



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 03:00 AM UTC

PDB ID : 8UPR / pdb_00008upr
EMDB ID : EMD-42454
Title : Escherichia coli transcription-translation coupled complex class A (TTC-A) containing RfaH bound to ops signal, mRNA with a 21 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 : 2023-10-23
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 ⓘ symbol.

The types of validation reports are described at

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

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

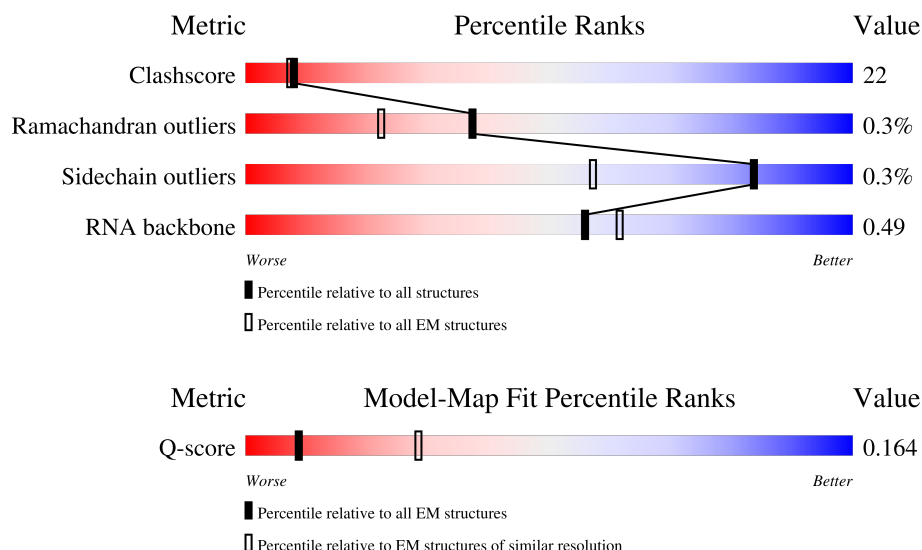
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 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.



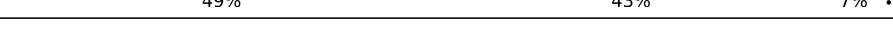
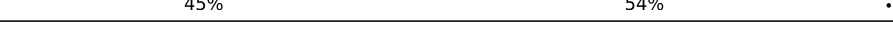
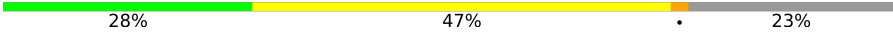
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	625 (4.80 - 5.80)

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

Mol	Chain	Length	Quality of chain
1	0	103	
2	1	110	
3	2	100	

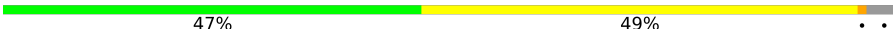
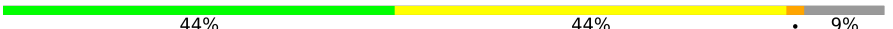
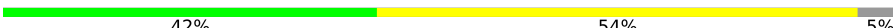
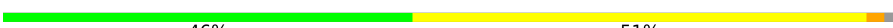
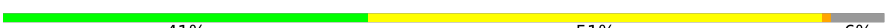
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Mol	Chain	Length	Quality of chain
4	3	104	
5	4	94	
6	5	38	
7	6	38	
8	7	38	
9	9	165	
10	A	76	
10	B	76	
11	AA	1342	
12	AB	162	
13	AC	329	
13	AD	329	
14	AE	1407	
15	AF	91	
16	C	75	
17	D	1542	
18	E	87	
19	F	71	
20	G	241	
21	H	557	
22	I	233	
23	J	206	
24	K	167	
25	L	135	
26	M	179	

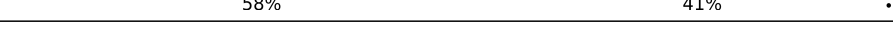
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Mol	Chain	Length	Quality of chain
27	N	130	
28	O	130	
29	P	103	
30	Q	129	
31	R	124	
32	S	101	
33	T	89	
34	U	82	
35	V	84	
36	W	92	
37	X	118	
38	Y	142	
39	Z	121	
40	a	2904	
41	b	85	
42	c	78	
43	d	120	
44	e	63	
45	f	59	
46	g	70	
47	h	273	
48	i	57	
49	j	209	
50	k	55	
51	l	201	

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Mol	Chain	Length	Quality of chain
52	m	46	 57% 43%
53	n	179	 44% 54% ...
54	o	65	 58% 35% 5% .
55	p	177	 68% 31% .
56	q	38	 61% 39%
57	r	149	 68% 32%
58	s	142	 55% 44% ..
59	t	123	 46% 54% .
60	u	144	 62% 37% .
61	v	136	 49% 49% .
62	w	127	 44% 46% . 6%
63	x	117	 63% 36% .
64	y	115	 63% 37% .
65	z	118	 58% 41% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
67	ZN	AE	1502	-	-	X	-

2 Entry composition [i](#)

There are 67 unique types of molecules in this entry. The entry contains 276059 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 ops.

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

- Molecule 7 is a DNA chain called T DNA ops.

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 21 nt long spacer.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	38	Total	C	N	O	P	0	0
			792	354	112	288	38		

- 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 tRNA (fMet).

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

- 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	218	Total	C	N	O	S	0	0
			1677	1048	297	326	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 30S ribosomal protein S18.

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

- Molecule 17 is a RNA chain called 16S rRNA.

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

- Molecule 18 is a protein called 30S ribosomal protein S20.

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

- Molecule 19 is a protein called 30S ribosomal protein S21.

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

- Molecule 20 is a protein called 30S ribosomal protein S2.

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

- Molecule 21 is a protein called 30S ribosomal protein S1.

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

- Molecule 22 is a protein called 30S ribosomal protein S3.

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

- Molecule 23 is a protein called 30S ribosomal protein S4.

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

- Molecule 24 is a protein called 30S ribosomal protein S5.

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

- Molecule 25 is a protein called 30S ribosomal protein S6.

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

- Molecule 26 is a protein called 30S ribosomal protein S7.

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

- Molecule 27 is a protein called 30S ribosomal protein S8.

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

- Molecule 28 is a protein called 30S ribosomal protein S9.

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

- Molecule 29 is a protein called 30S ribosomal protein S10.

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

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

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

- Molecule 31 is a protein called 30S ribosomal protein S12.

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

- Molecule 32 is a protein called 30S ribosomal protein S14.

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

- Molecule 33 is a protein called 30S ribosomal protein S15.

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

- Molecule 34 is a protein called 30S ribosomal protein S16.

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

- Molecule 35 is a protein called 30S ribosomal protein S17.

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

- Molecule 36 is a protein called 30S ribosomal protein S19.

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

- Molecule 37 is a protein called 30S ribosomal protein S13.

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

- Molecule 38 is a protein called 50S ribosomal protein L11.

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

- Molecule 39 is a protein called 50S ribosomal protein L7/L12.

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

- Molecule 40 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	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 41 is a protein called 50S ribosomal protein L27.

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

- Molecule 42 is a protein called 50S ribosomal protein L28.

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

- Molecule 43 is a RNA chain called 5S rRNA.

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

- Molecule 44 is a protein called 50S ribosomal protein L29.

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

- Molecule 45 is a protein called 50S ribosomal protein L30.

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

- Molecule 46 is a protein called 50S ribosomal protein L31.

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

- Molecule 47 is a protein called 50S ribosomal protein L2.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

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

- Molecule 49 is a protein called 50S ribosomal protein L3.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L4.

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

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

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

- Molecule 53 is a protein called 50S ribosomal protein L5.

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

- Molecule 54 is a protein called 50S ribosomal protein L35.

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

- Molecule 55 is a protein called 50S ribosomal protein L6.

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

- Molecule 56 is a protein called 50S ribosomal protein L36.

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

- Molecule 57 is a protein called 50S ribosomal protein L9.

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

- Molecule 58 is a protein called 50S ribosomal protein L13.

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

- Molecule 59 is a protein called 50S ribosomal protein L14.

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

- Molecule 60 is a protein called 50S ribosomal protein L15.

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

- Molecule 61 is a protein called 50S ribosomal protein L16.

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

- Molecule 62 is a protein called 50S ribosomal protein L17.

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

- Molecule 63 is a protein called 50S ribosomal protein L18.

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

- Molecule 64 is a protein called 50S ribosomal protein L19.

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

- Molecule 65 is a protein called 50S ribosomal protein L20.

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

- Molecule 66 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

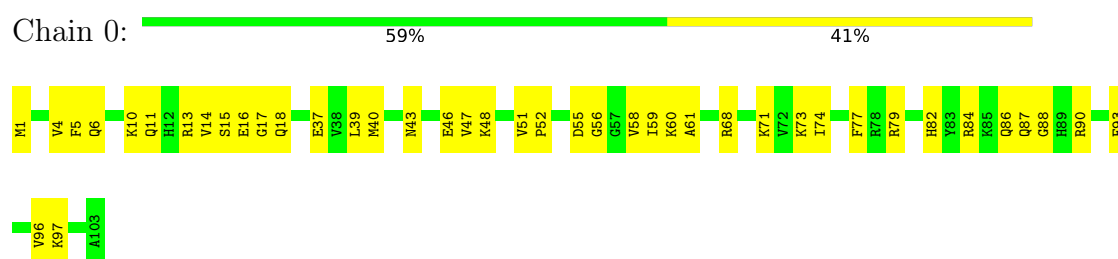
- Molecule 67 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

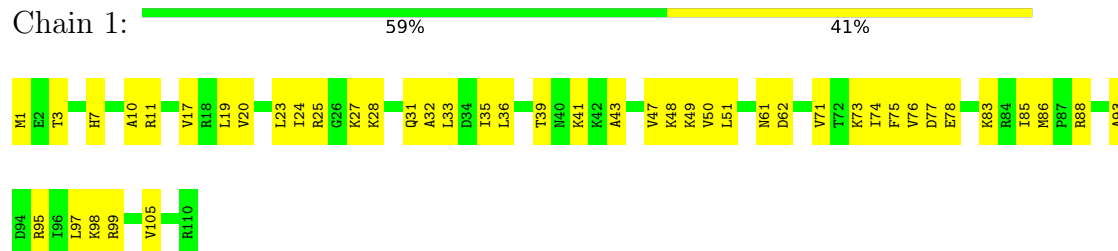
3 Residue-property plots

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.

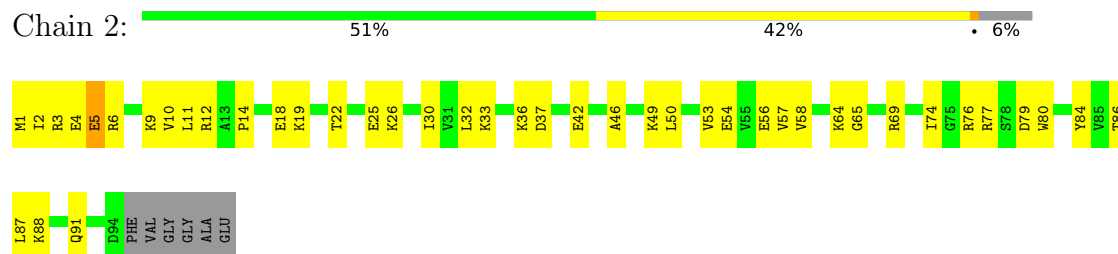
• Molecule 1: Ribosomal protein L21



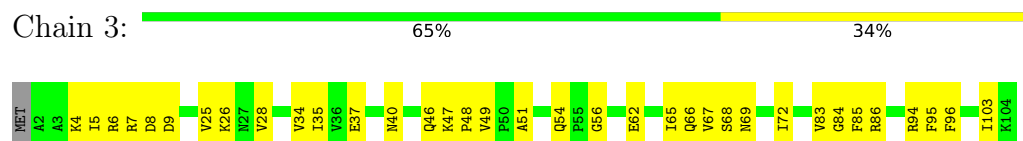
• Molecule 2: 50S ribosomal protein L22



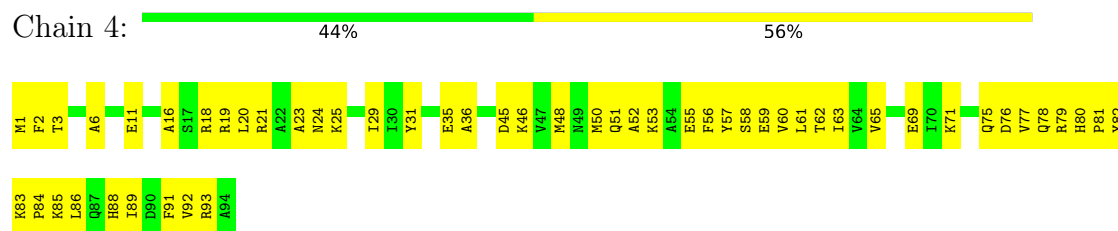
• Molecule 3: 50S ribosomal protein L23



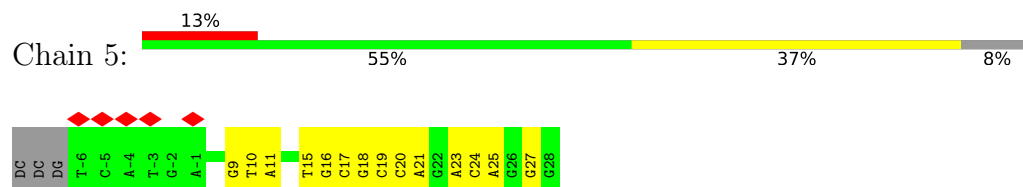
• Molecule 4: 50S ribosomal protein L24



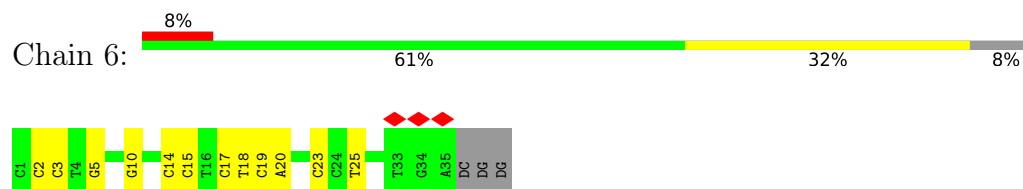
- Molecule 5: 50S ribosomal protein L25



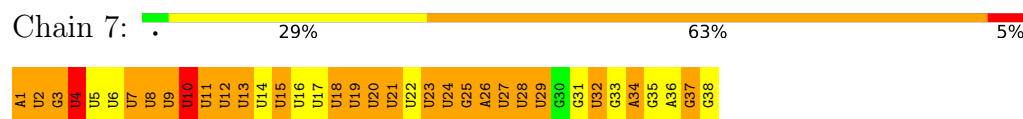
- Molecule 6: NT DNA ops



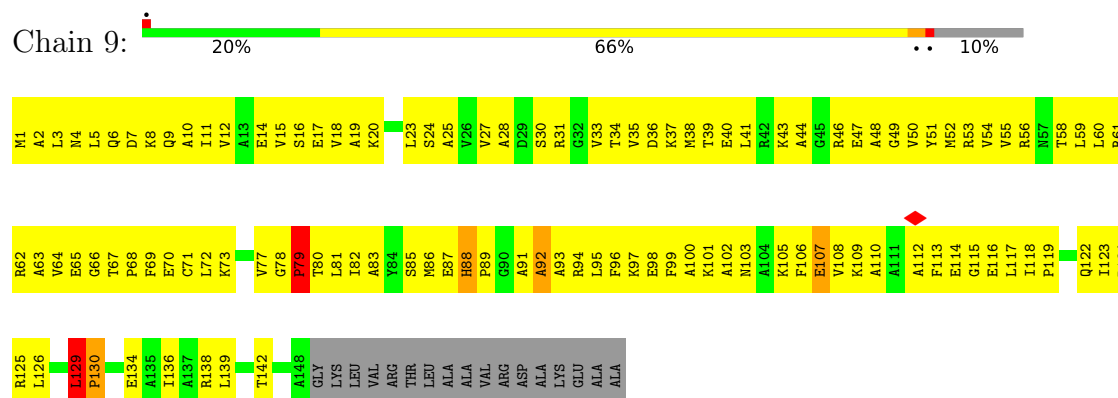
- Molecule 7: T DNA ops



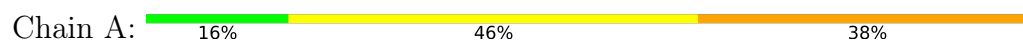
- Molecule 8: mRNA with 21 nt long spacer

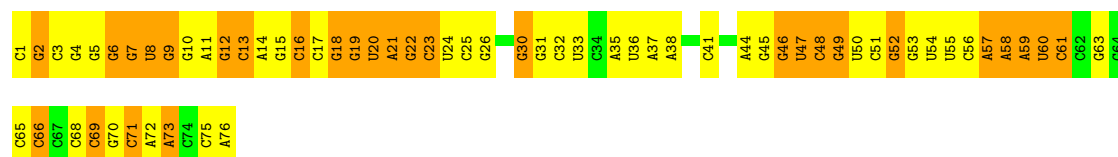


- Molecule 9: 50S ribosomal protein L10

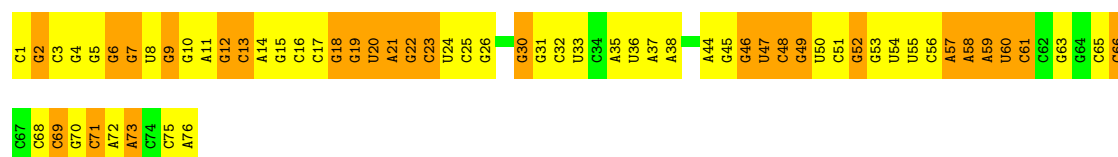
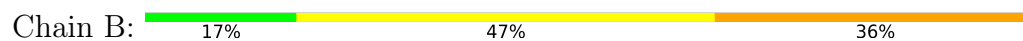


- Molecule 10: E-site and P-site tRNA (fMet)

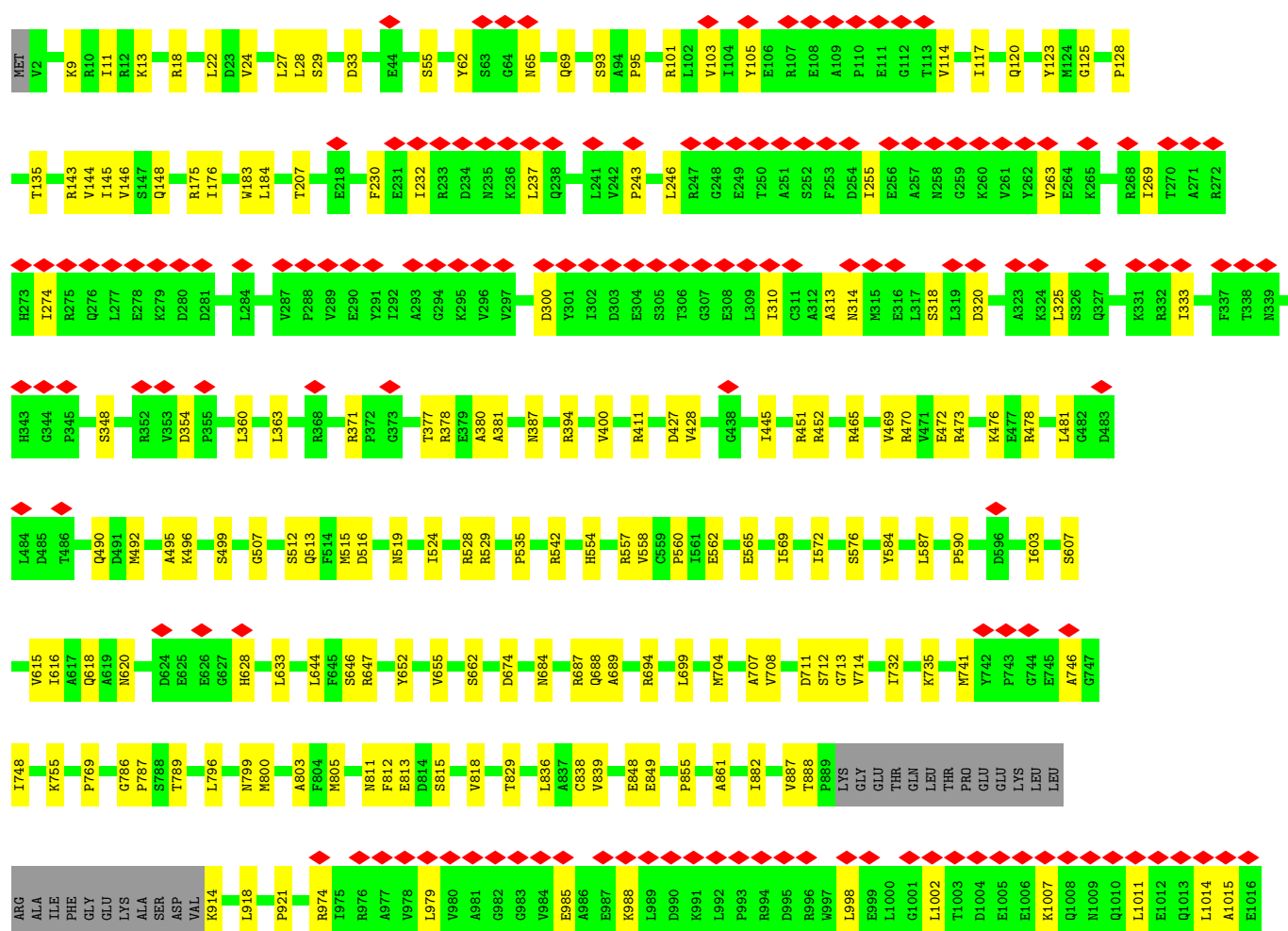
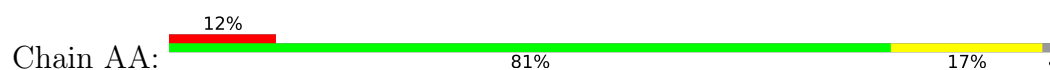




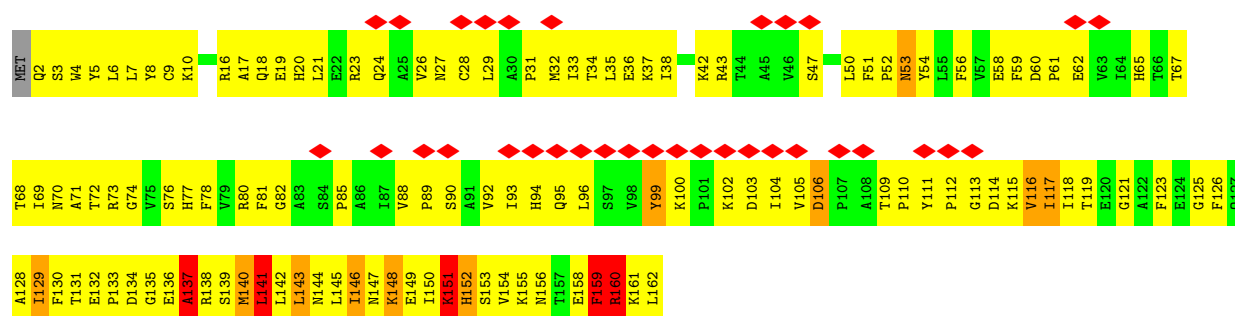
• Molecule 10: E-site and P-site tRNA (fMet)



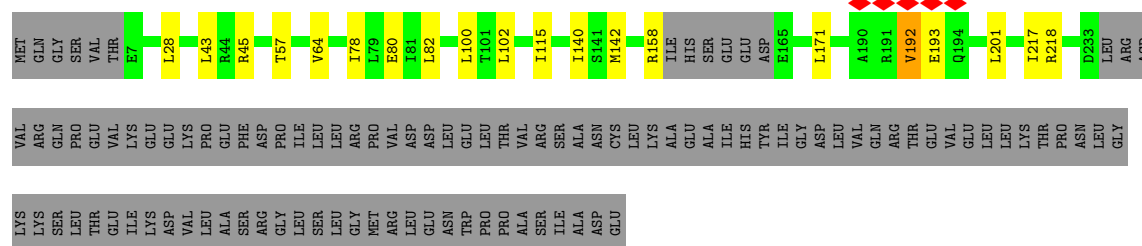
• Molecule 11: DNA-directed RNA polymerase subunit beta



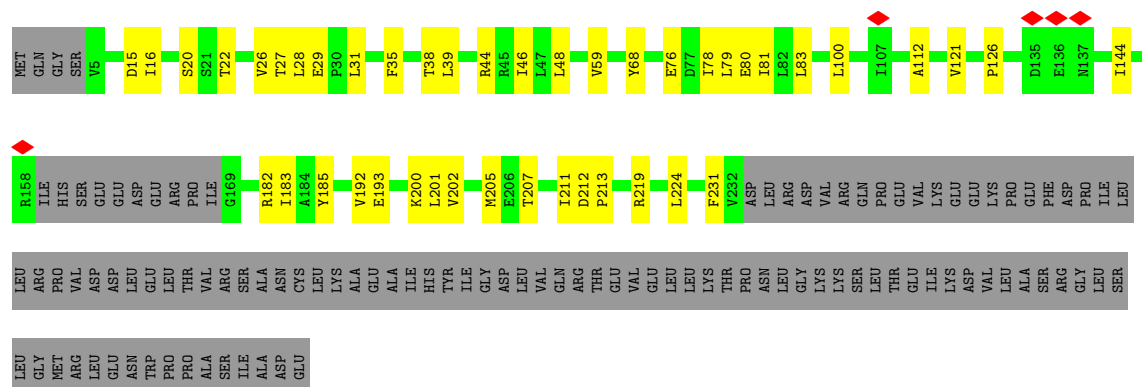
- Molecule 12: Transcription antitermination protein RfaH



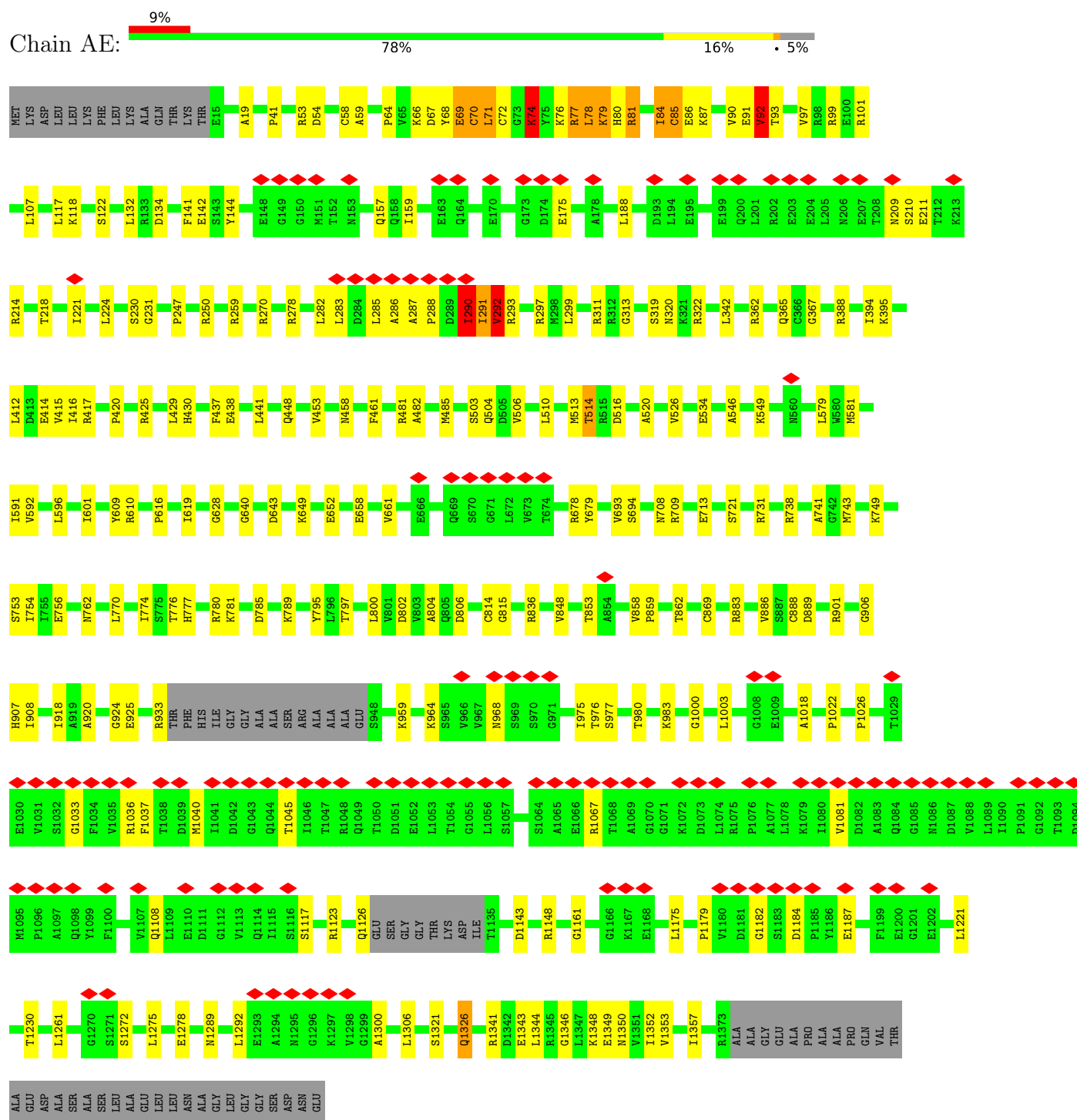
- Molecule 13: DNA-directed RNA polymerase subunit alpha

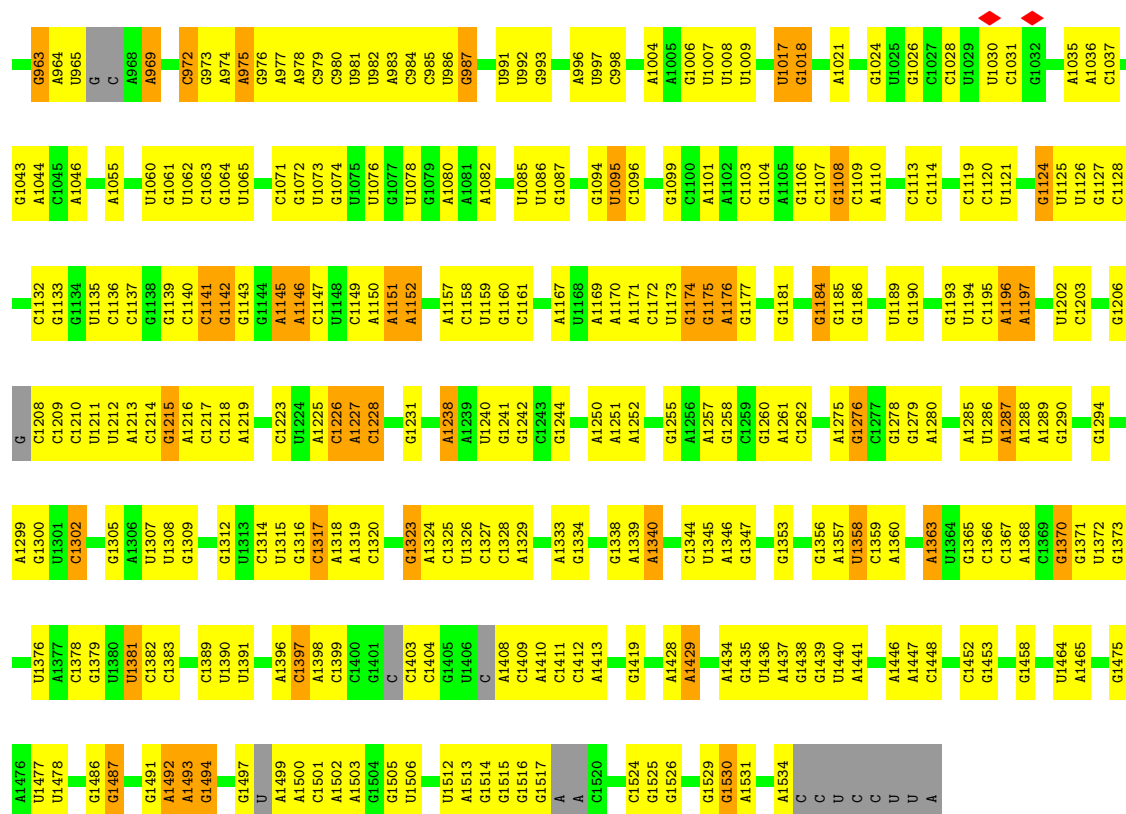


- Molecule 13: DNA-directed RNA polymerase subunit alpha

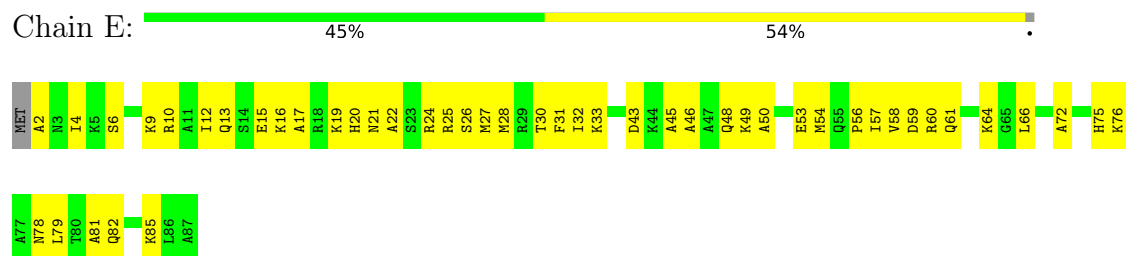


• Molecule 14: DNA-directed RNA polymerase subunit beta'

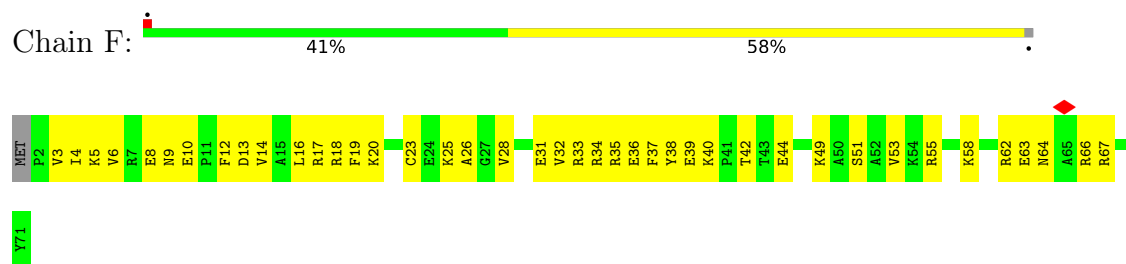




• Molecule 18: 30S ribosomal protein S20

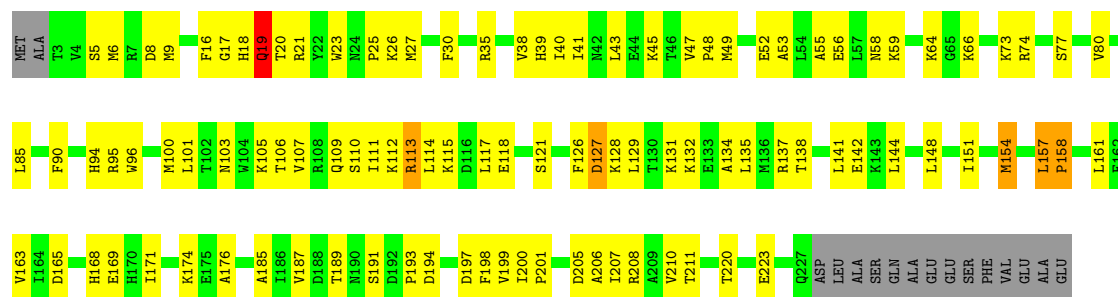


• Molecule 19: 30S ribosomal protein S21

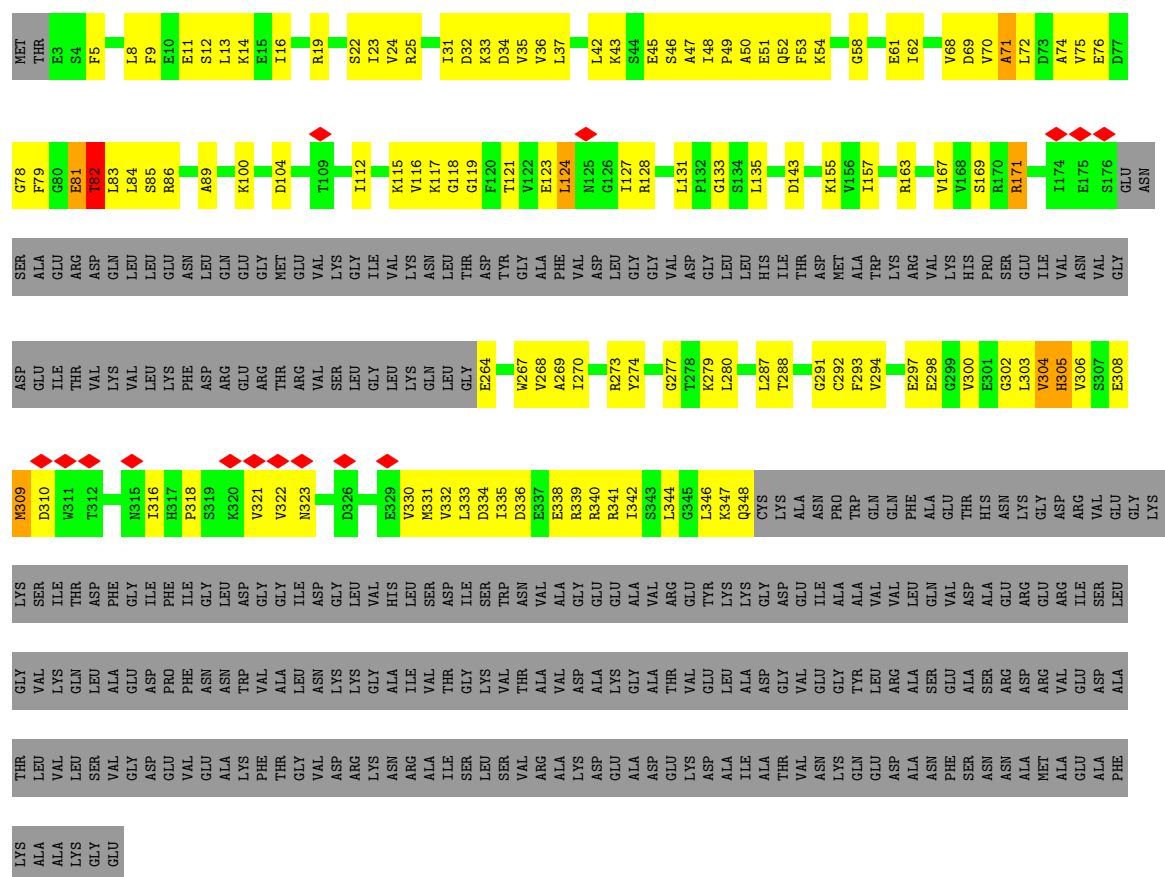


• Molecule 20: 30S ribosomal protein S2

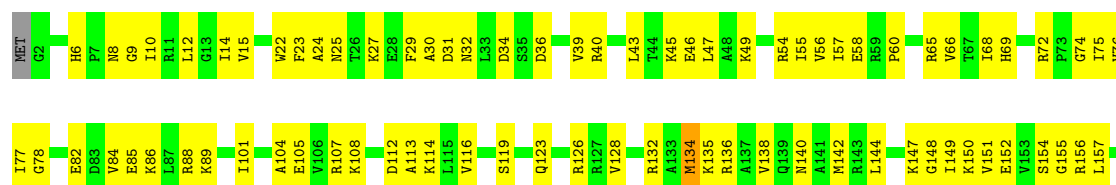




• Molecule 21: 30S ribosomal protein S1

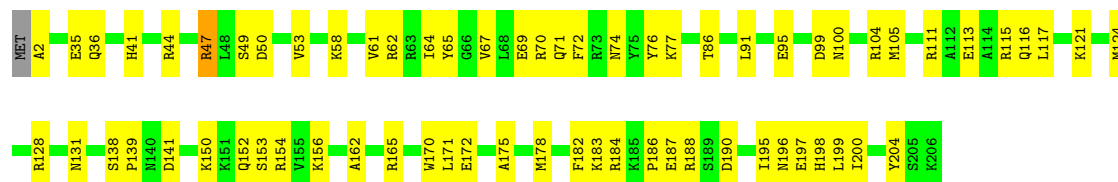


• Molecule 22: 30S ribosomal protein S3

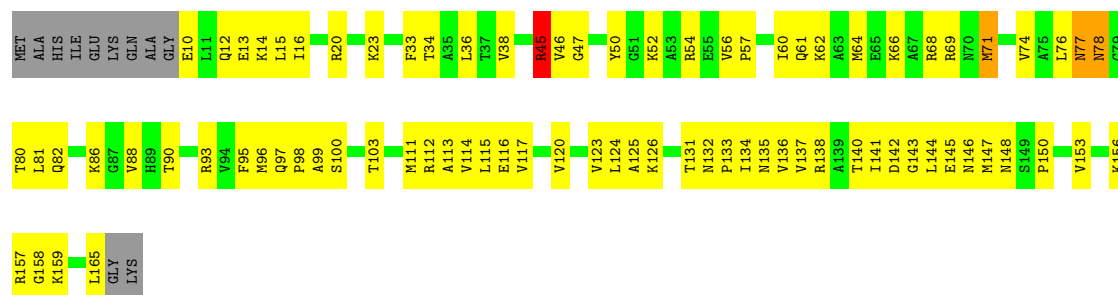




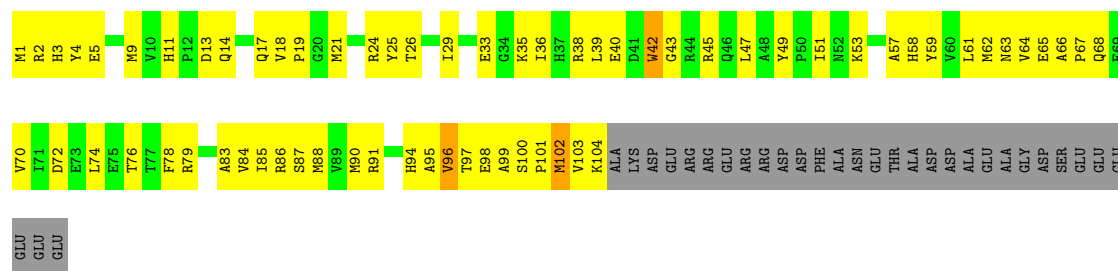
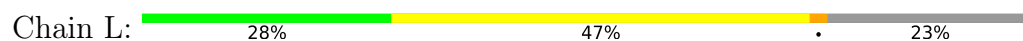
- Molecule 23: 30S ribosomal protein S4



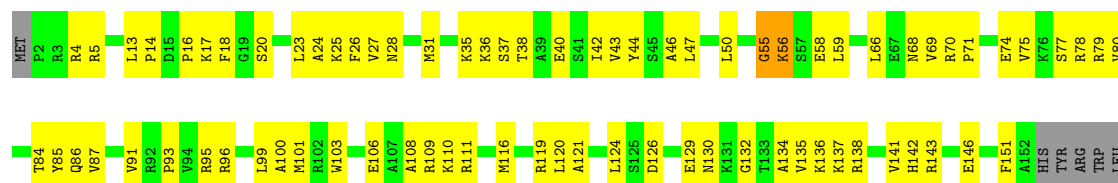
- Molecule 24: 30S ribosomal protein S5



- Molecule 25: 30S ribosomal protein S6



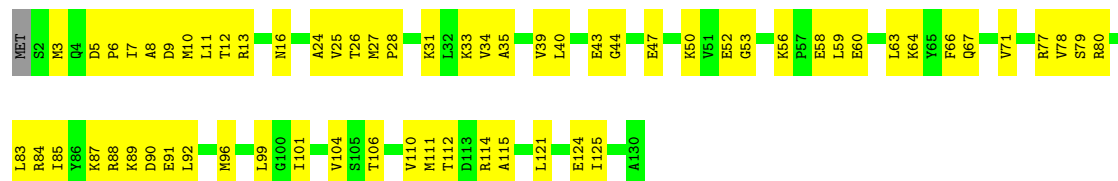
- Molecule 26: 30S ribosomal protein S7



SER
LEU
ARG
SER
PHE
SER
HIS
GLN
ALA
GLY
ALA
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SER
LYS
GLN
PRO
ALA
LEU
GLY
TYR
LEU
ASN

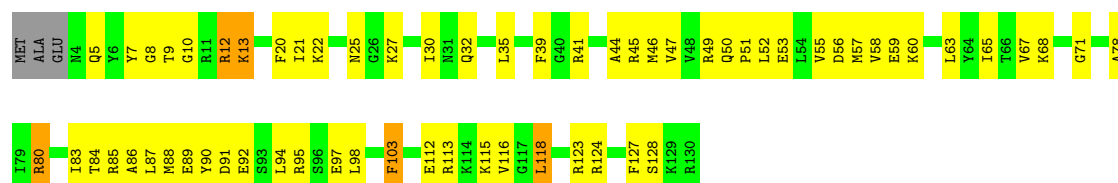
• Molecule 27: 30S ribosomal protein S8

Chain N: 51% 48%



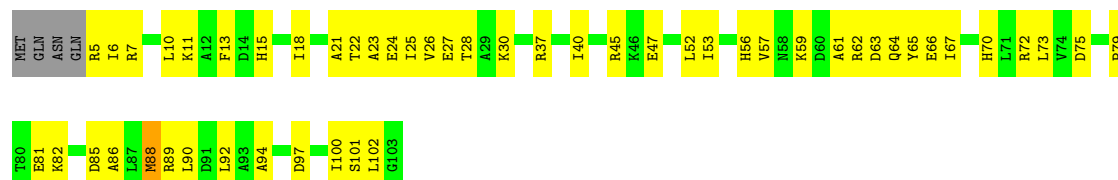
• Molecule 28: 30S ribosomal protein S9

Chain O: 49% 45%



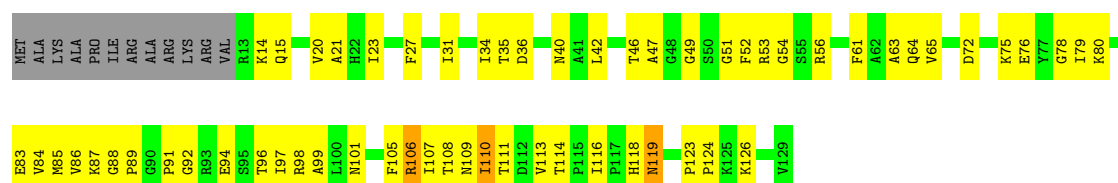
• Molecule 29: 30S ribosomal protein S10

Chain P: 47% 49%



• Molecule 30: 30S ribosomal protein S11

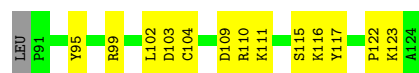
Chain Q: 44% 44% 9%



• Molecule 31: 30S ribosomal protein S12

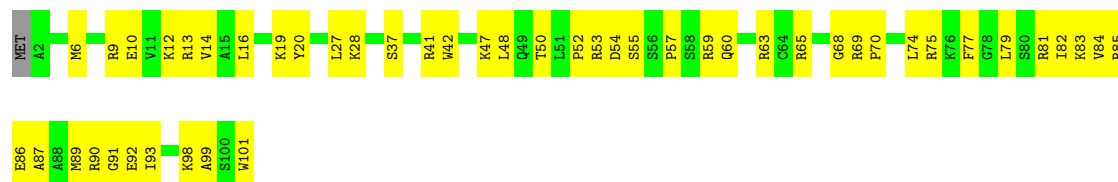
Chain R: 57% 40%





- Molecule 32: 30S ribosomal protein S14

Chain S: 51% 48%



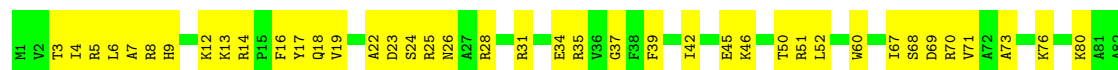
- Molecule 33: 30S ribosomal protein S15

Chain T: 42% 56%



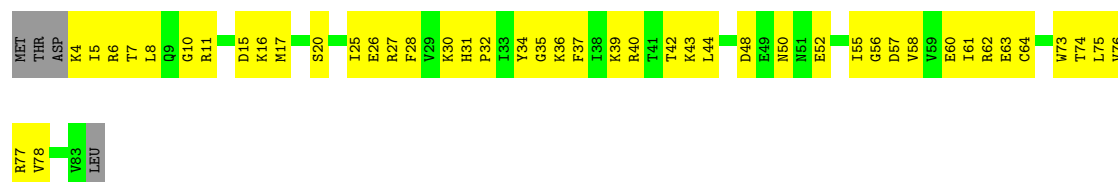
- Molecule 34: 30S ribosomal protein S16

Chain U: 51% 49%



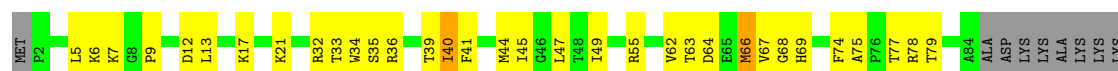
- Molecule 35: 30S ribosomal protein S17

Chain V: 42% 54% 5%



- Molecule 36: 30S ribosomal protein S19

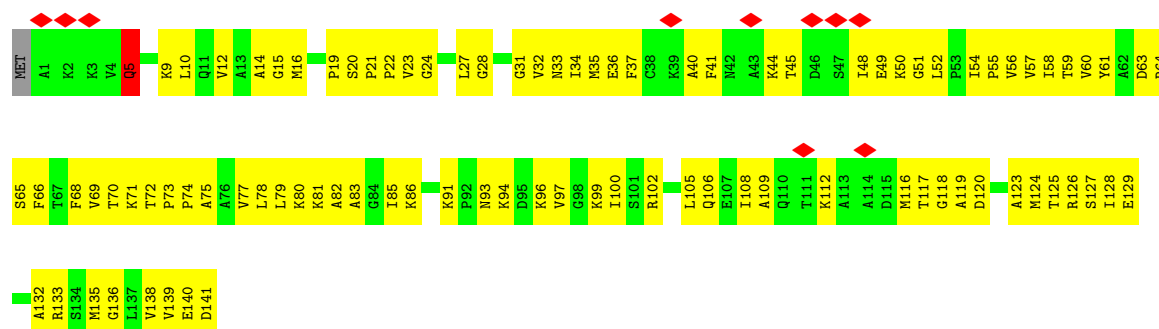
Chain W: 54% 34% 10%



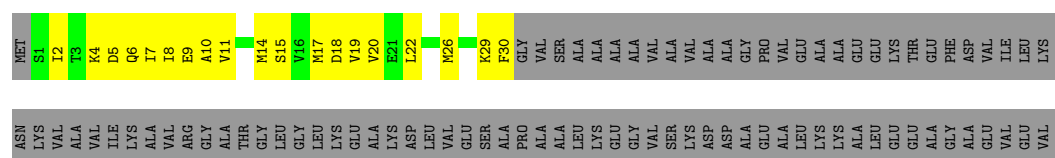
- Molecule 37: 30S ribosomal protein S13

[illegible]

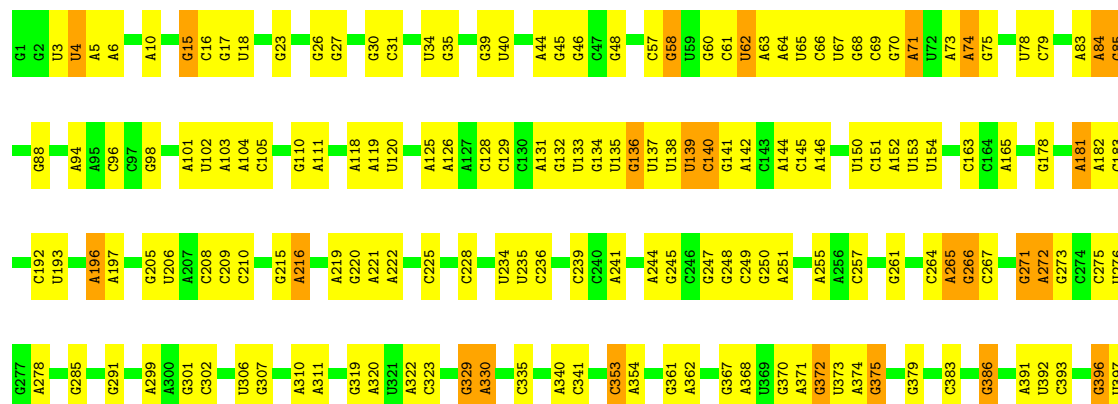
Chain Y: 7% 34% 65%



Chain Z: 9% 16% 75%



Chain a: 51% 41% 7%



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C1536	G1537	A1427	A1347	A1253	G1162	U1082	A1014	G940	U859	A764	G659	G585	A503	G400
A	G1617	C1428	C1348	G1256	C1167	A1084	U1019	A941	G860	C765	A666	C587	A504	A404
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G1649	A1548	A1433	A1353	G1266	U1172	A1089	G1024	C948	U872	G776	C672	U593	G410	G411
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G1651	G1361	G1441	G1361	A1269	A1175	A1085	G1026	G953	G874	A781	U677	U595	U521	A411
A1652	C1362	U1442	C1362	C1270	U1176	A1086	A1027	G954	U878	A782	A685	U596	A522	C413
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G1682	G1403	G1500	G1403	C1315	A1214	C1135	U1061	A990	A911	U826	U734	A632	G557	A475
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G1707	U1421	U1519	U1421	G1345	U1248	U1155	G1080	U932	A932	U843	U751	A652	U583	A492
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C2905	C2805	A2725	C2636	G2549	G2391	U2312	G2230	G2157	A2071	G1922	G1921	G1836	
U2903	U2903	A2726	U2637	G2550	U2473	C2313	G2231	C2158	C2072	U1923	U1923	A1754	A1754
U	U	U	U2638	C2551	C2475	A2314	U2236	G2159	C2073	C1924	C1924	G1840	A1755
			U2639	U2552	A2476	G2315	G2237	G2160	U2075	C2006	C1925	U1841	A1756
			U2640	U2554	U2477	C2396	G2238	G2161		U2007	U1926	G1842	U1758
					A2478	G2396	G2239	C2162	A2082		A1927	C1843	
					G2481	U2321	U2243	G2163	G2082	G2010	A1928	C1844	C1764
					A2482	A2322	U2244	A2163	G2083	U2011	A1936	G1845	
					C2483	G2325	U2245	C2164	G2086	G2012	U1937	G1846	G1770
					G2484	C2326	U2246	C2165	G2087	A2013	A1938	A1773	A1773
					G2485	A2327	A2247	G2168	C2091	A2014	U	C1774	C1774
						A2328	C2248	A2169	U2092	U2016	A1936	A1853	
						U2329	U2249	G2170	U2093	U2017	A1937	A1854	U1778
						G2330	G2250	A2171	G2093	G1930	A1938	U1855	U1779
						C2331	G	U2172	A2094	A2020	U	U1856	
						A2332	G2252	C2175	C2096	C2021	A1940	G1857	A1784
						C2333	G2253	A2176	A2097	C2022		A1785	A1785
						A2334	C2254	C2177	U2098	C2023		A1786	
						A2335	U2259	C2178	C2099	G2024	U1944	G1862	A1789
						C2339	G2260	C2179	G2100	U2026	U1946	G1863	C1790
							U2262	U2180	G2108	G2027	C1947	U1864	A1791
						G2345	C2263	U2181	A2108	U2028	A1953	G1869	G1792
						A2346	A2266	U2182	U2109	G2029	G1954	C1870	C1793
						C2347	A2267	A2183	G2110	A	U1955	A1794	A1794
						U2348	A2267	U2184	U2111	A2031	U1956	A1871	C1795
						G2349	A2268	U2185	G2112	G2032	U1956	A1872	C1796
						C2350	A2268	U2185	U2113	A2033	C1957	G1873	G1797
						G2351	A2273	U2189	A2114	U2034	C1958	C1874	U1798
							A2274	G2190	G2115	G2035	G1959	G1799	G1799
							C2275	A2191	G2116	C2036	A1960	C1800	C1800
							A2278	U2192	A2117	A2037	C	A1801	A1801
								G2193	U2118	G2038	U1963	A1802	A1802
								U2194	U2118	G2040	G1965	U1882	A1803
							C2283	U2197	G2121	U2041	C1966	U1883	A1808
							A2287	A2198	G2122	U2042	C1967	G1884	A1811
							U2288	A2199	G2123	U2043	U1963	A1885	
							G2289	C2200	G2124	C2044	C1967	A1885	G1811
							G2290	G2204	G2125			A1889	C1816
							U2291	A2205	G2126	G2049	A1970	G1817	C1816
							U2292	C2206	G2127	U2050	U1971	U1818	U1818
							U2293	A2205	G2128	A2051	G1972	U1819	A1819
							G2294	C2206	U2131	A2052		U1820	U1820
							C2295	A2211	U2132		A1981	G1906	G1906

- Molecule 41: 50S ribosomal protein L27

Chain b: 



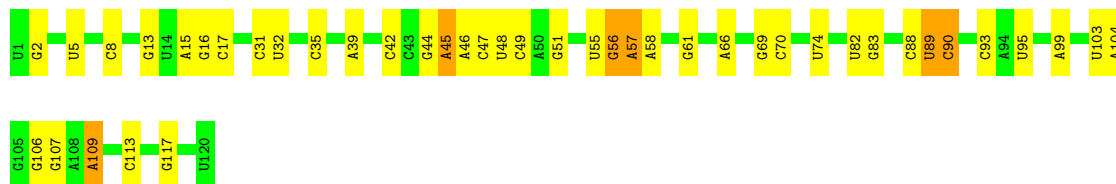
- Molecule 42: 50S ribosomal protein L28

Chain c: 



- Molecule 43: 5S rRNA

Chain d: 



- Molecule 44: 50S ribosomal protein L29

Chain e: 



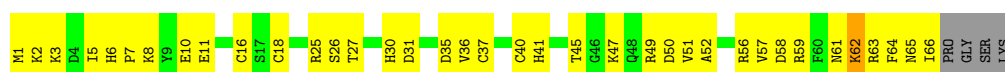
- Molecule 45: 50S ribosomal protein L30

Chain f: 



- Molecule 46: 50S ribosomal protein L31

Chain g: 



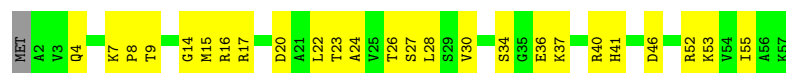
- Molecule 47: 50S ribosomal protein L2

Chain h: 



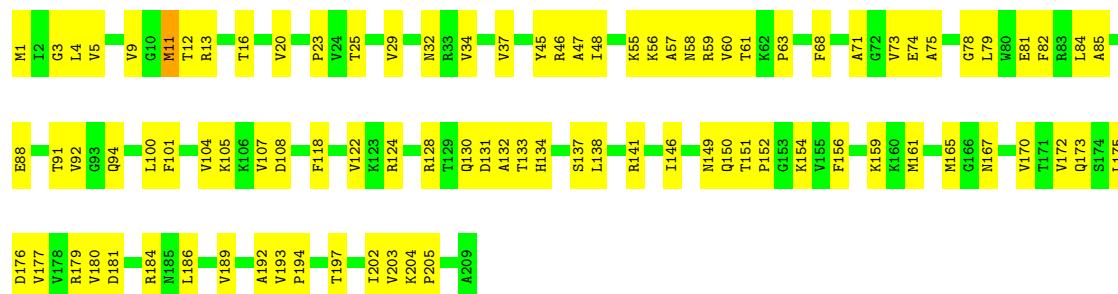
• Molecule 48: 50S ribosomal protein L32

Chain i: 54% 44%



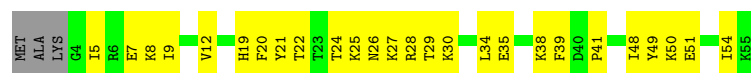
• Molecule 49: 50S ribosomal protein L3

Chain j: 56% 44%



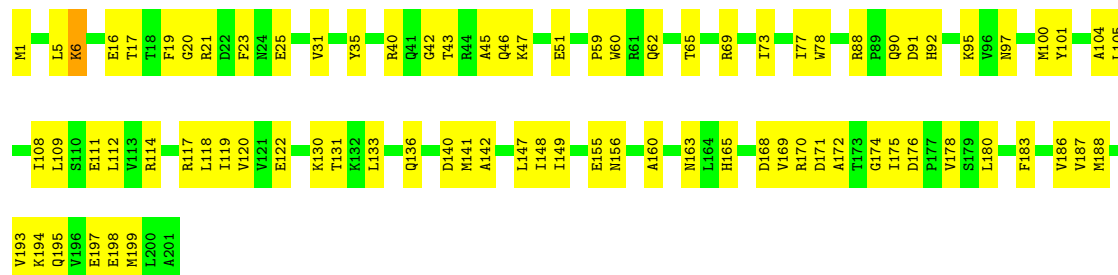
• Molecule 50: 50S ribosomal protein L33

Chain k: 47% 47%



• Molecule 51: 50S ribosomal protein L4

Chain l: 59% 40%

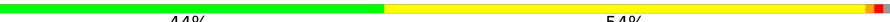


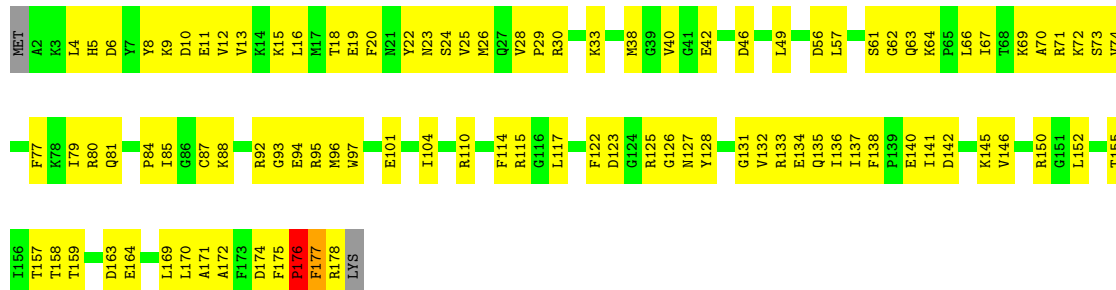
- Molecule 52: 50S ribosomal protein L34

Chain m:  57% 43%



- Molecule 53: 50S ribosomal protein L5

Chain n:  44% 54% ...



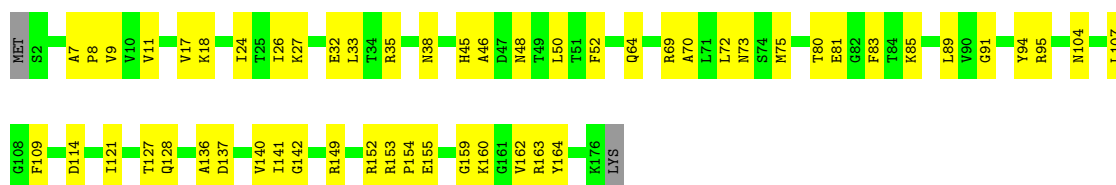
- Molecule 54: 50S ribosomal protein L35

Chain o:  58% 35% 5% •



- Molecule 55: 50S ribosomal protein L6

Chain p:  68% 31% •



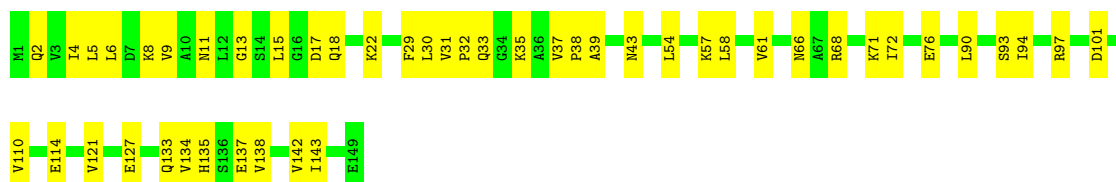
- Molecule 56: 50S ribosomal protein L36

Chain q:  61% 39%



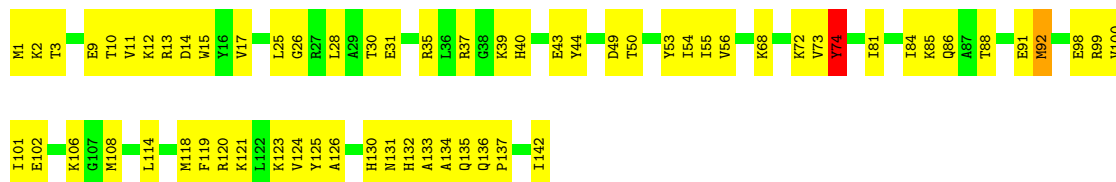
- Molecule 57: 50S ribosomal protein L9

Chain r:  68% 32%



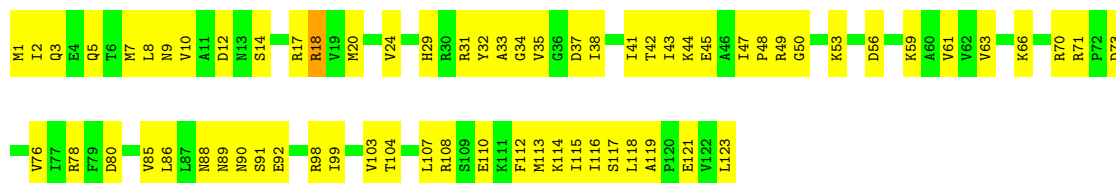
- Molecule 58: 50S ribosomal protein L13

Chain s: 55% 44% ..



- Molecule 59: 50S ribosomal protein L14

Chain t: 46% 54% .



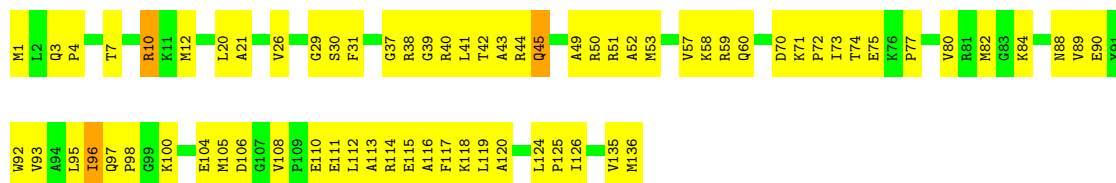
- Molecule 60: 50S ribosomal protein L15

Chain u: 62% 37% .



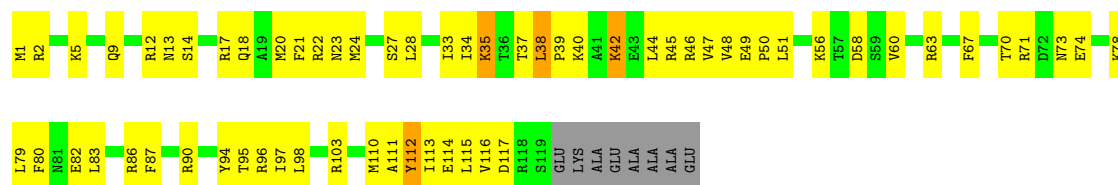
- Molecule 61: 50S ribosomal protein L16

Chain v: 49% 49% .



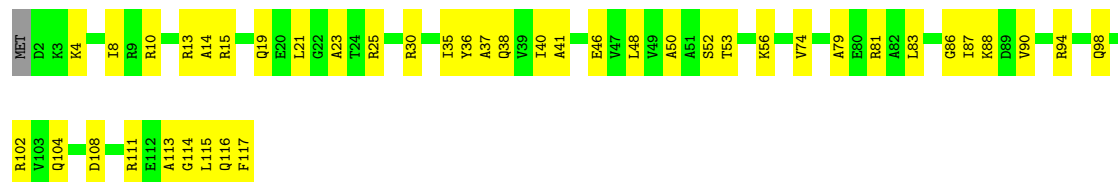
- Molecule 62: 50S ribosomal protein L17

Chain w: 44% 46% 6%



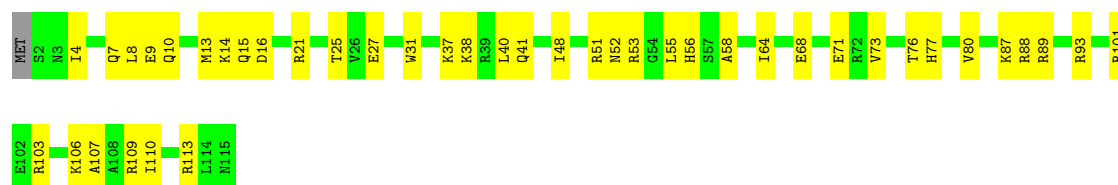
• Molecule 63: 50S ribosomal protein L18

Chain x: 63% 36%



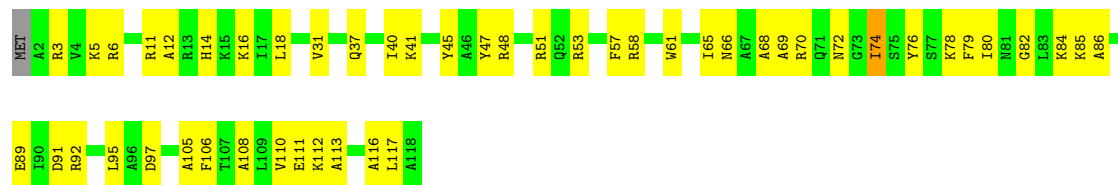
• Molecule 64: 50S ribosomal protein L19

Chain y: 63% 37%



• Molecule 65: 50S ribosomal protein L20

Chain z: 58% 41%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10509	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 ($e^-/\text{\AA}^2$)	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	0.032	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0025	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 ⓘ

5.1 Standard geometry ⓘ

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	0.43	0/829	0.51	0/1107
2	1	0.60	0/864	0.63	0/1156
3	2	0.55	1/752 (0.1%)	0.67	0/1005
4	3	0.35	0/796	0.49	0/1062
5	4	0.57	0/766	0.63	0/1025
6	5	0.56	0/816	0.77	0/1259
7	6	0.56	0/783	0.77	0/1203
8	7	0.56	2/879 (0.2%)	0.86	3/1364 (0.2%)
9	9	0.36	0/1131	0.74	2/1524 (0.1%)
10	A	0.27	0/1810	0.58	0/2821
10	B	0.27	0/1810	0.58	0/2821
11	AA	0.38	0/10547	0.62	0/14232
12	AB	0.46	0/1317	1.10	9/1786 (0.5%)
13	AC	0.38	0/1718	0.61	0/2328
13	AD	0.32	0/1696	0.60	0/2298
14	AE	0.39	0/10561	0.64	5/14258 (0.0%)
15	AF	0.29	0/652	0.61	0/879
16	C	0.67	0/553	0.81	1/743 (0.1%)
17	D	0.29	0/36610	0.41	9/57091 (0.0%)
18	E	0.61	0/675	0.72	0/895
19	F	0.53	0/597	0.60	0/792
20	G	0.68	5/1791 (0.3%)	0.79	8/2413 (0.3%)
21	H	0.38	0/1746	0.81	0/2382
22	I	0.57	1/1663 (0.1%)	0.68	4/2241 (0.2%)
23	J	0.46	0/1665	0.58	0/2227
24	K	0.72	2/1165 (0.2%)	0.86	6/1568 (0.4%)
25	L	0.68	1/867 (0.1%)	0.79	1/1171 (0.1%)
26	M	0.56	0/1195	0.69	2/1602 (0.1%)
27	N	0.50	0/989	0.58	0/1326
28	O	0.66	3/1034 (0.3%)	0.79	3/1375 (0.2%)
29	P	0.49	0/800	0.65	1/1082 (0.1%)
30	Q	0.72	2/893 (0.2%)	0.76	2/1205 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	R	0.49	0/952	0.59	0/1274
32	S	0.53	0/817	0.61	0/1088
33	T	0.57	1/722 (0.1%)	0.68	0/964
34	U	0.41	0/659	0.53	0/884
35	V	0.49	0/657	0.63	0/881
36	W	0.56	1/680 (0.1%)	0.62	1/915 (0.1%)
37	X	0.45	0/909	0.72	1/1215 (0.1%)
38	Y	0.38	2/1046 (0.2%)	0.66	2/1410 (0.1%)
39	Z	0.13	0/227	0.41	0/304
40	a	0.30	0/69247	0.43	10/107985 (0.0%)
41	b	0.42	0/589	0.56	0/779
42	c	0.51	0/635	0.61	0/848
43	d	0.25	0/2872	0.37	0/4478
44	e	0.69	2/502 (0.4%)	0.65	1/667 (0.1%)
45	f	0.52	0/452	0.57	0/605
46	g	0.45	1/531 (0.2%)	0.64	0/709
47	h	0.49	1/2121 (0.0%)	0.58	1/2852 (0.0%)
48	i	0.41	0/450	0.55	0/599
49	j	0.51	0/1586	0.57	1/2134 (0.0%)
50	k	0.45	0/433	0.62	0/576
51	l	0.51	1/1571 (0.1%)	0.62	0/2113
52	m	0.45	0/380	0.56	0/498
53	n	0.46	0/1434	0.66	1/1926 (0.1%)
54	o	0.51	0/513	0.71	1/676 (0.1%)
55	p	0.41	0/1333	0.62	2/1805 (0.1%)
56	q	0.46	0/303	0.64	0/397
57	r	0.28	0/1122	0.48	0/1515
58	s	0.70	2/1152 (0.2%)	0.74	2/1551 (0.1%)
59	t	0.52	0/955	0.75	3/1279 (0.2%)
60	u	0.43	0/1062	0.59	0/1413
61	v	0.60	1/1093 (0.1%)	0.77	3/1460 (0.2%)
62	w	0.83	3/964 (0.3%)	0.80	3/1289 (0.2%)
63	x	0.34	0/902	0.50	0/1209
64	y	0.41	0/929	0.54	0/1242
65	z	0.61	2/960 (0.2%)	0.62	0/1278
All	All	0.39	34/190730 (0.0%)	0.53	88/281059 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	9	0	3
12	AB	0	10
13	AC	0	1
13	AD	0	1
14	AE	0	4
20	G	0	1
21	H	0	5
22	I	0	1
24	K	0	2
28	O	0	1
37	X	0	1
38	Y	0	1
53	n	0	1
54	o	0	1
58	s	0	1
60	u	0	2
All	All	0	36

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	w	35	LYS	CE-NZ	-12.77	1.11	1.49
28	O	80	ARG	CD-NE	-10.47	1.31	1.46
62	w	42	LYS	CD-CE	-9.38	1.24	1.52
24	K	45	ARG	CG-CD	7.74	1.75	1.52
65	z	74	ILE	CG1-CD1	7.59	1.81	1.51

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	71	MET	CG-SD-CE	-11.34	75.95	100.90
20	G	158	PRO	N-CD-CG	-10.97	86.74	103.20
12	AB	141	LEU	CA-C-N	-10.59	106.28	122.16
12	AB	141	LEU	C-N-CA	-10.59	106.28	122.16
25	L	102	MET	CA-CB-CG	-9.59	94.91	114.10

There are no chirality outliers.

5 of 36 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
12	AB	106	ASP	Peptide
12	AB	116	VAL	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	816	839	839	54	0
2	1	857	922	922	68	0
3	2	746	811	811	61	0
4	3	788	844	844	45	0
5	4	753	780	780	88	0
6	5	726	0	392	110	0
7	6	703	0	396	35	0
8	7	792	0	392	109	0
9	9	1117	0	1155	257	0
10	A	1620	826	827	109	0
10	B	1620	814	827	111	0
11	AA	10381	0	10390	234	0
12	AB	1286	0	1300	345	0
13	AC	1698	0	1718	11	0
13	AD	1677	0	1713	28	0
14	AE	10404	0	10626	269	0
15	AF	650	0	658	15	0
16	C	544	559	560	109	0
17	D	32703	16423	16453	737	0
18	E	669	719	719	82	0
19	F	589	629	629	59	0
20	G	1760	1785	1787	154	0
21	H	1730	1454	1455	163	0
22	I	1636	1710	1710	133	0
23	J	1643	1707	1707	85	0
24	K	1152	1196	1196	117	0
25	L	848	846	846	104	0
26	M	1181	1235	1238	123	0
27	N	979	1031	1031	95	0
28	O	1022	1070	1070	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	P	790	831	831	137	0
30	Q	877	887	887	96	0
31	R	939	1001	1001	91	0
32	S	805	844	844	76	0
33	T	714	734	734	92	0
34	U	649	666	666	63	0
35	V	648	691	691	68	0
36	W	663	688	688	47	0
37	X	900	964	965	111	0
38	Y	1032	0	1088	214	0
39	Z	227	0	237	29	0
40	a	61841	31077	31120	1318	0
41	b	582	599	599	48	0
42	c	625	652	652	33	0
43	d	2569	1301	1301	43	0
44	e	501	531	531	45	0
45	f	448	488	488	38	0
46	g	522	520	520	65	0
47	h	2082	2154	2154	138	0
48	i	444	459	458	48	0
49	j	1565	1617	1616	123	0
50	k	426	464	464	44	0
51	l	1552	1619	1619	125	0
52	m	377	418	418	30	0
53	n	1410	1443	1444	155	0
54	o	504	572	572	52	0
55	p	1313	1358	1358	74	0
56	q	302	343	343	25	0
57	r	1111	1148	1148	52	0
58	s	1129	1162	1162	122	0
59	t	946	1023	1023	103	0
60	u	1053	1129	1129	79	0
61	v	1074	1157	1157	123	0
62	w	951	994	994	103	0
63	x	892	923	923	49	0
64	y	917	962	962	52	0
65	z	947	1020	1019	79	0
66	AE	1	0	0	0	0
67	AE	2	0	0	3	0
All	All	177420	98639	128797	6796	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

The worst 5 of 6796 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:K:45:ARG:CD	24:K:45:ARG:CG	1.75	1.59
14:AE:79:LYS:HA	14:AE:81:ARG:CZ	1.26	1.59
6:5:10:DT:C7	11:AA:62:TYR:CD2	1.84	1.58
6:5:9:DG:H5''	11:AA:473:ARG:CB	1.29	1.58
6:5:11:DA:C5'	12:AB:67:THR:HG22	1.20	1.58

There are no symmetry-related clashes.

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%)	101 (69%)	42 (29%)	3 (2%)	5	28
11	AA	1312/1342 (98%)	1199 (91%)	112 (8%)	1 (0%)	48	82
12	AB	159/162 (98%)	109 (69%)	45 (28%)	5 (3%)	3	21
13	AC	217/329 (66%)	203 (94%)	12 (6%)	2 (1%)	14	49
13	AD	214/329 (65%)	198 (92%)	16 (8%)	0	100	100
14	AE	1331/1407 (95%)	1210 (91%)	115 (9%)	6 (0%)	24	63
15	AF	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
16	C	64/75 (85%)	63 (98%)	1 (2%)	0	100	100
18	E	84/87 (97%)	83 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	F	68/71 (96%)	68 (100%)	0	0	100	100
20	G	223/241 (92%)	212 (95%)	10 (4%)	1 (0%)	30	67
21	H	255/557 (46%)	182 (71%)	66 (26%)	7 (3%)	4	24
22	I	206/233 (88%)	193 (94%)	13 (6%)	0	100	100
23	J	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
24	K	154/167 (92%)	145 (94%)	8 (5%)	1 (1%)	21	58
25	L	102/135 (76%)	97 (95%)	4 (4%)	1 (1%)	12	47
26	M	149/179 (83%)	140 (94%)	8 (5%)	1 (1%)	18	55
27	N	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
28	O	125/130 (96%)	116 (93%)	8 (6%)	1 (1%)	16	52
29	P	97/103 (94%)	89 (92%)	8 (8%)	0	100	100
30	Q	115/129 (89%)	107 (93%)	8 (7%)	0	100	100
31	R	117/124 (94%)	112 (96%)	5 (4%)	0	100	100
32	S	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
33	T	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
34	U	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
35	V	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
36	W	81/92 (88%)	80 (99%)	1 (1%)	0	100	100
37	X	114/118 (97%)	103 (90%)	9 (8%)	2 (2%)	6	32
38	Y	139/142 (98%)	101 (73%)	38 (27%)	0	100	100
39	Z	28/121 (23%)	22 (79%)	6 (21%)	0	100	100
41	b	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
42	c	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
44	e	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
45	f	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
46	g	64/70 (91%)	62 (97%)	2 (3%)	0	100	100
47	h	269/273 (98%)	255 (95%)	14 (5%)	0	100	100
48	i	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
49	j	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
50	k	50/55 (91%)	50 (100%)	0	0	100	100
51	l	199/201 (99%)	188 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	m	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
53	n	175/179 (98%)	161 (92%)	13 (7%)	1 (1%)	21	58
54	o	62/65 (95%)	57 (92%)	4 (6%)	1 (2%)	7	36
55	p	173/177 (98%)	162 (94%)	11 (6%)	0	100	100
56	q	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
57	r	147/149 (99%)	139 (95%)	8 (5%)	0	100	100
58	s	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
59	t	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
60	u	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
61	v	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
62	w	117/127 (92%)	112 (96%)	5 (4%)	0	100	100
63	x	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
64	y	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
65	z	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
All	All	9486/10558 (90%)	8740 (92%)	713 (8%)	33 (0%)	37	71

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	AB	141	LEU
12	AB	152	HIS
20	G	127	ASP
21	H	304	VAL
26	M	56	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	81 (100%)	0	100	100
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%)	112 (100%)	0	100	100
11	AA	1135/1157 (98%)	1130 (100%)	5 (0%)	84	83
12	AB	141/142 (99%)	139 (99%)	2 (1%)	59	71
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%)	1104 (98%)	18 (2%)	55	69
15	AF	70/75 (93%)	69 (99%)	1 (1%)	59	71
16	C	57/65 (88%)	57 (100%)	0	100	100
18	E	65/66 (98%)	65 (100%)	0	100	100
19	F	60/61 (98%)	60 (100%)	0	100	100
20	G	187/199 (94%)	187 (100%)	0	100	100
21	H	137/461 (30%)	137 (100%)	0	100	100
22	I	171/190 (90%)	171 (100%)	0	100	100
23	J	172/173 (99%)	171 (99%)	1 (1%)	78	81
24	K	119/126 (94%)	119 (100%)	0	100	100
25	L	91/116 (78%)	91 (100%)	0	100	100
26	M	124/147 (84%)	124 (100%)	0	100	100
27	N	104/105 (99%)	104 (100%)	0	100	100
28	O	105/107 (98%)	105 (100%)	0	100	100
29	P	86/90 (96%)	86 (100%)	0	100	100
30	Q	90/99 (91%)	90 (100%)	0	100	100
31	R	101/104 (97%)	101 (100%)	0	100	100
32	S	83/84 (99%)	83 (100%)	0	100	100
33	T	76/77 (99%)	76 (100%)	0	100	100
34	U	65/65 (100%)	65 (100%)	0	100	100
35	V	74/78 (95%)	74 (100%)	0	100	100
36	W	72/79 (91%)	72 (100%)	0	100	100
37	X	94/96 (98%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	Y	109/110 (99%)	109 (100%)	0	100	100
39	Z	26/85 (31%)	26 (100%)	0	100	100
41	b	58/63 (92%)	58 (100%)	0	100	100
42	c	67/68 (98%)	67 (100%)	0	100	100
44	e	54/55 (98%)	54 (100%)	0	100	100
45	f	48/49 (98%)	48 (100%)	0	100	100
46	g	59/62 (95%)	59 (100%)	0	100	100
47	h	216/218 (99%)	216 (100%)	0	100	100
48	i	47/48 (98%)	47 (100%)	0	100	100
49	j	164/164 (100%)	164 (100%)	0	100	100
50	k	47/49 (96%)	47 (100%)	0	100	100
51	l	165/165 (100%)	165 (100%)	0	100	100
52	m	38/38 (100%)	38 (100%)	0	100	100
53	n	148/150 (99%)	148 (100%)	0	100	100
54	o	51/52 (98%)	51 (100%)	0	100	100
55	p	136/138 (99%)	136 (100%)	0	100	100
56	q	34/34 (100%)	34 (100%)	0	100	100
57	r	114/114 (100%)	114 (100%)	0	100	100
58	s	116/116 (100%)	116 (100%)	0	100	100
59	t	104/104 (100%)	104 (100%)	0	100	100
60	u	103/103 (100%)	103 (100%)	0	100	100
61	v	109/109 (100%)	109 (100%)	0	100	100
62	w	99/103 (96%)	99 (100%)	0	100	100
63	x	86/87 (99%)	86 (100%)	0	100	100
64	y	99/100 (99%)	99 (100%)	0	100	100
65	z	89/90 (99%)	89 (100%)	0	100	100
All	All	7890/8723 (90%)	7863 (100%)	27 (0%)	84	84

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	AE	79	LYS
14	AE	85	CYS

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Mol	Chain	Res	Type
14	AE	1261	LEU
14	AE	84	ILE
14	AE	92	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
22	I	32	ASN
31	R	77	HIS
62	w	18	GLN
23	J	36	GLN
26	M	68	ASN

5.3.3 RNA ⓘ

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%)
17	D	1514/1542 (98%)	290 (19%)	20 (1%)
40	a	2859/2904 (98%)	511 (17%)	0
43	d	119/120 (99%)	15 (12%)	0
8	7	37/38 (97%)	28 (75%)	5 (13%)
All	All	4679/4756 (98%)	902 (19%)	41 (0%)

5 of 902 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
17	D	517	G
17	D	1213	A
17	D	991	U
17	D	1196	A

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Mol	Chain	Res	Type
17	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.

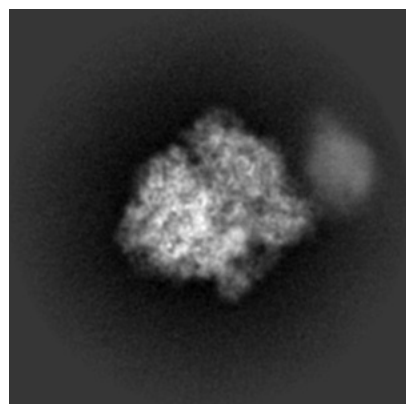
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42454. These allow visual inspection of the internal detail of the map and identification of artifacts.

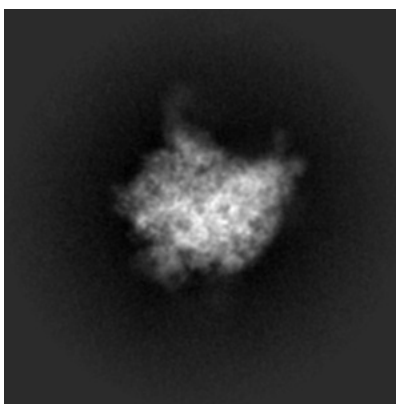
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

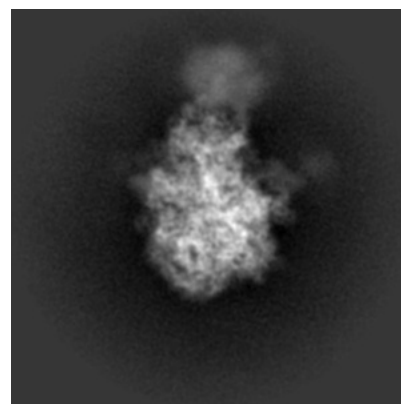
6.1.1 Primary map



X

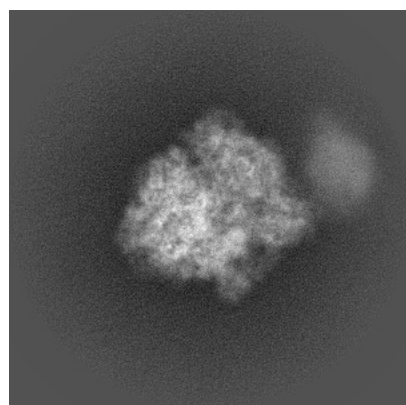


Y

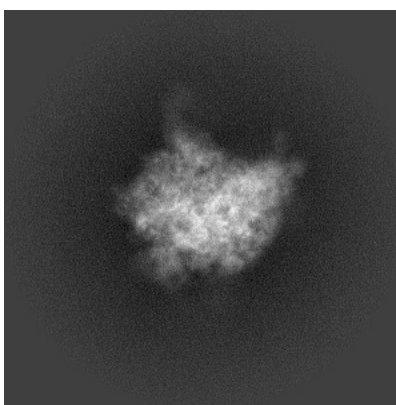


Z

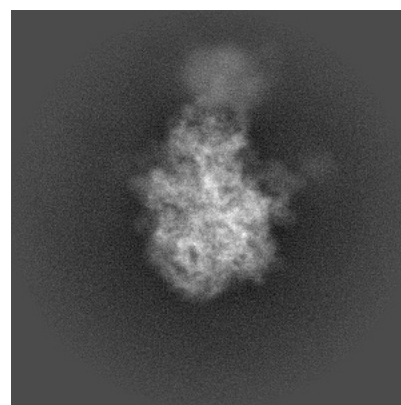
6.1.2 Raw map



X



Y

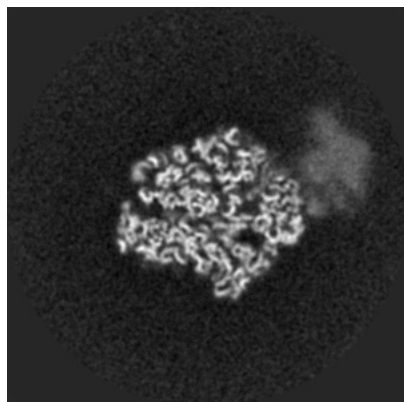


Z

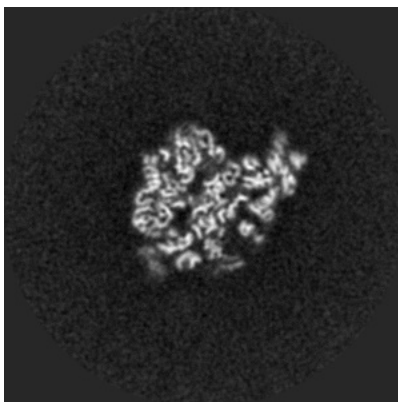
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

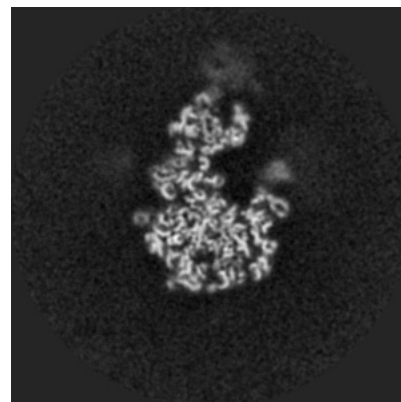
6.2.1 Primary map



X Index: 256

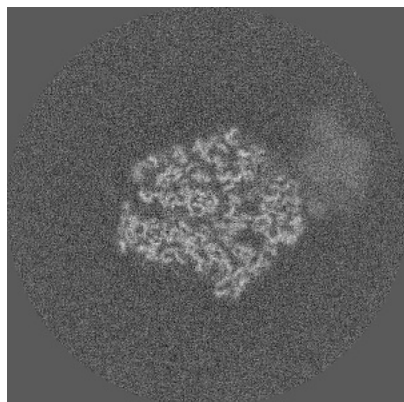


Y Index: 256

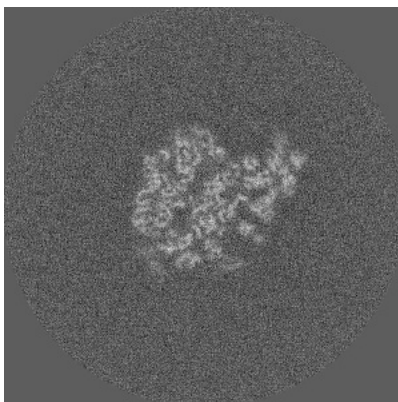


Z Index: 256

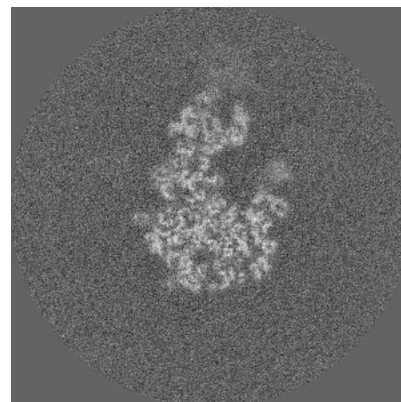
6.2.2 Raw map



X Index: 256



Y Index: 256

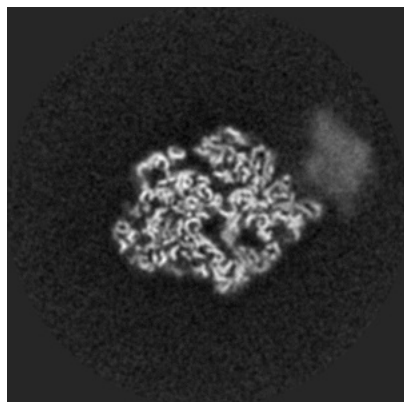


Z Index: 256

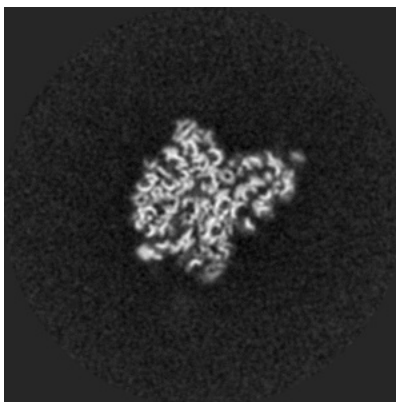
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

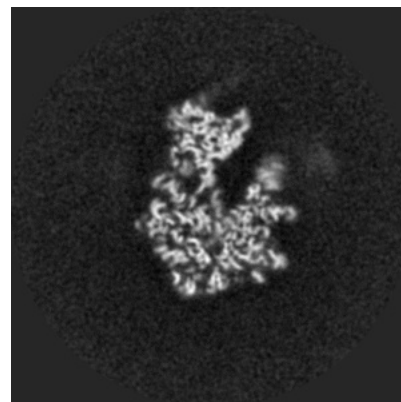
6.3.1 Primary map



X Index: 248

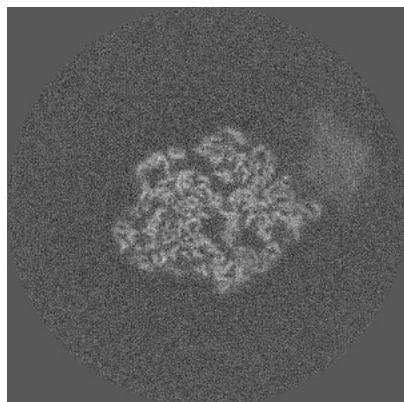


Y Index: 249

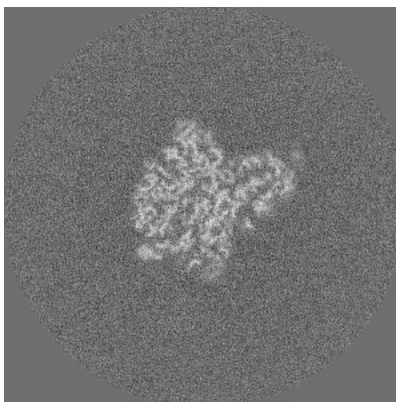


Z Index: 241

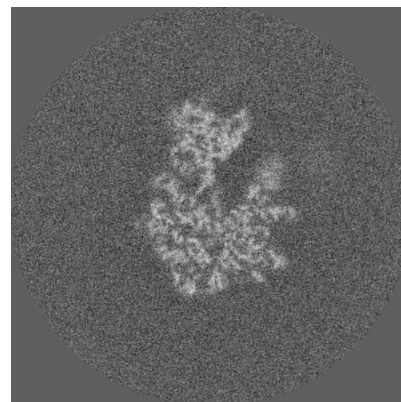
6.3.2 Raw map



X Index: 248



Y Index: 249

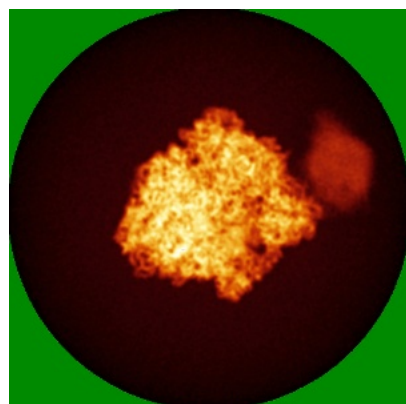


Z Index: 241

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

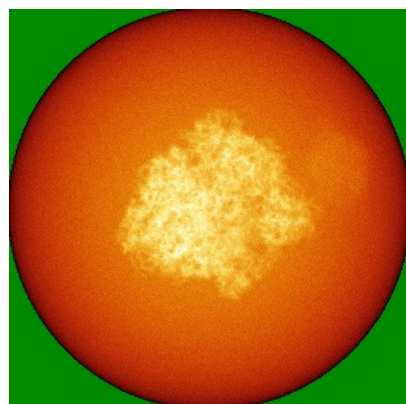


Y

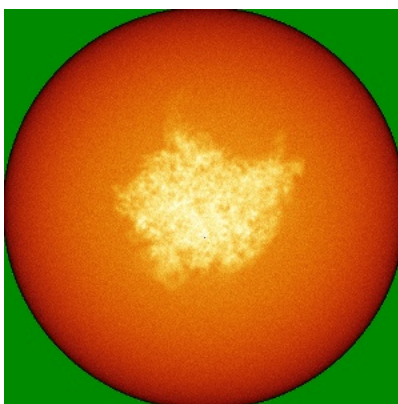


Z

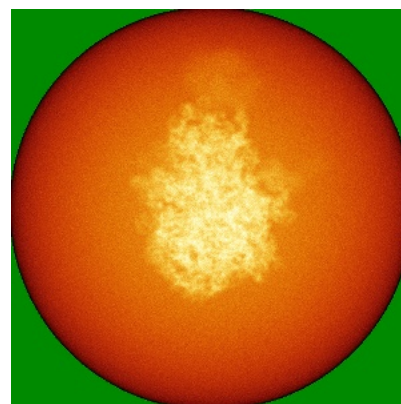
6.4.2 Raw map



X



Y

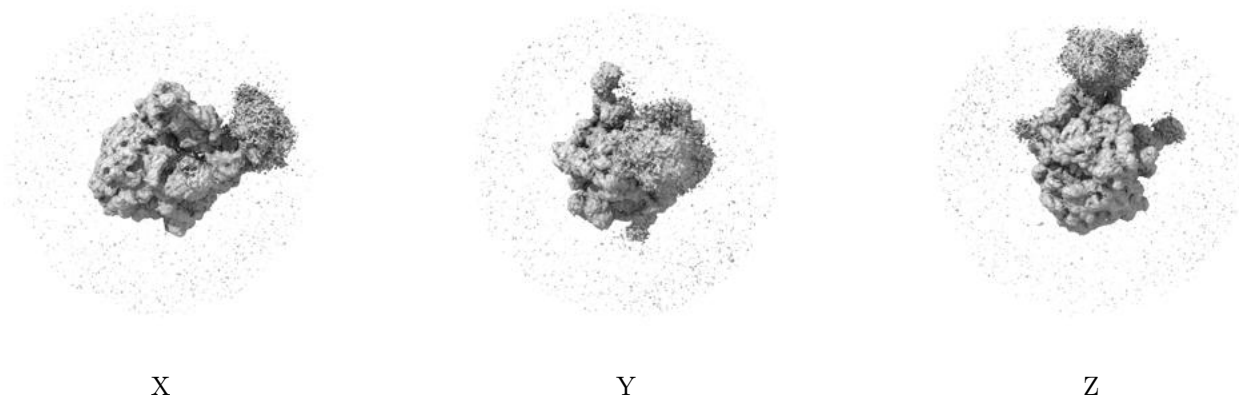


Z

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.

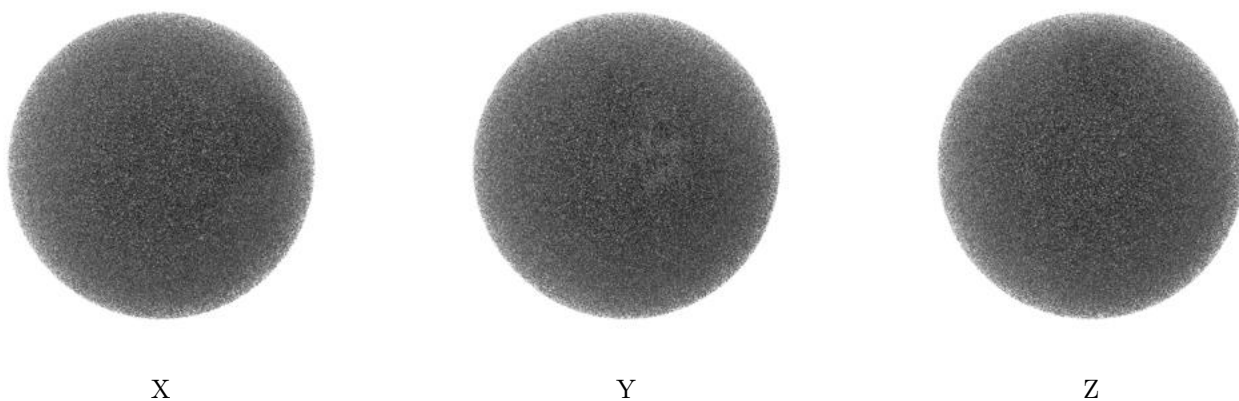
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0025. 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.

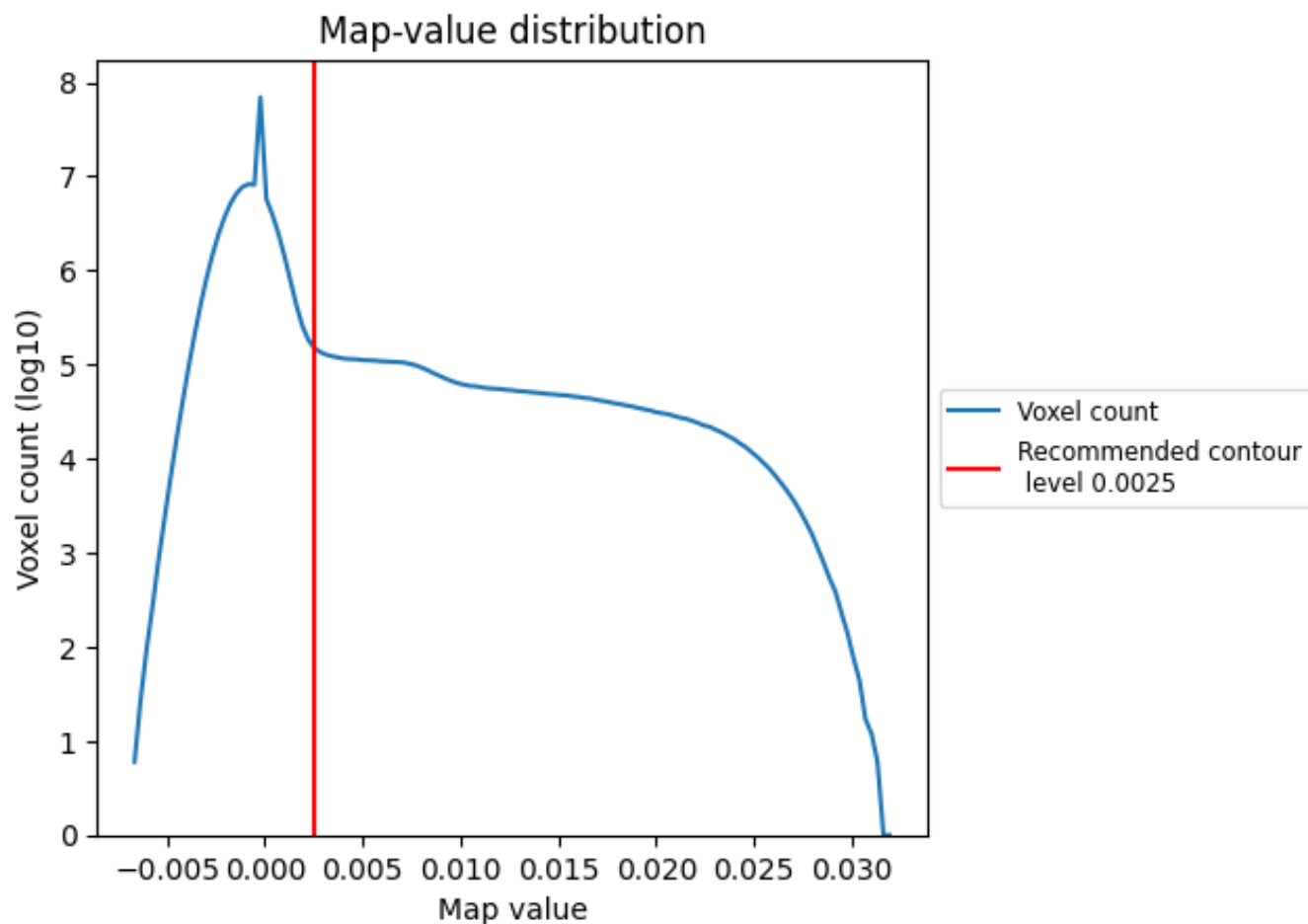
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

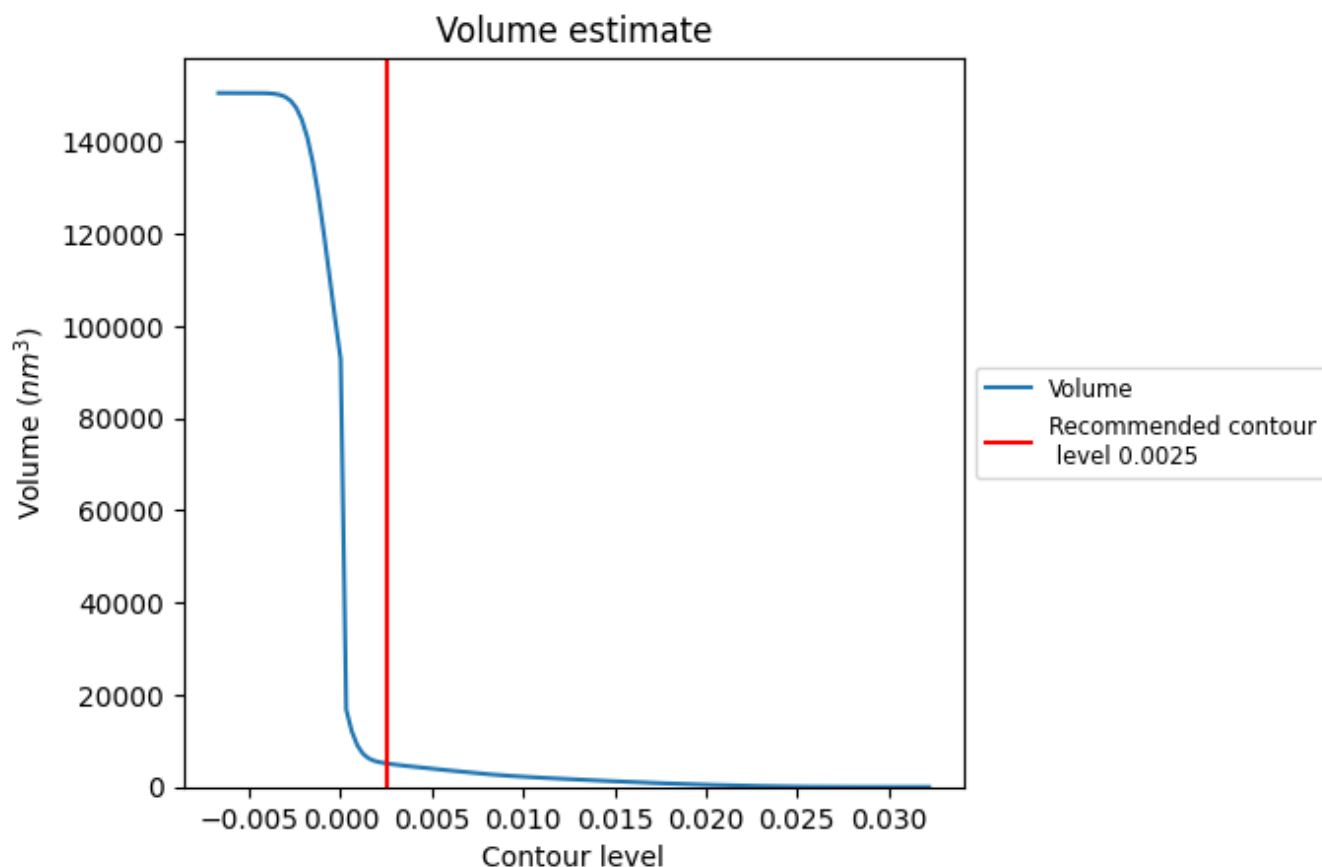
This section contains the results of statistical analysis of the map.

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.

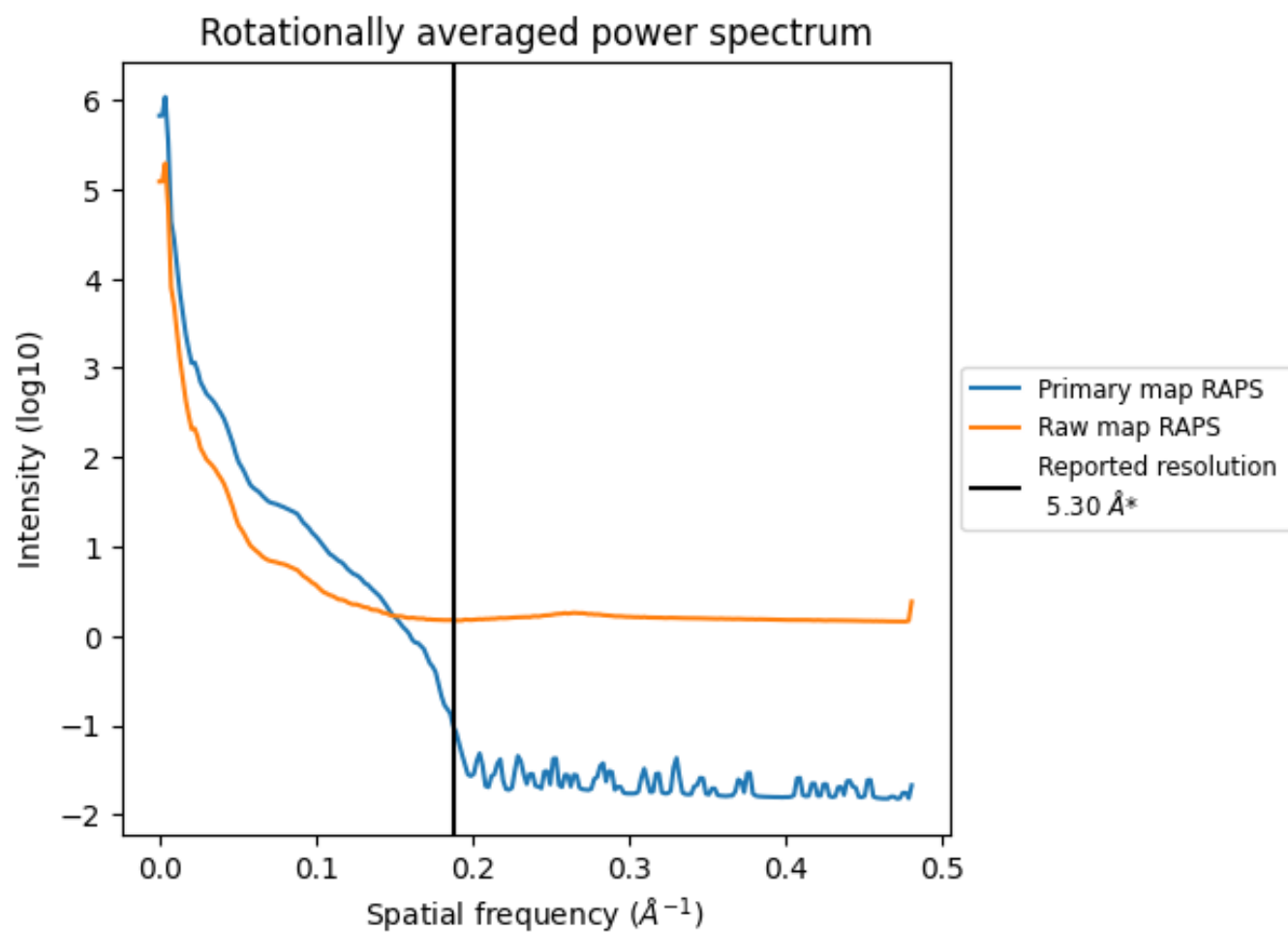
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5120 nm³; this corresponds to an approximate mass of 4625 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

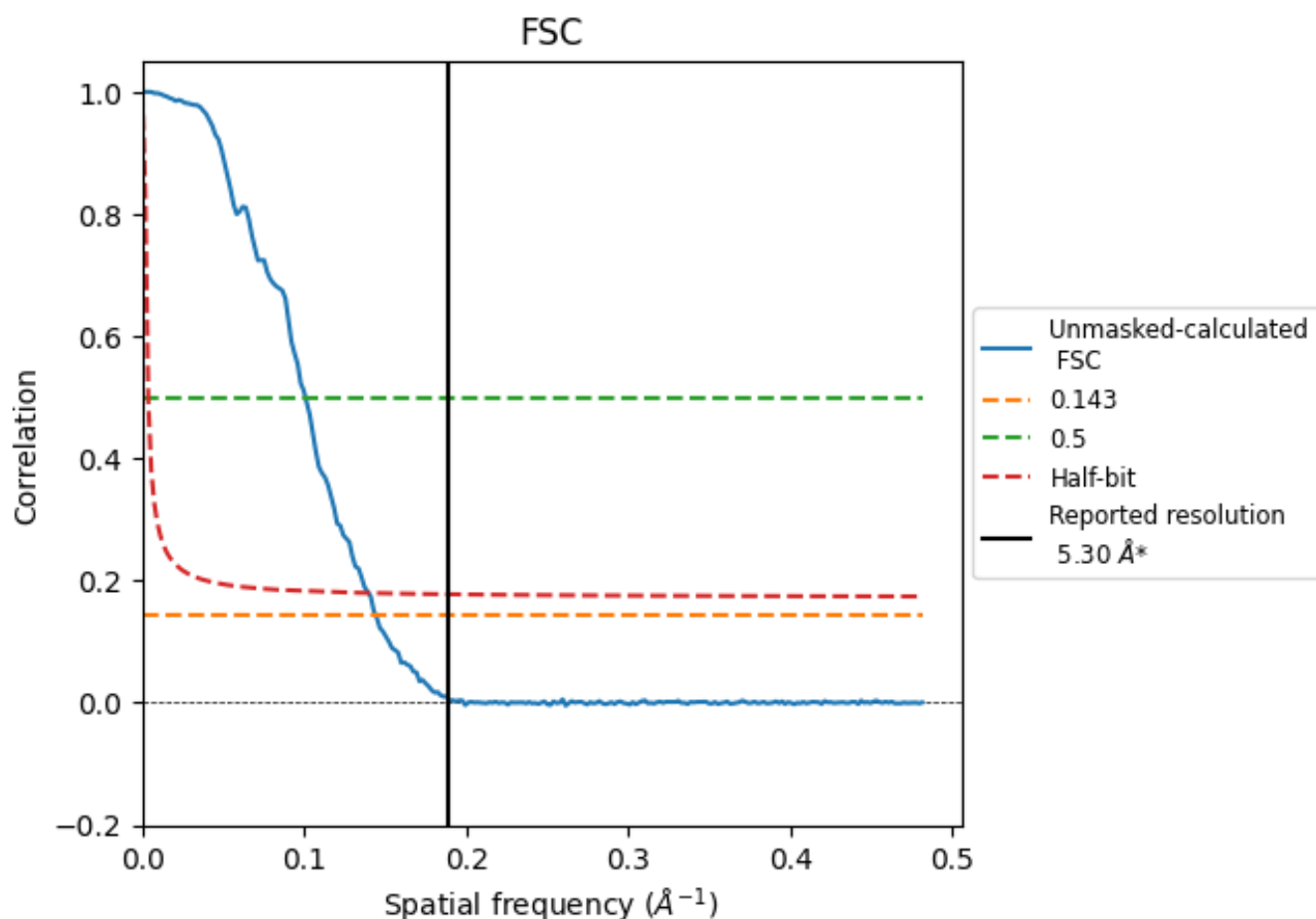


*Reported resolution corresponds to spatial frequency of 0.189 $\text{\AA}^{-1}$

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 0.189 Å⁻¹

8.2 Resolution estimates [i](#)

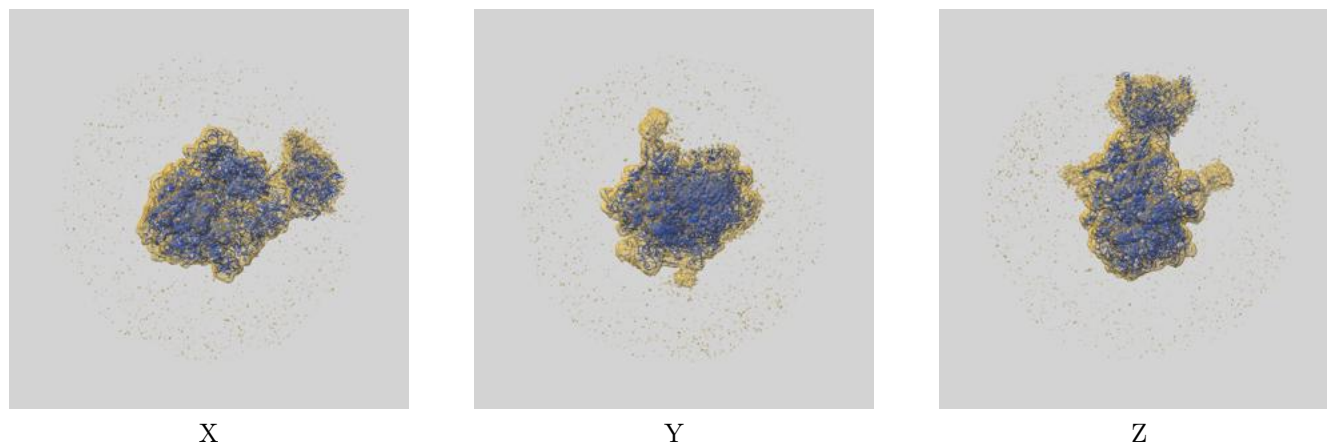
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.94	9.93	7.16

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

9 Map-model fit [i](#)

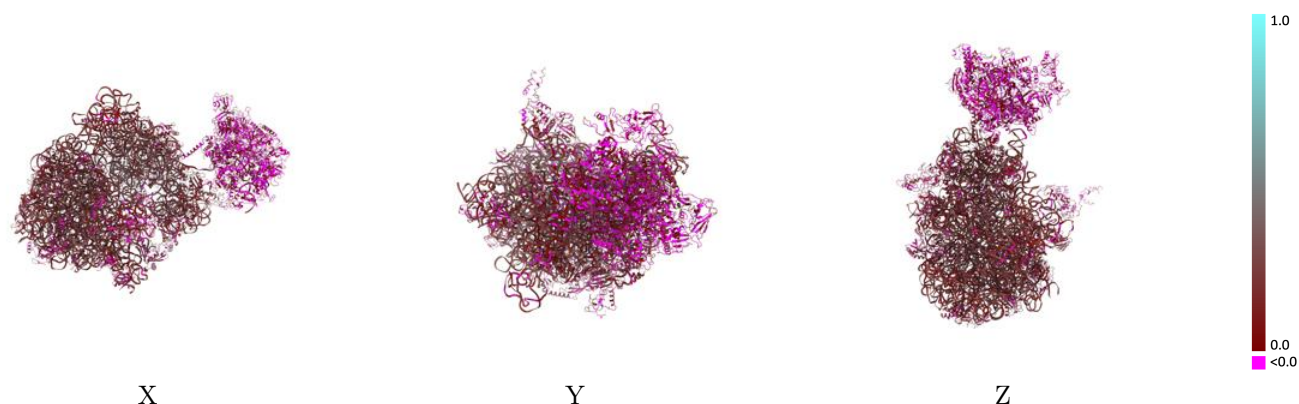
This section contains information regarding the fit between EMDB map EMD-42454 and PDB model 8UPR. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



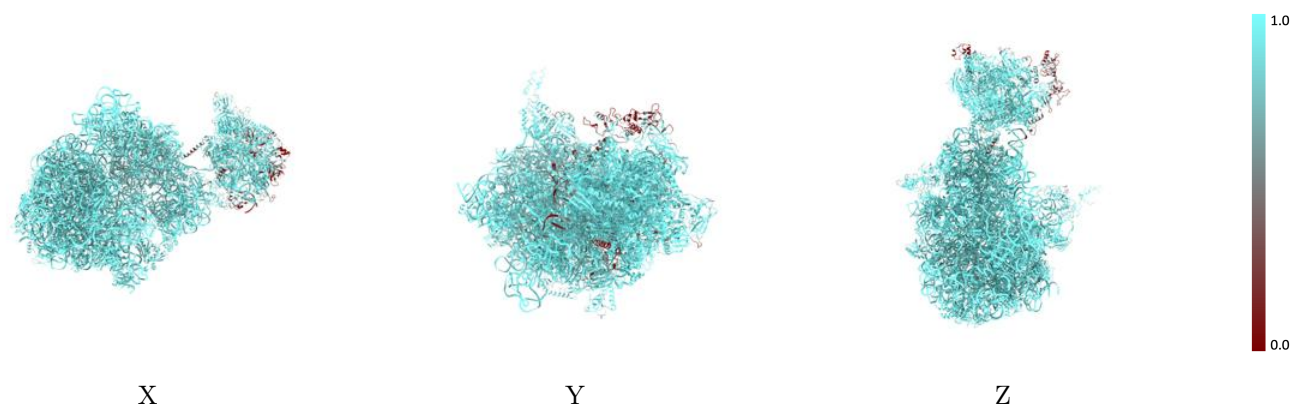
The images above show the 3D surface view of the map at the recommended contour level 0.0025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



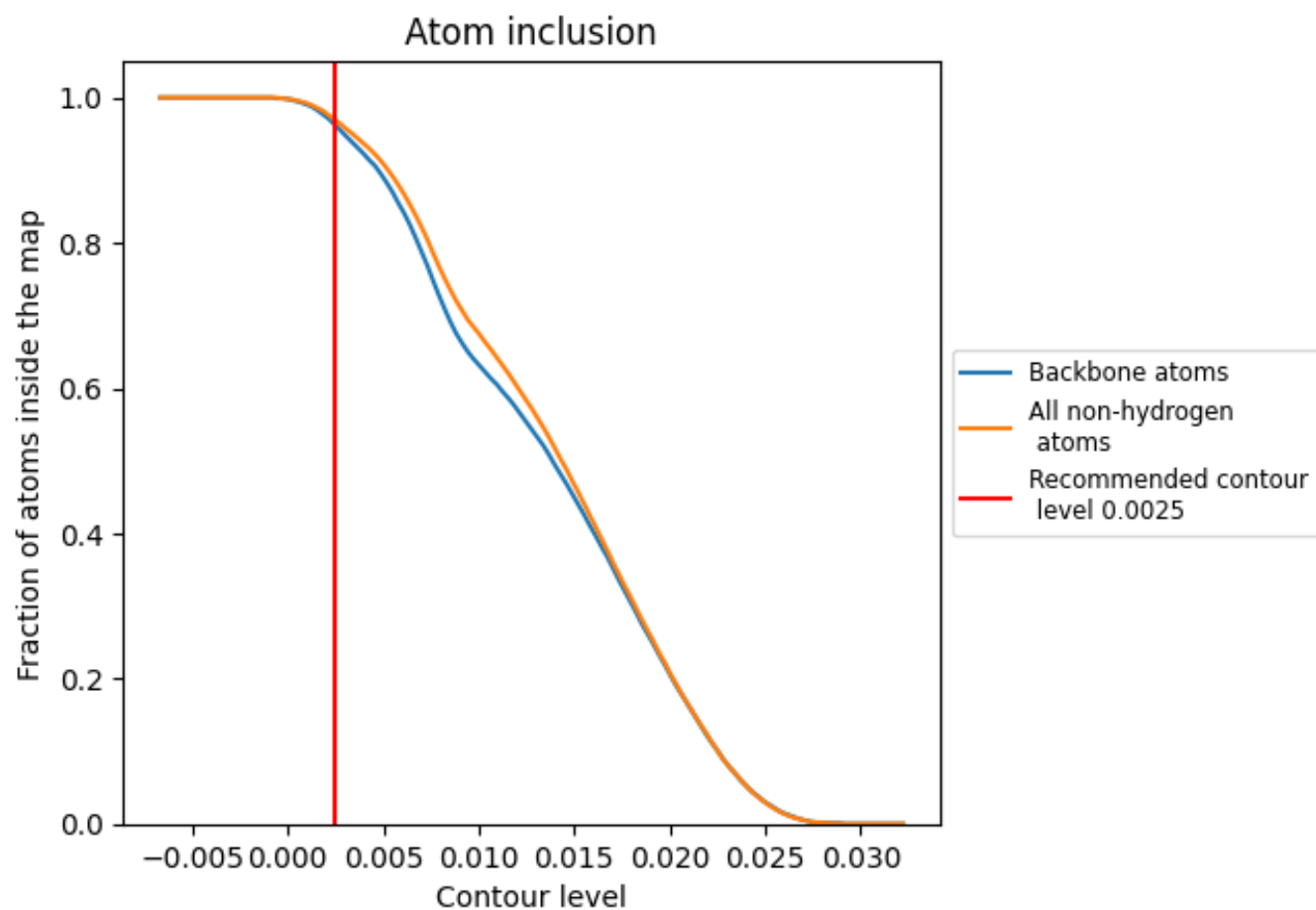
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 97% 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 (0.0025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9690	 0.1640
0	 0.9940	 0.1470
1	 0.9960	 0.1770
2	 0.9840	 0.1390
3	 0.9960	 0.1320
4	 0.9950	 0.1550
5	 0.8440	 0.0630
6	 0.8950	 0.0530
7	 0.9820	 0.0800
9	 0.9740	 0.0970
A	 1.0000	 0.1790
AA	 0.8530	 0.0180
AB	 0.7320	 0.0520
AC	 0.9780	 0.0280
AD	 0.9450	 0.0160
AE	 0.8920	 0.0320
AF	 0.7900	 0.0190
B	 0.9800	 0.1100
C	 0.9980	 0.1530
D	 0.9980	 0.2210
E	 0.9990	 0.1540
F	 0.9820	 0.1740
G	 0.9850	 0.1580
H	 0.9140	 0.0630
I	 0.9920	 0.1870
J	 0.9980	 0.1730
K	 0.9970	 0.2020
L	 1.0000	 0.1540
M	 0.9930	 0.1490
N	 0.9870	 0.1750
O	 0.9910	 0.1280
P	 1.0000	 0.1580
Q	 0.9970	 0.1510
R	 0.9980	 0.2050
S	 0.9970	 0.1650



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Chain	Atom inclusion	Q-score
T	 1.0000	 0.1490
U	 0.9980	 0.1610
V	 0.9910	 0.1670
W	 0.9750	 0.1230
X	 0.9930	 0.1390
Y	 0.9010	 0.0550
Z	 0.9690	 0.0340
a	 0.9990	 0.2090
b	 0.9970	 0.1270
c	 0.9920	 0.1580
d	 1.0000	 0.1810
e	 0.9920	 0.1320
f	 0.9930	 0.1740
g	 0.9940	 0.1140
h	 0.9930	 0.1500
i	 0.9910	 0.1870
j	 0.9960	 0.1550
k	 1.0000	 0.1360
l	 0.9890	 0.1340
m	 0.9940	 0.1680
n	 0.9880	 0.1240
o	 1.0000	 0.1240
p	 0.9980	 0.1480
q	 0.9970	 0.1410
r	 0.9660	 0.1120
s	 0.9960	 0.1710
t	 0.9900	 0.1740
u	 0.9940	 0.1280
v	 0.9920	 0.1800
w	 0.9950	 0.1510
x	 0.9820	 0.0900
y	 0.9940	 0.1690
z	 0.9970	 0.1390