



wwPDB EM Validation Summary Report ⓘ

Dec 18, 2024 – 07:13 pm GMT

PDB ID : 8P8M
EMDB ID : EMD-17549
Title : Yeast 60S ribosomal subunit, RPL39 deletion
Authors : Rabl, J.; Banerjee, A.; Boehringer, D.; Zavolan, M.
Deposited on : 2023-06-01
Resolution : 2.66 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:

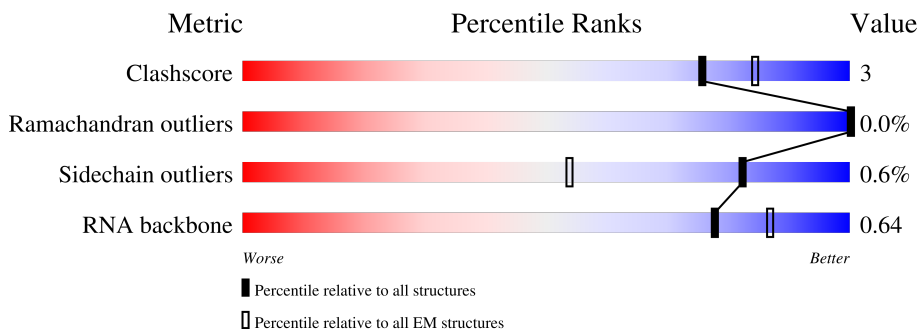
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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 2.66 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	3396	
2	QY	127	
3	JT	199	
4	QZ	136	
5	JU	138	
6	RA	149	
7	JV	204	

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Mol	Chain	Length	Quality of chain
8	RB	59	5% 81% 17% .
9	JW	199	. 94% 5% .
10	RC	105	5% 84% 9% 8%
11	LD	158	5% 81% 16% .
12	RD	113	76% 9% 15%
13	LE	121	. 84% 16%
14	RE	130	. 91% 7% .
15	LF	254	81% 15% .
16	RF	107	94% 5% .
17	LG	387	. 87% 12%
18	RG	121	. 79% 6% 15%
19	LH	362	. 92% 7%
20	RH	120	. 94% 5% .
21	LI	297	14% 89% 11%
22	RI	100	. 94% 5% .
23	LJ	176	. 75% 14% 11%
24	RJ	88	5% 91% 8% .
25	LK	244	. 82% 9% 9%
26	RM	78	17% 91% 8% .
27	LL	256	8% 82% 9% 9%
28	RO	128	. 35% . 61%
29	LM	191	6% 91% 9%
30	RQ	106	9% 83% 15% ..
31	LN	221	8% 84% 10% 7%
32	RT	92	. 89% 9% ..

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Mol	Chain	Length	Quality of chain
33	LO	174	
34	RV	312	
35	QO	184	
36	QP	186	
37	QQ	189	
38	QS	172	
39	QT	160	
40	QU	121	
41	QV	137	
42	QW	155	
43	QX	142	

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 119279 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 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	3035	64928	29001	11711	21181	3035	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2091	U	A	conflict	GB 834774822

- Molecule 2 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	QY	124	976	614	190	172	0	0

- Molecule 3 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	JT	189	1515	946	311	258	0	0

- Molecule 4 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	QZ	135	1092	710	202	180	0	0

- Molecule 5 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	JU	134	1039	666	196	175	2	0	0

- Molecule 6 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	RA	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 7 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	JV	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 8 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	RB	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 9 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	JW	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 10 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	RC	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 11 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LD	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 12 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	RD	96	Total	C	N	O	S	0	0
			782	503	151	127	1		

- Molecule 13 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
13	LE	121	2579	1152	461	845	121	0	0

- Molecule 14 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	RE	127	1020	647	205	167	1	0	0

- Molecule 15 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	LF	244	1855	1156	375	323	1	0	0

- Molecule 16 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	RF	106	850	540	165	144	1	0	0

- Molecule 17 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	LG	386	3078	1953	584	533	8	0	0

- Molecule 18 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	RG	103	811	503	167	137	4	0	0

- Molecule 19 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	LH	361	2748	1729	522	494	3	0	0

- Molecule 20 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	RH	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 21 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LI	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 22 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	RI	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 23 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LJ	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 24 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	RJ	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 25 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LK	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 26 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	RM	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 27 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LL	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 28 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	RO	50	Total	C	N	O	S	0	0
			401	247	84	65	5		

- Molecule 29 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LM	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 30 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	RQ	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 31 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LN	206	Total	C	N	O	S	0	0
			1674	1062	317	289	6		

- Molecule 32 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	RT	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 33 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LO	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 34 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	RV	7	54	32	12	9	1	0	0

- Molecule 35 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	QO	183	1420	882	281	257		0	0

- Molecule 36 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	QP	185	1441	908	290	241	2	0	0

- Molecule 37 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	QQ	147	1185	738	250	197		0	0

- Molecule 38 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	QS	172	1445	930	267	244	4	0	0

- Molecule 39 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	QT	159	1276	805	246	221	4	0	0

- Molecule 40 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	QU	100	796	516	131	149		0	0

- Molecule 41 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	QV	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 42 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	QW	61	Total	C	N	O	S	0	0
			509	328	100	80	1		

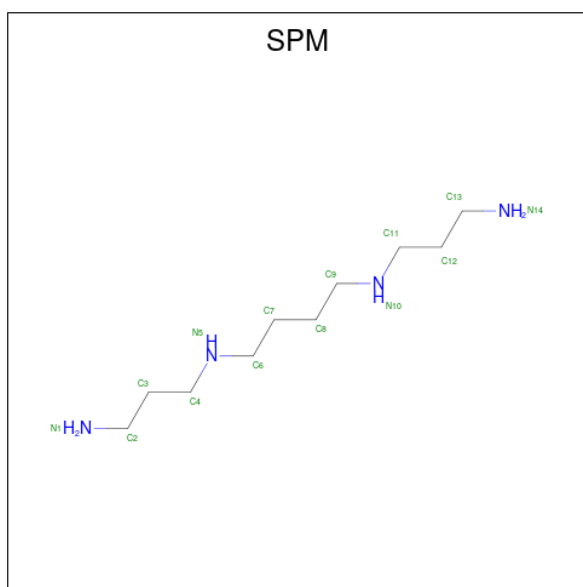
- Molecule 43 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	QX	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 44 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

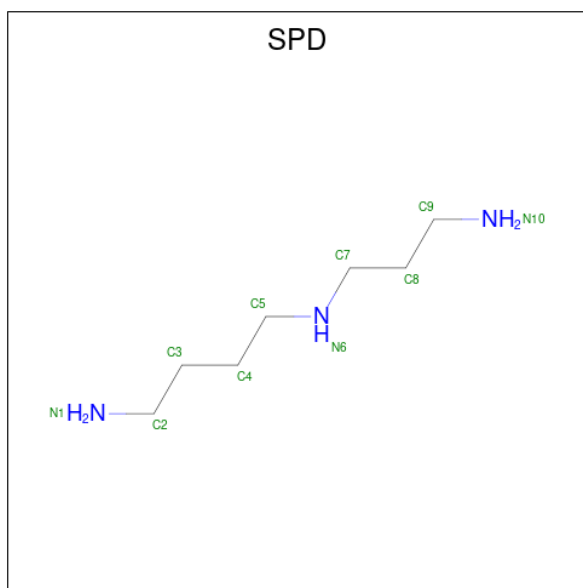
Mol	Chain	Residues	Atoms		AltConf
44	A	151	Total	Mg	0
			151	151	
44	JV	1	Total	Mg	0
			1	1	
44	LD	1	Total	Mg	0
			1	1	
44	LE	1	Total	Mg	0
			1	1	
44	QQ	1	Total	Mg	0
			1	1	
44	QV	1	Total	Mg	0
			1	1	

- Molecule 45 is SPERMINE (three-letter code: SPM) (formula: C₁₀H₂₆N₄).



Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	C	N	0
			14	10	4	

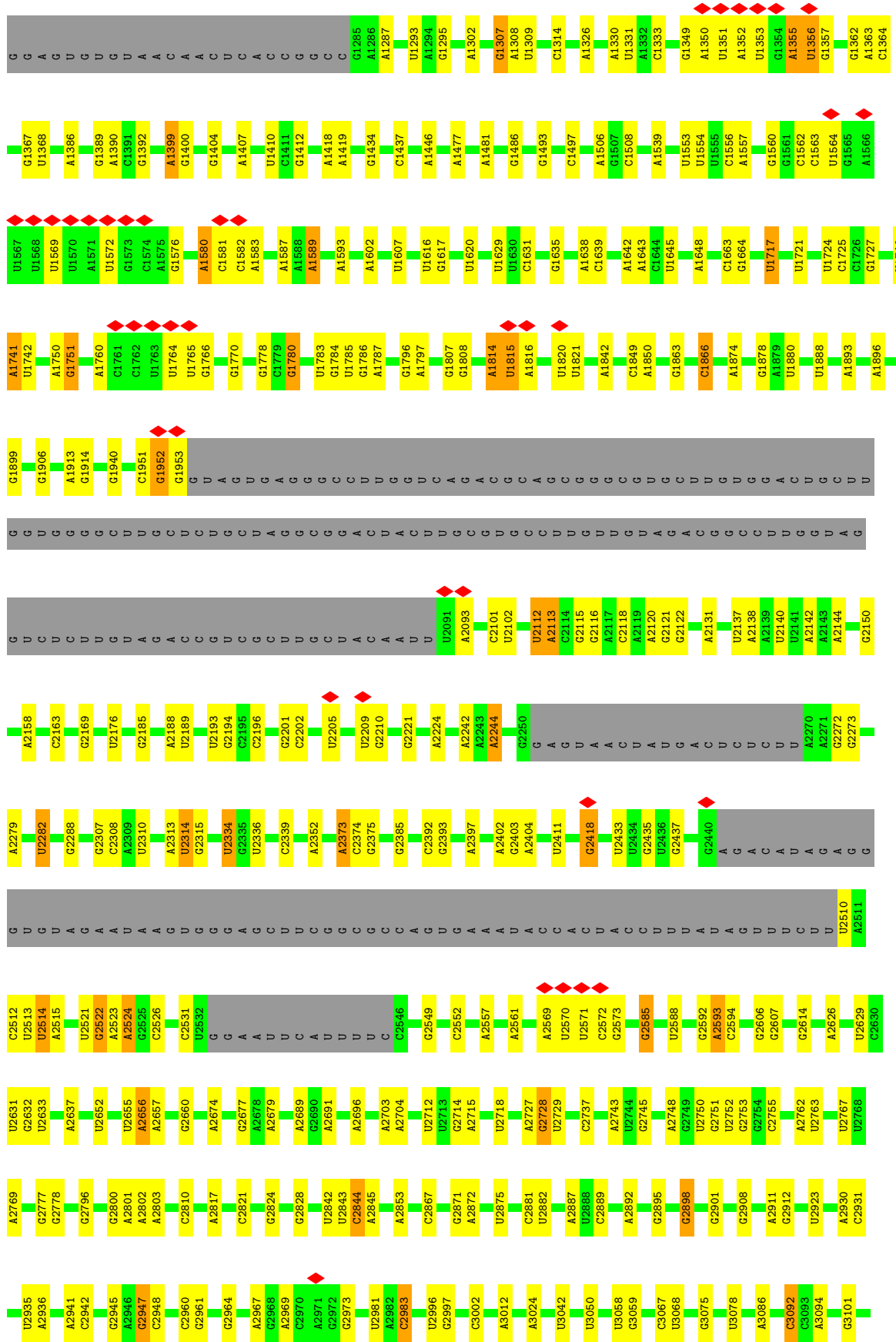
- Molecule 46 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).

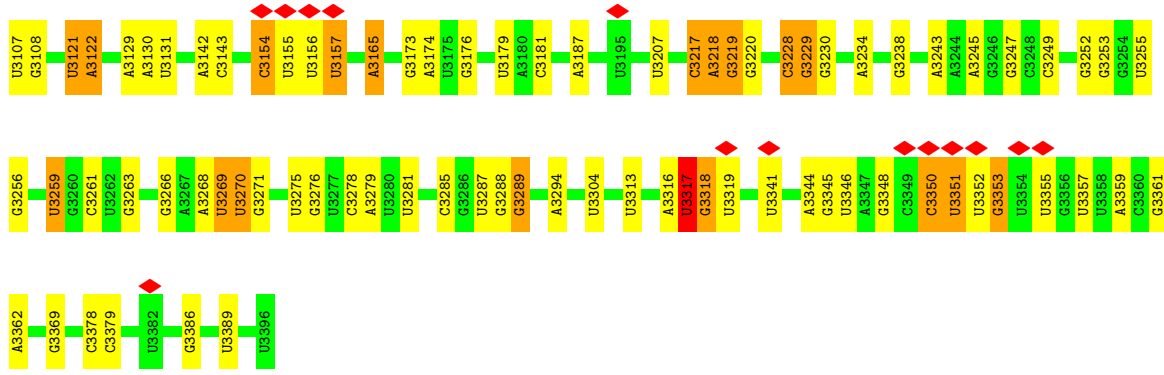


Mol	Chain	Residues	Atoms			AltConf
46	A	1	Total	C	N	0
			10	7	3	

- Molecule 47 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
47	RG	1	Total 1	Zn 1	0
47	RJ	1	Total 1	Zn 1	0
47	RO	1	Total 1	Zn 1	0
47	RQ	1	Total 1	Zn 1	0
47	RT	1	Total 1	Zn 1	0

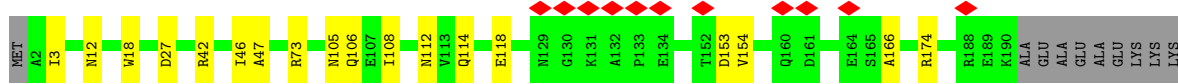
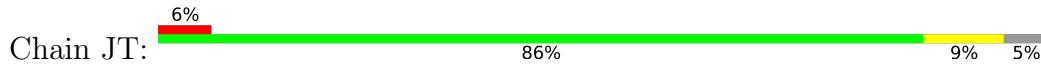




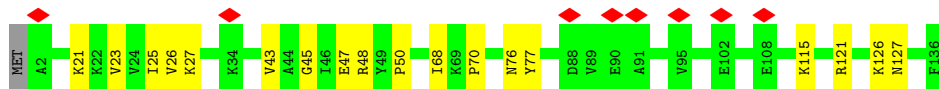
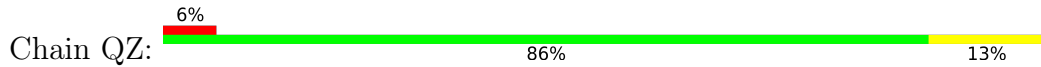
• Molecule 2: 60S ribosomal protein L26-A



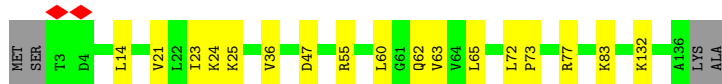
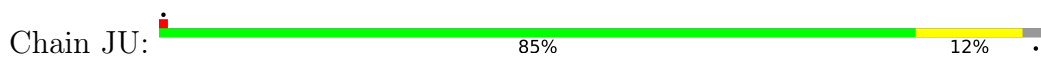
• Molecule 3: 60S ribosomal protein L13-A



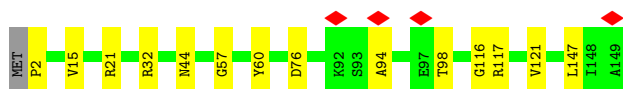
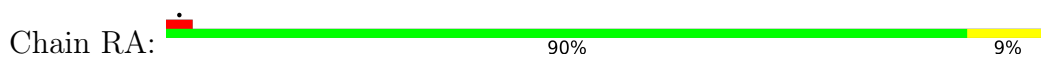
• Molecule 4: 60S ribosomal protein L27-A



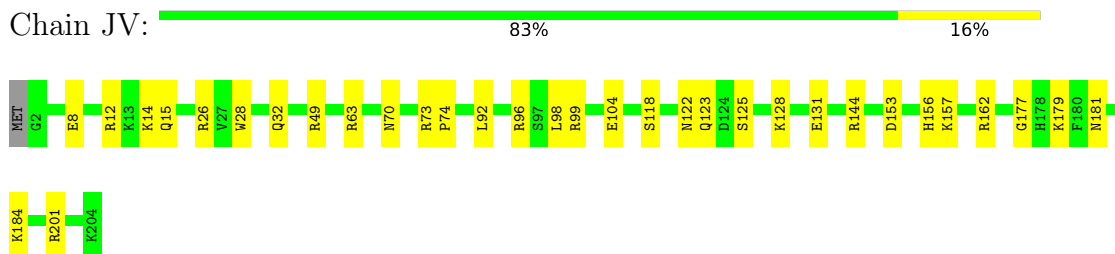
• Molecule 5: 60S ribosomal protein L14-A



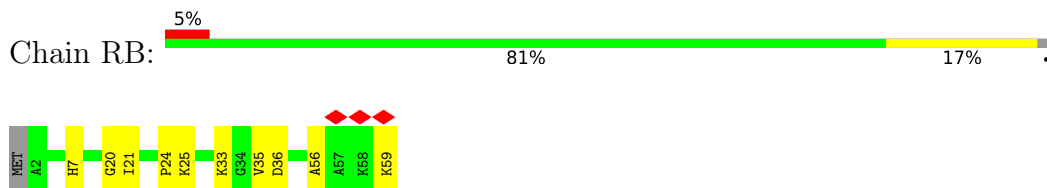
• Molecule 6: 60S ribosomal protein L28



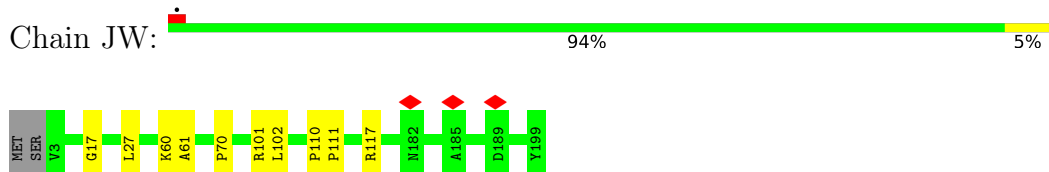
- Molecule 7: 60S ribosomal protein L15-A



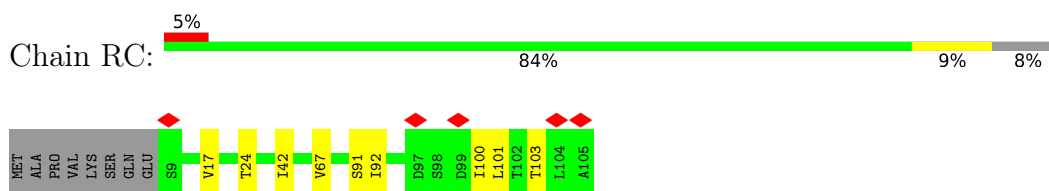
- Molecule 8: 60S ribosomal protein L29



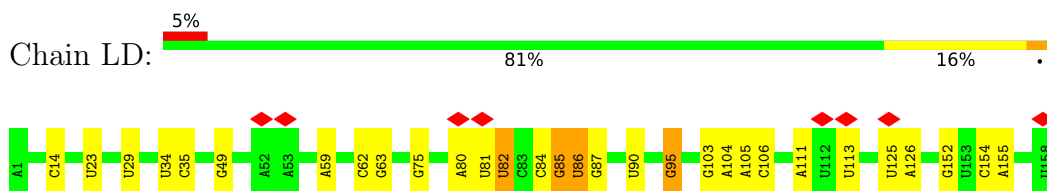
- Molecule 9: 60S ribosomal protein L16-A



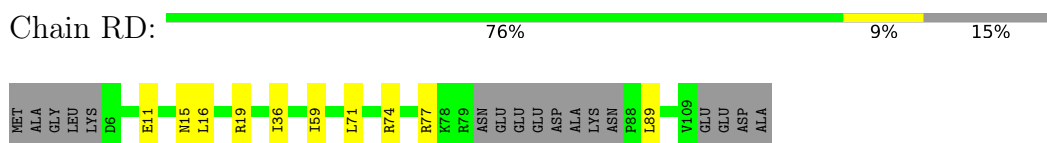
- Molecule 10: 60S ribosomal protein L30



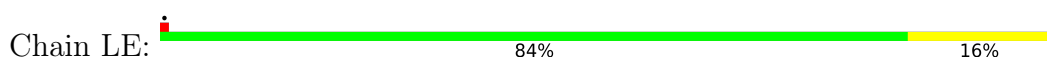
- Molecule 11: 5.8S rRNA



- Molecule 12: 60S ribosomal protein L31-A



- Molecule 13: 5S rRNA

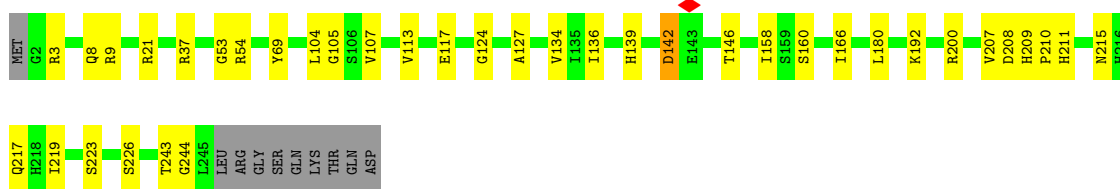
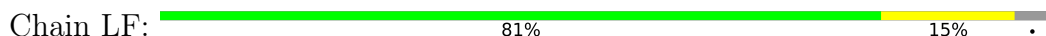




- Molecule 14: 60S ribosomal protein L32



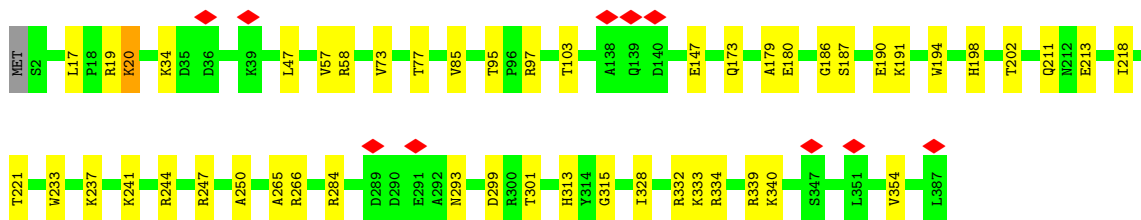
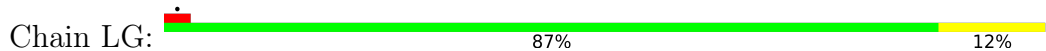
- Molecule 15: 60S ribosomal protein L2-A



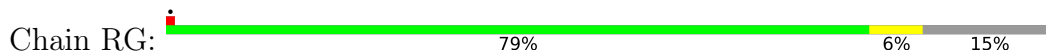
- Molecule 16: 60S ribosomal protein L33-A



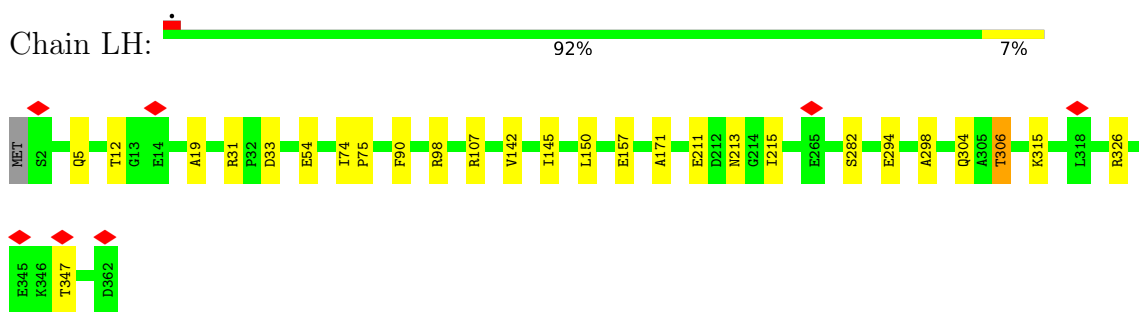
- Molecule 17: 60S ribosomal protein L3



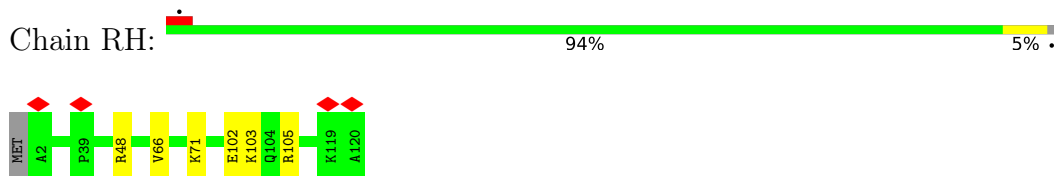
- Molecule 18: 60S ribosomal protein L34-A



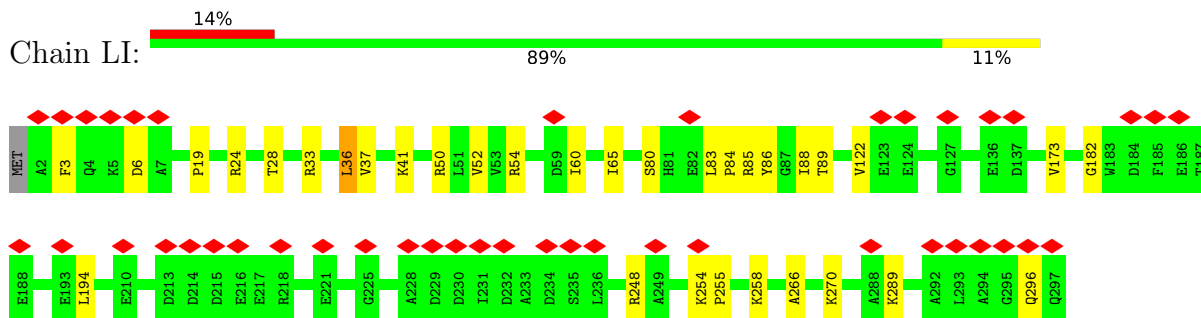
- Molecule 19: 60S ribosomal protein L4-A



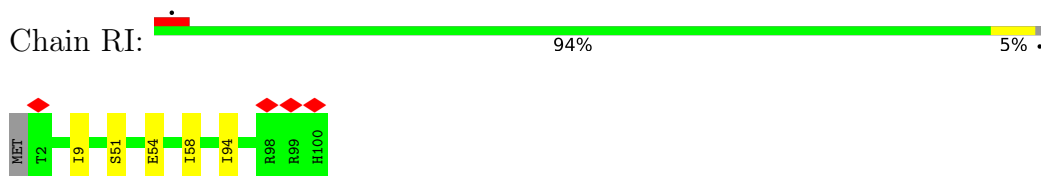
• Molecule 20: 60S ribosomal protein L35-A



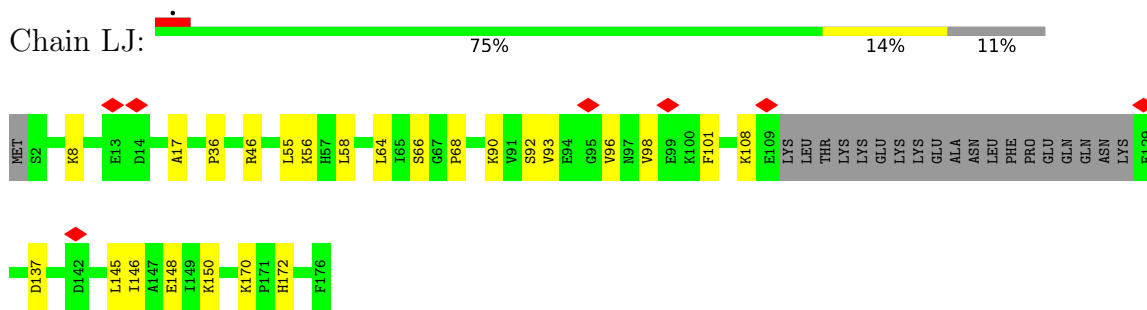
• Molecule 21: 60S ribosomal protein L5



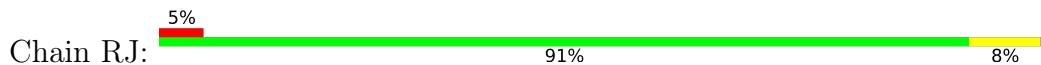
• Molecule 22: 60S ribosomal protein L36-A



• Molecule 23: 60S ribosomal protein L6-A

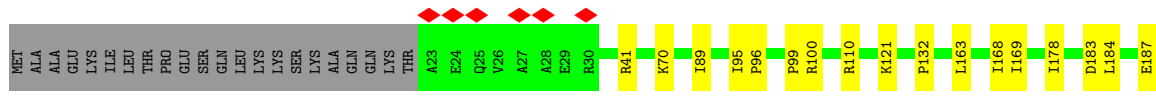
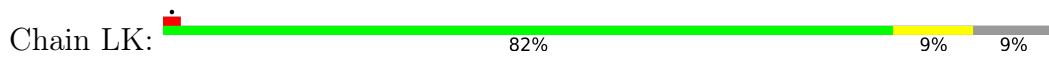


• Molecule 24: 60S ribosomal protein L37-A

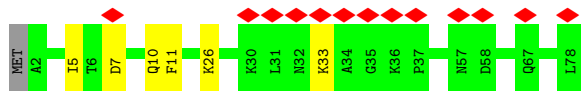
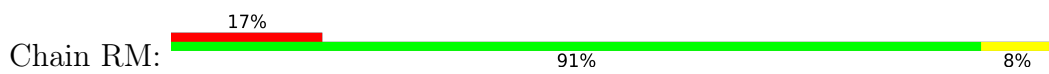




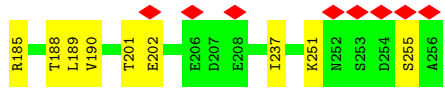
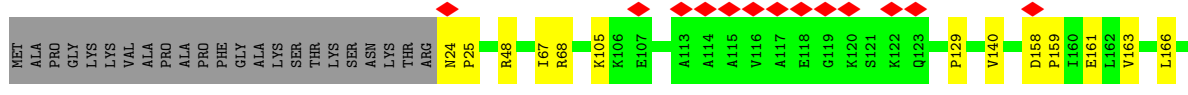
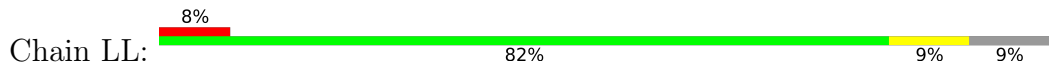
• Molecule 25: 60S ribosomal protein L7-A



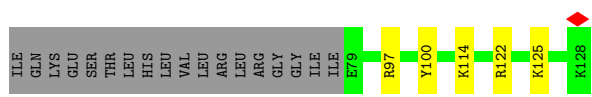
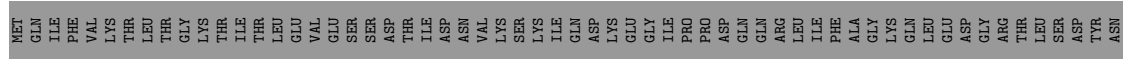
• Molecule 26: 60S ribosomal protein L38



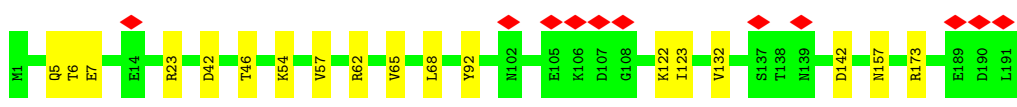
• Molecule 27: 60S ribosomal protein L8-A



• Molecule 28: Ubiquitin-60S ribosomal protein L40



• Molecule 29: 60S ribosomal protein L9-A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41172	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.483	Depositor
Minimum map value	-0.912	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.083	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	504.0, 504.0, 504.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.26, 1.26, 1.26	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: SPM, SPD, MG, ZN

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	0.18	0/72676	0.69	9/113300 (0.0%)
2	QY	0.24	0/987	0.51	0/1318
3	JT	0.24	0/1540	0.53	0/2068
4	QZ	0.24	0/1118	0.47	0/1497
5	JU	0.23	0/1054	0.47	0/1420
6	RA	0.23	0/1204	0.49	0/1612
7	JV	0.23	0/1757	0.56	0/2354
8	RB	0.22	0/473	0.46	0/629
9	JW	0.24	0/1585	0.47	0/2128
10	RC	0.24	0/751	0.43	0/1008
11	LD	0.17	0/3746	0.67	0/5832
12	RD	0.23	0/795	0.52	0/1065
13	LE	0.15	0/2883	0.66	0/4491
14	RE	0.23	0/1041	0.49	0/1394
15	LF	0.24	0/1889	0.54	0/2539
16	RF	0.25	0/868	0.52	0/1168
17	LG	0.24	0/3149	0.51	0/4233
18	RG	0.23	0/821	0.55	0/1097
19	LH	0.23	0/2800	0.49	0/3790
20	RH	0.23	0/978	0.47	0/1301
21	LI	0.24	0/2425	0.48	0/3271
22	RI	0.23	0/778	0.52	0/1034
23	LJ	0.24	0/1260	0.47	0/1694
24	RJ	0.24	0/696	0.54	0/923
25	LK	0.24	0/1821	0.46	0/2451
26	RM	0.24	0/618	0.51	0/826
27	LL	0.24	0/1836	0.44	0/2481
28	RO	0.24	0/407	0.53	0/540
29	LM	0.24	0/1539	0.48	0/2073
30	RQ	0.24	0/860	0.51	0/1136
31	LN	0.24	0/1709	0.50	0/2291
32	RT	0.23	0/701	0.54	0/934

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LO	0.23	0/1374	0.51	0/1842
34	RV	0.22	0/53	0.57	0/68
35	QO	0.23	0/1443	0.51	0/1944
36	QP	0.24	0/1465	0.53	0/1965
37	QQ	0.23	0/1202	0.51	0/1605
38	QS	0.25	0/1481	0.50	0/1990
39	QT	0.24	0/1300	0.49	0/1743
40	QU	0.24	0/812	0.44	0/1099
41	QV	0.25	0/1018	0.51	0/1369
42	QW	0.25	0/521	0.50	0/691
43	QX	0.24	0/979	0.47	0/1321
All	All	0.20	0/128413	0.63	9/189535 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	922	U	C2-N1-C1'	6.81	125.88	117.70
1	A	922	U	N1-C2-O2	5.64	126.75	122.80
1	A	1103	A	OP2-P-O3'	5.63	117.60	105.20
1	A	979	U	P-O3'-C3'	5.40	126.18	119.70
1	A	3317	U	OP2-P-O3'	5.27	116.79	105.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	64928	0	32626	260	0
2	QY	976	0	1064	7	0
3	JT	1515	0	1586	13	0
4	QZ	1092	0	1155	11	0
5	JU	1039	0	1131	14	0
6	RA	1173	0	1215	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	JV	1720	0	1778	23	0
8	RB	462	0	491	8	0
9	JW	1555	0	1659	6	0
10	RC	743	0	797	4	0
11	LD	3353	0	1695	9	0
12	RD	782	0	846	5	0
13	LE	2579	0	1304	8	0
14	RE	1020	0	1090	7	0
15	LF	1855	0	1919	26	0
16	RF	850	0	880	3	0
17	LG	3078	0	3153	31	0
18	RG	811	0	869	3	0
19	LH	2748	0	2859	21	0
20	RH	969	0	1078	5	0
21	LI	2375	0	2325	21	0
22	RI	771	0	849	3	0
23	LJ	1239	0	1326	13	0
24	RJ	681	0	683	7	0
25	LK	1784	0	1862	15	0
26	RM	612	0	682	3	0
27	LL	1804	0	1877	14	0
28	RO	401	0	433	5	0
29	LM	1518	0	1587	11	0
30	RQ	847	0	914	13	0
31	LN	1674	0	1710	14	0
32	RT	694	0	734	6	0
33	LO	1353	0	1383	28	0
34	RV	54	0	59	0	0
35	QO	1420	0	1437	9	0
36	QP	1441	0	1543	16	0
37	QQ	1185	0	1269	12	0
38	QS	1445	0	1487	14	0
39	QT	1276	0	1323	18	0
40	QU	796	0	812	4	0
41	QV	1003	0	1048	3	0
42	QW	509	0	537	3	0
43	QX	964	0	1025	1	0
44	A	151	0	0	0	0
44	JV	1	0	0	0	0
44	LD	1	0	0	0	0
44	LE	1	0	0	0	0
44	QQ	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	QV	1	0	0	0	0
45	A	14	0	26	0	0
46	A	10	0	19	1	0
47	RG	1	0	0	0	0
47	RJ	1	0	0	0	0
47	RO	1	0	0	0	0
47	RQ	1	0	0	0	0
47	RT	1	0	0	0	0
All	All	119279	0	86145	554	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 3.

The worst 5 of 554 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)
1:A:1874:A:N7	37:QQ:20:ARG:NH1	2.35	0.74
33:LO:92:ARG:HD3	33:LO:94:ARG:H	1.53	0.73
1:A:2969:A:N7	15:LF:215:ASN:ND2	2.37	0.73
30:RQ:17:CYS:SG	30:RQ:76:LYS:NZ	2.60	0.72
1:A:1213:G:H4'	38:QS:90:MET:HG3	1.70	0.72

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	QY	122/127 (96%)	122 (100%)	0	0	100 100
3	JT	187/199 (94%)	181 (97%)	6 (3%)	0	100 100
4	QZ	133/136 (98%)	125 (94%)	8 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	JU	132/138 (96%)	130 (98%)	2 (2%)	0	100	100
6	RA	146/149 (98%)	131 (90%)	14 (10%)	1 (1%)	19	31
7	JV	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
8	RB	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
9	JW	195/199 (98%)	194 (100%)	1 (0%)	0	100	100
10	RC	95/105 (90%)	95 (100%)	0	0	100	100
12	RD	92/113 (81%)	91 (99%)	1 (1%)	0	100	100
14	RE	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
15	LF	242/254 (95%)	231 (96%)	11 (4%)	0	100	100
16	RF	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
17	LG	384/387 (99%)	374 (97%)	9 (2%)	1 (0%)	37	53
18	RG	101/121 (84%)	100 (99%)	1 (1%)	0	100	100
19	LH	359/362 (99%)	346 (96%)	13 (4%)	0	100	100
20	RH	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
21	LI	294/297 (99%)	288 (98%)	6 (2%)	0	100	100
22	RI	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
23	LJ	152/176 (86%)	149 (98%)	3 (2%)	0	100	100
24	RJ	85/88 (97%)	84 (99%)	1 (1%)	0	100	100
25	LK	220/244 (90%)	215 (98%)	5 (2%)	0	100	100
26	RM	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
27	LL	231/256 (90%)	226 (98%)	5 (2%)	0	100	100
28	RO	48/128 (38%)	47 (98%)	1 (2%)	0	100	100
29	LM	189/191 (99%)	180 (95%)	9 (5%)	0	100	100
30	RQ	103/106 (97%)	97 (94%)	6 (6%)	0	100	100
31	LN	202/221 (91%)	199 (98%)	3 (2%)	0	100	100
32	RT	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
33	LO	167/174 (96%)	157 (94%)	10 (6%)	0	100	100
34	RV	5/312 (2%)	5 (100%)	0	0	100	100
35	QO	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
36	QP	183/186 (98%)	178 (97%)	5 (3%)	0	100	100
37	QQ	145/189 (77%)	144 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	QS	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
39	QT	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
40	QU	98/121 (81%)	96 (98%)	2 (2%)	0	100	100
41	QV	134/137 (98%)	134 (100%)	0	0	100	100
42	QW	59/155 (38%)	58 (98%)	1 (2%)	0	100	100
43	QX	119/142 (84%)	117 (98%)	2 (2%)	0	100	100
All	All	5994/6819 (88%)	5830 (97%)	162 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	LG	20	LYS
6	RA	15	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QY	107/110 (97%)	106 (99%)	1 (1%)	75	87
3	JT	152/159 (96%)	152 (100%)	0	100	100
4	QZ	115/116 (99%)	115 (100%)	0	100	100
5	JU	106/109 (97%)	106 (100%)	0	100	100
6	RA	118/119 (99%)	116 (98%)	2 (2%)	56	75
7	JV	175/176 (99%)	175 (100%)	0	100	100
8	RB	46/47 (98%)	46 (100%)	0	100	100
9	JW	160/162 (99%)	159 (99%)	1 (1%)	84	92
10	RC	81/88 (92%)	80 (99%)	1 (1%)	67	82
12	RD	84/97 (87%)	84 (100%)	0	100	100
14	RE	109/111 (98%)	109 (100%)	0	100	100
15	LF	187/196 (95%)	186 (100%)	1 (0%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	RF	90/91 (99%)	89 (99%)	1 (1%)	70	84
17	LG	321/323 (99%)	320 (100%)	1 (0%)	91	96
18	RG	88/103 (85%)	86 (98%)	2 (2%)	45	67
19	LH	288/289 (100%)	287 (100%)	1 (0%)	91	96
20	RH	104/105 (99%)	104 (100%)	0	100	100
21	LI	244/245 (100%)	241 (99%)	3 (1%)	67	82
22	RI	81/82 (99%)	81 (100%)	0	100	100
23	LJ	134/153 (88%)	132 (98%)	2 (2%)	60	77
24	RJ	70/71 (99%)	70 (100%)	0	100	100
25	LK	186/205 (91%)	186 (100%)	0	100	100
26	RM	68/69 (99%)	67 (98%)	1 (2%)	60	77
27	LL	187/208 (90%)	186 (100%)	1 (0%)	86	94
28	RO	45/116 (39%)	45 (100%)	0	100	100
29	LM	171/171 (100%)	171 (100%)	0	100	100
30	RQ	90/91 (99%)	89 (99%)	1 (1%)	70	84
31	LN	176/187 (94%)	175 (99%)	1 (1%)	84	92
32	RT	71/72 (99%)	70 (99%)	1 (1%)	62	79
33	LO	147/150 (98%)	146 (99%)	1 (1%)	81	90
34	RV	6/254 (2%)	6 (100%)	0	100	100
35	QO	140/146 (96%)	139 (99%)	1 (1%)	81	90
36	QP	150/151 (99%)	146 (97%)	4 (3%)	40	61
37	QQ	122/154 (79%)	122 (100%)	0	100	100
38	QS	156/156 (100%)	155 (99%)	1 (1%)	84	92
39	QT	136/137 (99%)	134 (98%)	2 (2%)	60	77
40	QU	87/107 (81%)	86 (99%)	1 (1%)	70	84
41	QV	104/105 (99%)	104 (100%)	0	100	100
42	QW	54/129 (42%)	54 (100%)	0	100	100
43	QX	104/118 (88%)	104 (100%)	0	100	100
All	All	5060/5678 (89%)	5029 (99%)	31 (1%)	82	92

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	LJ	98	VAL
38	QS	172	TYR
27	LL	163	VAL
39	QT	83	ARG
36	QP	98	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
25	LK	197	GLN
30	RQ	99	GLN
39	QT	122	GLN
25	LK	209	ASN
29	LM	139	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3027/3396 (89%)	379 (12%)	21 (0%)
11	LD	157/158 (99%)	21 (13%)	1 (0%)
13	LE	120/121 (99%)	9 (7%)	0
All	All	3304/3675 (89%)	409 (12%)	22 (0%)

5 of 409 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	40	A
1	A	43	A
1	A	49	A
1	A	59	G
1	A	60	A

5 of 22 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2512	C
1	A	3228	C
1	A	3218	A
1	A	3269	U
1	A	1103	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 163 ligands modelled in this entry, 161 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	$\# Z > 2$
46	SPD	A	3482	-	9,9,9	0.27	0	8,8,8	0.31	0
45	SPM	A	3476	-	13,13,13	0.35	0	12,12,12	0.88	0

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
46	SPD	A	3482	-	-	1/7/7/7	-
45	SPM	A	3476	-	-	1/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	3482	SPD	N6-C7-C8-C9
45	A	3476	SPM	C12-C11-N10-C9

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	A	3482	SPD	1	0

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.

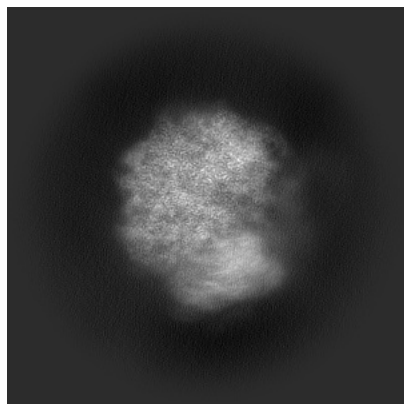
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17549. These allow visual inspection of the internal detail of the map and identification of artifacts.

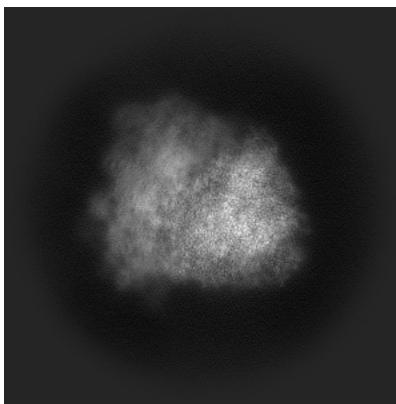
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

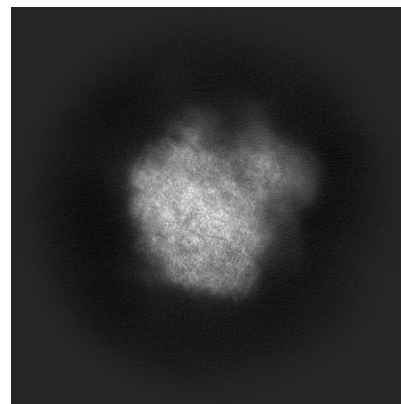
6.1.1 Primary map



X

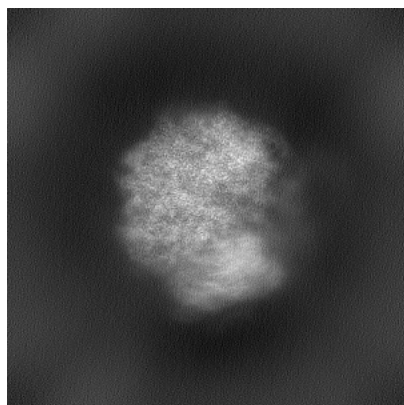


Y

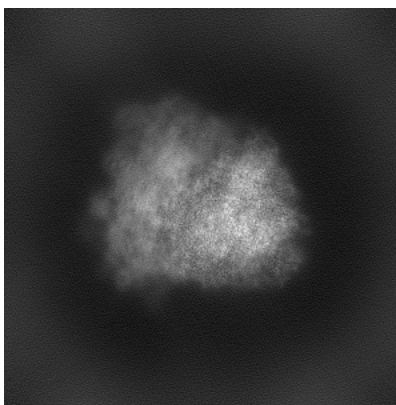


Z

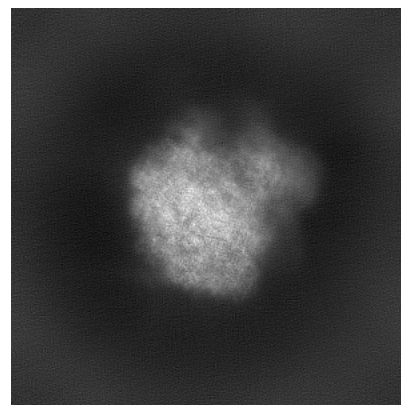
6.1.2 Raw map



X



Y

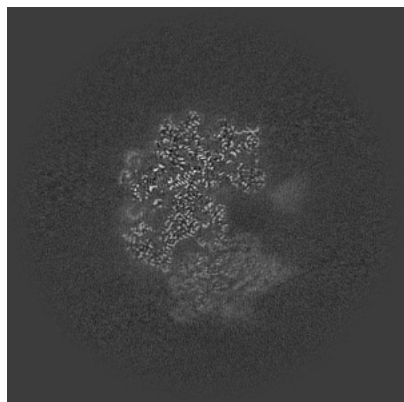


Z

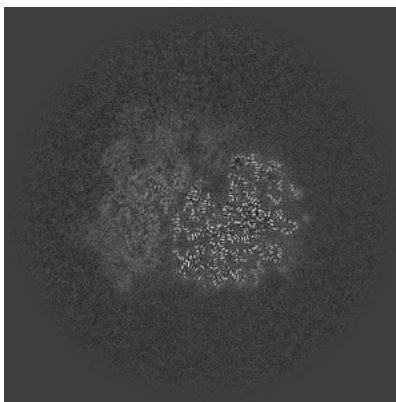
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

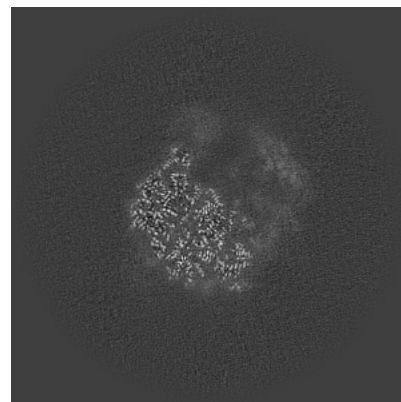
6.2.1 Primary map



X Index: 200

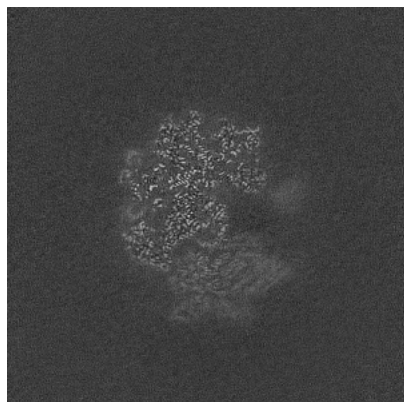


Y Index: 200

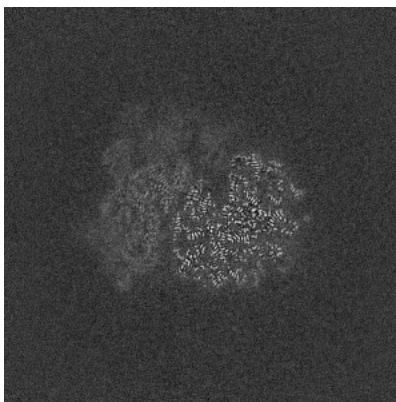


Z Index: 200

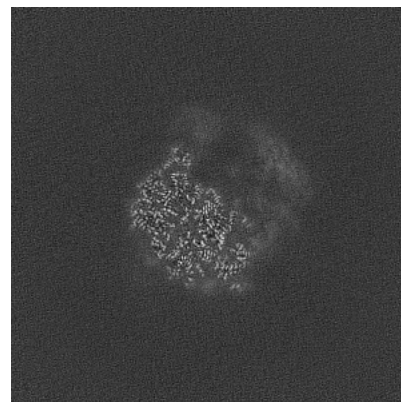
6.2.2 Raw map



X Index: 200



Y Index: 200

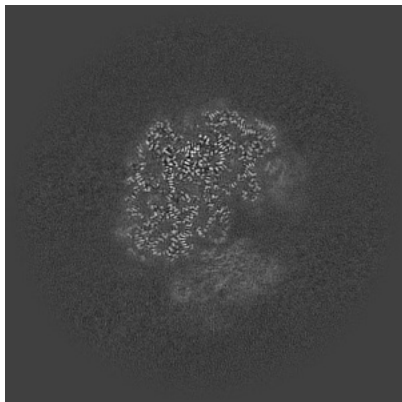


Z Index: 200

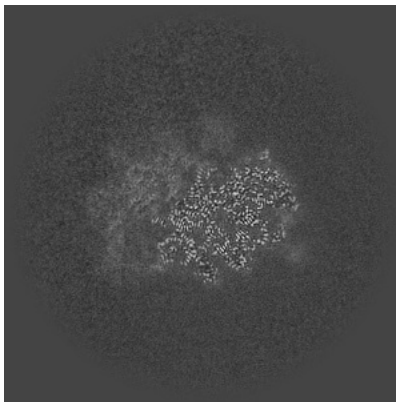
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

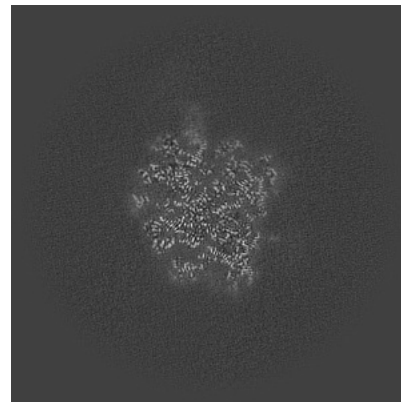
6.3.1 Primary map



X Index: 182

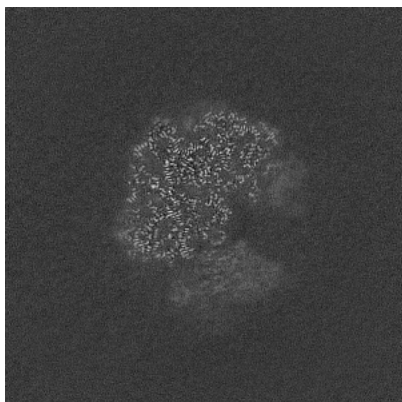


Y Index: 182

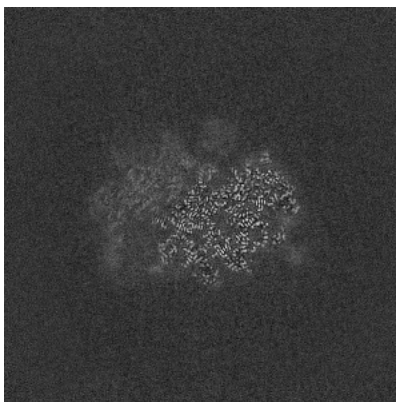


Z Index: 240

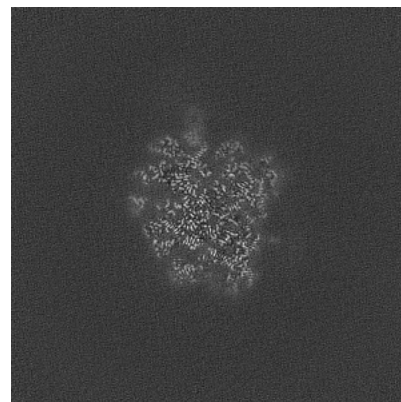
6.3.2 Raw map



X Index: 184



Y Index: 183

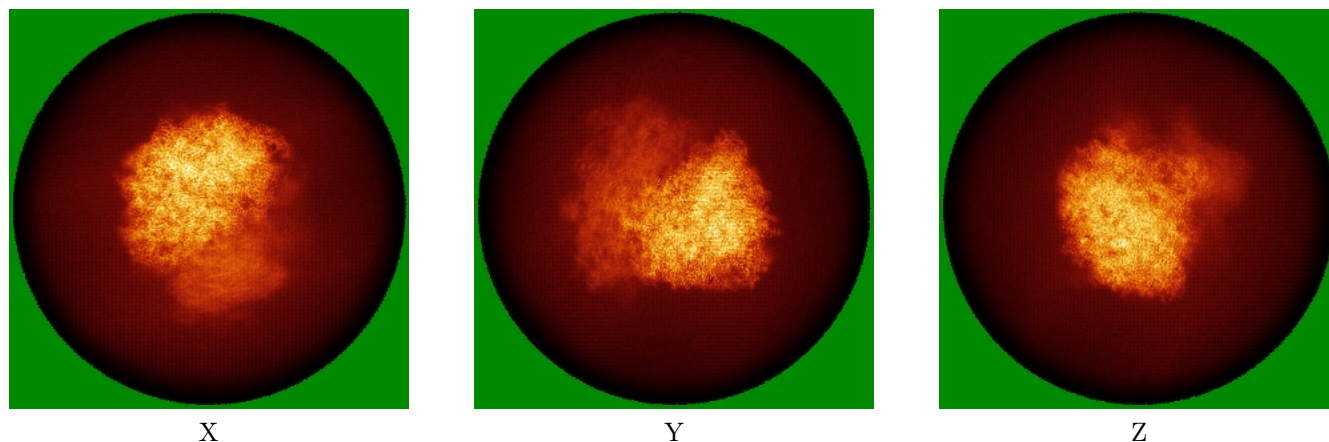


Z Index: 241

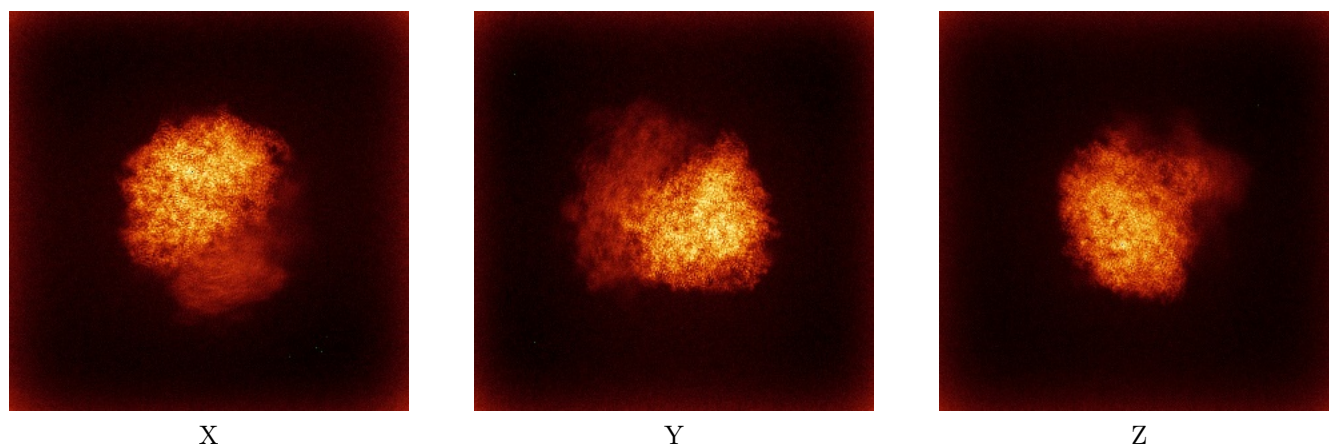
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



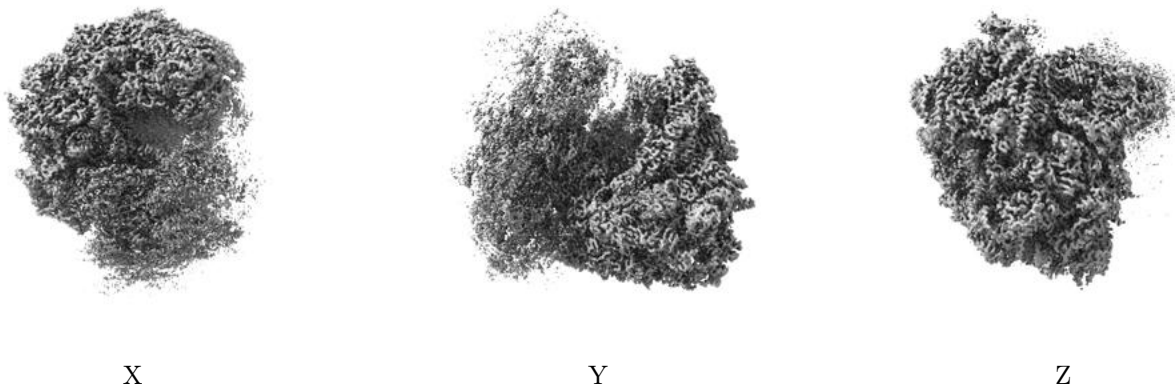
6.4.2 Raw map



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.

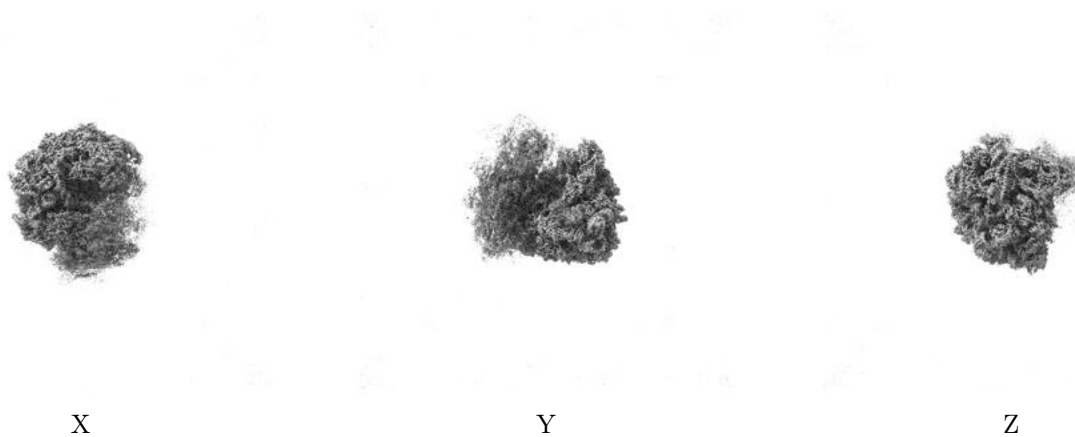
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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.

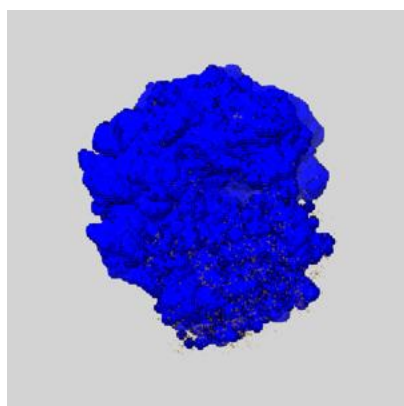
6.6 Mask visualisation [i](#)

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

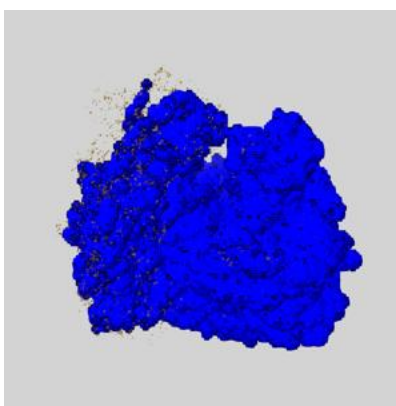
A mask typically either:

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

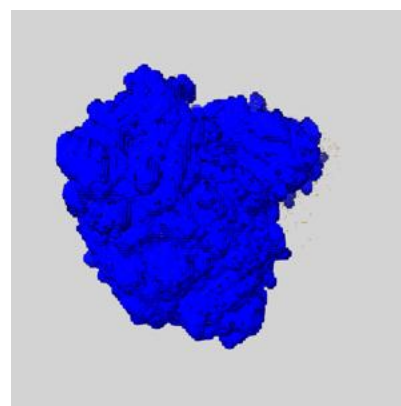
6.6.1 emd_17549_msk_1.map [i](#)



X



Y

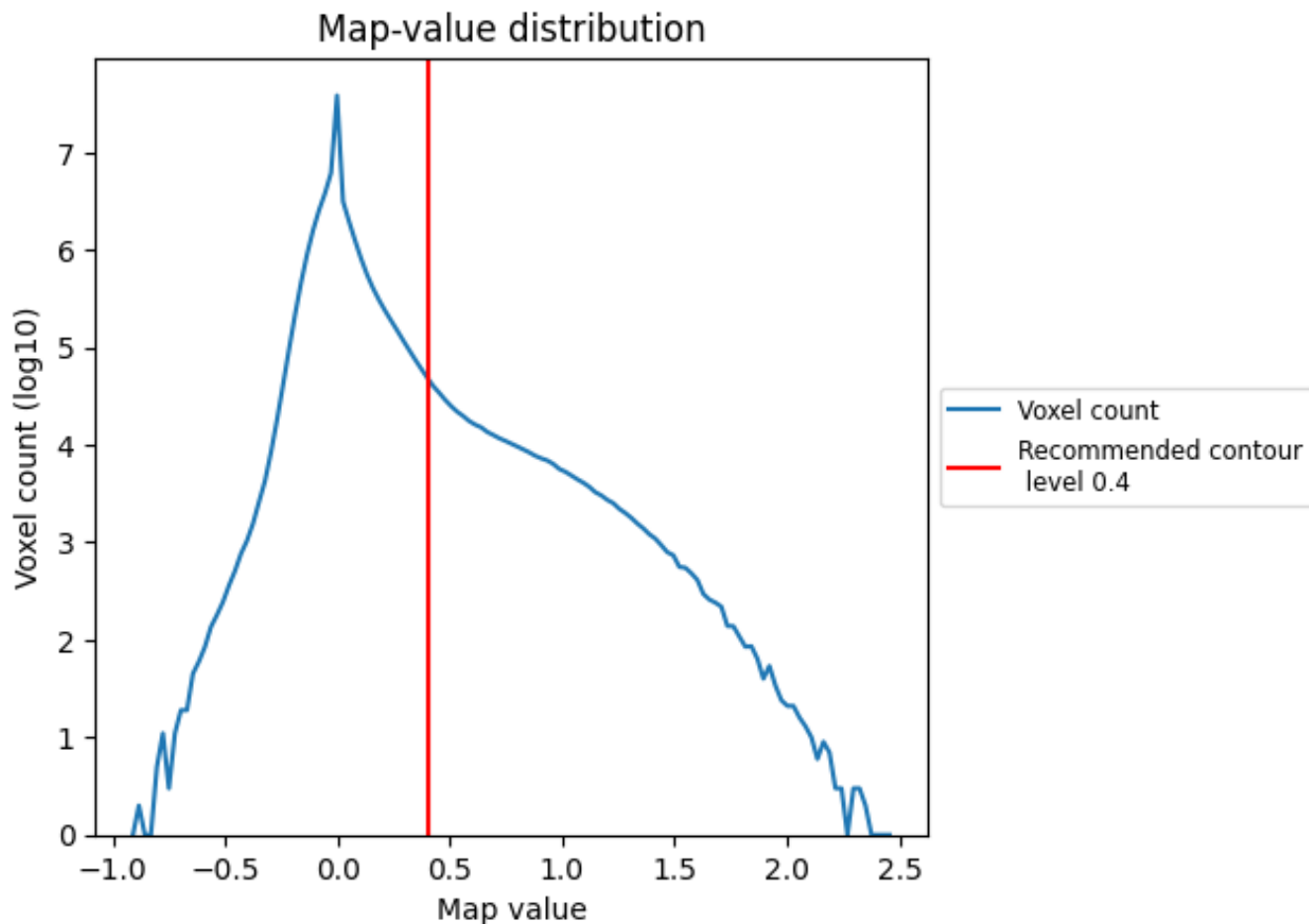


Z

7 Map analysis [i](#)

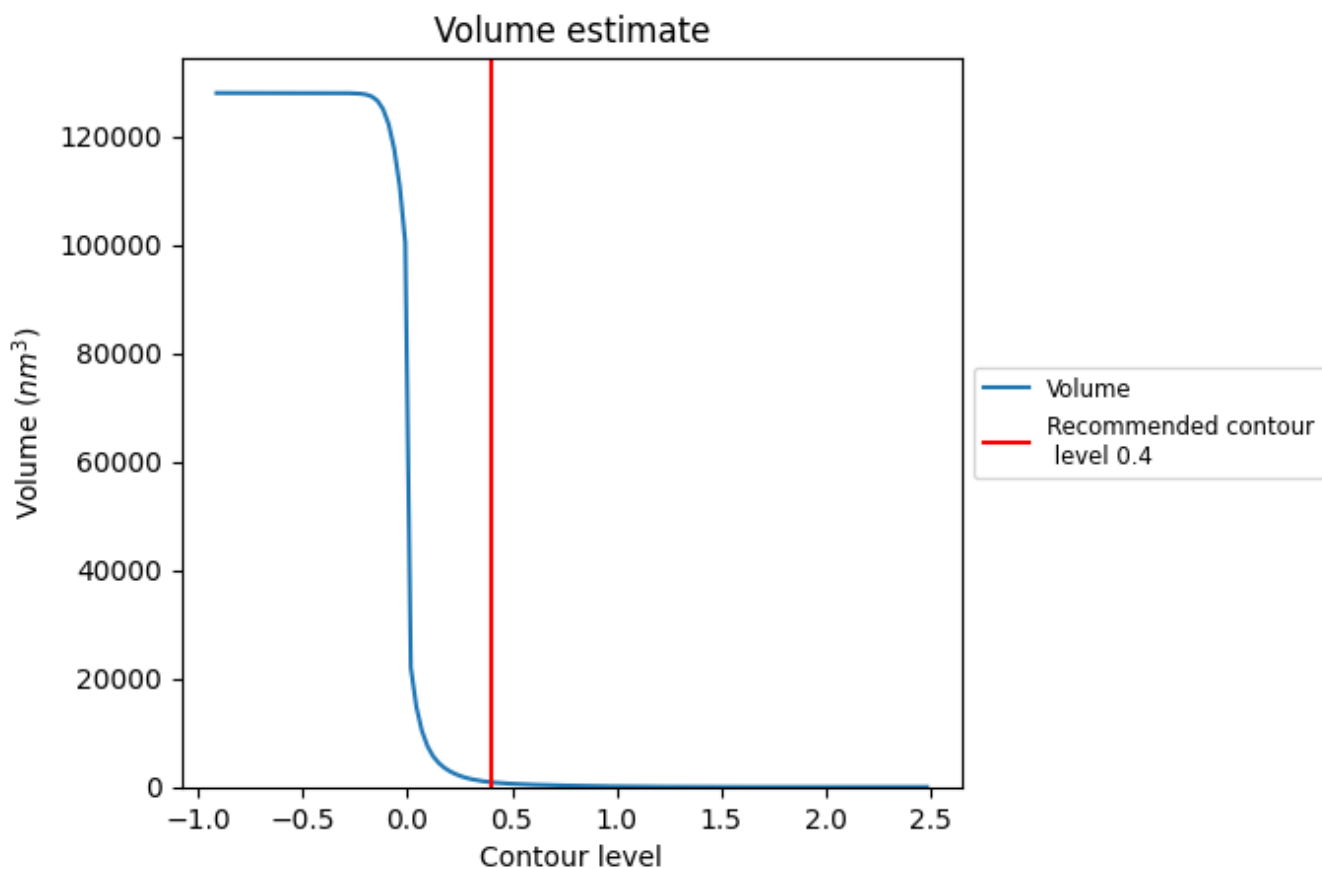
This section contains the results of statistical analysis of the map.

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.

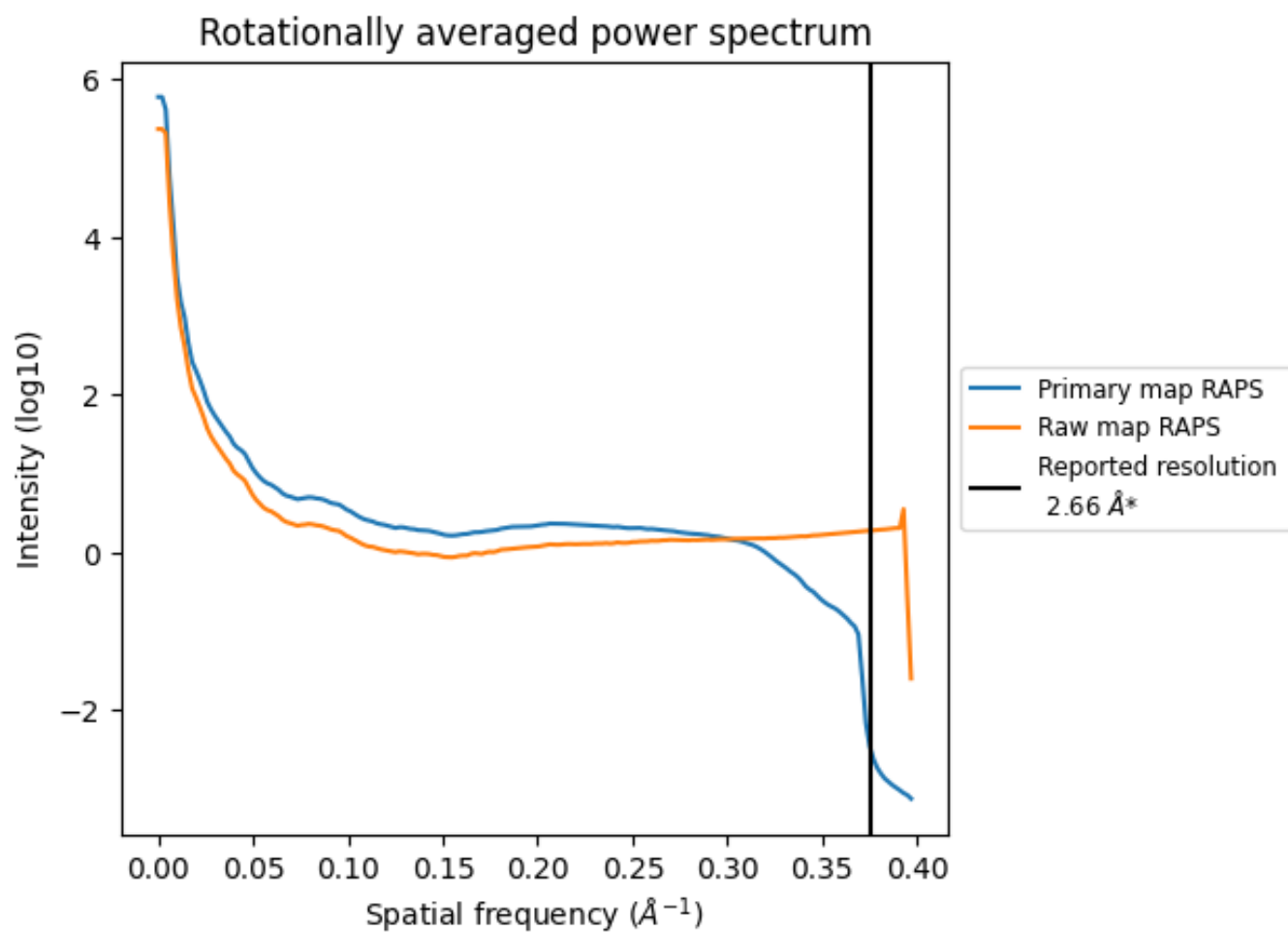
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 874 nm^3 ; this corresponds to an approximate mass of 790 kDa.

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

7.3 Rotationally averaged power spectrum i

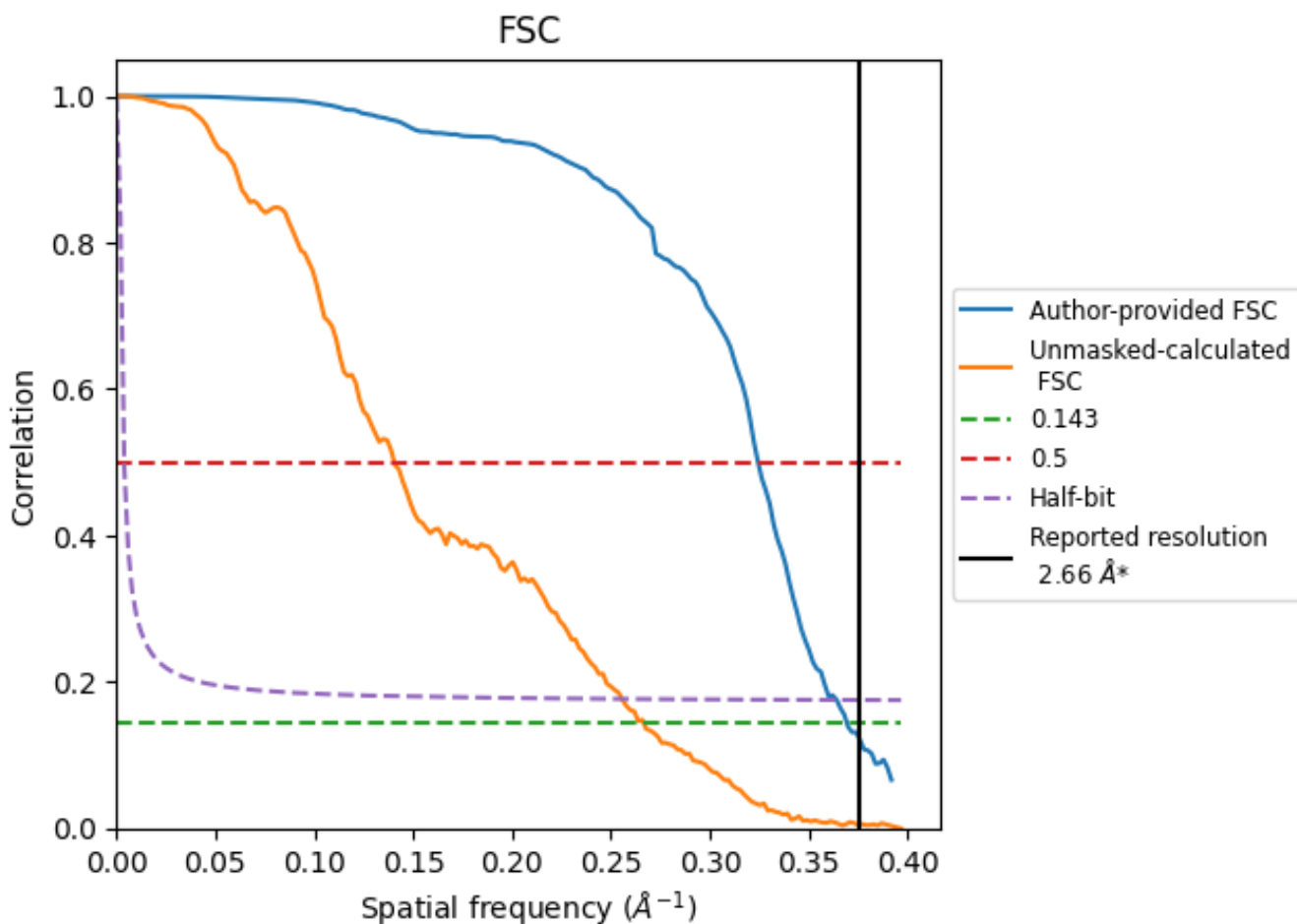


*Reported resolution corresponds to spatial frequency of 0.376 Å⁻¹

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 0.376 Å⁻¹

8.2 Resolution estimates [i](#)

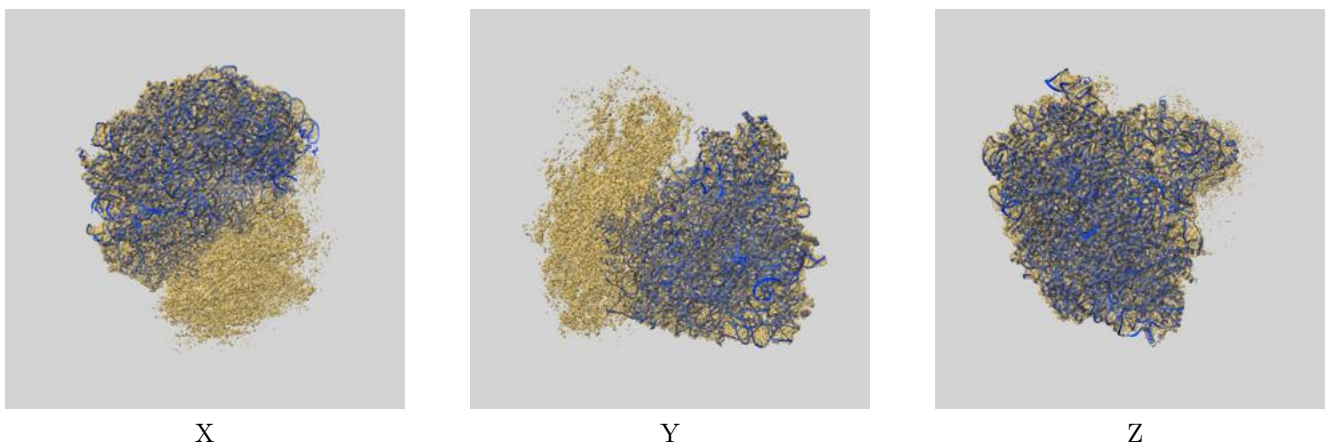
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	2.71	3.08	2.75
Unmasked-calculated*	3.75	7.12	3.91

*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 3.75 differs from the reported value 2.66 by more than 10 %

9 Map-model fit [i](#)

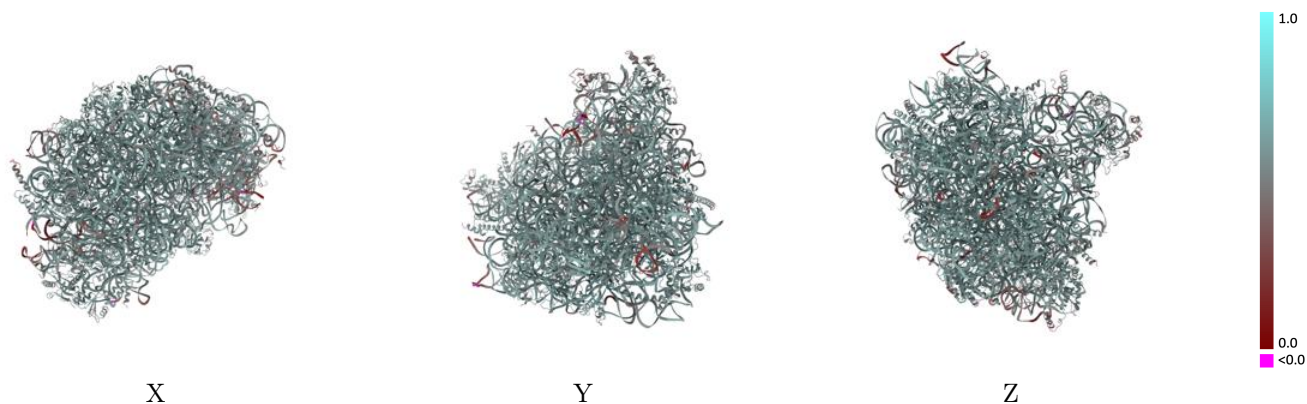
This section contains information regarding the fit between EMDB map EMD-17549 and PDB model 8P8M. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



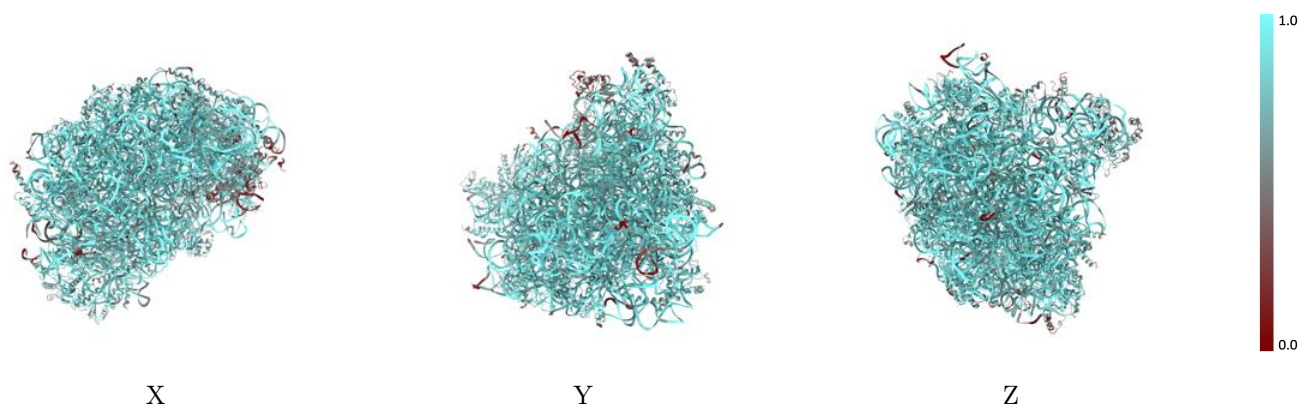
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



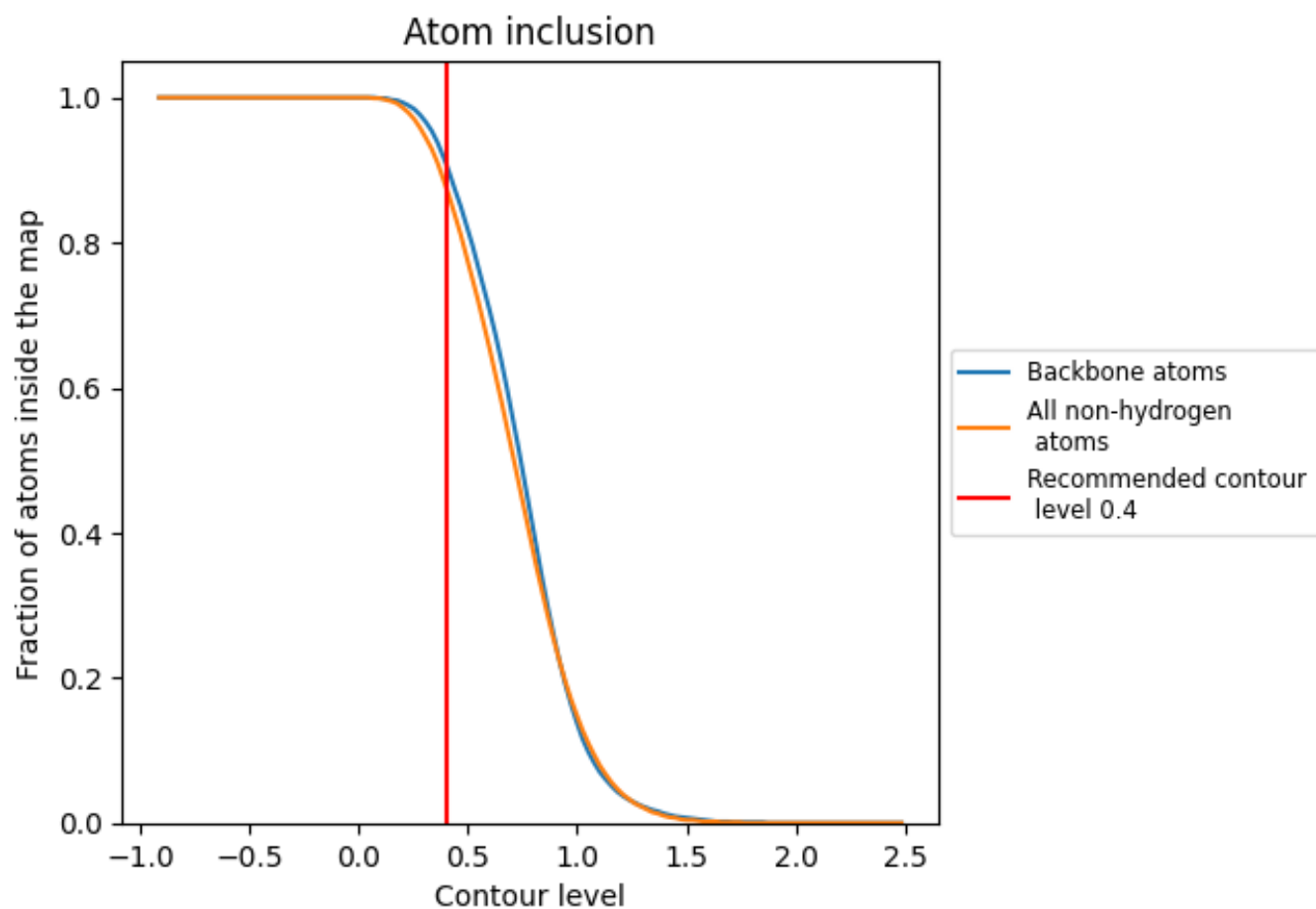
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8770	 0.5710
A	 0.9240	 0.5750
JT	 0.8360	 0.5630
JU	 0.8400	 0.5780
JV	 0.9290	 0.6020
JW	 0.8880	 0.5930
LD	 0.9060	 0.5590
LE	 0.9380	 0.5760
LF	 0.8540	 0.5890
LG	 0.8540	 0.5920
LH	 0.8480	 0.5820
LI	 0.6740	 0.5040
LJ	 0.7910	 0.5590
LK	 0.8490	 0.5710
LL	 0.7500	 0.5380
LM	 0.7670	 0.5560
LN	 0.7370	 0.5600
LO	 0.4740	 0.4590
QO	 0.8560	 0.5820
QP	 0.8820	 0.5870
QQ	 0.8410	 0.5830
QS	 0.8490	 0.5740
QT	 0.8150	 0.5640
QU	 0.6760	 0.5290
QV	 0.7370	 0.5720
QW	 0.8170	 0.5850
QX	 0.8220	 0.5720
QY	 0.8330	 0.5770
QZ	 0.7770	 0.5430
RA	 0.8780	 0.5920
RB	 0.7630	 0.5410
RC	 0.7510	 0.5420
RD	 0.8760	 0.5940
RE	 0.8710	 0.5950
RF	 0.9220	 0.6140



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Chain	Atom inclusion	Q-score
RG	 0.8820	 0.5910
RH	 0.8000	 0.5580
RI	 0.7560	 0.5390
RJ	 0.9050	 0.5960
RM	 0.6160	 0.5270
RO	 0.8120	 0.5730
RQ	 0.7660	 0.5370
RT	 0.7880	 0.5760
RV	 0.0770	 0.2640