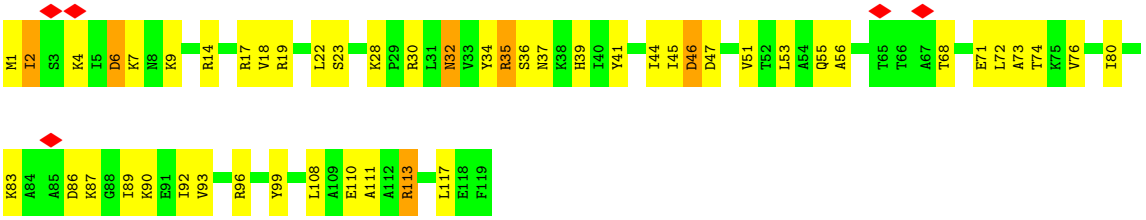
• Molecule 12: 50S ribosomal protein L17

Chain L:



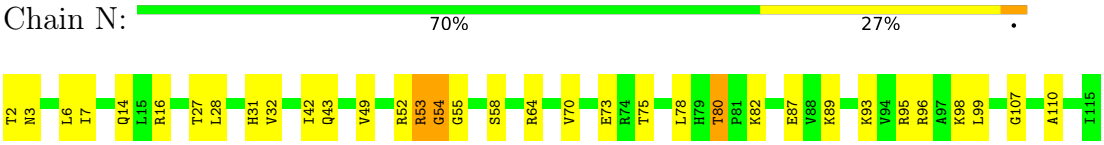
• Molecule 13: 50S ribosomal protein L18

Chain M:



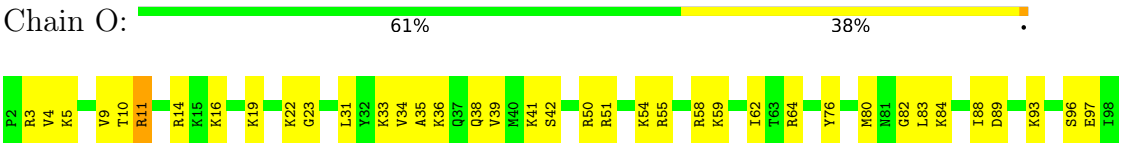
• Molecule 14: 50S ribosomal protein L19

Chain N:



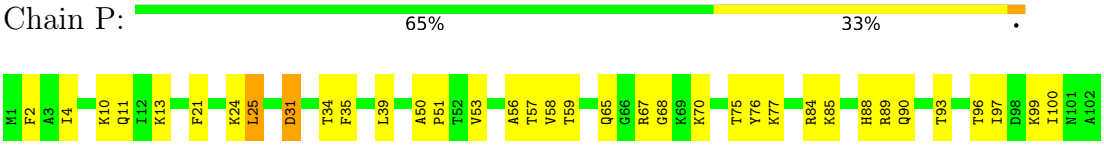
• Molecule 15: 50S ribosomal protein L20

Chain O:



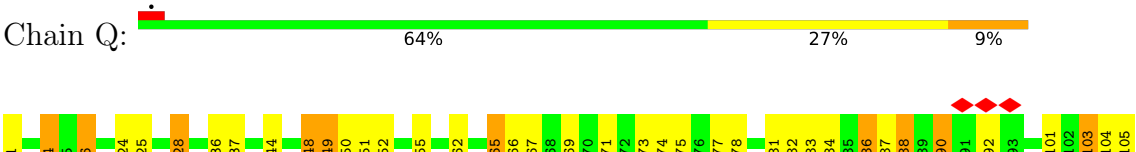
• Molecule 16: 50S ribosomal protein L21

Chain P:



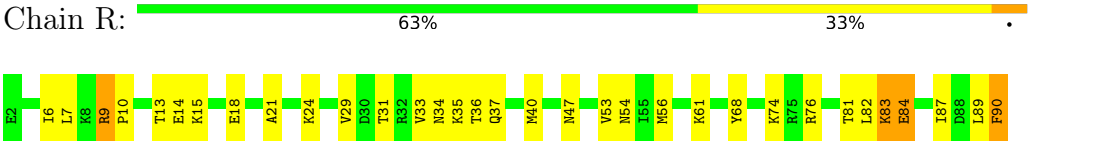
• Molecule 17: 50S ribosomal protein L22

Chain Q:



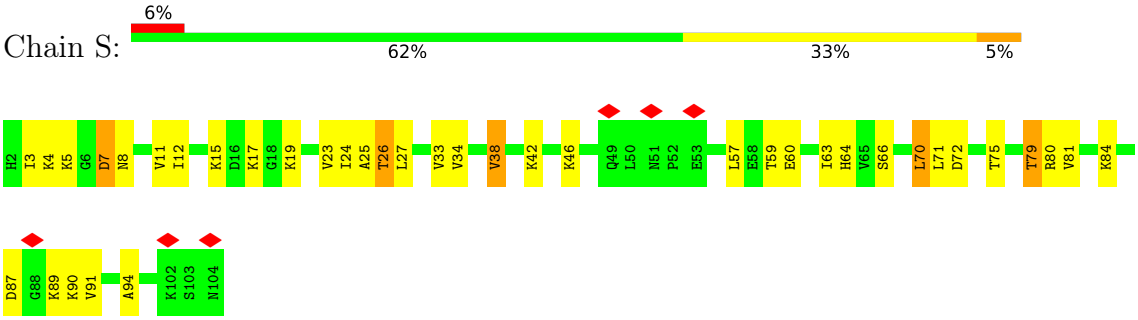
• Molecule 18: 50S ribosomal protein L23

Chain R:



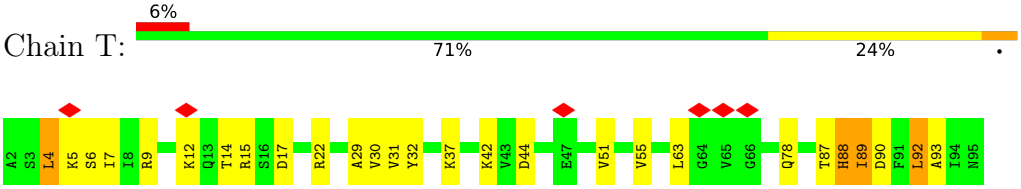
• Molecule 19: 50S ribosomal protein L24

Chain S:



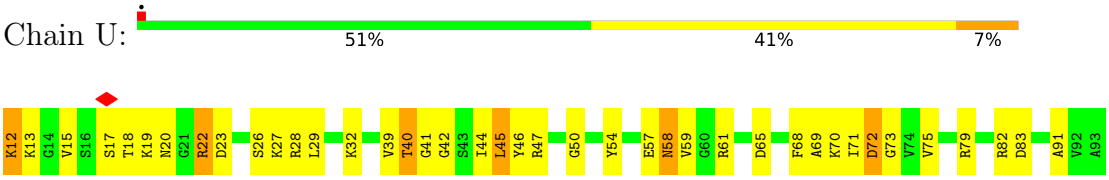
• Molecule 20: 50S ribosomal protein L25

Chain T:



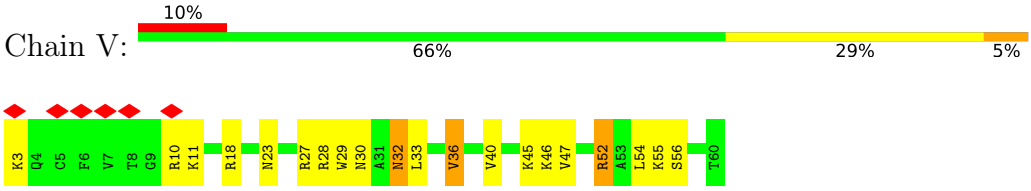
• Molecule 21: 50S ribosomal protein L27

Chain U:



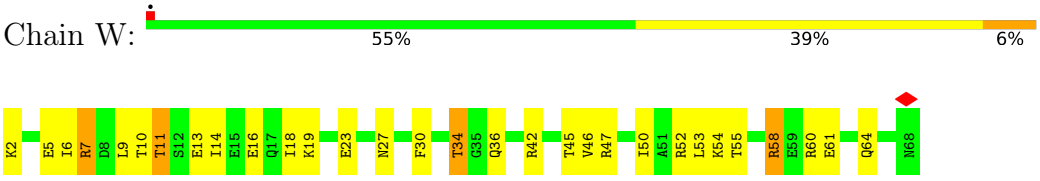
• Molecule 22: 50S ribosomal protein L28

Chain V:



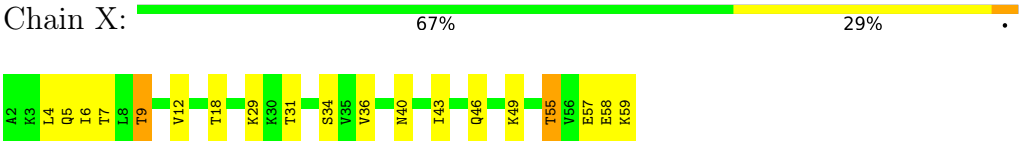
• Molecule 23: 50S ribosomal protein L29

Chain W:



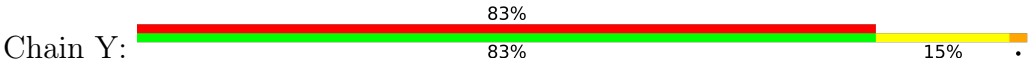
• Molecule 24: 50S ribosomal protein L30

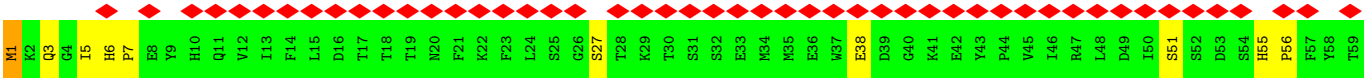
Chain X:



• Molecule 25: 50S ribosomal protein L31 type B

Chain Y:



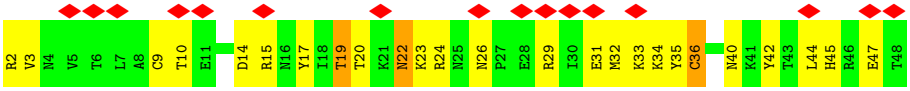


• Molecule 26: 50S ribosomal protein L32

Chain Z:

• Molecule 27: 50S ribosomal protein L33

Chain 1:

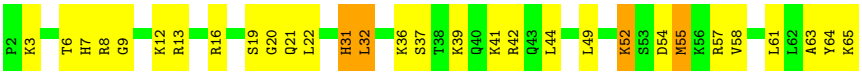


• Molecule 28: 50S ribosomal protein L34

Chain 2:

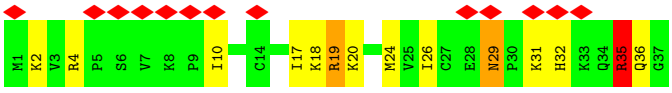
• Molecule 29: 50S ribosomal protein L35

Chain 3:



• Molecule 30: 50S ribosomal protein L36

Chain 4:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	145897	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.076	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	0.288	Depositor
Minimum map value	-0.161	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	426.80002, 426.80002, 426.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	1.75	217/69739 (0.3%)	1.56	1126/108751 (1.0%)
2	B	1.05	1/2733 (0.0%)	1.43	37/4257 (0.9%)
3	C	0.73	0/2125	0.75	1/2853 (0.0%)
4	D	0.87	1/1651 (0.1%)	0.71	1/2215 (0.0%)
5	E	0.79	0/1595	0.73	0/2154
6	F	0.35	0/1339	0.61	0/1805
7	G	0.34	0/1281	0.59	0/1736
8	H	0.82	0/1165	0.75	0/1570
9	I	0.78	0/925	0.79	0/1242
10	J	0.73	0/1100	0.73	0/1467
11	K	0.61	0/1095	0.70	1/1472 (0.1%)
12	L	0.73	0/936	0.79	2/1253 (0.2%)
13	M	0.48	0/900	0.69	0/1205
14	N	0.79	0/901	0.74	0/1209
15	O	0.90	0/954	0.76	0/1264
16	P	0.87	0/800	0.75	0/1070
17	Q	0.75	0/845	0.78	0/1140
18	R	0.72	0/723	0.69	0/966
19	S	0.58	0/779	0.66	0/1043
20	T	0.44	0/730	0.61	0/981
21	U	0.84	0/628	0.80	1/833 (0.1%)
22	V	0.54	0/451	0.74	0/603
23	W	0.50	0/542	0.63	0/722
24	X	0.82	0/451	0.70	0/606
25	Y	0.29	0/378	0.55	0/521
26	Z	0.75	0/366	0.86	3/489 (0.6%)
27	1	0.36	0/395	0.68	0/530
28	2	0.86	0/371	0.81	1/484 (0.2%)
29	3	0.67	0/526	0.81	0/690
30	4	0.48	0/298	0.80	0/392
All	All	1.54	219/96722 (0.2%)	1.41	1173/145523 (0.8%)

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
4	D	0	1
8	H	0	1
16	P	0	2
23	W	0	1
30	4	0	1
All	All	0	6

The worst 5 of 219 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	333	C	N1-C6	137.42	2.19	1.37
1	A	333	C	N3-C4	117.87	2.16	1.33
1	A	333	C	C2-N3	108.34	2.22	1.35
1	A	333	C	C4-C5	94.04	2.18	1.43
1	A	333	C	C5-C6	87.55	2.04	1.34

The worst 5 of 1173 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	393	G	C8-N9-C4	-101.37	65.85	106.40
1	A	393	G	N7-C8-N9	63.97	145.09	113.10
1	A	393	G	N9-C4-C5	53.72	126.89	105.40
1	A	393	G	N3-C4-C5	-41.56	107.82	128.60
1	A	393	G	C2-N3-C4	26.55	125.18	111.90

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	173	MET	Peptide
8	H	11	ASN	Peptide
16	P	50	ALA	Peptide
16	P	77	LYS	Peptide
23	W	34	THR	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62277	31296	31303	1057	0
2	B	2445	1240	1240	65	0
3	C	2090	2201	2201	73	0
4	D	1627	1667	1667	44	0
5	E	1572	1620	1619	57	0
6	F	1325	1342	1342	52	0
7	G	1263	1225	1225	40	0
8	H	1143	1134	1134	30	0
9	I	918	981	981	39	0
10	J	1086	1125	1125	23	0
11	K	1071	1123	1123	34	0
12	L	932	983	983	29	0
13	M	891	925	925	32	0
14	N	889	937	937	18	0
15	O	942	1014	1014	35	0
16	P	790	830	830	16	0
17	Q	837	887	887	24	0
18	R	715	748	748	23	0
19	S	770	809	809	27	0
20	T	722	766	766	19	0
21	U	622	643	643	26	0
22	V	445	466	466	15	0
23	W	541	563	563	21	0
24	X	449	491	491	9	0
25	Y	370	243	243	12	0
26	Z	360	358	358	21	0
27	1	390	394	394	26	0
28	2	367	415	415	16	0
29	3	521	586	586	23	0
30	4	295	340	340	18	0
All	All	88665	57352	57358	1616	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 1616 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:C:C5	1:A:333:C:C6	2.04	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2432:G:N2	1:A:2439:A:N7	1.69	1.35
1:A:333:C:C5	1:A:333:C:C4	2.18	1.31
1:A:1675:G:N3	1:A:1679:A:N6	1.87	1.22
1:A:1663:G:HO2'	28:2:2:VAL:N	1.39	1.18

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	272/274 (99%)	218 (80%)	54 (20%)	0	100	100
4	D	213/215 (99%)	179 (84%)	34 (16%)	0	100	100
5	E	204/206 (99%)	176 (86%)	28 (14%)	0	100	100
6	F	173/175 (99%)	142 (82%)	31 (18%)	0	100	100
7	G	173/175 (99%)	155 (90%)	18 (10%)	0	100	100
8	H	143/145 (99%)	126 (88%)	17 (12%)	0	100	100
9	I	120/122 (98%)	102 (85%)	18 (15%)	0	100	100
10	J	144/146 (99%)	123 (85%)	21 (15%)	0	100	100
11	K	135/137 (98%)	117 (87%)	18 (13%)	0	100	100
12	L	118/120 (98%)	105 (89%)	13 (11%)	0	100	100
13	M	117/119 (98%)	100 (86%)	17 (14%)	0	100	100
14	N	112/114 (98%)	97 (87%)	14 (12%)	1 (1%)	14	49
15	O	114/116 (98%)	107 (94%)	7 (6%)	0	100	100
16	P	100/102 (98%)	89 (89%)	10 (10%)	1 (1%)	13	47
17	Q	108/110 (98%)	94 (87%)	13 (12%)	1 (1%)	14	49
18	R	87/89 (98%)	72 (83%)	15 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	101/103 (98%)	83 (82%)	18 (18%)	0	100	100
20	T	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
21	U	80/82 (98%)	68 (85%)	12 (15%)	0	100	100
22	V	56/58 (97%)	48 (86%)	8 (14%)	0	100	100
23	W	65/67 (97%)	57 (88%)	8 (12%)	0	100	100
24	X	56/58 (97%)	49 (88%)	7 (12%)	0	100	100
25	Y	57/59 (97%)	48 (84%)	9 (16%)	0	100	100
26	Z	46/48 (96%)	33 (72%)	13 (28%)	0	100	100
27	1	45/47 (96%)	41 (91%)	4 (9%)	0	100	100
28	2	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
29	3	62/64 (97%)	52 (84%)	10 (16%)	0	100	100
30	4	35/37 (95%)	25 (71%)	10 (29%)	0	100	100
All	All	3069/3125 (98%)	2632 (86%)	434 (14%)	3 (0%)	50	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	Q	87	PRO
16	P	51	PRO
14	N	54	GLY

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	
3	C	220/221 (100%)	181 (82%)	39 (18%)	1	8
4	D	173/173 (100%)	152 (88%)	21 (12%)	4	19
5	E	168/168 (100%)	145 (86%)	23 (14%)	3	14
6	F	141/154 (92%)	122 (86%)	19 (14%)	3	15
7	G	124/153 (81%)	105 (85%)	19 (15%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	H	122/123 (99%)	105 (86%)	17 (14%)	3 14
9	I	100/100 (100%)	87 (87%)	13 (13%)	3 16
10	J	109/112 (97%)	94 (86%)	15 (14%)	3 14
11	K	108/114 (95%)	100 (93%)	8 (7%)	11 40
12	L	96/101 (95%)	86 (90%)	10 (10%)	5 25
13	M	86/95 (90%)	71 (83%)	15 (17%)	1 8
14	N	93/100 (93%)	82 (88%)	11 (12%)	4 20
15	O	96/96 (100%)	89 (93%)	7 (7%)	11 41
16	P	84/86 (98%)	72 (86%)	12 (14%)	2 13
17	Q	88/90 (98%)	68 (77%)	20 (23%)	0 3
18	R	78/80 (98%)	68 (87%)	10 (13%)	3 17
19	S	81/88 (92%)	67 (83%)	14 (17%)	1 8
20	T	78/82 (95%)	69 (88%)	9 (12%)	4 21
21	U	63/64 (98%)	47 (75%)	16 (25%)	0 2
22	V	44/49 (90%)	35 (80%)	9 (20%)	1 5
23	W	58/60 (97%)	48 (83%)	10 (17%)	1 8
24	X	52/52 (100%)	46 (88%)	6 (12%)	4 21
25	Y	23/56 (41%)	22 (96%)	1 (4%)	25 57
26	Z	35/44 (80%)	28 (80%)	7 (20%)	1 5
27	1	44/45 (98%)	38 (86%)	6 (14%)	3 15
28	2	39/39 (100%)	33 (85%)	6 (15%)	2 11
29	3	55/55 (100%)	48 (87%)	7 (13%)	3 17
30	4	35/35 (100%)	32 (91%)	3 (9%)	8 33
All	All	2493/2635 (95%)	2140 (86%)	353 (14%)	5 13

5 of 353 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Q	24	ILE
21	U	29	LEU
17	Q	65	ASN
19	S	8	ASN
22	V	29	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	106	GLN
15	O	72	HIS
13	M	55	GLN
17	Q	65	ASN
4	D	176	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2896/2905 (99%)	1040 (35%)	36 (1%)
2	B	114/115 (99%)	38 (33%)	0
All	All	3010/3020 (99%)	1078 (35%)	36 (1%)

5 of 1078 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	12	U
1	A	14	A
1	A	15	G
1	A	28	A
1	A	34	U

5 of 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2261	G
1	A	2878	U
1	A	2428	U
1	A	2462	A
1	A	688	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	A	8

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2207:U	O3'	2208:A	P	11.16
1	A	1939:A	O3'	1944:U	P	10.86
1	A	929:C	O3'	937:G	P	10.36
1	A	1096:C	O3'	1097:U	P	7.19
1	A	1153:C	O3'	1154:G	P	7.11

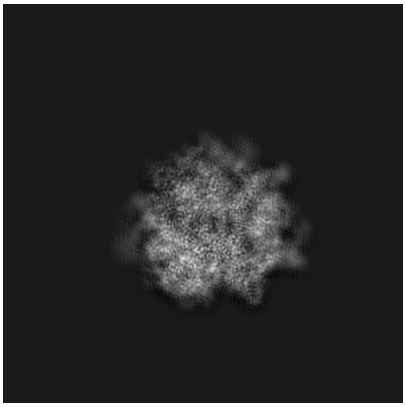
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10078. These allow visual inspection of the internal detail of the map and identification of artifacts.

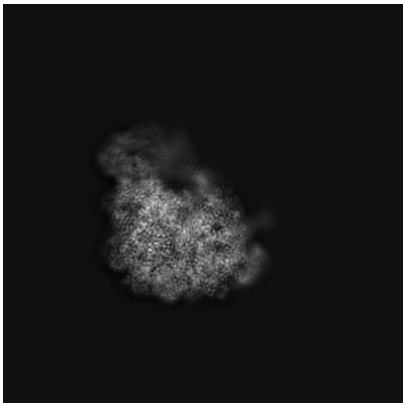
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

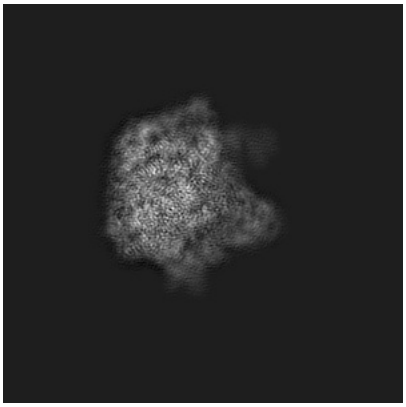
6.1.1 Primary map



X



Y

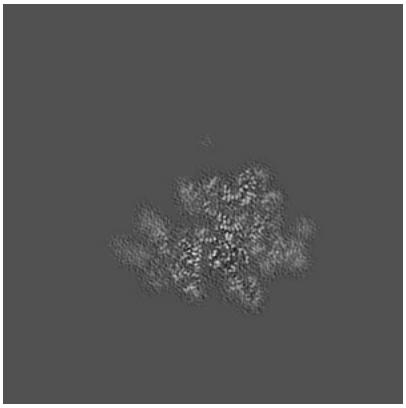


Z

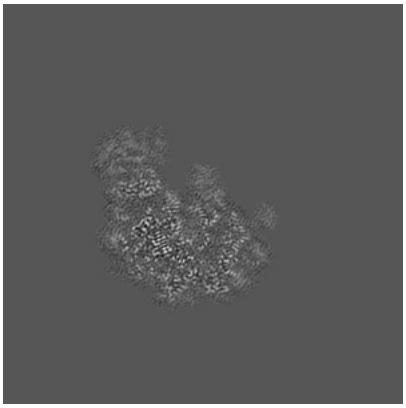
The images above show the map projected in three orthogonal directions.

6.2 Central slices

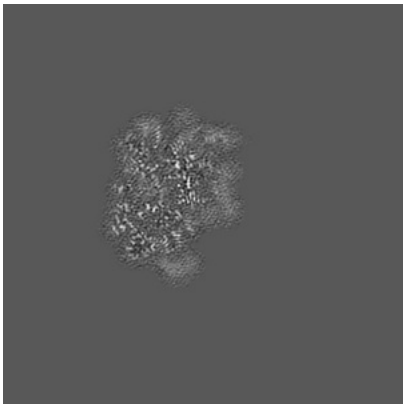
6.2.1 Primary map



X Index: 200



Y Index: 200

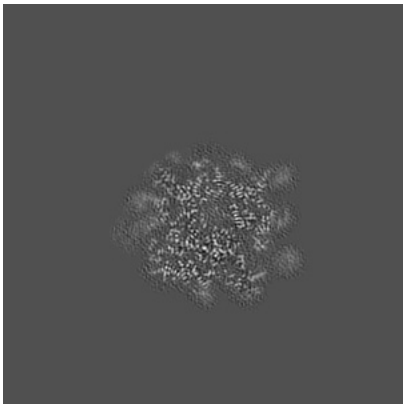


Z Index: 200

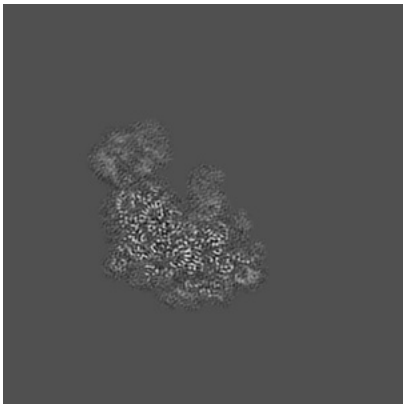
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

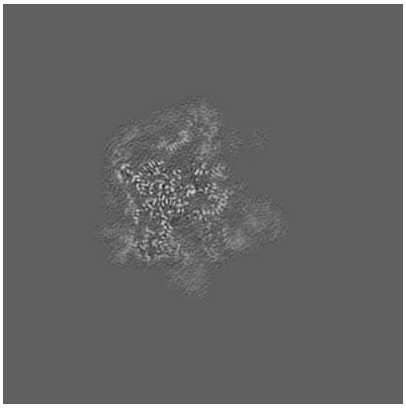
6.3.1 Primary map



X Index: 164



Y Index: 185

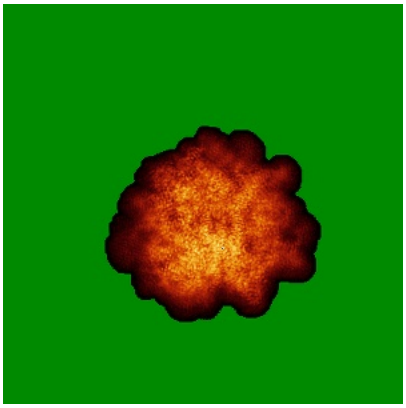


Z Index: 154

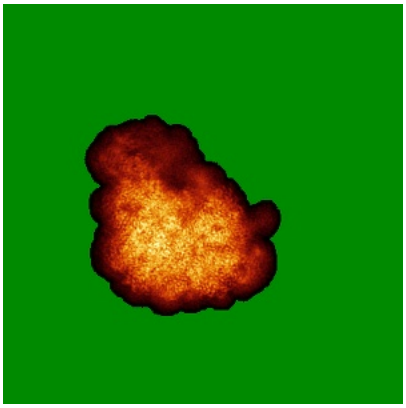
The images above show the largest variance slices of the map in three orthogonal directions.

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

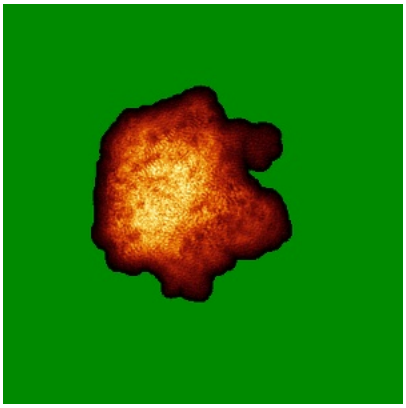
6.4.1 Primary map



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 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

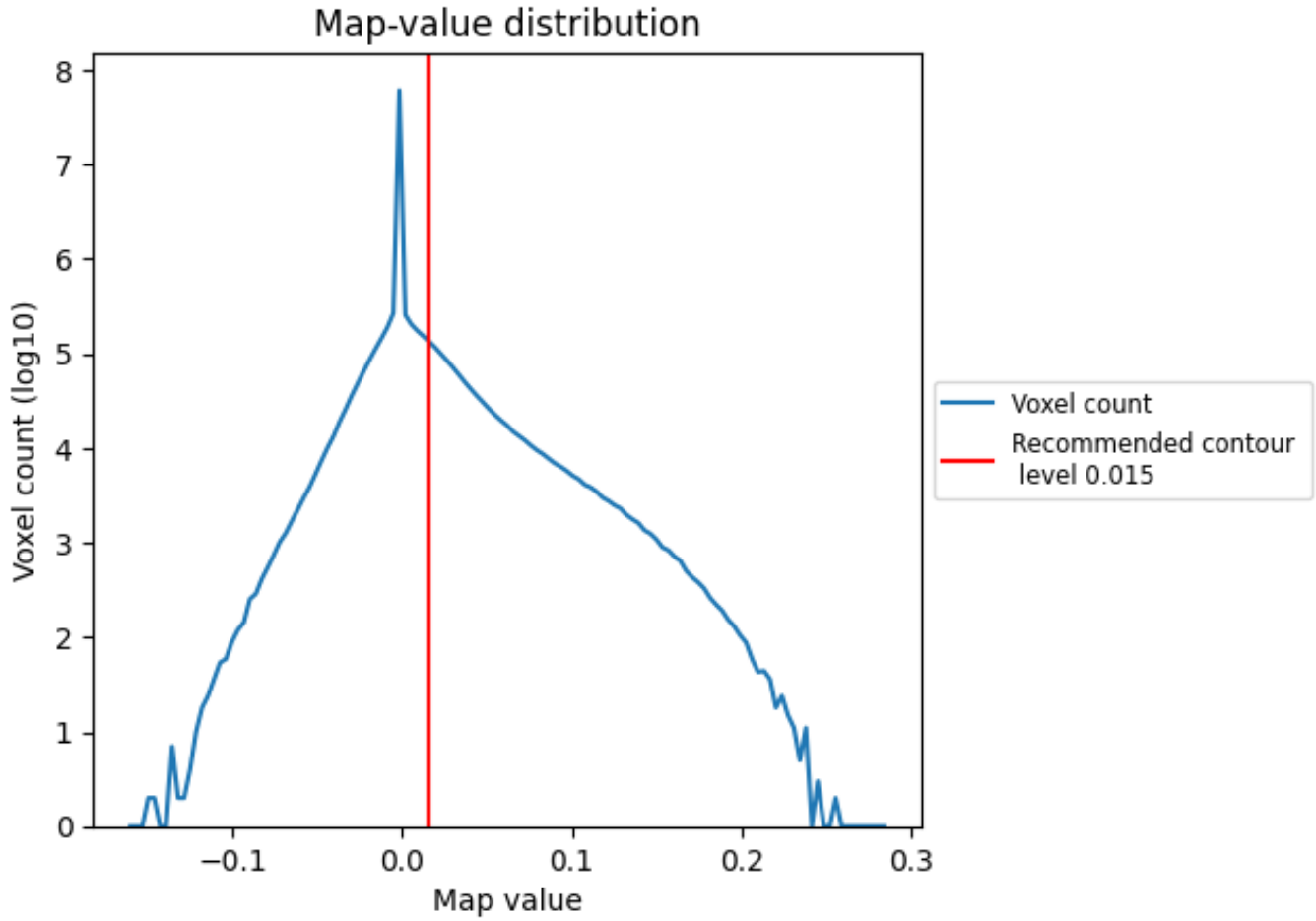
6.6 Mask visualisation (i)

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

7 Map analysis

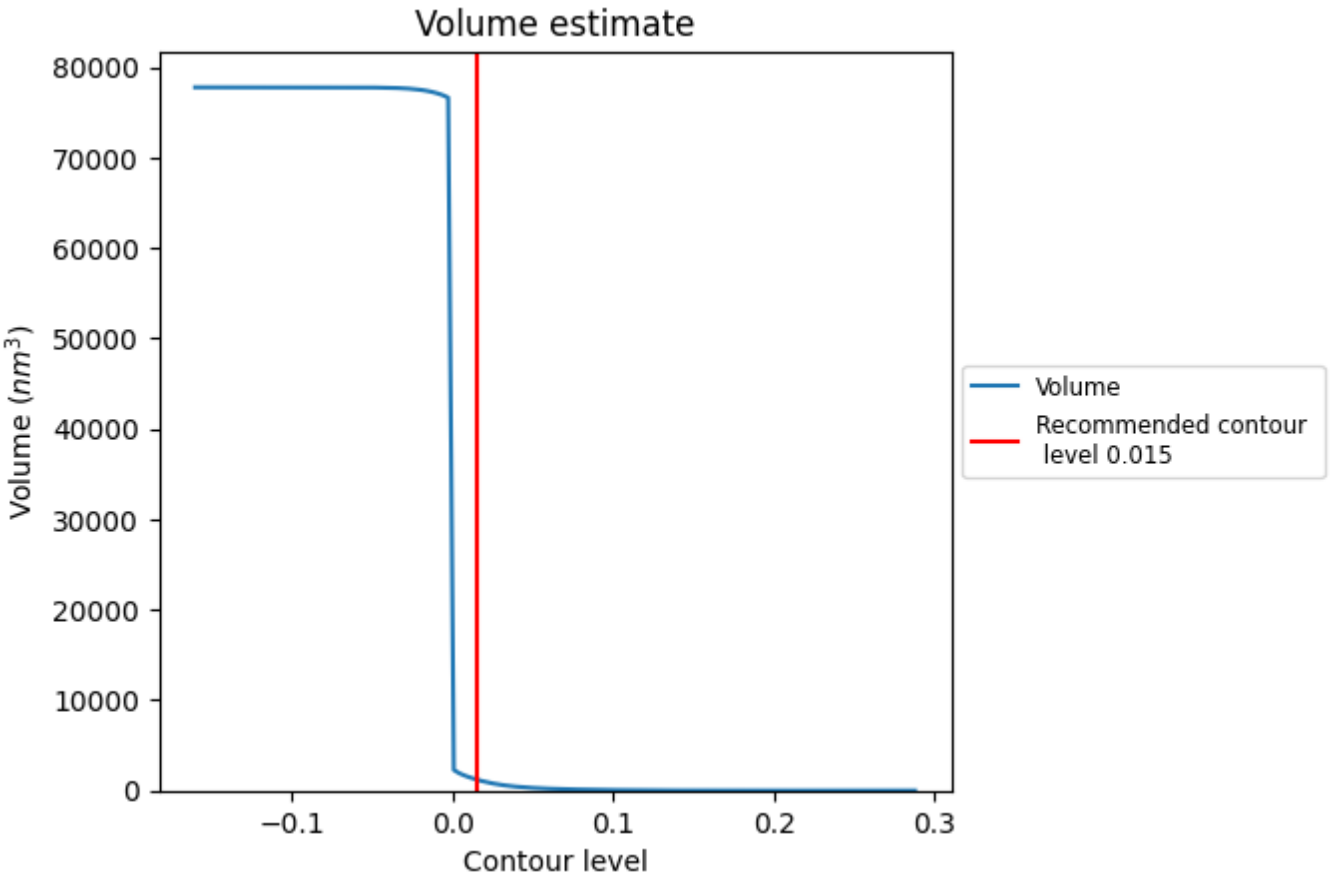
This section contains the results of statistical analysis of the map.

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.

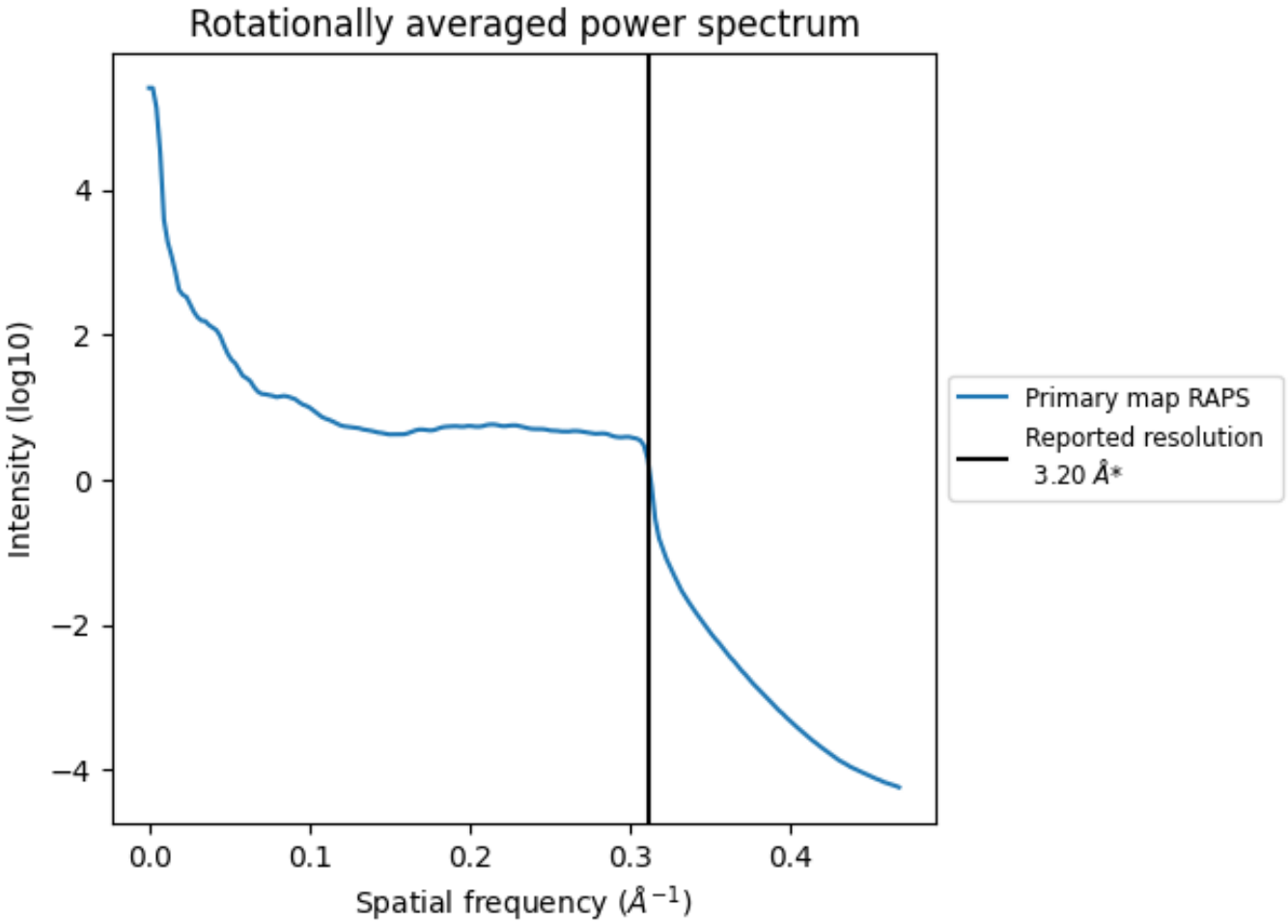
7.2 Volume estimate (i)



The volume at the recommended contour level is 1203 nm^3; this corresponds to an approximate mass of 1087 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 0.312 Å^{-1}

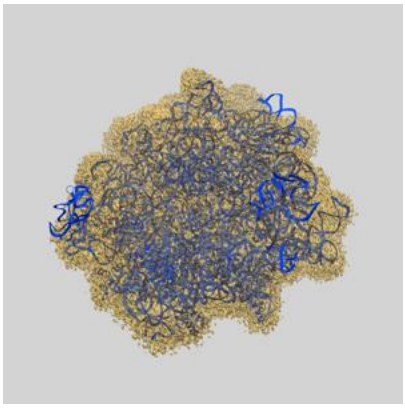
8 Fourier-Shell correlation (i)

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

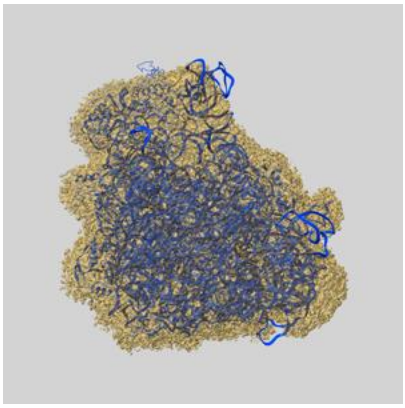
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10078 and PDB model 6S12. Per-residue inclusion information can be found in section 3 on page 9.

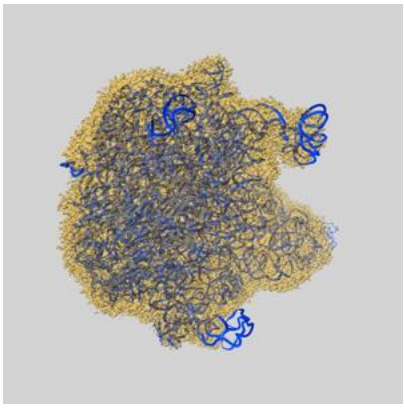
9.1 Map-model overlay



X



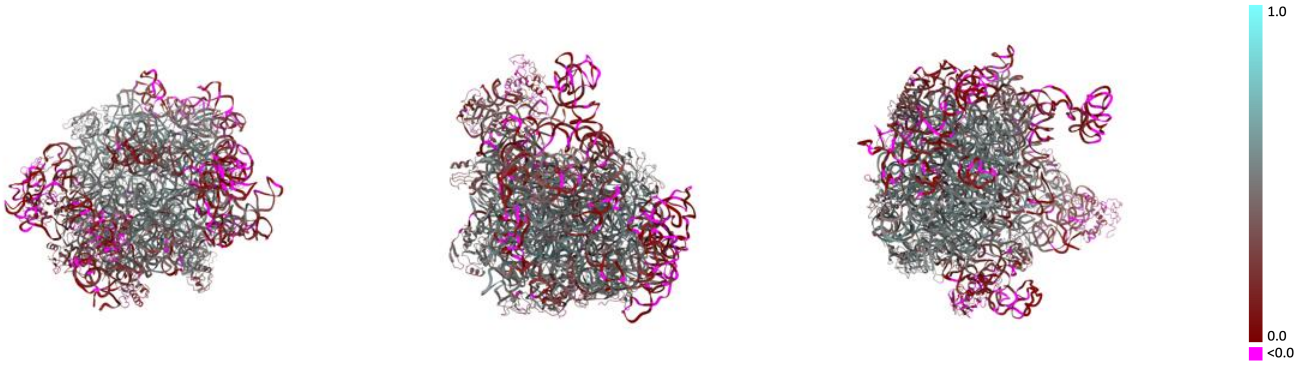
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

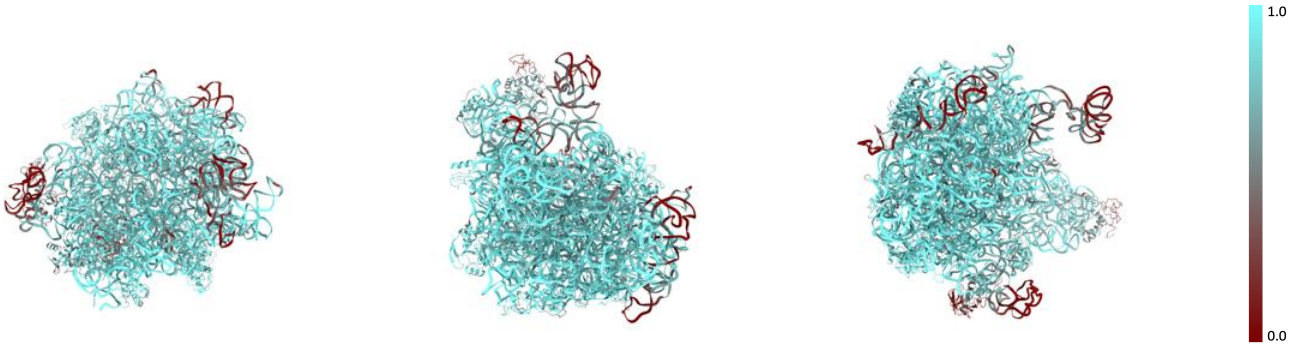
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

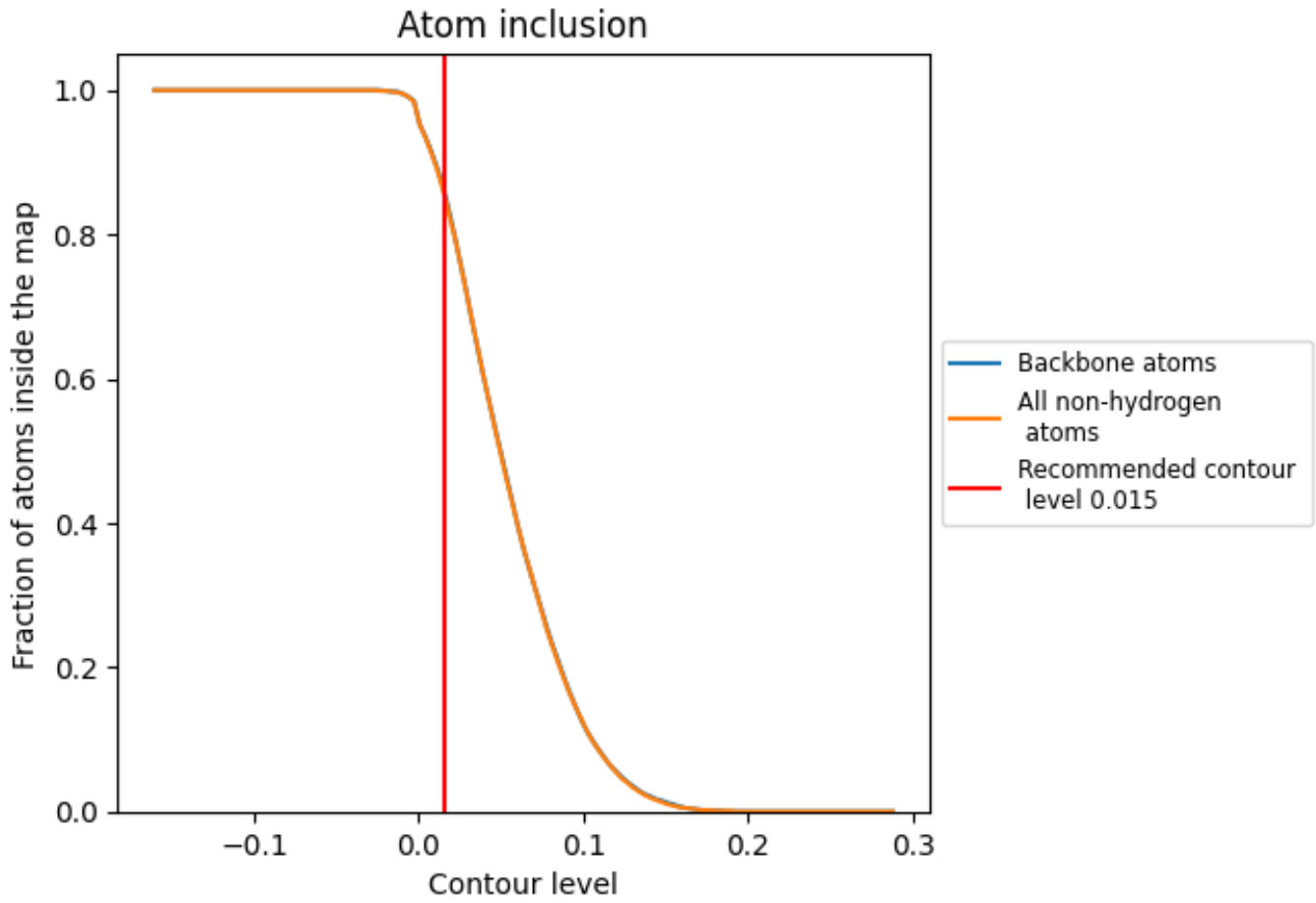
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8590	0.3640
1	0.5010	0.1650
2	0.9020	0.4630
3	0.8980	0.4510
4	0.5050	0.0530
A	0.8760	0.3690
B	0.9060	0.2130
C	0.8870	0.4390
D	0.9270	0.4850
E	0.9040	0.4640
F	0.6080	0.0970
G	0.3130	0.0670
H	0.9140	0.4760
I	0.8750	0.4380
J	0.9000	0.4190
K	0.8670	0.3600
L	0.8990	0.4580
M	0.8390	0.2650
N	0.9220	0.4640
O	0.9090	0.4850
P	0.9140	0.4630
Q	0.8700	0.4230
R	0.8860	0.3960
S	0.8390	0.3390
T	0.7120	0.2510
U	0.8890	0.4270
V	0.7740	0.3170
W	0.8440	0.2920
X	0.9090	0.4770
Y	0.2120	0.0390
Z	0.8470	0.3190