wwPDB EM Validation Summary Report (i)

Dec 14, 2024 – 10:10 PM EST

PDB ID	:	8UQM
EMDB ID	:	EMD-42474
Title	:	Escherichia coli transcription-translation coupled complex class B (TTC-B) containing RfaH in loaded state, NusA, mRNA with a 24 nt long spacer, and fMet-tRNAs in E-site and P-site of the ribosome
Authors	:	Molodtsov, V.; Wang, C.; Ebright, R.H.
Deposited on	:	2023-10-24
Resolution	:	5.30 Å(reported)

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

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

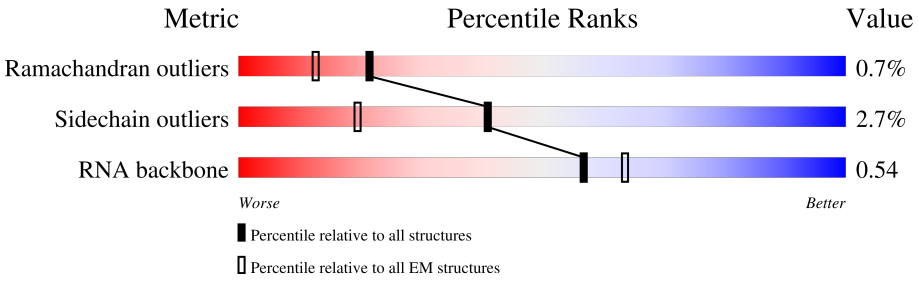
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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 5.30 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	0	103	100%
2	1	110	100%
3	2	100	91% · 6%
4	3	104	99% ·
5	4	94	98% ·
6	5	36	11% 53% 33% 14%
7	6	36	6% 72% 28%
8	7	41	17% 68% 5% 10%

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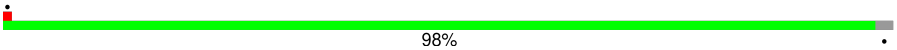
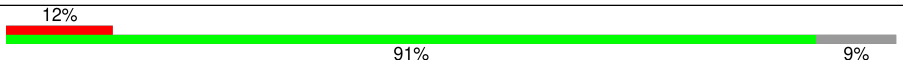
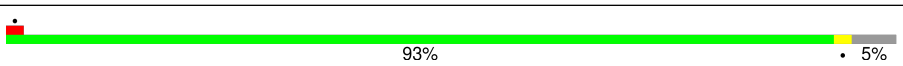
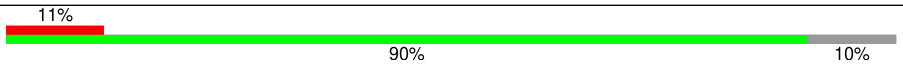
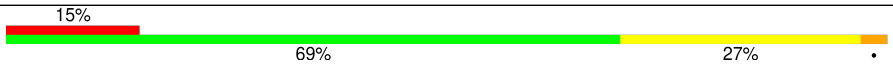
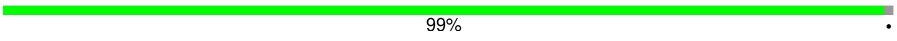
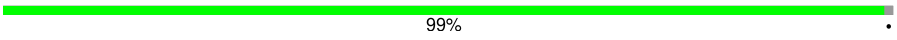
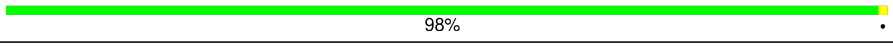
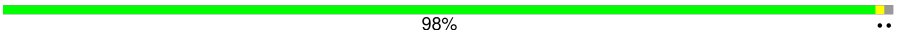
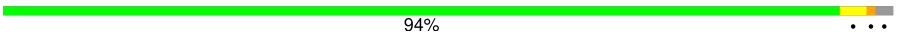
Mol	Chain	Length	Quality of chain
9	9	165	
10	A	76	
10	B	76	
11	AA	1342	
12	AB	162	
13	AC	329	
13	AD	329	
14	AE	1407	
15	AF	91	
16	AG	495	
17	C	75	
18	D	1542	
19	E	87	
20	F	71	
21	G	241	
22	H	557	
23	I	233	
24	J	206	
25	K	167	
26	L	135	
27	M	179	
28	N	130	
29	O	130	
30	P	103	
31	Q	129	

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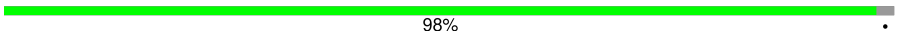
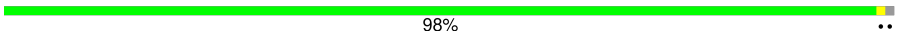
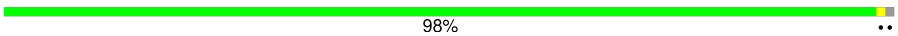
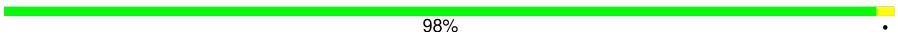
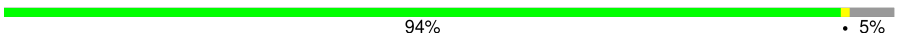
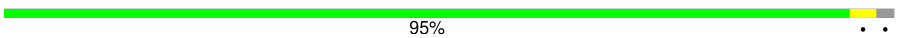
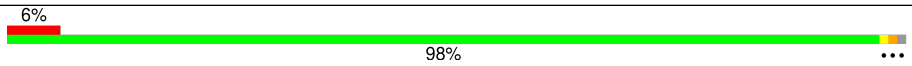
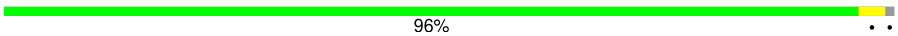
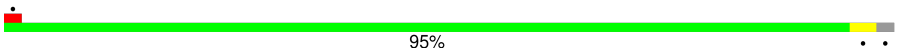
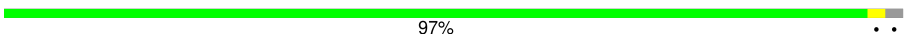
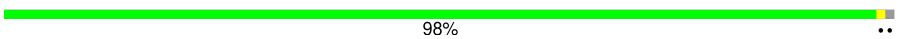
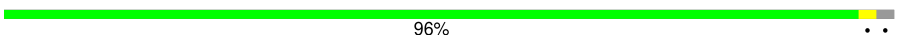
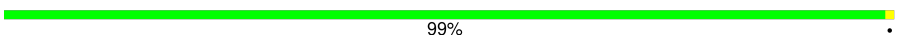
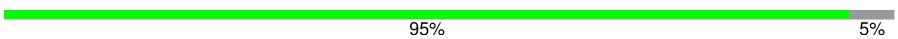
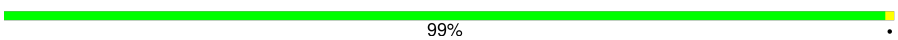
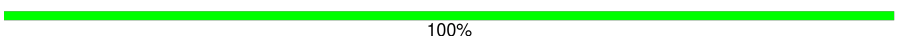
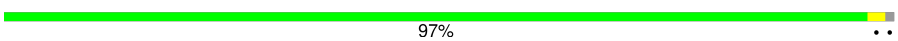
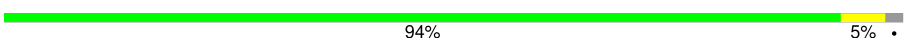
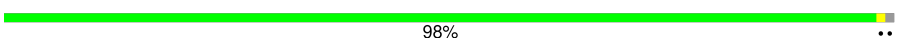
Mol	Chain	Length	Quality of chain
32	R	124	
33	S	101	
34	T	89	
35	U	82	
36	V	84	
37	W	92	
38	X	118	
39	Y	142	
40	Z	121	
41	a	2904	
42	b	85	
43	c	78	
44	d	120	
45	e	63	
46	f	59	
47	g	70	
48	h	273	
49	i	57	
50	j	209	
51	k	55	
52	l	201	
53	m	46	
54	n	179	
55	o	65	
56	p	177	

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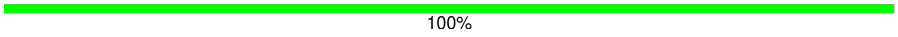
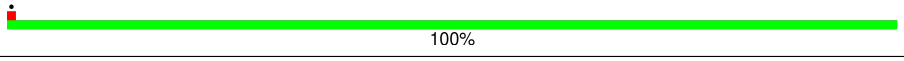
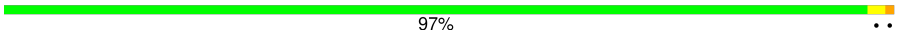
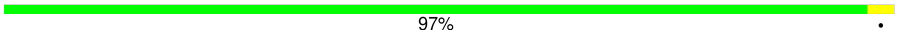
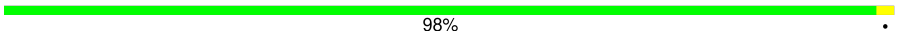
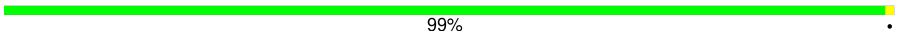
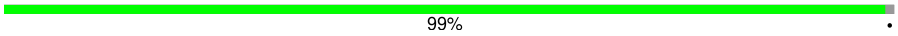
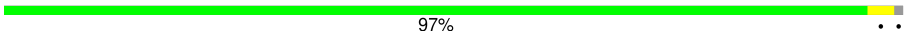
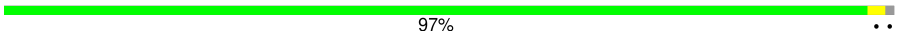
Mol	Chain	Length	Quality of chain
57	q	38	
58	r	149	
59	s	142	
60	t	123	
61	u	144	
62	v	136	
63	w	127	
64	x	117	
65	y	115	
66	z	118	

2 Entry composition (i)

There are 68 unique types of molecules in this entry. The entry contains 280205 atoms, of which 98639 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 protein called Ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	103	Total	C	H	N	O	S	0	0
			1655	516	839	153	145	2		

- Molecule 2 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1	110	Total	C	H	N	O	S	0	0
			1779	532	922	166	156	3		

- Molecule 3 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	2	94	Total	C	H	N	O	S	0	0
			1557	470	811	140	134	2		

- Molecule 4 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	103	Total	C	H	N	O	0	0
			1632	498	844	148	142		

- Molecule 5 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	4	94	Total	C	H	N	O	S	0	0
			1533	479	780	137	134	3		

- Molecule 6 is a DNA chain called NT DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	31	Total	C	N	O	P	0	0
			636	303	117	185	31		

- Molecule 7 is a DNA chain called T DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	36	Total	C	N	O	P	0	0
			706	337	119	215	35		

- Molecule 8 is a RNA chain called mRNA with 24 nt long spacer.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	37	Total	C	N	O	P	0	0
			772	345	110	280	37		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	148	Total	C	N	O	S	0	0
			1117	705	196	209	7		

- Molecule 10 is a RNA chain called E-site and P-site fMet-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	A	76	Total	C	H	N	O	P	0	0
			2446	723	826	295	527	75		
10	B	76	Total	C	H	N	O	P	0	0
			2434	723	814	295	527	75		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AA	1316	Total	C	N	O	S	0	0
			10381	6514	1810	2014	43		

- Molecule 12 is a protein called Transcription antitermination protein RfaH.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AB	161	Total	C	N	O	S	0	0
			1286	828	222	232	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AC	221	Total	C	N	O	S	0	0
			1698	1060	299	333	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	AD	299	Total	C	N	O	S	0	0
			2078	1287	378	407	6		

- Molecule 14 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AE	1337	Total	C	N	O	S	0	0
			10404	6535	1856	1963	50		

- Molecule 15 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AF	82	Total	C	N	O	S	0	0
			650	396	122	131	1		

- Molecule 16 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AG	495	Total	C	N	O	S	0	0
			3852	2396	669	774	13		

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	C	66	Total	C	H	N	O	S	0	0
			1103	344	559	102	97	1		

- Molecule 18 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	D	1524	Total	C	H	N	O	P	0	0
			49126	14585	16423	6003	10591	1524		

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	E	86	Total	C	H	N	O	S	0	0
			1388	414	719	138	114	3		

- Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	F	70	Total	C	H	N	O	S	0	0
			1218	366	629	125	97	1		

- Molecule 21 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	G	225	Total	C	H	N	O	S	0	0
			3545	1113	1785	316	323	8		

- Molecule 22 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	H	259	Total	C	H	N	O	S	0	0
			3184	1073	1454	305	349	3		

- Molecule 23 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	I	208	Total	C	H	N	O	S	0	0
			3346	1036	1710	307	290	3		

- Molecule 24 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	J	205	Total	C	H	N	O	S	0	0
			3350	1026	1707	315	298	4		

- Molecule 25 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	K	156	Total	C	H	N	O	S	0	0
			2348	717	1196	217	212	6		

- Molecule 26 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	L	104	Total	C	H	N	O	S	0	0
			1694	536	846	153	152	7		

- Molecule 27 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	M	151	Total	C	H	N	O	S	0	0
			2416	735	1235	227	215	4		

- Molecule 28 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	N	129	Total	C	H	N	O	S	0	0
			2010	616	1031	173	184	6		

- Molecule 29 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	O	127	Total	C	H	N	O	S	0	0
			2092	634	1070	206	179	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
30	P	99	Total	C	H	N	O	S	0	0
			1621	495	831	151	143	1		

- Molecule 31 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	Q	117	Total	C	H	N	O	S	0	0
			1764	540	887	174	160	3		

- Molecule 32 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	R	121	Total	C	H	N	O	S	0	0
			1940	580	1001	194	161	4		

- Molecule 33 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	S	100	Total	C	H	N	O	S	0	0
			1649	499	844	164	139	3		

- Molecule 34 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	T	88	Total	C	H	N	O	S	0	0
			1448	439	734	144	130	1		

- Molecule 35 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	U	82	Total	C	H	N	O	S	0	0
			1315	406	666	128	114	1		

- Molecule 36 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	V	80	Total	C	H	N	O	S	0	0
			1339	411	691	121	113	3		

- Molecule 37 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	W	83	Total	C	H	N	O	S	0	0
			1351	424	688	126	111	2		

- Molecule 38 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	X	116	Total	C	H	N	O	S	0	0
			1864	558	964	181	158	3		

- Molecule 39 is a protein called 50S ribosomal protein L11.

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

- Molecule 40 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Z	30	Total	C	N	O	S	0	0
			227	144	33	47	3		

- Molecule 41 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	a	2880	Total	C	H	N	O	P	0	0
			92918	27587	31077	11398	19976	2880		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	887	A	U	conflict	GB 937521852

- Molecule 42 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	b	76	Total	C	H	N	O	S	0	0
			1181	360	599	117	104	1		

- Molecule 43 is a protein called 50S ribosomal protein L28.

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

- Molecule 44 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	d	120	Total	C	H	N	O	P	0	0
			3870	1144	1301	468	837	120		

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
46	f	58	Total	C	H	N	O	S	0	0
			936	281	488	87	78	2		

- Molecule 47 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	g	66	Total	C	H	N	O	S	0	0
			1042	323	520	99	94	6		

- Molecule 48 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	h	271	Total	C	H	N	O	S	0	0
			4236	1288	2154	423	364	7		

- Molecule 49 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	i	56	Total	C	H	N	O	S	0	0
			903	269	459	94	80	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
50	j	209	Total	C	H	N	O	S	0	0
			3182	979	1617	288	294	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	k	52	Total	C	H	N	O	0	0
			890	275	464	78	73		

- Molecule 52 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	l	201	Total	C	H	N	O	S	0	0
			3171	974	1619	283	290	5		

- Molecule 53 is a protein called 50S ribosomal protein L34.

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

- Molecule 54 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	n	177	Total	C	H	N	O	S	0	0
			2853	899	1443	249	256	6		

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	o	64	Total	C	H	N	O	S	0	0
			1076	323	572	105	74	2		

- Molecule 56 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	p	175	Total	C	H	N	O	S	0	0
			2671	826	1358	241	244	2		

- Molecule 57 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	q	38	Total	C	H	N	O	S	0	0
			645	185	343	65	48	4		

- Molecule 58 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	r	149	Total	C	H	N	O	S	0	0
			2259	699	1148	197	214	1		

- Molecule 59 is a protein called 50S ribosomal protein L13.

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

- Molecule 60 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	t	123	Total	C	H	N	O	S	0	0
			1969	593	1023	181	166	6		

- Molecule 61 is a protein called 50S ribosomal protein L15.

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

- Molecule 62 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	v	136	Total	C	H	N	O	S	0	0
			2231	686	1157	205	177	6		

- Molecule 63 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	w	119	Total	C	H	N	O	S	0	0
			1945	588	994	195	163	5		

- Molecule 64 is a protein called 50S ribosomal protein L18.

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

- Molecule 65 is a protein called 50S ribosomal protein L19.

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

- Molecule 66 is a protein called 50S ribosomal protein L20.

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

- Molecule 67 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
67	AE	1	Total	Mg	0
			1	1	

- Molecule 68 is ZINC ION (three-letter code: ZN) (formula: Zn).

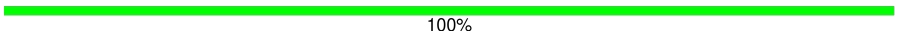
Mol	Chain	Residues	Atoms		AltConf
68	AE	2	Total	Zn	0
			2	2	

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: Ribosomal protein L21

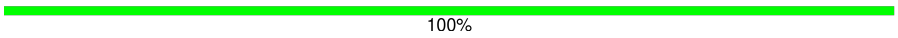
Chain 0:



There are no outlier residues recorded for this chain.

• Molecule 2: 50S ribosomal protein L22

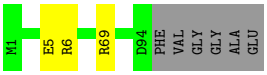
Chain 1:



There are no outlier residues recorded for this chain.

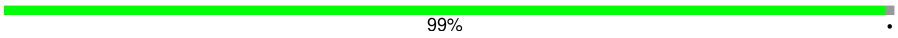
• Molecule 3: 50S ribosomal protein L23

Chain 2:



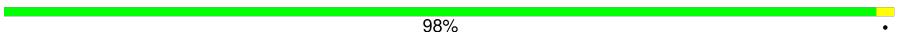
• Molecule 4: 50S ribosomal protein L24

Chain 3:



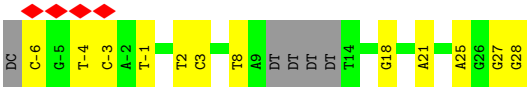
• Molecule 5: 50S ribosomal protein L25

Chain 4:



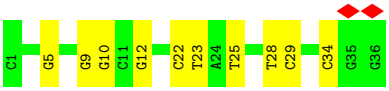
• Molecule 6: NT DNA

Chain 5:



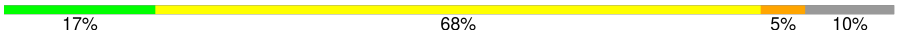
• Molecule 7: T DNA

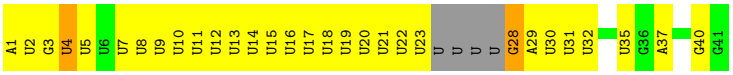
Chain 6:



• Molecule 8: mRNA with 24 nt long spacer

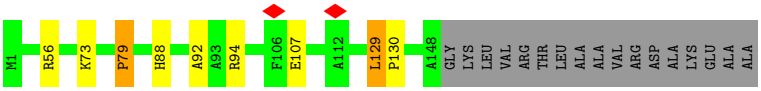
Chain 7:





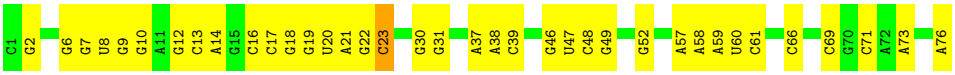
• Molecule 9: 50S ribosomal protein L10

Chain 9:



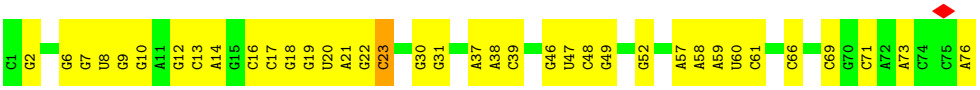
• Molecule 10: E-site and P-site fMet-tRNA

Chain A:



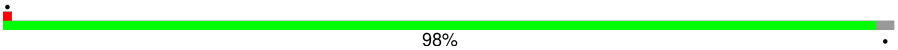
• Molecule 10: E-site and P-site fMet-tRNA

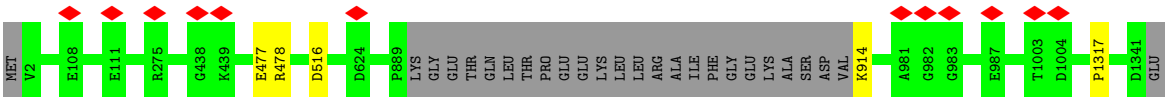
Chain B:



• Molecule 11: DNA-directed RNA polymerase subunit beta

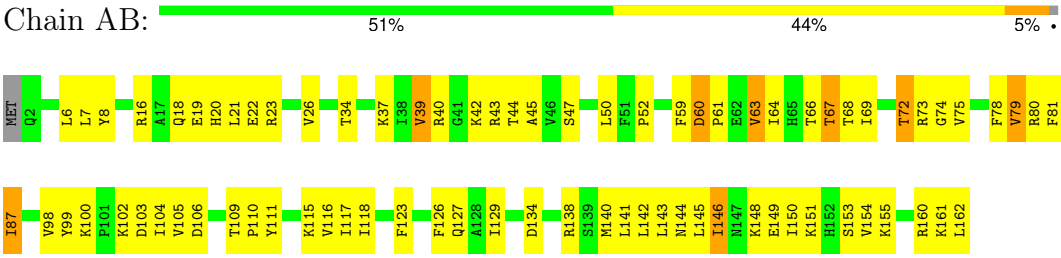
Chain AA:





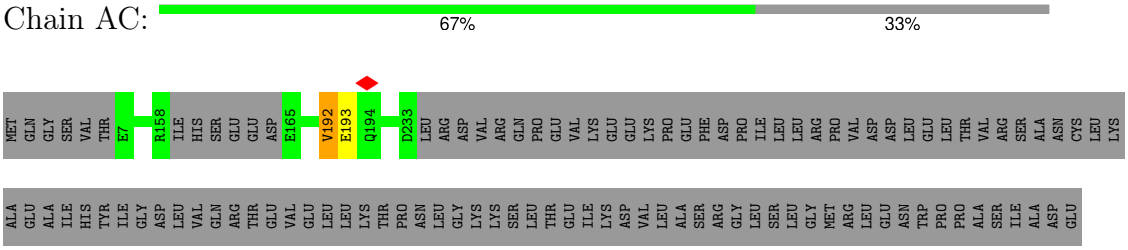
• Molecule 12: Transcription antitermination protein RfaH

Chain AB:



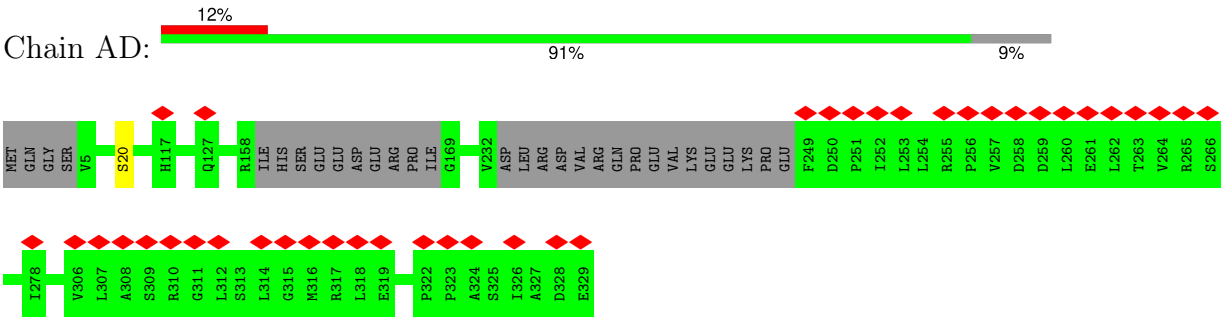
• Molecule 13: DNA-directed RNA polymerase subunit alpha

Chain AC:



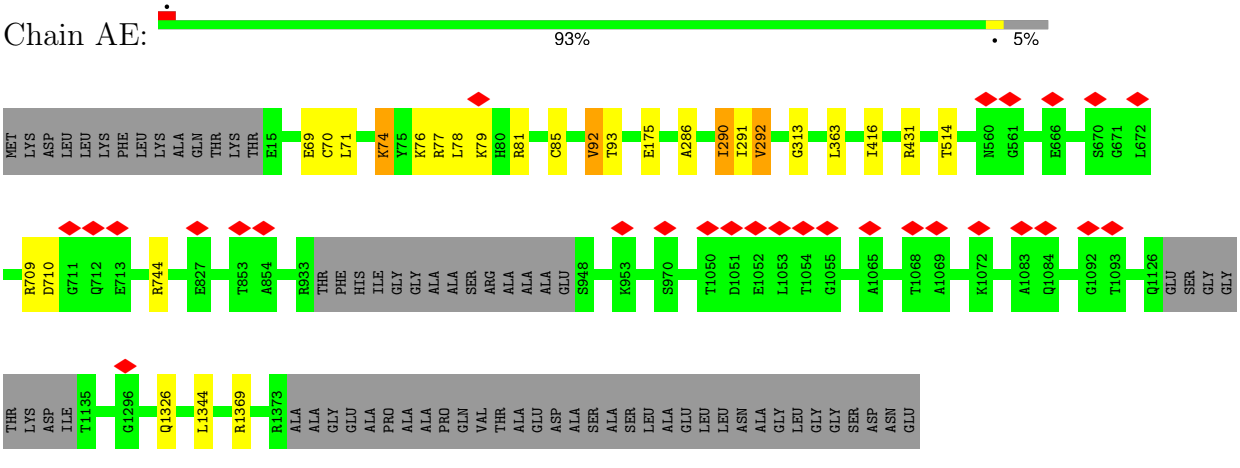
• Molecule 13: DNA-directed RNA polymerase subunit alpha

Chain AD:



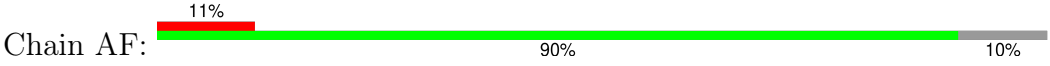
• Molecule 14: DNA-directed RNA polymerase subunit beta'

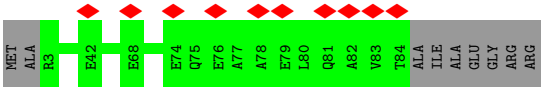
Chain AE:



• Molecule 15: DNA-directed RNA polymerase subunit omega

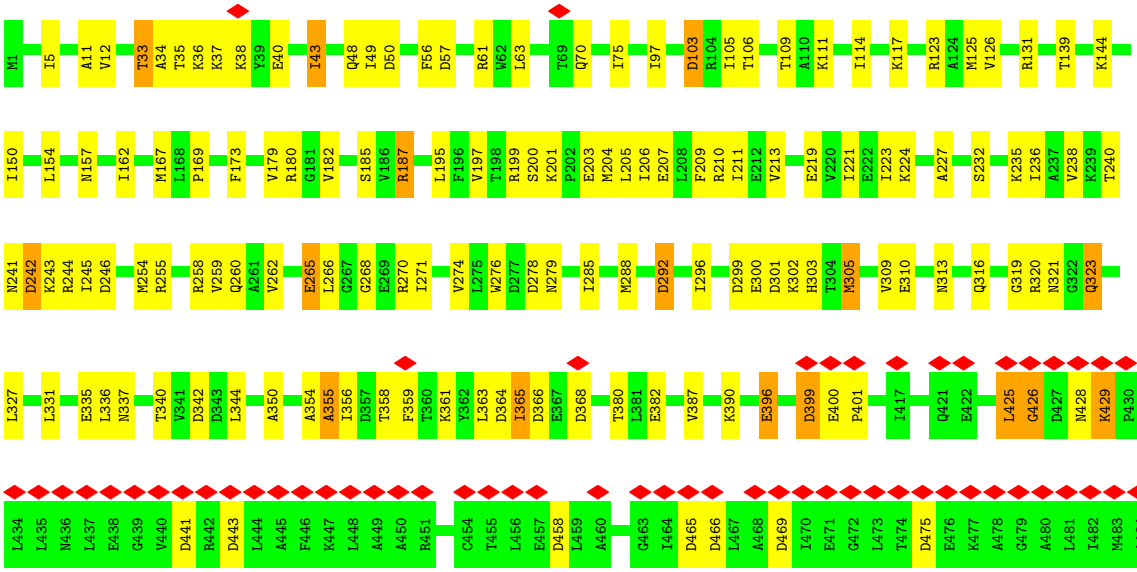
Chain AF:





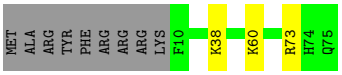
• Molecule 16: Transcription termination/antitermination protein NusA

Chain AG:



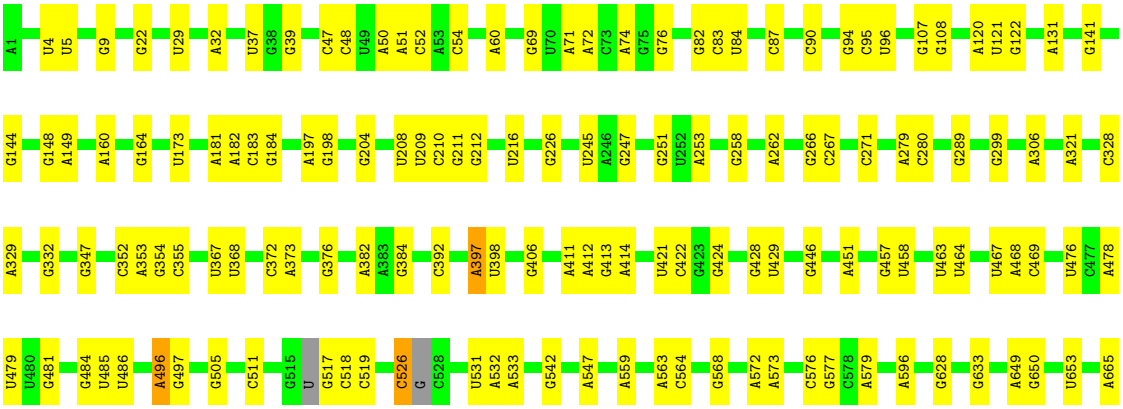
• Molecule 17: 30S ribosomal protein S18

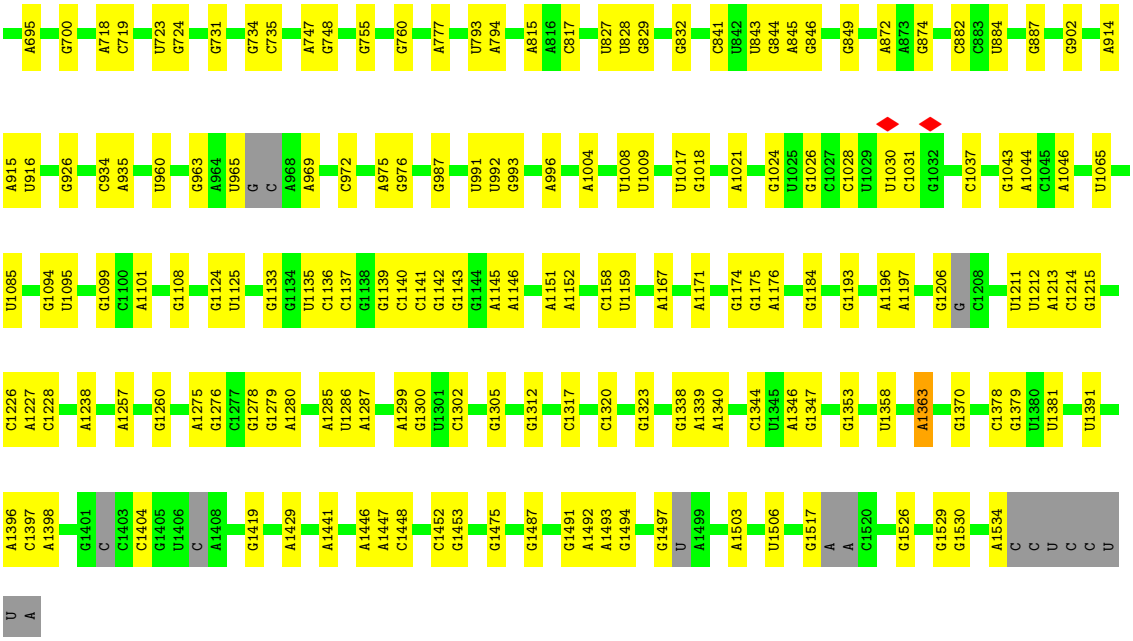
Chain C:



• Molecule 18: 16S rRNA

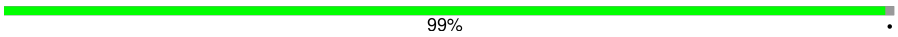
Chain D:





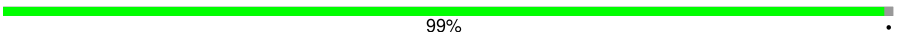
• Molecule 19: 30S ribosomal protein S20

Chain E:



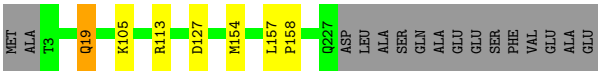
• Molecule 20: 30S ribosomal protein S21

Chain F:



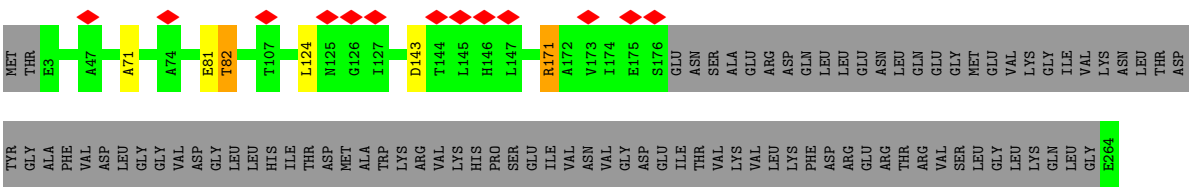
• Molecule 21: 30S ribosomal protein S2

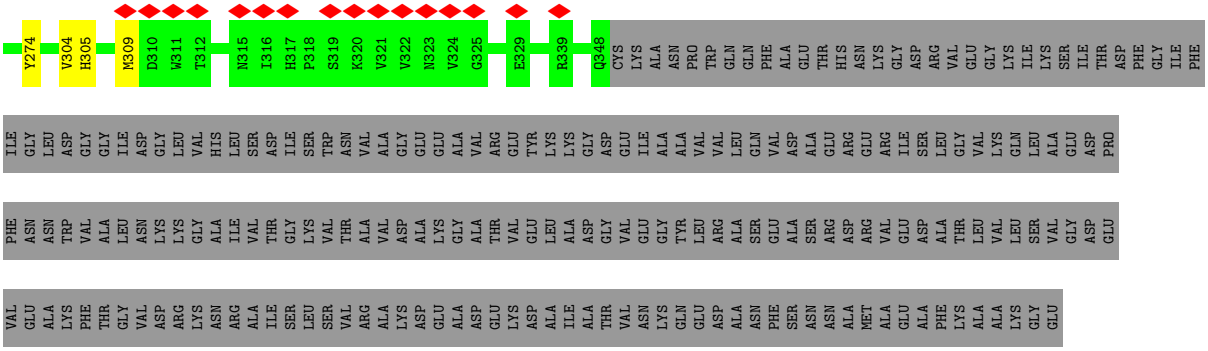
Chain G:



• Molecule 22: 30S ribosomal protein S1

Chain H:



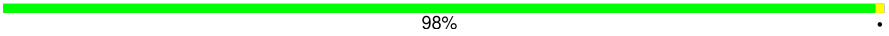


• Molecule 23: 30S ribosomal protein S3

Chain I:

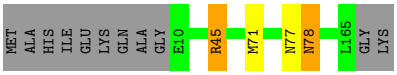
• Molecule 24: 30S ribosomal protein S4

Chain J:



• Molecule 25: 30S ribosomal protein S5

Chain K:



• Molecule 26: 30S ribosomal protein S6

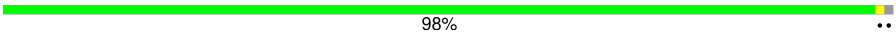
Chain L:

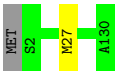
• Molecule 27: 30S ribosomal protein S7

Chain M:

• Molecule 28: 30S ribosomal protein S8

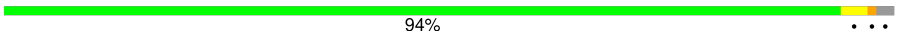
Chain N:

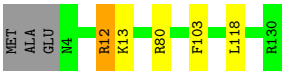




• Molecule 29: 30S ribosomal protein S9

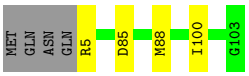
Chain O:





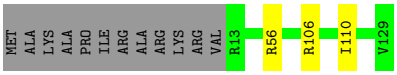
• Molecule 30: 30S ribosomal protein S10

Chain P:



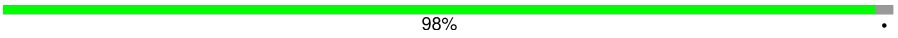
• Molecule 31: 30S ribosomal protein S11

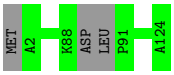
Chain Q:



• Molecule 32: 30S ribosomal protein S12

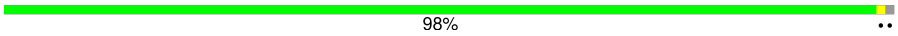
Chain R:





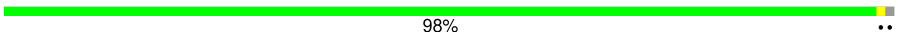
• Molecule 33: 30S ribosomal protein S14

Chain S:



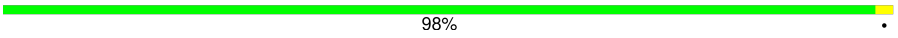
• Molecule 34: 30S ribosomal protein S15

Chain T:



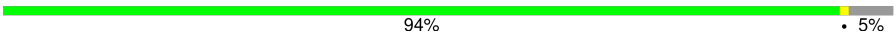
• Molecule 35: 30S ribosomal protein S16

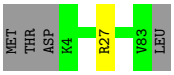
Chain U:



• Molecule 36: 30S ribosomal protein S17

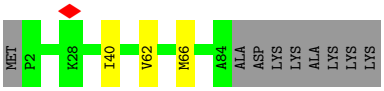
Chain V:





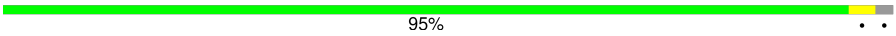
• Molecule 37: 30S ribosomal protein S19

Chain W:



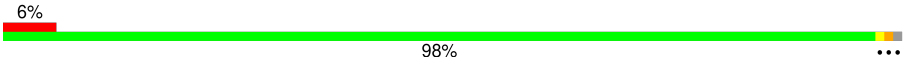
• Molecule 38: 30S ribosomal protein S13

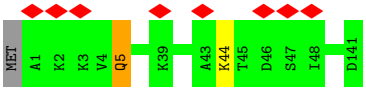
Chain X:



• Molecule 39: 50S ribosomal protein L11

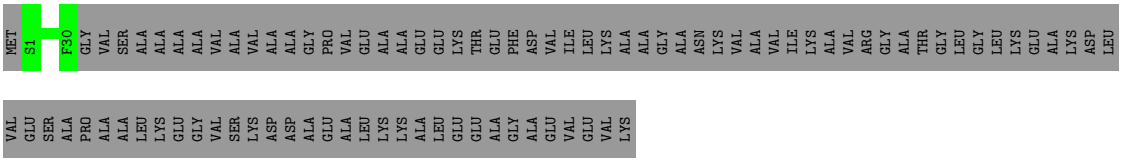
Chain Y:





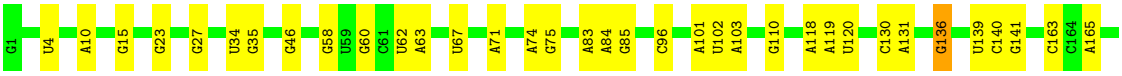
• Molecule 40: 50S ribosomal protein L7/L12

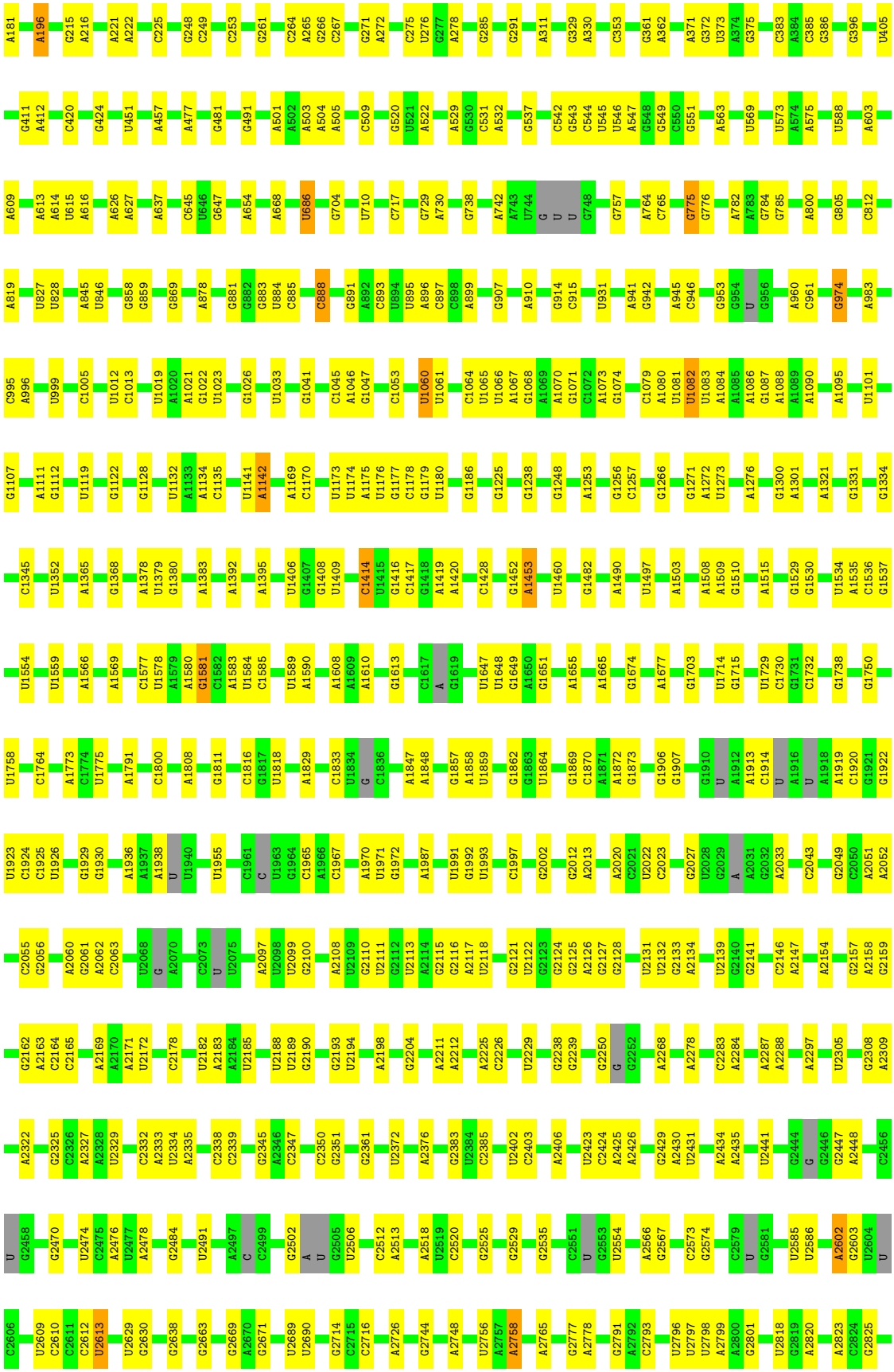
Chain Z:

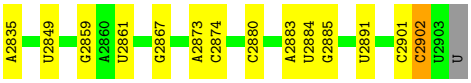


• Molecule 41: 23S rRNA

Chain a:

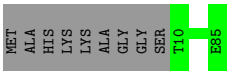



A181 A196 G215 A216 A221 A222 C225 G248 C249 C253 G261 C264 A265 G266 C267 G271 A272 C275 U276 G277 A278 G285 G291 A311 G329 A330 C353 G361 A362 A371 G372 U373 A374 G375 C383 A384 C385 G386 G396 U405
G411 A412 C420 G424 U451 A457 A477 G481 G491 A501 A502 A503 A504 A505 C509 G520 U521 A522 A529 G530 C531 A532 G537 C542 G543 C544 U545 U546 A547 G548 G549 C550 G551 A563 U569 U573 A574 A575 U588 A603
A609 A613 A614 U615 A616 A626 A627 A637 C645 U646 G647 A654 A668 U686 G704 U710 C717 G729 A730 G738 A742 A743 U744 G U U G748 G757 A764 C765 G775 G776 A782 A783 G784 G785 A800 G805 C812
A819 U827 U828 A845 U846 G858 G859 G869 A878 G881 G882 G883 U884 C885 C888 G891 A892 C893 U894 U895 A896 C897 C898 A899 G907 A910 G914 C915 U931 A941 G942 A945 C946 G953 G954 U G956 A960 C961 G974 A983
C995 A996 U999 C1005 U1012 C1013 U1019 A1020 A1021 G1022 U1023 G1026 U1033 G1041 C1045 A1046 G1047 C1053 U1060 U1061 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1090 A1095 U1101
G1107 A1111 G1112 U1119 G1122 G1128 U1132 A1133 A1134 C1135 U1141 A1142 A1169 C1170 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 G1186 G1225 G1238 G1248 A1253 G1256 C1257 G1266 G1271 A1272 U1273 A1276 G1300 A1301 A1321 G1331 G1334
C1345 U1352 A1365 G1368 A1378 U1379 G1380 A1383 A1392 A1395 U1406 G1407 G1408 U1409 C1414 U1415 G1416 C1417 G1418 A1419 A1420 C1428 G1452 A1453 U1460 G1482 A1490 U1497 A1503 A1508 A1509 G1510 A1515 G1529 G1530 U1534 A1535 C1536 G1537
U1554 U1559 A1566 A1569 C1577 U1578 A1579 A1580 G1581 C1582 A1583 U1584 C1585 U1589 A1590 A1608 A1609 A1610 G1613 C1617 A G1619 U1647 U1648 G1649 A1650 G1651 A1655 A1665 G1674 A1677 G1703 U1714 G1715 U1729 C1730 G1731 C1732 G1738 G1750
U1758 C1764 A1773 C1774 U1775 A1791 C1800 A1808 G1811 C1816 G1817 U1818 A1829 C1833 U1834 G C1836 A1847 A1848 G1857 A1858 U1859 G1862 G1863 U1864 G1869 C1870 A1871 A1872 G1873 G1906 G1907 G1910 U G1912 A1913 C1914 U A1916 U A1918 A1919 C1920 G1921 G1922
U1923 C1924 C1925 U1926 G1929 G1930 A1936 A1937 A1938 U U1940 U1955 C1961 C U1963 G1964 C1965 A1966 C1967 A1970 U1971 G1972 A1987 U1991 G1992 U1993 C1997 G2002 G2012 A2013 A2020 C2021 U2022 C2023 G2027 U2028 G2029 A A2031 G2032 A2033 C2043 G2049 C2050 A2051 A2052
C2055 G2056 A2060 G2061 A2062 C2063 U2068 G G A2070 C2073 U U2075 A2097 U2098 U2099 G2100 A2108 U2109 G2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 G2121 U2122 G2123 G2124 G2125 A2126 G2127 G2128 U2131 U2132 G2133 A2134 U2139 G2140 G2141 C2146 A2147 A2154 C2157 A2158 G2159
G2162 A2163 C2164 C2165 A2169 A2170 A2171 U2172 C2178 U2182 A2183 A2184 U2185 U2188 U2189 G2190 G2193 U2194 A2198 G2204 A2211 A2212 A2225 C2226 U2229 G2238 G2239 G2250 G G2252 A2268 A2278 C2283 A2284 A2287 A2288 A2297 U2305 G2308 A2309
A2322 G2325 C2326 A2327 A2328 U2329 C2332 A2333 U2334 A2335 C2338 C2339 G2345 A2346 C2347 C2350 G2351 G2361 U2372 A2376 G2383 U2384 C2385 U2402 C2403 A2406 U2423 C2424 A2425 A2426 G2429 A2430 U2431 A2434 A2435 U2441 G2444 G G2446 G2447 A2448 C2456
U G2458 G2470 U2474 C2475 A2476 U2477 A2478 G2484 U2491 A2497 C C2499 G2502 A U G2505 U2506 C2512 A2513 A2518 U2519 C2520 G2525 G2529 G2535 C2551 U G2553 U2554 A2566 G2567 C2573 G2574 C2579 U G2581 U2585 U2586 A2602 G2603 U2604 U
C2606 U2609 C2610 C2611 C2612 U2613 U2629 G2630 G2638 G2663 G2669 A2670 G2671 U2689 U2690 G2714 C2715 C2716 A2726 G2744 A2748 U2756 A2757 A2758 A2765 G2777 A2778 G2791 A2792 C2793 U2796 U2797 U2798 A2799 A2800 G2801 U2818 G2819 A2820 A2823 C2824 G2825



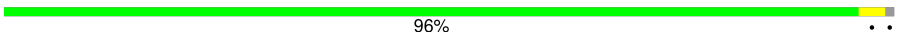
• Molecule 42: 50S ribosomal protein L27

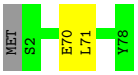
Chain b:



• Molecule 43: 50S ribosomal protein L28

Chain c:



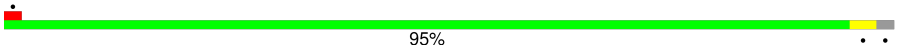


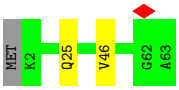
• Molecule 44: 5S rRNA

Chain d:

• Molecule 45: 50S ribosomal protein L29

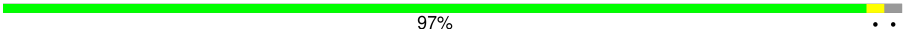
Chain e:

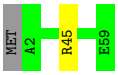




• Molecule 46: 50S ribosomal protein L30

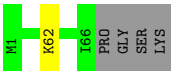
Chain f:





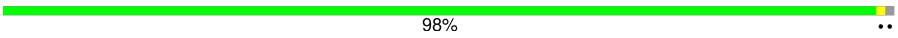
• Molecule 47: 50S ribosomal protein L31

Chain g:



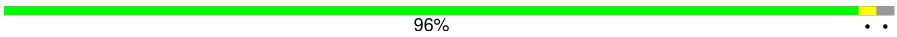
• Molecule 48: 50S ribosomal protein L2

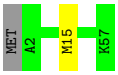
Chain h:



• Molecule 49: 50S ribosomal protein L32

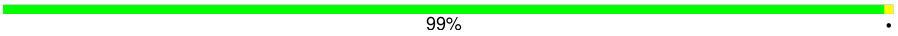
Chain i:





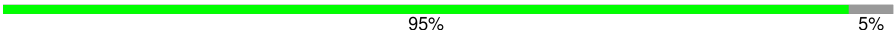
• Molecule 50: 50S ribosomal protein L3

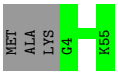
Chain j:



• Molecule 51: 50S ribosomal protein L33

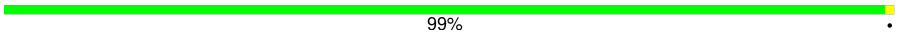
Chain k:

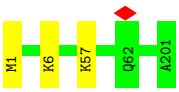




• Molecule 52: 50S ribosomal protein L4

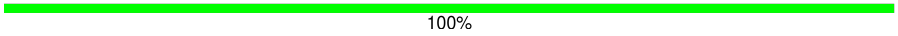
Chain l:





• Molecule 53: 50S ribosomal protein L34

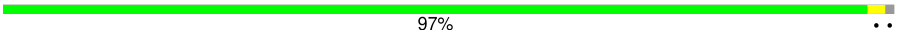
Chain m:



There are no outlier residues recorded for this chain.

• Molecule 54: 50S ribosomal protein L5

Chain n:

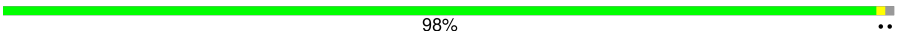


• Molecule 55: 50S ribosomal protein L35

Chain o:

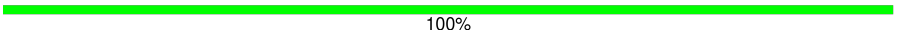
• Molecule 56: 50S ribosomal protein L6

Chain p:



• Molecule 57: 50S ribosomal protein L36

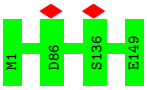
Chain q:



There are no outlier residues recorded for this chain.

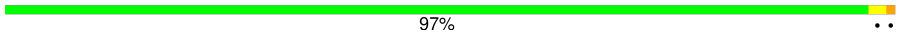
• Molecule 58: 50S ribosomal protein L9

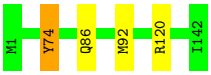
Chain r:



• Molecule 59: 50S ribosomal protein L13

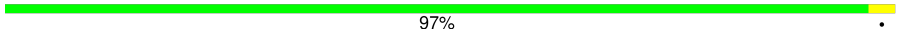
Chain s:

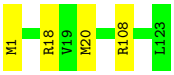




• Molecule 60: 50S ribosomal protein L14

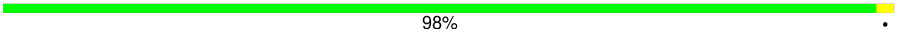
Chain t:

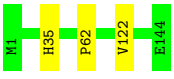




• Molecule 61: 50S ribosomal protein L15

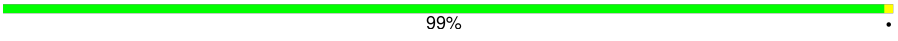
Chain u:





• Molecule 62: 50S ribosomal protein L16

Chain v:

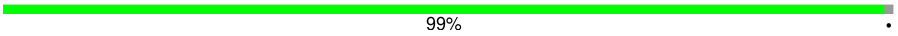


• Molecule 63: 50S ribosomal protein L17

Chain w:

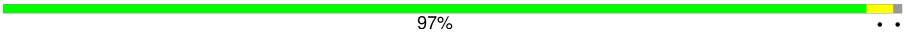
• Molecule 64: 50S ribosomal protein L18

Chain x:



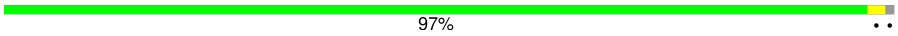
• Molecule 65: 50S ribosomal protein L19

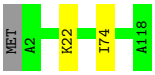
Chain y:



• Molecule 66: 50S ribosomal protein L20

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19976	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	28	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.030	Depositor
Minimum map value	-0.008	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0019	Depositor
Map size (Å)	531.968, 531.968, 531.968	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.039, 1.039, 1.039	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: MG, ZN

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	0	0.47	0/829	0.60	0/1107
2	1	0.58	0/864	0.69	0/1156
3	2	0.67	1/752 (0.1%)	0.71	1/1005 (0.1%)
4	3	0.41	0/796	0.55	0/1062
5	4	0.65	2/766 (0.3%)	0.69	0/1025
6	5	1.16	11/712 (1.5%)	1.12	1/1094 (0.1%)
7	6	1.12	8/786 (1.0%)	1.15	2/1206 (0.2%)
8	7	0.54	2/856 (0.2%)	0.89	4/1326 (0.3%)
9	9	0.36	0/1131	0.66	2/1524 (0.1%)
10	A	0.55	1/1810 (0.1%)	1.26	11/2821 (0.4%)
10	B	0.55	1/1810 (0.1%)	1.26	11/2821 (0.4%)
11	AA	0.43	0/10547	0.61	2/14232 (0.0%)
12	AB	0.63	0/1317	0.58	0/1786
13	AC	0.41	0/1718	0.62	0/2328
13	AD	0.34	0/2096	0.59	0/2854
14	AE	0.42	0/10561	0.63	3/14258 (0.0%)
15	AF	0.34	0/652	0.57	0/879
16	AG	0.64	2/3897 (0.1%)	0.79	22/5273 (0.4%)
17	C	0.70	0/553	0.93	4/743 (0.5%)
18	D	0.60	14/36610 (0.0%)	1.03	65/57091 (0.1%)
19	E	0.57	0/675	0.70	0/895
20	F	0.62	0/597	0.59	0/792
21	G	0.66	2/1791 (0.1%)	0.83	8/2413 (0.3%)
22	H	0.43	0/1746	0.70	0/2382
23	I	0.62	2/1663 (0.1%)	0.70	4/2241 (0.2%)
24	J	0.54	2/1665 (0.1%)	0.59	0/2227
25	K	0.69	1/1165 (0.1%)	0.86	4/1568 (0.3%)
26	L	0.79	3/867 (0.3%)	0.82	3/1171 (0.3%)
27	M	0.55	0/1195	0.70	2/1602 (0.1%)
28	N	0.52	0/989	0.63	1/1326 (0.1%)
29	O	0.67	4/1034 (0.4%)	0.82	4/1375 (0.3%)
30	P	0.52	0/800	0.67	1/1082 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	Q	0.71	1/893 (0.1%)	0.82	4/1205 (0.3%)
32	R	0.56	0/952	0.65	0/1274
33	S	0.63	1/817 (0.1%)	0.64	0/1088
34	T	0.56	0/722	0.72	1/964 (0.1%)
35	U	0.45	0/659	0.65	1/884 (0.1%)
36	V	0.56	0/657	0.70	0/881
37	W	0.56	1/680 (0.1%)	0.69	3/915 (0.3%)
38	X	0.48	0/909	0.72	1/1215 (0.1%)
39	Y	0.42	1/1046 (0.1%)	0.57	2/1410 (0.1%)
40	Z	0.23	0/227	0.38	0/304
41	a	0.61	14/69247 (0.0%)	1.03	132/107985 (0.1%)
42	b	0.47	0/589	0.57	0/779
43	c	0.57	1/635 (0.2%)	0.66	1/848 (0.1%)
44	d	0.50	0/2872	0.95	0/4478
45	e	0.81	2/502 (0.4%)	0.66	0/667
46	f	0.53	0/452	0.72	2/605 (0.3%)
47	g	0.50	1/531 (0.2%)	0.67	1/709 (0.1%)
48	h	0.53	2/2121 (0.1%)	0.67	6/2852 (0.2%)
49	i	0.42	0/450	0.65	1/599 (0.2%)
50	j	0.53	0/1586	0.64	2/2134 (0.1%)
51	k	0.51	0/433	0.68	0/576
52	l	0.54	1/1571 (0.1%)	0.64	1/2113 (0.0%)
53	m	0.43	0/380	0.60	0/498
54	n	0.51	0/1434	0.68	2/1926 (0.1%)
55	o	0.51	0/513	0.85	1/676 (0.1%)
56	p	0.50	0/1333	0.68	3/1805 (0.2%)
57	q	0.46	0/303	0.60	0/397
58	r	0.34	0/1122	0.52	0/1515
59	s	0.83	5/1152 (0.4%)	0.81	4/1551 (0.3%)
60	t	0.55	1/955 (0.1%)	0.89	5/1279 (0.4%)
61	u	0.47	1/1062 (0.1%)	0.63	0/1413
62	v	0.61	1/1093 (0.1%)	0.75	1/1460 (0.1%)
63	w	0.90	5/964 (0.5%)	0.95	9/1289 (0.7%)
64	x	0.42	0/902	0.57	0/1209
65	y	0.46	0/929	0.59	1/1242 (0.1%)
66	z	0.63	1/960 (0.1%)	0.60	0/1278
All	All	0.58	95/194903 (0.0%)	0.92	339/286688 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	9	0	3
13	AC	0	1
13	AD	0	1
14	AE	0	4
16	AG	0	3
21	G	0	1
22	H	0	5
23	I	0	1
25	K	0	2
29	O	0	1
38	X	0	1
39	Y	0	1
54	n	0	1
55	o	0	1
59	s	0	1
61	u	0	2
All	All	0	29

The worst 5 of 95 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	w	35	LYS	CE-NZ	-15.23	1.10	1.49
26	L	42	TRP	CB-CG	-12.33	1.28	1.50
3	2	5	GLU	CG-CD	-11.56	1.34	1.51
45	e	46	VAL	CB-CG1	-11.33	1.29	1.52
63	w	42	LYS	CD-CE	-10.77	1.24	1.51

The worst 5 of 339 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	a	1019	U	C5-C4-O4	30.65	144.29	125.90
41	a	1141	U	C5-C4-O4	29.47	143.58	125.90
18	D	1358	U	C5-C4-O4	29.31	143.49	125.90
18	D	37	U	C5-C4-O4	29.31	143.49	125.90
18	D	827	U	C5-C4-O4	28.70	143.12	125.90

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	9	107	GLU	Peptide
9	9	79	PRO	Peptide

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Mol	Chain	Res	Type	Group
9	9	92	ALA	Peptide
13	AC	192	VAL	Peptide
13	AD	20	SER	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
1	0	101/103 (98%)	97 (96%)	4 (4%)	0	100 100
2	1	108/110 (98%)	107 (99%)	1 (1%)	0	100 100
3	2	92/100 (92%)	87 (95%)	5 (5%)	0	100 100
4	3	101/104 (97%)	98 (97%)	3 (3%)	0	100 100
5	4	92/94 (98%)	89 (97%)	3 (3%)	0	100 100
9	9	146/165 (88%)	100 (68%)	43 (30%)	3 (2%)	5 29
11	AA	1312/1342 (98%)	1195 (91%)	116 (9%)	1 (0%)	48 83
12	AB	159/162 (98%)	112 (70%)	30 (19%)	17 (11%)	0 6
13	AC	217/329 (66%)	203 (94%)	12 (6%)	2 (1%)	14 51
13	AD	293/329 (89%)	269 (92%)	24 (8%)	0	100 100
14	AE	1331/1407 (95%)	1213 (91%)	112 (8%)	6 (0%)	25 64
15	AF	80/91 (88%)	77 (96%)	3 (4%)	0	100 100
16	AG	493/495 (100%)	376 (76%)	88 (18%)	29 (6%)	1 13
17	C	64/75 (85%)	63 (98%)	1 (2%)	0	100 100
19	E	84/87 (97%)	83 (99%)	1 (1%)	0	100 100
20	F	68/71 (96%)	68 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
21	G	223/241 (92%)	212 (95%)	10 (4%)	1 (0%)	30 68
22	H	255/557 (46%)	182 (71%)	66 (26%)	7 (3%)	4 25
23	I	206/233 (88%)	193 (94%)	13 (6%)	0	100 100
24	J	203/206 (98%)	201 (99%)	2 (1%)	0	100 100
25	K	154/167 (92%)	145 (94%)	8 (5%)	1 (1%)	22 60
26	L	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	13 49
27	M	149/179 (83%)	140 (94%)	8 (5%)	1 (1%)	19 56
28	N	127/130 (98%)	123 (97%)	4 (3%)	0	100 100
29	O	125/130 (96%)	116 (93%)	8 (6%)	1 (1%)	16 54
30	P	97/103 (94%)	89 (92%)	8 (8%)	0	100 100
31	Q	115/129 (89%)	107 (93%)	8 (7%)	0	100 100
32	R	117/124 (94%)	112 (96%)	5 (4%)	0	100 100
33	S	98/101 (97%)	97 (99%)	1 (1%)	0	100 100
34	T	86/89 (97%)	83 (96%)	3 (4%)	0	100 100
35	U	80/82 (98%)	76 (95%)	4 (5%)	0	100 100
36	V	78/84 (93%)	74 (95%)	4 (5%)	0	100 100
37	W	81/92 (88%)	80 (99%)	1 (1%)	0	100 100
38	X	114/118 (97%)	103 (90%)	9 (8%)	2 (2%)	7 33
39	Y	139/142 (98%)	101 (73%)	38 (27%)	0	100 100
40	Z	28/121 (23%)	22 (79%)	6 (21%)	0	100 100
42	b	74/85 (87%)	73 (99%)	1 (1%)	0	100 100
43	c	75/78 (96%)	72 (96%)	3 (4%)	0	100 100
45	e	60/63 (95%)	57 (95%)	3 (5%)	0	100 100
46	f	56/59 (95%)	52 (93%)	4 (7%)	0	100 100
47	g	64/70 (91%)	62 (97%)	2 (3%)	0	100 100
48	h	269/273 (98%)	255 (95%)	14 (5%)	0	100 100
49	i	54/57 (95%)	49 (91%)	5 (9%)	0	100 100
50	j	207/209 (99%)	198 (96%)	9 (4%)	0	100 100
51	k	50/55 (91%)	50 (100%)	0	0	100 100
52	l	199/201 (99%)	188 (94%)	11 (6%)	0	100 100
53	m	44/46 (96%)	43 (98%)	1 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
54	n	175/179 (98%)	160 (91%)	14 (8%)	1 (1%)	22 60
55	o	62/65 (95%)	57 (92%)	4 (6%)	1 (2%)	8 37
56	p	173/177 (98%)	162 (94%)	11 (6%)	0	100 100
57	q	36/38 (95%)	35 (97%)	1 (3%)	0	100 100
58	r	147/149 (99%)	139 (95%)	8 (5%)	0	100 100
59	s	140/142 (99%)	133 (95%)	7 (5%)	0	100 100
60	t	121/123 (98%)	114 (94%)	7 (6%)	0	100 100
61	u	142/144 (99%)	134 (94%)	8 (6%)	0	100 100
62	v	134/136 (98%)	129 (96%)	5 (4%)	0	100 100
63	w	117/127 (92%)	112 (96%)	5 (4%)	0	100 100
64	x	114/117 (97%)	107 (94%)	7 (6%)	0	100 100
65	y	112/115 (97%)	105 (94%)	7 (6%)	0	100 100
66	z	115/118 (98%)	111 (96%)	4 (4%)	0	100 100
All	All	10058/11053 (91%)	9187 (91%)	797 (8%)	74 (1%)	21 56

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	AB	52	PRO
12	AB	60	ASP
12	AB	87	ILE
12	AB	98	VAL
12	AB	109	THR

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
1	0	84/84 (100%)	84 (100%)	0	100 100
2	1	93/93 (100%)	93 (100%)	0	100 100
3	2	81/84 (96%)	80 (99%)	1 (1%)	67 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3	84/85 (99%)	84 (100%)	0	100	100
5	4	78/78 (100%)	78 (100%)	0	100	100
9	9	112/123 (91%)	109 (97%)	3 (3%)	40	59
11	AA	1135/1157 (98%)	1133 (100%)	2 (0%)	92	94
12	AB	141/142 (99%)	71 (50%)	70 (50%)	0	0
13	AC	186/286 (65%)	186 (100%)	0	100	100
13	AD	185/286 (65%)	185 (100%)	0	100	100
14	AE	1122/1168 (96%)	1103 (98%)	19 (2%)	56	72
15	AF	70/75 (93%)	70 (100%)	0	100	100
16	AG	409/409 (100%)	294 (72%)	115 (28%)	0	2
17	C	57/65 (88%)	57 (100%)	0	100	100
19	E	65/66 (98%)	65 (100%)	0	100	100
20	F	60/61 (98%)	60 (100%)	0	100	100
21	G	187/199 (94%)	186 (100%)	1 (0%)	86	89
22	H	137/461 (30%)	137 (100%)	0	100	100
23	I	171/190 (90%)	170 (99%)	1 (1%)	84	88
24	J	172/173 (99%)	171 (99%)	1 (1%)	84	88
25	K	119/126 (94%)	119 (100%)	0	100	100
26	L	91/116 (78%)	91 (100%)	0	100	100
27	M	124/147 (84%)	124 (100%)	0	100	100
28	N	104/105 (99%)	104 (100%)	0	100	100
29	O	105/107 (98%)	104 (99%)	1 (1%)	73	82
30	P	86/90 (96%)	83 (96%)	3 (4%)	31	51
31	Q	90/99 (91%)	90 (100%)	0	100	100
32	R	101/104 (97%)	101 (100%)	0	100	100
33	S	83/84 (99%)	83 (100%)	0	100	100
34	T	76/77 (99%)	76 (100%)	0	100	100
35	U	65/65 (100%)	64 (98%)	1 (2%)	60	75
36	V	74/78 (95%)	73 (99%)	1 (1%)	62	76
37	W	72/79 (91%)	72 (100%)	0	100	100
38	X	94/96 (98%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
39	Y	109/110 (99%)	108 (99%)	1 (1%)	75 83
40	Z	26/85 (31%)	26 (100%)	0	100 100
42	b	58/63 (92%)	58 (100%)	0	100 100
43	c	67/68 (98%)	67 (100%)	0	100 100
45	e	54/55 (98%)	54 (100%)	0	100 100
46	f	48/49 (98%)	48 (100%)	0	100 100
47	g	59/62 (95%)	59 (100%)	0	100 100
48	h	216/218 (99%)	216 (100%)	0	100 100
49	i	47/48 (98%)	47 (100%)	0	100 100
50	j	164/164 (100%)	164 (100%)	0	100 100
51	k	47/49 (96%)	47 (100%)	0	100 100
52	l	165/165 (100%)	164 (99%)	1 (1%)	84 88
53	m	38/38 (100%)	38 (100%)	0	100 100
54	n	148/150 (99%)	148 (100%)	0	100 100
55	o	51/52 (98%)	51 (100%)	0	100 100
56	p	136/138 (99%)	136 (100%)	0	100 100
57	q	34/34 (100%)	34 (100%)	0	100 100
58	r	114/114 (100%)	114 (100%)	0	100 100
59	s	116/116 (100%)	115 (99%)	1 (1%)	75 83
60	t	104/104 (100%)	103 (99%)	1 (1%)	73 82
61	u	103/103 (100%)	103 (100%)	0	100 100
62	v	109/109 (100%)	109 (100%)	0	100 100
63	w	99/103 (96%)	98 (99%)	1 (1%)	73 82
64	x	86/87 (99%)	86 (100%)	0	100 100
65	y	99/100 (99%)	97 (98%)	2 (2%)	50 68
66	z	89/90 (99%)	88 (99%)	1 (1%)	70 80
All	All	8299/9132 (91%)	8072 (97%)	227 (3%)	41 59

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	AG	117	LYS
59	s	86	GLN

Continued on next page...

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Mol	Chain	Res	Type
16	AG	210	ARG
39	Y	44	LYS
16	AG	361	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
26	L	3	HIS
54	n	5	HIS
27	M	68	ASN
45	e	31	GLN
62	v	45	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	75/76 (98%)	29 (38%)	8 (10%)
10	B	75/76 (98%)	29 (38%)	8 (10%)
18	D	1514/1542 (98%)	289 (19%)	20 (1%)
41	a	2859/2904 (98%)	508 (17%)	0
44	d	119/120 (99%)	15 (12%)	0
8	7	36/41 (87%)	26 (72%)	5 (13%)
All	All	4678/4759 (98%)	896 (19%)	41 (0%)

5 of 896 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	3	G
8	7	4	U
8	7	5	U
8	7	7	U
8	7	8	U

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
18	D	517	G
18	D	1213	A
18	D	991	U
18	D	1196	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	D	1447	A

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 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.

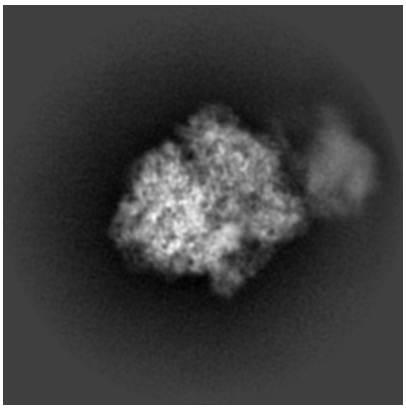
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42474. These allow visual inspection of the internal detail of the map and identification of artifacts.

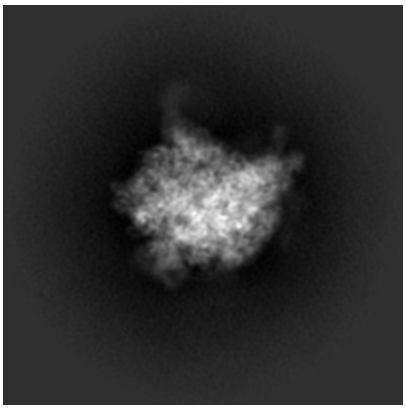
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

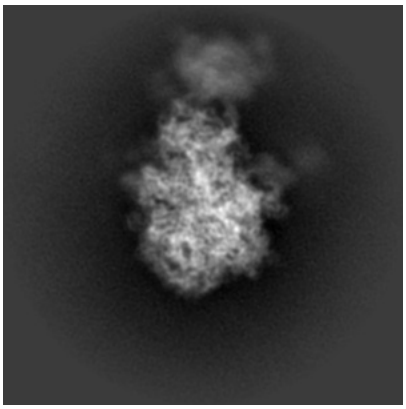
6.1.1 Primary map



X

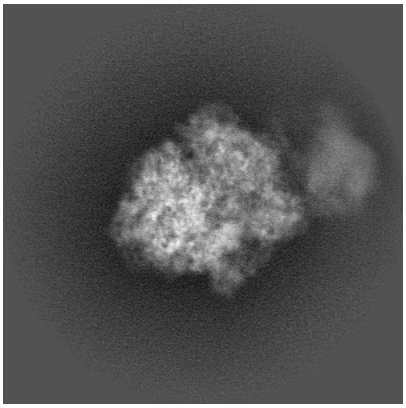


Y

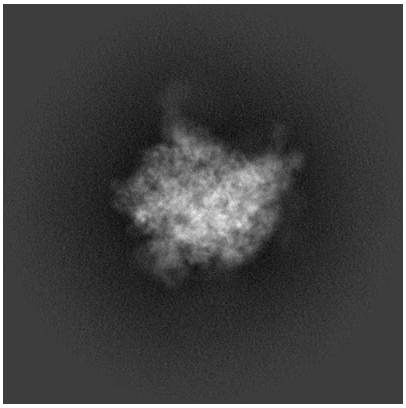


Z

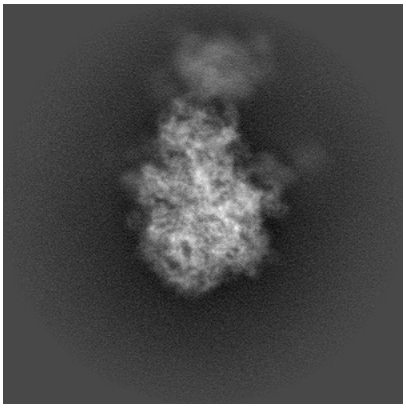
6.1.2 Raw map



X



Y

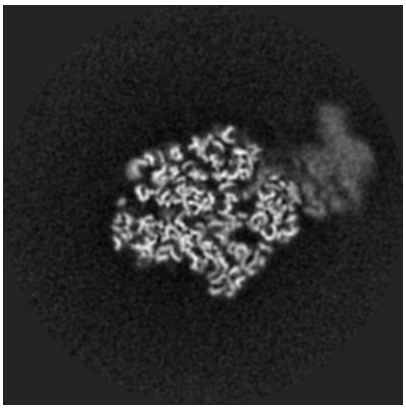


Z

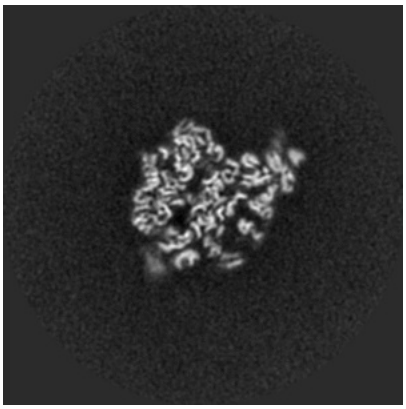
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

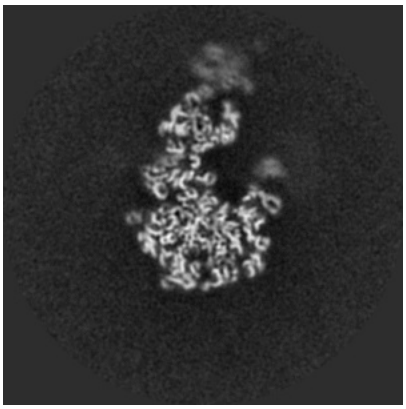
6.2.1 Primary map



X Index: 256

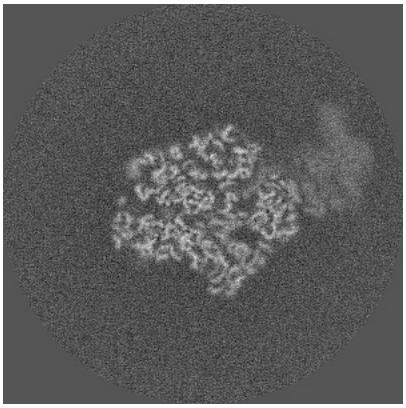


Y Index: 256

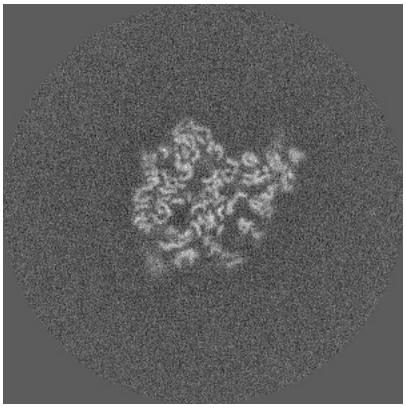


Z Index: 256

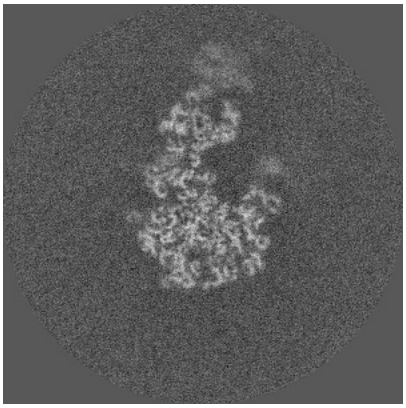
6.2.2 Raw map



X Index: 256



Y Index: 256

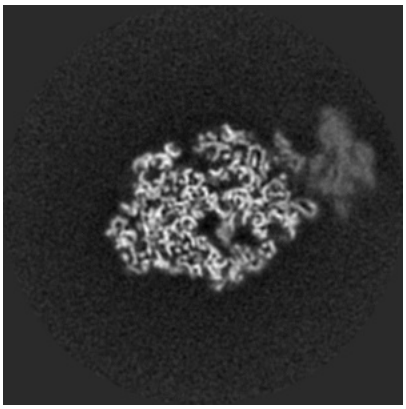


Z Index: 256

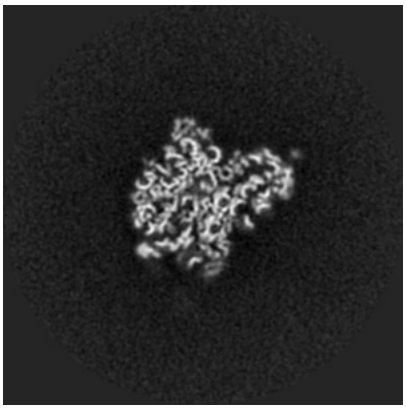
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

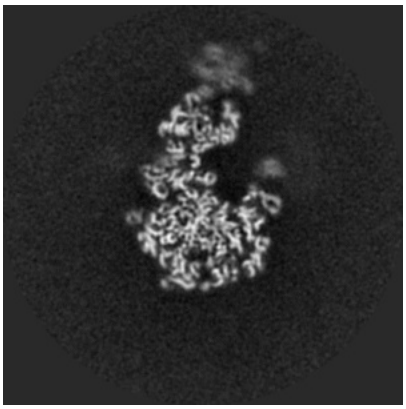
6.3.1 Primary map



X Index: 245

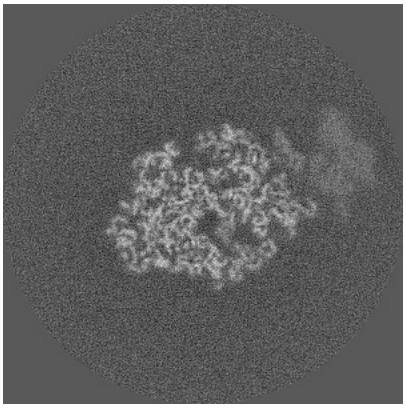


Y Index: 248

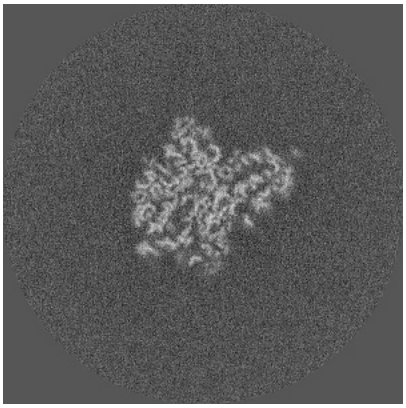


Z Index: 257

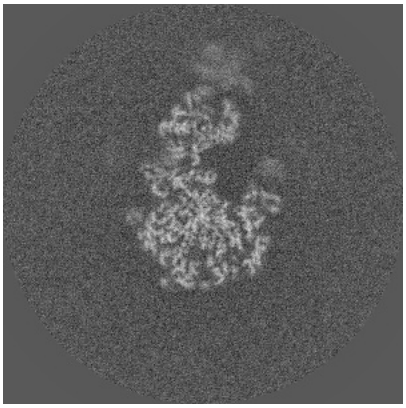
6.3.2 Raw map



X Index: 244



Y Index: 249

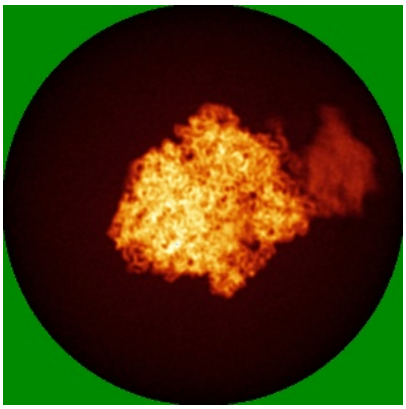


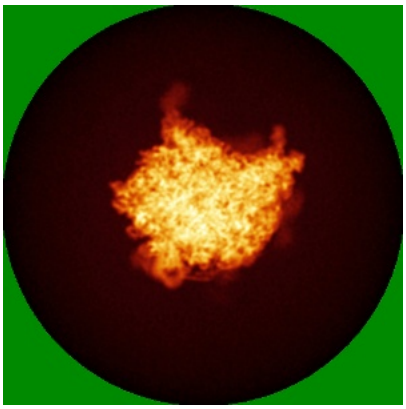
Z Index: 258

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

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

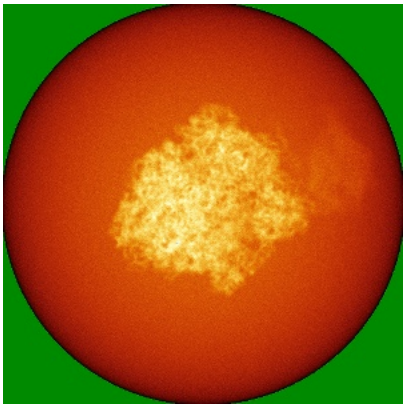
6.4.1 Primary map

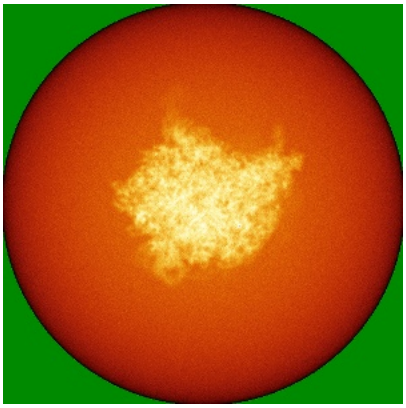

X

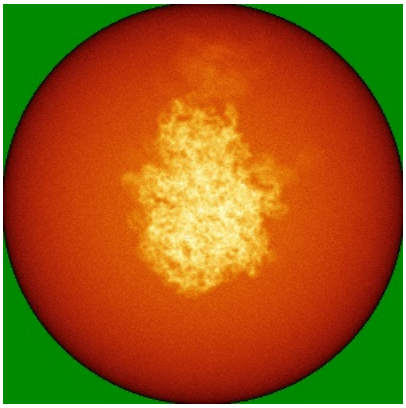

Y


Z

6.4.2 Raw map


X

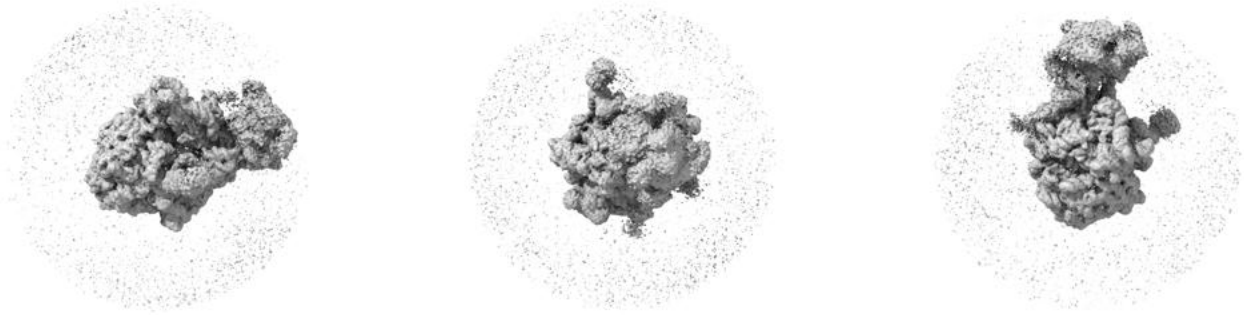

Y


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)

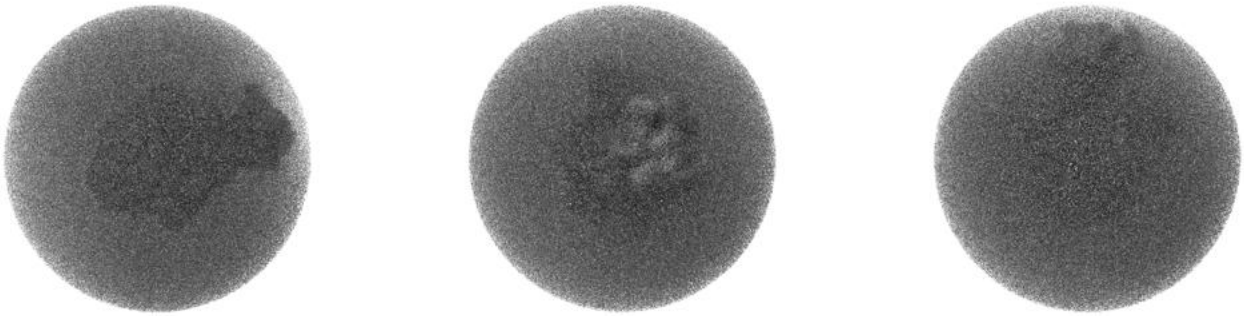
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0019. 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.

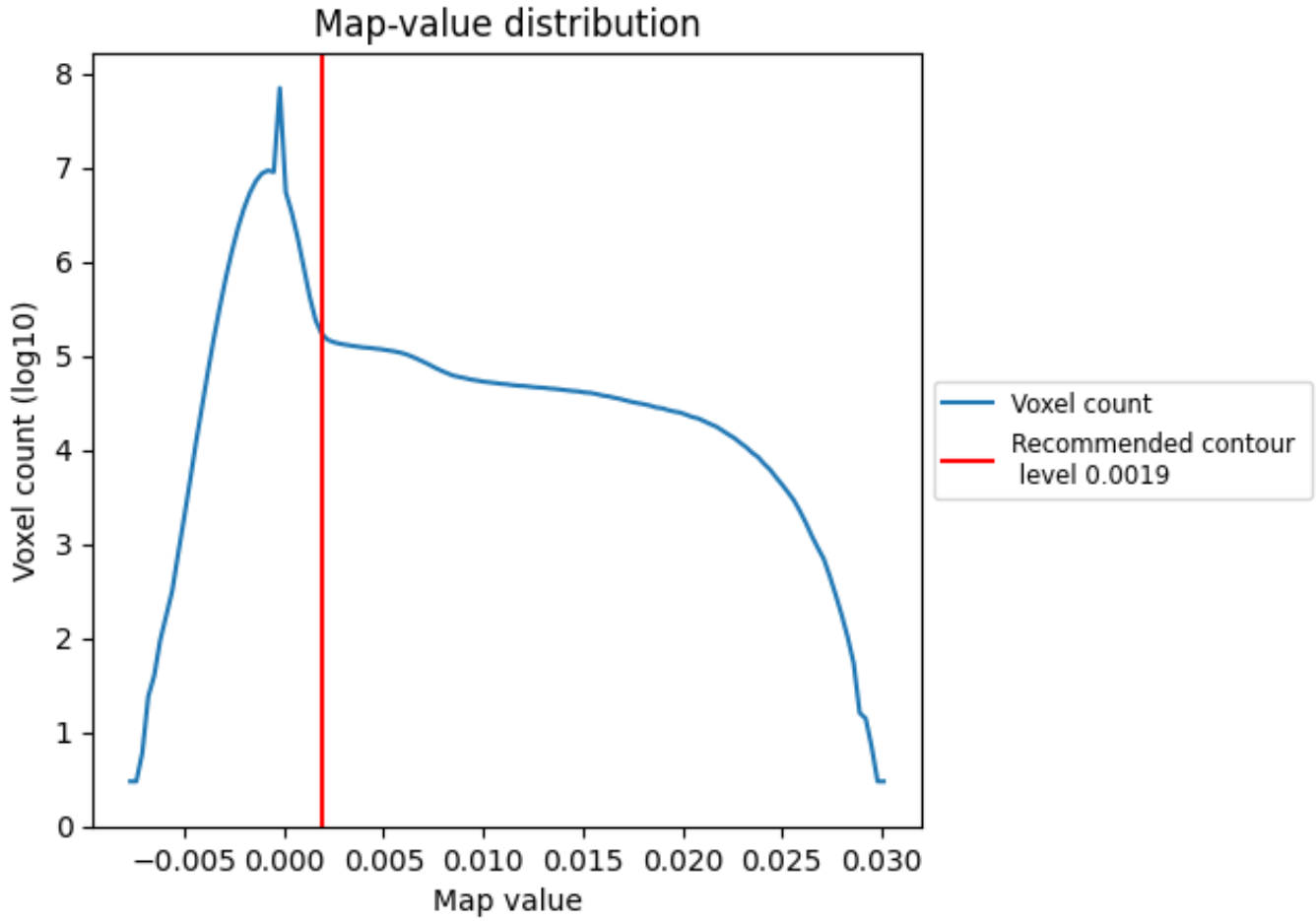
6.6 Mask visualisation (i)

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

7 Map analysis

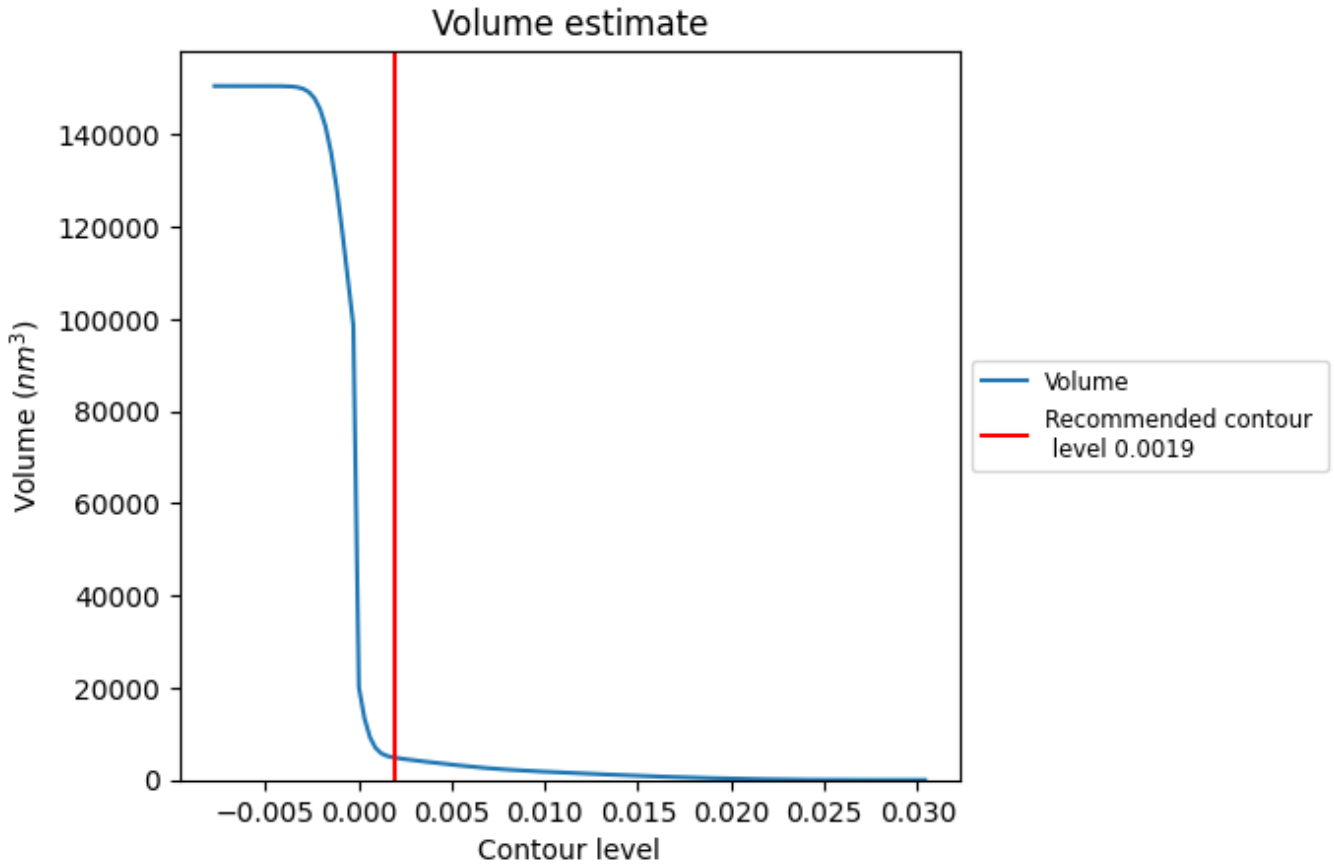
This section contains the results of statistical analysis of the map.

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.

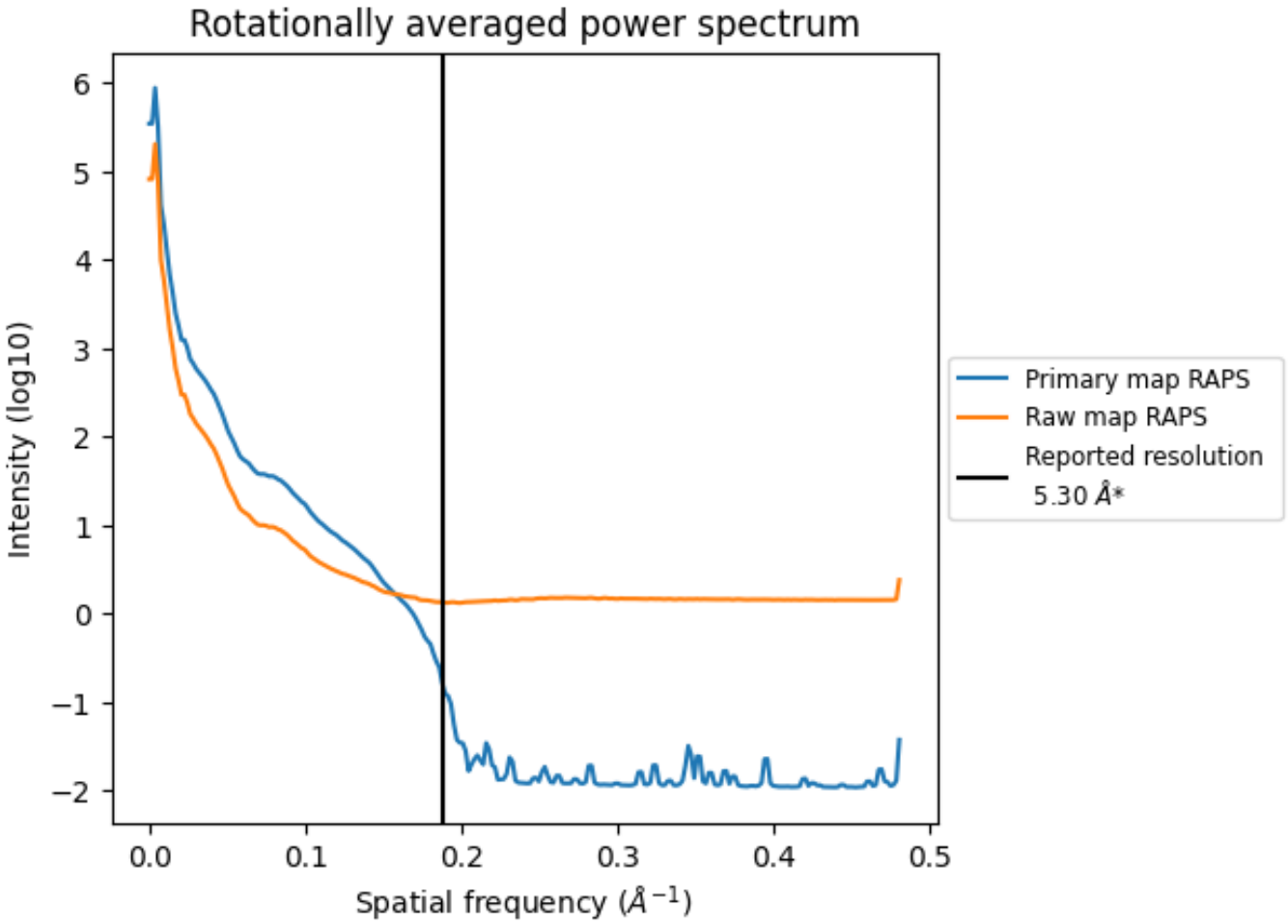
7.2 Volume estimate (i)



The volume at the recommended contour level is 4878 nm^3; this corresponds to an approximate mass of 4406 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)

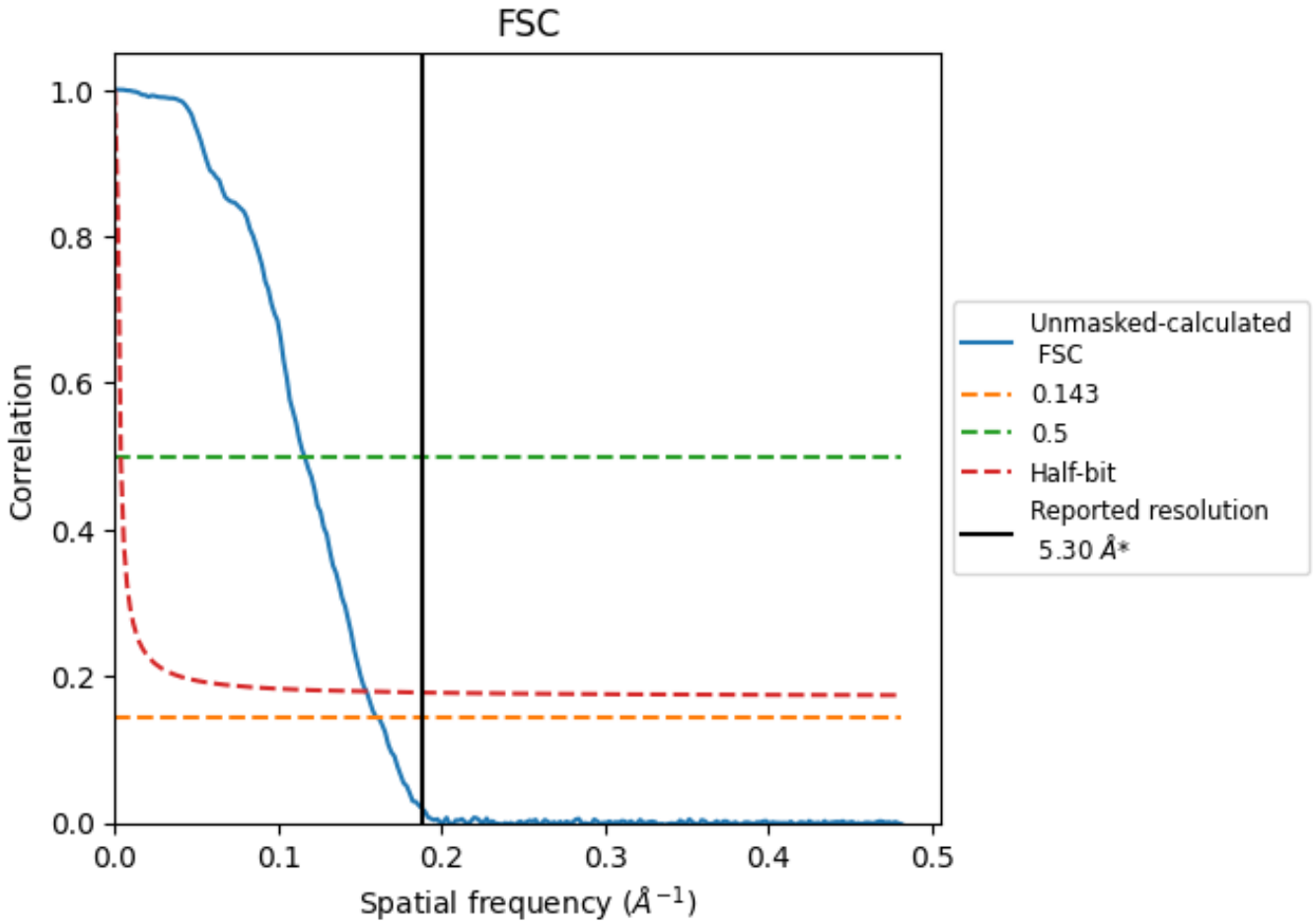


*Reported resolution corresponds to spatial frequency of 0.189 $Å^{-1}$

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 0.189 Å^{-1}

8.2 Resolution estimates (i)

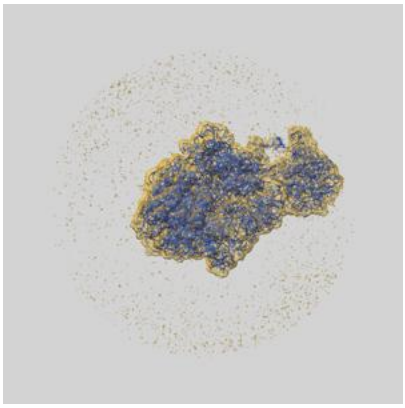
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.21	8.62	6.49

*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 6.21 differs from the reported value 5.3 by more than 10 %

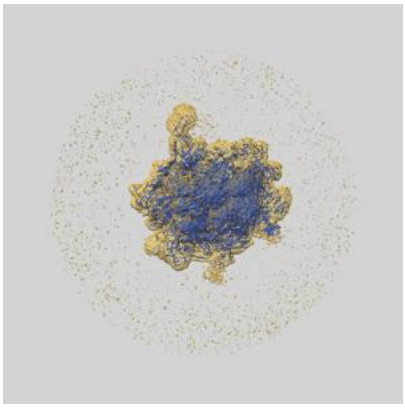
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42474 and PDB model 8UQM. Per-residue inclusion information can be found in section 3 on page 17.

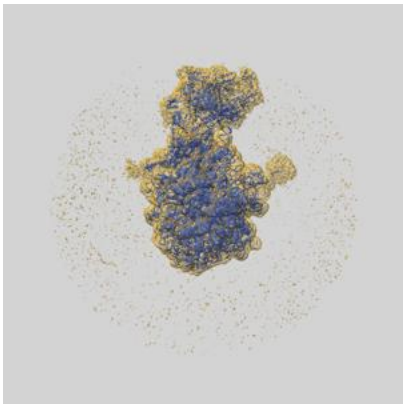
9.1 Map-model overlay



X



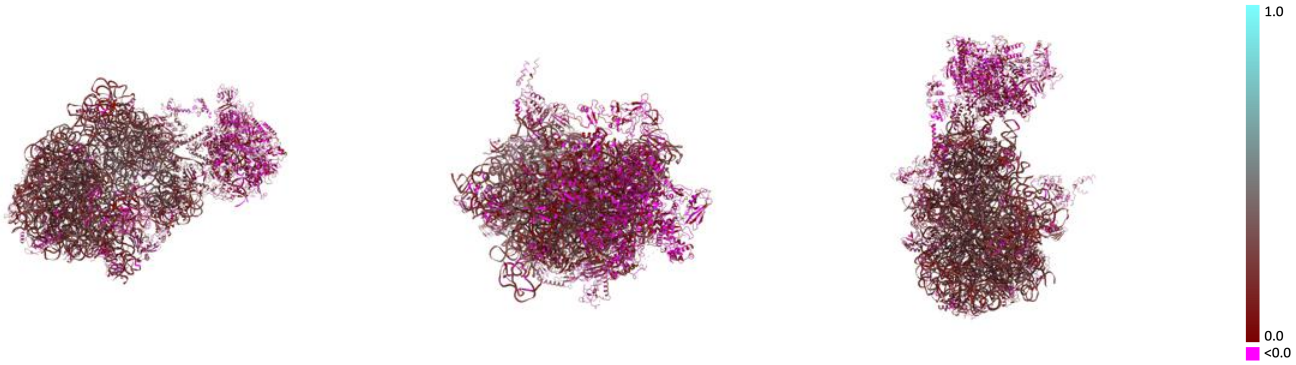
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

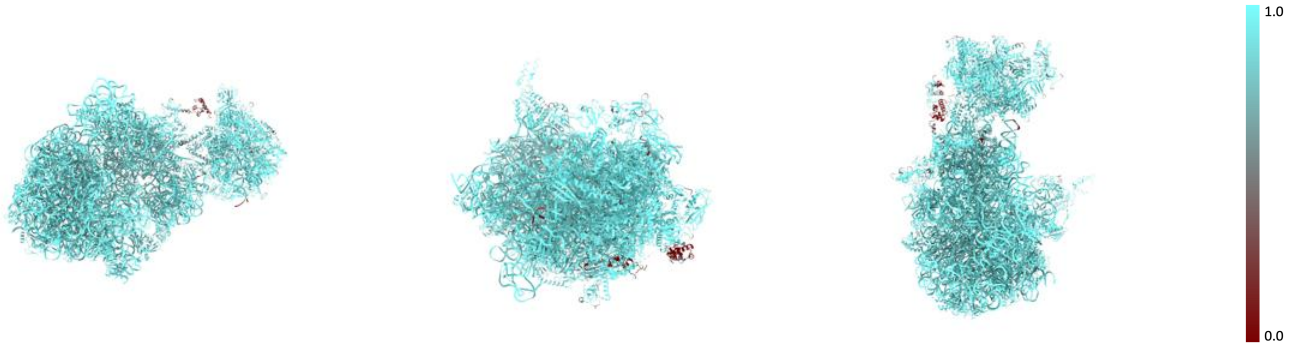
9.2 Q-score mapped to coordinate model



X Y Z

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

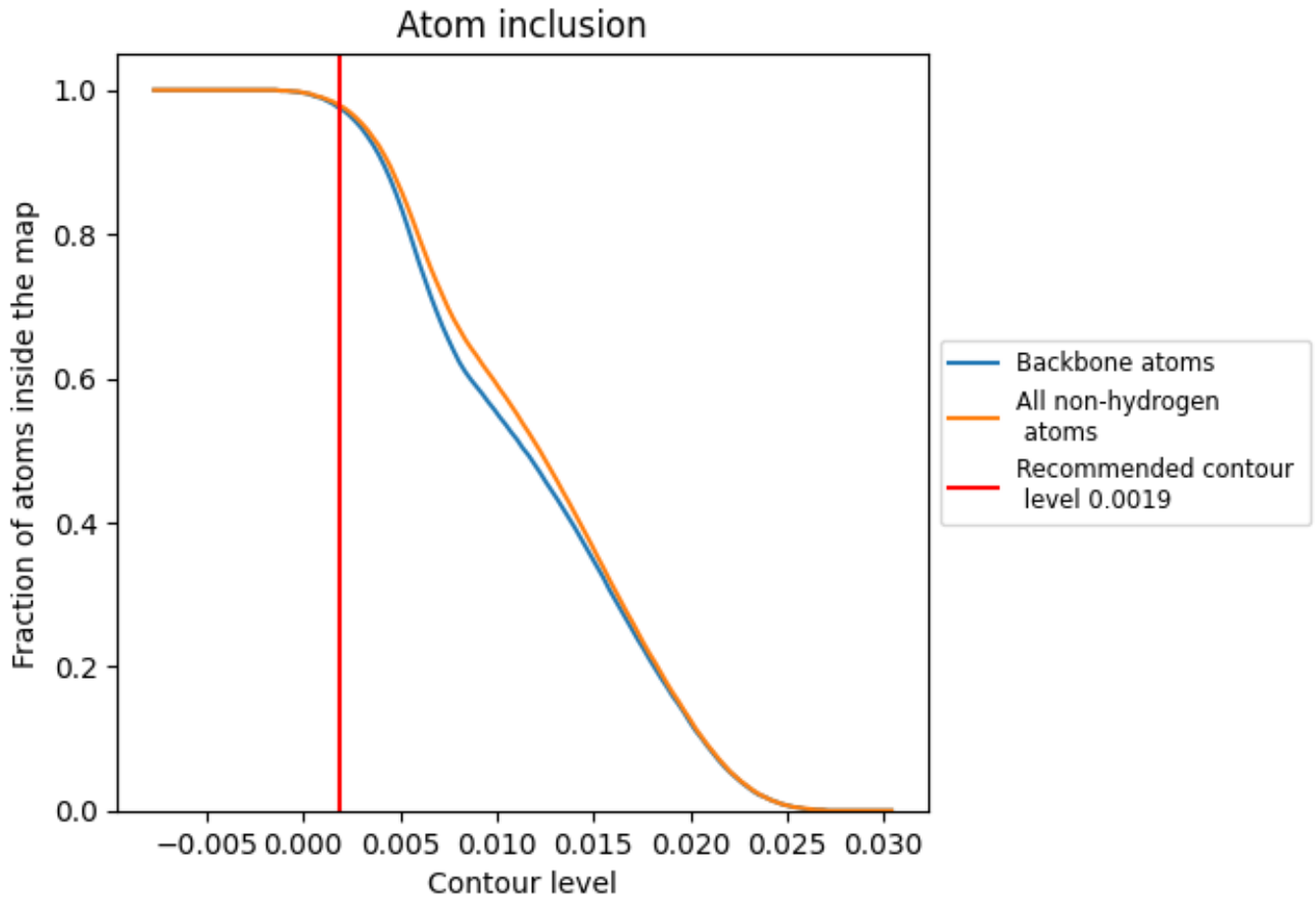
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0019).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 98% 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 (0.0019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9780	0.1740
0	0.9810	0.1530
1	0.9800	0.1790
2	0.9780	0.1490
3	0.9850	0.1330
4	0.9890	0.1570
5	0.8930	0.0610
6	0.9290	0.0700
7	0.9720	0.1090
9	0.9790	0.1000
A	0.9990	0.1900
AA	0.9770	0.0680
AB	0.9910	0.0890
AC	0.9870	0.0430
AD	0.8800	0.0530
AE	0.9670	0.0700
AF	0.8310	0.0770
AG	0.8160	0.1010
B	0.9540	0.1070
C	0.9940	0.1630
D	0.9980	0.2310
E	0.9910	0.1510
F	0.9790	0.1830
G	0.9690	0.1560
H	0.8700	0.0550
I	0.9790	0.1950
J	0.9920	0.1760
K	0.9950	0.2210
L	0.9920	0.1570
M	0.9900	0.1500
N	0.9780	0.1820
O	0.9870	0.1400
P	0.9860	0.1630
Q	0.9920	0.1620
R	0.9970	0.2230

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
S	0.9880	0.1630
T	0.9840	0.1590
U	0.9890	0.1670
V	0.9810	0.1740
W	0.9550	0.1120
X	0.9800	0.1400
Y	0.9170	0.0750
Z	1.0000	0.0220
a	0.9970	0.2170
b	0.9820	0.1350
c	0.9770	0.1630
d	0.9990	0.1810
e	0.9800	0.1280
f	0.9860	0.1660
g	0.9820	0.1030
h	0.9840	0.1620
i	0.9770	0.1880
j	0.9920	0.1680
k	0.9950	0.1450
l	0.9700	0.1340
m	0.9890	0.1710
n	0.9730	0.1220
o	0.9700	0.1310
p	0.9930	0.1540
q	0.9900	0.1570
r	0.9410	0.1140
s	0.9810	0.1790
t	0.9770	0.1910
u	0.9880	0.1440
v	0.9840	0.1890
w	0.9780	0.1670
x	0.9760	0.0960
y	0.9800	0.1750
z	0.9860	0.1440