



## Full wwPDB EM Validation Report ⓘ

Jun 1, 2026 – 01:18 PM EDT

PDB ID : 10QM / pdb\_000010qm  
EMDB ID : EMD-75389  
Title : E.coli 50S ribosomal subunit bound to compound 48a  
Authors : Raskar, T.; Lee, I.  
Deposited on : 2026-02-01  
Resolution : 2.49 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

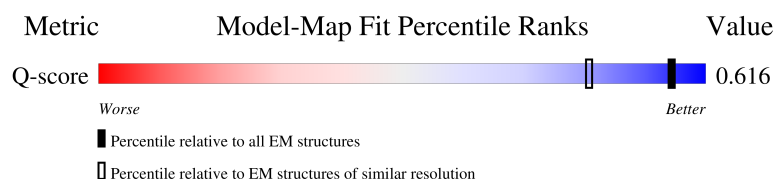
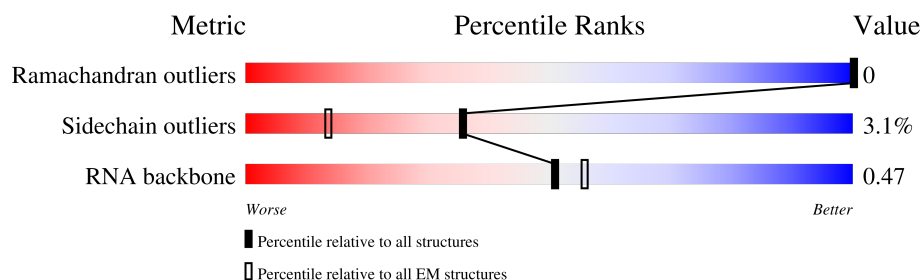
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.49 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	6237 ( 2.00 - 2.99 )

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  $\geq 3$ , 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	I	2904	<div> <div>17%</div> <div>83%</div> <div>17%</div> </div>
2	J	120	<div> <div>48%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
3	K	273	<div> <div>11%</div> <div>97%</div> <div>..</div> </div>
4	L	209	<div> <div>18%</div> <div>98%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
5	M	201	43% 99% 99%
6	N	179	95% 95%
7	O	177	84% 95% 5%
8	P	149	93% 98%
9	Q	134	100% 98%
10	R	142	11% 98%
11	S	123	28% 98%
12	T	144	27% 97%
13	U	136	22% 96%
14	V	127	7% 93% 6%
15	W	117	75% 96%
16	X	115	27% 96%
17	Y	118	8% 98%
18	Z	103	38% 95%
19	a	110	13% 97%
20	b	100	34% 92% 7%
21	c	104	60% 97%
22	d	94	57% 96%
23	e	85	11% 86% 12%
24	f	77	29% 100%
25	g	62	74% 97%
26	h	58	16% 98%
27	i	56	27% 98%
28	j	50	64% 96%
29	k	46	96%

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Mol	Chain	Length	Quality of chain
30	l	64	<div><div></div><div>6%</div><div>97%</div><div></div></div>
31	m	38	<div><div></div><div>24%</div><div>92%</div><div>8%</div></div>

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 107784 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	2898	Total	C	N	O	P	0	0
			62229	27768	11448	20115	2898		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	271	Total	C	N	O	S	1	0
			2093	1294	427	365	7		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 5 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 6 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 8 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 9 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 10 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 11 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 12 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	U	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 14 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 15 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 16 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

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

- Molecule 18 is a protein called Ribosomal protein L21.

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

- Molecule 19 is a protein called 50S ribosomal protein L22.

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

- Molecule 20 is a protein called 50S ribosomal protein L23.

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

- Molecule 21 is a protein called 50S ribosomal protein L24.

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

- Molecule 22 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	e	75	Total	C	N	O	S		
			575	356	116	102	1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L28.

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

- Molecule 25 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 26 is a protein called 50S ribosomal protein L30.

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

- Molecule 27 is a protein called 50S ribosomal protein L32.

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

- Molecule 28 is a protein called Large ribosomal subunit protein bL33.



Mol	Chain	Residues	Atoms				AltConf	Trace
28	j	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 29 is a protein called 50S ribosomal protein L34.

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

- Molecule 30 is a protein called Large ribosomal subunit protein bL35.

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

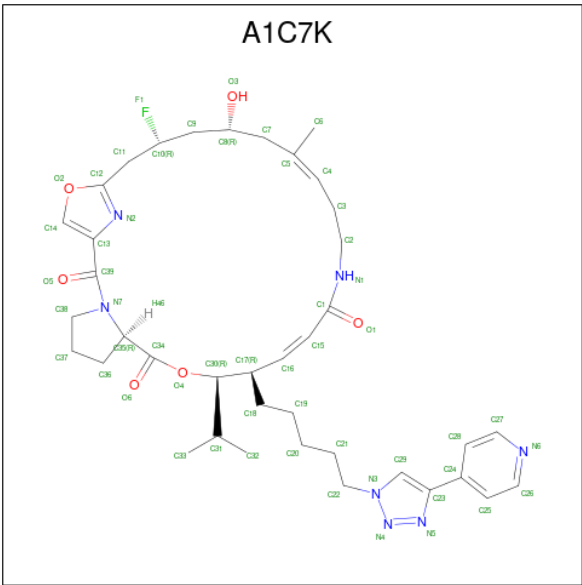
- Molecule 31 is a protein called 50S ribosomal protein L36.

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

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	I	183	Total	Mg	0
			183	183	
32	J	1	Total	Mg	0
			1	1	
32	V	1	Total	Mg	0
			1	1	

- Molecule 33 is (3R,4R,5E,11E,14R,16R,23R,26aR)-16-fluoro-14-hydroxy-12-methyl-3-(propan-2-yl)-4-{5-[4-(pyridin-4-yl)-1H-1,2,3-triazol-1-yl]pentyl}-3,4,8,9,10,13,14,15,16,17,24,25,26,26a-tetradecahydro-1H,7H,22H-21,18-(azeno)pyrrolo[2,1-c][1,8,4,19]dioxadiazacyclotetracosine-1,7,22-trione (CCD ID: A1C7K) (formula: C<sub>39</sub>H<sub>52</sub>FN<sub>7</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
33	I	1	Total	C	F	N	O	0
			53	39	1	7	6	

- Molecule 34 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
34	K	1	Total	Na	0
			1	1	

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
35	m	1	Total	Zn	0
			1	1	

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
36	I	11897	Total	O	0
			11897	11897	
36	J	549	Total	O	0
			549	549	
36	K	253	Total	O	0
			253	253	
36	L	221	Total	O	0
			221	221	

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Mol	Chain	Residues	Atoms		AltConf
36	M	201	Total 201	O 201	0
36	N	274	Total 274	O 274	0
36	O	292	Total 292	O 292	0
36	P	430	Total 430	O 430	0
36	Q	359	Total 359	O 359	0
36	R	142	Total 142	O 142	0
36	S	120	Total 120	O 120	0
36	T	142	Total 142	O 142	0
36	U	143	Total 143	O 143	0
36	V	101	Total 101	O 101	0
36	W	147	Total 147	O 147	0
36	X	153	Total 153	O 153	0
36	Y	95	Total 95	O 95	0
36	Z	112	Total 112	O 112	0
36	a	106	Total 106	O 106	0
36	b	115	Total 115	O 115	0
36	c	161	Total 161	O 161	0
36	d	123	Total 123	O 123	0
36	e	76	Total 76	O 76	0
36	f	86	Total 86	O 86	0
36	g	92	Total 92	O 92	0

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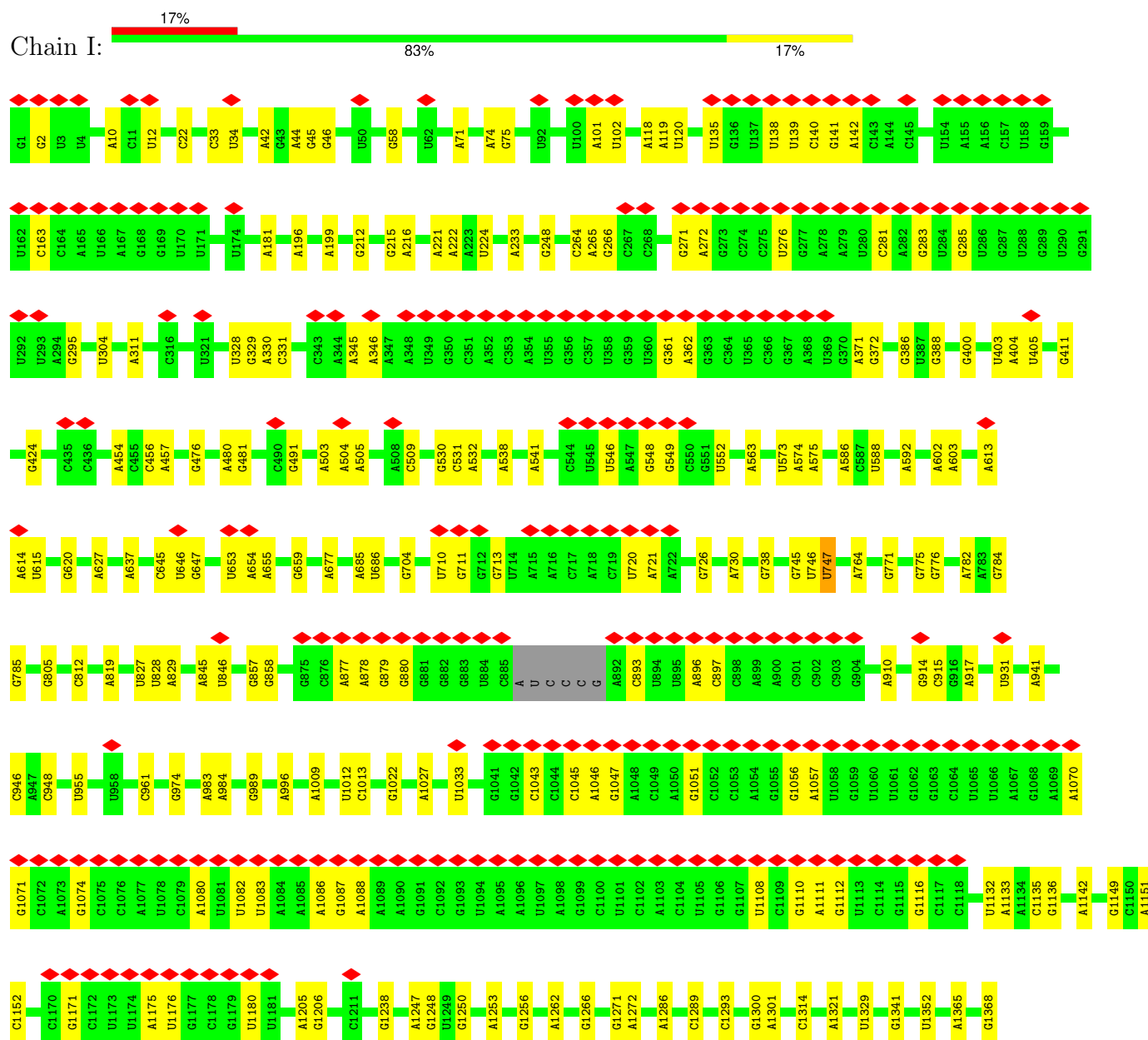
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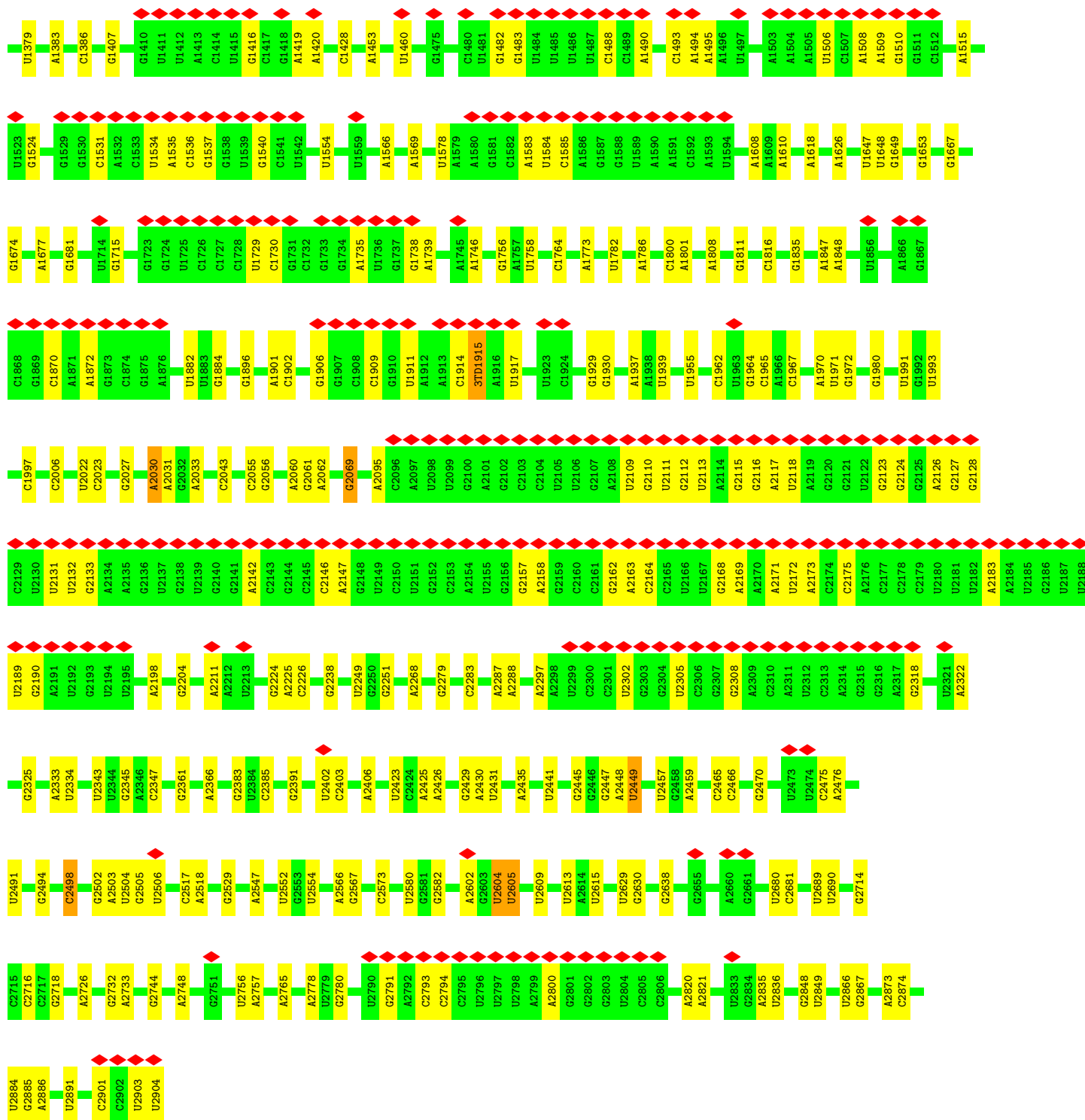
Mol	Chain	Residues	Atoms		AltConf
36	h	58	Total 58	O 58	0
36	i	70	Total 70	O 70	0
36	j	61	Total 61	O 61	0
36	k	59	Total 59	O 59	0
36	l	46	Total 46	O 46	0
36	m	30	Total 30	O 30	0

### 3 Residue-property plots

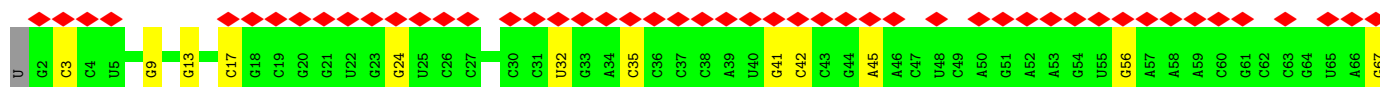
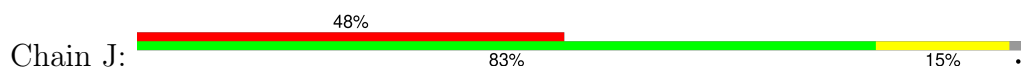
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

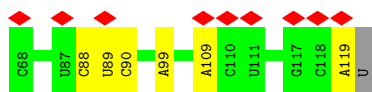
#### • Molecule 1: 23S ribosomal RNA



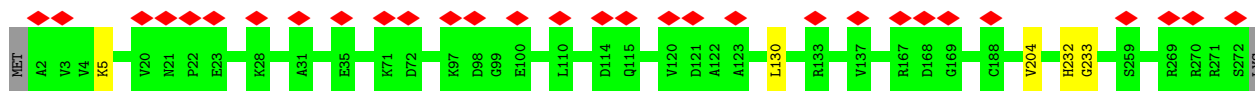


• Molecule 2: 5S ribosomal RNA

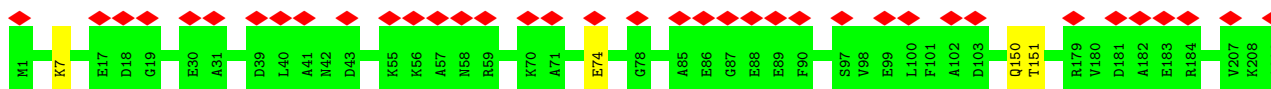




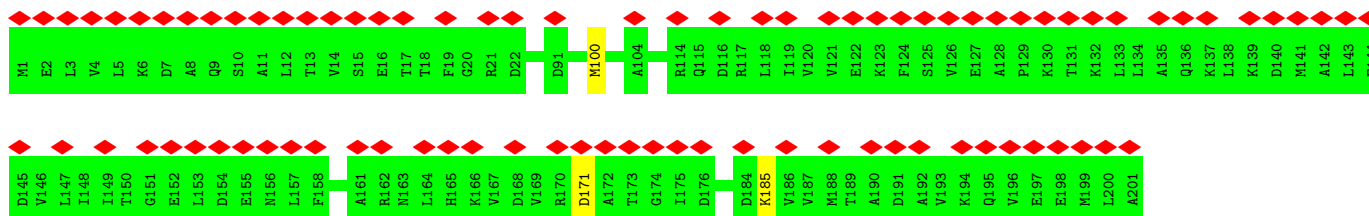
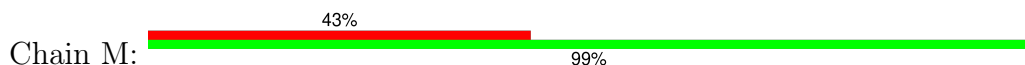
- Molecule 3: 50S ribosomal protein L2



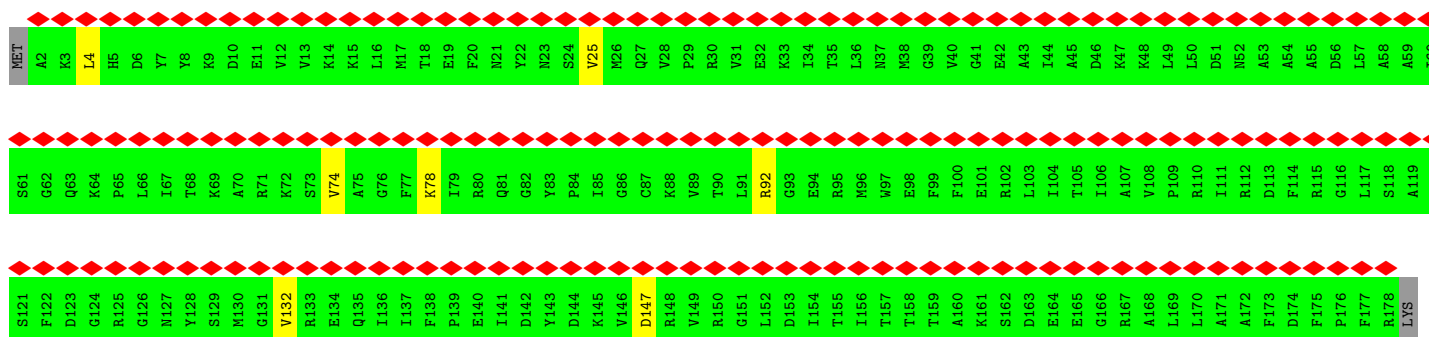
- Molecule 4: 50S ribosomal protein L3



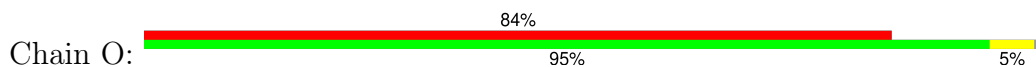
- Molecule 5: Large ribosomal subunit protein uL4

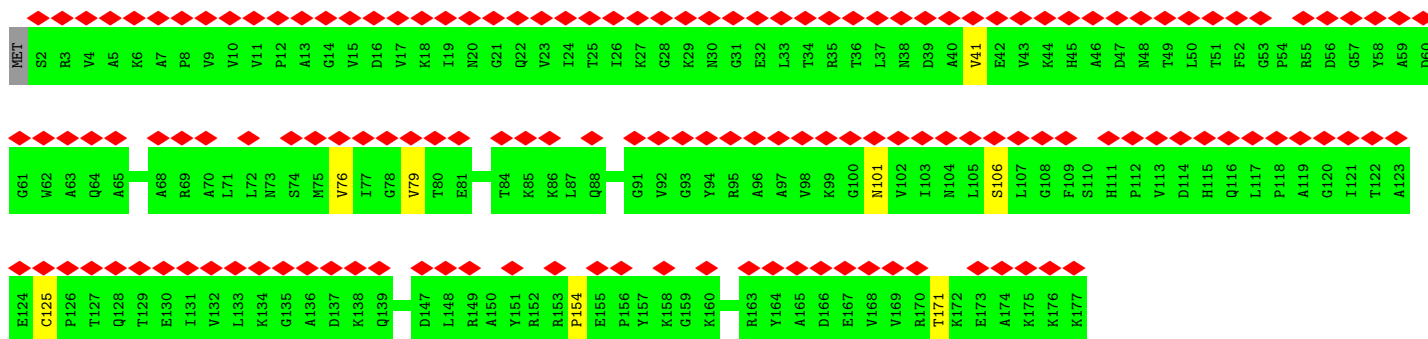


- Molecule 6: Large ribosomal subunit protein uL5

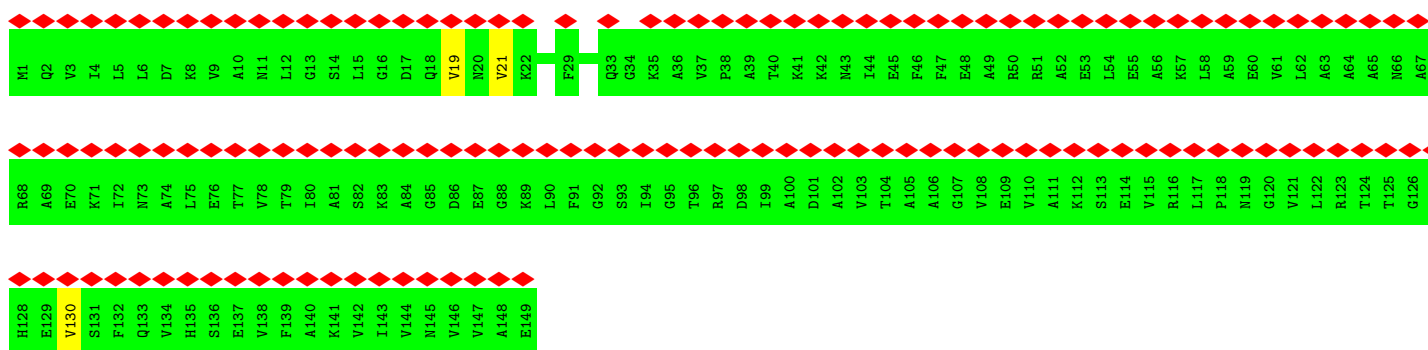


- Molecule 7: Large ribosomal subunit protein uL6

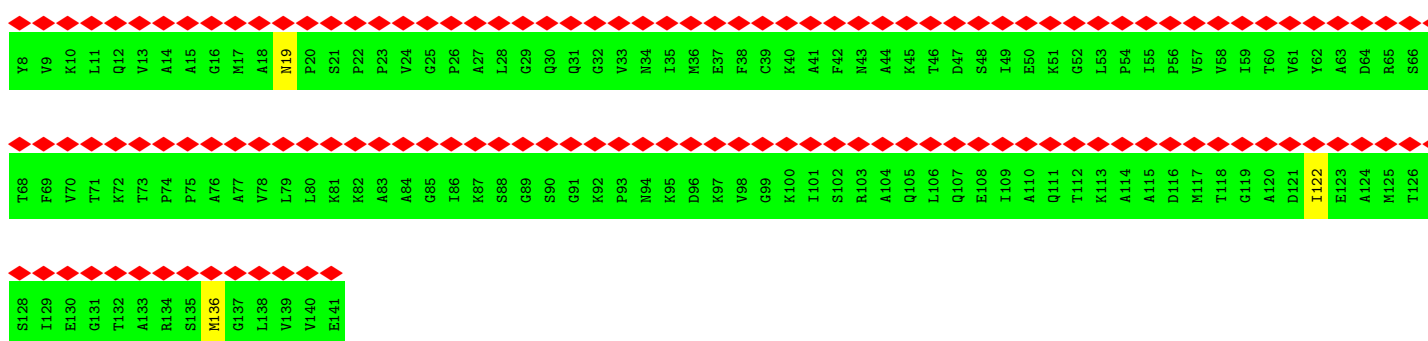




• Molecule 8: Large ribosomal subunit protein bL9



• Molecule 9: Large ribosomal subunit protein uL11



• Molecule 10: Large ribosomal subunit protein uL13



• Molecule 11: Large ribosomal subunit protein uL14

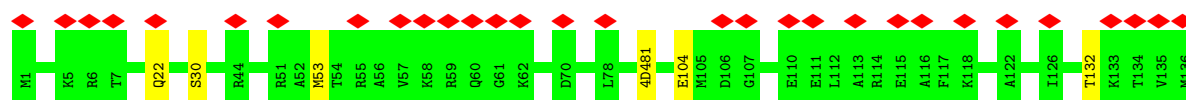




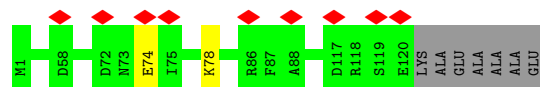
- Molecule 12: Large ribosomal subunit protein uL15



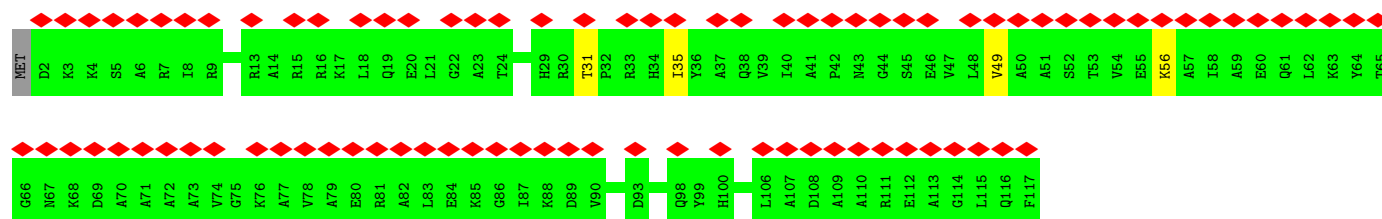
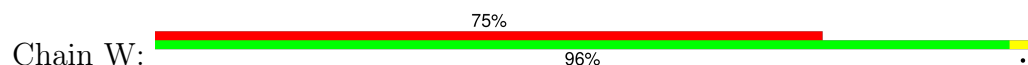
- Molecule 13: 50S ribosomal protein L16



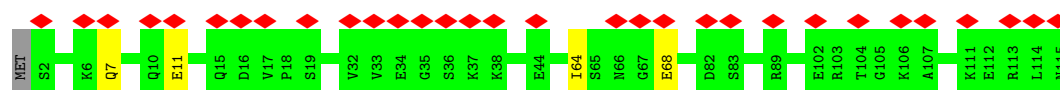
- Molecule 14: Large ribosomal subunit protein bL17



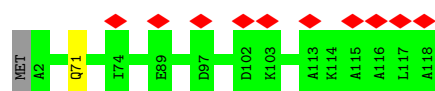
- Molecule 15: Large ribosomal subunit protein uL18



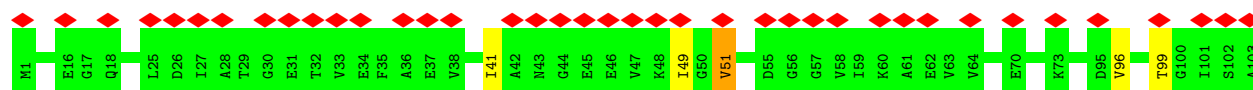
- Molecule 16: Large ribosomal subunit protein bL19



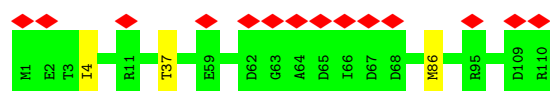
- Molecule 17: 50S ribosomal protein L20



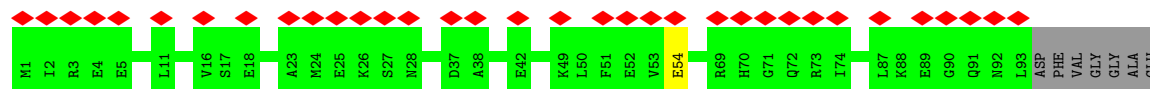
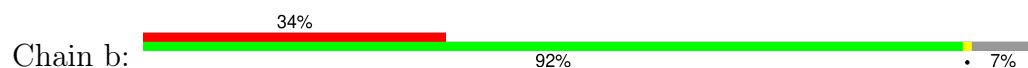
- Molecule 18: Ribosomal protein L21



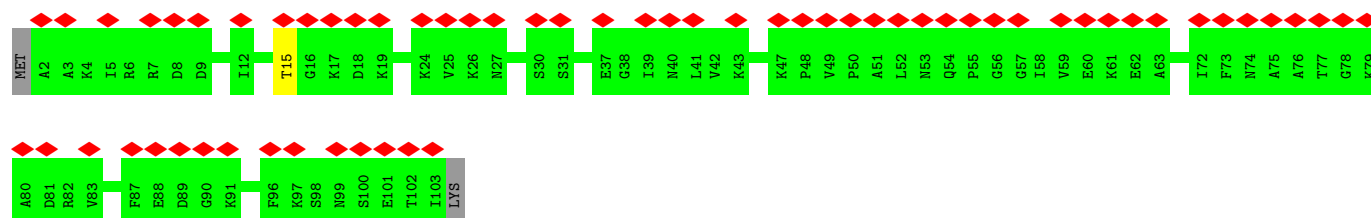
- Molecule 19: 50S ribosomal protein L22



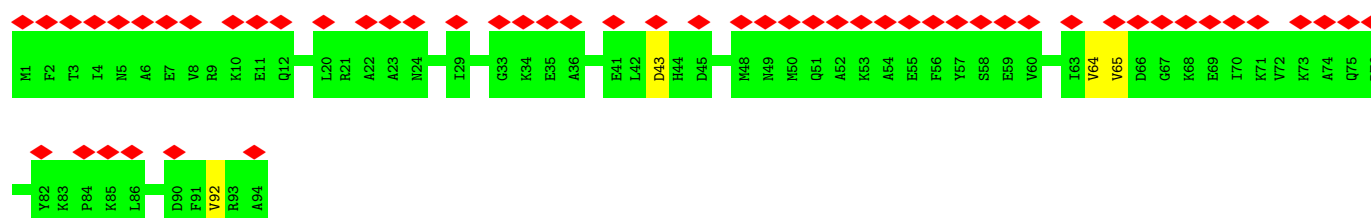
- Molecule 20: 50S ribosomal protein L23



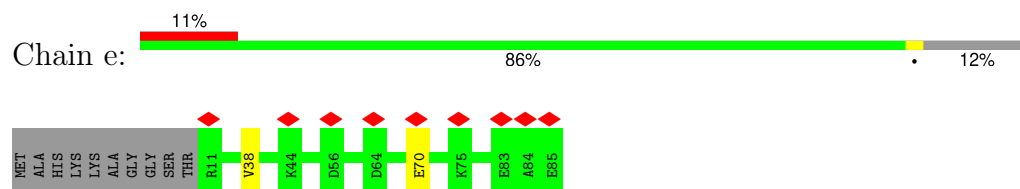
- Molecule 21: 50S ribosomal protein L24



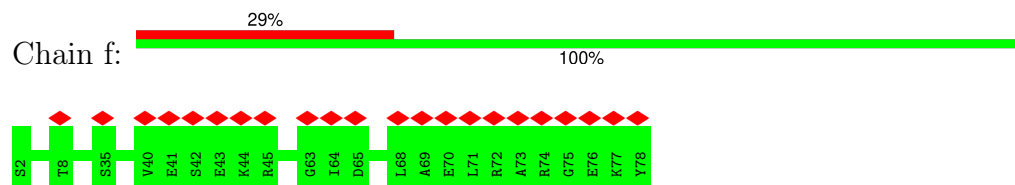
- Molecule 22: Large ribosomal subunit protein bL25



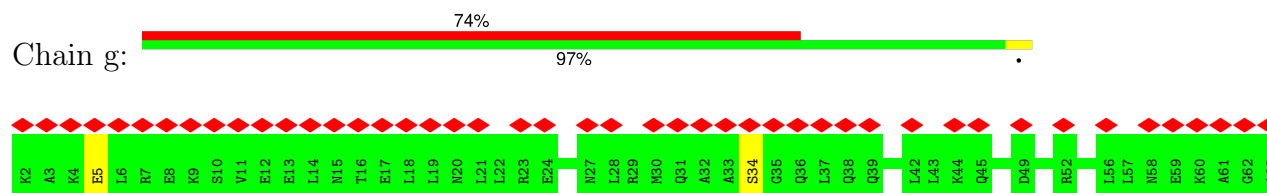
- Molecule 23: 50S ribosomal protein L27



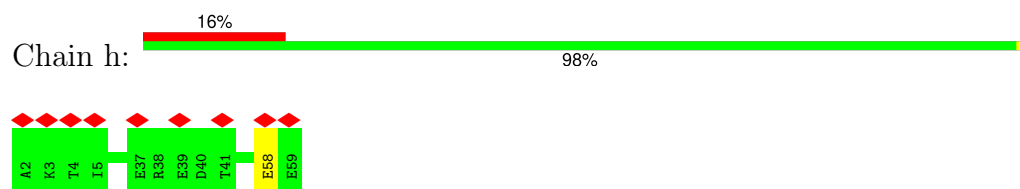
- Molecule 24: 50S ribosomal protein L28



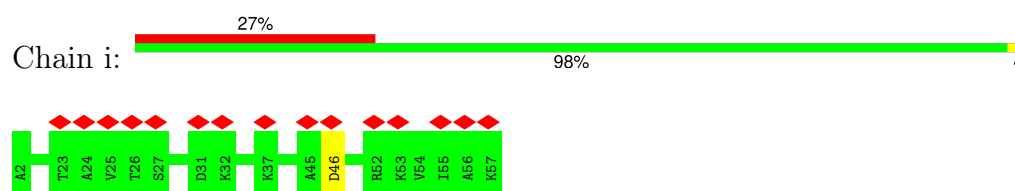
- Molecule 25: Large ribosomal subunit protein uL29



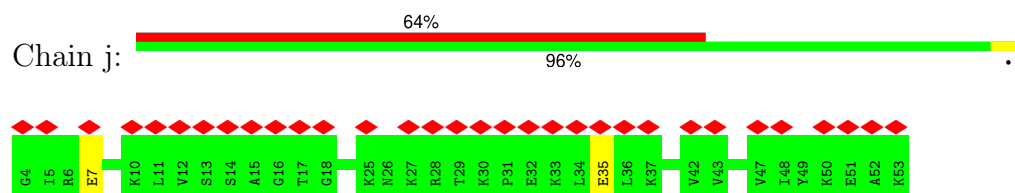
- Molecule 26: 50S ribosomal protein L30



- Molecule 27: 50S ribosomal protein L32

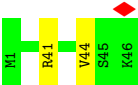


- Molecule 28: Large ribosomal subunit protein bL33

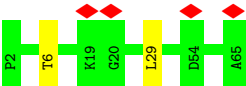


- Molecule 29: 50S ribosomal protein L34

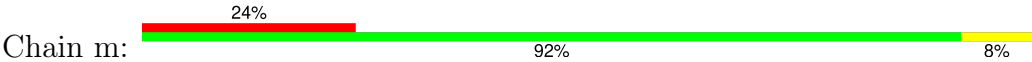




- Molecule 30: Large ribosomal subunit protein bL35



- Molecule 31: 50S ribosomal protein L36



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	569471	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.266	Depositor
Minimum map value	-1.344	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	429.24002, 429.24002, 429.24002	wwPDB
Map dimensions	588, 588, 588	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.73, 0.73, 0.73	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: A1C7K, NA, OMG, PSU, ZN, G7M, MG, 5MC, 4D4, 2MG, OMU, 2MA, 3TD, 5MU, H2U, 1MG, OMC, 6MZ

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	I	0.46	0/69121	0.42	0/107828
2	J	0.34	0/2828	0.34	0/4410
3	K	0.38	0/2132	0.53	1/2866 (0.0%)
4	L	0.38	0/1586	0.48	0/2134
5	M	0.35	0/1571	0.47	0/2113
6	N	0.26	0/1434	0.54	0/1926
7	O	0.27	0/1343	0.51	2/1816 (0.1%)
8	P	0.20	0/1121	0.49	0/1515
9	Q	0.21	0/993	0.50	0/1341
10	R	0.35	0/1152	0.43	0/1551
11	S	0.36	0/947	0.47	0/1268
12	T	0.36	0/1062	0.52	0/1413
13	U	0.35	0/1081	0.47	0/1443
14	V	0.39	0/973	0.50	0/1301
15	W	0.30	0/902	0.45	0/1209
16	X	0.34	0/929	0.45	0/1242
17	Y	0.38	0/960	0.44	0/1278
18	Z	0.36	0/829	0.46	0/1107
19	a	0.36	0/864	0.48	0/1156
20	b	0.32	0/744	0.44	0/994
21	c	0.34	0/787	0.49	0/1051
22	d	0.31	0/766	0.41	0/1025
23	e	0.35	0/582	0.48	0/769
24	f	0.32	0/635	0.46	0/848
25	g	0.28	0/502	0.44	0/667
26	h	0.34	0/453	0.42	0/605
27	i	0.37	0/450	0.48	0/599
28	j	0.30	0/416	0.47	0/554
29	k	0.41	0/380	0.55	0/498
30	l	0.39	0/513	0.50	0/676
31	m	0.36	0/303	0.46	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.43	0/98359	0.43	3/147600 (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
3	K	0	1
9	Q	0	1
18	Z	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	O	154	PRO	CA-C-N	-6.69	111.04	123.55
7	O	154	PRO	C-N-CA	-6.69	111.04	123.55
3	K	233	GLY	N-CA-C	5.21	120.56	111.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	232	HIS	Peptide
9	Q	19	ASN	Peptide
18	Z	51	VAL	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	
3	K	270/273 (99%)	255 (94%)	15 (6%)	0	100	100
4	L	207/209 (99%)	195 (94%)	12 (6%)	0	100	100
5	M	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
6	N	175/179 (98%)	155 (89%)	20 (11%)	0	100	100
7	O	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
8	P	147/149 (99%)	136 (92%)	11 (8%)	0	100	100
9	Q	132/134 (98%)	109 (83%)	23 (17%)	0	100	100
10	R	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
11	S	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
12	T	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
13	U	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
14	V	118/127 (93%)	113 (96%)	5 (4%)	0	100	100
15	W	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
16	X	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
17	Y	115/118 (98%)	115 (100%)	0	0	100	100
18	Z	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
19	a	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
20	b	91/100 (91%)	84 (92%)	7 (8%)	0	100	100
21	c	100/104 (96%)	92 (92%)	8 (8%)	0	100	100
22	d	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
23	e	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
24	f	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
25	g	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
26	h	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
27	i	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
28	j	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
29	k	44/46 (96%)	44 (100%)	0	0	100	100
30	l	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
31	m	36/38 (95%)	36 (100%)	0	0	100	100
All	All	3298/3391 (97%)	3123 (95%)	175 (5%)	0	100	100



There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	217/218 (100%)	214 (99%)	3 (1%)	59	81
4	L	164/164 (100%)	160 (98%)	4 (2%)	43	70
5	M	165/165 (100%)	162 (98%)	3 (2%)	51	77
6	N	148/150 (99%)	141 (95%)	7 (5%)	23	47
7	O	137/138 (99%)	130 (95%)	7 (5%)	21	43
8	P	114/114 (100%)	111 (97%)	3 (3%)	40	68
9	Q	104/104 (100%)	102 (98%)	2 (2%)	50	76
10	R	116/116 (100%)	113 (97%)	3 (3%)	40	68
11	S	103/104 (99%)	102 (99%)	1 (1%)	68	86
12	T	103/103 (100%)	98 (95%)	5 (5%)	22	45
13	U	108/108 (100%)	103 (95%)	5 (5%)	24	48
14	V	100/103 (97%)	98 (98%)	2 (2%)	48	75
15	W	86/87 (99%)	82 (95%)	4 (5%)	23	47
16	X	99/100 (99%)	95 (96%)	4 (4%)	28	54
17	Y	89/90 (99%)	88 (99%)	1 (1%)	65	84
18	Z	84/84 (100%)	79 (94%)	5 (6%)	17	36
19	a	93/93 (100%)	90 (97%)	3 (3%)	34	62
20	b	80/84 (95%)	79 (99%)	1 (1%)	61	82
21	c	83/85 (98%)	82 (99%)	1 (1%)	63	83
22	d	78/78 (100%)	74 (95%)	4 (5%)	21	43
23	e	57/63 (90%)	55 (96%)	2 (4%)	32	58
24	f	67/67 (100%)	67 (100%)	0	100	100
25	g	54/54 (100%)	52 (96%)	2 (4%)	30	57
26	h	48/48 (100%)	47 (98%)	1 (2%)	47	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	i	47/47 (100%)	46 (98%)	1 (2%)	47 74
28	j	45/45 (100%)	43 (96%)	2 (4%)	25 50
29	k	38/38 (100%)	36 (95%)	2 (5%)	20 42
30	l	51/51 (100%)	49 (96%)	2 (4%)	28 55
31	m	34/34 (100%)	31 (91%)	3 (9%)	9 20
All	All	2712/2735 (99%)	2629 (97%)	83 (3%)	36 62

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	5	LYS
3	K	130	LEU
3	K	204	VAL
4	L	7	LYS
4	L	74	GLU
4	L	150	GLN
4	L	151	THR
5	M	100	MET
5	M	171	ASP
5	M	185	LYS
6	N	4	LEU
6	N	25	VAL
6	N	74	VAL
6	N	78	LYS
6	N	92	ARG
6	N	132	VAL
6	N	147	ASP
7	O	41	VAL
7	O	76	VAL
7	O	79	VAL
7	O	101	ASN
7	O	106	SER
7	O	125	CYS
7	O	171	THR
8	P	19	VAL
8	P	21	VAL
8	P	130	VAL
9	Q	122	ILE
9	Q	136	MET
10	R	11	VAL

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Mol	Chain	Res	Type
10	R	90	GLU
10	R	128	ASN
11	S	6	THR
12	T	10	GLU
12	T	14	LYS
12	T	94	THR
12	T	106	GLU
12	T	129	LYS
13	U	22	GLN
13	U	30	SER
13	U	53	MET
13	U	104	GLU
13	U	132	THR
14	V	74	GLU
14	V	78	LYS
15	W	31	THR
15	W	35	ILE
15	W	49	VAL
15	W	56	LYS
16	X	7	GLN
16	X	11	GLU
16	X	64	ILE
16	X	68	GLU
17	Y	71	GLN
18	Z	41	ILE
18	Z	49	ILE
18	Z	51	VAL
18	Z	96	VAL
18	Z	99	THR
19	a	4	ILE
19	a	37	THR
19	a	86	MET
20	b	54	GLU
21	c	15	THR
22	d	43	ASP
22	d	64	VAL
22	d	65	VAL
22	d	92	VAL
23	e	38	VAL
23	e	70	GLU
25	g	5	GLU
25	g	34	SER

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Mol	Chain	Res	Type
26	h	58	GLU
27	i	46	ASP
28	j	7	GLU
28	j	35	GLU
29	k	41	ARG
29	k	44	VAL
30	l	6	THR
30	l	29	LEU
31	m	2	LYS
31	m	12	ARG
31	m	16	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
3	K	86	ASN
3	K	260	ASN
4	L	126	ASN
4	L	185	ASN
5	M	92	HIS
5	M	195	GLN
7	O	38	ASN
7	O	104	ASN
8	P	2	GLN
9	Q	19	ASN
9	Q	107	GLN
9	Q	111	GLN
11	S	5	GLN
11	S	9	ASN
11	S	29	HIS
12	T	35	HIS
14	V	9	GLN
14	V	31	HIS
15	W	100	HIS
16	X	66	ASN
17	Y	59	GLN
18	Z	43	ASN
19	a	7	HIS
21	c	69	ASN
22	d	5	ASN
22	d	12	GLN
23	e	76	ASN

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Mol	Chain	Res	Type
24	f	16	ASN
25	g	20	ASN
26	h	20	HIS
29	k	26	ASN
29	k	29	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	2896/2904 (99%)	464 (16%)	22 (0%)
2	J	117/120 (97%)	18 (15%)	0
All	All	3013/3024 (99%)	482 (15%)	22 (0%)

All (482) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	2	G
1	I	10	A
1	I	12	U
1	I	22	C
1	I	33	C
1	I	34	U
1	I	42	A
1	I	44	A
1	I	45	G
1	I	46	G
1	I	58	G
1	I	71	A
1	I	74	A
1	I	75	G
1	I	101	A
1	I	102	U
1	I	118	A
1	I	119	A
1	I	120	U
1	I	135	U
1	I	139	U
1	I	140	C
1	I	141	G
1	I	142	A
1	I	163	C

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Mol	Chain	Res	Type
1	I	181	A
1	I	196	A
1	I	199	A
1	I	212	G
1	I	215	G
1	I	216	A
1	I	221	A
1	I	222	A
1	I	224	U
1	I	233	A
1	I	248	G
1	I	264	C
1	I	265	A
1	I	266	G
1	I	272	A
1	I	276	U
1	I	281	C
1	I	283	G
1	I	285	G
1	I	295	G
1	I	304	U
1	I	311	A
1	I	328	U
1	I	329	G
1	I	330	A
1	I	331	C
1	I	345	A
1	I	346	A
1	I	361	G
1	I	362	A
1	I	371	A
1	I	372	G
1	I	386	G
1	I	388	G
1	I	400	G
1	I	403	U
1	I	405	U
1	I	411	G
1	I	424	G
1	I	454	A
1	I	456	C
1	I	457	A

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Mol	Chain	Res	Type
1	I	476	G
1	I	480	A
1	I	481	G
1	I	491	G
1	I	503	A
1	I	504	A
1	I	505	A
1	I	509	C
1	I	530	G
1	I	531	C
1	I	532	A
1	I	538	A
1	I	541	A
1	I	546	U
1	I	548	G
1	I	549	G
1	I	552	U
1	I	563	A
1	I	573	U
1	I	574	A
1	I	575	A
1	I	586	A
1	I	588	U
1	I	592	A
1	I	602	A
1	I	603	A
1	I	613	A
1	I	614	A
1	I	615	U
1	I	620	G
1	I	627	A
1	I	637	A
1	I	645	C
1	I	646	U
1	I	647	G
1	I	653	U
1	I	654	A
1	I	655	A
1	I	659	G
1	I	677	A
1	I	685	A
1	I	686	U

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Mol	Chain	Res	Type
1	I	704	G
1	I	710	U
1	I	711	G
1	I	713	G
1	I	720	U
1	I	721	A
1	I	726	G
1	I	730	A
1	I	738	G
1	I	747	5MU
1	I	764	A
1	I	771	G
1	I	775	G
1	I	776	G
1	I	782	A
1	I	784	G
1	I	785	G
1	I	805	G
1	I	812	C
1	I	819	A
1	I	827	U
1	I	828	U
1	I	829	A
1	I	845	A
1	I	846	U
1	I	857	G
1	I	858	G
1	I	877	A
1	I	878	A
1	I	879	G
1	I	880	G
1	I	893	C
1	I	896	A
1	I	897	C
1	I	910	A
1	I	914	G
1	I	915	C
1	I	917	A
1	I	931	U
1	I	941	A
1	I	946	C
1	I	948	C

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Mol	Chain	Res	Type
1	I	961	C
1	I	974	G
1	I	983	A
1	I	989	G
1	I	996	A
1	I	1009	A
1	I	1012	U
1	I	1013	C
1	I	1022	G
1	I	1027	A
1	I	1033	U
1	I	1043	C
1	I	1045	C
1	I	1046	A
1	I	1047	G
1	I	1051	G
1	I	1056	G
1	I	1057	A
1	I	1070	A
1	I	1071	G
1	I	1074	G
1	I	1080	A
1	I	1082	U
1	I	1083	U
1	I	1087	G
1	I	1088	A
1	I	1108	U
1	I	1110	G
1	I	1111	A
1	I	1112	G
1	I	1116	G
1	I	1132	U
1	I	1133	A
1	I	1135	C
1	I	1136	G
1	I	1142	A
1	I	1149	G
1	I	1151	A
1	I	1152	C
1	I	1171	G
1	I	1175	A
1	I	1176	U

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Mol	Chain	Res	Type
1	I	1180	U
1	I	1205	A
1	I	1206	G
1	I	1238	G
1	I	1247	A
1	I	1248	G
1	I	1250	G
1	I	1253	A
1	I	1256	G
1	I	1262	A
1	I	1266	G
1	I	1271	G
1	I	1272	A
1	I	1286	A
1	I	1289	C
1	I	1293	C
1	I	1300	G
1	I	1301	A
1	I	1314	C
1	I	1321	A
1	I	1329	U
1	I	1341	G
1	I	1352	U
1	I	1365	A
1	I	1368	G
1	I	1379	U
1	I	1383	A
1	I	1386	C
1	I	1407	G
1	I	1416	G
1	I	1419	A
1	I	1420	A
1	I	1428	C
1	I	1453	A
1	I	1460	U
1	I	1482	G
1	I	1483	G
1	I	1488	C
1	I	1490	A
1	I	1493	C
1	I	1494	A
1	I	1495	A

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Mol	Chain	Res	Type
1	I	1506	U
1	I	1508	A
1	I	1509	A
1	I	1510	G
1	I	1515	A
1	I	1524	G
1	I	1531	C
1	I	1534	U
1	I	1535	A
1	I	1536	C
1	I	1537	G
1	I	1540	G
1	I	1554	U
1	I	1566	A
1	I	1569	A
1	I	1578	U
1	I	1583	A
1	I	1584	U
1	I	1585	C
1	I	1608	A
1	I	1610	A
1	I	1626	A
1	I	1647	U
1	I	1648	U
1	I	1649	G
1	I	1653	G
1	I	1667	G
1	I	1674	G
1	I	1677	A
1	I	1681	G
1	I	1715	G
1	I	1729	U
1	I	1730	C
1	I	1735	A
1	I	1738	G
1	I	1739	A
1	I	1746	A
1	I	1756	G
1	I	1758	U
1	I	1764	C
1	I	1773	A
1	I	1782	U

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Mol	Chain	Res	Type
1	I	1786	A
1	I	1800	C
1	I	1801	A
1	I	1808	A
1	I	1811	G
1	I	1816	C
1	I	1848	A
1	I	1870	C
1	I	1872	A
1	I	1882	U
1	I	1884	G
1	I	1896	G
1	I	1901	A
1	I	1902	C
1	I	1906	G
1	I	1909	C
1	I	1914	C
1	I	1915	3TD
1	I	1929	G
1	I	1930	G
1	I	1937	A
1	I	1955	U
1	I	1964	G
1	I	1965	C
1	I	1967	C
1	I	1970	A
1	I	1971	U
1	I	1972	G
1	I	1980	G
1	I	1991	U
1	I	1993	U
1	I	1997	C
1	I	2006	C
1	I	2022	U
1	I	2023	C
1	I	2027	G
1	I	2030	6MZ
1	I	2031	A
1	I	2033	A
1	I	2043	C
1	I	2055	C
1	I	2056	G

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Mol	Chain	Res	Type
1	I	2060	A
1	I	2061	G
1	I	2062	A
1	I	2069	G7M
1	I	2095	A
1	I	2109	U
1	I	2110	G
1	I	2111	U
1	I	2112	G
1	I	2113	U
1	I	2115	G
1	I	2116	G
1	I	2117	A
1	I	2118	U
1	I	2123	G
1	I	2124	G
1	I	2126	A
1	I	2127	G
1	I	2128	G
1	I	2131	U
1	I	2132	U
1	I	2133	G
1	I	2142	A
1	I	2146	C
1	I	2147	A
1	I	2157	G
1	I	2158	A
1	I	2163	A
1	I	2164	C
1	I	2168	G
1	I	2169	A
1	I	2171	A
1	I	2172	U
1	I	2173	A
1	I	2175	C
1	I	2183	A
1	I	2189	U
1	I	2190	G
1	I	2198	A
1	I	2204	G
1	I	2211	A
1	I	2224	G

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Mol	Chain	Res	Type
1	I	2225	A
1	I	2226	C
1	I	2238	G
1	I	2249	U
1	I	2268	A
1	I	2279	G
1	I	2283	C
1	I	2287	A
1	I	2288	A
1	I	2297	A
1	I	2302	U
1	I	2305	U
1	I	2308	G
1	I	2318	G
1	I	2322	A
1	I	2325	G
1	I	2333	A
1	I	2334	U
1	I	2343	U
1	I	2345	G
1	I	2347	C
1	I	2361	G
1	I	2366	A
1	I	2383	G
1	I	2385	C
1	I	2391	G
1	I	2402	U
1	I	2403	C
1	I	2406	A
1	I	2423	U
1	I	2425	A
1	I	2426	A
1	I	2429	G
1	I	2430	A
1	I	2431	U
1	I	2435	A
1	I	2441	U
1	I	2448	A
1	I	2449	H2U
1	I	2459	A
1	I	2465	C
1	I	2466	C

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Mol	Chain	Res	Type
1	I	2470	G
1	I	2475	C
1	I	2476	A
1	I	2491	U
1	I	2494	G
1	I	2498	OMC
1	I	2502	G
1	I	2505	G
1	I	2506	U
1	I	2517	C
1	I	2518	A
1	I	2529	G
1	I	2547	A
1	I	2554	U
1	I	2566	A
1	I	2567	G
1	I	2573	C
1	I	2582	G
1	I	2602	A
1	I	2604	PSU
1	I	2605	PSU
1	I	2609	U
1	I	2613	U
1	I	2615	U
1	I	2629	U
1	I	2630	G
1	I	2638	G
1	I	2681	C
1	I	2689	U
1	I	2690	U
1	I	2714	G
1	I	2716	C
1	I	2718	G
1	I	2726	A
1	I	2732	G
1	I	2733	A
1	I	2744	G
1	I	2748	A
1	I	2757	A
1	I	2765	A
1	I	2778	A
1	I	2780	G

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Mol	Chain	Res	Type
1	I	2791	G
1	I	2793	C
1	I	2794	C
1	I	2800	A
1	I	2820	A
1	I	2821	A
1	I	2835	A
1	I	2836	U
1	I	2848	G
1	I	2849	U
1	I	2867	G
1	I	2873	A
1	I	2874	C
1	I	2884	U
1	I	2885	G
1	I	2886	A
1	I	2891	U
1	I	2901	C
1	I	2904	U
2	J	3	C
2	J	9	G
2	J	13	G
2	J	17	C
2	J	24	G
2	J	32	U
2	J	35	C
2	J	41	G
2	J	42	C
2	J	45	A
2	J	56	G
2	J	67	G
2	J	88	C
2	J	89	U
2	J	90	C
2	J	99	A
2	J	109	A
2	J	119	A

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	I	138	U

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Mol	Chain	Res	Type
1	I	271	G
1	I	404	A
1	I	504	A
1	I	764	A
1	I	784	G
1	I	984	A
1	I	1086	A
1	I	1738	G
1	I	1847	A
1	I	2116	G
1	I	2146	C
1	I	2162	G
1	I	2225	A
1	I	2425	A
1	I	2430	A
1	I	2447	G
1	I	2680	U
1	I	2756	U
1	I	2866	U
1	I	2873	A
1	I	2903	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	I	2504	1	18,21,22	1.28	3 (16%)	21,30,33	2.15	4 (19%)
1	5MU	I	1939	1	19,22,23	1.47	4 (21%)	27,32,35	2.24	6 (22%)
1	2MG	I	2445	1	23,26,27	1.16	3 (13%)	33,38,41	2.26	10 (30%)
1	PSU	I	1911	1	18,21,22	0.98	1 (5%)	21,30,33	2.06	4 (19%)
1	PSU	I	955	1	18,21,22	1.32	3 (16%)	21,30,33	2.18	4 (19%)
1	5MC	I	1962	1	19,22,23	1.39	3 (15%)	26,32,35	1.11	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMC	I	2498	32,1	19,22,23	1.05	2 (10%)	25,31,34	1.08	2 (8%)
1	PSU	I	2580	1	18,21,22	1.38	4 (22%)	21,30,33	2.27	7 (33%)
1	6MZ	I	2030	1	22,25,26	1.21	3 (13%)	29,36,39	2.34	9 (31%)
1	2MA	I	2503	32,1	22,25,26	1.41	4 (18%)	32,37,40	2.01	7 (21%)
1	PSU	I	1917	1	18,21,22	1.04	2 (11%)	21,30,33	2.02	3 (14%)
13	4D4	U	81	13	9,11,12	0.92	0	7,13,15	1.58	2 (28%)
1	1MG	I	745	1	23,26,27	1.18	3 (13%)	33,39,42	1.74	6 (18%)
1	H2U	I	2449	1	18,21,22	0.62	0	19,30,33	1.11	1 (5%)
1	PSU	I	2604	1	18,21,22	1.31	3 (16%)	21,30,33	2.32	6 (28%)
1	G7M	I	2069	1	23,26,27	0.67	0	34,39,42	0.87	1 (2%)
1	OMG	I	2251	1	23,26,27	0.99	2 (8%)	32,38,41	1.88	7 (21%)
1	5MU	I	747	1	19,22,23	1.30	3 (15%)	27,32,35	1.92	5 (18%)
1	2MG	I	1835	1	23,26,27	0.91	1 (4%)	33,38,41	2.03	8 (24%)
1	3TD	I	1915	1	19,22,23	1.23	4 (21%)	23,32,35	1.93	3 (13%)
1	PSU	I	2605	1	18,21,22	1.32	3 (16%)	21,30,33	2.23	6 (28%)
1	OMU	I	2552	1	19,22,23	1.39	4 (21%)	25,31,34	2.07	6 (24%)
1	PSU	I	746	1	18,21,22	1.38	4 (22%)	21,30,33	2.11	5 (23%)
1	6MZ	I	1618	1	22,25,26	1.27	2 (9%)	29,36,39	2.20	8 (27%)
1	PSU	I	2457	1	18,21,22	1.32	3 (16%)	21,30,33	2.33	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	I	2504	1	-	2/7/25/26	0/2/2/2
1	5MU	I	1939	1	-	0/7/25/26	0/2/2/2
1	2MG	I	2445	1	-	2/9/27/28	0/3/3/3
1	PSU	I	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	I	955	1	-	0/7/25/26	0/2/2/2
1	5MC	I	1962	1	-	2/7/25/26	0/2/2/2
1	OMC	I	2498	32,1	-	1/9/27/28	0/2/2/2
1	PSU	I	2580	1	-	0/7/25/26	0/2/2/2
1	6MZ	I	2030	1	-	2/9/27/28	0/3/3/3
1	2MA	I	2503	32,1	-	1/7/25/26	0/3/3/3
1	PSU	I	1917	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	4D4	U	81	13	-	0/11/12/14	-
1	1MG	I	745	1	-	0/7/25/26	0/3/3/3
1	H2U	I	2449	1	-	1/7/38/39	0/2/2/2
1	PSU	I	2604	1	-	2/7/25/26	0/2/2/2
1	G7M	I	2069	1	-	1/7/25/26	0/3/3/3
1	OMG	I	2251	1	-	1/9/27/28	0/3/3/3
1	5MU	I	747	1	-	0/7/25/26	0/2/2/2
1	2MG	I	1835	1	-	0/9/27/28	0/3/3/3
1	3TD	I	1915	1	-	2/7/25/26	0/2/2/2
1	PSU	I	2605	1	-	2/7/25/26	0/2/2/2
1	OMU	I	2552	1	-	0/9/27/28	0/2/2/2
1	PSU	I	746	1	-	0/7/25/26	0/2/2/2
1	6MZ	I	1618	1	-	0/9/27/28	0/3/3/3
1	PSU	I	2457	1	-	0/7/25/26	0/2/2/2

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2503	2MA	C5-N7	-3.59	1.32	1.39
1	I	1962	5MC	C5-C4	-3.52	1.41	1.44
1	I	1962	5MC	C2-N1	-3.41	1.32	1.40
1	I	2503	2MA	C6-N1	3.39	1.39	1.35
1	I	1939	5MU	C2-N1	-3.39	1.33	1.38
1	I	1618	6MZ	C6-N6	3.31	1.38	1.34
1	I	745	1MG	C6-N1	-3.13	1.33	1.40
1	I	2604	PSU	C4-N3	-3.07	1.33	1.38
1	I	2552	OMU	C4-N3	-3.06	1.33	1.38
1	I	2605	PSU	C4-N3	-3.03	1.33	1.38
1	I	747	5MU	C2-N1	-3.01	1.33	1.38
1	I	2580	PSU	C4-N3	-2.99	1.33	1.38
1	I	2445	2MG	C6-N1	-2.98	1.33	1.38
1	I	2552	OMU	C2-N1	-2.98	1.33	1.38
1	I	746	PSU	C2-N3	-2.96	1.32	1.37
1	I	955	PSU	C4-N3	-2.94	1.33	1.38
1	I	1939	5MU	C4-N3	-2.90	1.33	1.38
1	I	1939	5MU	C2-N3	-2.88	1.33	1.38
1	I	746	PSU	C4-N3	-2.88	1.33	1.38
1	I	2605	PSU	C2-N3	-2.84	1.32	1.37
1	I	2251	OMG	C6-N1	-2.83	1.33	1.38
1	I	2504	PSU	C4-N3	-2.77	1.33	1.38
1	I	2457	PSU	C4-N3	-2.75	1.33	1.38
1	I	747	5MU	C4-N3	-2.74	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	747	5MU	C2-N3	-2.68	1.33	1.38
1	I	2498	OMC	C2-N1	-2.68	1.34	1.40
1	I	2552	OMU	C2-N3	-2.68	1.33	1.38
1	I	2580	PSU	O4'-C1'	-2.62	1.40	1.43
1	I	1618	6MZ	C5-N7	-2.60	1.34	1.39
1	I	2030	6MZ	C5-N7	-2.58	1.34	1.39
1	I	2457	PSU	C2-N1	-2.55	1.33	1.36
1	I	2604	PSU	C2-N3	-2.54	1.33	1.37
1	I	955	PSU	C2-N3	-2.51	1.33	1.37
1	I	2030	6MZ	C6-N6	2.48	1.37	1.34
1	I	1835	2MG	C6-N1	-2.47	1.34	1.38
1	I	2503	2MA	C2-N3	-2.46	1.29	1.34
1	I	2580	PSU	C2-N3	-2.43	1.33	1.37
1	I	1915	3TD	C4-C5	-2.41	1.42	1.47
1	I	1915	3TD	O4'-C1'	-2.36	1.40	1.43
1	I	1939	5MU	C4-C5	-2.36	1.41	1.44
1	I	746	PSU	O4'-C1'	-2.35	1.40	1.43
1	I	1915	3TD	C4-N3	-2.34	1.35	1.40
1	I	2030	6MZ	C2-N3	-2.30	1.29	1.33
1	I	2580	PSU	C2-N1	-2.29	1.33	1.36
1	I	2445	2MG	C5-N7	-2.27	1.34	1.39
1	I	2504	PSU	C2-N3	-2.24	1.33	1.37
1	I	955	PSU	C2-N1	-2.22	1.33	1.36
1	I	1917	PSU	C4-N3	-2.21	1.34	1.38
1	I	2604	PSU	C2-N1	-2.20	1.33	1.36
1	I	2251	OMG	C5-N7	-2.20	1.34	1.39
1	I	2552	OMU	O4-C4	-2.20	1.20	1.24
1	I	745	1MG	C2-N3	-2.18	1.30	1.33
1	I	1915	3TD	C2-N1	-2.18	1.34	1.37
1	I	2504	PSU	C2-N1	-2.14	1.33	1.36
1	I	745	1MG	C5-N7	-2.14	1.34	1.39
1	I	746	PSU	C2-N1	-2.13	1.33	1.36
1	I	2445	2MG	O6-C6	-2.12	1.19	1.23
1	I	1962	5MC	C2-N3	-2.11	1.32	1.36
1	I	2457	PSU	C2-N3	-2.11	1.34	1.37
1	I	2605	PSU	C2-N1	-2.09	1.33	1.36
1	I	2503	2MA	C5-C6	2.07	1.46	1.41
1	I	1911	PSU	C4-N3	-2.03	1.35	1.38
1	I	1917	PSU	C2-N3	-2.02	1.34	1.37
1	I	2498	OMC	C2-N3	-2.01	1.32	1.36

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	2445	2MG	C2-N3-C4	7.42	121.28	112.00
1	I	1835	2MG	C2-N3-C4	6.87	120.59	112.00
1	I	2604	PSU	N1-C2-N3	6.72	122.26	115.17
1	I	2457	PSU	N1-C2-N3	6.70	122.24	115.17
1	I	2605	PSU	N1-C2-N3	6.61	122.14	115.17
1	I	2580	PSU	N1-C2-N3	6.50	122.03	115.17
1	I	1915	3TD	N1-C2-N3	6.46	120.83	116.13
1	I	955	PSU	N1-C2-N3	6.33	121.84	115.17
1	I	2503	2MA	C5-C4-N3	-6.23	120.62	127.18
1	I	746	PSU	N1-C2-N3	6.22	121.73	115.17
1	I	2504	PSU	N1-C2-N3	6.11	121.61	115.17
1	I	1939	5MU	C4-N3-C2	-5.74	119.81	127.34
1	I	2552	OMU	C4-N3-C2	-5.72	119.51	126.61
1	I	1618	6MZ	C5-C4-N3	-5.69	118.88	126.72
1	I	2445	2MG	C5-C4-N3	-5.68	119.36	128.39
1	I	1911	PSU	N1-C2-N3	5.67	121.15	115.17
1	I	1917	PSU	N1-C2-N3	5.62	121.09	115.17
1	I	1939	5MU	N3-C2-N1	5.56	122.14	114.89
1	I	2251	OMG	C5-C4-N3	-5.40	119.79	128.39
1	I	745	1MG	C5-C4-N3	-5.36	119.86	128.39
1	I	2552	OMU	N3-C2-N1	5.35	121.85	114.89
1	I	2030	6MZ	C5-C4-N3	-5.22	119.53	126.72
1	I	2604	PSU	C4-N3-C2	-5.16	119.27	126.37
1	I	2030	6MZ	C9-N6-C6	-5.12	118.10	122.85
1	I	746	PSU	C4-N3-C2	-5.10	119.35	126.37
1	I	2504	PSU	C4-N3-C2	-5.05	119.41	126.37
1	I	2457	PSU	C4-N3-C2	-5.04	119.44	126.37
1	I	1835	2MG	C5-C4-N3	-5.01	120.42	128.39
1	I	2251	OMG	C2-N3-C4	4.93	120.79	112.30
1	I	1618	6MZ	N3-C4-N9	4.84	135.41	127.17
1	I	955	PSU	C4-N3-C2	-4.79	119.78	126.37
1	I	2503	2MA	N3-C4-N9	4.76	133.03	126.99
1	I	1911	PSU	C4-N3-C2	-4.76	119.81	126.37
1	I	1939	5MU	C5-C4-N3	4.73	119.44	115.32
1	I	747	5MU	C4-N3-C2	-4.73	121.14	127.34
1	I	2605	PSU	C4-N3-C2	-4.72	119.86	126.37
1	I	1917	PSU	C4-N3-C2	-4.71	119.88	126.37
1	I	747	5MU	N3-C2-N1	4.70	121.01	114.89
1	I	747	5MU	C5-C4-N3	4.44	119.18	115.32
1	I	2580	PSU	C4-N3-C2	-4.43	120.27	126.37
1	I	2445	2MG	N9-C4-N3	4.38	134.71	125.95
1	I	2445	2MG	C2-N1-C6	-4.24	119.43	124.55
1	I	2030	6MZ	C5-N7-C8	4.19	110.03	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	745	1MG	C2-N3-C4	4.17	121.36	111.98
1	I	745	1MG	N9-C4-N3	4.15	134.26	125.95
1	I	1915	3TD	C4-N3-C2	-4.15	120.22	124.61
1	I	2457	PSU	O2-C2-N1	-4.14	118.52	122.79
1	I	2503	2MA	N6-C6-N1	4.03	122.47	117.03
1	I	1835	2MG	N9-C4-N3	4.01	133.96	125.95
1	I	2030	6MZ	N3-C4-N9	3.98	133.93	127.17
1	I	1939	5MU	C5-C6-N1	-3.97	119.00	123.31
1	I	2251	OMG	N9-C4-N3	3.97	133.89	125.95
1	I	1962	5MC	C5-C6-N1	-3.94	119.04	123.31
1	I	2030	6MZ	N1-C2-N3	-3.89	122.69	128.58
1	I	1618	6MZ	C5-N7-C8	3.81	109.44	103.45
1	I	1618	6MZ	N1-C2-N3	-3.78	122.86	128.58
1	I	2030	6MZ	C4-C5-N7	-3.73	106.32	110.58
1	I	2552	OMU	C5-C4-N3	3.72	120.01	114.80
1	I	2503	2MA	C5-N7-C8	3.68	109.23	103.45
1	I	1618	6MZ	C2-N3-C4	3.64	120.72	111.83
1	I	2030	6MZ	C2-N3-C4	3.51	120.41	111.83
1	I	747	5MU	C5-C6-N1	-3.48	119.54	123.31
1	I	2504	PSU	O2-C2-N1	-3.36	119.32	122.79
1	I	2449	H2U	C5-C4-N3	-3.28	113.20	116.69
1	I	2580	PSU	C6-N1-C2	-3.25	119.67	122.69
1	I	2604	PSU	O2-C2-N1	-3.25	119.44	122.79
1	I	2030	6MZ	C6-C5-N7	3.13	135.84	132.43
1	I	1917	PSU	O2-C2-N1	-3.12	119.58	122.79
1	I	1911	PSU	O2-C2-N1	-3.11	119.58	122.79
1	I	1835	2MG	C2-N1-C6	-3.05	120.86	124.55
1	I	2069	G7M	C8-N7-C5	-3.01	104.02	107.78
1	I	955	PSU	O2-C2-N1	-3.00	119.69	122.79
1	I	2503	2MA	N9-C8-N7	-2.96	109.74	113.94
1	I	745	1MG	C8-N7-C5	2.91	109.44	104.26
1	I	2580	PSU	O2-C2-N1	-2.89	119.81	122.79
1	I	2030	6MZ	N9-C8-N7	-2.88	109.85	113.94
1	I	1939	5MU	O4-C4-C5	-2.86	121.65	124.92
1	I	1618	6MZ	N9-C8-N7	-2.85	109.89	113.94
1	I	1618	6MZ	C4-C5-N7	-2.82	107.36	110.58
1	I	2552	OMU	CM2-O2'-C2'	-2.82	107.23	114.47
1	I	1618	6MZ	C9-N6-C6	-2.81	120.25	122.85
1	I	2498	OMC	O2-C2-N3	-2.80	117.92	122.33
1	I	2251	OMG	C8-N7-C5	2.79	109.23	104.26
1	I	2457	PSU	C6-N1-C2	-2.78	120.11	122.69
1	I	2445	2MG	C8-N7-C5	2.77	109.20	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	1915	3TD	C1'-C5-C4	2.76	121.80	117.61
1	I	2503	2MA	C4-C5-N7	-2.74	107.45	110.58
13	U	81	4D4	CG-CD-NE	-2.68	104.52	111.88
1	I	2552	OMU	O2-C2-N1	-2.67	119.32	122.80
1	I	2503	2MA	C5-C6-N1	-2.65	114.79	118.90
1	I	2580	PSU	O4'-C1'-C2'	2.64	108.80	105.15
1	I	955	PSU	C6-N1-C2	-2.63	120.25	122.69
1	I	2605	PSU	O2-C2-N3	-2.59	117.25	121.86
1	I	1939	5MU	O2-C2-N1	-2.58	119.43	122.80
1	I	2552	OMU	O4-C4-C5	-2.58	120.71	125.16
1	I	1835	2MG	C8-N7-C5	2.58	108.85	104.26
1	I	2605	PSU	C6-N1-C2	-2.57	120.31	122.69
1	I	2445	2MG	O6-C6-C5	-2.54	119.83	126.53
1	I	2251	OMG	C2-N1-C6	-2.53	120.53	125.11
1	I	746	PSU	C5-C6-N1	-2.45	118.74	122.14
1	I	2604	PSU	C5-C6-N1	-2.43	118.76	122.14
1	I	2605	PSU	C5-C6-N1	-2.43	118.77	122.14
1	I	2445	2MG	C5-C6-N1	2.42	119.41	113.25
1	I	747	5MU	O4-C4-C5	-2.41	122.16	124.92
1	I	746	PSU	O2-C2-N1	-2.36	120.36	122.79
1	I	2604	PSU	C6-N1-C2	-2.35	120.51	122.69
1	I	2504	PSU	C6-N1-C2	-2.34	120.52	122.69
1	I	1962	5MC	CM5-C5-C6	-2.33	119.70	122.85
1	I	1911	PSU	C6-N1-C2	-2.31	120.55	122.69
1	I	2251	OMG	C6-C5-N7	2.30	134.47	130.29
1	I	1835	2MG	C6-C5-N7	2.28	134.45	130.29
1	I	745	1MG	C6-C5-N7	2.28	134.42	129.36
1	I	2580	PSU	C6-C5-C4	2.25	119.69	118.17
1	I	2251	OMG	C4-C5-N7	-2.24	107.12	110.67
1	I	746	PSU	O2-C2-N3	-2.23	117.91	121.86
13	U	81	4D4	NE-CZ-NH2	2.20	124.45	120.67
1	I	1835	2MG	O6-C6-C5	-2.17	120.81	126.53
1	I	745	1MG	C4-C5-N7	-2.13	107.30	110.67
1	I	2605	PSU	O2-C2-N1	-2.11	120.61	122.79
1	I	2445	2MG	C6-C5-N7	2.09	134.10	130.29
1	I	2445	2MG	N9-C8-N7	-2.09	109.53	113.40
1	I	1835	2MG	C5-C6-N1	2.09	118.57	113.25
1	I	2580	PSU	O2-C2-N3	-2.08	118.16	121.86
1	I	2445	2MG	CM2-N2-C2	-2.07	119.20	123.65
1	I	2498	OMC	CM2-O2'-C2'	-2.04	109.25	114.47
1	I	2604	PSU	O2-C2-N3	-2.01	118.30	121.86

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	1915	3TD	O4'-C4'-C5'-O5'
1	I	2251	OMG	C1'-C2'-O2'-CM2
1	I	1915	3TD	C3'-C4'-C5'-O5'
1	I	2504	PSU	O4'-C4'-C5'-O5'
1	I	2604	PSU	C3'-C4'-C5'-O5'
1	I	2604	PSU	O4'-C4'-C5'-O5'
1	I	2030	6MZ	O4'-C4'-C5'-O5'
1	I	2030	6MZ	C3'-C4'-C5'-O5'
1	I	2445	2MG	C3'-C4'-C5'-O5'
1	I	2504	PSU	C3'-C4'-C5'-O5'
1	I	2605	PSU	C3'-C4'-C5'-O5'
1	I	2605	PSU	O4'-C4'-C5'-O5'
1	I	2445	2MG	O4'-C4'-C5'-O5'
1	I	2503	2MA	C4'-C5'-O5'-P
1	I	2498	OMC	O4'-C4'-C5'-O5'
1	I	1962	5MC	C2'-C1'-N1-C6
1	I	1962	5MC	O4'-C1'-N1-C6
1	I	2449	H2U	C4'-C5'-O5'-P
1	I	2069	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 188 ligands modelled in this entry, 187 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
33	A1C7K	I	3184	-	55,57,57	3.90	25 (45%)	67,77,77	1.94	14 (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
33	A1C7K	I	3184	-	-	13/60/70/70	0/4/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	I	3184	A1C7K	C39-N7	9.79	1.48	1.34
33	I	3184	A1C7K	C4-C5	8.61	1.52	1.33
33	I	3184	A1C7K	C7-C5	-8.24	1.35	1.51
33	I	3184	A1C7K	O6-C34	8.04	1.41	1.21
33	I	3184	A1C7K	C25-C26	7.72	1.53	1.38
33	I	3184	A1C7K	C25-C24	-7.11	1.28	1.39
33	I	3184	A1C7K	C1-N1	6.90	1.48	1.34
33	I	3184	A1C7K	C28-C24	6.80	1.49	1.39
33	I	3184	A1C7K	N5-N4	5.99	1.41	1.32
33	I	3184	A1C7K	C24-C23	5.75	1.56	1.47
33	I	3184	A1C7K	C27-N6	5.67	1.49	1.33
33	I	3184	A1C7K	C29-N3	5.54	1.43	1.34
33	I	3184	A1C7K	C3-C4	-5.24	1.34	1.50
33	I	3184	A1C7K	C13-C39	4.32	1.56	1.49
33	I	3184	A1C7K	O4-C34	-4.17	1.24	1.34
33	I	3184	A1C7K	C11-C12	4.16	1.56	1.49
33	I	3184	A1C7K	C15-C1	3.89	1.56	1.48
33	I	3184	A1C7K	O1-C1	-3.79	1.17	1.24
33	I	3184	A1C7K	C29-C23	3.70	1.43	1.37
33	I	3184	A1C7K	C14-C13	3.47	1.38	1.34
33	I	3184	A1C7K	C12-N2	3.03	1.32	1.29
33	I	3184	A1C7K	C28-C27	-2.99	1.32	1.38
33	I	3184	A1C7K	O5-C39	-2.19	1.18	1.23
33	I	3184	A1C7K	O4-C30	-2.15	1.41	1.44
33	I	3184	A1C7K	C26-N6	-2.09	1.28	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	I	3184	A1C7K	O2-C12-N2	-6.17	107.42	114.09
33	I	3184	A1C7K	C3-C4-C5	-5.38	115.31	127.62
33	I	3184	A1C7K	C36-C35-N7	4.75	109.98	103.02
33	I	3184	A1C7K	O2-C14-C13	-4.53	104.77	108.12
33	I	3184	A1C7K	C30-O4-C34	3.60	123.74	117.76
33	I	3184	A1C7K	C9-C8-C7	-3.49	105.83	112.96
33	I	3184	A1C7K	C9-C10-C11	-3.26	109.31	113.89
33	I	3184	A1C7K	O4-C34-C35	3.26	117.57	110.80
33	I	3184	A1C7K	C38-N7-C35	-3.03	107.26	112.01
33	I	3184	A1C7K	C8-C9-C10	-2.57	109.95	115.25
33	I	3184	A1C7K	C6-C5-C7	2.47	120.76	115.28
33	I	3184	A1C7K	C25-C24-C23	-2.43	118.15	120.87
33	I	3184	A1C7K	C25-C26-N6	-2.36	119.56	123.60
33	I	3184	A1C7K	C34-C35-N7	-2.26	107.63	112.08

There are no chirality outliers.

All (13) torsion outliers are listed below:

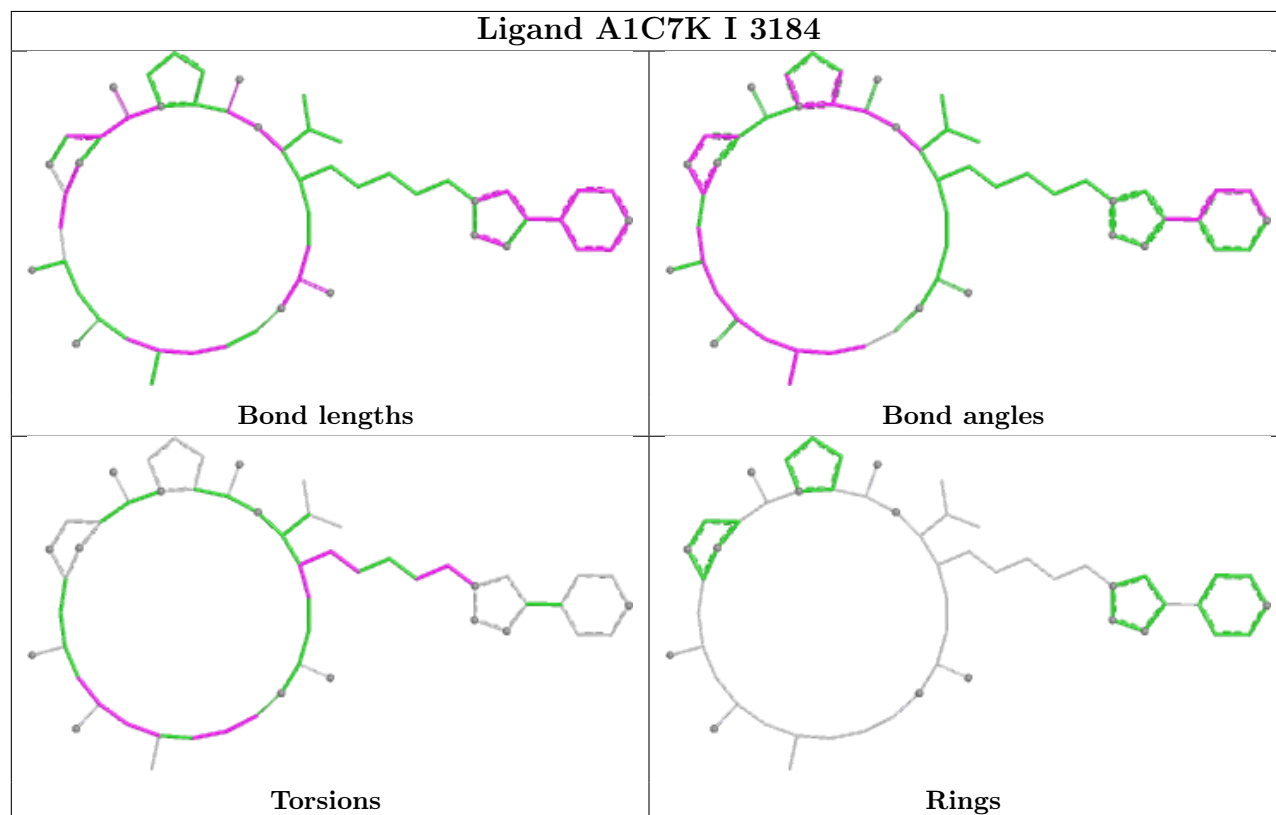
Mol	Chain	Res	Type	Atoms
33	I	3184	A1C7K	C4-C5-C7-C8
33	I	3184	A1C7K	C6-C5-C7-C8
33	I	3184	A1C7K	C5-C7-C8-C9
33	I	3184	A1C7K	C5-C7-C8-O3
33	I	3184	A1C7K	C15-C16-C17-C18
33	I	3184	A1C7K	C16-C17-C18-C19
33	I	3184	A1C7K	N1-C2-C3-C4
33	I	3184	A1C7K	C20-C21-C22-N3
33	I	3184	A1C7K	C2-C3-C4-C5
33	I	3184	A1C7K	O3-C8-C9-C10
33	I	3184	A1C7K	C30-C17-C18-C19
33	I	3184	A1C7K	C17-C18-C19-C20
33	I	3184	A1C7K	C21-C22-N3-C29

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.

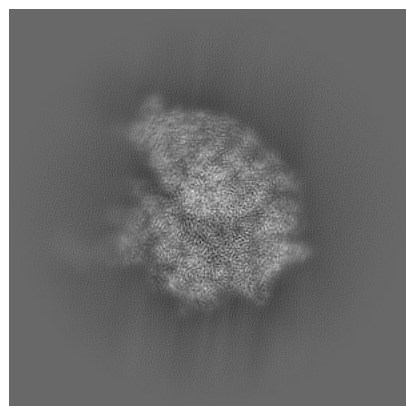
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75389. These allow visual inspection of the internal detail of the map and identification of artifacts.

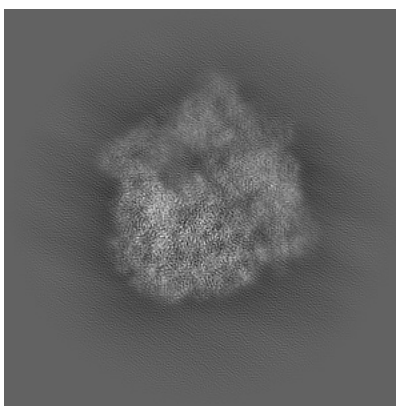
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

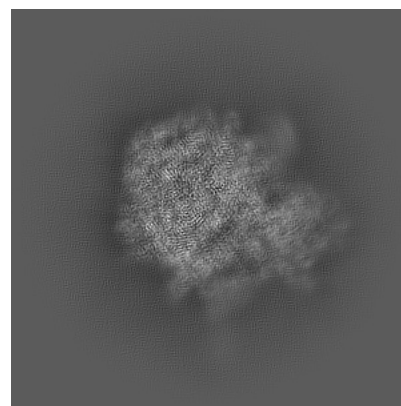
#### 6.1.1 Primary map



X

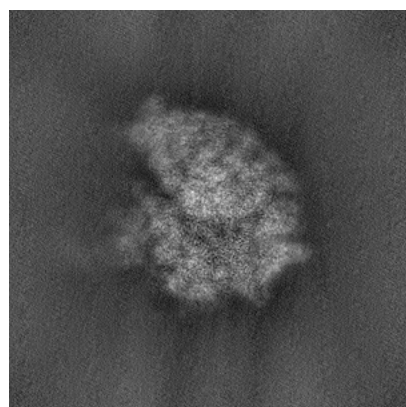


Y

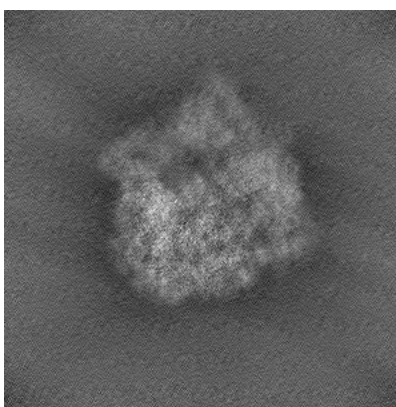


Z

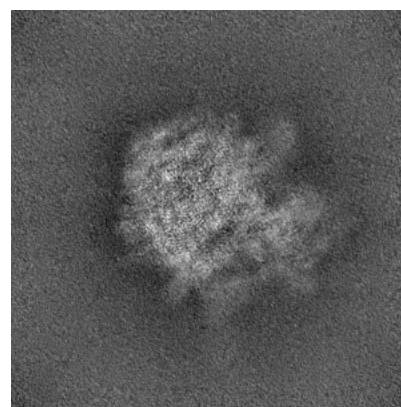
#### 6.1.2 Raw map



X



Y

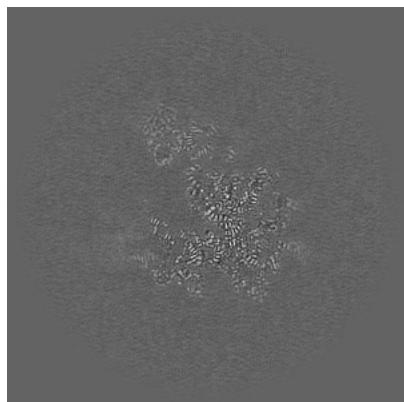


Z

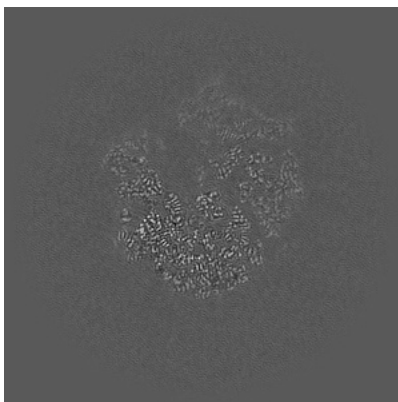
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

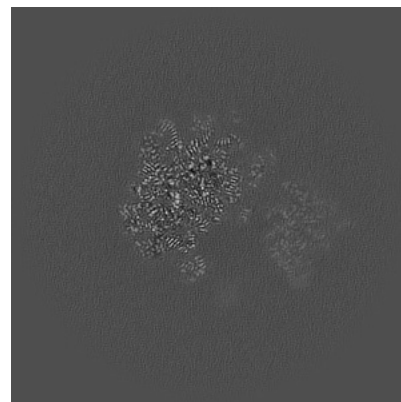
### 6.2.1 Primary map



X Index: 294

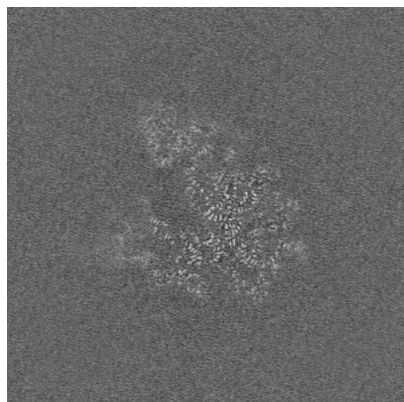


Y Index: 294

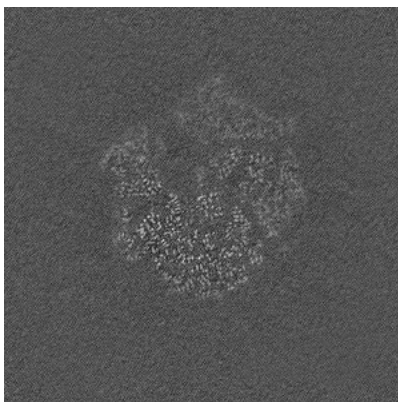


Z Index: 294

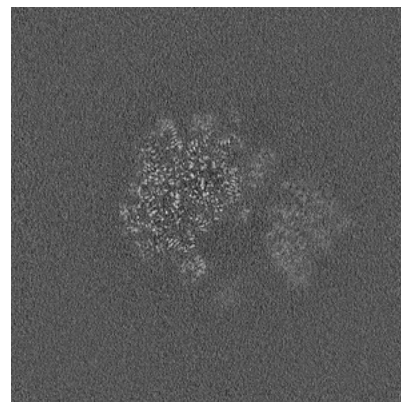
### 6.2.2 Raw map



X Index: 294



Y Index: 294



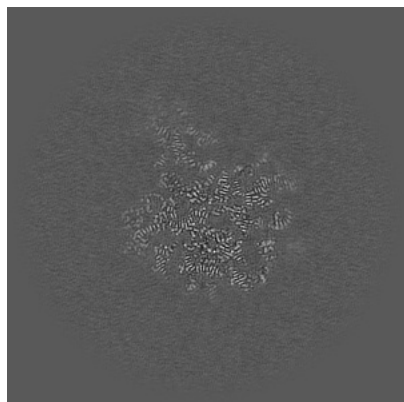
Z Index: 294

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

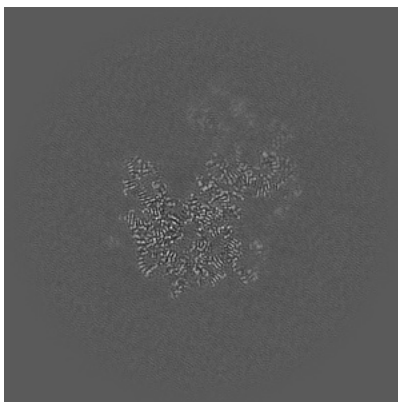


## 6.3 Largest variance slices [i](#)

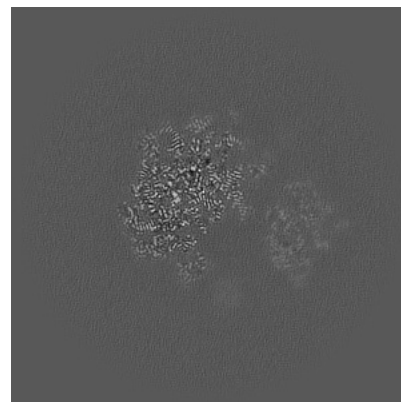
### 6.3.1 Primary map



X Index: 258

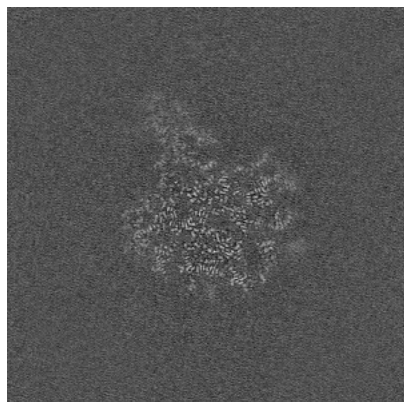


Y Index: 314

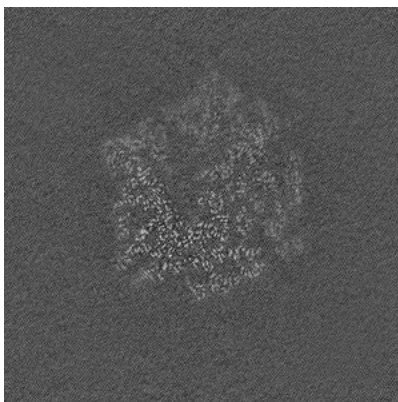


Z Index: 290

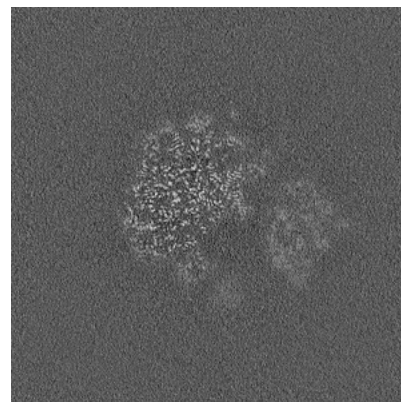
### 6.3.2 Raw map



X Index: 258



Y Index: 284

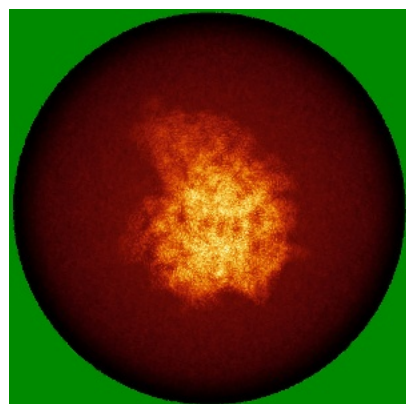


Z Index: 290

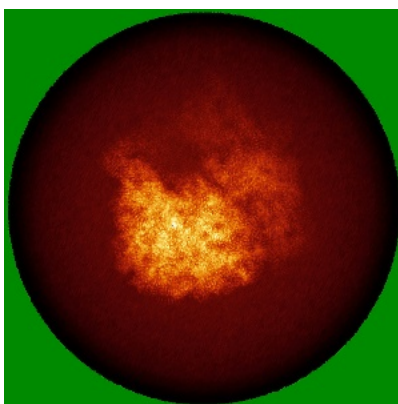
The images above show the largest variance slices of the map in three orthogonal directions.

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

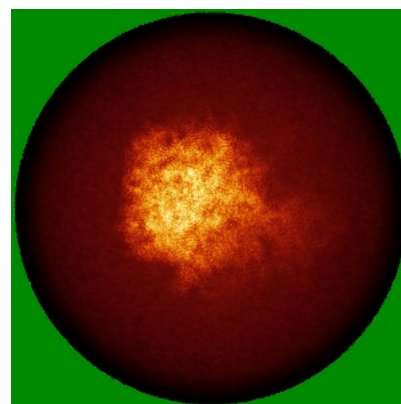
### 6.4.1 Primary map



X

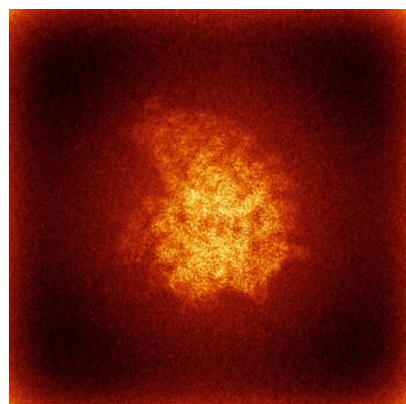


Y

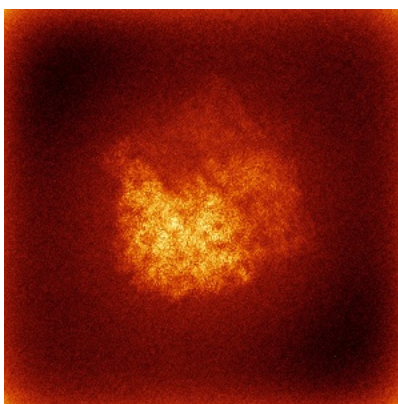


Z

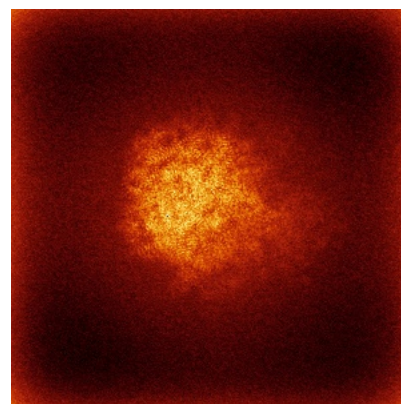
### 6.4.2 Raw map



X



Y

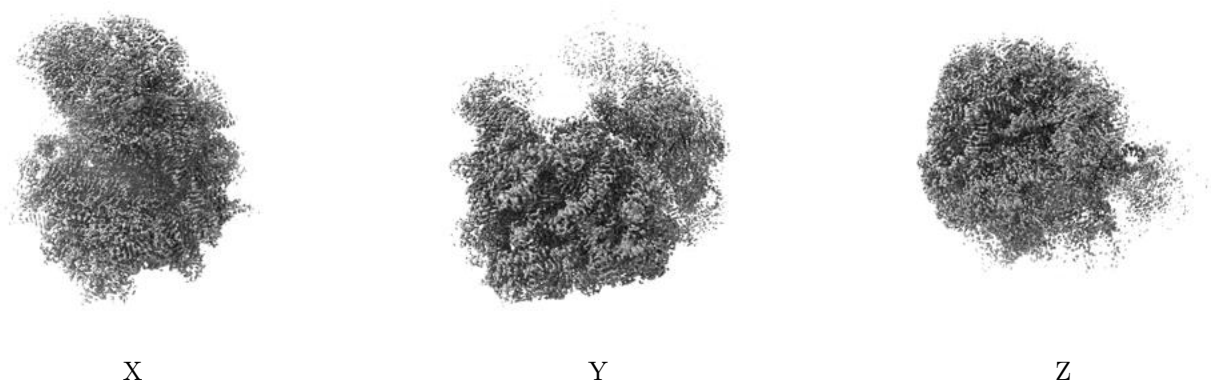


Z

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.

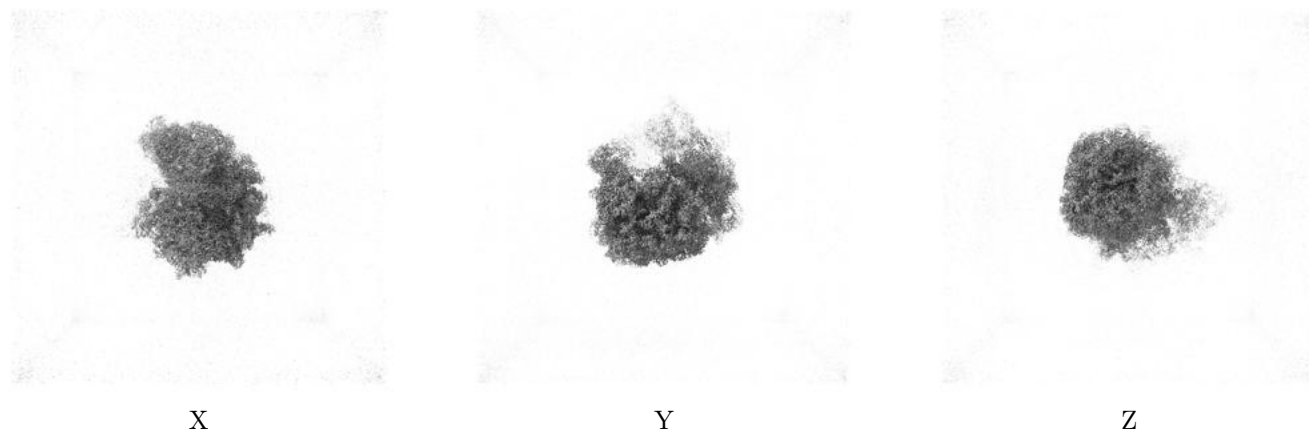
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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](#)

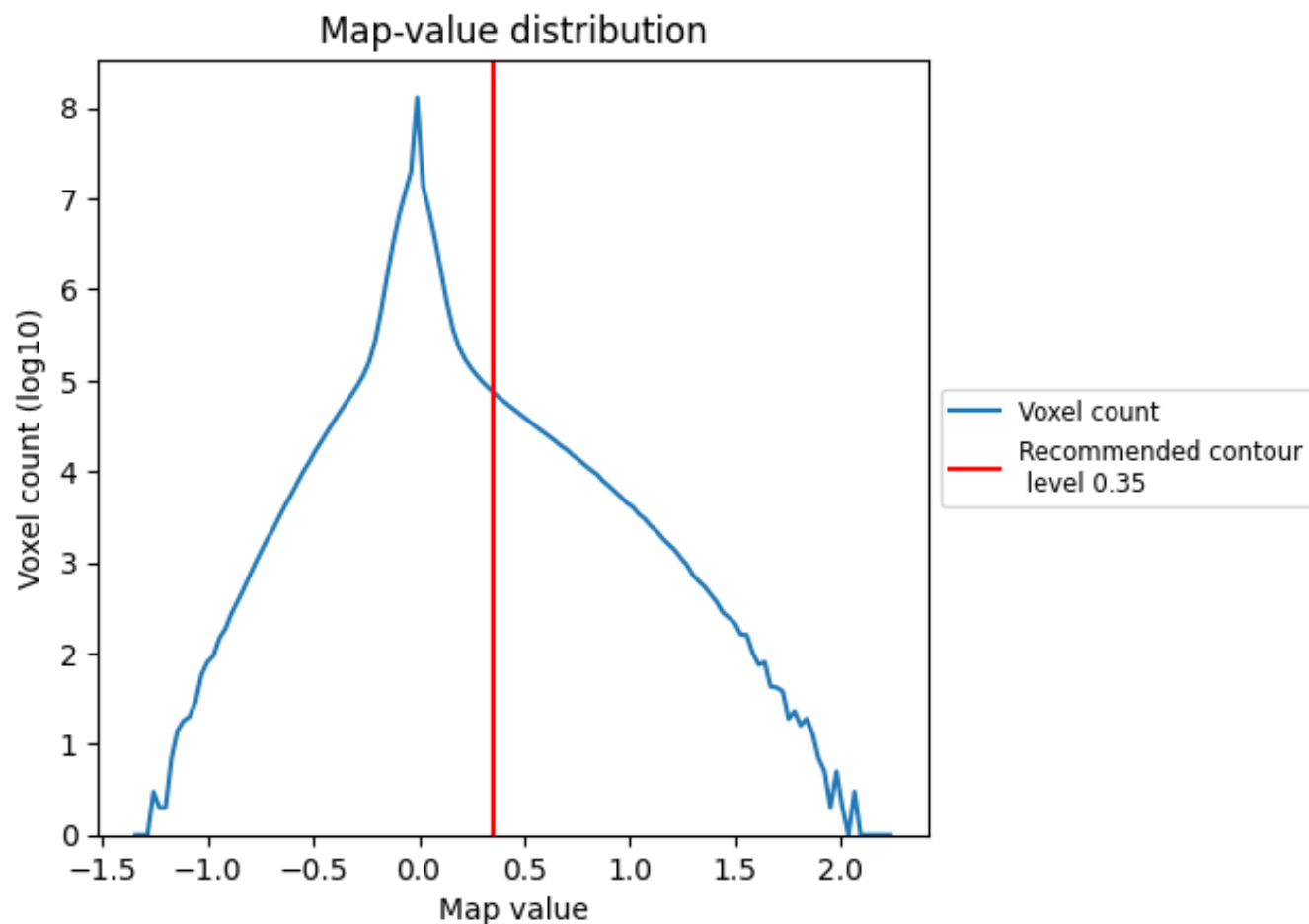
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

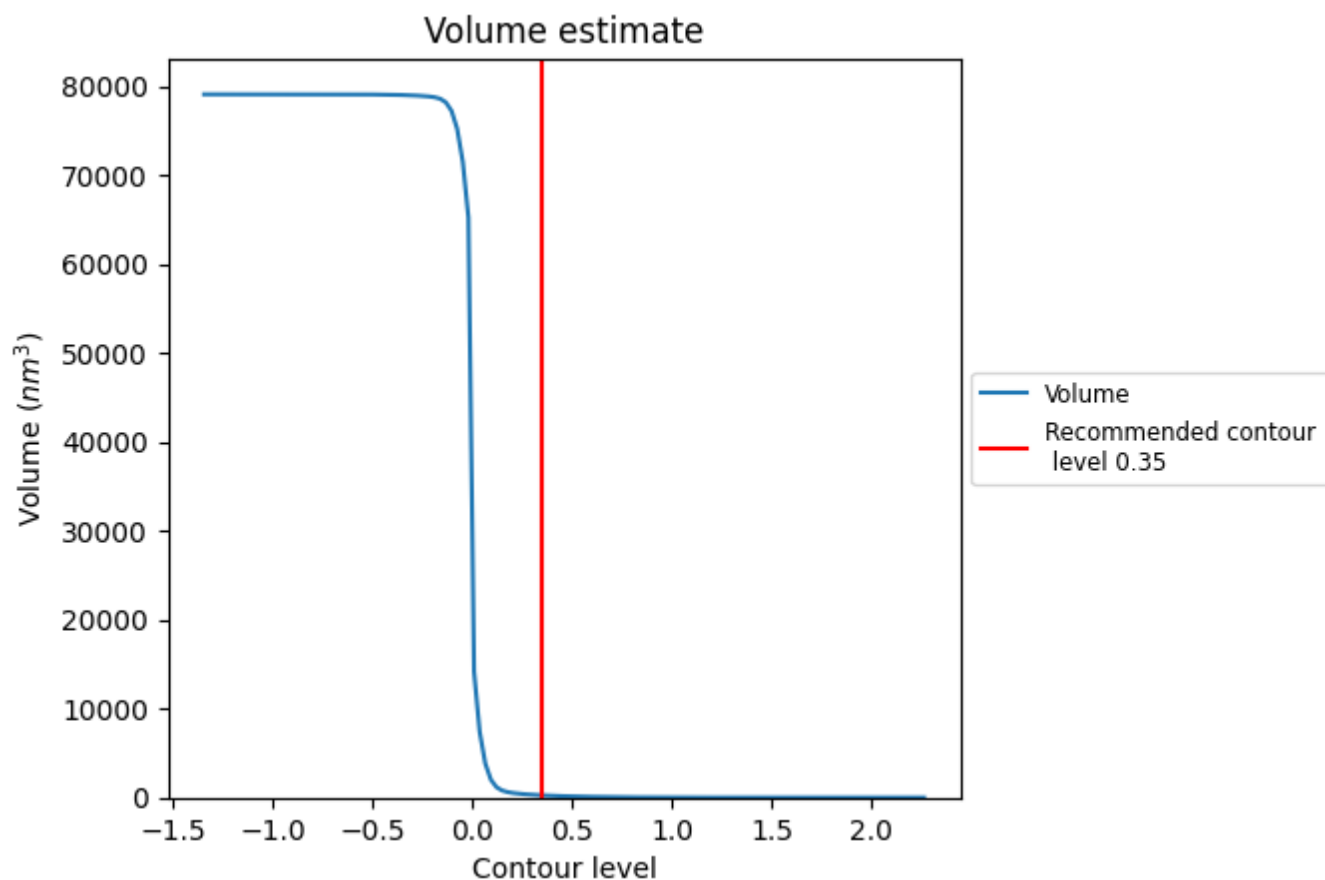
This section contains the results of statistical analysis of the map.

### 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.

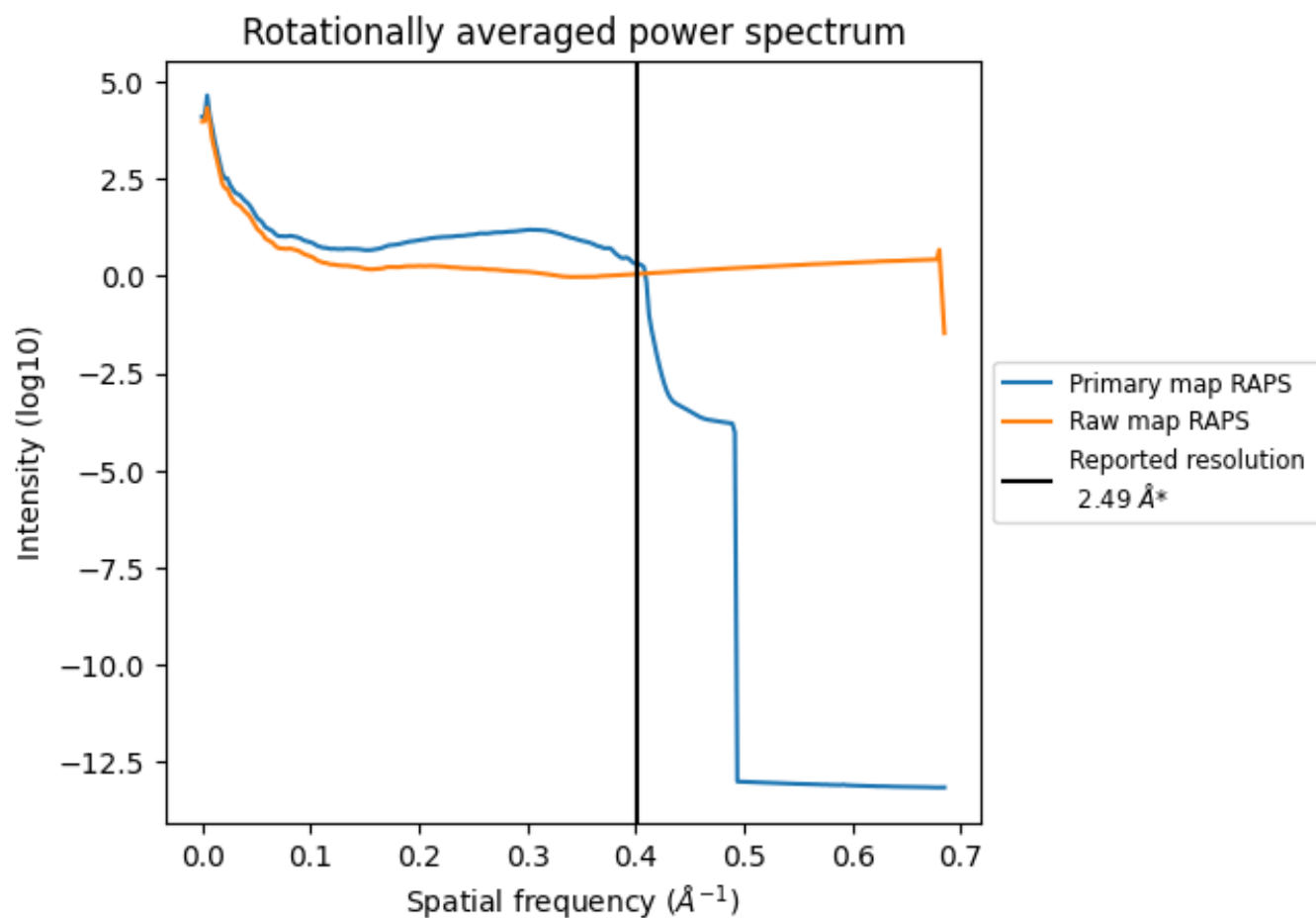
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 251 nm<sup>3</sup>; this corresponds to an approximate mass of 226 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

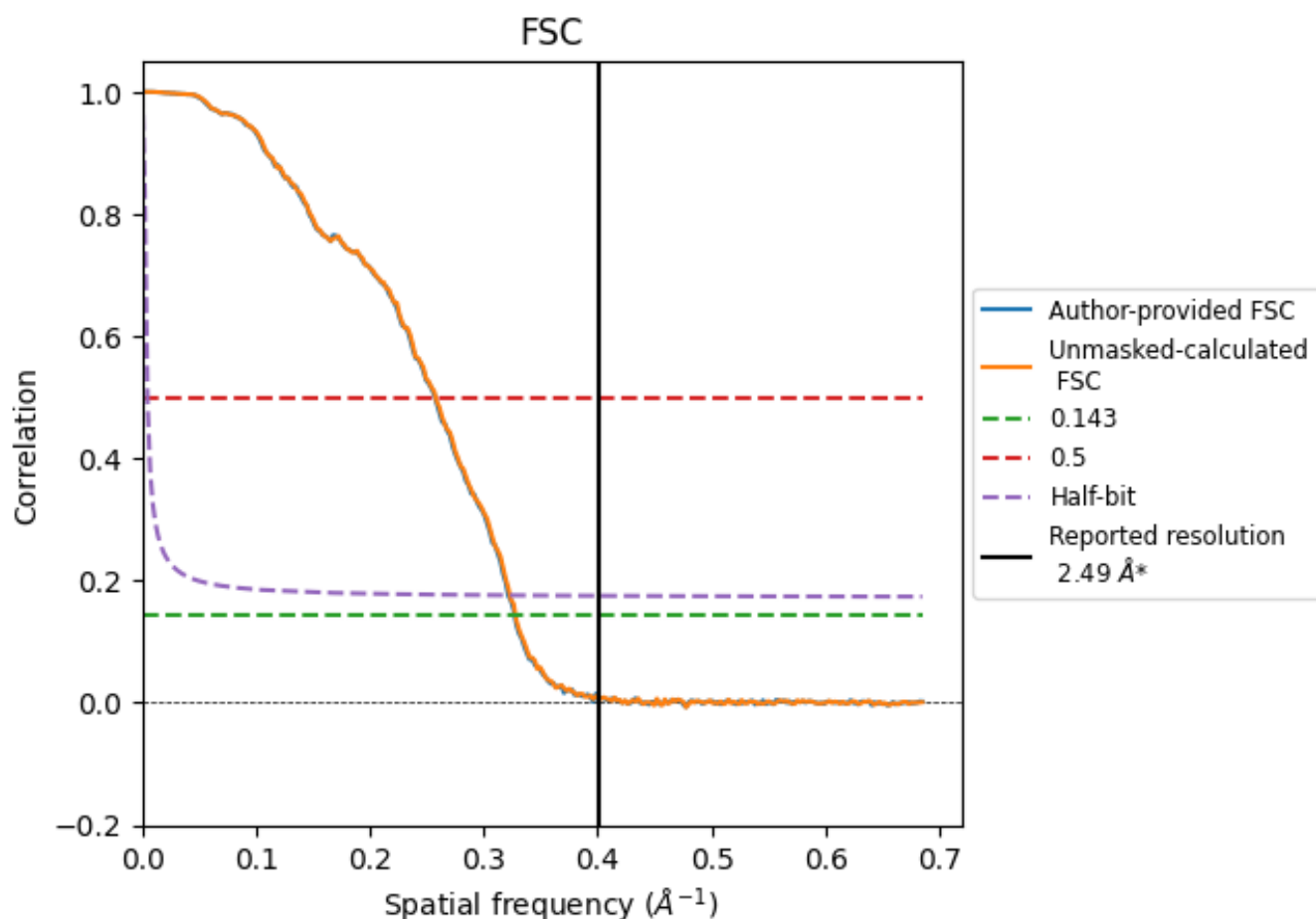


\*Reported resolution corresponds to spatial frequency of 0.402 Å<sup>-1</sup>

## 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 0.402  $\text{\AA}^{-1}$

## 8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.49	-	-
Author-provided FSC curve	3.06	3.89	3.11
Unmasked-calculated*	3.05	3.88	3.10

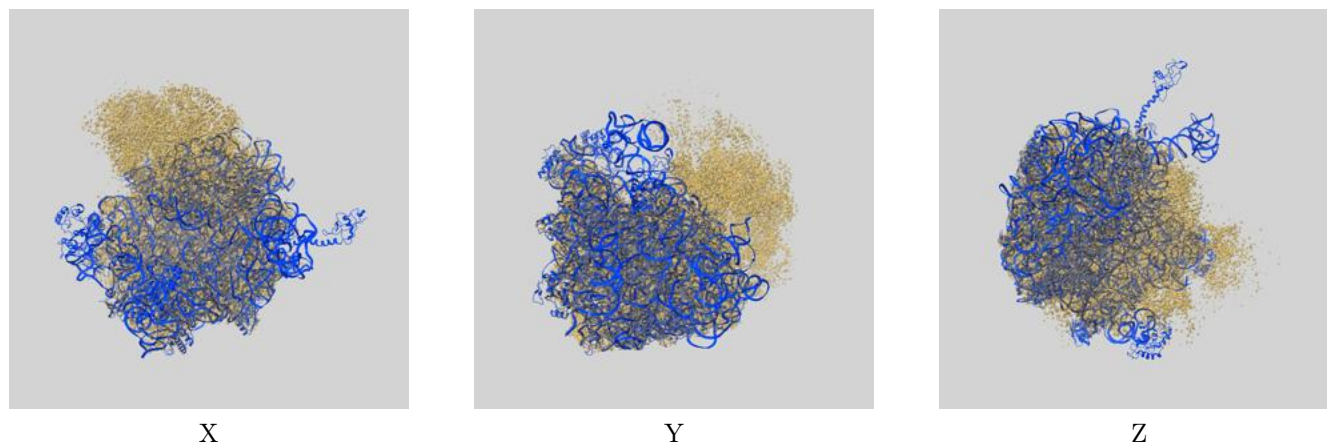
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.06 differs from the reported value 2.49 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.05 differs from the reported value 2.49 by more than 10 %

## 9 Map-model fit [i](#)

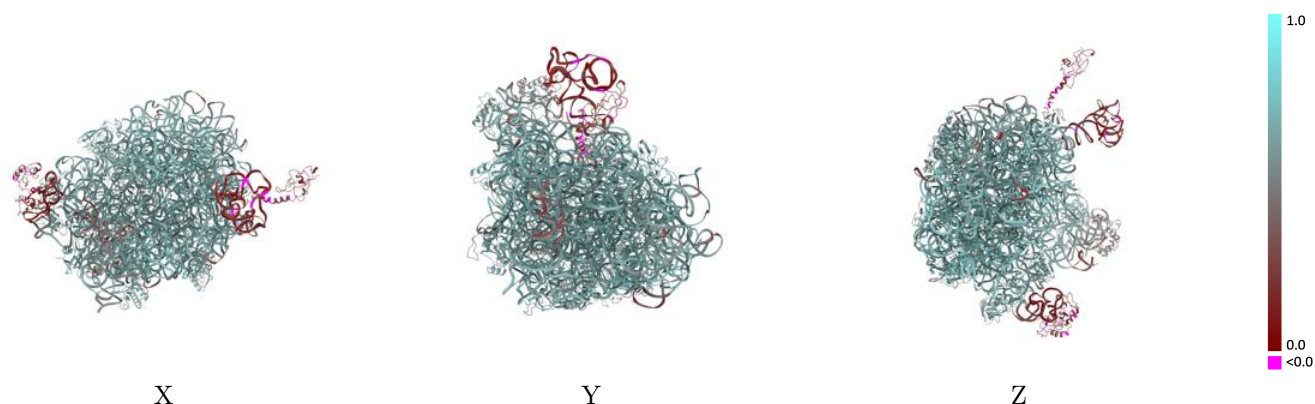
This section contains information regarding the fit between EMDB map EMD-75389 and PDB model 10QM. Per-residue inclusion information can be found in section 3 on page 13.

### 9.1 Map-model overlay [i](#)



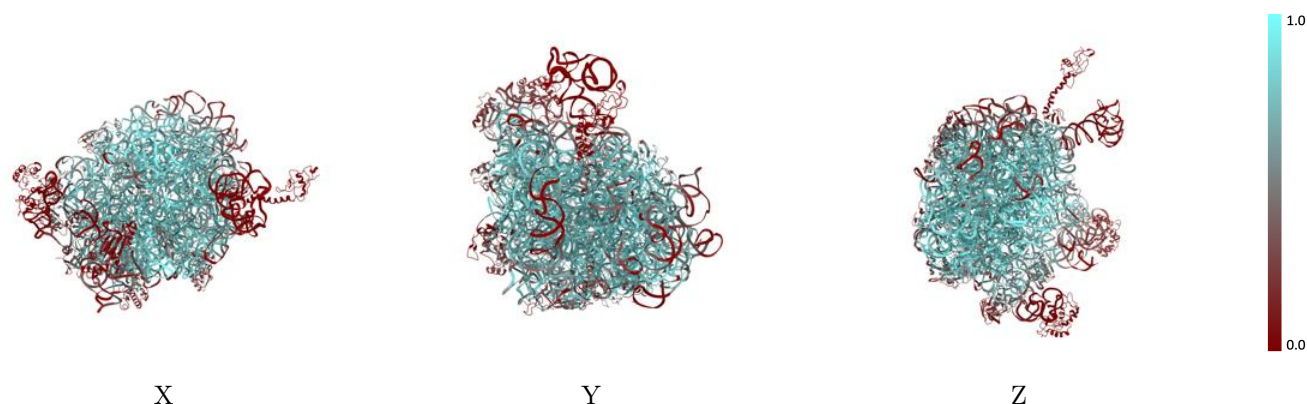
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



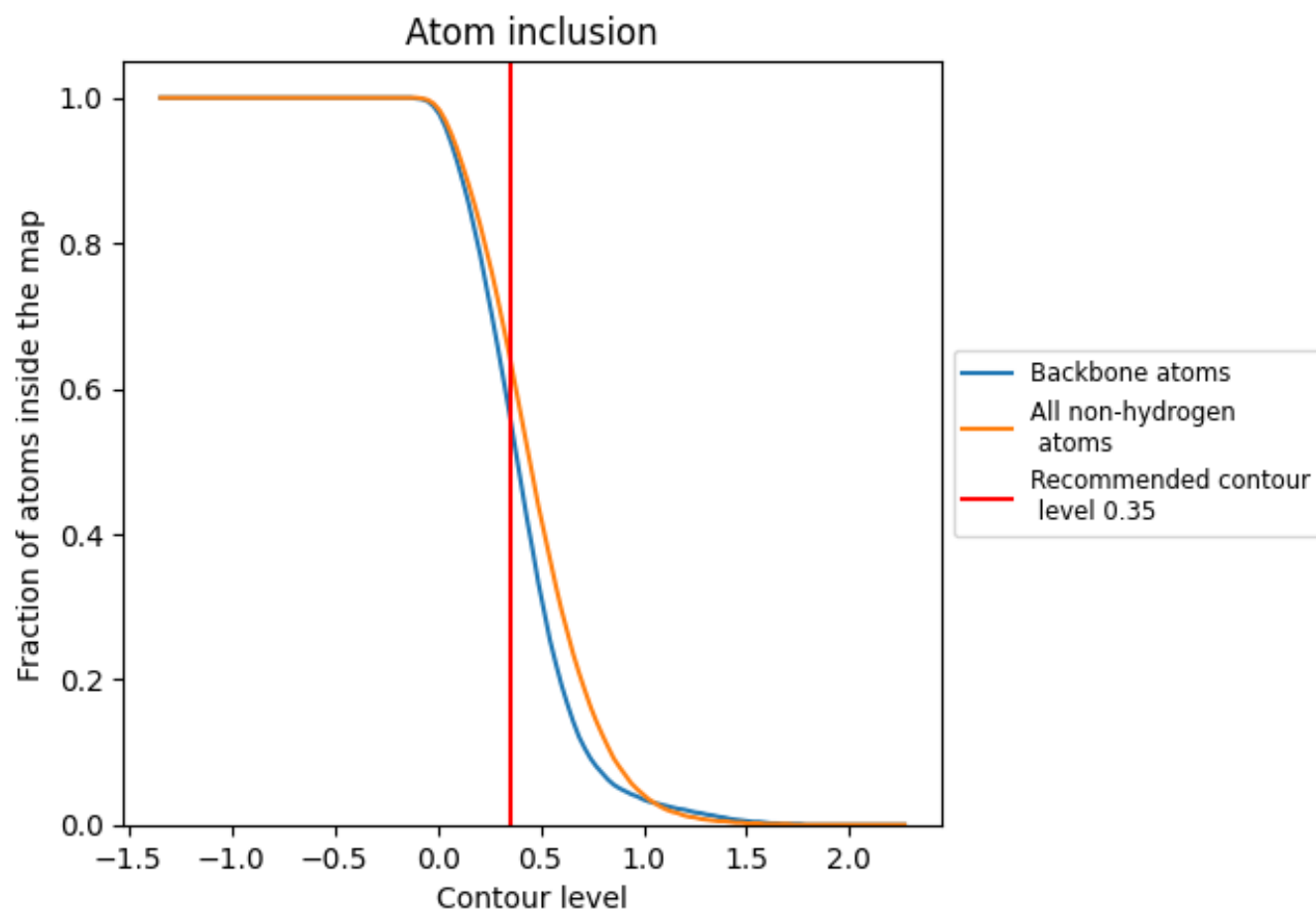
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

## 9.4 Atom inclusion [i](#)



































































At the recommended contour level, 56% of all backbone atoms, 64% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6450	 0.6160
I	 0.7110	 0.6220
J	 0.4630	 0.6030
K	 0.7330	 0.6750
L	 0.6910	 0.6690
M	 0.4920	 0.6290
N	 0.0160	 0.4160
O	 0.1710	 0.5680
P	 0.0570	 0.2780
Q	 0.0000	 0.1950
R	 0.7290	 0.6750
S	 0.6070	 0.6670
T	 0.6250	 0.6560
U	 0.6160	 0.6650
V	 0.7790	 0.6750
W	 0.2740	 0.5920
X	 0.5740	 0.6550
Y	 0.7850	 0.6850
Z	 0.5620	 0.6380
a	 0.6940	 0.6640
b	 0.5230	 0.6210
c	 0.3450	 0.5890
d	 0.4000	 0.6280
e	 0.7100	 0.6630
f	 0.6020	 0.6590
g	 0.2740	 0.5940
h	 0.6340	 0.6500
i	 0.6610	 0.6620
j	 0.3620	 0.6300
k	 0.8560	 0.6860
l	 0.7960	 0.6830
m	 0.6040	 0.6580

