wwPDB EM Validation Summary Report

Jun 24, 2026 – 11:32 AM EDT

PDB ID	:	11EL / pdb_000011el
EMDB ID	:	EMD-75650
Title	:	Chimeric Escherichia coli 70S ribosome containing an evolved 16S rRNA from Vibrio cholerae (VC-ST)
Authors	:	Raskar, T.
Deposited on	:	2026-02-19
Resolution	:	3.20 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:

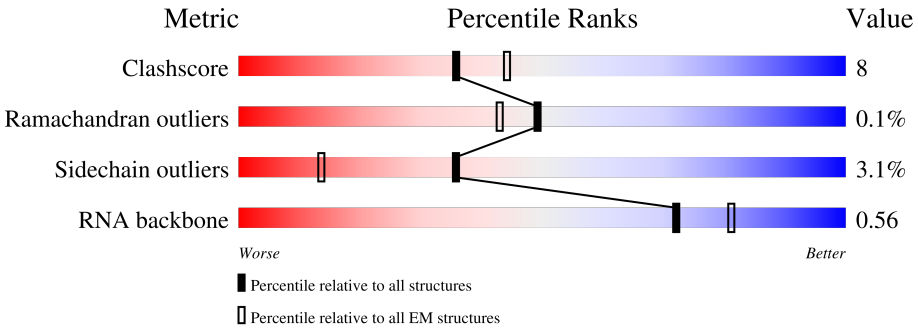
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

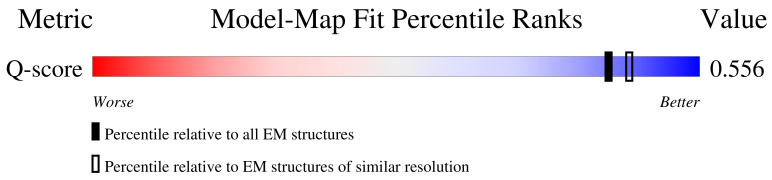
1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	0	55	11% 76% 16% 7%
2	1	46	87% 13%
3	2	65	77% 22%

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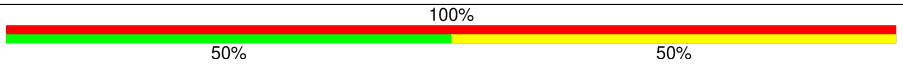
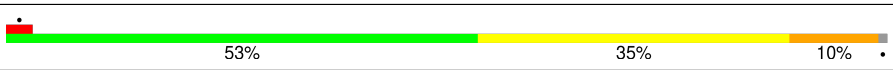
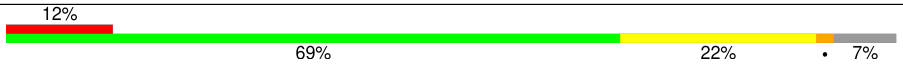
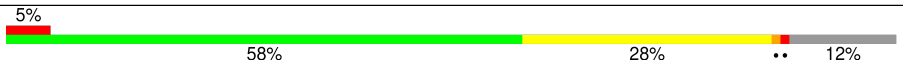
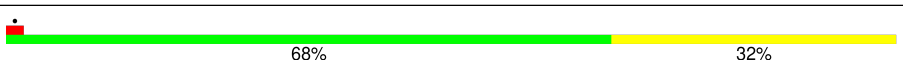
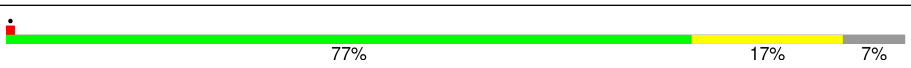
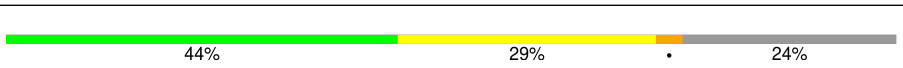
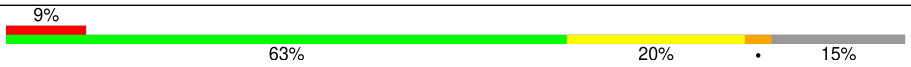
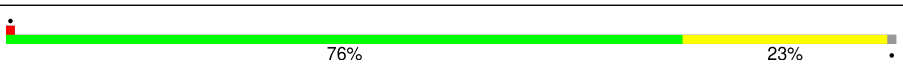
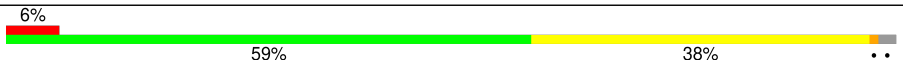
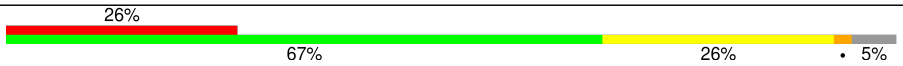
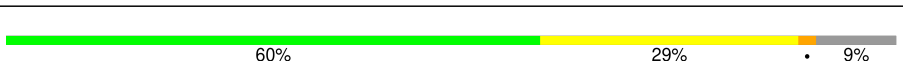
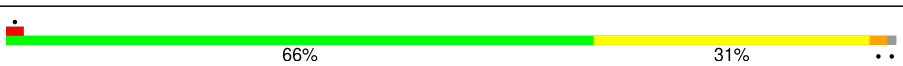
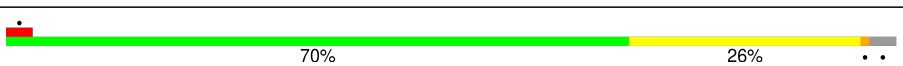
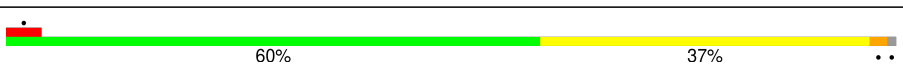
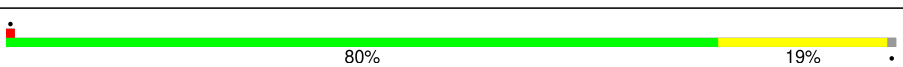
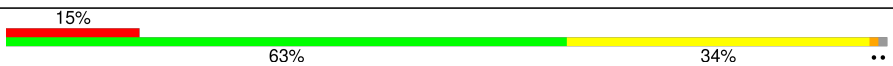
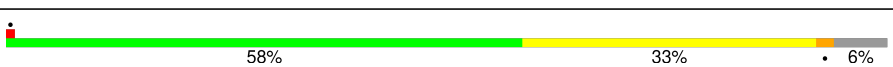
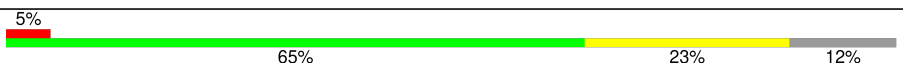
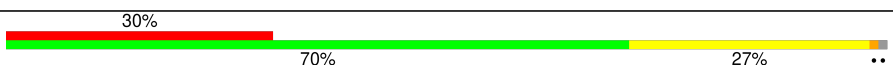
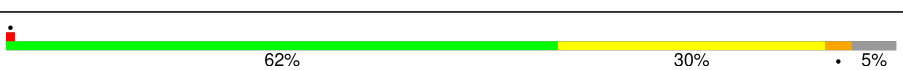
Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	5	2	
7	A	1543	
8	B	241	
9	C	233	
10	D	206	
11	E	167	
12	F	135	
13	G	179	
14	H	130	
15	I	130	
16	J	103	
17	K	129	
18	L	124	
19	M	118	
20	N	101	
21	O	89	
22	P	82	
23	Q	84	
24	R	75	
25	S	92	
26	T	87	
27	U	71	
28	a	2904	

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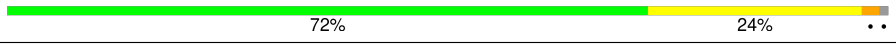
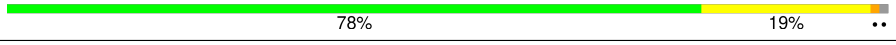
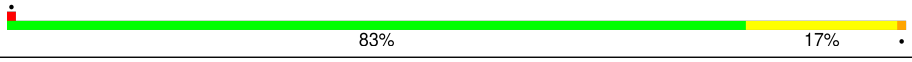
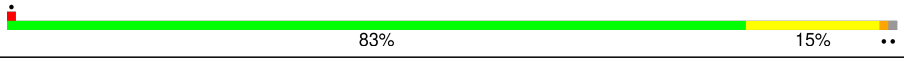
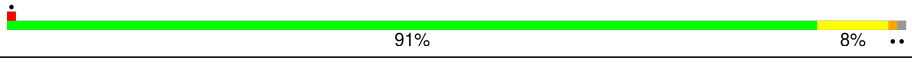
Mol	Chain	Length	Quality of chain
29	b	120	
30	c	273	
31	d	209	
32	e	201	
33	f	179	
34	g	177	
35	h	149	
36	i	142	
37	j	123	
38	k	144	
39	l	136	
40	m	127	
41	n	117	
42	o	115	
43	p	118	
44	q	103	
45	r	110	
46	s	100	
47	t	104	
48	u	94	
49	v	85	
50	w	78	
51	x	63	
52	y	59	
53	z	57	

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 138616 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

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

- Molecule 3 is a protein called 50S ribosomal protein L35.

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

- Molecule 4 is a protein called Large ribosomal subunit protein bL36A.

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

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

- Molecule 7 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	1520	Total	C	N	O	P	0	0
			32643	14567	5995	10561	1520		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	847	G	U	conflict	GB 3166933093

- Molecule 8 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 12 is a protein called Small ribosomal subunit protein bS6.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 17 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 18 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 19 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 20 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 21 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 22 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 23 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 24 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 25 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 26 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 27 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 28 is a RNA chain called 23S ribosomal RNA.

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

- Molecule 29 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 30 is a protein called 50S ribosomal protein L2.

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

- Molecule 31 is a protein called 50S ribosomal protein L3.

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

- Molecule 32 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 33 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 34 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 35 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 36 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 37 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 38 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 40 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 42 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 43 is a protein called 50S ribosomal protein L20.

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

- Molecule 44 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 45 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 46 is a protein called 50S ribosomal protein L23.

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

- Molecule 47 is a protein called 50S ribosomal protein L24.

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

- Molecule 48 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 49 is a protein called 50S ribosomal protein L27.

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

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

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

- Molecule 51 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 52 is a protein called 50S ribosomal protein L30.

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

- Molecule 53 is a protein called 50S ribosomal protein L32.

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

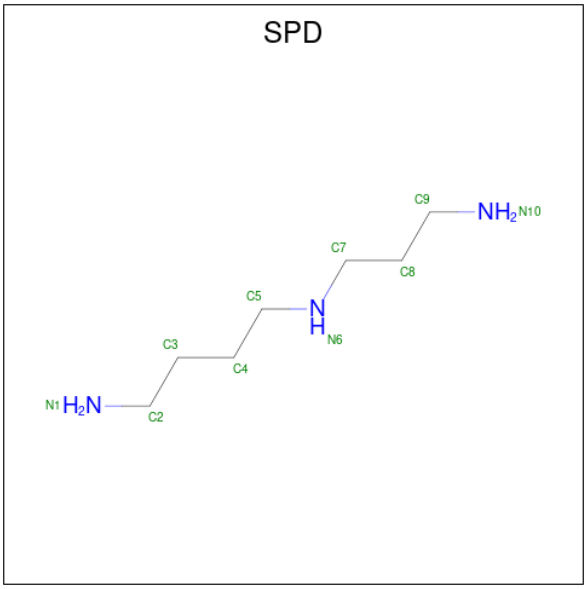
- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	3	1	Total	Zn	0
			1	1	
54	4	1	Total	Zn	0
			1	1	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
55	A	90	Total Mg 90 90	0
55	D	1	Total Mg 1 1	0
55	N	1	Total Mg 1 1	0
55	a	207	Total Mg 207 207	0
55	b	5	Total Mg 5 5	0
55	c	1	Total Mg 1 1	0
55	m	1	Total Mg 1 1	0
55	p	1	Total Mg 1 1	0
55	z	1	Total Mg 1 1	0

- Molecule 56 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	AltConf
56	A	1	Total C N 10 7 3	0
56	A	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0

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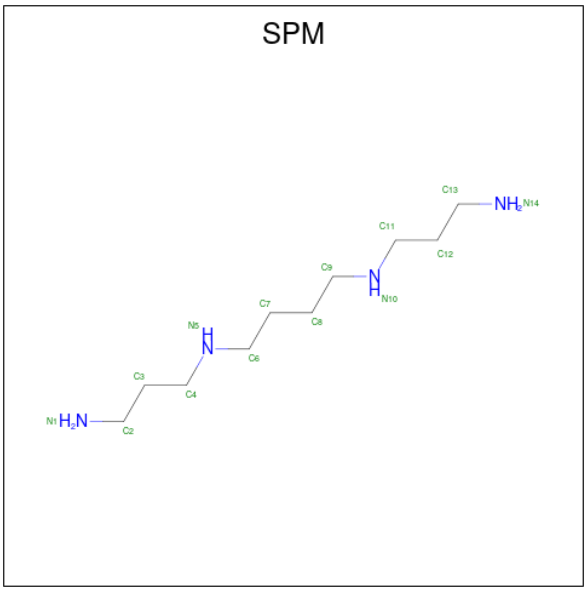
Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0
56	a	1	Total C N 10 7 3	0

- Molecule 57 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



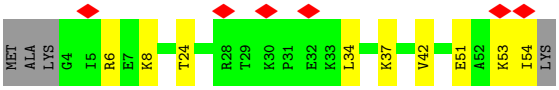
Mol	Chain	Residues	Atoms			AltConf
57	a	1	Total	C	N	0
			14	10	4	

3 Residue-property plots (i)

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

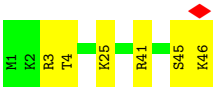
• Molecule 1: 50S ribosomal protein L33

Chain 0:



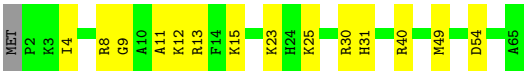
• Molecule 2: Large ribosomal subunit protein bL34

Chain 1:



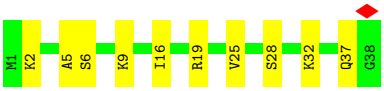
• Molecule 3: 50S ribosomal protein L35

Chain 2:



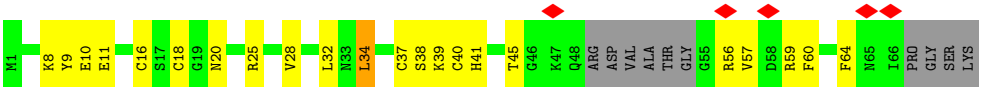
• Molecule 4: Large ribosomal subunit protein bL36A

Chain 3:



• Molecule 5: 50S ribosomal protein L31

Chain 4:

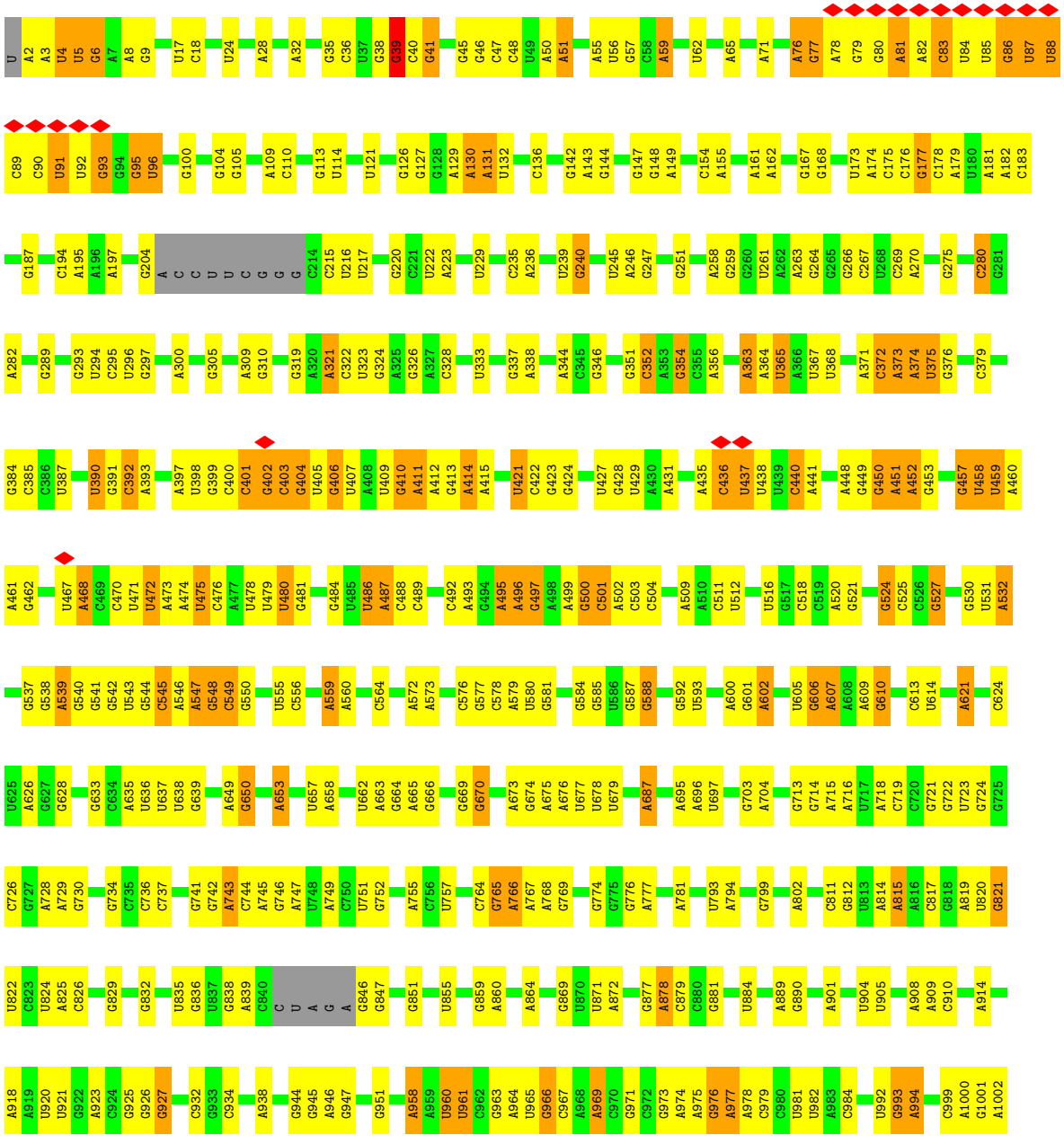


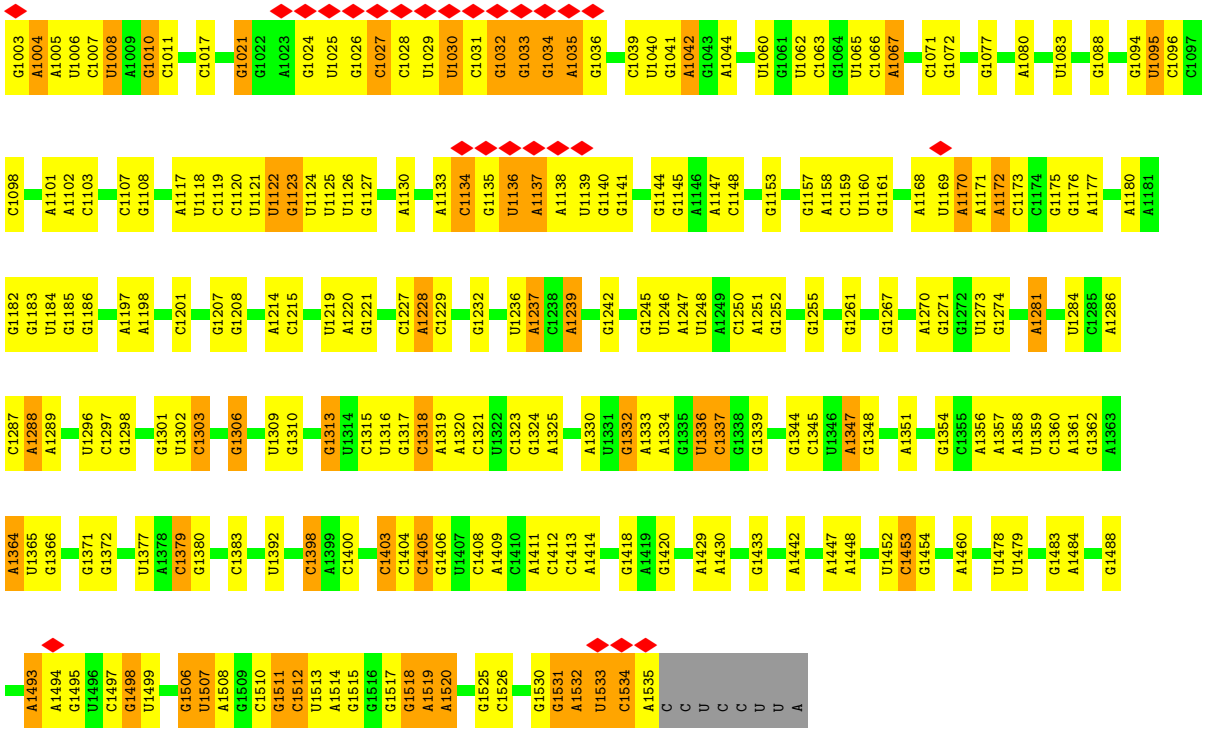
• Molecule 6: E-site tRNA

Chain 5:

• Molecule 7: 16S ribosomal RNA

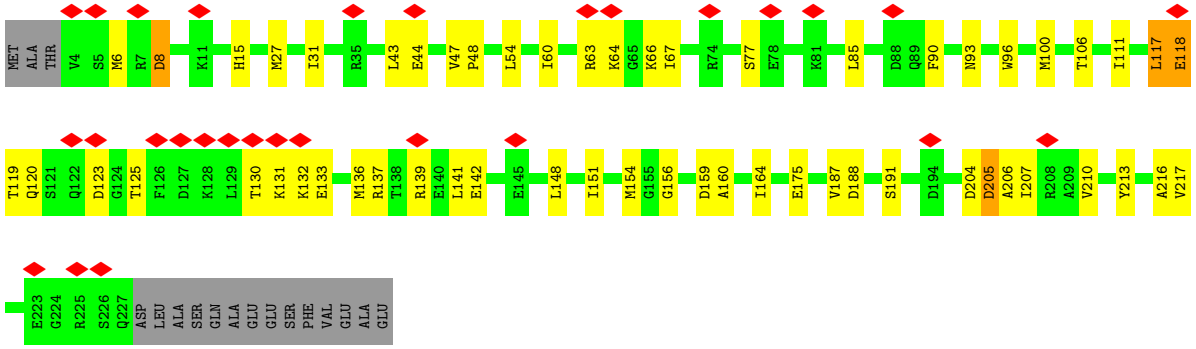
Chain A:





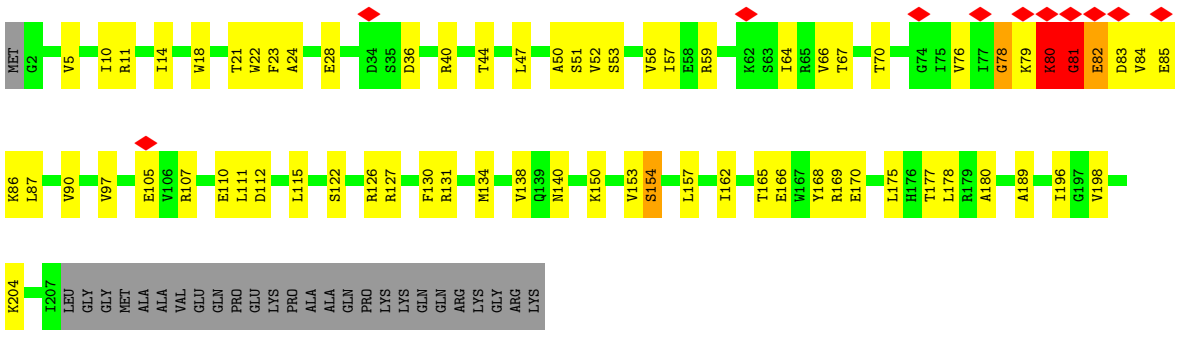
• Molecule 8: Small ribosomal subunit protein uS2

Chain B:



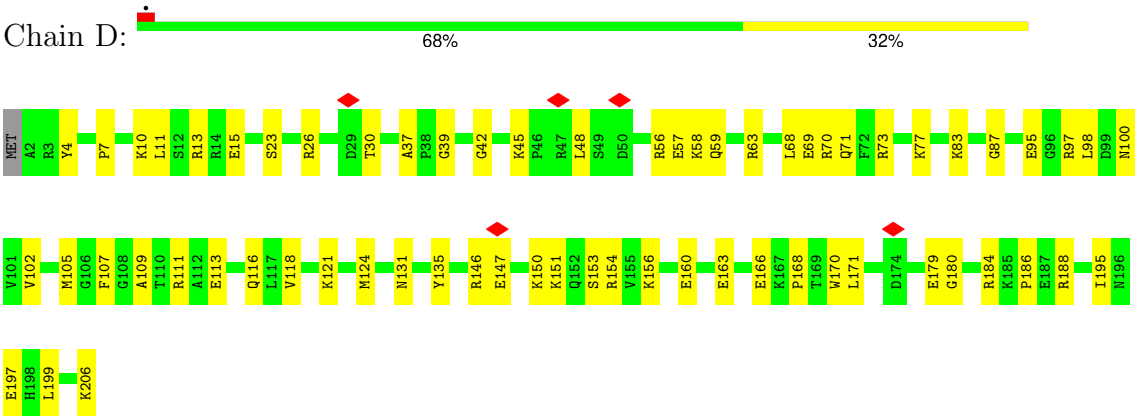
• Molecule 9: Small ribosomal subunit protein uS3

Chain C:



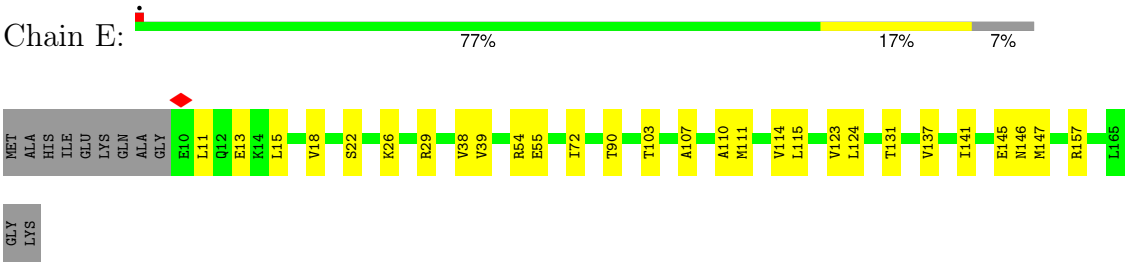
• Molecule 10: Small ribosomal subunit protein uS4

Chain D:



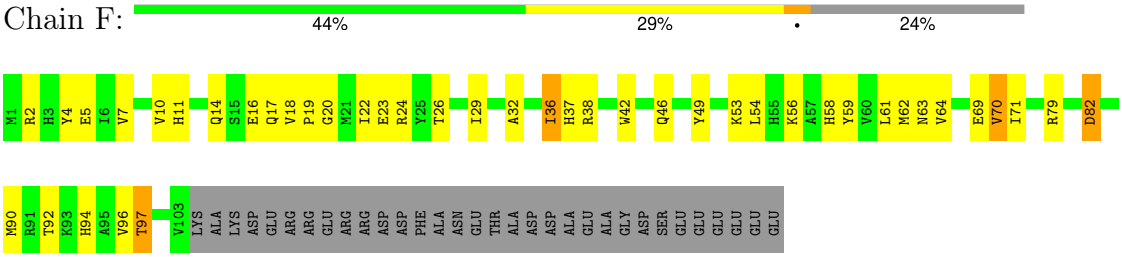
• Molecule 11: Small ribosomal subunit protein uS5

Chain E:



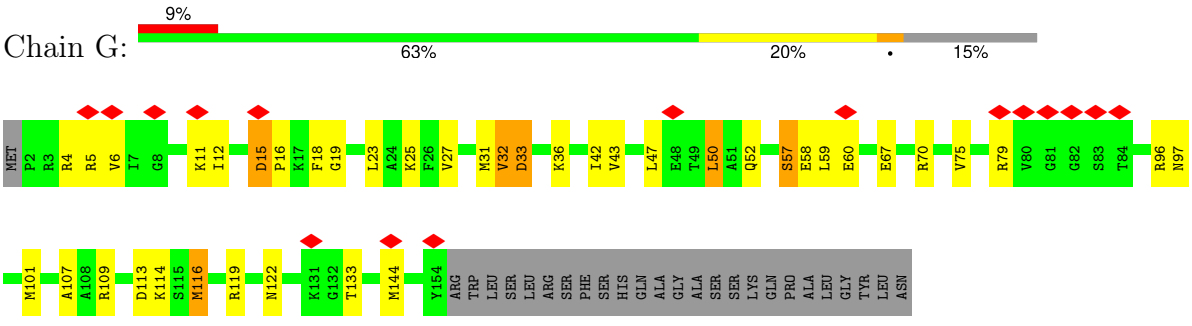
• Molecule 12: Small ribosomal subunit protein bS6

Chain F:



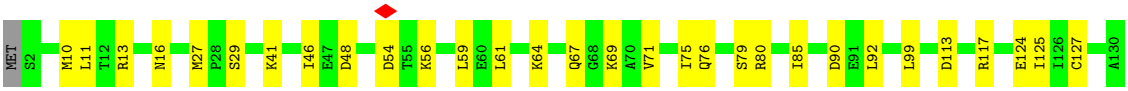
• Molecule 13: Small ribosomal subunit protein uS7

Chain G:



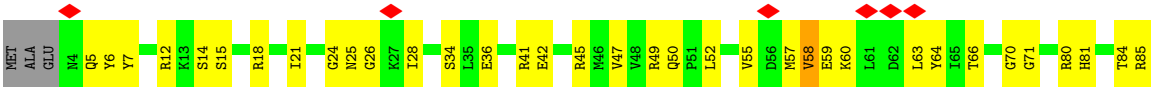
• Molecule 14: Small ribosomal subunit protein uS8

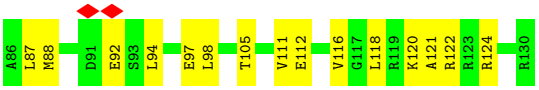
Chain H:



• Molecule 15: Small ribosomal subunit protein uS9

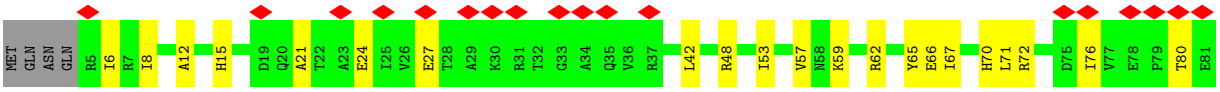
Chain I:

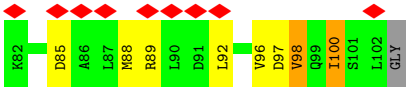




• Molecule 16: Small ribosomal subunit protein uS10

Chain J:



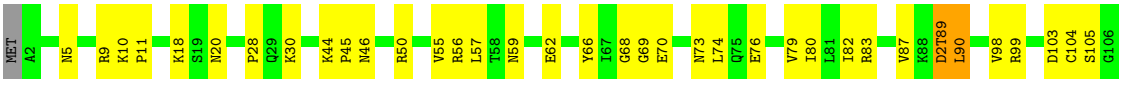


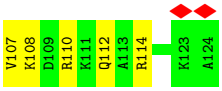
• Molecule 17: 30S ribosomal protein S11

Chain K:

• Molecule 18: Small ribosomal subunit protein uS12

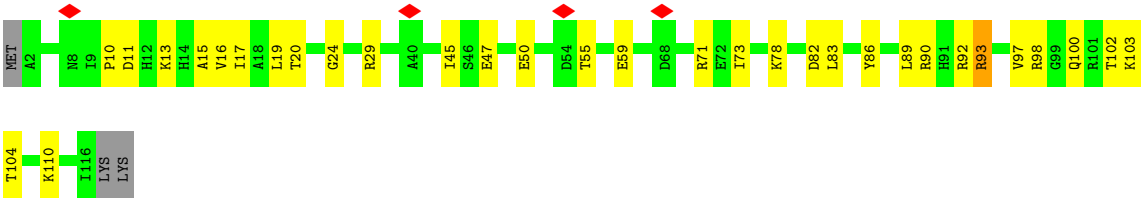
Chain L:





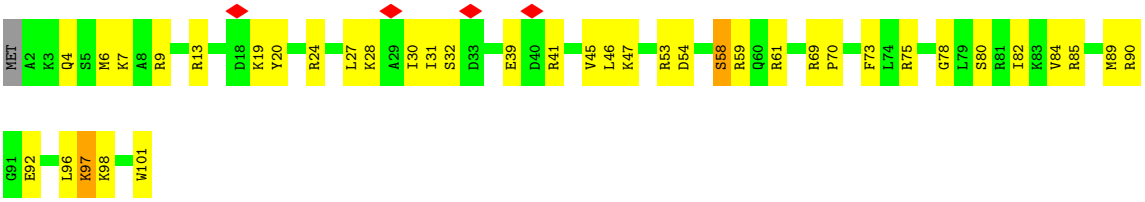
• Molecule 19: Small ribosomal subunit protein uS13

Chain M:



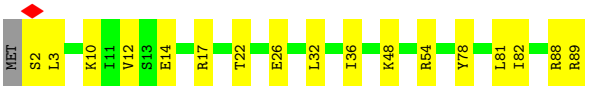
• Molecule 20: Small ribosomal subunit protein uS14

Chain N:



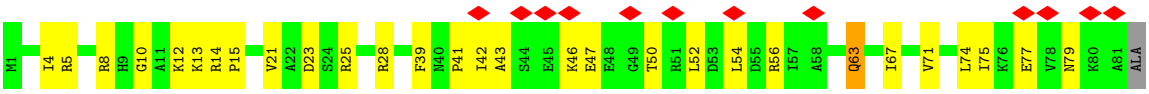
• Molecule 21: Small ribosomal subunit protein uS15

Chain O:



• Molecule 22: Small ribosomal subunit protein bS16

Chain P:



• Molecule 23: Small ribosomal subunit protein uS17

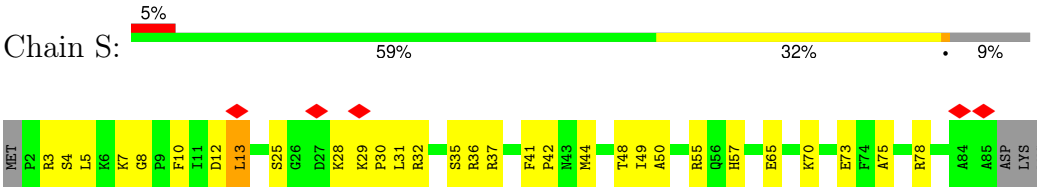
Chain Q:

• Molecule 24: Small ribosomal subunit protein bS18

Chain R:

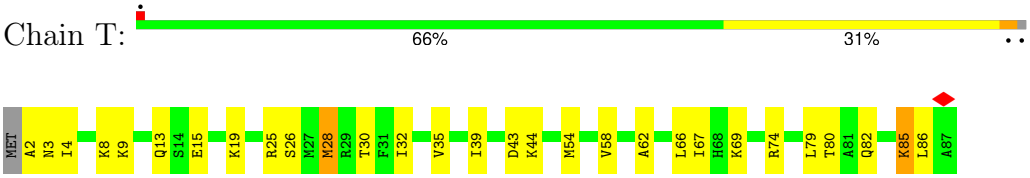
• Molecule 25: Small ribosomal subunit protein uS19

Chain S:



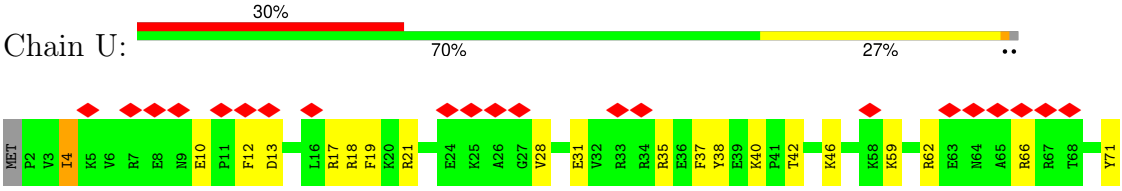
• Molecule 26: Small ribosomal subunit protein bS20

Chain T:



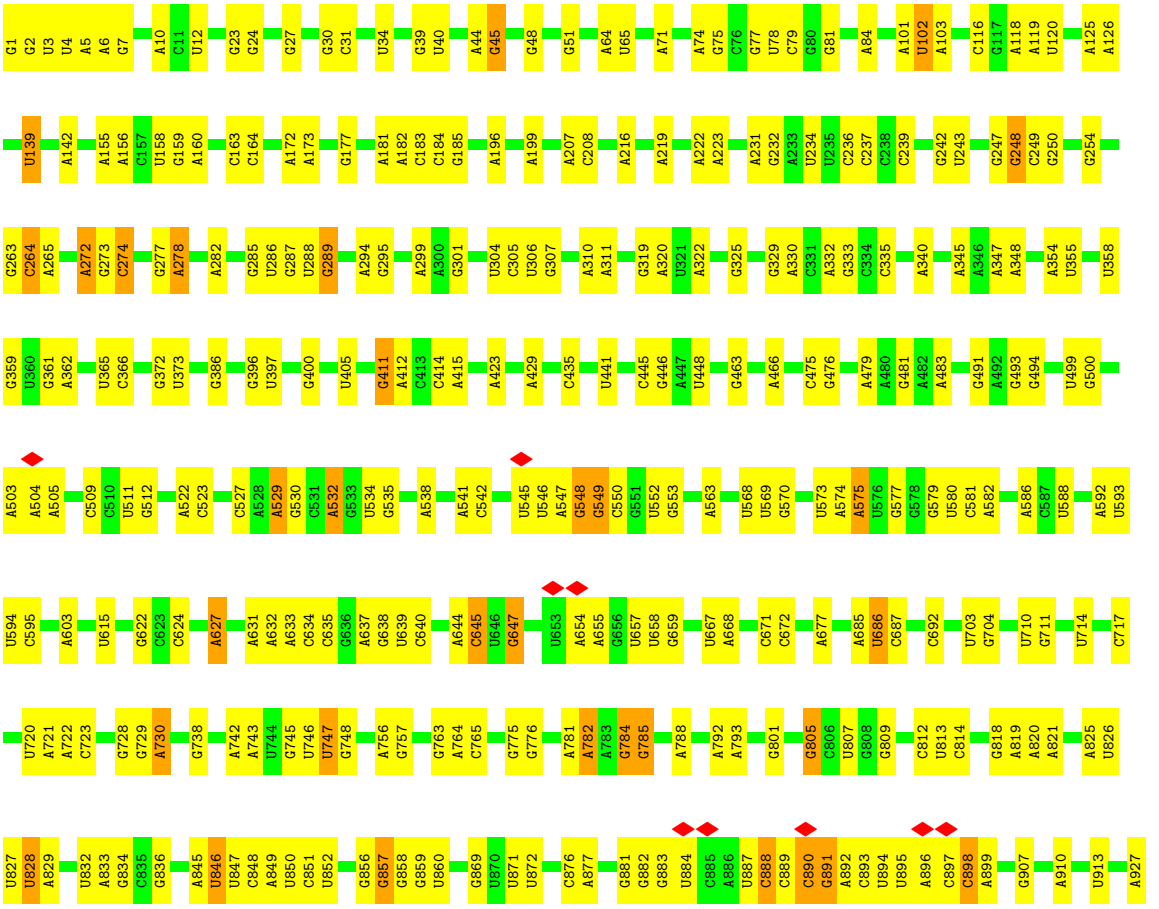
• Molecule 27: Small ribosomal subunit protein bS21

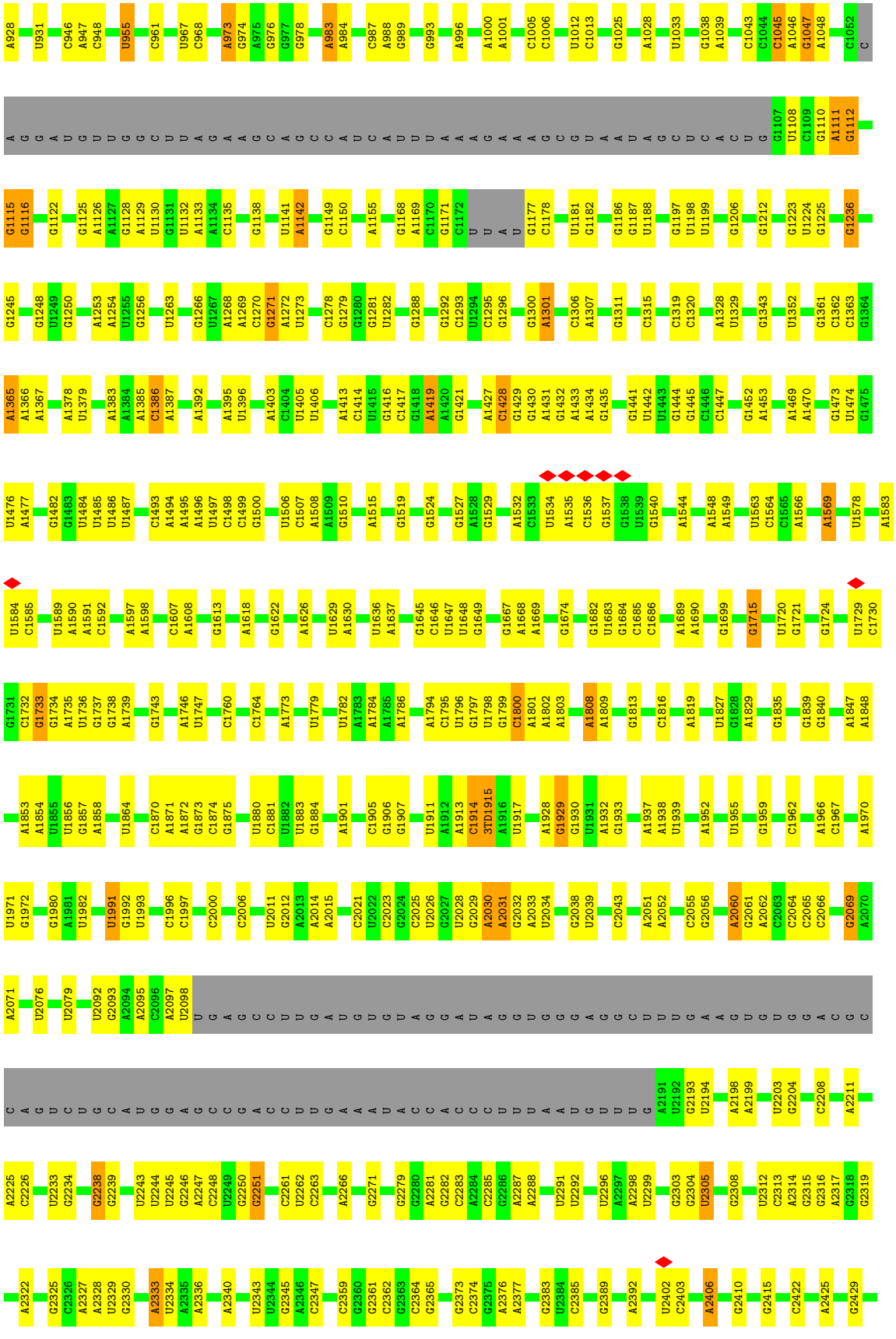
Chain U:

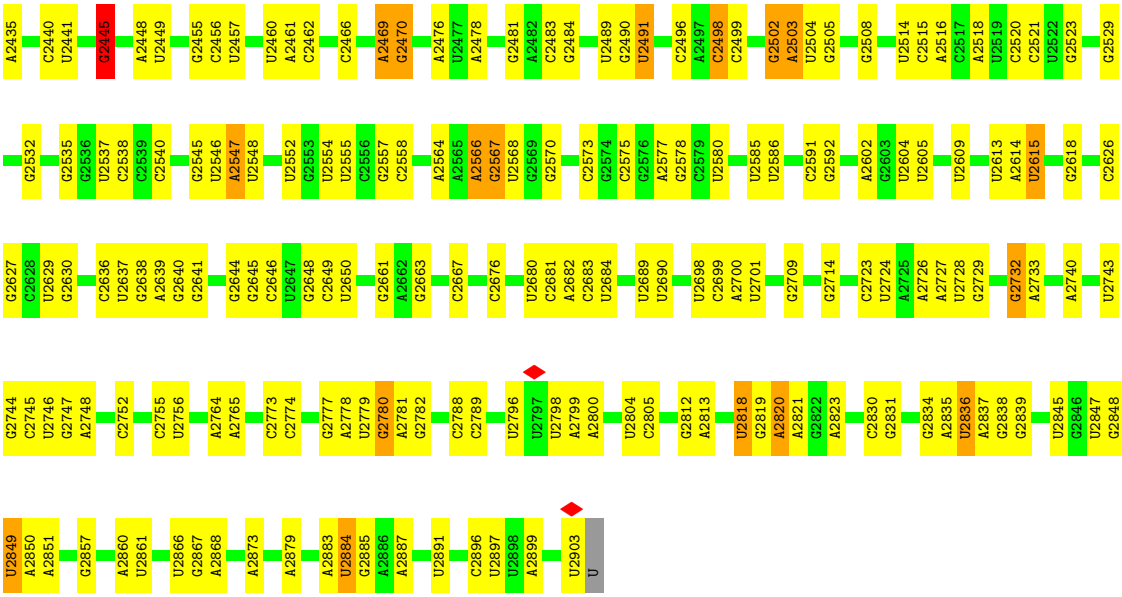


• Molecule 28: 23S ribosomal RNA

Chain a:

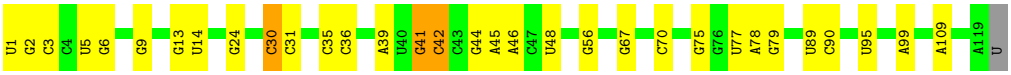






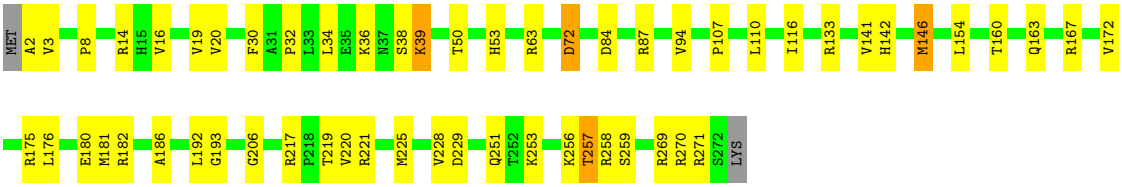
• Molecule 29: 5S ribosomal RNA

Chain b:



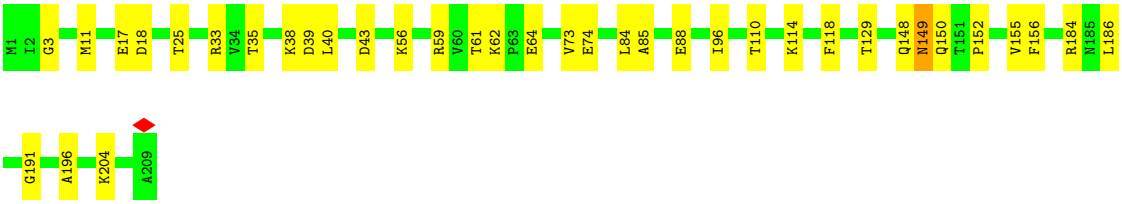
• Molecule 30: 50S ribosomal protein L2

Chain c:



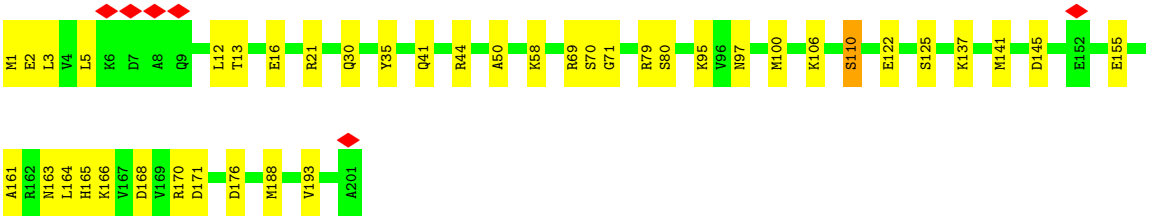
• Molecule 31: 50S ribosomal protein L3

Chain d:

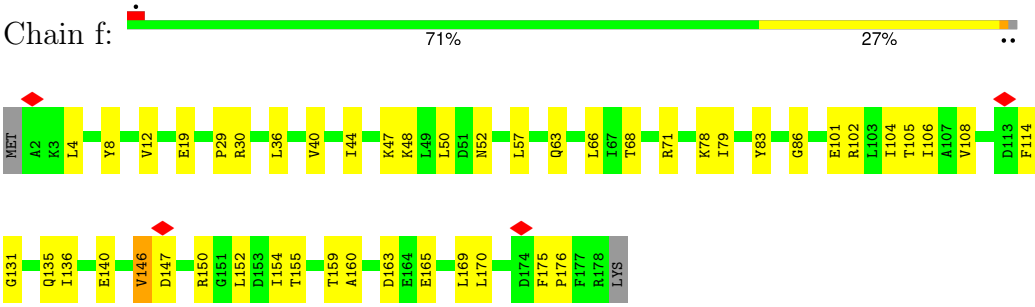


• Molecule 32: Large ribosomal subunit protein uL4

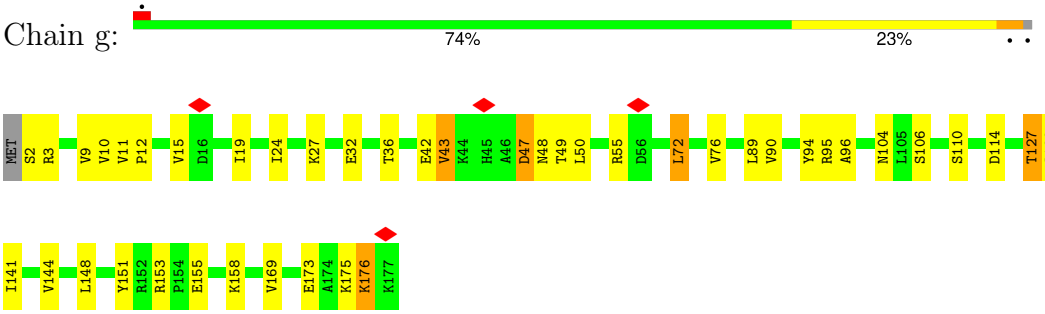
Chain e:



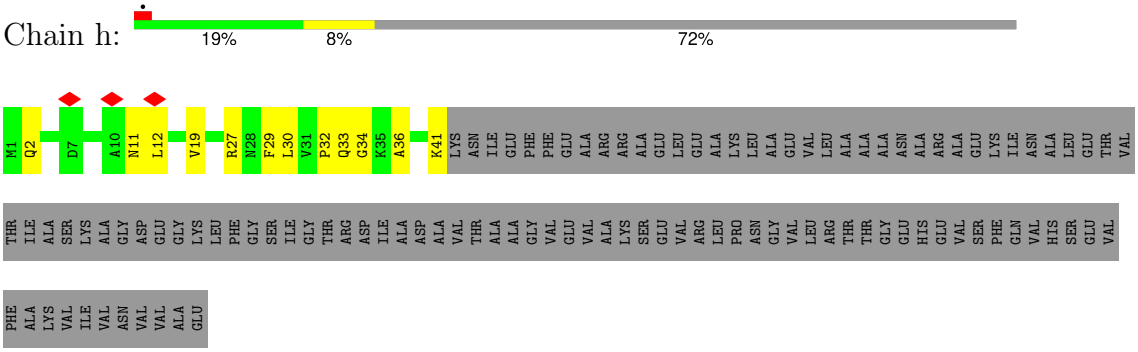
• Molecule 33: Large ribosomal subunit protein uL5



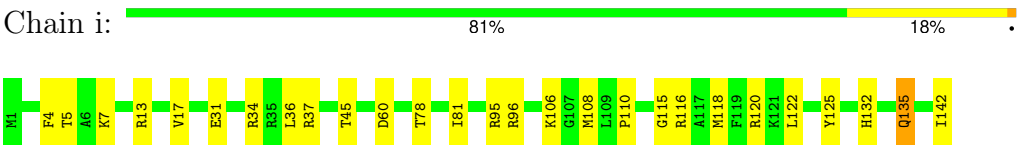
• Molecule 34: Large ribosomal subunit protein uL6



• Molecule 35: Large ribosomal subunit protein bL9

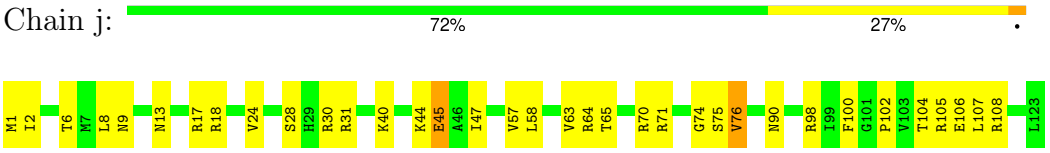


• Molecule 36: Large ribosomal subunit protein uL13



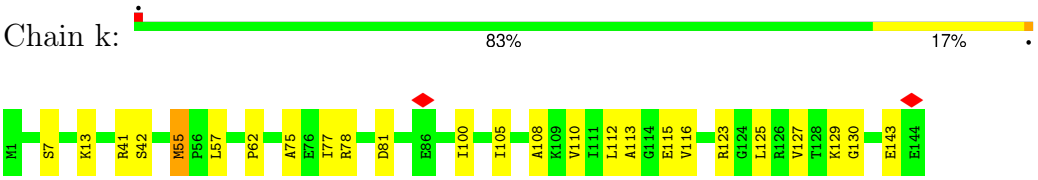
• Molecule 37: Large ribosomal subunit protein uL14

Chain j:



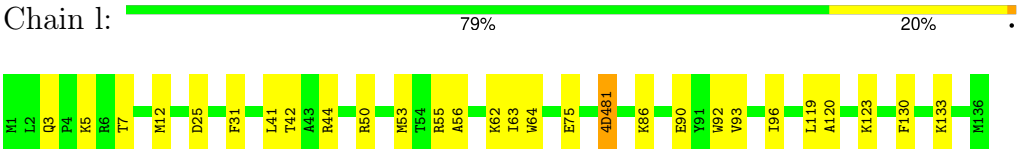
• Molecule 38: Large ribosomal subunit protein uL15

Chain k:



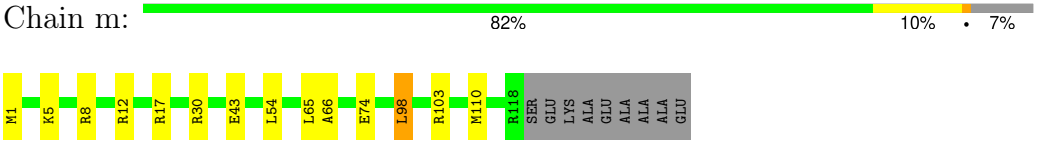
• Molecule 39: Large ribosomal subunit protein uL16

Chain l:



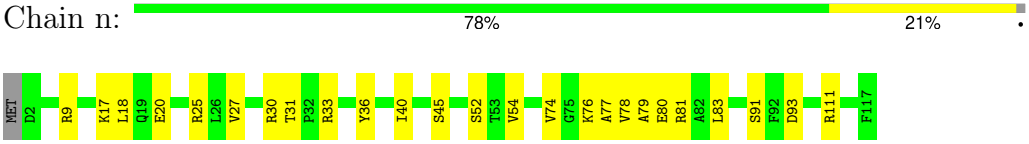
• Molecule 40: Large ribosomal subunit protein bL17

Chain m:



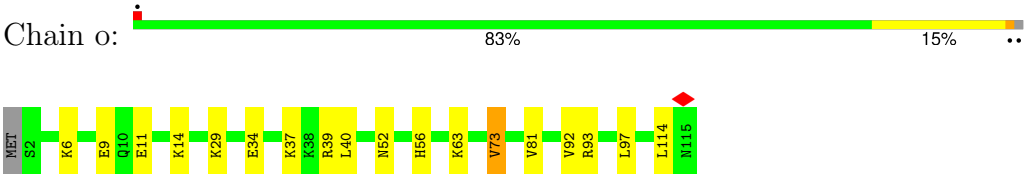
• Molecule 41: Large ribosomal subunit protein uL18

Chain n:



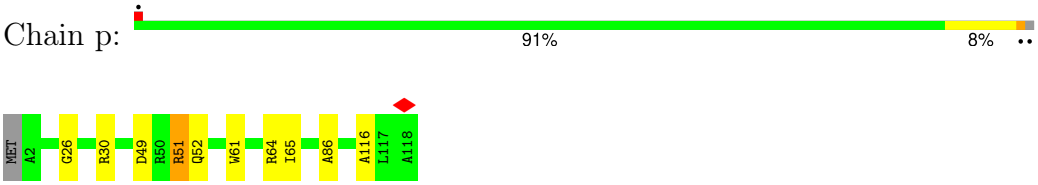
• Molecule 42: Large ribosomal subunit protein bL19

Chain o:



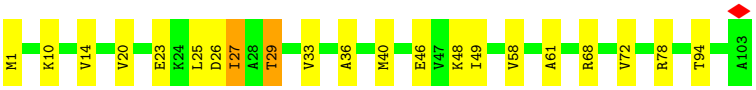
• Molecule 43: 50S ribosomal protein L20

Chain p:



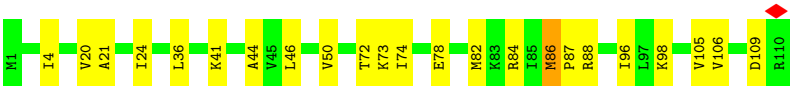
• Molecule 44: Large ribosomal subunit protein bL21

Chain q:



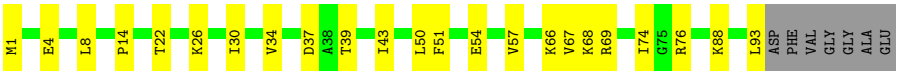
• Molecule 45: Large ribosomal subunit protein uL22

Chain r:



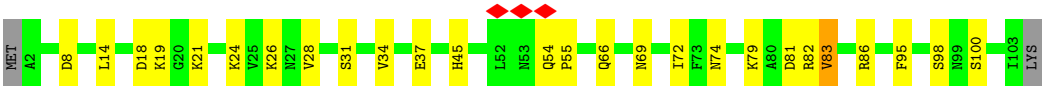
• Molecule 46: 50S ribosomal protein L23

Chain s:



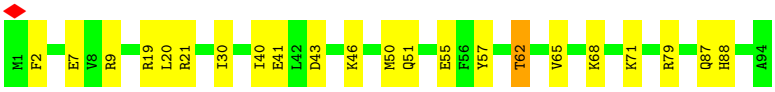
• Molecule 47: 50S ribosomal protein L24

Chain t:



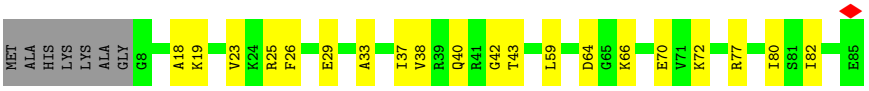
• Molecule 48: Large ribosomal subunit protein bL25

Chain u:



• Molecule 49: 50S ribosomal protein L27

Chain v:



• Molecule 50: 50S ribosomal protein L28

Chain w:

• Molecule 51: Large ribosomal subunit protein uL29

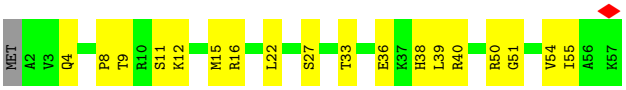
Chain x:

• Molecule 52: 50S ribosomal protein L30

Chain y:

• Molecule 53: 50S ribosomal protein L32

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	577128	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	27.798	Depositor
Minimum map value	-18.382	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	425.984, 425.984, 425.984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.17	0/424	0.30	0/565
2	1	0.36	0/380	0.30	0/498
3	2	0.32	0/513	0.32	0/676
4	3	0.32	0/303	0.31	0/397
5	4	0.19	0/488	0.39	0/649
6	5	0.10	0/46	0.09	0/69
7	A	0.31	2/36275 (0.0%)	0.34	2/56582 (0.0%)
8	B	0.19	0/1784	0.36	0/2403
9	C	0.26	0/1651	0.41	0/2225
10	D	0.22	0/1665	0.37	0/2227
11	E	0.29	0/1165	0.34	0/1568
12	F	0.24	0/858	0.41	0/1160
13	G	0.18	0/1219	0.33	0/1635
14	H	0.27	0/989	0.29	0/1326
15	I	0.21	0/1034	0.41	0/1375
16	J	0.20	0/796	0.40	0/1077
17	K	0.25	0/893	0.39	0/1205
18	L	0.28	0/960	0.35	0/1286
19	M	0.19	0/900	0.34	0/1204
20	N	0.23	0/817	0.39	0/1088
21	O	0.27	0/722	0.32	0/964
22	P	0.28	0/653	0.47	0/877
23	Q	0.26	0/650	0.49	0/871
24	R	0.25	0/553	0.33	0/742
25	S	0.20	0/685	0.33	0/922
26	T	0.26	0/676	0.35	0/895
27	U	0.17	0/597	0.27	0/792
28	a	0.36	0/65651	0.31	0/102413
29	b	0.27	0/2850	0.25	0/4444
30	c	0.36	0/2121	0.33	0/2852
31	d	0.34	0/1576	0.31	0/2119

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	e	0.27	0/1571	0.30	0/2113
33	f	0.20	0/1434	0.35	0/1926
34	g	0.21	0/1343	0.42	0/1816
35	h	0.22	0/306	0.48	0/413
36	i	0.30	0/1152	0.28	0/1551
37	j	0.34	0/955	0.30	0/1279
38	k	0.31	0/1062	0.32	0/1413
39	l	0.31	0/1073	0.30	0/1433
40	m	0.33	0/958	0.33	0/1281
41	n	0.22	0/902	0.35	0/1209
42	o	0.32	0/929	0.31	0/1242
43	p	0.35	0/960	0.28	0/1278
44	q	0.29	0/829	0.29	0/1107
45	r	0.30	0/864	0.28	0/1156
46	s	0.27	0/744	0.37	0/994
47	t	0.23	0/787	0.39	0/1051
48	u	0.26	0/766	0.29	0/1025
49	v	0.33	0/593	0.33	0/785
50	w	0.32	0/635	0.26	0/848
51	x	0.22	0/502	0.33	0/667
52	y	0.31	0/453	0.34	0/605
53	z	0.32	0/450	0.35	0/599
All	All	0.32	2/149162 (0.0%)	0.33	2/222897 (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	C	0	5
23	Q	0	1
34	g	0	1
39	l	0	1
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	39	G	C2-N2	-11.28	1.11	1.34
7	A	39	G	C6-N1	8.22	1.55	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	39	G	N1-C2-N2	-28.51	30.68	116.20
7	A	39	G	N3-C2-N2	-10.54	88.27	119.90

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	C	78	GLY	Peptide
9	C	80	LYS	Mainchain,Peptide
9	C	81	GLY	Peptide
9	C	82	GLU	Peptide
23	Q	16	LYS	Peptide

5.2 Too-close contacts (i)

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	417	0	451	4	0
2	1	377	0	418	6	0
3	2	504	0	572	14	0
4	3	302	0	340	7	0
5	4	480	0	478	19	0
6	5	42	0	23	0	0
7	A	32643	0	16433	452	0
8	B	1753	0	1780	39	0
9	C	1624	0	1696	51	0
10	D	1643	0	1707	49	0
11	E	1152	0	1196	20	0
12	F	839	0	833	33	0
13	G	1203	0	1254	29	0
14	H	979	0	1031	20	0
15	I	1022	0	1070	46	0
16	J	786	0	828	20	0
17	K	877	0	887	33	0
18	L	957	0	1017	29	0
19	M	891	0	952	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	N	805	0	844	36	0
21	O	714	0	734	13	0
22	P	643	0	661	27	0
23	Q	641	0	682	22	0
24	R	544	0	565	15	0
25	S	668	0	693	25	0
26	T	670	0	719	21	0
27	U	589	0	629	18	0
28	a	59130	0	29769	514	0
29	b	2549	0	1291	19	0
30	c	2082	0	2154	40	0
31	d	1566	0	1618	25	0
32	e	1552	0	1619	27	0
33	f	1410	0	1444	37	0
34	g	1323	0	1371	26	0
35	h	303	0	327	10	0
36	i	1129	0	1162	22	0
37	j	946	0	1023	23	0
38	k	1053	0	1129	17	0
39	l	1075	0	1145	18	0
40	m	945	0	989	8	0
41	n	892	0	923	15	0
42	o	917	0	962	15	0
43	p	947	0	1019	8	0
44	q	816	0	839	11	0
45	r	857	0	922	16	0
46	s	738	0	807	17	0
47	t	779	0	831	16	0
48	u	753	0	780	18	0
49	v	586	0	596	14	0
50	w	625	0	652	7	0
51	x	501	0	531	11	0
52	y	449	0	488	5	0
53	z	444	0	458	13	0
54	3	1	0	0	0	0
54	4	1	0	0	0	0
55	A	90	0	0	0	0
55	D	1	0	0	0	0
55	N	1	0	0	0	0
55	a	207	0	0	0	0
55	b	5	0	0	0	0
55	c	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	m	1	0	0	0	0
55	p	1	0	0	0	0
55	z	1	0	0	0	0
56	A	20	0	36	2	0
56	a	140	0	266	15	0
57	a	14	0	26	1	0
All	All	138616	0	93670	1767	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 8.

The worst 5 of 1767 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)
9:C:80:LYS:O	9:C:82:GLU:N	1.70	1.24
7:A:76:A:N6	7:A:93:G:H1	1.49	1.09
28:a:627:A:OP1	38:k:78:ARG:NH2	2.02	0.91
24:R:42:SER:HB2	24:R:52:GLN:HG3	1.55	0.89
5:4:16:CYS:SG	5:4:37:CYS:HB3	2.16	0.86

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	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
2	1	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
5	4	56/70 (80%)	55 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	B	222/241 (92%)	207 (93%)	15 (7%)	0	100	100
9	C	204/233 (88%)	191 (94%)	11 (5%)	2 (1%)	12	45
10	D	203/206 (98%)	186 (92%)	17 (8%)	0	100	100
11	E	154/167 (92%)	151 (98%)	3 (2%)	0	100	100
12	F	101/135 (75%)	94 (93%)	7 (7%)	0	100	100
13	G	151/179 (84%)	139 (92%)	12 (8%)	0	100	100
14	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
15	I	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
16	J	96/103 (93%)	91 (95%)	4 (4%)	1 (1%)	12	45
17	K	115/129 (89%)	108 (94%)	7 (6%)	0	100	100
18	L	120/124 (97%)	113 (94%)	7 (6%)	0	100	100
19	M	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
20	N	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
21	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
22	P	79/82 (96%)	70 (89%)	9 (11%)	0	100	100
23	Q	77/84 (92%)	73 (95%)	4 (5%)	0	100	100
24	R	64/75 (85%)	59 (92%)	5 (8%)	0	100	100
25	S	82/92 (89%)	80 (98%)	2 (2%)	0	100	100
26	T	84/87 (97%)	84 (100%)	0	0	100	100
27	U	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
30	c	269/273 (98%)	265 (98%)	4 (2%)	0	100	100
31	d	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	24	59
32	e	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
33	f	175/179 (98%)	170 (97%)	5 (3%)	0	100	100
34	g	174/177 (98%)	157 (90%)	16 (9%)	1 (1%)	21	56
35	h	39/149 (26%)	34 (87%)	5 (13%)	0	100	100
36	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
37	j	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
38	k	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
39	l	132/136 (97%)	130 (98%)	2 (2%)	0	100	100
40	m	116/127 (91%)	109 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	n	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
42	o	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
43	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
44	q	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
45	r	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
46	s	91/100 (91%)	86 (94%)	5 (6%)	0	100	100
47	t	100/104 (96%)	93 (93%)	7 (7%)	0	100	100
48	u	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
49	v	76/85 (89%)	73 (96%)	3 (4%)	0	100	100
50	w	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
51	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
52	y	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
53	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
All	All	5483/5913 (93%)	5243 (96%)	235 (4%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C	81	GLY
31	d	149	ASN
16	J	57	VAL
34	g	47	ASP
9	C	80	LYS

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	46/49 (94%)	43 (94%)	3 (6%)	15	47
2	1	38/38 (100%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	33 (97%)	1 (3%)	37	67
5	4	55/62 (89%)	54 (98%)	1 (2%)	51	74
8	B	186/199 (94%)	180 (97%)	6 (3%)	34	65
9	C	170/190 (90%)	166 (98%)	4 (2%)	43	70
10	D	172/173 (99%)	169 (98%)	3 (2%)	53	75
11	E	119/126 (94%)	117 (98%)	2 (2%)	53	75
12	F	90/116 (78%)	83 (92%)	7 (8%)	11	41
13	G	126/147 (86%)	116 (92%)	10 (8%)	11	40
14	H	104/105 (99%)	103 (99%)	1 (1%)	68	80
15	I	105/107 (98%)	98 (93%)	7 (7%)	15	47
16	J	86/90 (96%)	83 (96%)	3 (4%)	32	64
17	K	90/99 (91%)	86 (96%)	4 (4%)	25	59
18	L	102/103 (99%)	100 (98%)	2 (2%)	48	72
19	M	93/96 (97%)	87 (94%)	6 (6%)	15	47
20	N	83/84 (99%)	79 (95%)	4 (5%)	23	56
21	O	76/77 (99%)	76 (100%)	0	100	100
22	P	65/65 (100%)	64 (98%)	1 (2%)	57	76
23	Q	73/78 (94%)	68 (93%)	5 (7%)	14	46
24	R	57/65 (88%)	54 (95%)	3 (5%)	20	53
25	S	72/79 (91%)	71 (99%)	1 (1%)	59	77
26	T	65/66 (98%)	61 (94%)	4 (6%)	16	49
27	U	60/61 (98%)	58 (97%)	2 (3%)	33	65
30	c	216/218 (99%)	208 (96%)	8 (4%)	30	63
31	d	163/163 (100%)	157 (96%)	6 (4%)	30	63
32	e	165/165 (100%)	163 (99%)	2 (1%)	63	79
33	f	148/150 (99%)	145 (98%)	3 (2%)	48	72
34	g	137/138 (99%)	129 (94%)	8 (6%)	18	51
35	h	32/114 (28%)	32 (100%)	0	100	100
36	i	116/116 (100%)	114 (98%)	2 (2%)	53	75
37	j	104/104 (100%)	98 (94%)	6 (6%)	18	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
38	k	103/103 (100%)	100 (97%)	3 (3%)	37 67
39	l	107/107 (100%)	105 (98%)	2 (2%)	50 73
40	m	98/103 (95%)	96 (98%)	2 (2%)	48 72
41	n	86/87 (99%)	86 (100%)	0	100 100
42	o	99/100 (99%)	98 (99%)	1 (1%)	68 80
43	p	89/90 (99%)	88 (99%)	1 (1%)	65 79
44	q	84/84 (100%)	79 (94%)	5 (6%)	17 50
45	r	93/93 (100%)	92 (99%)	1 (1%)	65 79
46	s	80/84 (95%)	77 (96%)	3 (4%)	29 62
47	t	83/85 (98%)	81 (98%)	2 (2%)	43 70
48	u	78/78 (100%)	75 (96%)	3 (4%)	29 62
49	v	58/63 (92%)	57 (98%)	1 (2%)	53 75
50	w	67/68 (98%)	67 (100%)	0	100 100
51	x	54/55 (98%)	52 (96%)	2 (4%)	30 63
52	y	48/49 (98%)	48 (100%)	0	100 100
53	z	47/48 (98%)	45 (96%)	2 (4%)	26 59
All	All	4573/4826 (95%)	4430 (97%)	143 (3%)	36 66

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	k	7	SER
39	l	25	ASP
46	s	37	ASP
17	K	46	THR
16	J	100	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
47	t	45	HIS
48	u	49	ASN
52	y	20	HIS
21	O	40	GLN
17	K	119	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	a	2748/2904 (94%)	324 (11%)	0
29	b	118/120 (98%)	13 (11%)	0
6	5	1/2 (50%)	1 (100%)	0
7	A	1517/1543 (98%)	310 (20%)	17 (1%)
All	All	4384/4569 (95%)	648 (14%)	17 (0%)

5 of 648 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	5	76	A
7	A	3	A
7	A	4	U
7	A	5	U
7	A	6	G

5 of 17 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	1035	A
7	A	1533	U
7	A	500	G
7	A	548	G
7	A	606	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
31	MEQ	d	150	31	8,9,10	0.89	0	5,10,12	0.56	0
28	OMG	a	2251	28	23,26,27	0.85	2 (8%)	32,38,41	1.96	10 (31%)
28	G7M	a	2069	28	23,26,27	0.64	0	34,39,42	0.96	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	OMU	a	2552	28	19,22,23	1.24	3 (15%)	25,31,34	1.98	6 (24%)
28	5MU	a	747	28	19,22,23	1.33	4 (21%)	27,32,35	2.24	7 (25%)
7	2MG	A	966	7	23,26,27	0.80	0	33,38,41	2.25	12 (36%)
28	2MA	a	2503	28,55	22,25,26	1.31	4 (18%)	32,37,40	2.02	7 (21%)
7	2MG	A	1208	7	23,26,27	0.80	0	33,38,41	2.16	9 (27%)
28	5MC	a	1962	28	19,22,23	1.55	2 (10%)	26,32,35	1.23	3 (11%)
7	5MC	A	1408	7	19,22,23	1.62	2 (10%)	26,32,35	1.10	3 (11%)
28	OMC	a	2498	28,55	19,22,23	1.11	1 (5%)	25,31,34	1.22	2 (8%)
28	PSU	a	2504	28	18,21,22	1.14	3 (16%)	21,30,33	2.03	4 (19%)
28	PSU	a	2605	28	18,21,22	1.26	3 (16%)	21,30,33	2.01	4 (19%)
28	PSU	a	2457	28	18,21,22	1.22	4 (22%)	21,30,33	2.17	5 (23%)
28	H2U	a	2449	28	18,21,22	0.64	0	19,30,33	1.11	1 (5%)
28	2MG	a	1835	28	23,26,27	0.87	1 (4%)	33,38,41	2.30	13 (39%)
7	G7M	A	527	7	23,26,27	0.58	0	34,39,42	0.95	2 (5%)
7	5MC	A	967	7	19,22,23	1.41	2 (10%)	26,32,35	1.11	1 (3%)
7	PSU	A	516	7,55	18,21,22	1.16	3 (16%)	21,30,33	2.01	5 (23%)
28	PSU	a	1911	28	18,21,22	1.07	3 (16%)	21,30,33	2.03	4 (19%)
28	2MG	a	2445	28	23,26,27	0.93	2 (8%)	33,38,41	2.22	13 (39%)
28	3TD	a	1915	28	19,22,23	1.19	3 (15%)	23,32,35	1.92	3 (13%)
28	6MZ	a	1618	28	22,25,26	1.14	2 (9%)	29,36,39	2.28	9 (31%)
39	MS6	l	82	39	5,7,8	0.62	0	2,7,9	1.17	0
28	5MU	a	1939	28	19,22,23	1.33	4 (21%)	27,32,35	2.25	6 (22%)
28	PSU	a	2580	28	18,21,22	1.26	4 (22%)	21,30,33	2.12	5 (23%)
18	D2T	L	89	18	8,9,10	2.70	1 (12%)	6,11,13	1.43	1 (16%)
28	1MG	a	745	28	23,26,27	1.13	1 (4%)	33,39,42	1.81	6 (18%)
28	PSU	a	2604	28	18,21,22	1.20	3 (16%)	21,30,33	2.03	4 (19%)
7	MA6	A	1519	7	23,26,27	2.58	5 (21%)	33,38,41	2.84	7 (21%)
28	PSU	a	955	28	18,21,22	1.23	3 (16%)	21,30,33	2.03	4 (19%)
7	4OC	A	1403	7	20,23,24	2.35	4 (20%)	25,32,35	0.99	1 (4%)
28	PSU	a	746	28,55	18,21,22	1.13	3 (16%)	21,30,33	1.94	3 (14%)
28	PSU	a	1917	28	18,21,22	1.10	2 (11%)	21,30,33	1.91	4 (19%)
39	4D4	l	81	39	9,11,12	0.89	0	7,13,15	1.63	2 (28%)
7	MA6	A	1520	7	23,26,27	2.56	5 (21%)	33,38,41	2.81	7 (21%)
28	6MZ	a	2030	28	22,25,26	1.16	2 (9%)	29,36,39	2.37	10 (34%)
7	UR3	A	1499	7	19,22,23	3.79	6 (31%)	26,32,35	4.61	10 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	2MG	A	1517	7	23,26,27	0.85	1 (4%)	33,38,41	2.28	12 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	MEQ	d	150	31	-	2/8/9/11	-
28	OMG	a	2251	28	-	0/9/27/28	0/3/3/3
28	G7M	a	2069	28	-	0/7/25/26	0/3/3/3
28	OMU	a	2552	28	-	2/9/27/28	0/2/2/2
28	5MU	a	747	28	-	0/7/25/26	0/2/2/2
7	2MG	A	966	7	-	2/9/27/28	0/3/3/3
28	2MA	a	2503	28,55	-	1/7/25/26	0/3/3/3
7	2MG	A	1208	7	-	0/9/27/28	0/3/3/3
28	5MC	a	1962	28	-	0/7/25/26	0/2/2/2
7	5MC	A	1408	7	-	1/7/25/26	0/2/2/2
28	OMC	a	2498	28,55	-	0/9/27/28	0/2/2/2
28	PSU	a	2504	28	-	2/7/25/26	0/2/2/2
28	PSU	a	2605	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2457	28	-	0/7/25/26	0/2/2/2
28	H2U	a	2449	28	-	1/7/38/39	0/2/2/2
28	2MG	a	1835	28	-	2/9/27/28	0/3/3/3
7	G7M	A	527	7	-	2/7/25/26	0/3/3/3
7	5MC	A	967	7	-	0/7/25/26	0/2/2/2
7	PSU	A	516	7,55	-	0/7/25/26	0/2/2/2
28	PSU	a	1911	28	-	0/7/25/26	0/2/2/2
28	2MG	a	2445	28	-	2/9/27/28	0/3/3/3
28	3TD	a	1915	28	-	2/7/25/26	0/2/2/2
28	6MZ	a	1618	28	-	2/9/27/28	0/3/3/3
39	MS6	l	82	39	-	4/4/6/8	-
28	5MU	a	1939	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2580	28	-	2/7/25/26	0/2/2/2
18	D2T	L	89	18	-	1/7/12/14	-
28	1MG	a	745	28	-	0/7/25/26	0/3/3/3
28	PSU	a	2604	28	-	0/7/25/26	0/2/2/2
7	MA6	A	1519	7	-	0/11/29/30	0/3/3/3
28	PSU	a	955	28	-	0/7/25/26	0/2/2/2
7	4OC	A	1403	7	-	1/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PSU	a	746	28,55	-	1/7/25/26	0/2/2/2
28	PSU	a	1917	28	-	0/7/25/26	0/2/2/2
39	4D4	l	81	39	-	2/11/12/14	-
7	MA6	A	1520	7	-	2/11/29/30	0/3/3/3
28	6MZ	a	2030	28	-	1/9/27/28	0/3/3/3
7	UR3	A	1499	7	-	0/7/25/26	0/2/2/2
7	2MG	A	1517	7	-	0/9/27/28	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1499	UR3	C2-N1	13.61	1.57	1.38
7	A	1403	4OC	O2-C2	8.31	1.39	1.23
7	A	1520	MA6	C5-N7	7.60	1.53	1.39
7	A	1519	MA6	C5-N7	7.57	1.52	1.39
18	L	89	D2T	CB-CA	-6.99	1.52	1.54

The worst 5 of 206 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1499	UR3	C4-N3-C2	-14.64	112.80	124.58
7	A	1499	UR3	C6-N1-C2	-13.94	110.41	121.80
7	A	1519	MA6	C4-N9-C8	13.71	120.13	105.74
7	A	1520	MA6	C4-N9-C8	13.49	119.90	105.74
7	A	1499	UR3	C5-C4-N3	7.79	125.30	115.04

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	966	2MG	O4'-C4'-C5'-O5'
7	A	1520	MA6	O4'-C4'-C5'-O5'
28	a	1915	3TD	O4'-C4'-C5'-O5'
39	l	82	MS6	CA-CB-CG-SD
7	A	527	G7M	C3'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	d	150	MEQ	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	a	2251	OMG	1	0
28	a	2503	2MA	1	0
28	a	2445	2MG	1	0
28	a	1915	3TD	1	0
18	L	89	D2T	1	0
28	a	955	PSU	1	0
7	A	1403	4OC	1	0
28	a	2030	6MZ	3	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 327 ligands modelled in this entry, 310 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	SPD	a	6217	-	9,9,9	0.25	0	8,8,8	0.25	0
56	SPD	a	6220	-	9,9,9	0.28	0	8,8,8	0.32	0
56	SPD	a	6208	-	9,9,9	0.25	0	8,8,8	0.26	0
56	SPD	a	6212	-	9,9,9	0.28	0	8,8,8	0.29	0
56	SPD	a	6211	-	9,9,9	0.25	0	8,8,8	0.22	0
56	SPD	a	6213	-	9,9,9	0.25	0	8,8,8	0.26	0
56	SPD	a	6215	-	9,9,9	0.27	0	8,8,8	0.31	0
56	SPD	a	6214	-	9,9,9	0.28	0	8,8,8	0.24	0
56	SPD	a	6209	-	9,9,9	0.25	0	8,8,8	0.21	0
56	SPD	a	6218	-	9,9,9	0.26	0	8,8,8	0.43	0
56	SPD	a	6207	-	9,9,9	0.28	0	8,8,8	0.23	0
57	SPM	a	6221	-	13,13,13	0.35	0	12,12,12	0.94	0
56	SPD	a	6216	-	9,9,9	0.29	0	8,8,8	0.31	0
56	SPD	a	6219	-	9,9,9	0.27	0	8,8,8	0.34	0
56	SPD	a	6210	-	9,9,9	0.27	0	8,8,8	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
56	SPD	A	1691	-	9,9,9	0.25	0	8,8,8	0.26	0
56	SPD	A	1692	7	9,9,9	0.26	0	8,8,8	0.19	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	SPD	a	6217	-	-	2/7/7/7	-
56	SPD	a	6220	-	-	1/7/7/7	-
56	SPD	a	6208	-	-	3/7/7/7	-
56	SPD	a	6212	-	-	2/7/7/7	-
56	SPD	a	6211	-	-	4/7/7/7	-
56	SPD	a	6213	-	-	0/7/7/7	-
56	SPD	a	6215	-	-	4/7/7/7	-
56	SPD	a	6214	-	-	3/7/7/7	-
56	SPD	a	6209	-	-	2/7/7/7	-
56	SPD	a	6218	-	-	6/7/7/7	-
56	SPD	a	6207	-	-	4/7/7/7	-
57	SPM	a	6221	-	-	2/11/11/11	-
56	SPD	a	6216	-	-	3/7/7/7	-
56	SPD	a	6219	-	-	1/7/7/7	-
56	SPD	a	6210	-	-	1/7/7/7	-
56	SPD	A	1691	-	-	2/7/7/7	-
56	SPD	A	1692	7	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	A	1691	SPD	C3-C4-C5-N6
56	a	6207	SPD	C3-C4-C5-N6
56	a	6207	SPD	N6-C7-C8-C9
56	a	6208	SPD	N6-C7-C8-C9
56	a	6216	SPD	C3-C4-C5-N6

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	a	6217	SPD	2	0
56	a	6208	SPD	3	0
56	a	6212	SPD	1	0
56	a	6211	SPD	2	0
56	a	6215	SPD	1	0
56	a	6214	SPD	3	0
56	a	6218	SPD	2	0
57	a	6221	SPM	1	0
56	a	6216	SPD	1	0
56	A	1691	SPD	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	A	3
28	a	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	1914:C	O3'	1915:3TD	P	4.24
1	A	1402:G	O3'	1403:4OC	P	2.92
1	A	1498:G	O3'	1499:UR3	P	2.91
1	A	1518:G	O3'	1519:MA6	P	2.83

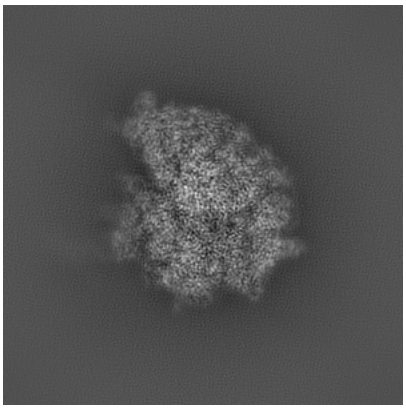
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-75650. These allow visual inspection of the internal detail of the map and identification of artifacts.

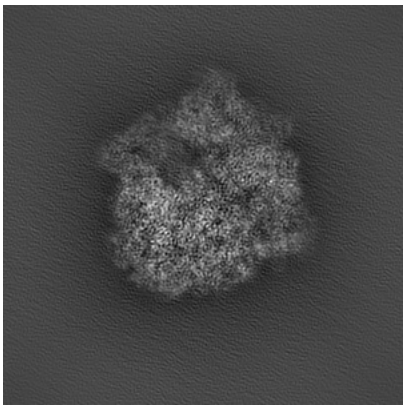
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

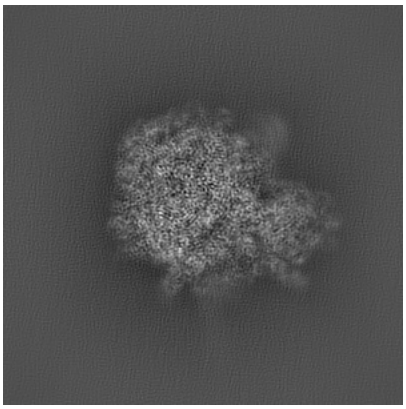
6.1.1 Primary map



X

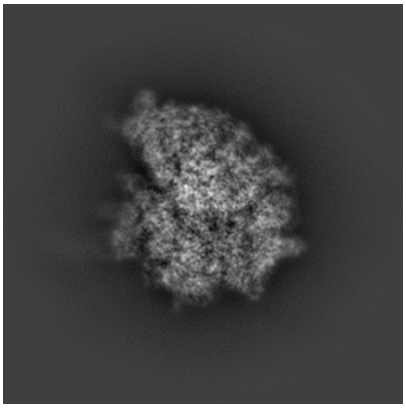


Y

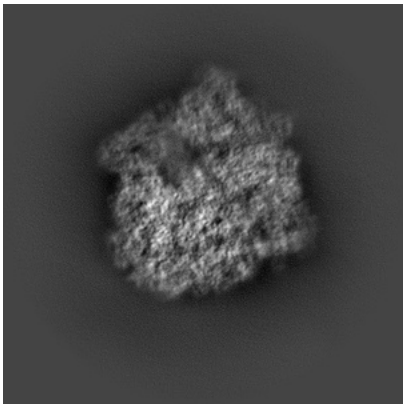


Z

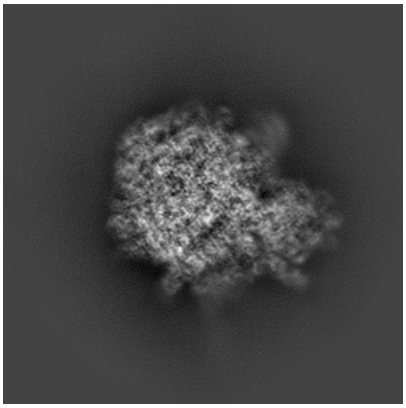
6.1.2 Raw map



X



Y

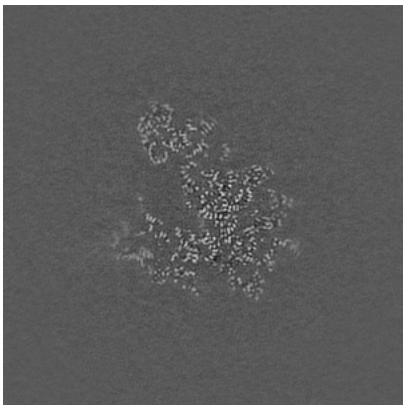


Z

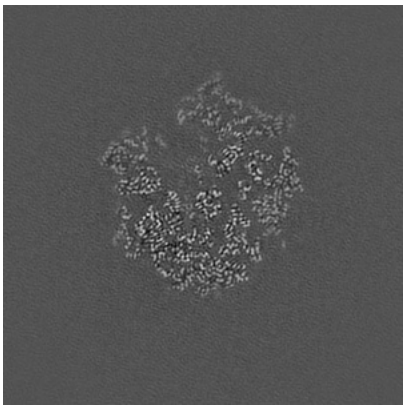
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

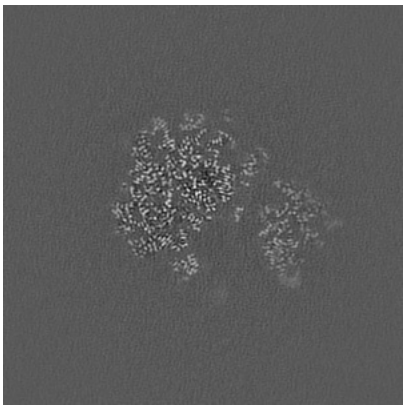
6.2.1 Primary map



X Index: 256

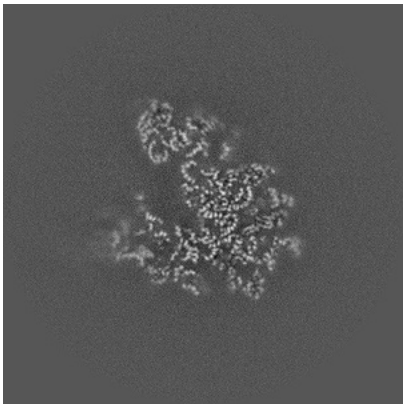


Y Index: 256

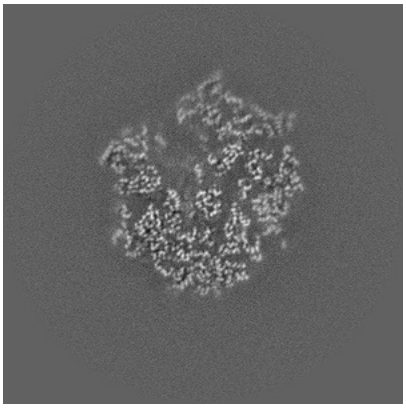


Z Index: 256

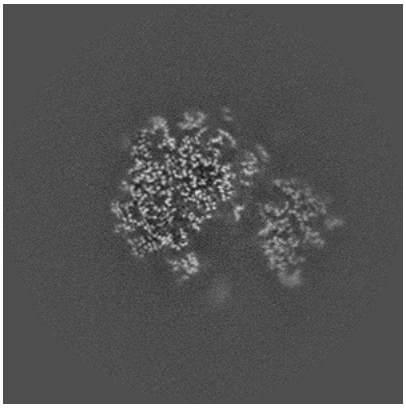
6.2.2 Raw map



X Index: 256



Y Index: 256

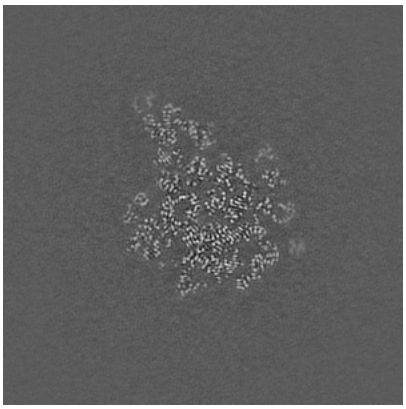


Z Index: 256

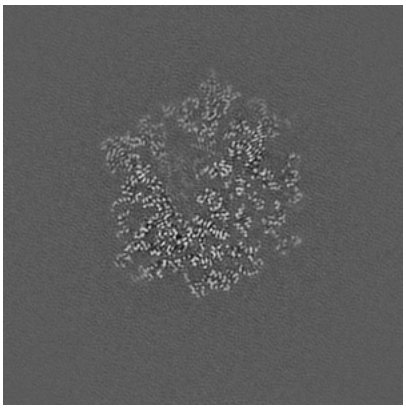
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

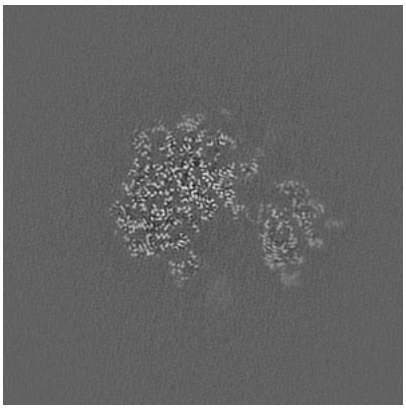
6.3.1 Primary map



X Index: 234

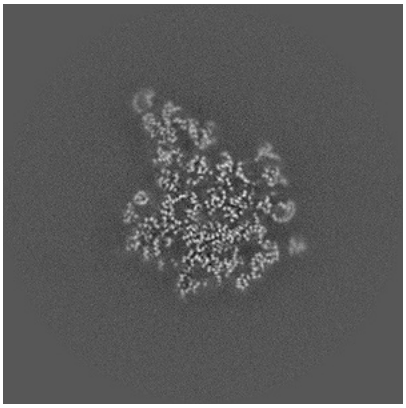


Y Index: 247

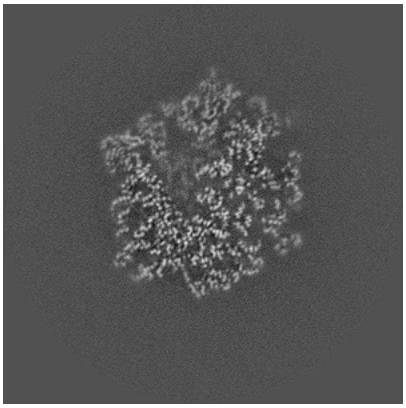


Z Index: 253

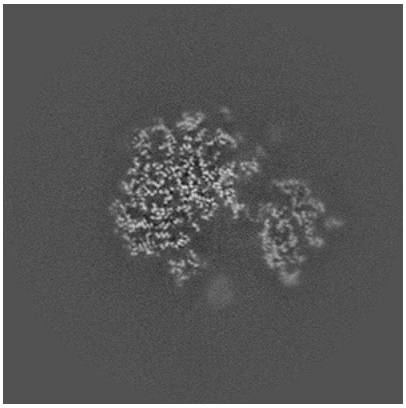
6.3.2 Raw map



X Index: 234



Y Index: 247

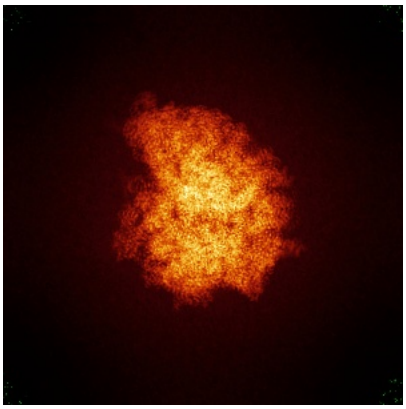


Z Index: 253

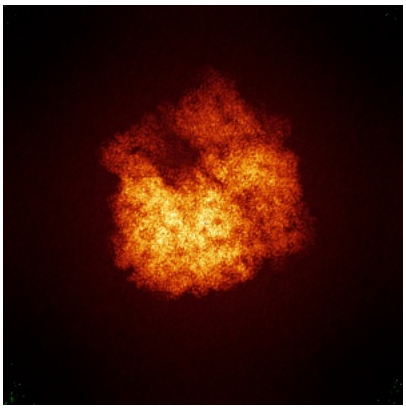
The images above show the largest variance slices of the map in three orthogonal directions.

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

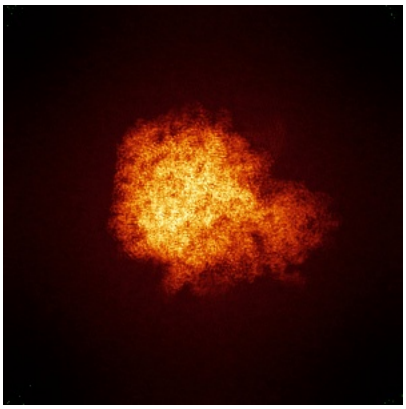
6.4.1 Primary map



X

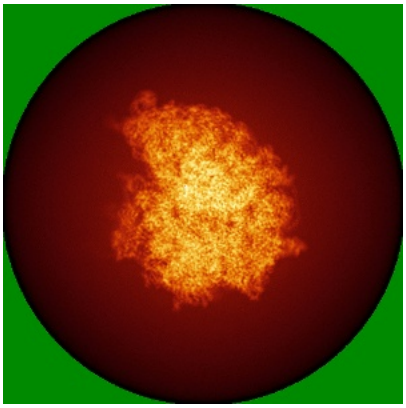


Y

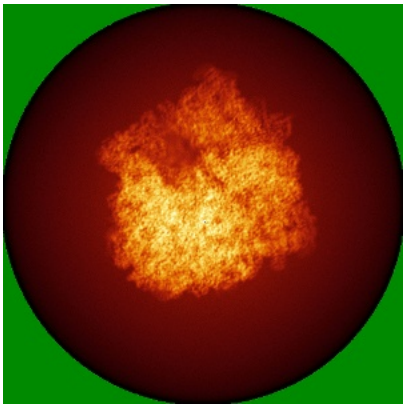


Z

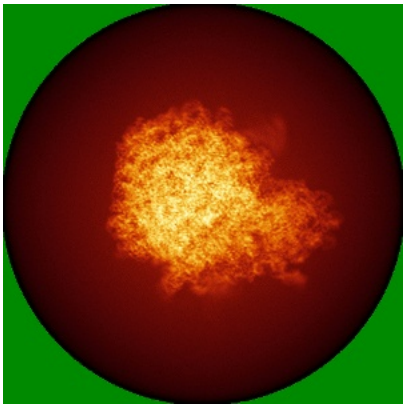
6.4.2 Raw map



X



Y



Z

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

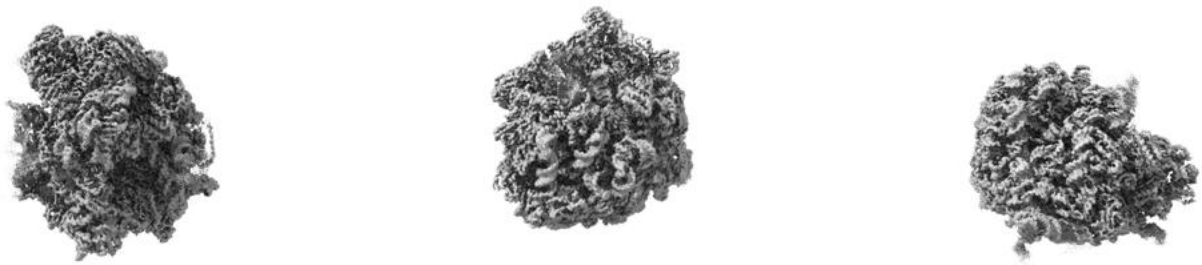
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

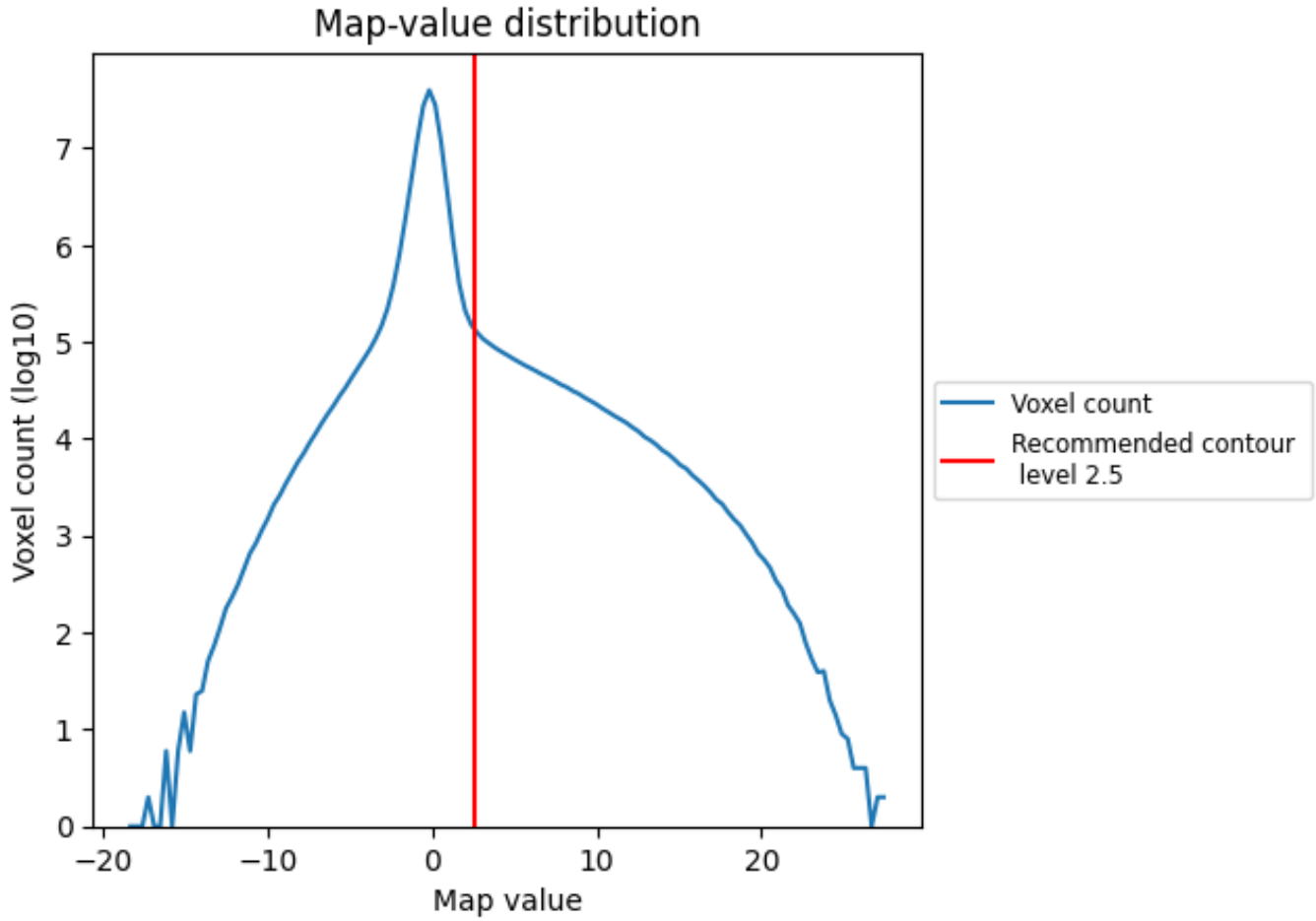
6.6 Mask visualisation (i)

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

7 Map analysis

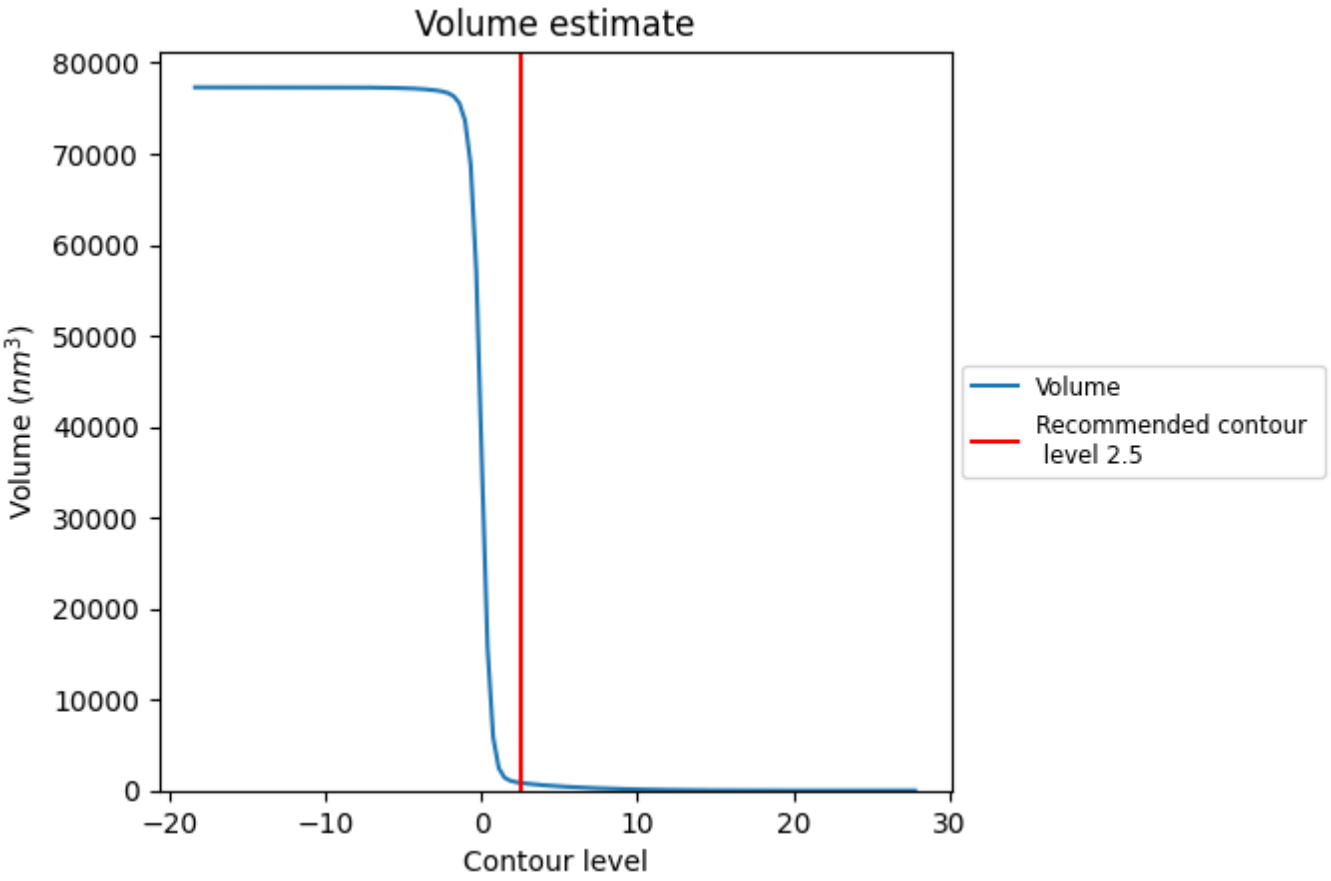
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

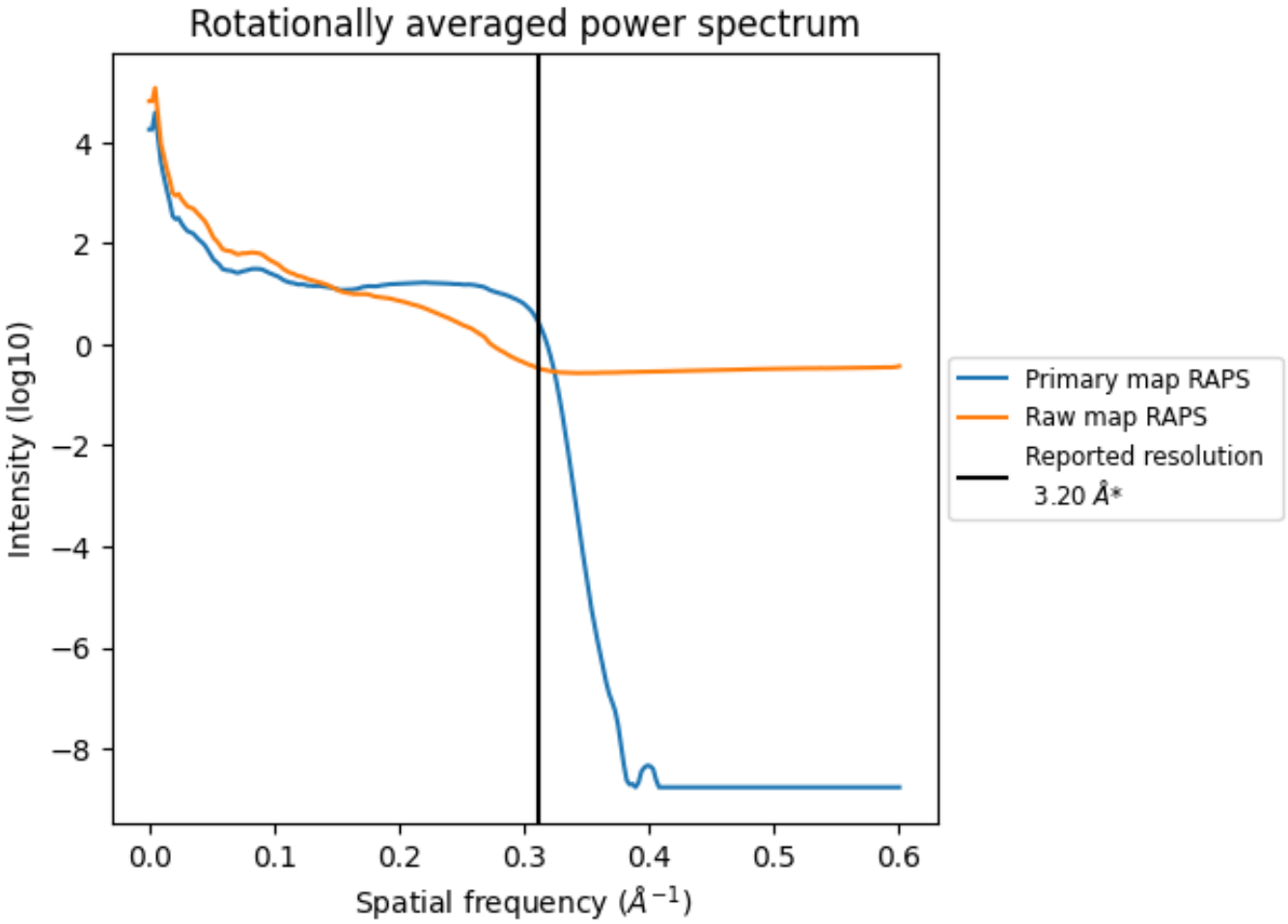
7.2 Volume estimate (i)



The volume at the recommended contour level is 852 nm^3; this corresponds to an approximate mass of 769 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)

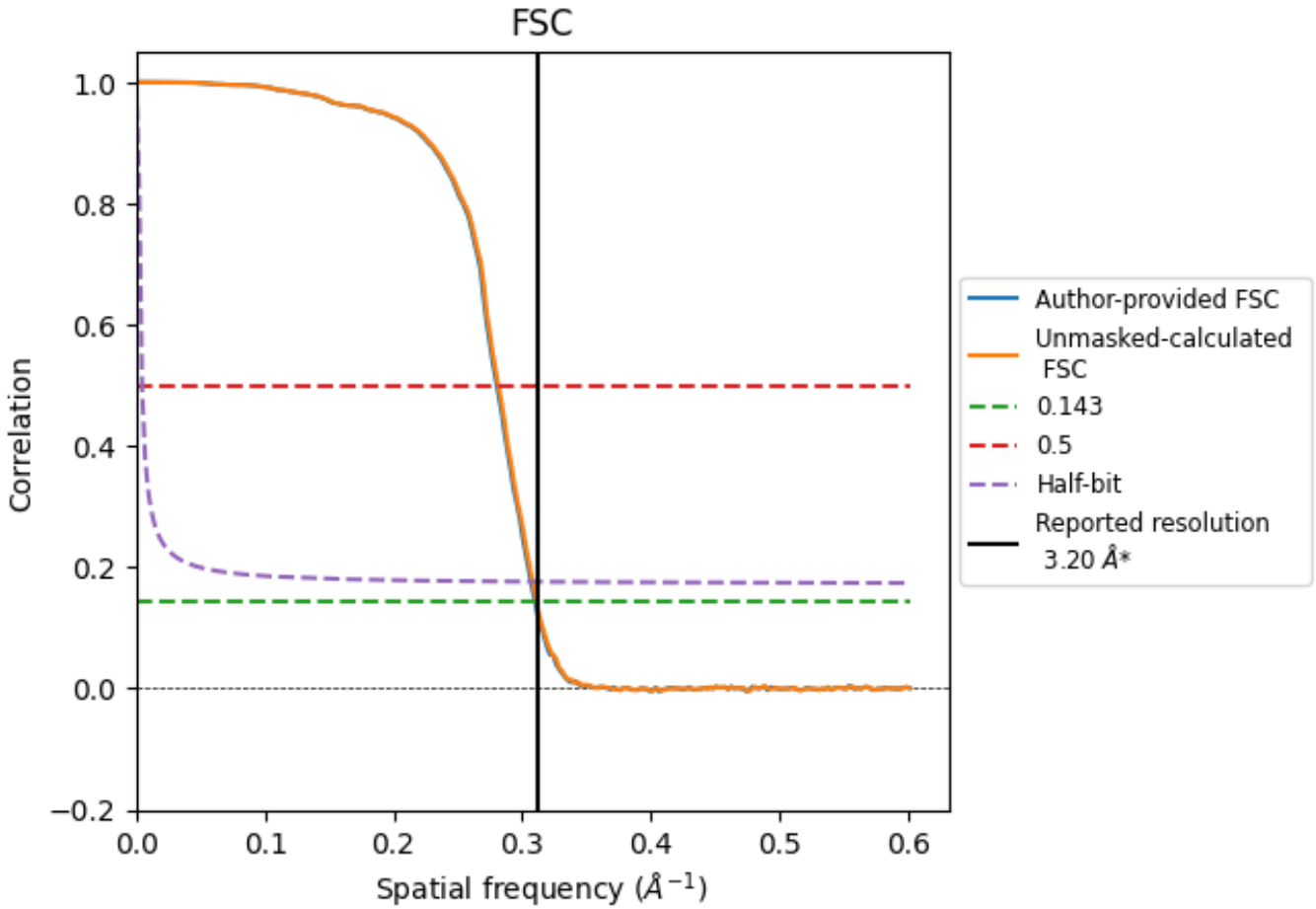


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

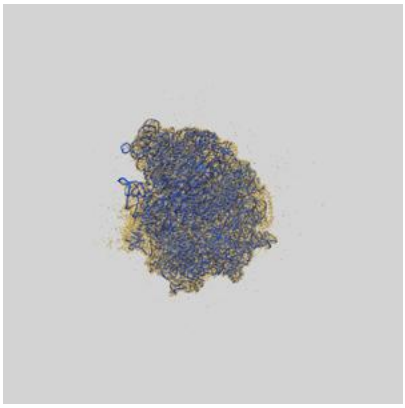
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.23	3.57	3.26
Unmasked-calculated*	3.21	3.55	3.25

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

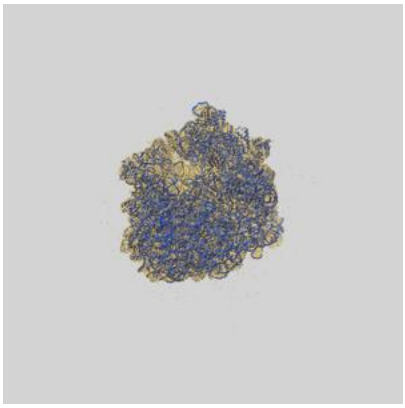
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-75650 and PDB model 11EL. Per-residue inclusion information can be found in section 3 on page 16.

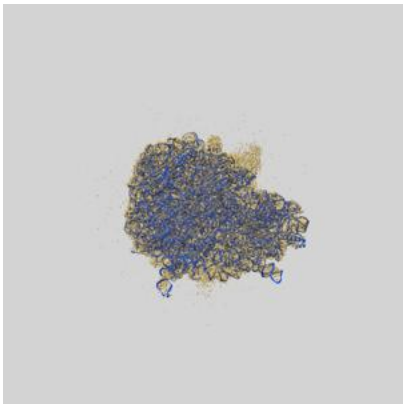
9.1 Map-model overlay



X



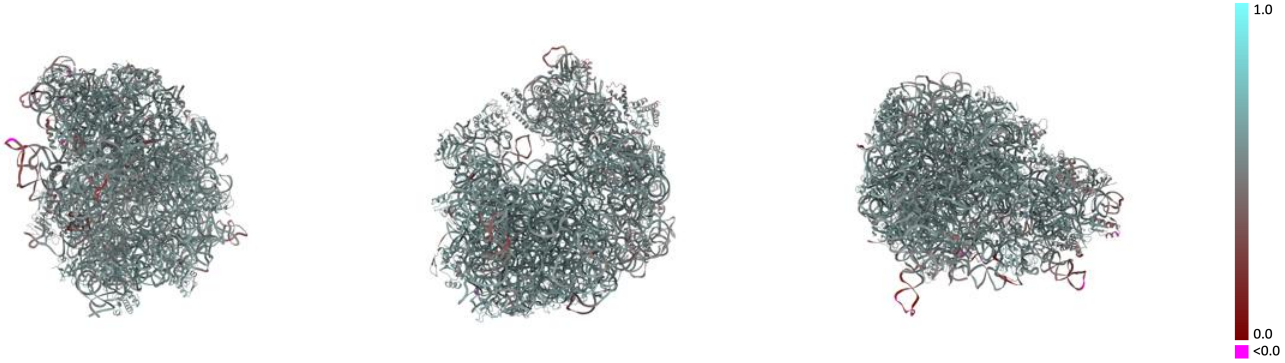
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

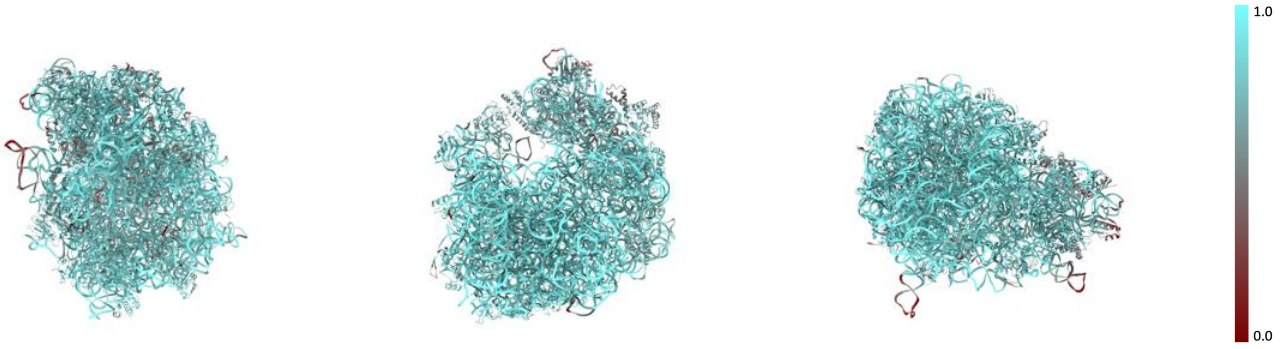
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

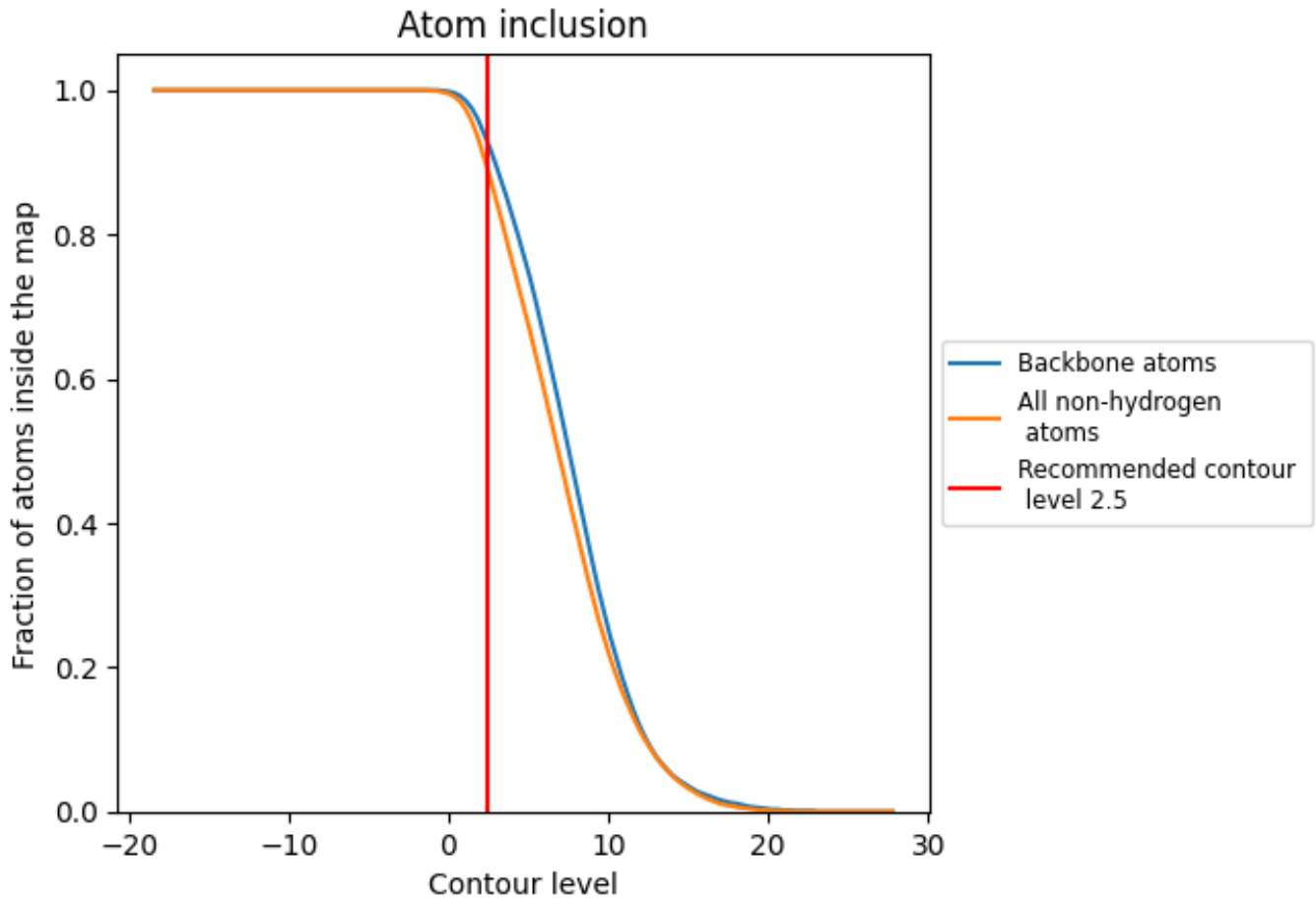
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 89% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8870	0.5560
0	0.6410	0.5560
1	0.9010	0.5960
2	0.9080	0.6030
3	0.8980	0.6060
4	0.7060	0.5010
5	0.0950	0.4890
A	0.8930	0.5350
B	0.6420	0.5180
C	0.7500	0.5470
D	0.7570	0.5480
E	0.8580	0.5740
F	0.8200	0.5440
G	0.6670	0.5000
H	0.8440	0.5760
I	0.6920	0.5260
J	0.5860	0.4920
K	0.8430	0.5570
L	0.8840	0.5780
M	0.7650	0.5410
N	0.7470	0.5370
O	0.8590	0.5700
P	0.6840	0.4320
Q	0.8160	0.5460
R	0.8300	0.5520
S	0.7640	0.5240
T	0.8260	0.5500
U	0.5080	0.4940
a	0.9370	0.5660
b	0.9170	0.5490
c	0.9250	0.5990
d	0.9050	0.5950
e	0.8200	0.5700
f	0.7500	0.5370
g	0.7800	0.5310

Continued on next page...

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Chain	Atom inclusion	Q-score
h	0.7370	0.5180
i	0.9050	0.5950
j	0.9010	0.5910
k	0.8790	0.5830
l	0.8880	0.5840
m	0.9010	0.5920
n	0.8300	0.5670
o	0.8910	0.5960
p	0.8930	0.5910
q	0.8700	0.5930
r	0.8640	0.5840
s	0.8410	0.5700
t	0.8200	0.5700
u	0.8540	0.5800
v	0.9000	0.5910
w	0.8950	0.5860
x	0.7950	0.5500
y	0.8580	0.5820
z	0.8880	0.5870