



Full wwPDB EM Validation Report ⓘ

Jun 17, 2024 – 09:32 pm BST

PDB ID : 9FBV
EMDB ID : EMD-50296
Title : 70S Escherichia coli ribosome with P-site initiator tRNA.
Authors : Koller, T.O.; Wilson, D.N.
Deposited on : 2024-05-14
Resolution : 2.40 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:

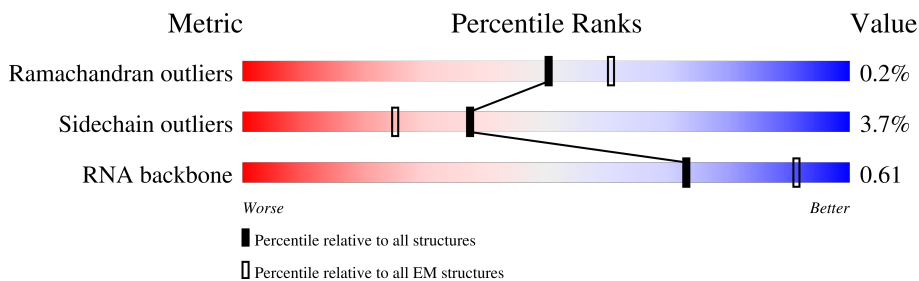
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.40 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	55	
2	1	46	
3	2	65	
4	3	38	
5	b	120	
6	c	273	
7	d	209	
8	e	201	

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Mol	Chain	Length	Quality of chain
9	f	179	22% 96%
10	g	177	25% 94% 5%
11	h	149	5% 26% 72%
12	i	142	100%
13	k	144	99%
14	l	136	99%
15	m	127	92% 7%
16	n	117	97%
17	o	115	5% 99%
18	p	118	97%
19	q	103	5% 98%
20	r	110	99%
21	s	100	7% 89% 7%
22	t	104	11% 89% 9%
23	u	94	9% 96%
24	v	85	9% 98%
25	w	78	5% 96%
26	x	63	11% 92% 6%
27	y	59	5% 97%
28	z	57	98%
29	4	70	37% 80% 6% 14%
30	a	2903	5% 83% 11% 5%
31	j	123	93%
32	B	241	39% 89% 7%
33	D	206	18% 87% 12%

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Mol	Chain	Length	Quality of chain
34	E	167	5% 92% 7%
35	F	135	13% 74% 24%
36	H	130	95% ..
37	K	129	8% 88% 9%
38	L	124	5% 89% 10% ..
39	O	89	99% .
40	P	82	11% 96% ..
41	Q	84	15% 92% 6%
42	R	75	13% 84% 12%
43	T	87	10% 98% ..
44	U	71	41% 93% 6% .
45	X	3	100%
46	C	233	12% 85% 12%
47	G	179	26% 80% 5% 15%
48	I	130	17% 95% ..
49	J	103	39% 91% 5%
50	M	118	14% 94% ..
51	N	101	13% 98% ..
52	S	92	22% 87% 9%
53	A	1534	7% 85% 14% .
54	Z	77	34% 77% 18% 5%

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 140031 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein bL33.

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

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

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

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

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

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

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

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

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

- Molecule 6 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 8 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 11 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 12 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 13 is a protein called 50S ribosomal protein L15.

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

- Molecule 14 is a protein called Large ribosomal subunit protein uL16.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 15 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 16 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 17 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 18 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 19 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 20 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 21 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 22 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 23 is a protein called 50S ribosomal protein L25.

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

- Molecule 24 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	v	83	629	388	128	112	1	0	0

- Molecule 25 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 26 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 27 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 28 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 29 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 30 is a RNA chain called 23S ribosomal RNA.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	118	Total	C	N	O	S	0	0
			901	567	170	158	6		

- Molecule 32 is a protein called 30S ribosomal protein S2.

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

- Molecule 33 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 34 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 35 is a protein called 30S ribosomal protein S6, fully modified isoform.

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

- Molecule 36 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 37 is a protein called Small ribosomal subunit protein uS11.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 38 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 39 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 40 is a protein called 30S ribosomal protein S16.

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

- Molecule 41 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 42 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 43 is a protein called 30S ribosomal protein S20.

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

- Molecule 44 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 45 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	X	3	Total	C	N	O	P	0	0
			65	29	12	21	3		

- Molecule 46 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 47 is a protein called 30S ribosomal protein S7.

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

- Molecule 48 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 49 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 50 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 51 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 52 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 53 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	A	1519	Total	C	N	O	P	0	0
			32608	14548	5986	10555	1519		

- Molecule 54 is a RNA chain called fMet-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
54	Z	73	1563	696	286	508	73	0	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	3	1	Total	Zn	0
			1	1	
55	4	1	Total	Zn	0
			1	1	

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	b	5	Total	Mg	0
			5	5	
56	c	1	Total	Mg	0
			1	1	
56	d	1	Total	Mg	0
			1	1	
56	k	1	Total	Mg	0
			1	1	
56	p	1	Total	Mg	0
			1	1	
56	z	1	Total	Mg	0
			1	1	
56	a	205	Total	Mg	0
			205	205	
56	A	91	Total	Mg	0
			91	91	

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
57	d	1	Total	K	0
			1	1	
57	a	1	Total	K	0
			1	1	
57	A	1	Total	K	0
			1	1	

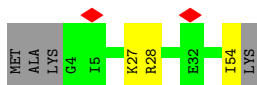
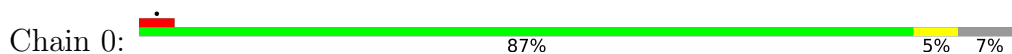
- Molecule 58 is water.

Mol	Chain	Residues	Atoms		AltConf
58	a	1	Total 1	O 1	0
58	X	7	Total 7	O 7	0
58	A	28	Total 28	O 28	0
58	Z	3	Total 3	O 3	0

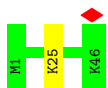
3 Residue-property plots [i](#)

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: Large ribosomal subunit protein bL33



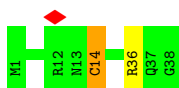
- Molecule 2: Large ribosomal subunit protein bL34



- Molecule 3: Large ribosomal subunit protein bL35



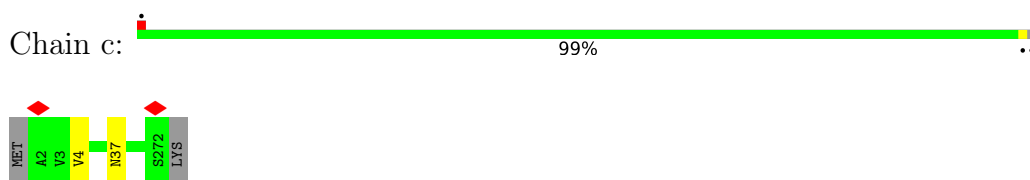
- Molecule 4: Large ribosomal subunit protein bL36A



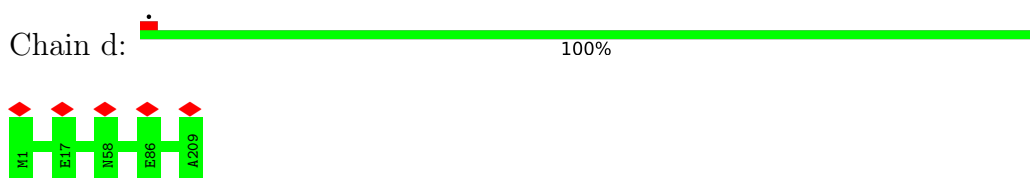
- Molecule 5: 5S ribosomal RNA



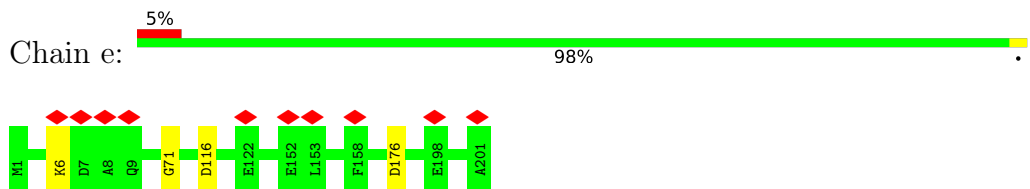
- Molecule 6: Large ribosomal subunit protein uL2



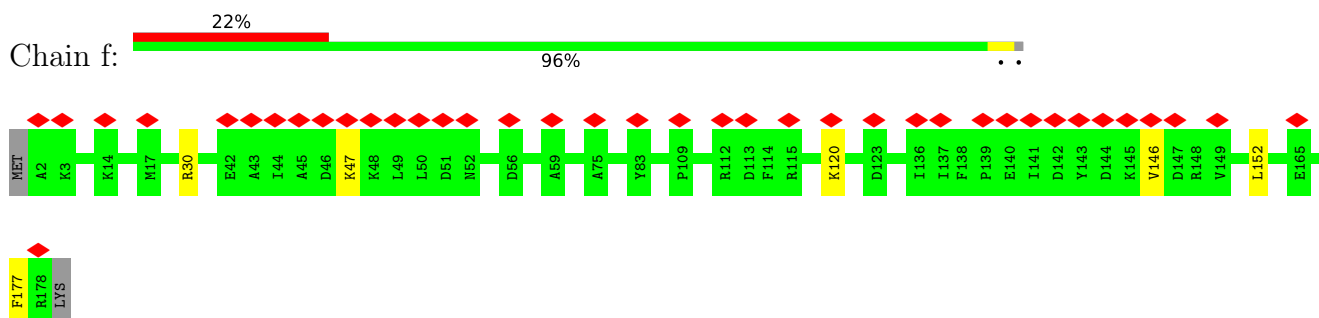
- Molecule 7: Large ribosomal subunit protein uL3



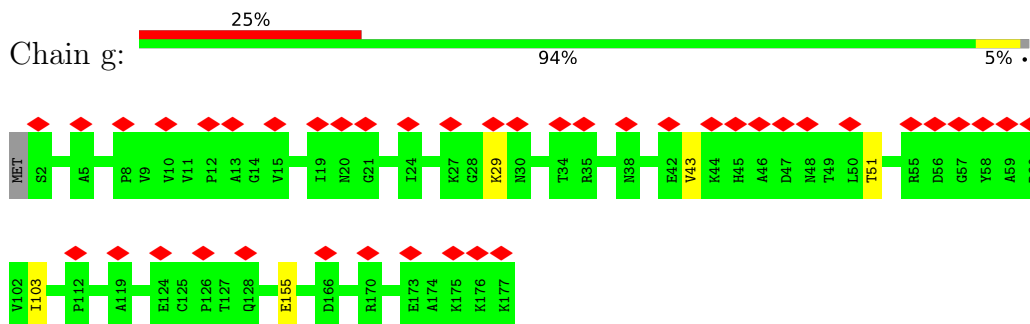
- Molecule 8: Large ribosomal subunit protein uL4



- Molecule 9: Large ribosomal subunit protein uL5

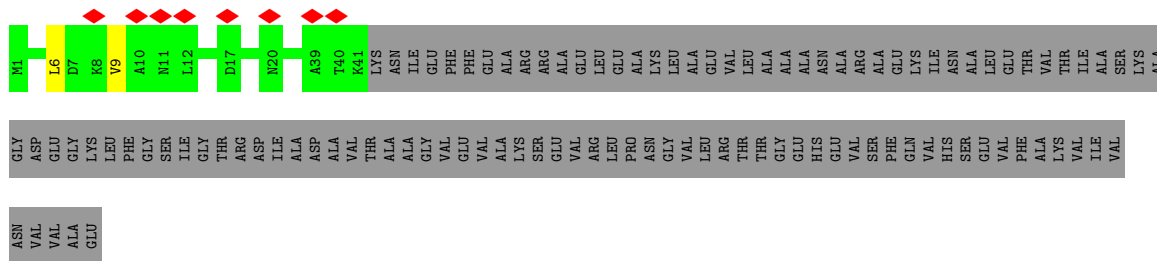


- Molecule 10: Large ribosomal subunit protein uL6

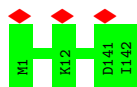


- Molecule 11: Large ribosomal subunit protein bL9

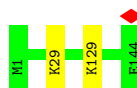




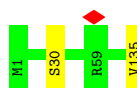
- Molecule 12: Large ribosomal subunit protein uL13



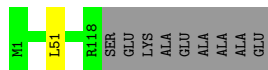
- Molecule 13: 50S ribosomal protein L15



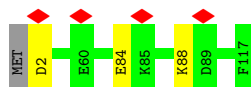
- Molecule 14: Large ribosomal subunit protein uL16



- Molecule 15: Large ribosomal subunit protein bL17

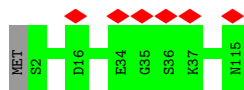


- Molecule 16: Large ribosomal subunit protein uL18



- Molecule 17: Large ribosomal subunit protein bL19

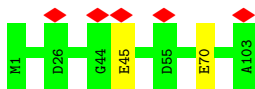




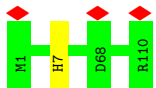
- Molecule 18: Large ribosomal subunit protein bL20



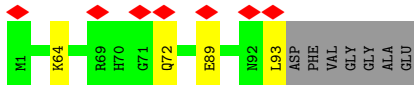
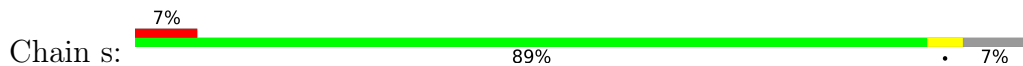
- Molecule 19: Large ribosomal subunit protein bL21



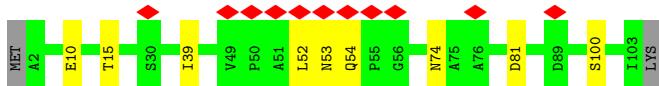
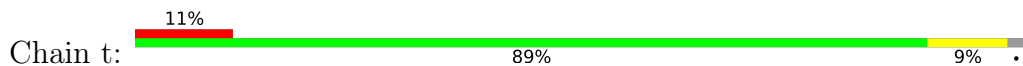
- Molecule 20: Large ribosomal subunit protein uL22



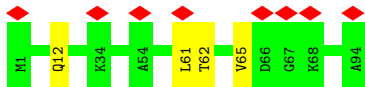
- Molecule 21: Large ribosomal subunit protein uL23



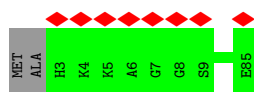
- Molecule 22: Large ribosomal subunit protein uL24



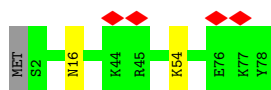
- Molecule 23: 50S ribosomal protein L25



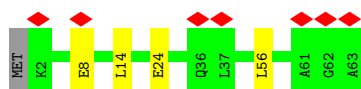
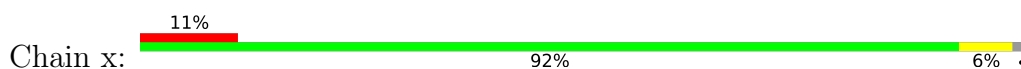
- Molecule 24: Large ribosomal subunit protein bL27



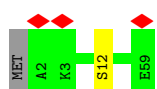
- Molecule 25: Large ribosomal subunit protein bL28



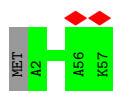
- Molecule 26: Large ribosomal subunit protein uL29



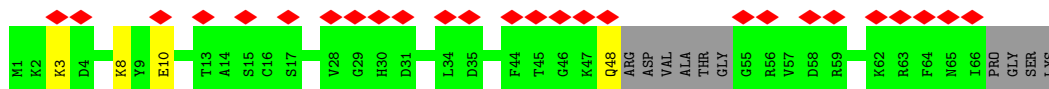
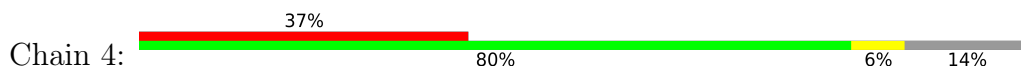
- Molecule 27: Large ribosomal subunit protein uL30



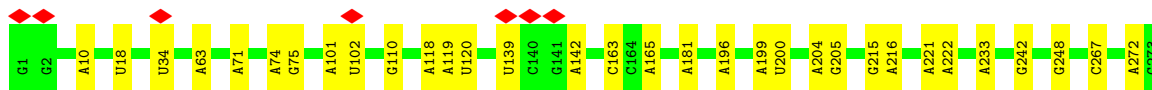
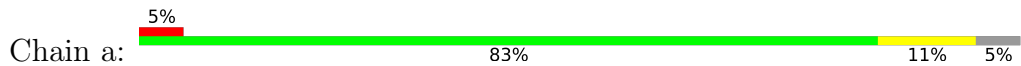
- Molecule 28: Large ribosomal subunit protein bL32

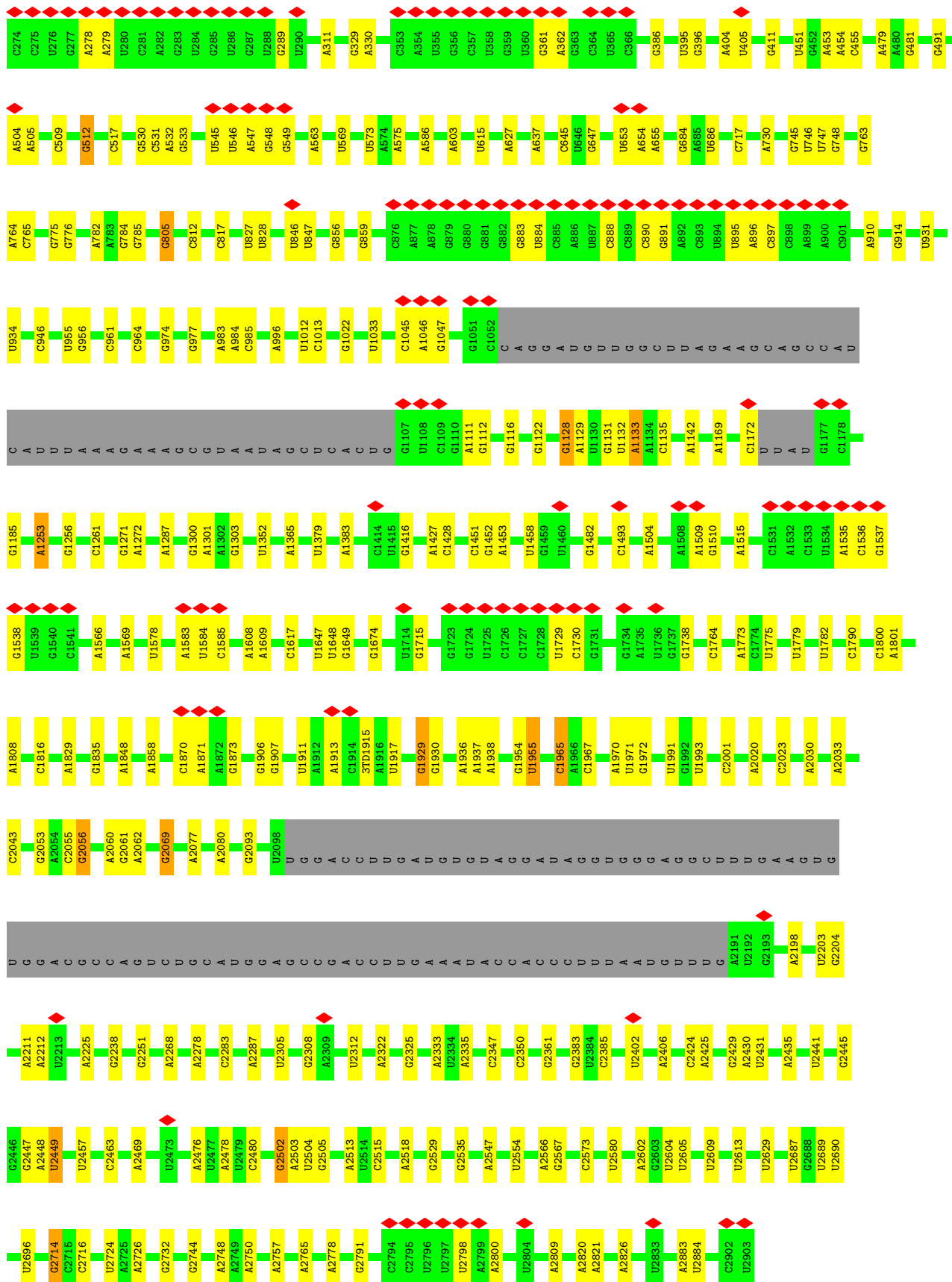


- Molecule 29: Large ribosomal subunit protein bL31A




- Molecule 30: 23S ribosomal RNA






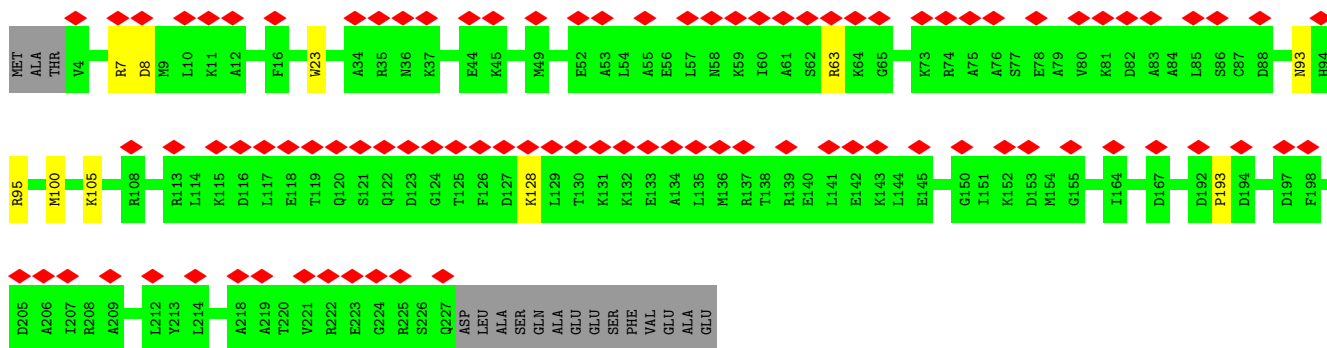
• Molecule 31: Large ribosomal subunit protein uL14

Chain j:  93%




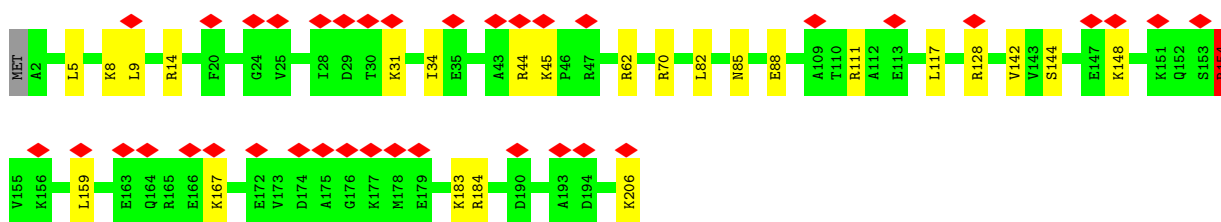
- Molecule 32: 30S ribosomal protein S2

Chain B:  39% 89% 7%

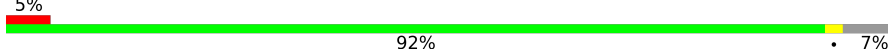


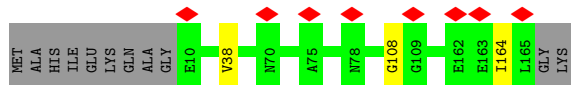
- Molecule 33: Small ribosomal subunit protein uS4

Chain D:  18% 87% 12%




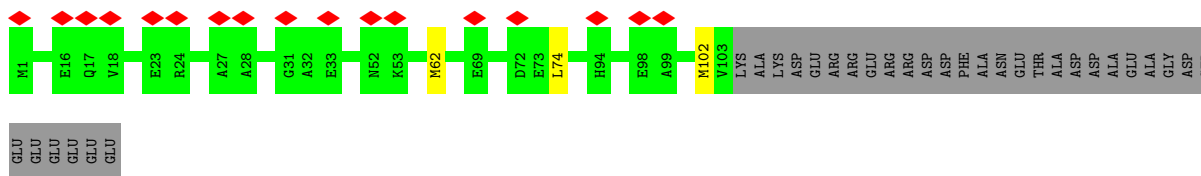
- Molecule 34: Small ribosomal subunit protein uS5

Chain E:  5% 92% 7%



- Molecule 35: 30S ribosomal protein S6, fully modified isoform

Chain F:  13% 74% 24%




- Molecule 36: Small ribosomal subunit protein uS8

Chain H:  95%




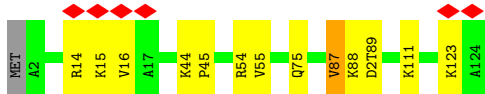
- Molecule 37: Small ribosomal subunit protein uS11

Chain K:  88% 9%



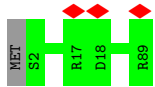
- Molecule 38: Small ribosomal subunit protein uS12

Chain L:  89% 10%



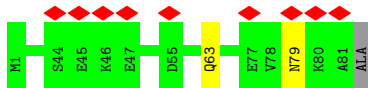
- Molecule 39: Small ribosomal subunit protein uS15

Chain O:  99%

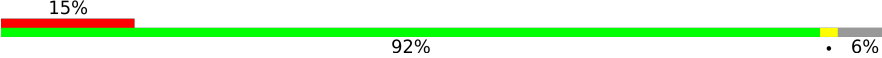


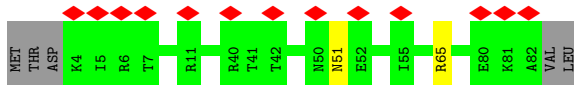
- Molecule 40: 30S ribosomal protein S16

Chain P:  96%




- Molecule 41: Small ribosomal subunit protein uS17

Chain Q:  92% 6%

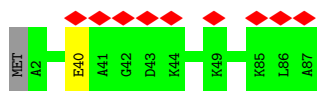


- Molecule 42: Small ribosomal subunit protein bS18

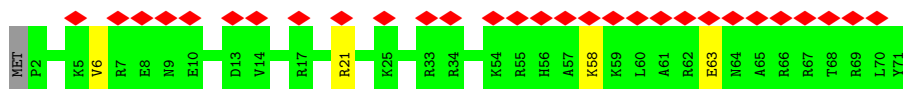
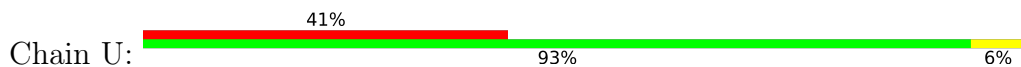
Chain R:  84% 12%



• Molecule 43: 30S ribosomal protein S20



• Molecule 44: Small ribosomal subunit protein bS21

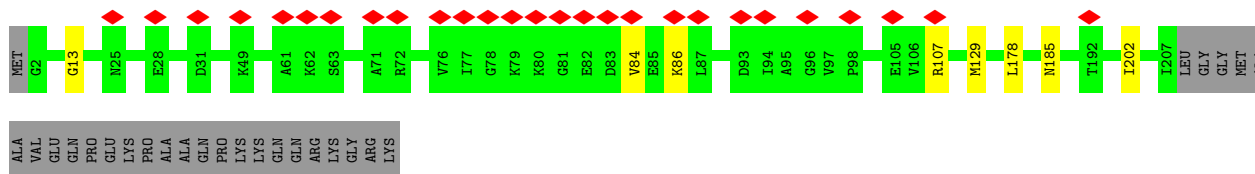
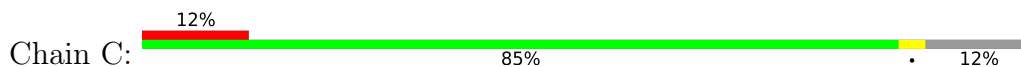


• Molecule 45: messenger RNA

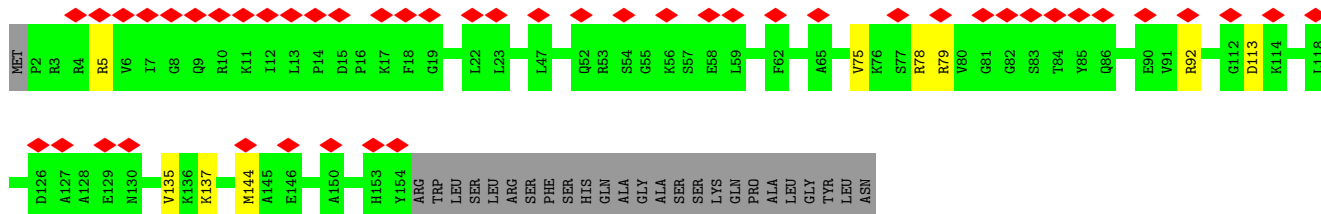
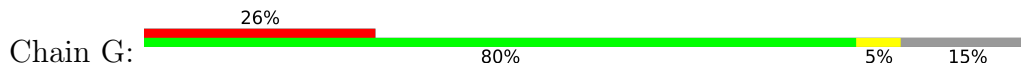


There are no outlier residues recorded for this chain.

• Molecule 46: Small ribosomal subunit protein uS3

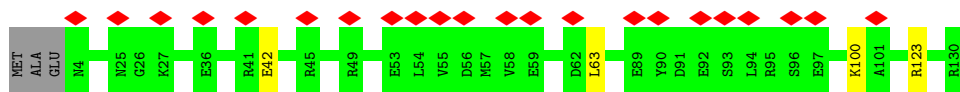


• Molecule 47: 30S ribosomal protein S7

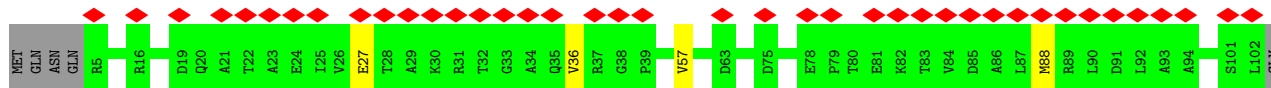
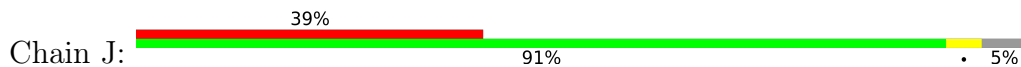


• Molecule 48: Small ribosomal subunit protein uS9

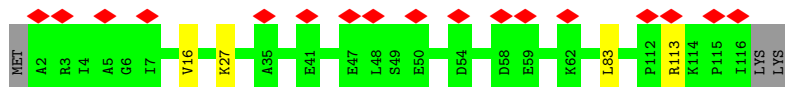




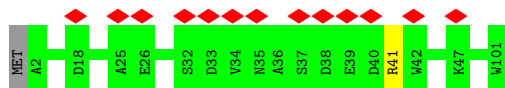
• Molecule 49: Small ribosomal subunit protein uS10



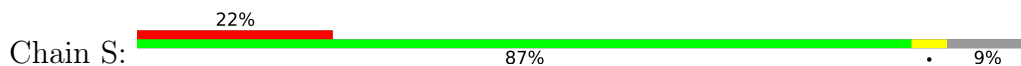
• Molecule 50: Small ribosomal subunit protein uS13



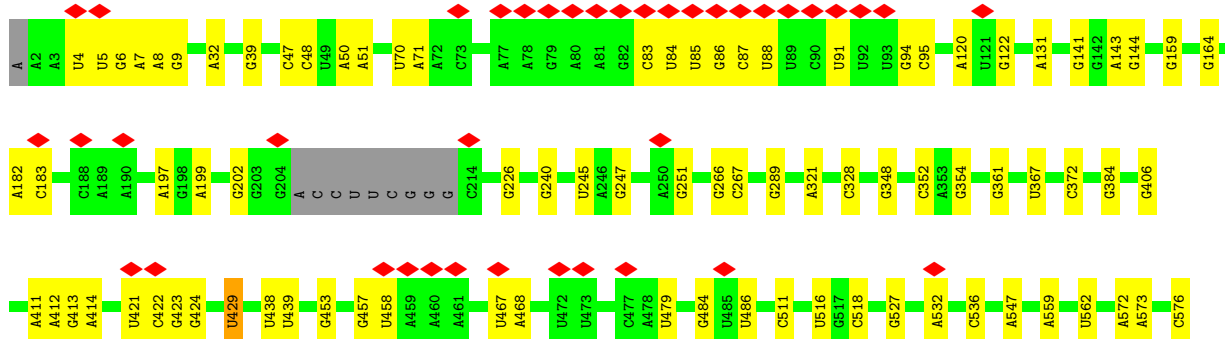
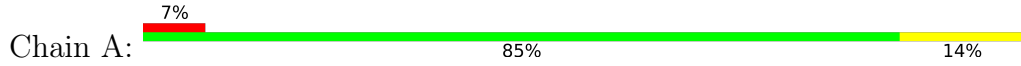
• Molecule 51: Small ribosomal subunit protein uS14

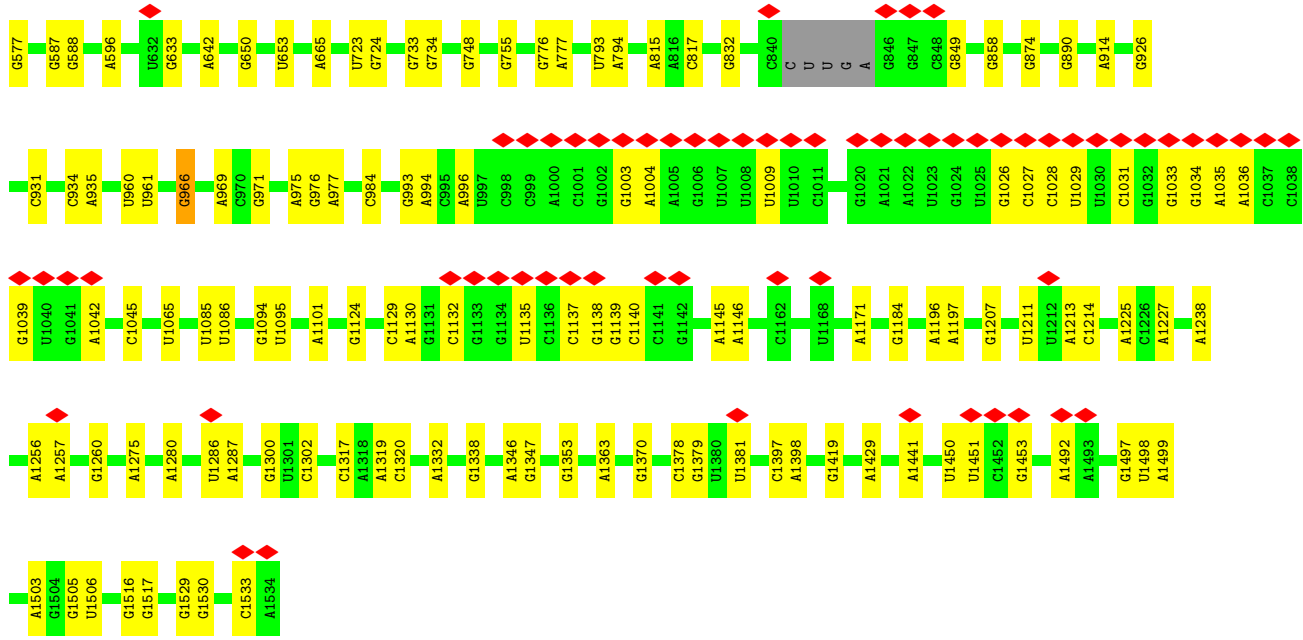


• Molecule 52: Small ribosomal subunit protein uS19

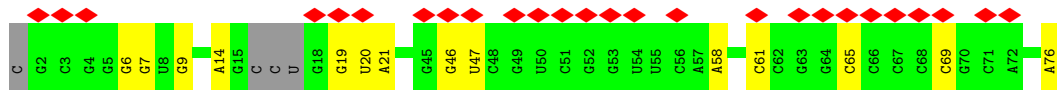
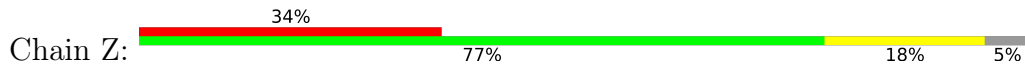


• Molecule 53: 16S ribosomal RNA





• Molecule 54: fMet-tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	84771	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (\AA)	480.0, 480.0, 480.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8, 0.8, 0.8	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: MS6, 4D4, OMG, PSU, OMC, ZN, 3TD, UR3, 2MA, OMU, H2U, 6MZ, G7M, 5MC, MEQ, 5MU, 2MG, IAS, K, 1MG, MG, 4OC, D2T

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.38	0/424	0.64	0/565
2	1	0.45	0/380	0.74	0/498
3	2	0.45	0/513	0.67	0/676
4	3	0.41	0/303	0.77	1/397 (0.3%)
5	b	0.52	0/2850	0.94	0/4444
6	c	0.43	0/2121	0.68	0/2852
7	d	0.41	0/1576	0.64	0/2119
8	e	0.39	0/1571	0.62	0/2113
9	f	0.35	0/1434	0.61	0/1926
10	g	0.36	0/1343	0.64	0/1816
11	h	0.37	0/306	0.64	0/413
12	i	0.38	0/1152	0.63	0/1551
13	k	0.45	0/1062	0.63	0/1413
14	l	0.37	0/1073	0.64	0/1433
15	m	0.41	0/958	0.68	0/1281
16	n	0.37	0/902	0.63	0/1209
17	o	0.39	0/929	0.65	0/1242
18	p	0.43	0/960	0.68	0/1278
19	q	0.40	0/829	0.65	0/1107
20	r	0.40	0/864	0.65	0/1156
21	s	0.36	0/744	0.59	0/994
22	t	0.36	0/787	0.64	0/1051
23	u	0.37	0/766	0.62	0/1025
24	v	0.43	0/637	0.61	0/841
25	w	0.40	0/635	0.67	0/848
26	x	0.34	0/502	0.58	0/667
27	y	0.36	0/453	0.62	0/605
28	z	0.42	0/450	0.67	0/599
29	4	0.40	0/488	0.61	0/649
30	a	0.60	0/65651	1.00	46/102413 (0.0%)
31	j	0.41	0/909	0.65	0/1217

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	B	0.35	0/1784	0.61	0/2403
33	D	0.37	0/1665	0.72	1/2227 (0.0%)
34	E	0.37	0/1165	0.61	0/1568
35	F	0.35	0/858	0.65	0/1160
36	H	0.36	0/989	0.63	0/1326
37	K	0.39	0/884	0.63	0/1191
38	L	0.41	1/960 (0.1%)	0.72	0/1286
39	O	0.37	0/722	0.61	0/964
40	P	0.35	0/653	0.68	0/877
41	Q	0.35	0/650	0.66	0/871
42	R	0.38	0/553	0.64	0/742
43	T	0.35	0/676	0.58	0/895
44	U	0.38	0/597	0.75	0/792
45	X	0.52	0/72	0.81	0/110
46	C	0.36	0/1651	0.61	0/2225
47	G	0.37	0/1219	0.62	0/1635
48	I	0.38	0/1034	0.66	0/1375
49	J	0.36	0/796	0.67	0/1077
50	M	0.36	0/900	0.65	0/1204
51	N	0.37	0/817	0.65	0/1088
52	S	0.39	0/685	0.61	0/922
53	A	0.53	0/36287	0.94	4/56602 (0.0%)
54	Z	0.59	0/1746	0.95	0/2719
All	All	0.53	1/150935 (0.0%)	0.90	52/225657 (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
25	w	0	1
30	a	0	5
32	B	0	1
33	D	0	1
34	E	0	1
36	H	0	1
38	L	0	1
46	C	0	1
51	N	0	1
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	L	87	VAL	C-N	5.24	1.46	1.34

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	2056	G	O5'-P-OP1	-8.52	98.03	105.70
30	a	1790	C	O5'-P-OP2	-8.06	98.45	105.70
30	a	1261	C	O5'-P-OP2	-8.05	98.45	105.70
30	a	2687	U	O5'-P-OP2	-7.42	99.02	105.70
30	a	1965	C	O5'-P-OP2	-7.16	99.26	105.70
30	a	517	C	O5'-P-OP2	-6.36	99.98	105.70
30	a	2515	C	O5'-P-OP2	-6.29	100.04	105.70
30	a	2447	G	O5'-P-OP1	-6.28	100.05	105.70
30	a	1128	G	C1'-O4'-C4'	-6.27	104.88	109.90
30	a	242	G	C3'-C2'-C1'	-6.13	96.60	101.50
30	a	18	U	O5'-P-OP2	-6.13	100.18	105.70
30	a	204	A	O3'-P-O5'	-6.08	92.44	104.00
30	a	1929	G	O3'-P-O5'	-5.85	92.89	104.00
30	a	569	U	O3'-P-O5'	-5.81	92.95	104.00
30	a	977	G	O5'-P-OP2	-5.81	100.47	105.70
30	a	1775	U	O5'-P-OP2	-5.79	100.48	105.70
33	D	154	ARG	CG-CD-NE	5.79	123.95	111.80
30	a	1936	A	C1'-O4'-C4'	-5.78	105.28	109.90
30	a	1185	G	O3'-P-O5'	-5.78	93.02	104.00
53	A	429	U	O3'-P-O5'	-5.73	93.11	104.00
30	a	1955	U	O5'-P-OP2	-5.66	100.61	105.70
30	a	763	G	O3'-P-O5'	-5.64	93.28	104.00
30	a	1936	A	O4'-C1'-N9	5.56	112.65	108.20
30	a	2513	A	O5'-P-OP2	-5.50	100.75	105.70
30	a	2502	G	O5'-P-OP1	-5.47	100.77	105.70
30	a	2053	G	O5'-P-OP2	-5.43	100.82	105.70
30	a	1617	C	O5'-P-OP2	-5.42	100.83	105.70
30	a	512	G	O4'-C1'-N9	5.37	112.50	108.20
30	a	2696	U	OP2-P-O3'	5.33	116.92	105.20
30	a	453	A	O5'-P-OP2	-5.30	100.93	105.70
30	a	1131	G	O3'-P-O5'	-5.25	94.03	104.00
4	3	14	CYS	CA-CB-SG	5.24	123.42	114.00
30	a	2001	C	O3'-P-O5'	-5.19	94.13	104.00
30	a	2714	G	OP1-P-O3'	5.19	116.62	105.20
30	a	805	G	OP1-P-O3'	5.18	116.61	105.20
30	a	2463	C	O3'-P-O5'	-5.16	94.20	104.00
30	a	684	G	OP2-P-O3'	5.14	116.50	105.20
30	a	1965	C	O5'-P-OP1	5.11	116.83	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A	1347	G	C3'-C2'-C1'	-5.09	97.43	101.50
30	a	817	C	O5'-P-OP2	-5.07	101.14	105.70
53	A	429	U	C2'-C3'-O3'	5.07	121.80	113.70
30	a	2724	U	O5'-P-OP2	-5.05	101.15	105.70
30	a	1779	U	O5'-P-OP2	-5.04	101.16	105.70
53	A	1499	A	OP1-P-O3'	5.03	116.27	105.20
30	a	2826	A	O3'-P-O5'	-5.03	94.44	104.00
30	a	512	G	C1'-O4'-C4'	-5.03	105.88	109.90
30	a	964	C	O3'-P-O5'	-5.02	94.45	104.00
30	a	748	G	C1'-O4'-C4'	-5.02	105.88	109.90
30	a	1133	A	C1'-O4'-C4'	-5.02	105.89	109.90
30	a	1954	G	OP2-P-O3'	5.02	116.24	105.20
30	a	479	A	C3'-C2'-C1'	-5.01	97.49	101.50
30	a	205	G	C3'-C2'-C1'	-5.01	97.50	101.50

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	B	193	PRO	Peptide
46	C	13	GLY	Peptide
33	D	154	ARG	Sidechain
34	E	108	GLY	Peptide
36	H	27	MET	Peptide
38	L	44	LYS	Peptide
51	N	41	ARG	Sidechain
30	a	1253	A	Sidechain
30	a	2732	G	Sidechain
30	a	395	U	Sidechain
30	a	512	G	Sidechain
30	a	956	G	Sidechain
25	w	16	ASN	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/55 (89%)	47 (96%)	2 (4%)	0	100	100
2	1	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
6	c	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
7	d	206/209 (99%)	201 (98%)	5 (2%)	0	100	100
8	e	199/201 (99%)	194 (98%)	4 (2%)	1 (0%)	29	41
9	f	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
10	g	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
11	h	39/149 (26%)	36 (92%)	3 (8%)	0	100	100
12	i	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
13	k	142/144 (99%)	136 (96%)	5 (4%)	1 (1%)	22	32
14	l	132/136 (97%)	128 (97%)	4 (3%)	0	100	100
15	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
16	n	114/117 (97%)	106 (93%)	7 (6%)	1 (1%)	17	25
17	o	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
18	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
19	q	101/103 (98%)	97 (96%)	3 (3%)	1 (1%)	15	23
20	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
21	s	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
22	t	100/104 (96%)	96 (96%)	3 (3%)	1 (1%)	15	23
23	u	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
24	v	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
25	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
26	x	60/63 (95%)	58 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
28	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
29	4	56/70 (80%)	52 (93%)	4 (7%)	0	100	100
31	j	114/123 (93%)	108 (95%)	5 (4%)	1 (1%)	17	25
32	B	222/241 (92%)	210 (95%)	12 (5%)	0	100	100
33	D	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
34	E	154/167 (92%)	150 (97%)	4 (3%)	0	100	100
35	F	101/135 (75%)	96 (95%)	5 (5%)	0	100	100
36	H	127/130 (98%)	122 (96%)	4 (3%)	1 (1%)	19	29
37	K	113/129 (88%)	108 (96%)	5 (4%)	0	100	100
38	L	120/124 (97%)	110 (92%)	9 (8%)	1 (1%)	19	29
39	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
40	P	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
41	Q	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
42	R	64/75 (85%)	60 (94%)	3 (5%)	1 (2%)	9	13
43	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
44	U	68/71 (96%)	66 (97%)	1 (2%)	1 (2%)	10	14
46	C	204/233 (88%)	192 (94%)	12 (6%)	0	100	100
47	G	151/179 (84%)	145 (96%)	6 (4%)	0	100	100
48	I	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
49	J	96/103 (93%)	91 (95%)	4 (4%)	1 (1%)	15	23
50	M	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
51	N	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
52	S	82/92 (89%)	78 (95%)	4 (5%)	0	100	100
All	All	5479/5913 (93%)	5271 (96%)	197 (4%)	11 (0%)	50	62

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	n	88	LYS
49	J	57	VAL
19	q	45	GLU
13	k	29	LYS
36	H	66	PHE

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Mol	Chain	Res	Type
44	U	6	VAL
31	j	5	GLN
42	R	22	ASP
22	t	39	ILE
38	L	45	PRO
8	e	71	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	
1	0	46/49 (94%)	43 (94%)	3 (6%)	17	27
2	1	38/38 (100%)	37 (97%)	1 (3%)	46	66
3	2	51/52 (98%)	48 (94%)	3 (6%)	19	32
4	3	34/34 (100%)	32 (94%)	2 (6%)	19	32
6	c	216/218 (99%)	214 (99%)	2 (1%)	78	90
7	d	163/163 (100%)	163 (100%)	0	100	100
8	e	165/165 (100%)	162 (98%)	3 (2%)	59	76
9	f	148/150 (99%)	142 (96%)	6 (4%)	30	48
10	g	137/138 (99%)	128 (93%)	9 (7%)	16	26
11	h	32/114 (28%)	30 (94%)	2 (6%)	18	28
12	i	116/116 (100%)	116 (100%)	0	100	100
13	k	103/103 (100%)	102 (99%)	1 (1%)	76	88
14	l	107/107 (100%)	105 (98%)	2 (2%)	57	75
15	m	98/103 (95%)	97 (99%)	1 (1%)	76	88
16	n	86/87 (99%)	84 (98%)	2 (2%)	50	70
17	o	99/100 (99%)	99 (100%)	0	100	100
18	p	89/90 (99%)	87 (98%)	2 (2%)	52	71
19	q	84/84 (100%)	83 (99%)	1 (1%)	71	85
20	r	93/93 (100%)	92 (99%)	1 (1%)	73	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	s	80/84 (95%)	76 (95%)	4 (5%)	24	40
22	t	83/85 (98%)	75 (90%)	8 (10%)	8	12
23	u	78/78 (100%)	74 (95%)	4 (5%)	24	39
24	v	62/63 (98%)	62 (100%)	0	100	100
25	w	67/68 (98%)	66 (98%)	1 (2%)	65	80
26	x	54/55 (98%)	50 (93%)	4 (7%)	13	22
27	y	48/49 (98%)	47 (98%)	1 (2%)	53	72
28	z	47/48 (98%)	47 (100%)	0	100	100
29	4	55/62 (89%)	51 (93%)	4 (7%)	14	22
31	j	99/104 (95%)	96 (97%)	3 (3%)	41	61
32	B	186/199 (94%)	177 (95%)	9 (5%)	25	41
33	D	172/173 (99%)	147 (86%)	25 (14%)	3	3
34	E	119/126 (94%)	117 (98%)	2 (2%)	60	78
35	F	90/116 (78%)	87 (97%)	3 (3%)	38	57
36	H	104/105 (99%)	100 (96%)	4 (4%)	33	51
37	K	89/98 (91%)	86 (97%)	3 (3%)	37	56
38	L	102/103 (99%)	92 (90%)	10 (10%)	8	11
39	O	76/77 (99%)	76 (100%)	0	100	100
40	P	65/65 (100%)	63 (97%)	2 (3%)	40	60
41	Q	73/78 (94%)	71 (97%)	2 (3%)	44	65
42	R	57/65 (88%)	55 (96%)	2 (4%)	36	55
43	T	65/66 (98%)	64 (98%)	1 (2%)	65	80
44	U	60/61 (98%)	57 (95%)	3 (5%)	24	40
46	C	170/190 (90%)	163 (96%)	7 (4%)	30	48
47	G	126/147 (86%)	117 (93%)	9 (7%)	14	23
48	I	105/107 (98%)	101 (96%)	4 (4%)	33	51
49	J	86/90 (96%)	83 (96%)	3 (4%)	36	55
50	M	93/96 (97%)	89 (96%)	4 (4%)	29	46
51	N	83/84 (99%)	83 (100%)	0	100	100
52	S	72/79 (91%)	68 (94%)	4 (6%)	21	34
All	All	4571/4825 (95%)	4404 (96%)	167 (4%)	37	53

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	27	LYS
1	0	28	ARG
1	0	54	ILE
2	1	25	LYS
3	2	31	HIS
3	2	47	LYS
3	2	57	LEU
4	3	14	CYS
4	3	36	ARG
6	c	4	VAL
6	c	37	ASN
8	e	6	LYS
8	e	116	ASP
8	e	176	ASP
9	f	30	ARG
9	f	47	LYS
9	f	120	LYS
9	f	146	VAL
9	f	152	LEU
9	f	177	PHE
10	g	29	LYS
10	g	43	VAL
10	g	51	THR
10	g	62	TRP
10	g	67	THR
10	g	72	LEU
10	g	90	VAL
10	g	103	ILE
10	g	155	GLU
11	h	6	LEU
11	h	9	VAL
13	k	129	LYS
14	l	30	SER
14	l	135	VAL
15	m	51	LEU
16	n	2	ASP
16	n	84	GLU
18	p	11	ARG
18	p	51	ARG
19	q	70	GLU
20	r	7	HIS
21	s	64	LYS

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Mol	Chain	Res	Type
21	s	72	GLN
21	s	89	GLU
21	s	93	LEU
22	t	10	GLU
22	t	15	THR
22	t	52	LEU
22	t	53	ASN
22	t	54	GLN
22	t	74	ASN
22	t	81	ASP
22	t	100	SER
23	u	12	GLN
23	u	61	LEU
23	u	62	THR
23	u	65	VAL
25	w	54	LYS
26	x	8	GLU
26	x	14	LEU
26	x	24	GLU
26	x	56	LEU
27	y	12	SER
29	4	3	LYS
29	4	8	LYS
29	4	10	GLU
29	4	48	GLN
31	j	49	ARG
31	j	58	LEU
31	j	93	GLN
32	B	7	ARG
32	B	8	ASP
32	B	23	TRP
32	B	63	ARG
32	B	93	ASN
32	B	95	ARG
32	B	100	MET
32	B	105	LYS
32	B	128	LYS
33	D	5	LEU
33	D	8	LYS
33	D	9	LEU
33	D	14	ARG
33	D	31	LYS

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Mol	Chain	Res	Type
33	D	34	ILE
33	D	44	ARG
33	D	45	LYS
33	D	62	ARG
33	D	70	ARG
33	D	82	LEU
33	D	85	ASN
33	D	88	GLU
33	D	111	ARG
33	D	117	LEU
33	D	128	ARG
33	D	142	VAL
33	D	144	SER
33	D	148	LYS
33	D	154	ARG
33	D	159	LEU
33	D	167	LYS
33	D	183	LYS
33	D	184	ARG
33	D	206	LYS
34	E	38	VAL
34	E	164	ILE
35	F	62	MET
35	F	74	LEU
35	F	102	MET
36	H	27	MET
36	H	50	LYS
36	H	56	LYS
36	H	89	LYS
37	K	38	GLN
37	K	72	ASP
37	K	94	GLU
38	L	14	ARG
38	L	15	LYS
38	L	16	VAL
38	L	54	ARG
38	L	55	VAL
38	L	75	GLN
38	L	87	VAL
38	L	88	LYS
38	L	111	LYS
38	L	123	LYS

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Mol	Chain	Res	Type
40	P	63	GLN
40	P	79	ASN
41	Q	51	ASN
41	Q	65	ARG
42	R	10	PHE
42	R	18	VAL
43	T	40	GLU
44	U	21	ARG
44	U	58	LYS
44	U	63	GLU
46	C	84	VAL
46	C	86	LYS
46	C	107	ARG
46	C	129	MET
46	C	178	LEU
46	C	185	ASN
46	C	202	ILE
47	G	5	ARG
47	G	75	VAL
47	G	78	ARG
47	G	79	ARG
47	G	92	ARG
47	G	113	ASP
47	G	135	VAL
47	G	137	LYS
47	G	144	MET
48	I	42	GLU
48	I	63	LEU
48	I	100	LYS
48	I	123	ARG
49	J	27	GLU
49	J	36	VAL
49	J	88	MET
50	M	16	VAL
50	M	27	LYS
50	M	83	LEU
50	M	113	ARG
52	S	42	PRO
52	S	43	ASN
52	S	55	ARG
52	S	63	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41)

such sidechains are listed below:

Mol	Chain	Res	Type
3	2	31	HIS
6	c	37	ASN
6	c	115	GLN
6	c	197	ASN
6	c	243	HIS
8	e	90	GLN
9	f	63	GLN
10	g	139	GLN
12	i	47	HIS
12	i	128	ASN
17	o	12	GLN
18	p	44	GLN
19	q	66	HIS
20	r	40	ASN
21	s	72	GLN
22	t	53	ASN
25	w	6	GLN
26	x	15	ASN
26	x	38	GLN
29	4	65	ASN
31	j	89	ASN
32	B	89	GLN
32	B	103	ASN
33	D	85	ASN
33	D	100	ASN
33	D	116	GLN
34	E	82	GLN
35	F	46	GLN
37	K	81	ASN
37	K	109	ASN
39	O	40	GLN
39	O	80	GLN
43	T	68	HIS
43	T	84	ASN
44	U	64	ASN
46	C	100	GLN
46	C	139	GLN
46	C	140	ASN
47	G	68	ASN
51	N	35	ASN
52	S	43	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	a	2745/2903 (94%)	285 (10%)	0
45	X	2/3 (66%)	0	0
5	b	118/120 (98%)	12 (10%)	0
53	A	1515/1534 (98%)	192 (12%)	25 (1%)
54	Z	71/77 (92%)	14 (19%)	3 (4%)
All	All	4451/4637 (95%)	503 (11%)	28 (0%)

All (503) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	b	34	A
5	b	35	C
5	b	36	C
5	b	37	C
5	b	44	G
5	b	45	A
5	b	56	G
5	b	88	C
5	b	89	U
5	b	90	C
5	b	99	A
5	b	109	A
30	a	10	A
30	a	34	U
30	a	63	A
30	a	71	A
30	a	74	A
30	a	75	G
30	a	101	A
30	a	102	U
30	a	110	G
30	a	118	A
30	a	119	A
30	a	120	U
30	a	139	U
30	a	142	A
30	a	163	C
30	a	165	A
30	a	181	A
30	a	196	A
30	a	199	A

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Mol	Chain	Res	Type
30	a	200	U
30	a	215	G
30	a	216	A
30	a	221	A
30	a	222	A
30	a	233	A
30	a	248	G
30	a	267	C
30	a	272	A
30	a	278	A
30	a	279	A
30	a	289	G
30	a	311	A
30	a	329	G
30	a	330	A
30	a	361	G
30	a	362	A
30	a	386	G
30	a	396	G
30	a	404	A
30	a	405	U
30	a	411	G
30	a	451	U
30	a	454	A
30	a	455	C
30	a	481	G
30	a	491	G
30	a	504	A
30	a	505	A
30	a	509	C
30	a	530	G
30	a	531	C
30	a	532	A
30	a	533	G
30	a	545	U
30	a	546	U
30	a	547	A
30	a	548	G
30	a	549	G
30	a	563	A
30	a	573	U
30	a	575	A

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Mol	Chain	Res	Type
30	a	586	A
30	a	603	A
30	a	615	U
30	a	627	A
30	a	637	A
30	a	645	C
30	a	647	G
30	a	653	U
30	a	654	A
30	a	655	A
30	a	686	U
30	a	717	C
30	a	730	A
30	a	747	5MU
30	a	764	A
30	a	765	C
30	a	775	G
30	a	776	G
30	a	782	A
30	a	784	G
30	a	785	G
30	a	805	G
30	a	812	C
30	a	827	U
30	a	828	U
30	a	846	U
30	a	847	U
30	a	856	G
30	a	859	G
30	a	883	G
30	a	884	U
30	a	888	C
30	a	890	C
30	a	891	G
30	a	895	U
30	a	896	A
30	a	897	C
30	a	910	A
30	a	914	G
30	a	931	U
30	a	934	U
30	a	946	C

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Mol	Chain	Res	Type
30	a	961	C
30	a	974	G
30	a	983	A
30	a	984	A
30	a	985	C
30	a	996	A
30	a	1012	U
30	a	1013	C
30	a	1022	G
30	a	1033	U
30	a	1045	C
30	a	1046	A
30	a	1047	G
30	a	1111	A
30	a	1112	G
30	a	1116	G
30	a	1122	G
30	a	1128	G
30	a	1129	A
30	a	1132	U
30	a	1133	A
30	a	1135	C
30	a	1142	A
30	a	1169	A
30	a	1172	C
30	a	1253	A
30	a	1256	G
30	a	1271	G
30	a	1272	A
30	a	1287	A
30	a	1300	G
30	a	1301	A
30	a	1303	G
30	a	1352	U
30	a	1365	A
30	a	1379	U
30	a	1383	A
30	a	1416	G
30	a	1427	A
30	a	1428	C
30	a	1451	C
30	a	1452	G

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Mol	Chain	Res	Type
30	a	1453	A
30	a	1458	U
30	a	1482	G
30	a	1493	C
30	a	1504	A
30	a	1509	A
30	a	1510	G
30	a	1515	A
30	a	1535	A
30	a	1536	C
30	a	1537	G
30	a	1538	G
30	a	1566	A
30	a	1569	A
30	a	1578	U
30	a	1583	A
30	a	1584	U
30	a	1585	C
30	a	1608	A
30	a	1609	A
30	a	1647	U
30	a	1648	U
30	a	1649	G
30	a	1674	G
30	a	1715	G
30	a	1729	U
30	a	1730	C
30	a	1738	G
30	a	1764	C
30	a	1773	A
30	a	1782	U
30	a	1800	C
30	a	1801	A
30	a	1808	A
30	a	1816	C
30	a	1829	A
30	a	1848	A
30	a	1858	A
30	a	1870	C
30	a	1871	A
30	a	1873	G
30	a	1906	G

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Mol	Chain	Res	Type
30	a	1907	G
30	a	1913	A
30	a	1929	G
30	a	1930	G
30	a	1937	A
30	a	1938	A
30	a	1955	U
30	a	1965	C
30	a	1967	C
30	a	1970	A
30	a	1971	U
30	a	1972	G
30	a	1991	U
30	a	1993	U
30	a	2020	A
30	a	2023	C
30	a	2033	A
30	a	2043	C
30	a	2055	C
30	a	2056	G
30	a	2060	A
30	a	2061	G
30	a	2062	A
30	a	2069	G7M
30	a	2077	A
30	a	2080	A
30	a	2093	G
30	a	2198	A
30	a	2203	U
30	a	2204	G
30	a	2211	A
30	a	2212	A
30	a	2225	A
30	a	2238	G
30	a	2268	A
30	a	2278	A
30	a	2283	C
30	a	2287	A
30	a	2305	U
30	a	2308	G
30	a	2312	U
30	a	2322	A

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Mol	Chain	Res	Type
30	a	2325	G
30	a	2333	A
30	a	2335	A
30	a	2347	C
30	a	2350	C
30	a	2361	G
30	a	2383	G
30	a	2385	C
30	a	2402	U
30	a	2406	A
30	a	2424	C
30	a	2425	A
30	a	2429	G
30	a	2430	A
30	a	2431	U
30	a	2435	A
30	a	2441	U
30	a	2448	A
30	a	2449	H2U
30	a	2469	A
30	a	2476	A
30	a	2478	A
30	a	2480	C
30	a	2502	G
30	a	2505	G
30	a	2518	A
30	a	2529	G
30	a	2535	G
30	a	2547	A
30	a	2554	U
30	a	2566	A
30	a	2567	G
30	a	2573	C
30	a	2602	A
30	a	2609	U
30	a	2613	U
30	a	2629	U
30	a	2689	U
30	a	2690	U
30	a	2714	G
30	a	2716	C
30	a	2726	A

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Mol	Chain	Res	Type
30	a	2744	G
30	a	2748	A
30	a	2750	A
30	a	2757	A
30	a	2765	A
30	a	2778	A
30	a	2791	G
30	a	2798	U
30	a	2800	A
30	a	2809	A
30	a	2820	A
30	a	2821	A
30	a	2883	A
30	a	2884	U
53	A	4	U
53	A	5	U
53	A	6	G
53	A	8	A
53	A	9	G
53	A	32	A
53	A	39	G
53	A	47	C
53	A	48	C
53	A	50	A
53	A	51	A
53	A	70	U
53	A	71	A
53	A	83	C
53	A	84	U
53	A	85	U
53	A	86	G
53	A	87	C
53	A	88	U
53	A	91	U
53	A	94	G
53	A	95	C
53	A	120	A
53	A	122	G
53	A	131	A
53	A	141	G
53	A	143	A
53	A	144	G

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Mol	Chain	Res	Type
53	A	159	G
53	A	164	G
53	A	182	A
53	A	183	C
53	A	197	A
53	A	202	G
53	A	226	G
53	A	240	G
53	A	245	U
53	A	247	G
53	A	251	G
53	A	266	G
53	A	267	C
53	A	289	G
53	A	321	A
53	A	328	C
53	A	348	G
53	A	352	C
53	A	354	G
53	A	367	U
53	A	372	C
53	A	384	G
53	A	406	G
53	A	411	A
53	A	412	A
53	A	413	G
53	A	414	A
53	A	421	U
53	A	422	C
53	A	423	G
53	A	424	G
53	A	429	U
53	A	438	U
53	A	439	U
53	A	453	G
53	A	457	G
53	A	458	U
53	A	467	U
53	A	468	A
53	A	479	U
53	A	484	G
53	A	486	U

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Mol	Chain	Res	Type
53	A	511	C
53	A	518	C
53	A	532	A
53	A	536	C
53	A	547	A
53	A	559	A
53	A	562	U
53	A	572	A
53	A	573	A
53	A	576	C
53	A	577	G
53	A	587	G
53	A	588	G
53	A	596	A
53	A	633	G
53	A	642	A
53	A	650	G
53	A	653	U
53	A	665	A
53	A	723	U
53	A	724	G
53	A	734	G
53	A	748	G
53	A	755	G
53	A	777	A
53	A	793	U
53	A	794	A
53	A	815	A
53	A	817	C
53	A	832	G
53	A	849	G
53	A	874	G
53	A	890	G
53	A	914	A
53	A	926	G
53	A	931	C
53	A	934	C
53	A	935	A
53	A	960	U
53	A	961	U
53	A	966	2MG
53	A	969	A

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Mol	Chain	Res	Type
53	A	971	G
53	A	975	A
53	A	976	G
53	A	977	A
53	A	984	C
53	A	993	G
53	A	994	A
53	A	996	A
53	A	1003	G
53	A	1004	A
53	A	1009	U
53	A	1027	C
53	A	1028	C
53	A	1029	U
53	A	1031	C
53	A	1033	G
53	A	1034	G
53	A	1036	A
53	A	1039	G
53	A	1042	A
53	A	1065	U
53	A	1085	U
53	A	1086	U
53	A	1094	G
53	A	1095	U
53	A	1101	A
53	A	1124	G
53	A	1129	C
53	A	1130	A
53	A	1132	C
53	A	1135	U
53	A	1137	C
53	A	1138	G
53	A	1140	C
53	A	1146	A
53	A	1171	A
53	A	1184	G
53	A	1196	A
53	A	1197	A
53	A	1213	A
53	A	1214	C
53	A	1227	A

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Mol	Chain	Res	Type
53	A	1238	A
53	A	1256	A
53	A	1257	A
53	A	1260	G
53	A	1275	A
53	A	1280	A
53	A	1286	U
53	A	1287	A
53	A	1300	G
53	A	1302	C
53	A	1317	C
53	A	1319	A
53	A	1320	C
53	A	1332	A
53	A	1338	G
53	A	1346	A
53	A	1353	G
53	A	1363	A
53	A	1370	G
53	A	1378	C
53	A	1379	G
53	A	1381	U
53	A	1397	C
53	A	1398	A
53	A	1419	G
53	A	1429	A
53	A	1441	A
53	A	1450	U
53	A	1451	U
53	A	1453	G
53	A	1492	A
53	A	1497	G
53	A	1503	A
53	A	1506	U
53	A	1517	G
53	A	1529	G
53	A	1530	G
53	A	1533	C
54	Z	6	G
54	Z	7	G
54	Z	9	G
54	Z	14	A

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Mol	Chain	Res	Type
54	Z	19	G
54	Z	20	U
54	Z	21	A
54	Z	46	G
54	Z	47	U
54	Z	58	A
54	Z	61	C
54	Z	65	C
54	Z	69	C
54	Z	76	A

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	A	7	A
53	A	70	U
53	A	86	G
53	A	94	G
53	A	199	A
53	A	361	G
53	A	438	U
53	A	547	A
53	A	587	G
53	A	733	G
53	A	776	G
53	A	793	U
53	A	858	G
53	A	993	G
53	A	1026	G
53	A	1035	A
53	A	1045	C
53	A	1124	G
53	A	1129	C
53	A	1139	G
53	A	1145	A
53	A	1211	U
53	A	1225	A
53	A	1319	A
53	A	1505	G
54	Z	6	G
54	Z	7	G
54	Z	47	U

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

37 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
30	PSU	a	955	30	18,21,22	0.83	1 (5%)	22,30,33	0.73	0
30	1MG	a	745	30	18,26,27	1.11	2 (11%)	19,39,42	0.52	0
30	5MU	a	1939	30	19,22,23	0.39	0	28,32,35	0.44	0
30	PSU	a	2605	30	18,21,22	0.94	1 (5%)	22,30,33	0.80	1 (4%)
53	5MC	A	967	53	18,22,23	0.38	0	26,32,35	0.59	0
30	2MG	a	2445	30	18,26,27	1.14	2 (11%)	16,38,41	0.75	1 (6%)
14	4D4	l	81	14	9,11,12	0.66	0	8,13,15	0.69	0
53	2MG	A	966	53	18,26,27	1.03	2 (11%)	16,38,41	0.63	0
30	5MU	a	747	30	19,22,23	0.35	0	28,32,35	0.39	0
30	5MC	a	1962	30	18,22,23	0.33	0	26,32,35	0.59	0
30	3TD	a	1915	30	18,22,23	1.07	1 (5%)	22,32,35	0.61	0
30	OMG	a	2251	54,30	18,26,27	1.05	3 (16%)	19,38,41	0.72	0
38	D2T	L	89	38	7,9,10	0.94	0	6,11,13	1.55	2 (33%)
7	MEQ	d	150	7	8,9,10	0.43	0	5,10,12	0.97	0
30	PSU	a	1917	30	18,21,22	0.96	1 (5%)	22,30,33	0.60	0
30	H2U	a	2449	30	18,21,22	0.59	0	21,30,33	1.10	3 (14%)
53	G7M	A	527	53	20,26,27	1.11	3 (15%)	17,39,42	0.50	0
30	6MZ	a	1618	30	18,25,26	0.83	0	16,36,39	0.79	0
30	6MZ	a	2030	30	18,25,26	0.75	0	16,36,39	0.83	1 (6%)
30	2MG	a	1835	30	18,26,27	1.14	2 (11%)	16,38,41	0.70	0
53	2MG	A	1207	53	18,26,27	1.09	2 (11%)	16,38,41	0.73	0
30	G7M	a	2069	30	20,26,27	1.29	3 (15%)	17,39,42	0.68	0
30	PSU	a	2457	30	18,21,22	1.05	1 (5%)	22,30,33	0.63	0
30	PSU	a	2604	30	18,21,22	0.89	1 (5%)	22,30,33	0.93	1 (4%)
53	2MG	A	1516	53	18,26,27	0.98	2 (11%)	16,38,41	0.90	0
30	OMU	a	2552	30	19,22,23	0.36	0	26,31,34	0.52	0
53	PSU	A	516	56,53	18,21,22	0.90	1 (5%)	22,30,33	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PSU	a	2504	57,30	18,21,22	0.95	1 (5%)	22,30,33	0.71	0
53	4OC	A	1402	53	20,23,24	0.40	0	26,32,35	0.57	0
30	PSU	a	746	56,30	18,21,22	0.93	1 (5%)	22,30,33	0.67	0
53	5MC	A	1407	53	18,22,23	0.36	0	26,32,35	0.66	0
30	PSU	a	1911	30	18,21,22	0.91	1 (5%)	22,30,33	0.63	0
30	OMC	a	2498	56,30	19,22,23	0.50	0	26,31,34	0.54	0
37	IAS	K	119	37	6,7,8	0.86	0	6,8,10	0.99	0
30	PSU	a	2580	30	18,21,22	0.94	1 (5%)	22,30,33	0.81	1 (4%)
30	2MA	a	2503	56,30	17,25,26	1.07	2 (11%)	17,37,40	0.82	0
53	UR3	A	1498	57,53	19,22,23	0.41	0	26,32,35	0.75	1 (3%)

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
30	PSU	a	955	30	-	0/7/25/26	0/2/2/2
30	1MG	a	745	30	-	0/3/25/26	0/3/3/3
30	5MU	a	1939	30	-	0/7/25/26	0/2/2/2
30	PSU	a	2605	30	-	0/7/25/26	0/2/2/2
53	5MC	A	967	53	-	0/7/25/26	0/2/2/2
30	2MG	a	2445	30	-	1/5/27/28	0/3/3/3
14	4D4	l	81	14	-	1/11/12/14	-
53	2MG	A	966	53	-	0/5/27/28	0/3/3/3
30	5MU	a	747	30	-	1/7/25/26	0/2/2/2
30	5MC	a	1962	30	-	2/7/25/26	0/2/2/2
30	3TD	a	1915	30	-	2/7/25/26	0/2/2/2
30	OMG	a	2251	54,30	-	1/5/27/28	0/3/3/3
38	D2T	L	89	38	-	2/7/12/14	-
7	MEQ	d	150	7	-	2/8/9/11	-
30	PSU	a	1917	30	-	0/7/25/26	0/2/2/2
30	H2U	a	2449	30	-	0/7/38/39	0/2/2/2
53	G7M	A	527	53	-	1/3/25/26	0/3/3/3
30	6MZ	a	1618	30	-	0/5/27/28	0/3/3/3
30	6MZ	a	2030	30	-	2/5/27/28	0/3/3/3
30	2MG	a	1835	30	-	0/5/27/28	0/3/3/3
53	2MG	A	1207	53	-	0/5/27/28	0/3/3/3
30	G7M	a	2069	30	-	2/3/25/26	0/3/3/3
30	PSU	a	2457	30	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PSU	a	2604	30	-	0/7/25/26	0/2/2/2
53	2MG	A	1516	53	-	0/5/27/28	0/3/3/3
30	OMU	a	2552	30	-	0/9/27/28	0/2/2/2
53	PSU	A	516	56,53	-	0/7/25/26	0/2/2/2
30	PSU	a	2504	57,30	-	0/7/25/26	0/2/2/2
53	4OC	A	1402	53	-	0/9/29/30	0/2/2/2
30	PSU	a	746	56,30	-	1/7/25/26	0/2/2/2
53	5MC	A	1407	53	-	0/7/25/26	0/2/2/2
30	PSU	a	1911	30	-	0/7/25/26	0/2/2/2
30	OMC	a	2498	56,30	-	0/9/27/28	0/2/2/2
37	IAS	K	119	37	-	0/7/7/8	-
30	PSU	a	2580	30	-	0/7/25/26	0/2/2/2
30	2MA	a	2503	56,30	-	1/3/25/26	0/3/3/3
53	UR3	A	1498	57,53	-	0/7/25/26	0/2/2/2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2457	PSU	C6-C5	4.05	1.40	1.35
30	a	1915	3TD	C6-C5	4.01	1.40	1.35
30	a	1911	PSU	C6-C5	3.58	1.39	1.35
30	a	1917	PSU	C6-C5	3.57	1.39	1.35
30	a	2605	PSU	C6-C5	3.43	1.39	1.35
53	A	516	PSU	C6-C5	3.39	1.39	1.35
30	a	746	PSU	C6-C5	3.36	1.39	1.35
30	a	2069	G7M	C8-N9	3.36	1.39	1.33
53	A	527	G7M	C8-N9	3.35	1.39	1.33
30	a	2580	PSU	C6-C5	3.32	1.39	1.35
30	a	2069	G7M	C8-N7	3.25	1.39	1.33
30	a	1835	2MG	C5-C6	-3.04	1.41	1.47
30	a	2604	PSU	C6-C5	3.03	1.38	1.35
30	a	2503	2MA	C2-N3	3.00	1.37	1.31
30	a	2445	2MG	C5-C6	-2.98	1.41	1.47
30	a	2504	PSU	C6-C5	2.96	1.38	1.35
30	a	2251	OMG	C5-C6	-2.67	1.42	1.47
30	a	955	PSU	C6-C5	2.55	1.38	1.35
30	a	745	1MG	C5-C4	-2.54	1.36	1.43
53	A	1207	2MG	C5-C6	-2.51	1.42	1.47
53	A	1516	2MG	C5-C6	-2.45	1.42	1.47
30	a	745	1MG	C5-C6	-2.42	1.40	1.47
30	a	2069	G7M	C5-C6	-2.36	1.39	1.45
53	A	966	2MG	C5-C6	-2.36	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2251	OMG	C5-C4	-2.30	1.37	1.43
53	A	527	G7M	C8-N7	2.30	1.37	1.33
30	a	2251	OMG	C8-N7	-2.24	1.31	1.35
53	A	1207	2MG	C8-N7	-2.23	1.31	1.35
53	A	966	2MG	C8-N7	-2.17	1.31	1.35
30	a	2445	2MG	C8-N7	-2.16	1.31	1.35
30	a	2503	2MA	C5-C4	-2.11	1.37	1.43
30	a	1835	2MG	C8-N7	-2.10	1.31	1.35
53	A	527	G7M	C5-C6	-2.06	1.40	1.45
53	A	1516	2MG	C5-C4	-2.03	1.37	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	2449	H2U	C4-N3-C2	-2.99	123.31	125.79
30	a	2449	H2U	O2-C2-N1	-2.49	119.98	123.11
30	a	2449	H2U	N3-C2-N1	2.45	119.24	116.65
30	a	2580	PSU	C3'-C2'-C1'	2.41	104.44	101.64
30	a	2030	6MZ	C2-N1-C6	2.35	118.61	116.59
30	a	2604	PSU	C2'-C3'-C4'	-2.35	98.07	102.64
53	A	1498	UR3	C6-N1-C2	-2.18	119.84	121.79
38	L	89	D2T	O-C-CA	-2.14	119.17	124.78
30	a	2605	PSU	C2'-C3'-C4'	-2.11	98.54	102.64
38	L	89	D2T	OD1-CG-CB	-2.08	118.08	122.44
30	a	2445	2MG	O6-C6-C5	2.02	128.31	124.37

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	L	89	D2T	SB-CB-CG-OD2
30	a	746	PSU	O4'-C1'-C5-C6
30	a	1915	3TD	C3'-C4'-C5'-O5'
30	a	1915	3TD	O4'-C4'-C5'-O5'
30	a	2251	OMG	C1'-C2'-O2'-CM2
30	a	2445	2MG	N3-C2-N2-CM2
7	d	150	MEQ	NE2-CD-CG-CB
7	d	150	MEQ	OE1-CD-CG-CB
30	a	2030	6MZ	O4'-C4'-C5'-O5'
38	L	89	D2T	CG-CB-SB-CB1
30	a	2069	G7M	C4'-C5'-O5'-P
53	A	527	G7M	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
30	a	747	5MU	C3'-C4'-C5'-O5'
30	a	2030	6MZ	C3'-C4'-C5'-O5'
30	a	1962	5MC	C2'-C1'-N1-C6
30	a	1962	5MC	O4'-C1'-N1-C6
30	a	2069	G7M	O4'-C4'-C5'-O5'
30	a	2503	2MA	O4'-C4'-C5'-O5'
14	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 311 ligands modelled in this entry, 311 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

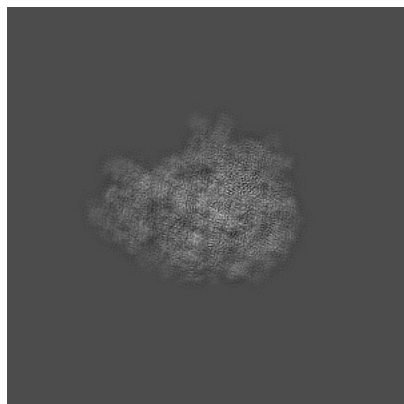
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50296. These allow visual inspection of the internal detail of the map and identification of artifacts.

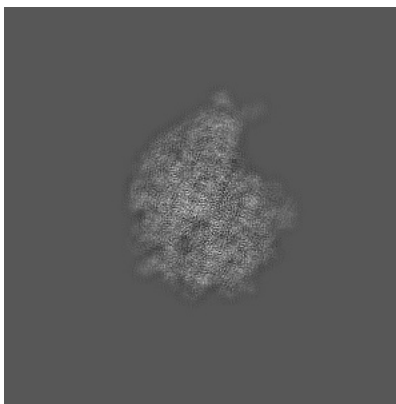
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

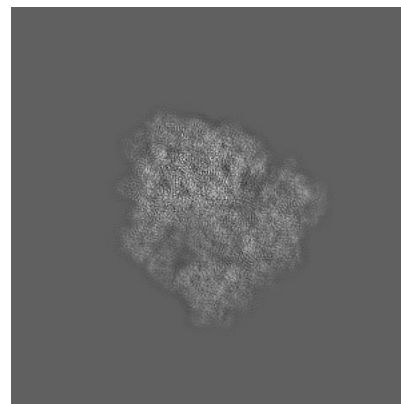
6.1.1 Primary map



X

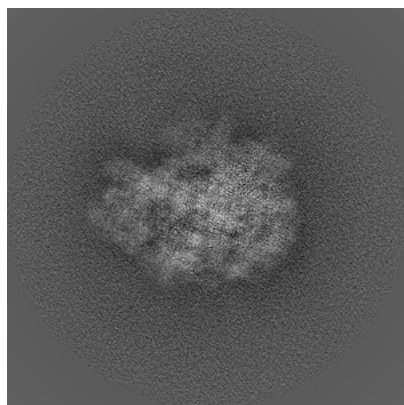


Y

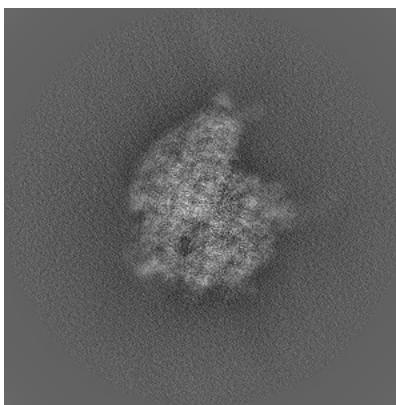


Z

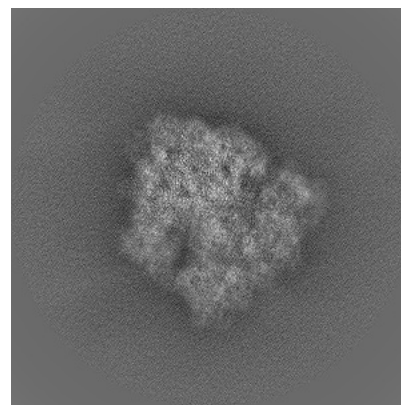
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

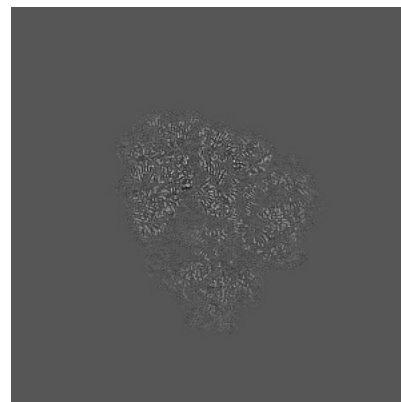
6.2.1 Primary map



X Index: 300

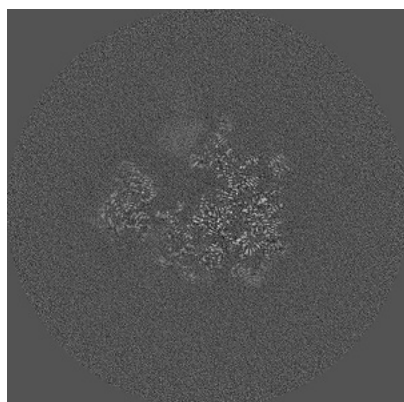


Y Index: 300

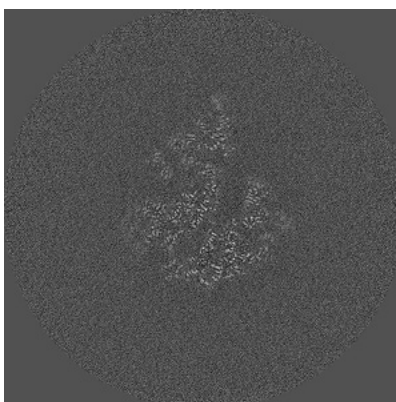


Z Index: 300

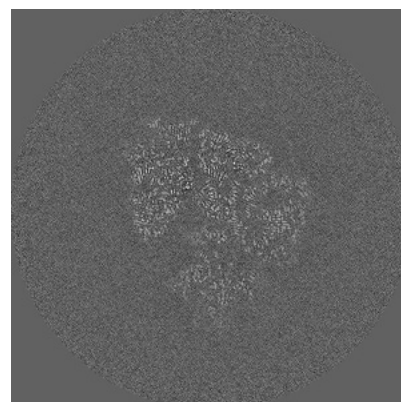
6.2.2 Raw map



X Index: 300



Y Index: 300

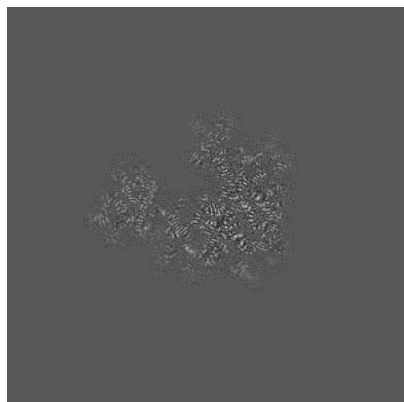


Z Index: 300

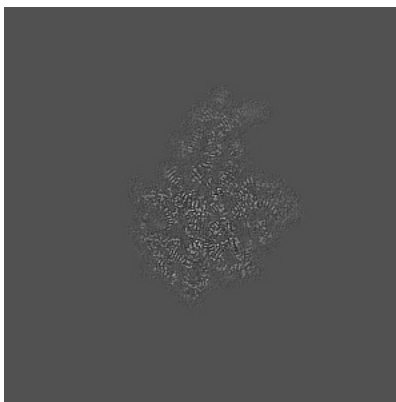
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

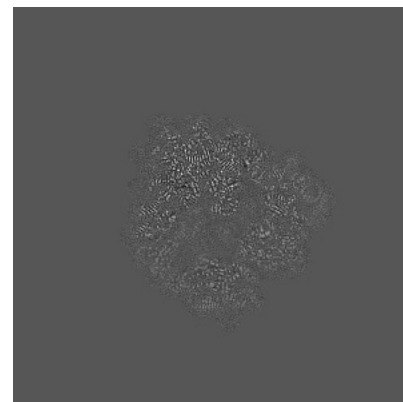
6.3.1 Primary map



X Index: 297

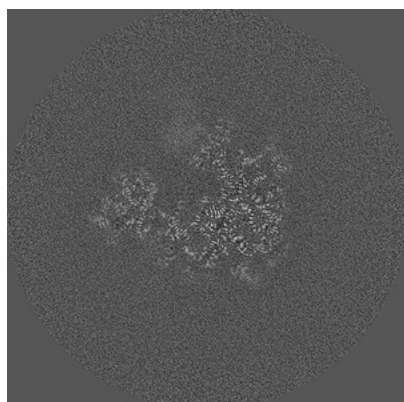


Y Index: 323

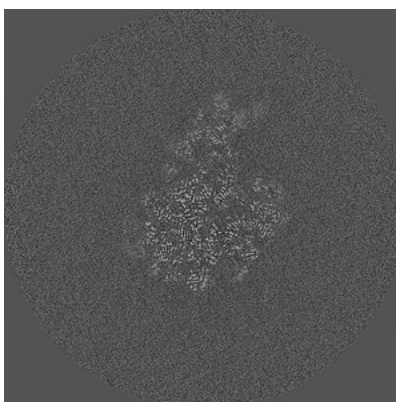


Z Index: 317

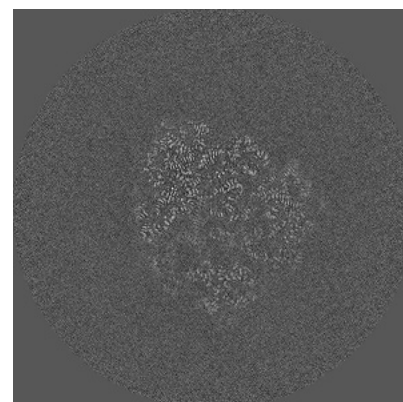
6.3.2 Raw map



X Index: 297



Y Index: 313

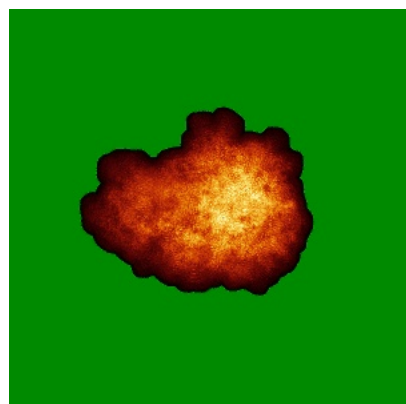


Z Index: 311

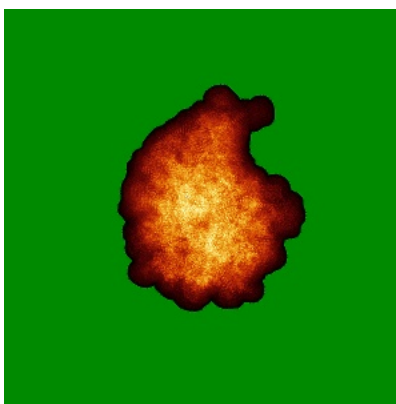
The images above show the largest variance slices of the map in three orthogonal directions.

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

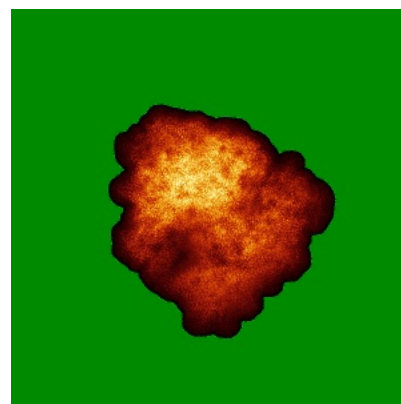
6.4.1 Primary map



X

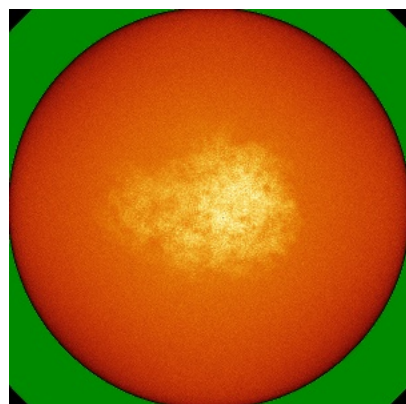


Y

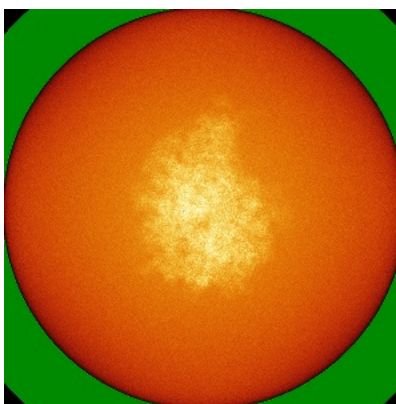


Z

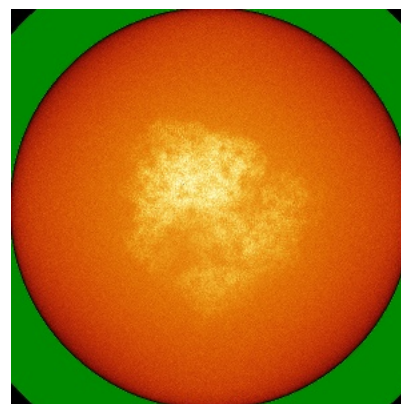
6.4.2 Raw map



X



Y

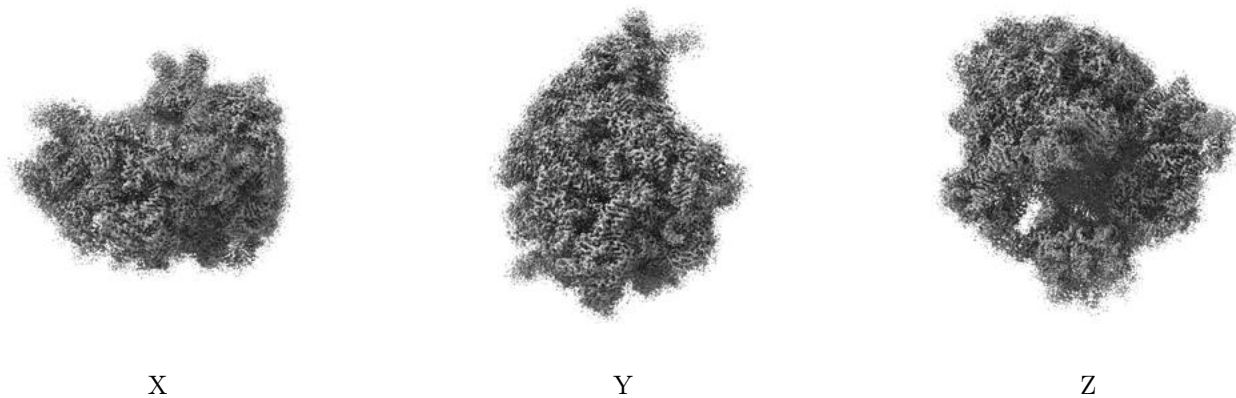


Z

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

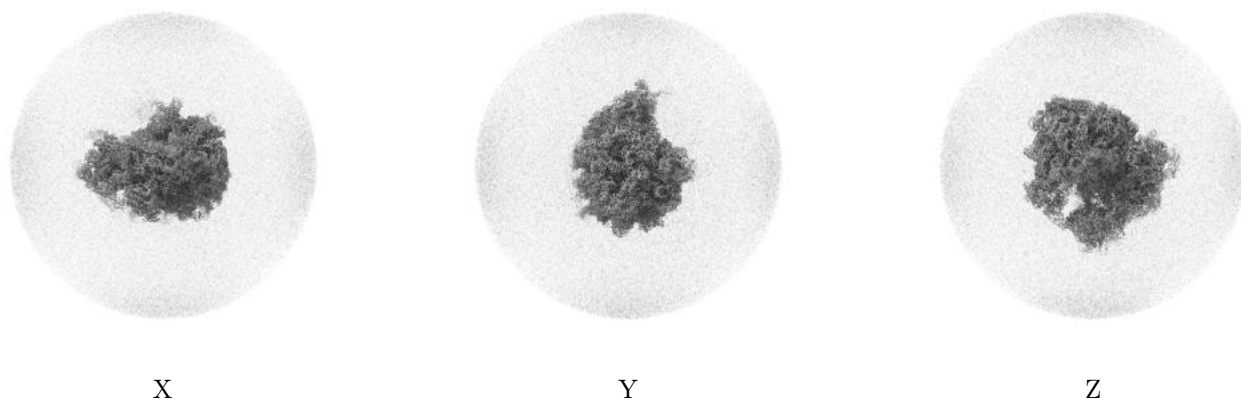
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

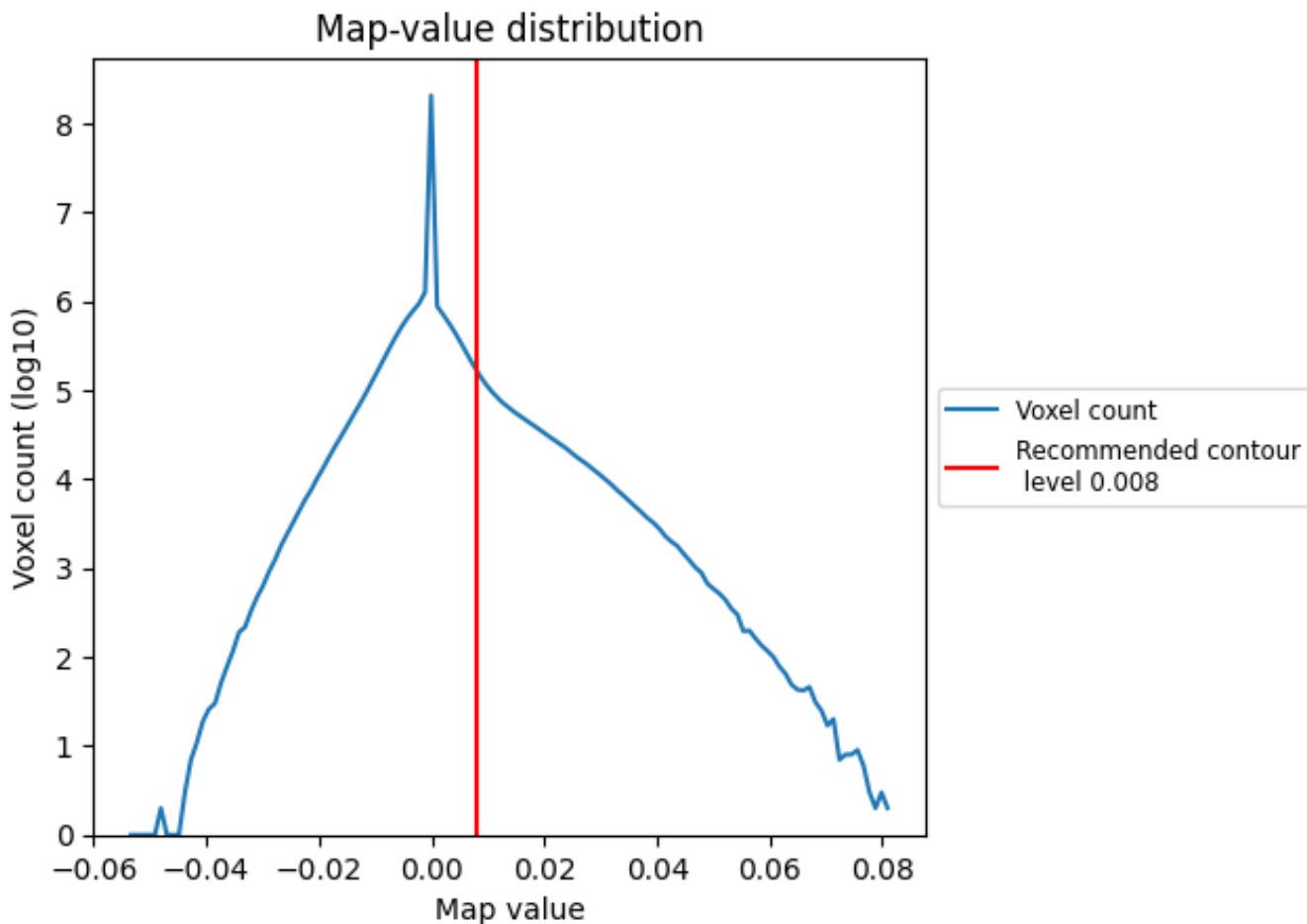
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

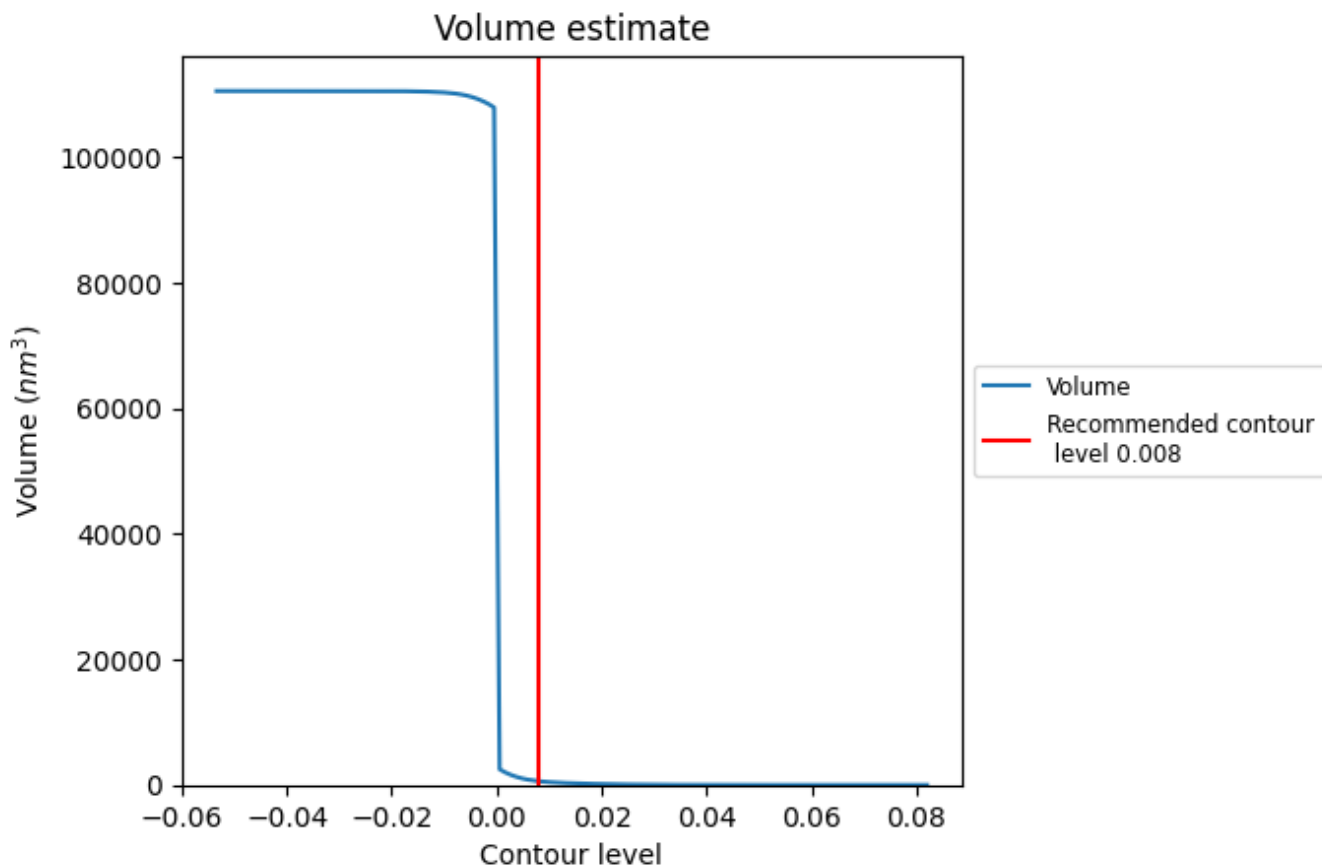
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

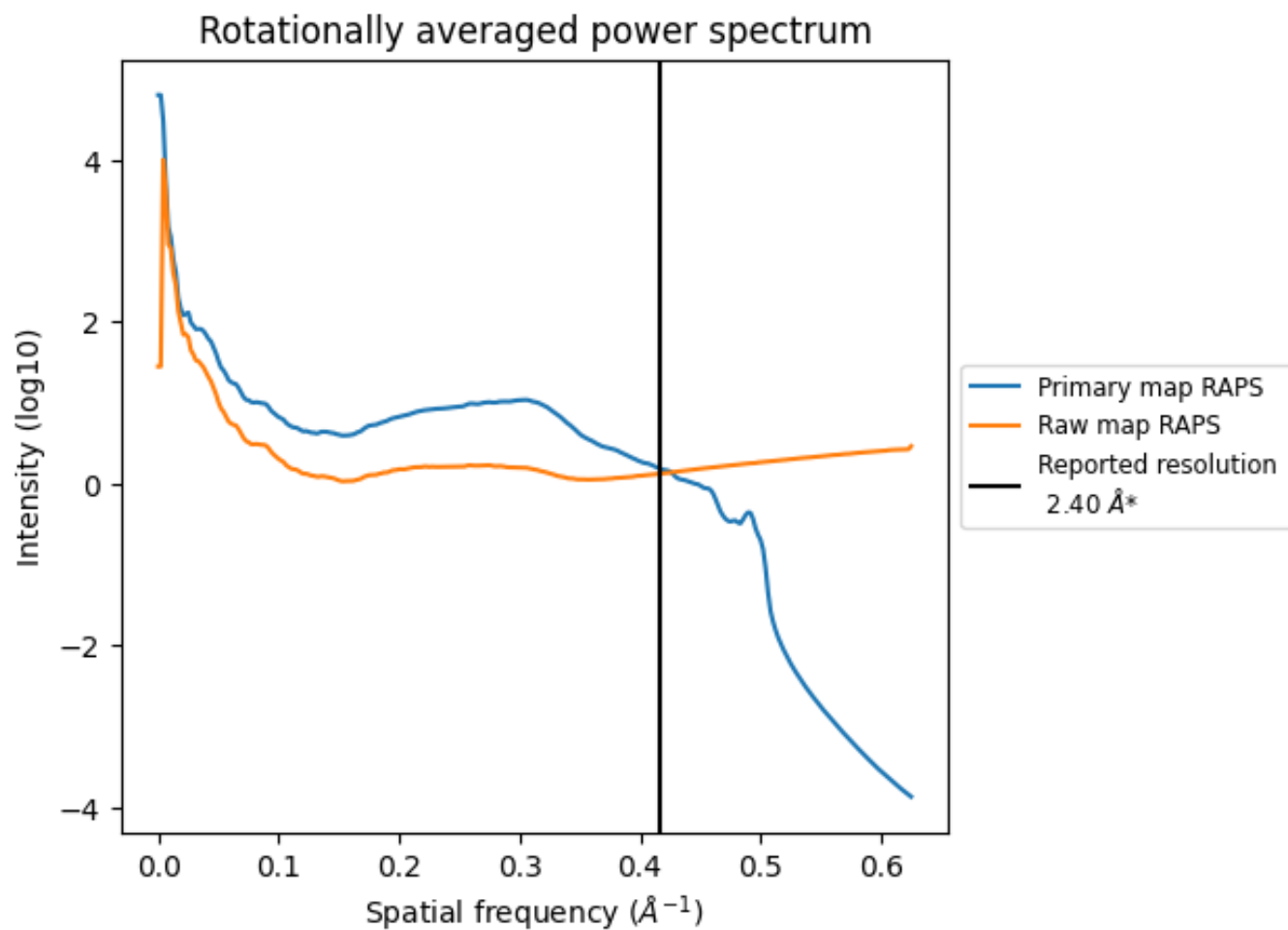
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 596 nm^3 ; this corresponds to an approximate mass of 539 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

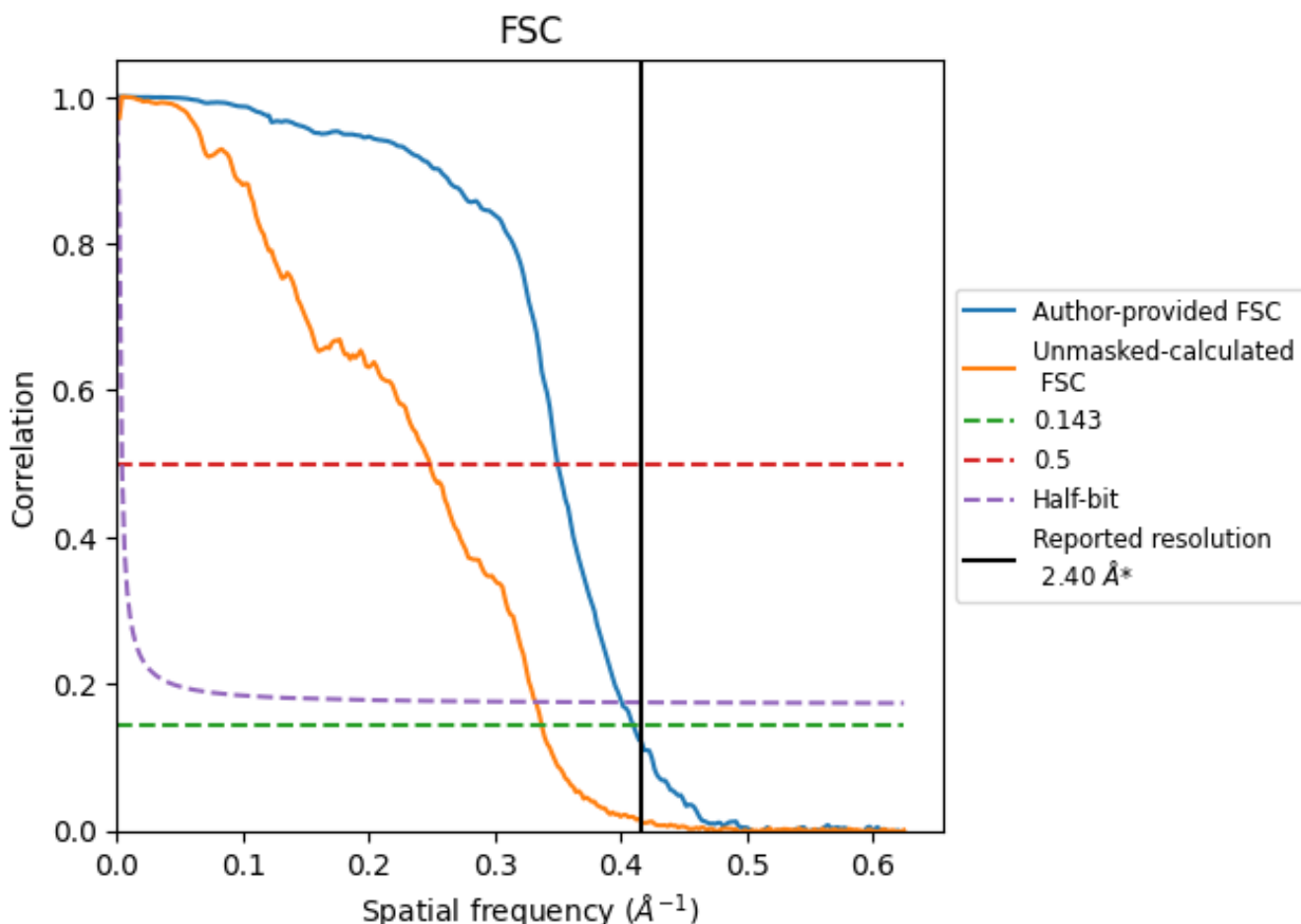


*Reported resolution corresponds to spatial frequency of 0.417 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8.2 Resolution estimates [i](#)

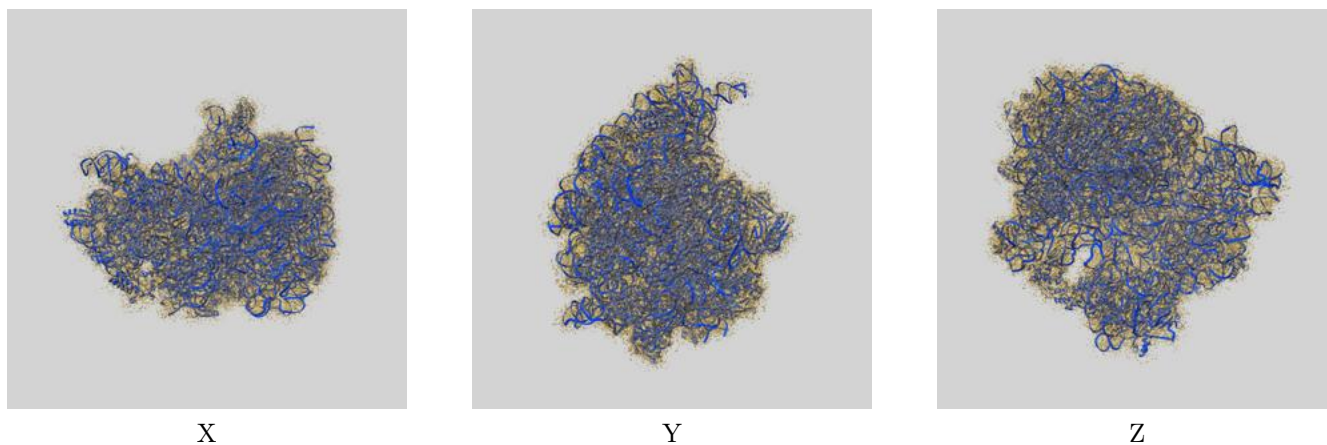
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.44	2.86	2.49
Unmasked-calculated*	2.96	4.02	3.01

*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 2.96 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

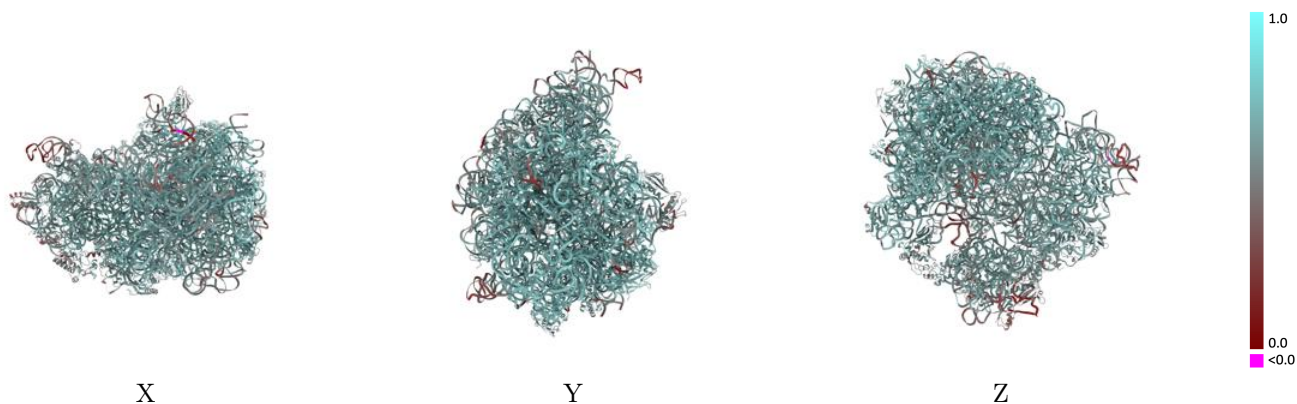
This section contains information regarding the fit between EMDB map EMD-50296 and PDB model 9FBV. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



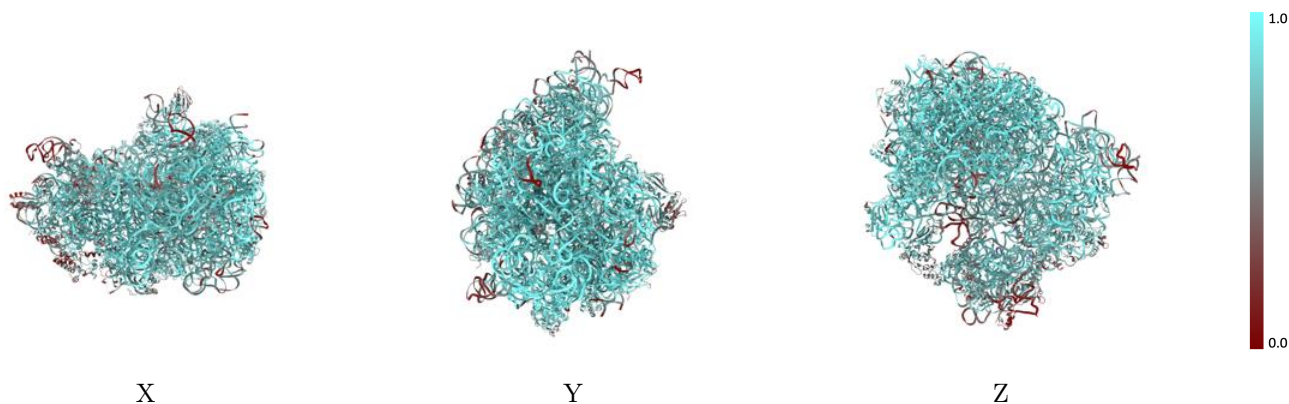
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



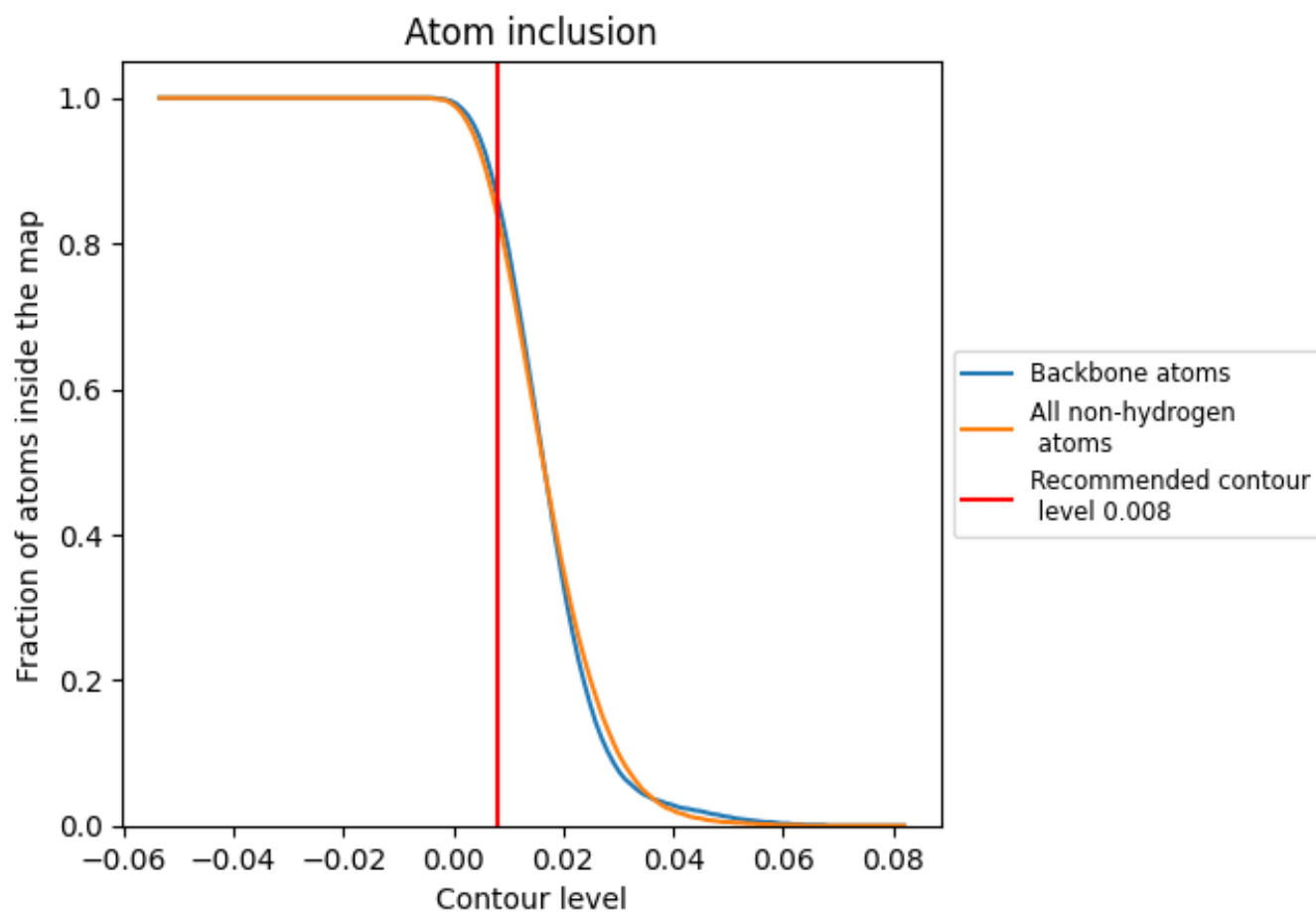
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8390	 0.6430
0	 0.8190	 0.6550
1	 0.9490	 0.7240
2	 0.9610	 0.7230
3	 0.8870	 0.6680
4	 0.4450	 0.4930
A	 0.8360	 0.6230
B	 0.4850	 0.5140
C	 0.7040	 0.5980
D	 0.6400	 0.5870
E	 0.8270	 0.6530
F	 0.6170	 0.5710
G	 0.5470	 0.5390
H	 0.8250	 0.6450
I	 0.6580	 0.5760
J	 0.5390	 0.5270
K	 0.7470	 0.6190
L	 0.7710	 0.6310
M	 0.6720	 0.5830
N	 0.7380	 0.6020
O	 0.7700	 0.6400
P	 0.7750	 0.6300
Q	 0.6700	 0.5910
R	 0.7190	 0.6030
S	 0.5910	 0.5510
T	 0.7560	 0.6100
U	 0.4940	 0.5050
X	 0.9230	 0.6770
Z	 0.5250	 0.5160
a	 0.9060	 0.6680
b	 0.8640	 0.6340
c	 0.9200	 0.7040
d	 0.9010	 0.6980
e	 0.8240	 0.6620
f	 0.6210	 0.5650



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Chain	Atom inclusion	Q-score
g	0.5730	0.5450
h	0.6470	0.5760
i	0.9110	0.6970
j	0.8740	0.6870
k	0.8980	0.6860
l	0.8790	0.6810
m	0.9500	0.7170
n	0.8240	0.6400
o	0.8720	0.6850
p	0.9570	0.7230
q	0.8410	0.6710
r	0.8910	0.6920
s	0.8140	0.6520
t	0.7600	0.6200
u	0.7600	0.6320
v	0.8400	0.6800
w	0.8520	0.6740
x	0.7180	0.6130
y	0.8670	0.6800
z	0.8650	0.6770