



wwPDB EM Validation Summary Report ⓘ

Oct 20, 2024 – 11:19 AM EDT

PDB ID : 6VWM
EMDB ID : EMD-21421
Title : 70S ribosome bound to HIV frameshifting stem-loop (FSS) and P-site tRNA (non-rotated conformation, Structure I)
Authors : Loerch, S.; Bao, C.; Ling, C.; Korostelev, A.A.; Grigorieff, N.; Ermolenko, D.M.
Deposited on : 2020-02-20
Resolution : 3.40 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:

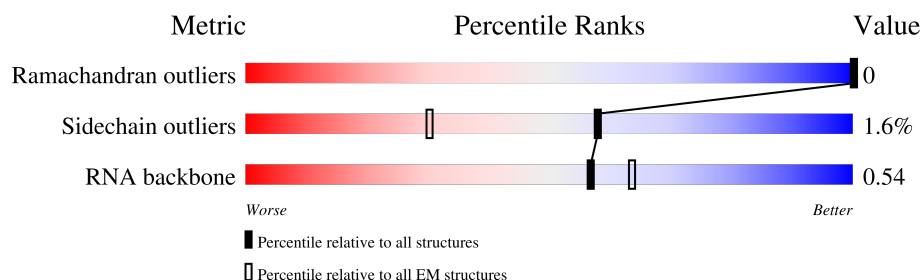
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) :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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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




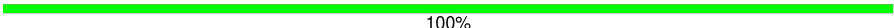
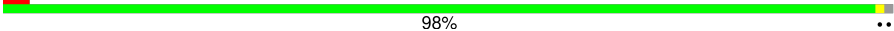
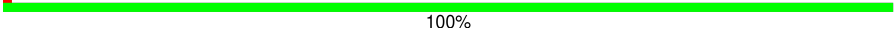

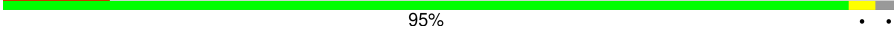
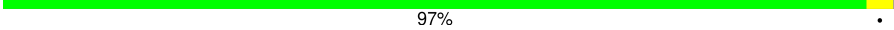
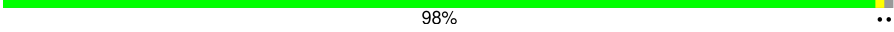
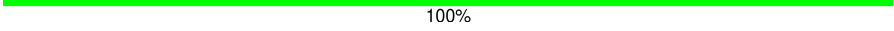
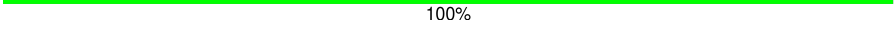


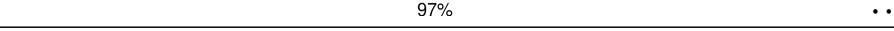

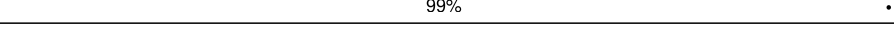
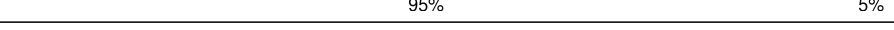
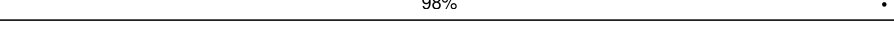
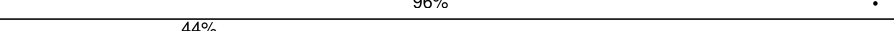

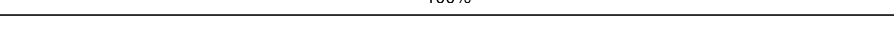
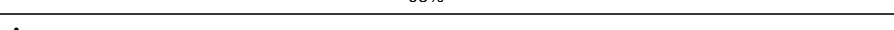
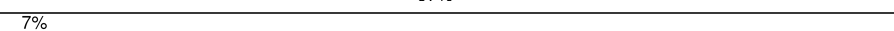



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	3	120	
2	5	76	
3	A	273	
4	B	209	
5	C	201	
6	D	179	
7	E	177	
8	G	149	

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Mol	Chain	Length	Quality of chain
9	H	142	 99%
10	I	123	 100%
11	J	144	 98%
12	K	136	 100%
13	L	127	 94% 6%
14	M	117	 95% 12%
15	N	115	 97%
16	O	118	 98%
17	P	103	 100% 5%
18	Q	110	 100%
19	R	100	 90% 10%
20	S	104	 91% 8%
21	T	94	 97% 6%
22	U	85	 86% 12%
23	V	78	 99%
24	W	63	 95% 5%
25	X	59	 98%
26	Y	57	 96%
27	Z	55	 87% 44% 13%
28	AA	46	 100%
29	AB	65	 95%
30	AC	38	 97%
31	2	2903	 78% 7% 19%
32	a	241	 90% 62% 9%
33	b	233	 84% 30% 15%

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Mol	Chain	Length	Quality of chain
34	c	206	
35	d	167	
36	e	135	
37	f	179	
38	g	130	
39	h	130	
40	i	103	
41	j	129	
42	k	124	
43	l	118	
44	m	101	
45	n	89	
46	o	82	
47	p	84	
48	q	75	
49	r	92	
50	s	87	
51	t	71	
52	1	1540	
53	4	93	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 140044 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 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	120	A	U	conflict	GB 984297099

- Molecule 2 is a RNA chain called tRNAPhe.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	76	Total	C	N	O	P	0	0
			1622	724	292	531	75		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	47	G	U	conflict	GB 984297099
5	48	U	C	conflict	GB 984297099

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	173	Total	C	N	O	S	0	0
			1298	817	238	241	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	48	Total	C	N	O	S	0	0
			368	238	63	66	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	114	Total	C	N	O		0	0
			875	542	175	158			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	117	Total	C	N	O		0	0
			947	604	192	151			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	90	Total	C	N	O	S	0	0
			714	449	136	128	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	96	Total	C	N	O	S	0	0
			735	464	138	133			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	93	Total	C	N	O	S	0	0
			745	474	136	133	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	60	Total	C	N	O	S	0	0
			491	303	96	91	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	48	Total	C	N	O		0	0
			396	255	72	69			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AA	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AB	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AC	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 31 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	2	2833	Total	C	N	O	P	0	0
			60819	27131	11192	19664	2832		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	208	C	-	insertion	GB 984297099
2	284	U	C	conflict	GB 984297099
2	285	G	A	conflict	GB 984297099
2	356	G	A	conflict	GB 984297099
2	542	C	U	conflict	GB 984297099
2	747	C	U	conflict	GB 984297099

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Chain	Residue	Modelled	Actual	Comment	Reference
2	1174	U	G	conflict	GB 984297099
2	1211	C	U	conflict	GB 984297099
2	1513	U	C	conflict	GB 984297099
2	1723	G	A	conflict	GB 984297099
2	1730	C	U	conflict	GB 984297099
2	1865	U	C	conflict	GB 984297099
2	2163	A	G	conflict	GB 984297099
2	2712	C	U	conflict	GB 984297099
2	2794	C	U	conflict	GB 984297099
2	2796	U	C	conflict	GB 984297099
2	2797	U	C	conflict	GB 984297099
2	2799	A	G	conflict	GB 984297099
2	2802	G	A	conflict	GB 984297099

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	220	Total	C	N	O	S	0	0
			1672	1062	293	310	7		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	197	Total	C	N	O	S	0	0
			1502	957	276	266	3		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	160	Total	C	N	O	S	0	0
			1280	801	241	235	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	47	ILE	LEU	conflict	UNP P0A7V8

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	157	Total	C	N	O	S	0	0
			1146	714	215	211	6		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	101	Total	C	N	O	S	0	0
			824	520	149	149	6		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	97	Total	C	N	O	S	0	0
			742	467	133	139	3		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	121	Total	C	N	O	S	0	0
			950	591	189	168	2		

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	89	Total	C	N	O	S	0	0
			726	455	141	129	1		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	111	Total	C	N	O	S	0	0
			867	535	180	148	4		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	111	Total	C	N	O	S	0	0
			859	531	172	153	3		

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	87	Total	C	N	O	S	0	0
			702	433	140	128	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	78	Total	C	N	O	S	0	0
			632	400	118	111	3		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	q	54	Total	C	N	O	0	0
			443	281	81	81		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	84	Total	C	N	O	S	0	0
			655	406	136	110	3		

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	68	Total	C	N	O	S	0	0
			566	351	120	94	1		

- Molecule 52 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	1	1508	Total	C	N	O	P	0	0
			32365	14434	5945	10478	1508		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	1517	A	G	conflict	GB 1726036237

- Molecule 53 is a RNA chain called HIV frameshift stimulating sequence mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	4	43	Total	C	N	O	P	0	0
			926	413	174	296	43		

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	A	1	Total	Mg	0
			1	1	
54	Y	1	Total	Mg	0
			1	1	
54	2	45	Total	Mg	0
			45	45	

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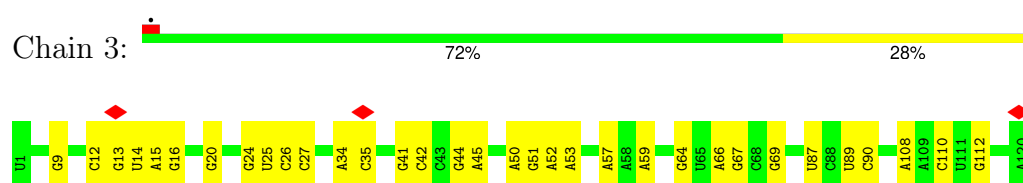
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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
54	1	6	6	6	0

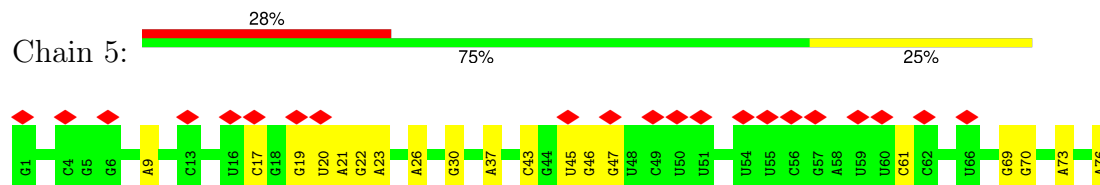
3 Residue-property plots [i](#)

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.

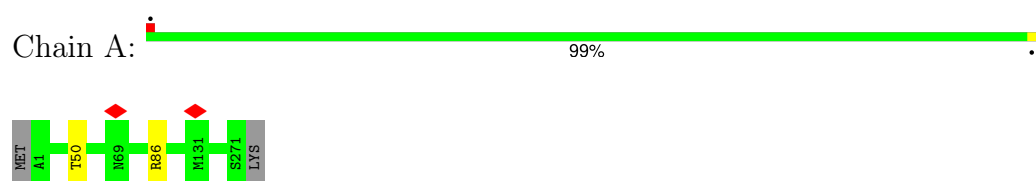
- Molecule 1: 5S ribosomal RNA



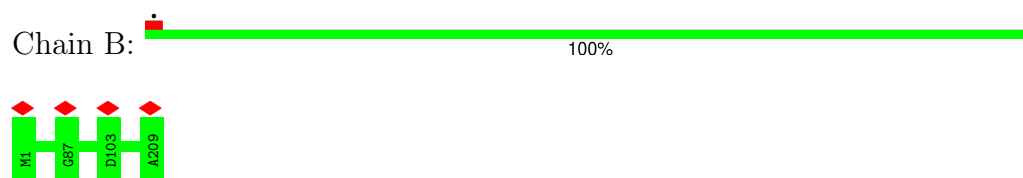
- Molecule 2: tRNAPhe



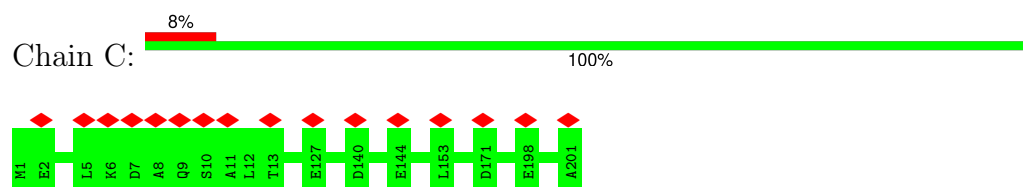
- Molecule 3: 50S ribosomal protein L2



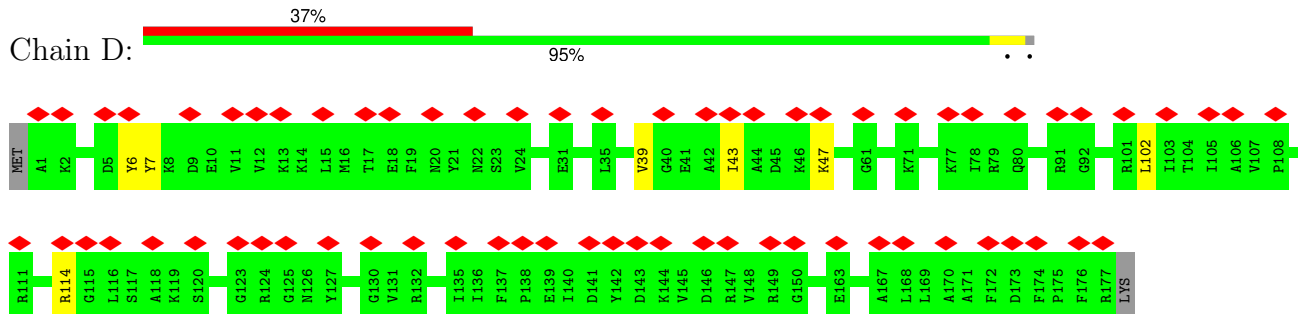
- Molecule 4: 50S ribosomal protein L3



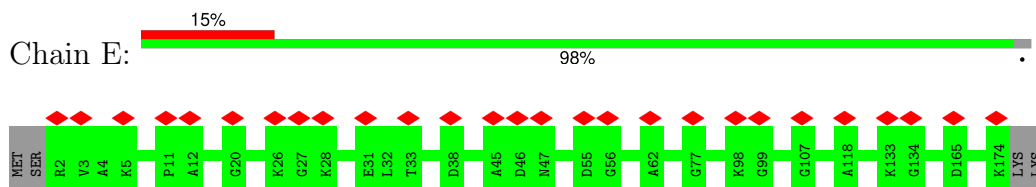
- Molecule 5: 50S ribosomal protein L4



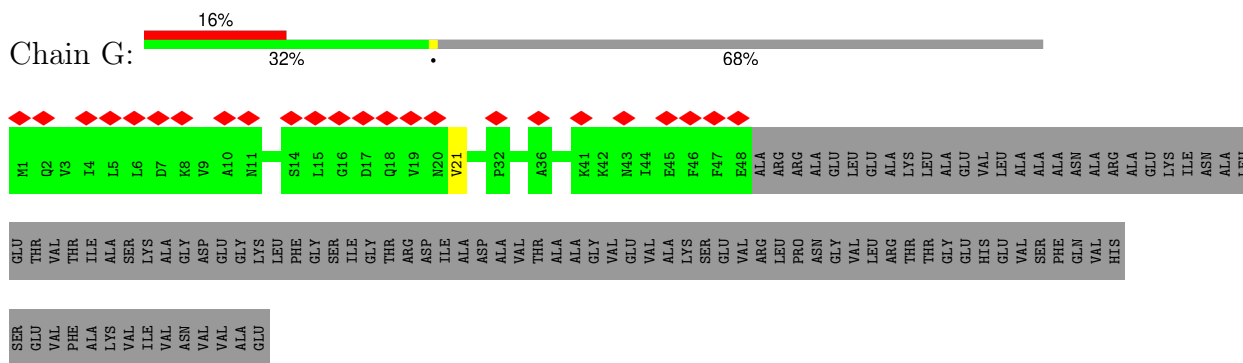
- Molecule 6: 50S ribosomal protein L5



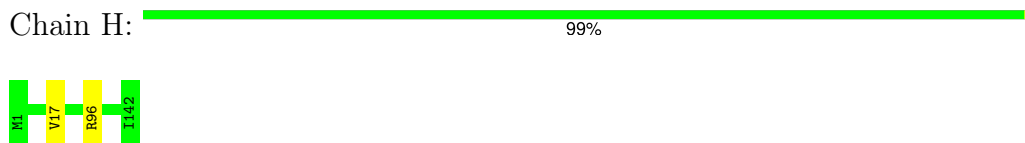
- Molecule 7: 50S ribosomal protein L6



- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13

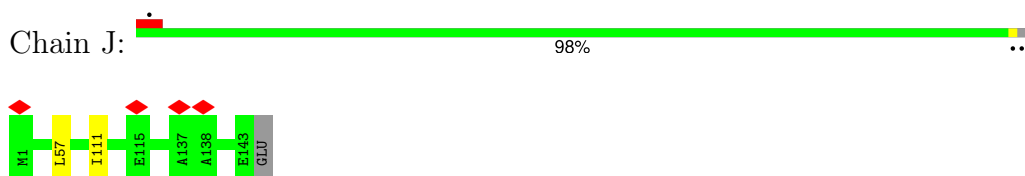


- Molecule 10: 50S ribosomal protein L14

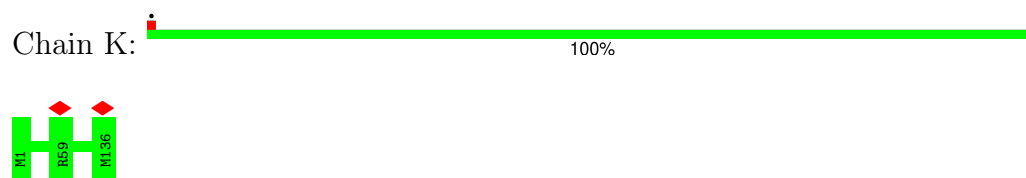


There are no outlier residues recorded for this chain.

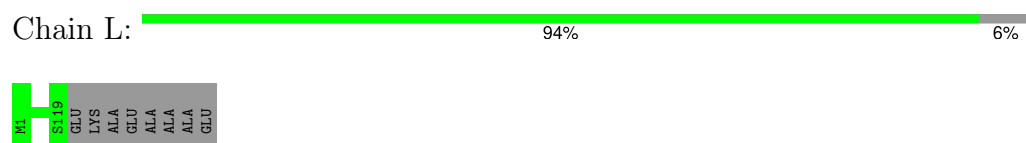
- Molecule 11: 50S ribosomal protein L15



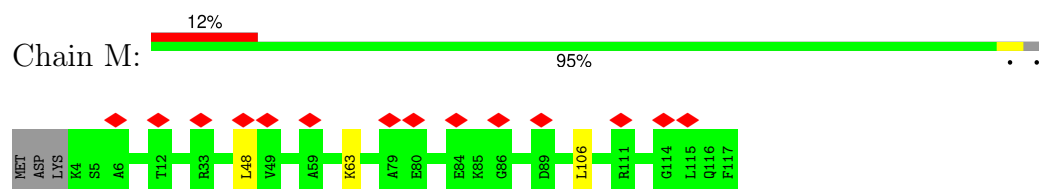
- Molecule 12: 50S ribosomal protein L16



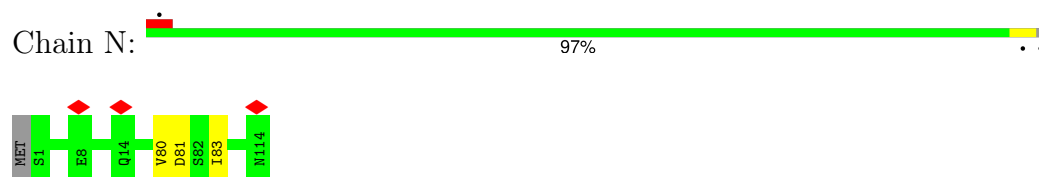
- Molecule 13: 50S ribosomal protein L17



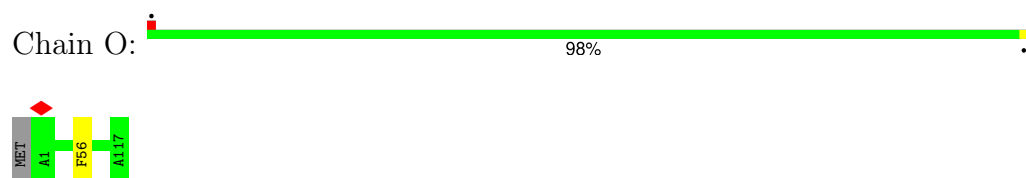
- Molecule 14: 50S ribosomal protein L18



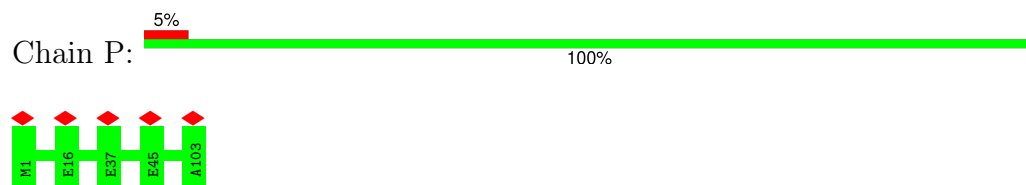
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20

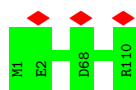


- Molecule 17: 50S ribosomal protein L21

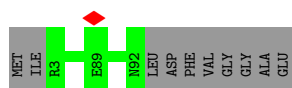


- Molecule 18: 50S ribosomal protein L22

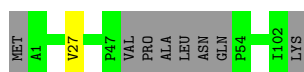
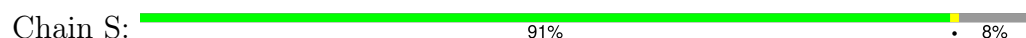




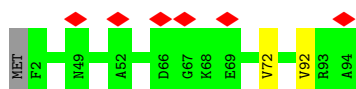
- Molecule 19: 50S ribosomal protein L23



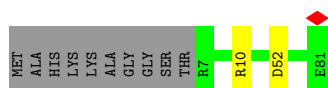
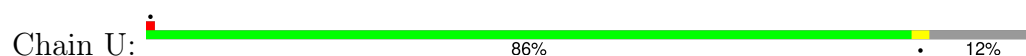
- Molecule 20: 50S ribosomal protein L24



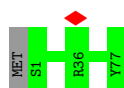
- Molecule 21: 50S ribosomal protein L25



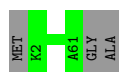
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28

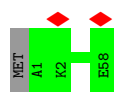


- Molecule 24: 50S ribosomal protein L29



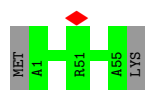
- Molecule 25: 50S ribosomal protein L30

Chain X:  98%




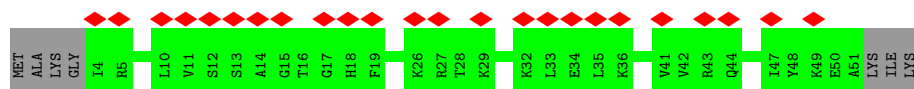
- Molecule 26: 50S ribosomal protein L32

Chain Y:  96%



- Molecule 27: 50S ribosomal protein L33

Chain Z:  44% 87% 13%



- Molecule 28: 50S ribosomal protein L34

Chain AA:  100%

There are no outlier residues recorded for this chain.

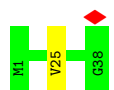
- Molecule 29: 50S ribosomal protein L35

Chain AB:  95%




- Molecule 30: 50S ribosomal protein L36

Chain AC:  97%

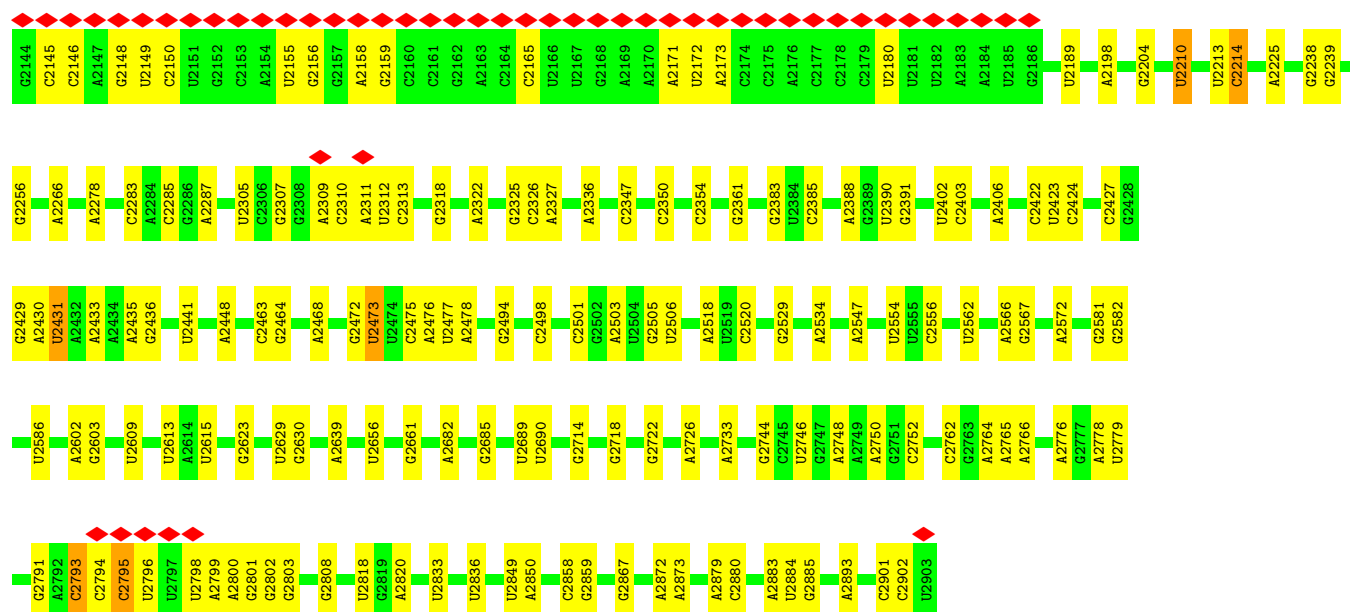


- Molecule 31: 23S ribosomal RNA

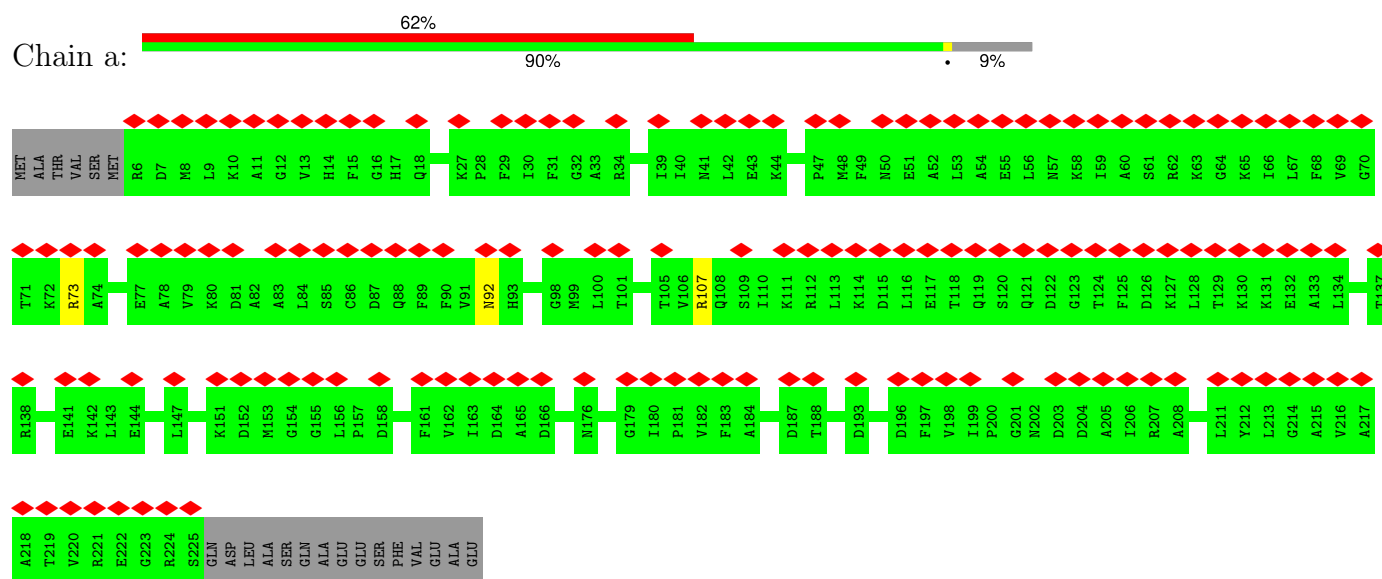
Chain 2:  7% 78% 19%



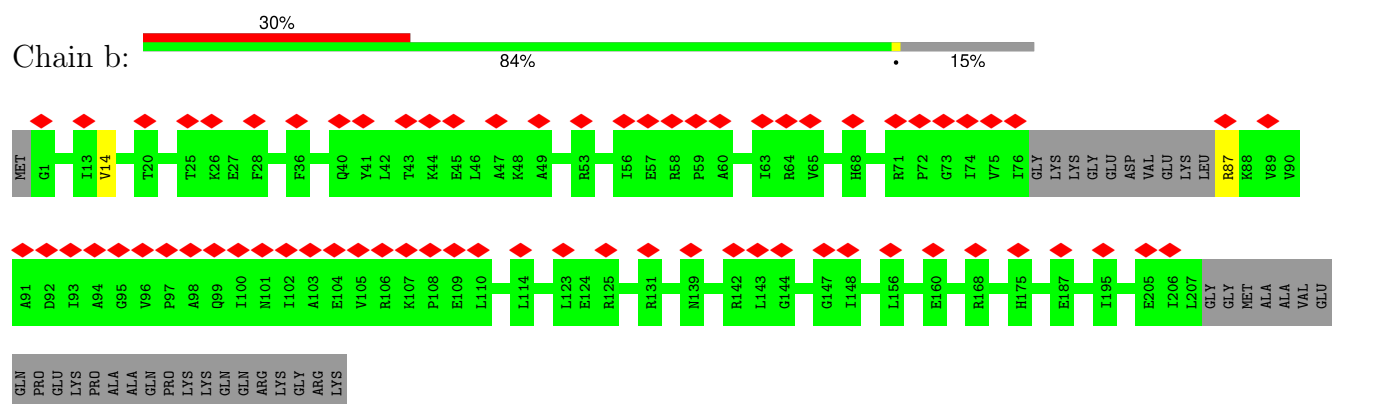




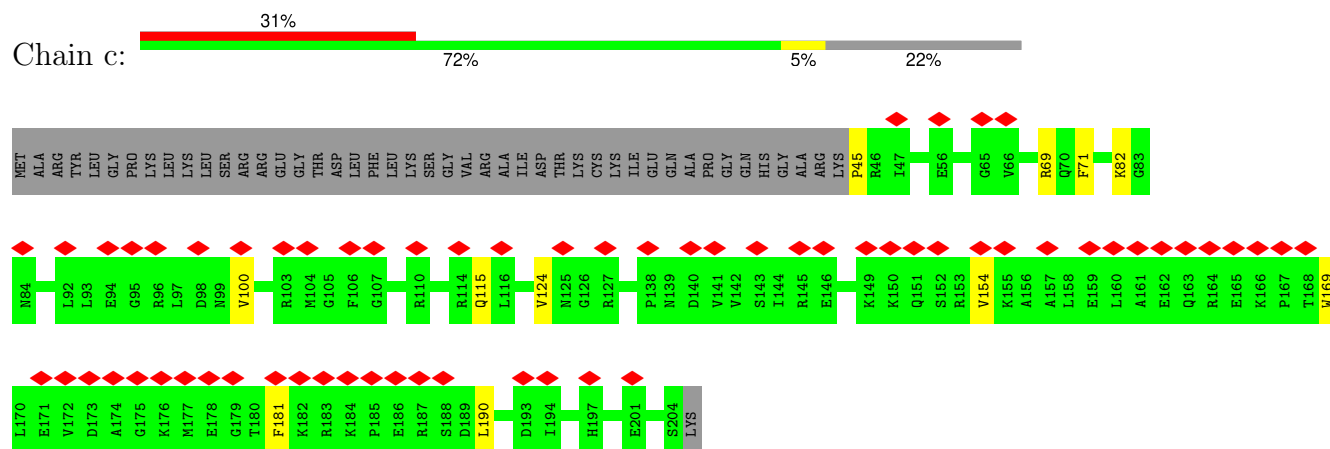
• Molecule 32: 30S ribosomal protein S2



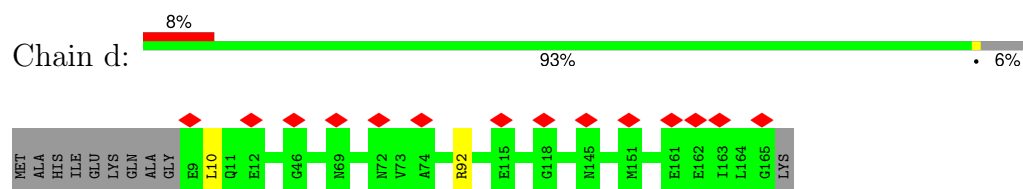
• Molecule 33: 30S ribosomal protein S3



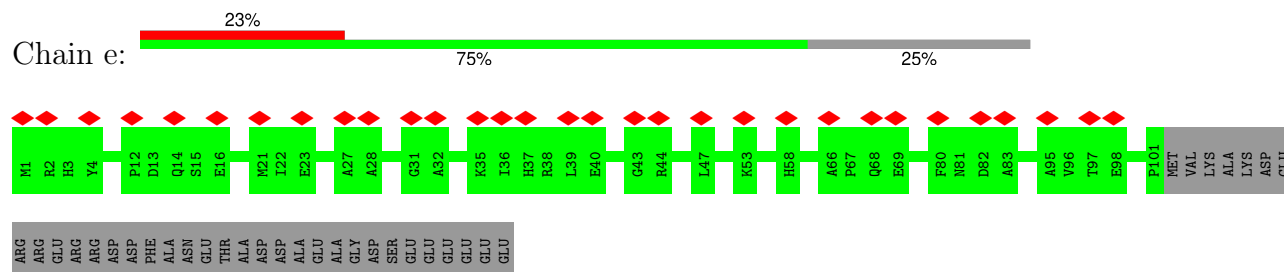
- Molecule 34: 30S ribosomal protein S4



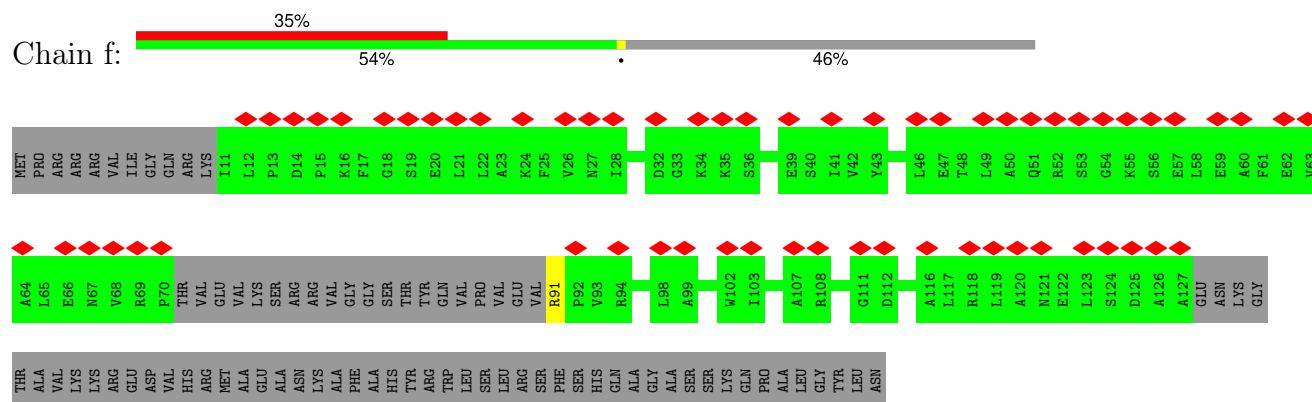
- Molecule 35: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S6

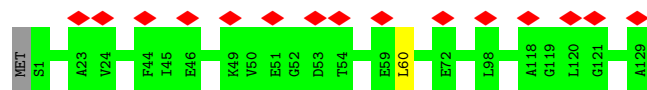


- Molecule 37: 30S ribosomal protein S7

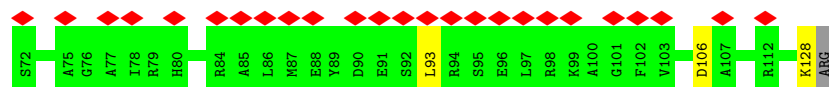
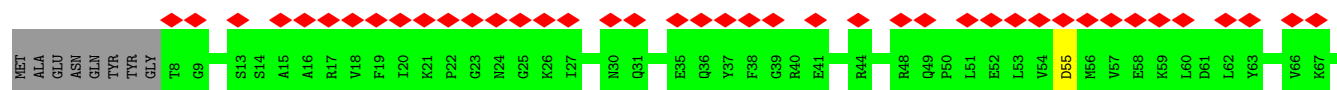
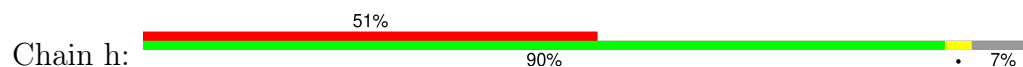


- Molecule 38: 30S ribosomal protein S8

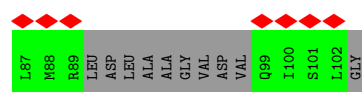
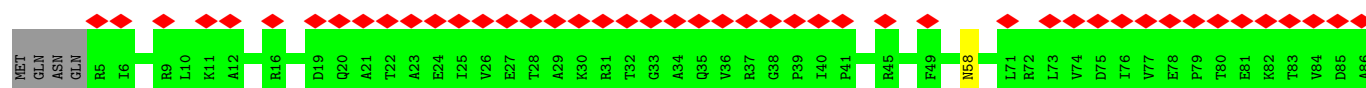
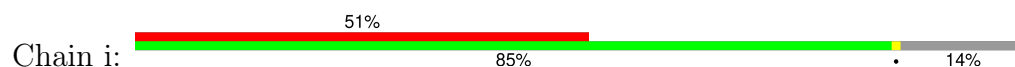




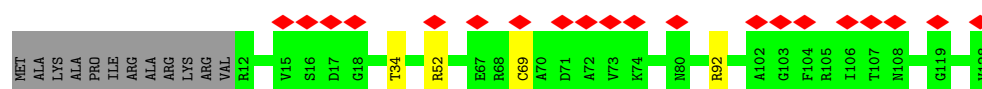
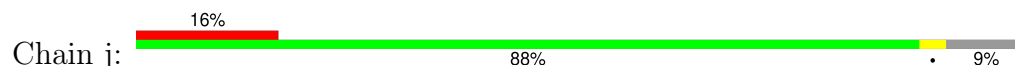
- Molecule 39: 30S ribosomal protein S9



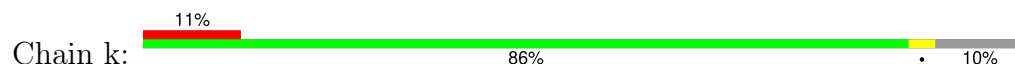
- Molecule 40: 30S ribosomal protein S10



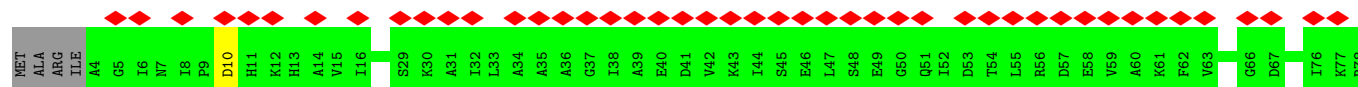
- Molecule 41: 30S ribosomal protein S11

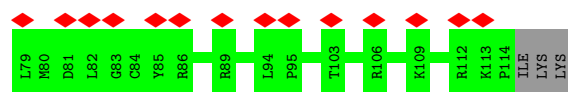


- Molecule 42: 30S ribosomal protein S12

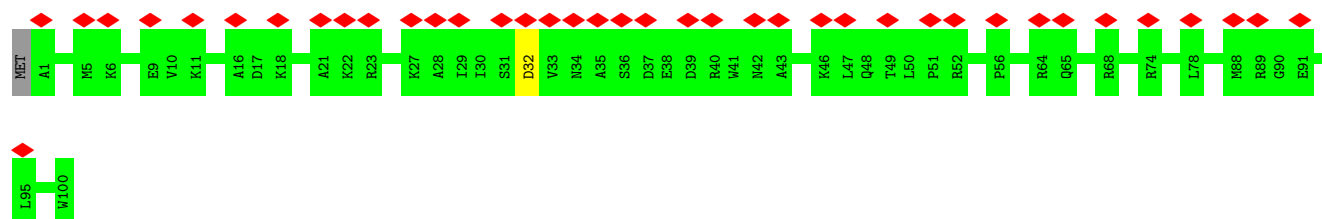
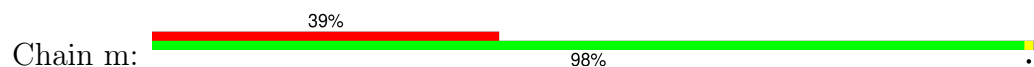


- Molecule 43: 30S ribosomal protein S13

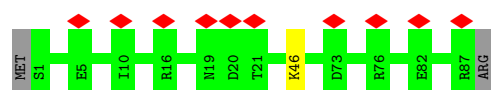




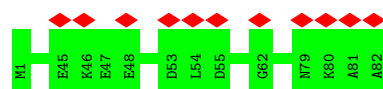
- Molecule 44: 30S ribosomal protein S14



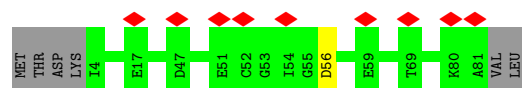
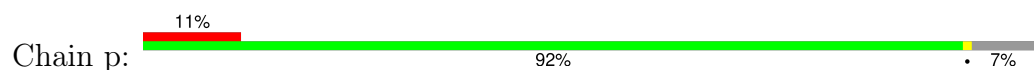
- Molecule 45: 30S ribosomal protein S15



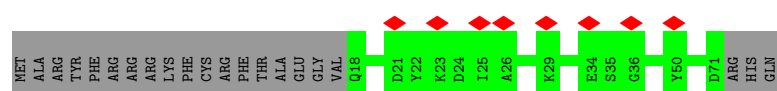
- Molecule 46: 30S ribosomal protein S16



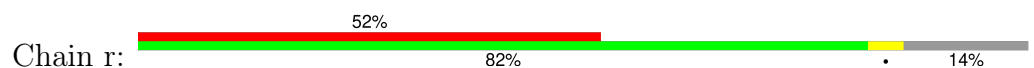
- Molecule 47: 30S ribosomal protein S17

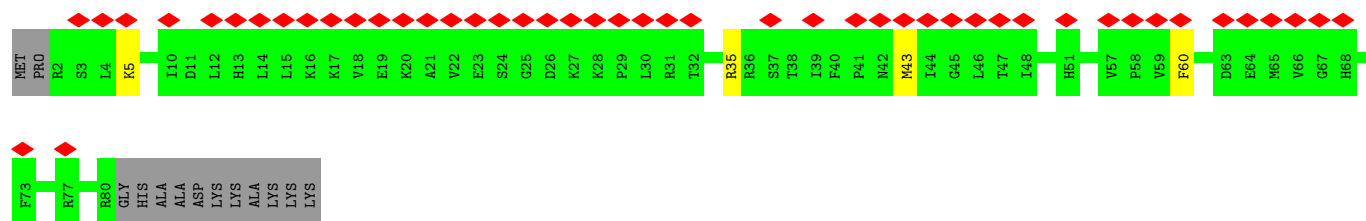


- Molecule 48: 30S ribosomal protein S18

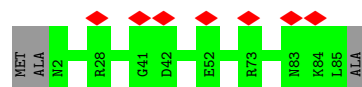


- Molecule 49: 30S ribosomal protein S19

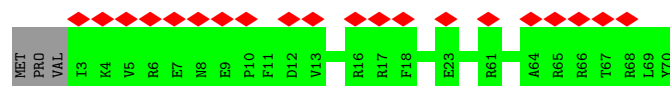




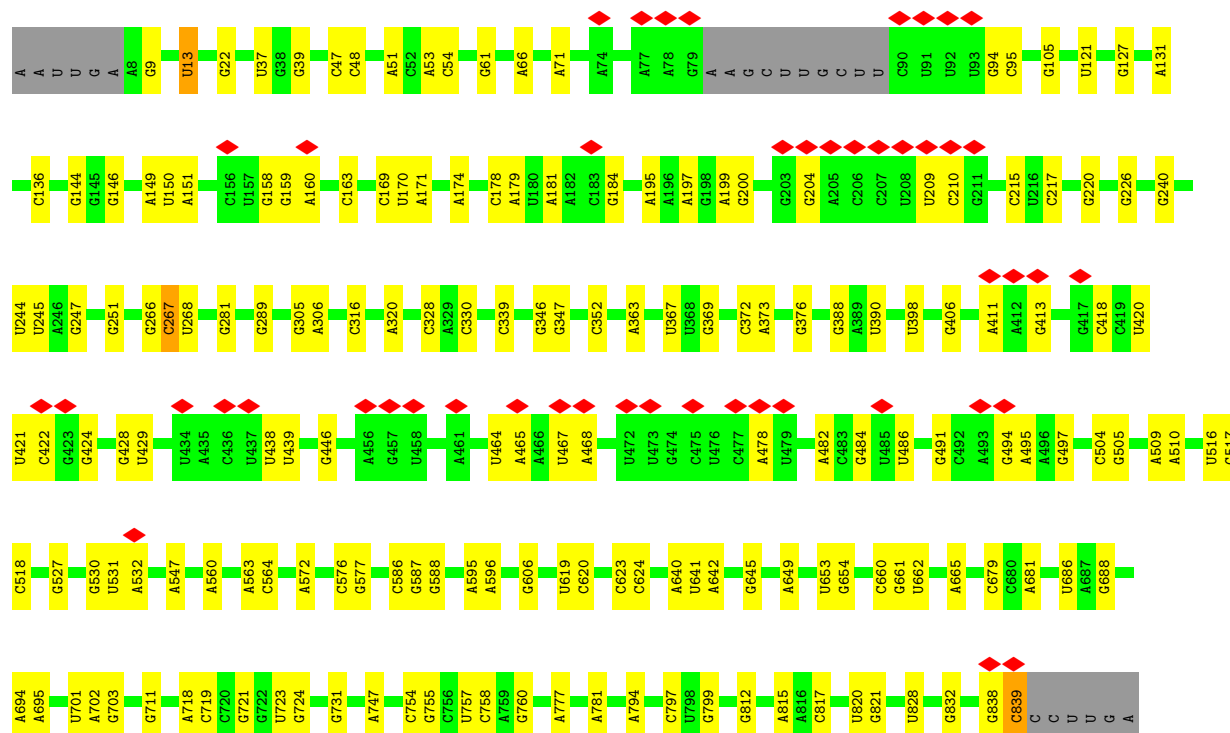
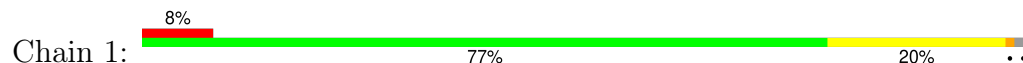
- Molecule 50: 30S ribosomal protein S20

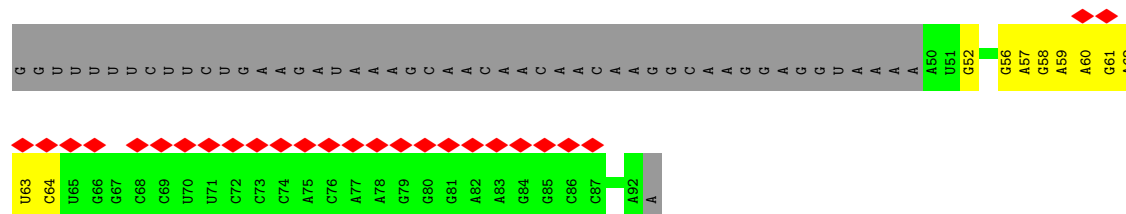


- Molecule 51: 30S ribosomal protein S21



- Molecule 52: 16S ribosomal RNA





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	640261	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	75	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	28.305	Depositor
Minimum map value	-9.165	Depositor
Average map value	0.187	Depositor
Map value standard deviation	1.136	Depositor
Recommended contour level	6	Depositor
Map size (Å)	654.48, 654.48, 654.48	wwPDB
Map dimensions	648, 648, 648	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.01, 1.01, 1.01	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	3	0.26	0/2872	0.87	0/4479
2	5	0.29	0/1813	0.98	0/2826
3	A	0.25	0/2121	0.44	0/2852
4	B	0.26	0/1586	0.46	0/2134
5	C	0.25	0/1571	0.42	0/2113
6	D	0.26	0/1434	0.48	1/1926 (0.1%)
7	E	0.25	0/1318	0.46	0/1786
8	G	0.26	0/373	0.44	0/502
9	H	0.25	0/1152	0.43	0/1551
10	I	0.25	0/956	0.46	0/1279
11	J	0.25	0/1052	0.45	0/1401
12	K	0.25	0/1093	0.43	0/1460
13	L	0.25	0/964	0.44	0/1289
14	M	0.25	0/885	0.46	0/1187
15	N	0.26	0/929	0.44	0/1242
16	O	0.25	0/960	0.36	0/1278
17	P	0.27	0/829	0.49	0/1107
18	Q	0.24	0/864	0.44	0/1156
19	R	0.24	0/720	0.43	0/962
20	S	0.26	0/741	0.44	0/984
21	T	0.25	0/758	0.42	0/1015
22	U	0.26	0/582	0.44	0/769
23	V	0.24	0/635	0.45	0/848
24	W	0.24	0/492	0.41	0/655
25	X	0.26	0/453	0.44	0/605
26	Y	0.24	0/440	0.47	0/588
27	Z	0.23	0/403	0.46	0/538
28	AA	0.23	0/380	0.41	0/498
29	AB	0.26	0/513	0.45	0/676
30	AC	0.24	0/303	0.44	0/397
31	2	0.29	0/68117	0.89	68/106268 (0.1%)
32	a	0.25	0/1703	0.45	0/2305

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.24	0/1528	0.43	0/2069
34	c	0.24	0/1297	0.43	0/1740
35	d	0.25	0/1159	0.47	0/1561
36	e	0.24	0/843	0.50	0/1140
37	f	0.24	0/750	0.43	0/1009
38	g	0.25	0/989	0.45	0/1326
39	h	0.24	0/960	0.49	0/1280
40	i	0.23	0/735	0.45	0/991
41	j	0.25	0/893	0.46	0/1205
42	k	0.25	0/878	0.51	0/1176
43	l	0.23	0/868	0.45	0/1161
44	m	0.24	0/817	0.44	0/1088
45	n	0.22	0/710	0.46	0/950
46	o	0.24	0/659	0.46	0/884
47	p	0.24	0/641	0.45	0/860
48	q	0.24	0/449	0.42	0/604
49	r	0.27	0/652	0.51	0/877
50	s	0.24	0/661	0.38	0/876
51	t	0.23	0/573	0.36	0/759
52	1	0.27	0/36240	0.90	40/56532 (0.1%)
53	4	0.27	0/1037	0.94	0/1616
All	All	0.28	0/152351	0.81	109/228380 (0.0%)

There are no bond length outliers.

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	2	2794	C	N3-C2-O2	-10.09	114.84	121.90
31	2	2210	U	C2-N1-C1'	9.21	128.75	117.70
31	2	2210	U	N1-C2-O2	8.95	129.06	122.80
52	1	1141	C	N3-C2-O2	-8.94	115.64	121.90
31	2	268	C	N3-C2-O2	-8.67	115.83	121.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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	A	269/273 (98%)	255 (95%)	14 (5%)	0	100	100
4	B	207/209 (99%)	200 (97%)	7 (3%)	0	100	100
5	C	199/201 (99%)	193 (97%)	6 (3%)	0	100	100
6	D	175/179 (98%)	161 (92%)	14 (8%)	0	100	100
7	E	171/177 (97%)	159 (93%)	12 (7%)	0	100	100
8	G	46/149 (31%)	44 (96%)	2 (4%)	0	100	100
9	H	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
10	I	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
11	J	141/144 (98%)	136 (96%)	5 (4%)	0	100	100
12	K	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
13	L	117/127 (92%)	110 (94%)	7 (6%)	0	100	100
14	M	112/117 (96%)	103 (92%)	9 (8%)	0	100	100
15	N	112/115 (97%)	101 (90%)	11 (10%)	0	100	100
16	O	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
17	P	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
18	Q	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
19	R	88/100 (88%)	85 (97%)	3 (3%)	0	100	100
20	S	92/104 (88%)	92 (100%)	0	0	100	100
21	T	91/94 (97%)	87 (96%)	4 (4%)	0	100	100
22	U	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
23	V	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
24	W	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
25	X	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
26	Y	53/57 (93%)	51 (96%)	2 (4%)	0	100	100
27	Z	46/55 (84%)	46 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	AA	44/46 (96%)	44 (100%)	0	0	100	100
29	AB	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
30	AC	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
32	a	218/241 (90%)	209 (96%)	9 (4%)	0	100	100
33	b	193/233 (83%)	186 (96%)	7 (4%)	0	100	100
34	c	158/206 (77%)	149 (94%)	9 (6%)	0	100	100
35	d	155/167 (93%)	149 (96%)	6 (4%)	0	100	100
36	e	99/135 (73%)	87 (88%)	12 (12%)	0	100	100
37	f	93/179 (52%)	88 (95%)	5 (5%)	0	100	100
38	g	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
39	h	119/130 (92%)	106 (89%)	13 (11%)	0	100	100
40	i	85/103 (82%)	81 (95%)	4 (5%)	0	100	100
41	j	115/129 (89%)	107 (93%)	8 (7%)	0	100	100
42	k	107/124 (86%)	95 (89%)	12 (11%)	0	100	100
43	l	109/118 (92%)	101 (93%)	8 (7%)	0	100	100
44	m	98/101 (97%)	92 (94%)	6 (6%)	0	100	100
45	n	85/89 (96%)	82 (96%)	3 (4%)	0	100	100
46	o	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
47	p	76/84 (90%)	66 (87%)	10 (13%)	0	100	100
48	q	52/75 (69%)	49 (94%)	3 (6%)	0	100	100
49	r	77/92 (84%)	65 (84%)	12 (16%)	0	100	100
50	s	82/87 (94%)	79 (96%)	3 (4%)	0	100	100
51	t	66/71 (93%)	63 (96%)	3 (4%)	0	100	100
All	All	5236/5843 (90%)	4975 (95%)	261 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	A	216/218 (99%)	214 (99%)	2 (1%)	75	86
4	B	164/164 (100%)	164 (100%)	0	100	100
5	C	165/165 (100%)	165 (100%)	0	100	100
6	D	148/150 (99%)	142 (96%)	6 (4%)	26	51
7	E	134/138 (97%)	134 (100%)	0	100	100
8	G	39/114 (34%)	38 (97%)	1 (3%)	41	64
9	H	116/116 (100%)	114 (98%)	2 (2%)	56	74
10	I	104/104 (100%)	104 (100%)	0	100	100
11	J	102/103 (99%)	100 (98%)	2 (2%)	50	70
12	K	109/109 (100%)	109 (100%)	0	100	100
13	L	99/103 (96%)	99 (100%)	0	100	100
14	M	84/87 (97%)	81 (96%)	3 (4%)	30	56
15	N	99/100 (99%)	96 (97%)	3 (3%)	36	61
16	O	89/90 (99%)	88 (99%)	1 (1%)	70	81
17	P	84/84 (100%)	84 (100%)	0	100	100
18	Q	93/93 (100%)	93 (100%)	0	100	100
19	R	77/84 (92%)	77 (100%)	0	100	100
20	S	78/85 (92%)	77 (99%)	1 (1%)	65	78
21	T	77/78 (99%)	75 (97%)	2 (3%)	41	64
22	U	57/63 (90%)	55 (96%)	2 (4%)	31	56
23	V	67/68 (98%)	67 (100%)	0	100	100
24	W	54/55 (98%)	54 (100%)	0	100	100
25	X	48/49 (98%)	48 (100%)	0	100	100
26	Y	46/48 (96%)	46 (100%)	0	100	100
27	Z	44/49 (90%)	44 (100%)	0	100	100
28	AA	38/38 (100%)	38 (100%)	0	100	100
29	AB	51/52 (98%)	49 (96%)	2 (4%)	27	53
30	AC	34/34 (100%)	33 (97%)	1 (3%)	37	61
32	a	171/199 (86%)	168 (98%)	3 (2%)	54	73
33	b	152/190 (80%)	150 (99%)	2 (1%)	65	78
34	c	134/173 (78%)	123 (92%)	11 (8%)	9	31
35	d	117/126 (93%)	115 (98%)	2 (2%)	56	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	e	88/116 (76%)	88 (100%)	0	100	100
37	f	77/147 (52%)	76 (99%)	1 (1%)	65	78
38	g	104/105 (99%)	103 (99%)	1 (1%)	73	83
39	h	97/107 (91%)	93 (96%)	4 (4%)	26	51
40	i	80/90 (89%)	79 (99%)	1 (1%)	65	78
41	j	90/99 (91%)	86 (96%)	4 (4%)	24	50
42	k	93/104 (89%)	89 (96%)	4 (4%)	25	50
43	l	90/96 (94%)	89 (99%)	1 (1%)	70	81
44	m	83/84 (99%)	82 (99%)	1 (1%)	67	80
45	n	75/77 (97%)	74 (99%)	1 (1%)	65	78
46	o	65/65 (100%)	65 (100%)	0	100	100
47	p	72/78 (92%)	71 (99%)	1 (1%)	62	77
48	q	47/65 (72%)	47 (100%)	0	100	100
49	r	70/79 (89%)	66 (94%)	4 (6%)	17	43
50	s	64/66 (97%)	64 (100%)	0	100	100
51	t	56/61 (92%)	56 (100%)	0	100	100
All	All	4341/4768 (91%)	4272 (98%)	69 (2%)	58	75

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	k	17	LYS
42	k	52	CYS
49	r	5	LYS
22	U	52	ASP
22	U	10	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
33	b	99	GLN
36	e	17	GLN
50	s	19	HIS
34	c	84	ASN
34	c	197	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3	119/120 (99%)	33 (27%)	1 (0%)
2	5	75/76 (98%)	19 (25%)	0
31	2	2831/2903 (97%)	550 (19%)	9 (0%)
52	1	1505/1540 (97%)	307 (20%)	6 (0%)
53	4	42/93 (45%)	10 (23%)	0
All	All	4572/4732 (96%)	919 (20%)	16 (0%)

5 of 919 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3	9	G
1	3	12	C
1	3	13	G
1	3	14	U
1	3	15	A

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	1	1201	A
52	1	1190	G
31	2	2581	G
52	1	509	A
31	2	1340	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 53 ligands modelled in this entry, 53 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

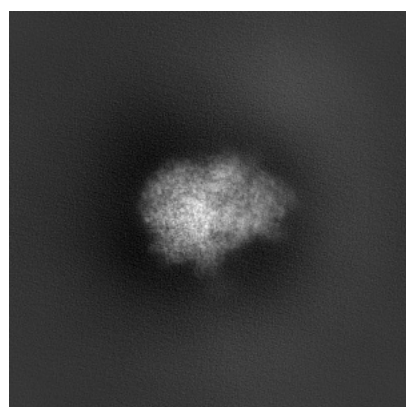
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21421. These allow visual inspection of the internal detail of the map and identification of artifacts.

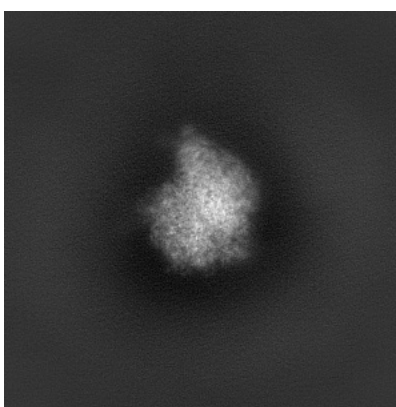
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

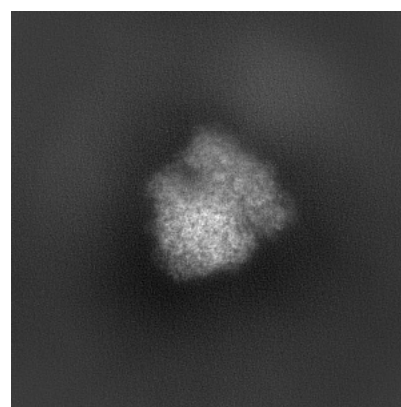
6.1.1 Primary map



X



Y

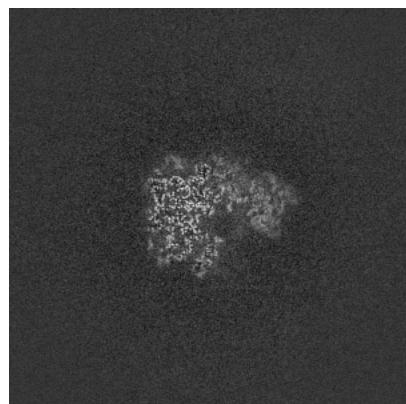


Z

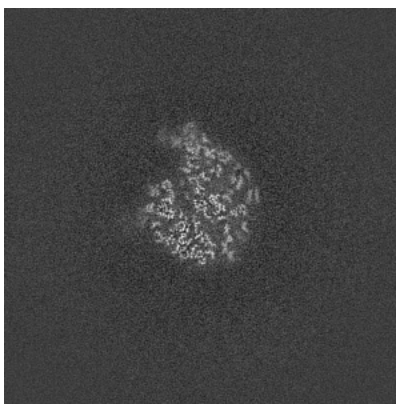
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

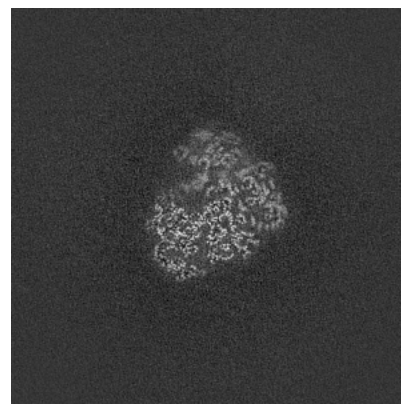
6.2.1 Primary map



X Index: 324



Y Index: 324

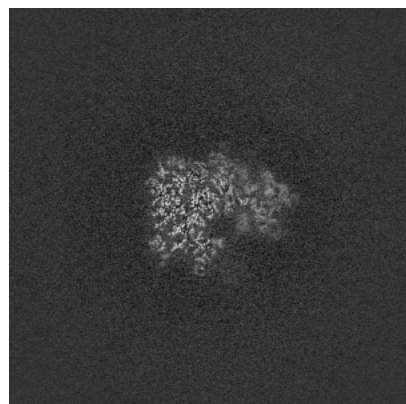


Z Index: 324

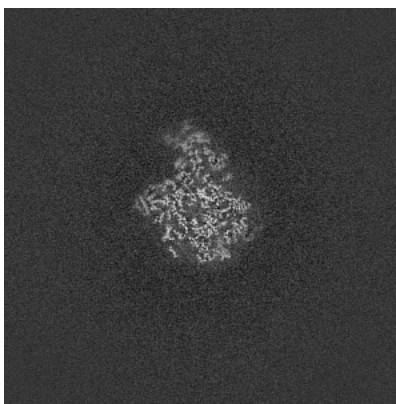
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

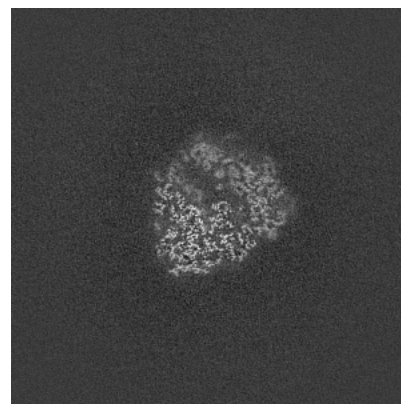
6.3.1 Primary map



X Index: 331



Y Index: 312

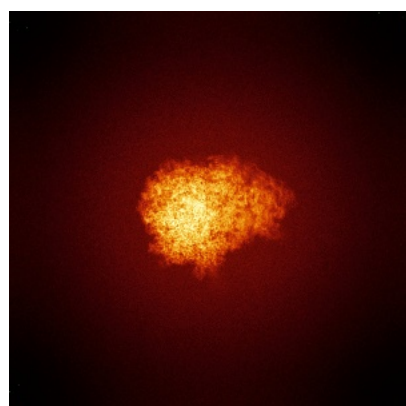


Z Index: 310

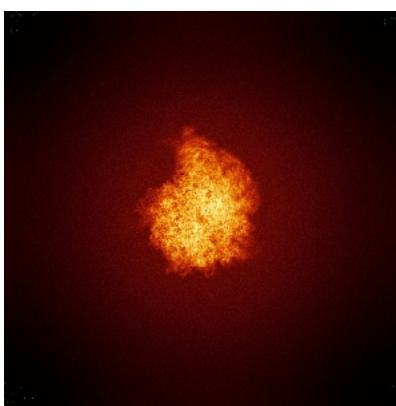
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

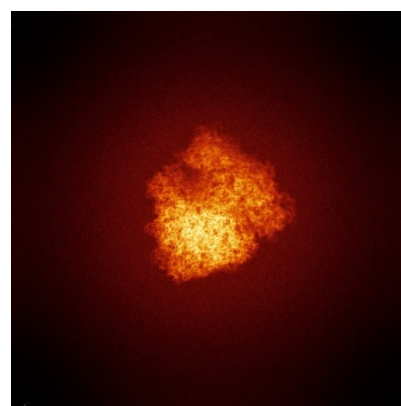
6.4.1 Primary map



X



Y

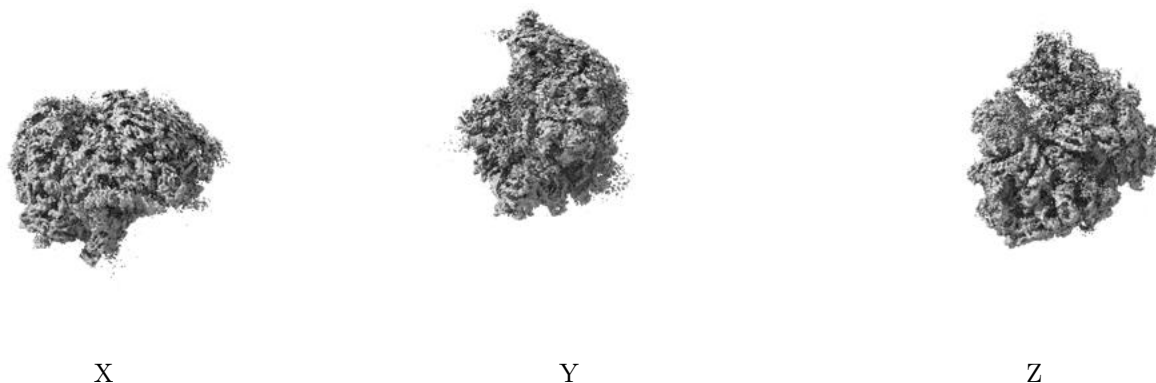


Z

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



The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

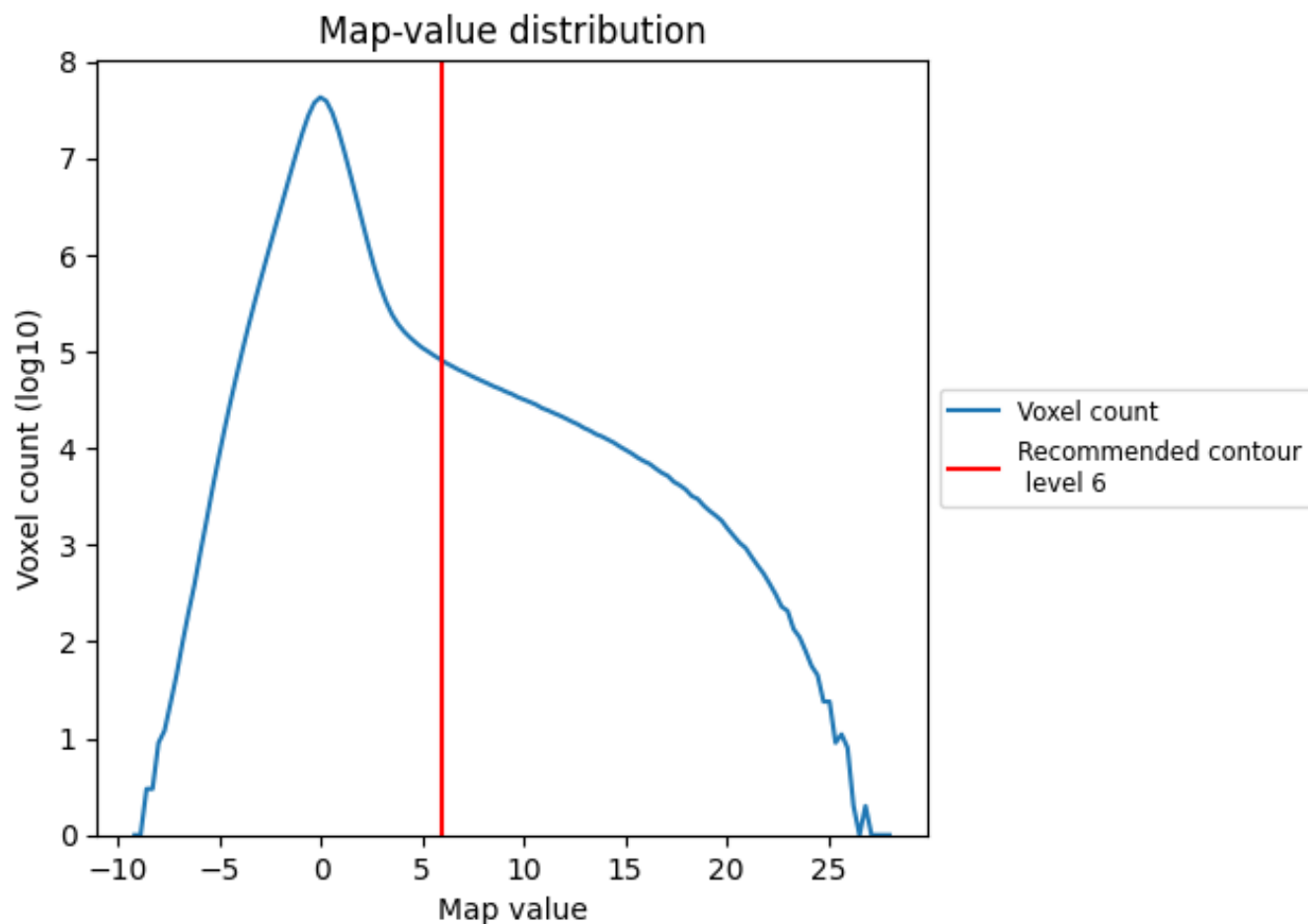
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

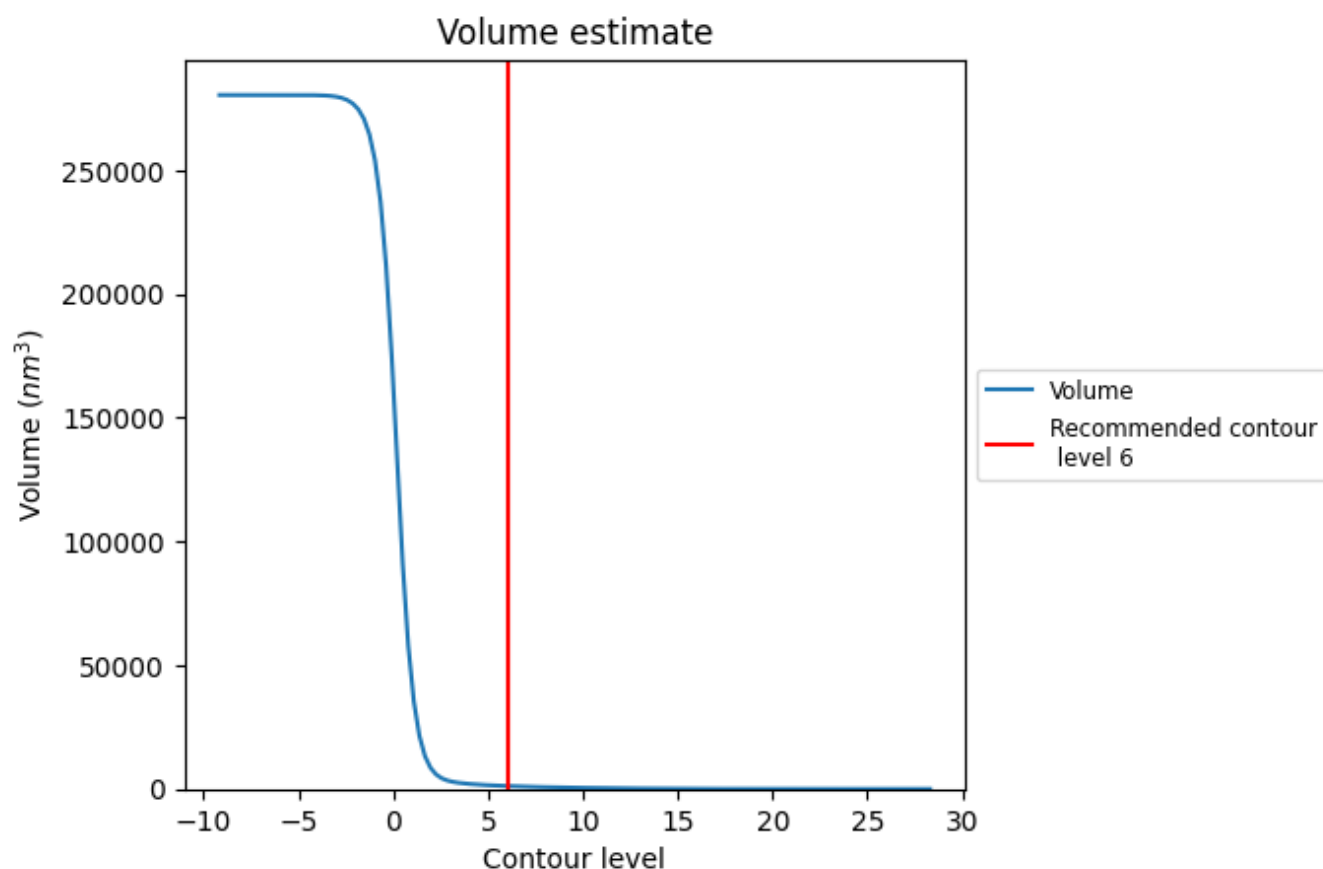
This section contains the results of statistical analysis of the map.

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.

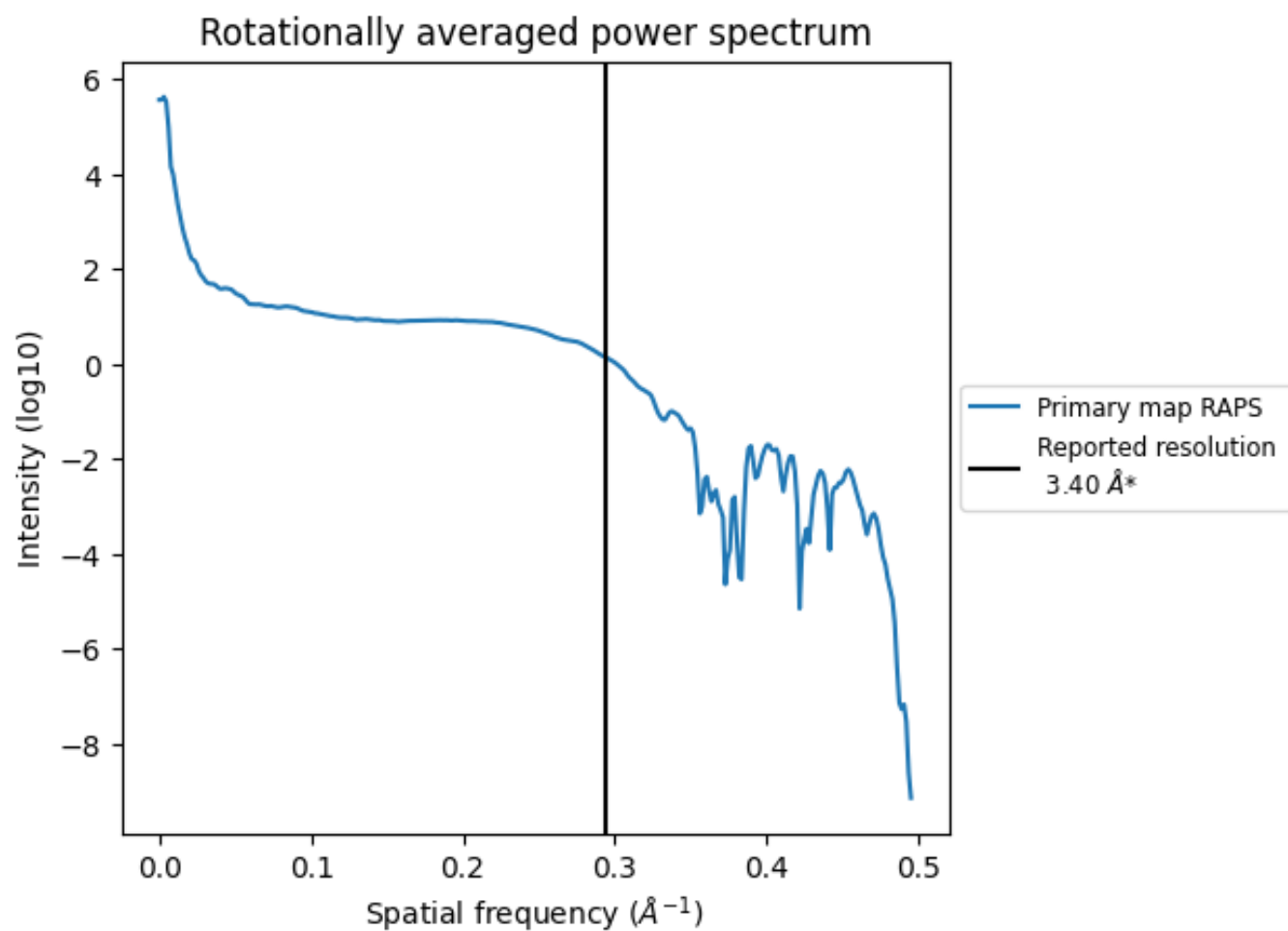
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1184 nm^3 ; this corresponds to an approximate mass of 1070 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 ⓘ

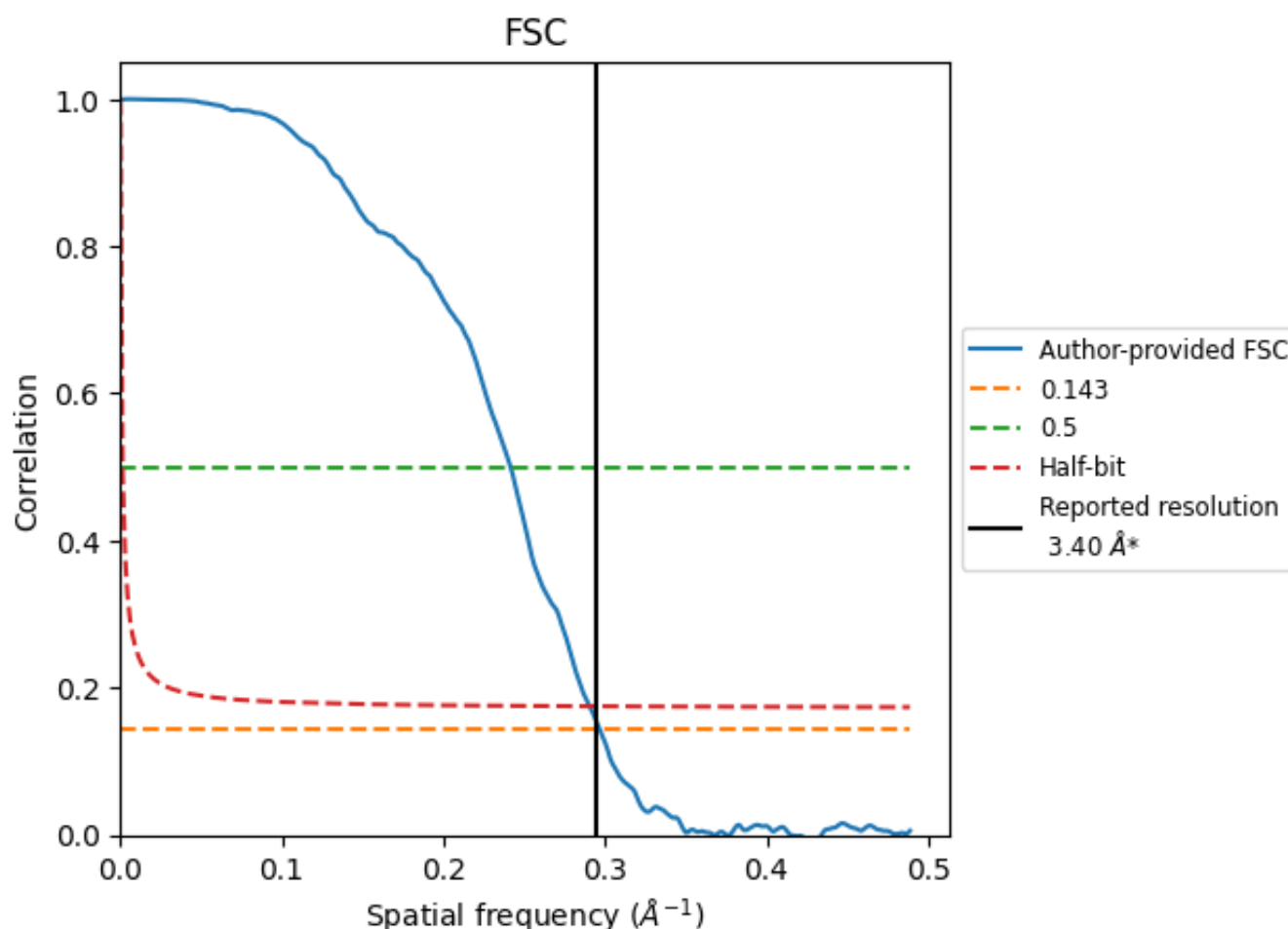


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

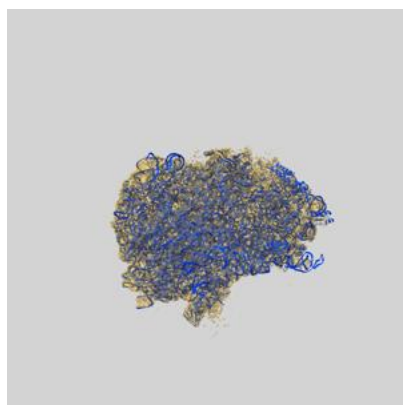
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.37	4.14	3.44
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

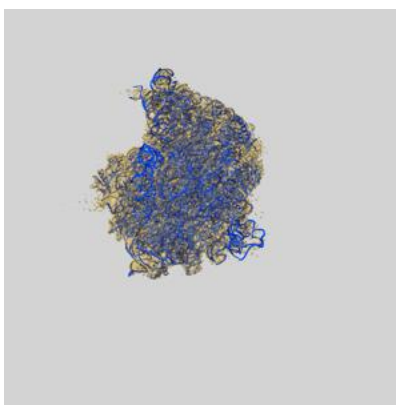
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21421 and PDB model 6VWM. Per-residue inclusion information can be found in section 3 on page 15.

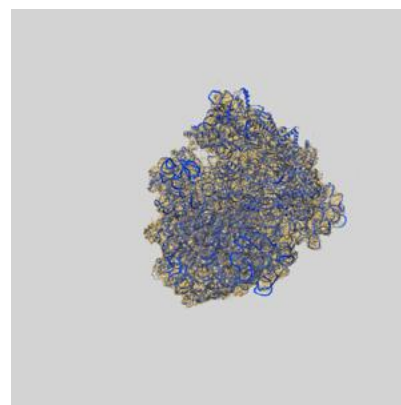
9.1 Map-model overlay [i](#)



X



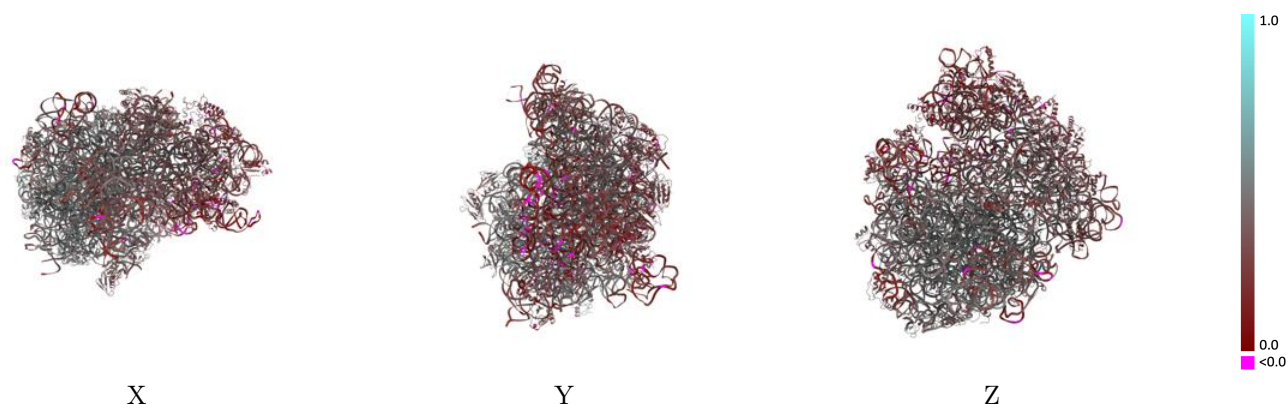
Y



Z

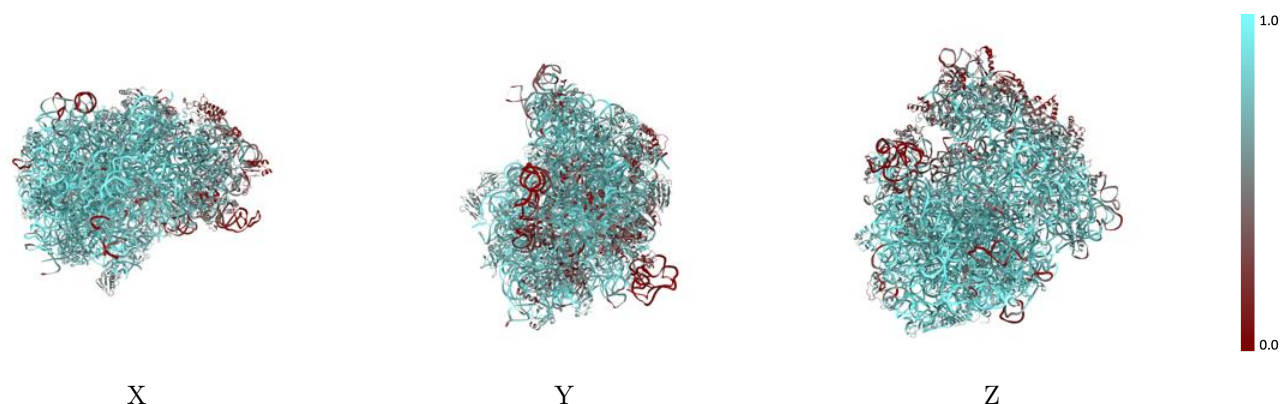
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



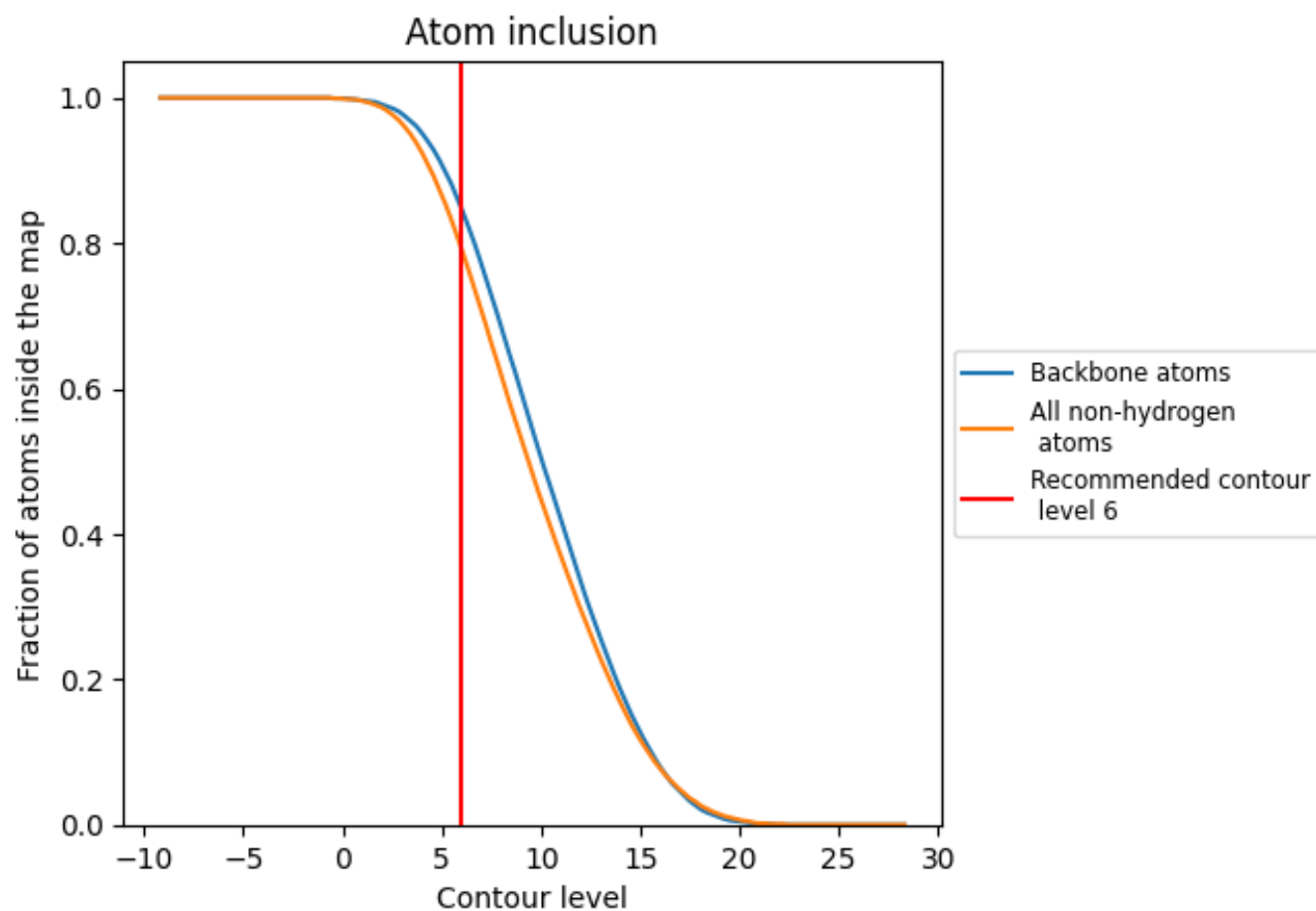
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 79% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7920	 0.3850
1	 0.8080	 0.3310
2	 0.8790	 0.4250
3	 0.8290	 0.3480
4	 0.3700	 0.1060
5	 0.6180	 0.2380
A	 0.8480	 0.4640
AA	 0.9320	 0.4860
AB	 0.8620	 0.4650
AC	 0.8320	 0.4320
B	 0.8030	 0.4750
C	 0.7450	 0.4490
D	 0.4620	 0.2700
E	 0.6090	 0.3710
G	 0.4110	 0.3160
H	 0.8320	 0.4730
I	 0.8320	 0.4750
J	 0.8140	 0.4700
K	 0.8380	 0.4630
L	 0.8470	 0.4740
M	 0.6680	 0.3500
N	 0.8040	 0.4520
O	 0.8460	 0.4690
P	 0.7580	 0.4700
Q	 0.8210	 0.4680
R	 0.7940	 0.4480
S	 0.7470	 0.4570
T	 0.7010	 0.4250
U	 0.8410	 0.4900
V	 0.8450	 0.4470
W	 0.7220	 0.4190
X	 0.7850	 0.4630
Y	 0.8350	 0.4720
Z	 0.3710	 0.3860
a	 0.3310	 0.2980



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Chain	Atom inclusion	Q-score
b	 0.5120	 0.2990
c	 0.4850	 0.2900
d	 0.7150	 0.3810
e	 0.5380	 0.3210
f	 0.3630	 0.2040
g	 0.6530	 0.3520
h	 0.3810	 0.2370
i	 0.3320	 0.2660
j	 0.6190	 0.3170
k	 0.6770	 0.3500
l	 0.3780	 0.2020
m	 0.4990	 0.2650
n	 0.6780	 0.3400
o	 0.6540	 0.3650
p	 0.7190	 0.3750
q	 0.6620	 0.3500
r	 0.3450	 0.2450
s	 0.7250	 0.3240
t	 0.5280	 0.3200