



Full wwPDB EM Validation Report ⓘ

Feb 27, 2024 – 03:07 PM EST

PDB ID : 8UU9
EMDB ID : EMD-42576
Title : Cryo-EM structure of the ratcheted *Listeria innocua* 70S ribosome (head-swiveled) in complex with HflXr and pe/E-tRNA (structure II-D)
Authors : Seely, S.M.; Basu, R.S.; Gagnon, M.G.
Deposited on : 2023-10-31
Resolution : 3.10 Å (reported)
Based on initial model : 7NHN

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:

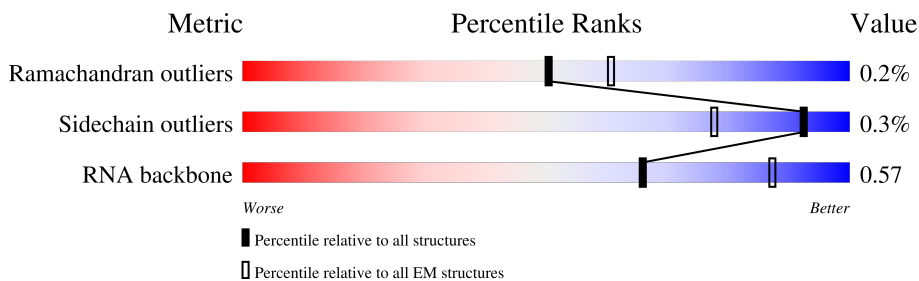
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	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	a	1550	
2	b	249	
3	c	218	
4	d	200	
5	e	167	
6	f	97	
7	g	156	
8	h	132	

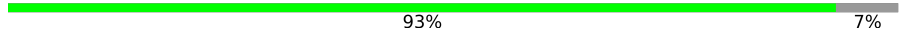

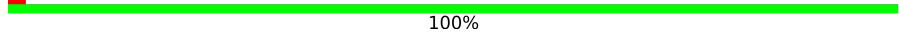
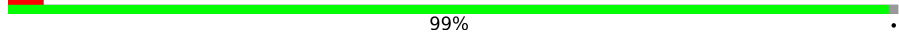
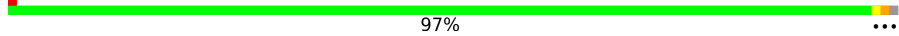
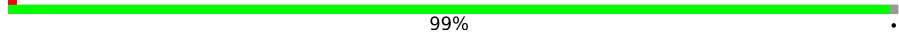
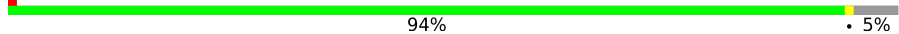
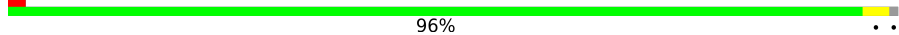
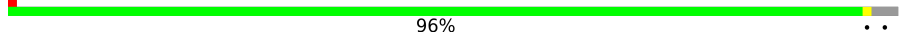

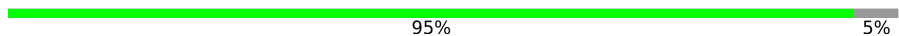
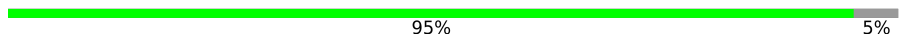
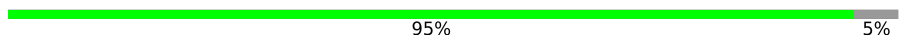


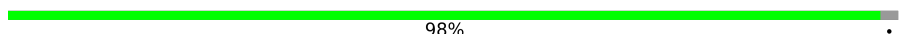
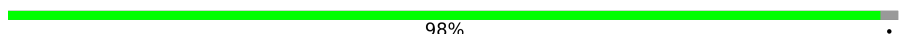
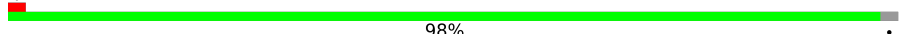
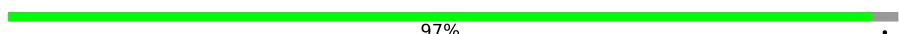
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Mol	Chain	Length	Quality of chain
9	i	130	17% 94% 5%
10	j	102	10% 93% 6%
11	k	129	12% 88% 12%
12	l	137	99%
13	m	121	54% 94% 6%
14	n	61	98%
15	o	89	98%
16	p	90	98%
17	q	87	93% 7%
18	r	79	81% 18%
19	s	92	55% 76% 20%
20	t	84	13% 95% 5%
21	x	76	63% 68% 26% 5%
22	w	21	24% 14% 24% 62%
23	v	418	5% 99%
24	A	2932	6% 82% 17%
25	B	116	89% 9%
26	C	277	99%
27	D	209	99%
28	E	207	99%
29	F	179	22% 97%
30	G	178	99%
31	L	145	97%
32	M	122	100%
33	N	146	100%

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Mol	Chain	Length	Quality of chain
34	O	144	 93% 7%
35	P	135	 90% 9%
36	Q	119	 100%
37	R	114	 99%
38	S	119	 97% ...
39	T	102	 99%
40	U	118	 94% 5%
41	V	94	 96% ..
42	W	103	 96% ..
43	Y	96	 79% 21%
44	Z	62	 95% 5%
45	1	63	 95% 5%
46	2	59	 95% 5%
47	3	81	 43% 86% 14%
48	4	57	 93% 7%
49	5	49	 98%
50	6	44	 98%
51	7	66	 98%
52	8	37	 97%

2 Entry composition i

There are 56 unique types of molecules in this entry. The entry contains 142177 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 Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1515	32493	14494	5955	10529	1515	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	1588	1011	279	292	6	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	204	1150	705	223	221	1	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	199	1537	961	286	288	2	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	155	1116	701	203	210	2	0	0

- Molecule 6 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	93	655	423	119	111	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	g	147	866	533	173	158	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	h	131	1022	651	180	189	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	i	123	833	520	163	149	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	j	96	608	376	116	115	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	k	114	824	508	158	155	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	l	135	1002	621	198	181	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	m	114	616	367	134	114	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	60	Total	C	N	O	S	0	0
			445	283	84	73	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	87	Total	C	N	O	S	0	0
			696	433	136	125	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	88	Total	C	N	O	S	0	0
			711	450	132	126	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	81	Total	C	N	O	S	0	0
			629	396	120	112	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	65	Total	C	N	O	S	0	0
			527	339	96	90	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
19	s	74	Total	C	N	O	0	0
			459	279	96	84		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	80	Total	C	N	O	S	0	0
			607	366	124	116	1		

- Molecule 21 is a RNA chain called pe/E Hybrid State Phenylalanine tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
21	x	74	Total	C	N	O	P	S	0	0
			1591	713	285	517	74	2		

- Molecule 22 is a RNA chain called F-Stop mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	w	8	Total	C	N	O	P	0	0
			168	76	29	55	8		

- Molecule 23 is a protein called GTPase HflX.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	v	416	Total	C	N	O	S	0	0
			3200	2015	558	619	8		

- Molecule 24 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	A	2899	Total	C	N	O	P	0	0
			62278	27794	11524	20061	2899		

- Molecule 25 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B	114	Total	C	N	O	P	0	0
			2428	1082	428	804	114		

- Molecule 26 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	C	273	Total	C	N	O	S	0	0
			2108	1307	415	379	7		

- Molecule 27 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	D	206	Total	C	N	O	S	0	0
			1545	974	287	280	4		

- Molecule 28 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	E	204	1564	989	288	287	0	0

- Molecule 29 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	F	175	1232	785	211	231	5	0	0

- Molecule 30 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	G	176	1318	830	244	243	1	0	0

- Molecule 31 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	L	143	1128	715	205	205	3	0	0

- Molecule 32 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	M	122	925	573	175	172	5	0	0

- Molecule 33 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	N	146	1112	687	216	208	1	0	0

- Molecule 34 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	O	134	1057	677	203	171	6	0	0

- Molecule 35 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	P	123	986	618	194	173	1	0	0

- Molecule 36 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	Q	119	867	530	172	164	1	0	0

- Molecule 37 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	R	113	879	557	168	153	1	0	0

- Molecule 38 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	S	118	953	605	188	156	4	0	0

- Molecule 39 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	T	101	785	506	134	144	1	0	0

- Molecule 40 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
40	U	112	864	544	162	158	0	0

- Molecule 41 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	V	93	760	482	132	143	3	0	0

- Molecule 42 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	W	100	Total	C	N	O	S	0	0
			734	465	137	129	3		

- Molecule 43 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Y	76	Total	C	N	O	S	0	0
			585	357	114	113	1		

- Molecule 44 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Z	59	Total	C	N	O	S	0	0
			462	286	97	77	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1	60	Total	C	N	O	S	0	0
			495	304	95	95	1		

- Molecule 46 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	2	56	Total	C	N	O	S	0	0
			433	272	82	78	1		

- Molecule 47 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	3	70	Total	C	N	O	0	0
			424	263	78	83		

- Molecule 48 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	4	53	Total	C	N	O	S	0	0
			425	259	87	74	5		

- Molecule 49 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	5	48	Total	C	N	O	S	0	0
			394	241	79	70	4		

- Molecule 50 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	6	43	Total	C	N	O	S	0	0
			365	222	88	53	2		

- Molecule 51 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	7	65	Total	C	N	O	S	0	0
			529	328	116	80	5		

- Molecule 52 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	8	36	Total	C	N	O	S	0	0
			292	183	59	44	6		

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	a	202	Total	Mg	0
			202	202	
53	c	1	Total	Mg	0
			1	1	
53	e	1	Total	Mg	0
			1	1	
53	i	1	Total	Mg	0
			1	1	
53	l	1	Total	Mg	0
			1	1	
53	m	1	Total	Mg	0
			1	1	
53	q	1	Total	Mg	0
			1	1	
53	v	3	Total	Mg	0
			3	3	
53	A	256	Total	Mg	0
			256	256	

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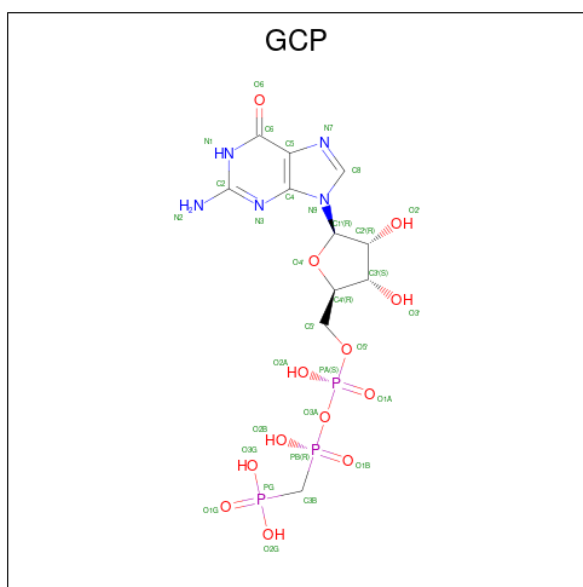
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Mol	Chain	Residues	Atoms		AltConf
53	B	4	Total	Mg	0
			4	4	
53	C	2	Total	Mg	0
			2	2	
53	V	1	Total	Mg	0
			1	1	
53	Y	1	Total	Mg	0
			1	1	

- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	n	1	Total	Zn	0
			1	1	
54	4	1	Total	Zn	0
			1	1	
54	5	1	Total	Zn	0
			1	1	
54	8	1	Total	Zn	0
			1	1	

- Molecule 55 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



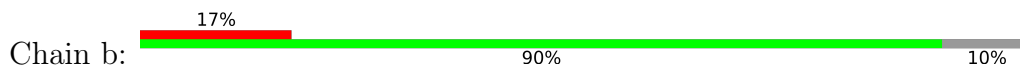
Mol	Chain	Residues	Atoms					AltConf
55	v	1	Total	C	N	O	P	0
			32	11	5	13	3	

- Molecule 56 is water.

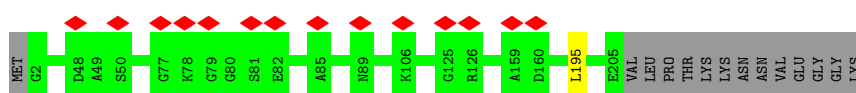
Mol	Chain	Residues	Atoms		AltConf
56	a	105	Total 105	O 105	0
56	c	1	Total 1	O 1	0
56	d	2	Total 2	O 2	0
56	e	1	Total 1	O 1	0
56	m	2	Total 2	O 2	0
56	n	2	Total 2	O 2	0
56	p	1	Total 1	O 1	0
56	v	2	Total 2	O 2	0
56	A	255	Total 255	O 255	0
56	B	5	Total 5	O 5	0
56	C	1	Total 1	O 1	0
56	N	4	Total 4	O 4	0
56	O	2	Total 2	O 2	0
56	P	1	Total 1	O 1	0
56	S	3	Total 3	O 3	0
56	T	1	Total 1	O 1	0
56	U	1	Total 1	O 1	0
56	V	3	Total 3	O 3	0
56	Y	1	Total 1	O 1	0
56	Z	2	Total 2	O 2	0
56	2	1	Total 1	O 1	0



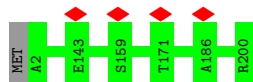
- Molecule 2: Small ribosomal subunit protein uS2



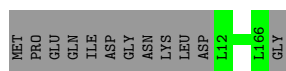
- Molecule 3: Small ribosomal subunit protein uS3



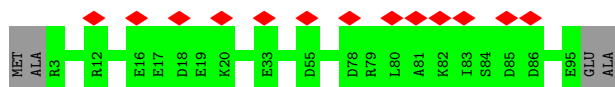
- Molecule 4: Small ribosomal subunit protein uS4



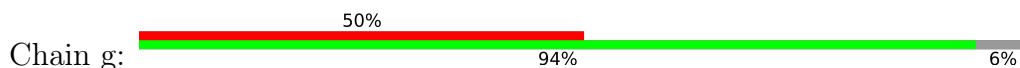
- Molecule 5: Small ribosomal subunit protein uS5

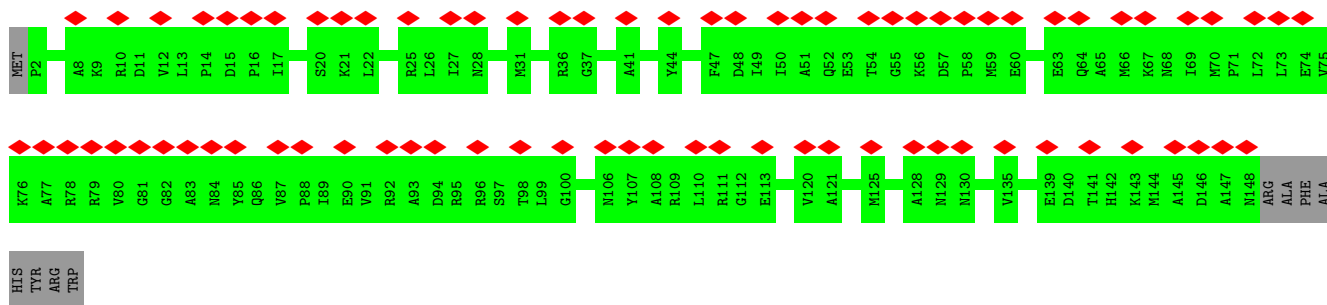


- Molecule 6: Small ribosomal subunit protein bS6



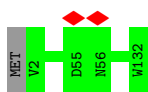
- Molecule 7: Small ribosomal subunit protein uS7





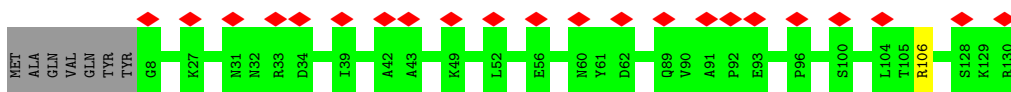
- Molecule 8: Small ribosomal subunit protein uS8

Chain h: 99%



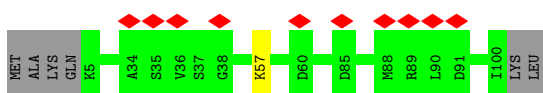
- Molecule 9: Small ribosomal subunit protein uS9

Chain i: 17% 94% 5%



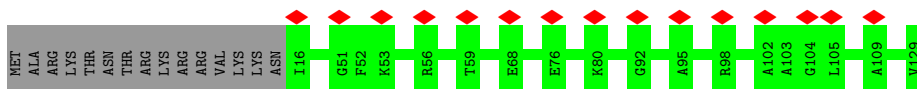
- Molecule 10: Small ribosomal subunit protein uS10

Chain j: 10% 93% 6%



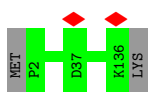
- Molecule 11: Small ribosomal subunit protein uS11

Chain k: 12% 88% 12%

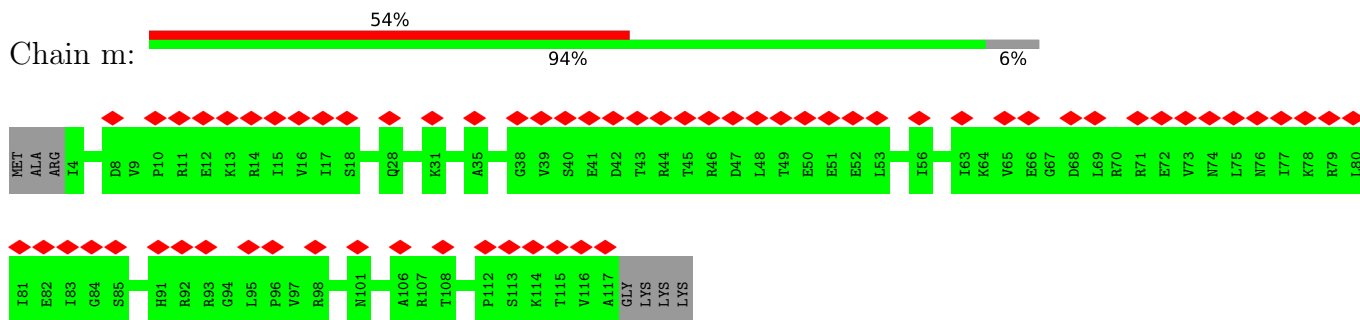


- Molecule 12: Small ribosomal subunit protein uS12

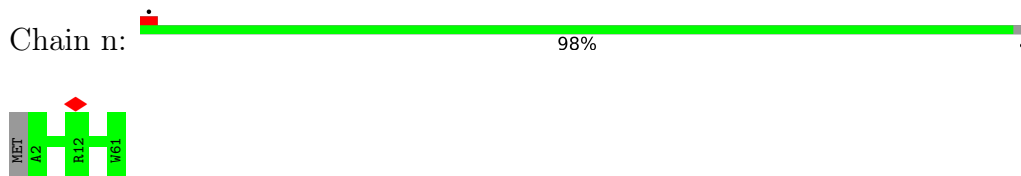
Chain l: 99%



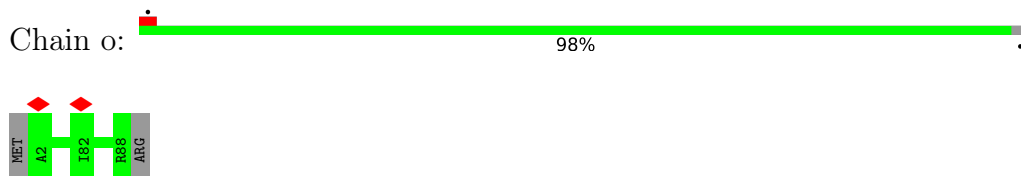
- Molecule 13: Small ribosomal subunit protein uS13



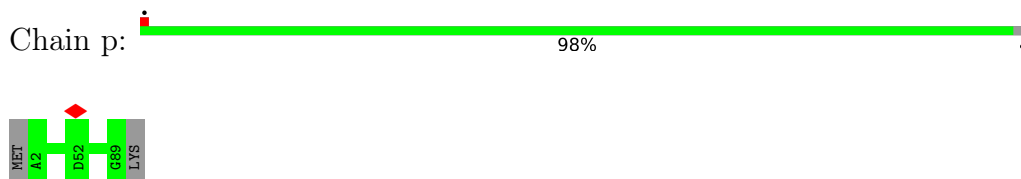
- Molecule 14: Small ribosomal subunit protein uS14



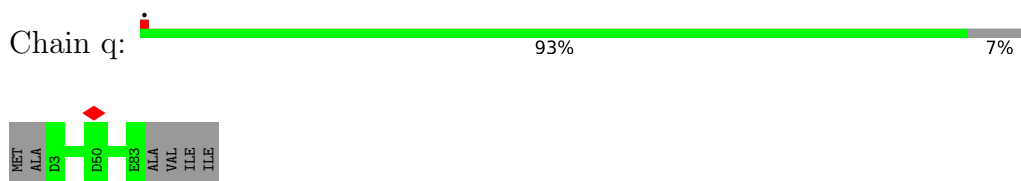
- Molecule 15: Small ribosomal subunit protein uS15



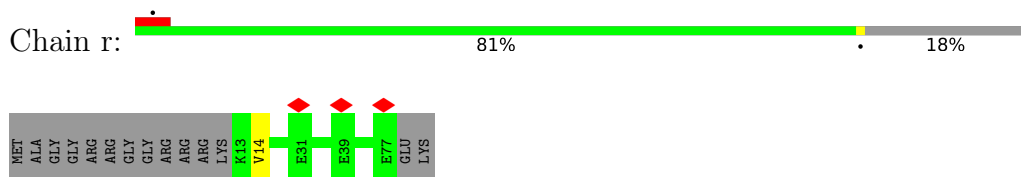
- Molecule 16: Small ribosomal subunit protein bS16



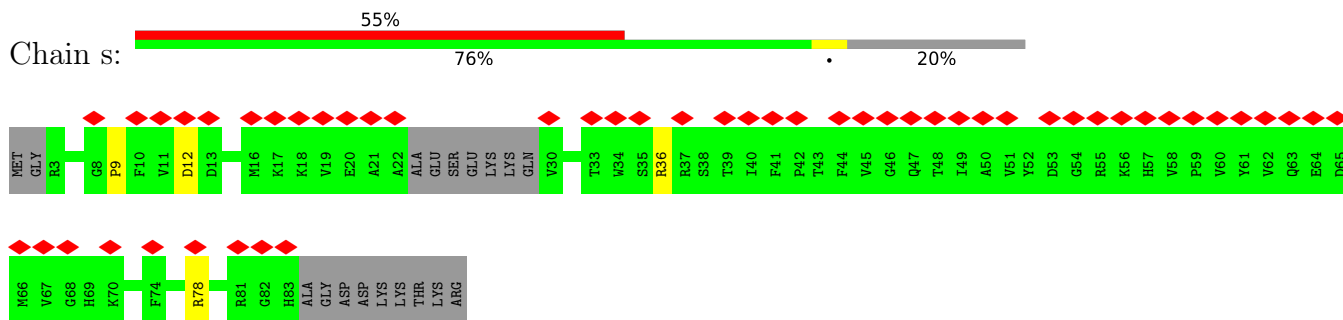
- Molecule 17: Small ribosomal subunit protein uS17



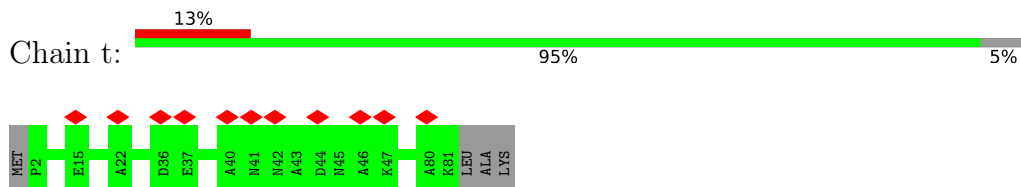
- Molecule 18: Small ribosomal subunit protein bS18



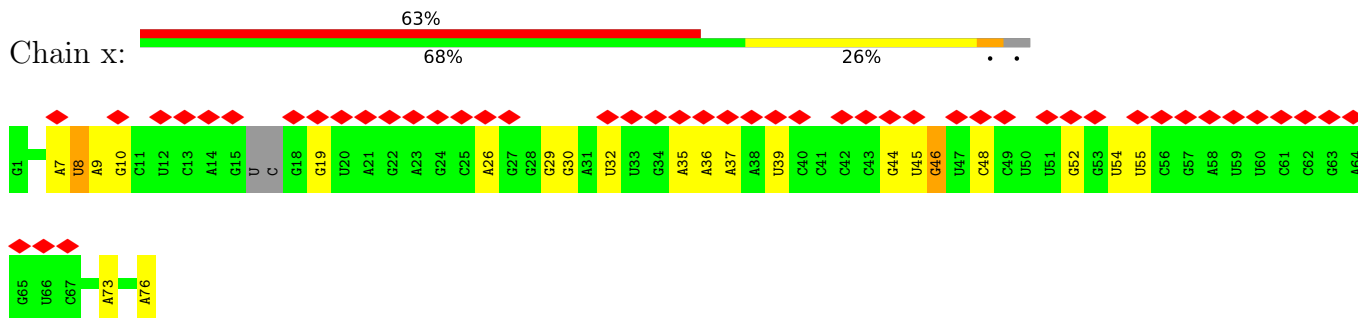
- Molecule 19: Small ribosomal subunit protein uS19



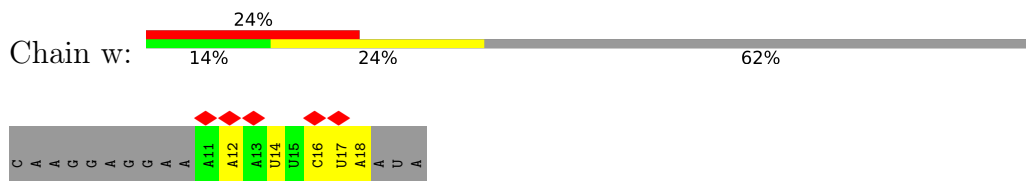
- Molecule 20: Small ribosomal subunit protein bS20



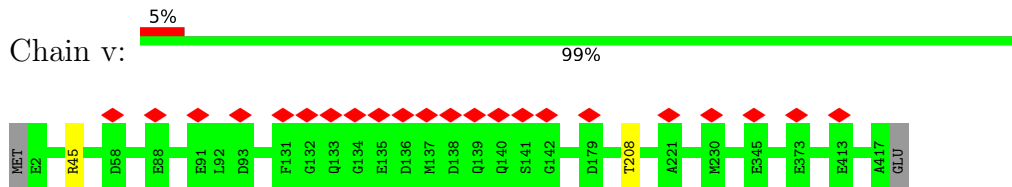
- Molecule 21: pe/E Hybrid State Phenylalanine tRNA



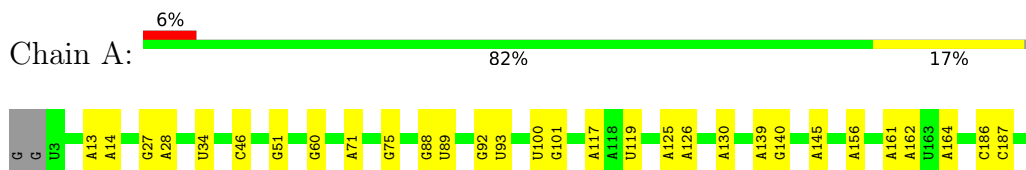
- Molecule 22: F-Stop mRNA

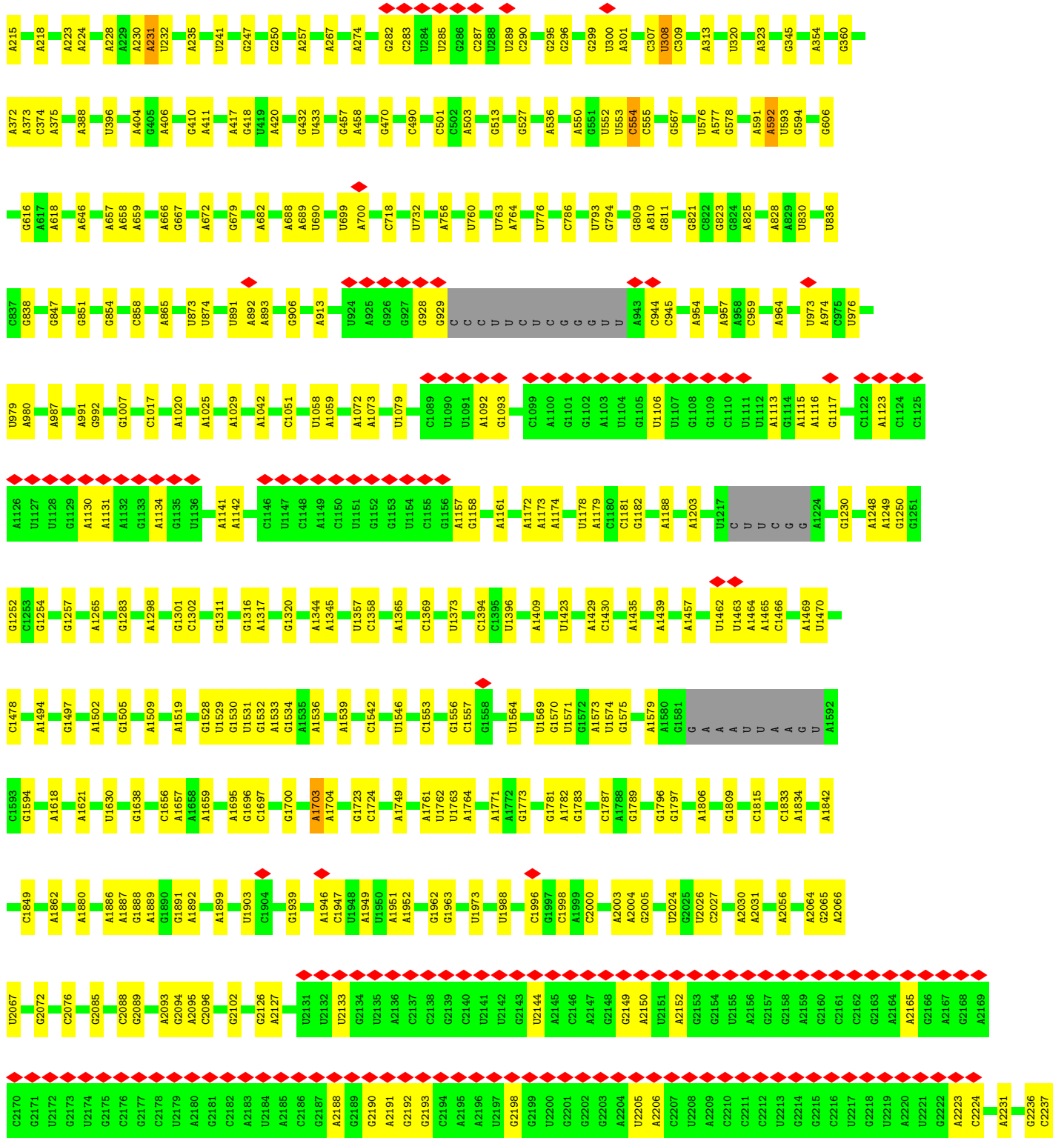


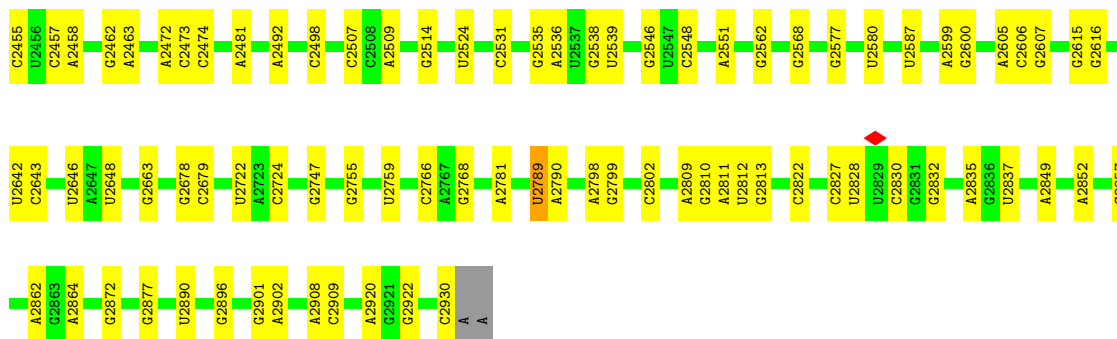
- Molecule 23: GTPase HflX



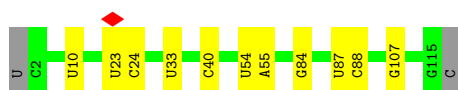
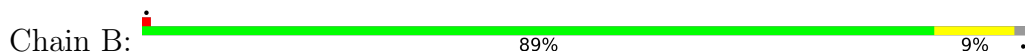
- Molecule 24: 23S Ribosomal RNA



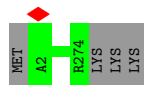




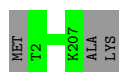
• Molecule 25: 5S Ribosomal RNA



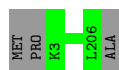
• Molecule 26: Large ribosomal subunit protein uL2



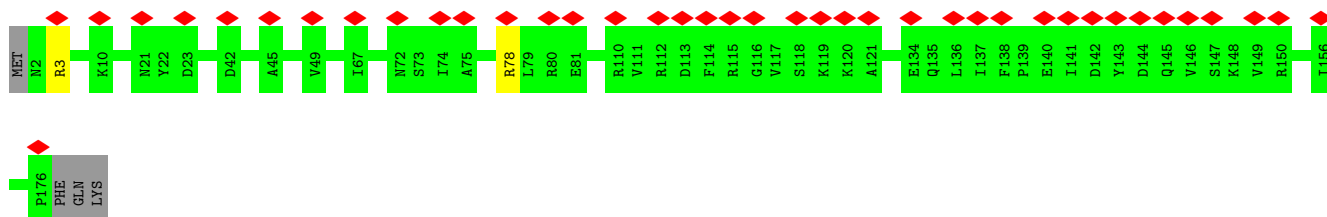
• Molecule 27: Large ribosomal subunit protein uL3



• Molecule 28: Large ribosomal subunit protein uL4

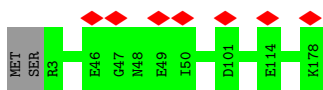


• Molecule 29: Large ribosomal subunit protein uL5



- Molecule 30: Large ribosomal subunit protein uL6

Chain G:  99%



- Molecule 31: Large ribosomal subunit protein uL13

Chain L:  97%



- Molecule 32: Large ribosomal subunit protein uL14

Chain M:  100%

There are no outlier residues recorded for this chain.

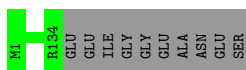
- Molecule 33: Large ribosomal subunit protein uL15

Chain N:  100%




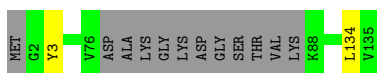
- Molecule 34: Large ribosomal subunit protein uL16

Chain O:  93% 7%



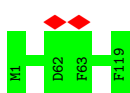
- Molecule 35: Large ribosomal subunit protein bL17

Chain P:  90% 9%



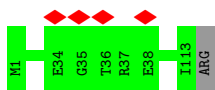
- Molecule 36: Large ribosomal subunit protein uL18

Chain Q:  100%



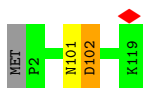
- Molecule 37: Large ribosomal subunit protein bL19

Chain R:  99%



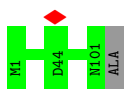
- Molecule 38: Large ribosomal subunit protein bL20

Chain S:  97%



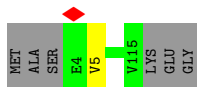
- Molecule 39: Large ribosomal subunit protein bL21

Chain T:  99%



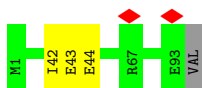
- Molecule 40: Large ribosomal subunit protein uL22

Chain U:  94%



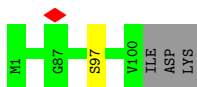
- Molecule 41: Large ribosomal subunit protein uL23

Chain V:  96%




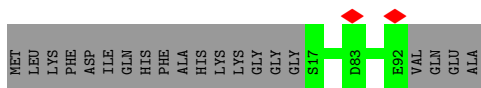
- Molecule 42: Large ribosomal subunit protein uL24

Chain W:  96%



- Molecule 43: Large ribosomal subunit protein bL27

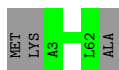
Chain Y:  79%



- Molecule 44: Large ribosomal subunit protein bL28



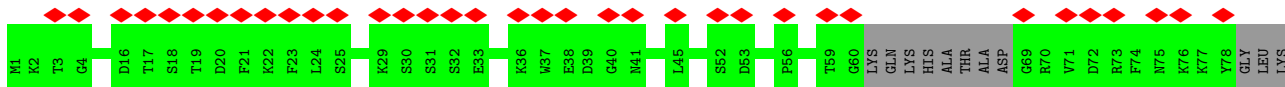
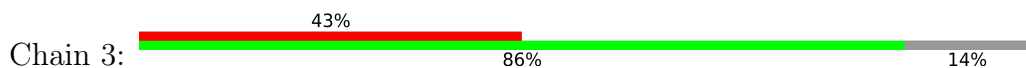
- Molecule 45: Large ribosomal subunit protein uL29



- Molecule 46: Large ribosomal subunit protein uL30



- Molecule 47: Large ribosomal subunit protein bL31B



- Molecule 48: Large ribosomal subunit protein bL32



- Molecule 49: Large ribosomal subunit protein bL33



- Molecule 50: Large ribosomal subunit protein bL34



- Molecule 51: Large ribosomal subunit protein bL35

Chain 7:  98%



- Molecule 52: Large ribosomal subunit protein bL36

Chain 8:  97%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	80381	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	31.784	Depositor
Minimum map value	-18.322	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	1.115	Depositor
Recommended contour level	3.4	Depositor
Map size (\AA)	435.2, 435.2, 435.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.85, 0.85, 0.85	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: MIA, GCP, ZN, PSU, 7MG, 4SU, MG, 5MU

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	0.58	0/36378	0.87	25/56739 (0.0%)
2	b	0.28	0/1612	0.46	0/2195
3	c	0.31	0/1160	0.55	1/1601 (0.1%)
4	d	0.33	0/1564	0.53	0/2109
5	e	0.33	0/1129	0.57	0/1530
6	f	0.29	0/666	0.52	0/909
7	g	0.28	0/871	0.55	0/1190
8	h	0.38	0/1035	0.56	0/1392
9	i	0.35	0/845	0.58	0/1146
10	j	0.37	0/617	0.55	0/845
11	k	0.28	0/838	0.53	0/1132
12	l	0.37	0/1017	0.61	0/1375
13	m	0.25	0/617	0.49	0/843
14	n	0.40	0/453	0.56	0/608
15	o	0.29	0/706	0.59	0/952
16	p	0.37	0/724	0.56	0/970
17	q	0.31	0/638	0.53	0/860
18	r	0.31	0/535	0.55	0/716
19	s	0.31	0/466	0.62	0/636
20	t	0.28	0/610	0.52	0/813
21	x	0.28	0/1605	0.82	0/2497
22	w	0.38	0/187	1.10	0/288
23	v	0.31	0/3240	0.52	0/4380
24	A	0.51	0/69775	0.80	10/108849 (0.0%)
25	B	0.31	0/2711	0.76	0/4224
26	C	0.32	0/2144	0.56	0/2875
27	D	0.34	0/1567	0.55	0/2111
28	E	0.31	0/1584	0.53	0/2134
29	F	0.28	0/1249	0.55	0/1704
30	G	0.28	0/1339	0.51	0/1811
31	L	0.33	0/1151	0.54	1/1546 (0.1%)
32	M	0.32	0/932	0.56	0/1248

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	N	0.30	0/1123	0.55	0/1492
34	O	0.32	0/1079	0.54	0/1442
35	P	0.32	0/997	0.60	1/1333 (0.1%)
36	Q	0.27	0/874	0.55	0/1175
37	R	0.31	0/891	0.55	0/1199
38	S	0.36	0/966	0.53	0/1284
39	T	0.35	0/798	0.49	0/1071
40	U	0.32	0/874	0.55	0/1182
41	V	0.35	0/769	0.56	0/1029
42	W	0.30	0/744	0.49	0/998
43	Y	0.35	0/592	0.60	0/788
44	Z	0.29	0/467	0.58	0/619
45	1	0.27	0/496	0.55	0/662
46	2	0.28	0/436	0.56	0/585
47	3	0.24	0/431	0.48	0/591
48	4	0.34	0/433	0.59	0/577
49	5	0.30	0/398	0.58	0/534
50	6	0.32	0/368	0.64	0/479
51	7	0.31	0/536	0.64	0/696
52	8	0.32	0/295	0.56	0/387
All	All	0.48	0/153532	0.76	38/230351 (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
19	s	0	1
31	L	0	1
All	All	0	2

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	308	U	C2-N1-C1'	6.86	125.93	117.70
1	a	970	U	C2-N3-C4	-6.73	122.96	127.00
24	A	1357	U	C2-N1-C1'	6.68	125.72	117.70
1	a	519	C	C2-N1-C1'	-6.61	111.53	118.80
1	a	1075	C	C2-N1-C1'	6.52	125.98	118.80
1	a	762	C	C2-N1-C1'	6.38	125.82	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	969	U	C2-N1-C1'	6.32	125.28	117.70
24	A	1703	A	O4'-C1'-N9	6.25	113.20	108.20
3	c	195	LEU	CA-CB-CG	6.08	129.27	115.30
1	a	1166	C	C2-N1-C1'	6.02	125.42	118.80
1	a	1366	C	C5-C6-N1	6.01	124.01	121.00
1	a	1366	C	C6-N1-C2	-5.98	117.91	120.30
1	a	970	U	N1-C2-N3	5.86	118.42	114.90
1	a	969	U	N1-C2-O2	5.73	126.81	122.80
24	A	554	C	C2-N1-C1'	5.65	125.01	118.80
24	A	231	A	O4'-C1'-N9	5.61	112.69	108.20
1	a	336	C	N1-C2-O2	5.52	122.21	118.90
1	a	993	C	C6-N1-C2	-5.50	118.10	120.30
1	a	67	C	C6-N1-C2	-5.46	118.12	120.30
1	a	1136	G	C4-N9-C1'	5.45	133.58	126.50
1	a	1208	A	P-O3'-C3'	5.44	126.23	119.70
24	A	2539	U	C2-N1-C1'	5.42	124.20	117.70
24	A	1358	C	C2-N1-C1'	5.39	124.73	118.80
1	a	336	C	C2-N1-C1'	5.33	124.67	118.80
1	a	1002	G	N3-C4-N9	5.28	129.17	126.00
24	A	2789	U	P-O3'-C3'	5.26	126.01	119.70
1	a	1136	G	C8-N9-C1'	-5.25	120.17	127.00
1	a	477	U	N3-C2-O2	-5.20	118.56	122.20
31	L	136	GLN	C-N-CA	5.19	134.67	121.70
35	P	134	LEU	CA-CB-CG	5.17	127.19	115.30
1	a	756	A	P-O3'-C3'	5.15	125.88	119.70
1	a	519	C	C6-N1-C1'	5.13	126.96	120.80
1	a	476	C	C2-N1-C1'	5.13	124.44	118.80
24	A	592	A	N1-C6-N6	-5.10	115.54	118.60
1	a	1110	A	P-O3'-C3'	5.07	125.78	119.70
1	a	1166	C	N1-C2-O2	5.07	121.94	118.90
1	a	1210	C	C5-C6-N1	5.07	123.53	121.00
24	A	308	U	C6-N1-C1'	-5.02	114.17	121.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	L	137	LYS	Peptide
19	s	36	ARG	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	222/249 (89%)	207 (93%)	15 (7%)	0	100	100
3	c	202/218 (93%)	171 (85%)	31 (15%)	0	100	100
4	d	197/200 (98%)	180 (91%)	17 (9%)	0	100	100
5	e	153/167 (92%)	142 (93%)	11 (7%)	0	100	100
6	f	91/97 (94%)	84 (92%)	7 (8%)	0	100	100
7	g	145/156 (93%)	122 (84%)	23 (16%)	0	100	100
8	h	129/132 (98%)	124 (96%)	5 (4%)	0	100	100
9	i	121/130 (93%)	111 (92%)	10 (8%)	0	100	100
10	j	94/102 (92%)	83 (88%)	10 (11%)	1 (1%)	14	46
11	k	112/129 (87%)	102 (91%)	10 (9%)	0	100	100
12	l	133/137 (97%)	126 (95%)	7 (5%)	0	100	100
13	m	112/121 (93%)	100 (89%)	12 (11%)	0	100	100
14	n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
15	o	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
16	p	86/90 (96%)	82 (95%)	4 (5%)	0	100	100
17	q	79/87 (91%)	74 (94%)	5 (6%)	0	100	100
18	r	63/79 (80%)	59 (94%)	3 (5%)	1 (2%)	9	37
19	s	70/92 (76%)	54 (77%)	14 (20%)	2 (3%)	4	24
20	t	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
23	v	414/418 (99%)	384 (93%)	30 (7%)	0	100	100
26	C	271/277 (98%)	258 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	D	204/209 (98%)	193 (95%)	11 (5%)	0	100	100
28	E	202/207 (98%)	189 (94%)	13 (6%)	0	100	100
29	F	173/179 (97%)	161 (93%)	12 (7%)	0	100	100
30	G	174/178 (98%)	163 (94%)	11 (6%)	0	100	100
31	L	141/145 (97%)	137 (97%)	3 (2%)	1 (1%)	22	57
32	M	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
33	N	144/146 (99%)	137 (95%)	7 (5%)	0	100	100
34	O	132/144 (92%)	128 (97%)	4 (3%)	0	100	100
35	P	119/135 (88%)	113 (95%)	5 (4%)	1 (1%)	19	54
36	Q	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
37	R	111/114 (97%)	106 (96%)	5 (4%)	0	100	100
38	S	116/119 (98%)	111 (96%)	4 (3%)	1 (1%)	17	52
39	T	99/102 (97%)	92 (93%)	7 (7%)	0	100	100
40	U	110/118 (93%)	105 (96%)	4 (4%)	1 (1%)	17	52
41	V	91/94 (97%)	84 (92%)	7 (8%)	0	100	100
42	W	98/103 (95%)	95 (97%)	2 (2%)	1 (1%)	15	49
43	Y	74/96 (77%)	67 (90%)	7 (10%)	0	100	100
44	Z	57/62 (92%)	52 (91%)	5 (9%)	0	100	100
45	1	58/63 (92%)	55 (95%)	3 (5%)	0	100	100
46	2	54/59 (92%)	51 (94%)	3 (6%)	0	100	100
47	3	66/81 (82%)	53 (80%)	13 (20%)	0	100	100
48	4	51/57 (90%)	48 (94%)	3 (6%)	0	100	100
49	5	46/49 (94%)	46 (100%)	0	0	100	100
50	6	41/44 (93%)	41 (100%)	0	0	100	100
51	7	63/66 (96%)	58 (92%)	5 (8%)	0	100	100
52	8	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
All	All	5610/5963 (94%)	5217 (93%)	384 (7%)	9 (0%)	50	79

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	s	9	PRO
31	L	137	LYS

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Mol	Chain	Res	Type
10	j	57	LYS
18	r	14	VAL
38	S	102	ASP
35	P	3	TYR
42	W	97	SER
19	s	12	ASP
40	U	5	VAL

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	138/214 (64%)	137 (99%)	1 (1%)	84	93
3	c	41/177 (23%)	41 (100%)	0	100	100
4	d	154/170 (91%)	154 (100%)	0	100	100
5	e	116/131 (88%)	116 (100%)	0	100	100
6	f	50/85 (59%)	50 (100%)	0	100	100
7	g	38/130 (29%)	38 (100%)	0	100	100
8	h	109/110 (99%)	109 (100%)	0	100	100
9	i	63/102 (62%)	62 (98%)	1 (2%)	62	84
10	j	35/93 (38%)	35 (100%)	0	100	100
11	k	83/100 (83%)	83 (100%)	0	100	100
12	l	105/118 (89%)	105 (100%)	0	100	100
13	m	13/102 (13%)	13 (100%)	0	100	100
14	n	41/52 (79%)	41 (100%)	0	100	100
15	o	72/81 (89%)	72 (100%)	0	100	100
16	p	78/80 (98%)	78 (100%)	0	100	100
17	q	65/78 (83%)	65 (100%)	0	100	100
18	r	58/67 (87%)	58 (100%)	0	100	100
19	s	21/78 (27%)	20 (95%)	1 (5%)	25	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	t	62/66 (94%)	62 (100%)	0	100	100
23	v	329/365 (90%)	327 (99%)	2 (1%)	86	94
26	C	221/225 (98%)	221 (100%)	0	100	100
27	D	159/171 (93%)	159 (100%)	0	100	100
28	E	170/174 (98%)	170 (100%)	0	100	100
29	F	114/155 (74%)	112 (98%)	2 (2%)	59	82
30	G	136/147 (92%)	136 (100%)	0	100	100
31	L	120/121 (99%)	120 (100%)	0	100	100
32	M	101/101 (100%)	101 (100%)	0	100	100
33	N	115/115 (100%)	115 (100%)	0	100	100
34	O	105/113 (93%)	105 (100%)	0	100	100
35	P	102/111 (92%)	102 (100%)	0	100	100
36	Q	83/97 (86%)	83 (100%)	0	100	100
37	R	92/99 (93%)	92 (100%)	0	100	100
38	S	96/97 (99%)	94 (98%)	2 (2%)	53	79
39	T	82/82 (100%)	82 (100%)	0	100	100
40	U	93/97 (96%)	93 (100%)	0	100	100
41	V	83/84 (99%)	80 (96%)	3 (4%)	35	67
42	W	78/88 (89%)	78 (100%)	0	100	100
43	Y	61/76 (80%)	61 (100%)	0	100	100
44	Z	50/53 (94%)	50 (100%)	0	100	100
45	1	53/55 (96%)	53 (100%)	0	100	100
46	2	50/52 (96%)	50 (100%)	0	100	100
47	3	27/73 (37%)	27 (100%)	0	100	100
48	4	47/50 (94%)	47 (100%)	0	100	100
49	5	44/48 (92%)	44 (100%)	0	100	100
50	6	39/39 (100%)	39 (100%)	0	100	100
51	7	55/56 (98%)	55 (100%)	0	100	100
52	8	35/35 (100%)	35 (100%)	0	100	100
All	All	4082/5013 (81%)	4070 (100%)	12 (0%)	92	96

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	169	GLU
9	i	106	ARG
19	s	78	ARG
23	v	45	ARG
23	v	208	THR
29	F	3	ARG
29	F	78	ARG
38	S	101	ASN
38	S	102	ASP
41	V	42	ILE
41	V	43	GLU
41	V	44	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	15	HIS
4	d	59	HIS
4	d	73	ASN
4	d	85	ASN
4	d	96	ASN
4	d	112	GLN
4	d	116	HIS
5	e	71	ASN
8	h	22	HIS
9	i	81	HIS
12	l	86	ASN
15	o	18	HIS
16	p	85	ASN
17	q	5	ASN
17	q	49	HIS
18	r	56	GLN
19	s	69	HIS
20	t	21	ASN
20	t	24	GLN
23	v	67	GLN
23	v	117	GLN
23	v	119	GLN
23	v	148	ASN
23	v	203	ASN
23	v	264	HIS
26	C	53	HIS
26	C	194	GLN

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Mol	Chain	Res	Type
27	D	50	GLN
27	D	68	HIS
27	D	152	ASN
28	E	119	ASN
30	G	20	ASN
30	G	51	ASN
30	G	97	GLN
31	L	97	ASN
31	L	136	GLN
32	M	4	GLN
33	N	27	ASN
39	T	90	GLN
40	U	107	HIS
41	V	73	ASN
42	W	67	ASN
43	Y	20	ASN
44	Z	16	ASN
44	Z	34	GLN
47	3	55	HIS
49	5	16	ASN
49	5	26	ASN
51	7	35	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1511/1550 (97%)	281 (18%)	0
21	x	71/76 (93%)	17 (23%)	0
22	w	7/21 (33%)	5 (71%)	0
24	A	2895/2932 (98%)	473 (16%)	28 (0%)
25	B	113/116 (97%)	11 (9%)	0
All	All	4597/4695 (97%)	787 (17%)	28 (0%)

All (787) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	9	G
1	a	22	G
1	a	31	G
1	a	32	A
1	a	39	G

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Mol	Chain	Res	Type
1	a	44	G
1	a	47	C
1	a	48	C
1	a	51	A
1	a	66	A
1	a	68	G
1	a	69	A
1	a	70	A
1	a	71	C
1	a	73	G
1	a	95	A
1	a	96	G
1	a	97	U
1	a	99	A
1	a	100	G
1	a	101	U
1	a	107	A
1	a	114	A
1	a	119	C
1	a	128	A
1	a	130	C
1	a	143	U
1	a	154	C
1	a	159	A
1	a	160	A
1	a	162	C
1	a	164	G
1	a	173	A
1	a	182	U
1	a	189	U
1	a	195	A
1	a	209	A
1	a	211	A
1	a	212	G
1	a	218	U
1	a	219	U
1	a	220	C
1	a	222	G
1	a	239	G
1	a	249	G
1	a	253	U
1	a	255	G

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Mol	Chain	Res	Type
1	a	259	G
1	a	265	A
1	a	274	G
1	a	275	C
1	a	288	C
1	a	297	G
1	a	329	A
1	a	336	C
1	a	340	G
1	a	351	U
1	a	353	C
1	a	354	G
1	a	355	G
1	a	360	C
1	a	362	G
1	a	372	A
1	a	373	U
1	a	375	U
1	a	380	C
1	a	381	A
1	a	392	G
1	a	400	G
1	a	412	G
1	a	414	G
1	a	416	A
1	a	417	U
1	a	420	A
1	a	421	G
1	a	423	A
1	a	429	U
1	a	430	C
1	a	431	G
1	a	432	G
1	a	437	U
1	a	441	G
1	a	447	U
1	a	454	A
1	a	456	A
1	a	457	A
1	a	460	A
1	a	461	C
1	a	462	A

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Mol	Chain	Res	Type
1	a	463	A
1	a	467	U
1	a	468	A
1	a	469	A
1	a	471	A
1	a	473	U
1	a	483	U
1	a	486	C
1	a	487	U
1	a	488	U
1	a	489	G
1	a	492	G
1	a	493	G
1	a	494	U
1	a	503	A
1	a	505	A
1	a	508	G
1	a	511	A
1	a	513	G
1	a	514	G
1	a	515	C
1	a	519	C
1	a	526	C
1	a	529	G
1	a	535	G
1	a	538	G
1	a	539	U
1	a	541	A
1	a	552	G
1	a	553	C
1	a	555	A
1	a	567	A
1	a	570	U
1	a	572	U
1	a	576	G
1	a	580	A
1	a	581	A
1	a	584	C
1	a	585	G
1	a	587	G
1	a	596	G
1	a	604	A

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Mol	Chain	Res	Type
1	a	628	U
1	a	643	A
1	a	657	G
1	a	661	G
1	a	673	A
1	a	679	G
1	a	683	A
1	a	695	A
1	a	702	A
1	a	711	G
1	a	712	A
1	a	729	A
1	a	731	U
1	a	739	G
1	a	741	G
1	a	742	A
1	a	750	G
1	a	757	A
1	a	763	G
1	a	768	G
1	a	786	G
1	a	789	A
1	a	801	U
1	a	802	A
1	a	825	C
1	a	829	G
1	a	848	G
1	a	855	C
1	a	881	A
1	a	923	A
1	a	935	G
1	a	936	G
1	a	940	C
1	a	943	C
1	a	944	A
1	a	954	G
1	a	957	C
1	a	965	U
1	a	966	U
1	a	969	U
1	a	970	U
1	a	974	A

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Mol	Chain	Res	Type
1	a	977	A
1	a	978	A
1	a	980	G
1	a	981	C
1	a	982	G
1	a	984	A
1	a	985	G
1	a	986	A
1	a	992	A
1	a	1001	U
1	a	1002	G
1	a	1003	A
1	a	1005	A
1	a	1010	U
1	a	1012	G
1	a	1013	A
1	a	1018	U
1	a	1022	G
1	a	1032	U
1	a	1033	U
1	a	1035	C
1	a	1046	C
1	a	1048	A
1	a	1050	G
1	a	1051	U
1	a	1052	G
1	a	1053	A
1	a	1055	A
1	a	1062	G
1	a	1063	C
1	a	1066	G
1	a	1067	G
1	a	1069	U
1	a	1074	U
1	a	1075	C
1	a	1090	G
1	a	1094	U
1	a	1103	G
1	a	1104	U
1	a	1110	A
1	a	1111	A
1	a	1133	G

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Mol	Chain	Res	Type
1	a	1135	U
1	a	1141	C
1	a	1142	A
1	a	1147	G
1	a	1148	U
1	a	1156	U
1	a	1165	A
1	a	1167	U
1	a	1176	A
1	a	1178	G
1	a	1181	G
1	a	1191	G
1	a	1203	A
1	a	1204	A
1	a	1208	A
1	a	1209	U
1	a	1219	U
1	a	1220	A
1	a	1231	U
1	a	1232	A
1	a	1233	C
1	a	1234	A
1	a	1235	C
1	a	1245	A
1	a	1264	C
1	a	1267	G
1	a	1274	C
1	a	1276	A
1	a	1287	A
1	a	1293	U
1	a	1294	A
1	a	1295	A
1	a	1306	A
1	a	1307	G
1	a	1308	U
1	a	1309	U
1	a	1312	G
1	a	1325	A
1	a	1329	C
1	a	1342	C
1	a	1343	C
1	a	1355	U

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Mol	Chain	Res	Type
1	a	1368	G
1	a	1371	U
1	a	1377	G
1	a	1388	U
1	a	1401	A
1	a	1405	A
1	a	1429	U
1	a	1447	U
1	a	1449	G
1	a	1453	A
1	a	1456	C
1	a	1495	G
1	a	1498	U
1	a	1500	A
1	a	1502	G
1	a	1514	U
1	a	1515	A
1	a	1525	G
1	a	1527	A
1	a	1537	G
1	a	1538	G
1	a	1539	A
1	a	1542	A
1	a	1545	U
21	x	7	A
21	x	8	4SU
21	x	9	A
21	x	10	G
21	x	19	G
21	x	26	A
21	x	29	G
21	x	30	G
21	x	35	A
21	x	36	A
21	x	44	G
21	x	45	U
21	x	46	7MG
21	x	48	C
21	x	52	G
21	x	73	A
21	x	76	A
22	w	12	A

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Mol	Chain	Res	Type
22	w	14	U
22	w	16	C
22	w	17	U
22	w	18	A
24	A	13	A
24	A	14	A
24	A	28	A
24	A	34	U
24	A	46	C
24	A	51	G
24	A	60	G
24	A	71	A
24	A	75	G
24	A	89	U
24	A	93	U
24	A	100	U
24	A	101	G
24	A	117	A
24	A	119	U
24	A	125	A
24	A	126	A
24	A	130	A
24	A	139	A
24	A	140	G
24	A	145	A
24	A	156	A
24	A	161	A
24	A	162	A
24	A	164	A
24	A	186	C
24	A	187	C
24	A	198	A
24	A	199	A
24	A	201	A
24	A	215	A
24	A	218	A
24	A	223	A
24	A	224	A
24	A	228	A
24	A	230	A
24	A	231	A
24	A	232	U

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Mol	Chain	Res	Type
24	A	235	A
24	A	241	U
24	A	247	G
24	A	250	G
24	A	257	A
24	A	267	A
24	A	274	A
24	A	282	G
24	A	283	C
24	A	285	U
24	A	287	C
24	A	289	U
24	A	290	C
24	A	295	G
24	A	296	G
24	A	299	G
24	A	300	U
24	A	301	A
24	A	307	C
24	A	308	U
24	A	309	C
24	A	313	A
24	A	320	U
24	A	323	A
24	A	345	G
24	A	354	A
24	A	360	G
24	A	372	A
24	A	373	A
24	A	374	C
24	A	375	A
24	A	388	A
24	A	396	U
24	A	404	A
24	A	406	A
24	A	410	G
24	A	411	A
24	A	417	A
24	A	418	G
24	A	420	A
24	A	432	G
24	A	433	U

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Mol	Chain	Res	Type
24	A	457	G
24	A	458	A
24	A	470	G
24	A	490	C
24	A	501	C
24	A	503	A
24	A	513	G
24	A	527	G
24	A	536	A
24	A	550	A
24	A	552	U
24	A	553	U
24	A	554	C
24	A	555	C
24	A	567	G
24	A	576	U
24	A	577	A
24	A	578	G
24	A	591	A
24	A	592	A
24	A	593	U
24	A	594	G
24	A	606	G
24	A	616	G
24	A	618	A
24	A	646	A
24	A	657	A
24	A	658	A
24	A	659	A
24	A	666	A
24	A	667	G
24	A	672	A
24	A	679	G
24	A	682	A
24	A	689	A
24	A	690	U
24	A	699	U
24	A	700	A
24	A	718	C
24	A	732	U
24	A	760	U
24	A	763	U

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Mol	Chain	Res	Type
24	A	764	A
24	A	776	U
24	A	786	C
24	A	793	U
24	A	794	G
24	A	810	A
24	A	811	G
24	A	821	G
24	A	823	G
24	A	825	A
24	A	828	A
24	A	830	U
24	A	836	U
24	A	838	G
24	A	851	G
24	A	858	C
24	A	865	A
24	A	873	U
24	A	874	U
24	A	891	U
24	A	892	A
24	A	893	A
24	A	906	G
24	A	913	A
24	A	928	G
24	A	929	G
24	A	944	C
24	A	945	C
24	A	954	A
24	A	957	A
24	A	959	C
24	A	964	A
24	A	973	U
24	A	974	A
24	A	976	U
24	A	979	U
24	A	980	A
24	A	987	A
24	A	991	A
24	A	992	G
24	A	1007	G
24	A	1020	A

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Mol	Chain	Res	Type
24	A	1025	A
24	A	1029	A
24	A	1042	A
24	A	1051	C
24	A	1058	U
24	A	1059	A
24	A	1072	A
24	A	1073	A
24	A	1079	U
24	A	1092	A
24	A	1093	G
24	A	1106	U
24	A	1113	A
24	A	1115	A
24	A	1116	A
24	A	1117	G
24	A	1123	A
24	A	1130	A
24	A	1131	A
24	A	1134	A
24	A	1141	A
24	A	1142	A
24	A	1157	A
24	A	1158	G
24	A	1161	A
24	A	1173	A
24	A	1174	A
24	A	1178	U
24	A	1179	A
24	A	1181	C
24	A	1182	G
24	A	1188	A
24	A	1203	A
24	A	1230	G
24	A	1249	A
24	A	1250	G
24	A	1252	G
24	A	1254	G
24	A	1257	G
24	A	1265	A
24	A	1283	G
24	A	1298	A

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Mol	Chain	Res	Type
24	A	1301	G
24	A	1302	C
24	A	1311	G
24	A	1316	G
24	A	1317	A
24	A	1320	G
24	A	1344	A
24	A	1345	A
24	A	1365	A
24	A	1369	C
24	A	1373	U
24	A	1394	C
24	A	1396	U
24	A	1409	A
24	A	1423	U
24	A	1429	A
24	A	1430	C
24	A	1435	A
24	A	1439	A
24	A	1457	A
24	A	1462	U
24	A	1463	U
24	A	1464	A
24	A	1465	A
24	A	1466	C
24	A	1469	A
24	A	1470	U
24	A	1478	C
24	A	1494	A
24	A	1502	A
24	A	1505	G
24	A	1509	A
24	A	1519	A
24	A	1528	G
24	A	1529	U
24	A	1530	G
24	A	1531	U
24	A	1532	G
24	A	1533	A
24	A	1534	G
24	A	1536	A
24	A	1539	A

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Mol	Chain	Res	Type
24	A	1542	C
24	A	1546	U
24	A	1553	C
24	A	1556	G
24	A	1557	C
24	A	1564	U
24	A	1570	G
24	A	1571	U
24	A	1573	A
24	A	1574	U
24	A	1575	G
24	A	1579	A
24	A	1594	G
24	A	1618	A
24	A	1621	A
24	A	1630	U
24	A	1638	G
24	A	1656	C
24	A	1657	A
24	A	1659	A
24	A	1695	A
24	A	1696	G
24	A	1697	C
24	A	1700	G
24	A	1703	A
24	A	1704	A
24	A	1723	G
24	A	1724	C
24	A	1749	A
24	A	1761	A
24	A	1762	U
24	A	1763	U
24	A	1764	A
24	A	1771	A
24	A	1773	G
24	A	1781	G
24	A	1782	A
24	A	1783	G
24	A	1787	C
24	A	1789	G
24	A	1796	G
24	A	1797	G

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Mol	Chain	Res	Type
24	A	1806	A
24	A	1809	G
24	A	1815	C
24	A	1833	C
24	A	1834	A
24	A	1842	A
24	A	1849	C
24	A	1862	A
24	A	1880	A
24	A	1886	A
24	A	1887	A
24	A	1889	A
24	A	1891	G
24	A	1892	A
24	A	1899	A
24	A	1903	U
24	A	1939	G
24	A	1946	A
24	A	1947	C
24	A	1949	A
24	A	1951	A
24	A	1952	A
24	A	1962	G
24	A	1963	G
24	A	1973	U
24	A	1988	U
24	A	1996	C
24	A	1998	C
24	A	2000	C
24	A	2003	A
24	A	2004	A
24	A	2005	G
24	A	2024	U
24	A	2026	U
24	A	2027	C
24	A	2030	A
24	A	2031	A
24	A	2056	A
24	A	2064	A
24	A	2065	G
24	A	2066	A
24	A	2067	U

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Mol	Chain	Res	Type
24	A	2072	G
24	A	2076	C
24	A	2085	G
24	A	2088	C
24	A	2089	G
24	A	2093	A
24	A	2094	G
24	A	2095	A
24	A	2096	C
24	A	2102	G
24	A	2126	G
24	A	2127	A
24	A	2133	U
24	A	2144	U
24	A	2149	G
24	A	2150	A
24	A	2152	A
24	A	2165	A
24	A	2188	A
24	A	2190	G
24	A	2191	A
24	A	2192	G
24	A	2193	G
24	A	2198	G
24	A	2205	U
24	A	2206	A
24	A	2223	A
24	A	2224	C
24	A	2231	A
24	A	2236	G
24	A	2237	C
24	A	2245	A
24	A	2256	A
24	A	2258	A
24	A	2259	C
24	A	2271	G
24	A	2272	G
24	A	2312	G
24	A	2316	C
24	A	2319	A
24	A	2320	A
24	A	2321	A

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Mol	Chain	Res	Type
24	A	2329	U
24	A	2338	A
24	A	2341	G
24	A	2343	A
24	A	2344	A
24	A	2353	A
24	A	2355	A
24	A	2358	G
24	A	2360	A
24	A	2367	C
24	A	2368	A
24	A	2380	C
24	A	2383	C
24	A	2394	A
24	A	2412	G
24	A	2416	G
24	A	2418	C
24	A	2420	U
24	A	2435	U
24	A	2439	C
24	A	2447	G
24	A	2455	C
24	A	2457	C
24	A	2458	A
24	A	2462	G
24	A	2463	A
24	A	2473	C
24	A	2474	C
24	A	2481	A
24	A	2492	A
24	A	2498	C
24	A	2507	C
24	A	2509	A
24	A	2514	G
24	A	2524	U
24	A	2531	C
24	A	2535	G
24	A	2536	A
24	A	2538	G
24	A	2546	G
24	A	2548	C
24	A	2551	A

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Mol	Chain	Res	Type
24	A	2562	G
24	A	2568	G
24	A	2577	G
24	A	2580	U
24	A	2587	U
24	A	2599	A
24	A	2600	G
24	A	2605	A
24	A	2606	C
24	A	2607	G
24	A	2615	G
24	A	2616	G
24	A	2642	U
24	A	2643	C
24	A	2646	U
24	A	2648	U
24	A	2663	G
24	A	2678	G
24	A	2679	C
24	A	2722	U
24	A	2724	C
24	A	2747	G
24	A	2755	G
24	A	2759	U
24	A	2766	C
24	A	2768	G
24	A	2781	A
24	A	2790	A
24	A	2798	A
24	A	2799	G
24	A	2802	C
24	A	2810	G
24	A	2811	A
24	A	2812	U
24	A	2813	G
24	A	2822	C
24	A	2827	C
24	A	2828	U
24	A	2830	C
24	A	2832	G
24	A	2835	A
24	A	2837	U

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Mol	Chain	Res	Type
24	A	2849	A
24	A	2852	A
24	A	2857	C
24	A	2862	A
24	A	2864	A
24	A	2872	G
24	A	2877	G
24	A	2890	U
24	A	2896	G
24	A	2901	G
24	A	2902	A
24	A	2909	C
24	A	2920	A
24	A	2922	G
24	A	2930	C
25	B	10	U
25	B	23	U
25	B	24	C
25	B	33	U
25	B	40	C
25	B	54	U
25	B	55	A
25	B	84	G
25	B	87	U
25	B	88	C
25	B	107	G

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	A	27	G
24	A	88	G
24	A	92	G
24	A	139	A
24	A	553	U
24	A	688	A
24	A	756	A
24	A	809	G
24	A	847	G
24	A	854	G
24	A	1017	C
24	A	1172	A

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Mol	Chain	Res	Type
24	A	1248	A
24	A	1249	A
24	A	1497	G
24	A	1528	G
24	A	1532	G
24	A	1533	A
24	A	1569	U
24	A	1886	A
24	A	1888	G
24	A	2320	A
24	A	2438	G
24	A	2472	A
24	A	2615	G
24	A	2789	U
24	A	2809	A
24	A	2908	A

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

7 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
21	7MG	x	46	21	22,26,27	1.31	3 (13%)	29,39,42	2.58	7 (24%)
21	PSU	x	55	21	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
21	PSU	x	39	21	18,21,22	1.27	2 (11%)	22,30,33	2.08	4 (18%)
21	4SU	x	8	21	18,21,22	1.77	5 (27%)	26,30,33	2.34	5 (19%)
21	PSU	x	32	21	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
21	5MU	x	54	21	19,22,23	1.39	5 (26%)	28,32,35	2.02	6 (21%)
21	MIA	x	37	21	24,31,32	2.22	3 (12%)	26,44,47	2.52	9 (34%)

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
21	7MG	x	46	21	-	5/7/37/38	0/3/3/3
21	PSU	x	55	21	-	0/7/25/26	0/2/2/2
21	PSU	x	39	21	-	0/7/25/26	0/2/2/2
21	4SU	x	8	21	-	0/7/25/26	0/2/2/2
21	PSU	x	32	21	-	0/7/25/26	0/2/2/2
21	5MU	x	54	21	-	0/7/25/26	0/2/2/2
21	MIA	x	37	21	-	2/11/33/34	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	x	37	MIA	C13-C14	7.11	1.52	1.32
21	x	37	MIA	C2-S10	-6.84	1.69	1.75
21	x	8	4SU	C4-S4	-4.56	1.59	1.68
21	x	8	4SU	C4-N3	-3.30	1.34	1.37
21	x	55	PSU	C6-C5	3.12	1.39	1.35
21	x	46	7MG	C5-C4	2.99	1.47	1.38
21	x	39	PSU	C6-C5	2.89	1.38	1.35
21	x	32	PSU	C6-C5	2.76	1.38	1.35
21	x	46	7MG	C4-N9	-2.76	1.34	1.37
21	x	54	5MU	C6-C5	2.69	1.39	1.34
21	x	32	PSU	C4-N3	-2.64	1.33	1.38
21	x	55	PSU	C4-N3	-2.61	1.34	1.38
21	x	54	5MU	C4-N3	-2.57	1.34	1.38
21	x	8	4SU	C5-C4	-2.51	1.39	1.42
21	x	37	MIA	C5-C4	2.50	1.47	1.40
21	x	46	7MG	C6-N1	-2.39	1.34	1.38
21	x	54	5MU	C2-N1	2.32	1.42	1.38
21	x	39	PSU	C4-N3	-2.31	1.34	1.38
21	x	54	5MU	C4-C5	2.24	1.48	1.44
21	x	54	5MU	C6-N1	-2.17	1.34	1.38
21	x	8	4SU	C2-N1	2.11	1.41	1.38
21	x	8	4SU	C2-N3	-2.08	1.34	1.38

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	x	46	7MG	N9-C4-N3	9.14	139.14	125.47
21	x	37	MIA	C12-C13-C14	-8.03	111.52	127.14
21	x	8	4SU	C4-N3-C2	-7.13	120.41	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	x	39	PSU	N1-C2-N3	6.32	122.29	115.13
21	x	8	4SU	C5-C4-N3	6.02	120.27	114.69
21	x	55	PSU	N1-C2-N3	5.94	121.86	115.13
21	x	32	PSU	N1-C2-N3	5.88	121.79	115.13
21	x	46	7MG	C5-C4-N3	-5.60	117.45	128.13
21	x	46	7MG	N9-C8-N7	-5.08	96.12	103.38
21	x	54	5MU	C4-N3-C2	-4.94	120.95	127.35
21	x	54	5MU	N3-C2-N1	4.83	121.31	114.89
21	x	39	PSU	C4-N3-C2	-4.59	119.72	126.34
21	x	46	7MG	C2-N3-C4	4.37	120.09	112.30
21	x	37	MIA	C2-N3-C4	4.29	121.24	115.32
21	x	39	PSU	O2-C2-N1	-4.23	118.13	122.79
21	x	54	5MU	C5-C4-N3	4.23	118.92	115.31
21	x	8	4SU	N3-C2-N1	4.19	120.45	114.89
21	x	37	MIA	C16-C14-C13	-4.08	110.86	122.65
21	x	54	5MU	O4-C4-C5	-4.06	120.20	124.90
21	x	55	PSU	C4-N3-C2	-4.04	120.51	126.34
21	x	8	4SU	C5-C4-S4	-4.01	119.31	124.47
21	x	37	MIA	C15-C14-C13	-3.96	111.21	122.65
21	x	32	PSU	O2-C2-N1	-3.87	118.53	122.79
21	x	32	PSU	C4-N3-C2	-3.82	120.84	126.34
21	x	37	MIA	C5-C6-N1	-3.63	117.79	120.81
21	x	55	PSU	O2-C2-N1	-3.46	118.98	122.79
21	x	54	5MU	C5-C6-N1	-3.38	119.86	123.34
21	x	37	MIA	C4-C5-N7	-2.76	106.52	109.40
21	x	46	7MG	C5-C6-N1	2.76	115.86	110.99
21	x	37	MIA	C11-S10-C2	-2.73	100.23	102.27
21	x	37	MIA	C2-N1-C6	2.65	121.93	117.19
21	x	46	7MG	C5-C4-N9	-2.27	103.40	106.35
21	x	37	MIA	N3-C2-N1	-2.23	122.88	126.98
21	x	46	7MG	O6-C6-C5	-2.19	122.18	127.54
21	x	39	PSU	C5-C6-N1	-2.03	119.07	122.11
21	x	8	4SU	C3'-C2'-C1'	2.02	105.27	101.43
21	x	54	5MU	O2-C2-N1	-2.00	120.12	122.79

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	x	37	MIA	C12-C13-C14-C16
21	x	46	7MG	O4'-C4'-C5'-O5'
21	x	46	7MG	O4'-C1'-N9-C4

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Mol	Chain	Res	Type	Atoms
21	x	46	7MG	C3'-C4'-C5'-O5'
21	x	46	7MG	O4'-C1'-N9-C8
21	x	37	MIA	N6-C12-C13-C14
21	x	46	7MG	C4'-C5'-O5'-P

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 480 ligands modelled in this entry, 479 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
55	GCP	v	502	53	27,34,34	1.42	5 (18%)	34,54,54	1.87	7 (20%)

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
55	GCP	v	502	53	-	5/15/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	502	GCP	C5-C6	3.77	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	502	GCP	PG-O3G	2.87	1.61	1.54
55	v	502	GCP	PG-O2G	2.67	1.61	1.54
55	v	502	GCP	PB-O3A	2.34	1.61	1.58
55	v	502	GCP	C5-C4	2.16	1.46	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	v	502	GCP	C2-N3-C4	4.39	120.37	115.36
55	v	502	GCP	C4-C5-C6	-4.30	116.69	120.80
55	v	502	GCP	C2-N1-C6	4.06	122.39	115.93
55	v	502	GCP	C5-C6-N1	-3.98	117.99	123.43
55	v	502	GCP	PB-O3A-PA	-3.43	121.69	132.56
55	v	502	GCP	N3-C2-N1	-3.20	122.96	127.22
55	v	502	GCP	C4-C5-N7	-2.58	106.71	109.40

There are no chirality outliers.

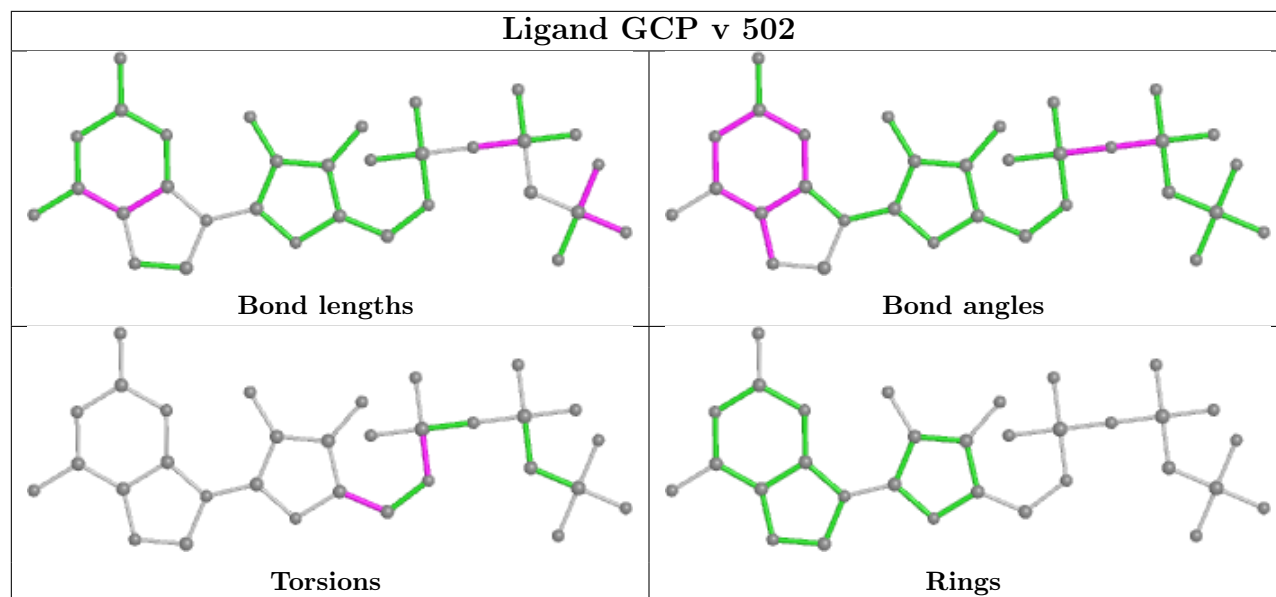
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	v	502	GCP	C5'-O5'-PA-O1A
55	v	502	GCP	C3'-C4'-C5'-O5'
55	v	502	GCP	O4'-C4'-C5'-O5'
55	v	502	GCP	C5'-O5'-PA-O3A
55	v	502	GCP	C5'-O5'-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

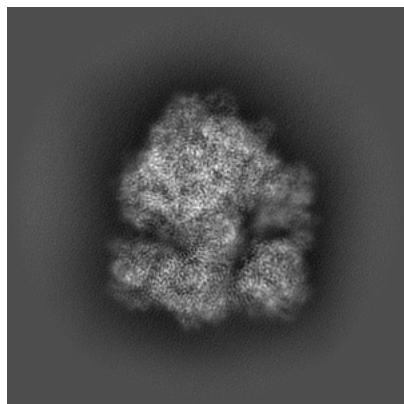
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42576. These allow visual inspection of the internal detail of the map and identification of artifacts.

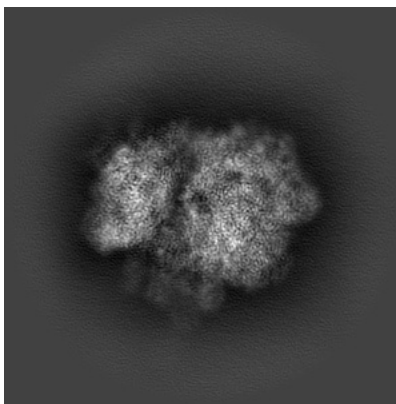
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

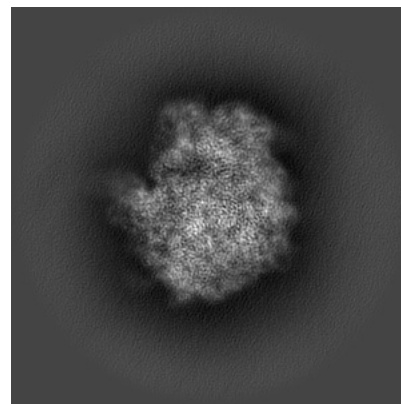
6.1.1 Primary map



X

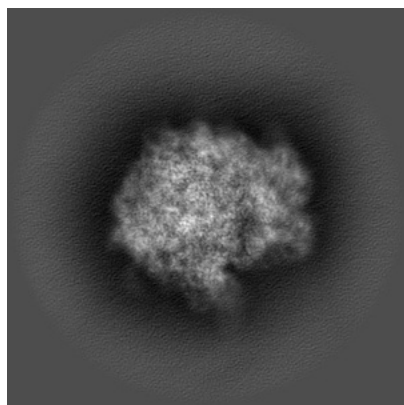


Y

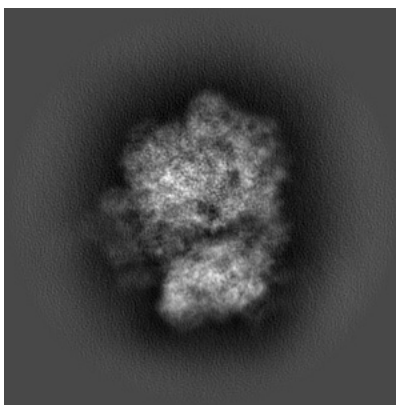


Z

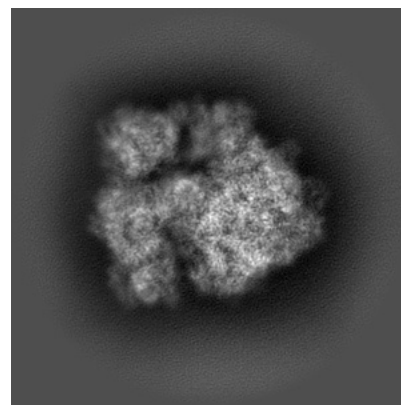
6.1.2 Raw map



X



Y

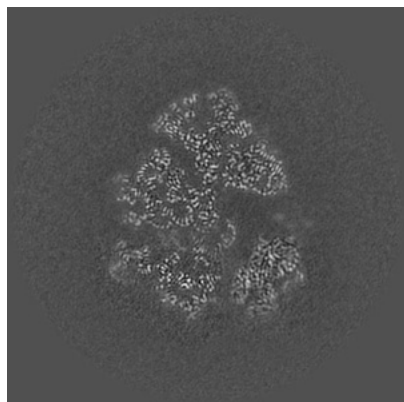


Z

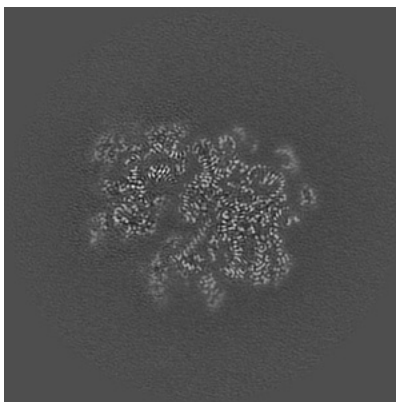
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

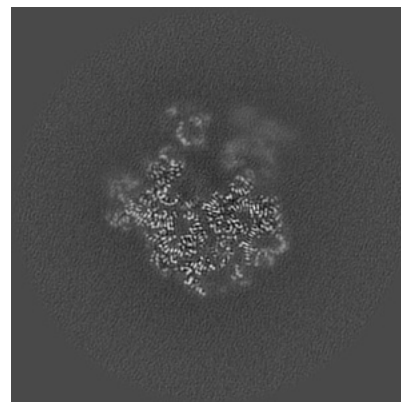
6.2.1 Primary map



X Index: 256

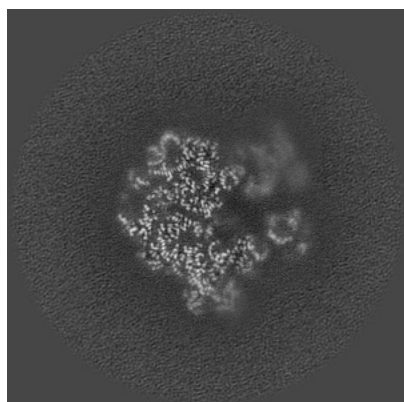


Y Index: 256

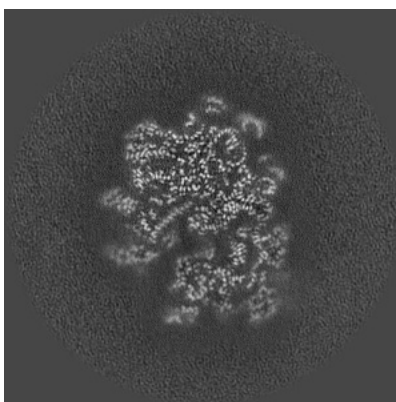


Z Index: 256

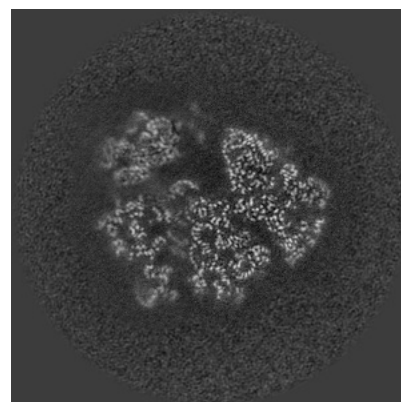
6.2.2 Raw map



X Index: 256



Y Index: 256

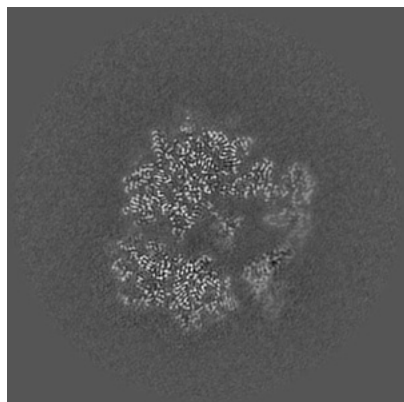


Z Index: 256

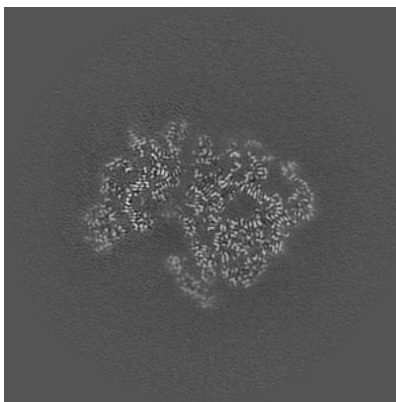
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

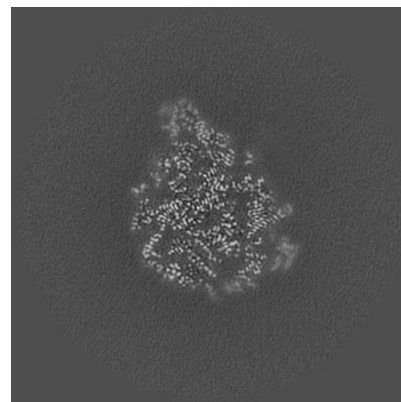
6.3.1 Primary map



X Index: 230

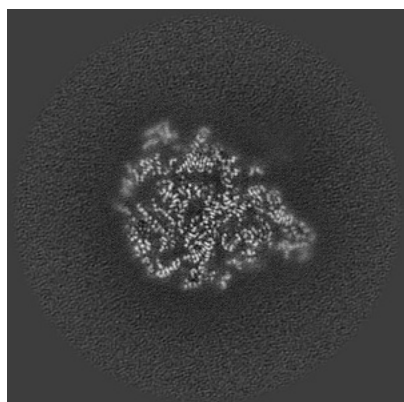


Y Index: 235

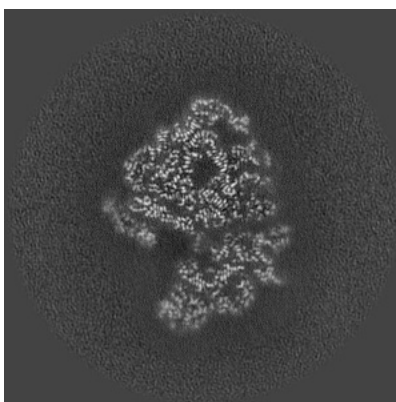


Z Index: 296

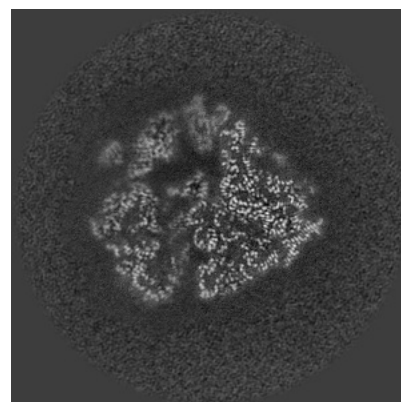
6.3.2 Raw map



X Index: 296



Y Index: 234

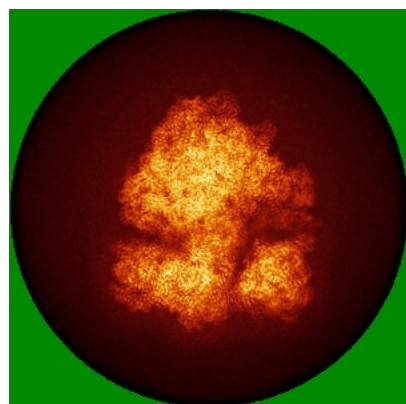


Z Index: 244

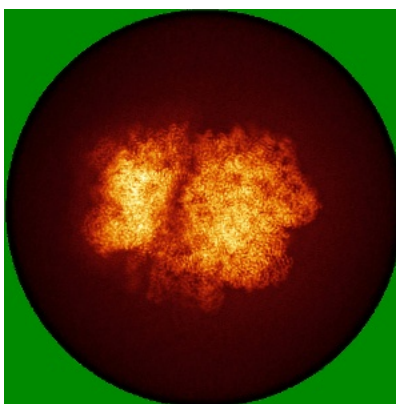
The images above show the largest variance slices of the map in three orthogonal directions.

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

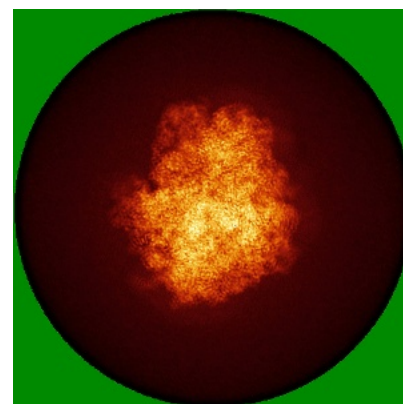
6.4.1 Primary map



X

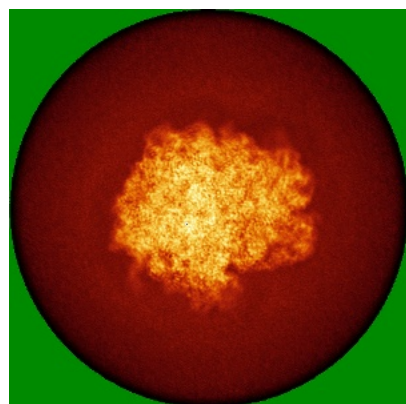


Y

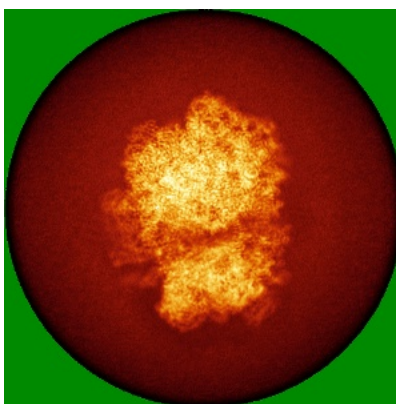


Z

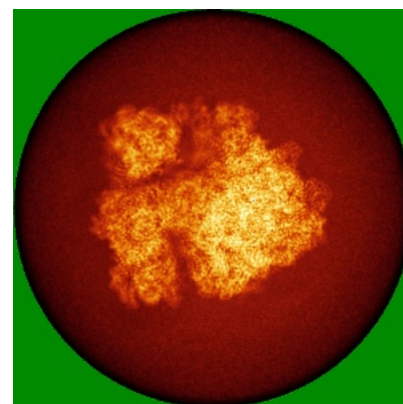
6.4.2 Raw map



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 3.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

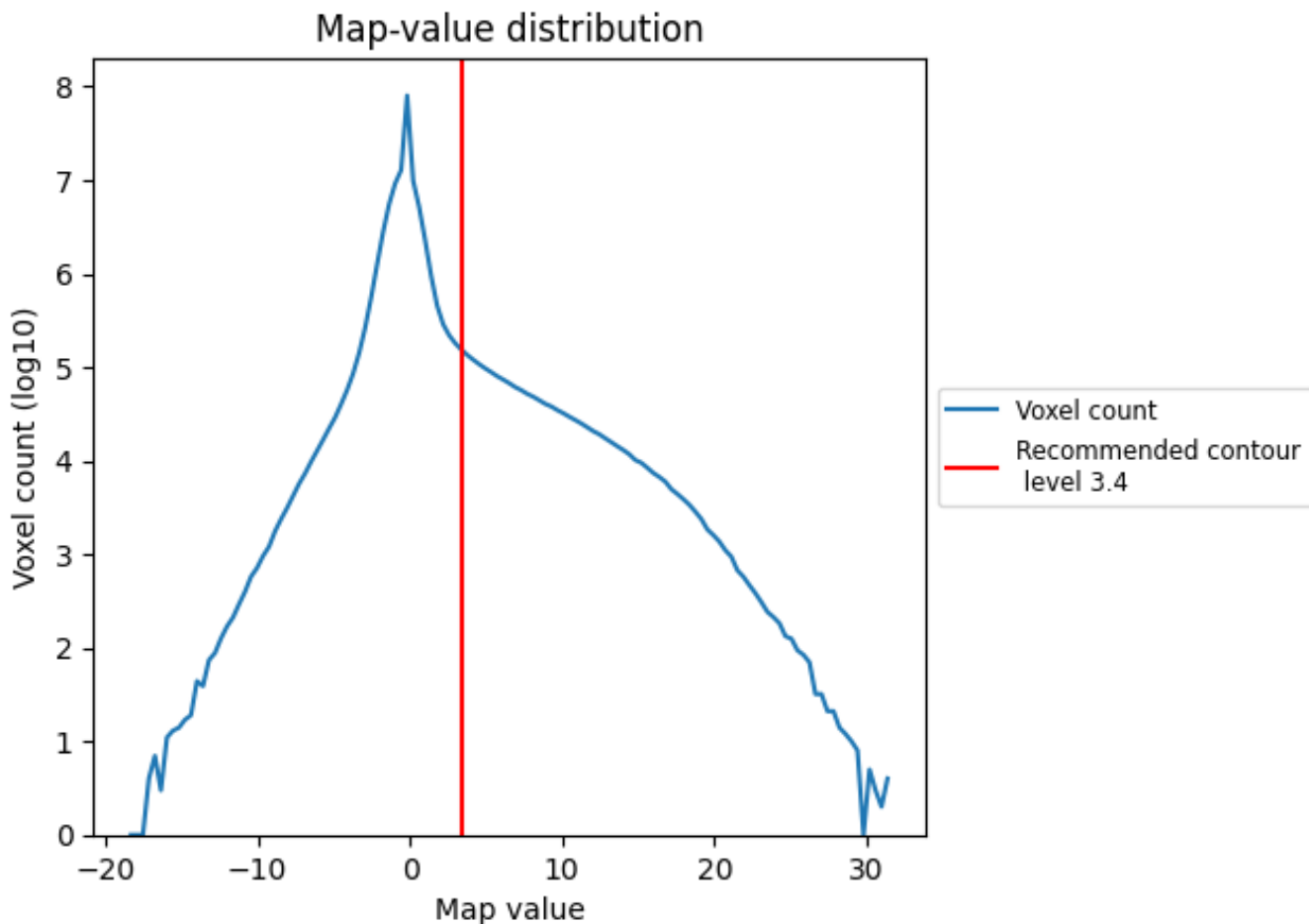
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

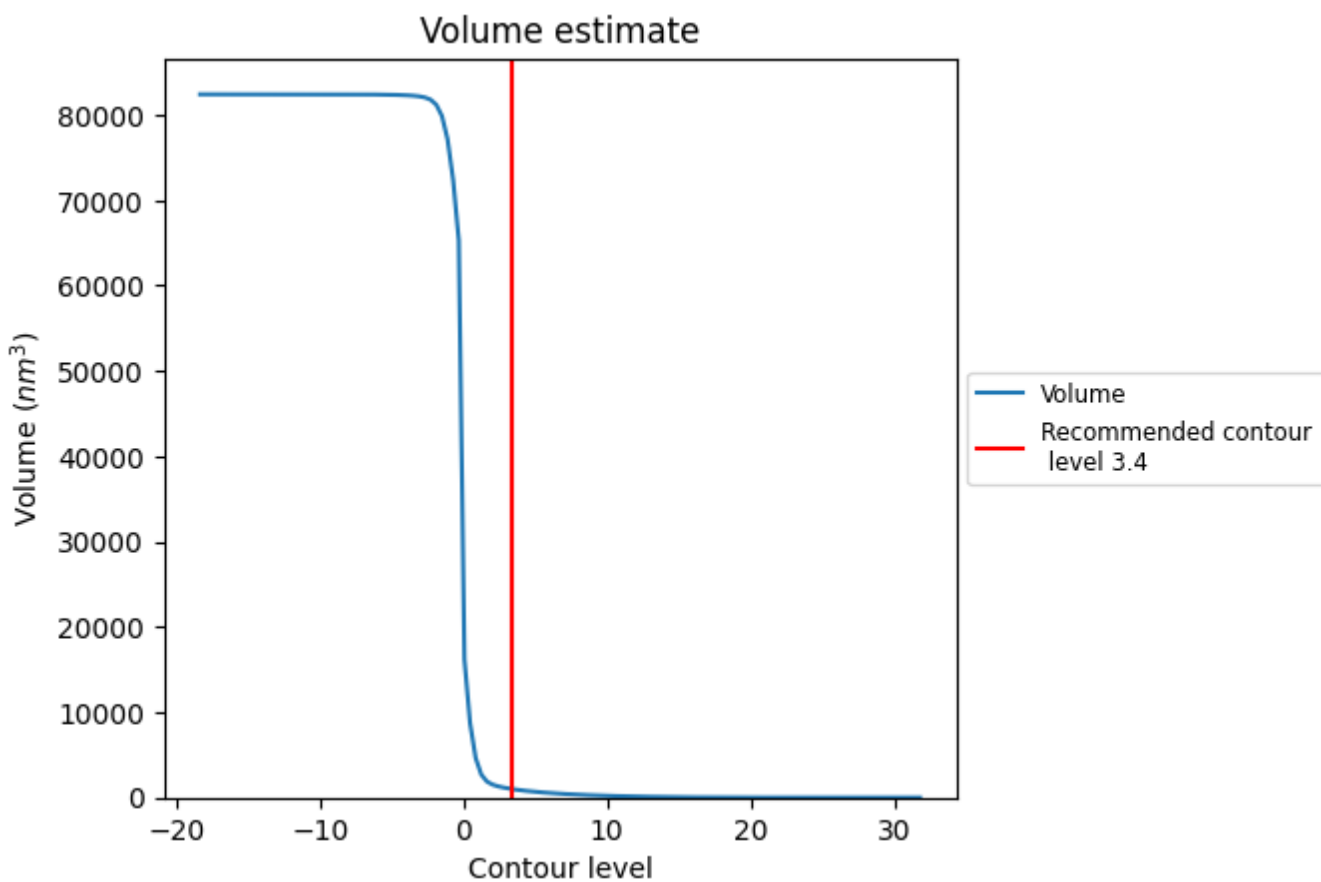
This section contains the results of statistical analysis of the map.

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.

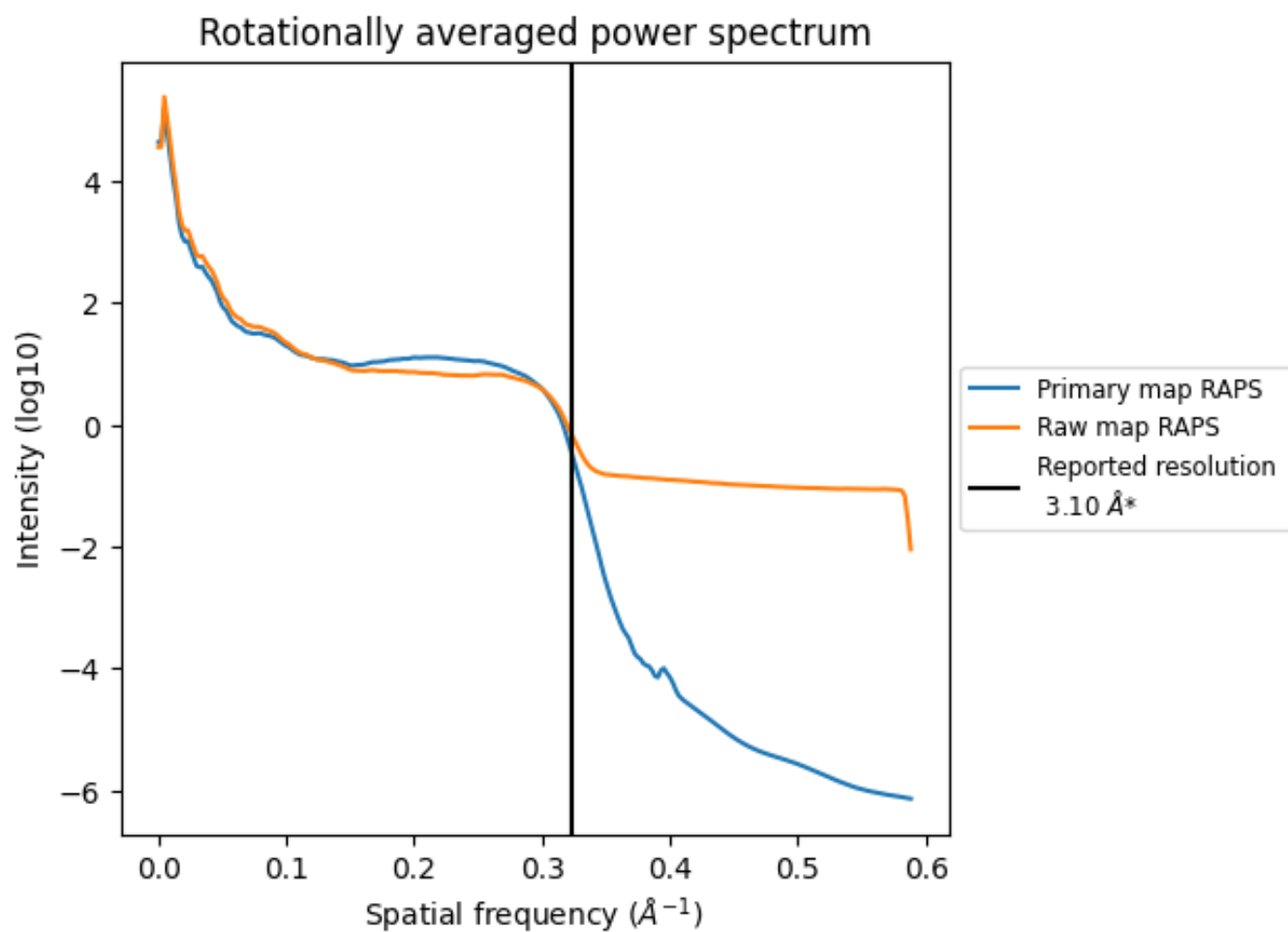
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 997 nm^3 ; this corresponds to an approximate mass of 901 kDa.

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

7.3 Rotationally averaged power spectrum i

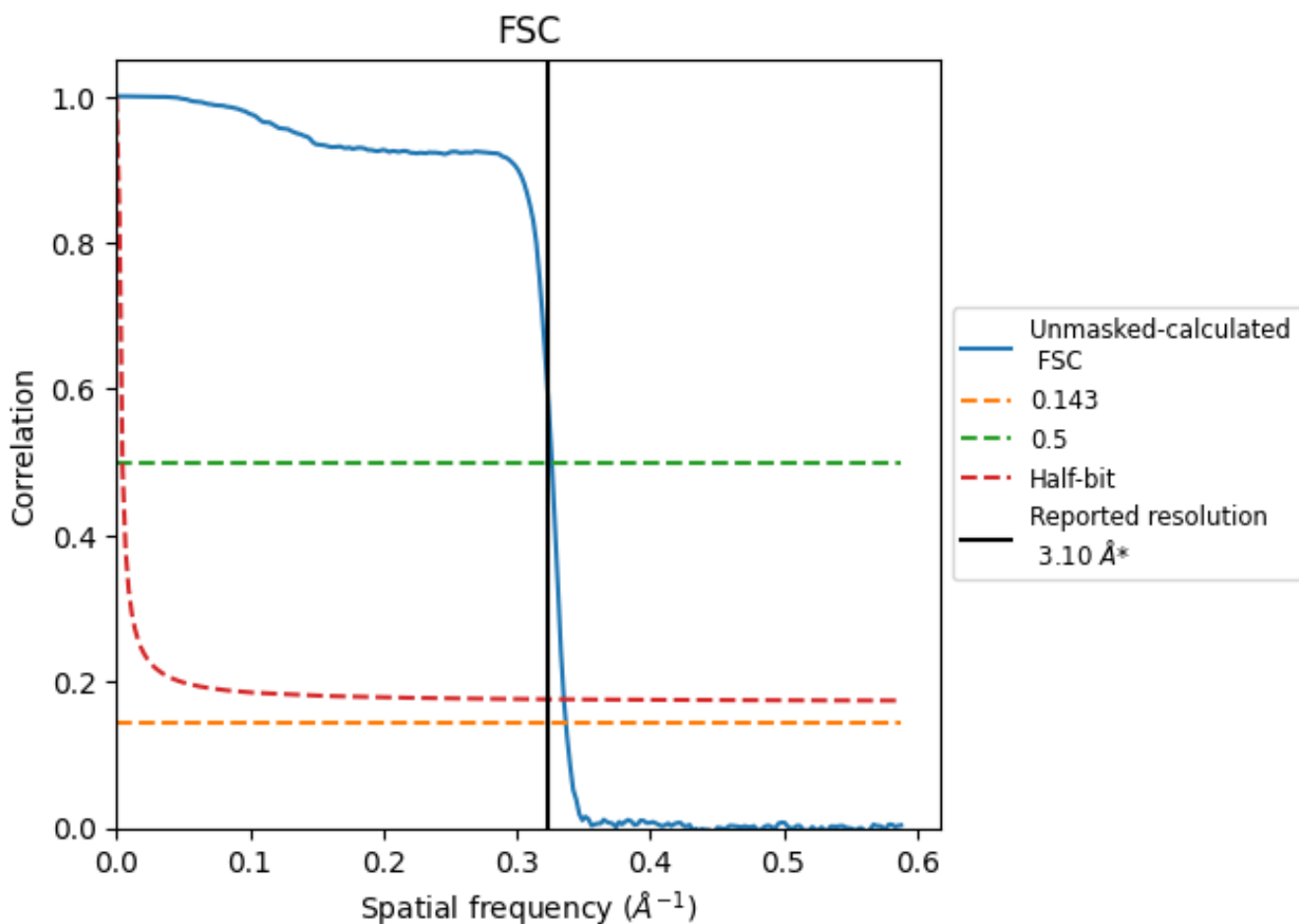


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

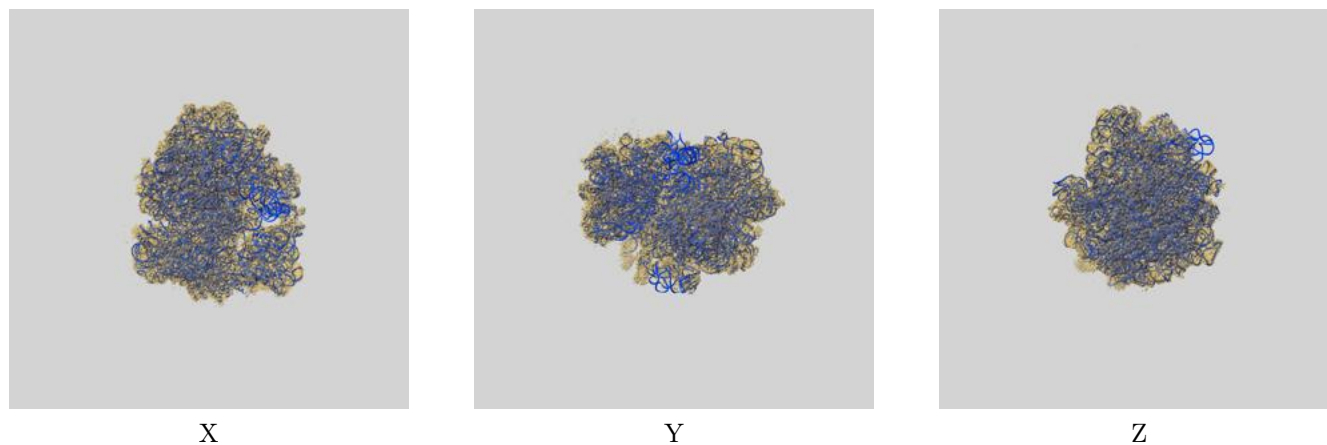
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.97	3.06	2.98

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

9 Map-model fit [i](#)

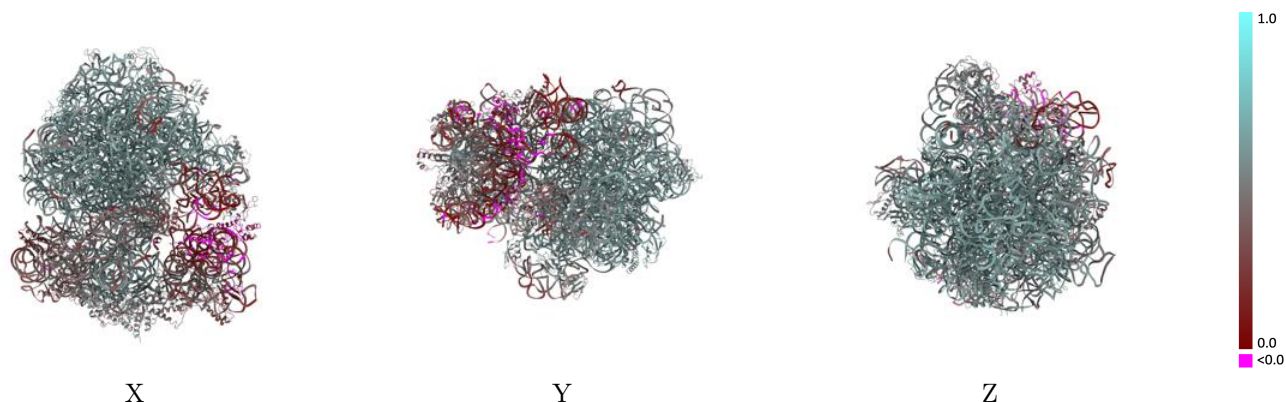
This section contains information regarding the fit between EMDB map EMD-42576 and PDB model 8UU9. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



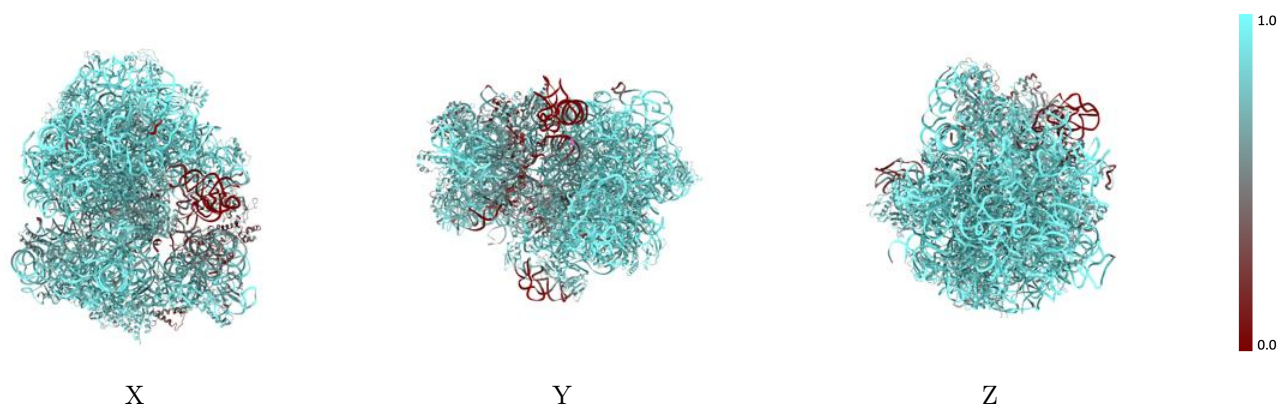
The images above show the 3D surface view of the map at the recommended contour level 3.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



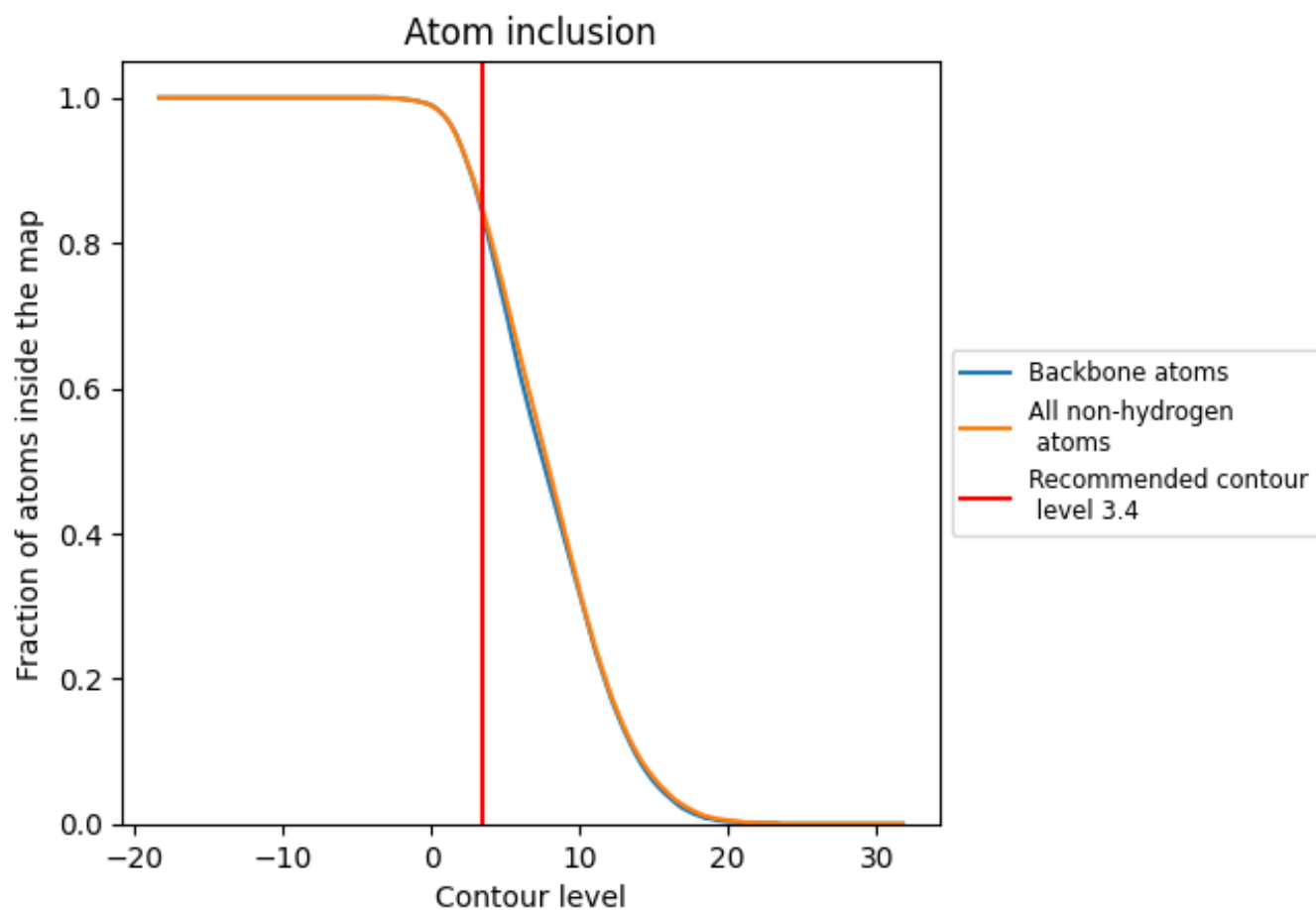
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.4).







































































9.4 Atom inclusion [i](#)

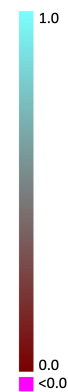


At the recommended contour level, 84% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





































The table lists the average atom inclusion at the recommended contour level (3.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8510	 0.4950
1	 0.8620	 0.5420
2	 0.8940	 0.5740
3	 0.4420	 0.3260
4	 0.8860	 0.5630
5	 0.8970	 0.5780
6	 0.9390	 0.6050
7	 0.9220	 0.6050
8	 0.8990	 0.5820
A	 0.9170	 0.5600
B	 0.9350	 0.5130
C	 0.8930	 0.5940
D	 0.9220	 0.5880
E	 0.8850	 0.5720
F	 0.5740	 0.4020
G	 0.7650	 0.5040
L	 0.9140	 0.5930
M	 0.8220	 0.5750
N	 0.8610	 0.5650
O	 0.8940	 0.5850
P	 0.8920	 0.5810
Q	 0.8180	 0.5200
R	 0.8480	 0.5760
S	 0.9230	 0.5910
T	 0.9110	 0.5880
U	 0.8910	 0.5860
V	 0.8520	 0.5620
W	 0.8420	 0.5490
Y	 0.9110	 0.5750
Z	 0.8640	 0.5700
a	 0.8150	 0.3880
b	 0.6720	 0.4670
c	 0.8160	 0.4320
d	 0.7840	 0.4280
e	 0.8550	 0.5450



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Chain	Atom inclusion	Q-score
f	 0.7170	 0.3850
g	 0.4440	 0.1330
h	 0.8600	 0.5120
i	 0.6920	 0.2370
j	 0.8110	 0.4170
k	 0.6440	 0.3450
l	 0.8610	 0.5340
m	 0.4220	 0.0750
n	 0.8370	 0.4080
o	 0.7150	 0.4320
p	 0.7400	 0.3670
q	 0.8090	 0.4140
r	 0.7680	 0.4390
s	 0.3210	 0.0980
t	 0.6540	 0.2830
v	 0.7920	 0.5180
w	 0.2740	 0.1830
x	 0.3410	 0.2300