



wwPDB EM Validation Summary Report ⓘ

Mar 22, 2026 – 03:54 PM UTC

PDB ID : 8ANA / pdb_00008ana
EMDB ID : EMD-15533
Title : Cryo-EM structure of the proline-rich antimicrobial peptide drosocin bound to the 50S ribosomal subunit
Authors : Koller, T.O.; Morici, M.; Wilson, D.N.
Deposited on : 2022-08-05
Resolution : 2.10 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:

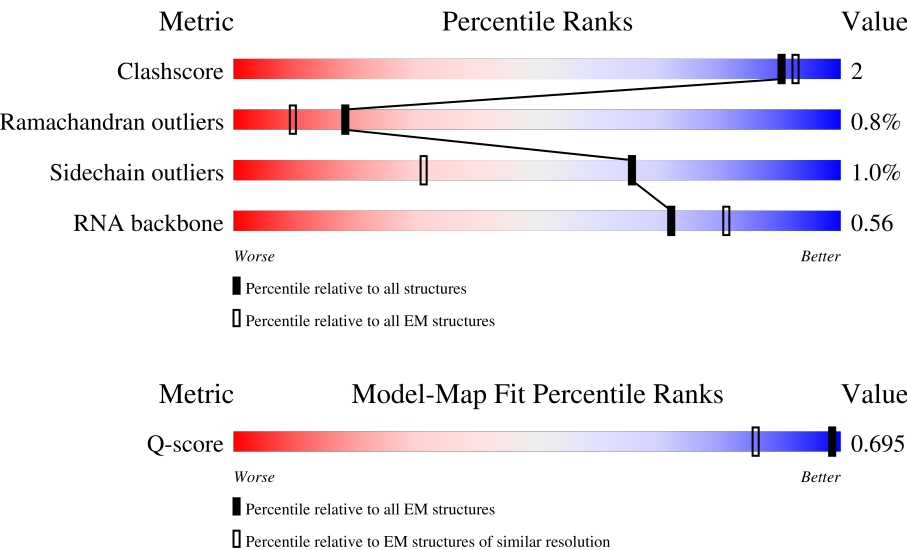
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	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	2317 (1.60 - 2.60)

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

Mol	Chain	Length	Quality of chain
1	0	55	
2	1	46	
3	2	65	

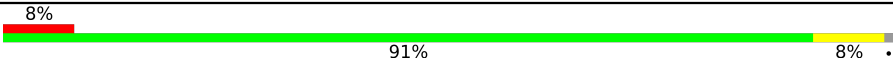
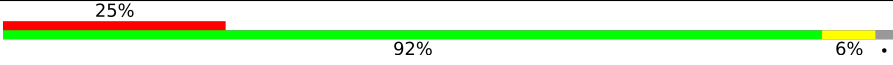
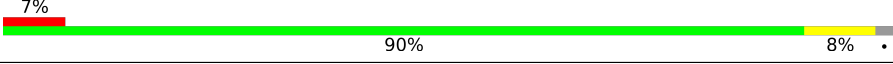
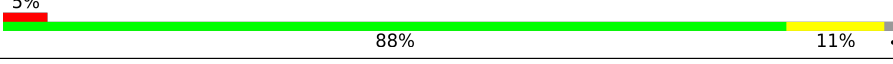
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Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	A	19	
7	a	2903	
8	b	120	
9	c	273	
10	d	209	
11	e	201	
12	f	179	
13	g	177	
14	h	149	
15	i	142	
16	j	123	
17	k	144	
18	l	136	
19	m	127	
20	n	117	
21	o	115	
22	p	118	
23	q	103	
24	r	110	
25	s	100	
26	t	104	
27	u	94	
28	v	85	

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Mol	Chain	Length	Quality of chain
29	w	78	 8% 91% 8%
30	x	63	 25% 92% 6%
31	y	59	 7% 90% 8%
32	z	57	 5% 88% 11%

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 86461 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L33.

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

- Molecule 2 is a protein called 50S ribosomal protein L34.

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

- Molecule 3 is a protein called 50S ribosomal protein L35.

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

- Molecule 4 is a protein called 50S ribosomal protein L36.

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

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a protein called Drosocin1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	A	19	Total	C	N	O	0	0
			155	98	34	23		

- Molecule 7 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	2733	Total	C	N	O	P	0	0
			58702	26191	10821	18957	2733		

- Molecule 8 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 9 is a protein called 50S ribosomal protein L2.

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

- Molecule 10 is a protein called 50S ribosomal protein L3.

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

- Molecule 11 is a protein called 50S ribosomal protein L4.

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

- Molecule 12 is a protein called 50S ribosomal protein L5.

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

- Molecule 13 is a protein called 50S ribosomal protein L6.

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

- Molecule 14 is a protein called 50S ribosomal protein L9.

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

- Molecule 15 is a protein called 50S ribosomal protein L13.

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

- Molecule 16 is a protein called 50S ribosomal protein L14.

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

- Molecule 17 is a protein called 50S ribosomal protein L15.

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

- Molecule 18 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	l	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 19 is a protein called 50S ribosomal protein L17.

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

- Molecule 20 is a protein called 50S ribosomal protein L18.

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

- Molecule 21 is a protein called 50S ribosomal protein L19.

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

- Molecule 22 is a protein called 50S ribosomal protein L20.

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

- Molecule 23 is a protein called 50S ribosomal protein L21.

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

- Molecule 24 is a protein called 50S ribosomal protein L22.

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

- Molecule 25 is a protein called 50S ribosomal protein L23.

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

- Molecule 26 is a protein called 50S ribosomal protein L24.

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

- Molecule 27 is a protein called 50S ribosomal protein L25.

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

- Molecule 28 is a protein called 50S ribosomal protein L27.

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

- Molecule 29 is a protein called 50S ribosomal protein L28.

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

- Molecule 30 is a protein called 50S ribosomal protein L29.

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

- Molecule 31 is a protein called 50S ribosomal protein L30.

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

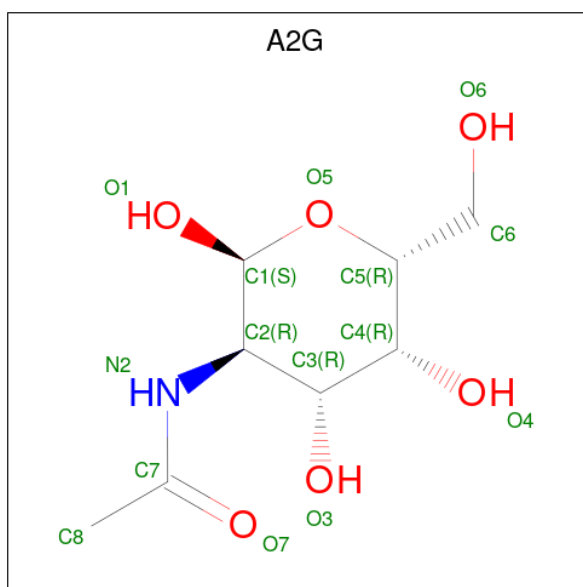
- Molecule 32 is a protein called 50S ribosomal protein L32.

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

- Molecule 33 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
33	3	1	Total	Zn	0
			1	1	
33	4	1	Total	Zn	0
			1	1	

- Molecule 34 is 2-acetamido-2-deoxy- α -D-galactopyranose (CCD ID: A2G) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

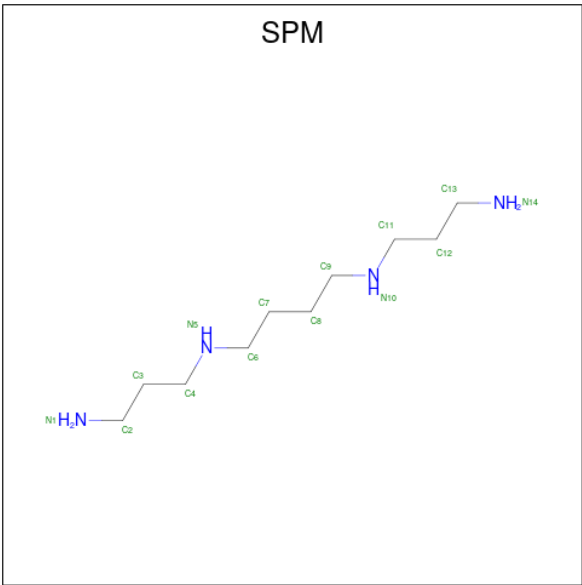


Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	a	208	Total	Mg	0
			208	208	
35	b	5	Total	Mg	0
			5	5	
35	c	1	Total	Mg	0
			1	1	
35	d	1	Total	Mg	0
			1	1	
35	z	1	Total	Mg	0
			1	1	

- Molecule 36 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).



Mol	Chain	Residues	Atoms			AltConf
36	a	1	Total	C	N	0
			14	10	4	

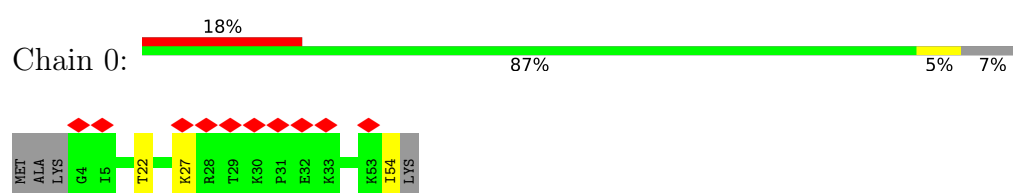
- Molecule 37 is water.

Mol	Chain	Residues	Atoms		AltConf
37	A	11	Total	O	0
			11	11	
37	a	27	Total	O	0
			27	27	
37	e	2	Total	O	0
			2	2	
37	r	2	Total	O	0
			2	2	

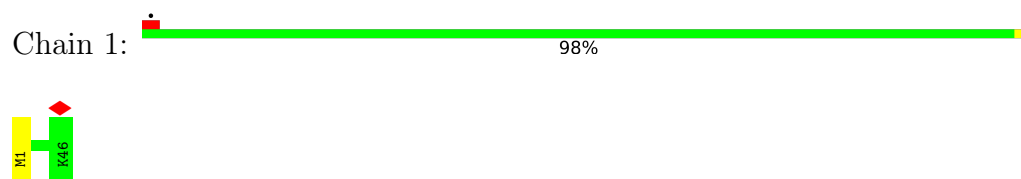
3 Residue-property plots [i](#)

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

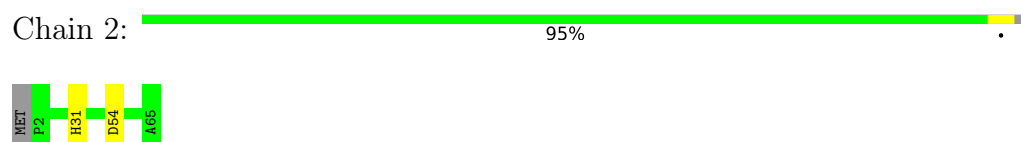
- Molecule 1: 50S ribosomal protein L33



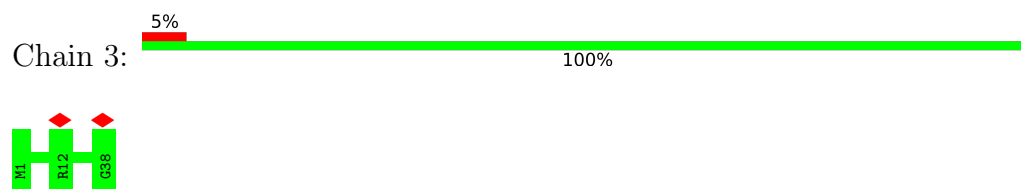
- Molecule 2: 50S ribosomal protein L34



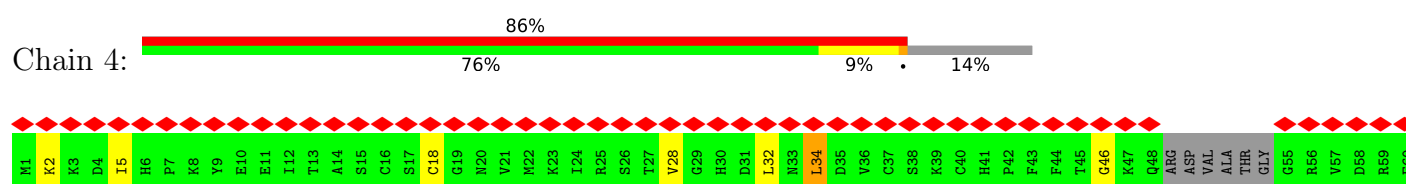
- Molecule 3: 50S ribosomal protein L35

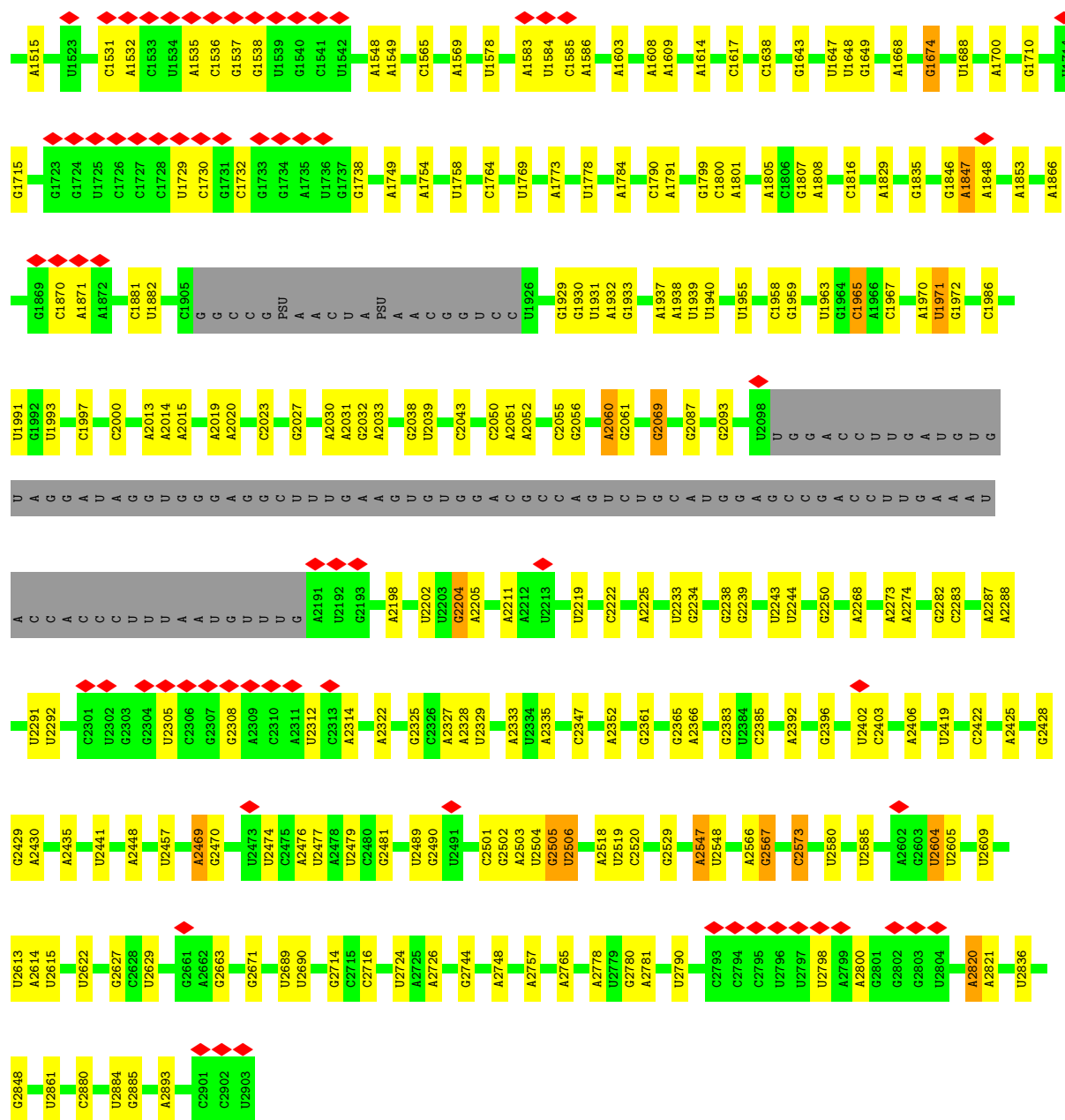


- Molecule 4: 50S ribosomal protein L36

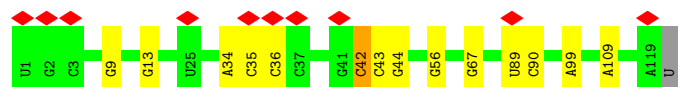
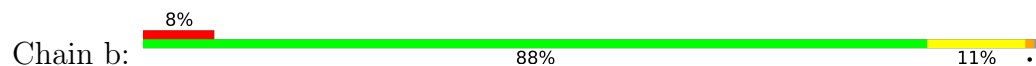


- Molecule 5: 50S ribosomal protein L31

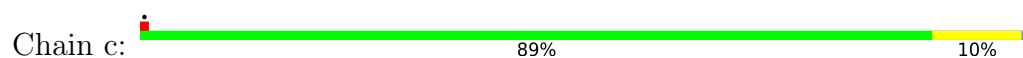


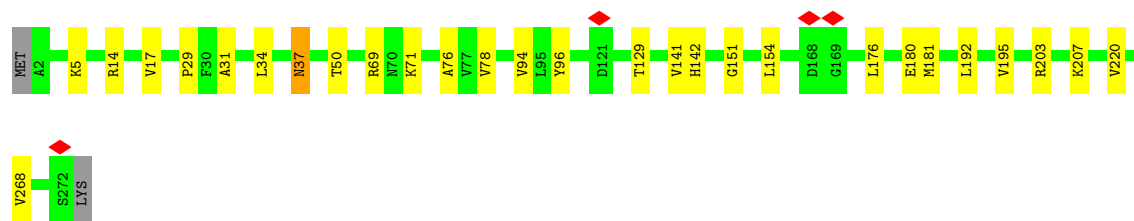


● Molecule 8: 5S ribosomal RNA

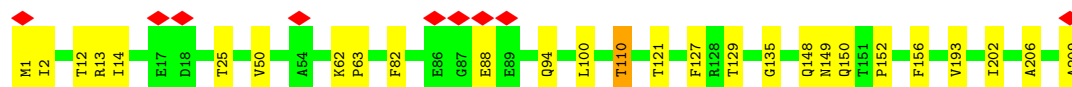
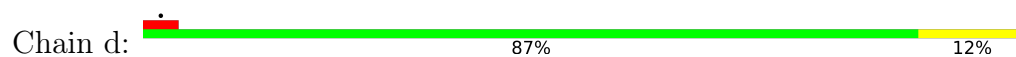


● Molecule 9: 50S ribosomal protein L2

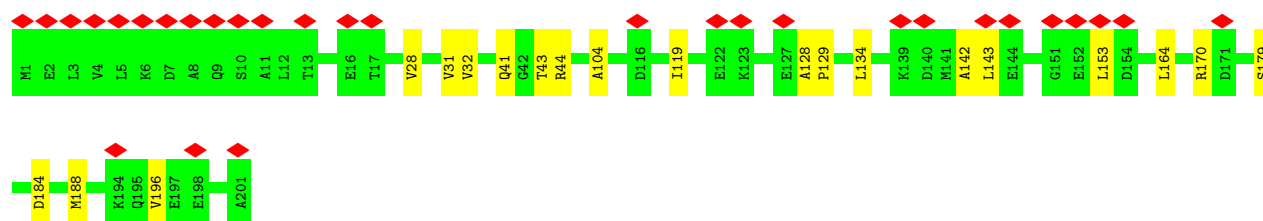
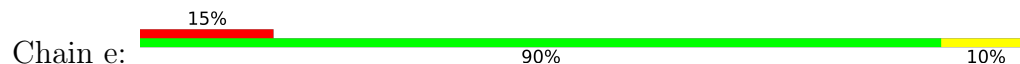




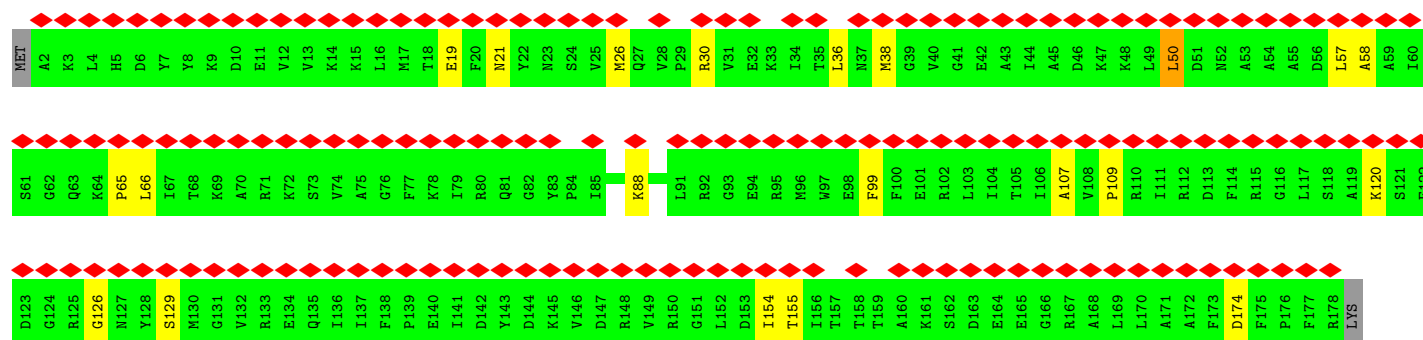
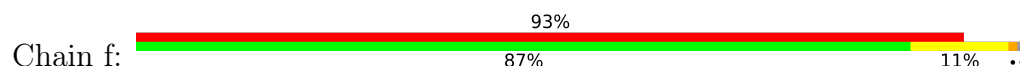
- Molecule 10: 50S ribosomal protein L3



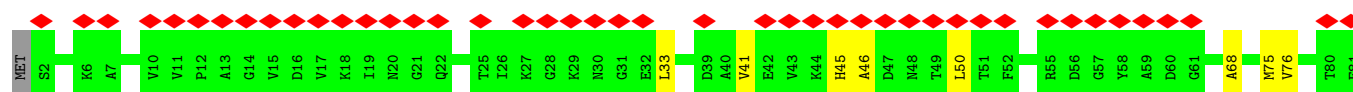
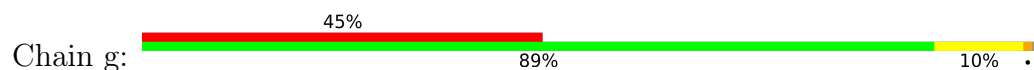
- Molecule 11: 50S ribosomal protein L4

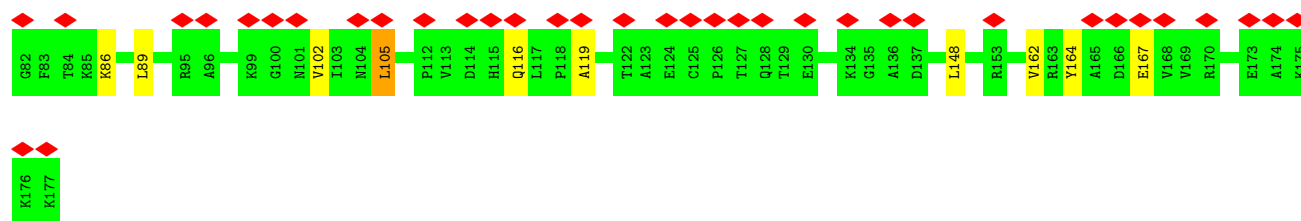


- Molecule 12: 50S ribosomal protein L5

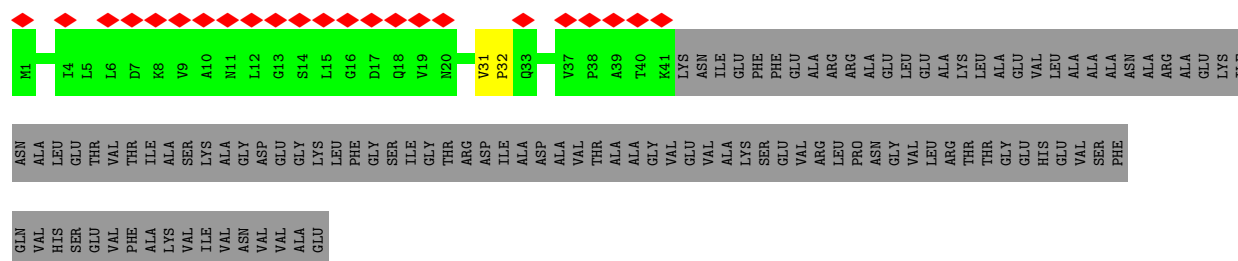


- Molecule 13: 50S ribosomal protein L6





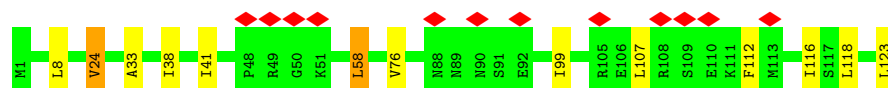
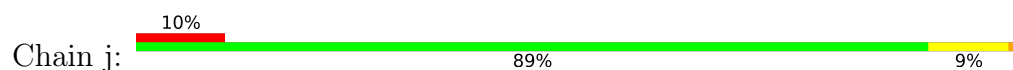
- Molecule 14: 50S ribosomal protein L9



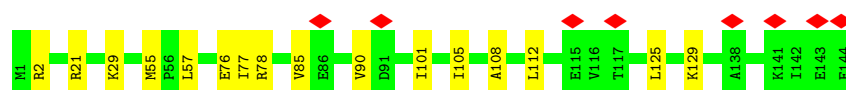
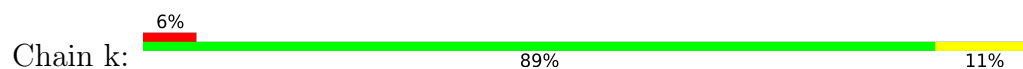
- Molecule 15: 50S ribosomal protein L13



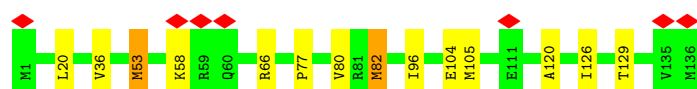
- Molecule 16: 50S ribosomal protein L14



- Molecule 17: 50S ribosomal protein L15



- Molecule 18: 50S ribosomal protein L16



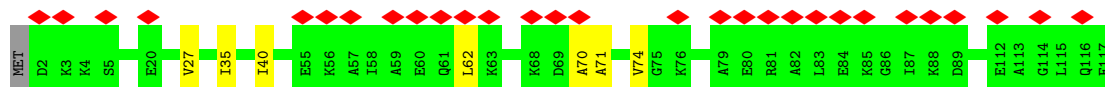
- Molecule 19: 50S ribosomal protein L17

Chain m:  80% 12% 7%

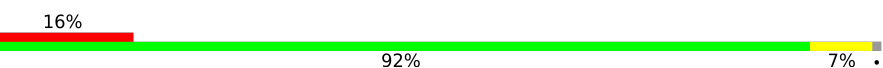


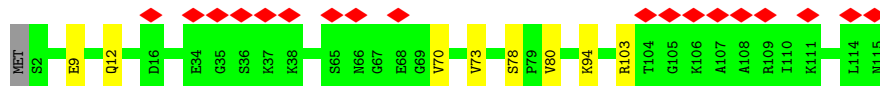
- Molecule 20: 50S ribosomal protein L18

Chain n:  25% 93% 6%



- Molecule 21: 50S ribosomal protein L19

Chain o:  16% 92% 7%

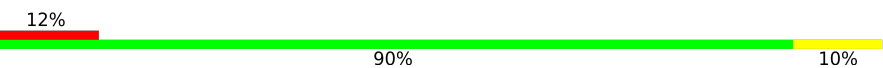


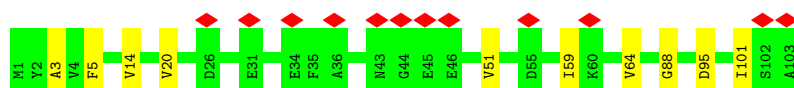
- Molecule 22: 50S ribosomal protein L20

Chain p:  86% 13%



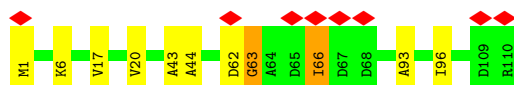
- Molecule 23: 50S ribosomal protein L21

Chain q:  12% 90% 10%



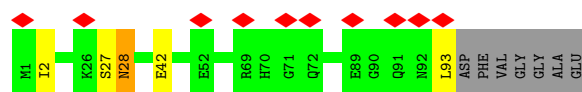
- Molecule 24: 50S ribosomal protein L22

Chain r:  7% 90% 8%

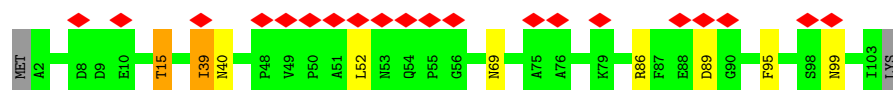
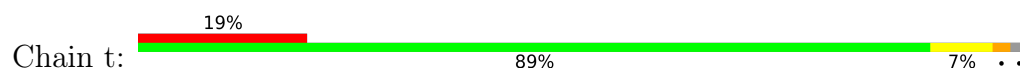


- Molecule 25: 50S ribosomal protein L23

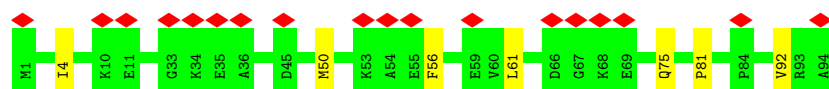
Chain s:  10% 88% 7%



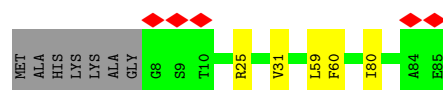
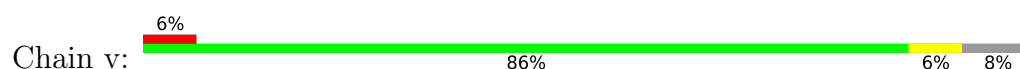
- Molecule 26: 50S ribosomal protein L24



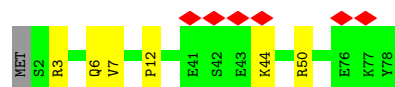
- Molecule 27: 50S ribosomal protein L25



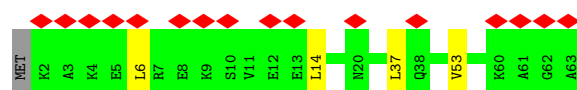
- Molecule 28: 50S ribosomal protein L27



- Molecule 29: 50S ribosomal protein L28



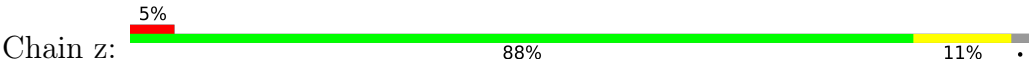
- Molecule 30: 50S ribosomal protein L29



- Molecule 31: 50S ribosomal protein L30



- Molecule 32: 50S ribosomal protein L32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	159749	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.115	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	480.0, 480.0, 480.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8, 0.8, 0.8	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, 2MA, OMC, PSU, OMU, 1MG, G7M, H2U, 5MU, A2G, OMG, MEQ, MG, SPM, ZN, 2MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.40	0/424	0.71	0/565
2	1	0.43	0/380	0.76	0/498
3	2	0.45	0/513	0.78	0/676
4	3	0.45	0/303	0.67	0/397
5	4	0.43	0/488	0.73	0/649
6	A	0.59	0/162	0.99	1/221 (0.5%)
7	a	0.54	1/65294 (0.0%)	0.87	29/101861 (0.0%)
8	b	0.84	0/2850	0.86	0/4444
9	c	1.01	0/2121	1.32	1/2852 (0.0%)
10	d	1.01	0/1576	1.35	0/2119
11	e	1.03	0/1571	1.45	0/2113
12	f	1.06	0/1434	1.35	0/1926
13	g	1.06	0/1343	1.39	0/1816
14	h	1.08	0/306	1.47	0/413
15	i	0.98	0/1152	1.35	0/1551
16	j	1.05	0/955	1.33	0/1279
17	k	1.02	0/1062	1.40	0/1413
18	l	1.00	0/1093	1.37	0/1460
19	m	0.97	0/958	1.45	0/1281
20	n	1.05	0/902	1.53	0/1209
21	o	1.01	0/929	1.29	0/1242
22	p	0.94	0/960	1.56	0/1278
23	q	1.03	0/829	1.23	0/1107
24	r	1.02	0/864	1.41	0/1156
25	s	1.03	0/744	1.36	0/994
26	t	1.10	0/787	1.35	0/1051
27	u	1.02	0/766	1.26	0/1025
28	v	1.04	0/593	1.31	0/785
29	w	0.97	0/635	1.39	0/848
30	x	0.98	0/502	1.59	0/667
31	y	1.02	0/453	1.41	0/605
32	z	1.01	0/450	1.38	0/599

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.70	1/93399 (0.0%)	1.00	31/140100 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	2069	G7M	O3'-P	5.07	1.61	1.56

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	781	A	O3'-P-O5'	-7.65	92.53	104.00
7	a	2050	C	O3'-P-O5'	-6.83	93.75	104.00
7	a	1971	U	O3'-P-O5'	-6.07	94.90	104.00
7	a	204	A	O3'-P-O5'	-6.01	94.99	104.00
7	a	1617	C	P-O3'-C3'	-5.92	111.32	120.20

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	0	417	0	451	1	0
2	1	377	0	418	0	0
3	2	504	0	572	1	0
4	3	302	0	340	0	0
5	4	480	0	478	3	0
6	A	155	0	164	1	0
7	a	58702	0	29546	105	0
8	b	2549	0	1291	1	0
9	c	2082	0	2154	17	0
10	d	1566	0	1618	18	0
11	e	1552	0	1619	12	0
12	f	1410	0	1444	11	0
13	g	1323	0	1371	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	h	303	0	327	1	0
15	i	1129	0	1162	7	0
16	j	946	0	1023	10	0
17	k	1053	0	1129	14	0
18	l	1074	0	1157	9	0
19	m	945	0	989	10	0
20	n	892	0	923	4	0
21	o	917	0	962	8	0
22	p	947	0	1019	10	0
23	q	816	0	839	6	0
24	r	857	0	922	8	0
25	s	738	0	807	2	0
26	t	779	0	831	3	0
27	u	753	0	780	4	0
28	v	586	0	596	3	0
29	w	625	0	652	2	0
30	x	501	0	531	3	0
31	y	449	0	488	4	0
32	z	444	0	458	5	0
33	3	1	0	0	0	0
33	4	1	0	0	0	0
34	A	14	0	12	1	0
35	a	208	0	0	0	0
35	b	5	0	0	0	0
35	c	1	0	0	0	0
35	d	1	0	0	0	0
35	z	1	0	0	0	0
36	a	14	0	26	0	0
37	A	11	0	0	0	0
37	a	27	0	0	0	0
37	e	2	0	0	0	0
37	r	2	0	0	0	0
All	All	86461	0	57099	245	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 2.

The worst 5 of 245 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)
12:f:38:MET:HE3	12:f:57:LEU:HD13	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:1252:G:H1	22:p:37:GLN:HE21	1.15	0.90
10:d:110:THR:HG23	10:d:202:ILE:HB	1.64	0.79
7:a:12:U:H2'	7:a:12:U:O2	1.89	0.71
18:l:20:LEU:HD13	27:u:81:PRO:HG2	1.72	0.70

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	
1	0	49/55 (89%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	47 (84%)	7 (12%)	2 (4%)	2	1
6	A	17/19 (90%)	17 (100%)	0	0	100	100
9	c	269/273 (98%)	256 (95%)	12 (4%)	1 (0%)	30	28
10	d	206/209 (99%)	196 (95%)	8 (4%)	2 (1%)	12	9
11	e	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	24	22
12	f	175/179 (98%)	146 (83%)	22 (13%)	7 (4%)	2	0
13	g	174/177 (98%)	158 (91%)	14 (8%)	2 (1%)	11	8
14	h	39/149 (26%)	35 (90%)	4 (10%)	0	100	100
15	i	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
16	j	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
17	k	142/144 (99%)	128 (90%)	13 (9%)	1 (1%)	18	15
18	l	134/136 (98%)	125 (93%)	8 (6%)	1 (1%)	18	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	m	116/127 (91%)	104 (90%)	12 (10%)	0	100	100
20	n	114/117 (97%)	102 (90%)	12 (10%)	0	100	100
21	o	112/115 (97%)	106 (95%)	6 (5%)	0	100	100
22	p	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
23	q	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
24	r	108/110 (98%)	101 (94%)	6 (6%)	1 (1%)	14	10
25	s	91/100 (91%)	84 (92%)	6 (7%)	1 (1%)	11	8
26	t	100/104 (96%)	86 (86%)	11 (11%)	3 (3%)	3	1
27	u	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
28	v	76/85 (89%)	74 (97%)	2 (3%)	0	100	100
29	w	75/78 (96%)	73 (97%)	0	2 (3%)	4	1
30	x	60/63 (95%)	56 (93%)	3 (5%)	1 (2%)	7	3
31	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
32	z	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
All	All	3133/3356 (93%)	2928 (94%)	180 (6%)	25 (1%)	18	12

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	f	174	ASP
24	r	63	GLY
26	t	99	ASN
12	f	50	LEU
18	l	58	LYS

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	
1	0	46/49 (94%)	44 (96%)	2 (4%)	26	27
2	1	38/38 (100%)	37 (97%)	1 (3%)	40	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	2	51/52 (98%)	50 (98%)	1 (2%)	48	56
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	55/62 (89%)	54 (98%)	1 (2%)	51	60
6	A	18/18 (100%)	18 (100%)	0	100	100
9	c	216/218 (99%)	215 (100%)	1 (0%)	81	88
10	d	163/163 (100%)	161 (99%)	2 (1%)	63	72
11	e	165/165 (100%)	163 (99%)	2 (1%)	63	72
12	f	148/150 (99%)	146 (99%)	2 (1%)	59	67
13	g	137/138 (99%)	135 (98%)	2 (2%)	57	65
14	h	32/114 (28%)	32 (100%)	0	100	100
15	i	116/116 (100%)	116 (100%)	0	100	100
16	j	104/104 (100%)	102 (98%)	2 (2%)	50	58
17	k	103/103 (100%)	101 (98%)	2 (2%)	50	58
18	l	109/109 (100%)	107 (98%)	2 (2%)	51	60
19	m	98/103 (95%)	97 (99%)	1 (1%)	68	76
20	n	86/87 (99%)	86 (100%)	0	100	100
21	o	99/100 (99%)	99 (100%)	0	100	100
22	p	89/90 (99%)	88 (99%)	1 (1%)	65	74
23	q	84/84 (100%)	84 (100%)	0	100	100
24	r	93/93 (100%)	92 (99%)	1 (1%)	65	74
25	s	80/84 (95%)	79 (99%)	1 (1%)	61	69
26	t	83/85 (98%)	81 (98%)	2 (2%)	43	49
27	u	78/78 (100%)	78 (100%)	0	100	100
28	v	58/63 (92%)	58 (100%)	0	100	100
29	w	67/68 (98%)	67 (100%)	0	100	100
30	x	54/55 (98%)	54 (100%)	0	100	100
31	y	48/49 (98%)	48 (100%)	0	100	100
32	z	47/48 (98%)	47 (100%)	0	100	100
All	All	2599/2720 (96%)	2573 (99%)	26 (1%)	65	76

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	j	24	VAL
17	k	129	LYS
26	t	15	THR
17	k	112	LEU
18	l	53	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
18	l	60	GLN
22	p	52	GLN
20	n	29	HIS
21	o	10	GLN
24	r	31	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	a	2728/2903 (93%)	305 (11%)	0
8	b	118/120 (98%)	14 (11%)	0
All	All	2846/3023 (94%)	319 (11%)	0

5 of 319 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	a	10	A
7	a	12	U
7	a	15	G
7	a	34	U
7	a	63	A

There are no RNA pucker outliers to report.

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

20 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	$\# Z > 2$
7	2MA	a	2503	7,35	22,25,26	0.93	1 (4%)	32,37,40	1.11	4 (12%)
7	OMG	a	2251	7,35	23,26,27	0.31	0	32,38,41	0.40	0
7	PSU	a	2580	7,35	18,21,22	1.07	1 (5%)	21,30,33	0.72	1 (4%)
7	5MU	a	1939	7	19,22,23	0.30	0	27,32,35	0.37	0
7	5MC	a	1962	7	19,22,23	0.54	0	26,32,35	0.48	0
7	H2U	a	2449	7	18,21,22	0.65	0	19,30,33	0.46	0
7	5MU	a	747	7	19,22,23	0.27	0	27,32,35	0.35	0
7	PSU	a	746	7,35	18,21,22	0.97	1 (5%)	21,30,33	0.69	0
7	2MG	a	2445	7	23,26,27	0.45	0	33,38,41	0.49	0
7	PSU	a	2605	7	18,21,22	1.10	1 (5%)	21,30,33	0.77	0
10	MEQ	d	150	10	8,9,10	0.49	0	5,10,12	0.56	0
7	1MG	a	745	7	23,26,27	0.66	0	33,39,42	0.66	0
7	PSU	a	2504	7	18,21,22	0.99	1 (5%)	21,30,33	0.75	0
7	PSU	a	955	7	18,21,22	0.97	1 (5%)	21,30,33	0.69	0
7	PSU	a	2457	7	18,21,22	1.08	1 (5%)	21,30,33	0.72	0
7	OMC	a	2498	7,35	19,22,23	0.29	0	25,31,34	0.54	0
7	OMU	a	2552	7	19,22,23	0.22	0	25,31,34	0.42	0
7	2MG	a	1835	7	23,26,27	1.00	1 (4%)	33,38,41	0.46	0
7	G7M	a	2069	7	23,26,27	0.74	1 (4%)	34,39,42	0.63	1 (2%)
7	PSU	a	2604	7	18,21,22	1.02	1 (5%)	21,30,33	0.79	1 (4%)

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
7	2MA	a	2503	7,35	-	2/7/25/26	0/3/3/3
7	OMG	a	2251	7,35	-	0/9/27/28	0/3/3/3
7	PSU	a	2580	7,35	-	0/7/25/26	0/2/2/2
7	5MU	a	1939	7	-	0/7/25/26	0/2/2/2
7	5MC	a	1962	7	-	0/7/25/26	0/2/2/2
7	H2U	a	2449	7	-	0/7/38/39	0/2/2/2
7	5MU	a	747	7	-	1/7/25/26	0/2/2/2
7	PSU	a	746	7,35	-	2/7/25/26	0/2/2/2
7	2MG	a	2445	7	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PSU	a	2605	7	-	0/7/25/26	0/2/2/2
10	MEQ	d	150	10	-	2/8/9/11	-
7	1MG	a	745	7	-	0/7/25/26	0/3/3/3
7	PSU	a	2504	7	-	0/7/25/26	0/2/2/2
7	PSU	a	955	7	-	0/7/25/26	0/2/2/2
7	PSU	a	2457	7	-	0/7/25/26	0/2/2/2
7	OMC	a	2498	7,35	-	0/9/27/28	0/2/2/2
7	OMU	a	2552	7	-	0/9/27/28	0/2/2/2
7	2MG	a	1835	7	-	0/9/27/28	0/3/3/3
7	G7M	a	2069	7	-	1/7/25/26	0/3/3/3
7	PSU	a	2604	7	-	0/7/25/26	0/2/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	2605	PSU	C6-C5	4.31	1.40	1.35
7	a	1835	2MG	CM2-N2	4.28	1.53	1.45
7	a	2580	PSU	C6-C5	4.12	1.39	1.35
7	a	2604	PSU	C6-C5	3.98	1.39	1.35
7	a	2457	PSU	C6-C5	3.97	1.39	1.35

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	2503	2MA	C5-C4-N3	-3.01	124.01	127.18
7	a	2503	2MA	CM2-C2-N1	2.64	121.09	117.13
7	a	2503	2MA	N3-C2-N1	-2.33	121.65	125.77
7	a	2503	2MA	C2-N1-C6	2.32	121.67	118.10
7	a	2604	PSU	C2'-C3'-C4'	-2.27	98.23	102.61

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	d	150	MEQ	NE2-CD-CG-CB
10	d	150	MEQ	OE1-CD-CG-CB
7	a	2069	G7M	C4'-C5'-O5'-P
7	a	2445	2MG	C3'-C4'-C5'-O5'
7	a	746	PSU	O4'-C1'-C5-C6

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	a	1939	5MU	1	0
7	a	747	5MU	1	0
10	d	150	MEQ	1	0
7	a	2604	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 220 ligands modelled in this entry, 218 are monoatomic - leaving 2 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	$\# Z > 2$
36	SPM	a	6209	-	13,13,13	0.22	0	12,12,12	0.31	0
34	A2G	A	101	6	14,14,15	0.47	0	17,19,21	1.02	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	SPM	a	6209	-	-	6/11/11/11	-
34	A2G	A	101	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	A	101	A2G	O5-C1-C2	-3.40	106.03	111.29

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

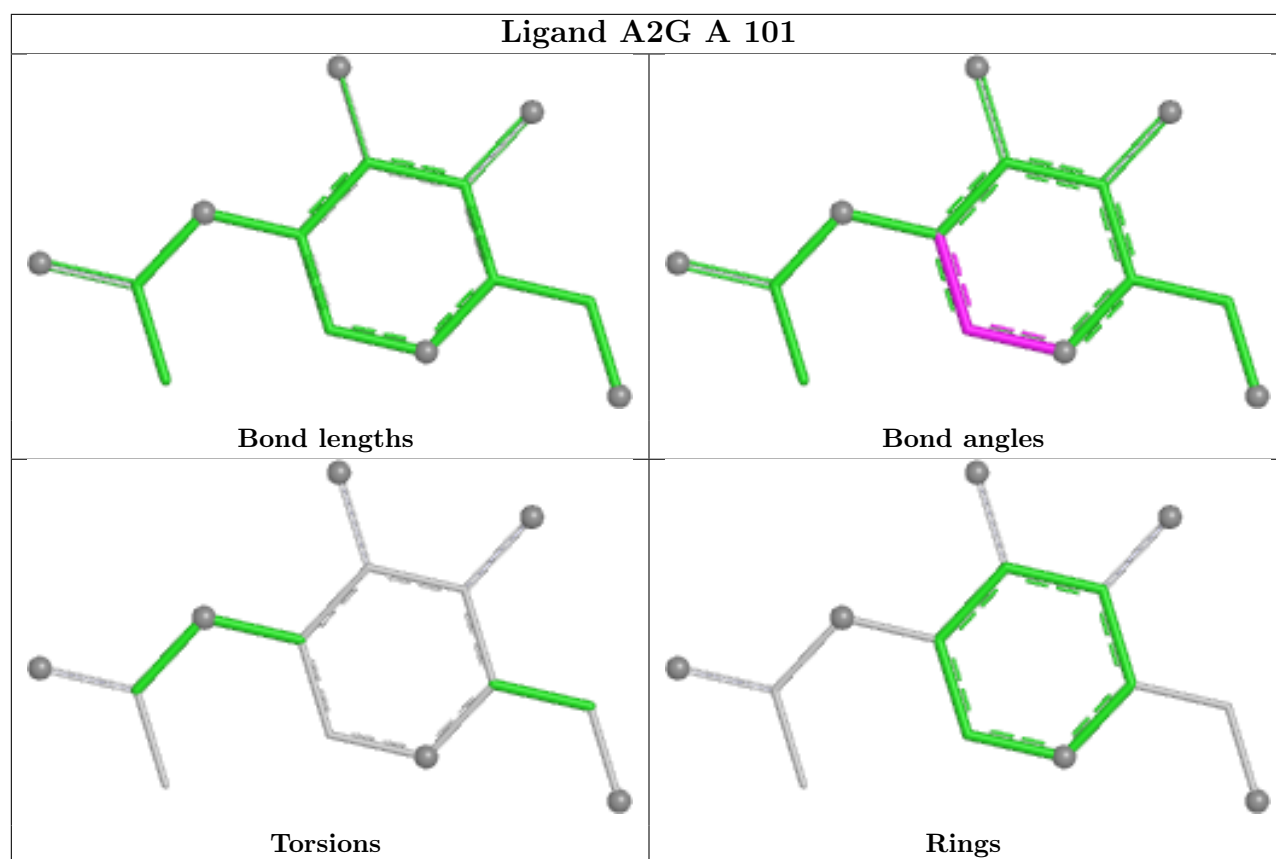
Mol	Chain	Res	Type	Atoms
36	a	6209	SPM	N10-C11-C12-C13
36	a	6209	SPM	C6-C7-C8-C9
36	a	6209	SPM	C8-C9-N10-C11
36	a	6209	SPM	C3-C4-N5-C6
36	a	6209	SPM	C7-C6-N5-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	A	101	A2G	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.

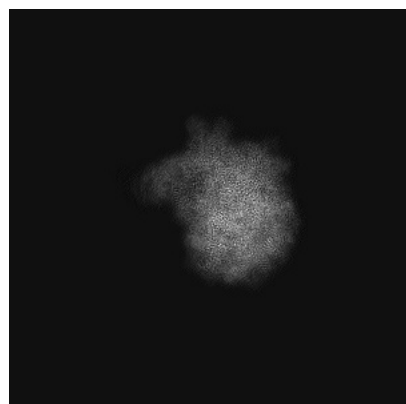
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15533. These allow visual inspection of the internal detail of the map and identification of artifacts.

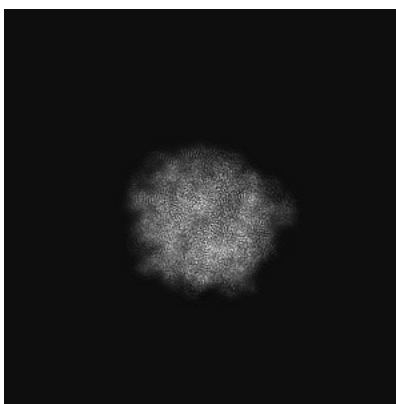
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

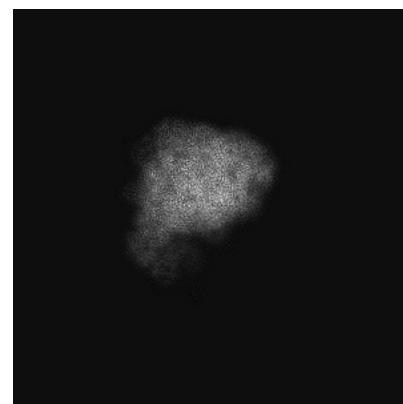
6.1.1 Primary map



X

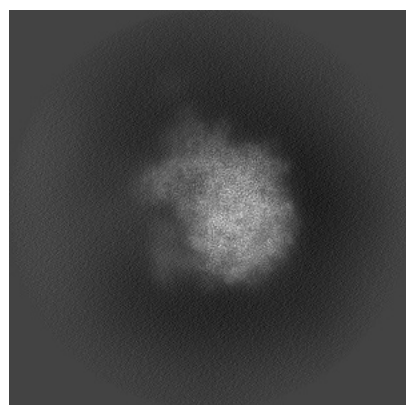


Y

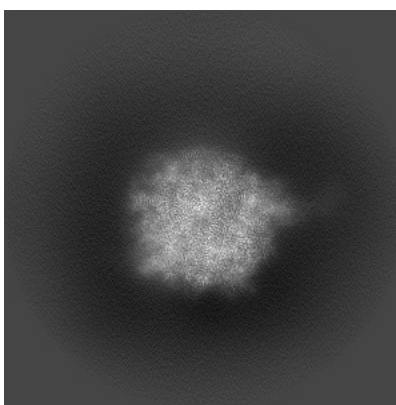


Z

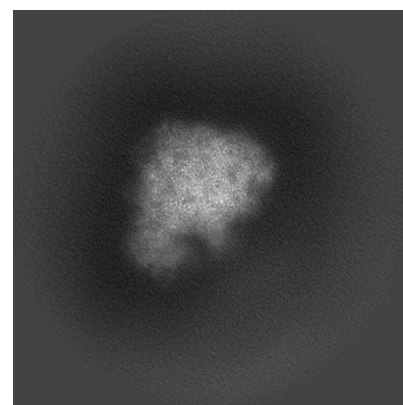
6.1.2 Raw map



X



Y



Z

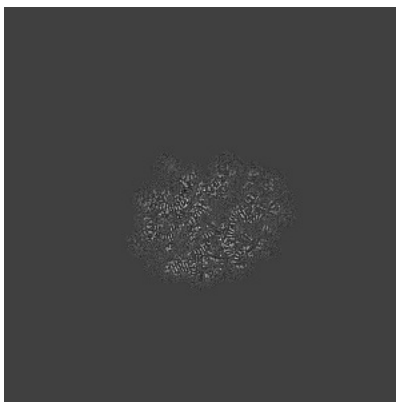
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 300

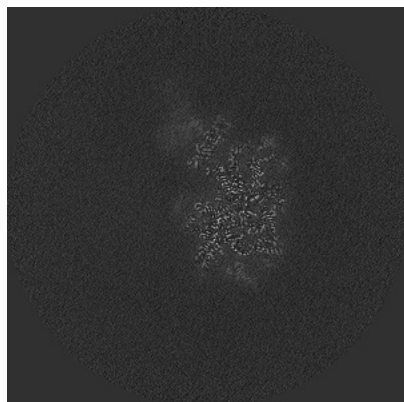


Y Index: 300

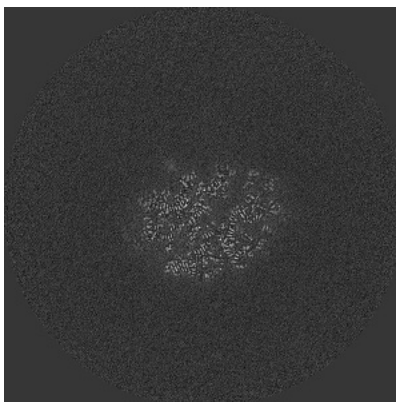


Z Index: 300

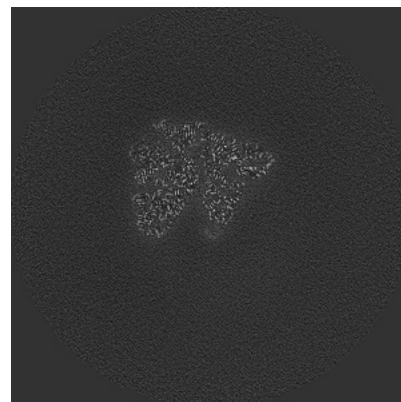
6.2.2 Raw map



X Index: 300



Y Index: 300



Z Index: 300

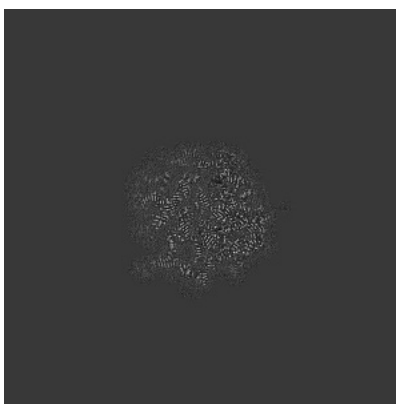
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 311

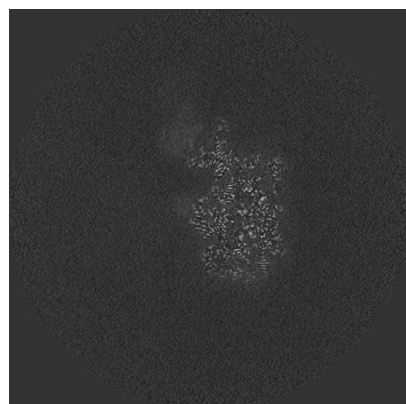


Y Index: 344

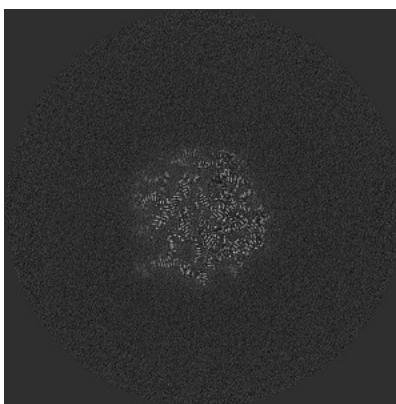


Z Index: 309

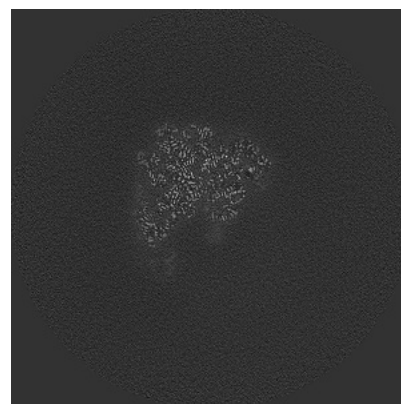
6.3.2 Raw map



X Index: 311



Y Index: 344

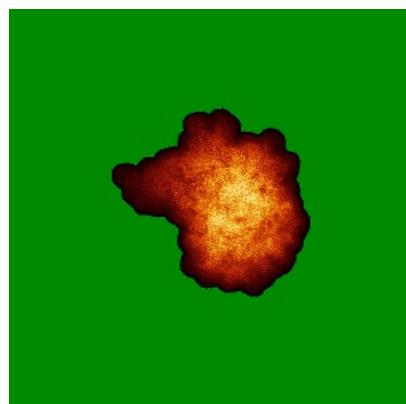


Z Index: 309

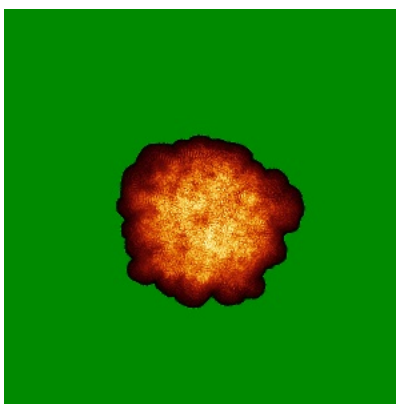
The images above show the largest variance slices of the map in three orthogonal directions.

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

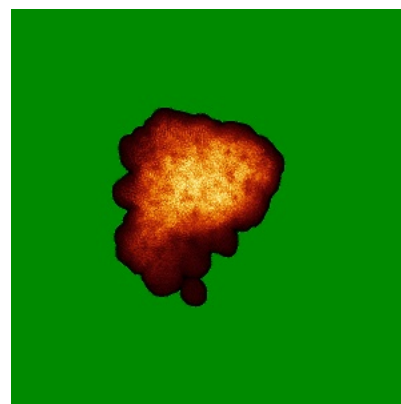
6.4.1 Primary map



X

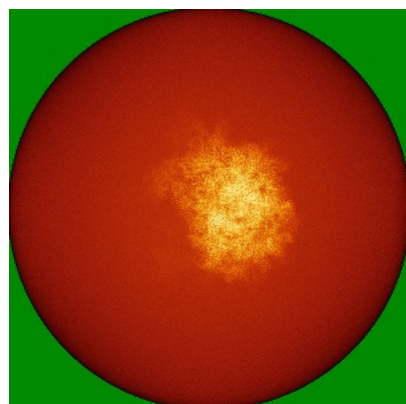


Y

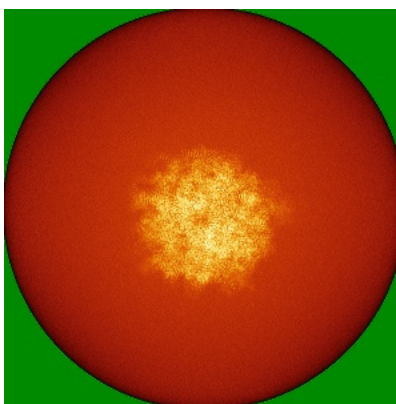


Z

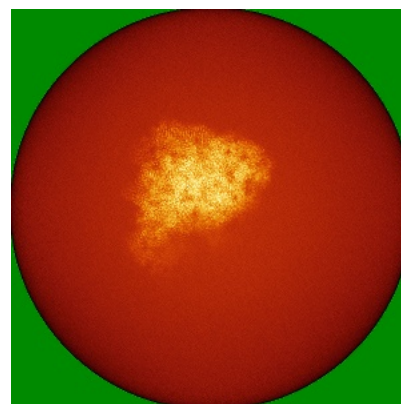
6.4.2 Raw map



X



Y

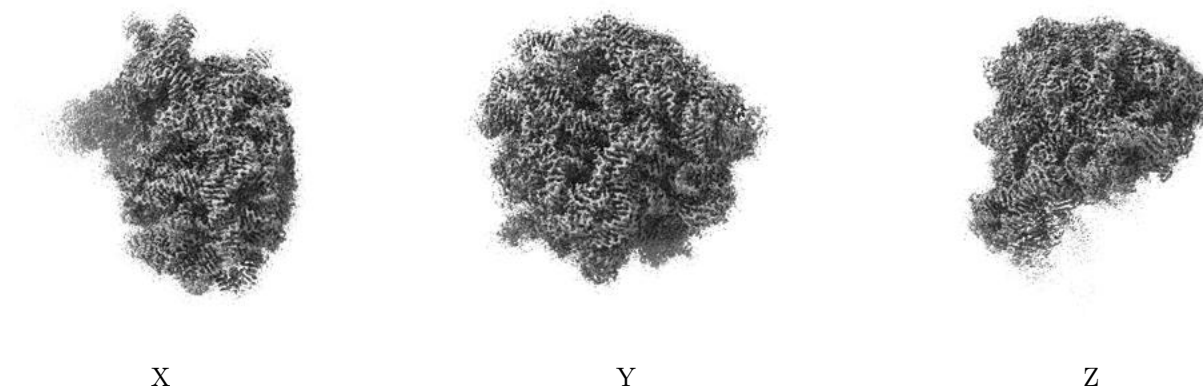


Z

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.

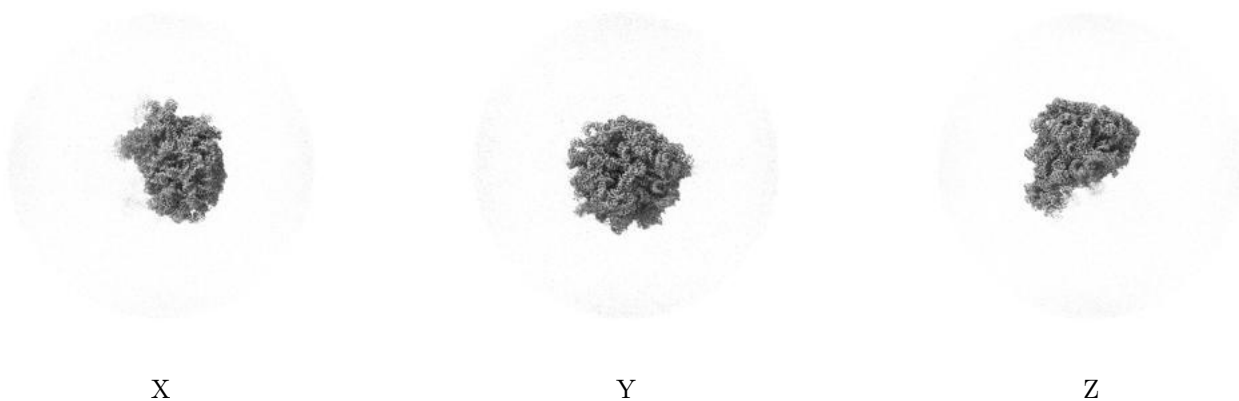
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. 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.

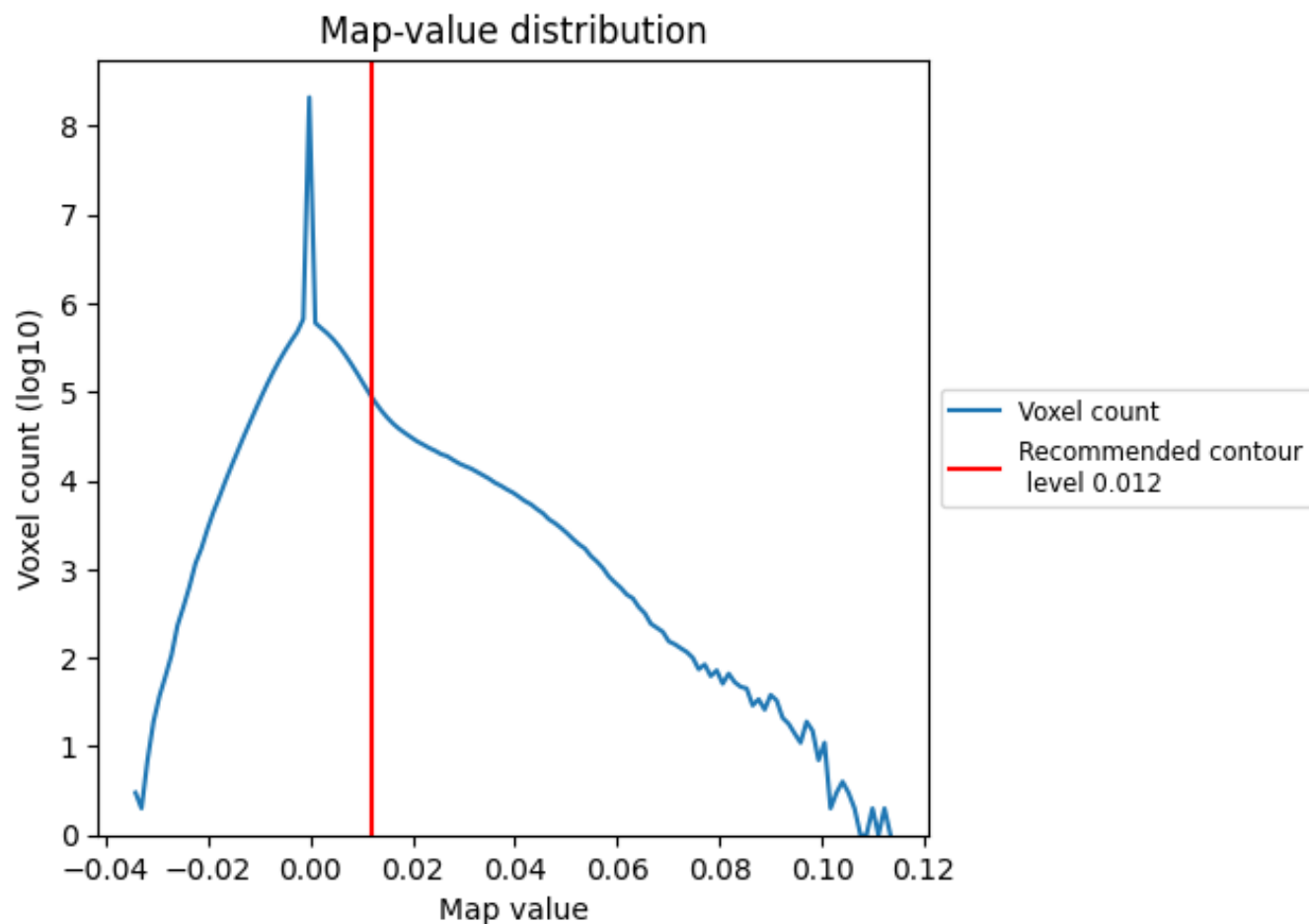
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

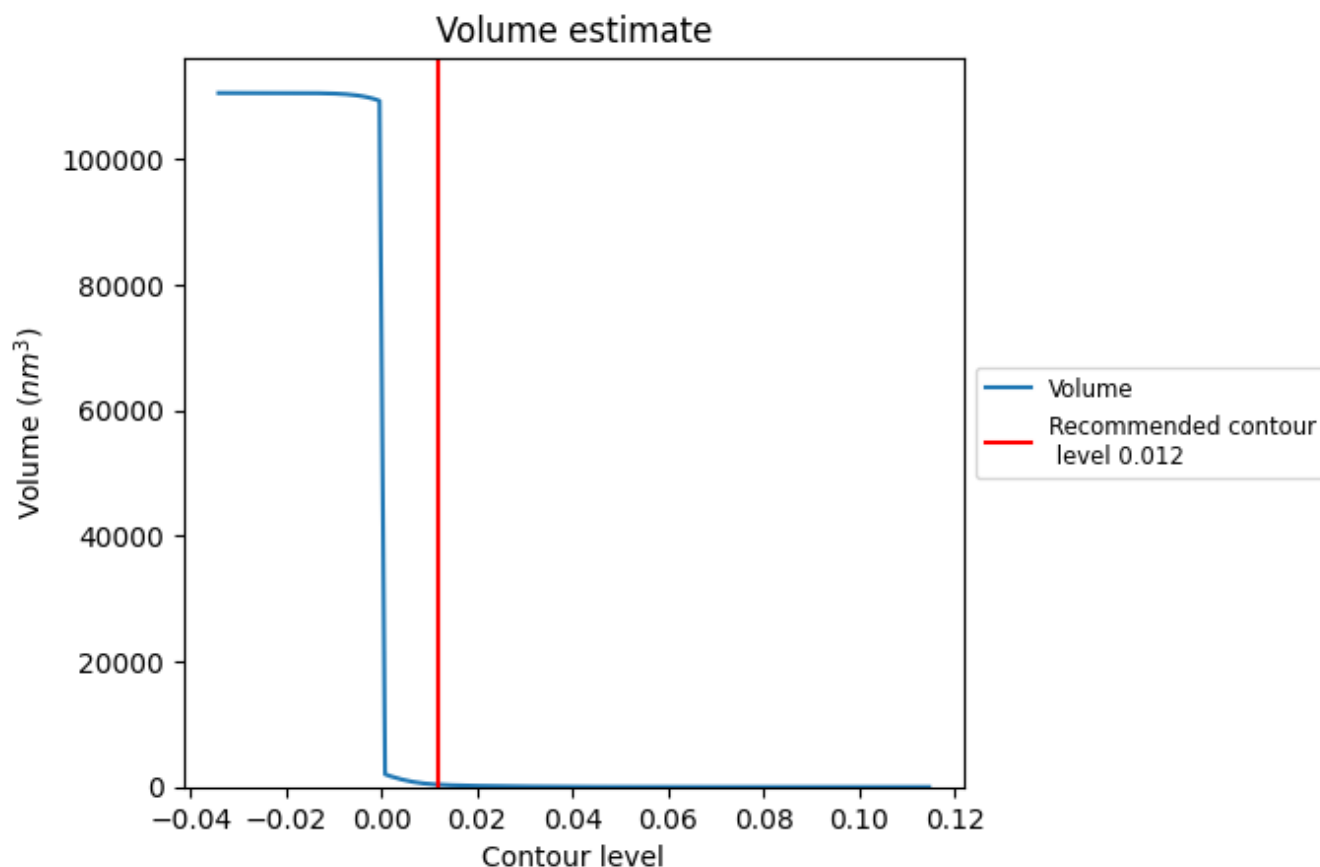
This section contains the results of statistical analysis of the map.

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.

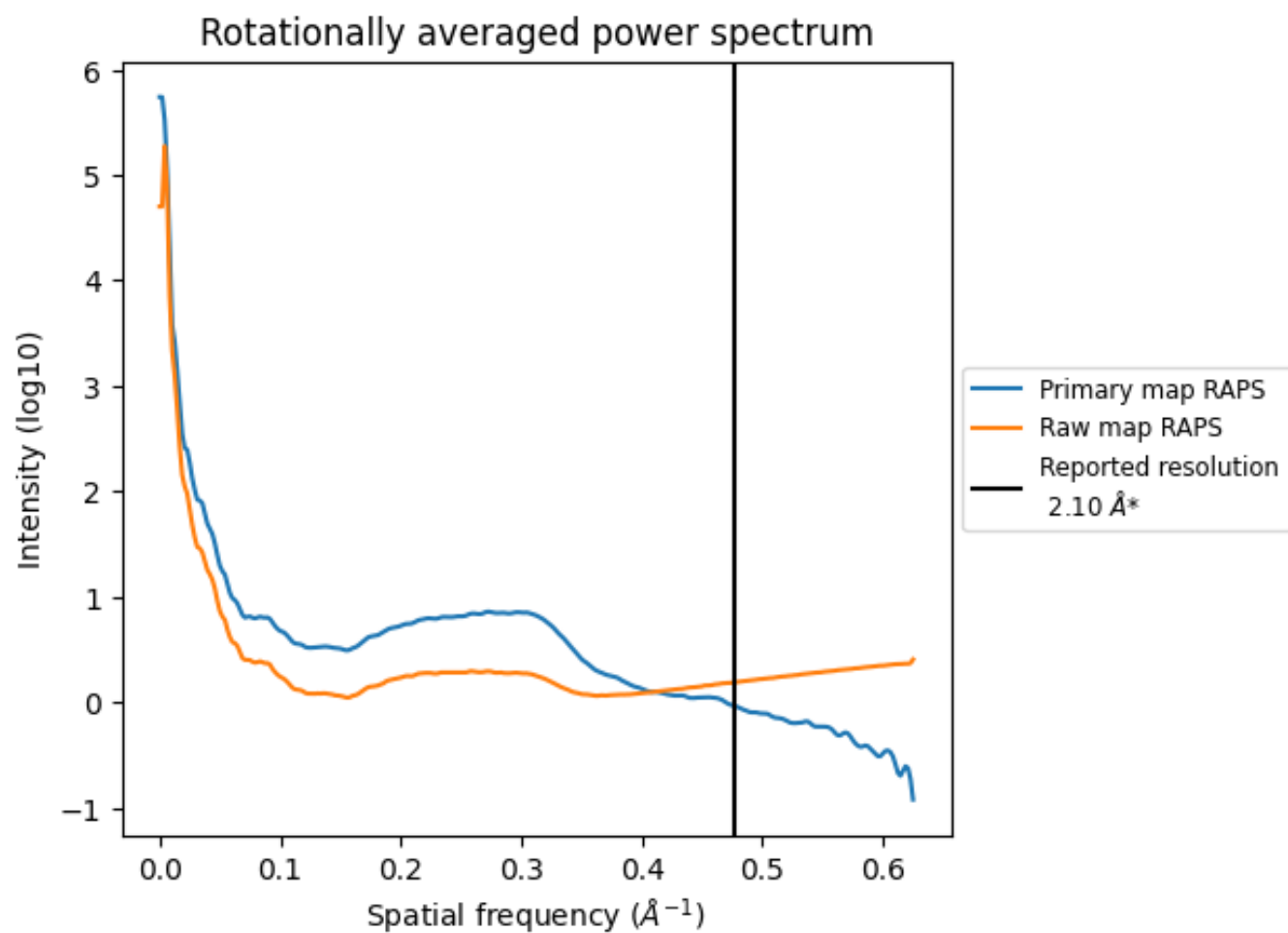
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 364 nm^3 ; this corresponds to an approximate mass of 329 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 ⓘ

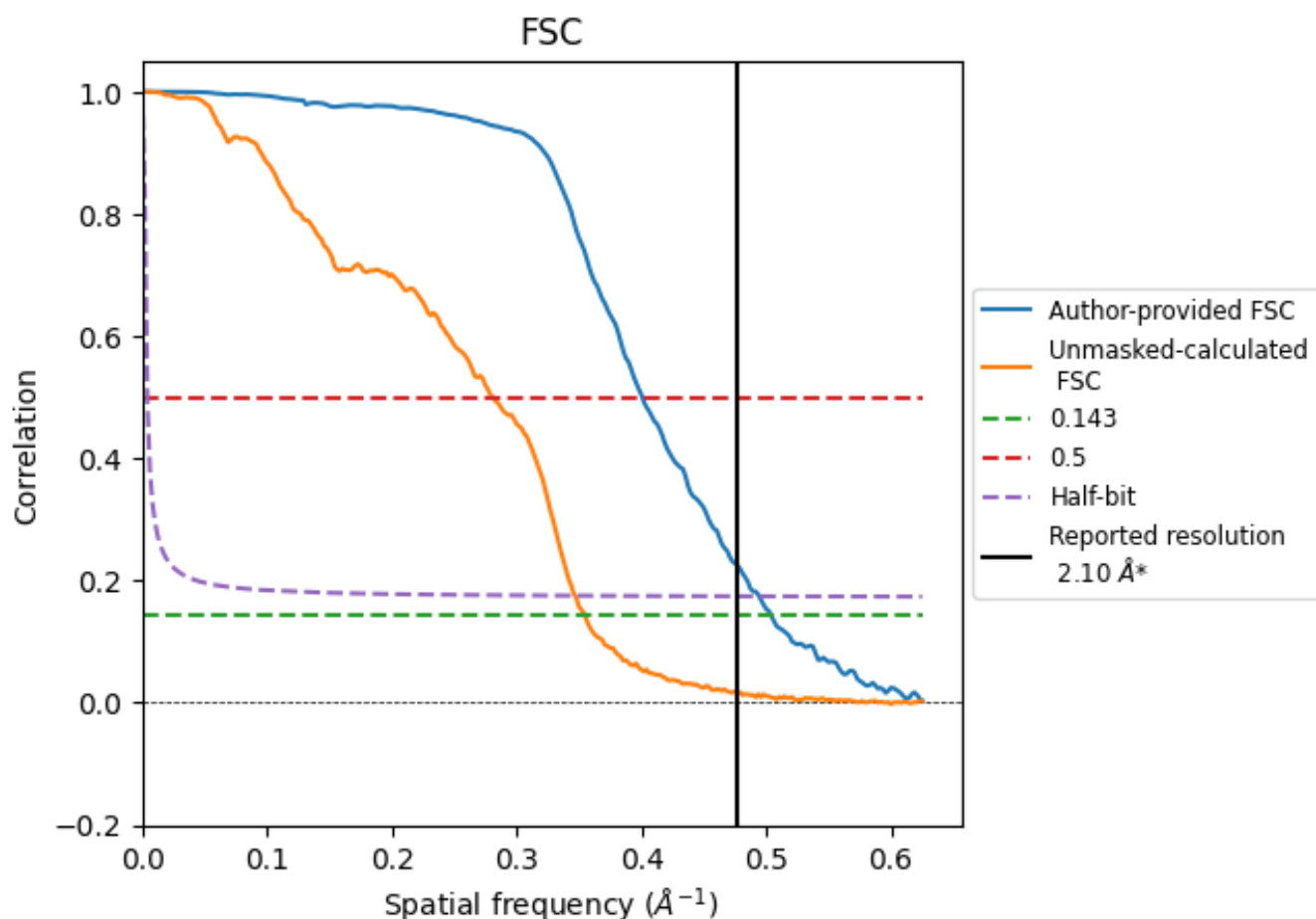


*Reported resolution corresponds to spatial frequency of 0.476 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.476 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

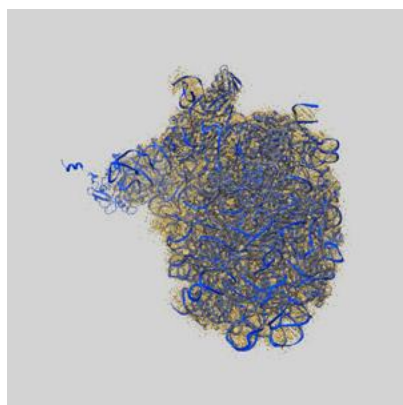
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	1.98	2.50	2.02
Unmasked-calculated*	2.82	3.56	2.88

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.82 differs from the reported value 2.1 by more than 10 %

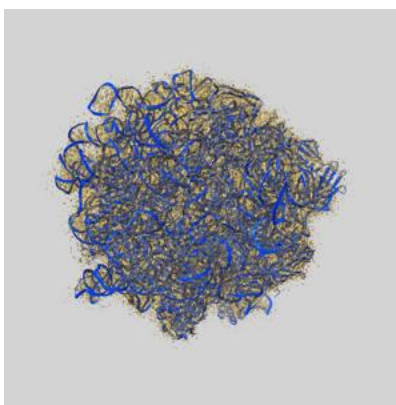
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15533 and PDB model 8ANA. Per-residue inclusion information can be found in section [3](#) on page [12](#).

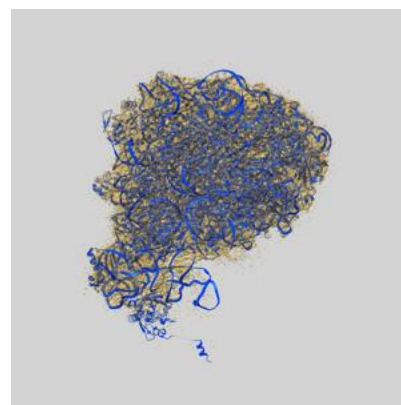
9.1 Map-model overlay [i](#)



X



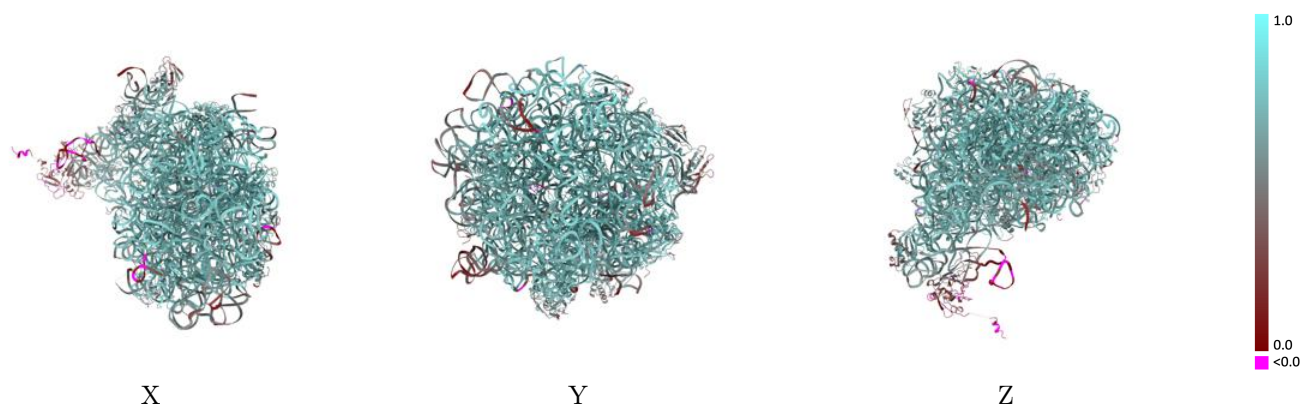
Y



Z

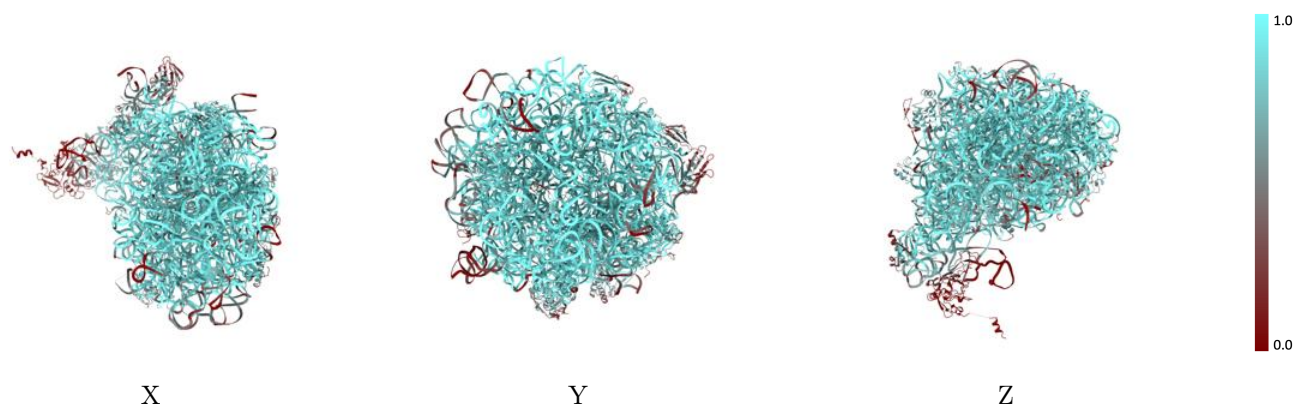
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



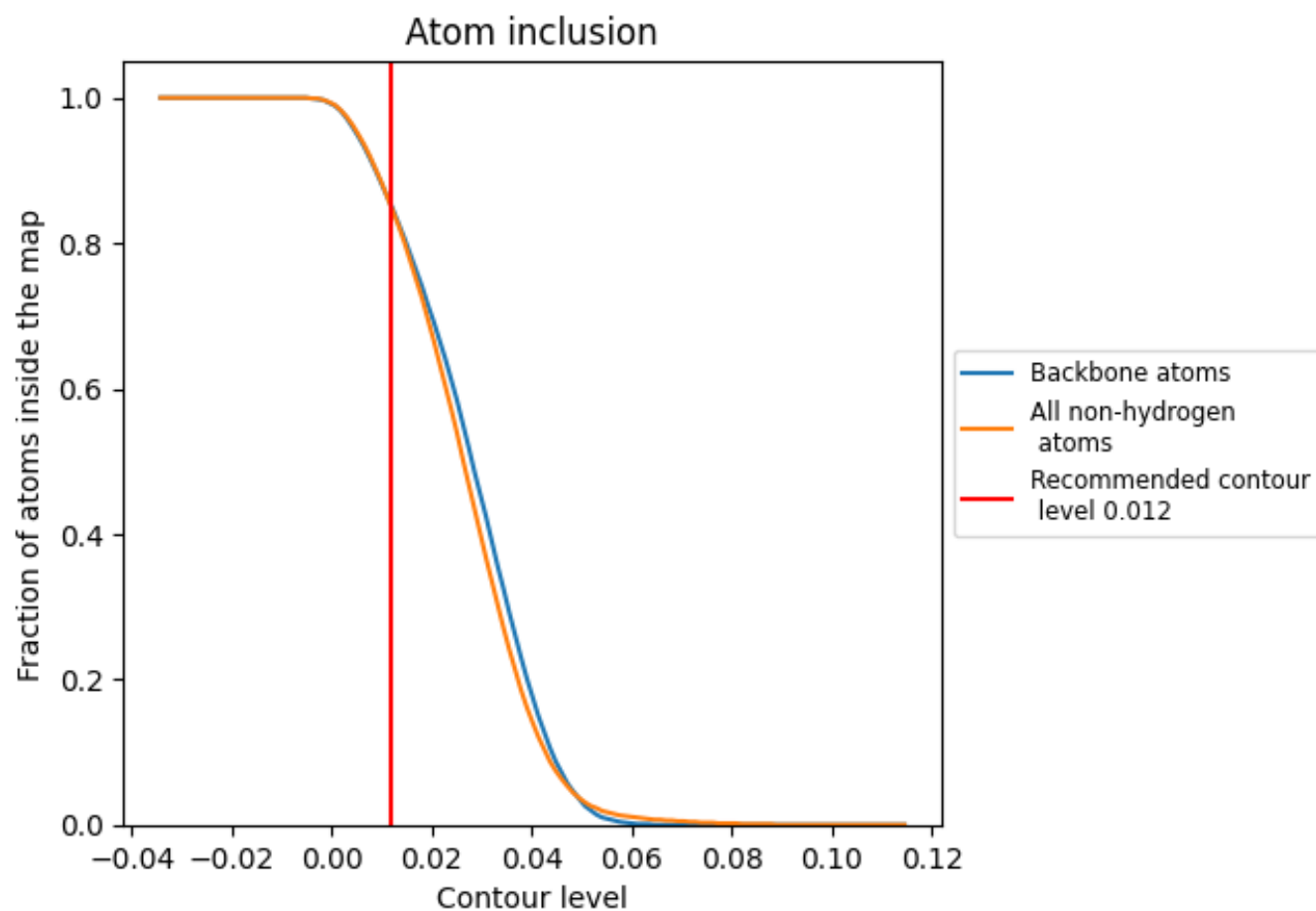
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8490	 0.6950
0	 0.7460	 0.6550
1	 0.9520	 0.7800
2	 0.9570	 0.7840
3	 0.9010	 0.7220
4	 0.0130	 0.1330
A	 0.9630	 0.7670
a	 0.8970	 0.7160
b	 0.7460	 0.6190
c	 0.9100	 0.7370
d	 0.8880	 0.7420
e	 0.7550	 0.6670
f	 0.1100	 0.2750
g	 0.4540	 0.5050
h	 0.4170	 0.4530
i	 0.9080	 0.7470
j	 0.8030	 0.6800
k	 0.8360	 0.7040
l	 0.8590	 0.7160
m	 0.9590	 0.7770
n	 0.6190	 0.5610
o	 0.7580	 0.6540
p	 0.9390	 0.7810
q	 0.7750	 0.6750
r	 0.8730	 0.7320
s	 0.7810	 0.6580
t	 0.6820	 0.5950
u	 0.6790	 0.6220
v	 0.8600	 0.7200
w	 0.8420	 0.7030
x	 0.6540	 0.5860
y	 0.8560	 0.7060
z	 0.8420	 0.7140

