



## wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 10:49 AM EDT

PDB ID : 8URY  
EMDB ID : EMD-42504  
Title : Escherichia coli transcription-translation coupled complex class B (TTC-B) containing RfaH bound to ops signal, NusA, mRNA with a 30 nt long spacer, and fMet-tRNA in E-site and P-site of the ribosome  
Authors : Molodtsov, V.; Wang, C.; Ebright, R.H.  
Deposited on : 2023-10-27  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

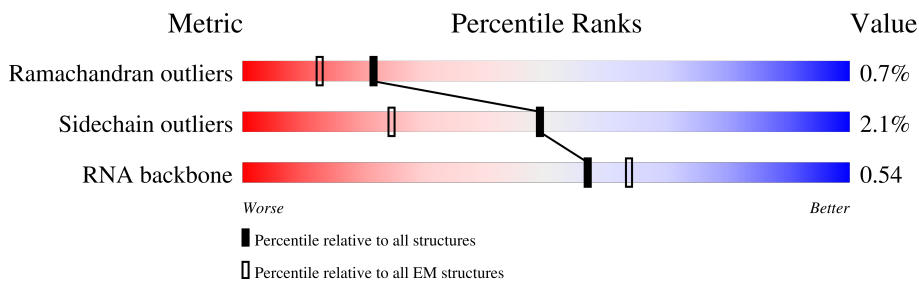
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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.



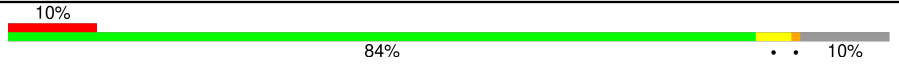


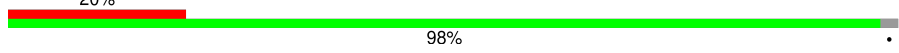



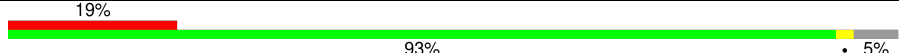
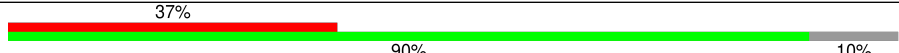
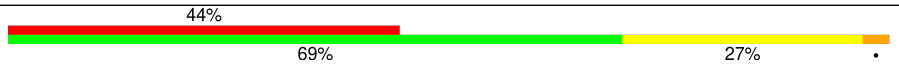


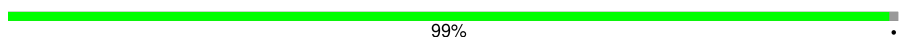
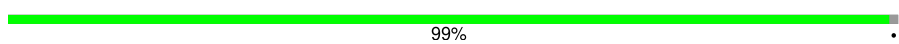


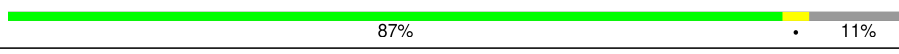
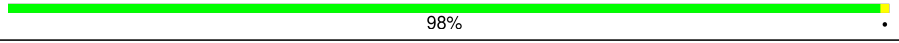
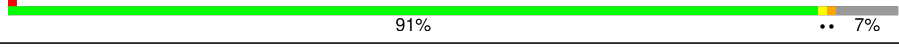
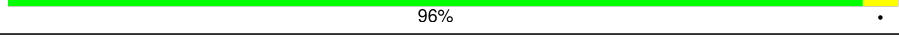

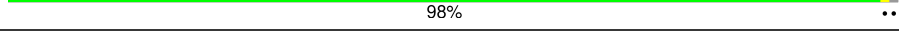
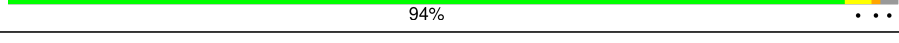
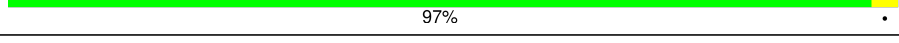
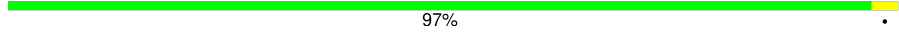
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	0	103	
2	1	110	
3	2	100	
4	3	104	
5	4	94	
6	5	38	
7	6	38	
8	7	47	

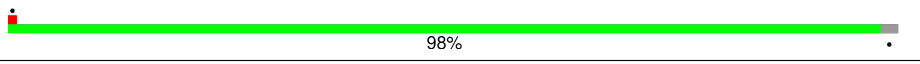
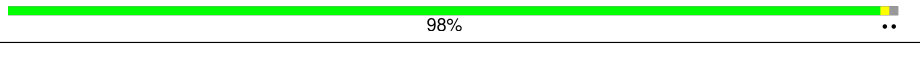
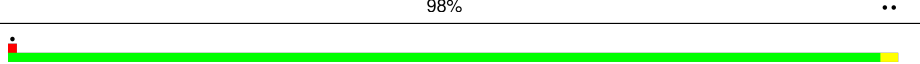
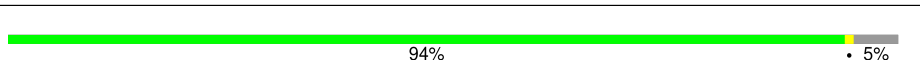

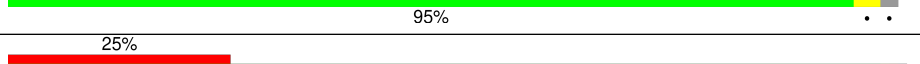
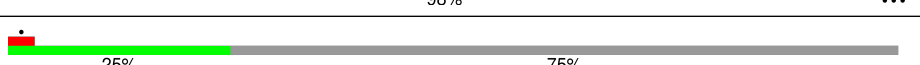

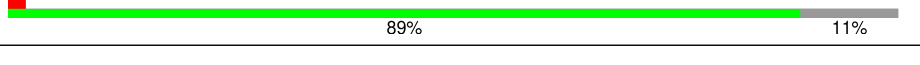
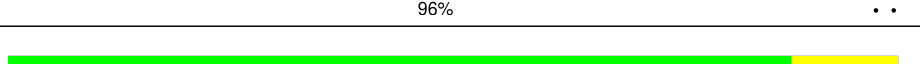
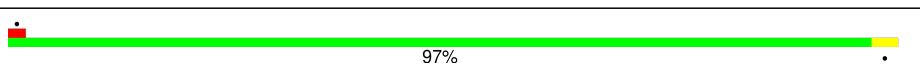
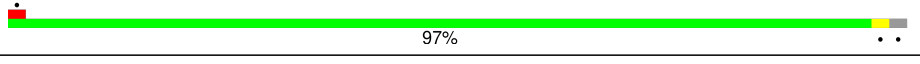
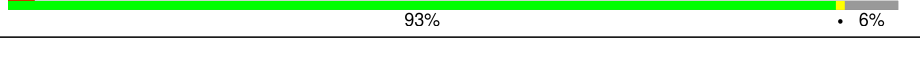
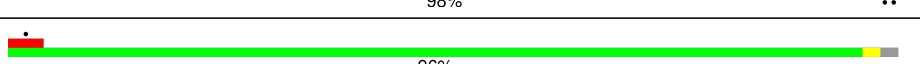
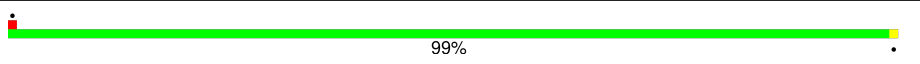
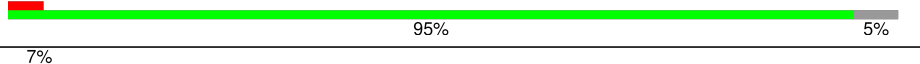
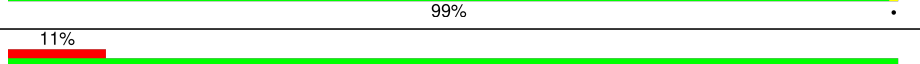
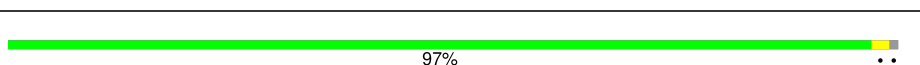
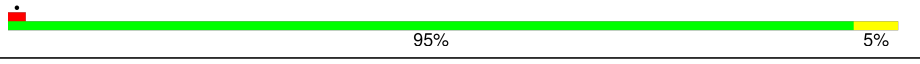
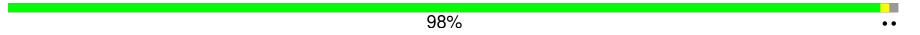



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Mol	Chain	Length	Quality of chain
9	9	165	
10	A	76	
10	B	76	
11	AA	1342	
12	AB	162	
13	AC	329	
13	AD	329	
14	AE	1407	
15	AF	91	
16	AG	495	
17	C	75	
18	D	1542	
19	E	87	
20	F	71	
21	G	241	
22	H	557	
23	I	233	
24	J	206	
25	K	167	
26	L	104	
27	M	179	
28	N	130	
29	O	130	
30	P	99	
31	Q	117	

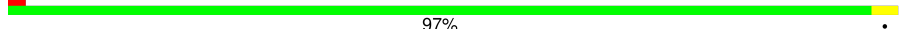
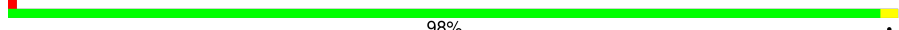

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Mol	Chain	Length	Quality of chain
32	R	124	 98%
33	S	101	 98%
34	T	89	 98%
35	U	82	 98%
36	V	84	 94% 5%
37	W	92	 87% 10%
38	X	118	 95%
39	Y	142	 25% 98%
40	Z	121	 25% 75%
41	a	2904	 80% 19%
42	b	85	 89% 11%
43	c	78	 96%
44	d	120	 88% 12%
45	e	62	 97%
46	f	59	 97%
47	g	70	 93% 6%
48	h	273	 98%
49	i	57	 96%
50	j	209	 99%
51	k	55	 95% 5%
52	l	201	 7% 99%
53	m	46	 11% 100%
54	n	179	 97%
55	o	64	95% 5%
56	p	177	98%

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Mol	Chain	Length	Quality of chain
57	q	38	 100%
58	r	149	 5% 100%
59	s	142	 97% ..
60	t	123	 97% .
61	u	144	 98% .
62	v	136	 99% .
63	w	127	 89% 5% 6%
64	x	117	 99% .
65	y	115	 97% ..
66	z	118	 97% ..

## 2 Entry composition [i](#)

There are 68 unique types of molecules in this entry. The entry contains 280292 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 50S ribosomal protein L21.

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

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

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

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

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

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

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

- Molecule 5 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 6 is a DNA chain called NT DNA ops.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	5	35	726	342	141	208	35	0	0

- Molecule 7 is a DNA chain called T DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	35	Total	C	N	O	P	0	0
			703	336	117	215	35		

- Molecule 8 is a RNA chain called mRNA with 30 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
			Total	C	N	O	S		
13	AD	299	2078	1287	378	407	6	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- 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 Small ribosomal subunit protein bS1.

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	
			Total	C	H	N	O			S
27	M	151	2416	735	1235	227	215	4	0	0

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

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

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

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

- Molecule 30 is a protein called Small ribosomal subunit protein uS10.

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

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

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

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

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

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

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

- 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
			Total	C	H	N	O	P		
41	a	2880	92918	27587	31077	11398	19976	2880	0	0

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 Large ribosomal subunit protein bL27.

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

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

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

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

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL29.

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

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

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

- Molecule 47 is a protein called Large ribosomal subunit protein bL31.

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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 Large ribosomal subunit protein bL35.

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 Large ribosomal subunit protein uL13.

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 Large ribosomal subunit protein bL19.

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).

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
68	AE	2	Total 2	Zn 2	0



### 3 Residue-property plots

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

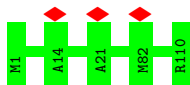
- Molecule 1: 50S ribosomal protein L21

Chain 0:  100%

There are no outlier residues recorded for this chain.

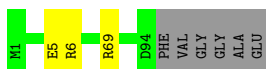
- Molecule 2: 50S ribosomal protein L22

Chain 1:  100%



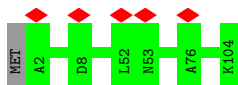
- Molecule 3: 50S ribosomal protein L23

Chain 2:  91% 6%



- Molecule 4: 50S ribosomal protein L24

Chain 3:  5% 99%

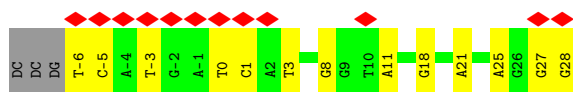


- Molecule 5: Large ribosomal subunit protein bL25

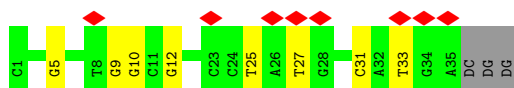
Chain 4:  98%



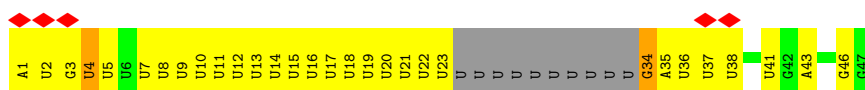
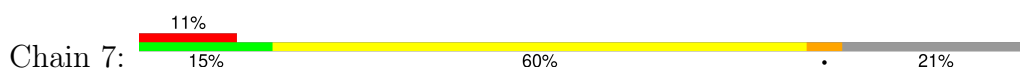
- Molecule 6: NT DNA ops



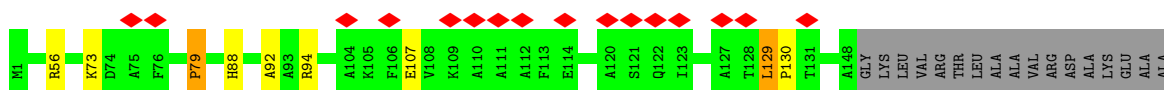
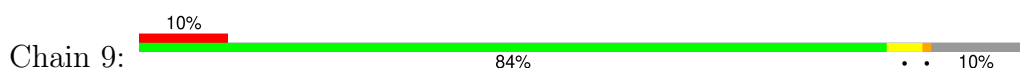
• Molecule 7: T DNA



• Molecule 8: mRNA with 30 nt long spacer



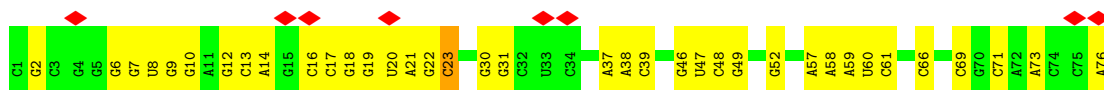
• Molecule 9: 50S ribosomal protein L10



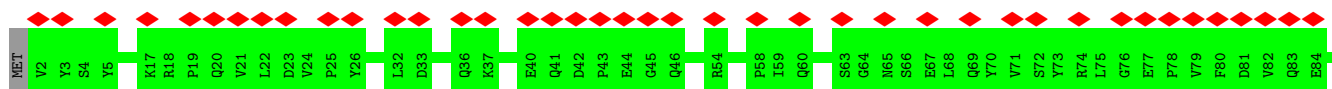
• Molecule 10: E-site and P-site fMet-tRNA

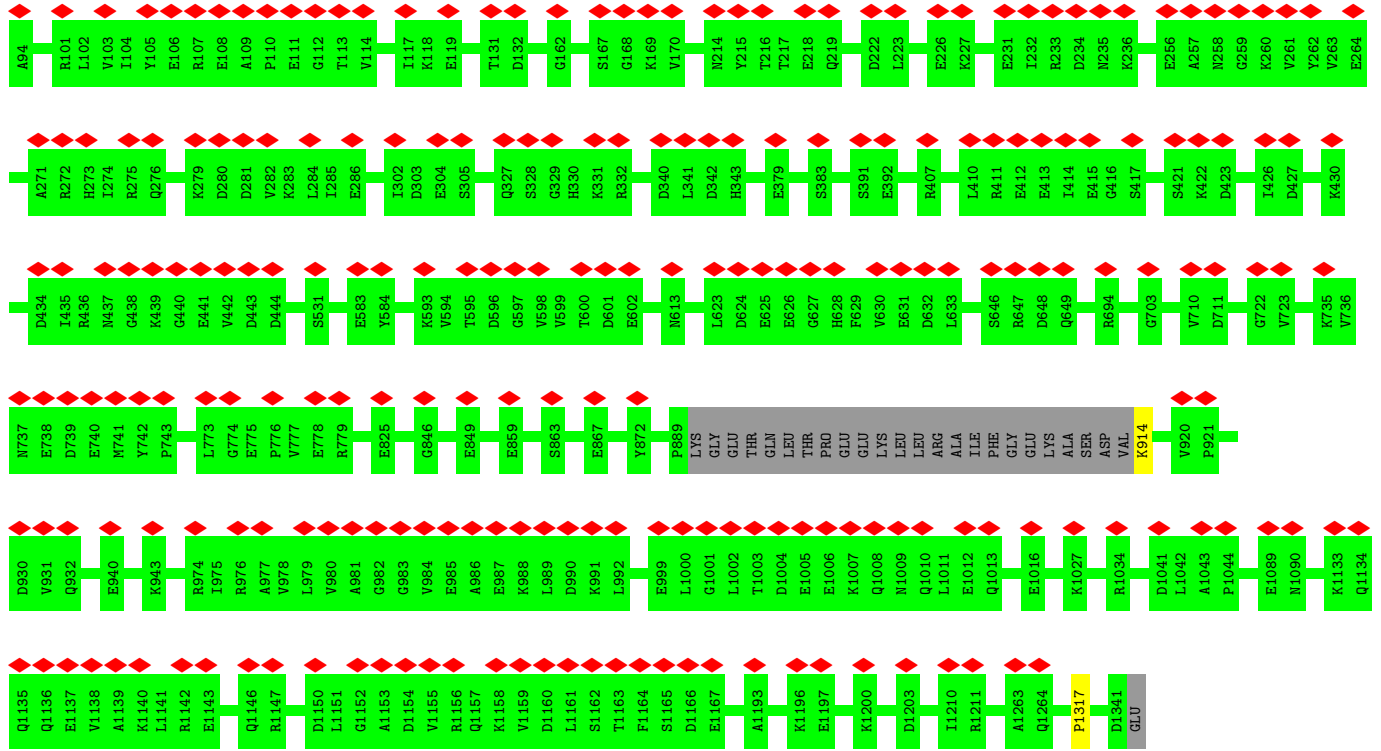


• Molecule 10: E-site and P-site fMet-tRNA

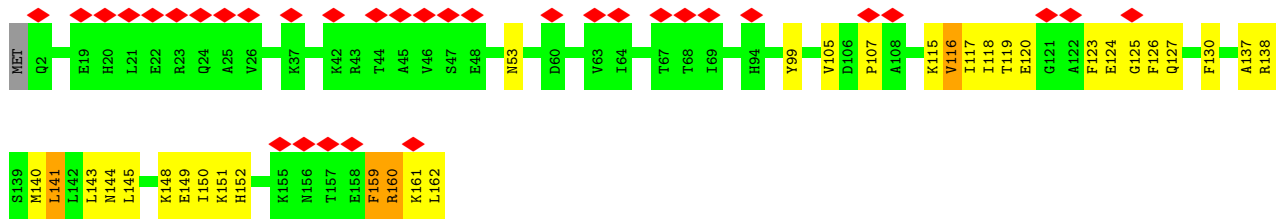
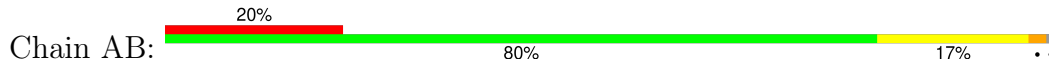


• Molecule 11: DNA-directed RNA polymerase subunit beta

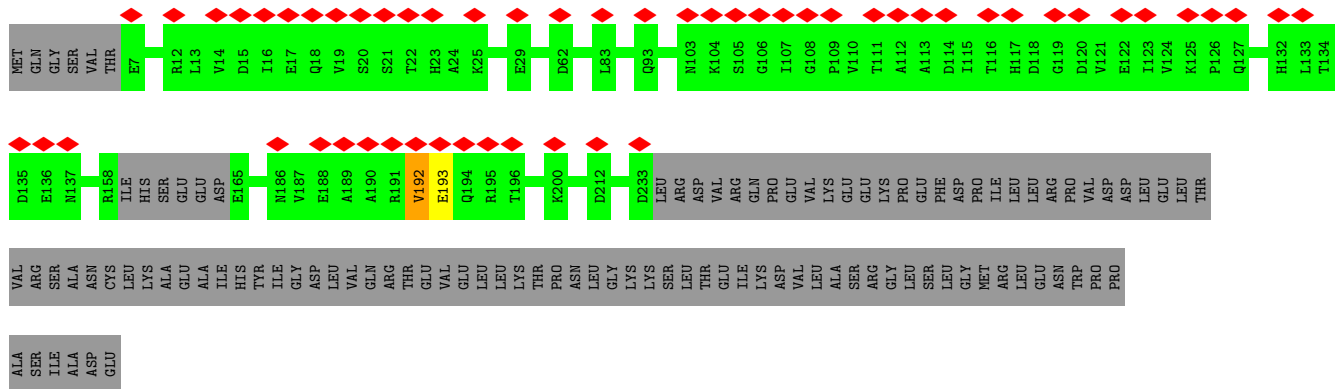




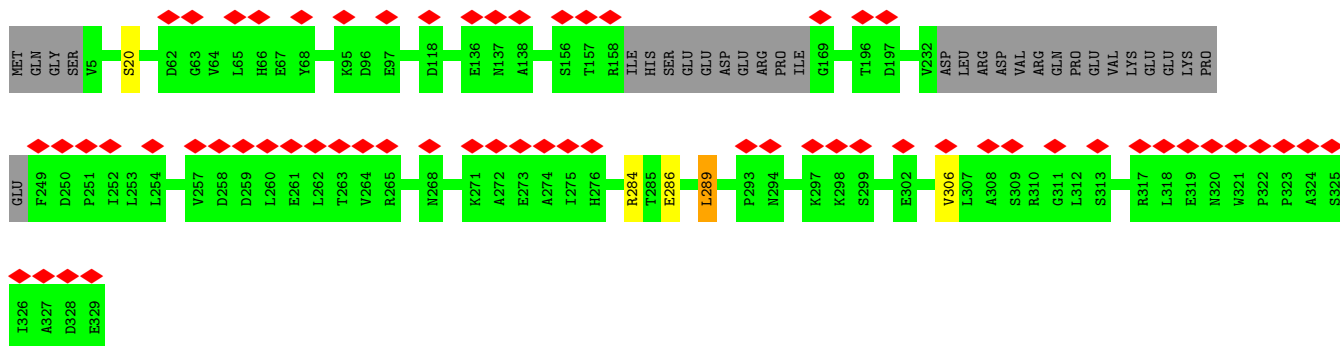
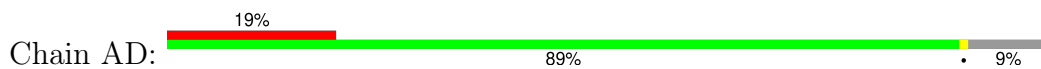
● Molecule 12: Transcription antitermination protein RfaH



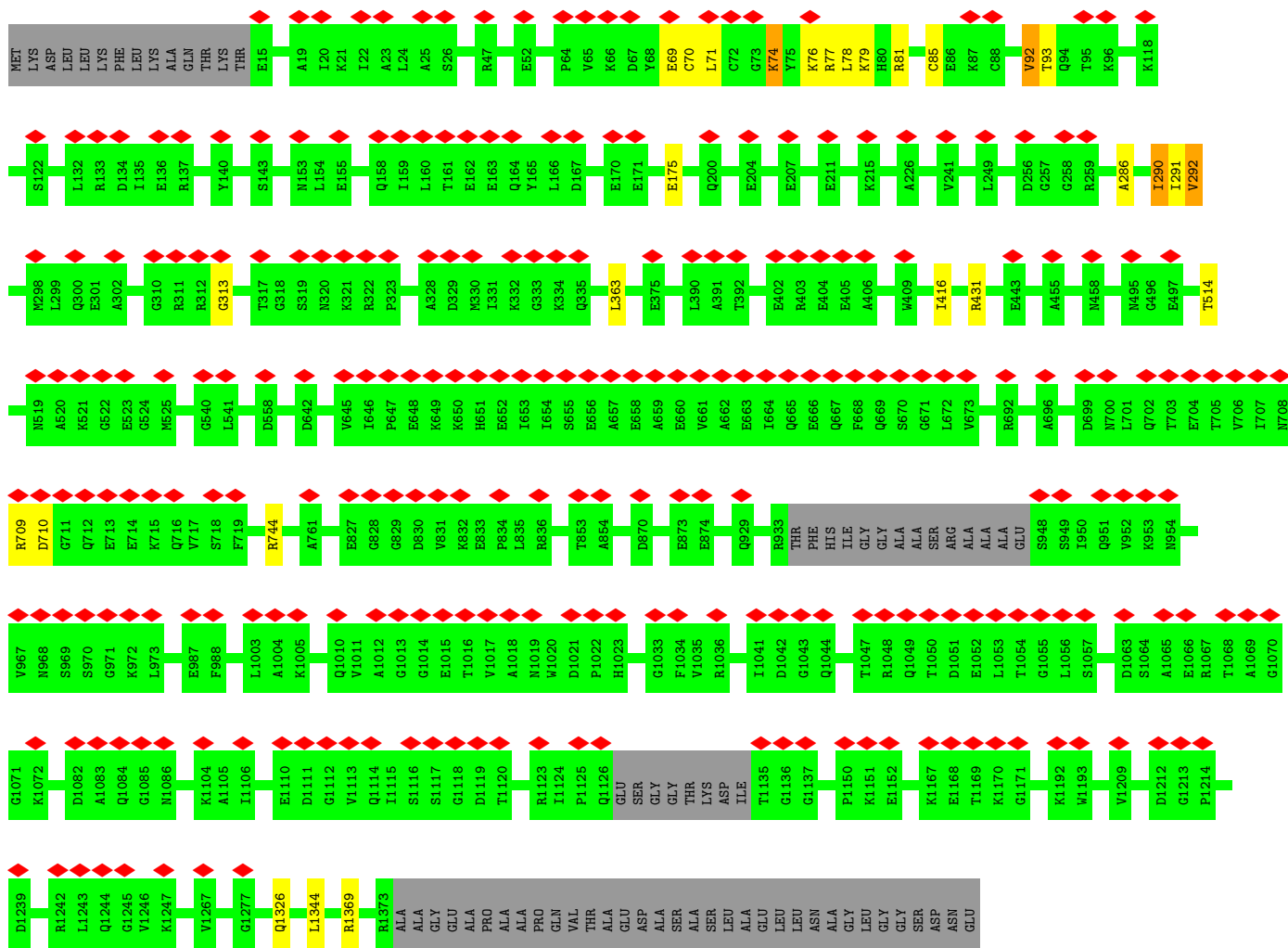
● Molecule 13: DNA-directed RNA polymerase subunit alpha



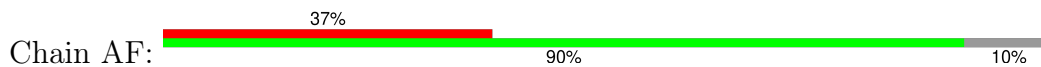
● Molecule 13: DNA-directed RNA polymerase subunit alpha

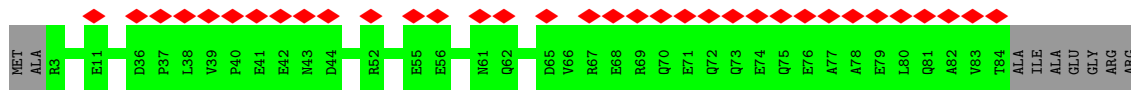


• Molecule 14: DNA-directed RNA polymerase subunit beta'

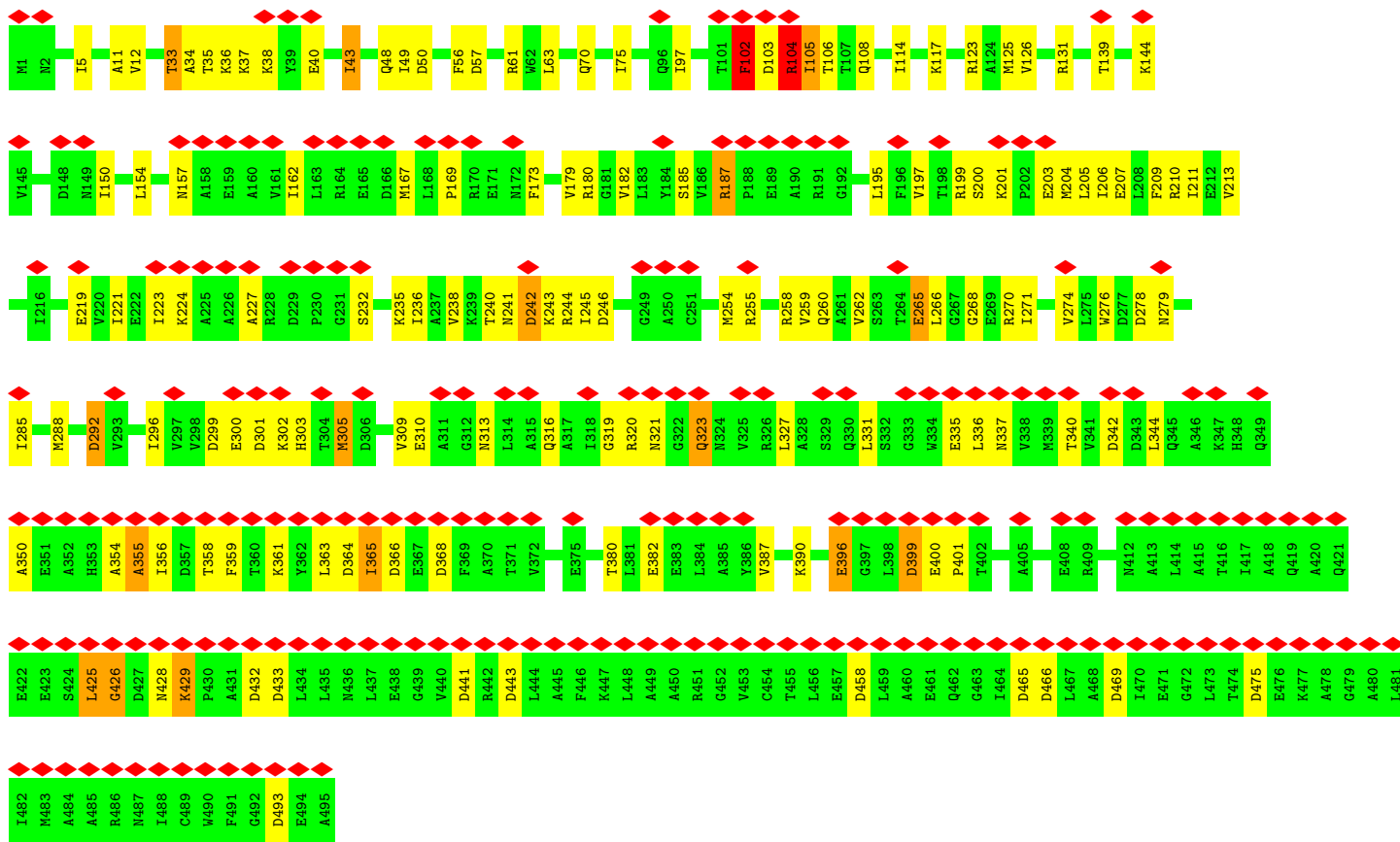
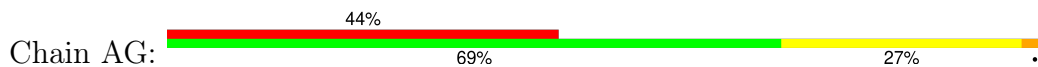


• Molecule 15: DNA-directed RNA polymerase subunit omega

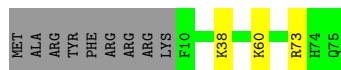
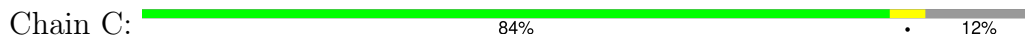




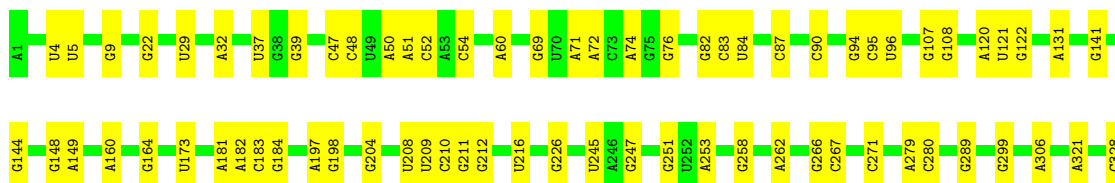
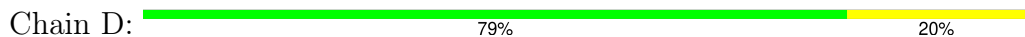
• Molecule 16: Transcription termination/antitermination protein NusA

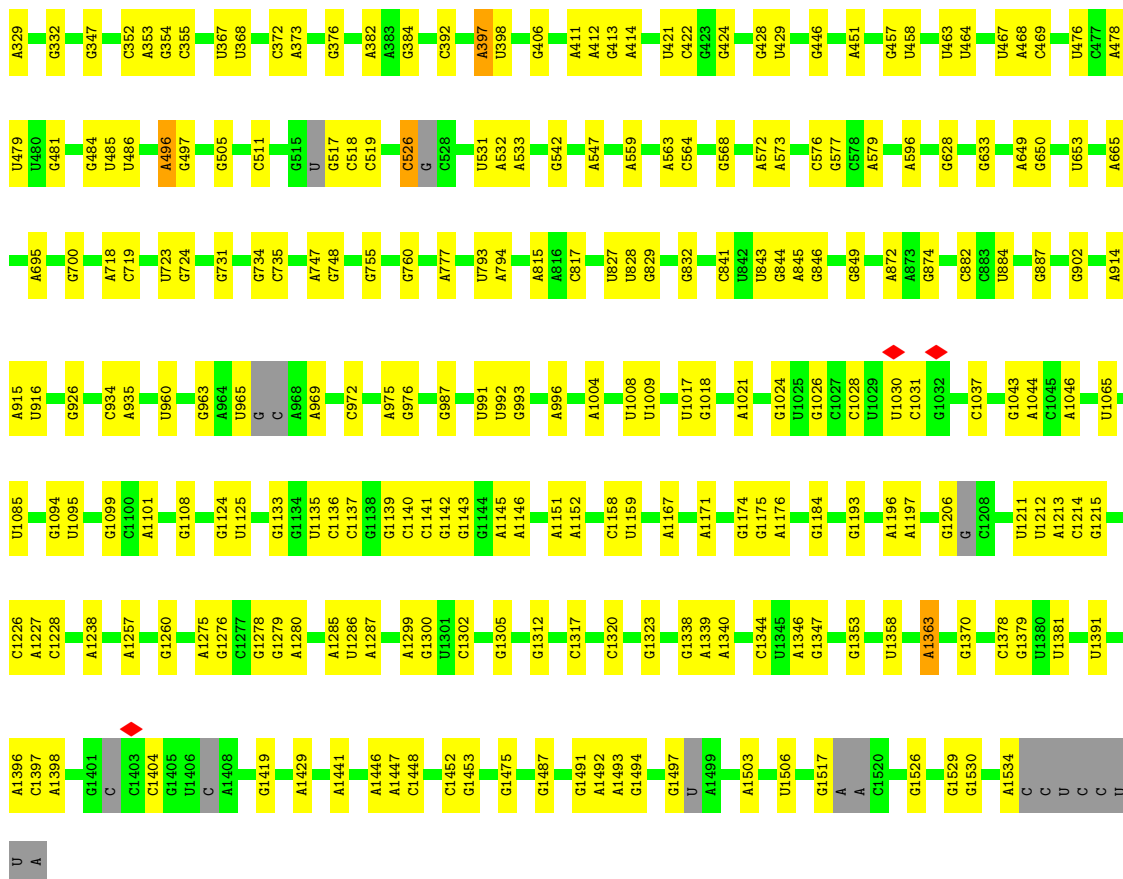


• Molecule 17: 30S ribosomal protein S18



• Molecule 18: 16S rRNA





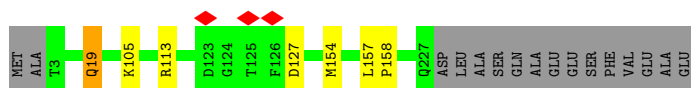
- Molecule 19: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S21



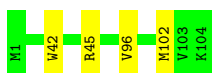
- Molecule 21: 30S ribosomal protein S2




- Molecule 22: Small ribosomal subunit protein bS1

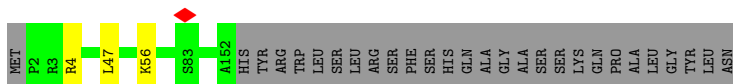


Chain L:  96%



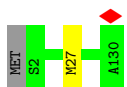
- Molecule 27: 30S ribosomal protein S7

Chain M:  83% 16%



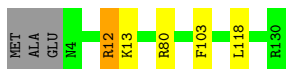
- Molecule 28: 30S ribosomal protein S8

Chain N:  98%



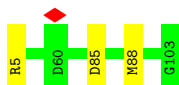
- Molecule 29: 30S ribosomal protein S9

Chain O:  94%



- Molecule 30: Small ribosomal subunit protein uS10

Chain P:  97%



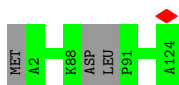
- Molecule 31: 30S ribosomal protein S11

Chain Q:  97%



- Molecule 32: 30S ribosomal protein S12

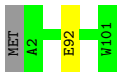
Chain R:  98%





- Molecule 33: 30S ribosomal protein S14

Chain S:  98% ..



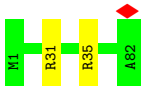
- Molecule 34: 30S ribosomal protein S15

Chain T:  98% ..



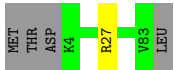
- Molecule 35: 30S ribosomal protein S16

Chain U:  98% .




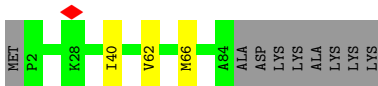
- Molecule 36: 30S ribosomal protein S17

Chain V:  94% • 5%



- Molecule 37: 30S ribosomal protein S19

Chain W:  87% • 10%



- Molecule 38: 30S ribosomal protein S13

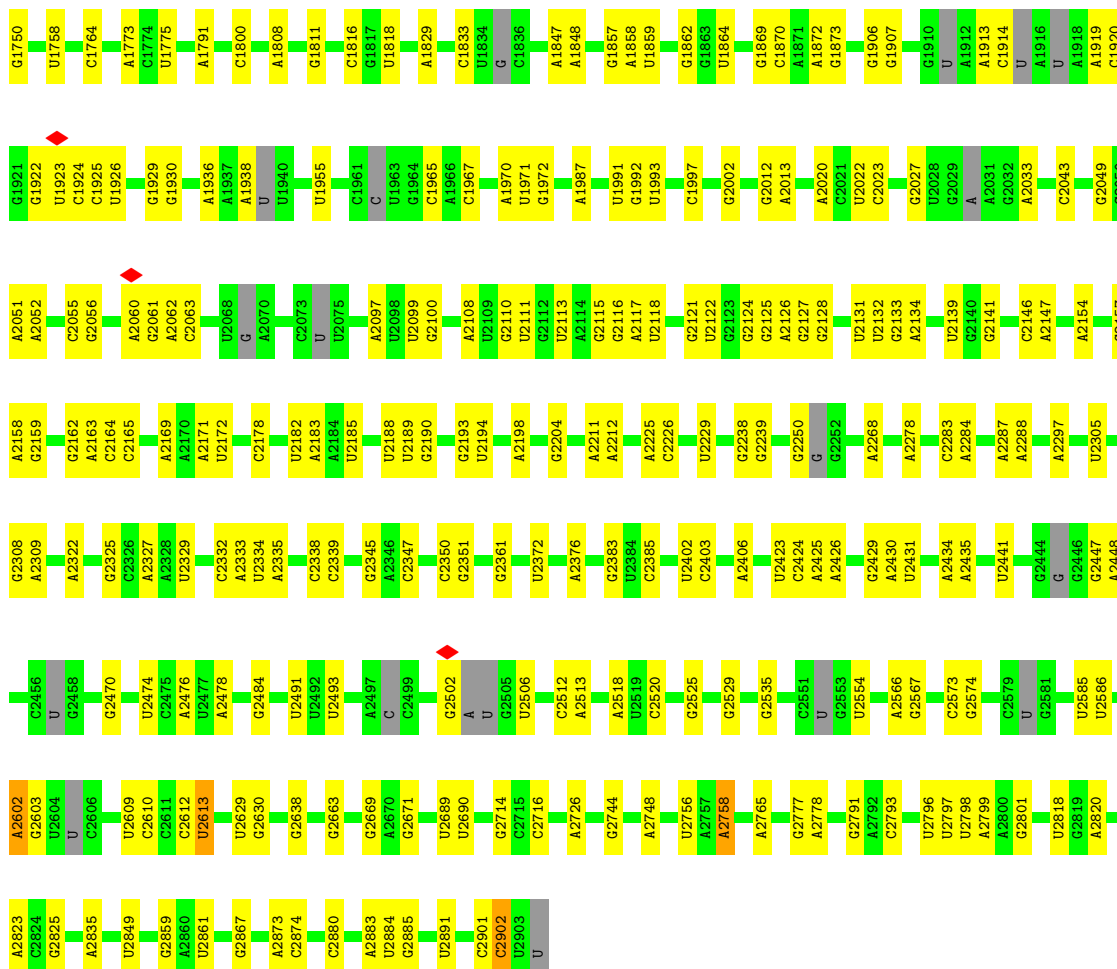
Chain X:  95% ..



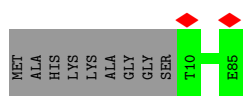
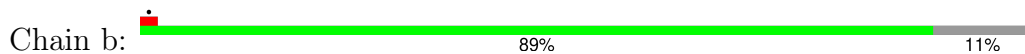
- Molecule 39: 50S ribosomal protein L11

Chain Y:  25% 98% ...





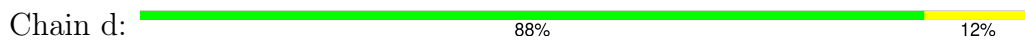
• Molecule 42: Large ribosomal subunit protein bL27



• Molecule 43: 50S ribosomal protein L28



• Molecule 44: 5S rRNA



- Molecule 45: Large ribosomal subunit protein uL29

Chain e:  97%



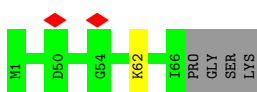
- Molecule 46: 50S ribosomal protein L30

Chain f:  97%



- Molecule 47: Large ribosomal subunit protein bL31

Chain g:  93% • 6%



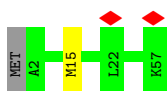
- Molecule 48: 50S ribosomal protein L2

Chain h:  98%



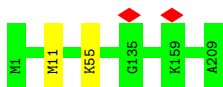
- Molecule 49: 50S ribosomal protein L32

Chain i:  96%



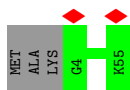
- Molecule 50: 50S ribosomal protein L3

Chain j:  99%

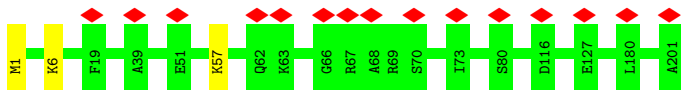


- Molecule 51: 50S ribosomal protein L33

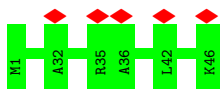
Chain k:  95% 5%



- Molecule 52: 50S ribosomal protein L4



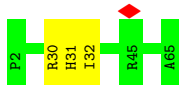
- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L5



- Molecule 55: Large ribosomal subunit protein bL35



- Molecule 56: 50S ribosomal protein L6



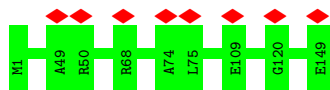
- Molecule 57: 50S ribosomal protein L36



There are no outlier residues recorded for this chain.

- Molecule 58: 50S ribosomal protein L9





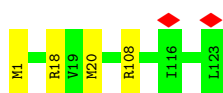
- Molecule 59: Large ribosomal subunit protein uL13

Chain s: 97%



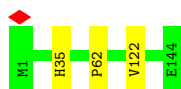
- Molecule 60: 50S ribosomal protein L14

Chain t: 97%



- Molecule 61: 50S ribosomal protein L15

Chain u: 98%



- Molecule 62: 50S ribosomal protein L16

Chain v: 99%



- Molecule 63: 50S ribosomal protein L17

Chain w: 89% 5% 6%



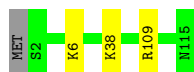
- Molecule 64: 50S ribosomal protein L18

Chain x: 99%



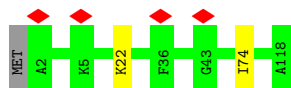
- Molecule 65: Large ribosomal subunit protein bL19

Chain y:  97% ..



- Molecule 66: 50S ribosomal protein L20

Chain z:  97% ..



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12096	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.056	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0048	Depositor
Map size ( $\text{\AA}$ )	563.2, 563.2, 563.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0, 1.0, 1.0	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: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	0	0.47	0/829	0.61	0/1107
2	1	0.58	0/864	0.69	0/1156
3	2	0.67	1/752 (0.1%)	0.72	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	1.14	11/816 (1.3%)	1.13	2/1259 (0.2%)
7	6	1.12	8/783 (1.0%)	1.10	0/1203
8	7	0.53	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	12/2821 (0.4%)
11	AA	0.43	0/10547	0.61	0/14232
12	AB	0.47	0/1317	0.86	5/1786 (0.3%)
13	AC	0.41	0/1718	0.62	0/2328
13	AD	0.37	0/2096	0.62	1/2854 (0.0%)
14	AE	0.42	0/10561	0.63	3/14258 (0.0%)
15	AF	0.34	0/652	0.57	0/879
16	AG	0.66	2/3897 (0.1%)	0.89	31/5273 (0.6%)
17	C	0.70	0/553	0.92	4/743 (0.5%)
18	D	0.59	14/36610 (0.0%)	1.03	67/57091 (0.1%)
19	E	0.57	0/675	0.71	0/895
20	F	0.62	0/597	0.59	0/792
21	G	0.66	2/1791 (0.1%)	0.83	7/2413 (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	0.68	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	0.57	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	134/107985 (0.1%)
42	b	0.47	0/589	0.57	0/779
43	c	0.56	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	0.71	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	0.86	1/676 (0.1%)
56	p	0.50	0/1333	0.68	3/1805 (0.2%)
57	q	0.46	0/303	0.61	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	0.62	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	95/195004 (0.0%)	0.92	355/286850 (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
12	AB	0	2
13	AC	0	1
13	AD	0	2
14	AE	0	4
16	AG	0	6
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	35

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	-15.16	1.11	1.49
26	L	42	TRP	CB-CG	-12.34	1.28	1.50
3	2	5	GLU	CG-CD	-11.59	1.34	1.51
45	e	46	VAL	CB-CG1	-11.30	1.29	1.52
63	w	42	LYS	CD-CE	-10.79	1.24	1.51

The worst 5 of 355 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
41	a	1019	U	C5-C4-O4	30.68	144.31	125.90
41	a	1141	U	C5-C4-O4	29.52	143.62	125.90
18	D	37	U	C5-C4-O4	29.46	143.58	125.90
18	D	1358	U	C5-C4-O4	29.25	143.45	125.90
18	D	827	U	C5-C4-O4	28.61	143.06	125.90

There are no chirality outliers.

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	9	107	GLU	Peptide

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Mol	Chain	Res	Type	Group
9	9	79	PRO	Peptide
9	9	92	ALA	Peptide
12	AB	140	MET	Peptide
12	AB	151	LYS	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	25
11	AA	1312/1342 (98%)	1198 (91%)	113 (9%)	1 (0%)	48	79
12	AB	159/162 (98%)	105 (66%)	43 (27%)	11 (7%)	1	5
13	AC	217/329 (66%)	203 (94%)	12 (6%)	2 (1%)	14	45
13	AD	293/329 (89%)	263 (90%)	27 (9%)	3 (1%)	13	42
14	AE	1331/1407 (95%)	1212 (91%)	113 (8%)	6 (0%)	25	58
15	AF	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
16	AG	493/495 (100%)	375 (76%)	87 (18%)	31 (6%)	1	7
17	C	64/75 (85%)	63 (98%)	1 (2%)	0	100	100
19	E	84/87 (97%)	83 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	F	68/71 (96%)	68 (100%)	0	0	100	100
21	G	223/241 (92%)	212 (95%)	10 (4%)	1 (0%)	30	63
22	H	255/557 (46%)	182 (71%)	66 (26%)	7 (3%)	4	21
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	53
26	L	102/104 (98%)	97 (95%)	4 (4%)	1 (1%)	13	42
27	M	149/179 (83%)	140 (94%)	8 (5%)	1 (1%)	19	51
28	N	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
29	O	125/130 (96%)	116 (93%)	8 (6%)	1 (1%)	16	48
30	P	97/99 (98%)	88 (91%)	9 (9%)	0	100	100
31	Q	115/117 (98%)	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	29
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	60/62 (97%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	m	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
54	n	175/179 (98%)	160 (91%)	14 (8%)	1 (1%)	22	53
55	o	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	8	31
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	10058/11004 (91%)	9174 (91%)	811 (8%)	73 (1%)	21	51

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	AB	107	PRO
12	AB	125	GLY
12	AB	130	PHE
12	AB	137	ALA
12	AB	141	LEU

### 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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	2	81/84 (96%)	80 (99%)	1 (1%)	67	83
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	67
11	AA	1135/1157 (98%)	1134 (100%)	1 (0%)	92	97
12	AB	141/142 (99%)	122 (86%)	19 (14%)	3	13
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	78
15	AF	70/75 (93%)	70 (100%)	0	100	100
16	AG	409/409 (100%)	297 (73%)	112 (27%)	0	1
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	92
22	H	137/461 (30%)	137 (100%)	0	100	100
23	I	171/190 (90%)	170 (99%)	1 (1%)	84	91
24	J	172/173 (99%)	171 (99%)	1 (1%)	84	91
25	K	119/126 (94%)	119 (100%)	0	100	100
26	L	91/91 (100%)	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	86
30	P	86/86 (100%)	84 (98%)	2 (2%)	45	70
31	Q	90/90 (100%)	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	80
36	V	74/78 (95%)	73 (99%)	1 (1%)	62	81
37	W	72/79 (91%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	X	94/96 (98%)	94 (100%)	0	100	100
39	Y	109/110 (99%)	108 (99%)	1 (1%)	75	88
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	54/54 (100%)	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	91
53	m	38/38 (100%)	38 (100%)	0	100	100
54	n	148/150 (99%)	148 (100%)	0	100	100
55	o	51/51 (100%)	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	88
60	t	104/104 (100%)	103 (99%)	1 (1%)	73	86
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	86
64	x	86/87 (99%)	86 (100%)	0	100	100
65	y	99/100 (99%)	97 (98%)	2 (2%)	50	74
66	z	89/90 (99%)	88 (99%)	1 (1%)	70	84
All	All	8299/9092 (91%)	8128 (98%)	171 (2%)	49	72

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	AG	276	TRP

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Mol	Chain	Res	Type
16	AG	359	PHE
16	AG	296	ILE
16	AG	320	ARG
16	AG	399	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
35	U	26	ASN
62	v	97	GLN
45	e	25	GLN
53	m	29	GLN
65	y	10	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	36/47 (76%)	26 (72%)	5 (13%)
All	All	4678/4765 (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

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Mol	Chain	Res	Type
18	D	1196	A
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.

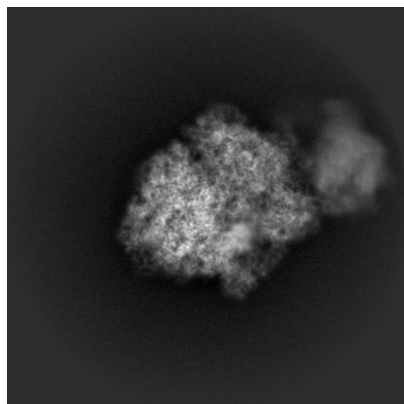
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42504. These allow visual inspection of the internal detail of the map and identification of artifacts.

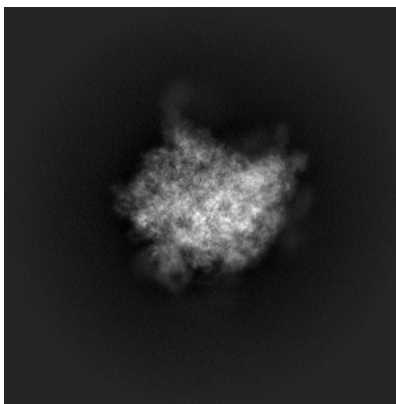
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

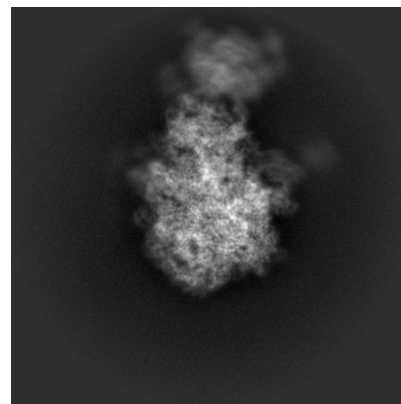
#### 6.1.1 Primary map



X

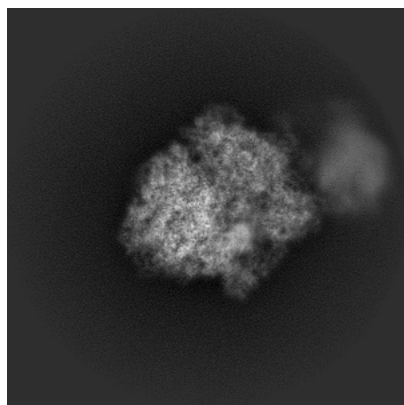


Y

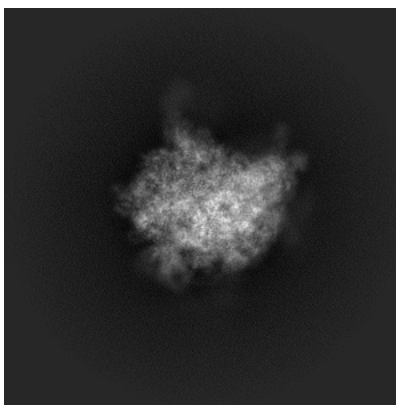


Z

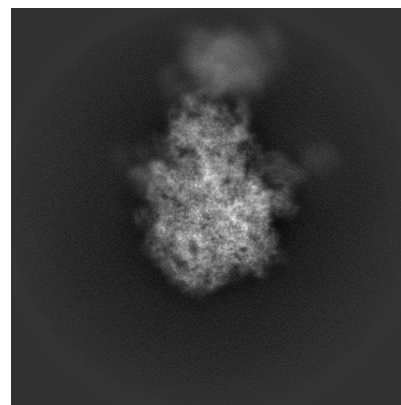
#### 6.1.2 Raw map



X



Y

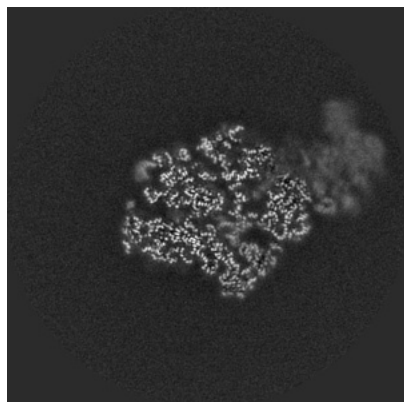


Z

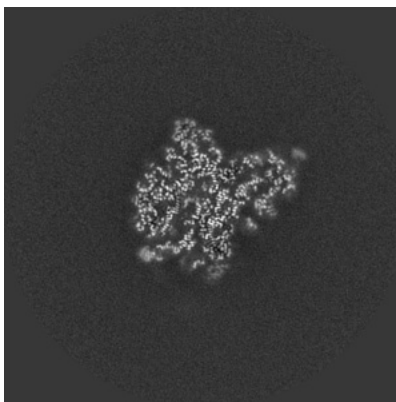
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

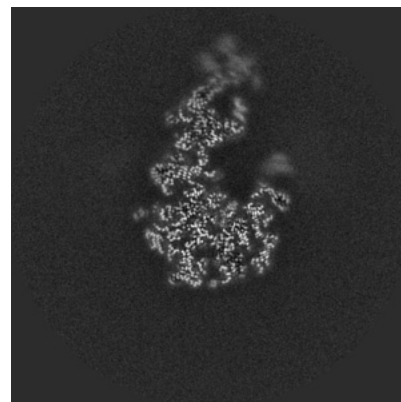
### 6.2.1 Primary map



X Index: 256

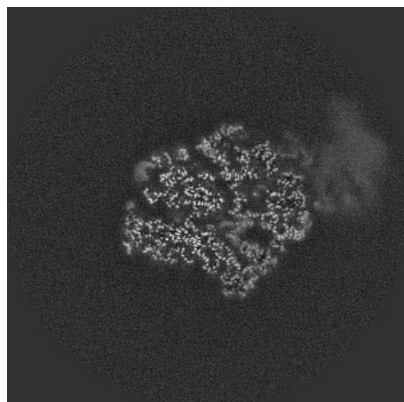


Y Index: 256

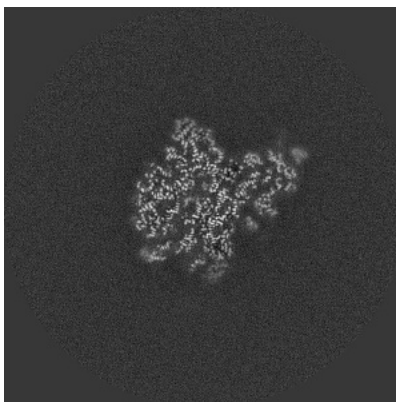


Z Index: 256

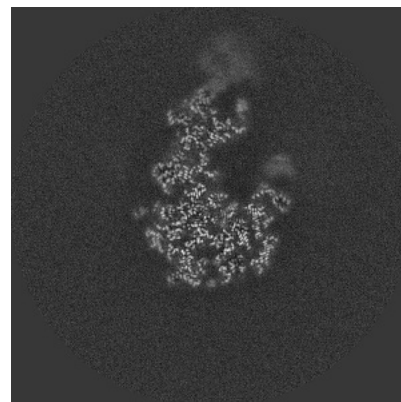
### 6.2.2 Raw map



X Index: 256



Y Index: 256

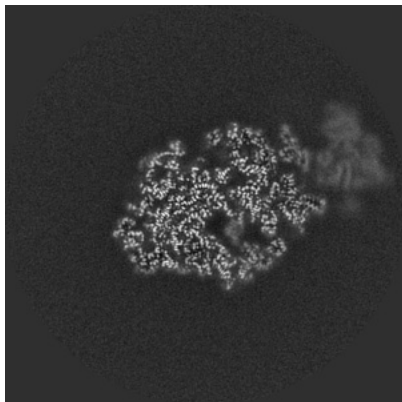


Z Index: 256

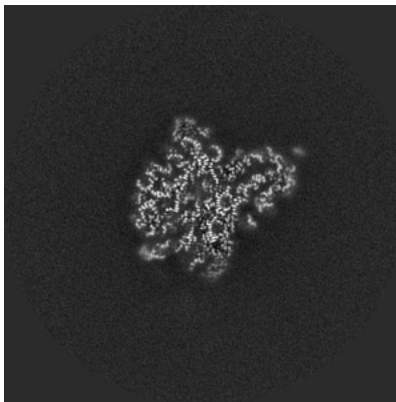
The images above show central slices of the map in three orthogonal directions.

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

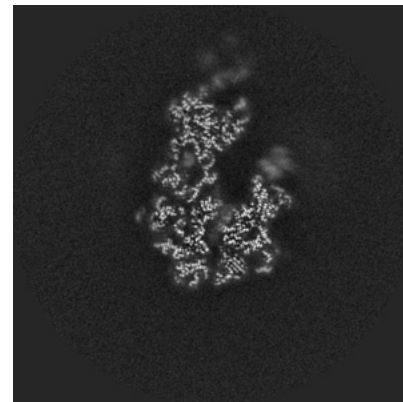
### 6.3.1 Primary map



X Index: 243

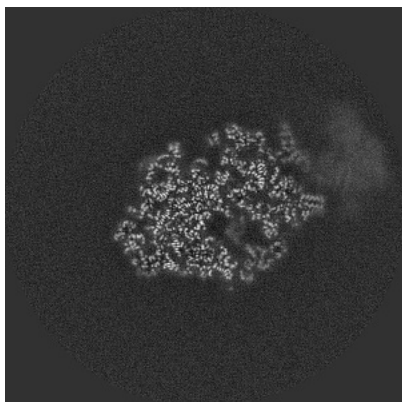


Y Index: 254

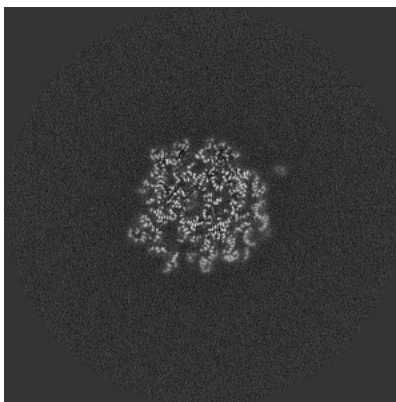


Z Index: 247

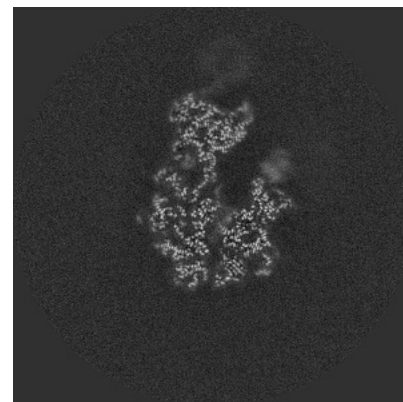
### 6.3.2 Raw map



X Index: 242



Y Index: 220



Z Index: 246

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

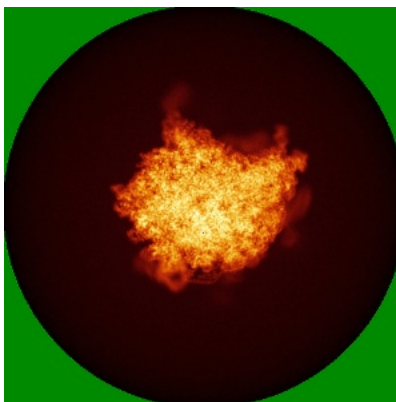


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



X

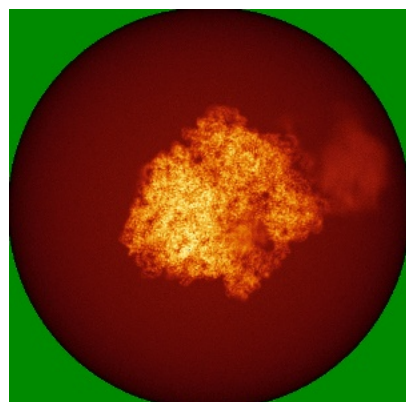


Y

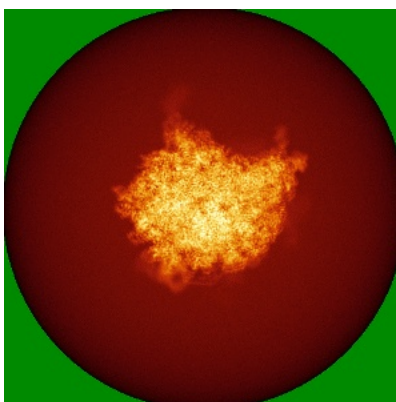


Z

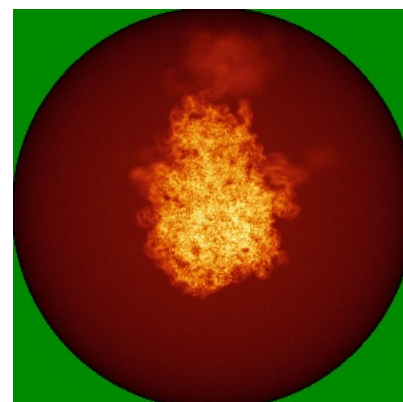
### 6.4.2 Raw map



X



Y

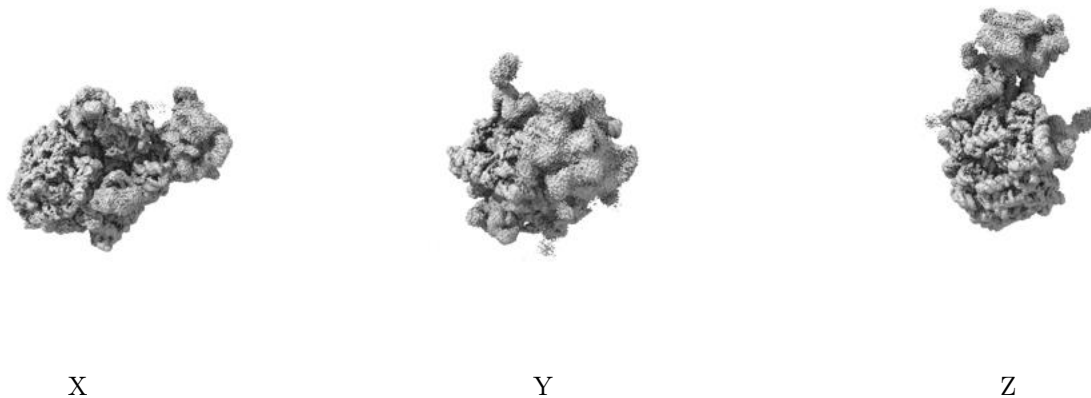


Z

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.

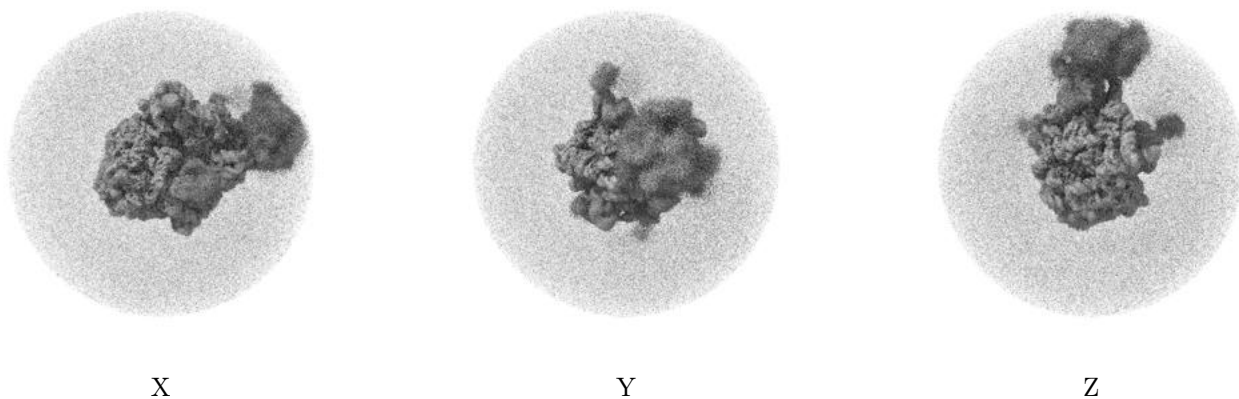
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0048. 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



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.

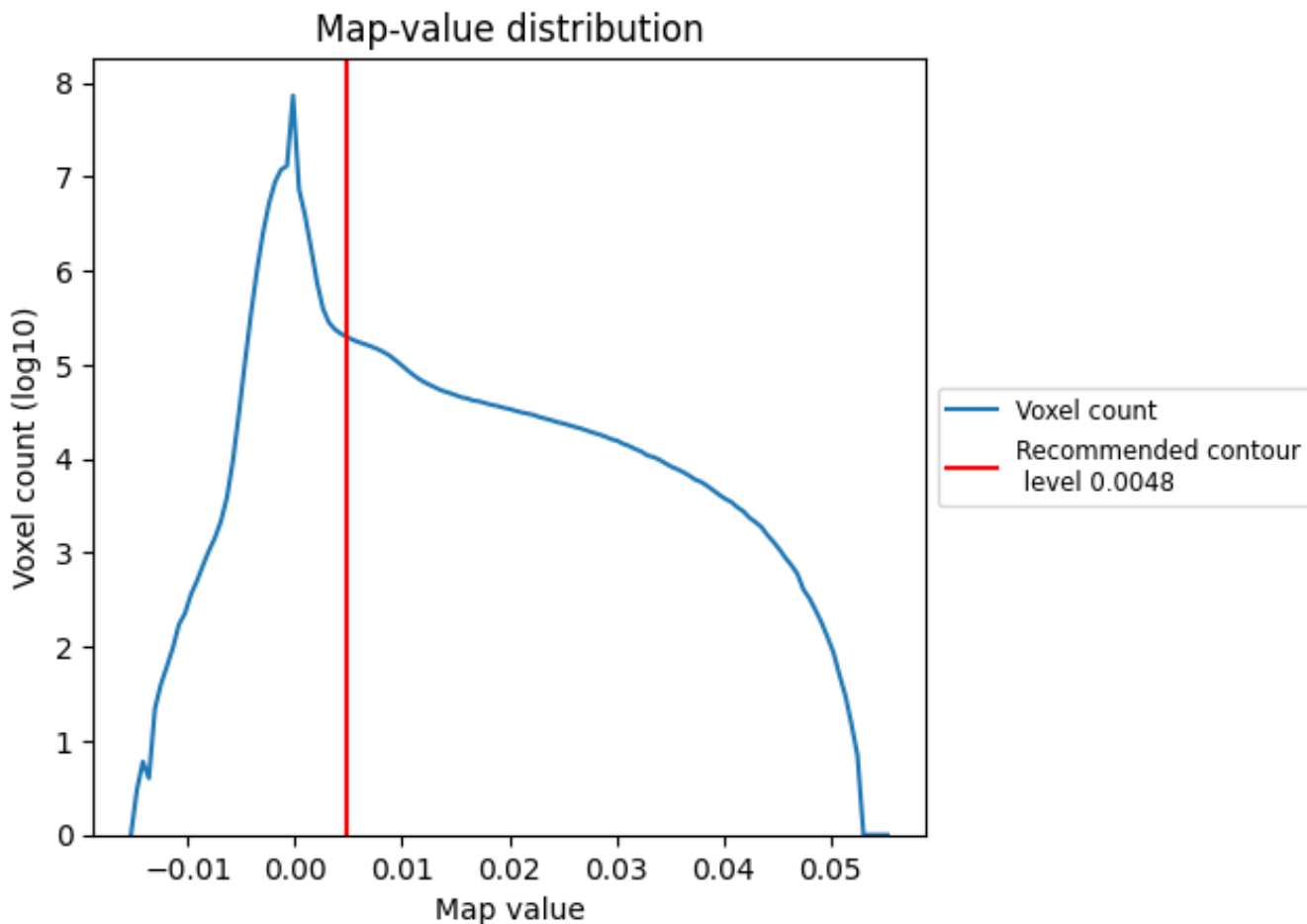
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

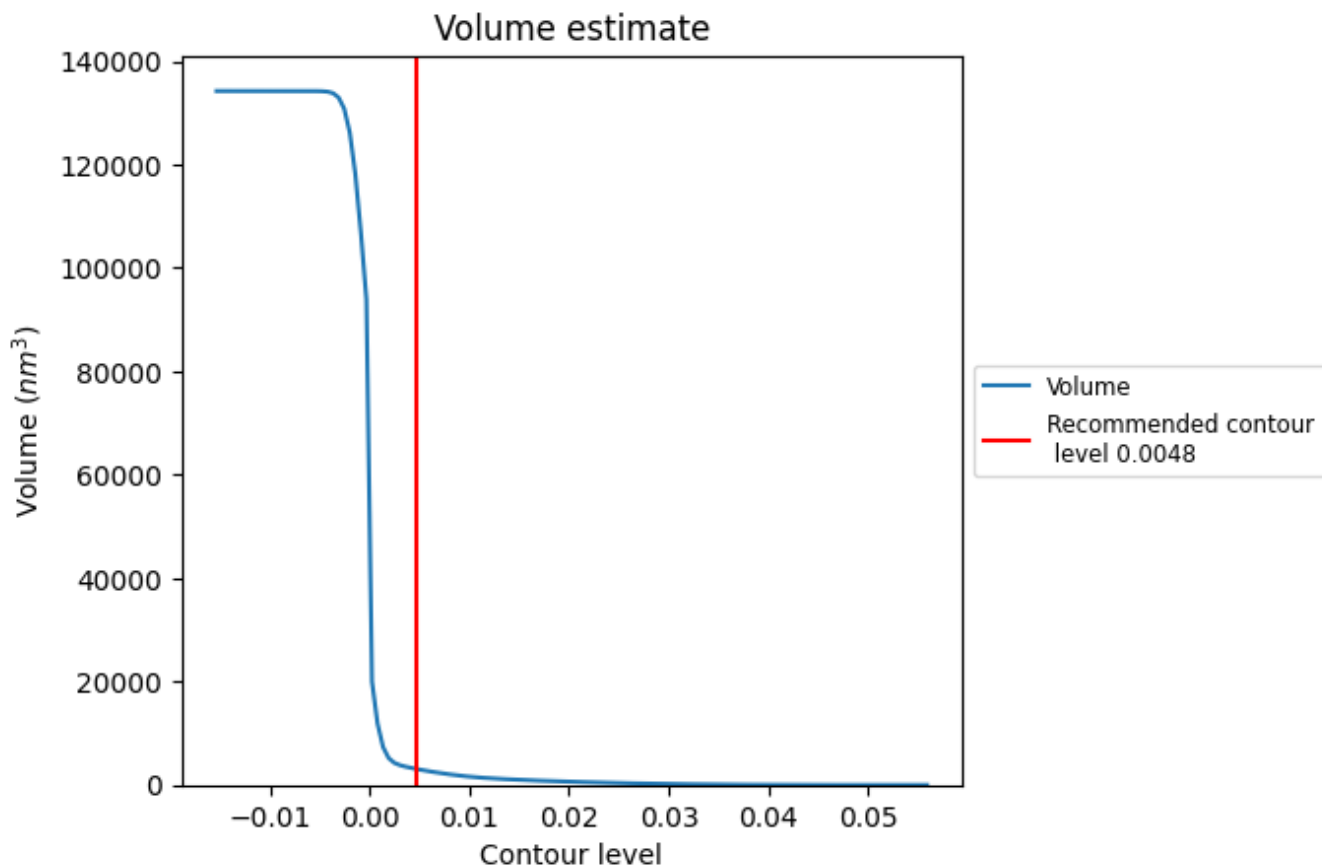
### 7.1 Map-value distribution [i](#)



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



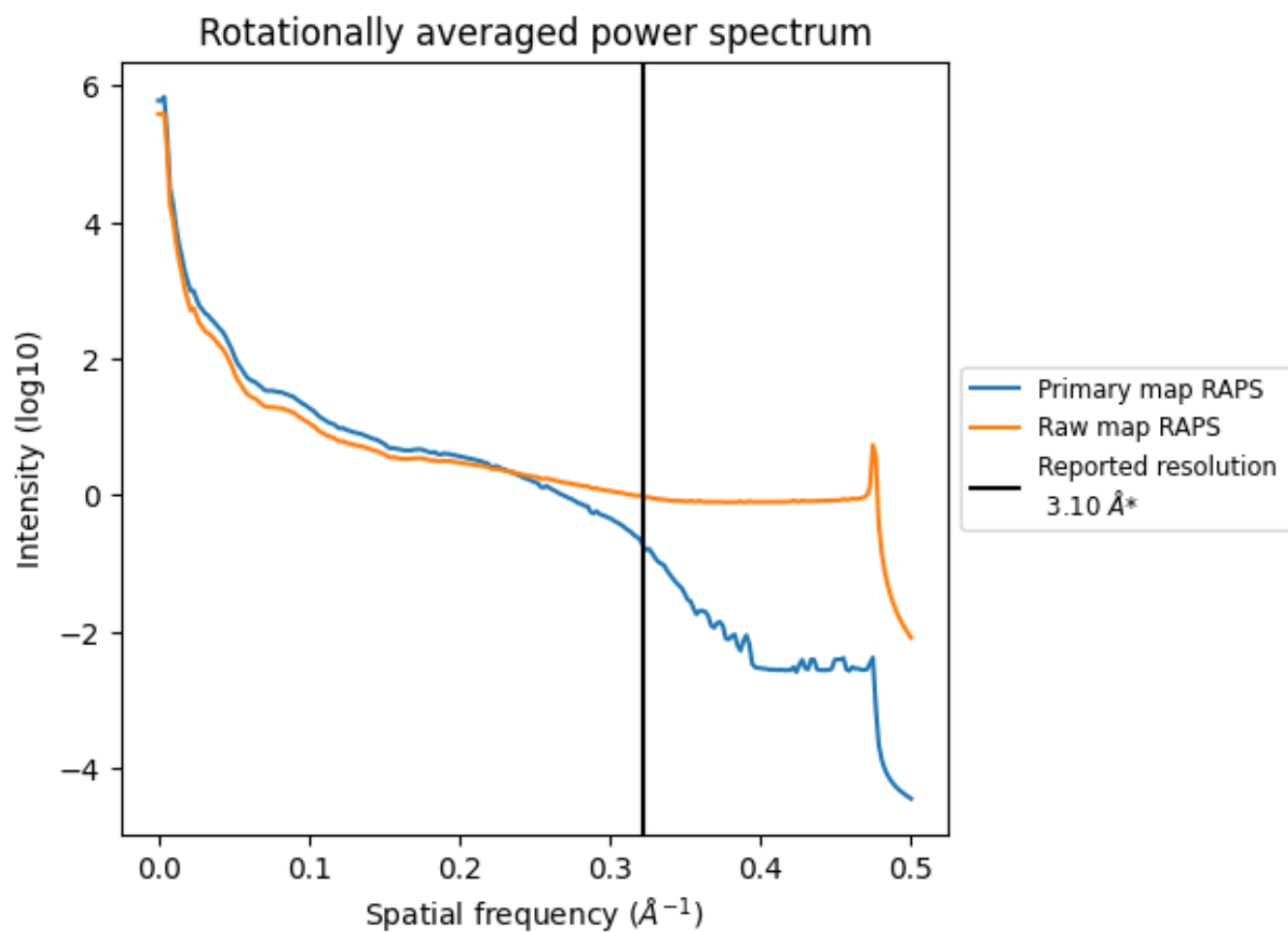
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 3048  $\text{nm}^3$ ; this corresponds to an approximate mass of 2753 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](#)

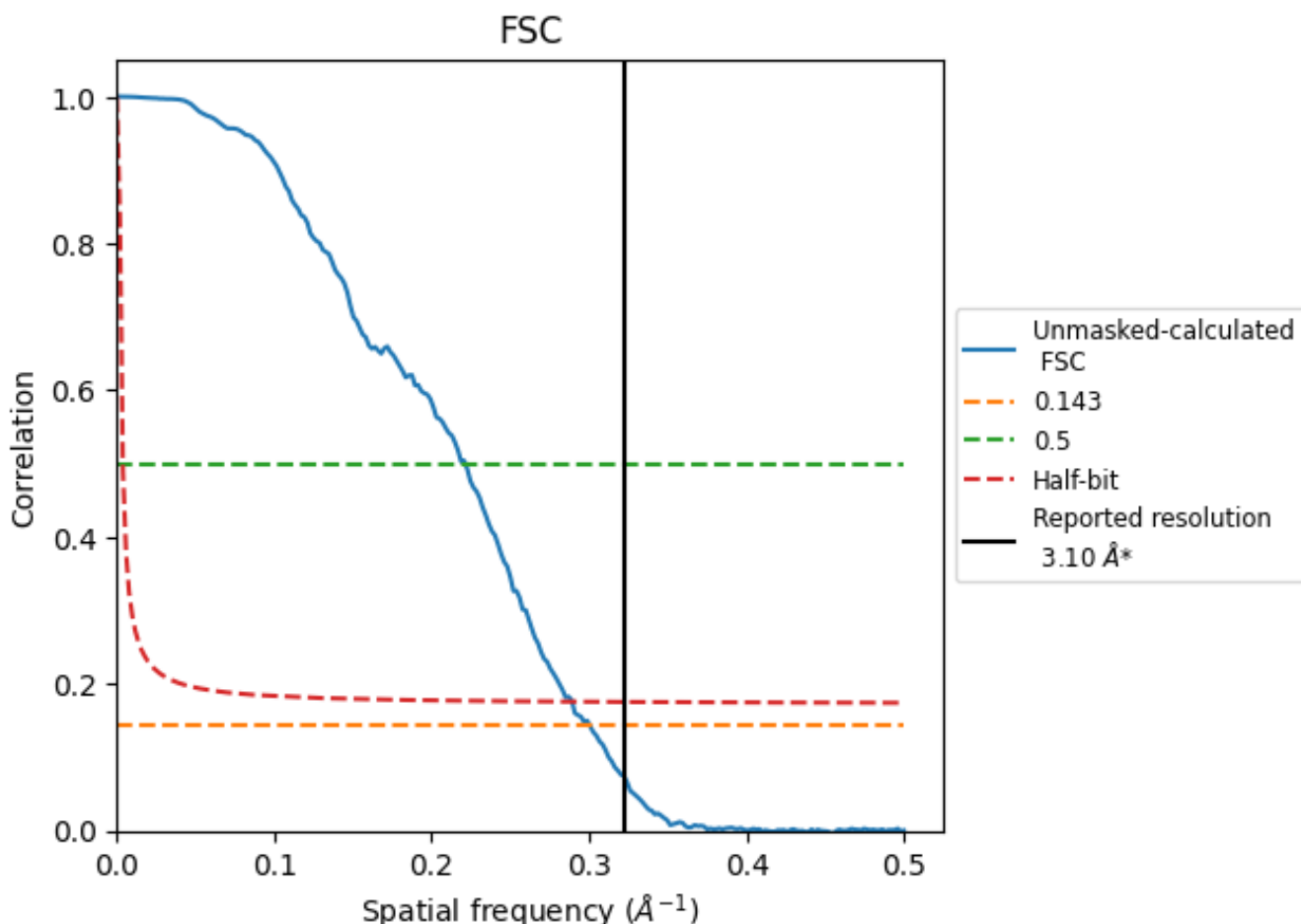


\*Reported resolution corresponds to spatial frequency of  $0.323 \text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.323  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

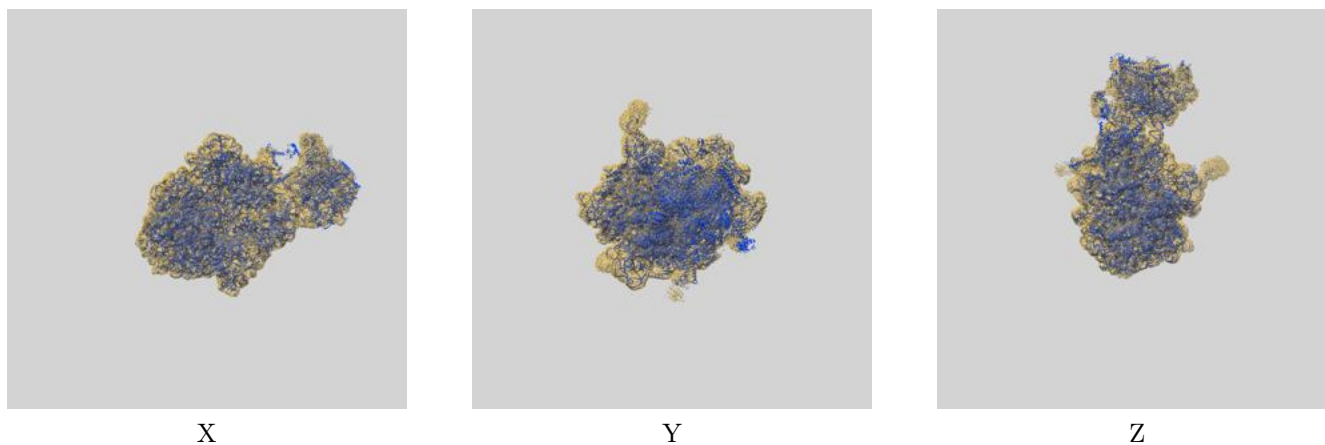
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.33	4.52	3.46

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

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

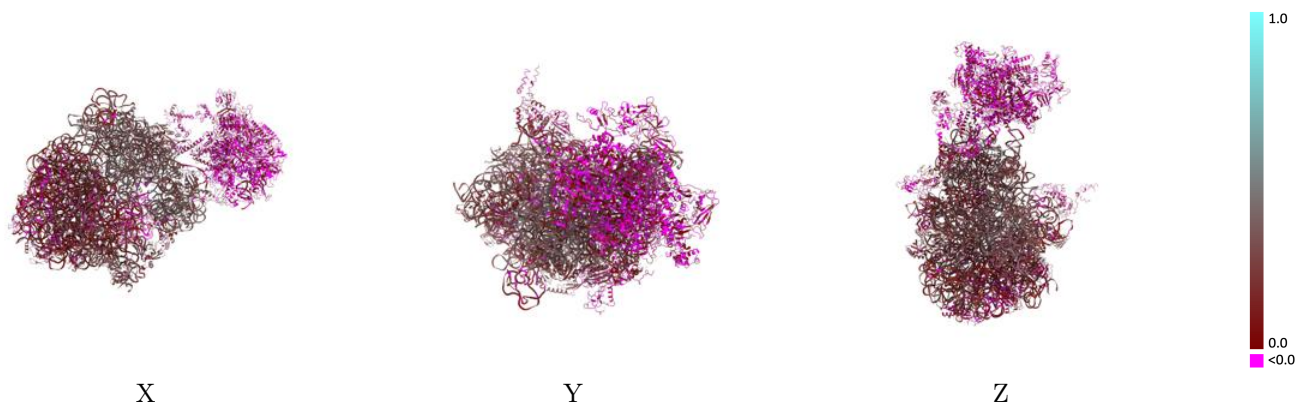
This section contains information regarding the fit between EMDB map EMD-42504 and PDB model 8URY. Per-residue inclusion information can be found in section 3 on page 17.

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



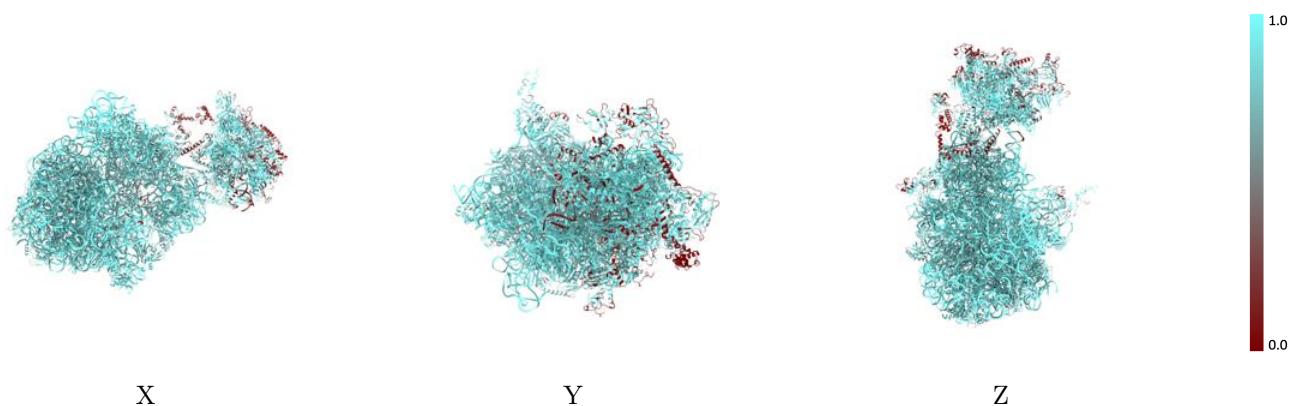
The images above show the 3D surface view of the map at the recommended contour level 0.0048 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



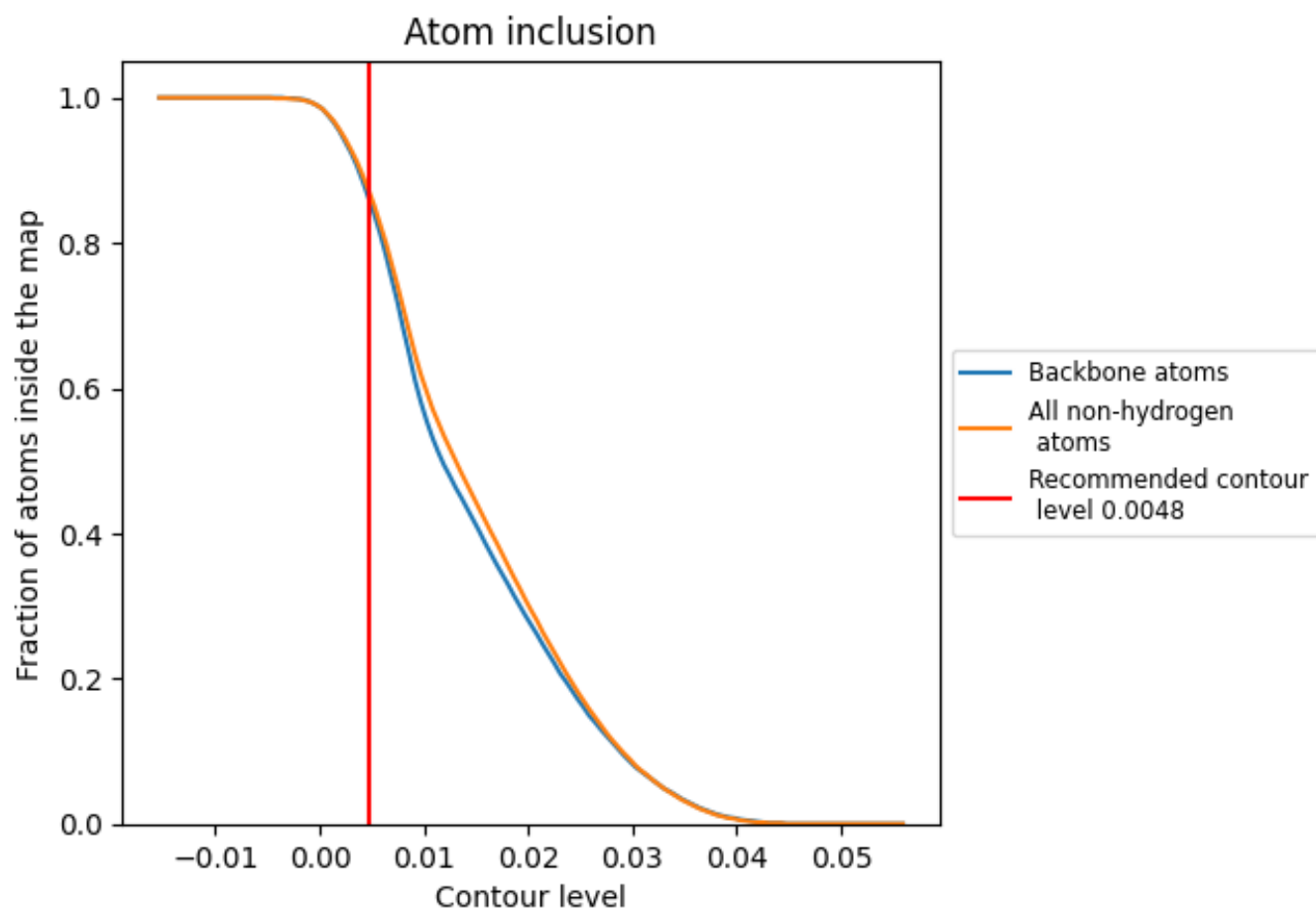
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0048).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% 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 (0.0048) and Q-score for the entire model and for each chain.





































































Chain	Atom inclusion	Q-score
All	 0.8690	 0.1690
0	 0.8390	 0.1200
1	 0.7740	 0.0580
2	 0.8160	 0.1040
3	 0.8240	 0.0530
4	 0.9230	 0.2810
5	 0.5950	 0.0250
6	 0.6810	 0.0070
7	 0.7860	 0.0090
9	 0.8650	 0.0920
A	 0.9580	 0.1850
AA	 0.7470	 0.0010
AB	 0.7460	 0.0140
AC	 0.7300	 0.0220
AD	 0.7870	 0.0640
AE	 0.7590	 0.0100
AF	 0.5270	 0.0320
AG	 0.5150	 0.0260
B	 0.8050	 0.0850
C	 0.8530	 0.1750
D	 0.9850	 0.3160
E	 0.9220	 0.2900
F	 0.8520	 0.1970
G	 0.8680	 0.2300
H	 0.5840	 0.0480
I	 0.8920	 0.2990
J	 0.8910	 0.2570
K	 0.8530	 0.2130
L	 0.8360	 0.1670
M	 0.9060	 0.2950
N	 0.8580	 0.2190
O	 0.9170	 0.2780
P	 0.8990	 0.2740
Q	 0.8990	 0.2380
R	 0.9250	 0.3070



*Continued on next page...*



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Chain	Atom inclusion	Q-score
S	 0.9200	 0.3230
T	 0.8770	 0.2350
U	 0.9070	 0.2980
V	 0.8910	 0.2580
W	 0.8980	 0.2080
X	 0.8870	 0.1690
Y	 0.6890	 0.0410
Z	 0.8060	 -0.0280
a	 0.9450	 0.1560
b	 0.8430	 0.1990
c	 0.8300	 0.1330
d	 0.9840	 0.2930
e	 0.8040	 0.1230
f	 0.8600	 0.1710
g	 0.8940	 0.2080
h	 0.8670	 0.2110
i	 0.8010	 0.1080
j	 0.8240	 0.1130
k	 0.8520	 0.1610
l	 0.7900	 0.1090
m	 0.7690	 0.1080
n	 0.8950	 0.1930
o	 0.8230	 0.1430
p	 0.9090	 0.1930
q	 0.8800	 0.2140
r	 0.8050	 0.1810
s	 0.8900	 0.2230
t	 0.8320	 0.1700
u	 0.8360	 0.1430
v	 0.8790	 0.1830
w	 0.8070	 0.0960
x	 0.9110	 0.2280
y	 0.8540	 0.1450
z	 0.7950	 0.1120