wwPDB EM Validation Summary Report

Nov 4, 2023 – 09:24 AM EDT

PDB ID	:	7LVK
EMDB ID	:	EMD-23539
Title	:	Cfr-modified 50S subunit from Escherichia coli
Authors	:	Stojkovic, V.; Myasnikov, A.G.; Frost, A.; Fujimori, D.G.
Deposited on	:	2021-02-25
Resolution	:	2.20 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 ⓘ 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 ⓘ) were used in the production of this report:

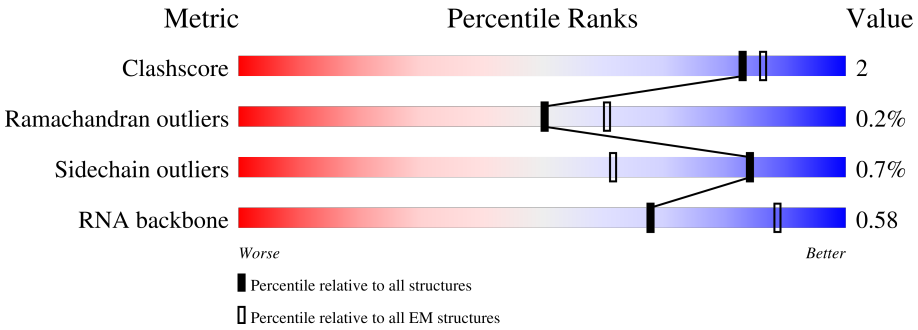
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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	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	I	2904	9% 79% 18%
2	J	120	77% 18%
3	K	273	86% 12%
4	L	209	91% 9%
5	M	201	95%
6	N	179	47% 92% 7%
7	O	177	15% 93% 7%

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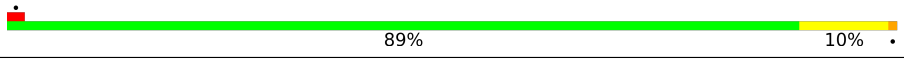
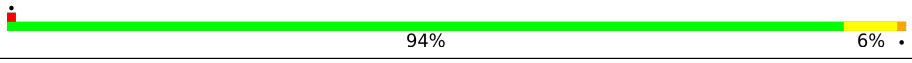
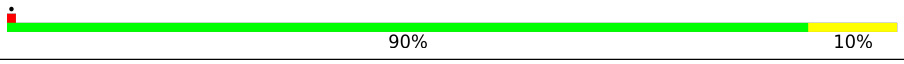
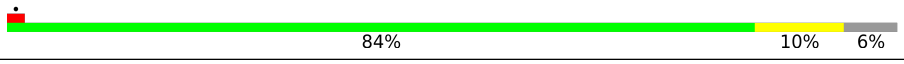
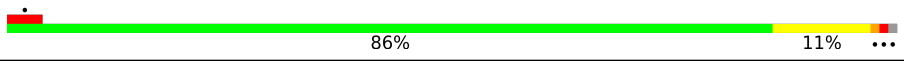
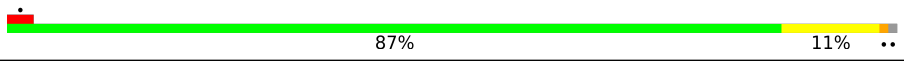
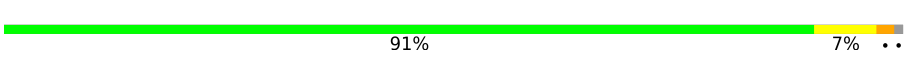
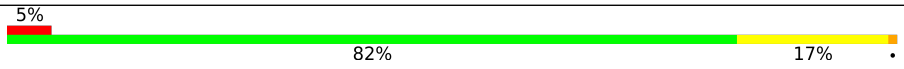
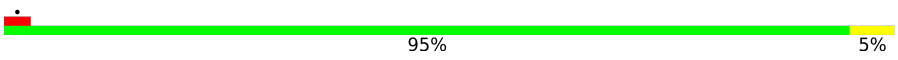
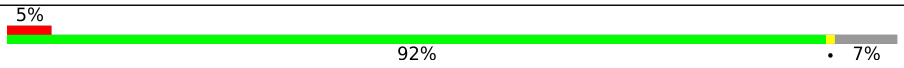
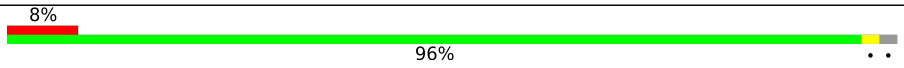
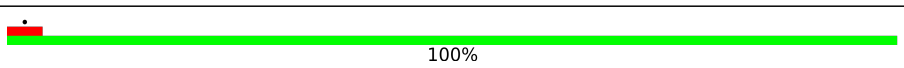
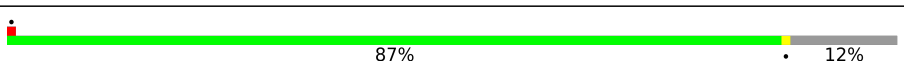
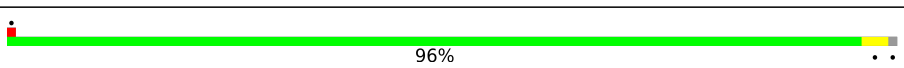
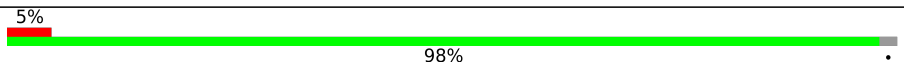
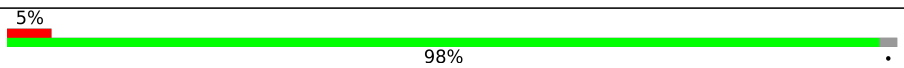
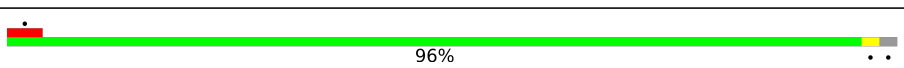
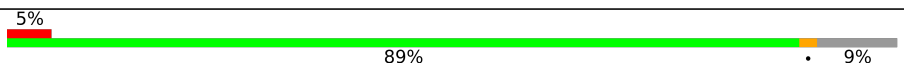
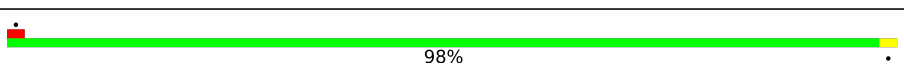
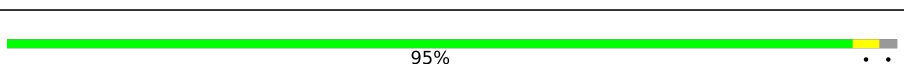
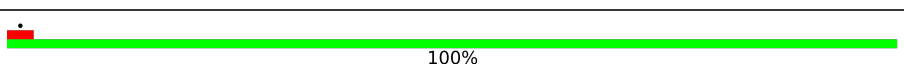
Mol	Chain	Length	Quality of chain
8	P	149	
9	R	142	
10	S	123	
11	T	144	
12	U	136	
13	V	127	
14	W	117	
15	X	115	
16	Y	118	
17	Z	103	
18	a	110	
19	b	100	
20	c	104	
21	d	94	
22	e	85	
23	f	78	
24	g	63	
25	h	59	
26	i	57	
27	j	55	
28	k	46	
29	l	65	
30	m	38	

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 151692 atoms, of which 58960 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 rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	I	2898	93535	27769	31305	11448	20115	2898	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	J	118	3809	1126	1280	464	821	118	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	K	271	4236	1288	2154	423	364	7	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	L	209	3182	979	1617	288	294	4	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	M	201	3171	974	1619	283	290	5	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	N	177	2854	899	1444	249	256	6	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	O	176	Total	C	H	N	O	S	0	0
			2694	832	1371	243	246	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	P	149	Total	C	H	N	O	S	0	0
			2258	699	1148	197	213	1		

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	R	142	Total	C	H	N	O	S	0	0
			2291	714	1162	212	199	4		

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	S	122	Total	C	H	N	O	S	0	0
			1950	587	1012	180	165	6		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	T	144	Total	C	H	N	O	S	0	0
			2182	654	1129	207	190	2		

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	U	136	Total	C	H	N	O	S	0	0
			2229	686	1154	205	178	6		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	V	120	Total	C	H	N	O	S	0	0
			1960	593	1000	196	166	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	116	Total	C	H	N	O	0	0
			1815	552	923	178	162		

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	X	114	Total	C	H	N	O	S	0	0
			1879	574	962	179	163	1		

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Y	117	Total	C	H	N	O	0	0
			1967	604	1020	192	151		

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Z	103	Total	C	H	N	O	S	0	0
			1655	516	839	153	145	2		

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	a	110	Total	C	H	N	O	S	0	0
			1779	532	922	166	156	3		

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	b	93	Total	C	H	N	O	S	0	0
			1545	466	807	139	131	2		

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	c	102	Total	C	H	N	O	0	0
			1610	492	831	146	141		

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	d	94	Total	C	H	N	O	S	0	0
			1533	479	780	137	134	3		

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	e	75	Total	C	H	N	O	S	0	0
			1150	353	581	113	102	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	f	77	Total	C	H	N	O	S	0	0
			1277	388	652	129	106	2		

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	g	62	Total	C	H	N	O	S	0	0
			1032	308	531	98	94	1		

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	h	58	Total	C	H	N	O	S	0	0
			937	281	488	87	79	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
26	i	56	Total	C	H	N	O	S	0	0
			902	269	458	94	80	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	j	50	Total	C	H	N	O	0	0
			849	263	440	75	71		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
28	k	46	Total	C	H	N	O	S	0	0
			795	228	418	90	57	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
29	l	64	Total	C	H	N	O	S	0	0
			1077	323	573	105	74	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
30	m	38	Total	C	H	N	O	S	0	0
			642	185	340	65	48	4		

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
31	I	175	Total	Mg	0
			175	175	
31	J	1	Total	Mg	0
			1	1	
31	K	1	Total	Mg	0
			1	1	
31	L	1	Total	Mg	0
			1	1	
31	W	1	Total	Mg	0
			1	1	

- Molecule 32 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
32	K	1	Total	Na	0
			1	1	

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
33	m	1	Total	Zn	0
			1	1	

- Molecule 34 is water.

Mol	Chain	Residues	Atoms	AltConf
34	I	2340	Total O 2340 2340	0
34	J	34	Total O 34 34	0
34	K	58	Total O 58 58	0
34	L	44	Total O 44 44	0
34	M	22	Total O 22 22	0
34	P	1	Total O 1 1	0
34	R	10	Total O 10 10	0
34	S	11	Total O 11 11	0
34	T	28	Total O 28 28	0
34	U	20	Total O 20 20	0
34	V	15	Total O 15 15	0
34	W	1	Total O 1 1	0
34	X	14	Total O 14 14	0
34	Y	16	Total O 16 16	0
34	Z	12	Total O 12 12	0
34	a	16	Total O 16 16	0
34	b	6	Total O 6 6	0
34	c	1	Total O 1 1	0
34	d	3	Total O 3 3	0
34	e	13	Total O 13 13	0
34	f	6	Total O 6 6	0
34	h	5	Total O 5 5	0

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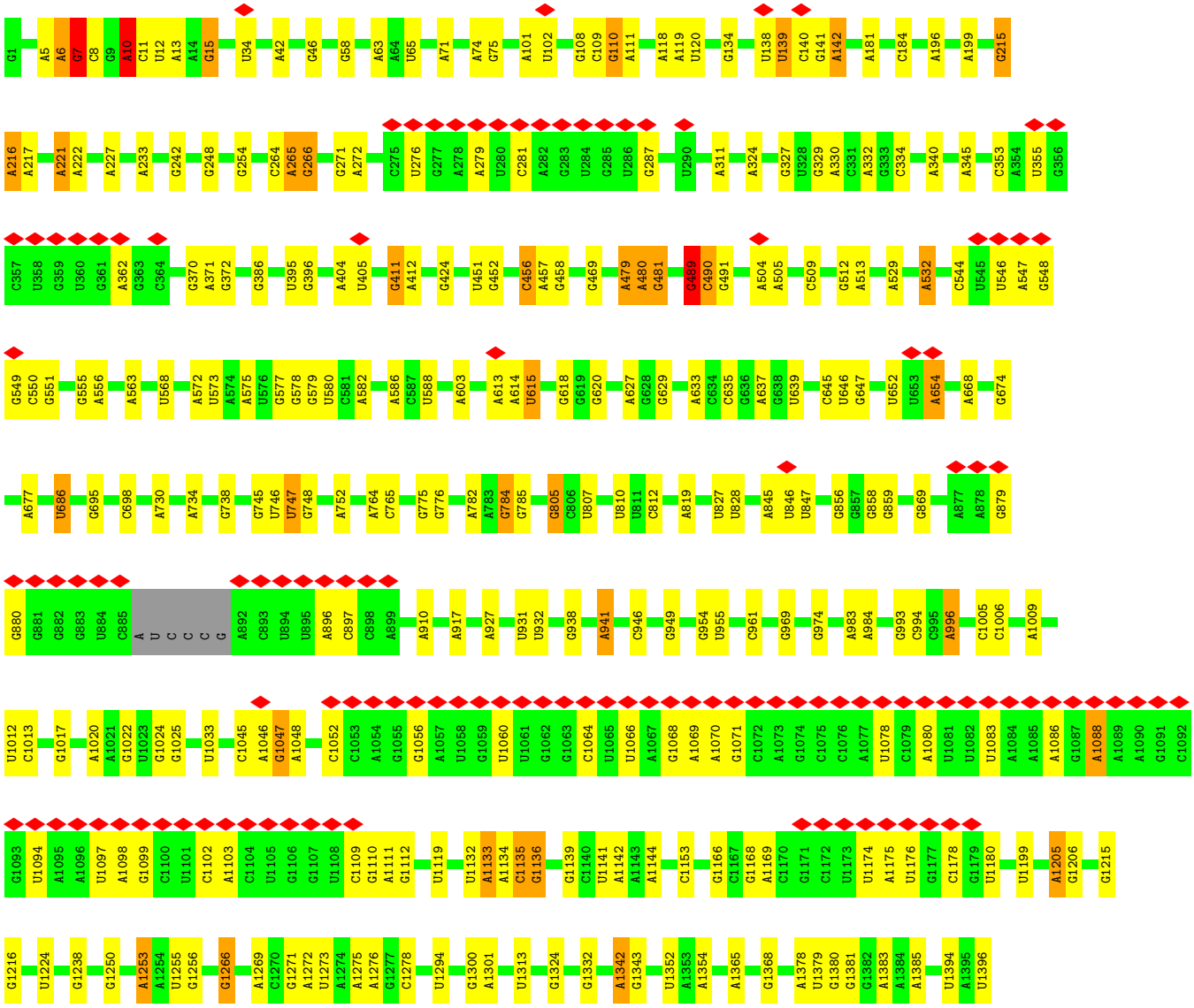
Mol	Chain	Residues	Atoms	AltConf
34	i	10	Total O 10 10	0
34	j	2	Total O 2 2	0
34	k	11	Total O 11 11	0
34	l	13	Total O 13 13	0
34	m	4	Total O 4 4	0

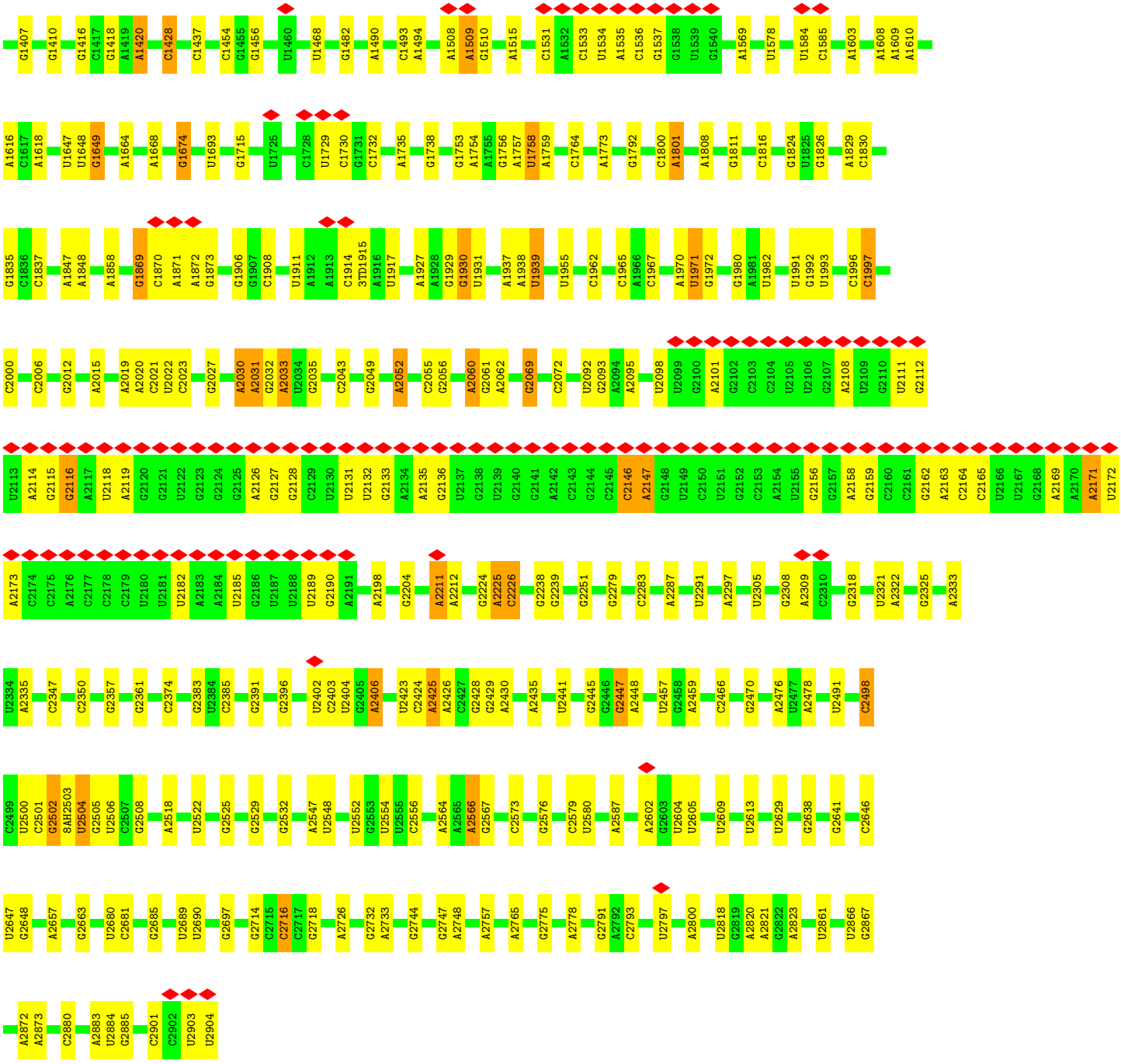
3 Residue-property plots (i)

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

- Molecule 1: 23S rRNA

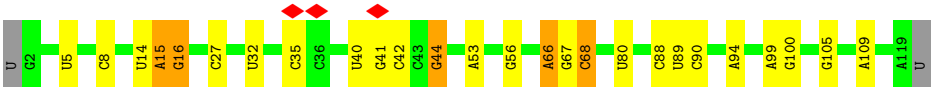
Chain I:





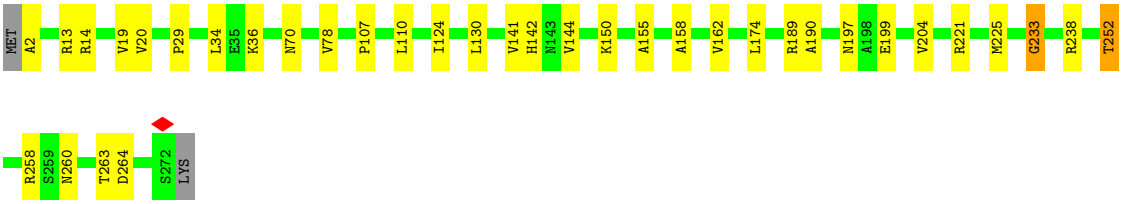
• Molecule 2: 5S rRNA

Chain J:

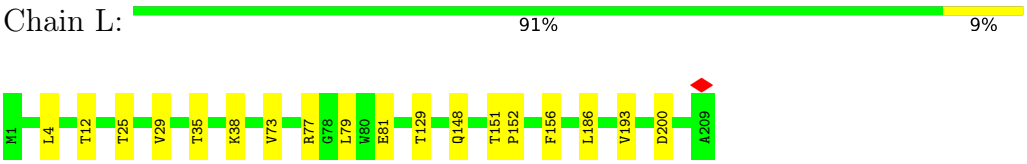


• Molecule 3: 50S ribosomal protein L2

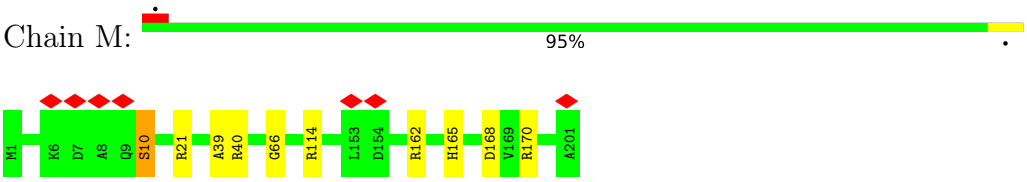
Chain K:



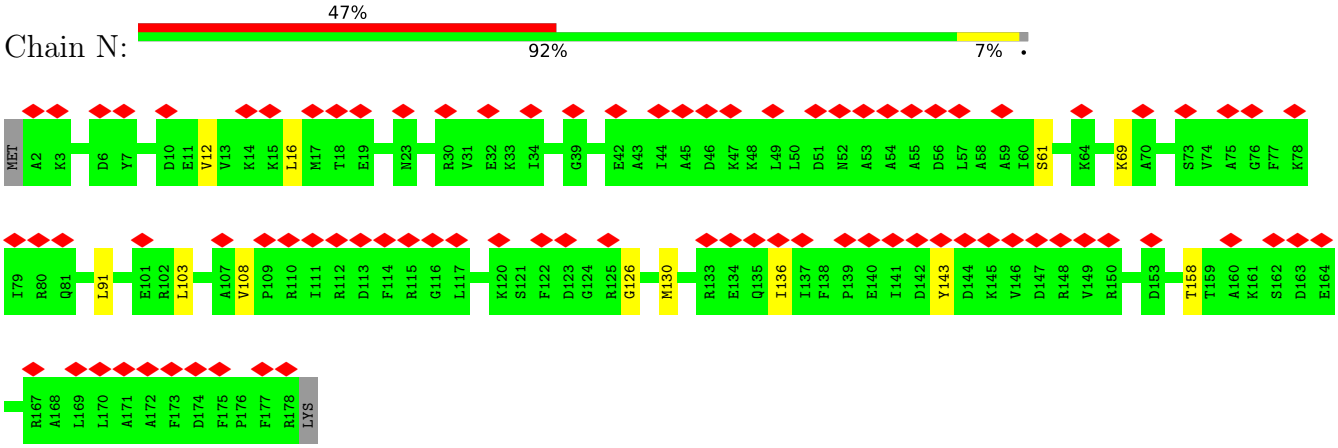
• Molecule 4: 50S ribosomal protein L3



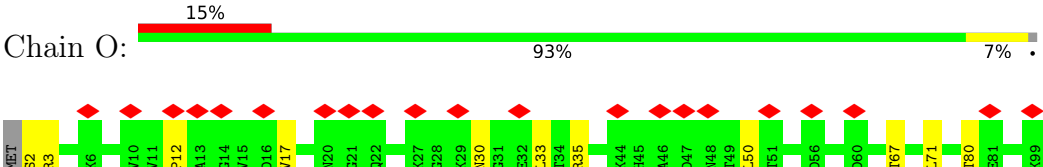
• Molecule 5: 50S ribosomal protein L4



• Molecule 6: 50S ribosomal protein L5

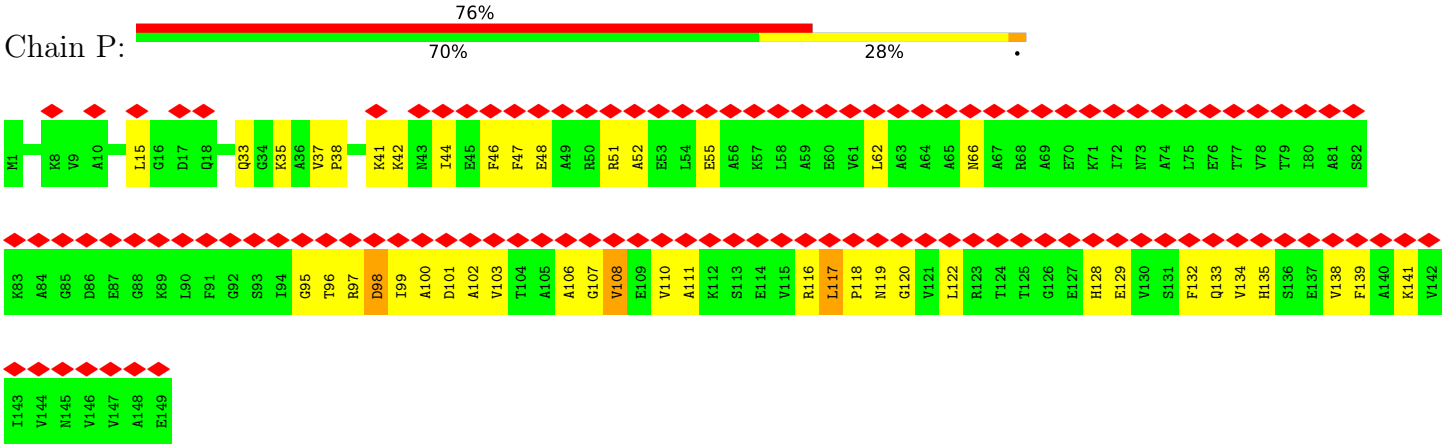


• Molecule 7: 50S ribosomal protein L6



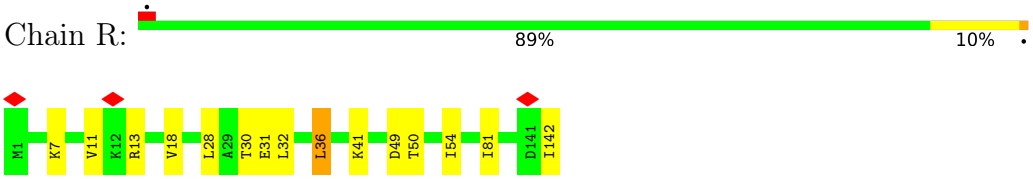
• Molecule 8: 50S ribosomal protein L9

Chain P:



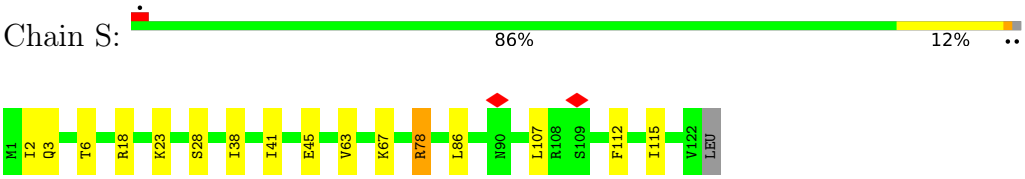
• Molecule 9: 50S ribosomal protein L13

Chain R:



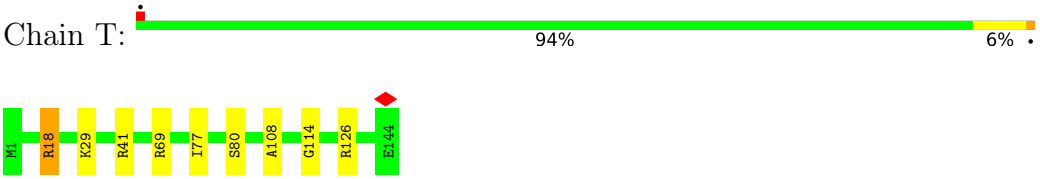
• Molecule 10: 50S ribosomal protein L14

Chain S:



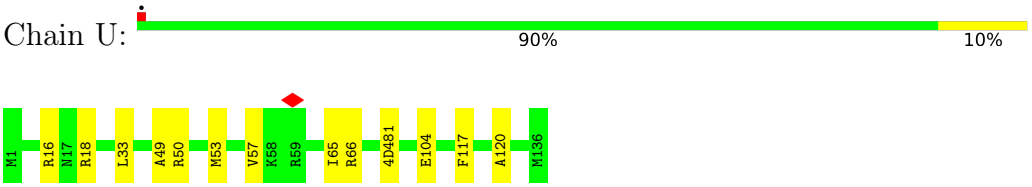
• Molecule 11: 50S ribosomal protein L15

Chain T:



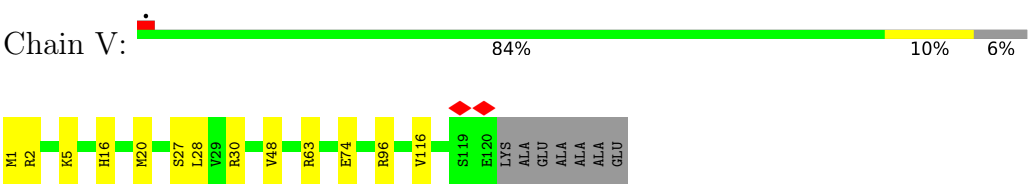
• Molecule 12: 50S ribosomal protein L16

Chain U:



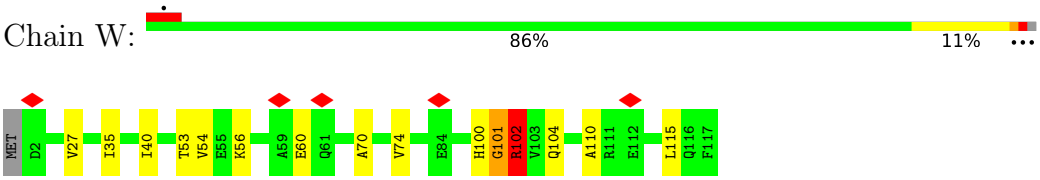
• Molecule 13: 50S ribosomal protein L17

Chain V:



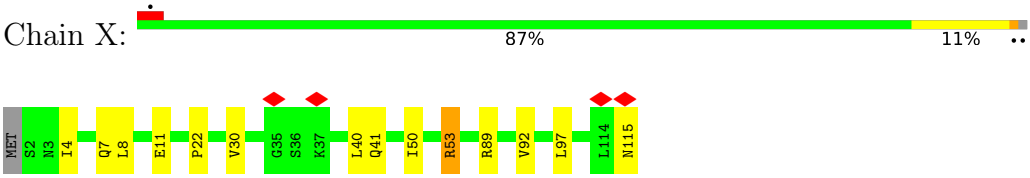
• Molecule 14: 50S ribosomal protein L18

Chain W:



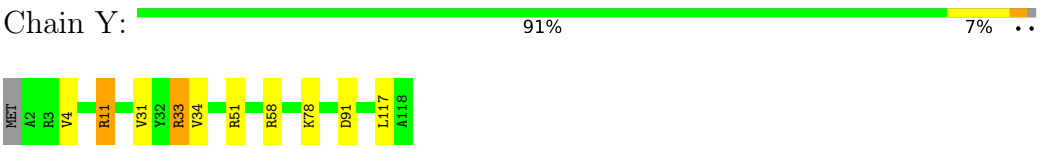
• Molecule 15: 50S ribosomal protein L19

Chain X:



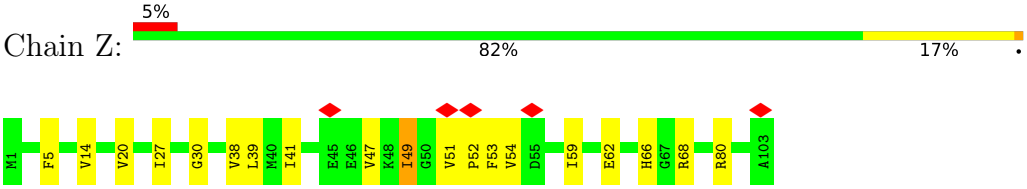
• Molecule 16: 50S ribosomal protein L20

Chain Y:



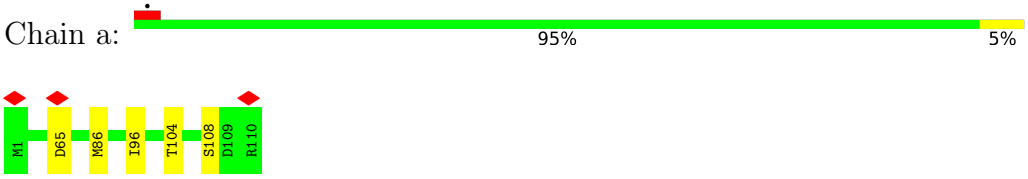
• Molecule 17: 50S ribosomal protein L21

Chain Z:



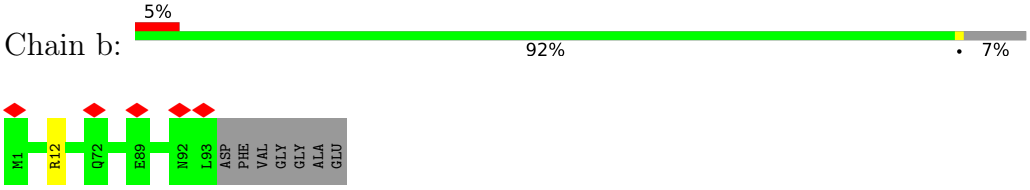
• Molecule 18: 50S ribosomal protein L22

Chain a:



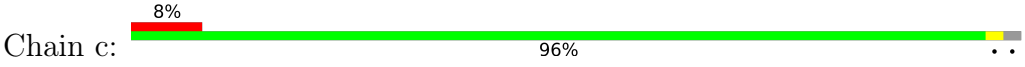
• Molecule 19: 50S ribosomal protein L23

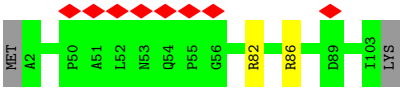
Chain b:



• Molecule 20: 50S ribosomal protein L24

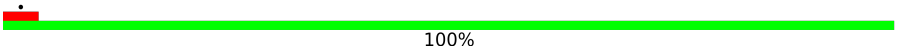
Chain c:

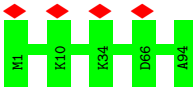




• Molecule 21: 50S ribosomal protein L25

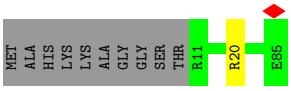
Chain d:





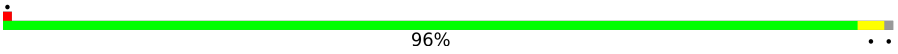
• Molecule 22: 50S ribosomal protein L27

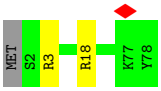
Chain e:



• Molecule 23: 50S ribosomal protein L28

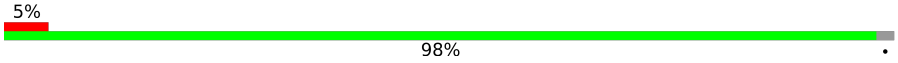
Chain f:

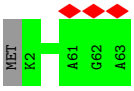




• Molecule 24: 50S ribosomal protein L29

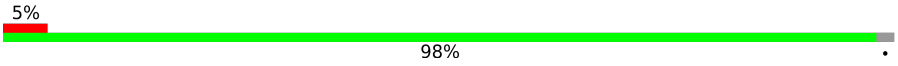
Chain g:

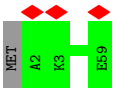




• Molecule 25: 50S ribosomal protein L30

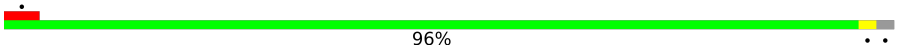
Chain h:

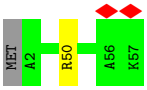




• Molecule 26: 50S ribosomal protein L32

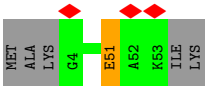
Chain i:





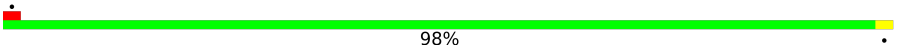
• Molecule 27: 50S ribosomal protein L33

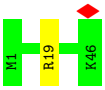
Chain j:



• Molecule 28: 50S ribosomal protein L34

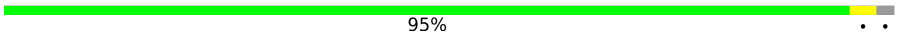
Chain k:





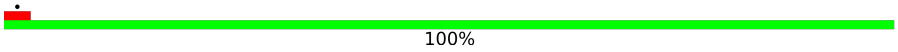
• Molecule 29: 50S ribosomal protein L35

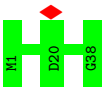
Chain l:



• Molecule 30: 50S ribosomal protein L36

Chain m:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	141549	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.226	Depositor
Minimum map value	-0.114	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	420.864, 420.864, 420.864	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, 5MU, 6MZ, 2MG, G7M, MG, OMU, 8AH, 4D4, OMG, PSU, ZN, NA, 3TD, OMC, 1MG

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	I	0.94	5/69165 (0.0%)	0.97	51/107896 (0.0%)
2	J	0.72	0/2828	0.92	4/4410 (0.1%)
3	K	0.53	1/2121 (0.0%)	0.79	3/2852 (0.1%)
4	L	0.57	1/1586 (0.1%)	0.73	3/2134 (0.1%)
5	M	0.47	0/1571	0.65	1/2113 (0.0%)
6	N	0.32	0/1434	0.62	0/1926
7	O	0.35	0/1343	0.57	0/1816
8	P	0.37	0/1121	0.77	2/1515 (0.1%)
9	R	0.48	0/1152	0.67	2/1551 (0.1%)
10	S	0.48	0/947	0.71	2/1268 (0.2%)
11	T	0.49	0/1062	0.72	1/1413 (0.1%)
12	U	0.47	0/1081	0.66	0/1443
13	V	0.48	0/973	0.72	1/1301 (0.1%)
14	W	0.54	1/902 (0.1%)	0.79	2/1209 (0.2%)
15	X	0.45	0/929	0.69	2/1242 (0.2%)
16	Y	0.56	0/960	0.77	4/1278 (0.3%)
17	Z	0.53	0/829	0.73	0/1107
18	a	0.54	0/864	0.75	0/1156
19	b	0.40	0/744	0.64	0/994
20	c	0.43	0/787	0.70	2/1051 (0.2%)
21	d	0.44	0/766	0.62	0/1025
22	e	0.50	0/576	0.72	2/762 (0.3%)
23	f	0.48	0/635	0.80	2/848 (0.2%)
24	g	0.35	0/502	0.59	0/667
25	h	0.37	0/453	0.65	0/605
26	i	0.45	0/450	0.87	2/599 (0.3%)
27	j	0.50	0/416	0.77	1/554 (0.2%)
28	k	0.48	0/380	0.89	1/498 (0.2%)
29	l	0.54	0/513	0.79	2/676 (0.3%)
30	m	0.46	0/303	0.67	0/397
All	All	0.83	8/97393 (0.0%)	0.92	90/146306 (0.1%)

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
8	P	0	7
14	W	0	1
All	All	0	8

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	W	101	GLY	C-O	-9.96	1.07	1.23
1	I	1757	A	O3'-P	8.88	1.71	1.61
4	L	151	THR	C-O	-7.90	1.08	1.23
1	I	108	G	O3'-P	5.99	1.68	1.61
1	I	2500	U	O3'-P	5.49	1.67	1.61

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	111	A	N9-C1'-C2'	-9.82	101.20	112.00
1	I	6	A	N9-C1'-C2'	-9.36	101.70	112.00
2	J	16	G	N9-C1'-C2'	-9.23	101.84	112.00
1	I	1136	G	N9-C1'-C2'	-8.69	102.44	112.00
2	J	14	U	P-O3'-C3'	8.57	129.99	119.70

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	P	100	ALA	Peptide
8	P	102	ALA	Peptide
8	P	108	VAL	Peptide
8	P	116	ARG	Peptide
8	P	47	PHE	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	I	62230	31305	31306	138	0
2	J	2529	1280	1281	8	0
3	K	2082	2154	2154	30	0
4	L	1565	1617	1616	9	0
5	M	1552	1619	1619	6	0
6	N	1410	1444	1444	7	0
7	O	1323	1371	1371	8	0
8	P	1110	1148	1148	31	0
9	R	1129	1162	1162	11	0
10	S	938	1012	1012	14	0
11	T	1053	1129	1129	8	0
12	U	1075	1154	1154	7	0
13	V	960	1000	1000	9	0
14	W	892	923	923	9	0
15	X	917	962	962	8	0
16	Y	947	1020	1019	8	0
17	Z	816	839	839	20	0
18	a	857	922	922	0	0
19	b	738	807	807	0	0
20	c	779	831	831	0	0
21	d	753	780	780	0	0
22	e	569	581	581	0	0
23	f	625	652	652	0	0
24	g	501	531	531	0	0
25	h	449	488	488	0	0
26	i	444	458	458	0	0
27	j	409	440	440	0	0
28	k	377	418	418	0	0
29	l	504	573	572	0	0
30	m	302	340	340	0	0
31	I	175	0	0	0	0
31	J	1	0	0	0	0
31	K	1	0	0	0	0
31	L	1	0	0	0	0
31	W	1	0	0	0	0
32	K	1	0	0	0	0
33	m	1	0	0	0	0
34	I	2340	0	0	22	0
34	J	34	0	0	2	0
34	K	58	0	0	1	0
34	L	44	0	0	0	0
34	M	22	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	P	1	0	0	0	0
34	R	10	0	0	0	0
34	S	11	0	0	0	0
34	T	28	0	0	0	0
34	U	20	0	0	0	0
34	V	15	0	0	0	0
34	W	1	0	0	0	0
34	X	14	0	0	0	0
34	Y	16	0	0	0	0
34	Z	12	0	0	0	0
34	a	16	0	0	0	0
34	b	6	0	0	0	0
34	c	1	0	0	0	0
34	d	3	0	0	0	0
34	e	13	0	0	0	0
34	f	6	0	0	0	0
34	h	5	0	0	0	0
34	i	10	0	0	0	0
34	j	2	0	0	0	0
34	k	11	0	0	0	0
34	l	13	0	0	0	0
34	m	4	0	0	0	0
All	All	92732	58960	58959	290	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 2.

The worst 5 of 290 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)
14:W:56:LYS:O	14:W:60:GLU:HG2	1.20	1.27
3:K:124:ILE:CD1	3:K:130:LEU:HD11	1.71	1.19
1:I:1250:G:N7	11:T:18:ARG:NH1	1.92	1.16
3:K:124:ILE:HD13	3:K:130:LEU:HD11	1.31	1.09
8:P:108:VAL:O	8:P:139:PHE:O	1.77	1.02

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	K	269/273 (98%)	259 (96%)	10 (4%)	0	100	100
4	L	207/209 (99%)	198 (96%)	8 (4%)	1 (0%)	29	31
5	M	199/201 (99%)	193 (97%)	6 (3%)	0	100	100
6	N	175/179 (98%)	162 (93%)	13 (7%)	0	100	100
7	O	174/177 (98%)	162 (93%)	12 (7%)	0	100	100
8	P	147/149 (99%)	108 (74%)	39 (26%)	0	100	100
9	R	140/142 (99%)	140 (100%)	0	0	100	100
10	S	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
11	T	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
12	U	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
13	V	118/127 (93%)	115 (98%)	3 (2%)	0	100	100
14	W	114/117 (97%)	108 (95%)	5 (4%)	1 (1%)	17	16
15	X	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
16	Y	115/118 (98%)	115 (100%)	0	0	100	100
17	Z	101/103 (98%)	95 (94%)	5 (5%)	1 (1%)	15	14
18	a	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	17	16
19	b	91/100 (91%)	88 (97%)	3 (3%)	0	100	100
20	c	100/104 (96%)	91 (91%)	9 (9%)	0	100	100
21	d	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
22	e	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
23	f	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
24	g	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
25	h	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
26	i	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
27	j	48/55 (87%)	45 (94%)	2 (4%)	1 (2%)	7	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
28	k	44/46 (96%)	43 (98%)	1 (2%)	0	100 100
29	l	62/65 (95%)	59 (95%)	3 (5%)	0	100 100
30	m	36/38 (95%)	33 (92%)	3 (8%)	0	100 100
All	All	3165/3267 (97%)	3000 (95%)	160 (5%)	5 (0%)	50 55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	W	102	ARG
18	a	65	ASP
17	Z	52	PRO
27	j	51	GLU
4	L	152	PRO

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	K	216/218 (99%)	214 (99%)	2 (1%)	78 88
4	L	164/164 (100%)	163 (99%)	1 (1%)	86 93
5	M	165/165 (100%)	163 (99%)	2 (1%)	71 83
6	N	148/150 (99%)	148 (100%)	0	100 100
7	O	137/138 (99%)	137 (100%)	0	100 100
8	P	114/114 (100%)	113 (99%)	1 (1%)	78 88
9	R	116/116 (100%)	116 (100%)	0	100 100
10	S	103/104 (99%)	103 (100%)	0	100 100
11	T	103/103 (100%)	102 (99%)	1 (1%)	76 86
12	U	108/108 (100%)	108 (100%)	0	100 100
13	V	100/103 (97%)	98 (98%)	2 (2%)	55 69
14	W	86/87 (99%)	85 (99%)	1 (1%)	71 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	X	99/100 (99%)	98 (99%)	1 (1%)	76 86
16	Y	89/90 (99%)	89 (100%)	0	100 100
17	Z	84/84 (100%)	82 (98%)	2 (2%)	49 62
18	a	93/93 (100%)	89 (96%)	4 (4%)	29 36
19	b	80/84 (95%)	79 (99%)	1 (1%)	69 81
20	c	83/85 (98%)	83 (100%)	0	100 100
21	d	78/78 (100%)	78 (100%)	0	100 100
22	e	56/63 (89%)	56 (100%)	0	100 100
23	f	67/68 (98%)	67 (100%)	0	100 100
24	g	54/55 (98%)	54 (100%)	0	100 100
25	h	48/49 (98%)	48 (100%)	0	100 100
26	i	47/48 (98%)	47 (100%)	0	100 100
27	j	45/49 (92%)	45 (100%)	0	100 100
28	k	38/38 (100%)	38 (100%)	0	100 100
29	l	51/52 (98%)	50 (98%)	1 (2%)	55 69
30	m	34/34 (100%)	34 (100%)	0	100 100
All	All	2606/2640 (99%)	2587 (99%)	19 (1%)	84 91

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	a	96	ILE
19	b	12	ARG
29	l	31	HIS
18	a	108	SER
13	V	20	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	2892/2904 (99%)	391 (13%)	30 (1%)
2	J	117/120 (97%)	16 (13%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	3009/3024 (99%)	407 (13%)	31 (1%)

5 of 407 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	7	G
1	I	10	A
1	I	15	G
1	I	34	U
1	I	42	A

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	I	1758	U
1	I	2866	U
1	I	2031	A
1	I	2903	U
1	I	2501	C

5.4 Non-standard residues in protein, DNA, RNA chains (i)

23 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	I	2580	1	18,21,22	1.77	6 (33%)	22,30,33	1.72	5 (22%)
1	OMG	I	2251	1	18,26,27	2.30	8 (44%)	19,38,41	1.34	3 (15%)
1	PSU	I	1911	1	18,21,22	1.45	4 (22%)	22,30,33	1.86	3 (13%)
1	OMC	I	2498	31,1	19,22,23	2.65	7 (36%)	26,31,34	0.72	0
12	4D4	U	81	12	9,11,12	2.52	2 (22%)	8,13,15	0.61	0
1	1MG	I	745	1	18,26,27	2.81	5 (27%)	19,39,42	1.48	4 (21%)
1	8AH	I	2503	31,1	20,26,27	3.78	6 (30%)	23,39,42	1.81	4 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	I	2504	1	18,21,22	1.44	3 (16%)	22,30,33	2.32	8 (36%)
1	PSU	I	955	1	18,21,22	1.60	5 (27%)	22,30,33	1.71	4 (18%)
1	PSU	I	746	1	18,21,22	1.54	5 (27%)	22,30,33	1.74	4 (18%)
1	6MZ	I	1618	1	18,25,26	1.80	2 (11%)	16,36,39	2.57	2 (12%)
1	2MG	I	2445	1	18,26,27	2.19	7 (38%)	16,38,41	1.09	2 (12%)
1	PSU	I	1917	1	18,21,22	1.41	3 (16%)	22,30,33	1.88	4 (18%)
1	PSU	I	2457	1	18,21,22	1.67	4 (22%)	22,30,33	1.75	3 (13%)
1	3TD	I	1915	1	18,22,23	4.25	8 (44%)	22,32,35	1.60	2 (9%)
1	5MU	I	1939	1	19,22,23	4.58	7 (36%)	28,32,35	3.61	9 (32%)
1	2MG	I	1835	1	18,26,27	2.28	7 (38%)	16,38,41	1.18	3 (18%)
1	5MU	I	747	1	19,22,23	4.67	7 (36%)	28,32,35	3.58	8 (28%)
1	G7M	I	2069	1	20,26,27	2.12	7 (35%)	17,39,42	1.29	2 (11%)
1	OMU	I	2552	1	19,22,23	2.84	7 (36%)	26,31,34	1.67	4 (15%)
1	5MC	I	1962	1	18,22,23	3.16	7 (38%)	26,32,35	1.03	2 (7%)
1	6MZ	I	2030	1	18,25,26	1.88	4 (22%)	16,36,39	2.65	6 (37%)
1	PSU	I	2605	1	18,21,22	1.67	4 (22%)	22,30,33	1.64	4 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	I	2580	1	-	0/7/25/26	0/2/2/2
1	OMG	I	2251	1	-	0/5/27/28	0/3/3/3
1	PSU	I	1911	1	-	0/7/25/26	0/2/2/2
1	OMC	I	2498	31,1	-	0/9/27/28	0/2/2/2
12	4D4	U	81	12	-	1/11/12/14	-
1	1MG	I	745	1	-	0/3/25/26	0/3/3/3
1	8AH	I	2503	31,1	-	2/3/25/26	0/3/3/3
1	PSU	I	2504	1	-	2/7/25/26	0/2/2/2
1	PSU	I	955	1	-	0/7/25/26	0/2/2/2
1	PSU	I	746	1	-	1/7/25/26	0/2/2/2
1	6MZ	I	1618	1	-	0/5/27/28	0/3/3/3
1	2MG	I	2445	1	-	1/5/27/28	0/3/3/3
1	PSU	I	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2457	1	-	0/7/25/26	0/2/2/2
1	3TD	I	1915	1	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	I	1939	1	-	0/7/25/26	0/2/2/2
1	2MG	I	1835	1	-	2/5/27/28	0/3/3/3
1	5MU	I	747	1	-	0/7/25/26	0/2/2/2
1	G7M	I	2069	1	-	2/3/25/26	0/3/3/3
1	OMU	I	2552	1	-	0/9/27/28	0/2/2/2
1	5MC	I	1962	1	-	0/7/25/26	0/2/2/2
1	6MZ	I	2030	1	-	2/5/27/28	0/3/3/3
1	PSU	I	2605	1	-	0/7/25/26	0/2/2/2

The worst 5 of 125 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	1915	3TD	C6-C5	12.42	1.49	1.35
1	I	2503	8AH	O4'-C1'	-10.59	1.26	1.41
1	I	747	5MU	C2-N1	10.30	1.55	1.38
1	I	747	5MU	C6-N1	10.28	1.55	1.38
1	I	1939	5MU	C6-N1	9.94	1.55	1.38

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	1939	5MU	C5-C4-N3	11.90	125.47	115.31
1	I	747	5MU	C5-C4-N3	11.63	125.24	115.31
1	I	1939	5MU	C5-C6-N1	-9.85	113.20	123.34
1	I	747	5MU	C5-C6-N1	-9.45	113.62	123.34
1	I	1618	6MZ	C1'-N9-C4	-8.68	111.38	126.64

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	2030	6MZ	O4'-C4'-C5'-O5'
1	I	2030	6MZ	C3'-C4'-C5'-O5'
1	I	2504	PSU	C3'-C4'-C5'-O5'
1	I	2504	PSU	O4'-C4'-C5'-O5'
1	I	2445	2MG	C3'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	2498	OMC	1	0
1	I	1939	5MU	1	0
1	I	2030	6MZ	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 181 ligands modelled in this entry, 181 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

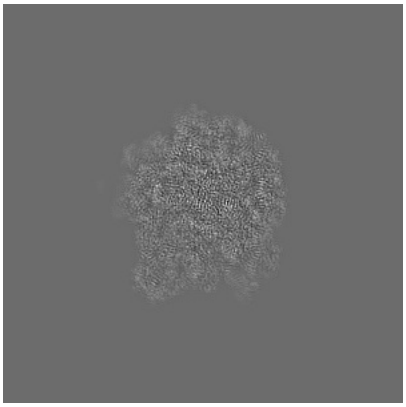
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23539. These allow visual inspection of the internal detail of the map and identification of artifacts.

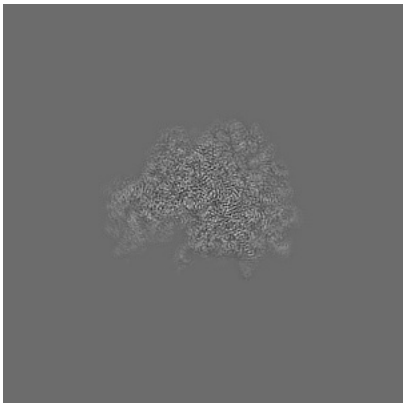
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

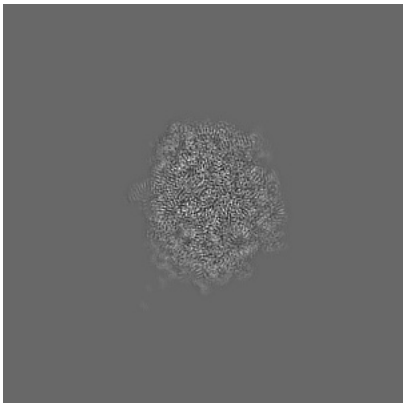
6.1.1 Primary map



X



Y

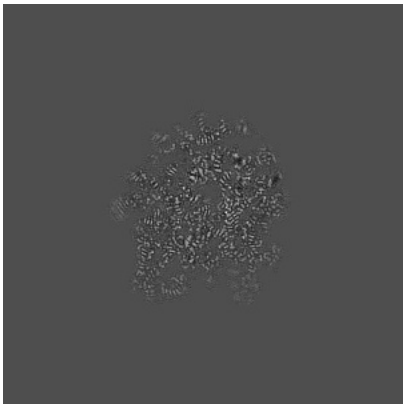


Z

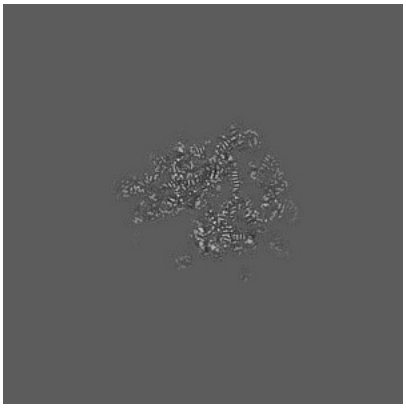
The images above show the map projected in three orthogonal directions.

6.2 Central slices

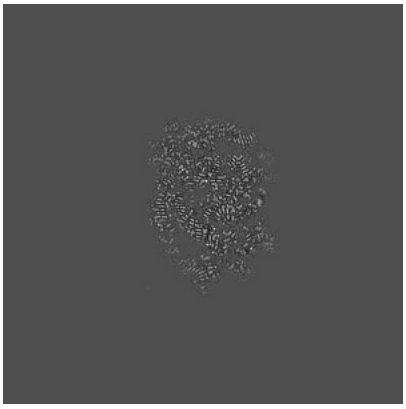
6.2.1 Primary map



X Index: 256



Y Index: 256



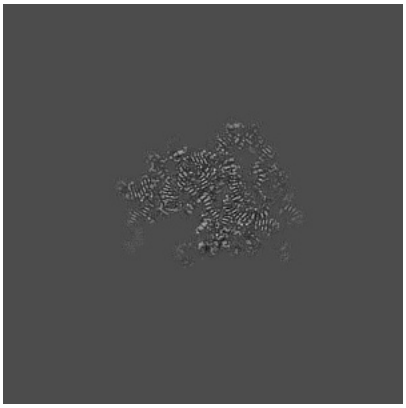
Z Index: 256

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

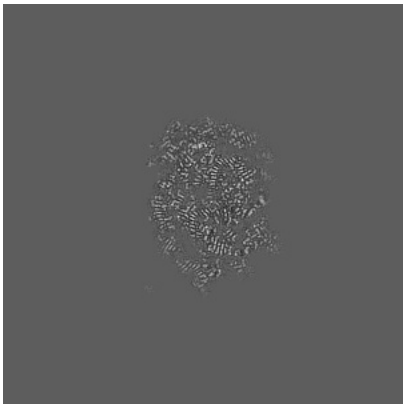
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 265



Y Index: 247

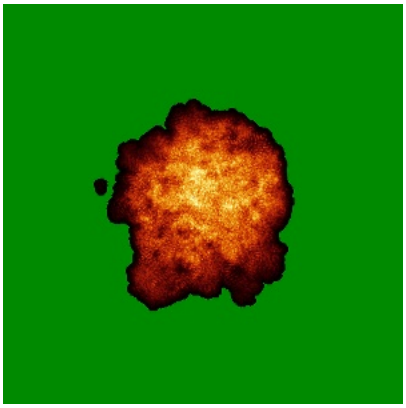


Z Index: 259

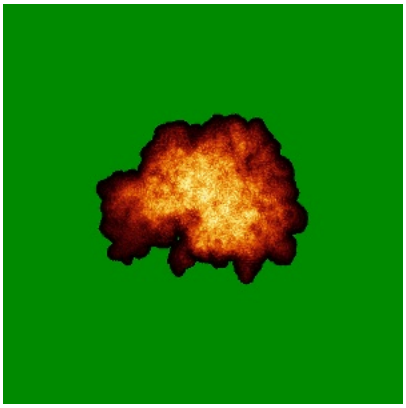
The images above show the largest variance slices of the map in three orthogonal directions.

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

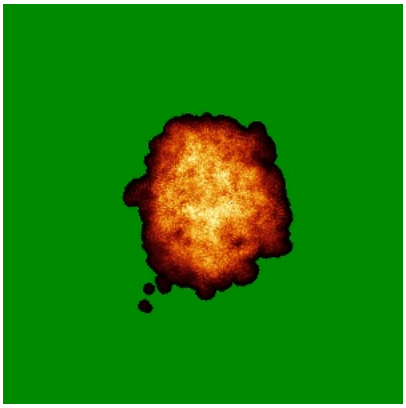
6.4.1 Primary map



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.

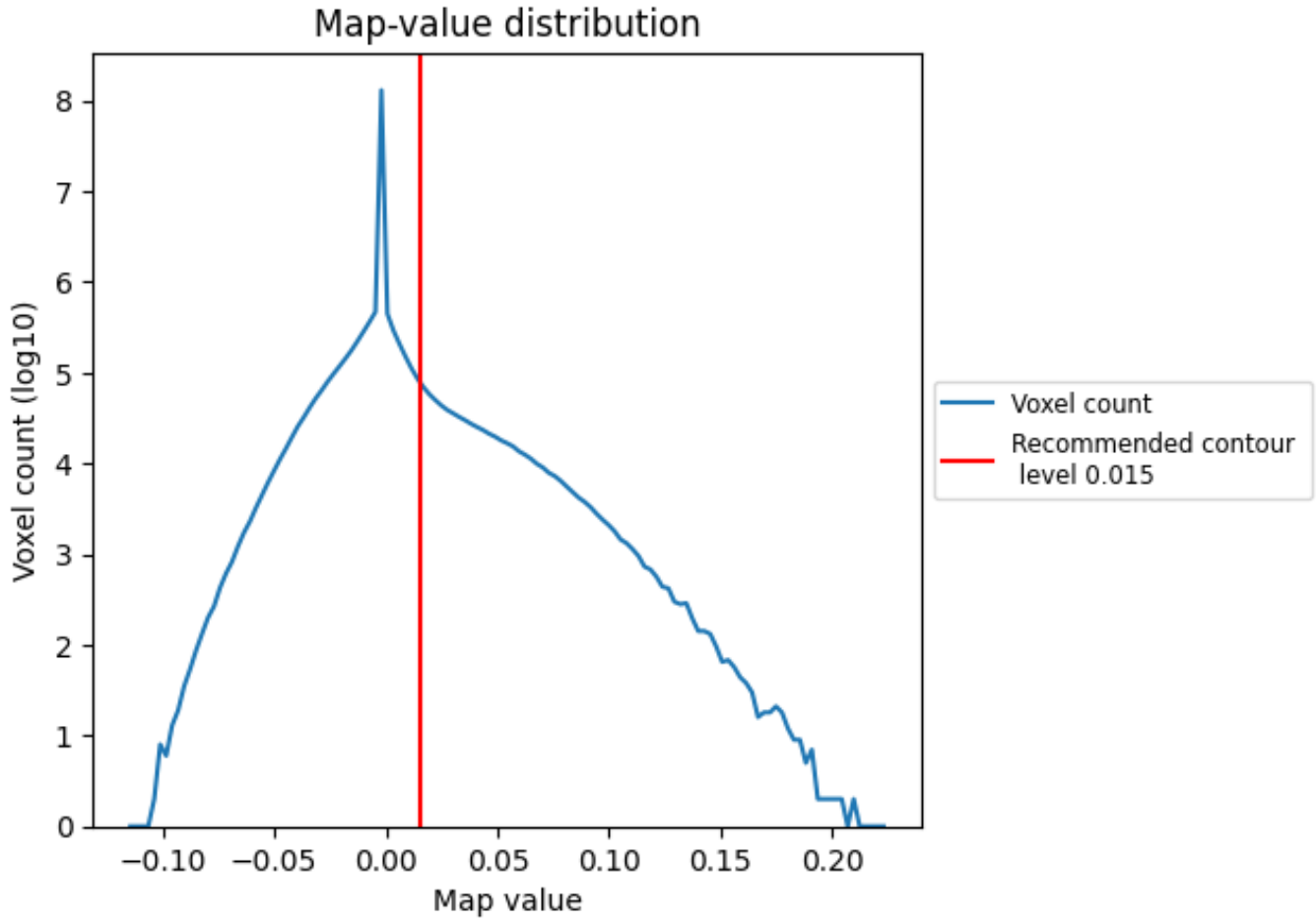
6.6 Mask visualisation (i)

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

7 Map analysis

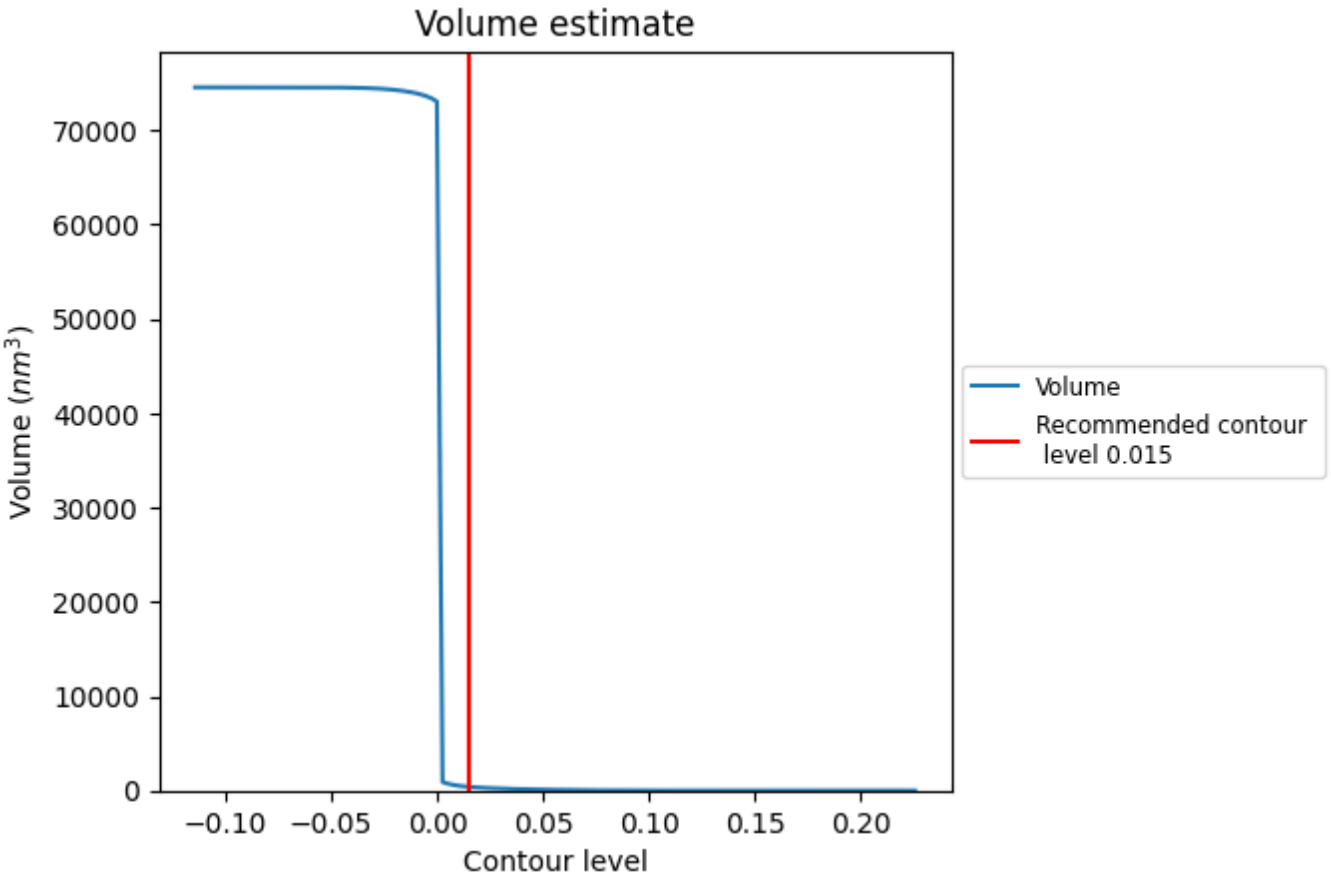
This section contains the results of statistical analysis of the map.

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.

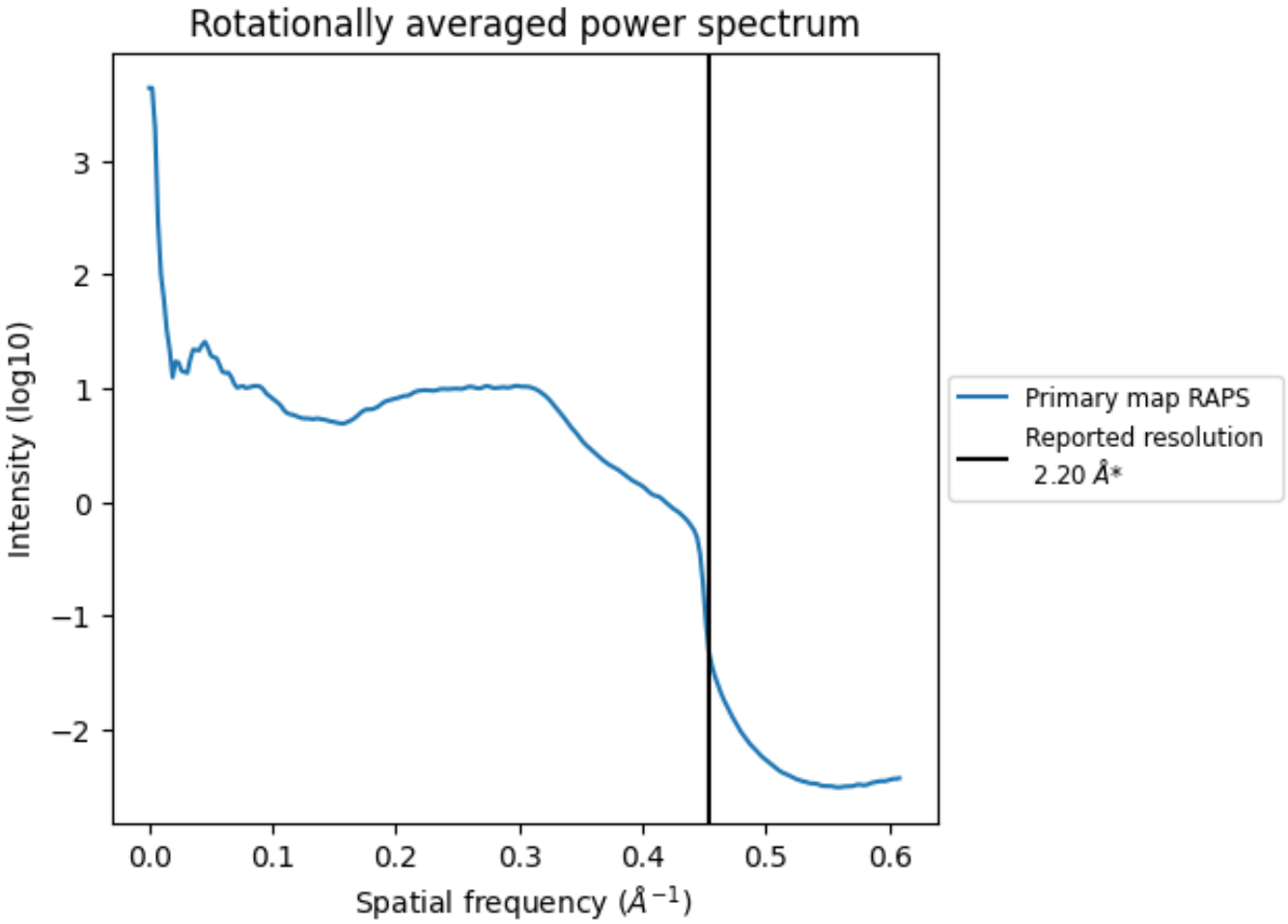
7.2 Volume estimate (i)



The volume at the recommended contour level is 389 nm^3; this corresponds to an approximate mass of 352 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 0.455 Å^{-1}

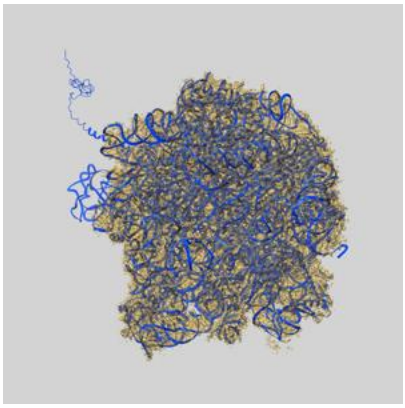
8 Fourier-Shell correlation (i)

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

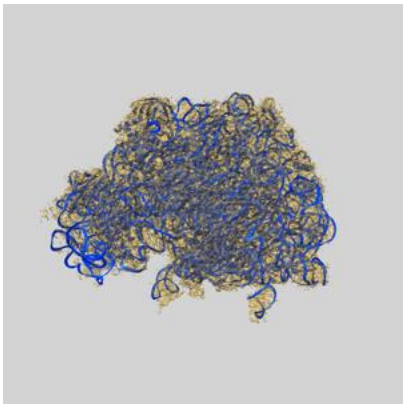
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23539 and PDB model 7LVK. Per-residue inclusion information can be found in section 3 on page 11.

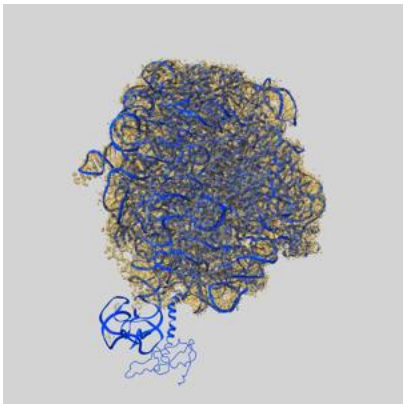
9.1 Map-model overlay



X



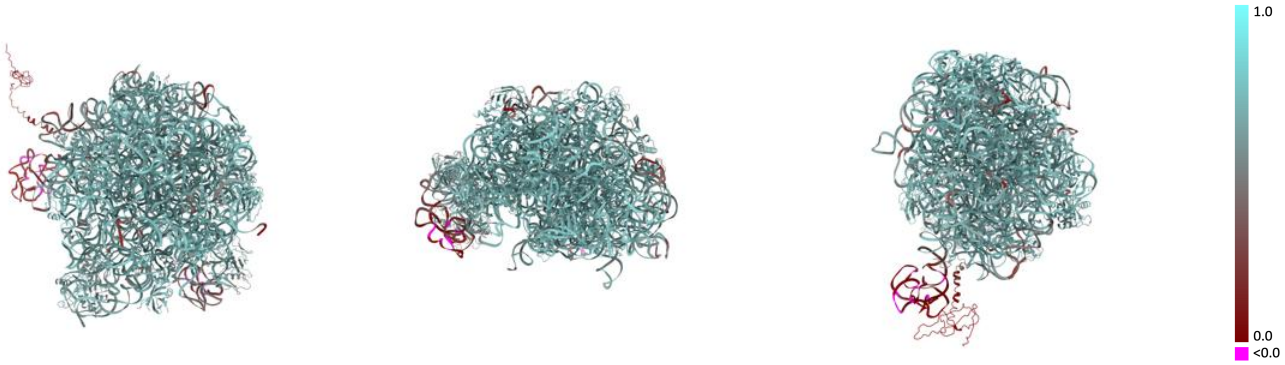
Y



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.

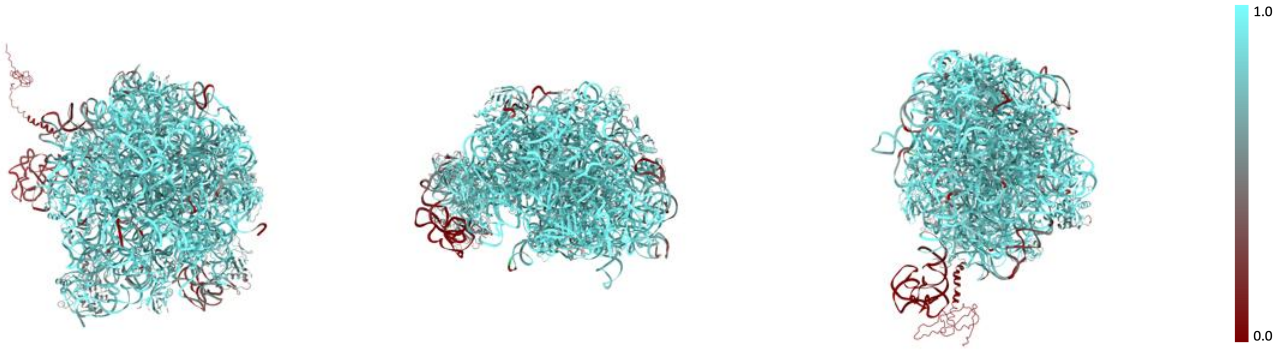
9.2 Q-score mapped to coordinate model



X Y Z

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

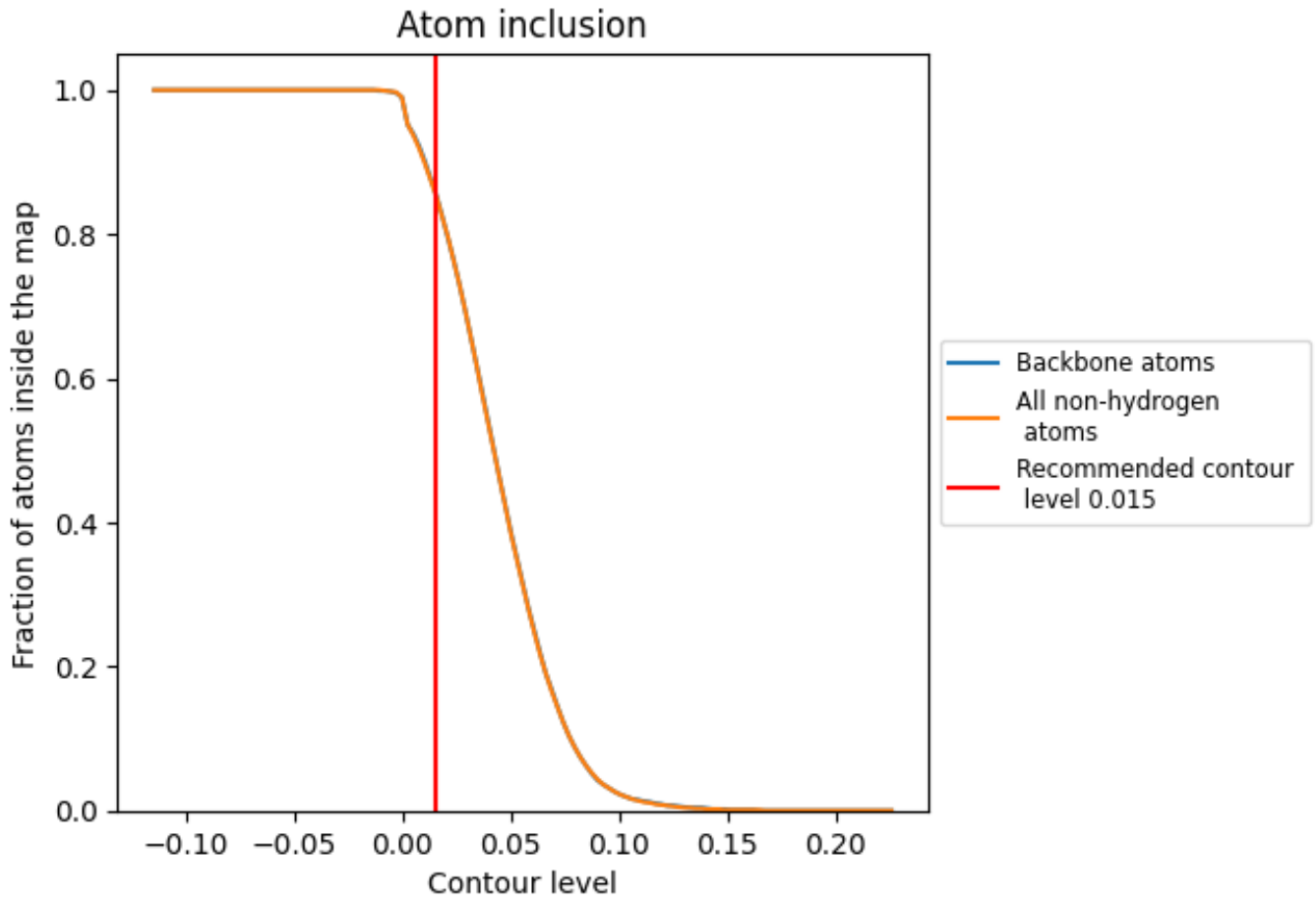
9.3 Atom inclusion mapped to coordinate model



X Y Z

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

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	0.6460
I	0.8760	0.6460
J	0.8650	0.6430
K	0.9270	0.7040
L	0.9050	0.6950
M	0.8520	0.6740
N	0.4640	0.5220
O	0.6740	0.5900
P	0.2050	0.1920
R	0.9140	0.7020
S	0.8830	0.6800
T	0.8960	0.6870
U	0.9010	0.6880
V	0.9360	0.7120
W	0.8080	0.6490
X	0.8790	0.6870
Y	0.9470	0.7200
Z	0.8620	0.6530
a	0.8820	0.6840
b	0.8170	0.6460
c	0.7930	0.6310
d	0.8250	0.6580
e	0.9100	0.7020
f	0.8920	0.6940
g	0.7910	0.6410
h	0.8760	0.6720
i	0.8900	0.6850
j	0.8000	0.6360
k	0.9520	0.7180
l	0.9510	0.7190
m	0.9010	0.6850