Full wwPDB EM Validation Report ⓘ

Apr 17, 2024 – 12:04 pm BST

PDB ID	:	8PVA
EMDB ID	:	EMD-17959
Title	:	Structure of bacterial ribosome determined by cryoEM at 100 keV
Authors	:	McMullan, G.; Naydenova, K.; Mihaylov, D.; Peet, M.J.; Wilson, H.; Yamashita, K.; Dickerson, J.L.; Chen, S.; Cannone, G.; Lee, Y.; Hutchings, K.A.; Gittins, O.; Sobhy, M.; Wells, T.; El-Gomati, M.M.; Dalby, J.; Meffert, M.; Schulze-Briese, C.; Henderson, R.; Russo, C.J.
Deposited on	:	2023-07-17
Resolution	:	4.50 Å(reported)
Based on initial model	:	7k00

This is a Full wwPDB EM Validation 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:

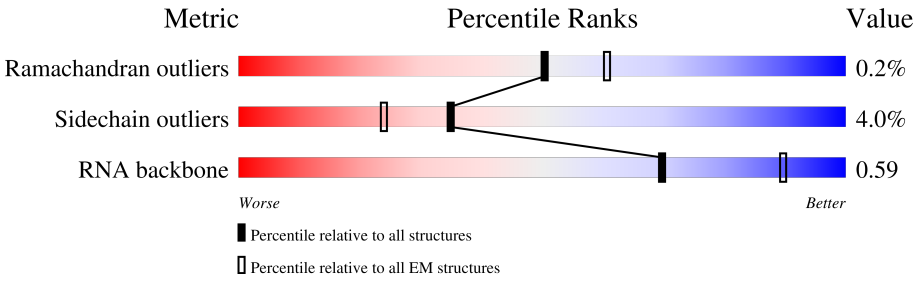
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	1542	83% 15%
2	B	241	30% 87% 6% 7%
3	C	233	38% 85% 12%
4	D	206	54% 93% 6%
5	E	167	26% 92% 7%
6	F	135	16% 74% 24%
7	G	179	30% 79% 6% 15%
8	H	130	25% 97%

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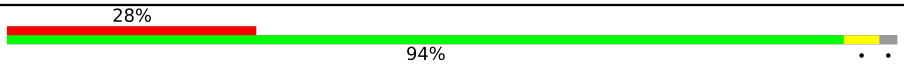
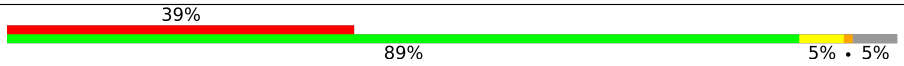
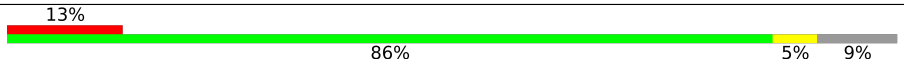
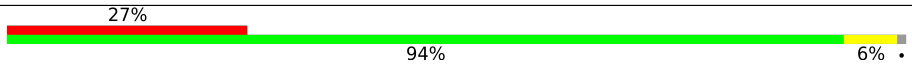
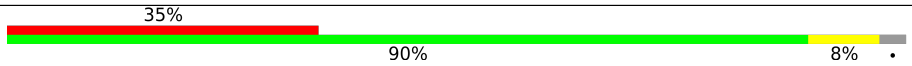
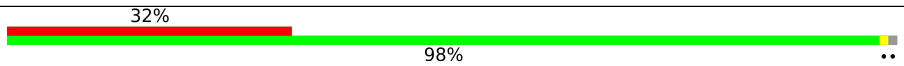
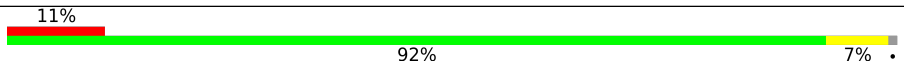
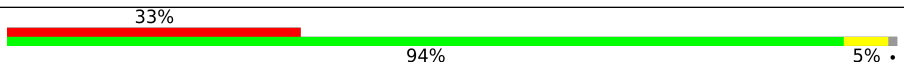
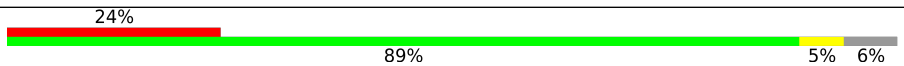
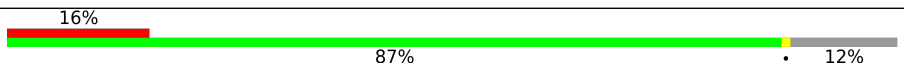
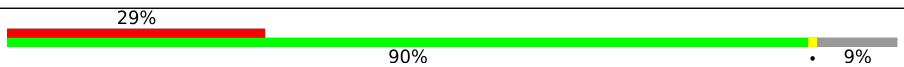
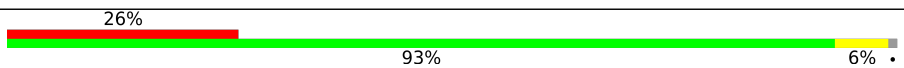
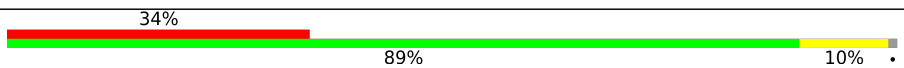
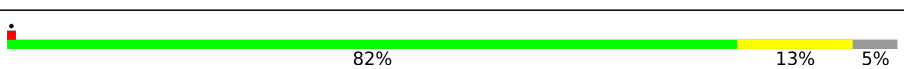
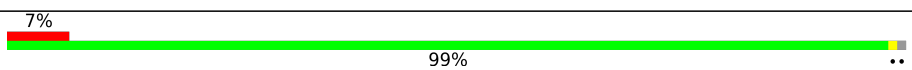
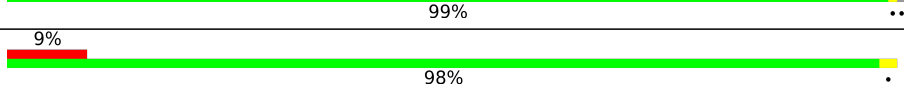
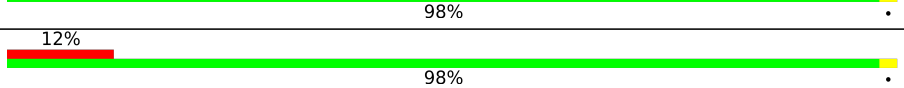
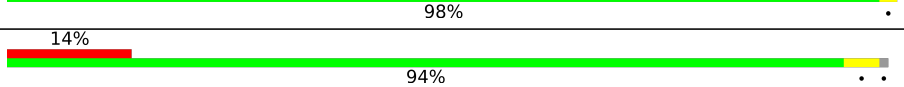
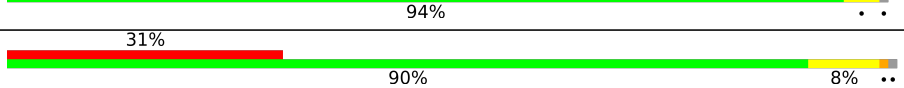
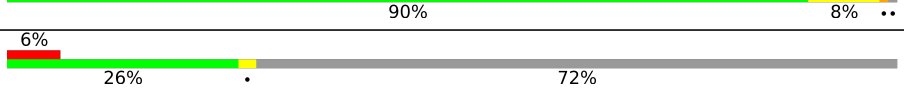
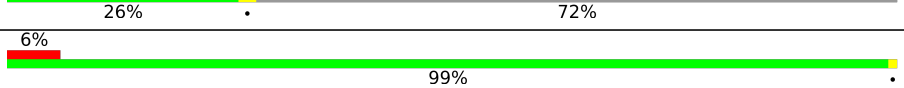
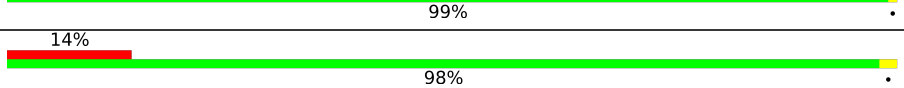
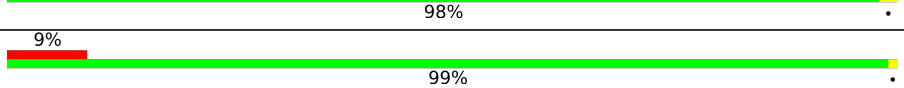
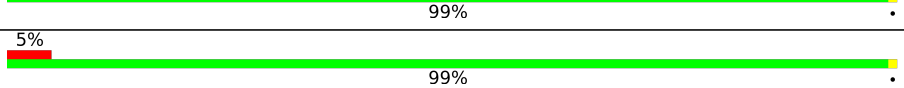
Mol	Chain	Length	Quality of chain
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	a	2904	
23	b	120	
24	c	273	
25	d	209	
26	e	201	
27	f	179	
28	g	177	
29	h	149	
30	i	142	
31	j	123	
32	k	144	
33	l	136	

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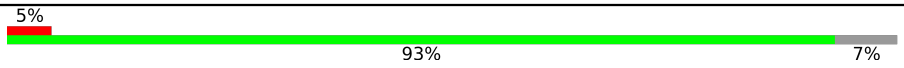
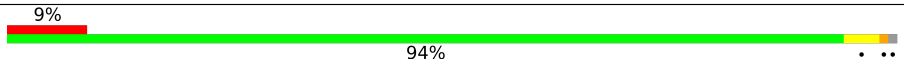
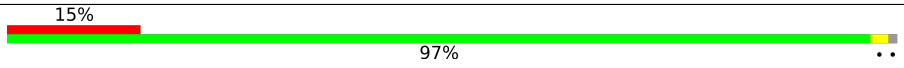
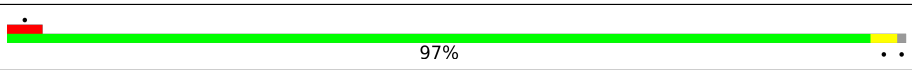
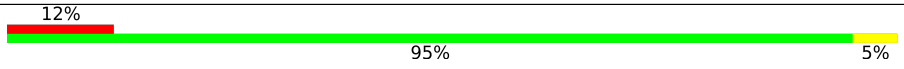
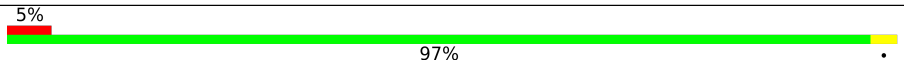
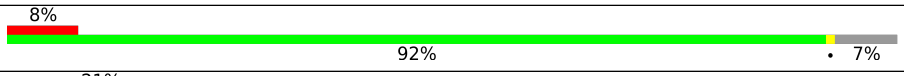
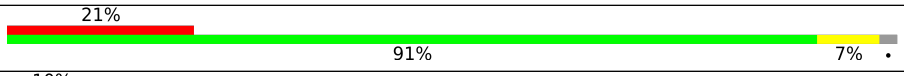
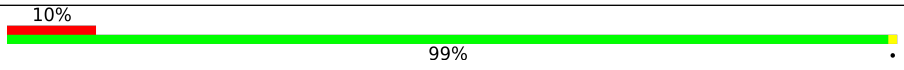
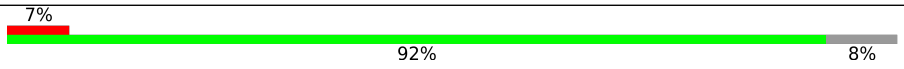
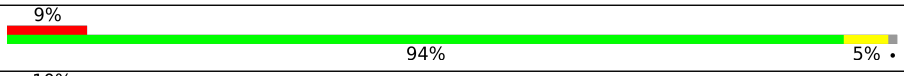
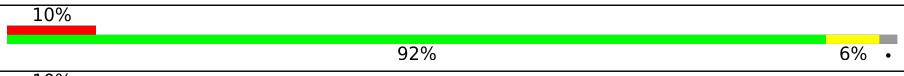
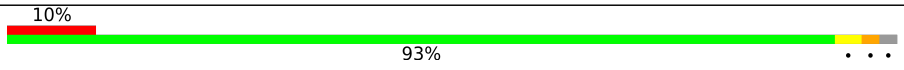
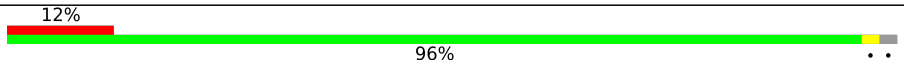
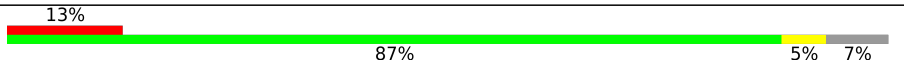
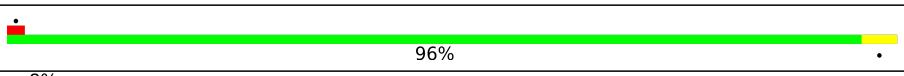
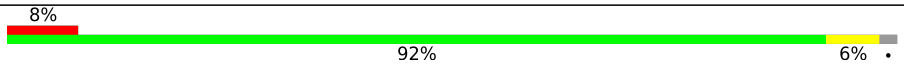
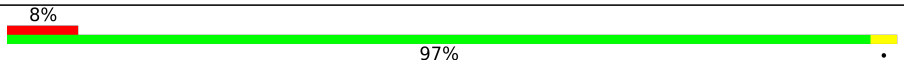
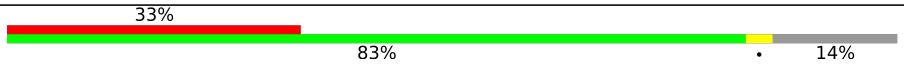
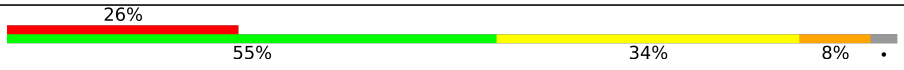
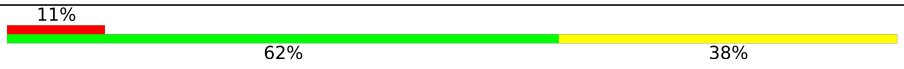
Mol	Chain	Length	Quality of chain
34	m	127	
35	n	117	
36	o	115	
37	p	118	
38	q	103	
39	r	110	
40	s	100	
41	t	104	
42	u	94	
43	v	85	
44	w	78	
45	x	63	
46	y	59	
47	z	57	
48	0	55	
49	1	46	
50	2	65	
51	3	38	
52	4	70	
53	X	28	
54	Y	76	
55	Z	76	
56	5	2	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 141565 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

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

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 6 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

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

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

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

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

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

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

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

- Molecule 24 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 25 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 26 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 27 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 28 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 29 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 30 is a protein called Large ribosomal subunit protein uL13.

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

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

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

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

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

- Molecule 33 is a protein called Large ribosomal subunit protein uL16.

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 52 is a protein called Large ribosomal subunit protein bL31A.

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

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	X	12	Total	C	N	O	P	0	0
			260	117	51	80	12		

- Molecule 54 is a RNA chain called A-site tRNA-val.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Y	74	Total	C	N	O	P	0	0
			1579	705	287	514	73		

- Molecule 55 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Z	76	Total	C	N	O	P	0	0
			1623	723	294	530	76		

- Molecule 56 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	5	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

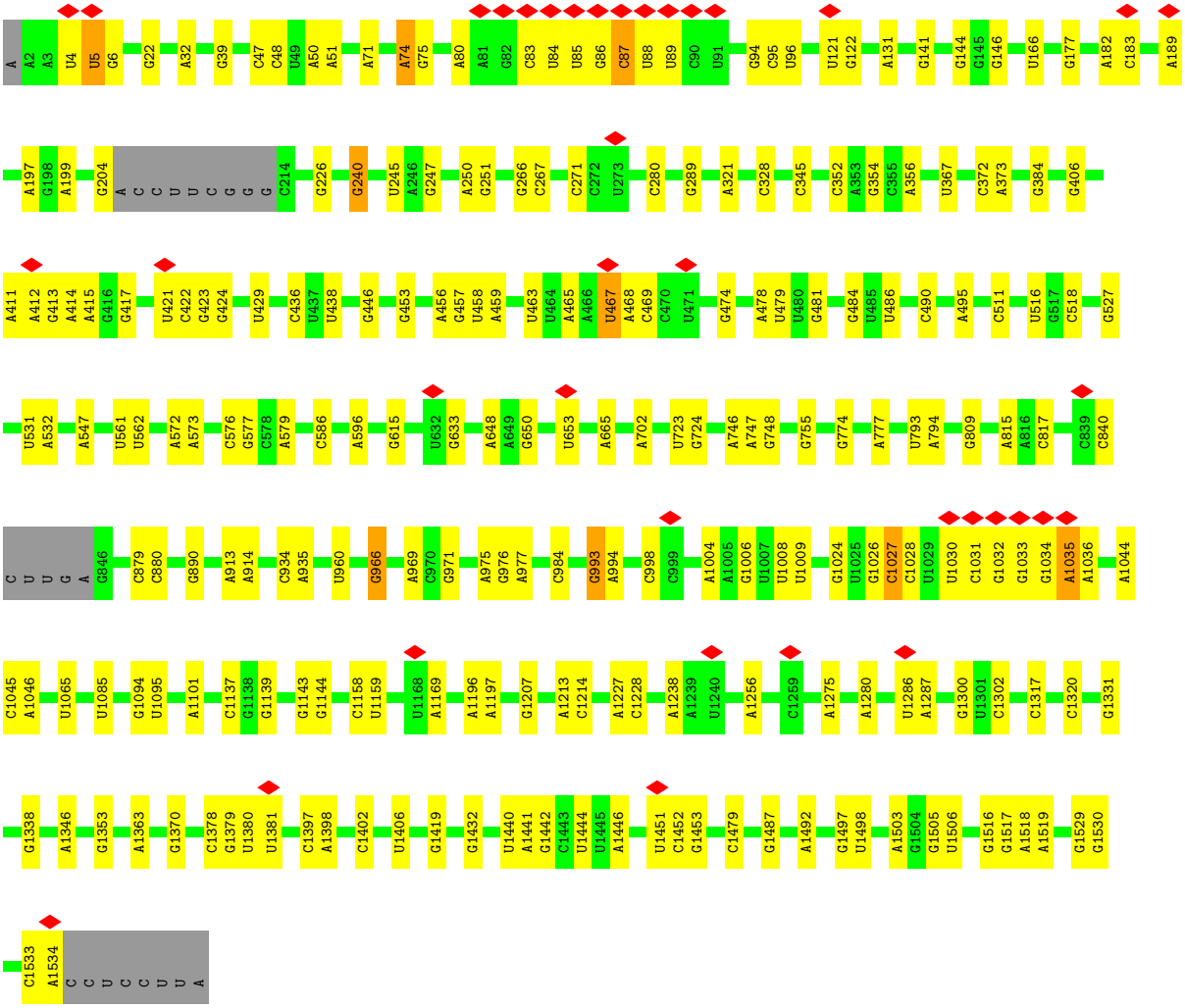
Mol	Chain	Residues	Atoms		AltConf
57	3	1	Total	Zn	0
			1	1	
57	4	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

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

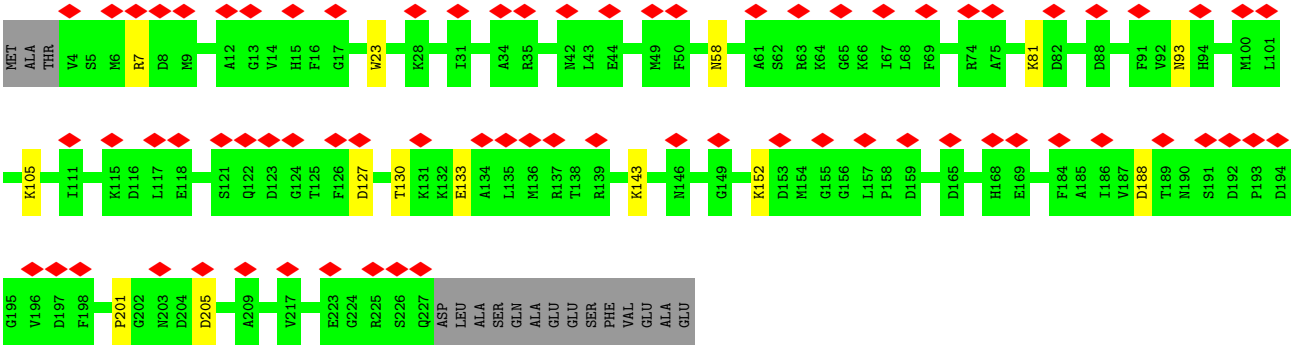
- Molecule 1: 16S rRNA

Chain A:



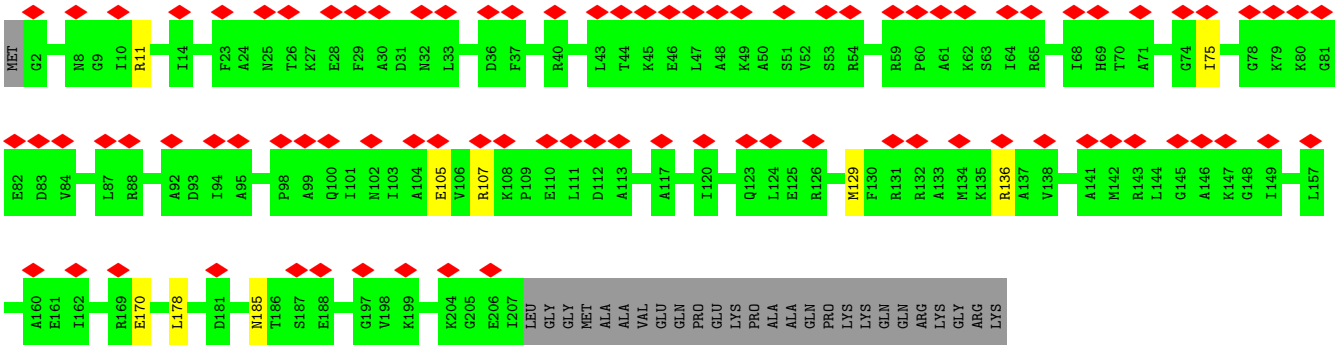
- Molecule 2: Small ribosomal subunit protein uS2

Chain B:



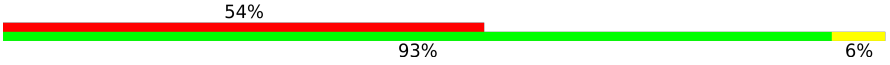
• Molecule 3: Small ribosomal subunit protein uS3

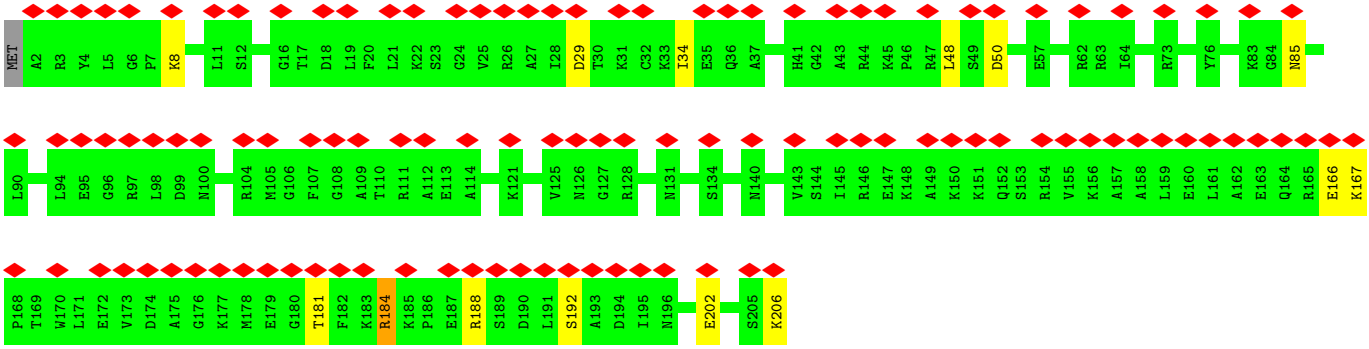
Chain C:



• Molecule 4: Small ribosomal subunit protein uS4

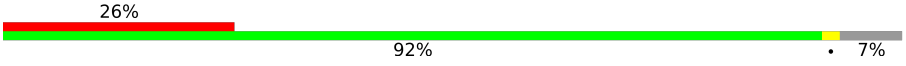
Chain D:

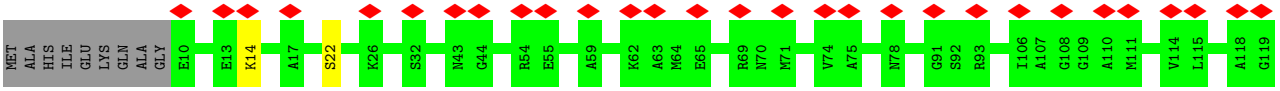


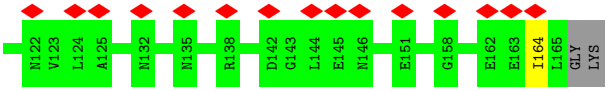


• Molecule 5: Small ribosomal subunit protein uS5

Chain E:

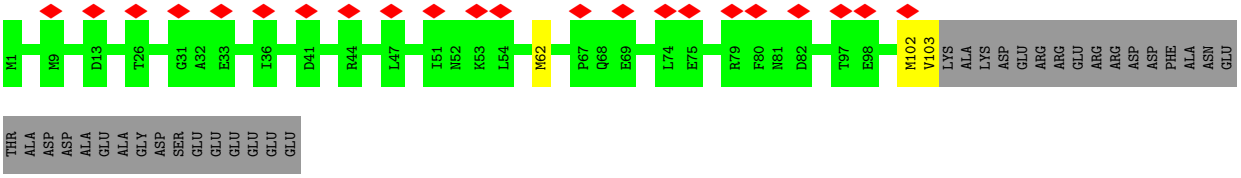






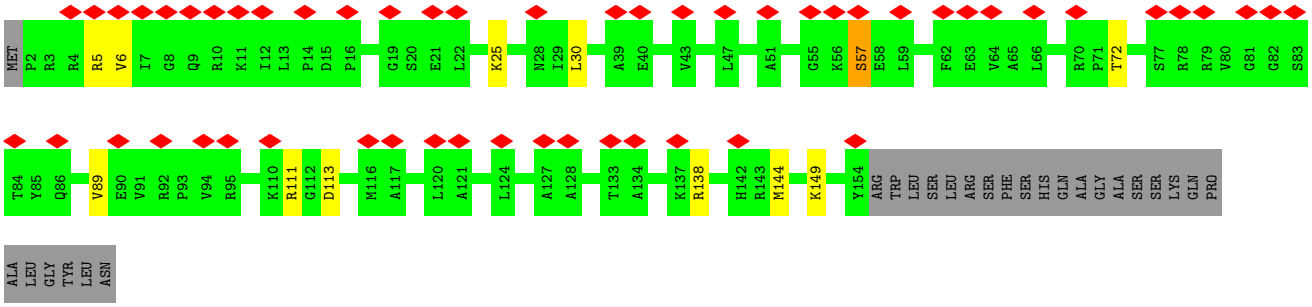
• Molecule 6: Small ribosomal subunit protein bS6, fully modified isoform

Chain F:



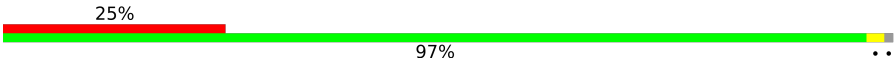
• Molecule 7: Small ribosomal subunit protein uS7

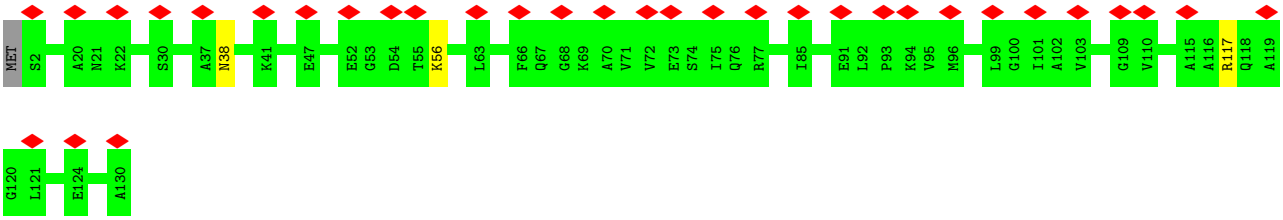
Chain G:



• Molecule 8: Small ribosomal subunit protein uS8

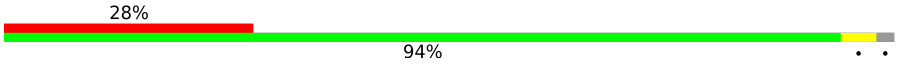
Chain H:

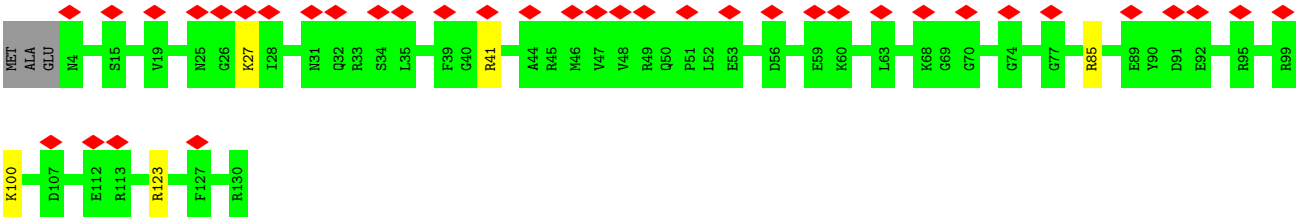




• Molecule 9: Small ribosomal subunit protein uS9

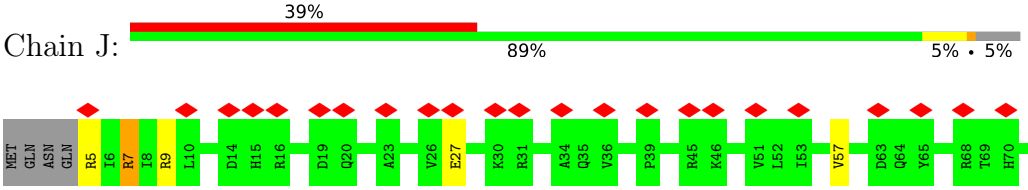
Chain I:





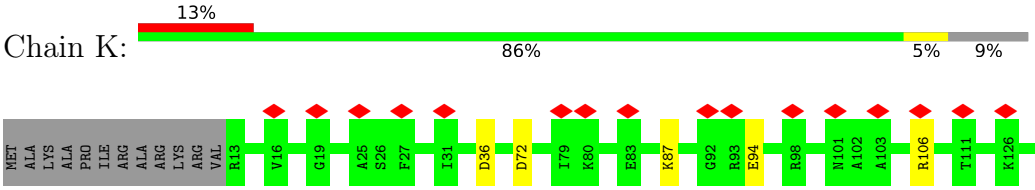
• Molecule 10: Small ribosomal subunit protein uS10

Chain J:



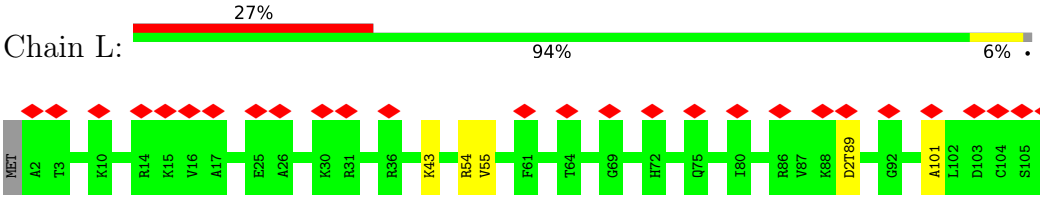
• Molecule 11: Small ribosomal subunit protein uS11

Chain K:



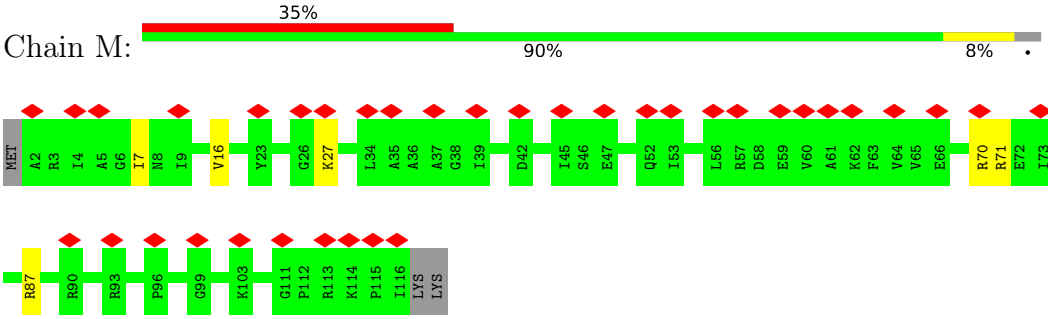
• Molecule 12: Small ribosomal subunit protein uS12

Chain L:



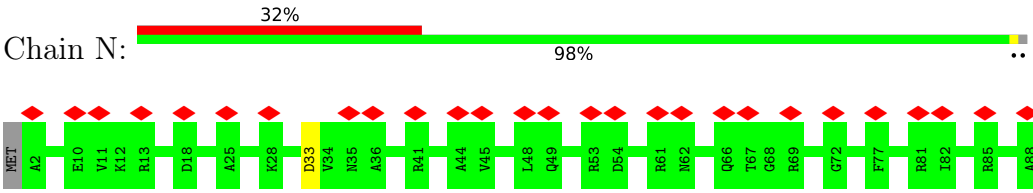
• Molecule 13: Small ribosomal subunit protein uS13

Chain M:



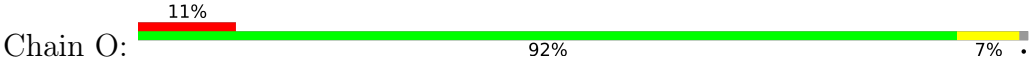
• Molecule 14: Small ribosomal subunit protein uS14

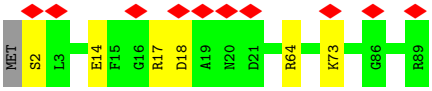
Chain N:



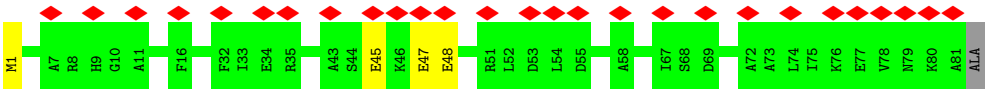
• Molecule 15: Small ribosomal subunit protein uS15

Chain O:

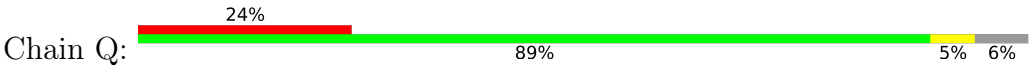


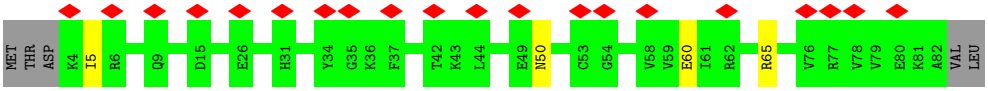


• Molecule 16: Small ribosomal subunit protein bS16

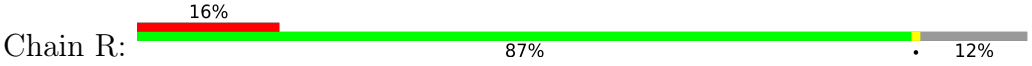


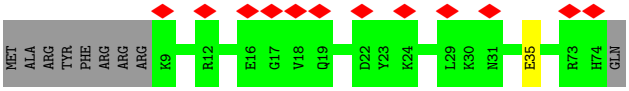
• Molecule 17: Small ribosomal subunit protein uS17



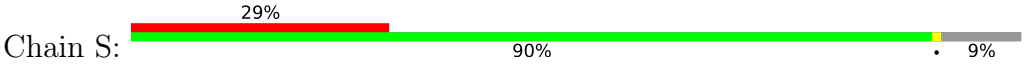


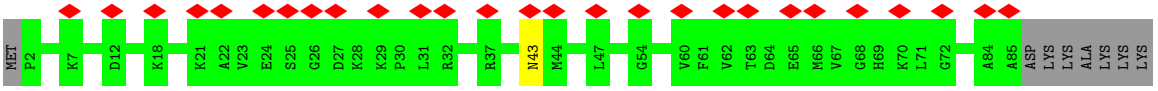
• Molecule 18: Small ribosomal subunit protein bS18



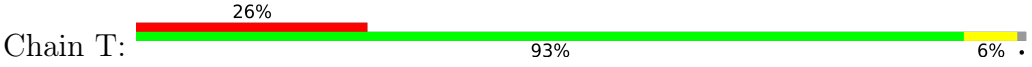


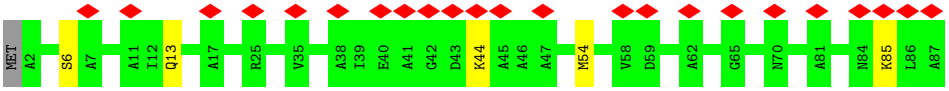
• Molecule 19: Small ribosomal subunit protein uS19



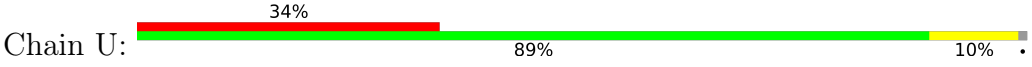


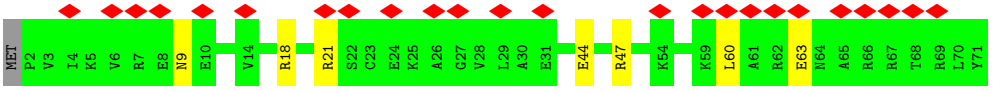
• Molecule 20: Small ribosomal subunit protein bS20





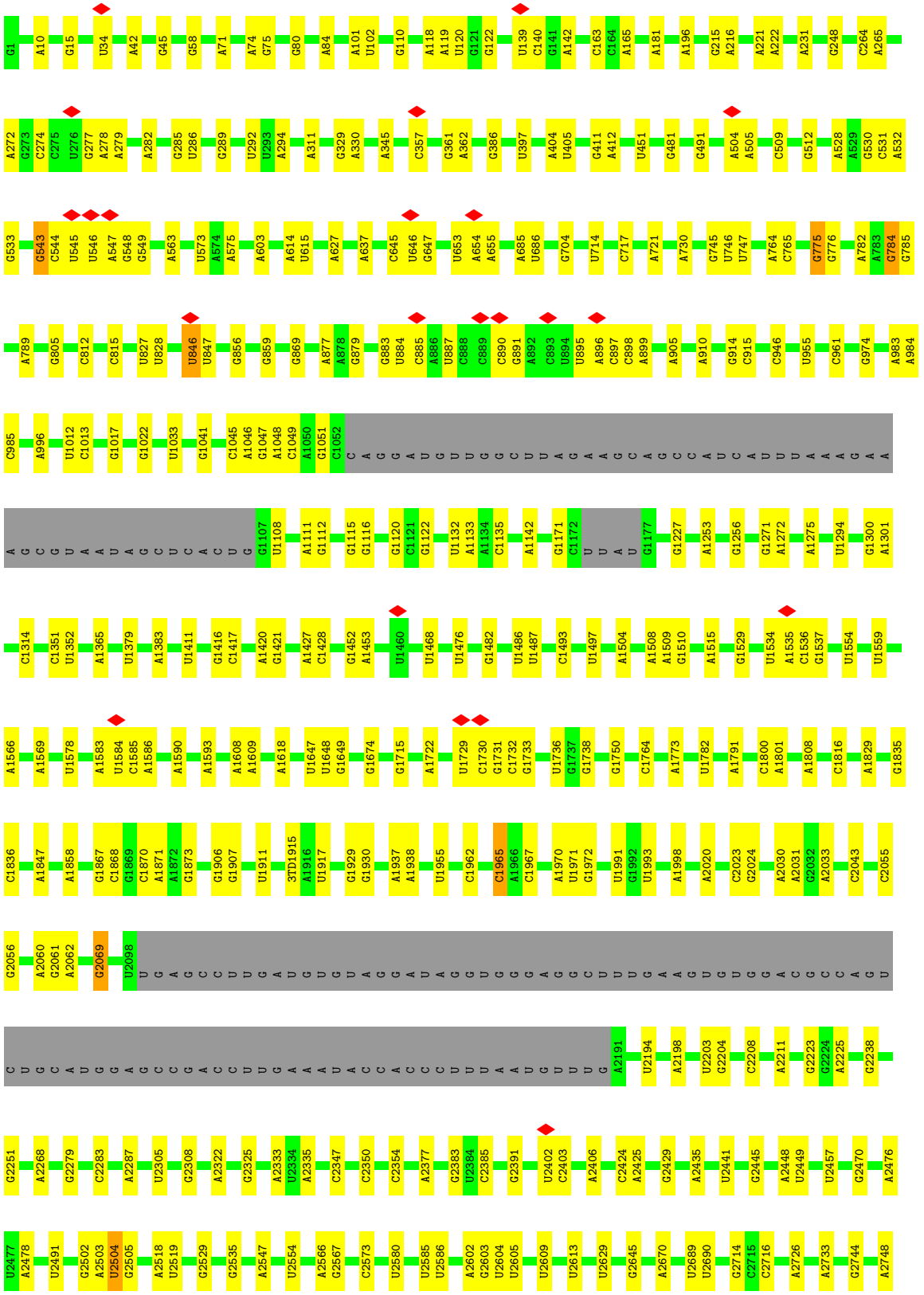
• Molecule 21: Small ribosomal subunit protein bS21

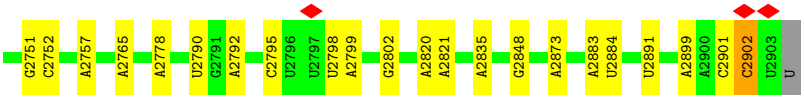




• Molecule 22: 23S rRNA

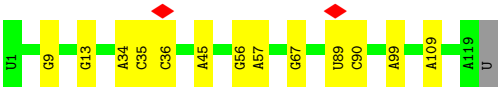
Chain a:





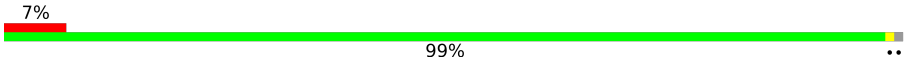
• Molecule 23: 5S rRNA

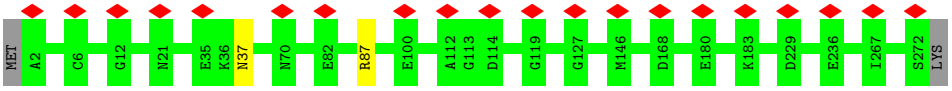
Chain b:



• Molecule 24: Large ribosomal subunit protein uL2

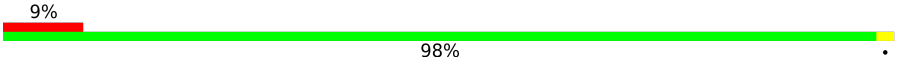
Chain c:

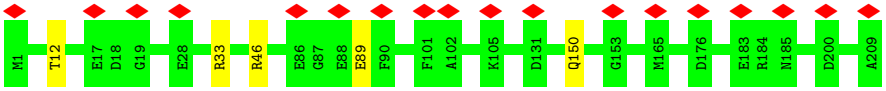




• Molecule 25: Large ribosomal subunit protein uL3

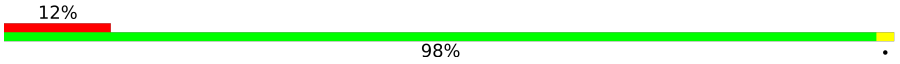
Chain d:

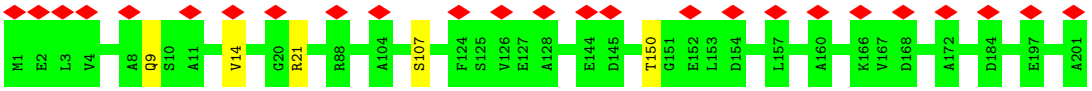




• Molecule 26: Large ribosomal subunit protein uL4

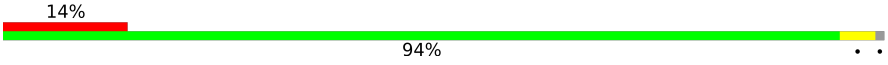
Chain e:

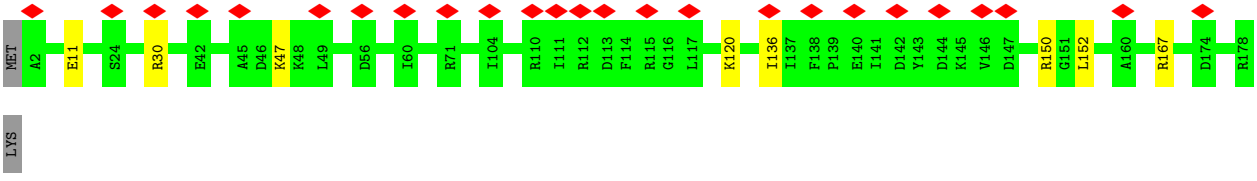




• Molecule 27: Large ribosomal subunit protein uL5

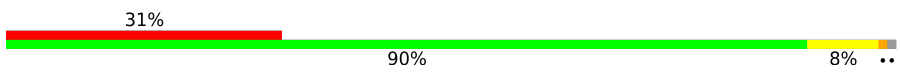
Chain f:

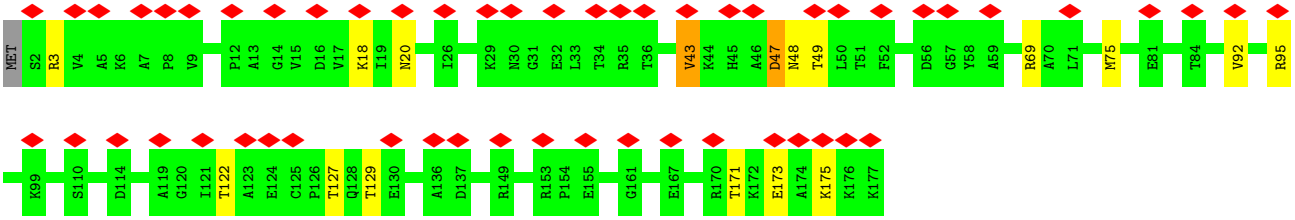




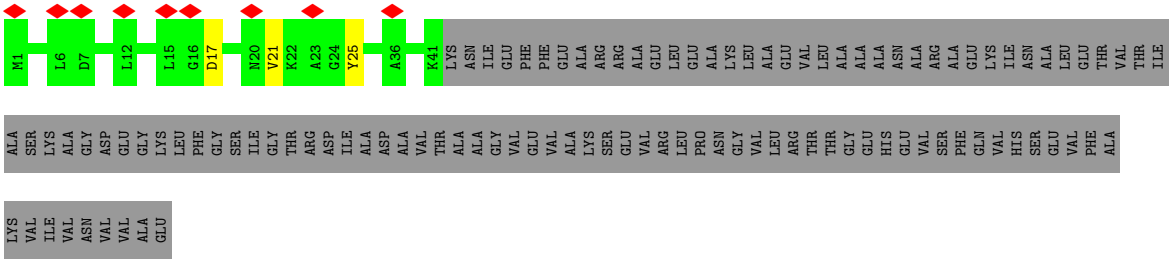
• Molecule 28: Large ribosomal subunit protein uL6

Chain g:

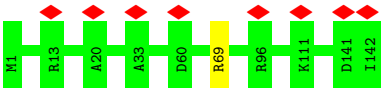




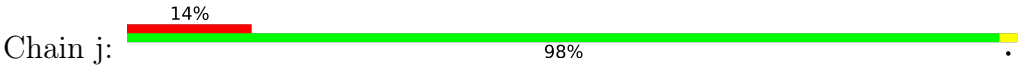
• Molecule 29: Large ribosomal subunit protein bL9

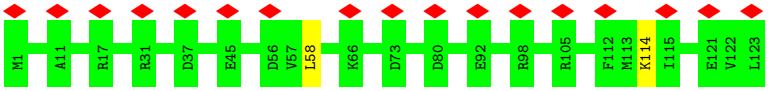


• Molecule 30: Large ribosomal subunit protein uL13

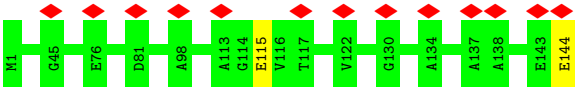


• Molecule 31: 50S ribosomal protein L14

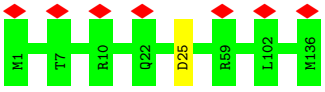




• Molecule 32: 50S ribosomal protein L15

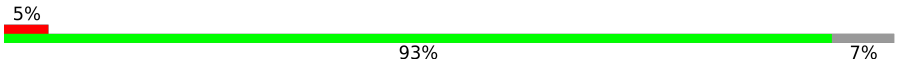


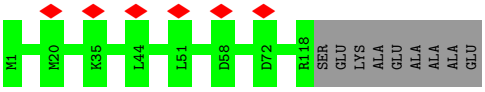
• Molecule 33: Large ribosomal subunit protein uL16



• Molecule 34: 50S ribosomal protein L17

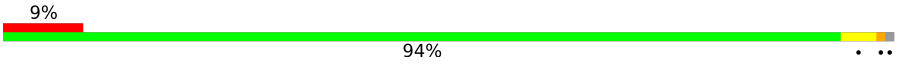
Chain m:

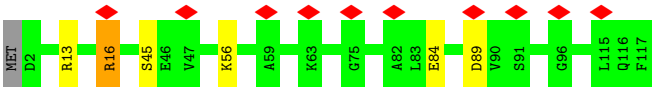




• Molecule 35: 50S ribosomal protein L18

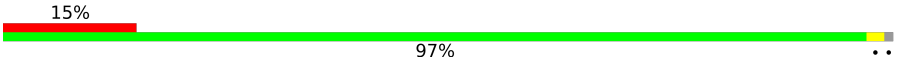
Chain n:

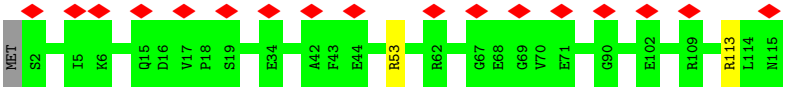




• Molecule 36: 50S ribosomal protein L19

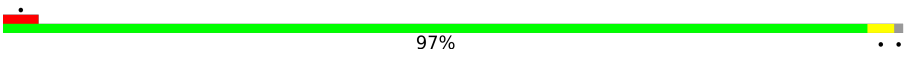
Chain o:

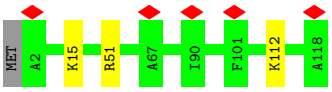




• Molecule 37: 50S ribosomal protein L20

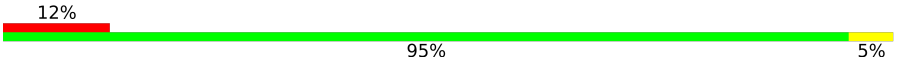
Chain p:

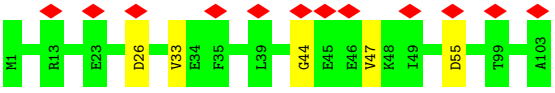




• Molecule 38: 50S ribosomal protein L21

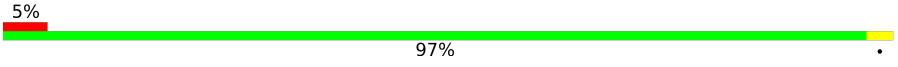
Chain q:





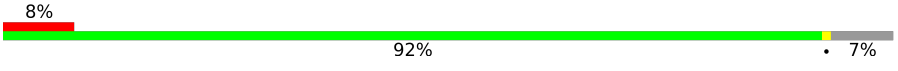
• Molecule 39: 50S ribosomal protein L22

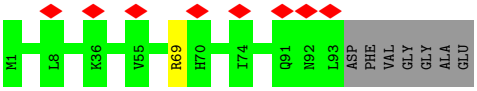
Chain r:



• Molecule 40: 50S ribosomal protein L23

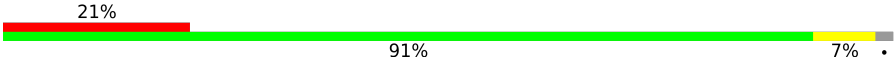
Chain s:

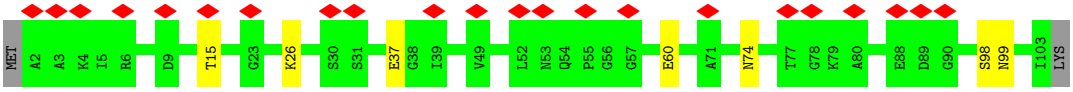




• Molecule 41: 50S ribosomal protein L24

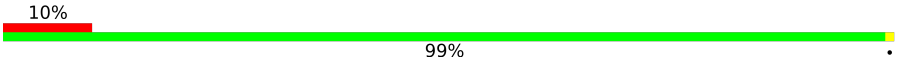
Chain t:

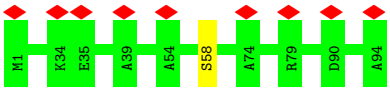




• Molecule 42: 50S ribosomal protein L25

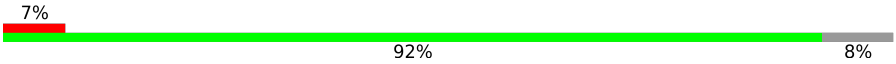
Chain u:

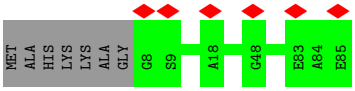




• Molecule 43: 50S ribosomal protein L27

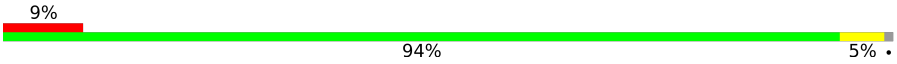
Chain v:

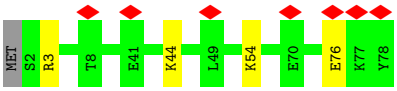




• Molecule 44: 50S ribosomal protein L28

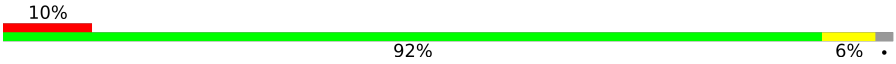
Chain w:

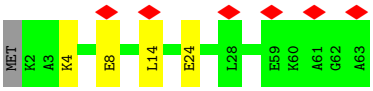




• Molecule 45: 50S ribosomal protein L29

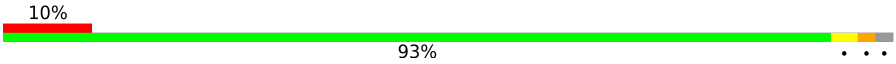
Chain x:

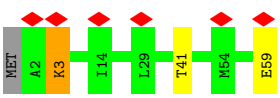




• Molecule 46: 50S ribosomal protein L30

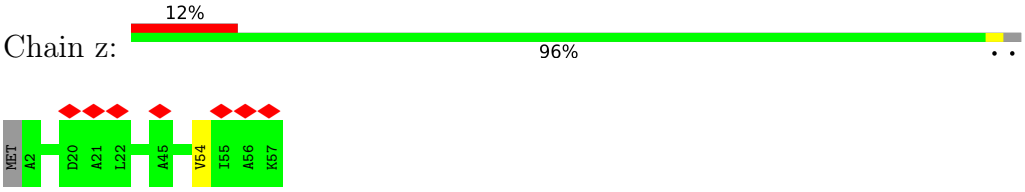
Chain y:





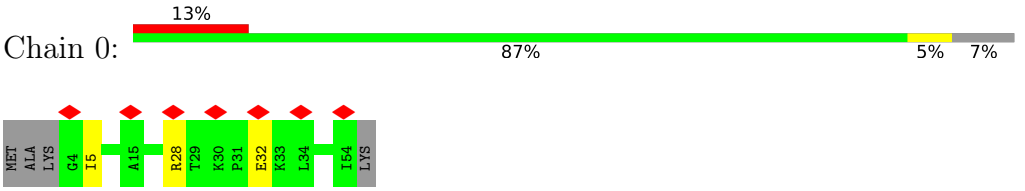
• Molecule 47: 50S ribosomal protein L32

Chain z:



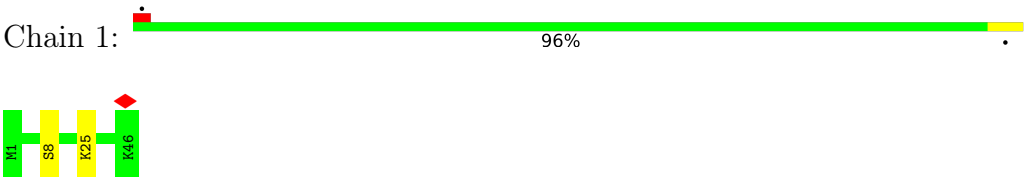
• Molecule 48: 50S ribosomal protein L33

Chain 0:



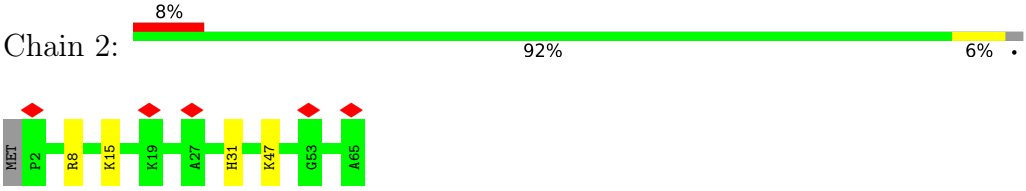
• Molecule 49: 50S ribosomal protein L34

Chain 1:



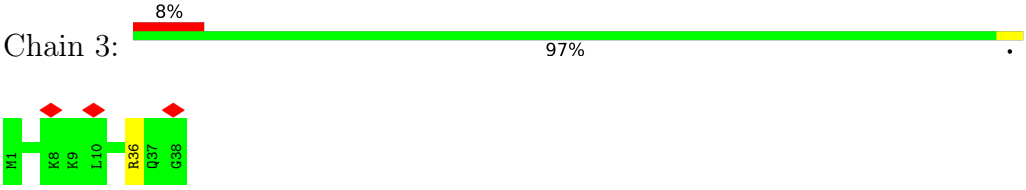
• Molecule 50: 50S ribosomal protein L35

Chain 2:



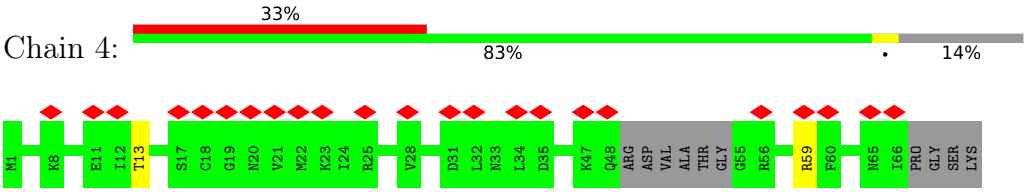
• Molecule 51: 50S ribosomal protein L36

Chain 3:



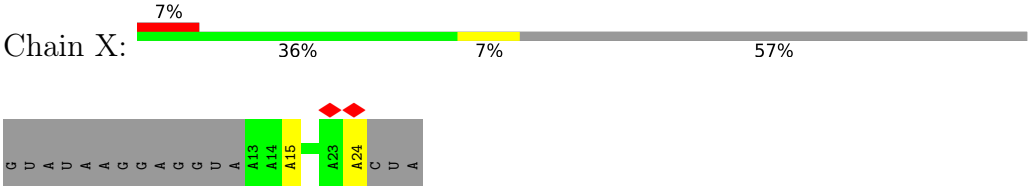
• Molecule 52: Large ribosomal subunit protein bL31A

Chain 4:



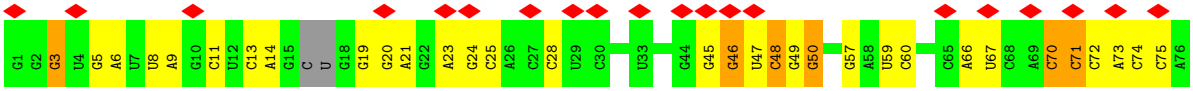
• Molecule 53: mRNA

Chain X:



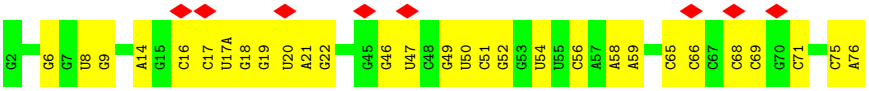
• Molecule 54: A-site tRNA-val

Chain Y:



• Molecule 55: P-site tRNA-fMet

Chain Z:



• Molecule 56: E-site tRNA

Chain 5:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11872	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 1400/HR + YPS FEG	Depositor
Voltage (kV)	100	Depositor
Electron dose ($e^-/Å^2$)	24	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	DECTRIS SINGLA (1k x 1k)	Depositor
Maximum map value	0.050	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	412.4, 412.4, 412.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.031, 1.031, 1.031	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.66	0/36236	1.17	24/56520 (0.0%)
2	B	0.45	0/1784	0.85	0/2403
3	C	0.43	0/1651	0.84	2/2225 (0.1%)
4	D	0.44	0/1665	0.88	1/2227 (0.0%)
5	E	0.44	0/1165	0.84	0/1568
6	F	0.45	0/858	0.85	0/1160
7	G	0.44	0/1219	0.95	1/1635 (0.1%)
8	H	0.43	0/989	0.83	1/1326 (0.1%)
9	I	0.44	0/1034	0.90	2/1375 (0.1%)
10	J	0.42	0/796	0.97	3/1077 (0.3%)
11	K	0.43	0/884	0.84	0/1191
12	L	0.43	0/960	0.89	1/1286 (0.1%)
13	M	0.46	0/900	0.99	5/1204 (0.4%)
14	N	0.42	0/817	0.81	0/1088
15	O	0.42	0/722	0.78	0/964
16	P	0.42	0/653	0.87	0/877
17	Q	0.42	0/650	0.86	0/871
18	R	0.43	0/553	0.89	0/742
19	S	0.45	0/685	0.83	0/922
20	T	0.41	0/676	0.83	0/895
21	U	0.43	0/597	1.01	2/792 (0.3%)
22	a	0.64	0/65651	1.18	31/102413 (0.0%)
23	b	0.68	0/2850	1.20	0/4444
24	c	0.43	0/2121	0.86	1/2852 (0.0%)
25	d	0.41	0/1576	0.80	1/2119 (0.0%)
26	e	0.41	0/1571	0.80	0/2113
27	f	0.45	0/1434	0.83	1/1926 (0.1%)
28	g	0.45	0/1343	0.91	1/1816 (0.1%)
29	h	0.48	0/306	0.96	0/413
30	i	0.42	0/1152	0.81	1/1551 (0.1%)
31	j	0.42	0/955	0.87	0/1279

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	k	0.45	0/1062	0.83	0/1413
33	l	0.41	0/1073	0.85	0/1433
34	m	0.41	0/958	0.86	0/1281
35	n	0.43	0/902	0.88	1/1209 (0.1%)
36	o	0.41	0/929	0.87	1/1242 (0.1%)
37	p	0.40	0/960	0.80	0/1278
38	q	0.43	0/829	0.87	0/1107
39	r	0.40	0/864	0.84	0/1156
40	s	0.41	0/744	0.87	1/994 (0.1%)
41	t	0.43	0/787	0.88	0/1051
42	u	0.42	0/766	0.86	0/1025
43	v	0.43	0/593	0.84	0/785
44	w	0.43	0/635	0.88	1/848 (0.1%)
45	x	0.44	0/502	0.83	0/667
46	y	0.41	0/453	0.86	0/605
47	z	0.42	0/450	0.84	0/599
48	0	0.44	0/424	0.90	0/565
49	1	0.40	0/380	0.88	0/498
50	2	0.41	0/513	0.91	1/676 (0.1%)
51	3	0.41	0/303	0.91	0/397
52	4	0.45	0/488	0.82	0/649
53	X	0.71	0/292	1.10	0/453
54	Y	0.75	0/1764	1.43	10/2747 (0.4%)
55	Z	0.74	0/1813	1.31	2/2825 (0.1%)
56	5	0.99	0/46	1.12	0/69
All	All	0.60	0/152983	1.11	95/228846 (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
2	B	0	1
12	L	0	1
28	g	0	2
46	y	0	1
All	All	0	5

There are no bond length outliers.

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	M	71	ARG	NE-CZ-NH1	10.38	125.49	120.30
22	a	512	G	O4'-C1'-N9	9.34	115.67	108.20
54	Y	46	G	O4'-C1'-N9	8.20	114.76	108.20
22	a	122	G	O5'-P-OP2	-8.18	98.33	105.70
54	Y	70	C	C6-N1-C2	-7.59	117.26	120.30
22	a	404	A	P-O3'-C3'	7.34	128.51	119.70
13	M	71	ARG	NE-CZ-NH2	-7.09	116.76	120.30
22	a	397	U	O5'-P-OP2	-7.00	99.40	105.70
1	A	1035	A	P-O3'-C3'	6.78	127.84	119.70
22	a	784	G	P-O3'-C3'	6.75	127.80	119.70
22	a	277	G	P-O3'-C3'	6.72	127.77	119.70
54	Y	3	G	O4'-C1'-N9	6.60	113.48	108.20
1	A	1331	G	O4'-C1'-N9	6.58	113.47	108.20
22	a	846	U	OP1-P-O3'	6.48	119.47	105.20
22	a	815	C	O5'-P-OP2	-6.46	99.89	105.70
22	a	877	A	O5'-P-OP2	-6.38	99.96	105.70
54	Y	71	C	C6-N1-C2	-6.29	117.78	120.30
22	a	1049	C	C6-N1-C2	-6.28	117.79	120.30
1	A	1479	C	O5'-P-OP2	-6.25	100.07	105.70
22	a	846	U	P-O3'-C3'	6.16	127.09	119.70
1	A	74	A	O4'-C1'-N9	6.16	113.12	108.20
54	Y	50	G	O5'-P-OP1	-6.14	100.17	105.70
10	J	5	ARG	NE-CZ-NH1	6.12	123.36	120.30
54	Y	3	G	C8-N9-C4	-6.10	103.96	106.40
22	a	1965	C	O5'-P-OP2	-6.09	100.22	105.70
22	a	2024	G	O5'-P-OP2	-6.08	100.23	105.70
21	U	18	ARG	NE-CZ-NH1	6.04	123.32	120.30
21	U	47	ARG	NE-CZ-NH1	6.02	123.31	120.30
54	Y	3	G	N9-C4-C5	5.97	107.79	105.40
1	A	87	C	C6-N1-C2	-5.90	117.94	120.30
40	s	69	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	809	G	O5'-P-OP2	-5.81	100.47	105.70
4	D	184	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	A	561	U	O3'-P-O5'	-5.81	92.97	104.00
28	g	69	ARG	NE-CZ-NH1	5.76	123.18	120.30
22	a	2519	U	O3'-P-O5'	-5.74	93.10	104.00
54	Y	72	C	C6-N1-C2	-5.65	118.04	120.30
22	a	2848	G	O4'-C1'-N9	5.64	112.71	108.20
1	A	5	U	P-O3'-C3'	5.64	126.47	119.70
3	C	11	ARG	NE-CZ-NH1	5.62	123.11	120.30
27	f	167	ARG	NE-CZ-NH1	5.62	123.11	120.30
22	a	2645	G	O4'-C1'-N9	5.61	112.69	108.20
44	w	3	ARG	NE-CZ-NH2	5.61	123.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	136	ARG	NE-CZ-NH1	5.52	123.06	120.30
25	d	46	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	438	U	O4'-C1'-N1	5.46	112.56	108.20
1	A	586	C	O4'-C1'-N1	5.46	112.56	108.20
22	a	784	G	OP1-P-O3'	5.46	117.20	105.20
1	A	1406	U	O4'-C1'-N1	5.45	112.56	108.20
50	2	8	ARG	NE-CZ-NH1	5.45	123.03	120.30
22	a	775	G	O4'-C1'-N9	5.45	112.56	108.20
1	A	1158	C	C6-N1-C2	-5.40	118.14	120.30
35	n	16	ARG	NE-CZ-NH2	5.39	123.00	120.30
22	a	2902	C	C6-N1-C2	-5.38	118.15	120.30
7	G	138	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	1027	C	C6-N1-C2	-5.35	118.16	120.30
1	A	1228	C	O5'-P-OP2	-5.32	100.91	105.70
1	A	1028	C	C6-N1-C2	-5.32	118.17	120.30
55	Z	75	C	C6-N1-C2	-5.32	118.17	120.30
10	J	7	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	879	C	O4'-C1'-N1	5.31	112.45	108.20
9	I	85	ARG	NE-CZ-NH1	5.30	122.95	120.30
13	M	79	ARG	NE-CZ-NH1	5.29	122.95	120.30
36	o	113	ARG	NE-CZ-NH1	5.27	122.93	120.30
8	H	117	ARG	NE-CZ-NH1	5.24	122.92	120.30
22	a	704	G	O4'-C1'-N9	5.22	112.38	108.20
1	A	880	C	O4'-C1'-N1	5.22	112.38	108.20
22	a	1836	C	OP1-P-O3'	5.22	116.67	105.20
22	a	231	A	O5'-P-OP2	-5.21	101.01	105.70
1	A	240	G	O5'-P-OP2	-5.18	101.03	105.70
54	Y	28	C	C6-N1-C2	-5.17	118.23	120.30
22	a	1314	C	C6-N1-C2	-5.17	118.23	120.30
24	c	87	ARG	NE-CZ-NH1	5.17	122.88	120.30
54	Y	48	C	C3'-C2'-C1'	5.17	105.63	101.50
30	i	69	ARG	NE-CZ-NH1	5.17	122.88	120.30
55	Z	51	C	C6-N1-C2	-5.17	118.23	120.30
9	I	41	ARG	NE-CZ-NH1	5.14	122.87	120.30
22	a	1351	C	O4'-C1'-N1	5.13	112.31	108.20
10	J	9	ARG	NE-CZ-NH1	5.12	122.86	120.30
12	L	114	ARG	NE-CZ-NH1	5.12	122.86	120.30
22	a	1998	A	O5'-P-OP2	-5.10	101.11	105.70
13	M	87	ARG	NE-CZ-NH1	5.09	122.84	120.30
22	a	543	G	C8-N9-C4	-5.07	104.37	106.40
1	A	1380	U	O5'-P-OP2	-5.06	101.14	105.70
1	A	993	G	C4-N9-C1'	5.06	133.08	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	846	U	C2-N1-C1'	5.06	123.77	117.70
13	M	70	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	356	A	O4'-C1'-N9	5.05	112.24	108.20
1	A	467	U	P-O3'-C3'	5.05	125.76	119.70
1	A	1028	C	C5-C6-N1	5.05	123.53	121.00
1	A	913	A	O3'-P-O5'	-5.05	94.41	104.00
22	a	548	G	C8-N9-C4	-5.03	104.39	106.40
22	a	887	U	OP2-P-O3'	5.02	116.25	105.20
22	a	2354	C	O4'-C1'-N1	5.01	112.21	108.20
22	a	2391	G	O4'-C1'-N9	5.01	112.21	108.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	130	THR	Peptide
12	L	101	ALA	Peptide
28	g	43	VAL	Peptide
28	g	47	ASP	Peptide
46	y	3	LYS	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	222/241 (92%)	208 (94%)	14 (6%)	0	100	100
3	C	204/233 (88%)	196 (96%)	8 (4%)	0	100	100
4	D	203/206 (98%)	195 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	154/167 (92%)	150 (97%)	4 (3%)	0	100	100
6	F	101/135 (75%)	96 (95%)	5 (5%)	0	100	100
7	G	151/179 (84%)	138 (91%)	10 (7%)	3 (2%)	7	40
8	H	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
9	I	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
10	J	96/103 (93%)	92 (96%)	3 (3%)	1 (1%)	15	54
11	K	113/129 (88%)	108 (96%)	5 (4%)	0	100	100
12	L	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
13	M	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
14	N	98/101 (97%)	95 (97%)	2 (2%)	1 (1%)	15	54
15	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
16	P	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
17	Q	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
18	R	64/75 (85%)	59 (92%)	5 (8%)	0	100	100
19	S	82/92 (89%)	80 (98%)	2 (2%)	0	100	100
20	T	84/87 (97%)	84 (100%)	0	0	100	100
21	U	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
24	c	269/273 (98%)	258 (96%)	11 (4%)	0	100	100
25	d	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
26	e	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
27	f	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
28	g	174/177 (98%)	152 (87%)	19 (11%)	3 (2%)	9	43
29	h	39/149 (26%)	35 (90%)	4 (10%)	0	100	100
30	i	140/142 (99%)	140 (100%)	0	0	100	100
31	j	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
32	k	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
33	l	132/136 (97%)	130 (98%)	2 (2%)	0	100	100
34	m	116/127 (91%)	114 (98%)	2 (2%)	0	100	100
35	n	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
36	o	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
37	p	115/118 (98%)	115 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
38	q	101/103 (98%)	99 (98%)	1 (1%)	1 (1%)	15 54
39	r	108/110 (98%)	107 (99%)	1 (1%)	0	100 100
40	s	91/100 (91%)	85 (93%)	6 (7%)	0	100 100
41	t	100/104 (96%)	90 (90%)	9 (9%)	1 (1%)	15 54
42	u	92/94 (98%)	92 (100%)	0	0	100 100
43	v	76/85 (89%)	75 (99%)	1 (1%)	0	100 100
44	w	75/78 (96%)	75 (100%)	0	0	100 100
45	x	60/63 (95%)	58 (97%)	2 (3%)	0	100 100
46	y	56/59 (95%)	54 (96%)	2 (4%)	0	100 100
47	z	54/57 (95%)	52 (96%)	2 (4%)	0	100 100
48	0	49/55 (89%)	48 (98%)	1 (2%)	0	100 100
49	1	44/46 (96%)	44 (100%)	0	0	100 100
50	2	62/65 (95%)	60 (97%)	2 (3%)	0	100 100
51	3	36/38 (95%)	36 (100%)	0	0	100 100
52	4	56/70 (80%)	53 (95%)	3 (5%)	0	100 100
All	All	5481/5913 (93%)	5273 (96%)	198 (4%)	10 (0%)	50 81

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	g	47	ASP
28	g	92	VAL
7	G	57	SER
10	J	57	VAL
14	N	33	ASP
41	t	99	ASN
28	g	48	ASN
7	G	6	VAL
7	G	5	ARG
38	q	44	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	186/199 (94%)	173 (93%)	13 (7%)	15	41
3	C	170/190 (90%)	163 (96%)	7 (4%)	30	56
4	D	172/173 (99%)	158 (92%)	14 (8%)	11	37
5	E	119/126 (94%)	116 (98%)	3 (2%)	47	68
6	F	90/116 (78%)	87 (97%)	3 (3%)	38	61
7	G	126/147 (86%)	117 (93%)	9 (7%)	14	41
8	H	104/105 (99%)	102 (98%)	2 (2%)	57	75
9	I	105/107 (98%)	102 (97%)	3 (3%)	42	64
10	J	86/90 (96%)	83 (96%)	3 (4%)	36	60
11	K	89/98 (91%)	83 (93%)	6 (7%)	16	43
12	L	102/103 (99%)	98 (96%)	4 (4%)	32	57
13	M	93/96 (97%)	88 (95%)	5 (5%)	22	49
14	N	83/84 (99%)	83 (100%)	0	100	100
15	O	76/77 (99%)	70 (92%)	6 (8%)	12	38
16	P	65/65 (100%)	61 (94%)	4 (6%)	18	45
17	Q	73/78 (94%)	69 (94%)	4 (6%)	21	49
18	R	57/65 (88%)	56 (98%)	1 (2%)	59	77
19	S	72/79 (91%)	71 (99%)	1 (1%)	67	81
20	T	65/66 (98%)	60 (92%)	5 (8%)	13	39
21	U	60/61 (98%)	55 (92%)	5 (8%)	11	36
24	c	216/218 (99%)	215 (100%)	1 (0%)	88	93
25	d	163/163 (100%)	160 (98%)	3 (2%)	59	77
26	e	165/165 (100%)	160 (97%)	5 (3%)	41	63
27	f	148/150 (99%)	141 (95%)	7 (5%)	26	52
28	g	137/138 (99%)	124 (90%)	13 (10%)	8	29
29	h	32/114 (28%)	29 (91%)	3 (9%)	8	30
30	i	116/116 (100%)	116 (100%)	0	100	100
31	j	104/104 (100%)	102 (98%)	2 (2%)	57	75
32	k	103/103 (100%)	101 (98%)	2 (2%)	57	75
33	l	107/107 (100%)	106 (99%)	1 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	m	98/103 (95%)	98 (100%)	0	100	100
35	n	86/87 (99%)	80 (93%)	6 (7%)	15	41
36	o	99/100 (99%)	98 (99%)	1 (1%)	76	86
37	p	89/90 (99%)	86 (97%)	3 (3%)	37	61
38	q	84/84 (100%)	80 (95%)	4 (5%)	25	52
39	r	93/93 (100%)	90 (97%)	3 (3%)	39	62
40	s	80/84 (95%)	80 (100%)	0	100	100
41	t	83/85 (98%)	77 (93%)	6 (7%)	14	41
42	u	78/78 (100%)	77 (99%)	1 (1%)	69	82
43	v	58/63 (92%)	58 (100%)	0	100	100
44	w	67/68 (98%)	64 (96%)	3 (4%)	27	54
45	x	54/55 (98%)	50 (93%)	4 (7%)	13	40
46	y	48/49 (98%)	45 (94%)	3 (6%)	18	44
47	z	47/48 (98%)	46 (98%)	1 (2%)	53	72
48	0	46/49 (94%)	43 (94%)	3 (6%)	17	44
49	1	38/38 (100%)	36 (95%)	2 (5%)	22	49
50	2	51/52 (98%)	48 (94%)	3 (6%)	19	47
51	3	34/34 (100%)	33 (97%)	1 (3%)	42	64
52	4	55/62 (89%)	53 (96%)	2 (4%)	35	60
All	All	4572/4825 (95%)	4391 (96%)	181 (4%)	35	56

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	ARG
2	B	23	TRP
2	B	58	ASN
2	B	81	LYS
2	B	93	ASN
2	B	105	LYS
2	B	127	ASP
2	B	133	GLU
2	B	143	LYS
2	B	152	LYS
2	B	188	ASP

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Mol	Chain	Res	Type
2	B	201	PRO
2	B	205	ASP
3	C	75	ILE
3	C	105	GLU
3	C	107	ARG
3	C	129	MET
3	C	170	GLU
3	C	178	LEU
3	C	185	ASN
4	D	8	LYS
4	D	29	ASP
4	D	34	ILE
4	D	48	LEU
4	D	50	ASP
4	D	85	ASN
4	D	166	GLU
4	D	167	LYS
4	D	181	THR
4	D	184	ARG
4	D	188	ARG
4	D	192	SER
4	D	202	GLU
4	D	206	LYS
5	E	14	LYS
5	E	22	SER
5	E	164	ILE
6	F	62	MET
6	F	102	MET
6	F	103	VAL
7	G	25	LYS
7	G	30	LEU
7	G	57	SER
7	G	72	THR
7	G	89	VAL
7	G	111	ARG
7	G	113	ASP
7	G	144	MET
7	G	149	LYS
8	H	38	ASN
8	H	56	LYS
9	I	27	LYS
9	I	100	LYS

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Mol	Chain	Res	Type
9	I	123	ARG
10	J	7	ARG
10	J	27	GLU
10	J	85	ASP
11	K	36	ASP
11	K	72	ASP
11	K	87	LYS
11	K	94	GLU
11	K	106	ARG
11	K	129	VAL
12	L	43	LYS
12	L	54	ARG
12	L	55	VAL
12	L	109	ASP
13	M	7	ILE
13	M	16	VAL
13	M	27	LYS
13	M	75	MET
13	M	82	ASP
15	O	2	SER
15	O	14	GLU
15	O	17	ARG
15	O	18	ASP
15	O	64	ARG
15	O	73	LYS
16	P	1	MET
16	P	45	GLU
16	P	47	GLU
16	P	48	GLU
17	Q	5	ILE
17	Q	50	ASN
17	Q	60	GLU
17	Q	65	ARG
18	R	35	GLU
19	S	43	ASN
20	T	6	SER
20	T	13	GLN
20	T	44	LYS
20	T	54	MET
20	T	85	LYS
21	U	9	ASN
21	U	21	ARG

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Mol	Chain	Res	Type
21	U	44	GLU
21	U	60	LEU
21	U	63	GLU
24	c	37	ASN
25	d	12	THR
25	d	33	ARG
25	d	89	GLU
26	e	9	GLN
26	e	14	VAL
26	e	21	ARG
26	e	107	SER
26	e	150	THR
27	f	11	GLU
27	f	30	ARG
27	f	47	LYS
27	f	120	LYS
27	f	136	ILE
27	f	150	ARG
27	f	152	LEU
28	g	3	ARG
28	g	18	LYS
28	g	20	ASN
28	g	43	VAL
28	g	49	THR
28	g	75	MET
28	g	95	ARG
28	g	122	THR
28	g	127	THR
28	g	129	THR
28	g	171	THR
28	g	173	GLU
28	g	175	LYS
29	h	17	ASP
29	h	21	VAL
29	h	25	TYR
31	j	58	LEU
31	j	114	LYS
32	k	115	GLU
32	k	144	GLU
33	l	25	ASP
35	n	13	ARG
35	n	16	ARG

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Mol	Chain	Res	Type
35	n	45	SER
35	n	56	LYS
35	n	84	GLU
35	n	89	ASP
36	o	53	ARG
37	p	15	LYS
37	p	51	ARG
37	p	112	LYS
38	q	26	ASP
38	q	33	VAL
38	q	47	VAL
38	q	55	ASP
39	r	7	HIS
39	r	66	ILE
39	r	83	LYS
41	t	15	THR
41	t	26	LYS
41	t	37	GLU
41	t	60	GLU
41	t	74	ASN
41	t	98	SER
42	u	58	SER
44	w	44	LYS
44	w	54	LYS
44	w	76	GLU
45	x	4	LYS
45	x	8	GLU
45	x	14	LEU
45	x	24	GLU
46	y	3	LYS
46	y	41	THR
46	y	59	GLU
47	z	54	VAL
48	0	5	ILE
48	0	28	ARG
48	0	32	GLU
49	1	8	SER
49	1	25	LYS
50	2	15	LYS
50	2	31	HIS
50	2	47	LYS
51	3	36	ARG

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Mol	Chain	Res	Type
52	4	13	THR
52	4	59	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	89	GLN
2	B	103	ASN
2	B	109	GLN
3	C	123	GLN
3	C	140	ASN
4	D	40	GLN
4	D	71	GLN
4	D	100	ASN
4	D	131	ASN
4	D	136	GLN
4	D	152	GLN
4	D	196	ASN
5	E	73	ASN
5	E	82	GLN
5	E	146	ASN
7	G	68	ASN
9	I	31	ASN
10	J	56	HIS
12	L	112	GLN
13	M	8	ASN
14	N	35	ASN
14	N	43	ASN
15	O	40	GLN
19	S	52	HIS
19	S	83	HIS
20	T	48	GLN
20	T	68	HIS
20	T	84	ASN
24	c	115	GLN
24	c	117	GLN
24	c	197	ASN
28	g	38	ASN
28	g	48	ASN
28	g	115	HIS
28	g	139	GLN
29	h	20	ASN

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Mol	Chain	Res	Type
30	i	128	ASN
33	l	60	GLN
36	o	12	GLN
37	p	37	GLN
37	p	44	GLN
37	p	52	GLN
38	q	43	ASN
39	r	31	GLN
40	s	48	GLN
41	t	53	ASN
41	t	74	ASN
42	u	5	ASN
44	w	6	GLN
45	x	15	ASN
47	z	4	GLN
47	z	6	ASN
50	2	31	HIS
52	4	41	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1513/1542 (98%)	207 (13%)	6 (0%)
22	a	2745/2904 (94%)	344 (12%)	0
23	b	118/120 (98%)	13 (11%)	0
53	X	11/28 (39%)	2 (18%)	0
54	Y	72/76 (94%)	29 (40%)	6 (8%)
55	Z	75/76 (98%)	27 (36%)	1 (1%)
56	5	1/2 (50%)	1 (100%)	0
All	All	4535/4748 (95%)	623 (13%)	13 (0%)

All (623) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	5	U
1	A	6	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	47	C

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Mol	Chain	Res	Type
1	A	48	C
1	A	50	A
1	A	51	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	80	A
1	A	83	C
1	A	84	U
1	A	85	U
1	A	86	G
1	A	87	C
1	A	88	U
1	A	89	U
1	A	94	G
1	A	95	C
1	A	96	U
1	A	121	U
1	A	122	G
1	A	131	A
1	A	141	G
1	A	144	G
1	A	146	G
1	A	166	U
1	A	177	G
1	A	182	A
1	A	183	C
1	A	189	A
1	A	197	A
1	A	204	G
1	A	226	G
1	A	240	G
1	A	245	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	271	C
1	A	280	C
1	A	289	G
1	A	321	A
1	A	328	C

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Mol	Chain	Res	Type
1	A	345	C
1	A	352	C
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	384	G
1	A	406	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	414	A
1	A	415	A
1	A	417	G
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	429	U
1	A	436	C
1	A	446	G
1	A	453	G
1	A	456	A
1	A	457	G
1	A	458	U
1	A	459	A
1	A	463	U
1	A	465	A
1	A	467	U
1	A	468	A
1	A	469	C
1	A	474	G
1	A	478	A
1	A	479	U
1	A	481	G
1	A	484	G
1	A	486	U
1	A	490	C
1	A	495	A
1	A	511	C
1	A	518	C
1	A	531	U

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Mol	Chain	Res	Type
1	A	532	A
1	A	547	A
1	A	562	U
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	579	A
1	A	596	A
1	A	615	G
1	A	633	G
1	A	648	A
1	A	650	G
1	A	653	U
1	A	665	A
1	A	702	A
1	A	723	U
1	A	724	G
1	A	746	A
1	A	747	A
1	A	748	G
1	A	755	G
1	A	774	G
1	A	777	A
1	A	793	U
1	A	794	A
1	A	815	A
1	A	817	C
1	A	840	C
1	A	890	G
1	A	914	A
1	A	934	C
1	A	935	A
1	A	960	U
1	A	966	2MG
1	A	969	A
1	A	971	G
1	A	975	A
1	A	976	G
1	A	977	A
1	A	984	C
1	A	993	G

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Mol	Chain	Res	Type
1	A	994	A
1	A	998	C
1	A	1004	A
1	A	1006	G
1	A	1008	U
1	A	1009	U
1	A	1024	G
1	A	1027	C
1	A	1030	U
1	A	1031	C
1	A	1032	G
1	A	1033	G
1	A	1034	G
1	A	1036	A
1	A	1044	A
1	A	1045	C
1	A	1046	A
1	A	1065	U
1	A	1085	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1137	C
1	A	1139	G
1	A	1143	G
1	A	1144	G
1	A	1159	U
1	A	1169	A
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1214	C
1	A	1227	A
1	A	1238	A
1	A	1256	A
1	A	1275	A
1	A	1280	A
1	A	1286	U
1	A	1287	A
1	A	1300	G
1	A	1302	C
1	A	1317	C

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Mol	Chain	Res	Type
1	A	1320	C
1	A	1338	G
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1370	G
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1397	C
1	A	1398	A
1	A	1419	G
1	A	1432	G
1	A	1440	U
1	A	1441	A
1	A	1442	G
1	A	1444	U
1	A	1446	A
1	A	1451	U
1	A	1452	C
1	A	1453	G
1	A	1487	G
1	A	1492	A
1	A	1497	G
1	A	1503	A
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
1	A	1533	C
1	A	1534	A
22	a	10	A
22	a	15	G
22	a	34	U
22	a	42	A
22	a	45	G
22	a	58	G
22	a	71	A
22	a	74	A
22	a	75	G
22	a	80	G

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Mol	Chain	Res	Type
22	a	84	A
22	a	101	A
22	a	102	U
22	a	110	G
22	a	118	A
22	a	119	A
22	a	120	U
22	a	139	U
22	a	140	C
22	a	142	A
22	a	163	C
22	a	165	A
22	a	181	A
22	a	196	A
22	a	215	G
22	a	216	A
22	a	221	A
22	a	222	A
22	a	248	G
22	a	264	C
22	a	265	A
22	a	272	A
22	a	274	C
22	a	278	A
22	a	279	A
22	a	282	A
22	a	285	G
22	a	286	U
22	a	289	G
22	a	292	U
22	a	294	A
22	a	311	A
22	a	329	G
22	a	330	A
22	a	345	A
22	a	357	C
22	a	361	G
22	a	362	A
22	a	386	G
22	a	405	U
22	a	411	G
22	a	412	A

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Mol	Chain	Res	Type
22	a	451	U
22	a	481	G
22	a	491	G
22	a	504	A
22	a	505	A
22	a	509	C
22	a	528	A
22	a	530	G
22	a	531	C
22	a	532	A
22	a	533	G
22	a	543	G
22	a	544	C
22	a	545	U
22	a	546	U
22	a	547	A
22	a	549	G
22	a	563	A
22	a	573	U
22	a	575	A
22	a	603	A
22	a	614	A
22	a	615	U
22	a	627	A
22	a	637	A
22	a	645	C
22	a	646	U
22	a	647	G
22	a	653	U
22	a	654	A
22	a	655	A
22	a	685	A
22	a	686	U
22	a	714	U
22	a	717	C
22	a	721	A
22	a	730	A
22	a	747	5MU
22	a	764	A
22	a	765	C
22	a	775	G
22	a	776	G

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Mol	Chain	Res	Type
22	a	782	A
22	a	784	G
22	a	785	G
22	a	789	A
22	a	805	G
22	a	812	C
22	a	827	U
22	a	828	U
22	a	846	U
22	a	847	U
22	a	856	G
22	a	859	G
22	a	869	G
22	a	879	G
22	a	883	G
22	a	884	U
22	a	885	C
22	a	890	C
22	a	891	G
22	a	895	U
22	a	896	A
22	a	897	C
22	a	898	C
22	a	899	A
22	a	905	A
22	a	910	A
22	a	914	G
22	a	915	C
22	a	946	C
22	a	961	C
22	a	974	G
22	a	983	A
22	a	984	A
22	a	985	C
22	a	996	A
22	a	1012	U
22	a	1013	C
22	a	1017	G
22	a	1022	G
22	a	1033	U
22	a	1041	G
22	a	1045	C

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Mol	Chain	Res	Type
22	a	1046	A
22	a	1047	G
22	a	1048	A
22	a	1051	G
22	a	1108	U
22	a	1111	A
22	a	1112	G
22	a	1115	G
22	a	1116	G
22	a	1120	G
22	a	1122	G
22	a	1132	U
22	a	1133	A
22	a	1135	C
22	a	1142	A
22	a	1171	G
22	a	1227	G
22	a	1253	A
22	a	1256	G
22	a	1271	G
22	a	1272	A
22	a	1275	A
22	a	1294	U
22	a	1300	G
22	a	1301	A
22	a	1352	U
22	a	1365	A
22	a	1379	U
22	a	1383	A
22	a	1411	U
22	a	1416	G
22	a	1417	C
22	a	1420	A
22	a	1421	G
22	a	1427	A
22	a	1428	C
22	a	1452	G
22	a	1453	A
22	a	1468	U
22	a	1476	U
22	a	1482	G
22	a	1486	U

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Mol	Chain	Res	Type
22	a	1487	U
22	a	1493	C
22	a	1497	U
22	a	1504	A
22	a	1508	A
22	a	1509	A
22	a	1510	G
22	a	1515	A
22	a	1529	G
22	a	1534	U
22	a	1535	A
22	a	1536	C
22	a	1537	G
22	a	1554	U
22	a	1559	U
22	a	1566	A
22	a	1569	A
22	a	1578	U
22	a	1583	A
22	a	1584	U
22	a	1585	C
22	a	1586	A
22	a	1590	A
22	a	1593	A
22	a	1608	A
22	a	1609	A
22	a	1647	U
22	a	1648	U
22	a	1649	G
22	a	1674	G
22	a	1715	G
22	a	1722	A
22	a	1729	U
22	a	1730	C
22	a	1731	G
22	a	1732	C
22	a	1733	G
22	a	1736	U
22	a	1738	G
22	a	1750	G
22	a	1764	C
22	a	1773	A

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Mol	Chain	Res	Type
22	a	1782	U
22	a	1791	A
22	a	1800	C
22	a	1801	A
22	a	1808	A
22	a	1816	C
22	a	1829	A
22	a	1847	A
22	a	1858	A
22	a	1867	G
22	a	1868	C
22	a	1870	C
22	a	1871	A
22	a	1873	G
22	a	1906	G
22	a	1907	G
22	a	1929	G
22	a	1930	G
22	a	1937	A
22	a	1938	A
22	a	1955	U
22	a	1965	C
22	a	1967	C
22	a	1970	A
22	a	1971	U
22	a	1972	G
22	a	1991	U
22	a	1993	U
22	a	2020	A
22	a	2023	C
22	a	2031	A
22	a	2033	A
22	a	2043	C
22	a	2055	C
22	a	2056	G
22	a	2060	A
22	a	2061	G
22	a	2062	A
22	a	2069	G7M
22	a	2194	U
22	a	2198	A
22	a	2203	U

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Mol	Chain	Res	Type
22	a	2204	G
22	a	2208	C
22	a	2211	A
22	a	2223	G
22	a	2225	A
22	a	2238	G
22	a	2268	A
22	a	2279	G
22	a	2283	C
22	a	2287	A
22	a	2305	U
22	a	2308	G
22	a	2322	A
22	a	2325	G
22	a	2333	A
22	a	2335	A
22	a	2347	C
22	a	2350	C
22	a	2377	A
22	a	2383	G
22	a	2385	C
22	a	2402	U
22	a	2403	C
22	a	2406	A
22	a	2424	C
22	a	2425	A
22	a	2429	G
22	a	2435	A
22	a	2441	U
22	a	2448	A
22	a	2470	G
22	a	2476	A
22	a	2478	A
22	a	2491	U
22	a	2502	G
22	a	2504	PSU
22	a	2505	G
22	a	2518	A
22	a	2529	G
22	a	2535	G
22	a	2547	A
22	a	2554	U

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Mol	Chain	Res	Type
22	a	2566	A
22	a	2567	G
22	a	2573	C
22	a	2585	U
22	a	2586	U
22	a	2602	A
22	a	2603	G
22	a	2609	U
22	a	2613	U
22	a	2629	U
22	a	2670	A
22	a	2689	U
22	a	2690	U
22	a	2714	G
22	a	2716	C
22	a	2726	A
22	a	2733	A
22	a	2744	G
22	a	2748	A
22	a	2751	G
22	a	2752	C
22	a	2757	A
22	a	2765	A
22	a	2778	A
22	a	2790	U
22	a	2792	A
22	a	2795	C
22	a	2798	U
22	a	2799	A
22	a	2802	G
22	a	2820	A
22	a	2821	A
22	a	2835	A
22	a	2873	A
22	a	2883	A
22	a	2884	U
22	a	2891	U
22	a	2899	A
22	a	2901	C
22	a	2902	C
23	b	9	G
23	b	13	G

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Mol	Chain	Res	Type
23	b	34	A
23	b	35	C
23	b	36	C
23	b	45	A
23	b	56	G
23	b	57	A
23	b	67	G
23	b	89	U
23	b	90	C
23	b	99	A
23	b	109	A
53	X	15	A
53	X	24	A
54	Y	3	G
54	Y	5	G
54	Y	6	A
54	Y	8	U
54	Y	9	A
54	Y	11	C
54	Y	13	C
54	Y	14	A
54	Y	19	G
54	Y	20	G
54	Y	21	A
54	Y	23	A
54	Y	24	G
54	Y	25	C
54	Y	45	G
54	Y	46	G
54	Y	47	U
54	Y	48	C
54	Y	49	G
54	Y	50	G
54	Y	57	G
54	Y	59	U
54	Y	66	A
54	Y	67	U
54	Y	70	C
54	Y	71	C
54	Y	73	A
54	Y	74	C
54	Y	75	C

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Mol	Chain	Res	Type
55	Z	6	G
55	Z	8	U
55	Z	9	G
55	Z	14	A
55	Z	16	C
55	Z	17	C
55	Z	17(A)	U
55	Z	18	G
55	Z	19	G
55	Z	20	U
55	Z	21	A
55	Z	22	G
55	Z	46	G
55	Z	47	U
55	Z	49	G
55	Z	50	U
55	Z	52	G
55	Z	54	U
55	Z	56	C
55	Z	58	A
55	Z	59	A
55	Z	65	C
55	Z	66	C
55	Z	68	C
55	Z	69	C
55	Z	71	C
55	Z	76	A
56	5	76	A

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	199	A
1	A	250	A
1	A	993	G
1	A	1026	G
1	A	1035	A
54	Y	13	C
54	Y	19	G
54	Y	45	G
54	Y	46	G

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Mol	Chain	Res	Type
54	Y	48	C
54	Y	60	C
55	Z	58	A

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	$\#\|Z\| > 2$
1	5MC	A	967	1	18,22,23	0.44	0	26,32,35	0.77	0
22	OMU	a	2552	22	19,22,23	0.36	0	26,31,34	0.50	0
22	PSU	a	2605	22	18,21,22	1.03	1 (5%)	22,30,33	0.89	0
1	MA6	A	1518	1	18,26,27	0.85	1 (5%)	19,38,41	0.47	0
22	2MG	a	2445	22	18,26,27	1.04	2 (11%)	16,38,41	0.78	0
22	PSU	a	955	22	18,21,22	0.99	1 (5%)	22,30,33	0.75	0
22	6MZ	a	1618	22	18,25,26	0.74	0	16,36,39	0.84	1 (6%)
22	5MC	a	1962	22	18,22,23	0.44	0	26,32,35	0.84	1 (3%)
22	PSU	a	2457	22	18,21,22	1.00	1 (5%)	22,30,33	0.75	0
22	3TD	a	1915	22	19,22,23	1.03	1 (5%)	21,32,35	1.00	2 (9%)
22	PSU	a	2580	22	18,21,22	1.00	1 (5%)	22,30,33	0.83	1 (4%)
22	PSU	a	746	22	18,21,22	1.16	1 (5%)	22,30,33	0.84	0
1	5MC	A	1407	1	18,22,23	0.45	0	26,32,35	0.86	0
22	G7M	a	2069	22	20,26,27	1.07	2 (10%)	17,39,42	0.75	0
22	PSU	a	1911	22	18,21,22	1.02	1 (5%)	22,30,33	0.74	0
1	2MG	A	966	1	18,26,27	1.07	2 (11%)	16,38,41	0.67	0
22	5MU	a	747	22	19,22,23	0.44	0	28,32,35	0.51	0
22	5MU	a	1939	22	19,22,23	0.42	0	28,32,35	0.50	0
22	OMG	a	2251	55,22	18,26,27	1.02	2 (11%)	19,38,41	0.74	0
22	PSU	a	1917	22	18,21,22	1.01	1 (5%)	22,30,33	0.77	1 (4%)
1	PSU	A	516	1	18,21,22	1.02	1 (5%)	22,30,33	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	4D4	l	81	33	9,11,12	0.50	0	8,13,15	0.70	0
22	PSU	a	2604	22	18,21,22	1.03	1 (5%)	22,30,33	0.90	0
1	UR3	A	1498	1	19,22,23	0.41	0	26,32,35	0.83	2 (7%)
12	D2T	L	89	12	7,9,10	1.04	0	6,11,13	1.64	3 (50%)
22	H2U	a	2449	22	18,21,22	0.86	1 (5%)	21,30,33	0.78	1 (4%)
1	2MG	A	1207	1	18,26,27	1.02	1 (5%)	16,38,41	0.79	0
1	4OC	A	1402	1	20,23,24	0.49	0	26,32,35	0.82	1 (3%)
22	OMC	a	2498	22	19,22,23	0.42	0	26,31,34	0.74	0
22	PSU	a	2504	22	18,21,22	0.98	1 (5%)	22,30,33	0.74	0
1	G7M	A	527	1	20,26,27	1.12	2 (10%)	17,39,42	0.72	0
1	MA6	A	1519	1	18,26,27	0.85	1 (5%)	19,38,41	0.79	0
25	MEQ	d	150	25	8,9,10	0.45	0	5,10,12	1.71	2 (40%)
22	1MG	a	745	22	18,26,27	1.07	2 (11%)	19,39,42	0.49	0
22	2MG	a	1835	22	18,26,27	1.02	2 (11%)	16,38,41	0.67	0
1	2MG	A	1516	1	18,26,27	1.03	1 (5%)	16,38,41	0.80	0
11	IAS	K	119	11	6,7,8	0.94	0	6,8,10	1.02	0
22	6MZ	a	2030	22	18,25,26	0.70	0	16,36,39	0.87	1 (6%)
22	2MA	a	2503	22	17,25,26	1.03	1 (5%)	17,37,40	0.90	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
22	OMU	a	2552	22	-	1/9/27/28	0/2/2/2
22	PSU	a	2605	22	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
22	2MG	a	2445	22	-	1/5/27/28	0/3/3/3
22	PSU	a	955	22	-	0/7/25/26	0/2/2/2
22	6MZ	a	1618	22	-	0/5/27/28	0/3/3/3
22	5MC	a	1962	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2457	22	-	0/7/25/26	0/2/2/2
22	3TD	a	1915	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2580	22	-	0/7/25/26	0/2/2/2
22	PSU	a	746	22	-	1/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
22	G7M	a	2069	22	-	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	a	1911	22	-	0/7/25/26	0/2/2/2
1	2MG	A	966	1	-	0/5/27/28	0/3/3/3
22	5MU	a	747	22	-	0/7/25/26	0/2/2/2
22	5MU	a	1939	22	-	0/7/25/26	0/2/2/2
22	OMG	a	2251	55,22	-	0/5/27/28	0/3/3/3
22	PSU	a	1917	22	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
33	4D4	l	81	33	-	1/11/12/14	-
22	PSU	a	2604	22	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
12	D2T	L	89	12	-	2/7/12/14	-
22	H2U	a	2449	22	-	0/7/38/39	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	A	1402	1	-	0/9/29/30	0/2/2/2
22	OMC	a	2498	22	-	0/9/27/28	0/2/2/2
22	PSU	a	2504	22	-	2/7/25/26	0/2/2/2
1	G7M	A	527	1	-	1/3/25/26	0/3/3/3
1	MA6	A	1519	1	-	2/7/29/30	0/3/3/3
25	MEQ	d	150	25	-	2/8/9/11	-
22	1MG	a	745	22	-	0/3/25/26	0/3/3/3
22	2MG	a	1835	22	-	0/5/27/28	0/3/3/3
1	2MG	A	1516	1	-	0/5/27/28	0/3/3/3
11	IAS	K	119	11	-	0/7/7/8	-
22	6MZ	a	2030	22	-	2/5/27/28	0/3/3/3
22	2MA	a	2503	22	-	2/3/25/26	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	746	PSU	C6-C5	4.46	1.40	1.35
22	a	2605	PSU	C6-C5	4.07	1.40	1.35
1	A	516	PSU	C6-C5	4.06	1.40	1.35
22	a	1911	PSU	C6-C5	4.04	1.40	1.35
22	a	2580	PSU	C6-C5	4.02	1.40	1.35
22	a	1917	PSU	C6-C5	4.00	1.40	1.35
22	a	2604	PSU	C6-C5	3.97	1.39	1.35
22	a	2457	PSU	C6-C5	3.96	1.39	1.35
22	a	1915	3TD	C6-C5	3.93	1.39	1.35
22	a	955	PSU	C6-C5	3.91	1.39	1.35
22	a	2504	PSU	C6-C5	3.91	1.39	1.35
1	A	527	G7M	C8-N9	3.62	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2069	G7M	C8-N9	3.51	1.39	1.33
22	a	2503	2MA	C2-N3	2.90	1.37	1.31
22	a	745	1MG	C6-N1	2.68	1.44	1.39
22	a	2251	OMG	C5-C6	-2.57	1.42	1.47
1	A	1519	MA6	C6-N1	2.42	1.36	1.33
1	A	1518	MA6	C6-N1	2.40	1.36	1.33
22	a	2445	2MG	C5-C6	-2.34	1.42	1.47
1	A	966	2MG	C5-C6	-2.33	1.42	1.47
22	a	2449	H2U	C2-N1	2.31	1.38	1.35
22	a	745	1MG	C5-C4	-2.30	1.37	1.43
22	a	2069	G7M	C8-N7	2.28	1.37	1.33
1	A	527	G7M	C8-N7	2.28	1.37	1.33
22	a	1835	2MG	C5-C6	-2.27	1.42	1.47
1	A	1516	2MG	C5-C6	-2.24	1.42	1.47
22	a	2251	OMG	C8-N7	-2.17	1.31	1.35
1	A	966	2MG	C8-N7	-2.16	1.31	1.35
22	a	1835	2MG	C8-N7	-2.13	1.31	1.35
1	A	1207	2MG	C5-C6	-2.12	1.43	1.47
22	a	2445	2MG	C8-N7	-2.03	1.31	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	2503	2MA	CM2-C2-N1	2.69	122.22	116.23
22	a	2030	6MZ	C2-N1-C6	2.49	118.72	116.59
25	d	150	MEQ	CG-CD-NE2	2.31	119.50	116.29
25	d	150	MEQ	OE1-CD-CG	-2.30	117.81	122.02
12	L	89	D2T	O-C-CA	-2.29	118.77	124.78
1	A	1498	UR3	C4-N3-C2	-2.29	122.41	124.56
12	L	89	D2T	OD2-CG-CB	2.25	118.01	113.15
1	A	1498	UR3	C6-N1-C2	-2.22	119.80	121.79
12	L	89	D2T	OD1-CG-CB	-2.16	117.91	122.44
22	a	2449	H2U	C4-N3-C2	-2.16	124.00	125.79
22	a	1915	3TD	C4-N3-C2	-2.15	122.28	124.61
1	A	1402	4OC	O2'-C2'-C1'	2.14	113.25	109.08
22	a	1915	3TD	O2'-C2'-C3'	2.12	118.69	111.82
22	a	1618	6MZ	C2-N1-C6	2.11	118.40	116.59
22	a	1917	PSU	O2'-C2'-C3'	2.10	118.63	111.82
22	a	1962	5MC	CM5-C5-C6	-2.08	120.07	122.85
22	a	2580	PSU	C3'-C2'-C1'	2.04	104.02	101.64

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	L	89	D2T	CG-CB-SB-CB1
22	a	2030	6MZ	O4'-C4'-C5'-O5'
25	d	150	MEQ	NE2-CD-CG-CB
25	d	150	MEQ	OE1-CD-CG-CB
22	a	2030	6MZ	C3'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
22	a	2504	PSU	O4'-C4'-C5'-O5'
22	a	2069	G7M	C4'-C5'-O5'-P
12	L	89	D2T	CA-CB-SB-CB1
22	a	2503	2MA	C4'-C5'-O5'-P
22	a	2445	2MG	C3'-C4'-C5'-O5'
22	a	2504	PSU	C3'-C4'-C5'-O5'
22	a	746	PSU	O4'-C1'-C5-C6
1	A	527	G7M	C4'-C5'-O5'-P
22	a	2552	OMU	C3'-C2'-O2'-CM2
1	A	1519	MA6	C3'-C4'-C5'-O5'
22	a	2069	G7M	O4'-C4'-C5'-O5'
22	a	2503	2MA	O4'-C4'-C5'-O5'
33	l	81	4D4	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

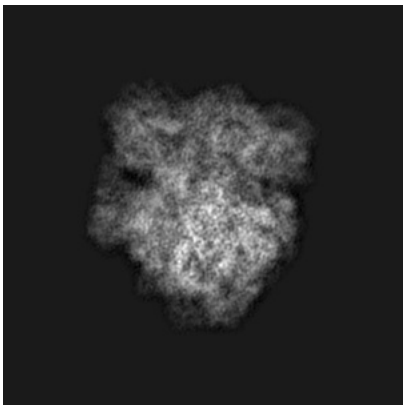
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17959. These allow visual inspection of the internal detail of the map and identification of artifacts.

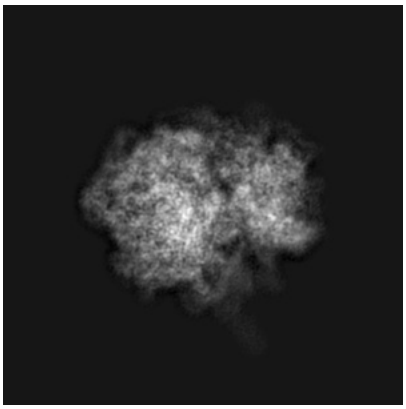
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

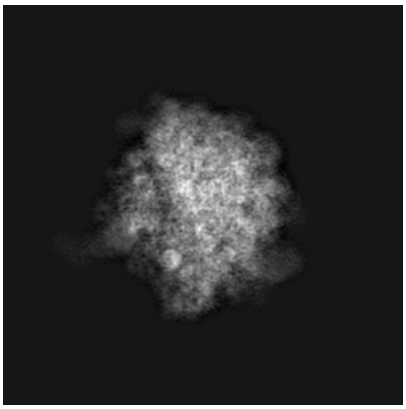
6.1.1 Primary map



X

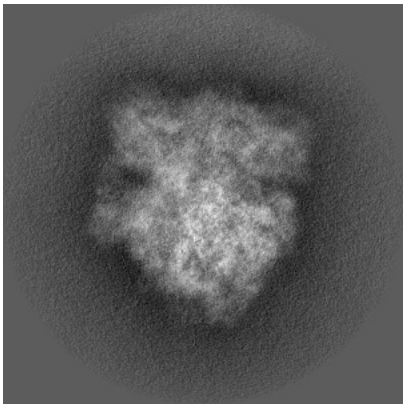


Y

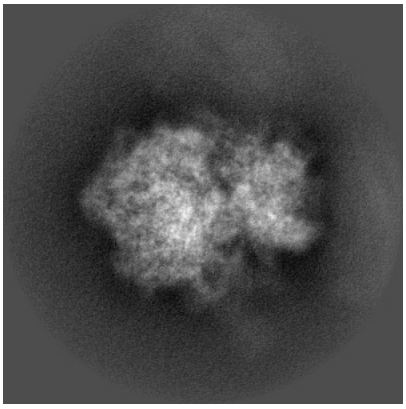


Z

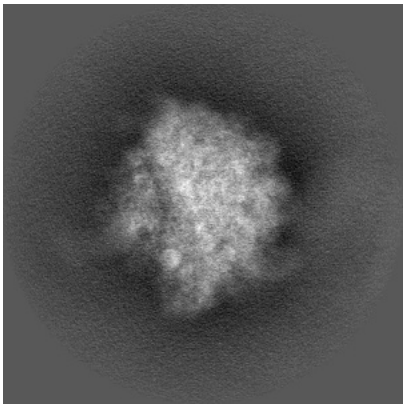
6.1.2 Raw map



X



Y

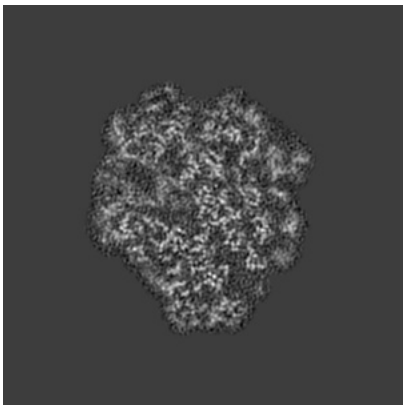


Z

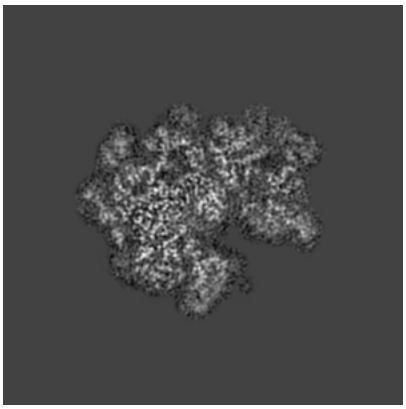
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

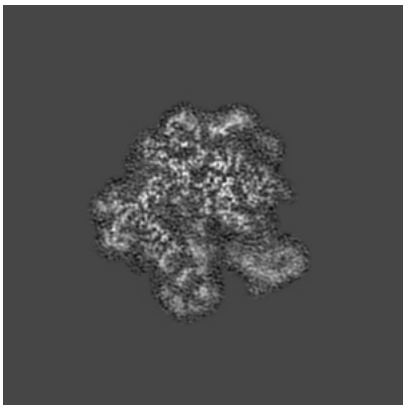
6.2.1 Primary map



X Index: 200

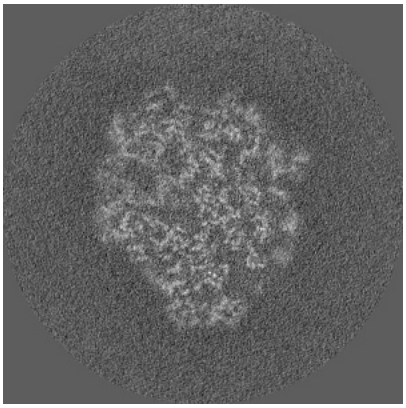


Y Index: 200

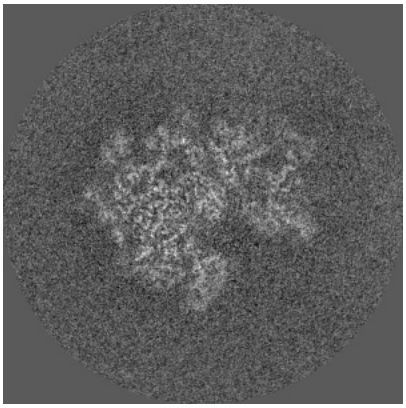


Z Index: 200

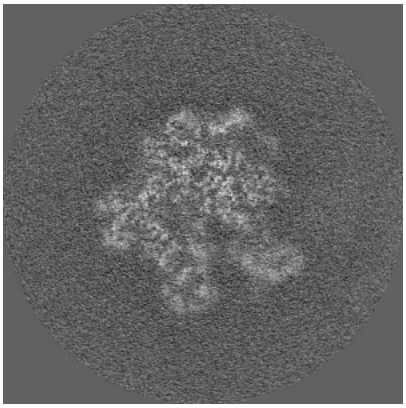
6.2.2 Raw map



X Index: 200



Y Index: 200

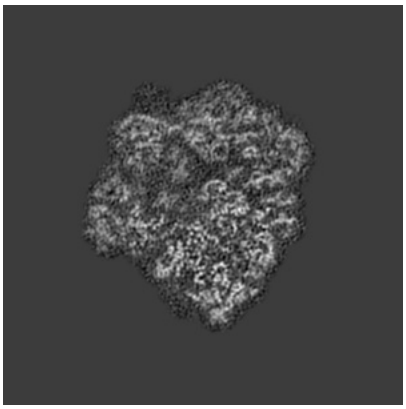


Z Index: 200

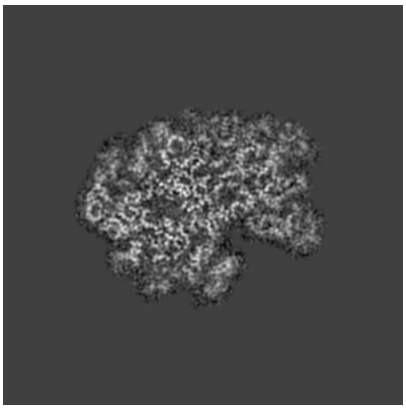
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

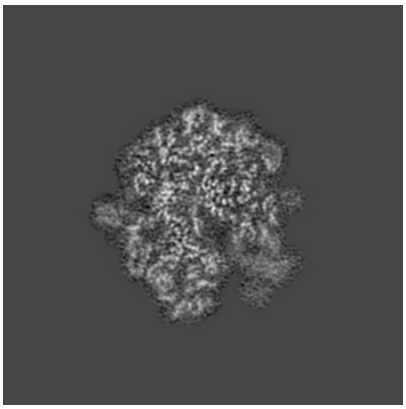
6.3.1 Primary map



X Index: 185

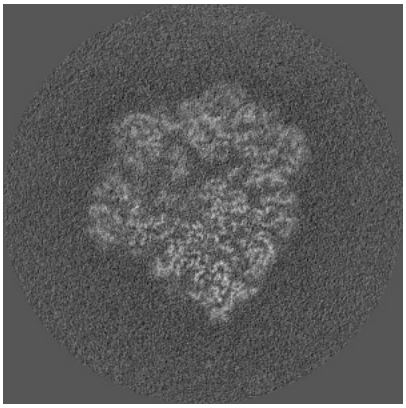


Y Index: 214

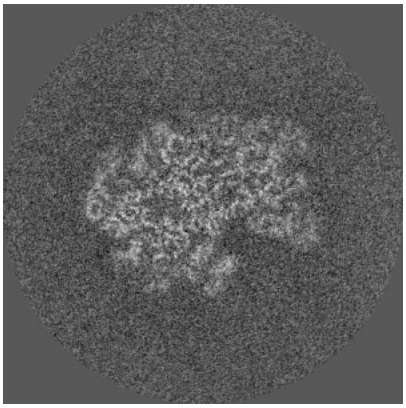


Z Index: 184

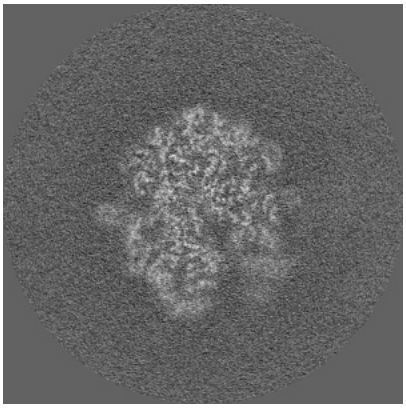
6.3.2 Raw map



X Index: 184



Y Index: 214

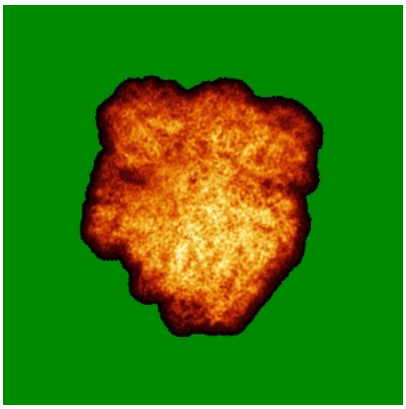


Z Index: 183

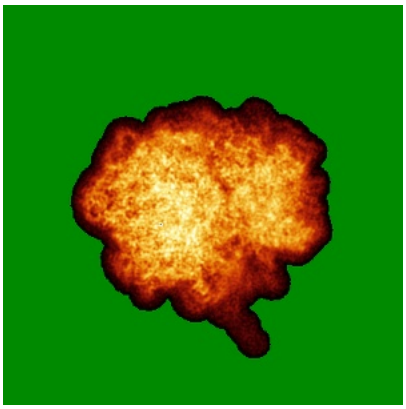
The images above show the largest variance slices of the map in three orthogonal directions.

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

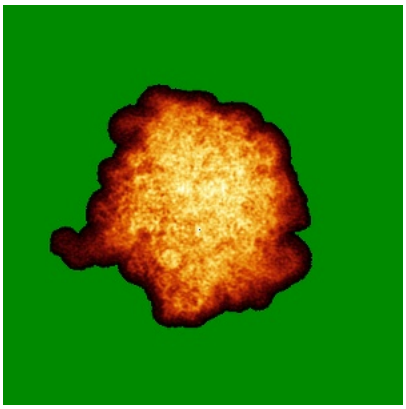
6.4.1 Primary map



X

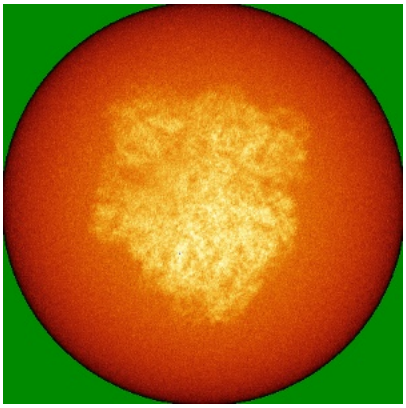


Y

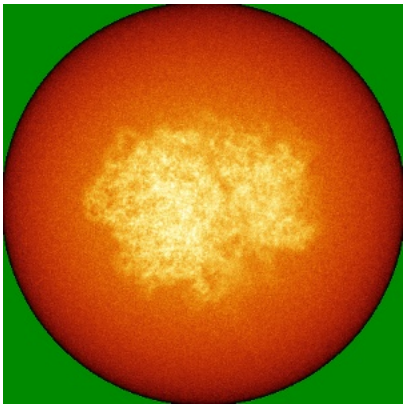


Z

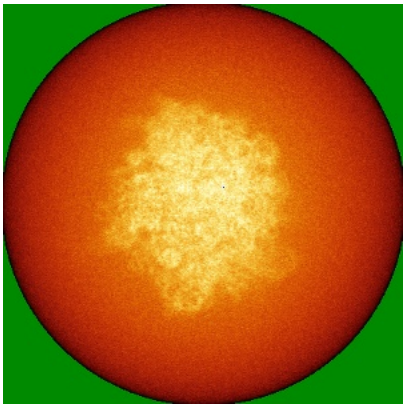
6.4.2 Raw map



X



Y



Z

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

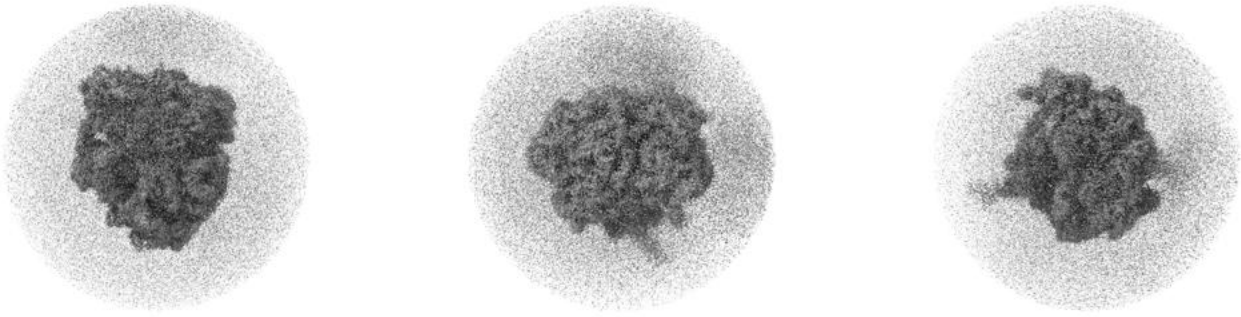
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

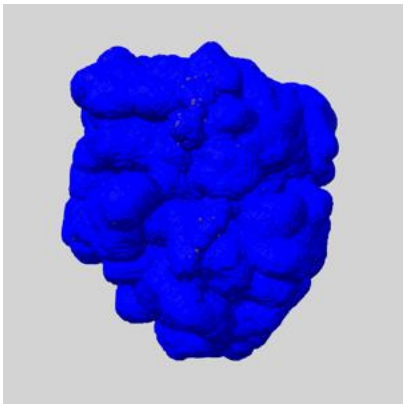
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

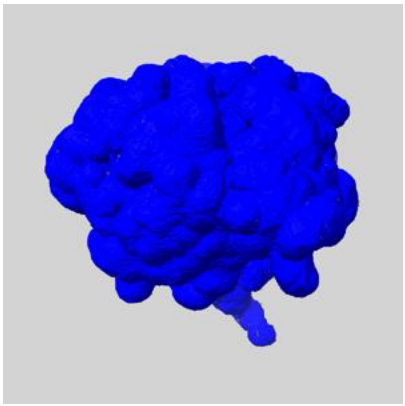
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

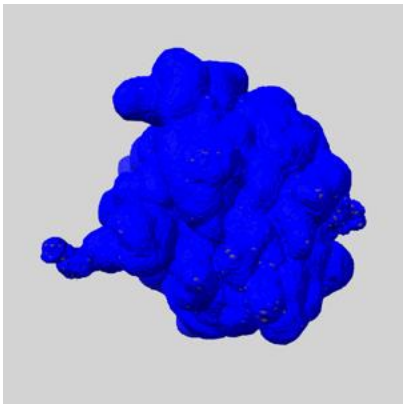
6.6.1 emd_17959_msk_1.map (i)



X



Y

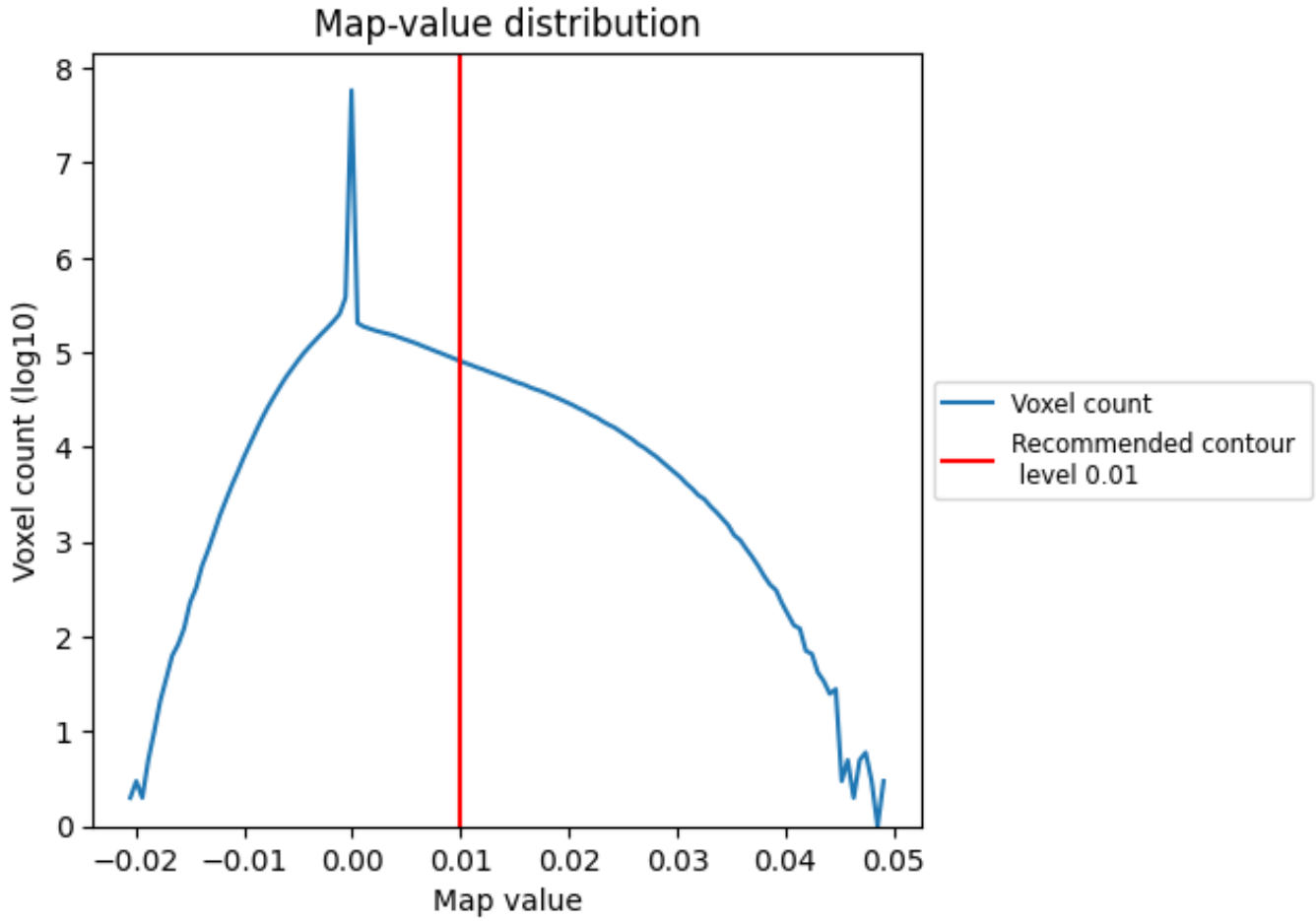


Z

7 Map analysis

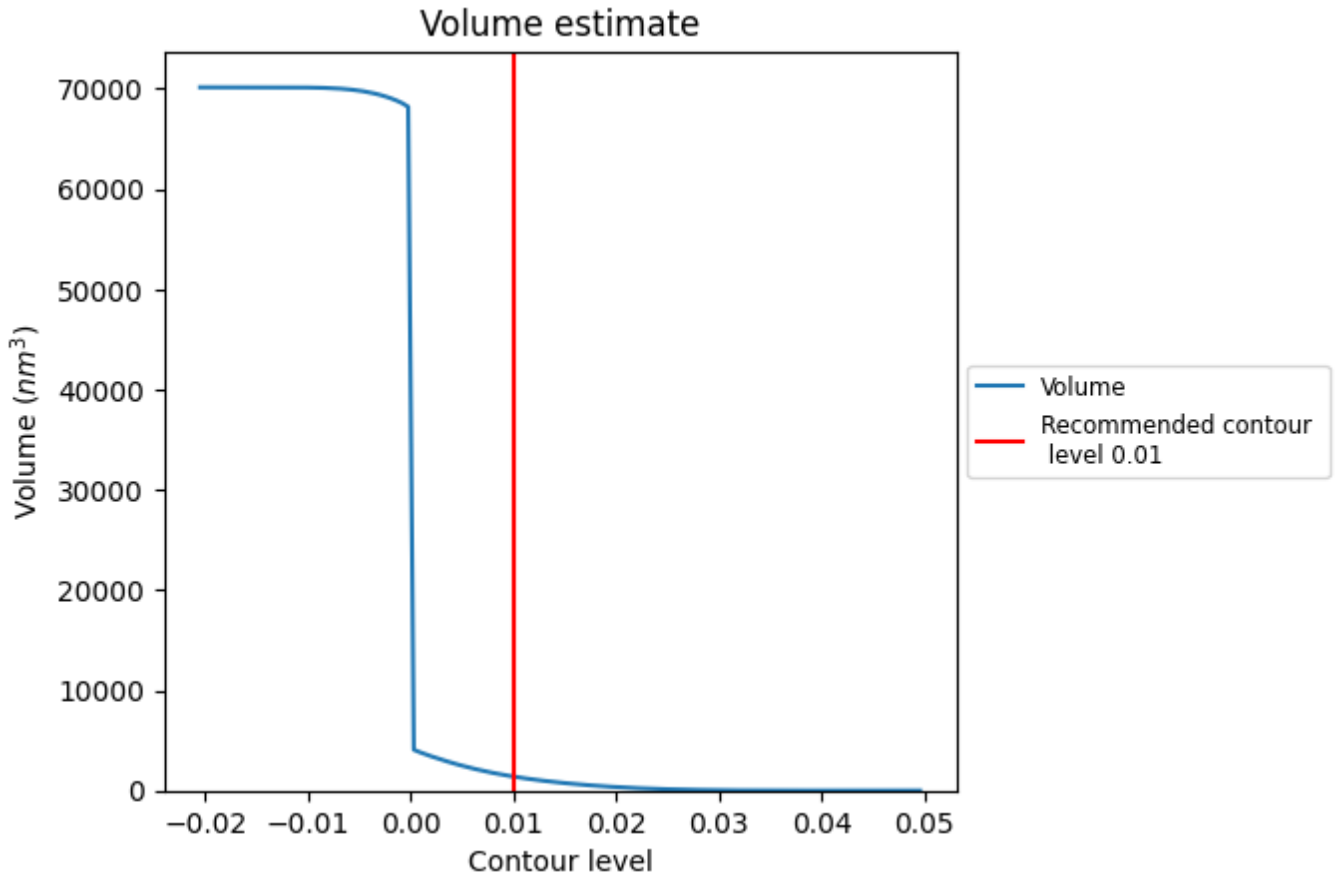
This section contains the results of statistical analysis of the map.

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.

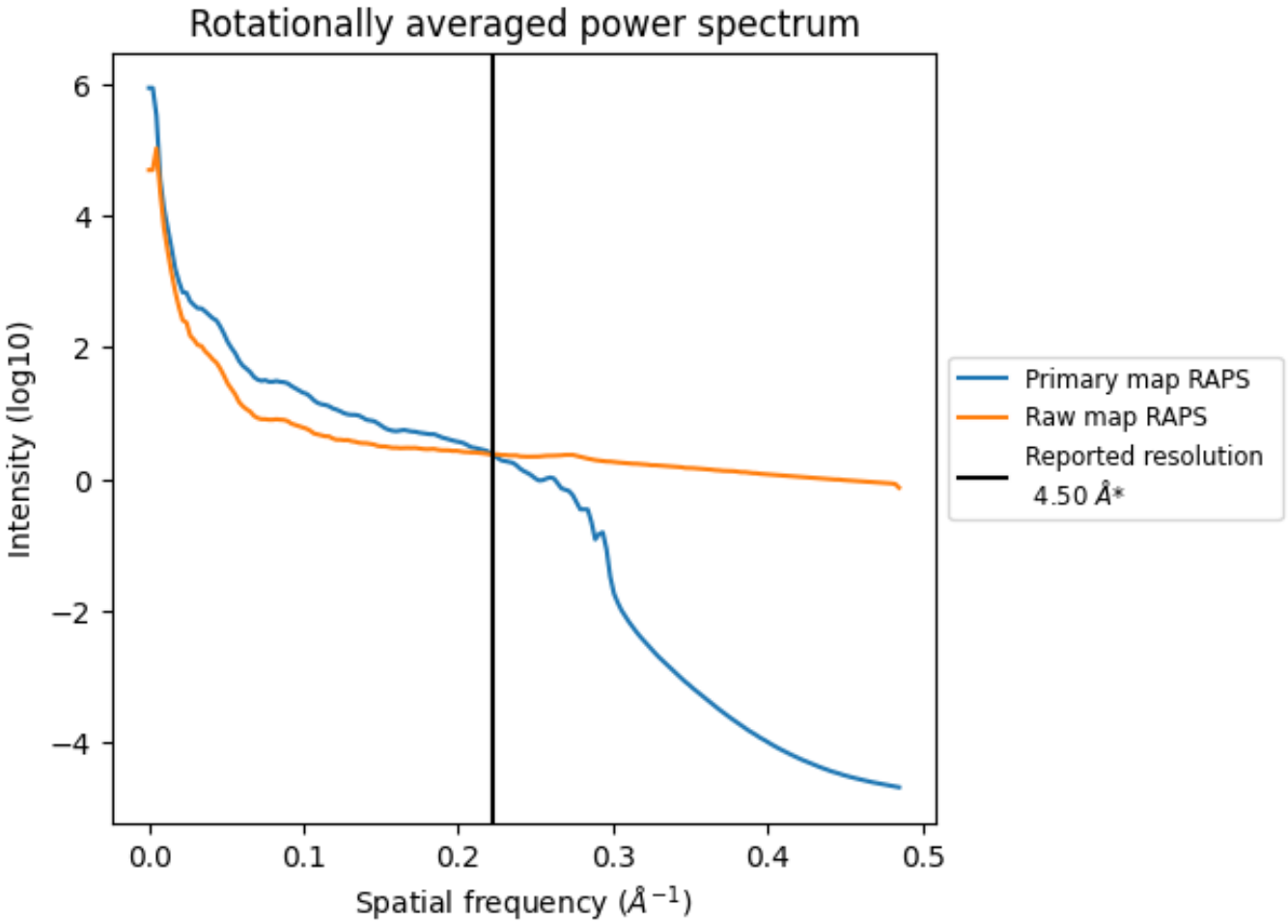
7.2 Volume estimate



The volume at the recommended contour level is 1400 nm^3; this corresponds to an approximate mass of 1264 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)

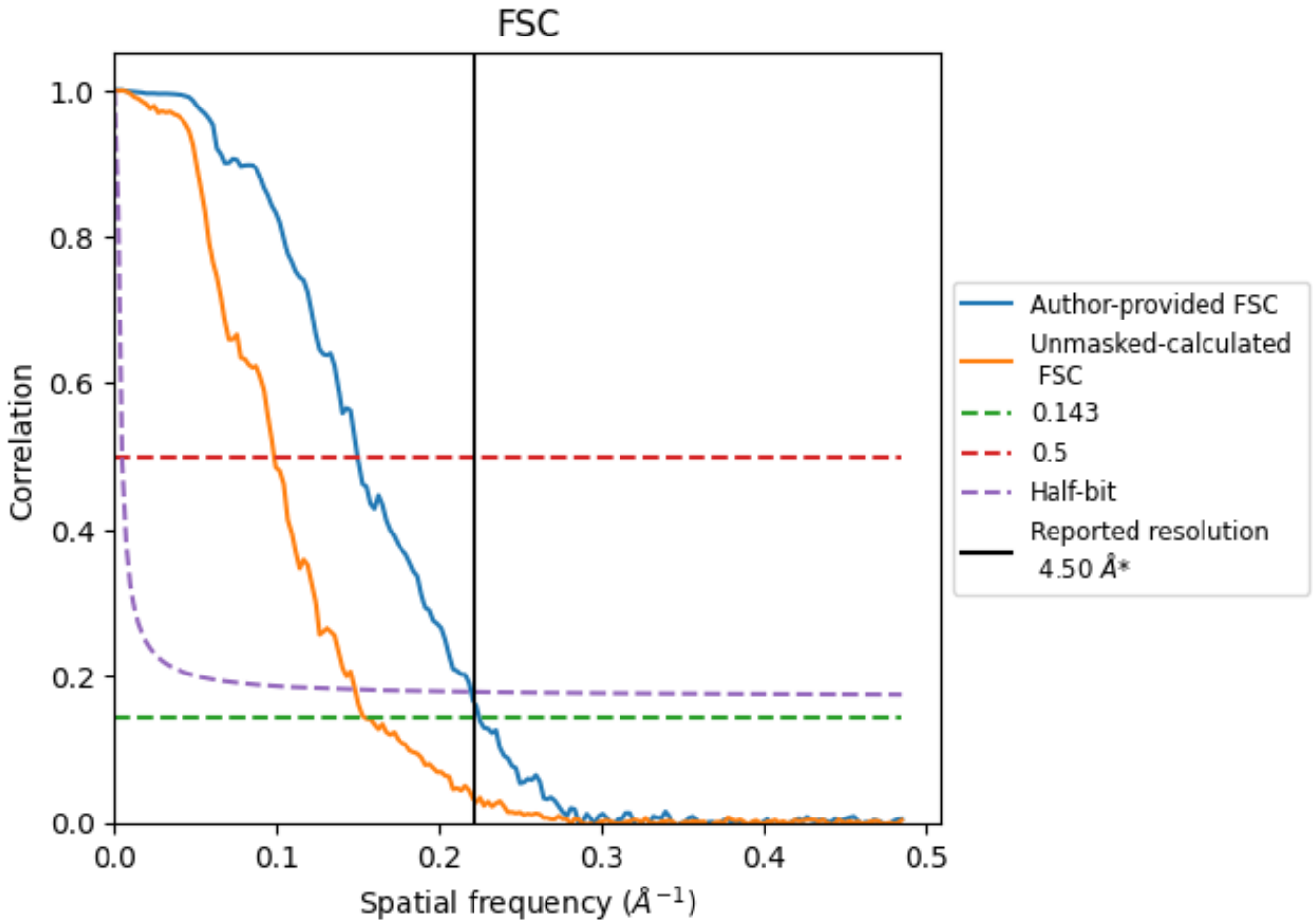


*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

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 0.222 Å^{-1}

8.2 Resolution estimates (i)

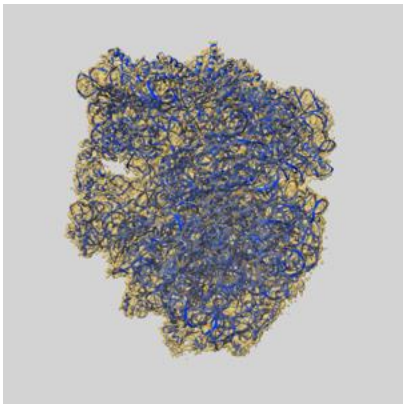
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.44	6.68	4.56
Unmasked-calculated*	6.47	10.16	6.74

*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 6.47 differs from the reported value 4.5 by more than 10 %

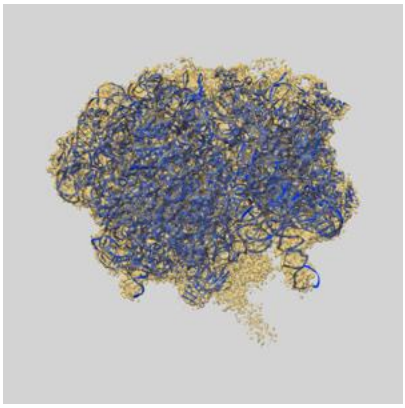
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17959 and PDB model 8PVA. Per-residue inclusion information can be found in section 3 on page 14.

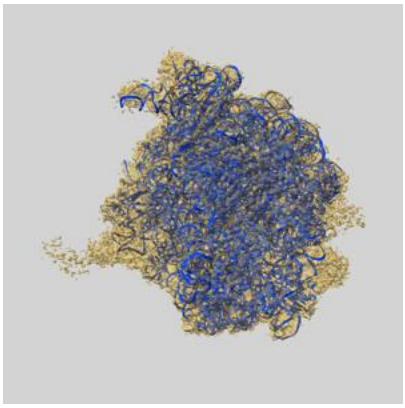
9.1 Map-model overlay



X



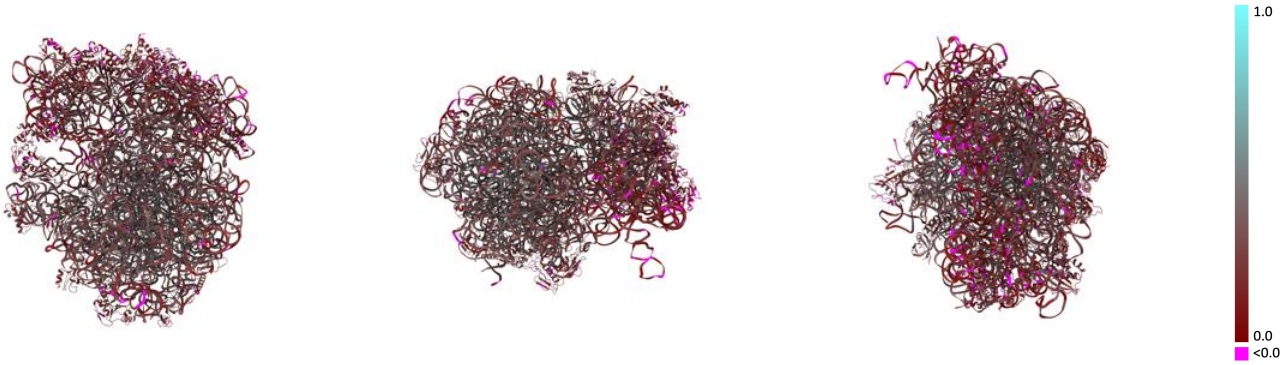
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

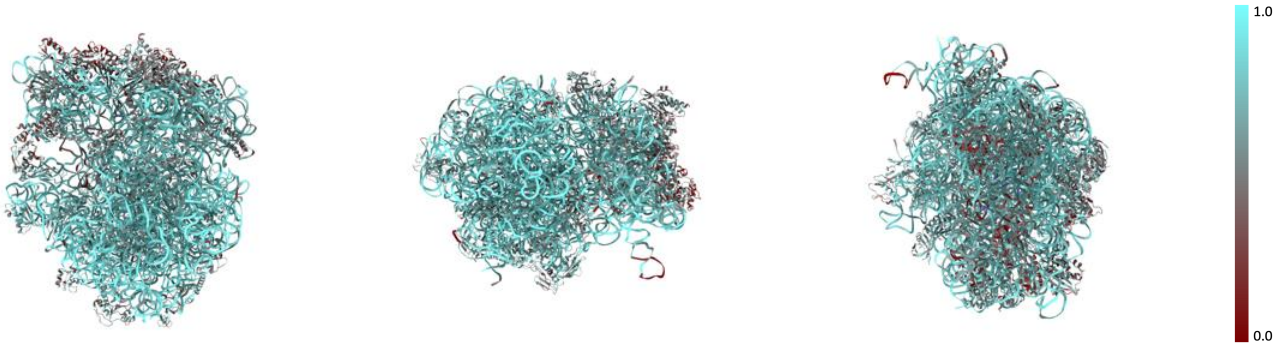
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

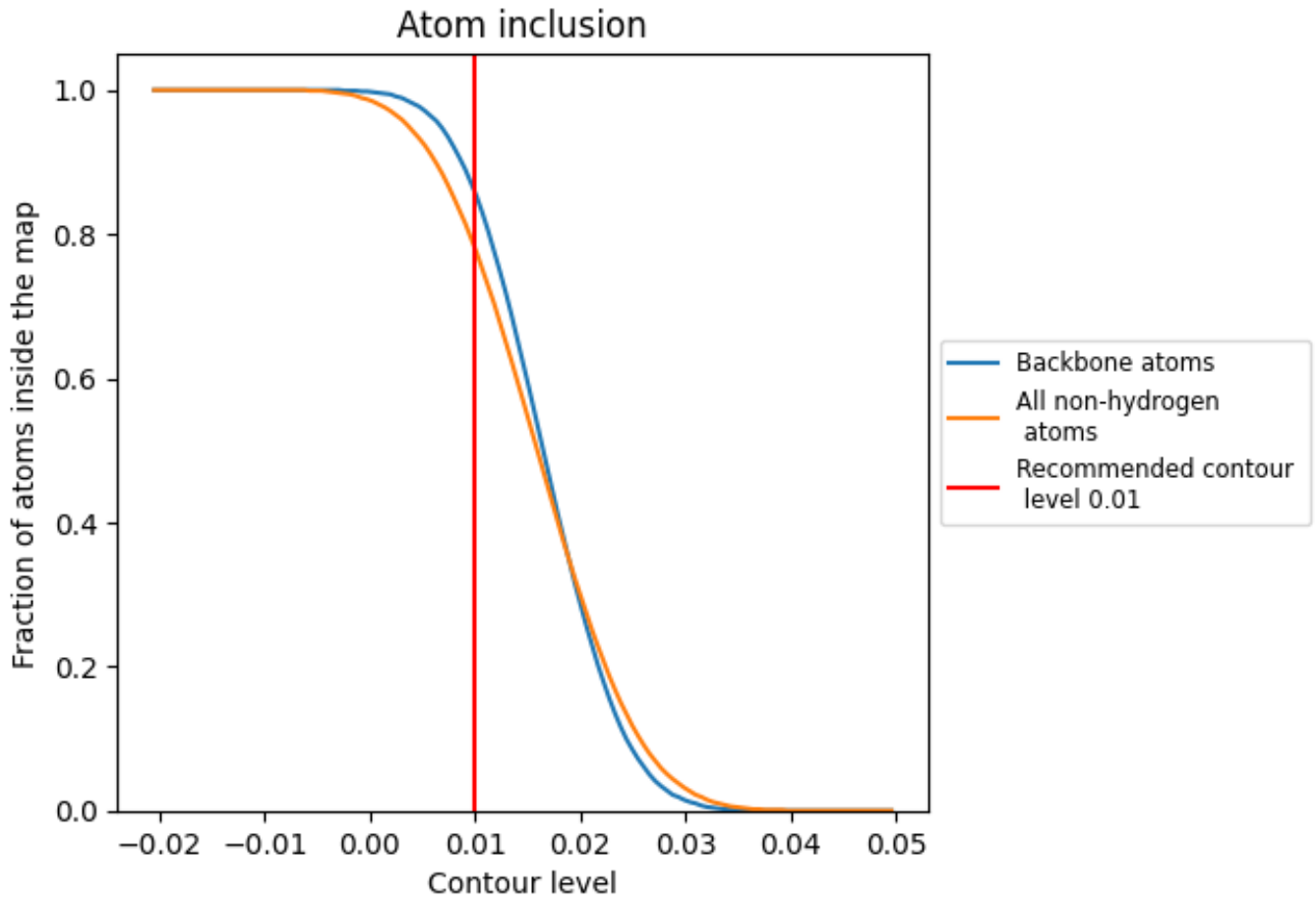
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 78% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7810	0.2870
0	0.6240	0.2300
1	0.7520	0.3560
2	0.6970	0.3600
3	0.6890	0.2800
4	0.4750	0.1650
5	0.7140	0.3100
A	0.8230	0.2540
B	0.4910	0.1880
C	0.4500	0.1830
D	0.3740	0.1230
E	0.5410	0.2140
F	0.5560	0.2540
G	0.5080	0.1960
H	0.5710	0.2020
I	0.5300	0.2130
J	0.4440	0.1720
K	0.6160	0.2990
L	0.5500	0.1700
M	0.5060	0.1700
N	0.5210	0.1640
O	0.6380	0.2370
P	0.4890	0.1670
Q	0.5440	0.1790
R	0.5990	0.2830
S	0.5260	0.1360
T	0.5510	0.1550
U	0.4870	0.2210
X	0.6310	0.2330
Y	0.5350	0.1650
Z	0.6540	0.1760
a	0.9000	0.3420
b	0.9030	0.2940
c	0.6910	0.3340
d	0.6800	0.3160

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Chain	Atom inclusion	Q-score
e	0.6350	0.3010
f	0.5920	0.2150
g	0.5580	0.1870
h	0.5600	0.2410
i	0.6840	0.3120
j	0.6240	0.2950
k	0.6620	0.3060
l	0.6810	0.3210
m	0.7120	0.3350
n	0.6780	0.2530
o	0.6240	0.2560
p	0.7070	0.3250
q	0.6300	0.2810
r	0.6670	0.3410
s	0.6370	0.3190
t	0.5710	0.2560
u	0.6640	0.2610
v	0.7010	0.3210
w	0.6570	0.3140
x	0.6320	0.2360
y	0.6290	0.2930
z	0.6710	0.3170