wwPDB EM Validation Summary Report (i)

Dec 11, 2022 – 01:05 pm GMT

PDB ID	:	6SPD
EMDB ID	:	EMD-10282
Title	:	Pseudomonas aeruginosa 50s ribosome from a clinical isolate
Authors	:	Halfon, Y.; Jimenez-Fernande, A.; La Ros, R.; Espinos, R.; Krogh Johansen, H.; Matzov, D.; Eyal, Z.; Bashan, A.; Zimmerman, E.; Belousoff, M.; Molin, S.; Yonath, A.
Deposited on	:	2019-09-01
Resolution	:	3.28 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:

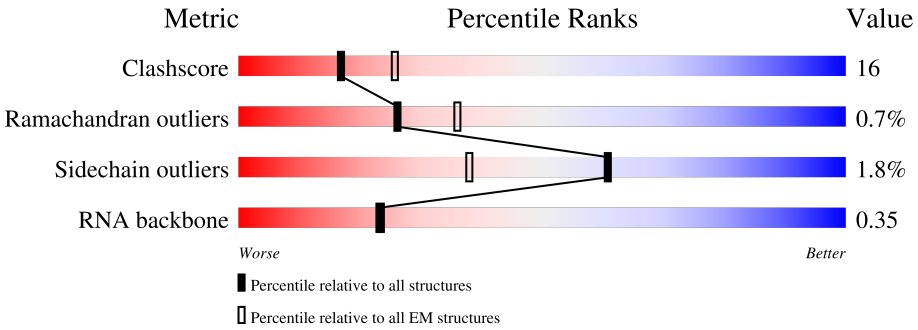
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.28 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	2888	6% 48% 34% 16%
2	B	116	64% 27% 9%
3	C	271	50% 85% 15%
4	D	207	86% 11%
5	E	199	57% 86% 11%
6	F	175	14% 79% 18%
7	G	173	6% 83% 16%

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Mol	Chain	Length	Quality of chain
8	H	147	99% 84% 15%
9	I	140	93% 81% 19%
10	J	141	92% 8%
11	K	120	7% 82% 18%
12	L	143	38% 91% 8%
13	M	135	93% 7%
14	N	118	92% 7%
15	O	115	10% 94% 6%
16	P	113	5% 86% 12%
17	Q	117	17% 89% 11%
18	R	103	26% 79% 19%
19	S	109	15% 94% 5%
20	T	92	45% 90% 9%
21	U	103	53% 88% 12%
22	V	188	8% 77% 20%
23	W	76	5% 82% 14%
24	X	77	66% 81% 19%
25	Y	60	42% 87% 10%
26	Z	57	14% 84% 16%
27	1	31	10% 87% 13%
28	2	53	8% 92% 8%
29	3	50	32% 76% 24%
30	4	44	48% 77% 23%
31	5	63	29% 83% 16%
32	6	38	89% 11%

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 90352 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2851	61164	27299	11236	19786	2843	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	361	A	G	conflict	REF 470469287

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	116	2469	1104	442	808	115	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	271	2067	1273	425	363	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	207	1557	964	297	291	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	199	1516	951	282	281	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	175	Total	C	N	O	S	0	0
			1402	896	248	254	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	7	LEU	ILE	conflict	UNP A0A072ZMU2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	173	Total	C	N	O	S	0	0
			1308	823	240	243	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	147	Total	C	N	O	0	0
			1086	681	193	212		

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	140	Total	C	N	O	S	0	0
			1026	642	183	198	3		

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	141	Total	C	N	O	S	0	0
			1122	713	205	201	3		

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	120	Total	C	N	O	S	0	0
			922	576	178	162	6		

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	143	Total	C	N	O	S	0	0
			1058	649	214	193	2		

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	135	Total	C	N	O	S	0	0
			1069	679	209	178	3		

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	118	Total	C	N	O	S	0	0
			945	590	190	160	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	115	Total	C	N	O	S	0	0
			881	544	174	161	2		

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	113	Total	C	N	O	S	0	0
			894	564	169	160	1		

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	117	Total	C	N	O	0	0
			936	592	196	148		

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	103	Total	C	N	O	S	0	0
			822	521	156	143	2		

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	109	Total	C	N	O	S	0	0
			825	510	160	152	3		

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	T	92	Total	C	N	O	0	0
			701	449	124	128		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	103	Total	C	N	O	S	0	0
			801	503	152	144	2		

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	188	Total	C	N	O	S	0	0
			1405	893	255	255	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	6	VAL	LEU	conflict	UNP A0A072ZBM5
V	71	VAL	ALA	conflict	UNP A0A072ZBM5

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	W	76	Total	C	N	O	0	0
			574	365	110	99		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	40	LEU	GLN	conflict	UNP A0A071LFT4

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	77	Total 630	C 391	N 134	O 103	S 2	0	0

- Molecule 25 is a protein called Ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	60	Total 476	C 290	N 96	O 89	S 1	0	0

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	57	Total 445	C 277	N 87	O 79	S 2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1	31	Total 232	C 144	N 40	O 45	S 3	0	0

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	2	53	Total 423	C 254	N 90	O 78	S 1	0	0

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	3	50	Total 418	C 267	N 77	O 74	0	0

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	44	Total 365	C 222	N 87	O 54	S 2	0	0

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	5	63	Total	C	N	O	S	0	0
			506	314	108	81	3		

- Molecule 32 is a protein called 50S ribosomal protein L36.

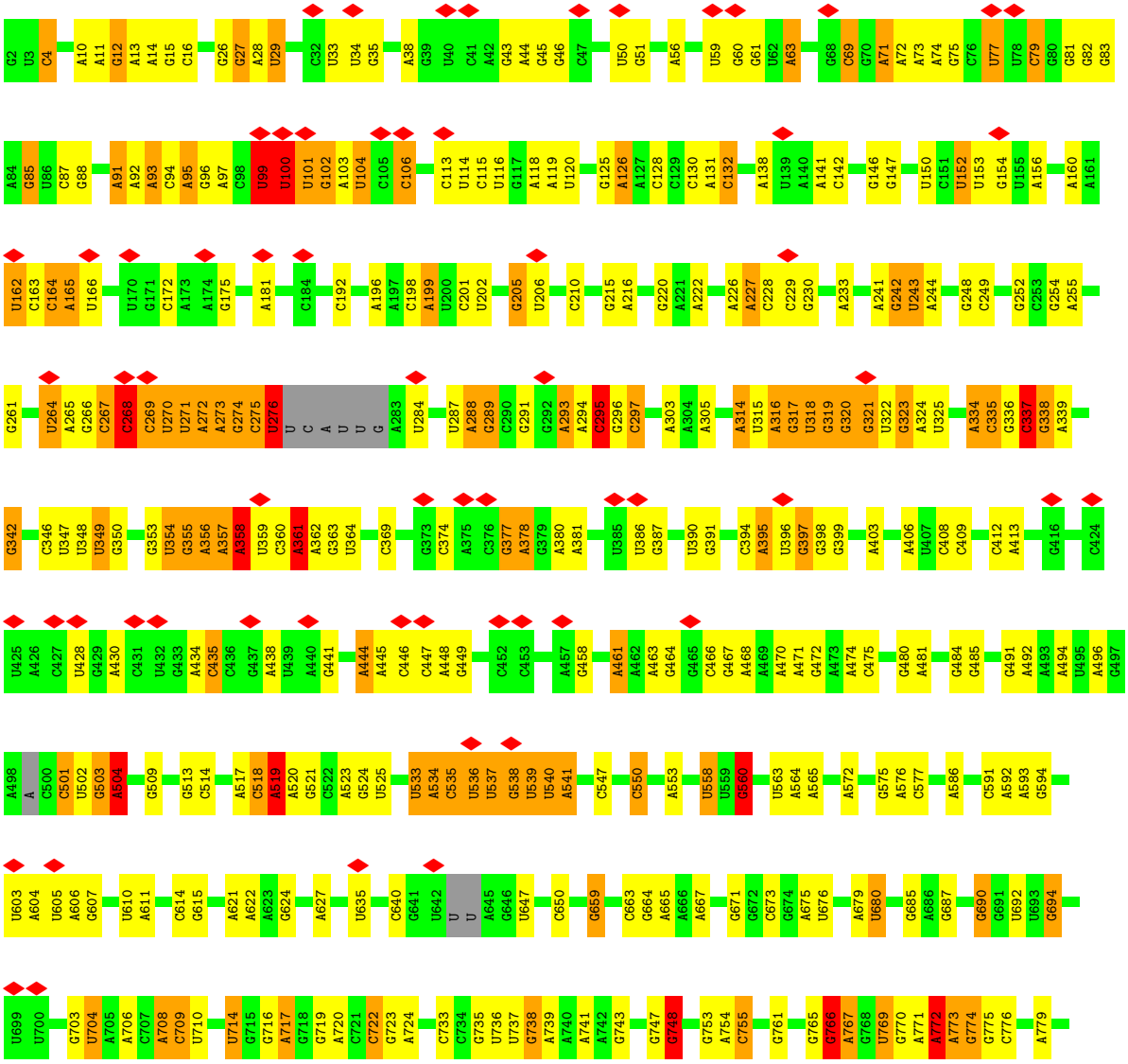
Mol	Chain	Residues	Atoms					AltConf	Trace
32	6	38	Total	C	N	O	S	0	0
			307	186	69	48	4		

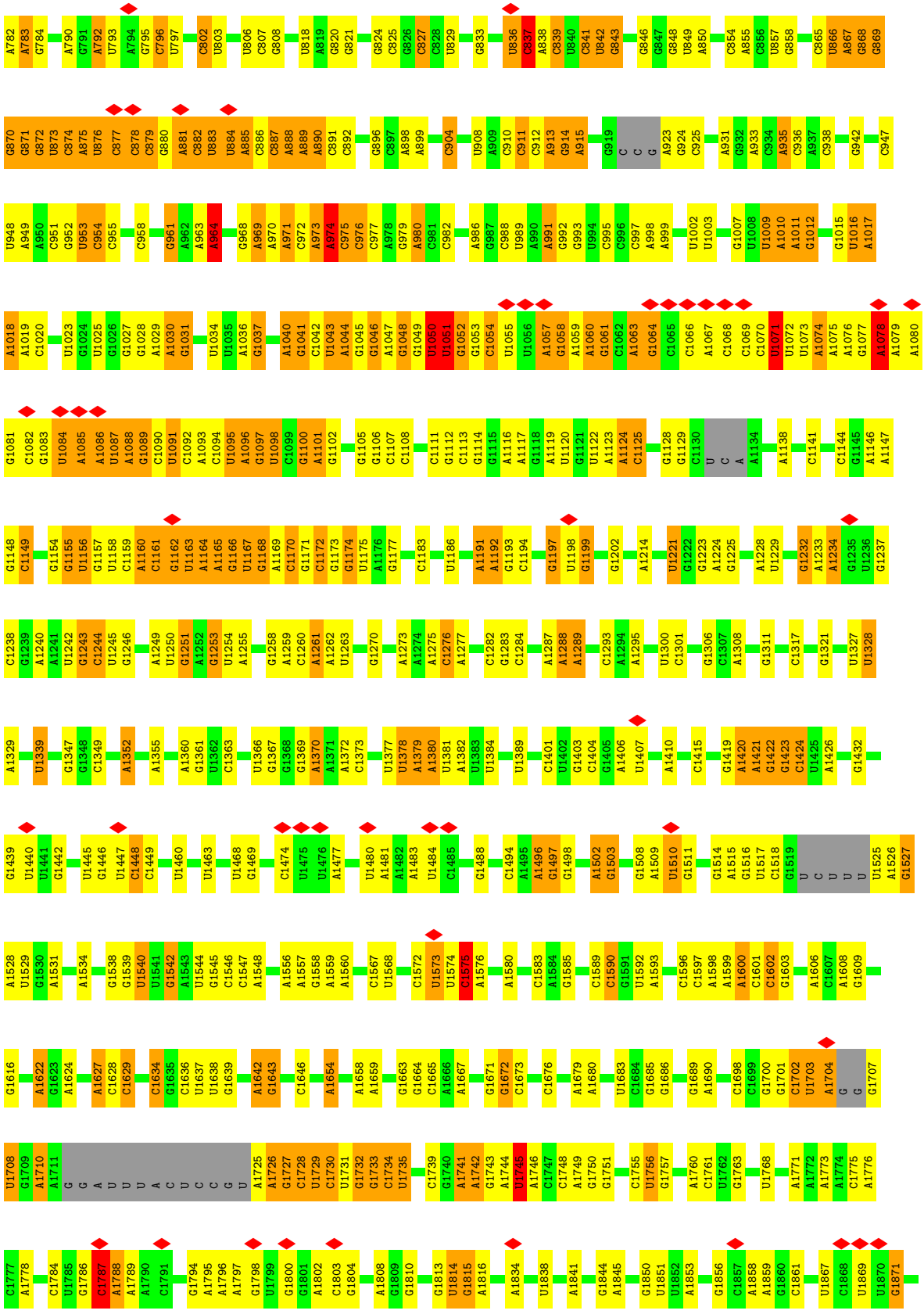
3 Residue-property plots (i)

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:

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G833
U836 C837 A838 C839 U840 C841 U842 G843
G846 G847 G848 U849 A850
C854 A855 C856 U857 G858
C865 U866 A867 G868 G869
G870 G871 G872 U873 C874 A875 U876 C877 C878 C879 G880
A881 C882 U883 U884 A885 C886 C887 A888 A889 A890 C891 C892
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G919 C C G
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G942 C947
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C958
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G1015 U1016 A1017
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U1071 U1072 U1073 A1074 A1075 A1076 G1077 A1078 A1079 A1080
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U1084 A1085 A1086 U1087 A1088 G1089 C1090 U1091
C1092 A1093 C1094
U1095 A1096 G1097 U1098 G1099 G1100 A1101 G1102
G1105 G1106 C1107 C1108
C1111 G1112 C1113 G1114 G1115 A1116 A1117 G1118 A1119 U1120 G1121 U1122 A1123 A1124 C1125
G1128 G1129 C1130 U C A A1134
A1138
C1141
C1144 G1145 A1146 A1147
G1148 C1149
G1154 G1155 U1156 G1157 U1158 C1159 A1160 C1161 G1162 U1163 A1164 A1165 G1166 U1167 G1168 A1169 C1170 G1171 C1172 G1173 G1174 U1175 A1176 G1177
C1183
U1186
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G1197 U1198 G1199
G1202
A1214
U1221 G1222 G1223 A1224 G1225
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A1355
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G1671 G1672 C1673
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G1689 A1690
C1698 C1699 G1700 G1701 C1702 U1703 A1704 G G G1707
U1708 G1709 A1710 A1711 G A U U U A C U C C G U
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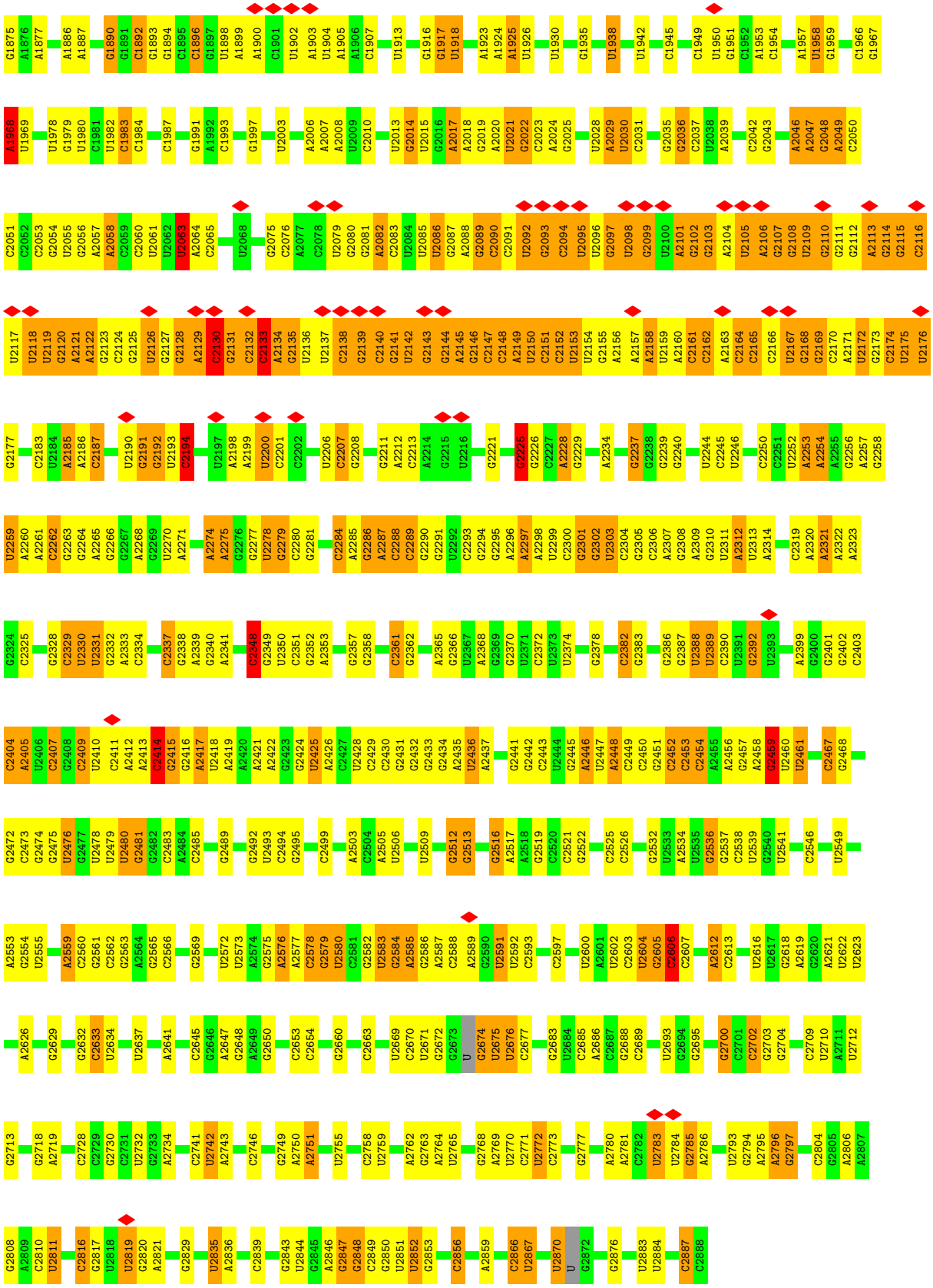
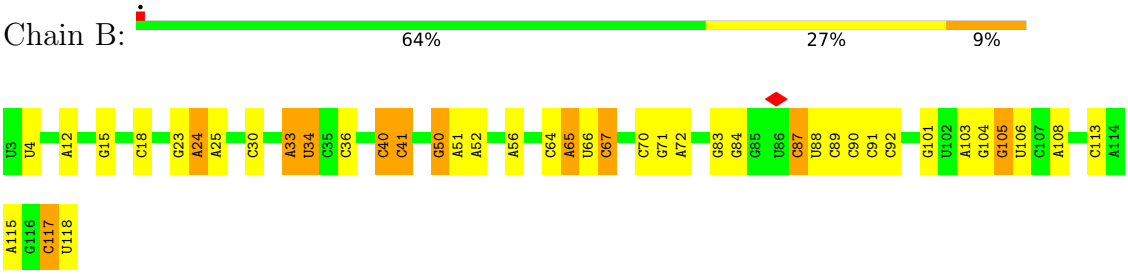


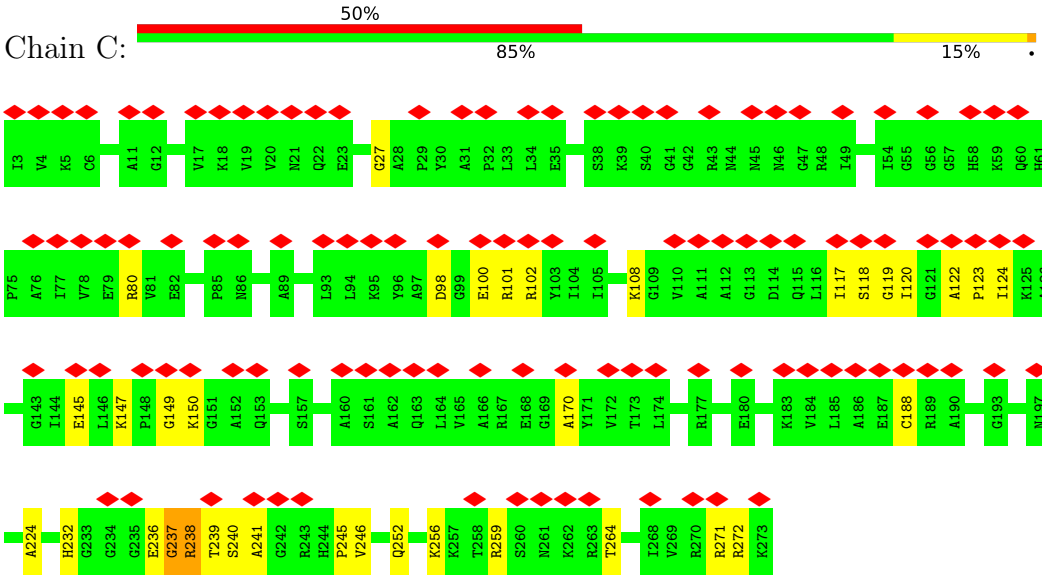
• Molecule 2: 5S ribosomal RNA

Chain B:



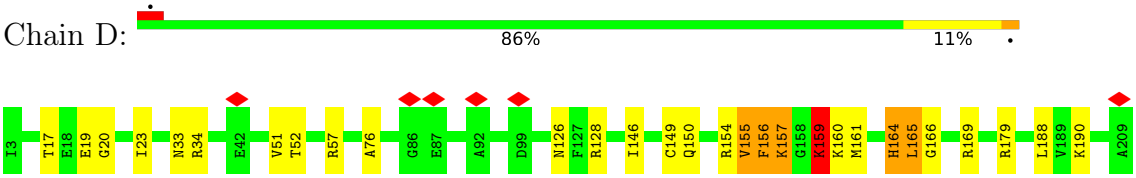
• Molecule 3: 50S ribosomal protein L2

Chain C:



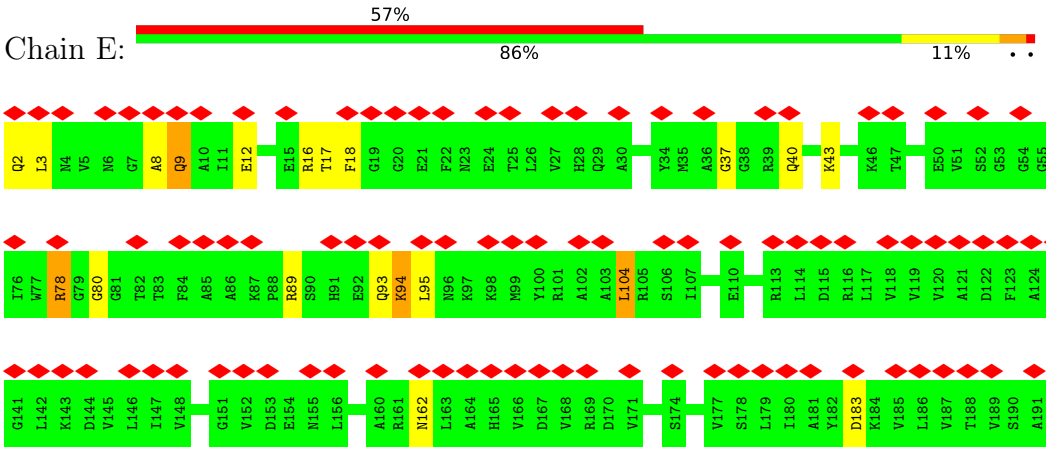
• Molecule 4: 50S ribosomal protein L3

Chain D:



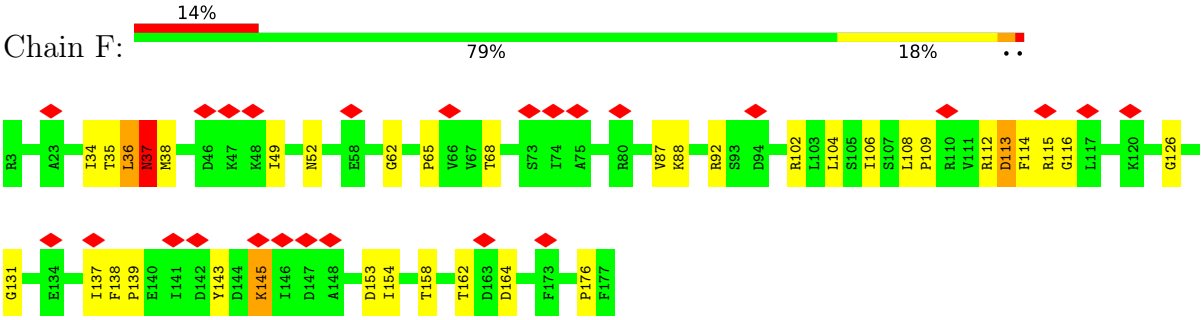
• Molecule 5: 50S ribosomal protein L4

Chain E:



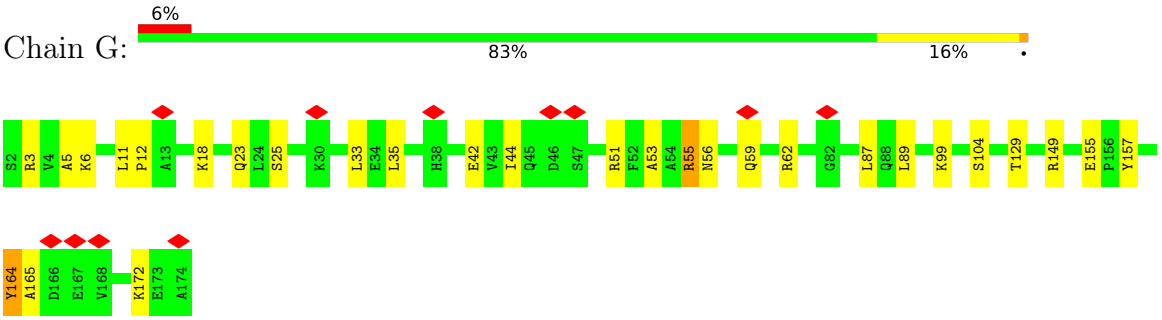
• Molecule 6: 50S ribosomal protein L5

Chain F:



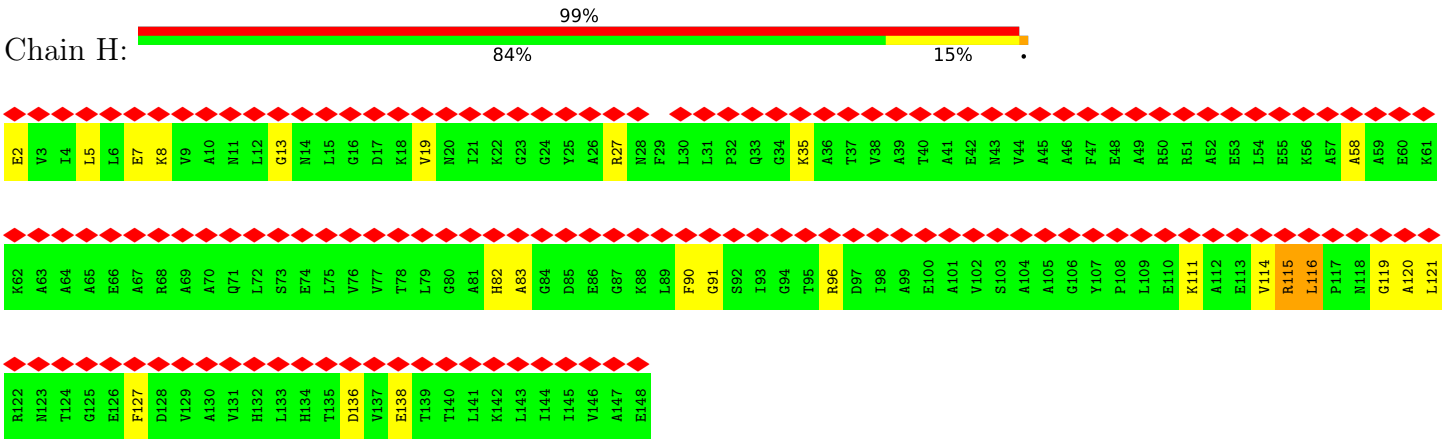
• Molecule 7: 50S ribosomal protein L6

Chain G:



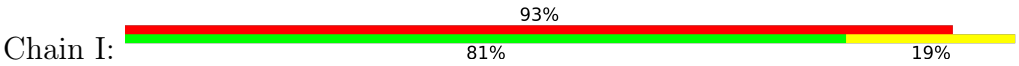
• Molecule 8: 50S ribosomal protein L9

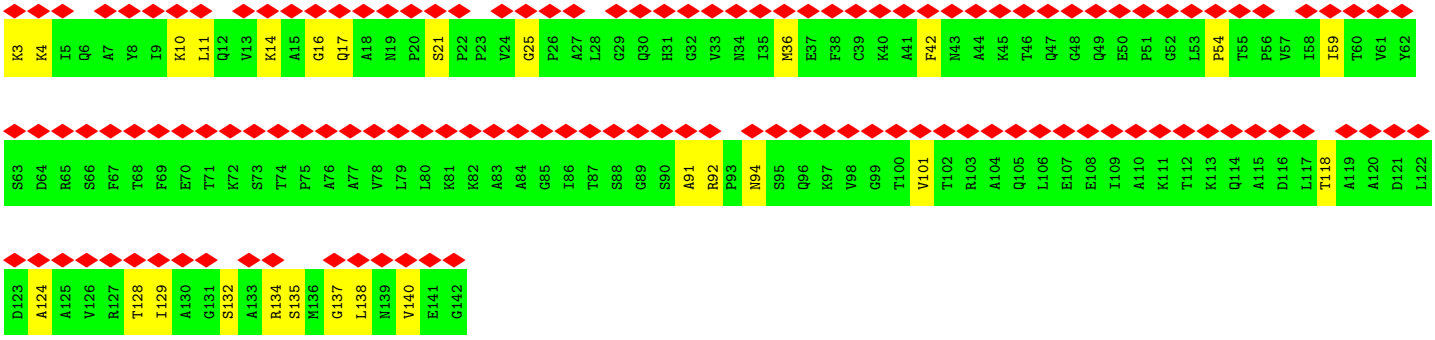
Chain H:



• Molecule 9: 50S ribosomal protein L11

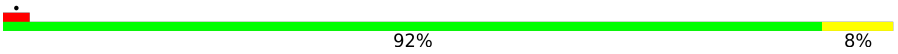
Chain I:

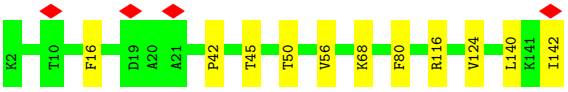




• Molecule 10: 50S ribosomal protein L13

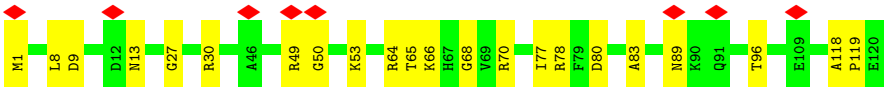
Chain J:





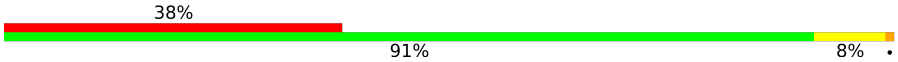
• Molecule 11: 50S ribosomal protein L14

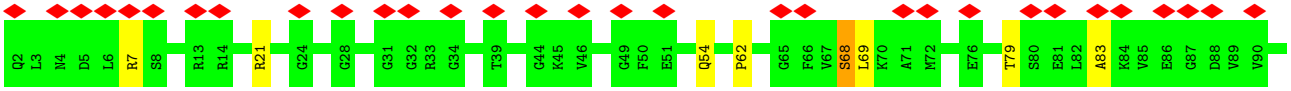
Chain K:

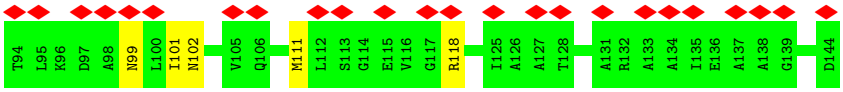


• Molecule 12: 50S ribosomal protein L15

Chain L:

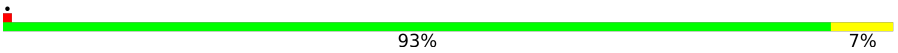


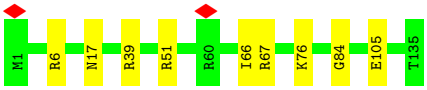




• Molecule 13: 50S ribosomal protein L16

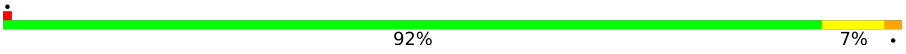
Chain M:

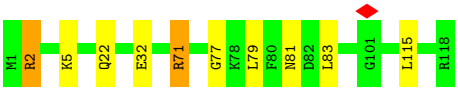




• Molecule 14: 50S ribosomal protein L17

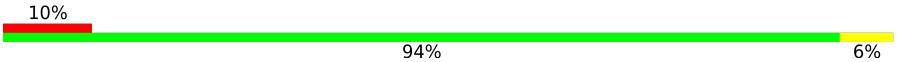
Chain N:

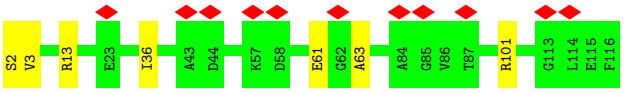




• Molecule 15: 50S ribosomal protein L18

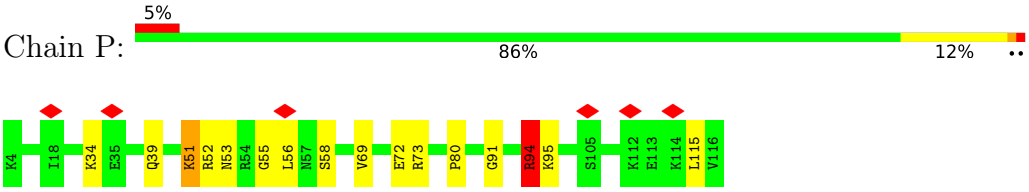
Chain O:





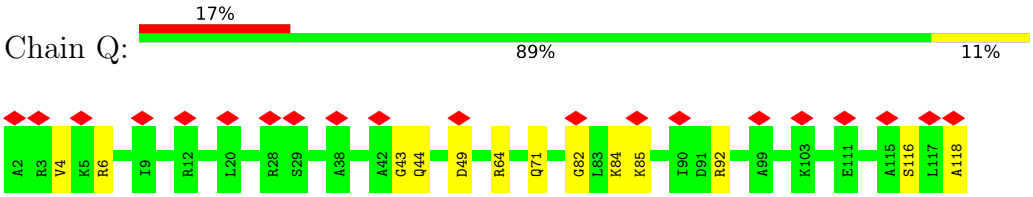
• Molecule 16: 50S ribosomal protein L19

Chain P:



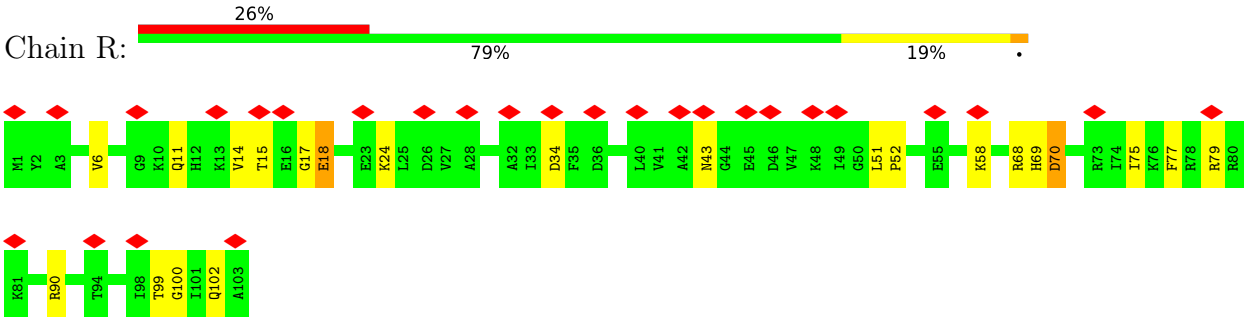
• Molecule 17: 50S ribosomal protein L20

Chain Q:



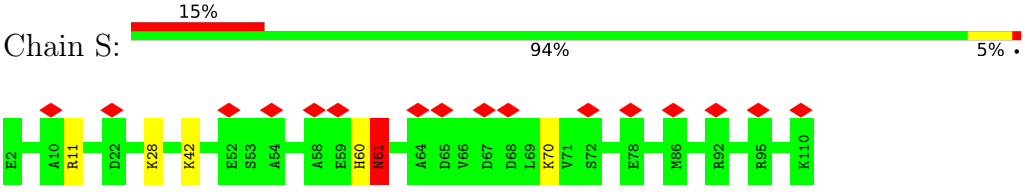
• Molecule 18: 50S ribosomal protein L21

Chain R:



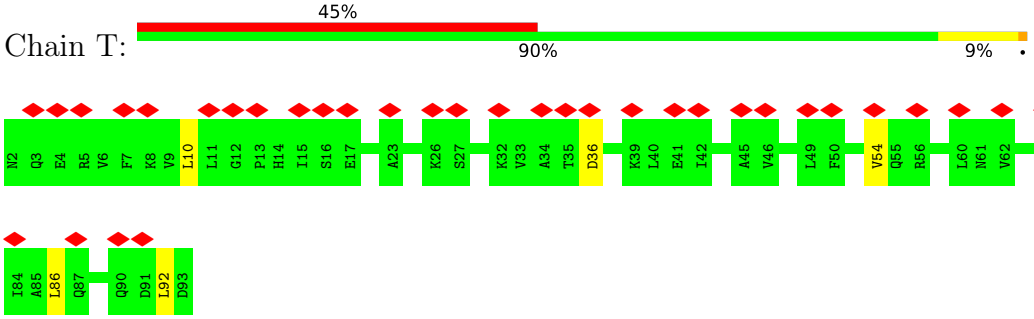
• Molecule 19: 50S ribosomal protein L22

Chain S:



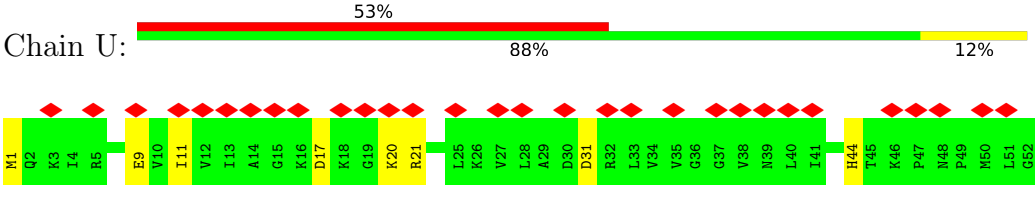
• Molecule 20: 50S ribosomal protein L23

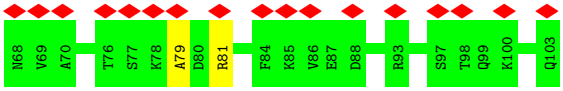
Chain T:



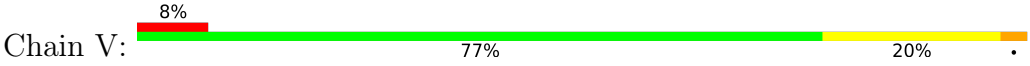
• Molecule 21: 50S ribosomal protein L24

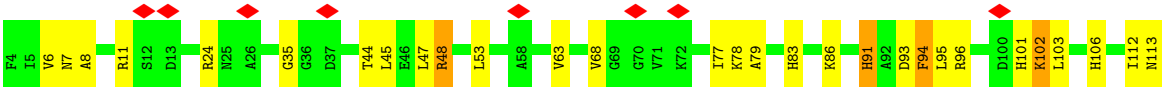
Chain U:

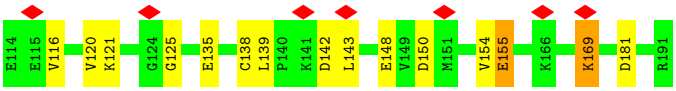




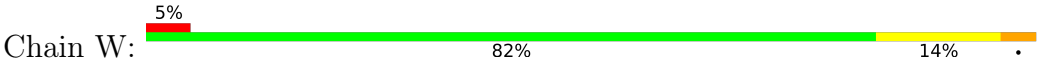
• Molecule 22: 50S ribosomal protein L25

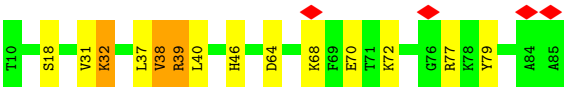




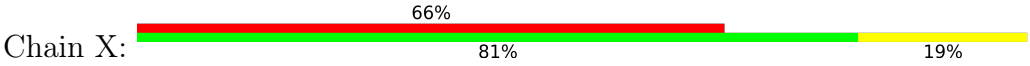


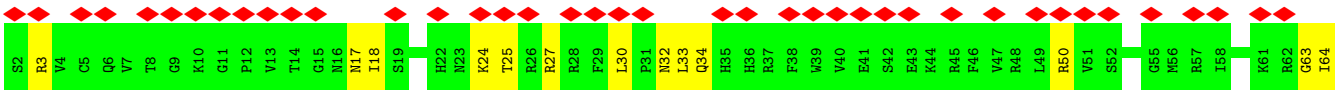
• Molecule 23: 50S ribosomal protein L27

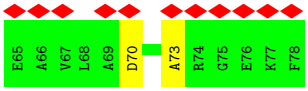




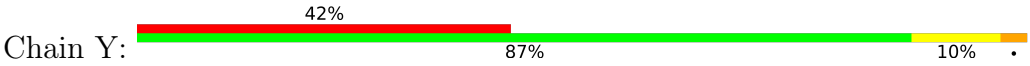
• Molecule 24: 50S ribosomal protein L28

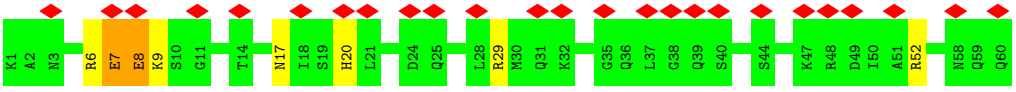




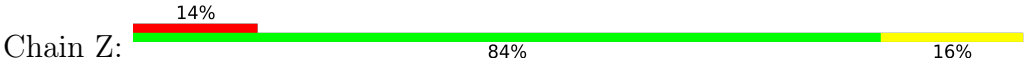


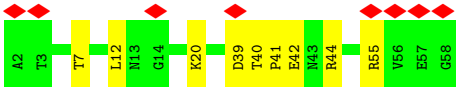
• Molecule 25: Ribosomal protein uL29





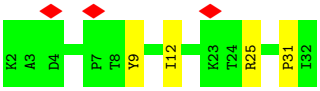
• Molecule 26: 50S ribosomal protein L30





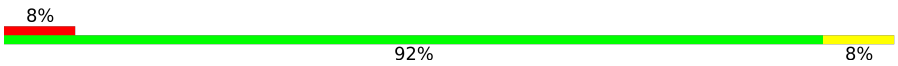
• Molecule 27: 50S ribosomal protein L31

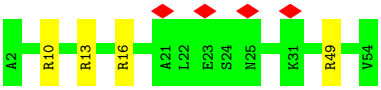
Chain 1:



• Molecule 28: 50S ribosomal protein L32

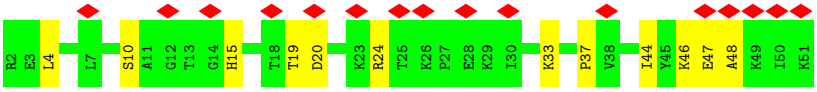
Chain 2:





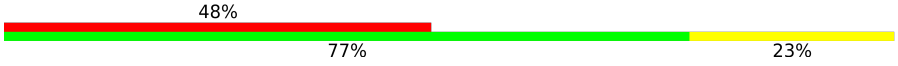
• Molecule 29: 50S ribosomal protein L33

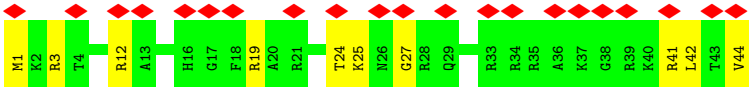
Chain 3:



• Molecule 30: 50S ribosomal protein L34

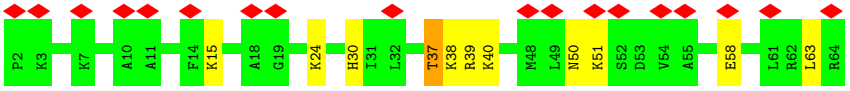
Chain 4:





• Molecule 31: 50S ribosomal protein L35

Chain 5:



• Molecule 32: 50S ribosomal protein L36

Chain 6:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	128795	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 ($e^-/Å^2$)	1.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.514	Depositor
Minimum map value	-0.233	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.0566	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	1.20	26/68494 (0.0%)	1.21	564/106830 (0.5%)
2	B	0.94	0/2760	1.19	29/4300 (0.7%)
3	C	0.55	0/2103	0.67	0/2824
4	D	0.57	0/1580	0.69	0/2128
5	E	0.50	0/1536	0.72	1/2069 (0.0%)
6	F	0.39	0/1423	0.74	1/1911 (0.1%)
7	G	0.42	0/1326	0.65	1/1787 (0.1%)
8	H	0.29	0/1097	0.54	1/1482 (0.1%)
9	I	0.32	0/1041	0.63	0/1408
10	J	0.59	0/1148	0.62	0/1549
11	K	0.51	0/931	0.71	1/1247 (0.1%)
12	L	0.49	0/1070	0.69	0/1426
13	M	0.55	0/1089	0.62	0/1456
14	N	0.53	0/960	0.64	0/1282
15	O	0.42	0/888	0.61	0/1183
16	P	0.55	0/903	0.72	1/1207 (0.1%)
17	Q	0.66	0/946	0.64	0/1257
18	R	0.48	0/835	0.72	1/1117 (0.1%)
19	S	0.47	0/829	0.65	1/1104 (0.1%)
20	T	0.52	0/710	0.66	0/953
21	U	0.46	0/809	0.72	1/1079 (0.1%)
22	V	0.46	0/1428	0.70	0/1936
23	W	0.57	0/582	0.93	3/773 (0.4%)
24	X	0.49	0/641	0.66	1/854 (0.1%)
25	Y	0.42	0/479	0.65	0/640
26	Z	0.49	0/449	0.64	0/602
27	1	0.37	0/235	0.60	0/318
28	2	0.49	0/429	0.64	0/572
29	3	0.42	0/425	0.65	0/566
30	4	0.59	0/368	0.73	1/482 (0.2%)
31	5	0.49	0/511	0.68	0/668
32	6	0.51	0/308	0.64	0/404
All	All	1.04	26/98333 (0.0%)	1.10	607/147414 (0.4%)

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
3	C	0	5
4	D	0	3
5	E	0	4
6	F	0	5
7	G	0	2
11	K	0	1
12	L	0	1
16	P	0	3
18	R	0	7
19	S	0	1
22	V	0	5
24	X	0	1
25	Y	0	2
29	3	0	1
All	All	0	41

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	519	A	N9-C4	-7.40	1.33	1.37
1	A	838	A	N9-C4	-6.92	1.33	1.37
1	A	2254	A	N9-C4	-6.58	1.33	1.37
1	A	2192	G	N9-C4	-6.58	1.32	1.38
1	A	1234	A	N9-C4	-6.46	1.33	1.37

The worst 5 of 607 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2021	U	N3-C2-O2	-11.84	113.91	122.20
1	A	2674	G	C2-N3-C4	11.69	117.74	111.90
1	A	1510	U	C2-N1-C1'	11.62	131.65	117.70
1	A	1448	C	C6-N1-C2	-11.57	115.67	120.30
1	A	1262	A	O4'-C1'-N9	11.43	117.34	108.20

There are no chirality outliers.

5 of 41 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	118	SER	Peptide
3	C	119	GLY	Peptide
3	C	122	ALA	Peptide
3	C	123	PRO	Peptide
3	C	27	GLY	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	61164	0	30774	1981	0
2	B	2469	0	1252	5	0
3	C	2067	0	2147	31	0
4	D	1557	0	1568	30	0
5	E	1516	0	1571	18	0
6	F	1402	0	1468	22	0
7	G	1308	0	1362	15	0
8	H	1086	0	1110	17	0
9	I	1026	0	1063	19	0
10	J	1122	0	1148	14	0
11	K	922	0	992	12	0
12	L	1058	0	1100	6	0
13	M	1069	0	1139	4	0
14	N	945	0	989	5	0
15	O	881	0	920	4	0
16	P	894	0	954	10	0
17	Q	936	0	1025	11	0
18	R	822	0	858	8	0
19	S	825	0	885	2	0
20	T	701	0	735	7	0
21	U	801	0	864	7	0
22	V	1405	0	1432	37	0
23	W	574	0	601	14	0
24	X	630	0	653	6	0
25	Y	476	0	497	5	0
26	Z	445	0	472	5	0
27	1	232	0	238	5	0
28	2	423	0	420	5	0
29	3	418	0	445	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	4	365	0	409	5	0
31	5	506	0	569	10	0
32	6	307	0	345	2	0
All	All	90352	0	60005	2230	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 16.

The worst 5 of 2230 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:2123:G:H2'	1:A:2124:C:C5	1.21	1.70
1:A:1093:A:H3'	1:A:1094:C:C6	1.37	1.57
1:A:1166:G:N2	1:A:1167:U:C2	1.82	1.47
1:A:2123:G:C2	1:A:2124:C:C4	2.02	1.47
1:A:2123:G:N3	1:A:2124:C:C4	1.85	1.44

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	269/271 (99%)	240 (89%)	27 (10%)	2 (1%)	22 56
4	D	205/207 (99%)	166 (81%)	37 (18%)	2 (1%)	15 48
5	E	197/199 (99%)	164 (83%)	29 (15%)	4 (2%)	7 34
6	F	173/175 (99%)	140 (81%)	31 (18%)	2 (1%)	13 44
7	G	171/173 (99%)	149 (87%)	22 (13%)	0	100 100
8	H	145/147 (99%)	131 (90%)	14 (10%)	0	100 100
9	I	138/140 (99%)	118 (86%)	20 (14%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
11	K	118/120 (98%)	107 (91%)	10 (8%)	1 (1%)	19	52
12	L	141/143 (99%)	117 (83%)	22 (16%)	2 (1%)	11	40
13	M	133/135 (98%)	123 (92%)	10 (8%)	0	100	100
14	N	116/118 (98%)	100 (86%)	15 (13%)	1 (1%)	17	50
15	O	113/115 (98%)	103 (91%)	10 (9%)	0	100	100
16	P	111/113 (98%)	90 (81%)	19 (17%)	2 (2%)	8	36
17	Q	115/117 (98%)	108 (94%)	7 (6%)	0	100	100
18	R	101/103 (98%)	85 (84%)	14 (14%)	2 (2%)	7	34
19	S	107/109 (98%)	103 (96%)	3 (3%)	1 (1%)	17	50
20	T	90/92 (98%)	78 (87%)	12 (13%)	0	100	100
21	U	101/103 (98%)	94 (93%)	7 (7%)	0	100	100
22	V	186/188 (99%)	160 (86%)	23 (12%)	3 (2%)	9	38
23	W	74/76 (97%)	48 (65%)	26 (35%)	0	100	100
24	X	75/77 (97%)	69 (92%)	5 (7%)	1 (1%)	12	42
25	Y	58/60 (97%)	52 (90%)	5 (9%)	1 (2%)	9	37
26	Z	55/57 (96%)	51 (93%)	4 (7%)	0	100	100
27	1	29/31 (94%)	25 (86%)	4 (14%)	0	100	100
28	2	51/53 (96%)	46 (90%)	5 (10%)	0	100	100
29	3	48/50 (96%)	42 (88%)	6 (12%)	0	100	100
30	4	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
31	5	61/63 (97%)	53 (87%)	8 (13%)	0	100	100
32	6	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
All	All	3398/3458 (98%)	2961 (87%)	413 (12%)	24 (1%)	26	56

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	60	ARG
6	F	37	ASN
16	P	95	LYS
18	R	70	ASP
3	C	237	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	212/212 (100%)	209 (99%)	3 (1%)	67 82
4	D	159/159 (100%)	151 (95%)	8 (5%)	24 55
5	E	157/157 (100%)	153 (98%)	4 (2%)	47 72
6	F	150/150 (100%)	148 (99%)	2 (1%)	69 82
7	G	137/137 (100%)	135 (98%)	2 (2%)	65 81
8	H	106/106 (100%)	105 (99%)	1 (1%)	78 87
9	I	108/108 (100%)	106 (98%)	2 (2%)	57 77
10	J	118/118 (100%)	116 (98%)	2 (2%)	60 78
11	K	100/100 (100%)	98 (98%)	2 (2%)	55 76
12	L	105/105 (100%)	103 (98%)	2 (2%)	57 77
13	M	108/108 (100%)	106 (98%)	2 (2%)	57 77
14	N	97/97 (100%)	96 (99%)	1 (1%)	76 85
15	O	86/86 (100%)	86 (100%)	0	100 100
16	P	95/95 (100%)	95 (100%)	0	100 100
17	Q	87/87 (100%)	87 (100%)	0	100 100
18	R	86/86 (100%)	84 (98%)	2 (2%)	50 73
19	S	86/86 (100%)	84 (98%)	2 (2%)	50 73
20	T	73/77 (95%)	72 (99%)	1 (1%)	67 82
21	U	88/88 (100%)	88 (100%)	0	100 100
22	V	146/153 (95%)	141 (97%)	5 (3%)	37 65
23	W	56/56 (100%)	55 (98%)	1 (2%)	59 78
24	X	66/66 (100%)	64 (97%)	2 (3%)	41 68
25	Y	53/53 (100%)	53 (100%)	0	100 100
26	Z	48/48 (100%)	47 (98%)	1 (2%)	53 75
27	1	27/27 (100%)	27 (100%)	0	100 100
28	2	46/46 (100%)	46 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
29	3	46/46 (100%)	45 (98%)	1 (2%)	52 74
30	4	37/37 (100%)	35 (95%)	2 (5%)	22 53
31	5	54/54 (100%)	53 (98%)	1 (2%)	57 77
32	6	34/34 (100%)	33 (97%)	1 (3%)	42 68
All	All	2771/2782 (100%)	2721 (98%)	50 (2%)	61 78

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	6	ARG
20	T	77	ASN
32	6	8	LYS
13	M	76	LYS
18	R	79	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
11	K	89	ASN
26	Z	33	HIS
18	R	43	ASN
22	V	113	ASN
17	Q	44	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2840/2888 (98%)	1042 (36%)	72 (2%)
2	B	115/116 (99%)	28 (24%)	2 (1%)
All	All	2955/3004 (98%)	1070 (36%)	74 (2%)

5 of 1070 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	C
1	A	10	A
1	A	12	G
1	A	13	A
1	A	14	A

5 of 74 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2149	A
1	A	2852	U
1	A	2228	A
1	A	2604	U
1	A	868	G

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)

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	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2605:G	O3'	2606:C	P	4.42

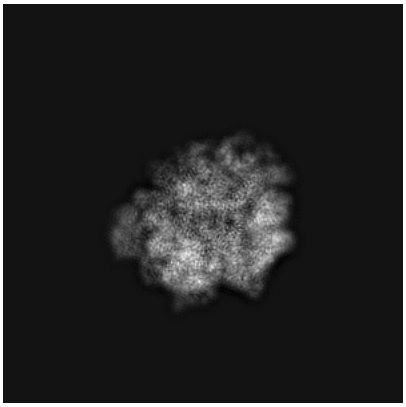
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10282. These allow visual inspection of the internal detail of the map and identification of artifacts.

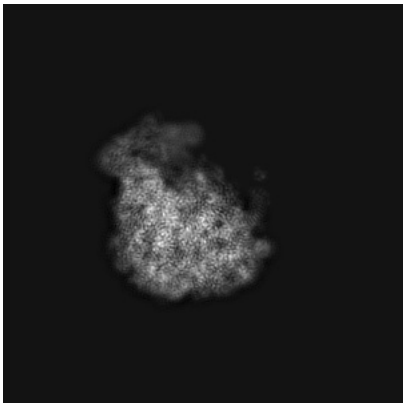
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

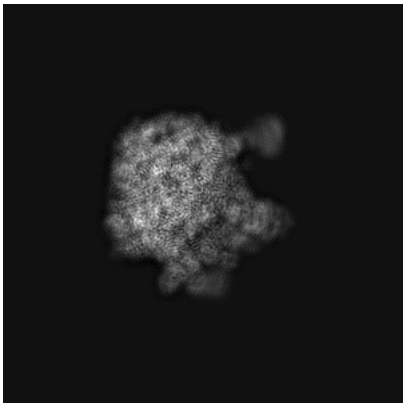
6.1.1 Primary map



X



Y

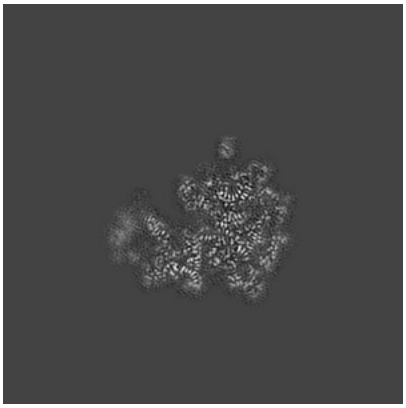


Z

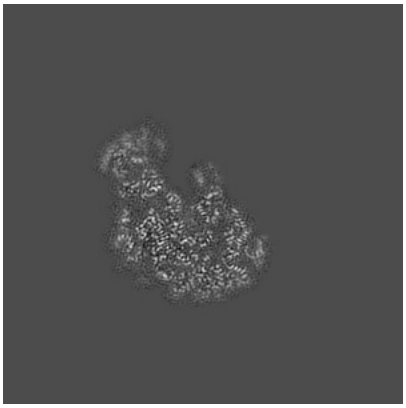
The images above show the map projected in three orthogonal directions.

6.2 Central slices

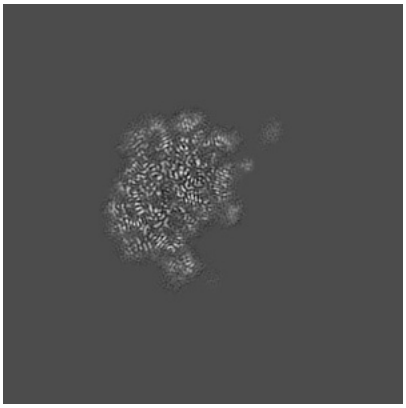
6.2.1 Primary map



X Index: 200



Y Index: 200

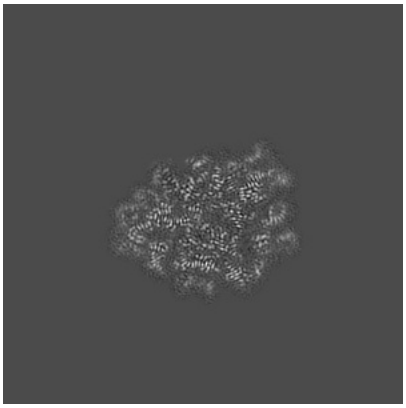


Z Index: 200

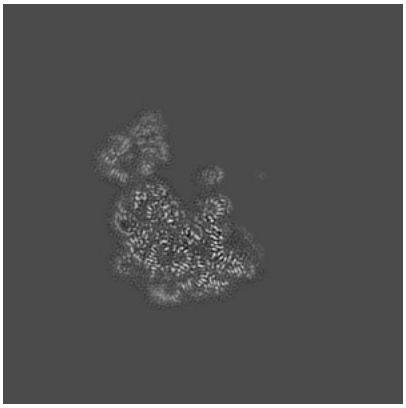
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

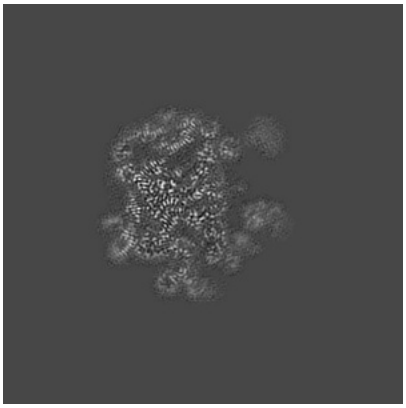
6.3.1 Primary map



X Index: 172



Y Index: 182

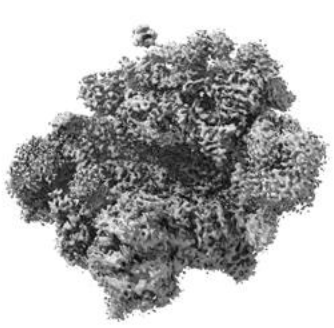


Z Index: 159

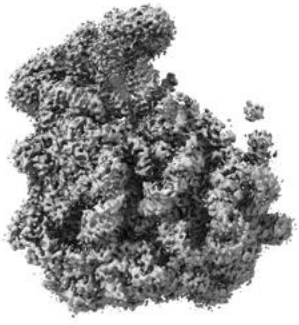
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

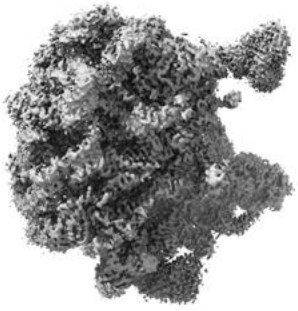
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0566. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

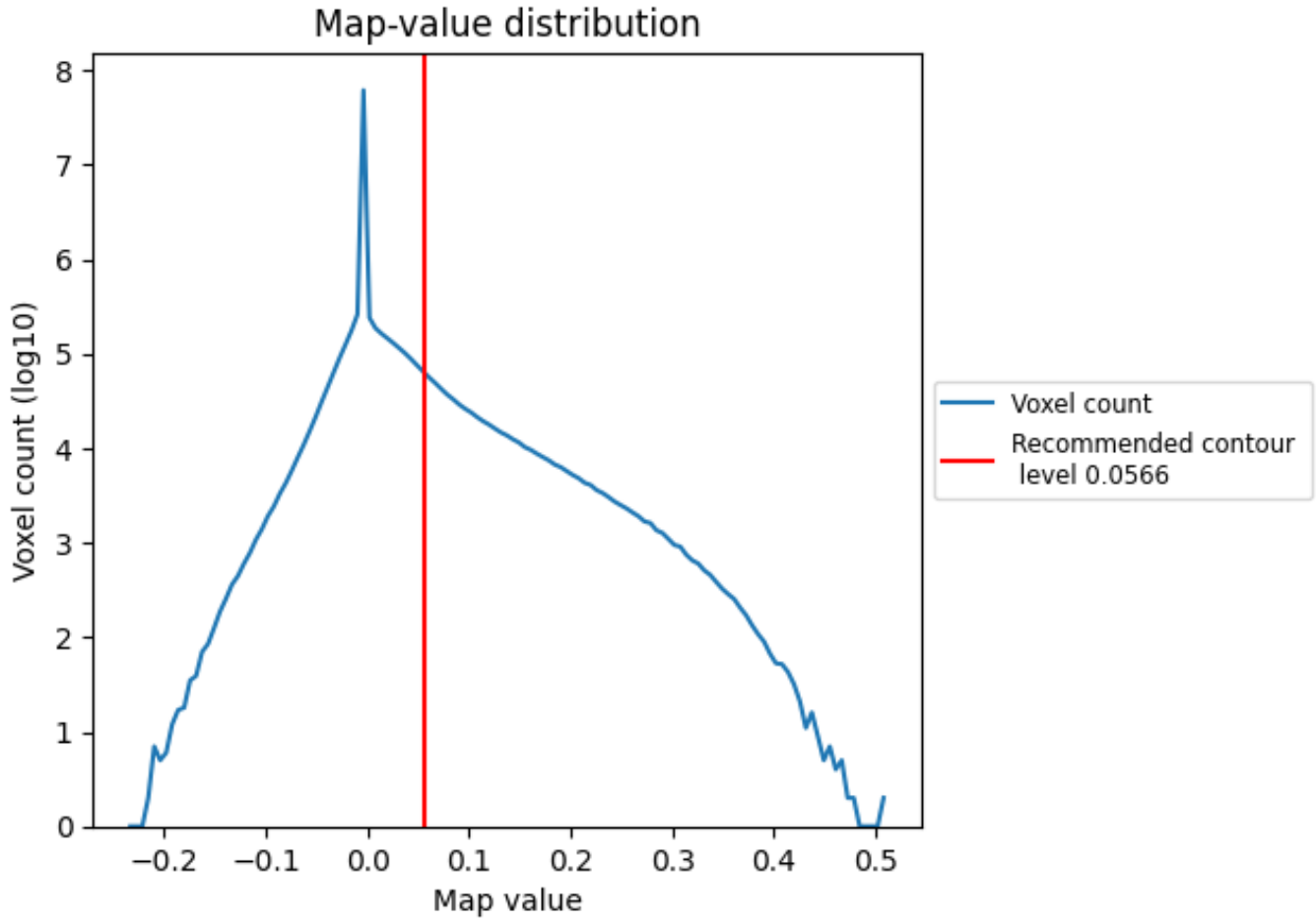
6.5 Mask visualisation (i)

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

7 Map analysis

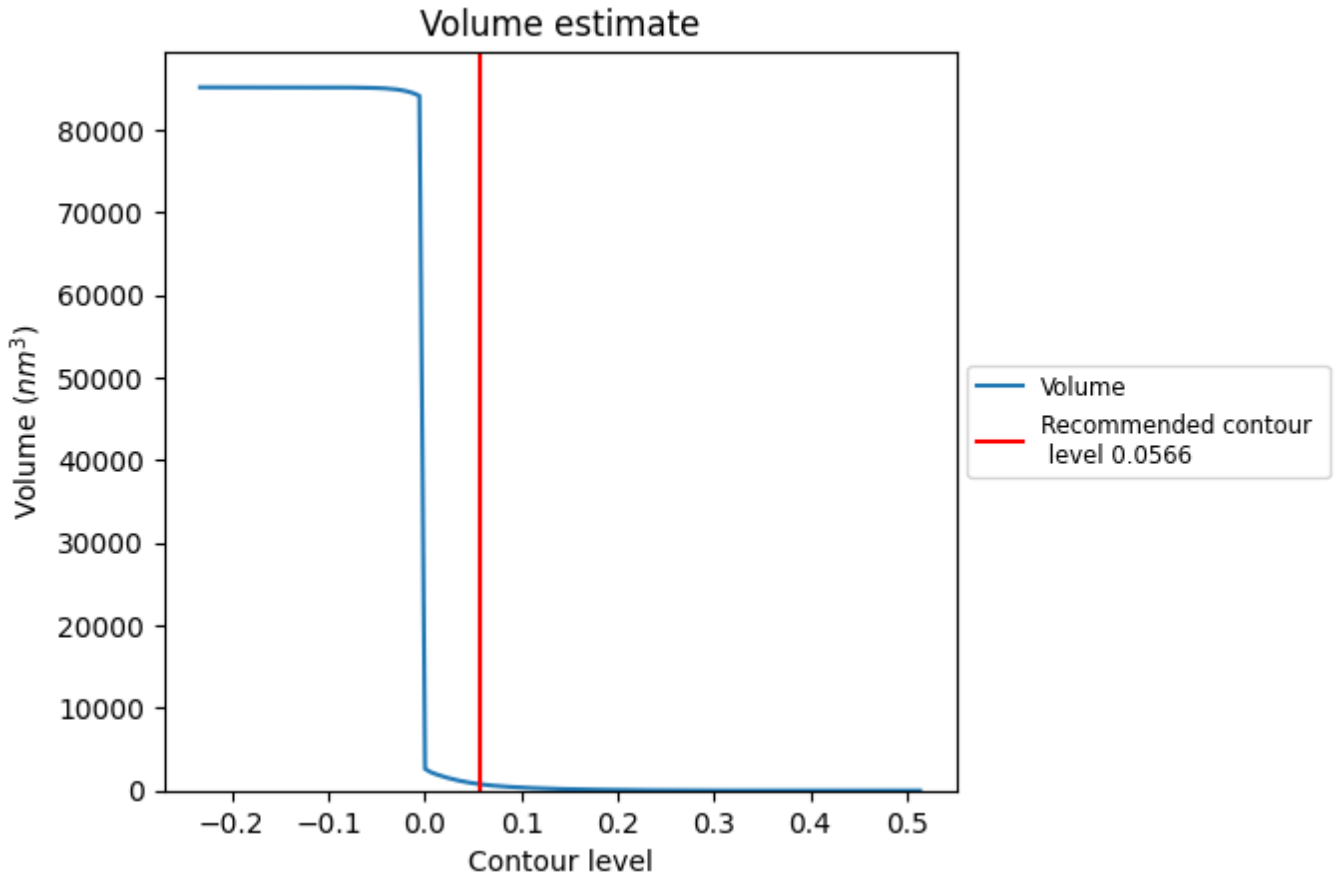
This section contains the results of statistical analysis of the map.

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.

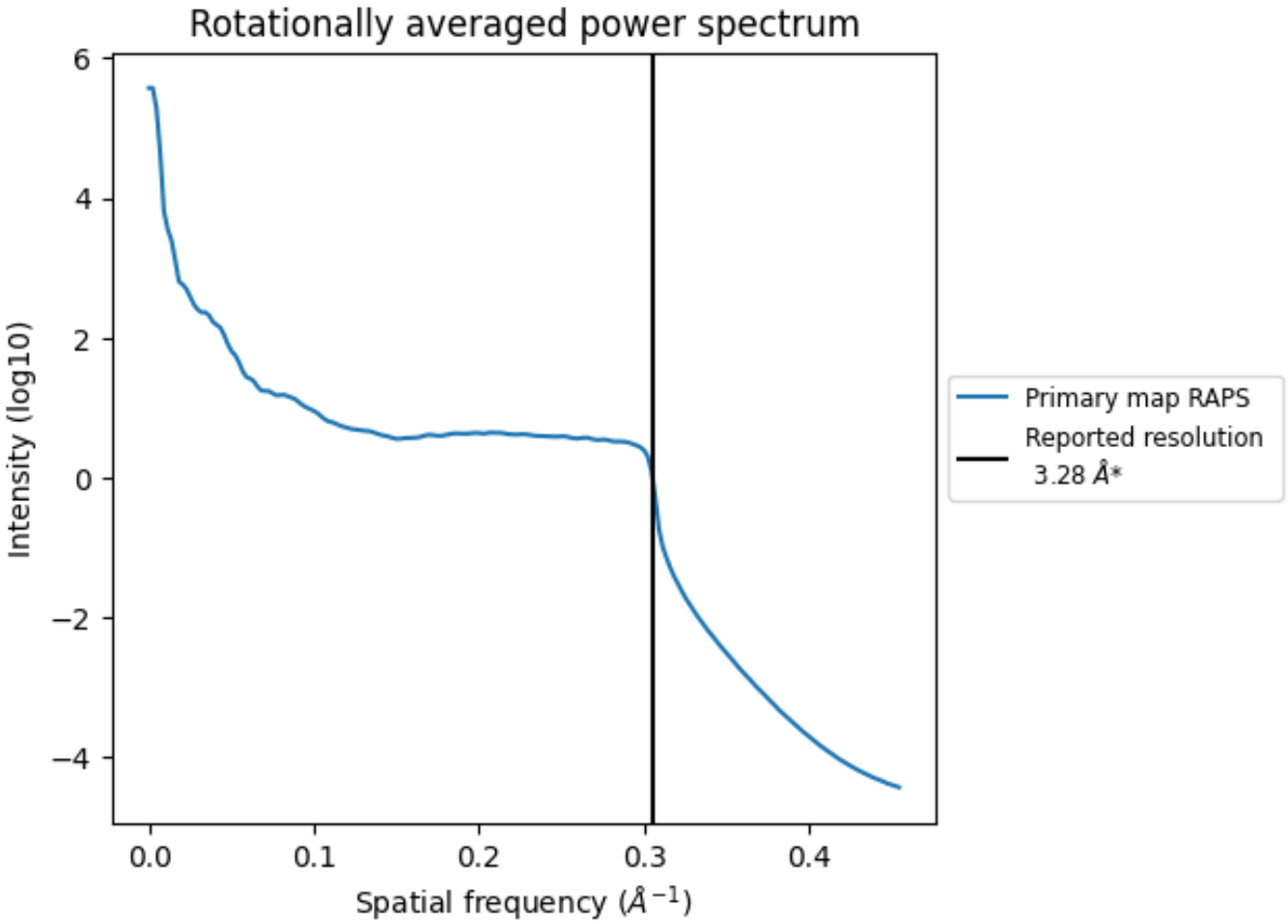
7.2 Volume estimate (i)



The volume at the recommended contour level is 783 nm^3; this corresponds to an approximate mass of 707 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 0.305 Å^{-1}

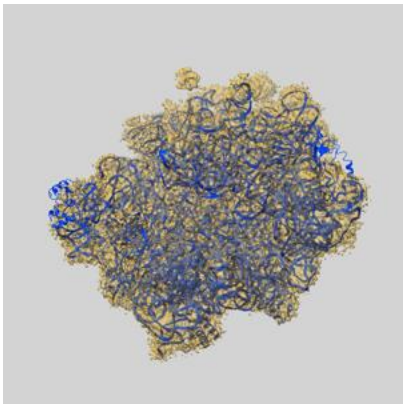
8 Fourier-Shell correlation (i)

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

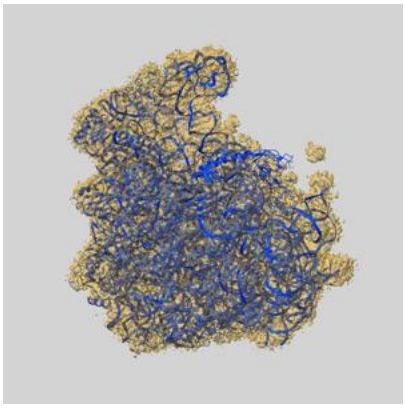
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10282 and PDB model 6SPD. Per-residue inclusion information can be found in section 3 on page 10.

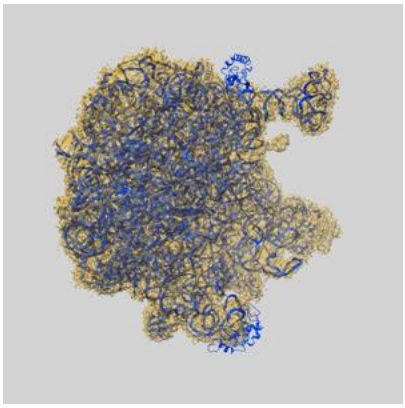
9.1 Map-model overlay



X



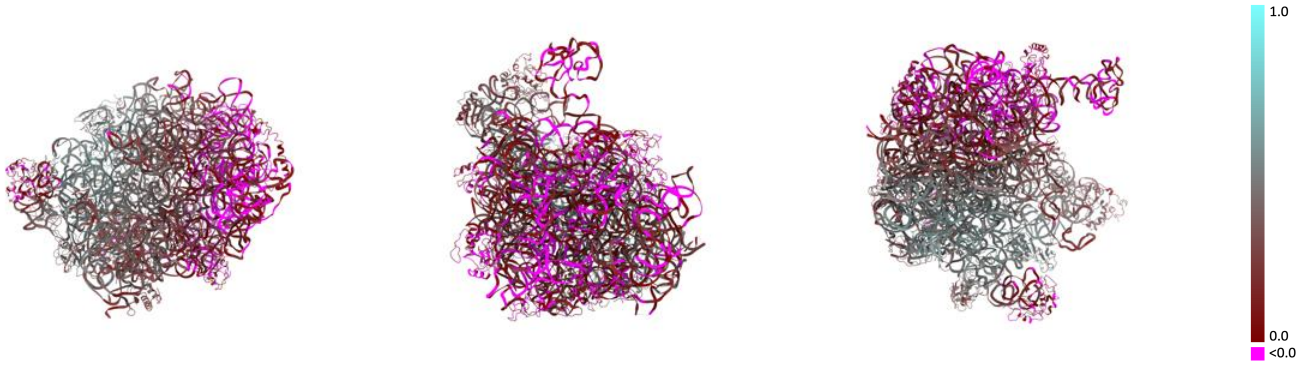
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0566 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.

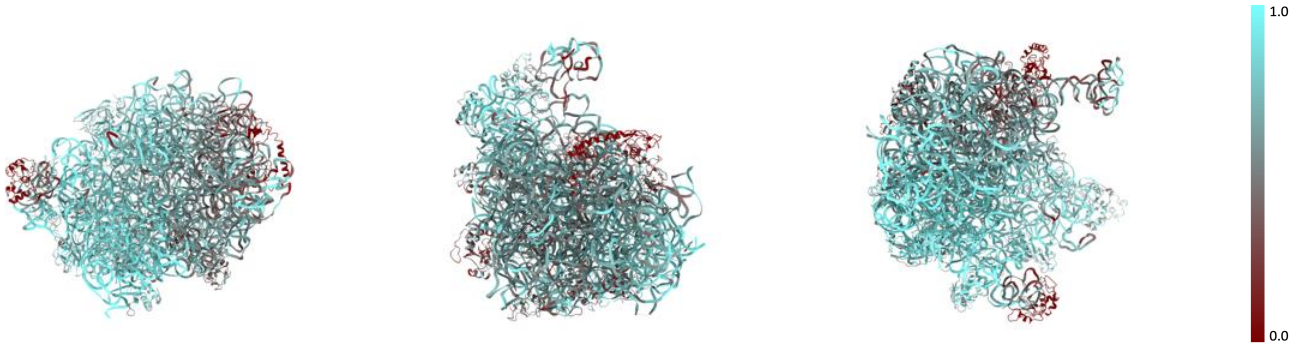
9.2 Q-score mapped to coordinate model (i)



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.

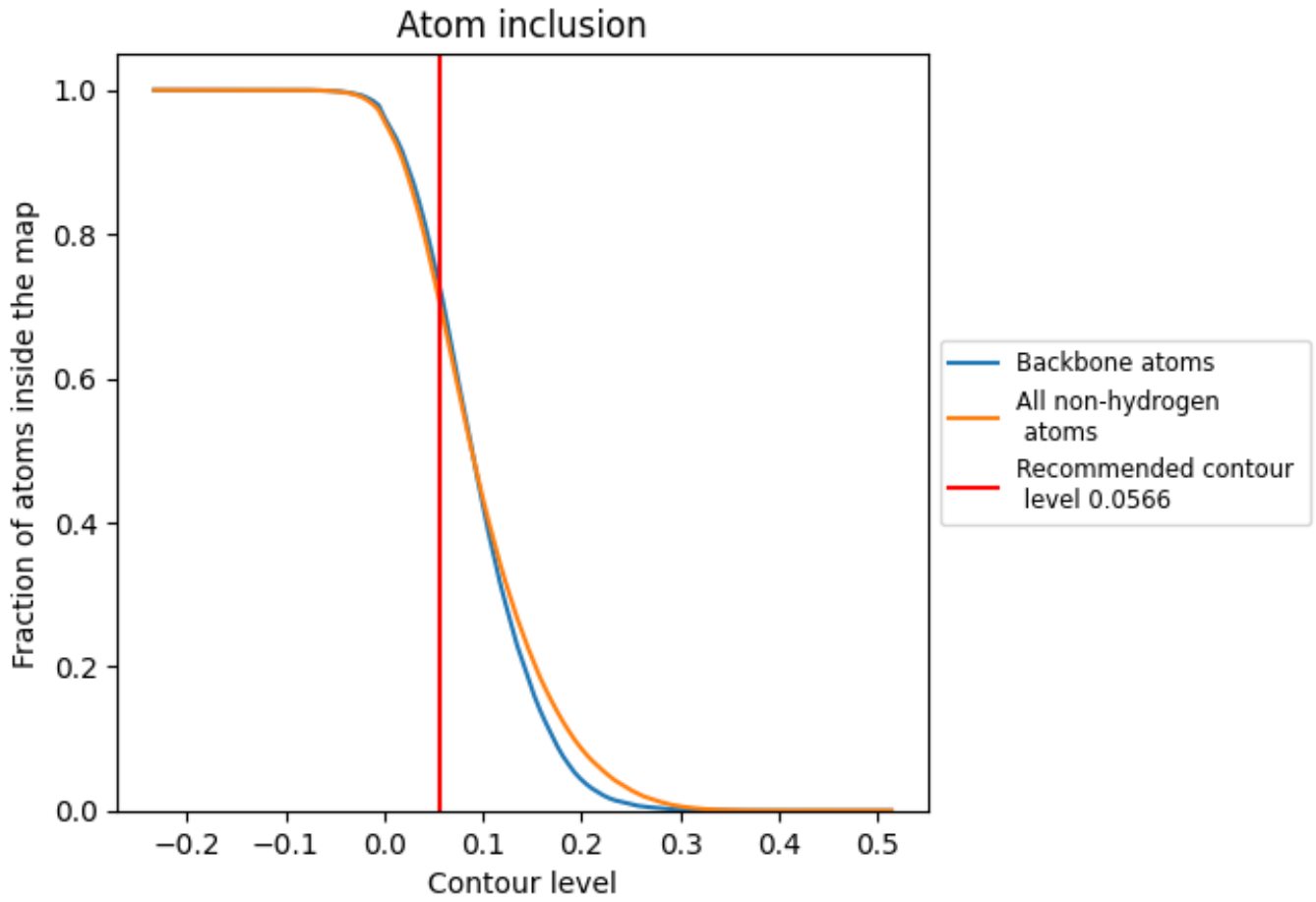
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0566).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 70% 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 (0.0566) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7024	0.2490
1	0.6376	0.1720
2	0.7083	0.3080
3	0.5209	0.1630
4	0.4490	0.0840
5	0.5143	0.1780
6	0.8464	0.5070
A	0.7472	0.2440
B	0.9202	0.4050
C	0.4176	0.0830
D	0.8255	0.4700
E	0.3858	0.0320
F	0.6364	0.2640
G	0.7301	0.3730
H	0.0243	-0.0140
I	0.0957	0.0860
J	0.7336	0.3510
K	0.7703	0.4830
L	0.4825	0.1190
M	0.8250	0.5190
N	0.8143	0.4380
O	0.7336	0.3130
P	0.7733	0.4860
Q	0.6309	0.2300
R	0.5460	0.1660
S	0.5973	0.2540
T	0.4473	0.0790
U	0.3914	0.0230
V	0.7507	0.4350
W	0.7125	0.3460
X	0.3306	0.0010
Y	0.4421	0.0280
Z	0.6420	0.2840