wwPDB EM Validation Summary Report

Feb 4, 2025 – 05:03 PM JST

PDB ID	:	8HSP
EMDB ID	:	EMD-35001
Title	:	E. coli 70S ribosome complexed with tRNA_Ile2 bearing L34 and t6A37 in classical state
Authors	:	Akiyama, N.; Ishiguro, K.; Yokoyama, T.; Shirouzu, M.; Suzuki, T.
Deposited on	:	2022-12-20
Resolution	:	2.32 Å(reported)
Based on initial model	:	7K00

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

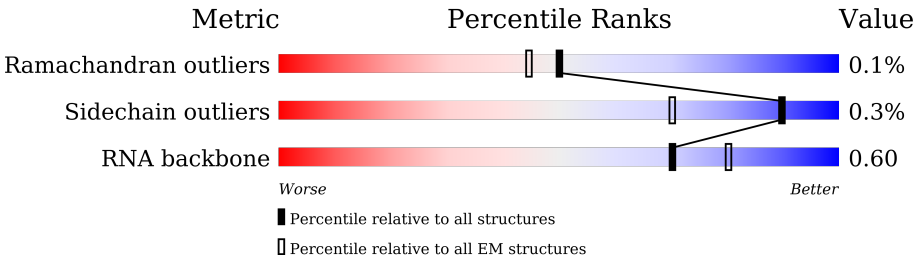
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.32 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 <=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	1542	5% 84% 15%
2	B	241	30% 93% 7%
3	C	233	6% 88% 12%
4	D	206	17% 100%
5	E	167	93% 7%
6	F	135	9% 76% 24%
7	G	179	12% 85% 15%
8	H	130	99%

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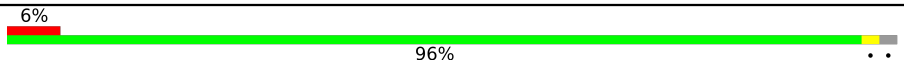
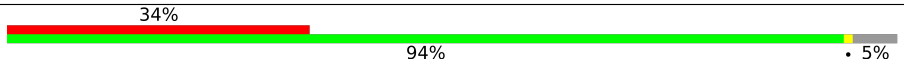
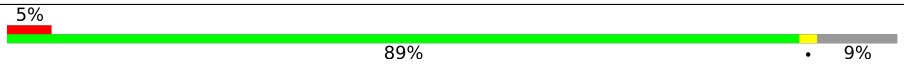
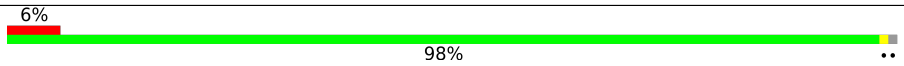
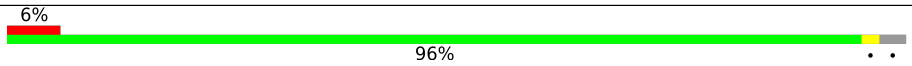
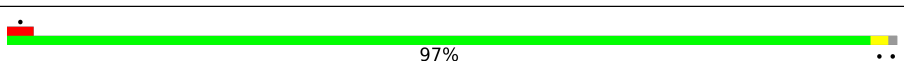
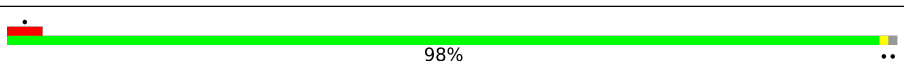
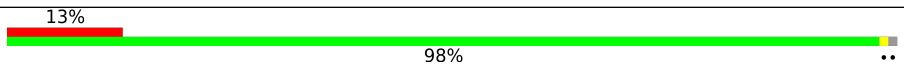
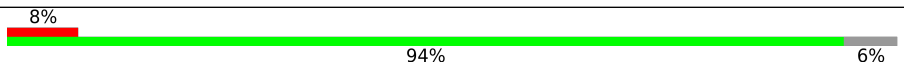
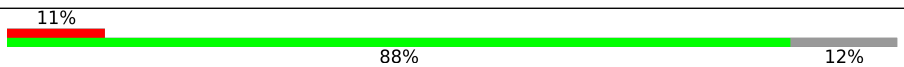
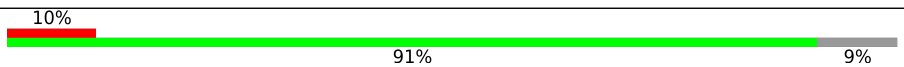
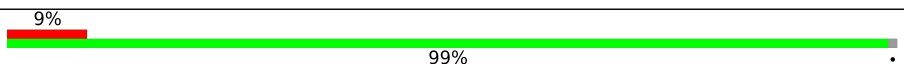
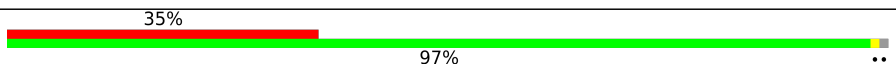
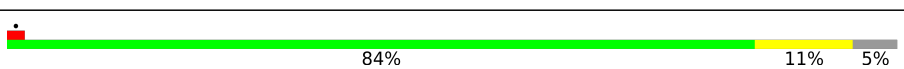
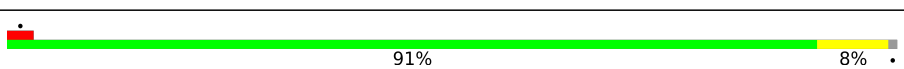
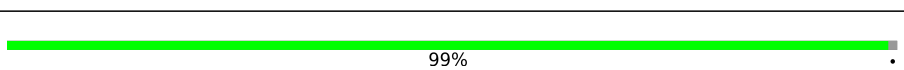
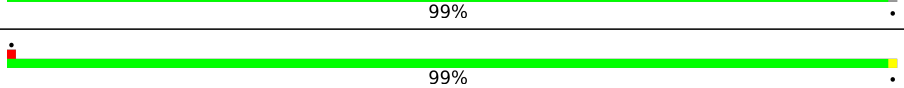
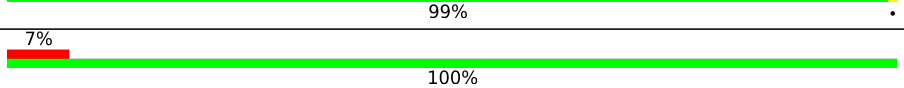
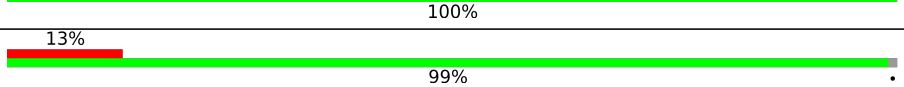
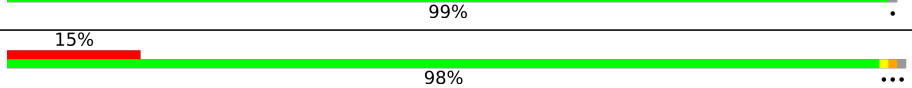
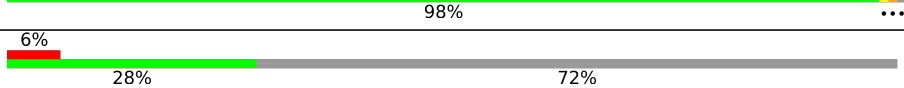
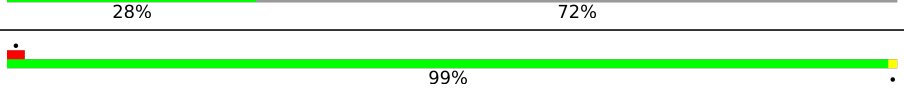
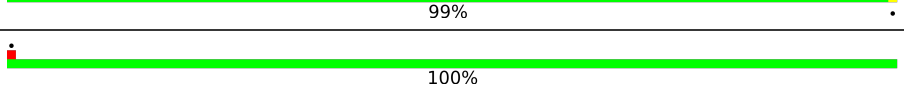
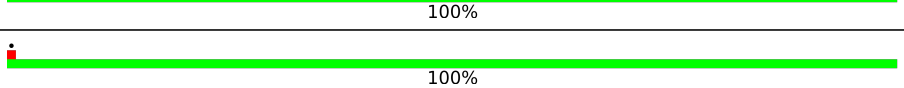
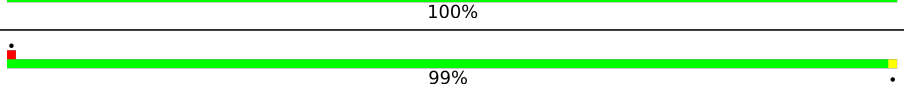
Mol	Chain	Length	Quality of chain
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	a	2904	
23	b	120	
24	c	273	
25	d	209	
26	e	201	
27	f	179	
28	g	177	
29	h	149	
30	i	142	
31	j	123	
32	k	144	
33	l	136	

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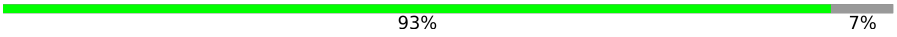
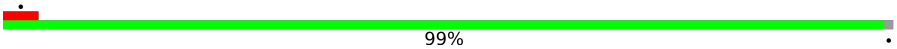
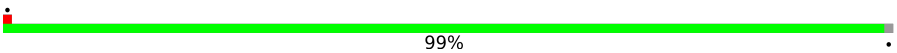
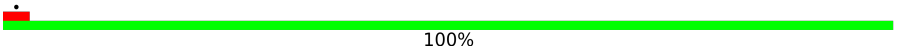
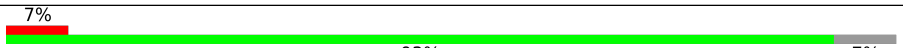
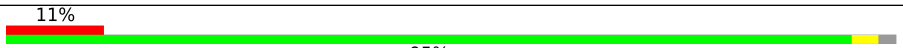
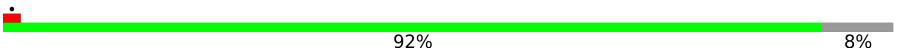
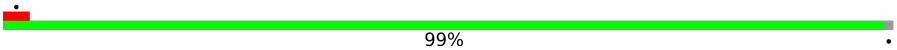
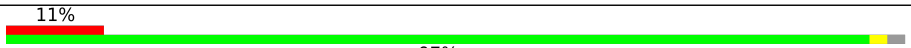
Mol	Chain	Length	Quality of chain
34	m	127	
35	n	117	
36	o	115	
37	p	118	
38	q	103	
39	r	110	
40	s	100	
41	t	104	
42	u	94	
43	v	85	
44	w	78	
45	x	63	
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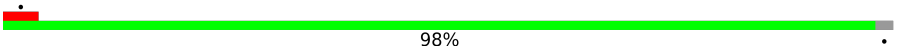
47	z	57	
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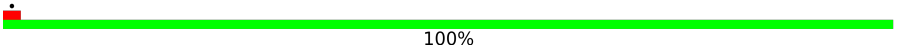
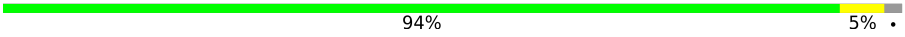
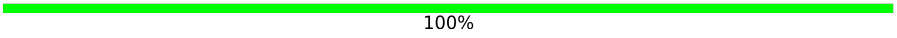
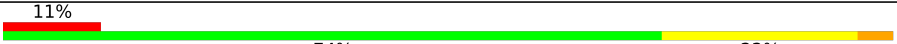
49	1	46	
50	2	65	
51	3	38	
52	4	70	
53	V	76	
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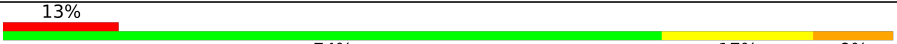
55	X	76	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 141877 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1519	32612	14552	5986	10555	1519	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	224	1753	1109	315	321	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	206	1624	1028	305	288	3	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	156	1152	717	217	212	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	103	839	530	151	151	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	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
			786	493	150	142	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP P0A7R9

- 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
			957	591	196	165	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	115	Total 891	C 552	N 179	O 157	S 3	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	81	Total 643	C 403	N 127	O 112	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	79	Total 641	C 406	N 120	O 112	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	66	Total 544	C 345	N 102	O 96	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	84	Total 668	C 427	N 127	O 112	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	2753	Total	C	N	O	P	0	0
			59130	26384	10897	19096	2753		

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 24 is a protein called 50S ribosomal protein L2.

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

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

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

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 30 is a protein called 50S ribosomal protein L13.

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

- Molecule 31 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 32 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 33 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	conflict	UNP P0ADY7

- Molecule 34 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 35 is a protein called 50S ribosomal protein L18.

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

- Molecule 36 is a protein called 50S ribosomal protein L19.

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

- Molecule 37 is a protein called 50S ribosomal protein L20.

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

- Molecule 38 is a protein called 50S ribosomal protein L21.

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

- Molecule 39 is a protein called 50S ribosomal protein L22.

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

- Molecule 40 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	s	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 41 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	t	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 42 is a protein called 50S ribosomal protein L25.

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

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

- Molecule 44 is a protein called 50S ribosomal protein L28.

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

- Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 46 is a protein called 50S ribosomal protein L30.

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

- Molecule 47 is a protein called 50S ribosomal protein L32.

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

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 53 is a RNA chain called P-site tRNA_Glu.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	V	76	Total	C	N	O	P	S	0	0
			1619	724	288	530	76	1		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	W	11	Total 236	C 106	N 44	O 75	P 11	0	0

- Molecule 55 is a RNA chain called A-site tRNA_Ile2.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	X	76	Total 1647	C 740	N 292	O 538	P 76	S 1	0	0

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	A	93	Total 93	Mg 93	0
56	a	208	Total 208	Mg 208	0
56	b	5	Total 5	Mg 5	0
56	c	1	Total 1	Mg 1	0
56	d	1	Total 1	Mg 1	0
56	z	1	Total 1	Mg 1	0
56	V	2	Total 2	Mg 2	0
56	W	2	Total 2	Mg 2	0
56	X	2	Total 2	Mg 2	0

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

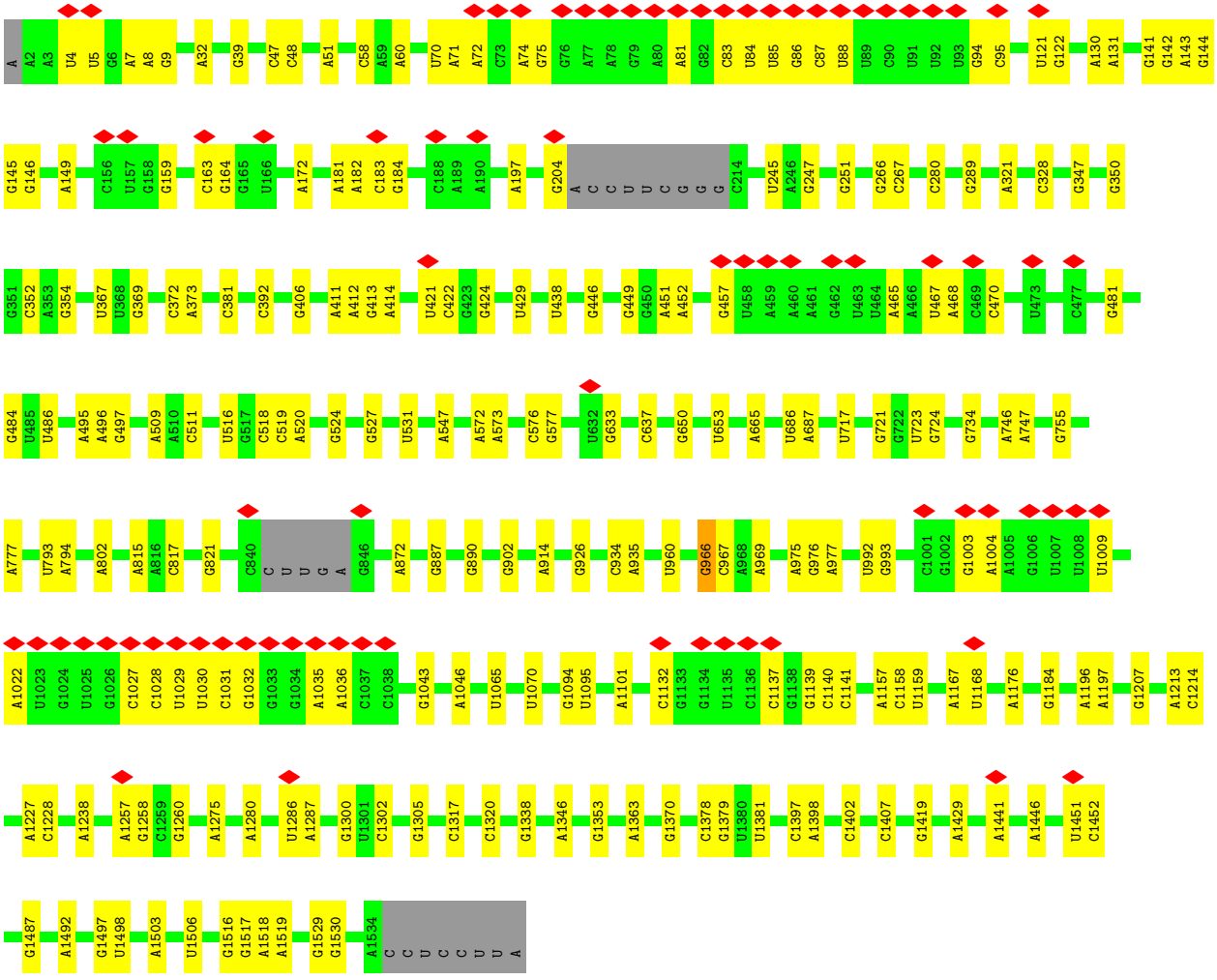
Mol	Chain	Residues	Atoms		AltConf
57	A	1	Total 1	K 1	0

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.

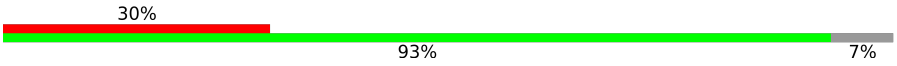
- Molecule 1: 16S rRNA

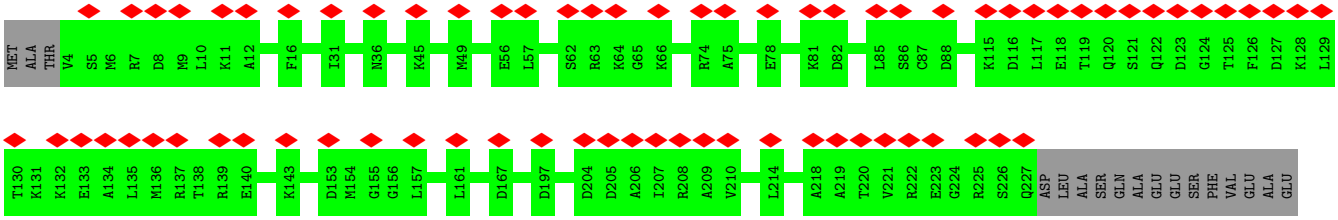
Chain A:



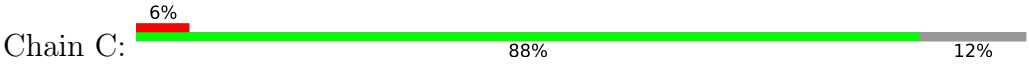
- Molecule 2: 30S ribosomal protein S2

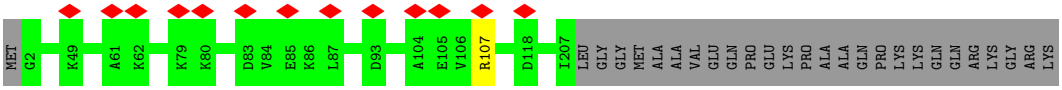
Chain B:



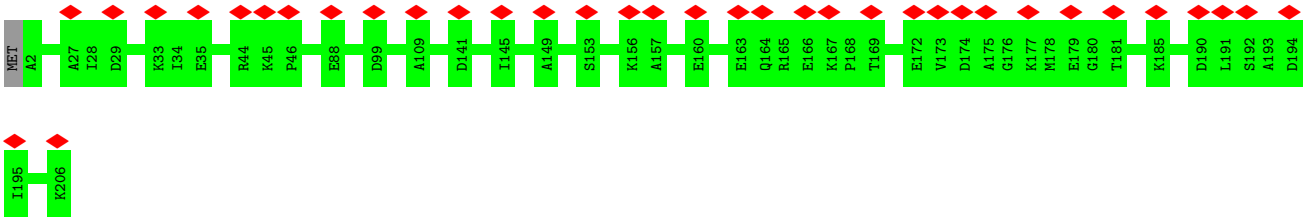


• Molecule 3: 30S ribosomal protein S3

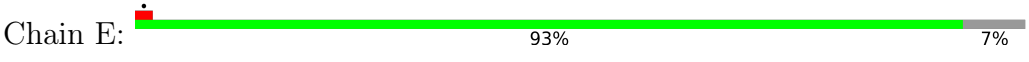


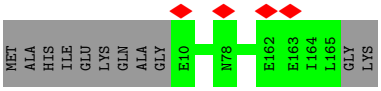


• Molecule 4: 30S ribosomal protein S4



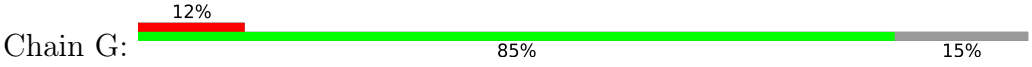
• Molecule 5: 30S ribosomal protein S5

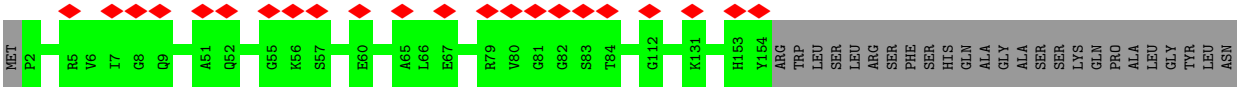




• Molecule 6: 30S ribosomal protein S6, fully modified isoform

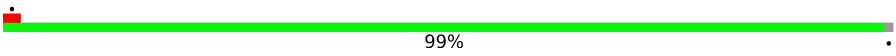
• Molecule 7: 30S ribosomal protein S7

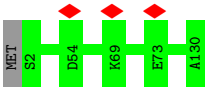




• Molecule 8: 30S ribosomal protein S8

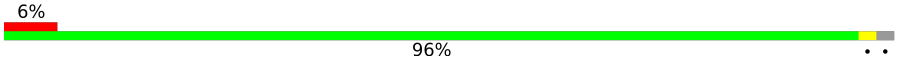
Chain H:

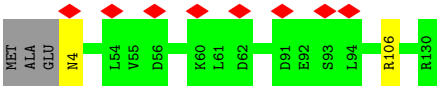




• Molecule 9: 30S ribosomal protein S9

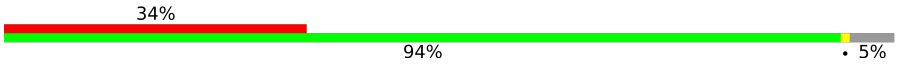
Chain I:

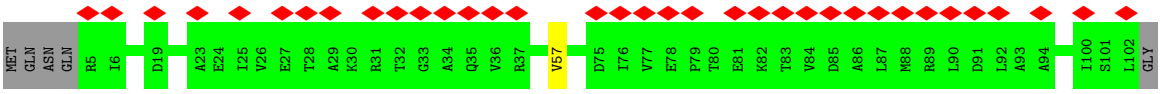




• Molecule 10: 30S ribosomal protein S10

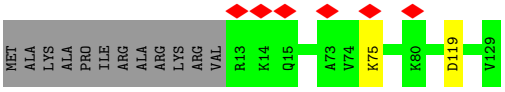
Chain J:





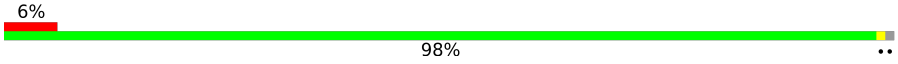
• Molecule 11: 30S ribosomal protein S11

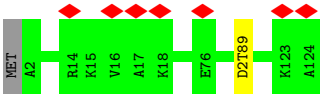
Chain K:



• Molecule 12: 30S ribosomal protein S12

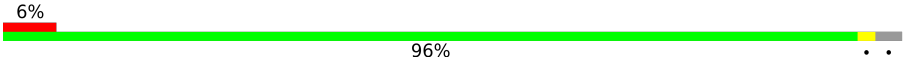
Chain L:

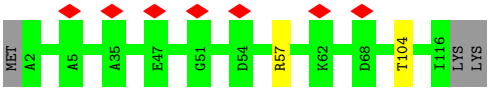




• Molecule 13: 30S ribosomal protein S13

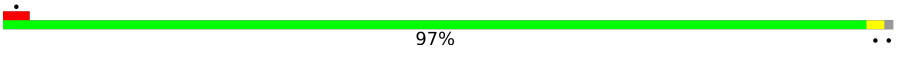
Chain M:

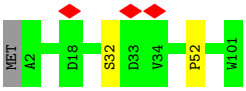




• Molecule 14: 30S ribosomal protein S14

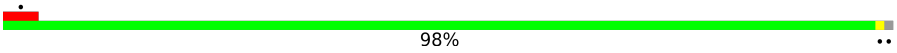
Chain N:

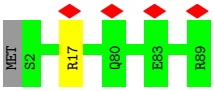




• Molecule 15: 30S ribosomal protein S15

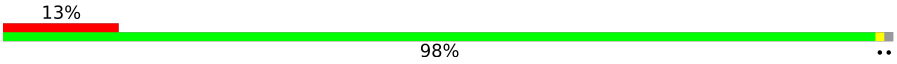
Chain O:

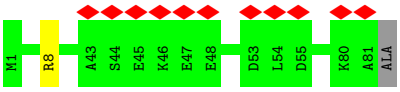




• Molecule 16: 30S ribosomal protein S16

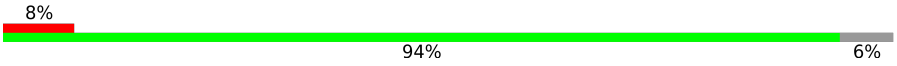
Chain P:

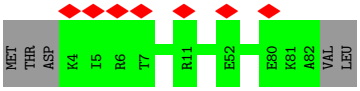




• Molecule 17: 30S ribosomal protein S17

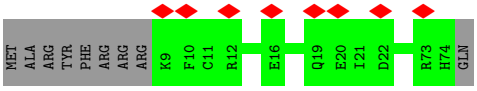
Chain Q:





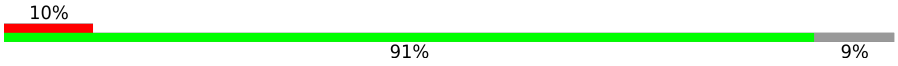
• Molecule 18: 30S ribosomal protein S18

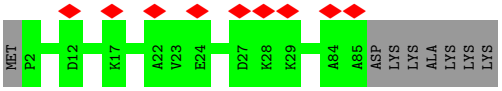
Chain R:



• Molecule 19: 30S ribosomal protein S19

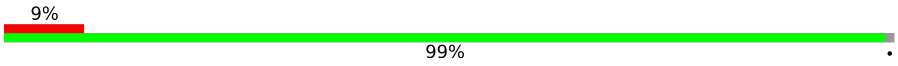
Chain S:

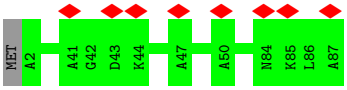




• Molecule 20: 30S ribosomal protein S20

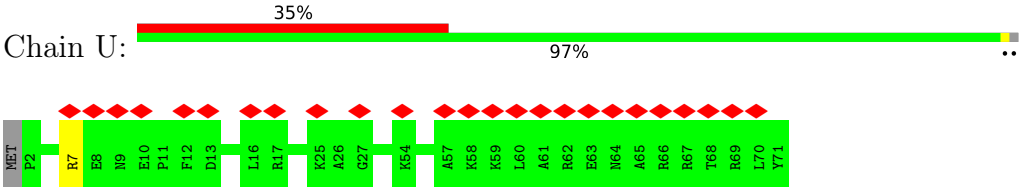
Chain T:





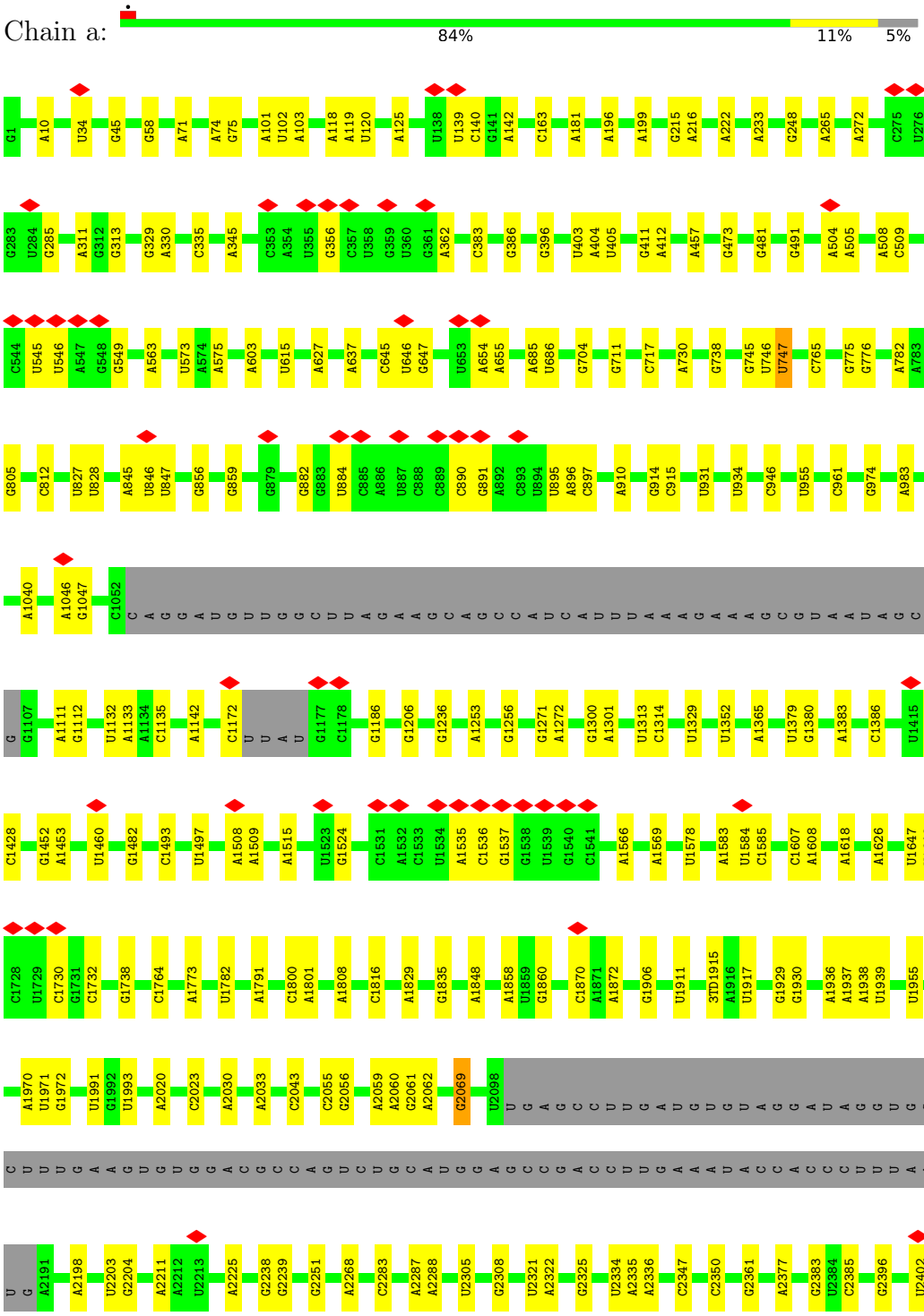
• Molecule 21: 30S ribosomal protein S21

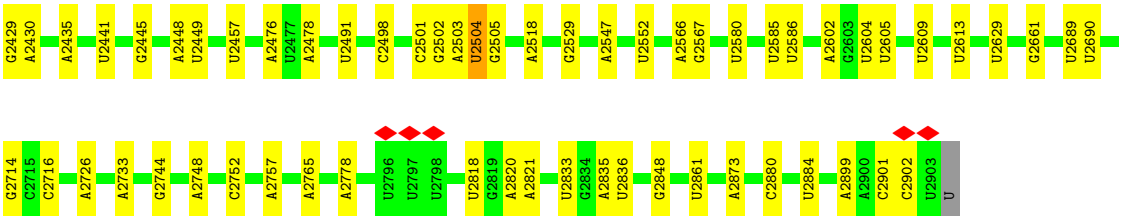
Chain U:



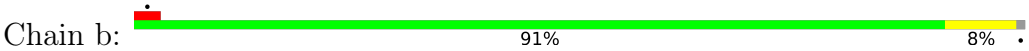
• Molecule 22: 23S rRNA

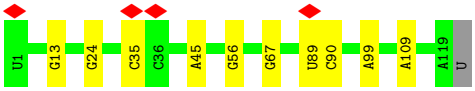
Chain a:



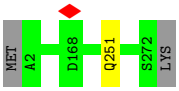


• Molecule 23: 5S rRNA

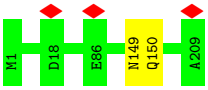




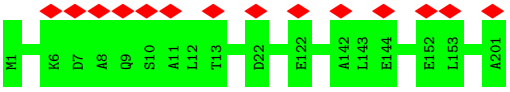
• Molecule 24: 50S ribosomal protein L2



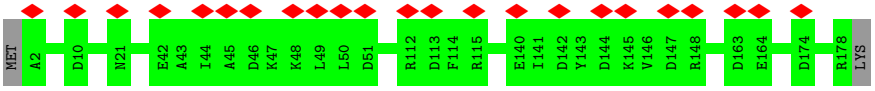
• Molecule 25: 50S ribosomal protein L3



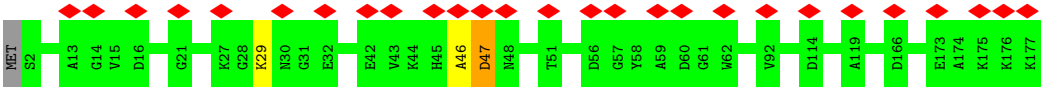
• Molecule 26: 50S ribosomal protein L4



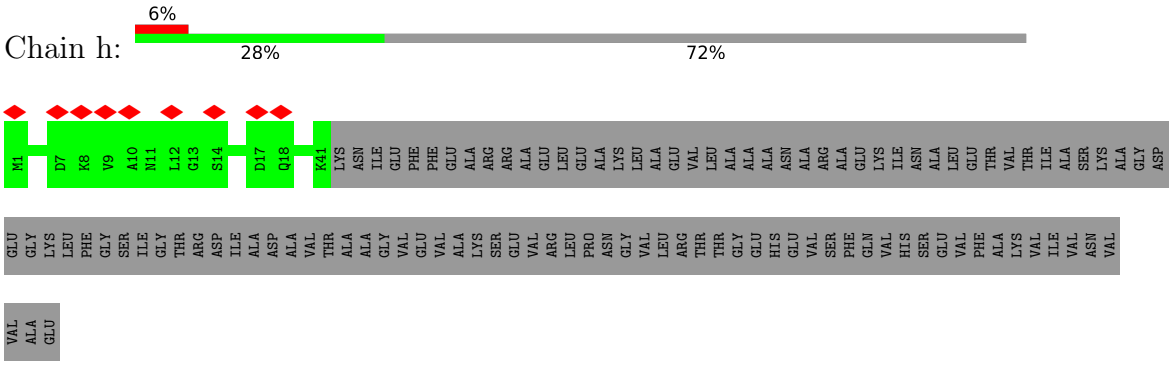
• Molecule 27: 50S ribosomal protein L5



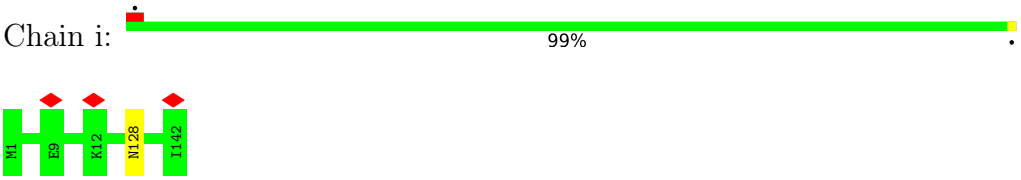
• Molecule 28: 50S ribosomal protein L6



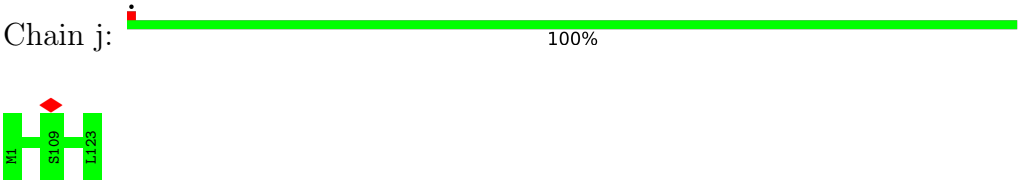
• Molecule 29: 50S ribosomal protein L9



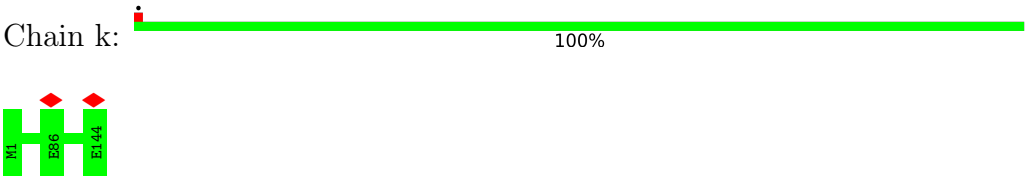
• Molecule 30: 50S ribosomal protein L13



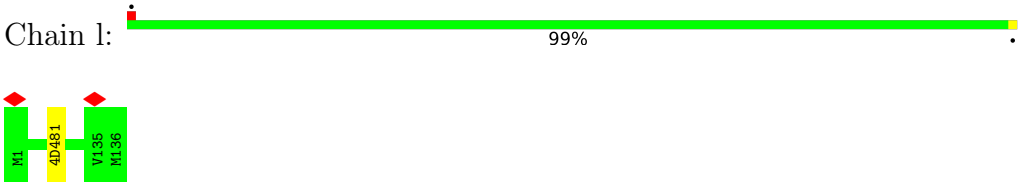
• Molecule 31: 50S ribosomal protein L14



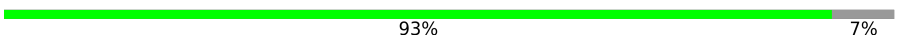
• Molecule 32: 50S ribosomal protein L15

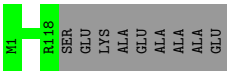


• Molecule 33: 50S ribosomal protein L16



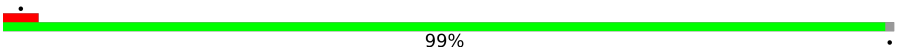
• Molecule 34: 50S ribosomal protein L17

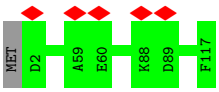




• Molecule 35: 50S ribosomal protein L18

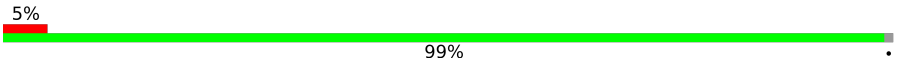
Chain n:

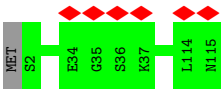




• Molecule 36: 50S ribosomal protein L19

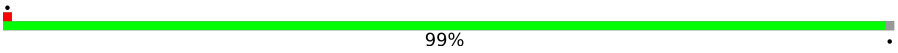
Chain o:





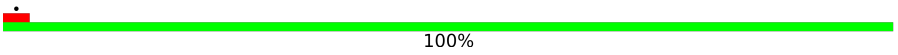
• Molecule 37: 50S ribosomal protein L20

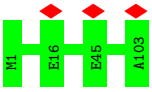
Chain p:



• Molecule 38: 50S ribosomal protein L21

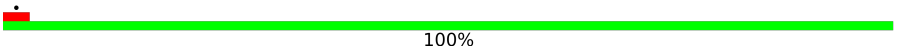
Chain q:

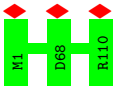




• Molecule 39: 50S ribosomal protein L22

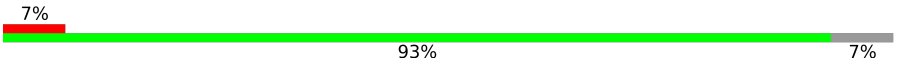
Chain r:

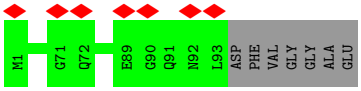




• Molecule 40: 50S ribosomal protein L23

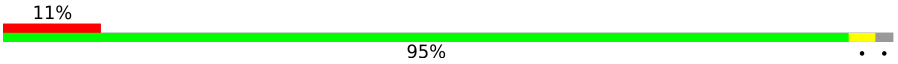
Chain s:

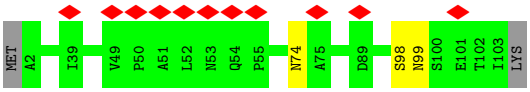




• Molecule 41: 50S ribosomal protein L24

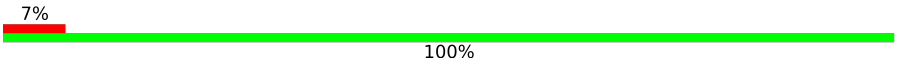
Chain t:

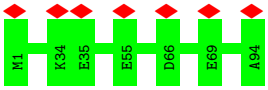




• Molecule 42: 50S ribosomal protein L25

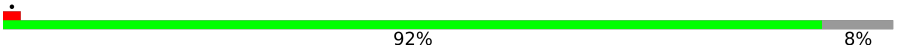
Chain u:

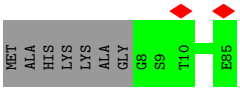




• Molecule 43: 50S ribosomal protein L27

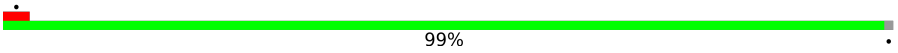
Chain v:

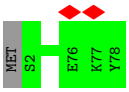




• Molecule 44: 50S ribosomal protein L28

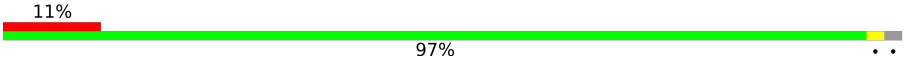
Chain w:

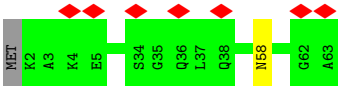




• Molecule 45: 50S ribosomal protein L29

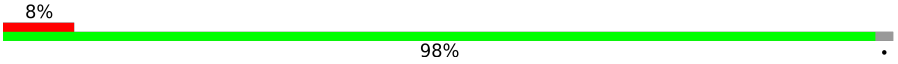
Chain x:

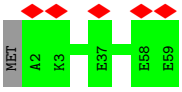




• Molecule 46: 50S ribosomal protein L30

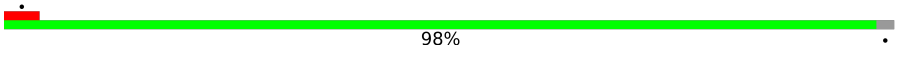
Chain y:

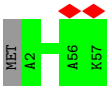




• Molecule 47: 50S ribosomal protein L32

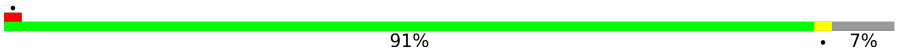
Chain z:

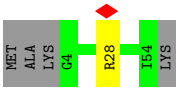




• Molecule 48: 50S ribosomal protein L33

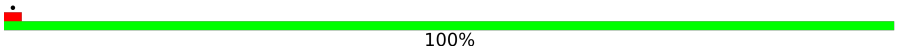
Chain 0:





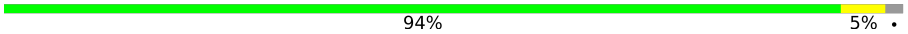
• Molecule 49: 50S ribosomal protein L34

Chain 1:



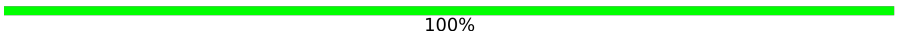
• Molecule 50: 50S ribosomal protein L35

Chain 2:



• Molecule 51: 50S ribosomal protein L36

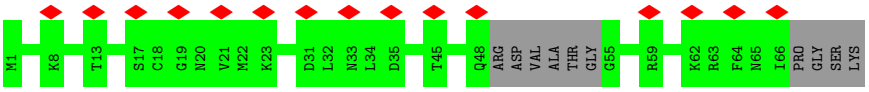
Chain 3:



There are no outlier residues recorded for this chain.

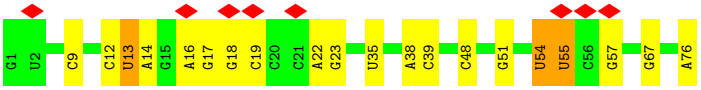
• Molecule 52: 50S ribosomal protein L31

Chain 4:



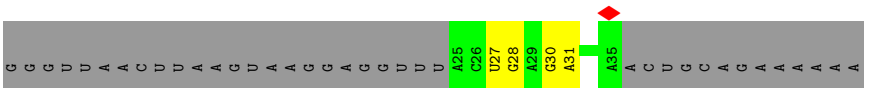
• Molecule 53: P-site tRNA_Glu

Chain V:

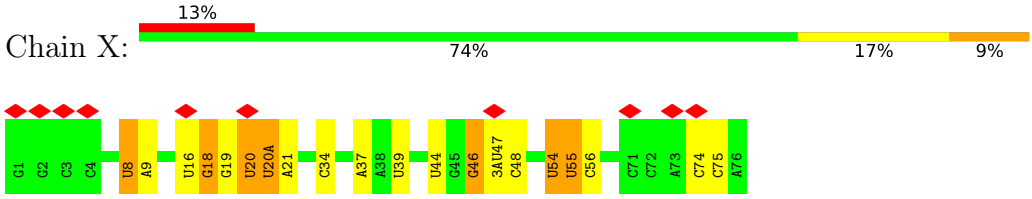


• Molecule 54: mRNA

Chain W:



• Molecule 55: A-site tRNA_Ile2



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	201764	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.187	Depositor
Minimum map value	-0.075	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0176	Depositor
Map size (Å)	439.10498, 439.10498, 439.10498	wwPDB
Map dimensions	530, 530, 530	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8285, 0.8285, 0.8285	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 2MA, T6A, MA6, MS6, IAS, OMC, PSU, 3TD, MEQ, 6MZ, OMG, OMU, 4SU, U8U, M3X, H2U, 5MC, 5MU, D2T, K, G7M, UR3, 4OC, 1MG, MG, 4D4, 3AU, 2MG

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	0.42	0/36236	0.81	5/56520 (0.0%)
2	B	0.28	0/1784	0.52	0/2403
3	C	0.27	0/1651	0.55	0/2225
4	D	0.27	0/1665	0.56	0/2227
5	E	0.31	0/1165	0.56	0/1568
6	F	0.28	0/858	0.56	0/1160
7	G	0.29	0/1219	0.59	0/1635
8	H	0.28	0/989	0.54	0/1326
9	I	0.27	0/1034	0.62	0/1375
10	J	0.29	0/796	0.62	0/1077
11	K	0.31	0/884	0.59	0/1191
12	L	0.31	0/960	0.61	0/1286
13	M	0.27	0/900	0.64	0/1204
14	N	0.29	0/817	0.62	1/1088 (0.1%)
15	O	0.30	0/722	0.58	0/964
16	P	0.28	0/653	0.59	0/877
17	Q	0.28	0/650	0.55	0/871
18	R	0.29	0/553	0.54	0/742
19	S	0.28	0/685	0.53	0/922
20	T	0.27	0/676	0.51	0/895
21	U	0.30	0/597	0.62	0/792
22	a	0.48	0/65651	0.82	10/102413 (0.0%)
23	b	0.41	0/2850	0.80	0/4444
24	c	0.29	0/2121	0.60	0/2852
25	d	0.29	0/1576	0.56	0/2119
26	e	0.28	0/1571	0.52	0/2113
27	f	0.28	0/1434	0.54	0/1926
28	g	0.29	0/1343	0.57	0/1816
29	h	0.27	0/306	0.56	0/413
30	i	0.30	0/1152	0.51	0/1551
31	j	0.31	0/955	0.60	0/1279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	k	0.28	0/1062	0.61	0/1413
33	l	0.30	0/1073	0.58	0/1433
34	m	0.28	0/958	0.61	0/1281
35	n	0.28	0/902	0.58	0/1209
36	o	0.29	0/929	0.57	0/1242
37	p	0.31	0/960	0.55	0/1278
38	q	0.29	0/829	0.57	0/1107
39	r	0.29	0/864	0.55	0/1156
40	s	0.27	0/744	0.54	0/994
41	t	0.29	0/787	0.58	1/1051 (0.1%)
42	u	0.28	0/766	0.53	0/1025
43	v	0.29	0/593	0.54	0/785
44	w	0.28	0/635	0.58	0/848
45	x	0.28	0/502	0.59	0/667
46	y	0.28	0/453	0.58	0/605
47	z	0.28	0/450	0.62	0/599
48	0	0.27	0/424	0.55	0/565
49	1	0.27	0/380	0.69	0/498
50	2	0.28	0/513	0.58	0/676
51	3	0.29	0/303	0.60	0/397
52	4	0.26	0/488	0.52	0/649
53	V	0.35	0/1686	0.82	0/2621
54	W	0.45	0/264	0.89	0/409
55	X	0.34	0/1552	0.85	0/2413
All	All	0.42	0/152570	0.76	17/228195 (0.0%)

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
13	M	0	1
14	N	0	1
28	g	0	2
50	2	0	1
All	All	0	5

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	512	G	O4'-C1'-N9	9.46	115.77	108.20
14	N	52	PRO	CA-N-CD	-6.83	101.93	111.50
1	A	1141	C	N3-C2-O2	-6.83	117.12	121.90
22	a	1313	U	C2-N1-C1'	6.16	125.09	117.70
22	a	2321	U	C2-N1-C1'	5.83	124.70	117.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
50	2	31	HIS	Peptide
13	M	104	THR	Peptide
14	N	32	SER	Peptide
28	g	46	ALA	Peptide
28	g	47	ASP	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	222/241 (92%)	211 (95%)	11 (5%)	0	100	100
3	C	204/233 (88%)	195 (96%)	9 (4%)	0	100	100
4	D	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
5	E	154/167 (92%)	147 (96%)	7 (4%)	0	100	100
6	F	101/135 (75%)	96 (95%)	5 (5%)	0	100	100
7	G	151/179 (84%)	142 (94%)	9 (6%)	0	100	100
8	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
10	J	96/103 (93%)	88 (92%)	7 (7%)	1 (1%)	13	14
11	K	113/129 (88%)	106 (94%)	7 (6%)	0	100	100
12	L	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
13	M	113/118 (96%)	106 (94%)	7 (6%)	0	100	100
14	N	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
15	O	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
16	P	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
17	Q	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
18	R	64/75 (85%)	59 (92%)	5 (8%)	0	100	100
19	S	82/92 (89%)	79 (96%)	3 (4%)	0	100	100
20	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	U	68/71 (96%)	68 (100%)	0	0	100	100
24	c	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
25	d	206/209 (99%)	201 (98%)	4 (2%)	1 (0%)	25	31
26	e	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
27	f	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
28	g	174/177 (98%)	160 (92%)	13 (8%)	1 (1%)	22	26
29	h	39/149 (26%)	32 (82%)	7 (18%)	0	100	100
30	i	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
31	j	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
32	k	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
33	l	132/136 (97%)	128 (97%)	4 (3%)	0	100	100
34	m	116/127 (91%)	109 (94%)	7 (6%)	0	100	100
35	n	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
36	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
37	p	115/118 (98%)	115 (100%)	0	0	100	100
38	q	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
39	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
40	s	91/100 (91%)	86 (94%)	5 (6%)	0	100	100
41	t	100/104 (96%)	91 (91%)	8 (8%)	1 (1%)	13	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
42	u	92/94 (98%)	90 (98%)	2 (2%)	0	100 100
43	v	76/85 (89%)	75 (99%)	1 (1%)	0	100 100
44	w	75/78 (96%)	74 (99%)	1 (1%)	0	100 100
45	x	60/63 (95%)	55 (92%)	5 (8%)	0	100 100
46	y	56/59 (95%)	54 (96%)	2 (4%)	0	100 100
47	z	54/57 (95%)	54 (100%)	0	0	100 100
48	0	49/55 (89%)	49 (100%)	0	0	100 100
49	1	44/46 (96%)	44 (100%)	0	0	100 100
50	2	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	8 7
51	3	36/38 (95%)	36 (100%)	0	0	100 100
52	4	56/70 (80%)	51 (91%)	5 (9%)	0	100 100
All	All	5481/5913 (93%)	5258 (96%)	218 (4%)	5 (0%)	50 60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	57	VAL
25	d	149	ASN
28	g	47	ASP
50	2	32	ILE
41	t	99	ASN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	186/199 (94%)	186 (100%)	0	100 100
3	C	170/190 (90%)	169 (99%)	1 (1%)	84 92
4	D	172/173 (99%)	172 (100%)	0	100 100
5	E	119/126 (94%)	119 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	90/116 (78%)	90 (100%)	0	100	100
7	G	126/147 (86%)	126 (100%)	0	100	100
8	H	104/105 (99%)	104 (100%)	0	100	100
9	I	105/107 (98%)	103 (98%)	2 (2%)	52	68
10	J	86/90 (96%)	86 (100%)	0	100	100
11	K	89/98 (91%)	88 (99%)	1 (1%)	70	83
12	L	102/103 (99%)	102 (100%)	0	100	100
13	M	93/96 (97%)	92 (99%)	1 (1%)	70	83
14	N	83/84 (99%)	83 (100%)	0	100	100
15	O	76/77 (99%)	75 (99%)	1 (1%)	65	78
16	P	65/65 (100%)	64 (98%)	1 (2%)	60	75
17	Q	73/78 (94%)	73 (100%)	0	100	100
18	R	57/65 (88%)	57 (100%)	0	100	100
19	S	72/79 (91%)	72 (100%)	0	100	100
20	T	65/66 (98%)	65 (100%)	0	100	100
21	U	60/61 (98%)	59 (98%)	1 (2%)	56	71
24	c	216/218 (99%)	215 (100%)	1 (0%)	86	93
25	d	163/163 (100%)	163 (100%)	0	100	100
26	e	165/165 (100%)	165 (100%)	0	100	100
27	f	148/150 (99%)	148 (100%)	0	100	100
28	g	137/138 (99%)	136 (99%)	1 (1%)	81	90
29	h	32/114 (28%)	32 (100%)	0	100	100
30	i	116/116 (100%)	115 (99%)	1 (1%)	75	86
31	j	104/104 (100%)	104 (100%)	0	100	100
32	k	103/103 (100%)	103 (100%)	0	100	100
33	l	107/107 (100%)	107 (100%)	0	100	100
34	m	98/103 (95%)	98 (100%)	0	100	100
35	n	86/87 (99%)	86 (100%)	0	100	100
36	o	99/100 (99%)	99 (100%)	0	100	100
37	p	89/90 (99%)	89 (100%)	0	100	100
38	q	84/84 (100%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	r	93/93 (100%)	93 (100%)	0	100 100
40	s	80/84 (95%)	80 (100%)	0	100 100
41	t	83/85 (98%)	82 (99%)	1 (1%)	67 80
42	u	78/78 (100%)	78 (100%)	0	100 100
43	v	58/63 (92%)	58 (100%)	0	100 100
44	w	67/68 (98%)	67 (100%)	0	100 100
45	x	54/55 (98%)	53 (98%)	1 (2%)	52 68
46	y	48/49 (98%)	48 (100%)	0	100 100
47	z	47/48 (98%)	47 (100%)	0	100 100
48	0	46/49 (94%)	45 (98%)	1 (2%)	47 63
49	1	38/38 (100%)	38 (100%)	0	100 100
50	2	51/52 (98%)	50 (98%)	1 (2%)	50 67
51	3	34/34 (100%)	34 (100%)	0	100 100
52	4	55/62 (89%)	55 (100%)	0	100 100
All	All	4572/4825 (95%)	4557 (100%)	15 (0%)	90 95

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	U	7	ARG
48	0	28	ARG
24	c	251	GLN
50	2	52	LYS
41	t	74	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	71	GLN
6	F	11	HIS
7	G	86	GLN
28	g	143	GLN
31	j	5	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1513/1542 (98%)	208 (13%)	4 (0%)
22	a	2745/2904 (94%)	296 (10%)	0
23	b	118/120 (98%)	10 (8%)	0
53	V	73/76 (96%)	18 (24%)	0
54	W	10/48 (20%)	3 (30%)	1 (10%)
55	X	73/76 (96%)	16 (21%)	1 (1%)
All	All	4532/4766 (95%)	551 (12%)	6 (0%)

5 of 551 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	U
1	A	7	A
1	A	8	A
1	A	9	G

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1397	C
54	W	30	G
55	X	46	G7M
1	A	519	C
1	A	451	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MC	A	1407	1	18,22,23	3.68	8 (44%)	26,32,35	1.05	1 (3%)
55	M3X	X	34	54,55	24,30,31	2.00	4 (16%)	26,41,44	1.18	2 (7%)
22	PSU	a	2580	22	18,21,22	3.82	7 (38%)	22,30,33	1.98	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	OMU	a	2552	22	19,22,23	2.83	6 (31%)	26,31,34	1.78	5 (19%)
11	IAS	K	119	11	6,7,8	1.08	0	6,8,10	1.35	1 (16%)
22	PSU	a	1911	22	18,21,22	3.84	6 (33%)	22,30,33	1.80	5 (22%)
1	2MG	A	966	1	18,26,27	2.17	6 (33%)	16,38,41	1.47	4 (25%)
22	2MG	a	2445	22	18,26,27	2.14	6 (33%)	16,38,41	1.40	3 (18%)
12	D2T	L	89	12	7,9,10	1.99	2 (28%)	6,11,13	1.93	3 (50%)
1	MA6	A	1518	1	18,26,27	1.01	1 (5%)	19,38,41	1.60	3 (15%)
22	5MU	a	1939	22	19,22,23	4.59	6 (31%)	28,32,35	3.79	10 (35%)
33	4D4	l	81	33	9,11,12	1.40	2 (22%)	8,13,15	1.97	3 (37%)
22	6MZ	a	1618	22	18,25,26	2.01	3 (16%)	16,36,39	2.02	3 (18%)
22	OMG	a	2251	56,53,22	18,26,27	2.81	8 (44%)	19,38,41	1.51	4 (21%)
55	PSU	X	55	55	18,21,22	3.88	6 (33%)	22,30,33	1.91	5 (22%)
22	PSU	a	2504	22	18,21,22	3.83	6 (33%)	22,30,33	1.70	4 (18%)
1	2MG	A	1207	1	18,26,27	2.17	6 (33%)	16,38,41	1.42	3 (18%)
22	PSU	a	2457	22	18,21,22	3.83	6 (33%)	22,30,33	1.90	6 (27%)
22	2MA	a	2503	56,22	17,25,26	2.51	5 (29%)	17,37,40	1.32	2 (11%)
1	MA6	A	1519	1	18,26,27	0.96	1 (5%)	19,38,41	1.68	2 (10%)
22	5MU	a	747	22	19,22,23	4.64	6 (31%)	28,32,35	3.60	9 (32%)
1	2MG	A	1516	1	18,26,27	2.17	6 (33%)	16,38,41	1.42	3 (18%)
1	UR3	A	1498	1	19,22,23	2.78	8 (42%)	26,32,35	1.32	3 (11%)
22	H2U	a	2449	22	18,21,22	1.09	2 (11%)	21,30,33	0.80	0
55	H2U	X	20(A)	55	18,21,22	1.00	2 (11%)	21,30,33	1.03	3 (14%)
1	PSU	A	516	56,1	18,21,22	3.81	6 (33%)	22,30,33	1.83	6 (27%)
22	PSU	a	2604	22	18,21,22	3.77	6 (33%)	22,30,33	1.64	3 (13%)
53	2MA	V	38	53	17,25,26	2.45	5 (29%)	17,37,40	1.27	2 (11%)
22	1MG	a	745	22	18,26,27	2.55	7 (38%)	19,39,42	1.32	2 (10%)
22	PSU	a	746	56,22	18,21,22	3.80	7 (38%)	22,30,33	1.82	5 (22%)
55	H2U	X	20	55	18,21,22	1.06	2 (11%)	21,30,33	1.09	1 (4%)
55	PSU	X	39	55	18,21,22	3.84	6 (33%)	22,30,33	1.83	5 (22%)
1	4OC	A	1402	56,1	20,23,24	3.07	8 (40%)	26,32,35	1.01	1 (3%)
53	PSU	V	55	53	18,21,22	3.88	5 (27%)	22,30,33	1.88	5 (22%)
22	PSU	a	2605	22	18,21,22	3.81	6 (33%)	22,30,33	1.80	5 (22%)
22	6MZ	a	2030	22	18,25,26	1.90	3 (16%)	16,36,39	2.20	3 (18%)
55	4SU	X	8	55	18,21,22	3.72	8 (44%)	26,30,33	2.24	4 (15%)
22	OMC	a	2498	56,22	19,22,23	2.88	8 (42%)	26,31,34	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	2MG	a	1835	22	18,26,27	2.16	6 (33%)	16,38,41	1.38	3 (18%)
22	3TD	a	1915	22	19,22,23	3.93	6 (31%)	21,32,35	1.75	3 (14%)
53	U8U	V	35	54,53	19,24,25	2.57	6 (31%)	23,34,37	1.05	2 (8%)
55	3AU	X	47	55	24,28,29	2.73	9 (37%)	33,40,43	1.35	4 (12%)
55	G7M	X	46	55	20,26,27	2.74	7 (35%)	17,39,42	1.18	2 (11%)
55	T6A	X	37	55	27,34,35	2.35	7 (25%)	29,49,52	2.05	5 (17%)
55	5MU	X	54	55	19,22,23	4.70	6 (31%)	28,32,35	3.62	9 (32%)
22	5MC	a	1962	22	18,22,23	3.70	8 (44%)	26,32,35	1.04	2 (7%)
22	G7M	a	2069	22	20,26,27	2.63	7 (35%)	17,39,42	1.19	2 (11%)
53	PSU	V	13	53	18,21,22	3.87	6 (33%)	22,30,33	1.90	6 (27%)
55	OMG	X	18	55	18,26,27	2.81	8 (44%)	19,38,41	1.48	4 (21%)
25	MEQ	d	150	25	8,9,10	1.07	1 (12%)	5,10,12	1.48	2 (40%)
22	PSU	a	1917	22	18,21,22	3.83	6 (33%)	22,30,33	1.78	4 (18%)
1	G7M	A	527	1	20,26,27	2.71	7 (35%)	17,39,42	1.00	1 (5%)
1	5MC	A	967	1	18,22,23	3.76	8 (44%)	26,32,35	0.98	1 (3%)
22	PSU	a	955	22	18,21,22	3.81	6 (33%)	22,30,33	1.92	5 (22%)
53	5MU	V	54	53	19,22,23	4.68	6 (31%)	28,32,35	3.61	9 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
55	M3X	X	34	54,55	-	4/17/37/38	0/2/2/2
22	PSU	a	2580	22	-	0/7/25/26	0/2/2/2
22	OMU	a	2552	22	-	0/9/27/28	0/2/2/2
11	IAS	K	119	11	-	0/7/7/8	-
22	PSU	a	1911	22	-	0/7/25/26	0/2/2/2
1	2MG	A	966	1	-	2/5/27/28	0/3/3/3
22	2MG	a	2445	22	-	2/5/27/28	0/3/3/3
12	D2T	L	89	12	-	2/7/12/14	-
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
22	5MU	a	1939	22	-	0/7/25/26	0/2/2/2
33	4D4	l	81	33	-	0/11/12/14	-
22	6MZ	a	1618	22	-	0/5/27/28	0/3/3/3
22	OMG	a	2251	56,53,22	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PSU	X	55	55	-	2/7/25/26	0/2/2/2
22	PSU	a	2504	22	-	2/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
22	PSU	a	2457	22	-	0/7/25/26	0/2/2/2
22	2MA	a	2503	56,22	-	2/3/25/26	0/3/3/3
1	MA6	A	1519	1	-	2/7/29/30	0/3/3/3
22	5MU	a	747	22	-	0/7/25/26	0/2/2/2
1	2MG	A	1516	1	-	0/5/27/28	0/3/3/3
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
22	H2U	a	2449	22	-	0/7/38/39	0/2/2/2
55	H2U	X	20(A)	55	-	1/7/38/39	0/2/2/2
1	PSU	A	516	56,1	-	0/7/25/26	0/2/2/2
22	PSU	a	2604	22	-	0/7/25/26	0/2/2/2
53	2MA	V	38	53	-	0/3/25/26	0/3/3/3
22	1MG	a	745	22	-	0/3/25/26	0/3/3/3
22	PSU	a	746	56,22	-	3/7/25/26	0/2/2/2
55	H2U	X	20	55	-	1/7/38/39	0/2/2/2
55	PSU	X	39	55	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	56,1	-	0/9/29/30	0/2/2/2
53	PSU	V	55	53	-	0/7/25/26	0/2/2/2
22	PSU	a	2605	22	-	0/7/25/26	0/2/2/2
22	6MZ	a	2030	22	-	2/5/27/28	0/3/3/3
55	4SU	X	8	55	-	0/7/25/26	0/2/2/2
22	OMC	a	2498	56,22	-	0/9/27/28	0/2/2/2
22	2MG	a	1835	22	-	0/5/27/28	0/3/3/3
22	3TD	a	1915	22	-	2/7/25/26	0/2/2/2
53	U8U	V	35	54,53	-	0/9/28/29	0/2/2/2
55	3AU	X	47	55	-	4/16/34/35	0/2/2/2
55	G7M	X	46	55	-	3/3/25/26	0/3/3/3
55	T6A	X	37	55	-	4/19/41/42	0/3/3/3
55	5MU	X	54	55	-	0/7/25/26	0/2/2/2
22	5MC	a	1962	22	-	2/7/25/26	0/2/2/2
22	G7M	a	2069	22	-	1/3/25/26	0/3/3/3
53	PSU	V	13	53	-	2/7/25/26	0/2/2/2
55	OMG	X	18	55	-	2/5/27/28	0/3/3/3
25	MEQ	d	150	25	-	4/8/9/11	-
22	PSU	a	1917	22	-	0/7/25/26	0/2/2/2
1	G7M	A	527	1	-	2/3/25/26	0/3/3/3
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	a	955	22	-	0/7/25/26	0/2/2/2
53	5MU	V	54	53	-	3/7/25/26	0/2/2/2

The worst 5 of 306 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	1915	3TD	C6-C5	12.01	1.49	1.35
53	V	54	5MU	C6-N1	10.75	1.56	1.38
55	X	54	5MU	C6-N1	10.69	1.56	1.38
22	a	747	5MU	C6-N1	10.64	1.56	1.38
55	X	54	5MU	C2-N1	10.47	1.55	1.38

The worst 5 of 199 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	1939	5MU	C5-C4-N3	12.23	125.75	115.31
53	V	54	5MU	C5-C4-N3	12.05	125.60	115.31
22	a	747	5MU	C5-C4-N3	11.97	125.53	115.31
55	X	54	5MU	C5-C4-N3	11.86	125.44	115.31
22	a	1939	5MU	C5-C6-N1	-10.61	112.42	123.34

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	L	89	D2T	SB-CB-CG-OD2
25	d	150	MEQ	C-CA-CB-CG
22	a	746	PSU	C2'-C1'-C5-C4
22	a	1915	3TD	C3'-C4'-C5'-O5'
22	a	2251	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 316 ligands modelled in this entry, 316 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

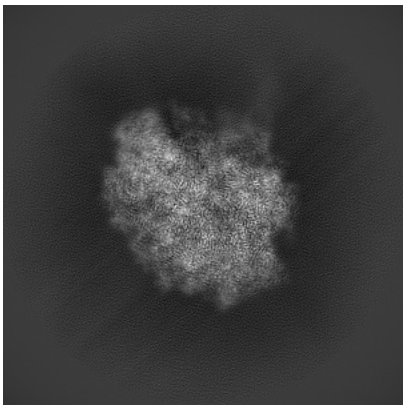
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35001. These allow visual inspection of the internal detail of the map and identification of artifacts.

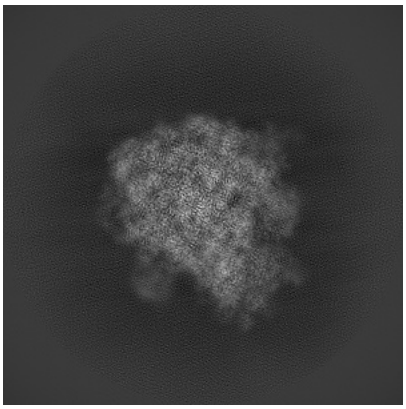
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

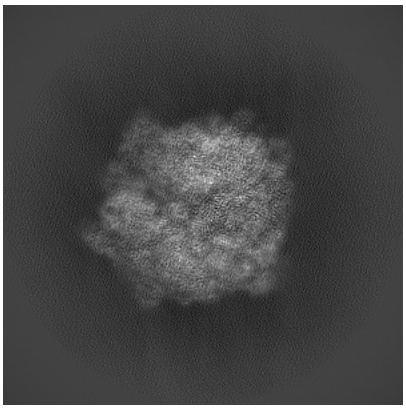
6.1.1 Primary map



X

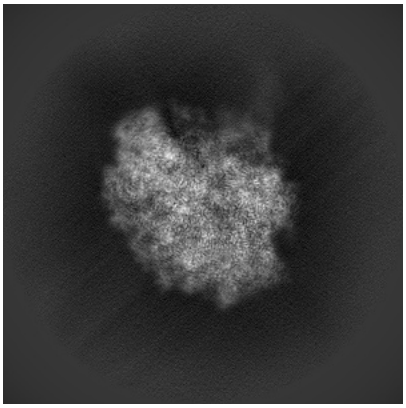


Y

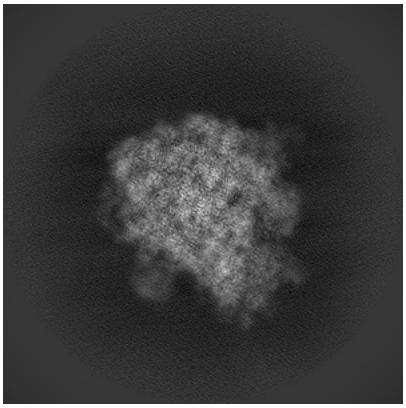


Z

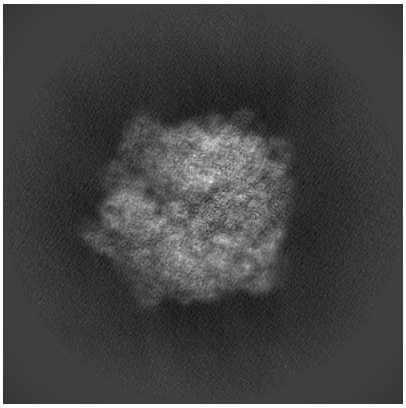
6.1.2 Raw map



X



Y

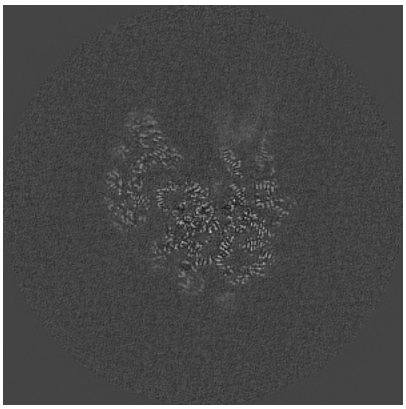


Z

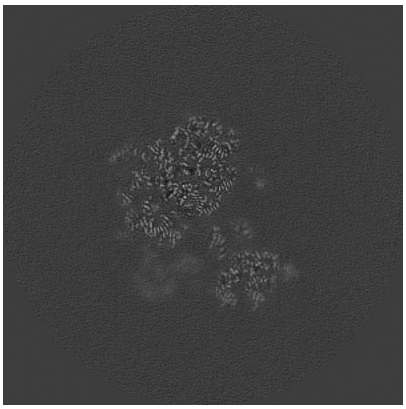
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

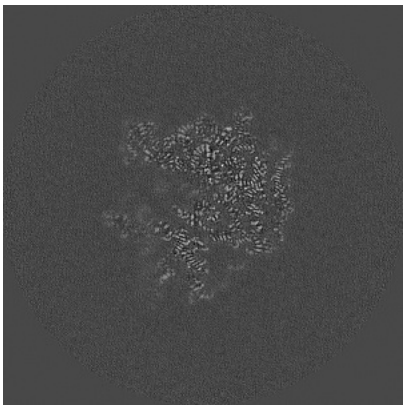
6.2.1 Primary map



X Index: 265

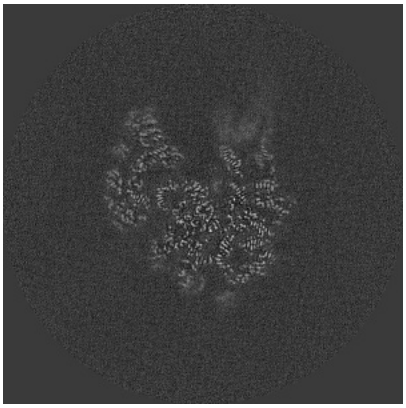


Y Index: 265

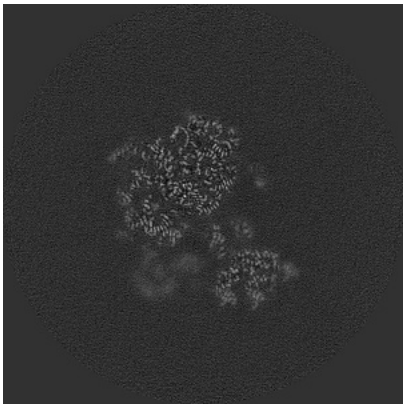


Z Index: 265

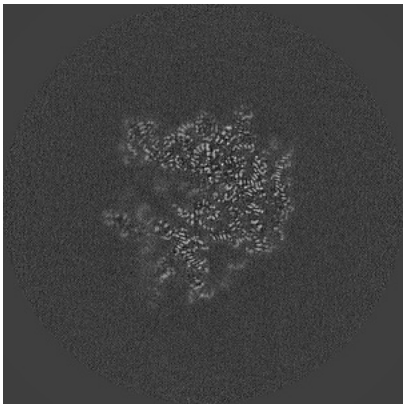
6.2.2 Raw map



X Index: 265



Y Index: 265

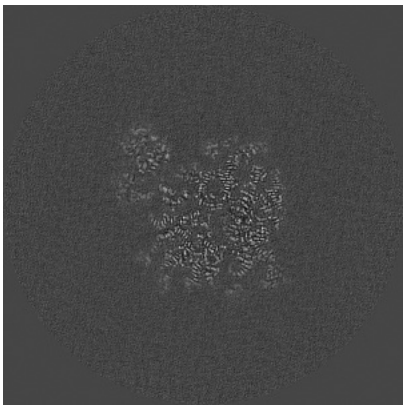


Z Index: 265

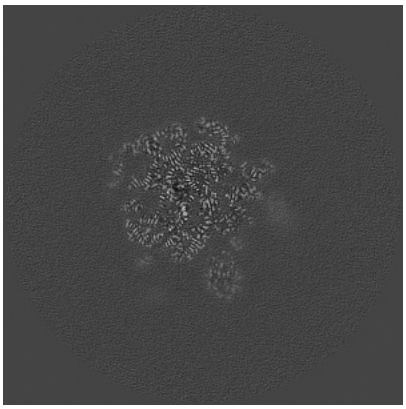
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

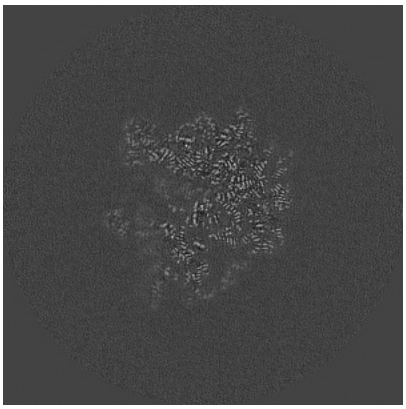
6.3.1 Primary map



X Index: 296

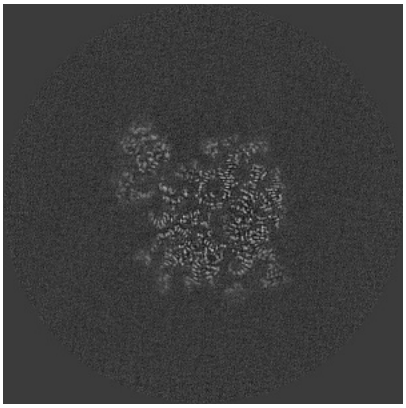


Y Index: 316

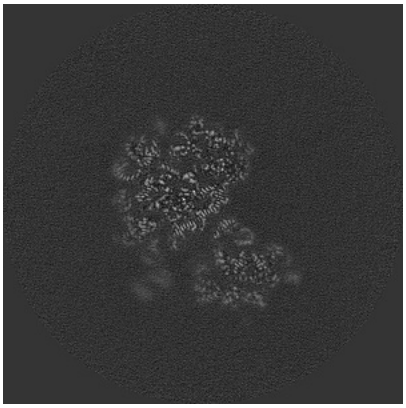


Z Index: 268

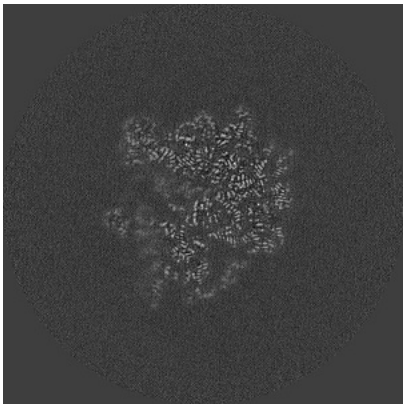
6.3.2 Raw map



X Index: 296



Y Index: 249

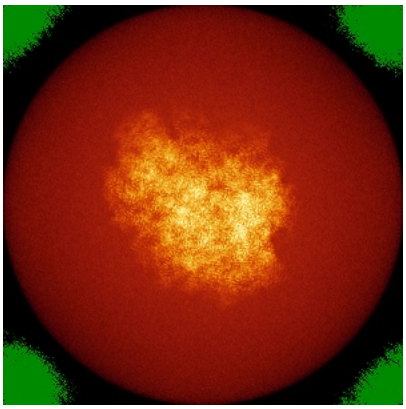


Z Index: 268

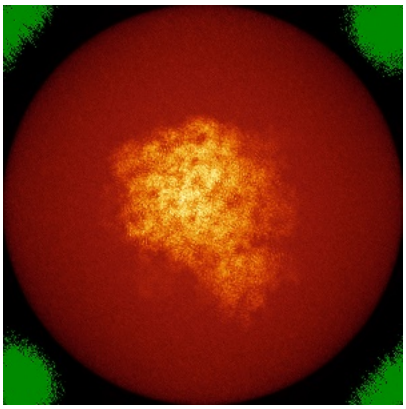
The images above show the largest variance slices of the map in three orthogonal directions.

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

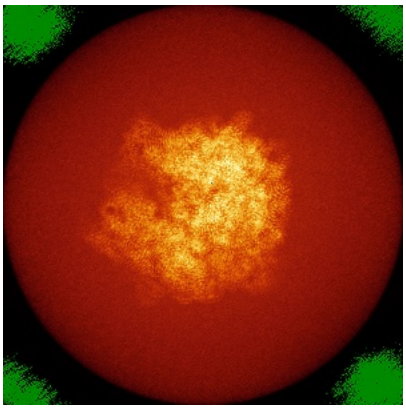
6.4.1 Primary map



X

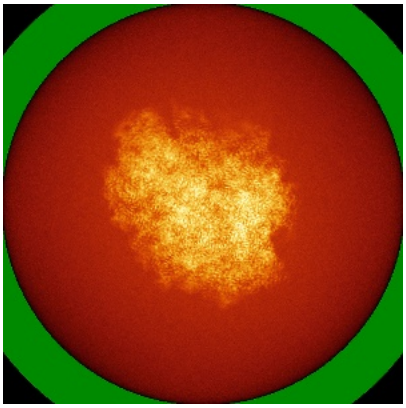


Y

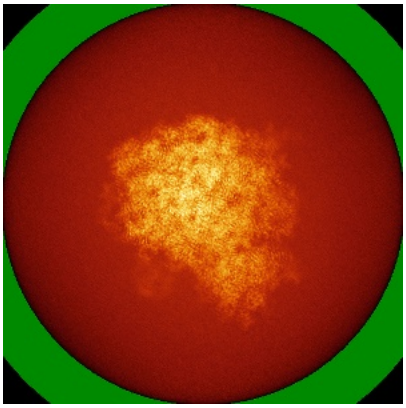


Z

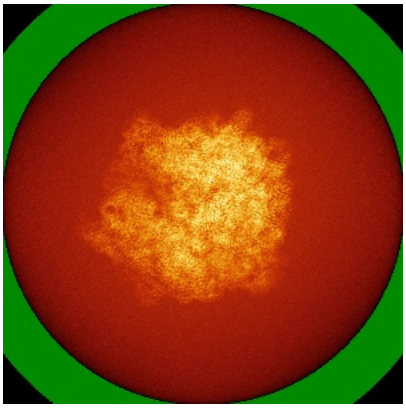
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

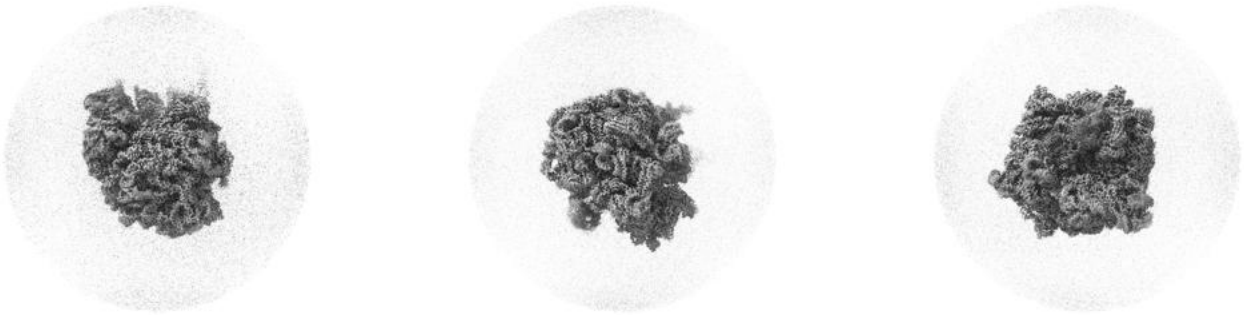
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0176. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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.

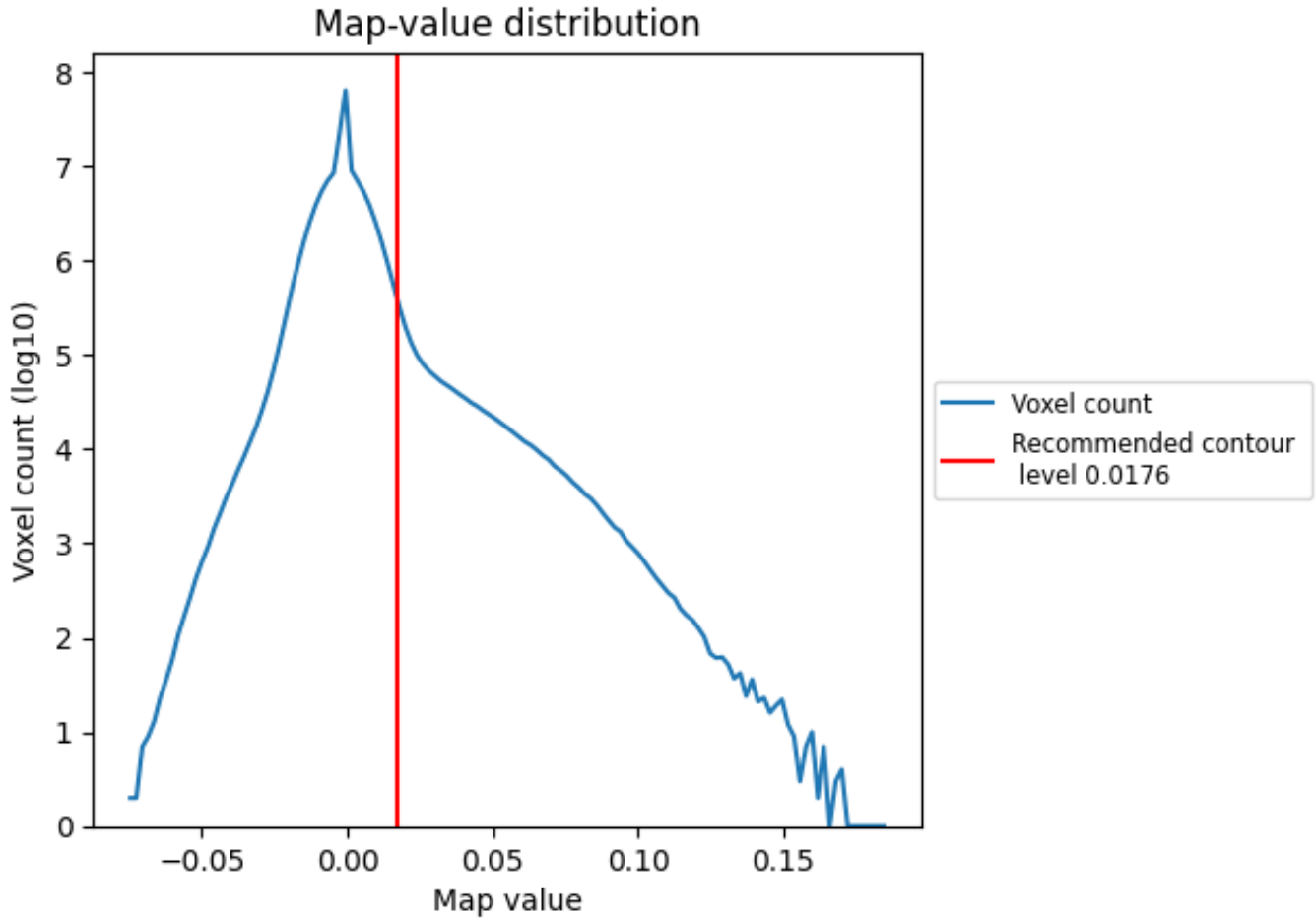
6.6 Mask visualisation (i)

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

7 Map analysis

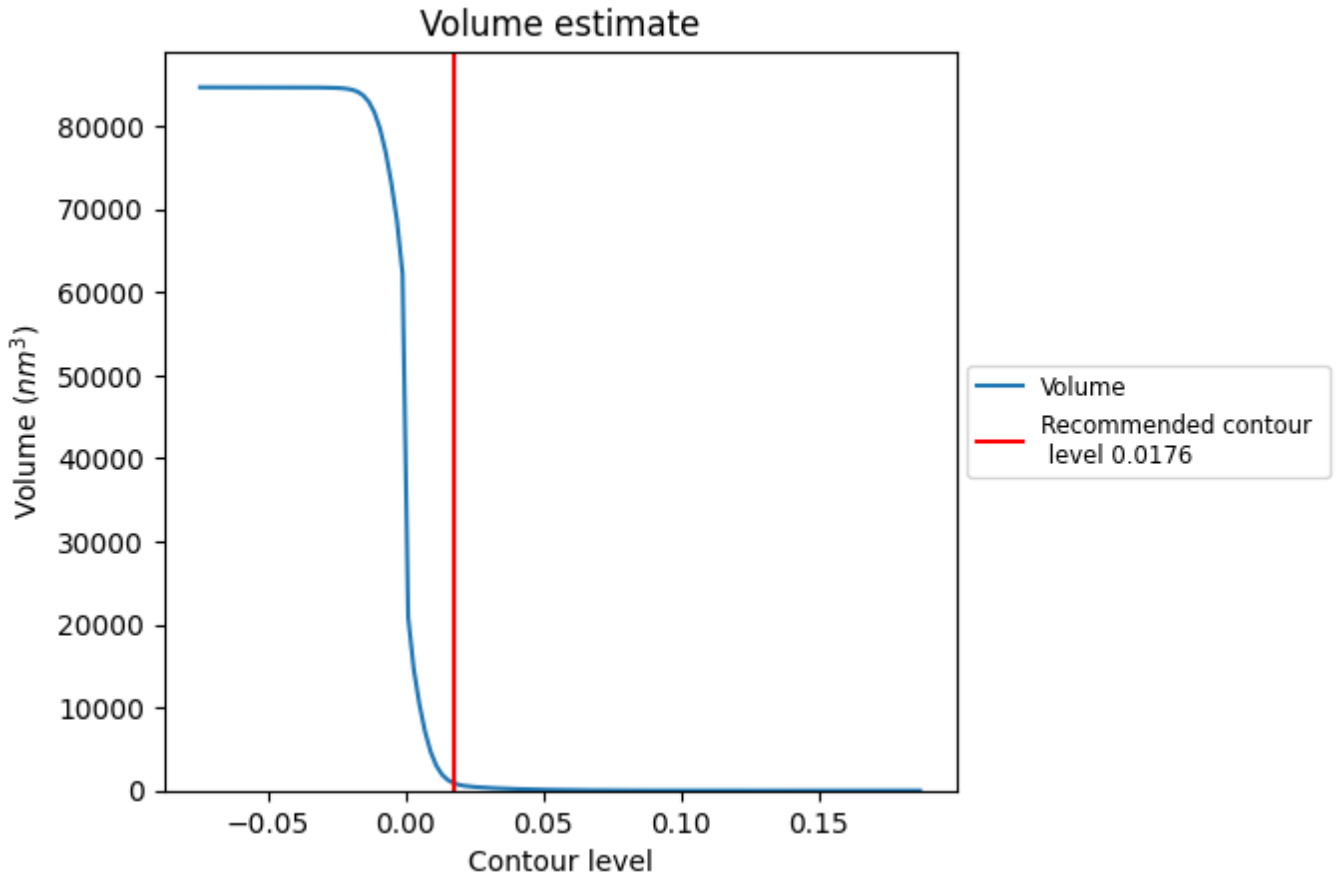
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

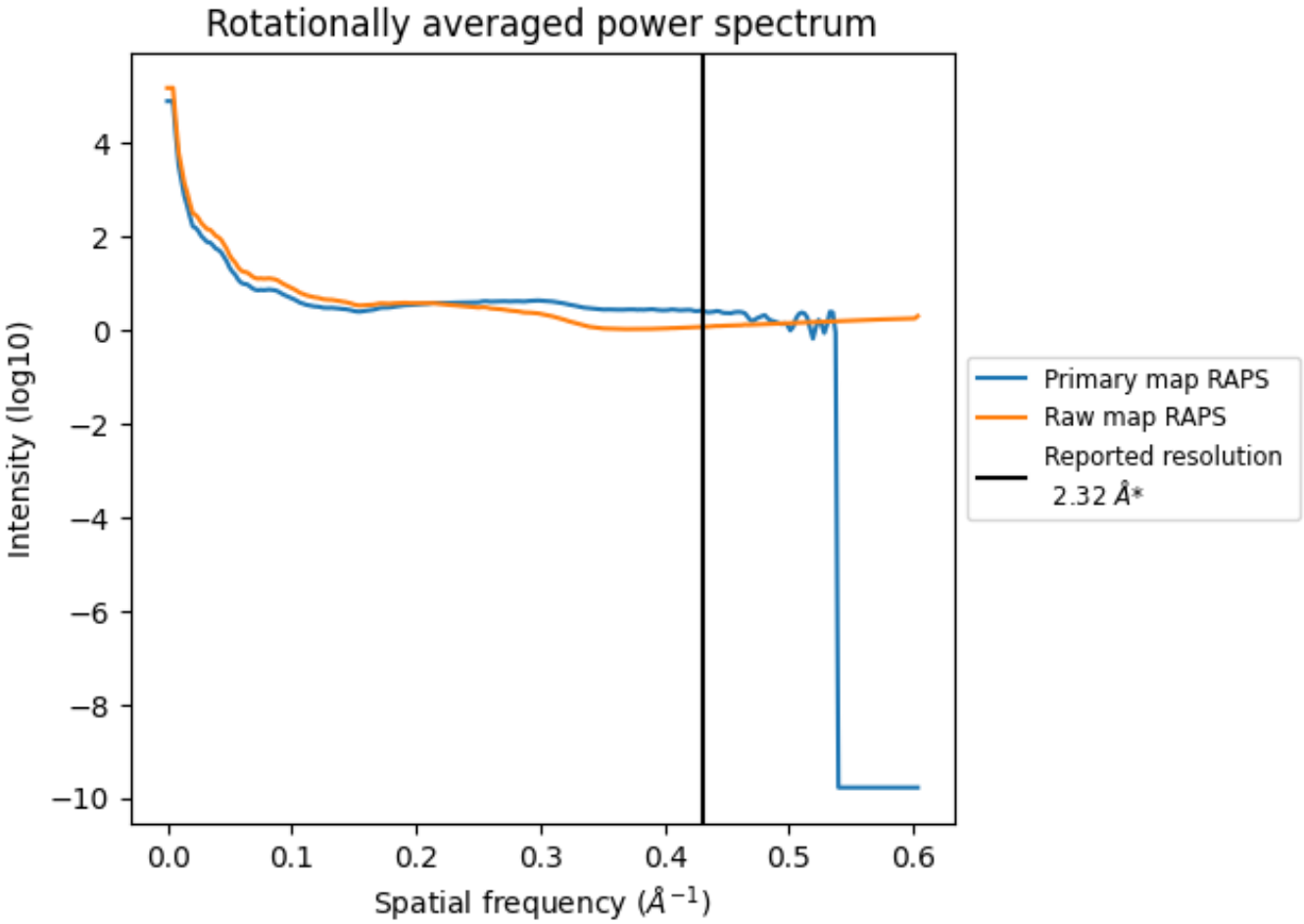
7.2 Volume estimate (i)



The volume at the recommended contour level is 885 nm^3; this corresponds to an approximate mass of 800 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

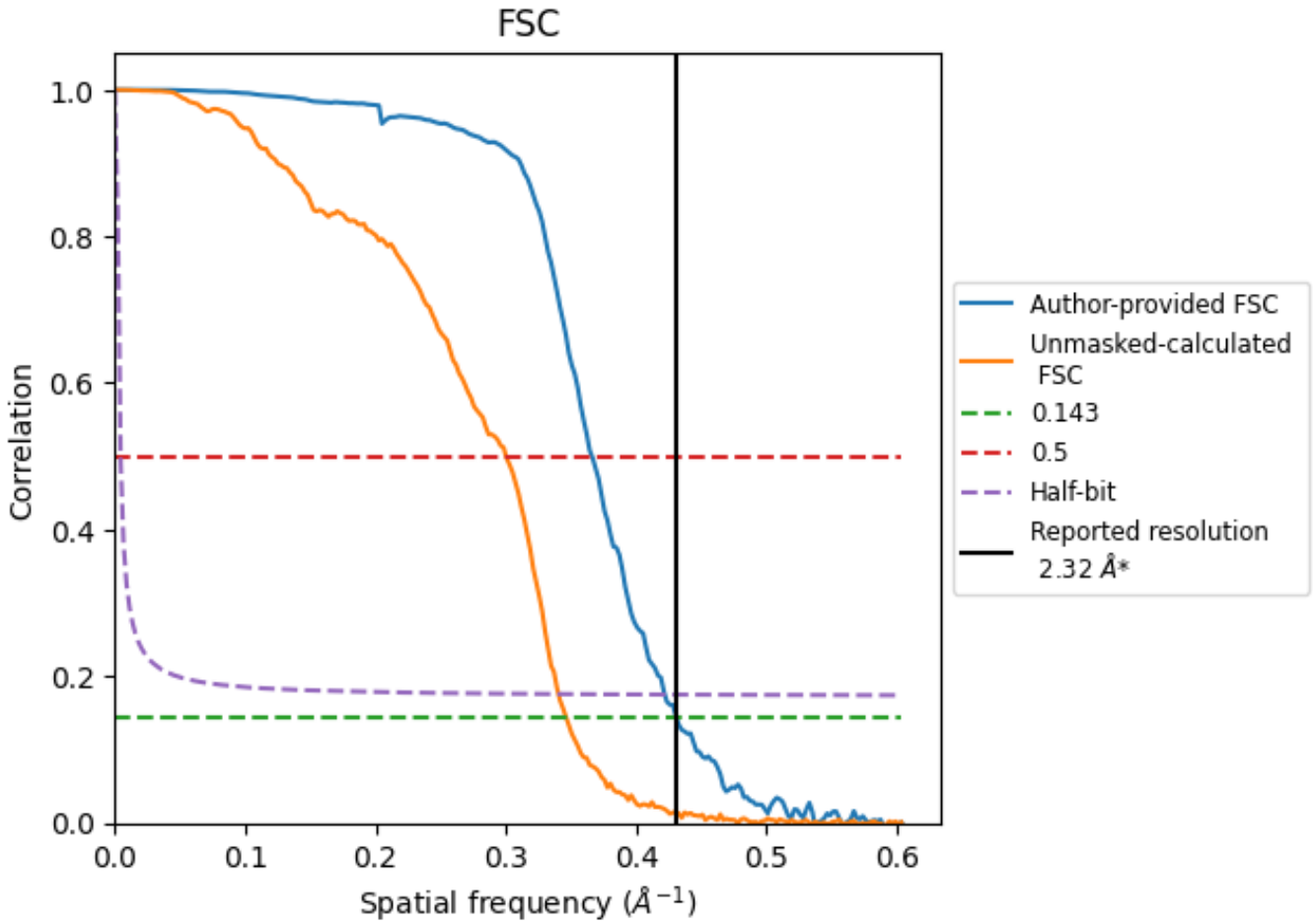


*Reported resolution corresponds to spatial frequency of 0.431 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.431 Å^{-1}

8.2 Resolution estimates (i)

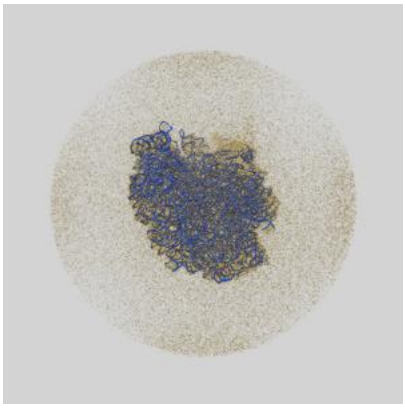
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.32	-	-
Author-provided FSC curve	2.32	2.73	2.37
Unmasked-calculated*	2.89	3.33	2.94

*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 2.89 differs from the reported value 2.32 by more than 10 %

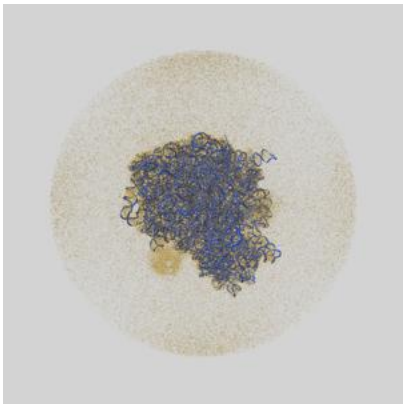
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35001 and PDB model 8HSP. Per-residue inclusion information can be found in section 3 on page 14.

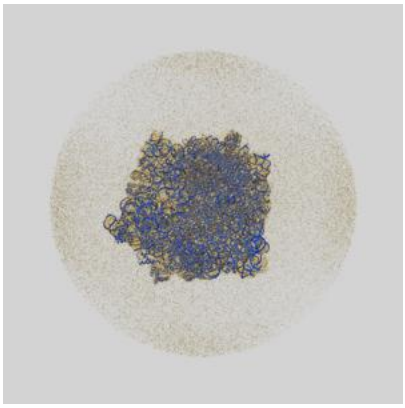
9.1 Map-model overlay



X



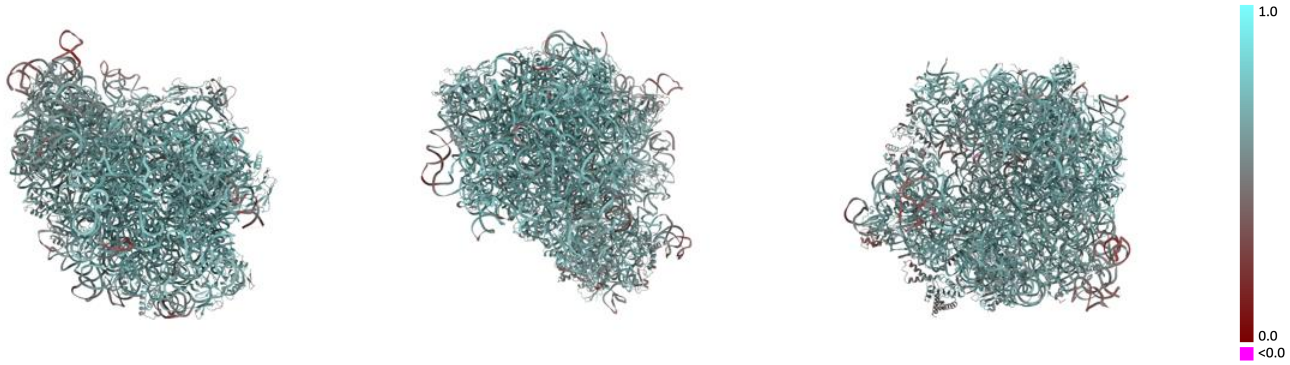
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0176 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

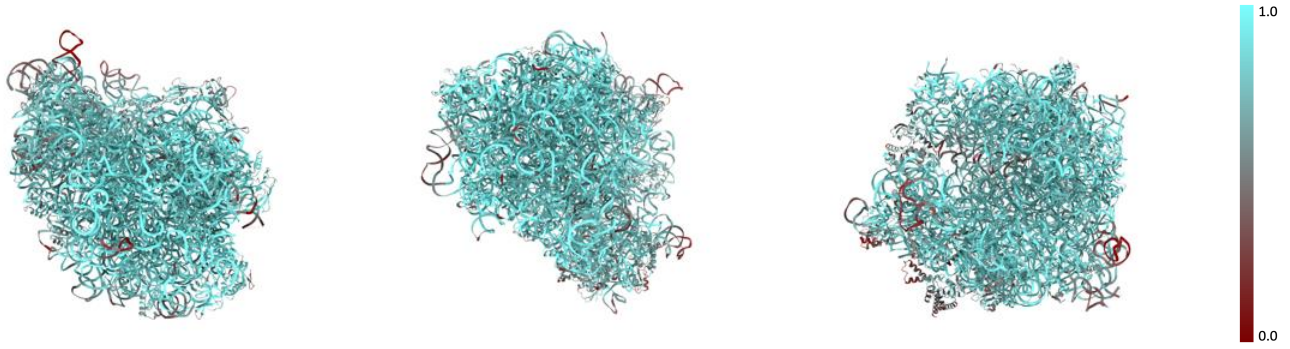
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

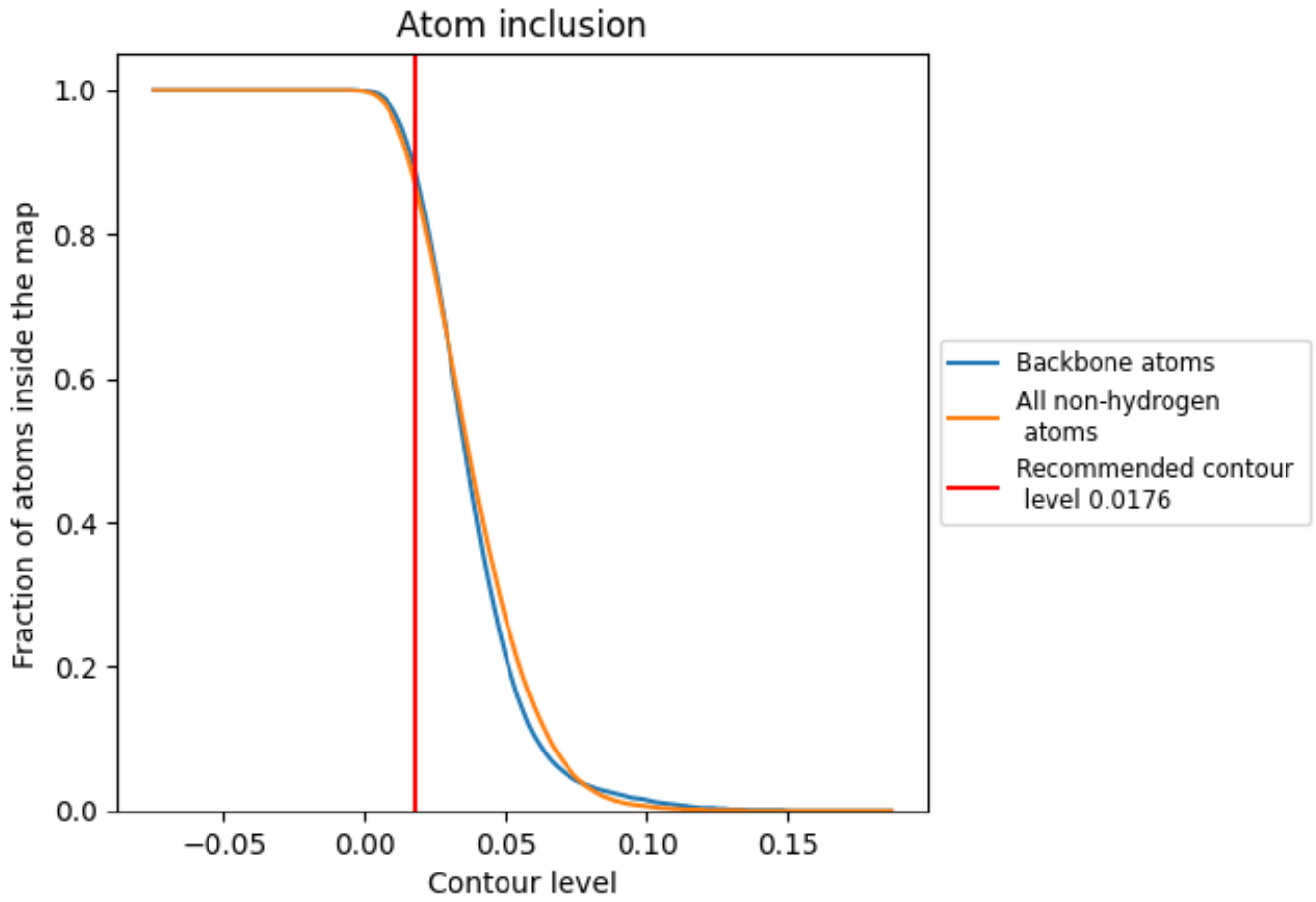
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0176).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 87% 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 (0.0176) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8740	0.6490
0	0.8510	0.6590
1	0.9550	0.7210
2	0.9570	0.7190
3	0.9250	0.6770
4	0.5650	0.5210
A	0.8790	0.6300
B	0.5390	0.5390
C	0.7720	0.6230
D	0.6580	0.5870
E	0.8300	0.6550
F	0.6970	0.5700
G	0.6730	0.5740
H	0.8380	0.6500
I	0.7480	0.6040
J	0.5780	0.5260
K	0.7950	0.6230
L	0.8470	0.6620
M	0.7280	0.5900
N	0.8140	0.6300
O	0.8130	0.6430
P	0.7340	0.5790
Q	0.7520	0.6030
R	0.7840	0.6150
S	0.7550	0.6080
T	0.6990	0.5790
U	0.5190	0.5250
V	0.7190	0.5600
W	0.8660	0.6380
X	0.7070	0.5500
a	0.9360	0.6760
b	0.9010	0.6370
c	0.9430	0.7100
d	0.9060	0.6970
e	0.8200	0.6550

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Chain	Atom inclusion	Q-score
f	0.6990	0.5780
g	0.6550	0.5510
h	0.5900	0.5480
i	0.9130	0.6980
j	0.8870	0.6910
k	0.8970	0.6840
l	0.9080	0.7010
m	0.9560	0.7090
n	0.8370	0.6370
o	0.8640	0.6760
p	0.9530	0.7200
q	0.8630	0.6630
r	0.8930	0.6850
s	0.7800	0.6340
t	0.7380	0.5910
u	0.8020	0.6390
v	0.9090	0.7060
w	0.8970	0.6770
x	0.7080	0.5880
y	0.8740	0.6650
z	0.8700	0.6830