



## wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 10:13 am GMT

PDB ID : 5LZA  
EMDB ID : EMD-4121  
Title : Structure of the 70S ribosome with SECIS-mRNA and P-site tRNA (Initial complex, IC)  
Authors : Fischer, N.; Neumann, P.; Bock, L.V.; Maracci, C.; Wang, Z.; Paleskava, A.; Konevega, A.L.; Schroeder, G.F.; Grubmueller, H.; Ficner, R.; Rodnina, M.V.; Stark, H.  
Deposited on : 2016-09-29  
Resolution : 3.60 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

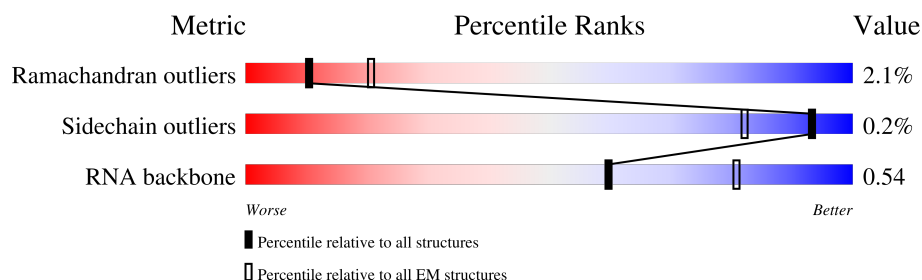
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 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 3.60 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	a	1539	
2	b	218	
3	c	206	
4	d	205	
5	e	157	
6	f	100	
7	g	151	
8	h	129	

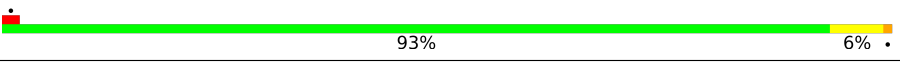
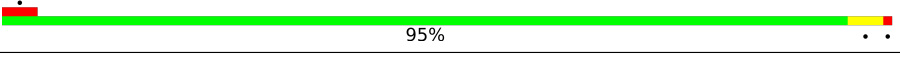
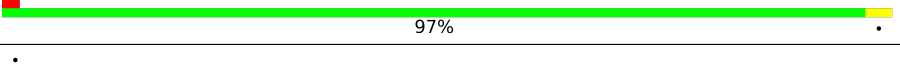
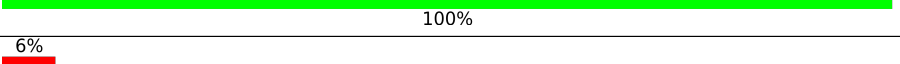
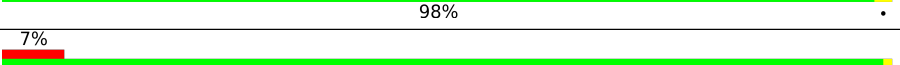
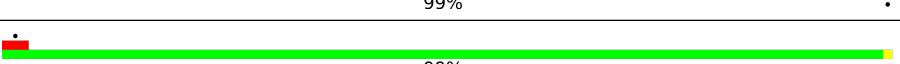
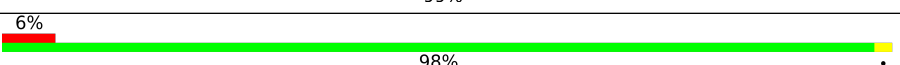
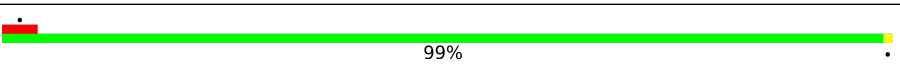
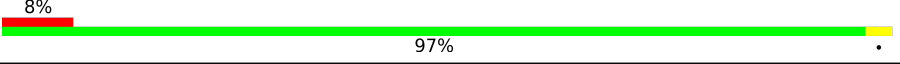
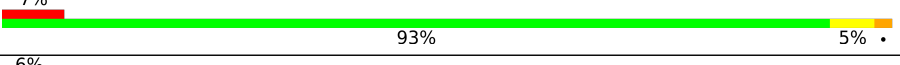
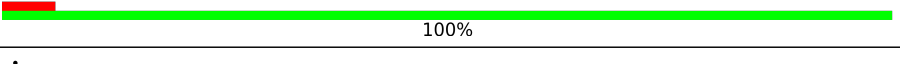
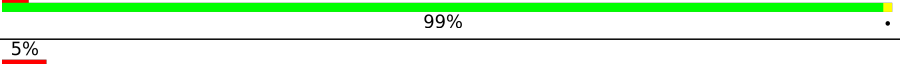
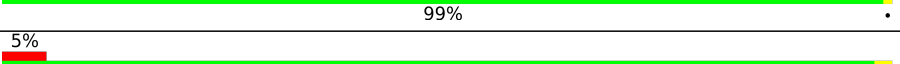
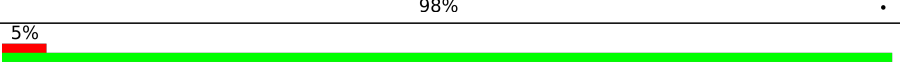
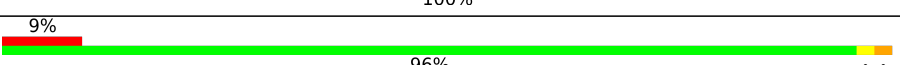
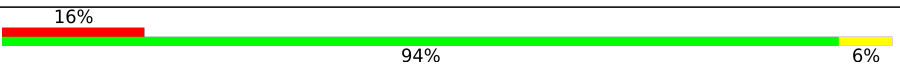
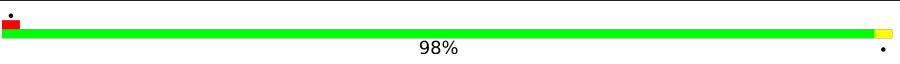
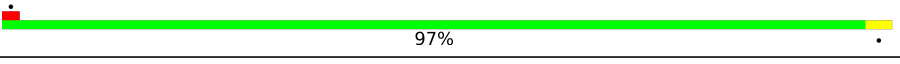
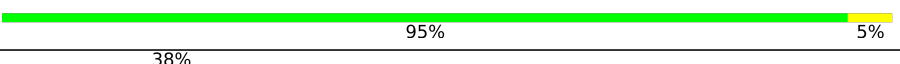
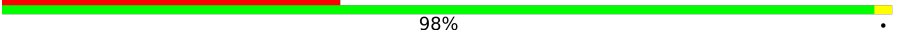


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Mol	Chain	Length	Quality of chain
9	i	127	
10	j	98	
11	k	116	
12	l	123	
13	m	114	
14	n	100	
15	o	88	
16	p	82	
17	q	80	
18	r	65	
19	s	79	
20	t	85	
21	u	65	
22	v	77	
23	x	48	
24	A	2903	
25	B	120	
26	C	271	
27	D	209	
28	E	201	
29	F	177	
30	G	176	
31	I	141	
32	H	149	
33	J	142	

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Mol	Chain	Length	Quality of chain
34	K	122	
35	L	143	
36	M	136	
37	N	120	
38	O	116	
39	P	114	
40	Q	117	
41	R	103	
42	S	110	
43	T	93	
44	U	102	
45	V	94	
46	W	75	
47	X	77	
48	Y	63	
49	Z	58	
50	0	56	
51	1	50	
52	2	46	
53	3	64	
54	4	38	
55	6	66	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	G7M	a	527	X	-	-	-
24	G7M	A	2069	X	-	-	-

## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 146037 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1539	Total	C	N	O	P	4	0
			33119	14778	6072	10726	1543		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			794	495	164	132	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	65	Total	C	N	O	0	0
			505	317	96	92		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	65	Total	C	N	O	S	0	0
			496	307	100	88	1		

- Molecule 22 is a RNA chain called fMet-tRNA<sup>fMet</sup>.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	v	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		

- Molecule 23 is a RNA chain called SECIS mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	x	48	Total	C	N	O	P	0	0
			1025	457	183	337	48		

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	A	2900	Total	C	N	O	P	1	0
			62296	27797	11464	20134	2901		

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	C	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 27 is a protein called 50S ribosomal protein L3.

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

- Molecule 28 is a protein called 50S ribosomal protein L4.

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

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 31 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	K	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	N	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	O	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	T	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	U	102	Total	C	N	O		0	0
			780	492	146	142			

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 46 is a protein called 50S ribosomal protein L27.

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

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1	50	Total	C	N	O	S	0	0
			410	263	75	72			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 55 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	6	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

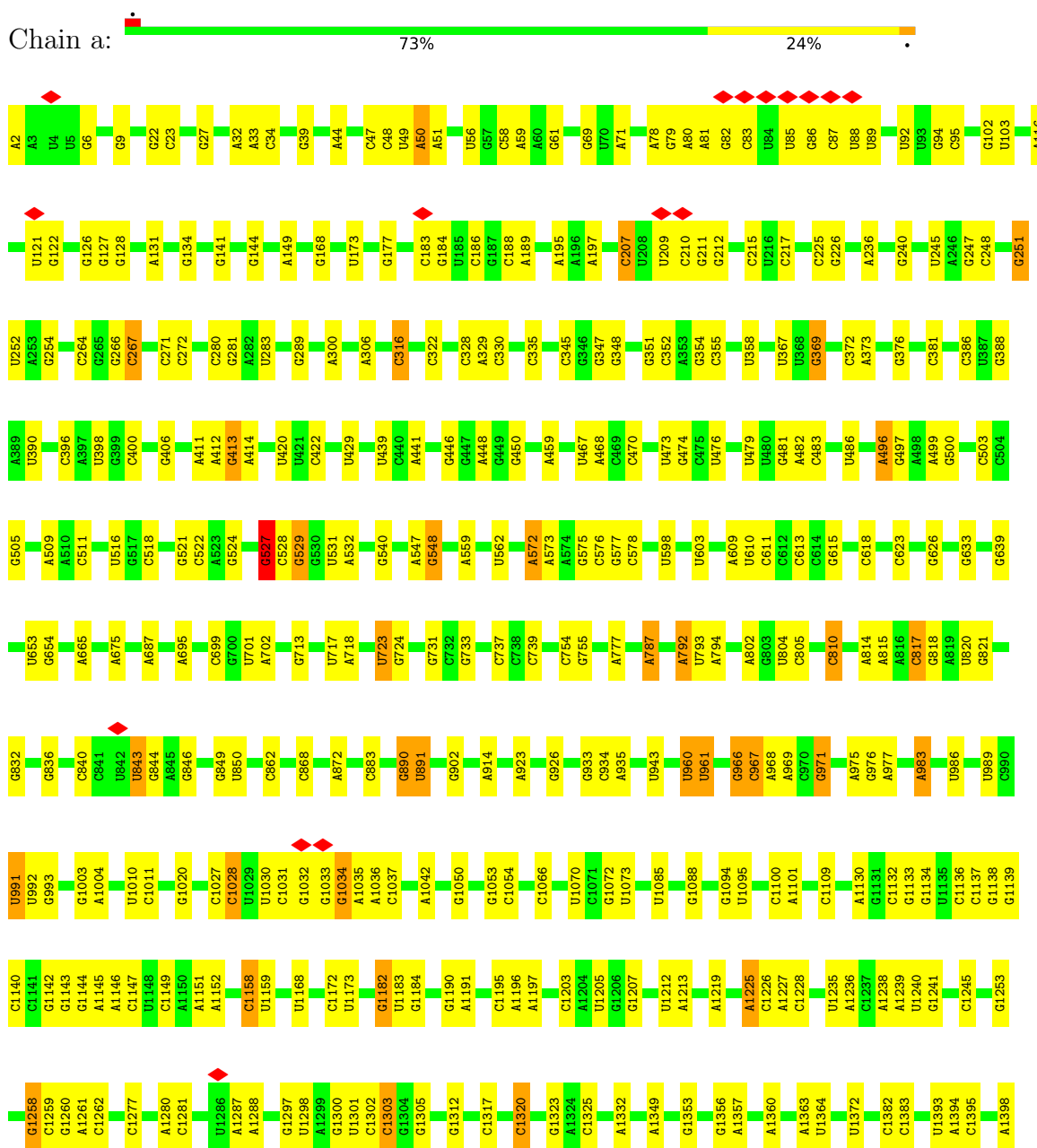
- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

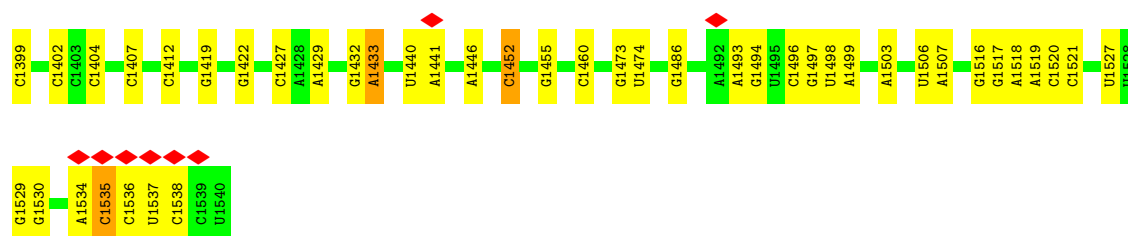
Mol	Chain	Residues	Atoms		AltConf
56	4	1	Total 1	Zn 1	0
56	6	1	Total 1	Zn 1	0

### 3 Residue-property plots

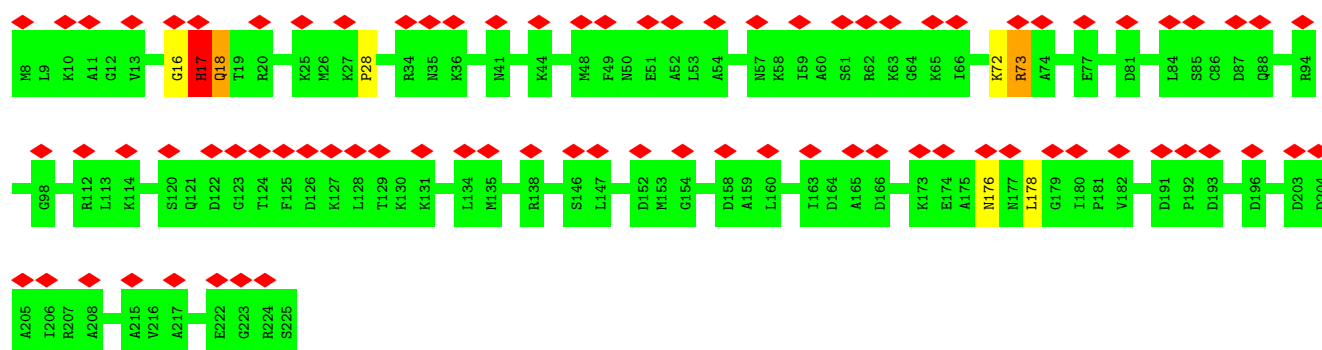
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

#### • Molecule 1: 16S ribosomal RNA

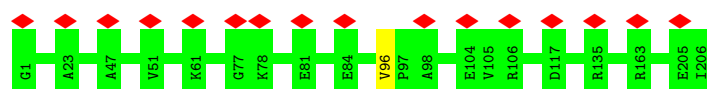




• Molecule 2: 30S ribosomal protein S2



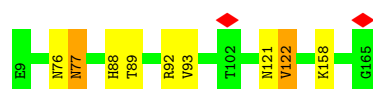
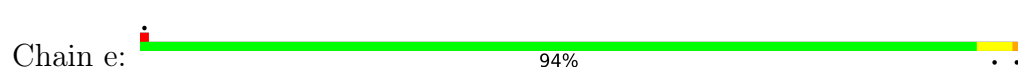
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5



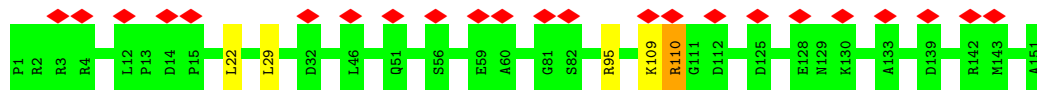
• Molecule 6: 30S ribosomal protein S6



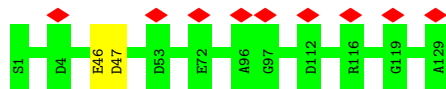




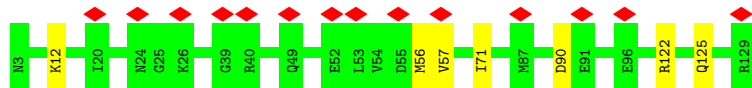
- Molecule 7: 30S ribosomal protein S7



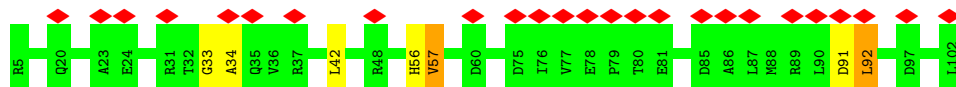
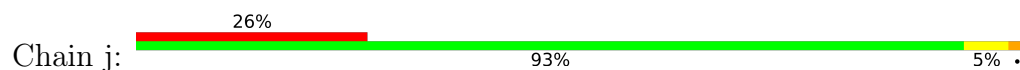
- Molecule 8: 30S ribosomal protein S8



- Molecule 9: 30S ribosomal protein S9



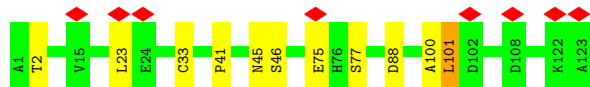
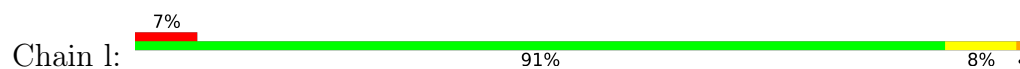
- Molecule 10: 30S ribosomal protein S10



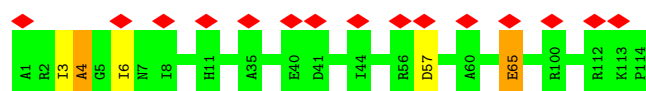
- Molecule 11: 30S ribosomal protein S11



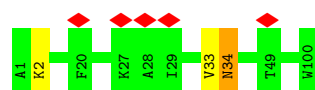
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



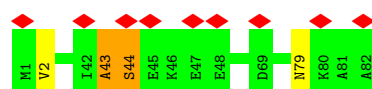
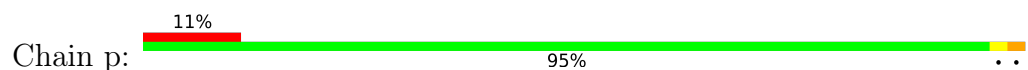
- Molecule 14: 30S ribosomal protein S14



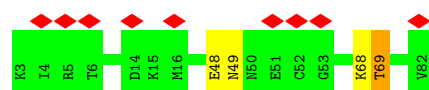
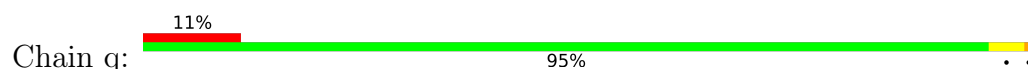
- Molecule 15: 30S ribosomal protein S15



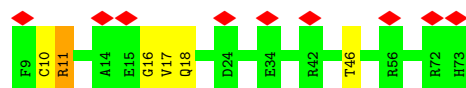
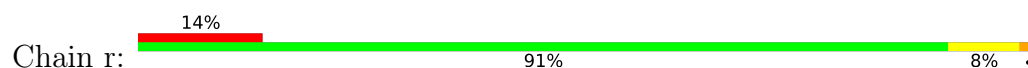
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18

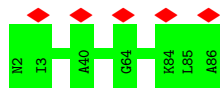


- Molecule 19: 30S ribosomal protein S19

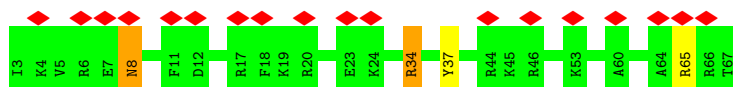




- Molecule 20: 30S ribosomal protein S20



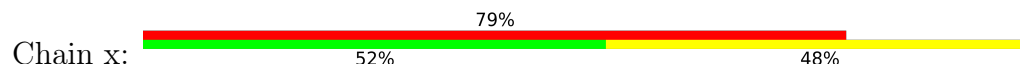
- Molecule 21: 30S ribosomal protein S21



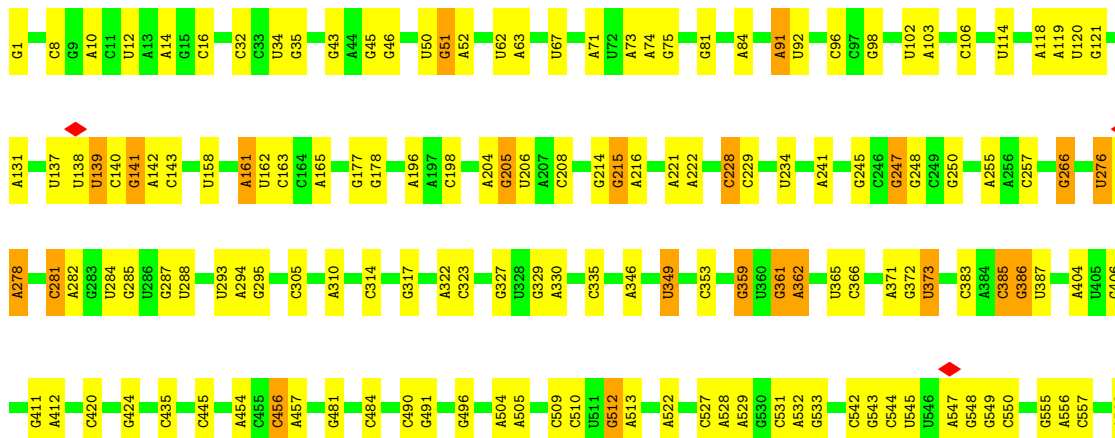
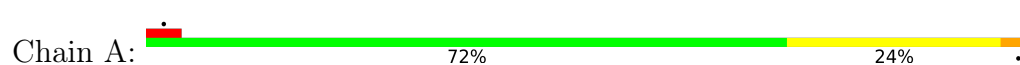
- Molecule 22: fMet-tRNAfMet

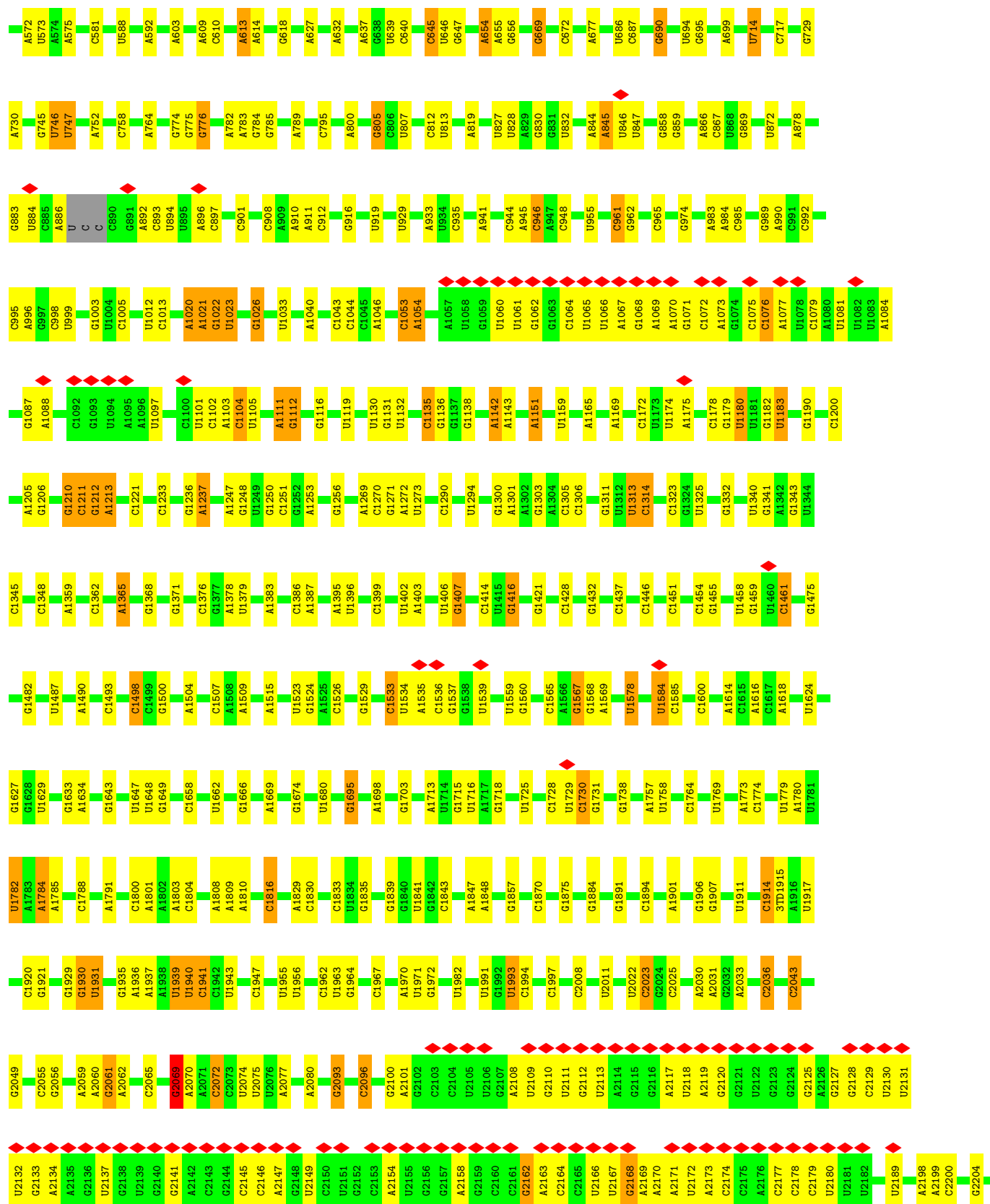


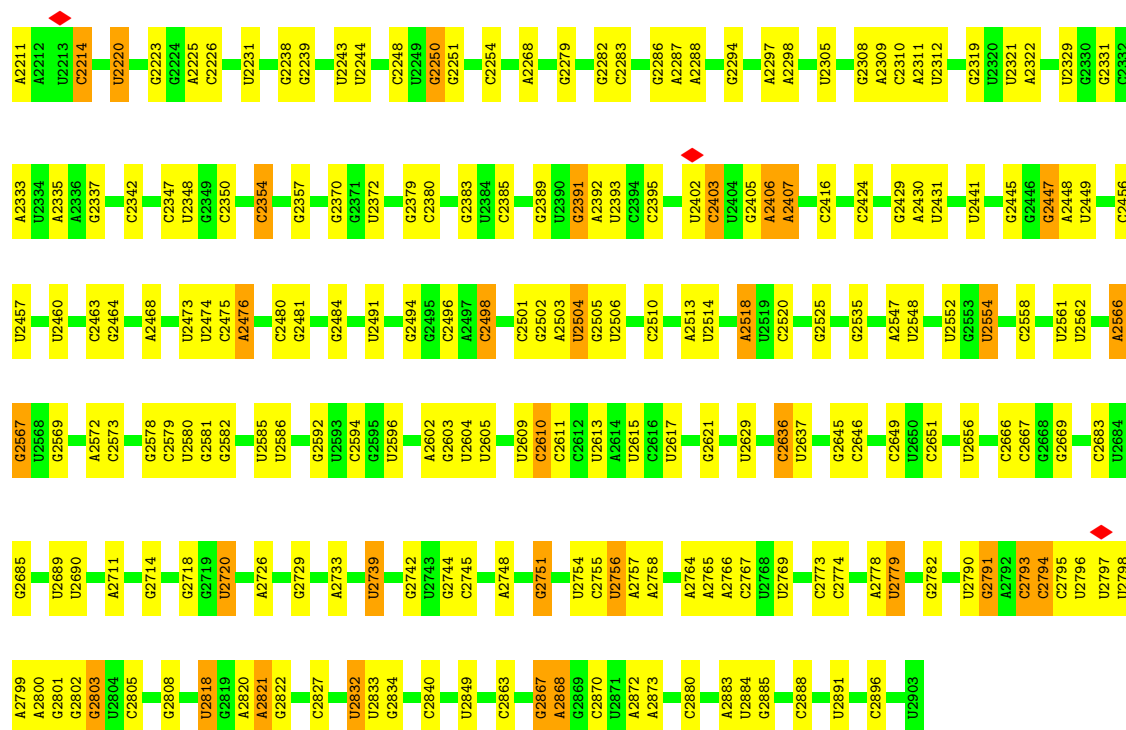
- Molecule 23: SECIS mRNA



- Molecule 24: 23S ribosomal RNA



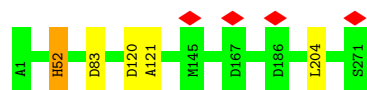




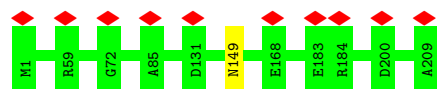
• Molecule 25: 5S ribosomal RNA



• Molecule 26: 50S ribosomal protein L2

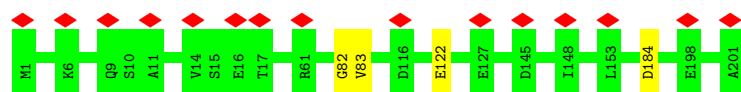


• Molecule 27: 50S ribosomal protein L3

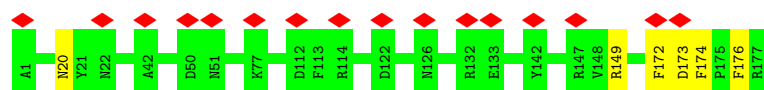


• Molecule 28: 50S ribosomal protein L4

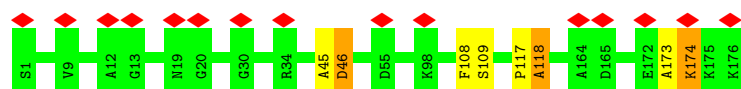




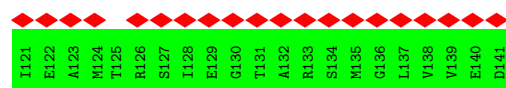
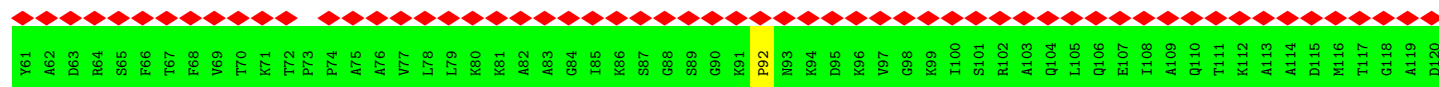
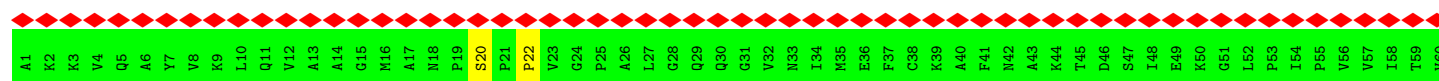
- Molecule 29: 50S ribosomal protein L5



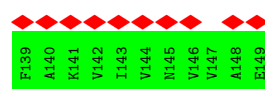
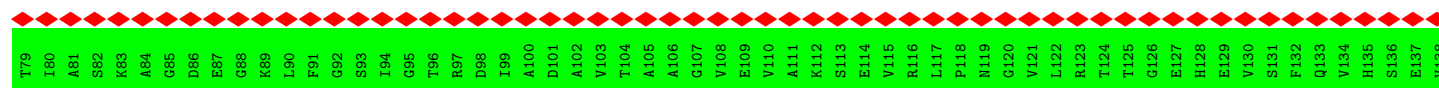
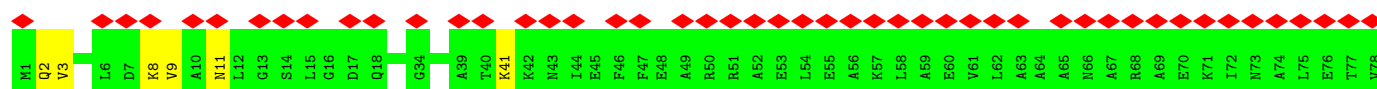
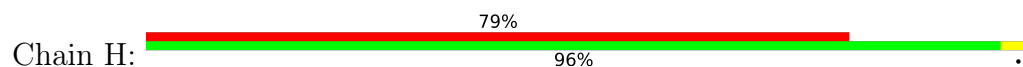
- Molecule 30: 50S ribosomal protein L6



- Molecule 31: 50S ribosomal protein L11

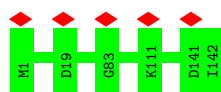


- Molecule 32: 50S ribosomal protein L9



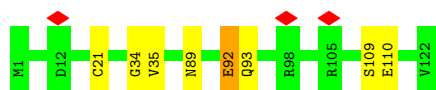
- Molecule 33: 50S ribosomal protein L13

Chain J:  100%



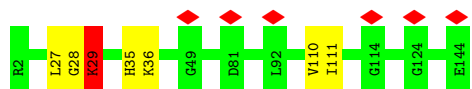
- Molecule 34: 50S ribosomal protein L14

Chain K:  93% 6%



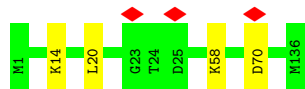
- Molecule 35: 50S ribosomal protein L15

Chain L:  95%



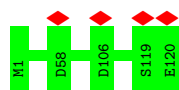
- Molecule 36: 50S ribosomal protein L16

Chain M:  97%



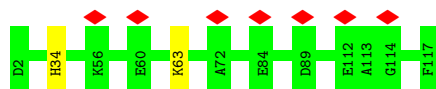
- Molecule 37: 50S ribosomal protein L17

Chain N:  100%



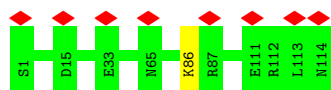
- Molecule 38: 50S ribosomal protein L18

Chain O:  98% 6%



- Molecule 39: 50S ribosomal protein L19

Chain P:  99% 7%



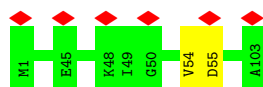
- Molecule 40: 50S ribosomal protein L20

Chain Q:  99%



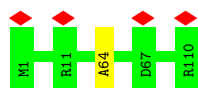
- Molecule 41: 50S ribosomal protein L21

Chain R:  98%



- Molecule 42: 50S ribosomal protein L22

Chain S:  99%




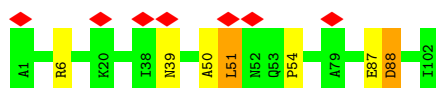
- Molecule 43: 50S ribosomal protein L23

Chain T:  97%



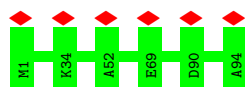
- Molecule 44: 50S ribosomal protein L24

Chain U:  93% 5%



- Molecule 45: 50S ribosomal protein L25

Chain V:  100%



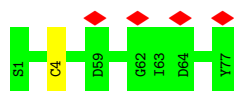
- Molecule 46: 50S ribosomal protein L27

Chain W:  99%





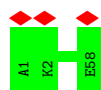
- Molecule 47: 50S ribosomal protein L28



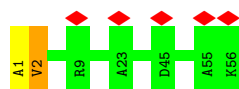
- Molecule 48: 50S ribosomal protein L29



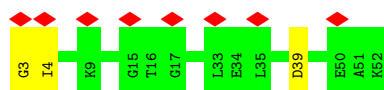
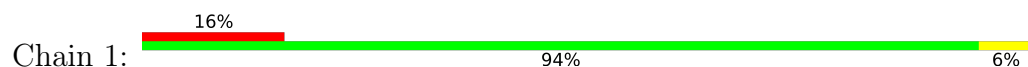
- Molecule 49: 50S ribosomal protein L30



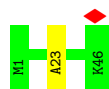
- Molecule 50: 50S ribosomal protein L32



- Molecule 51: 50S ribosomal protein L33

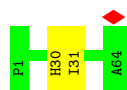


- Molecule 52: 50S ribosomal protein L34



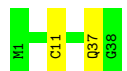
- Molecule 53: 50S ribosomal protein L35

Chain 3:  97%




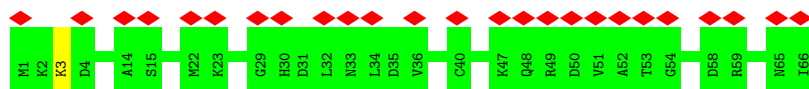
- Molecule 54: 50S ribosomal protein L36

Chain 4:  95%



- Molecule 55: 50S ribosomal protein L31

Chain 6:  38% 98%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75176	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; Local CTF correction, after MSA based classification and averaging of local power spectra	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	3.934	Depositor
Minimum map value	-2.060	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.265	Depositor
Recommended contour level	0.52	Depositor
Map size ( $\text{\AA}$ )	315.52, 315.52, 315.52	wwPDB
Map dimensions	272, 272, 272	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.16, 1.16, 1.16	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: G7M, 2MG, 4SU, 2MA, 5MU, 5MC, ZN, 6MZ, UR3, OMC, 4OC, H2U, PSU, 1MG, OMU, OMG, MA6, 3TD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	a	0.61	4/36803 (0.0%)	1.26	322/57406 (0.6%)
2	b	0.43	0/1736	0.66	3/2338 (0.1%)
3	c	0.40	0/1652	0.60	0/2225
4	d	0.43	0/1665	0.62	0/2227
5	e	0.44	0/1170	0.80	2/1573 (0.1%)
6	f	0.49	0/836	0.83	2/1128 (0.2%)
7	g	0.43	0/1196	0.70	3/1602 (0.2%)
8	h	0.42	0/989	0.66	0/1326
9	i	0.41	0/1034	0.69	0/1375
10	j	0.37	0/797	0.74	0/1077
11	k	0.40	0/886	0.71	0/1195
12	l	0.43	0/969	0.82	2/1300 (0.2%)
13	m	0.46	0/893	0.78	3/1193 (0.3%)
14	n	0.45	0/806	0.66	1/1074 (0.1%)
15	o	0.40	0/722	0.61	0/964
16	p	0.45	0/659	0.70	1/884 (0.1%)
17	q	0.45	0/658	0.78	1/881 (0.1%)
18	r	0.42	0/512	0.70	0/689
19	s	0.41	0/653	0.75	1/877 (0.1%)
20	t	0.42	0/671	0.60	0/888
21	u	0.53	0/501	0.84	1/668 (0.1%)
22	v	0.55	1/1747 (0.1%)	1.29	19/2721 (0.7%)
23	x	0.58	1/1145 (0.1%)	1.09	1/1781 (0.1%)
24	A	0.66	9/69196 (0.0%)	1.26	616/107943 (0.6%)
25	B	0.59	1/2873 (0.0%)	1.25	29/4478 (0.6%)
26	C	0.48	0/2122	0.73	1/2852 (0.0%)
27	D	0.44	0/1586	0.67	0/2134
28	E	0.43	0/1571	0.63	0/2113
29	F	0.43	0/1435	0.71	2/1926 (0.1%)
30	G	0.42	0/1343	0.67	4/1816 (0.2%)
31	I	0.38	0/1046	0.61	0/1410

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	H	0.38	0/1122	0.63	0/1515
33	J	0.46	0/1152	0.61	0/1551
34	K	0.46	0/948	0.69	0/1268
35	L	0.44	0/1054	0.74	1/1403 (0.1%)
36	M	0.46	0/1093	0.72	1/1460 (0.1%)
37	N	0.44	0/974	0.65	0/1301
38	O	0.42	0/902	0.59	0/1209
39	P	0.45	0/929	0.67	0/1242
40	Q	0.47	0/960	0.60	1/1278 (0.1%)
41	R	0.45	0/829	0.72	0/1107
42	S	0.40	0/864	0.62	0/1156
43	T	0.40	0/745	0.63	0/994
44	U	0.44	0/788	0.78	2/1051 (0.2%)
45	V	0.40	0/766	0.60	0/1025
46	W	0.41	0/582	0.62	0/769
47	X	0.38	0/635	0.59	0/848
48	Y	0.42	0/510	0.64	0/677
49	Z	0.40	0/453	0.60	0/605
50	0	0.41	0/450	0.72	0/599
51	1	0.42	0/417	0.84	1/554 (0.2%)
52	2	0.41	0/380	0.67	0/498
53	3	0.47	0/513	0.65	0/676
54	4	0.67	1/303 (0.3%)	0.78	0/397
55	6	0.42	0/532	0.62	0/709
All	All	0.59	17/157773 (0.0%)	1.14	1020/235956 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	2	0
2	b	0	4
5	e	0	4
6	f	0	1
7	g	0	2
8	h	0	1
9	i	0	1
10	j	0	5
12	l	0	1
13	m	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	p	0	1
17	q	0	2
18	r	0	3
19	s	0	1
21	u	0	1
24	A	2	0
26	C	0	1
28	E	0	1
30	G	0	3
32	H	0	2
34	K	0	3
35	L	0	4
42	S	0	1
44	U	0	3
48	Y	0	1
50	0	0	2
51	1	0	1
53	3	0	1
All	All	4	51

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	x	87	A	OP3-P	-10.73	1.48	1.61
24	A	1	G	OP3-P	-10.59	1.48	1.61
25	B	1	U	OP3-P	-10.53	1.48	1.61
22	v	1	C	OP3-P	-10.52	1.48	1.61
1	a	2	A	OP3-P	-10.51	1.48	1.61

The worst 5 of 1020 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1313	U	N3-C2-O2	-14.71	111.90	122.20
24	A	2072	C	C6-N1-C2	-14.04	114.69	120.30
1	a	89	U	C5-C4-O4	-13.94	117.53	125.90
1	a	529	G	C5-C6-O6	-13.71	120.38	128.60
24	A	62	U	N1-C2-O2	13.14	132.00	122.80

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C4',C3'

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Mol	Chain	Res	Type	Atom
24	A	2069	G7M	C4',C3'

5 of 51 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	b	16	GLY	Peptide
2	b	17	HIS	Mainchain,Peptide
2	b	72	LYS	Peptide
5	e	76	ASN	Peptide
5	e	88	HIS	Peptide

## 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 [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	
2	b	216/218 (99%)	189 (88%)	23 (11%)	4 (2%)	8	42
3	c	204/206 (99%)	190 (93%)	13 (6%)	1 (0%)	29	68
4	d	203/205 (99%)	187 (92%)	14 (7%)	2 (1%)	15	55
5	e	155/157 (99%)	134 (86%)	16 (10%)	5 (3%)	4	31
6	f	98/100 (98%)	82 (84%)	10 (10%)	6 (6%)	1	17
7	g	149/151 (99%)	135 (91%)	11 (7%)	3 (2%)	7	41
8	h	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	19	59
9	i	125/127 (98%)	104 (83%)	15 (12%)	6 (5%)	2	22
10	j	96/98 (98%)	82 (85%)	10 (10%)	4 (4%)	3	25
11	k	114/116 (98%)	100 (88%)	11 (10%)	3 (3%)	5	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	l	121/123 (98%)	98 (81%)	14 (12%)	9 (7%)	1	13
13	m	112/114 (98%)	97 (87%)	12 (11%)	3 (3%)	5	35
14	n	98/100 (98%)	83 (85%)	13 (13%)	2 (2%)	7	41
15	o	86/88 (98%)	73 (85%)	11 (13%)	2 (2%)	6	38
16	p	80/82 (98%)	71 (89%)	6 (8%)	3 (4%)	3	27
17	q	78/80 (98%)	66 (85%)	10 (13%)	2 (3%)	5	35
18	r	63/65 (97%)	57 (90%)	2 (3%)	4 (6%)	1	17
19	s	77/79 (98%)	70 (91%)	6 (8%)	1 (1%)	12	50
20	t	83/85 (98%)	77 (93%)	6 (7%)	0	100	100
21	u	63/65 (97%)	50 (79%)	9 (14%)	4 (6%)	1	17
26	C	269/271 (99%)	246 (91%)	20 (7%)	3 (1%)	14	53
27	D	207/209 (99%)	193 (93%)	13 (6%)	1 (0%)	29	68
28	E	199/201 (99%)	184 (92%)	12 (6%)	3 (2%)	10	47
29	F	175/177 (99%)	158 (90%)	13 (7%)	4 (2%)	6	38
30	G	174/176 (99%)	157 (90%)	11 (6%)	6 (3%)	3	31
31	I	139/141 (99%)	121 (87%)	15 (11%)	3 (2%)	6	39
32	H	147/149 (99%)	129 (88%)	14 (10%)	4 (3%)	5	35
33	J	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
34	K	120/122 (98%)	105 (88%)	10 (8%)	5 (4%)	3	25
35	L	141/143 (99%)	129 (92%)	9 (6%)	3 (2%)	7	40
36	M	134/136 (98%)	124 (92%)	7 (5%)	3 (2%)	6	39
37	N	118/120 (98%)	106 (90%)	12 (10%)	0	100	100
38	O	114/116 (98%)	104 (91%)	8 (7%)	2 (2%)	8	43
39	P	112/114 (98%)	104 (93%)	7 (6%)	1 (1%)	17	57
40	Q	115/117 (98%)	108 (94%)	7 (6%)	0	100	100
41	R	101/103 (98%)	91 (90%)	8 (8%)	2 (2%)	7	41
42	S	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
43	T	91/93 (98%)	81 (89%)	7 (8%)	3 (3%)	4	31
44	U	100/102 (98%)	89 (89%)	6 (6%)	5 (5%)	2	21
45	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
46	W	73/75 (97%)	68 (93%)	4 (6%)	1 (1%)	11	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	X	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
48	Y	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
49	Z	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
50	0	54/56 (96%)	49 (91%)	4 (7%)	1 (2%)	8	42
51	1	48/50 (96%)	45 (94%)	2 (4%)	1 (2%)	7	40
52	2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	6	38
53	3	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	9	46
54	4	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	5	34
55	6	64/66 (97%)	59 (92%)	4 (6%)	1 (2%)	9	46
All	All	5717/5817 (98%)	5150 (90%)	447 (8%)	120 (2%)	10	40

5 of 120 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	17	HIS
2	b	18	GLN
2	b	73	ARG
4	d	192	ALA
5	e	77	ASN

### 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	
2	b	180/180 (100%)	178 (99%)	2 (1%)	73	88
3	c	170/170 (100%)	170 (100%)	0	100	100
4	d	172/172 (100%)	171 (99%)	1 (1%)	86	94
5	e	119/119 (100%)	119 (100%)	0	100	100
6	f	87/87 (100%)	87 (100%)	0	100	100
7	g	124/124 (100%)	124 (100%)	0	100	100
8	h	104/104 (100%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	i	105/105 (100%)	105 (100%)	0	100	100
10	j	86/86 (100%)	86 (100%)	0	100	100
11	k	89/89 (100%)	89 (100%)	0	100	100
12	l	103/103 (100%)	102 (99%)	1 (1%)	76	88
13	m	92/92 (100%)	92 (100%)	0	100	100
14	n	79/83 (95%)	78 (99%)	1 (1%)	69	86
15	o	76/76 (100%)	76 (100%)	0	100	100
16	p	65/65 (100%)	64 (98%)	1 (2%)	65	84
17	q	74/74 (100%)	74 (100%)	0	100	100
18	r	48/56 (86%)	48 (100%)	0	100	100
19	s	70/70 (100%)	70 (100%)	0	100	100
20	t	65/65 (100%)	65 (100%)	0	100	100
21	u	44/55 (80%)	44 (100%)	0	100	100
26	C	216/216 (100%)	215 (100%)	1 (0%)	88	95
27	D	164/164 (100%)	164 (100%)	0	100	100
28	E	165/165 (100%)	165 (100%)	0	100	100
29	F	148/148 (100%)	148 (100%)	0	100	100
30	G	137/137 (100%)	137 (100%)	0	100	100
31	I	109/109 (100%)	109 (100%)	0	100	100
32	H	114/114 (100%)	114 (100%)	0	100	100
33	J	116/116 (100%)	116 (100%)	0	100	100
34	K	103/103 (100%)	102 (99%)	1 (1%)	76	88
35	L	102/102 (100%)	101 (99%)	1 (1%)	76	88
36	M	109/109 (100%)	109 (100%)	0	100	100
37	N	100/100 (100%)	100 (100%)	0	100	100
38	O	86/86 (100%)	86 (100%)	0	100	100
39	P	99/99 (100%)	99 (100%)	0	100	100
40	Q	89/89 (100%)	89 (100%)	0	100	100
41	R	84/84 (100%)	84 (100%)	0	100	100
42	S	93/93 (100%)	93 (100%)	0	100	100
43	T	80/80 (100%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	U	83/83 (100%)	83 (100%)	0	100	100
45	V	78/78 (100%)	78 (100%)	0	100	100
46	W	57/57 (100%)	57 (100%)	0	100	100
47	X	67/67 (100%)	66 (98%)	1 (2%)	65	84
48	Y	55/55 (100%)	55 (100%)	0	100	100
49	Z	48/48 (100%)	48 (100%)	0	100	100
50	0	47/47 (100%)	46 (98%)	1 (2%)	53	78
51	1	45/45 (100%)	45 (100%)	0	100	100
52	2	38/38 (100%)	38 (100%)	0	100	100
53	3	51/51 (100%)	51 (100%)	0	100	100
54	4	34/34 (100%)	34 (100%)	0	100	100
55	6	59/59 (100%)	59 (100%)	0	100	100
All	All	4728/4751 (100%)	4717 (100%)	11 (0%)	93	98

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	K	21	CYS
35	L	27	LEU
50	0	2	VAL
47	X	4	CYS
14	n	34	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
44	U	39	ASN
37	N	81	ASN
27	D	49	GLN
37	N	62	ASN
26	C	44	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1531/1539 (99%)	260 (16%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	v	76/77 (98%)	15 (19%)	0
23	x	47/48 (97%)	21 (44%)	0
24	A	2893/2903 (99%)	540 (18%)	34 (1%)
25	B	119/120 (99%)	17 (14%)	3 (2%)
All	All	4666/4687 (99%)	853 (18%)	37 (0%)

5 of 853 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	6	G
1	a	9	G
1	a	22	G
1	a	32	A
1	a	39	G

5 of 37 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	A	2566	A
25	B	66	A
24	A	2610	C
24	A	2832	U
24	A	1070	A

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

39 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
24	OMU	A	2552	24	19,22,23	1.23	2 (10%)	26,31,34	1.94	7 (26%)
24	PSU	A	746	24	18,21,22	1.34	2 (11%)	22,30,33	1.74	4 (18%)
24	PSU	A	2504	24	18,21,22	1.44	3 (16%)	22,30,33	1.84	3 (13%)
24	3TD	A	1915	24	18,22,23	4.06	7 (38%)	22,32,35	1.79	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	2MA	A	2503	24	17,25,26	1.00	1 (5%)	17,37,40	0.96	2 (11%)
1	5MC	a	967	1	18,22,23	0.92	2 (11%)	26,32,35	1.10	3 (11%)
24	OMG	A	2251	22,24	18,26,27	1.01	1 (5%)	19,38,41	1.19	2 (10%)
22	4SU	v	8	22	18,21,22	1.80	4 (22%)	26,30,33	2.35	5 (19%)
22	5MU	v	54	22	19,22,23	1.40	6 (31%)	28,32,35	2.05	6 (21%)
24	PSU	A	955	24	18,21,22	1.42	4 (22%)	22,30,33	1.94	3 (13%)
1	MA6	a	1519	1	19,26,27	0.93	1 (5%)	18,38,41	1.89	4 (22%)
1	MA6	a	1518	1	19,26,27	0.99	1 (5%)	18,38,41	1.74	4 (22%)
24	PSU	A	2580	24	18,21,22	1.51	3 (16%)	22,30,33	1.94	3 (13%)
1	2MG	a	1207	1	18,26,27	1.02	1 (5%)	16,38,41	1.04	2 (12%)
24	PSU	A	2604	24	18,21,22	1.48	3 (16%)	22,30,33	1.84	4 (18%)
24	5MU	A	1939	24	19,22,23	1.45	4 (21%)	28,32,35	2.18	5 (17%)
24	OMC	A	2498	24	19,22,23	0.88	1 (5%)	26,31,34	1.13	2 (7%)
1	UR3	a	1498	1	19,22,23	1.13	2 (10%)	26,32,35	2.06	5 (19%)
24	2MG	A	2445	24	18,26,27	0.98	1 (5%)	16,38,41	1.19	3 (18%)
24	6MZ	A	1618	24	18,25,26	0.94	1 (5%)	16,36,39	2.35	4 (25%)
24	5MC	A	1962	24	18,22,23	1.00	1 (5%)	26,32,35	1.49	3 (11%)
24	1MG	A	745	24	18,26,27	0.81	1 (5%)	19,39,42	1.07	2 (10%)
22	PSU	v	55	22	18,21,22	1.38	3 (16%)	22,30,33	1.86	4 (18%)
24	6MZ	A	2030	24	18,25,26	0.95	1 (5%)	16,36,39	2.69	4 (25%)
24	PSU	A	2605	24	18,21,22	1.40	3 (16%)	22,30,33	1.90	4 (18%)
1	4OC	a	1402	1	20,23,24	0.77	0	26,32,35	0.98	2 (7%)
24	PSU	A	1911	24	18,21,22	1.38	3 (16%)	22,30,33	1.94	3 (13%)
1	2MG	a	1516	1	18,26,27	0.89	1 (5%)	16,38,41	1.15	2 (12%)
1	5MC	a	1407	1	18,22,23	0.89	2 (11%)	26,32,35	1.19	3 (11%)
24	H2U	A	2449	24	18,21,22	1.05	2 (11%)	21,30,33	1.76	3 (14%)
1	G7M	a	527	1	20,26,27	1.74	5 (25%)	17,39,42	1.94	6 (35%)
1	PSU	a	516	1	18,21,22	1.39	3 (16%)	22,30,33	1.87	4 (18%)
24	2MG	A	1835	24	18,26,27	0.91	1 (5%)	16,38,41	1.22	3 (18%)
1	2MG	a	966	1	18,26,27	0.91	1 (5%)	16,38,41	1.22	2 (12%)
24	G7M	A	2069	24	20,26,27	1.41	3 (15%)	17,39,42	1.59	2 (11%)
22	H2U	v	20	22	18,21,22	0.94	2 (11%)	21,30,33	1.26	3 (14%)
24	5MU	A	747	24	19,22,23	1.42	5 (26%)	28,32,35	2.06	8 (28%)
24	PSU	A	2457	24	18,21,22	1.55	4 (22%)	22,30,33	2.11	5 (22%)
24	PSU	A	1917	24	18,21,22	1.42	3 (16%)	22,30,33	1.93	3 (13%)

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
24	OMU	A	2552	24	-	2/9/27/28	0/2/2/2
24	PSU	A	746	24	-	2/7/25/26	0/2/2/2
24	PSU	A	2504	24	-	2/7/25/26	0/2/2/2
24	3TD	A	1915	24	-	5/7/25/26	0/2/2/2
24	2MA	A	2503	24	-	2/3/25/26	0/3/3/3
1	5MC	a	967	1	-	2/7/25/26	0/2/2/2
24	OMG	A	2251	22,24	-	3/5/27/28	0/3/3/3
22	4SU	v	8	22	-	0/7/25/26	0/2/2/2
22	5MU	v	54	22	-	0/7/25/26	0/2/2/2
1	MA6	a	1519	1	-	3/7/29/30	0/3/3/3
24	PSU	A	955	24	-	0/7/25/26	0/2/2/2
1	MA6	a	1518	1	-	3/7/29/30	0/3/3/3
24	PSU	A	2580	24	-	2/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	0/5/27/28	0/3/3/3
24	PSU	A	2604	24	-	1/7/25/26	0/2/2/2
24	5MU	A	1939	24	-	2/7/25/26	0/2/2/2
24	OMC	A	2498	24	-	2/9/27/28	0/2/2/2
1	UR3	a	1498	1	-	2/7/25/26	0/2/2/2
24	2MG	A	2445	24	-	3/5/27/28	0/3/3/3
24	6MZ	A	1618	24	-	0/5/27/28	0/3/3/3
24	5MC	A	1962	24	-	4/7/25/26	0/2/2/2
24	1MG	A	745	24	-	0/3/25/26	0/3/3/3
22	PSU	v	55	22	-	2/7/25/26	0/2/2/2
24	6MZ	A	2030	24	-	3/5/27/28	0/3/3/3
24	PSU	A	2605	24	-	0/7/25/26	0/2/2/2
1	4OC	a	1402	1	-	0/9/29/30	0/2/2/2
24	PSU	A	1911	24	-	0/7/25/26	0/2/2/2
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
24	H2U	A	2449	24	-	0/7/38/39	0/2/2/2
1	G7M	a	527	1	2/2/5/5	1/3/25/26	0/3/3/3
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
24	2MG	A	1835	24	-	2/5/27/28	0/3/3/3
1	2MG	a	966	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	G7M	A	2069	24	2/2/5/5	2/3/25/26	0/3/3/3
22	H2U	v	20	22	-	0/7/38/39	0/2/2/2
24	5MU	A	747	24	-	1/7/25/26	0/2/2/2
24	PSU	A	2457	24	-	2/7/25/26	0/2/2/2
24	PSU	A	1917	24	-	0/7/25/26	0/2/2/2

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1915	3TD	C6-C5	11.98	1.49	1.35
24	A	1915	3TD	C2-N1	8.97	1.48	1.37
24	A	1915	3TD	C6-N1	5.66	1.45	1.36
1	a	527	G7M	C5-C4	4.81	1.48	1.39
22	v	8	4SU	C4-S4	-4.62	1.59	1.68

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	2030	6MZ	C9-N6-C6	-7.16	116.71	122.87
24	A	2457	PSU	N1-C2-N3	6.97	123.03	115.13
22	v	8	4SU	C4-N3-C2	-6.82	120.71	127.34
24	A	1618	6MZ	C2-N1-C6	6.65	122.29	116.59
24	A	2449	H2U	C4-N3-C2	-6.55	120.36	125.79

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C4'
1	a	527	G7M	C3'
24	A	2069	G7M	C4'
24	A	2069	G7M	C3'

5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	967	5MC	O4'-C4'-C5'-O5'
1	a	967	5MC	C3'-C4'-C5'-O5'
1	a	1498	UR3	O4'-C1'-N1-C6
1	a	1498	UR3	O4'-C1'-N1-C2
1	a	1518	MA6	C5-C6-N6-C9

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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.



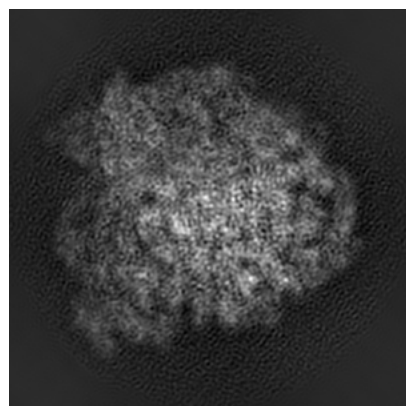
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4121. These allow visual inspection of the internal detail of the map and identification of artifacts.

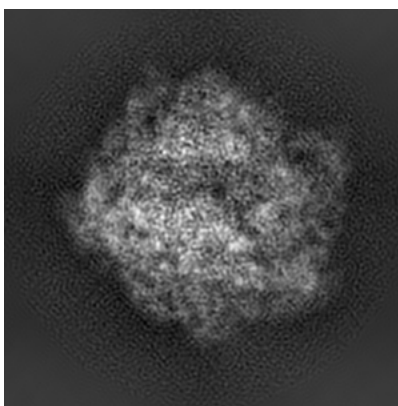
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

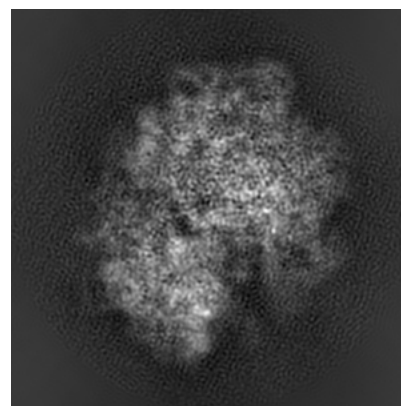
#### 6.1.1 Primary map



X

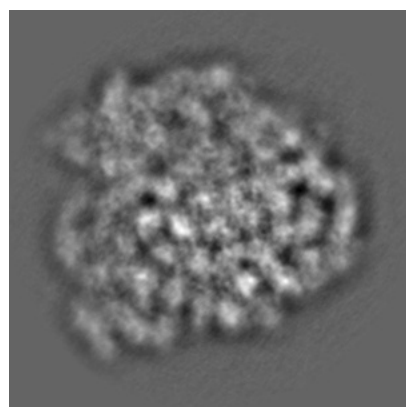


Y

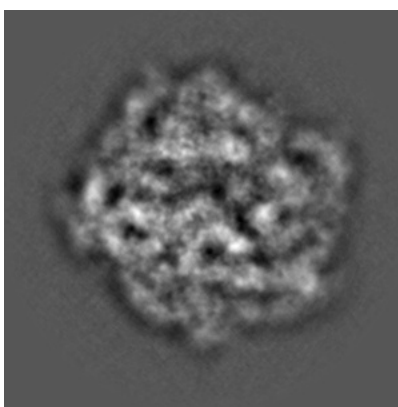


Z

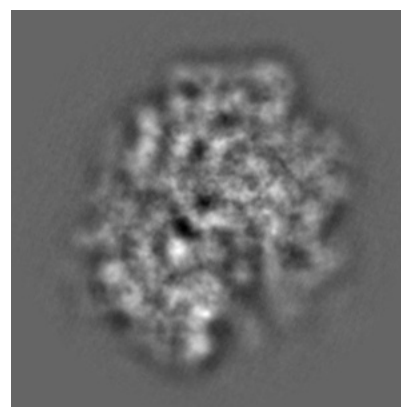
#### 6.1.2 Raw map



X



Y

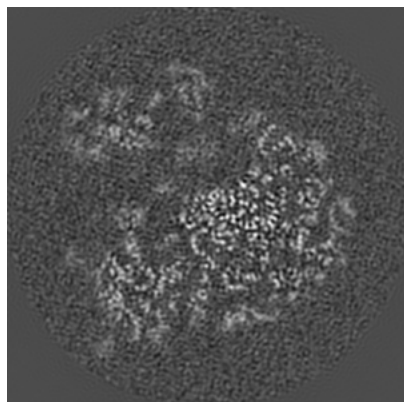


Z

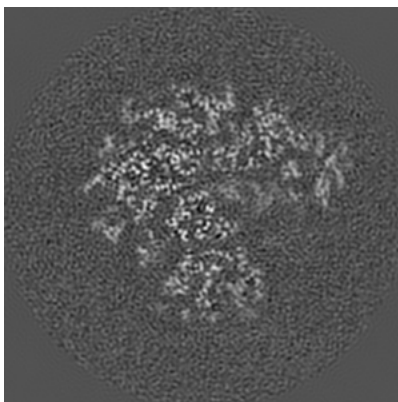
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

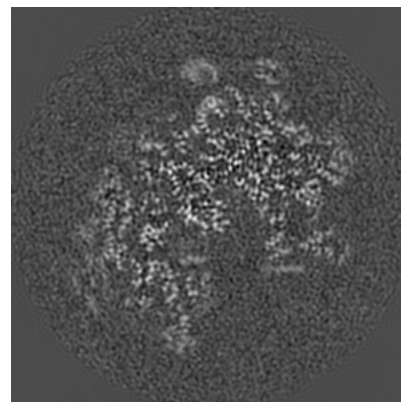
### 6.2.1 Primary map



X Index: 136

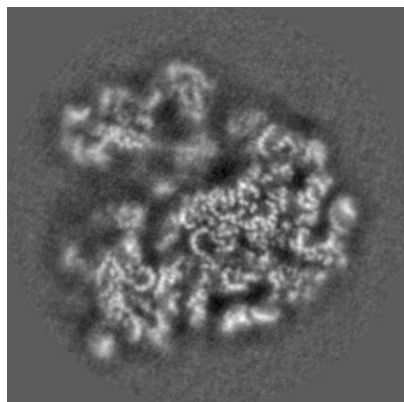


Y Index: 136

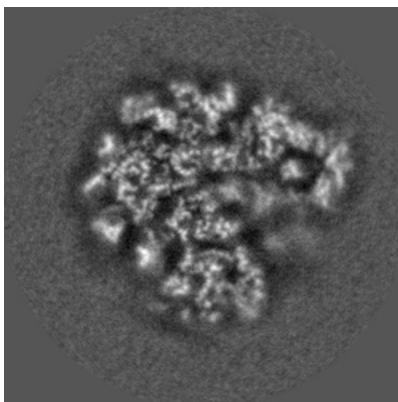


Z Index: 136

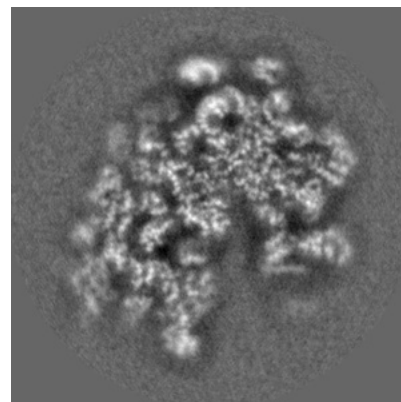
### 6.2.2 Raw map



X Index: 136



Y Index: 136

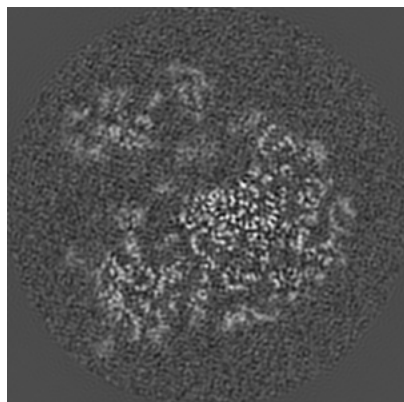


Z Index: 136

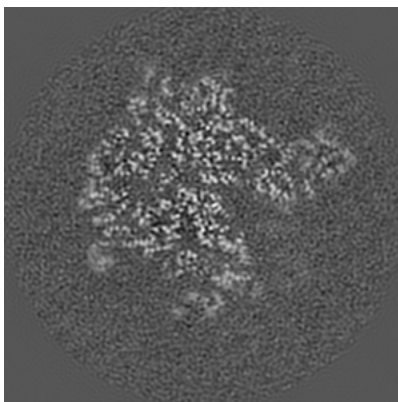
The images above show central slices of the map in three orthogonal directions.

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

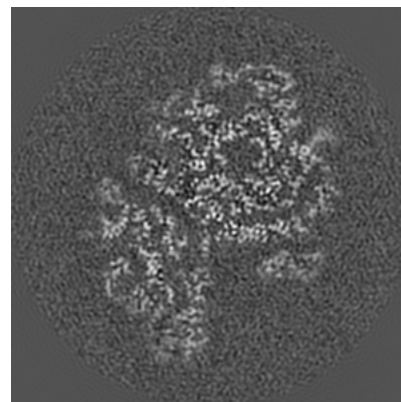
### 6.3.1 Primary map



X Index: 136

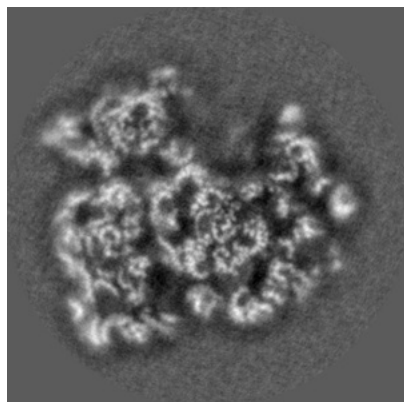


Y Index: 152

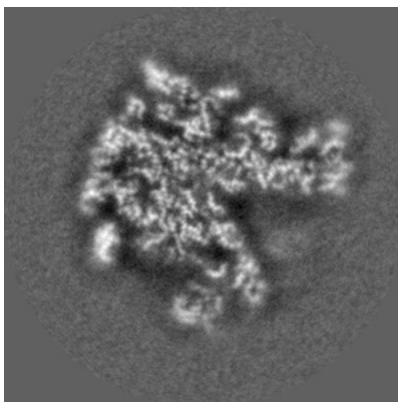


Z Index: 119

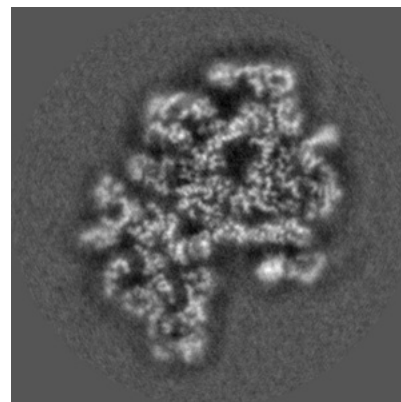
### 6.3.2 Raw map



X Index: 125



Y Index: 146

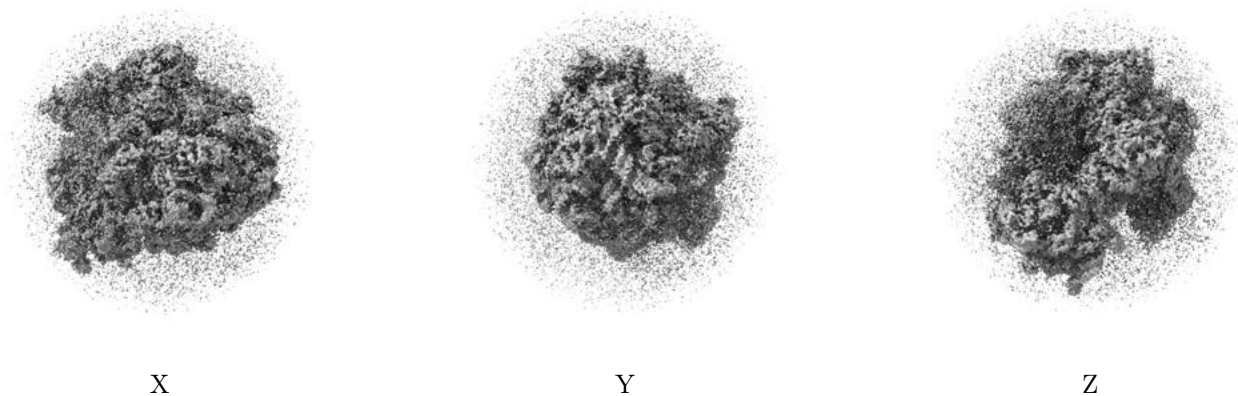


Z Index: 121

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.52. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

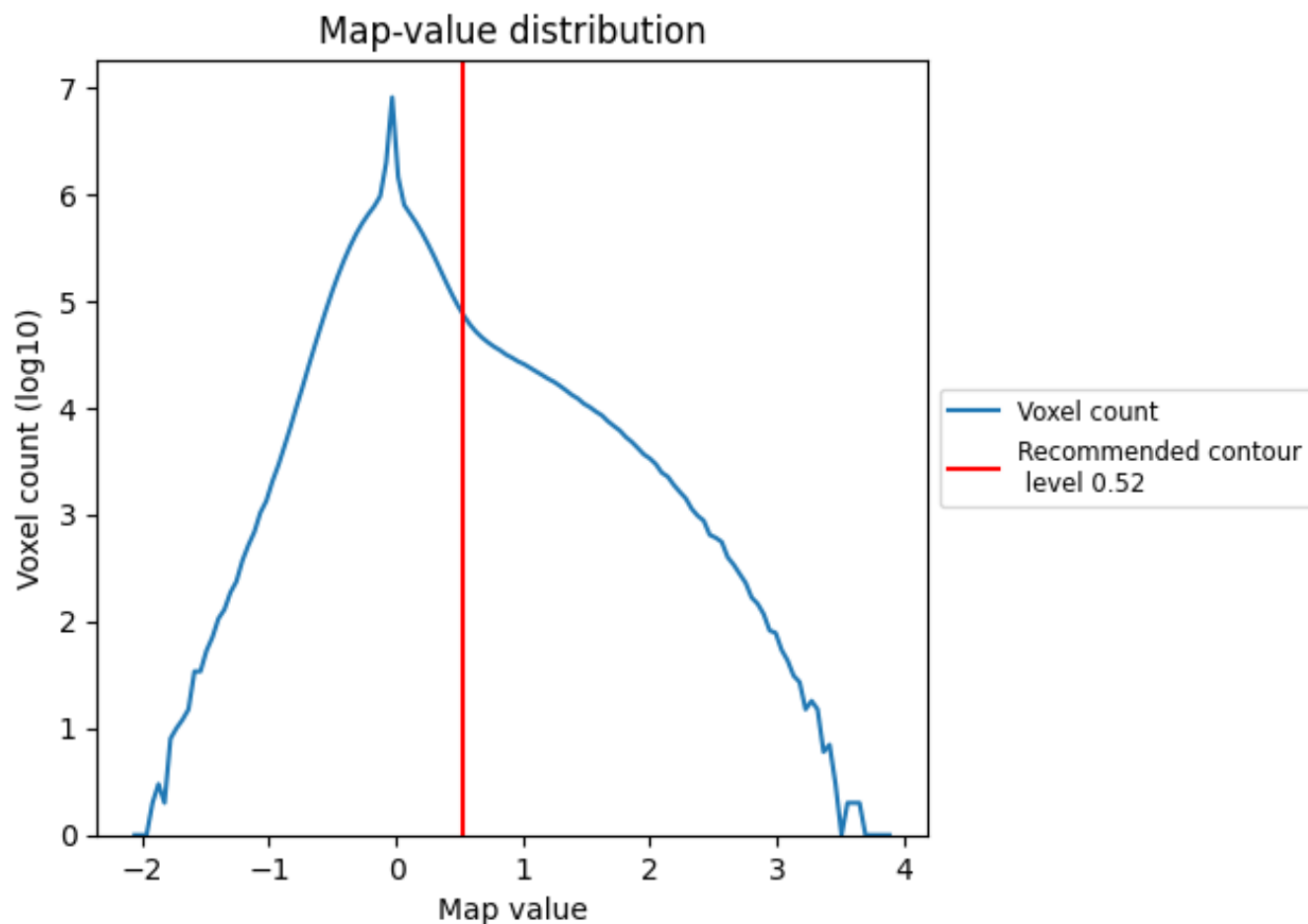
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

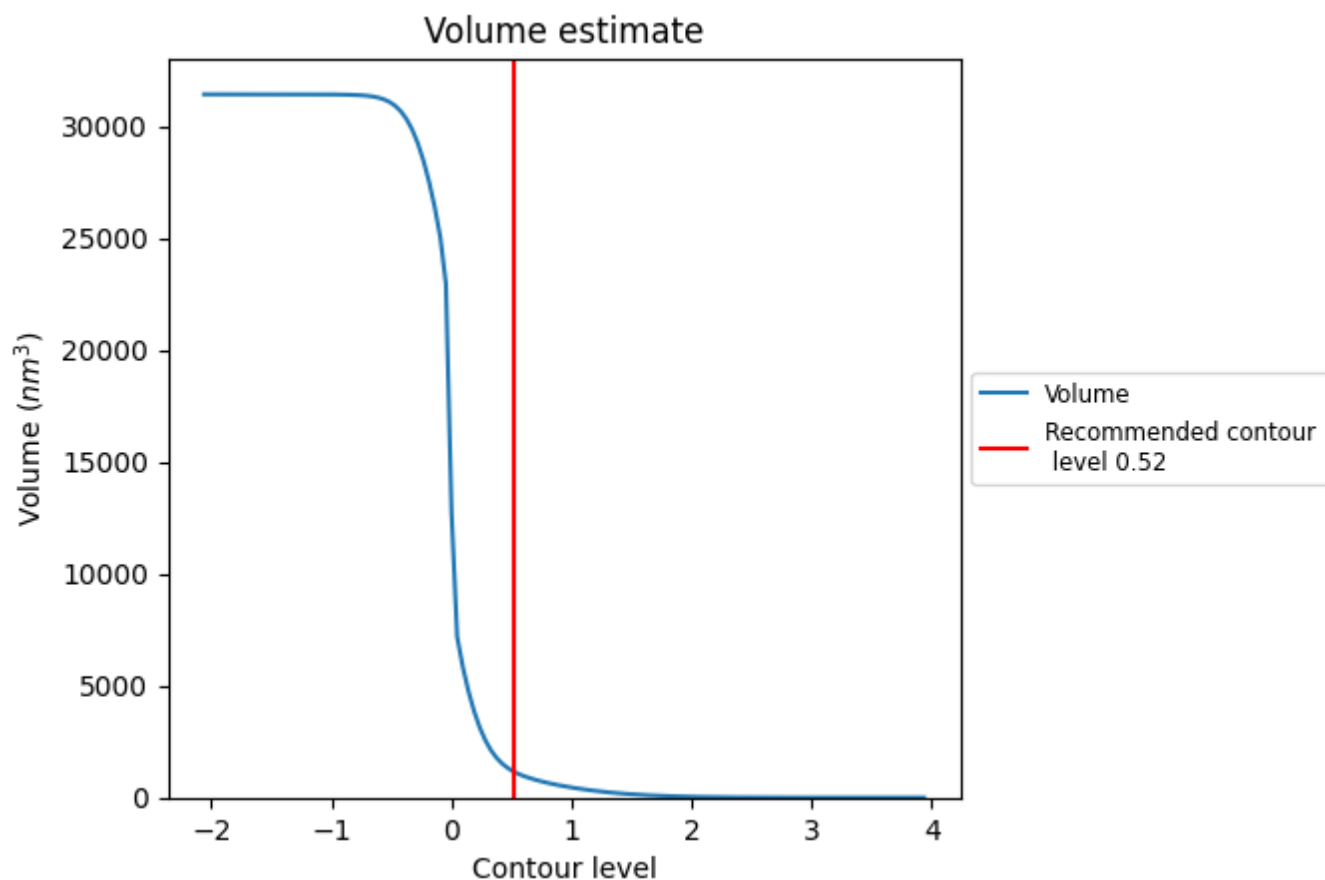
This section contains the results of statistical analysis of the map.

### 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](#)

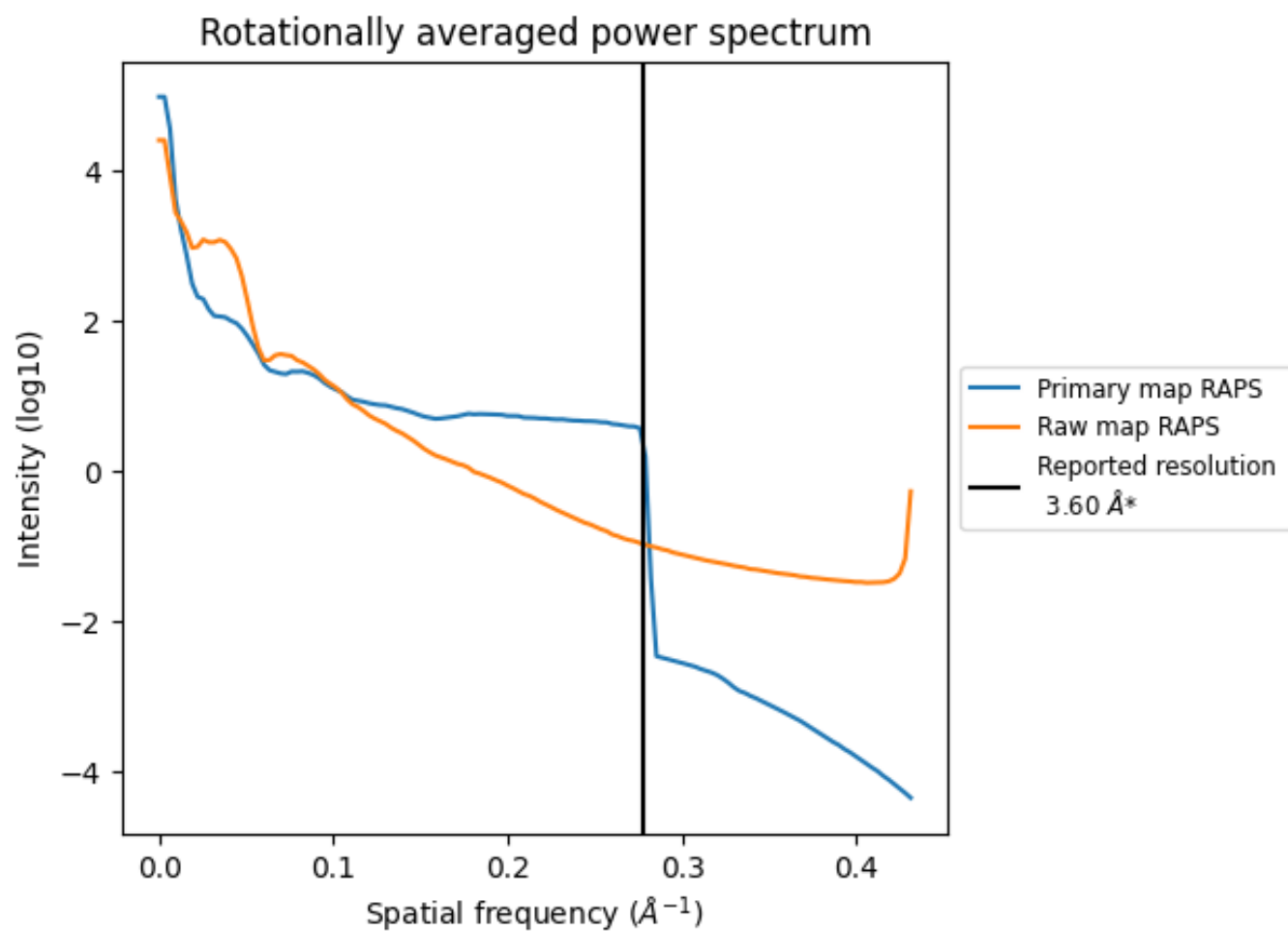


The volume at the recommended contour level is 1155 nm<sup>3</sup>; this corresponds to an approximate mass of 1043 kDa.

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 ⓘ

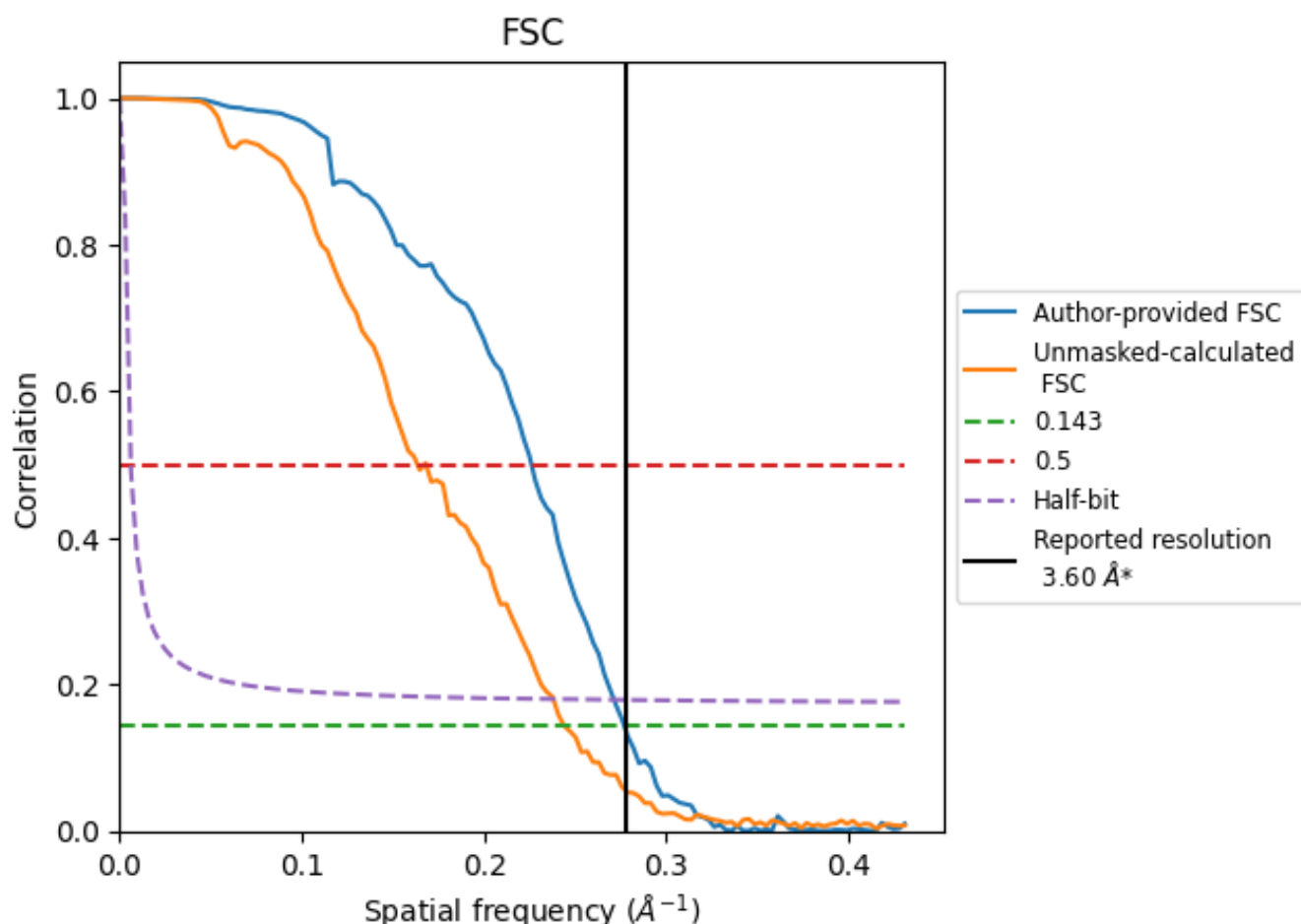


\*Reported resolution corresponds to spatial frequency of  $0.278 \text{ \AA}^{-1}$

## 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 0.278 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

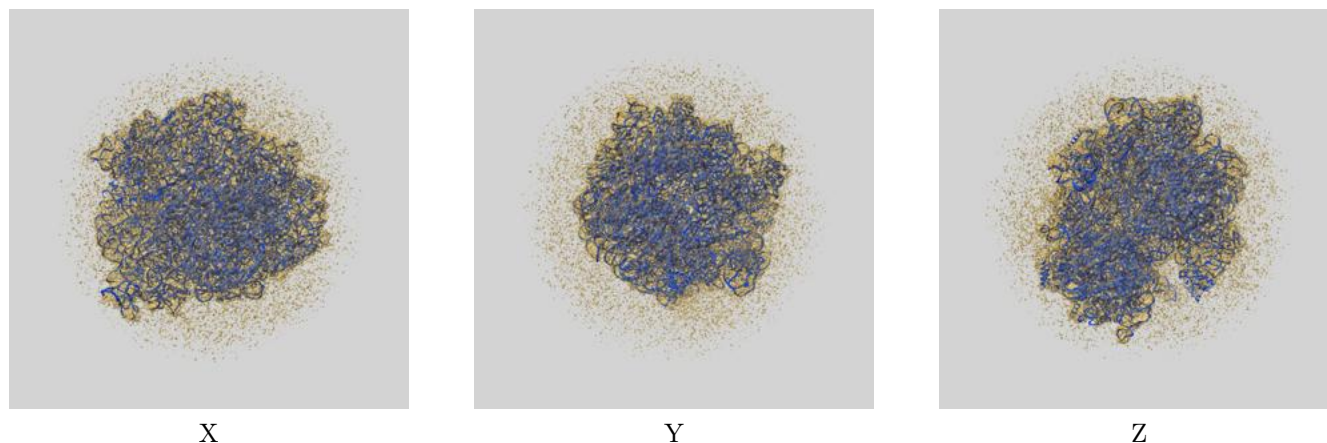
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.61	4.42	3.68
Unmasked-calculated*	4.10	6.12	4.20

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.10 differs from the reported value 3.6 by more than 10 %

## 9 Map-model fit [i](#)

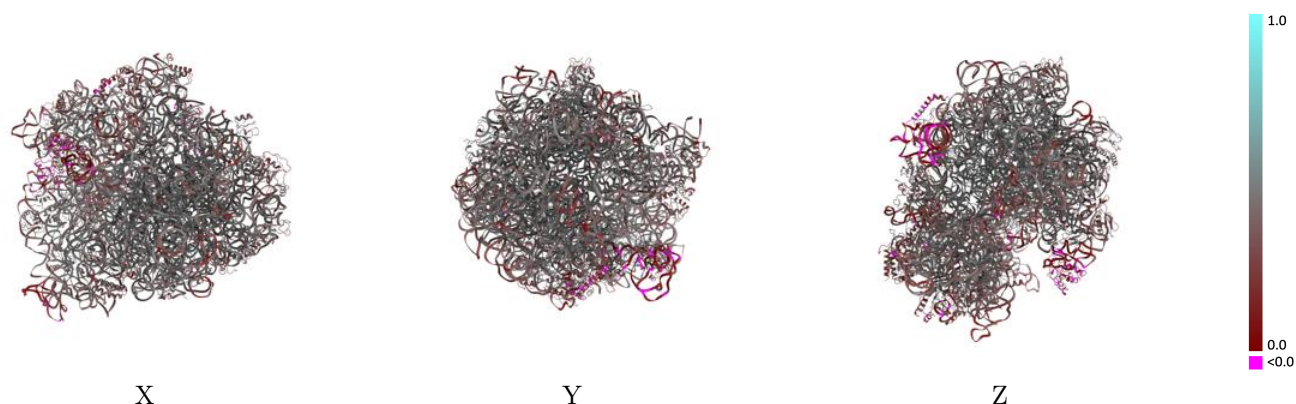
This section contains information regarding the fit between EMDB map EMD-4121 and PDB model 5LZA. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

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



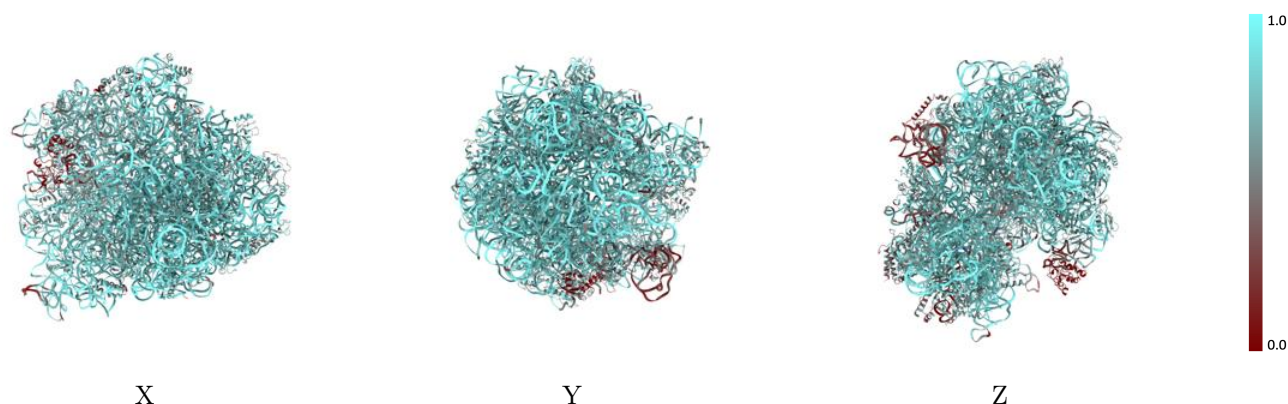
The images above show the 3D surface view of the map at the recommended contour level 0.52 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



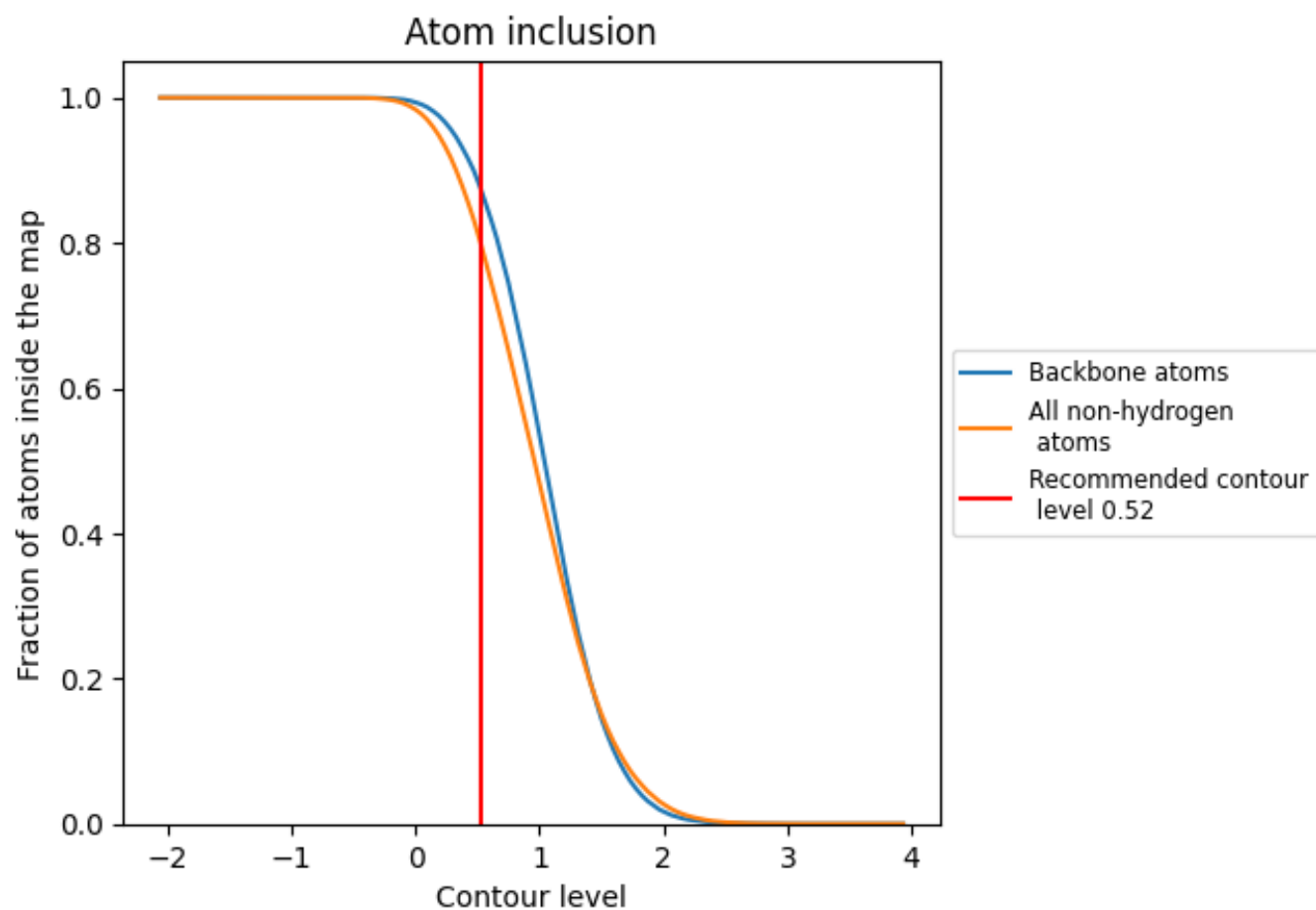
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.52).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 80% 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 (0.52) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8022	 0.4070
0	 0.7313	 0.4610
1	 0.6119	 0.3830
2	 0.7944	 0.4860
3	 0.7637	 0.4790
4	 0.7270	 0.4640
6	 0.5107	 0.2440
A	 0.8745	 0.4260
B	 0.8942	 0.4000
C	 0.7714	 0.4680
D	 0.7256	 0.4450
E	 0.6776	 0.3990
F	 0.6638	 0.3560
G	 0.6685	 0.3660
H	 0.2190	 0.2180
I	 0.0499	 0.0810
J	 0.7218	 0.4380
K	 0.7177	 0.4370
L	 0.7323	 0.4350
M	 0.7418	 0.4440
N	 0.7411	 0.4440
O	 0.6674	 0.3800
P	 0.7140	 0.4120
Q	 0.7335	 0.4480
R	 0.7189	 0.4200
S	 0.7045	 0.4270
T	 0.6722	 0.3980
U	 0.6628	 0.3880
V	 0.6911	 0.3840
W	 0.7335	 0.4540
X	 0.7171	 0.4400
Y	 0.6660	 0.3720
Z	 0.7048	 0.4150
a	 0.8815	 0.4160
b	 0.4785	 0.3010



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Chain	Atom inclusion	Q-score
c	 0.6523	 0.3940
d	 0.6126	 0.3520
e	 0.6960	 0.4120
f	 0.6863	 0.3480
g	 0.6341	 0.3380
h	 0.6896	 0.4030
i	 0.6118	 0.3400
j	 0.5486	 0.3390
k	 0.7104	 0.3950
l	 0.7242	 0.4100
m	 0.6643	 0.3530
n	 0.6920	 0.3970
o	 0.7246	 0.4000
p	 0.6746	 0.4080
q	 0.6540	 0.3540
r	 0.6975	 0.4040
s	 0.6576	 0.3670
t	 0.6831	 0.3690
u	 0.5199	 0.2610
v	 0.7141	 0.3550
x	 0.1990	 0.1580