



## wwPDB EM Validation Summary Report ⓘ

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

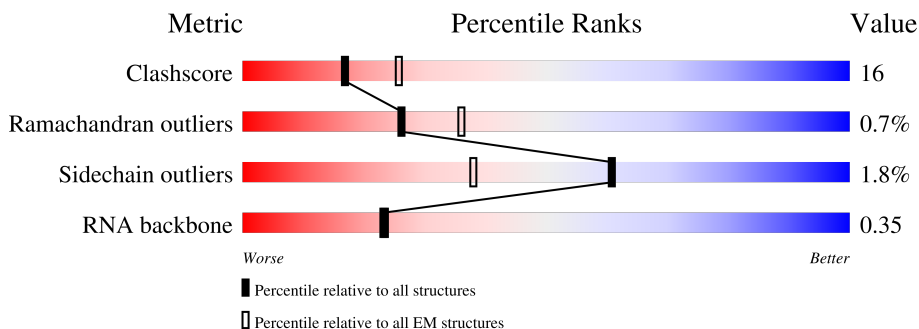
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP)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

# 1 Overall quality at a glance

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2888	
2	B	116	
3	C	271	
4	D	207	
5	E	199	
6	F	175	
7	G	173	

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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
			Total	C	N	O	S		
6	F	175	1402	896	248	254	4	0	0

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
			Total	C	N	O	S		
7	G	173	1308	823	240	243	2	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O		
23	W	76	574	365	110	99	0	0

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	C	N	O	S	0	0
			630	391	134	103	2		

- Molecule 25 is a protein called Ribosomal protein uL29.

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

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

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

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

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

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

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

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

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

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

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

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



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

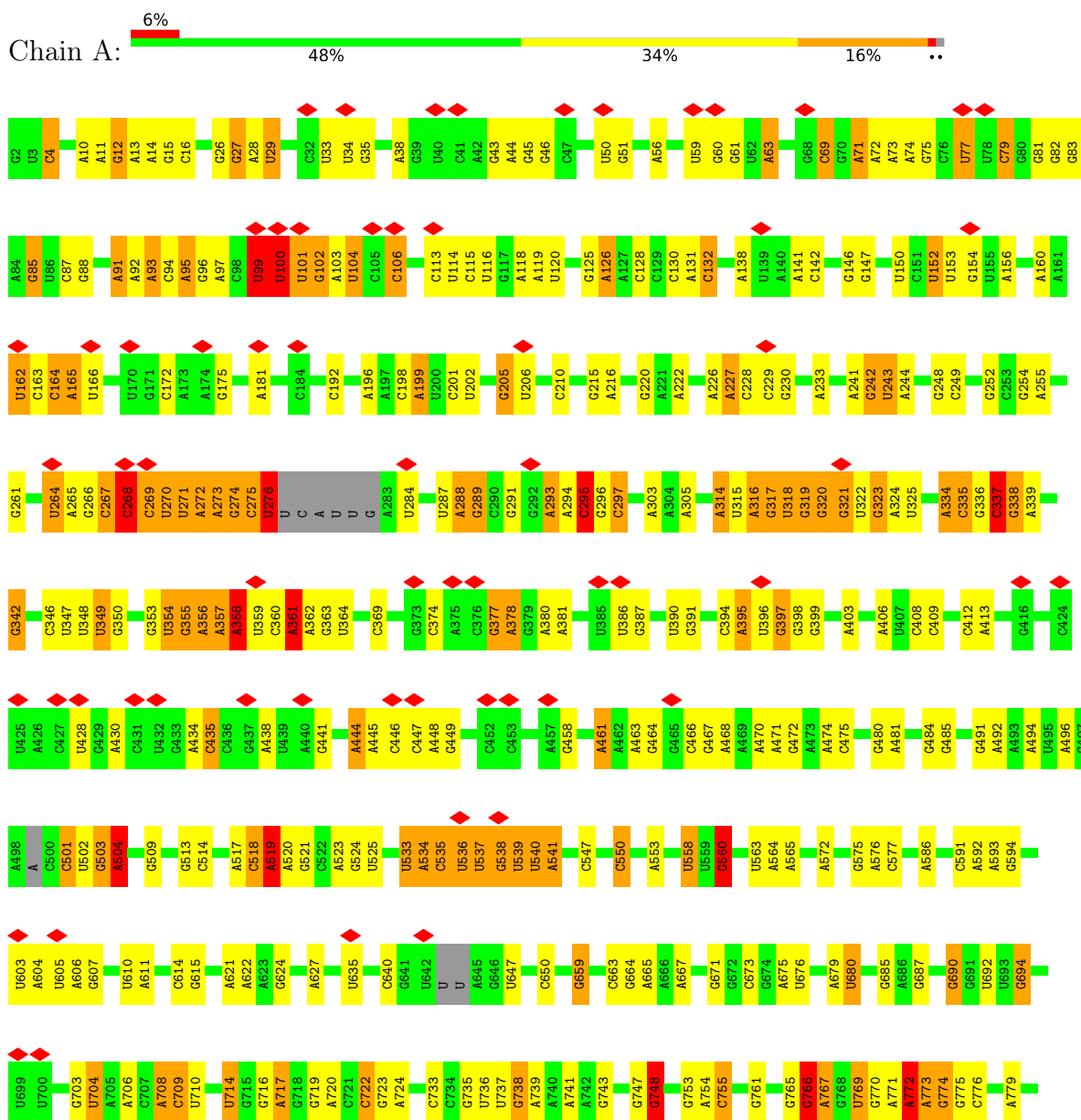
- Molecule 32 is a protein called 50S ribosomal protein L36.

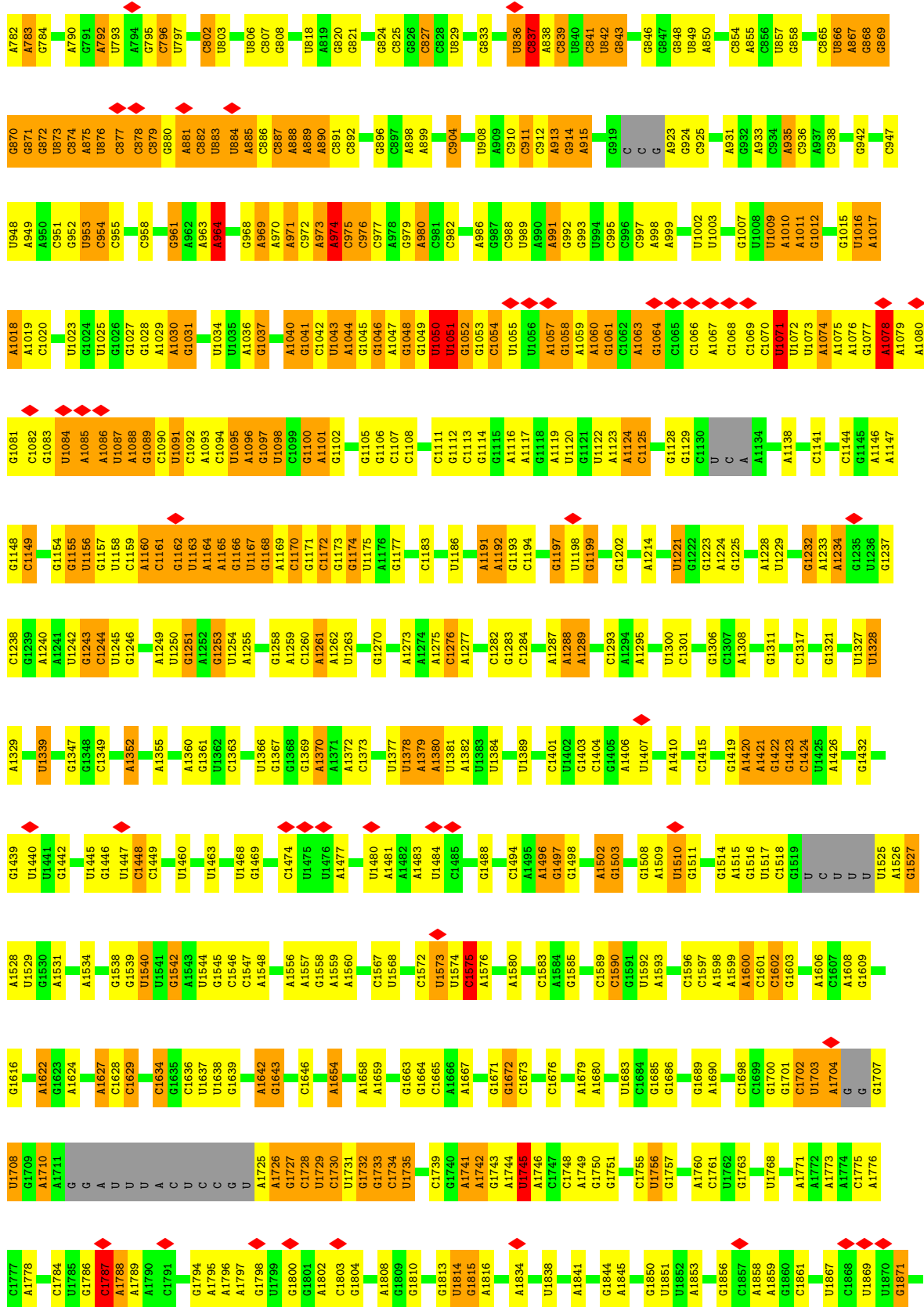
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	6	38	307	186	69	48	4	0	0

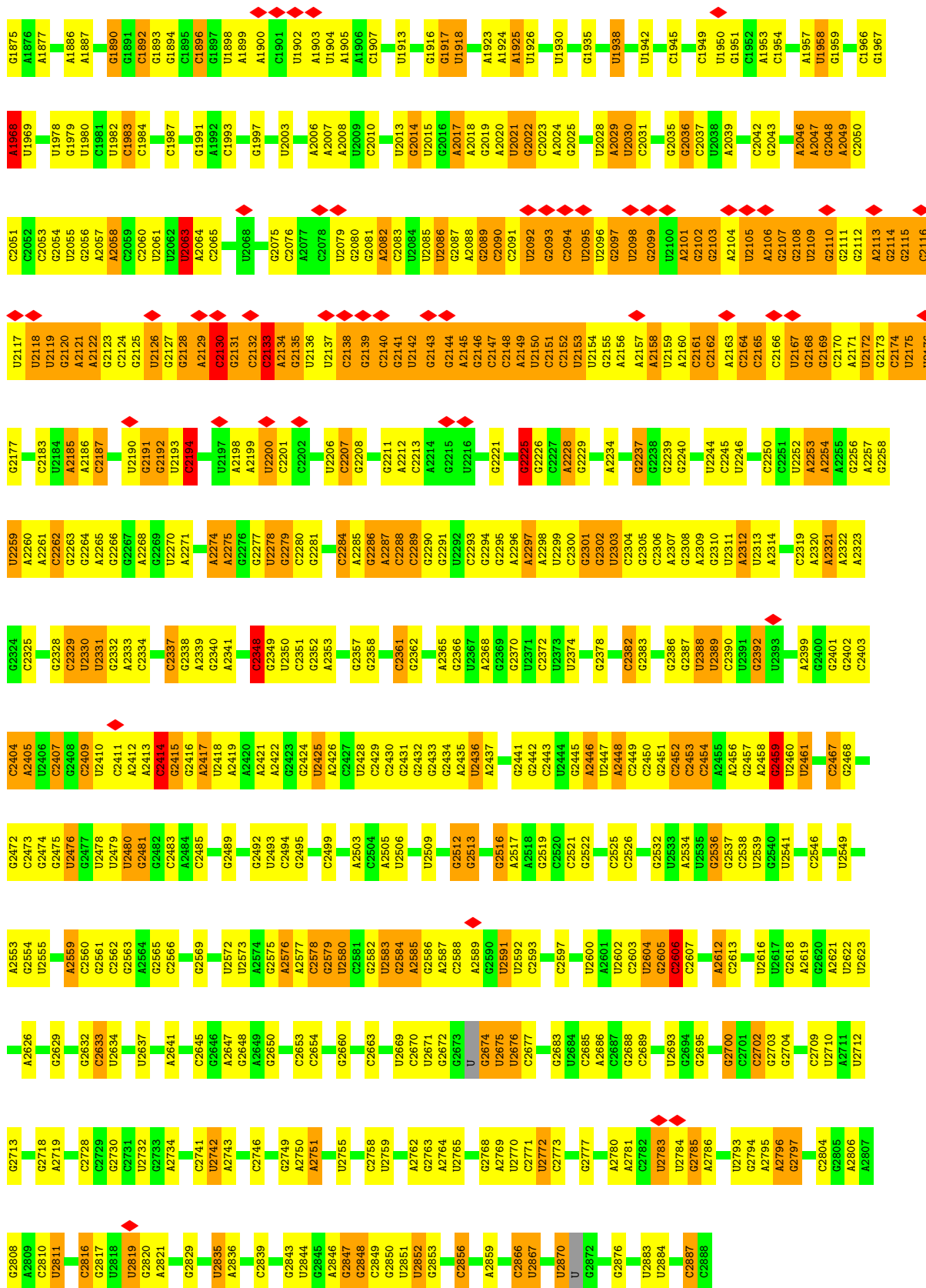
### 3 Residue-property plots

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



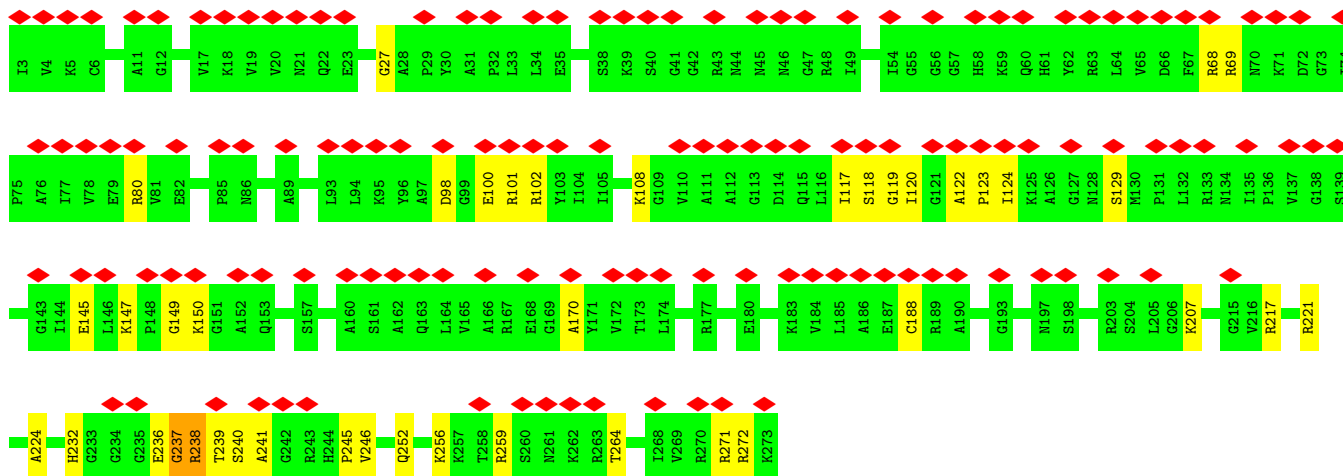
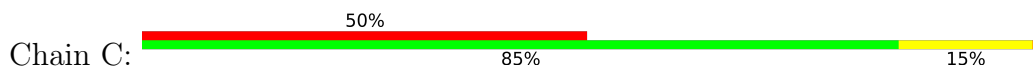




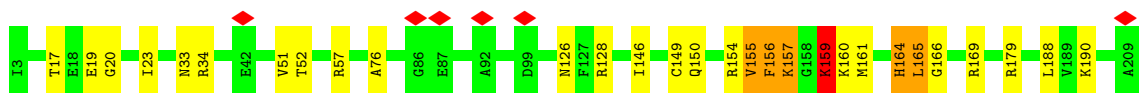
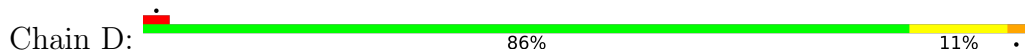
• Molecule 2: 5S ribosomal RNA



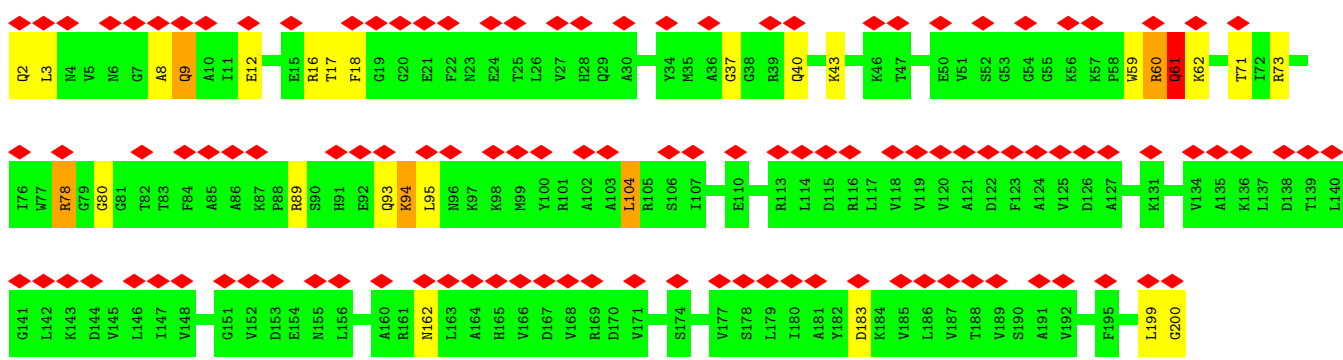
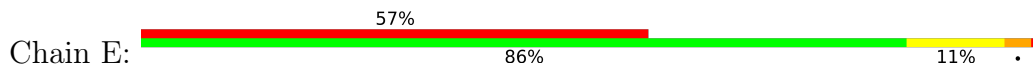
• Molecule 3: 50S ribosomal protein L2



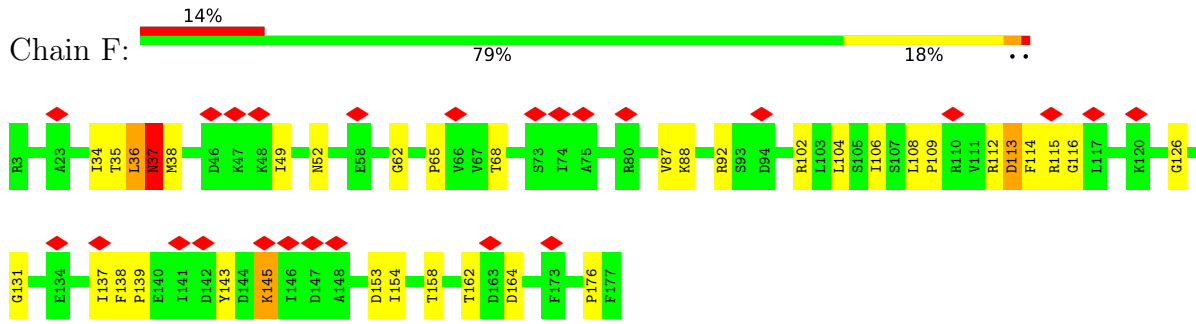
• Molecule 4: 50S ribosomal protein L3



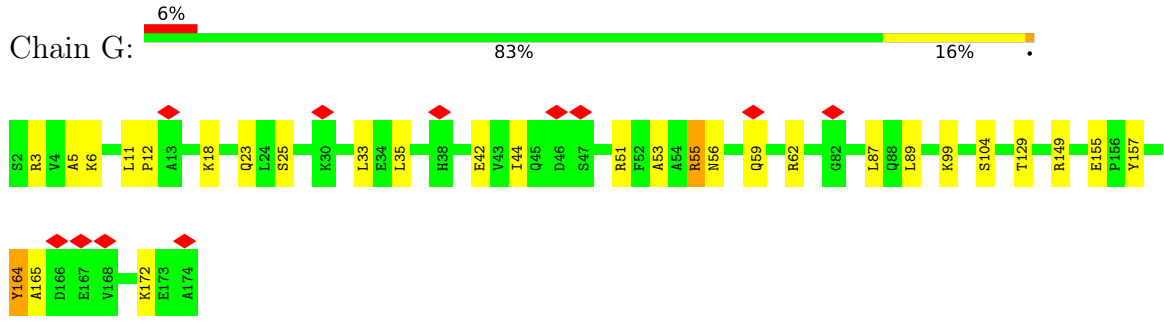
• Molecule 5: 50S ribosomal protein L4



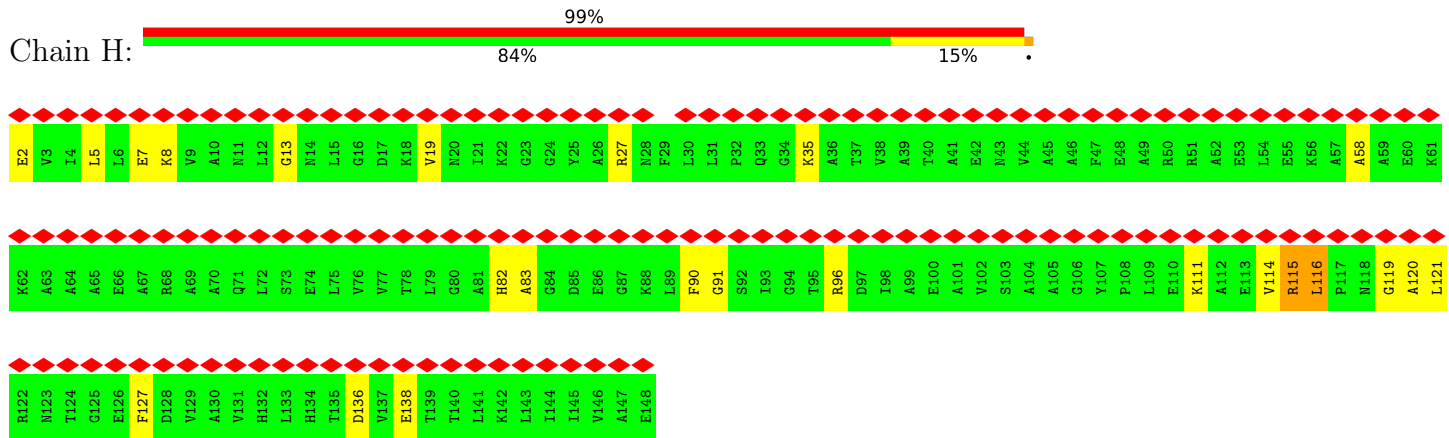
• Molecule 6: 50S ribosomal protein L5



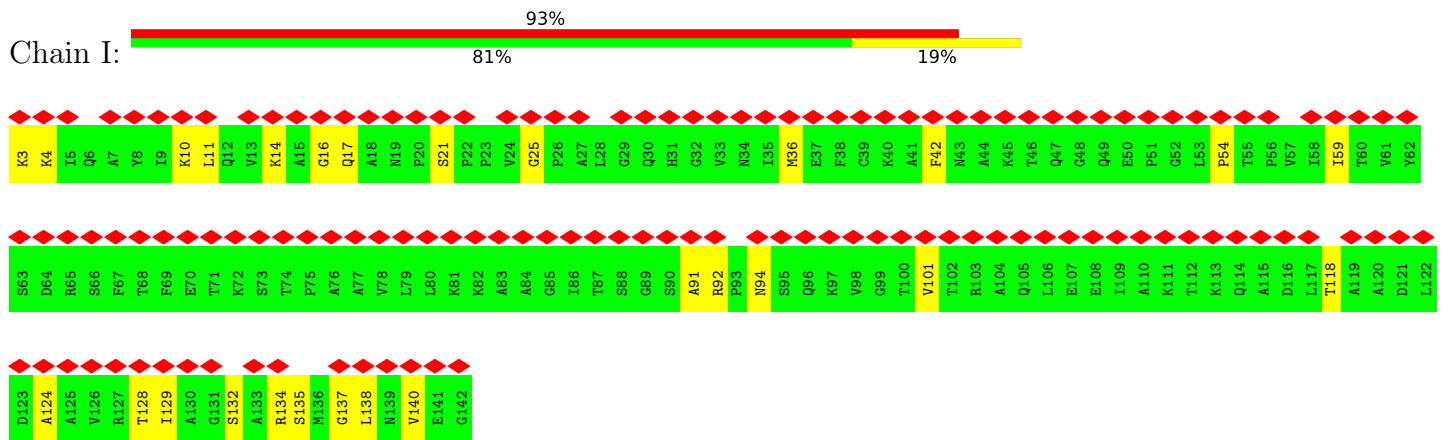
• Molecule 7: 50S ribosomal protein L6



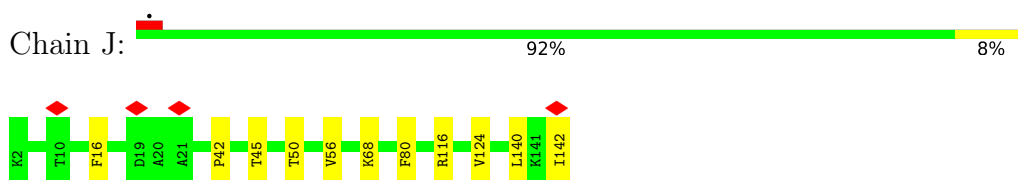
• Molecule 8: 50S ribosomal protein L9



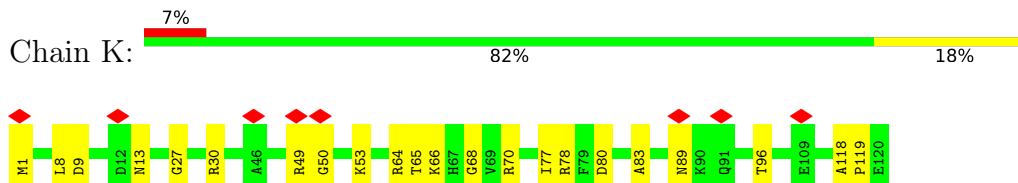
• Molecule 9: 50S ribosomal protein L11



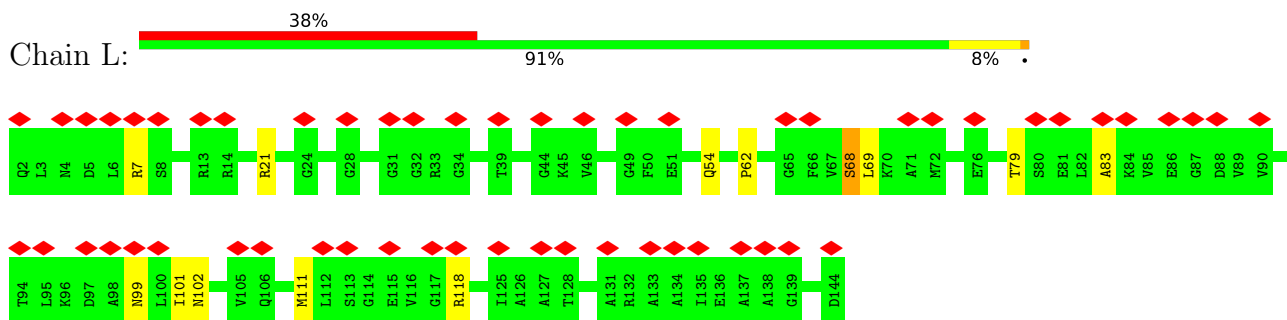
- Molecule 10: 50S ribosomal protein L13



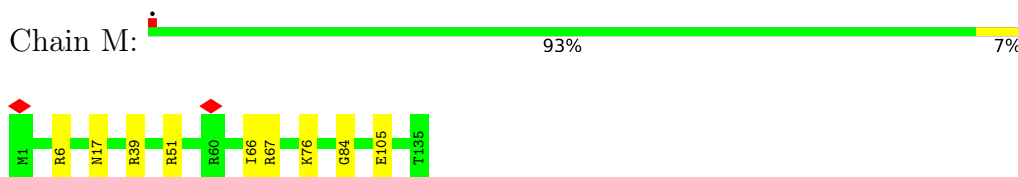
- Molecule 11: 50S ribosomal protein L14



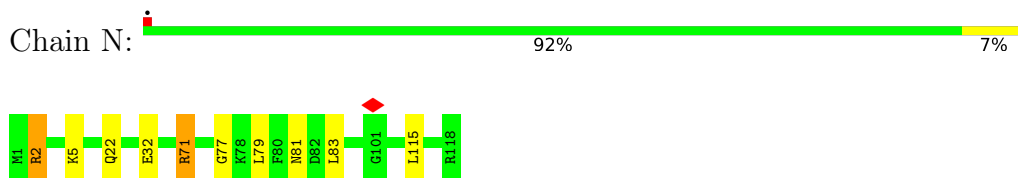
- Molecule 12: 50S ribosomal protein L15



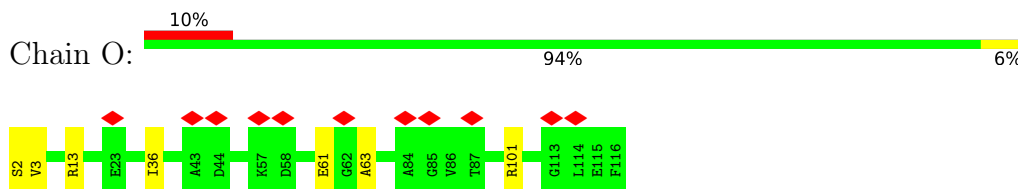
- Molecule 13: 50S ribosomal protein L16



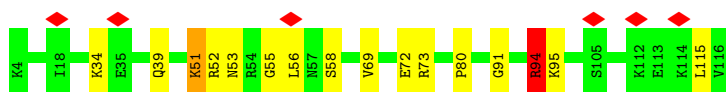
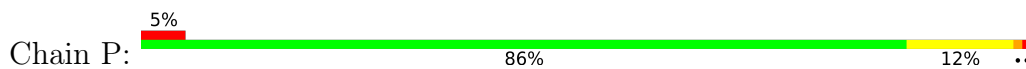
- Molecule 14: 50S ribosomal protein L17



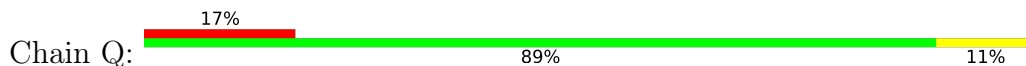
- Molecule 15: 50S ribosomal protein L18



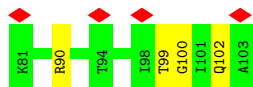
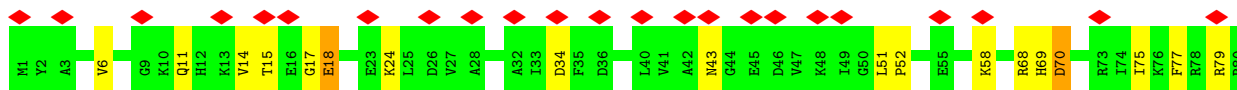
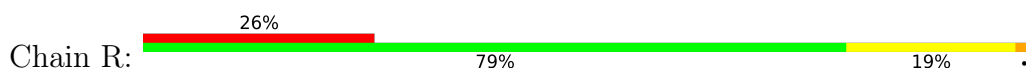
- Molecule 16: 50S ribosomal protein L19



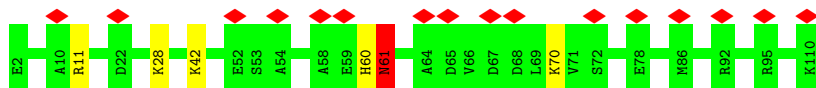
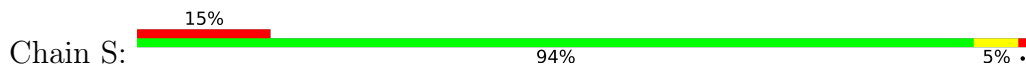
- Molecule 17: 50S ribosomal protein L20



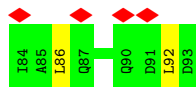
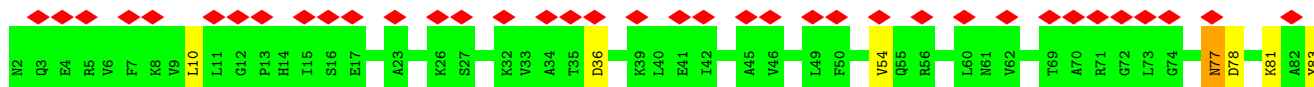
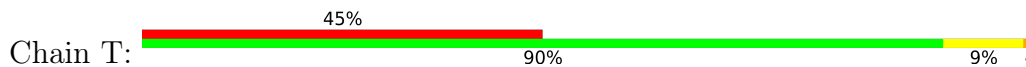
- Molecule 18: 50S ribosomal protein L21



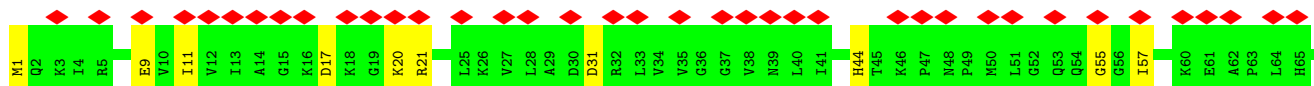
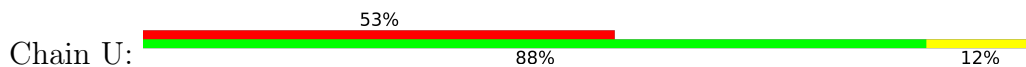
- Molecule 19: 50S ribosomal protein L22



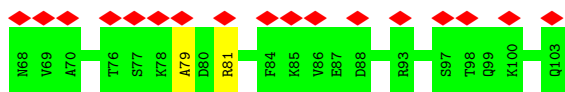
- Molecule 20: 50S ribosomal protein L23



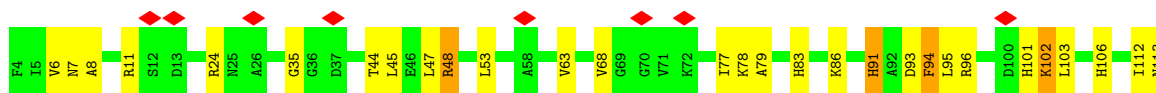
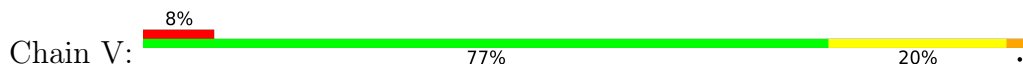
- Molecule 21: 50S ribosomal protein L24



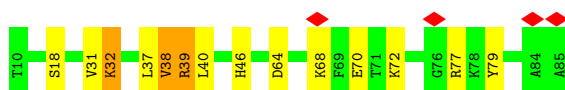
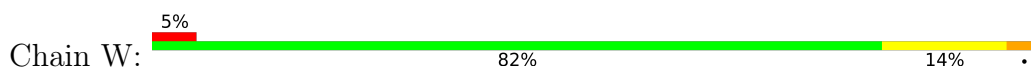




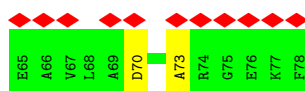
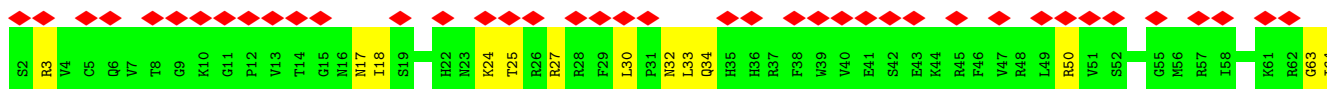
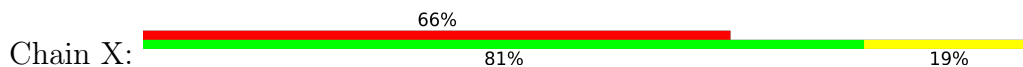
- Molecule 22: 50S ribosomal protein L25



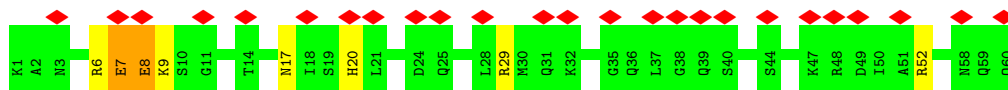
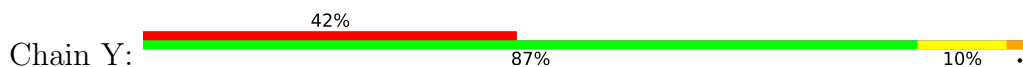
- Molecule 23: 50S ribosomal protein L27



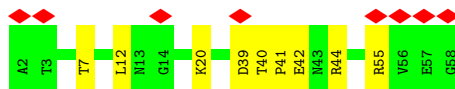
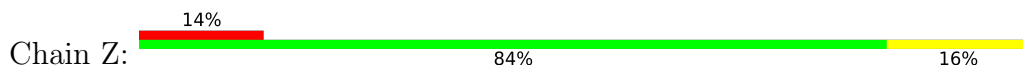
- Molecule 24: 50S ribosomal protein L28



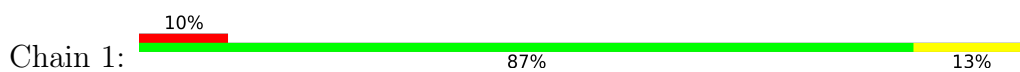
- Molecule 25: Ribosomal protein uL29



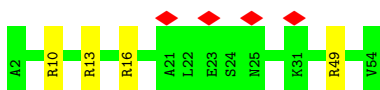
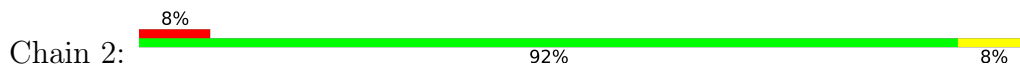
- Molecule 26: 50S ribosomal protein L30



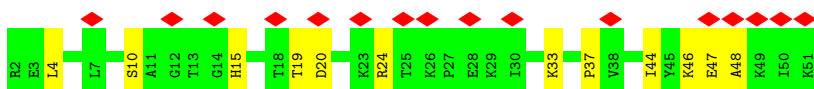
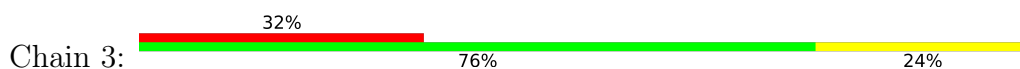
- Molecule 27: 50S ribosomal protein L31



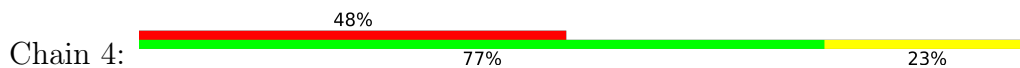
- Molecule 28: 50S ribosomal protein L32



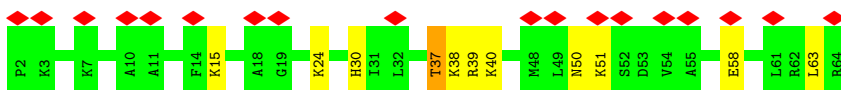
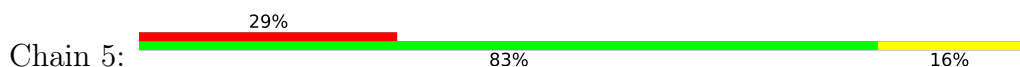
- Molecule 29: 50S ribosomal protein L33



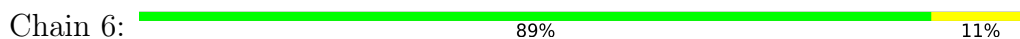
- Molecule 30: 50S ribosomal protein L34



- Molecule 31: 50S ribosomal protein L35



- Molecule 32: 50S ribosomal protein L36



## 4 Experimental information

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 ( $e^-/\text{\AA}^2$ )	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 ( $\text{\AA}$ )	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1, 1.1, 1.1	Depositor

## 5 Model quality

### 5.1 Standard geometry

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(°)	Ideal(°)
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

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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

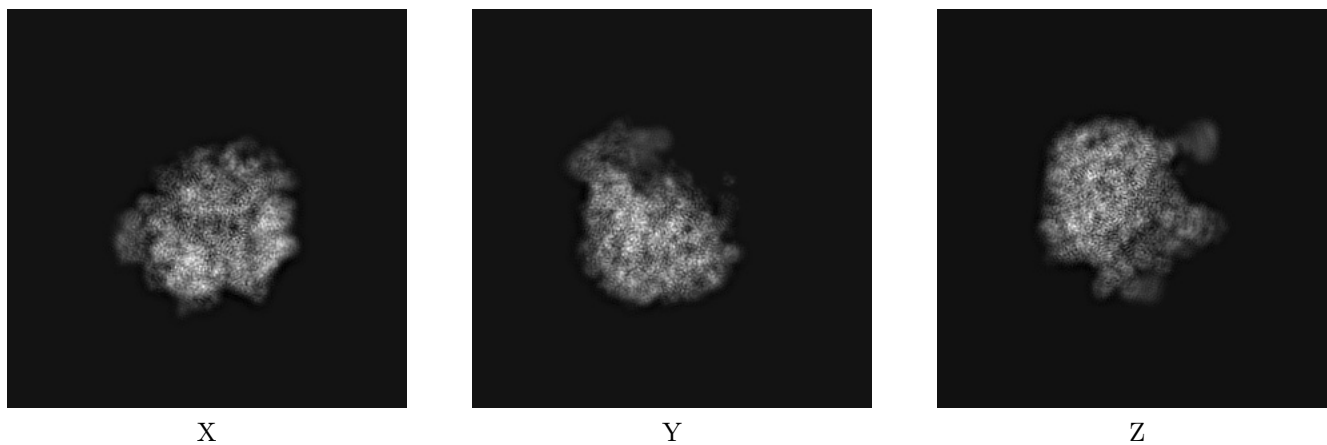
## 6 Map visualisation [i](#)

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 [i](#)

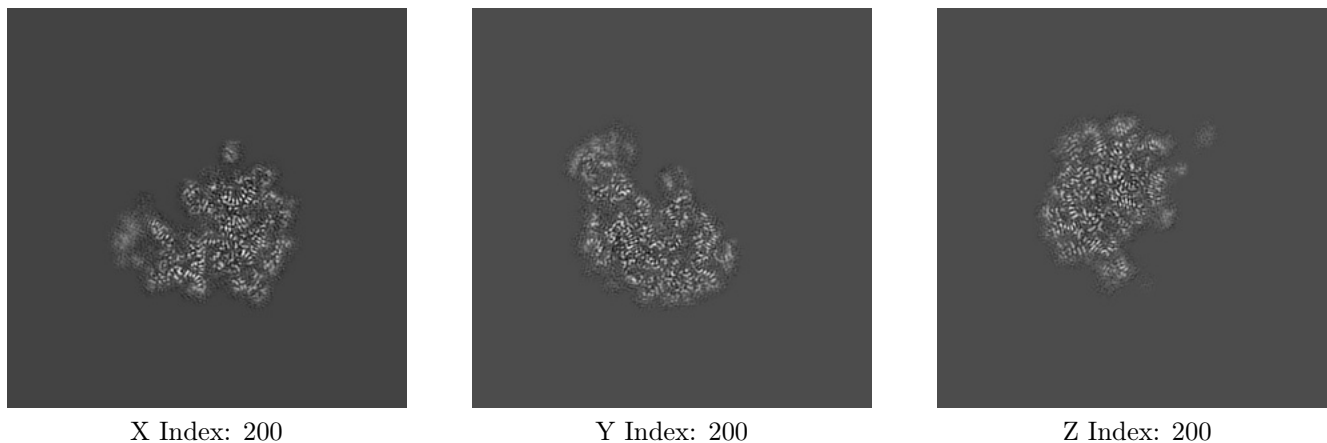
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

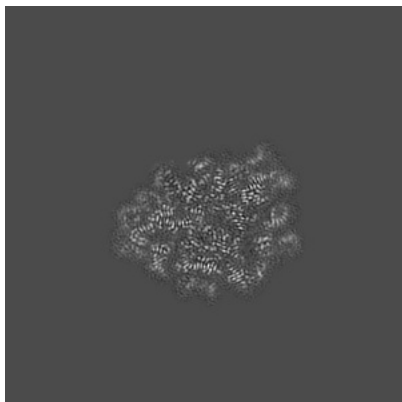
#### 6.2.1 Primary map



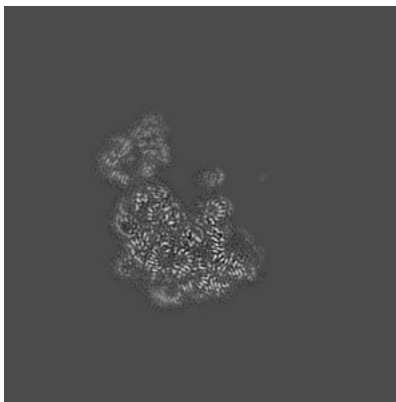
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

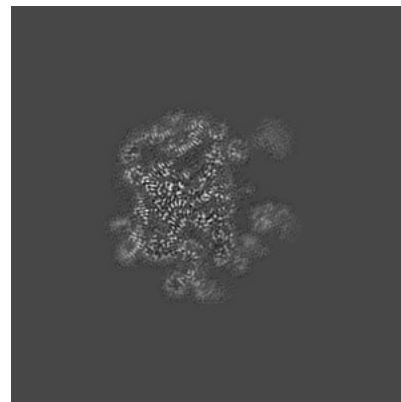
### 6.3.1 Primary map



X Index: 172



Y Index: 182

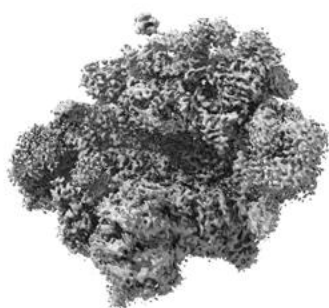


Z Index: 159

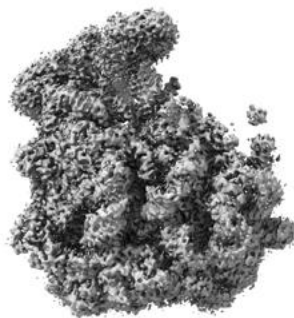
The images above show the largest variance slices of the map in three orthogonal directions.

## 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.

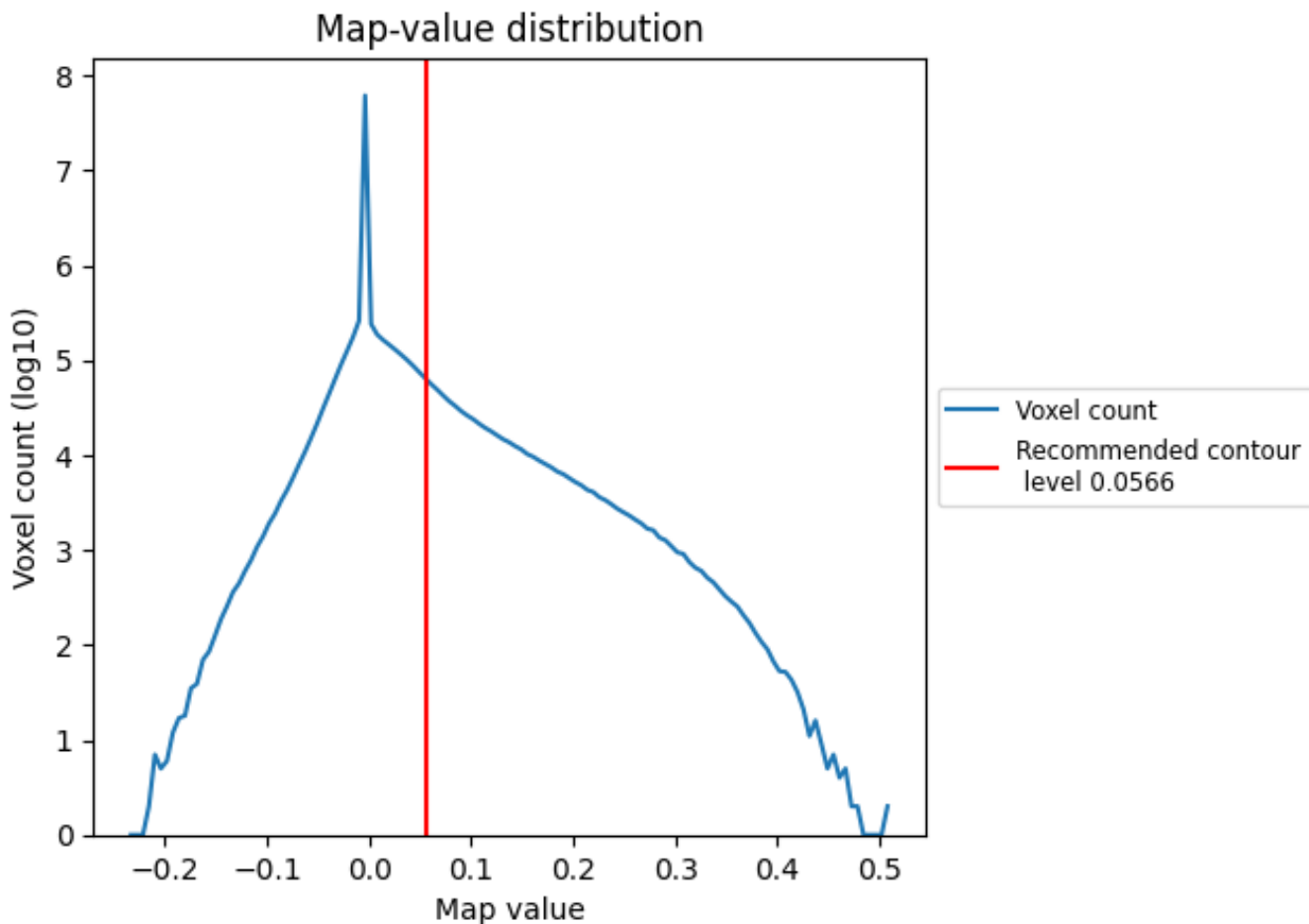
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

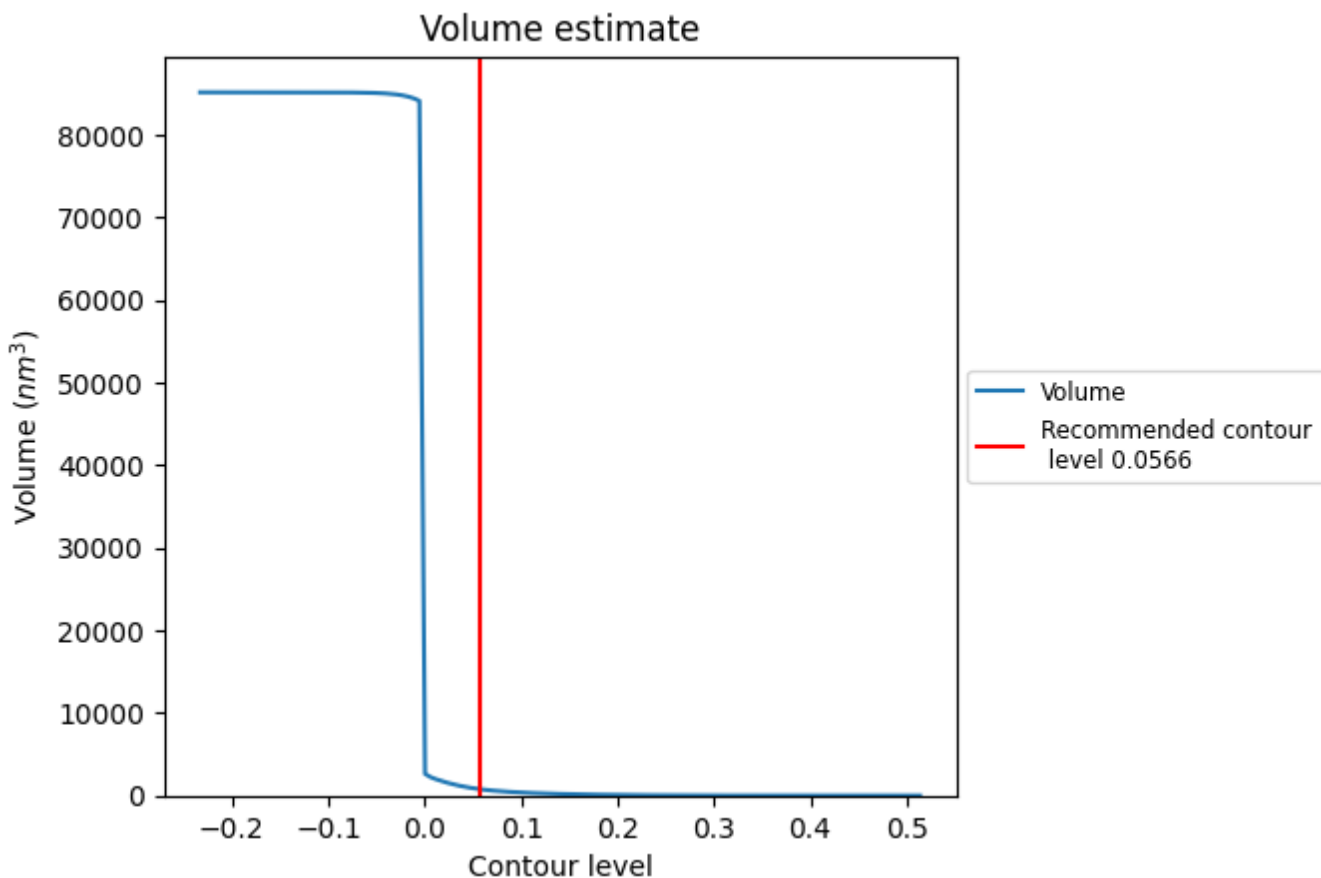
This section contains the results of statistical analysis of the map.

### 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 [\(i\)](#)

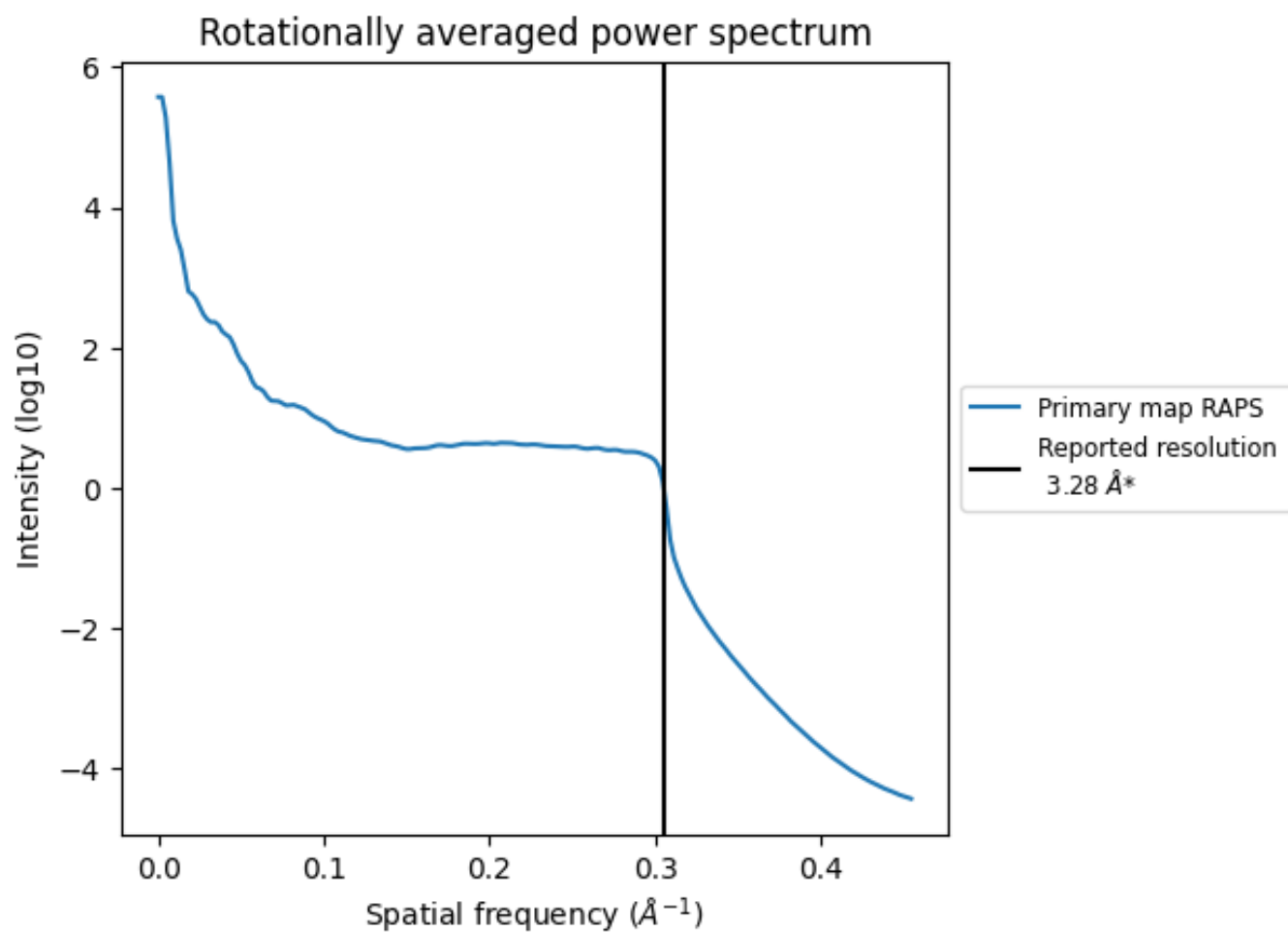


The volume at the recommended contour level is 783  $\text{nm}^3$ ; this corresponds to an approximate mass of 707 kDa.

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  $0.305 \text{\AA}^{-1}$

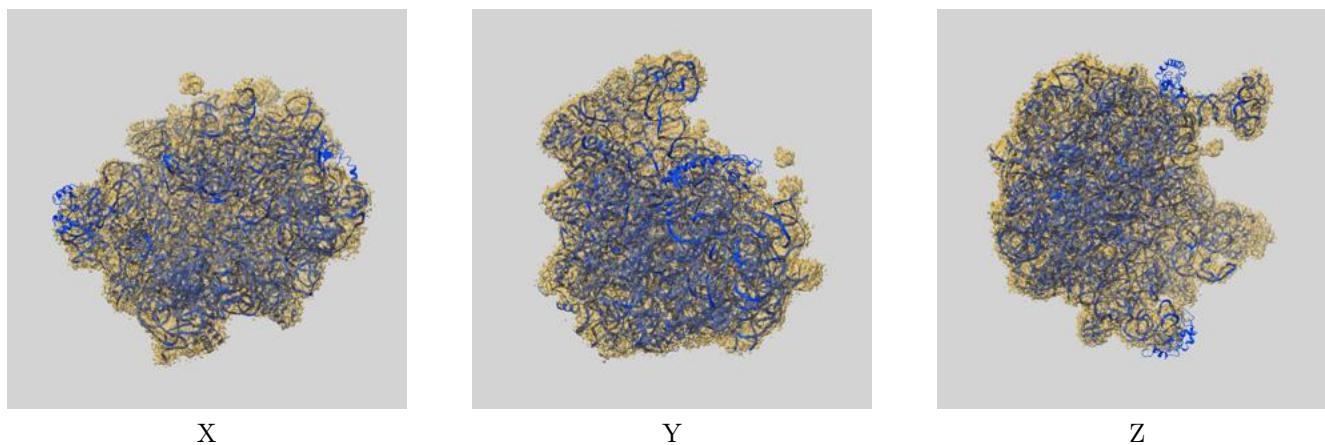
## 8 Fourier-Shell correlation

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-10282 and PDB model 6SPD. Per-residue inclusion information can be found in section 3 on page 10.

### 9.1 Map-model overlay [i](#)



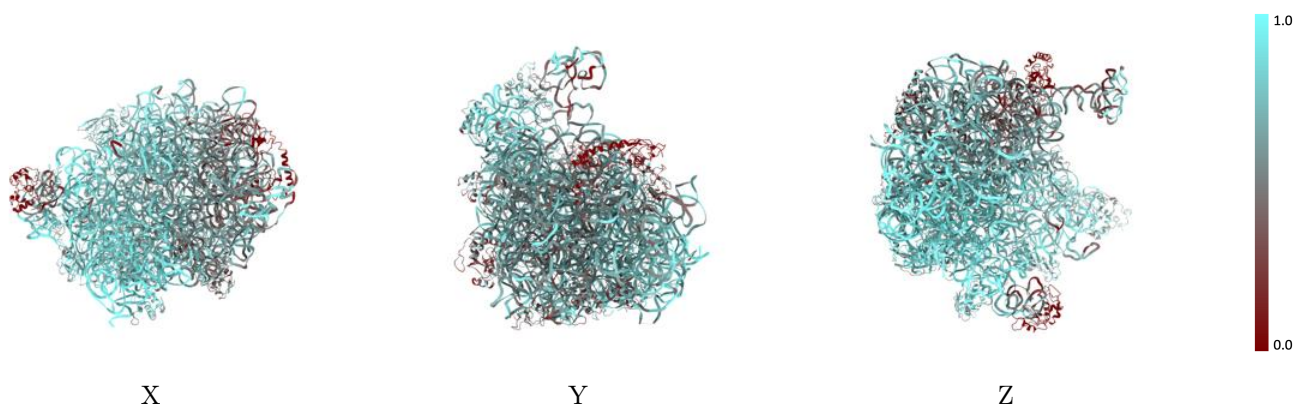
The images above show the 3D surface view of the map at the recommended contour level 0.0566 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



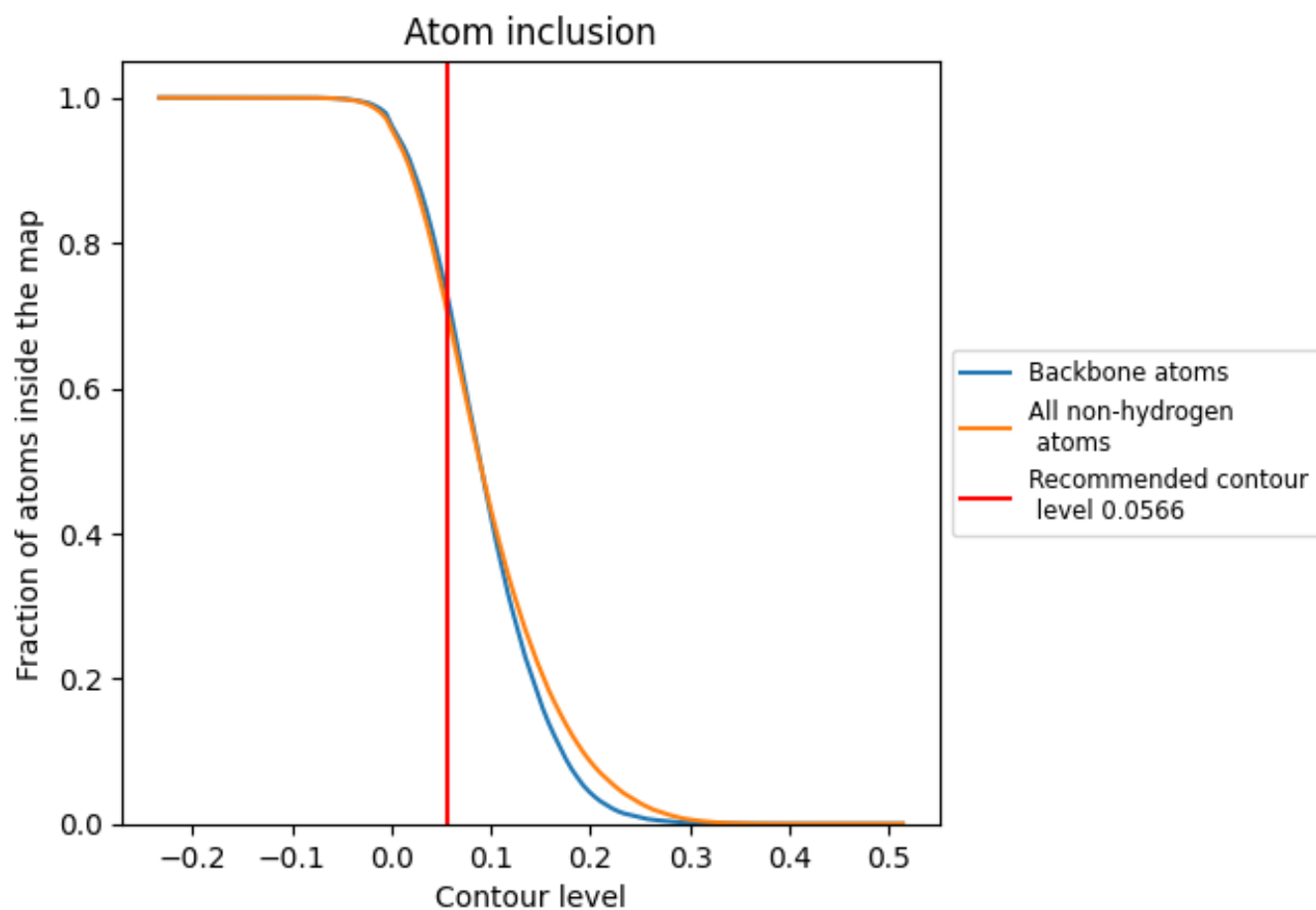
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0566).



































































## 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

