



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 10:08 PM UTC

PDB ID : 8Y36 / pdb_00008y36
EMDB ID : EMD-38873
Title : cryo-EM structure of Staphylococcus aureus(ATCC 29213) 50S ribosome in complex with MCX-190.
Authors : Li, Y.; Lu, G.; Li, J.; Pei, X.; Lin, J.
Deposited on : 2024-01-28
Resolution : 2.65 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

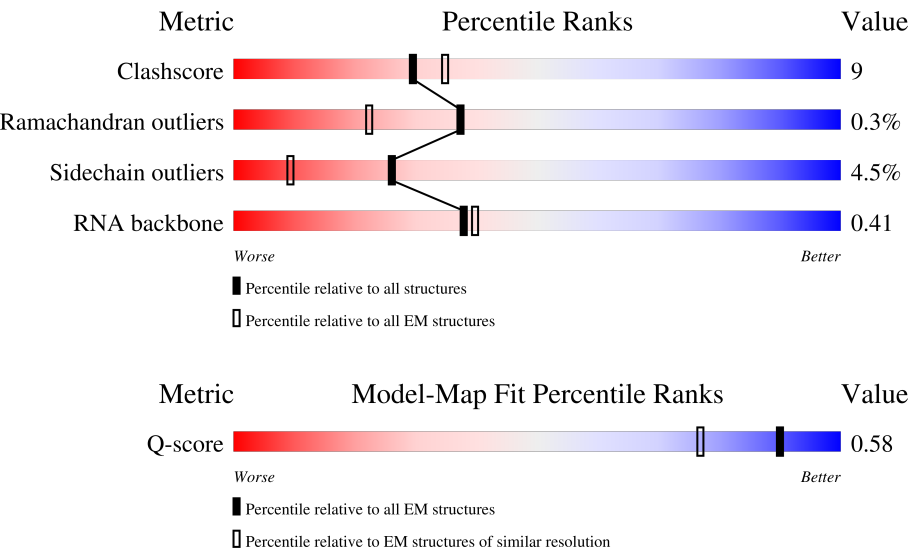
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	9050 (2.15 - 3.15)

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	2921	
2	1	47	
3	2	43	

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Mol	Chain	Length	Quality of chain
4	3	64	
5	4	37	
6	B	115	
7	C	274	
8	D	215	
9	E	206	
10	F	175	
11	G	175	
12	H	145	
13	I	122	
14	J	146	
15	K	137	
16	L	120	
17	M	119	
18	N	114	
19	O	116	
20	P	102	
21	Q	117	
22	R	89	
23	S	103	
24	T	94	
25	U	82	
26	V	58	
27	W	67	
28	X	58	

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Mol	Chain	Length	Quality of chain
29	Y	59	97% 80% 14% 5%
30	Z	48	83% 17%

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 88318 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	A	2885	Total	C	N	O	P	0	0
			61864	27621	11316	20042	2885		

- Molecule 2 is a protein called Large ribosomal subunit protein bL33B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	47	Total	C	N	O	S	0	0
			390	238	78	70	4		

- Molecule 3 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

- Molecule 4 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 5 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

- Molecule 6 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	115	Total	C	N	O	P	0	0
			2445	1094	436	801	114		

- Molecule 7 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	274	Total	C	N	O	S	0	0
			2090	1301	415	369	5		

- Molecule 8 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	215	Total	C	N	O	S	0	0
			1627	1018	299	305	5		

- Molecule 9 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	206	Total	C	N	O	S	0	0
			1572	986	288	296	2		

- Molecule 10 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	175	Total	C	N	O	S	0	0
			1315	832	224	253	6		

- Molecule 11 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	175	Total	C	N	O	S	0	0
			1259	788	239	229	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	145	Total	C	N	O	S	0	0
			1143	714	208	218	3		

- Molecule 13 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	122	Total	C	N	O	S	0	0
			918	572	174	168	4		

- Molecule 14 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	146	Total	C	N	O	S	0	0
			1086	674	214	197	1		

- Molecule 15 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	137	Total	C	N	O	S	0	0
			1071	689	203	175	4		

- Molecule 16 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	120	Total	C	N	O	S	0	0
			932	576	182	173	1		

- Molecule 17 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	119	Total	C	N	O	S	0	0
			891	557	174	159	1		

- Molecule 18 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	114	Total	C	N	O		0	0
			889	563	175	151			

- Molecule 19 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	116	Total	C	N	O	S	0	0
			942	593	189	156	4		

- Molecule 20 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	102	Total	C	N	O	S	0	0
			790	503	142	144	1		

- Molecule 21 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	112	Total	C	N	O	S	0	0
			853	532	163	155	3		

- Molecule 22 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	89	Total	C	N	O	S	0	0
			715	453	127	131	4		

- Molecule 23 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	103	Total	C	N	O	S	0	0
			770	486	142	141	1		

- Molecule 24 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	94	Total	C	N	O		0	0
			715	459	128	128			

- Molecule 25 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	82	Total	C	N	O		0	0
			615	380	121	114			

- Molecule 26 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	58	Total	C	N	O		0	0
			445	277	96	72			

- Molecule 27 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	67	Total	C	N	O		0	0
			541	333	102	106			

- Molecule 28 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	X	58	Total	C	N	O	0	0
			449	280	85	84		

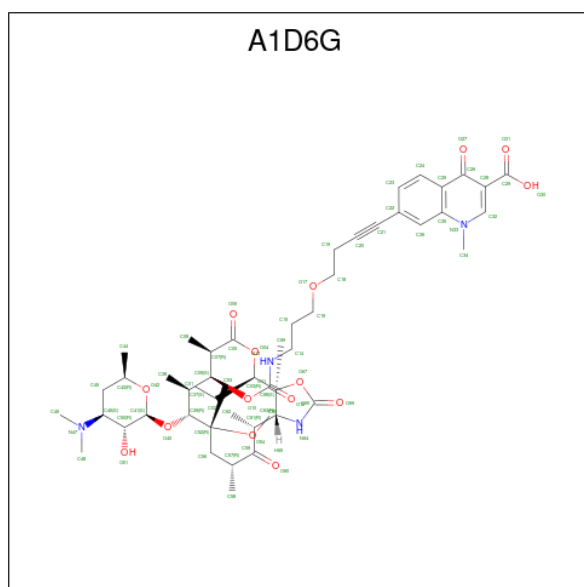
- Molecule 29 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	59	Total	C	N	O	S	0	0
			363	219	68	75	1		

- Molecule 30 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	48	Total	C	N	O	S	0	0
			361	222	77	59	3		

- Molecule 31 is 7-[4-[3-[(1 {S},2 {R},5 {R},6 {S},7 {S},8 {R},9 {R},11 {R},13 {R},14 {R})-8-[(2 {S},3 {R},4 {S},6 {R})-4-(dimethylamino)-6-methyl-3-oxidanyl-oxan-2-yl]oxy-2-ethyl-9-methoxy-1,5,7,9,11,13-hexamethyl-4,12,16-tris(oxidanylidene)-3,17-dioxo-15-azabicyclo[1 2.3.0]heptadecan-6-yl]oxycarbonylamino]propoxy]but-1-ynyl]-1-methyl-4-oxidanylidene-quinoline-3-carboxylic acid (CCD ID: A1D6G) (formula: C₅₀H₇₂N₄O₁₅).



Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	C	N	O	0
			69	50	4	15	

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

Mol	Chain	Residues	Atoms		AltConf
32	A	11	Total	Mg	0
			11	11	

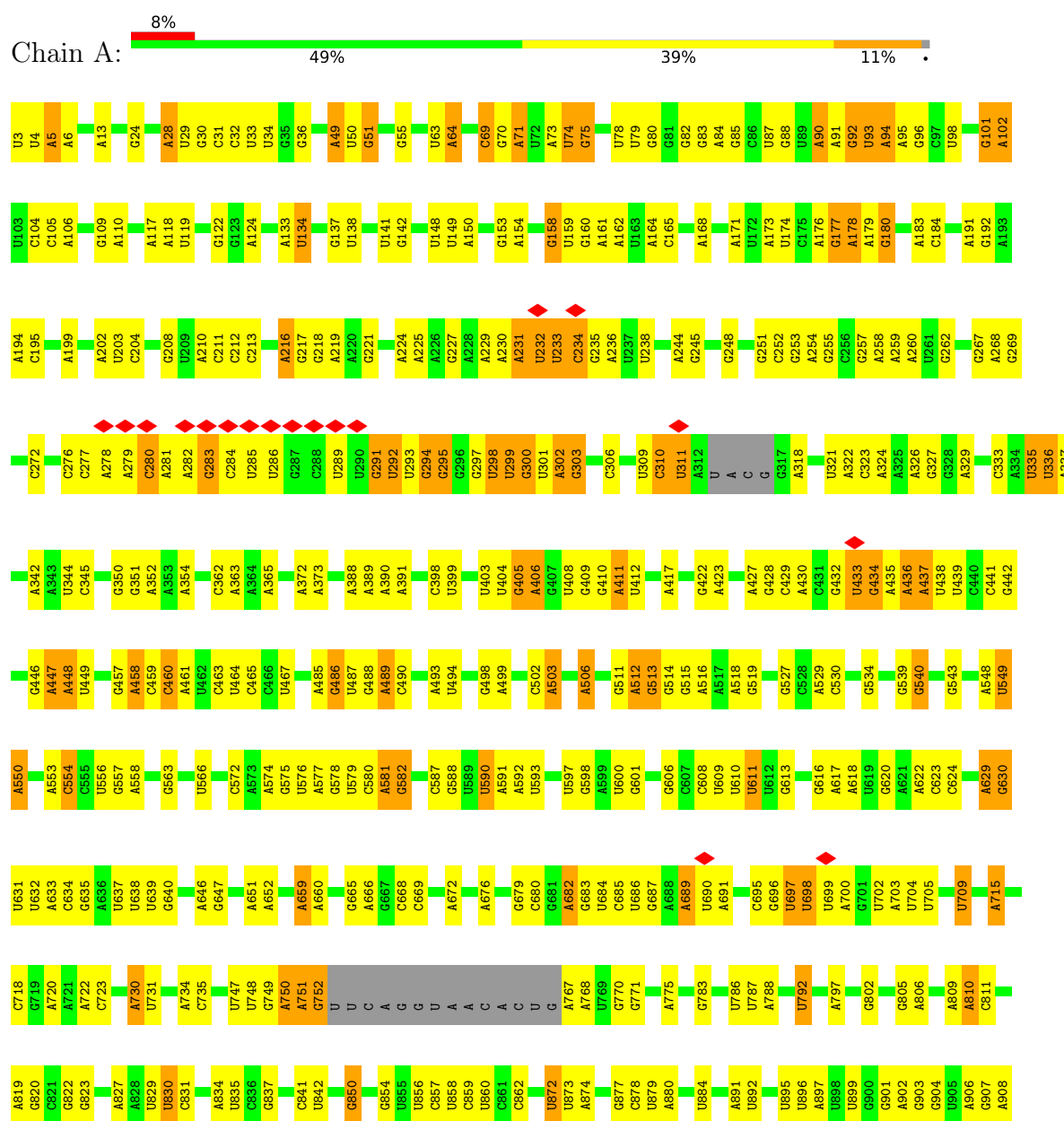
- Molecule 33 is water.

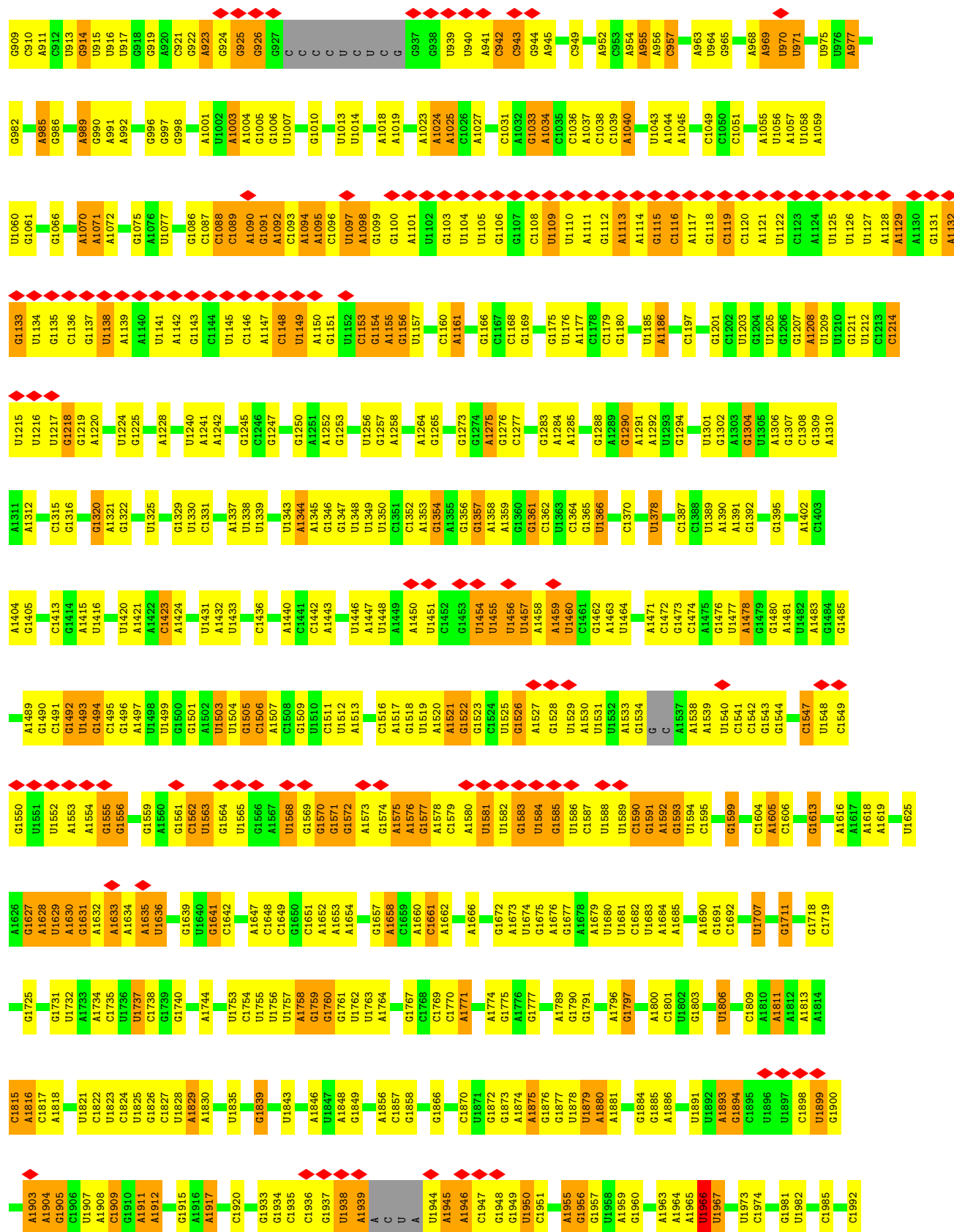
Mol	Chain	Residues	Atoms		AltConf
33	A	3	Total	O	0
			3	3	

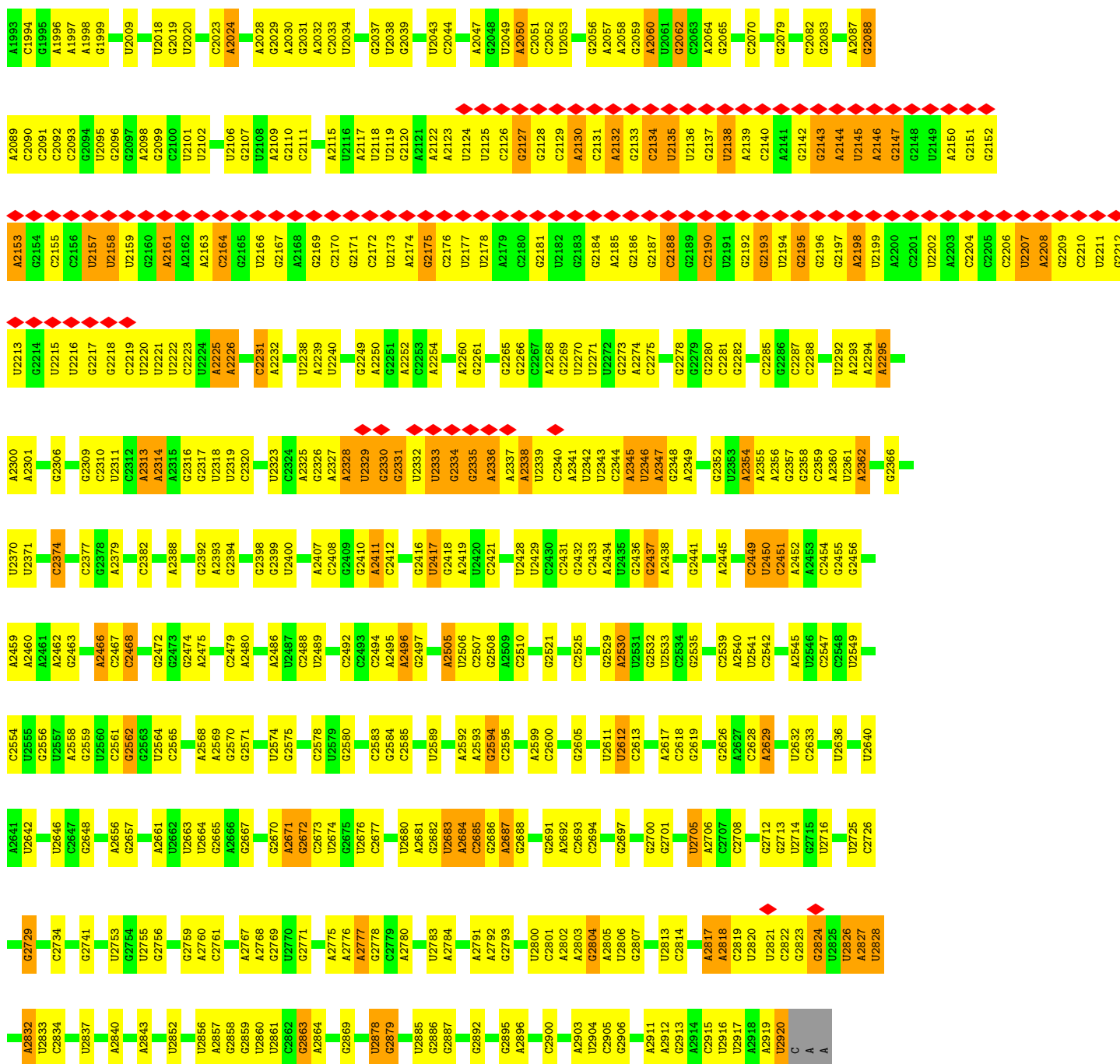
3 Residue-property plots

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









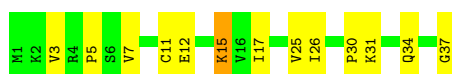
- Molecule 4: Large ribosomal subunit protein bL35

Chain 3: 73% 27%



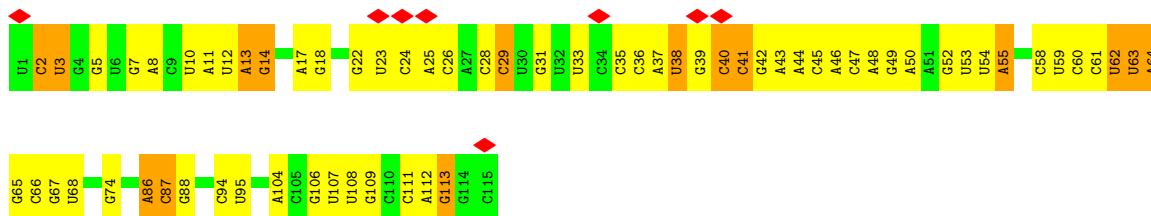
- Molecule 5: Large ribosomal subunit protein bL36

Chain 4: 65% 32% .



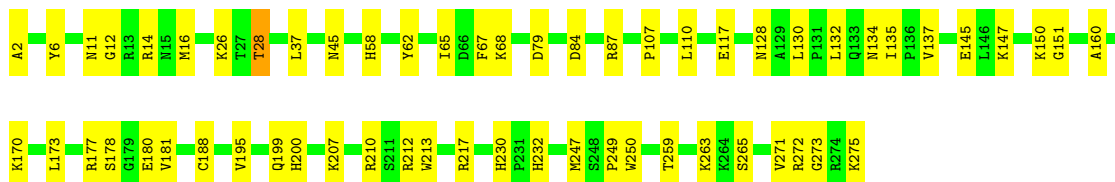
- Molecule 6: 5S ribosomal RNA

Chain B: 7% 43% 44% 13%



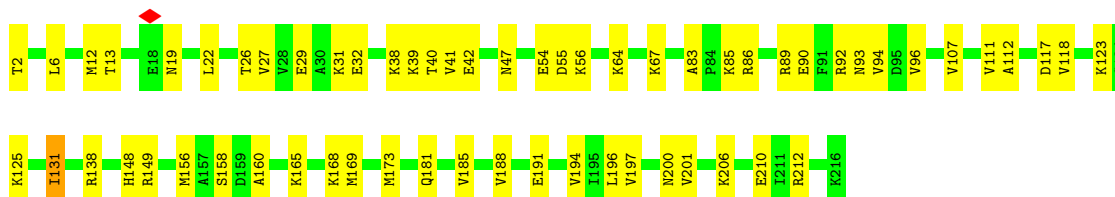
- Molecule 7: Large ribosomal subunit protein uL2

Chain C: 78% 21%



- Molecule 8: Large ribosomal subunit protein uL3

Chain D: 72% 28%



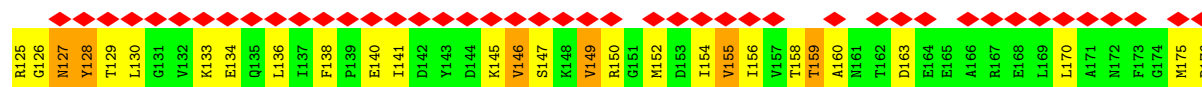
- Molecule 9: Large ribosomal subunit protein uL4

Chain E:  85% 14%



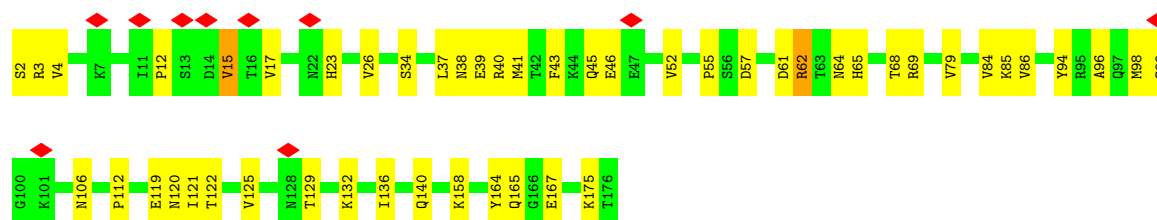
- Molecule 10: Large ribosomal subunit protein uL5

Chain F:  81% 52% 43% 5%



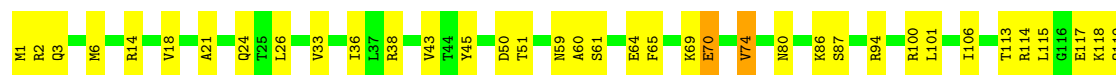
- Molecule 11: Large ribosomal subunit protein uL6

Chain G:  6% 71% 27%



- Molecule 12: Large ribosomal subunit protein uL13

Chain H:  71% 28%

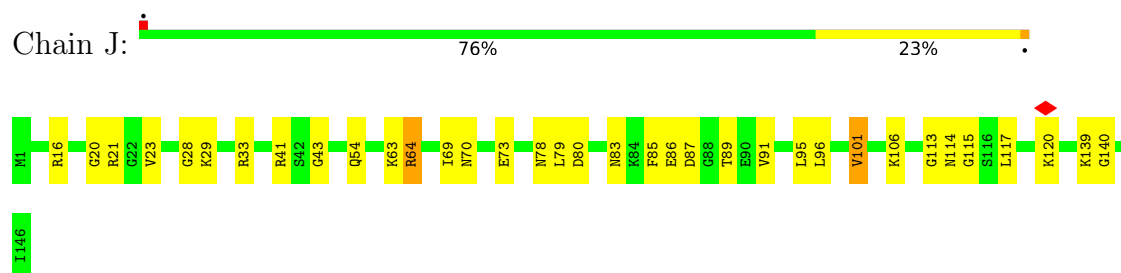


- Molecule 13: Large ribosomal subunit protein uL14

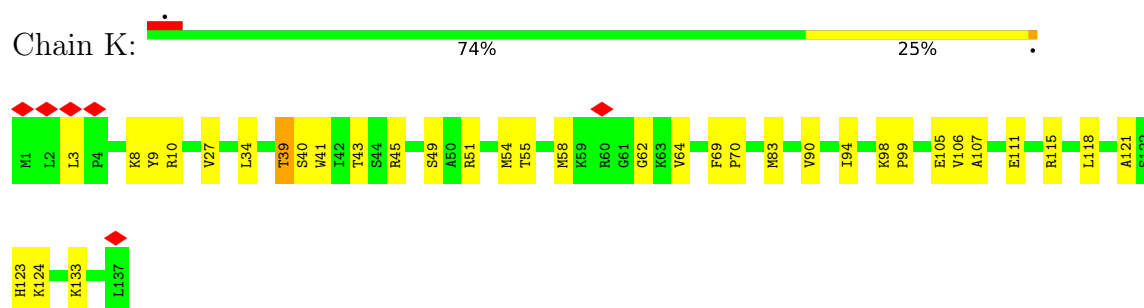
Chain I:  76% 23%



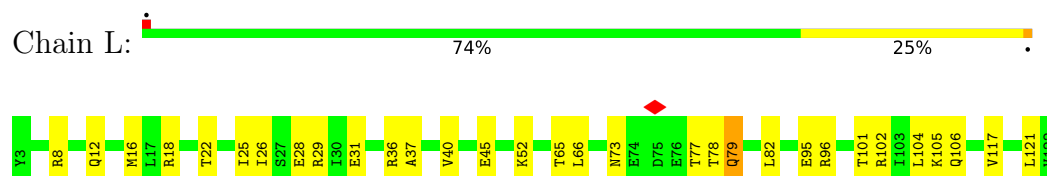
- Molecule 14: Large ribosomal subunit protein uL15



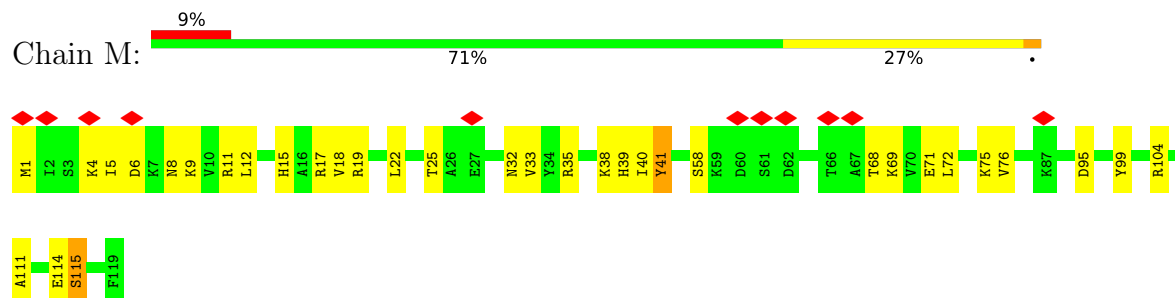
- Molecule 15: Large ribosomal subunit protein uL16



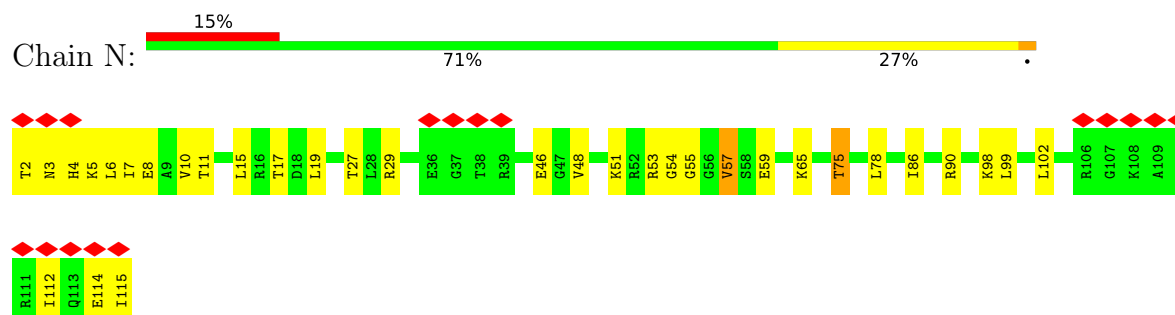
- Molecule 16: Large ribosomal subunit protein bL17



- Molecule 17: Large ribosomal subunit protein uL18



- Molecule 18: Large ribosomal subunit protein bL19



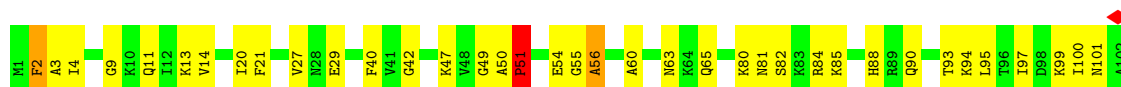
- Molecule 19: Large ribosomal subunit protein bL20

Chain O:  83% 17%



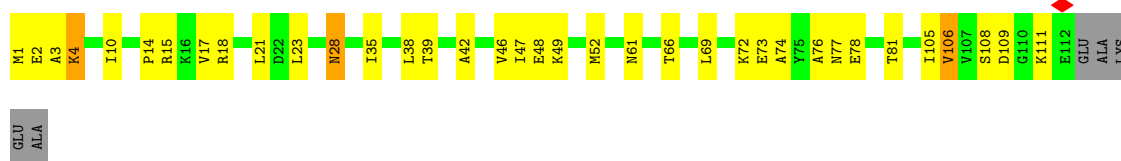
- Molecule 20: Large ribosomal subunit protein bL21

Chain P:  64% 33% ..



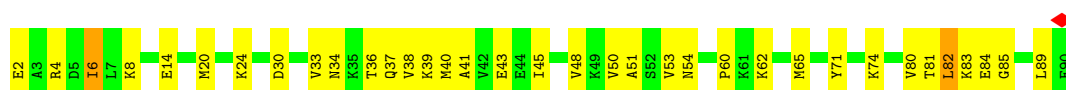
- Molecule 21: Large ribosomal subunit protein uL22

Chain Q:  65% 28% ..



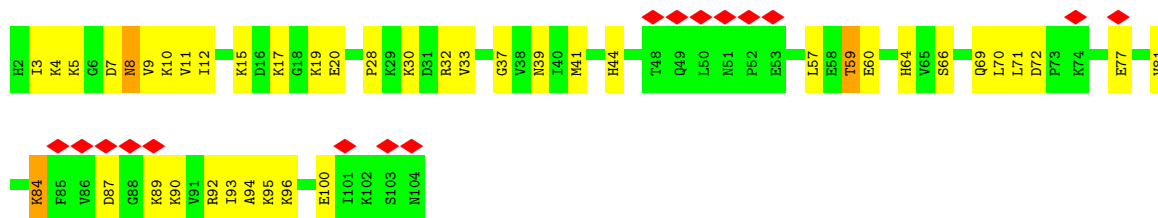
- Molecule 22: Large ribosomal subunit protein uL23

Chain R:  61% 37% .



- Molecule 23: Large ribosomal subunit protein uL24

Chain S:  16% 59% 38% .



- Molecule 24: Large ribosomal subunit protein bL25

Chain T:  5% 73% 23% .



- Molecule 25: Large ribosomal subunit protein bL27

Chain U:  79% 21%



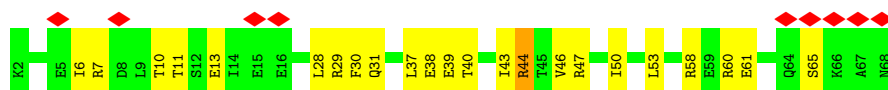
- Molecule 26: Large ribosomal subunit protein bL28

Chain V:  79% 19%



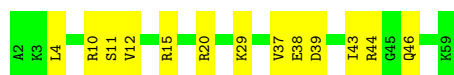
- Molecule 27: Large ribosomal subunit protein uL29

Chain W:  13% 66% 33%



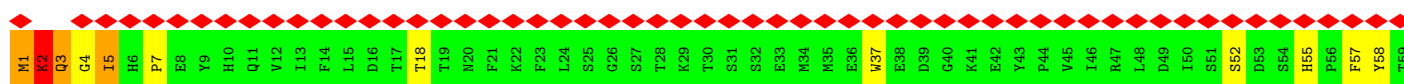
- Molecule 28: Large ribosomal subunit protein uL30

Chain X:  78% 22%



- Molecule 29: Large ribosomal subunit protein bL31B

Chain Y:  97% 80% 14% 5%



- Molecule 30: Large ribosomal subunit protein bL32

Chain Z:  83% 17%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	163945	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.040	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size ($\text{\AA}$)	395.52, 395.52, 395.52	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.824, 0.824, 0.824	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, 2MG, 5MU, A1D6G, 2MA, MG

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	0.36	0/69155	0.46	9/107848 (0.0%)
2	1	0.30	0/395	0.44	0/530
3	2	0.29	0/371	0.45	0/484
4	3	0.32	0/526	0.50	0/690
5	4	0.32	0/299	0.68	0/393
6	B	0.28	0/2733	0.40	0/4257
7	C	0.41	0/2125	0.59	0/2853
8	D	0.36	0/1651	0.59	0/2215
9	E	0.29	0/1595	0.43	0/2154
10	F	0.33	0/1329	0.64	0/1793
11	G	0.35	0/1277	0.58	0/1731
12	H	0.34	0/1165	0.52	0/1570
13	I	0.39	0/925	0.62	0/1242
14	J	0.32	0/1100	0.55	0/1467
15	K	0.32	0/1095	0.50	0/1472
16	L	0.33	0/936	0.56	0/1253
17	M	0.28	0/900	0.52	0/1205
18	N	0.31	0/901	0.53	0/1209
19	O	0.35	0/954	0.50	0/1264
20	P	0.43	0/800	0.69	2/1070 (0.2%)
21	Q	0.30	0/861	0.47	0/1161
22	R	0.29	0/723	0.53	0/966
23	S	0.39	0/779	0.69	1/1043 (0.1%)
24	T	0.25	0/723	0.45	0/973
25	U	0.34	0/621	0.55	0/825
26	V	0.28	0/451	0.51	0/603
27	W	0.23	0/542	0.47	0/722
28	X	0.28	0/451	0.47	0/606
29	Y	0.43	0/370	0.77	2/510 (0.4%)
30	Z	0.33	0/367	0.47	0/490
All	All	0.36	0/96120	0.48	14/144599 (0.0%)

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y	2	LYS	N-CA-C	-7.84	101.42	111.92
1	A	2466	A	C2'-C3'-O3'	7.49	120.74	109.50
20	P	51	PRO	N-CA-C	-6.66	98.75	112.47
1	A	298	U	C2'-C3'-O3'	-6.38	104.13	113.70
1	A	1760	G	C4'-C3'-O3'	6.00	118.39	109.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	61864	0	31099	784	0
2	1	390	0	394	10	0
3	2	367	0	415	5	0
4	3	521	0	586	14	0
5	4	296	0	342	10	0
6	B	2445	0	1240	49	0
7	C	2090	0	2201	42	0
8	D	1627	0	1667	38	0
9	E	1572	0	1619	25	0
10	F	1315	0	1327	81	0
11	G	1259	0	1221	29	0
12	H	1143	0	1134	34	0
13	I	918	0	981	20	0
14	J	1086	0	1125	25	0
15	K	1071	0	1123	27	0
16	L	932	0	983	18	0
17	M	891	0	925	25	0
18	N	889	0	937	26	0
19	O	942	0	1014	17	0
20	P	790	0	830	30	0
21	Q	853	0	905	24	0
22	R	715	0	748	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	S	770	0	809	31	0
24	T	715	0	751	17	0
25	U	615	0	622	12	0
26	V	445	0	466	10	0
27	W	541	0	563	16	0
28	X	449	0	491	8	0
29	Y	363	0	236	18	0
30	Z	361	0	361	7	0
31	A	69	0	0	1	0
32	A	11	0	0	0	0
33	A	3	0	0	1	0
All	All	88318	0	57115	1315	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 1315 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:54:VAL:O	10:F:58:GLU:HB3	1.78	0.83
13:I:63:VAL:HG12	13:I:106:LEU:HD11	1.62	0.81
1:A:2421:C:H42	1:A:2449:C:H41	1.27	0.81
27:W:11:THR:OG1	27:W:60:ARG:NH1	2.14	0.81
1:A:1570:G:N2	1:A:1571:G:O6	2.15	0.79

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	1	45/47 (96%)	43 (96%)	2 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
4	3	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
5	4	35/37 (95%)	35 (100%)	0	0	100	100
7	C	272/274 (99%)	262 (96%)	10 (4%)	0	100	100
8	D	213/215 (99%)	199 (93%)	13 (6%)	1 (0%)	24	39
9	E	204/206 (99%)	197 (97%)	7 (3%)	0	100	100
10	F	173/175 (99%)	152 (88%)	20 (12%)	1 (1%)	21	34
11	G	173/175 (99%)	165 (95%)	7 (4%)	1 (1%)	21	34
12	H	143/145 (99%)	134 (94%)	9 (6%)	0	100	100
13	I	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
14	J	144/146 (99%)	137 (95%)	7 (5%)	0	100	100
15	K	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
16	L	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
17	M	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
18	N	112/114 (98%)	104 (93%)	8 (7%)	0	100	100
19	O	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
20	P	100/102 (98%)	92 (92%)	5 (5%)	3 (3%)	3	5
21	Q	110/117 (94%)	105 (96%)	5 (4%)	0	100	100
22	R	87/89 (98%)	82 (94%)	5 (6%)	0	100	100
23	S	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
24	T	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
25	U	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
26	V	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
27	W	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
28	X	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
29	Y	57/59 (97%)	48 (84%)	7 (12%)	2 (4%)	3	4
30	Z	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
All	All	3071/3132 (98%)	2898 (94%)	165 (5%)	8 (0%)	37	52

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	D	160	ALA

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Mol	Chain	Res	Type
11	G	55	PRO
20	P	51	PRO
20	P	56	ALA
10	F	76	THR

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	
2	1	44/45 (98%)	41 (93%)	3 (7%)	14	25
3	2	39/39 (100%)	38 (97%)	1 (3%)	40	63
4	3	55/55 (100%)	55 (100%)	0	100	100
5	4	35/35 (100%)	32 (91%)	3 (9%)	10	16
7	C	220/221 (100%)	214 (97%)	6 (3%)	39	61
8	D	173/173 (100%)	164 (95%)	9 (5%)	21	36
9	E	168/168 (100%)	163 (97%)	5 (3%)	36	57
10	F	139/154 (90%)	127 (91%)	12 (9%)	10	16
11	G	123/153 (80%)	116 (94%)	7 (6%)	18	32
12	H	122/123 (99%)	118 (97%)	4 (3%)	33	55
13	I	100/100 (100%)	94 (94%)	6 (6%)	17	30
14	J	109/112 (97%)	105 (96%)	4 (4%)	30	50
15	K	108/114 (95%)	107 (99%)	1 (1%)	70	82
16	L	96/101 (95%)	93 (97%)	3 (3%)	35	56
17	M	86/95 (90%)	81 (94%)	5 (6%)	18	31
18	N	93/100 (93%)	89 (96%)	4 (4%)	26	44
19	O	96/96 (100%)	94 (98%)	2 (2%)	47	69
20	P	84/86 (98%)	82 (98%)	2 (2%)	43	65
21	Q	89/94 (95%)	84 (94%)	5 (6%)	19	32
22	R	78/80 (98%)	75 (96%)	3 (4%)	29	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	S	81/88 (92%)	74 (91%)	7 (9%)	10	16
24	T	76/82 (93%)	72 (95%)	4 (5%)	20	35
25	U	60/64 (94%)	57 (95%)	3 (5%)	22	37
26	V	44/49 (90%)	41 (93%)	3 (7%)	14	25
27	W	58/60 (97%)	55 (95%)	3 (5%)	21	36
28	X	52/52 (100%)	48 (92%)	4 (8%)	12	20
29	Y	22/56 (39%)	19 (86%)	3 (14%)	3	5
30	Z	36/44 (82%)	36 (100%)	0	100	100
All	All	2486/2639 (94%)	2374 (96%)	112 (4%)	26	42

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	J	64	ARG
29	Y	2	LYS
18	N	57	VAL
29	Y	1	MET
26	V	25	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
21	Q	61	ASN
23	S	69	GLN
10	F	9	ASN
8	D	192	ASN
24	T	38	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2879/2921 (98%)	780 (27%)	32 (1%)
6	B	114/115 (99%)	33 (28%)	0
All	All	2993/3036 (98%)	813 (27%)	32 (1%)

5 of 813 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	A
1	A	13	A
1	A	28	A
1	A	34	U
1	A	36	G

5 of 32 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2449	C
1	A	2466	A
1	A	872	U
1	A	809	A
1	A	2783	U

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

5 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	2MG	A	2472	1	23,26,27	1.29	4 (17%)	33,38,41	2.27	10 (30%)
1	OMG	A	2278	1	23,26,27	1.23	3 (13%)	32,38,41	2.00	6 (18%)
1	2MA	A	2530	1,32	22,25,26	1.46	5 (22%)	32,37,40	2.45	10 (31%)
1	5MU	A	1966	1	19,22,23	1.38	5 (26%)	27,32,35	2.18	7 (25%)
1	5MU	A	792	1	19,22,23	1.42	5 (26%)	27,32,35	2.16	9 (33%)

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	2MG	A	2472	1	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	A	2278	1	-	0/9/27/28	0/3/3/3
1	2MA	A	2530	1,32	-	3/7/25/26	0/3/3/3
1	5MU	A	1966	1	-	2/7/25/26	0/2/2/2
1	5MU	A	792	1	-	0/7/25/26	0/2/2/2

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2530	2MA	C5-C4	3.88	1.46	1.39
1	A	792	5MU	C4-N3	-3.14	1.33	1.38
1	A	2278	OMG	C6-N1	-2.93	1.33	1.38
1	A	2472	2MG	C6-N1	-2.85	1.33	1.38
1	A	2278	OMG	C5-C4	2.84	1.46	1.38

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2530	2MA	C5-C4-N3	-8.66	118.06	127.18
1	A	2472	2MG	C2-N3-C4	7.24	121.06	112.00
1	A	2530	2MA	N3-C4-N9	6.92	135.77	126.99
1	A	2278	OMG	C5-C4-N3	-6.54	117.99	128.39
1	A	2472	2MG	C5-C4-N3	-6.11	118.66	128.39

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1966	5MU	C3'-C4'-C5'-O5'
1	A	2530	2MA	O4'-C4'-C5'-O5'
1	A	1966	5MU	O4'-C4'-C5'-O5'
1	A	2472	2MG	C3'-C4'-C5'-O5'
1	A	2530	2MA	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1966	5MU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 11 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	$\# Z > 2$
31	A1D6G	A	3001	32	72,73,73	2.40	25 (34%)	97,107,107	1.75	20 (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
31	A1D6G	A	3001	32	-	8/82/113/113	0/5/5/5

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	3001	A1D6G	C65-N64	8.75	1.45	1.33
31	A	3001	A1D6G	C11-N13	7.63	1.50	1.34
31	A	3001	A1D6G	O10-C11	4.93	1.43	1.35
31	A	3001	A1D6G	O67-C65	4.82	1.43	1.36
31	A	3001	A1D6G	C22-C21	4.56	1.55	1.44

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	3001	A1D6G	O10-C11-N13	5.68	120.27	111.01
31	A	3001	A1D6G	C02-C03-C68	-5.64	107.46	115.23
31	A	3001	A1D6G	C63-N64-C65	-4.14	106.99	112.39
31	A	3001	A1D6G	O04-C05-C07	3.88	119.83	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	3001	A1D6G	C52-C39-C37	-3.54	108.13	113.54

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

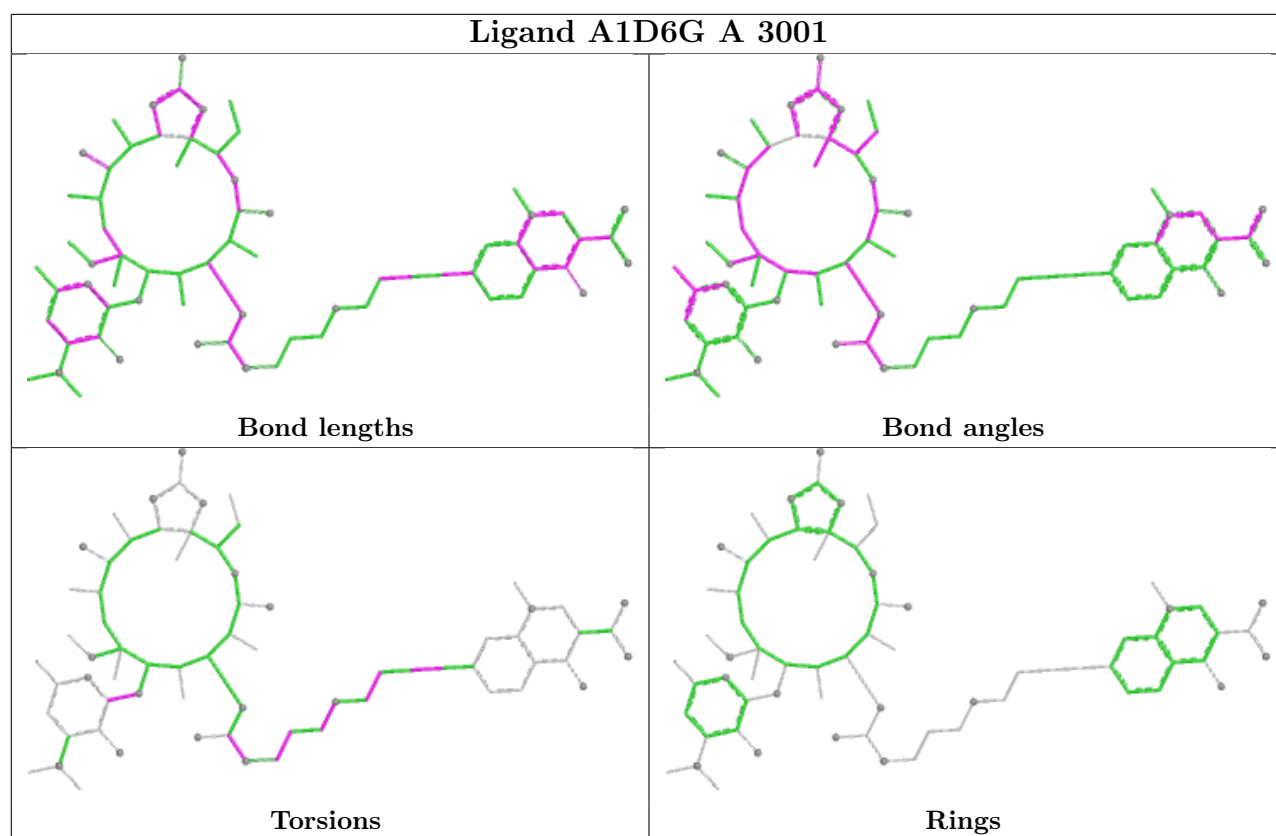
Mol	Chain	Res	Type	Atoms
31	A	3001	A1D6G	N13-C14-C15-C16
31	A	3001	A1D6G	O10-C11-N13-C14
31	A	3001	A1D6G	O12-C11-N13-C14
31	A	3001	A1D6G	O17-C18-C19-C20
31	A	3001	A1D6G	O42-C41-O40-C39

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	3001	A1D6G	1	0

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.

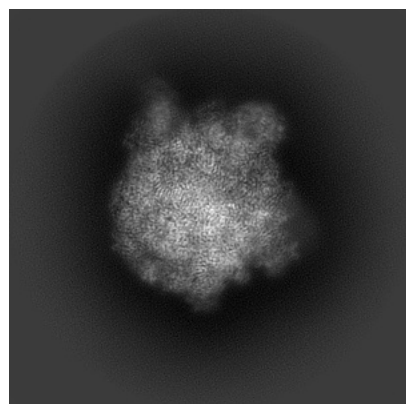
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38873. These allow visual inspection of the internal detail of the map and identification of artifacts.

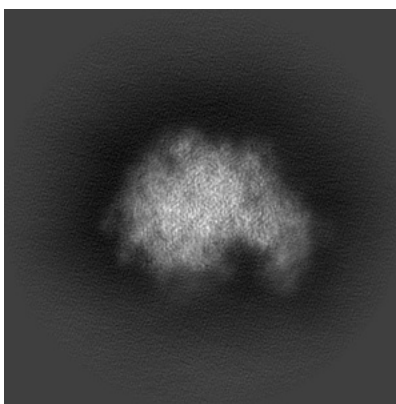
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

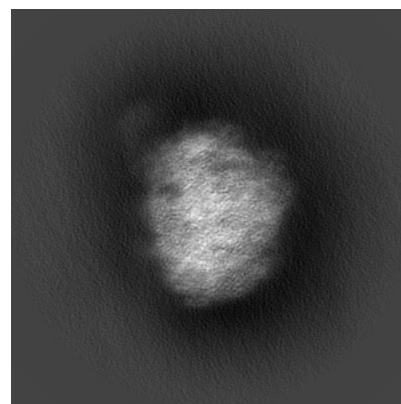
6.1.1 Primary map



X

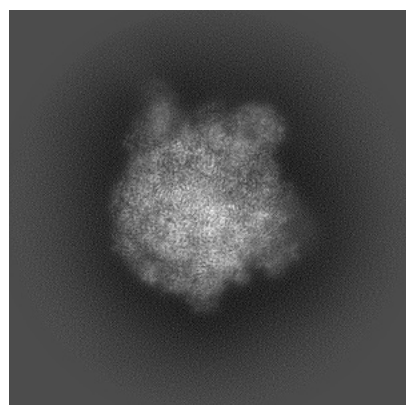


Y

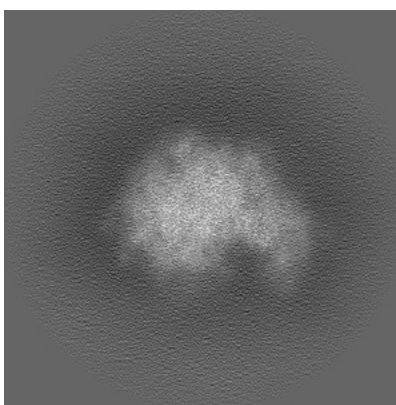


Z

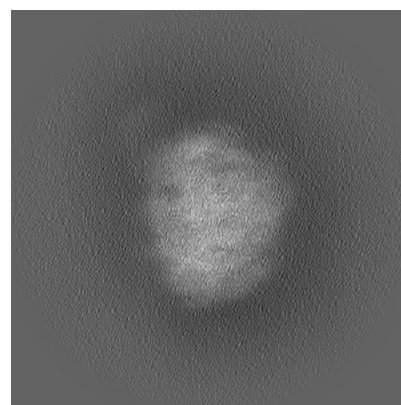
6.1.2 Raw map



X



Y

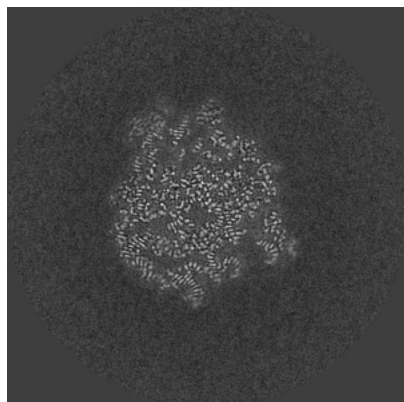


Z

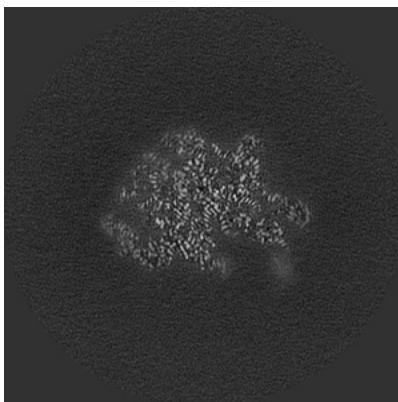
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

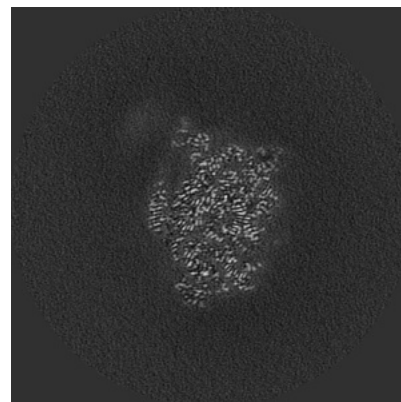
6.2.1 Primary map



X Index: 240

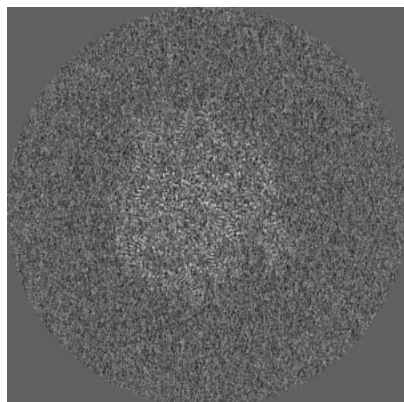


Y Index: 240

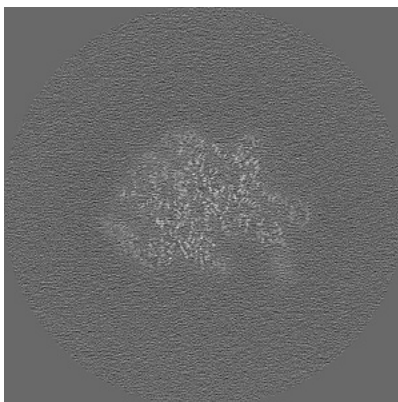


Z Index: 240

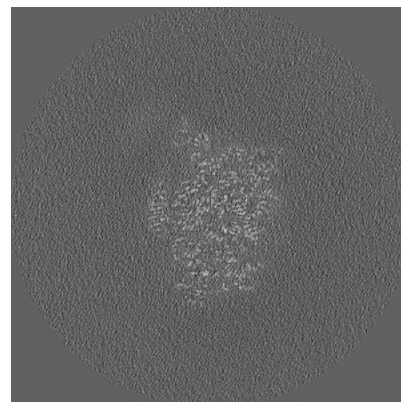
6.2.2 Raw map



X Index: 240



Y Index: 240

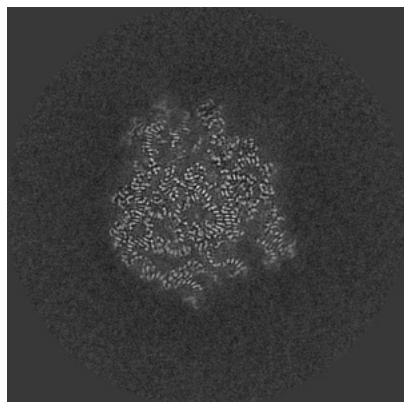


Z Index: 240

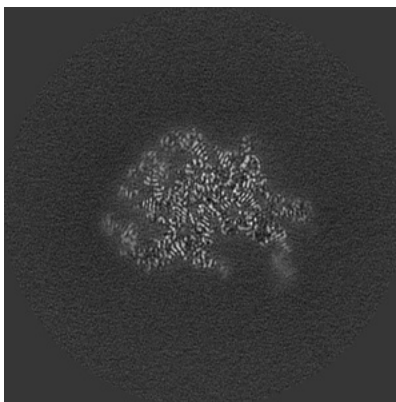
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

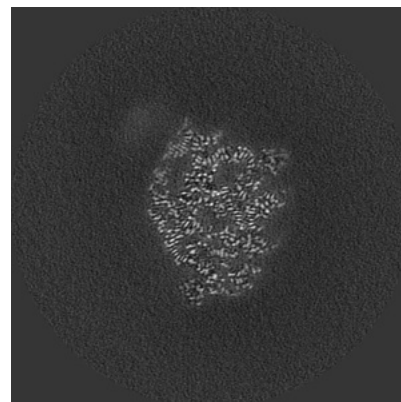
6.3.1 Primary map



X Index: 237

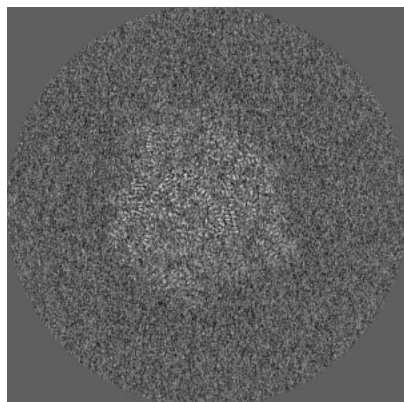


Y Index: 243

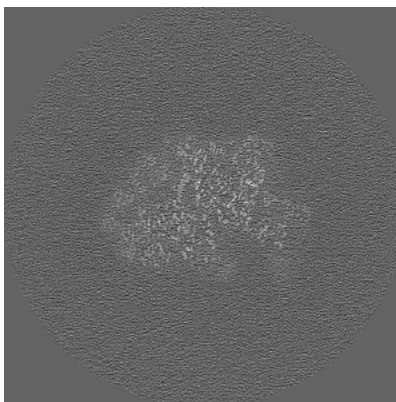


Z Index: 235

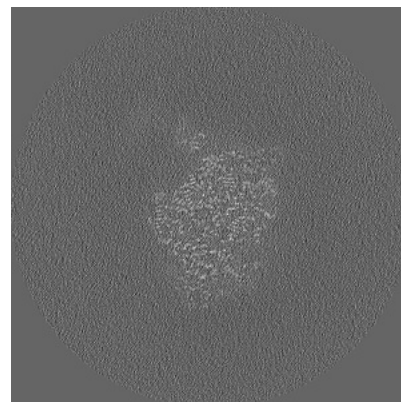
6.3.2 Raw map



X Index: 236



Y Index: 234

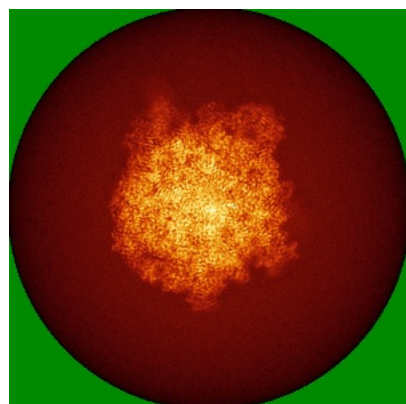


Z Index: 243

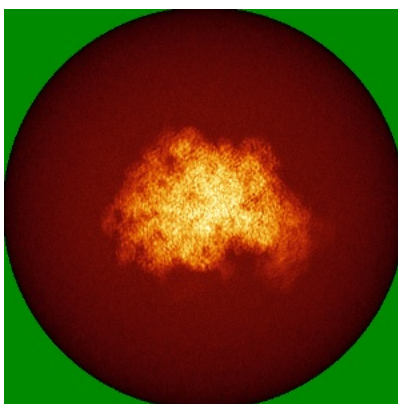
The images above show the largest variance slices of the map in three orthogonal directions.

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

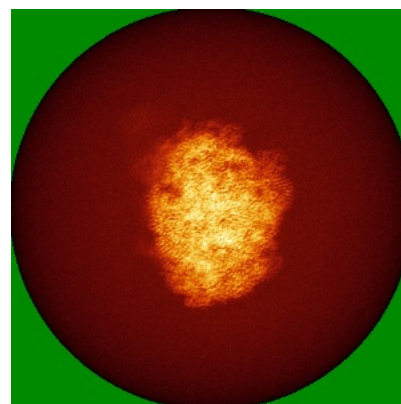
6.4.1 Primary map



X

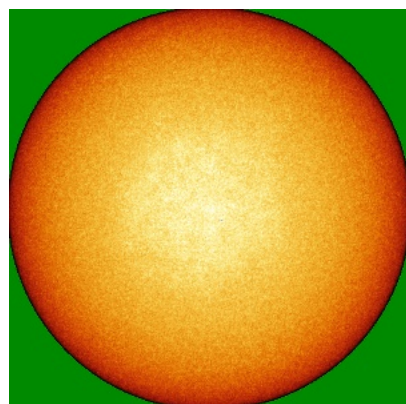


Y

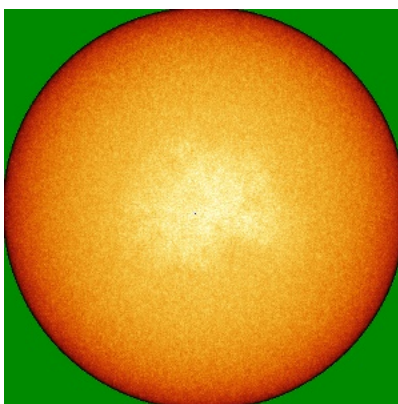


Z

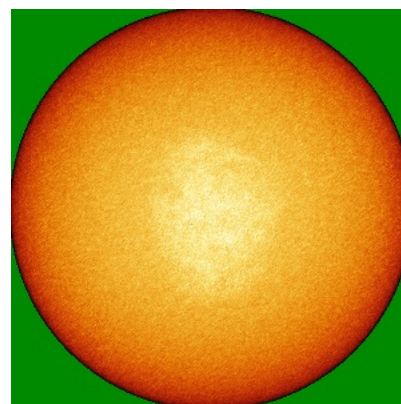
6.4.2 Raw map



X



Y

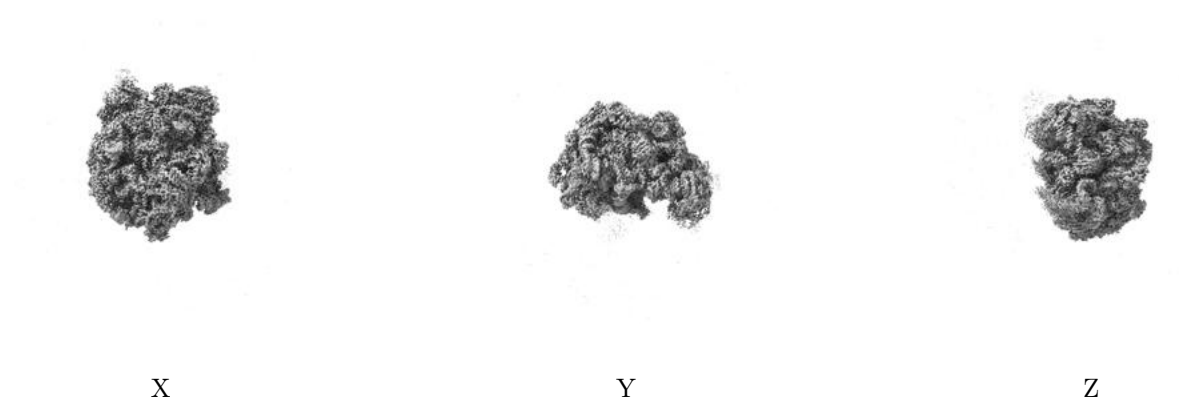


Z

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.

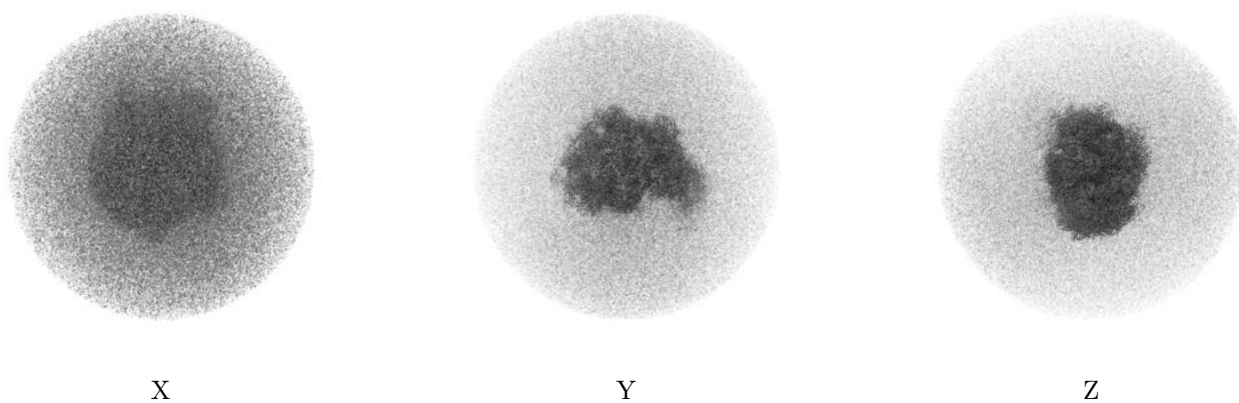
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

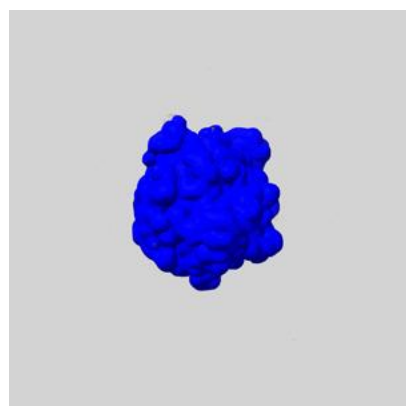
6.6 Mask visualisation [i](#)

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

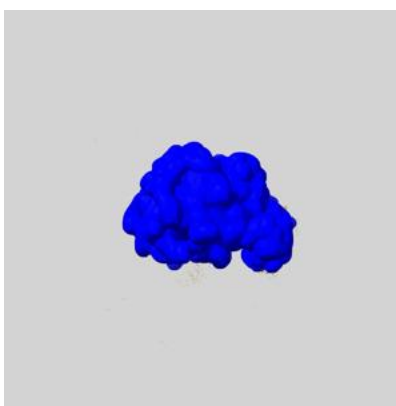
A mask typically either:

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

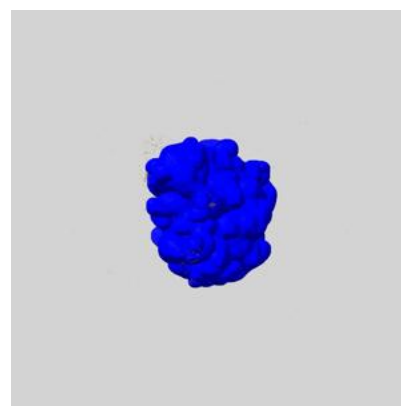
6.6.1 emd_38873_msk_1.map [i](#)



X



Y

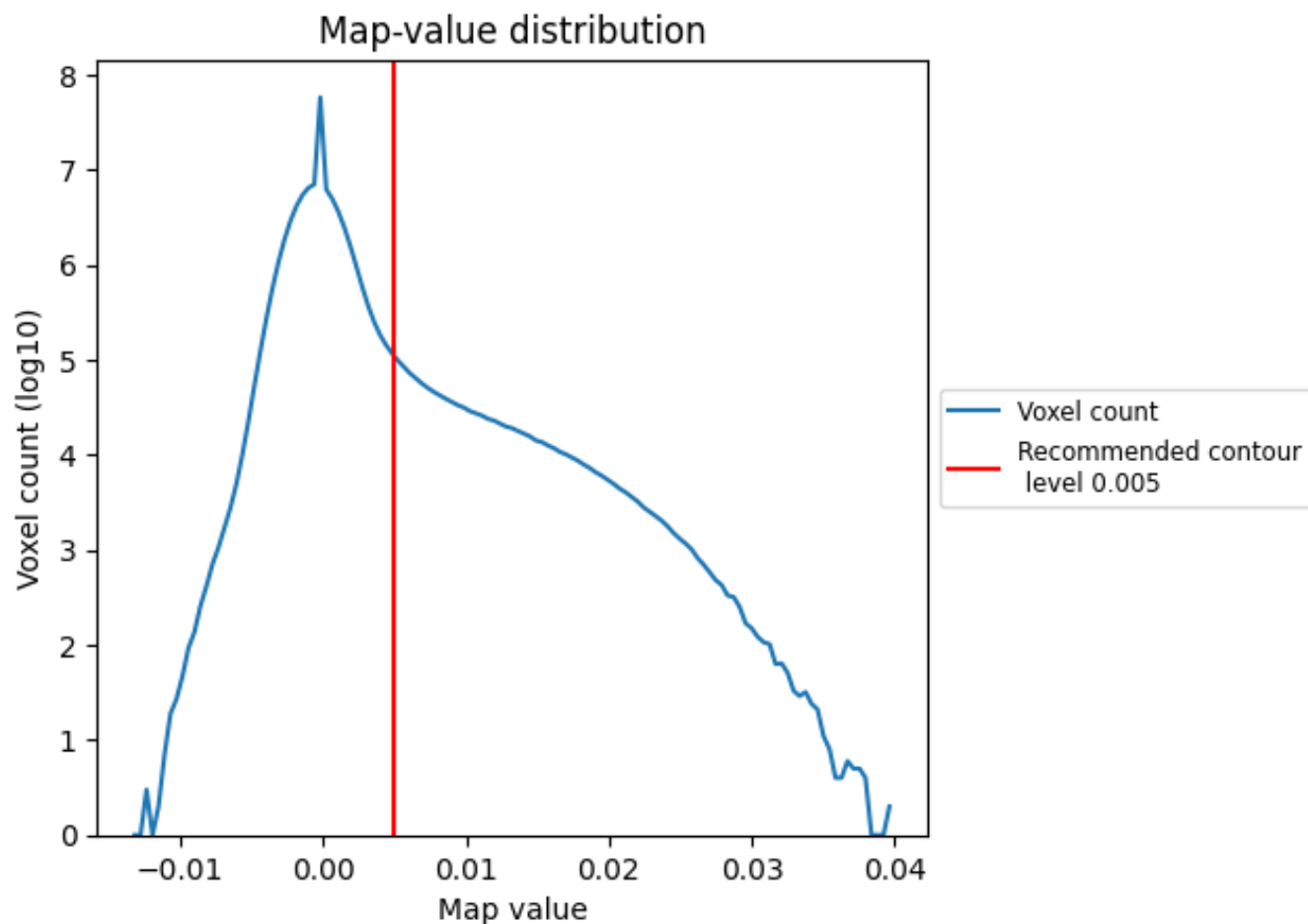


Z

7 Map analysis [i](#)

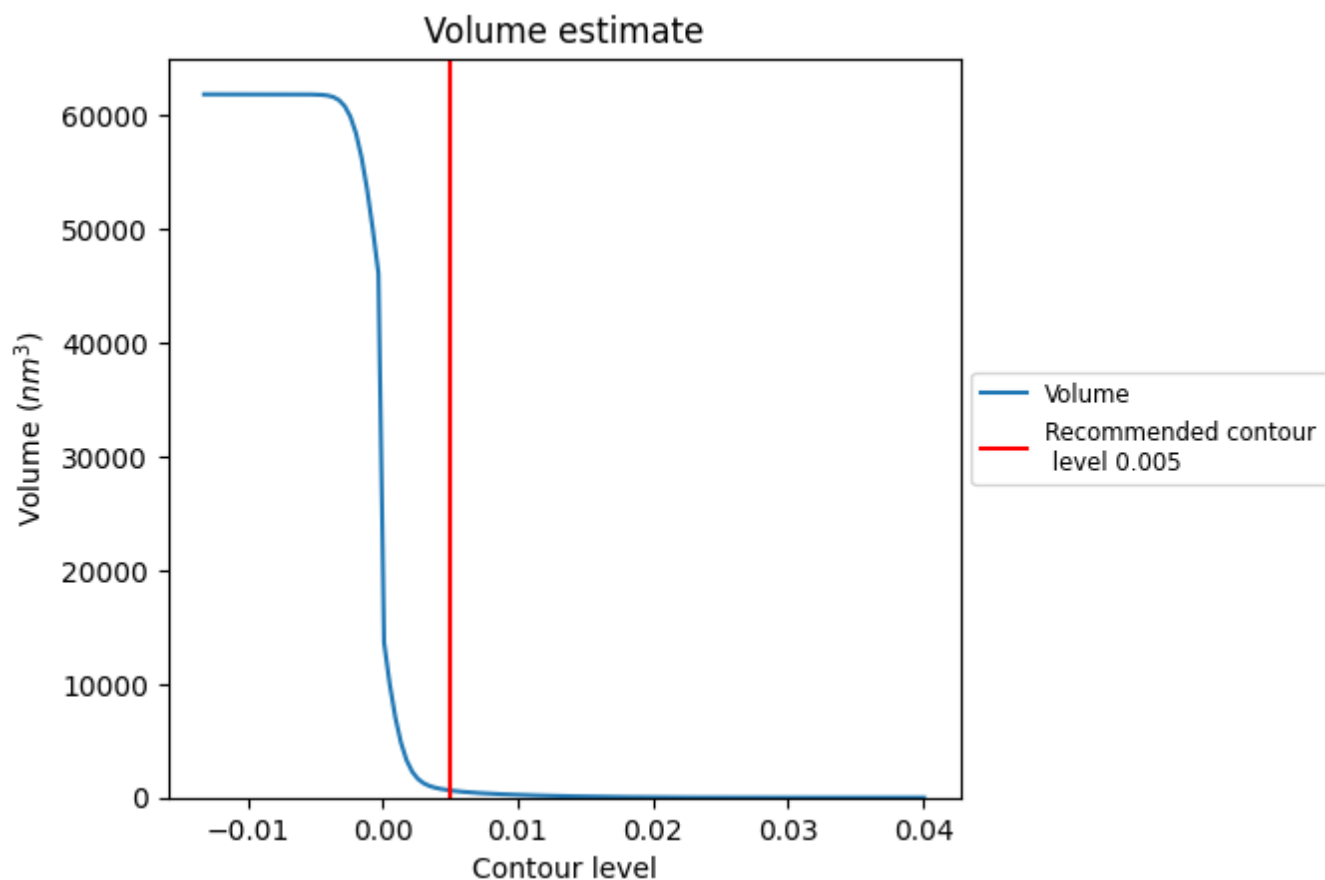
This section contains the results of statistical analysis of the map.

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.

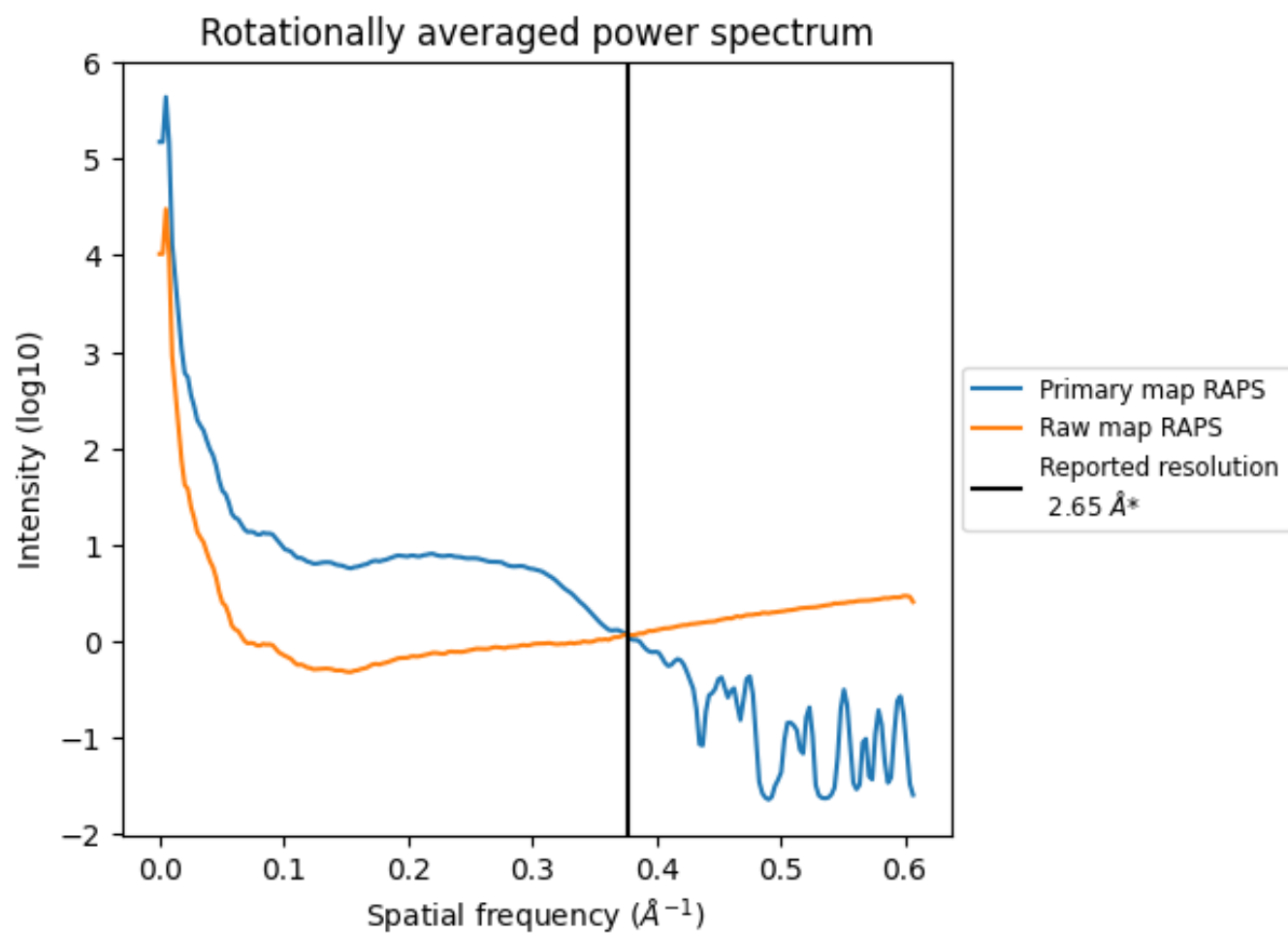
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 630 nm³; this corresponds to an approximate mass of 569 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 ⓘ

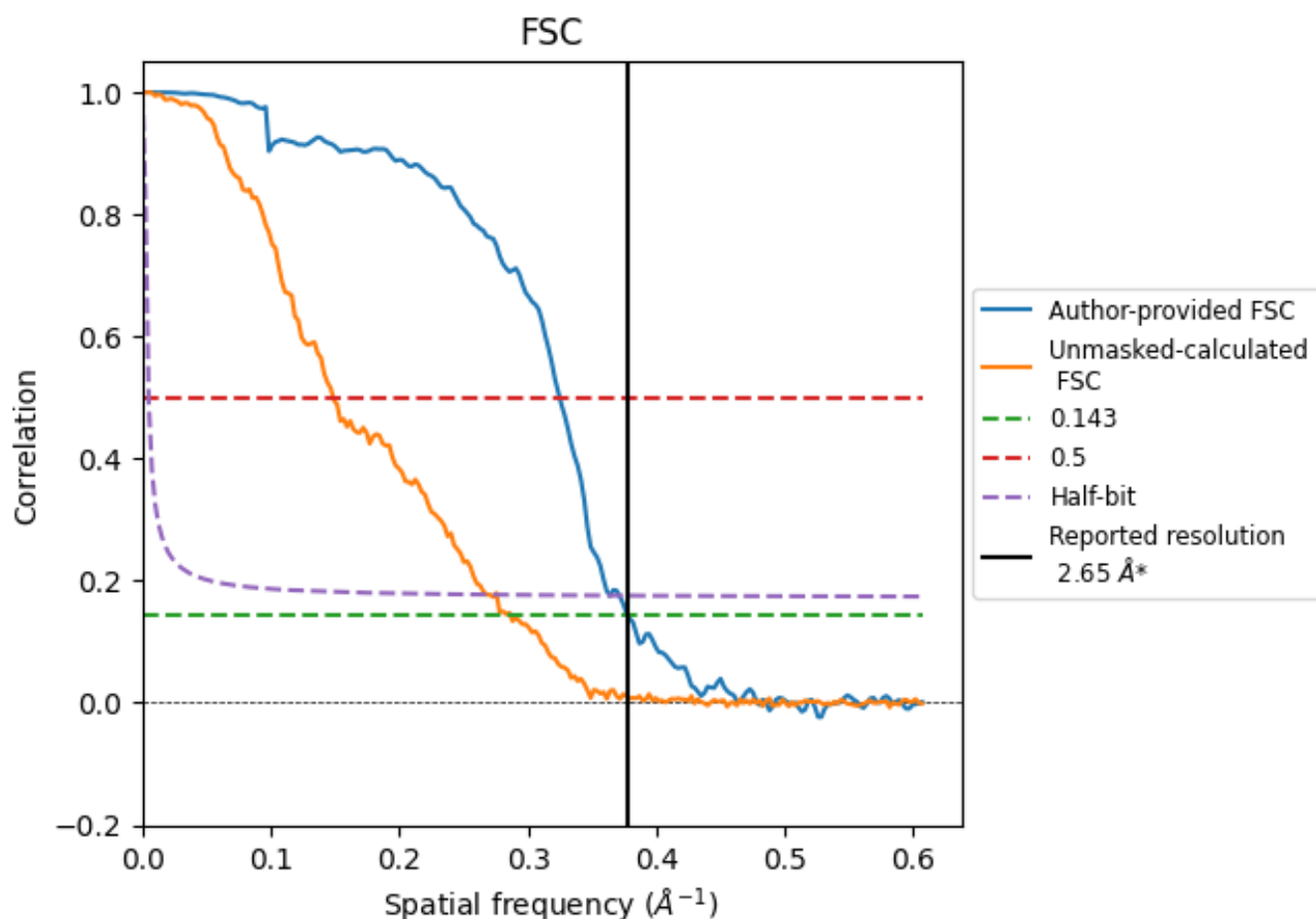


*Reported resolution corresponds to spatial frequency of 0.377 Å⁻¹

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 0.377 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

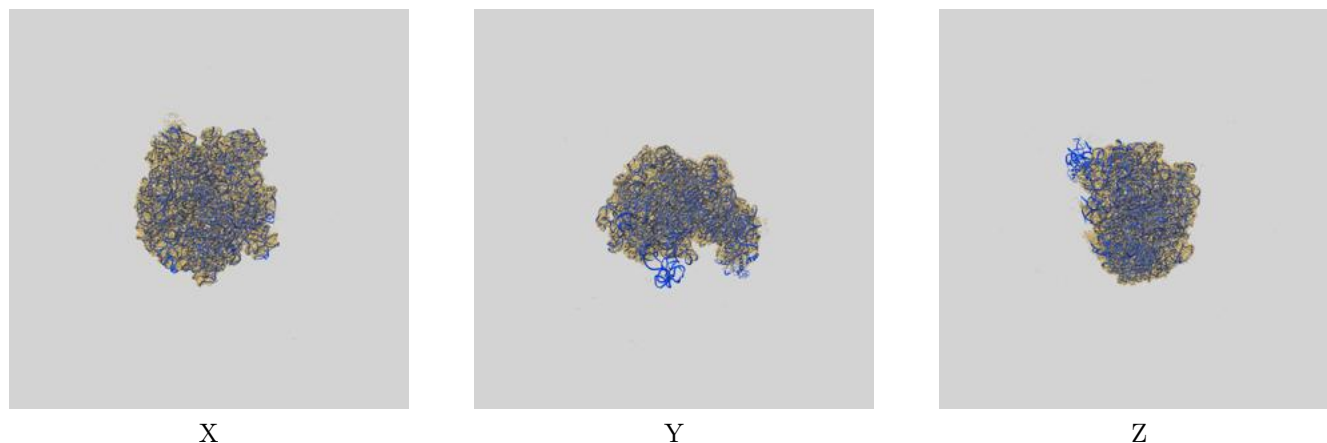
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.65	-	-
Author-provided FSC curve	2.65	3.08	2.75
Unmasked-calculated*	3.49	6.73	3.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.49 differs from the reported value 2.65 by more than 10 %

9 Map-model fit [i](#)

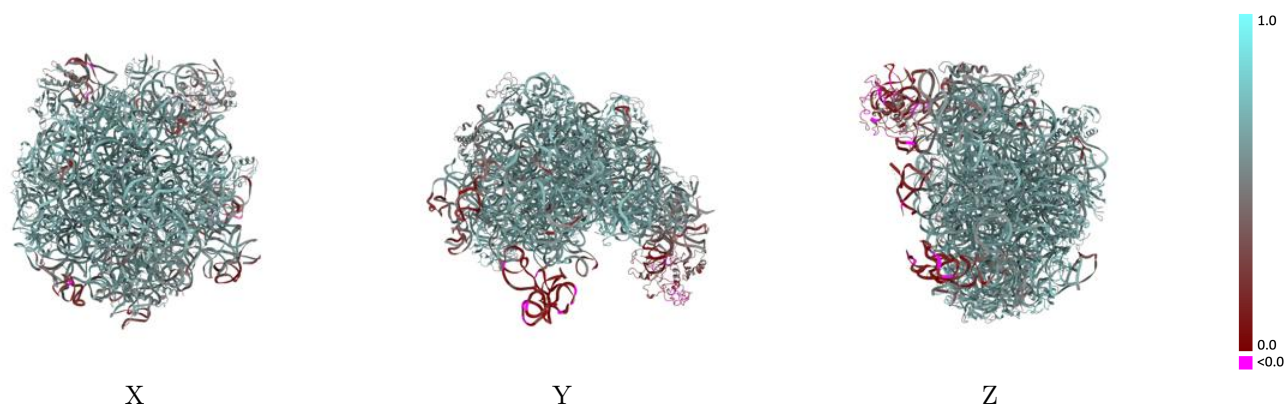
This section contains information regarding the fit between EMDB map EMD-38873 and PDB model 8Y36. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



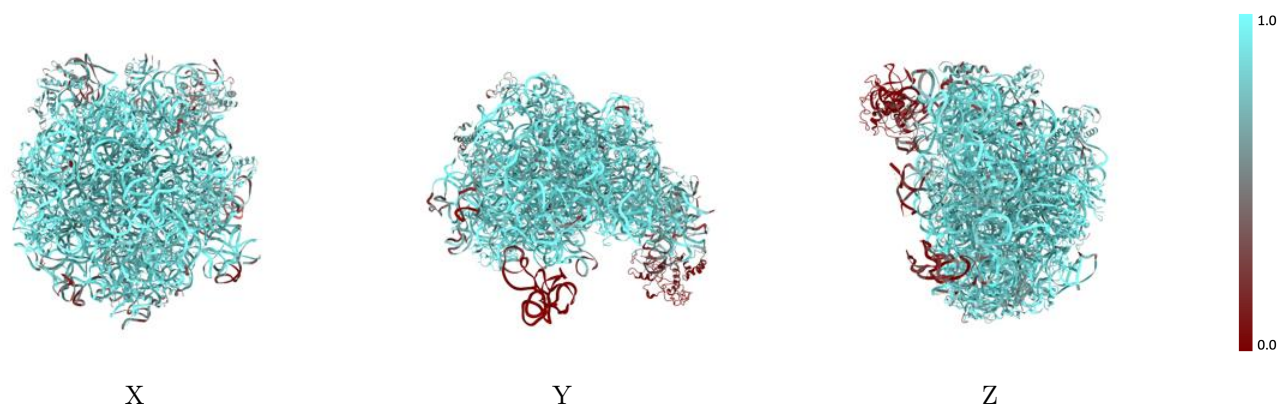
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



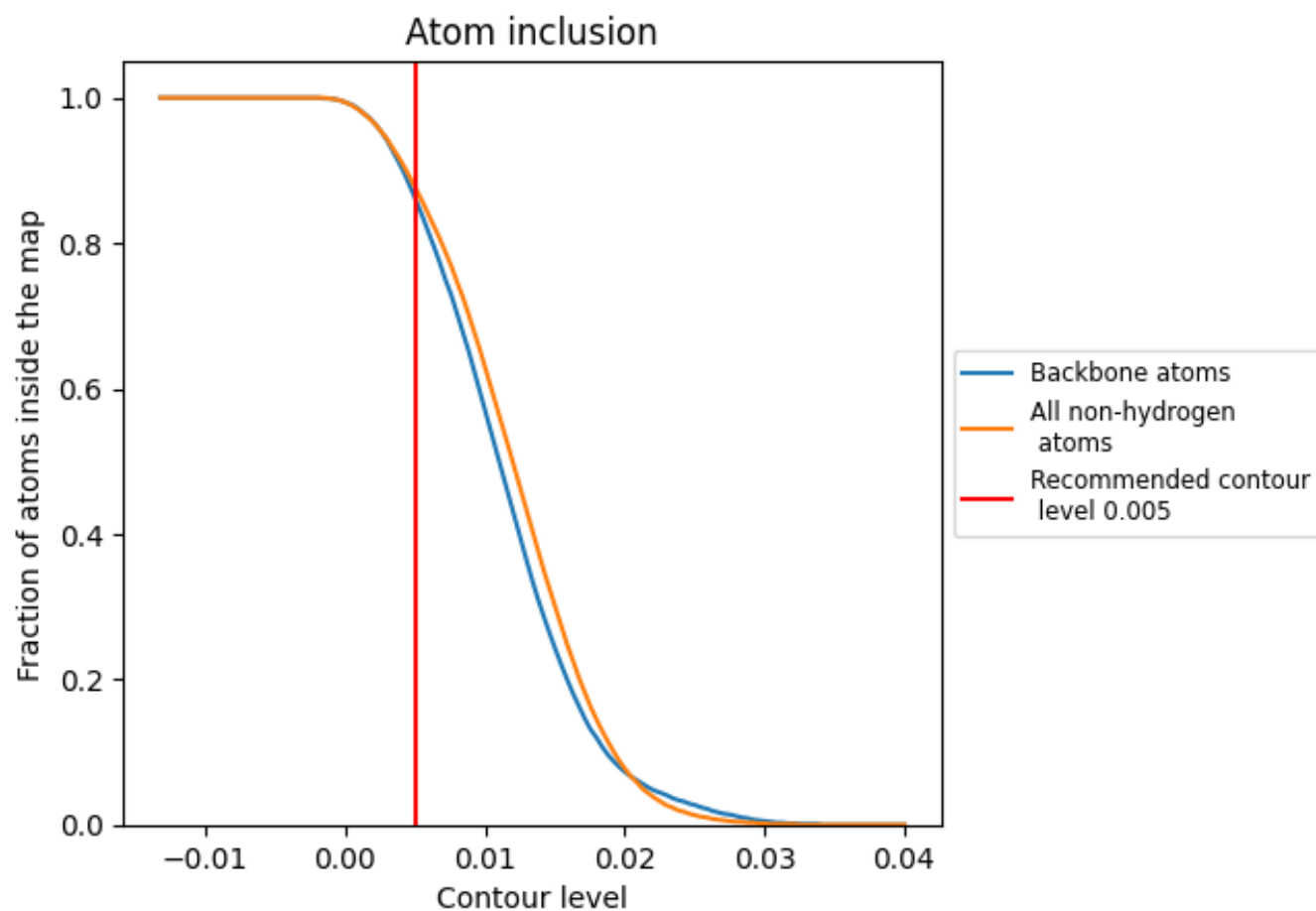
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 88% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8780	 0.5800
1	 0.9360	 0.6350
2	 0.9880	 0.6600
3	 0.9940	 0.6690
4	 0.9620	 0.6500
A	 0.8940	 0.5770
B	 0.8380	 0.5180
C	 0.9440	 0.6490
D	 0.9430	 0.6510
E	 0.8820	 0.6280
F	 0.2190	 0.3030
G	 0.7680	 0.5540
H	 0.9660	 0.6550
I	 0.8980	 0.6290
J	 0.9060	 0.6180
K	 0.9320	 0.6410
L	 0.9350	 0.6320
M	 0.7410	 0.5210
N	 0.7890	 0.5960
O	 0.9630	 0.6520
P	 0.9230	 0.6210
Q	 0.9540	 0.6490
R	 0.8960	 0.6020
S	 0.7040	 0.5230
T	 0.7620	 0.5800
U	 0.9280	 0.6350
V	 0.9490	 0.6250
W	 0.7280	 0.5350
X	 0.9360	 0.6360
Y	 0.0440	 0.1450
Z	 0.9800	 0.6560

