



Full wwPDB EM Validation Report ⓘ

Apr 24, 2023 – 09:42 pm BST

PDB ID : 8BJQ
EMDB ID : EMD-16090
Title : Structure of a yeast 80S ribosome-bound N-Acetyltransferase B complex
Authors : Knorr, A.G.; Mackens-Kiani, T.; Musial, J.; Berninghausen, O.; Becker, T.;
Beatrix, B.; Beckmann, R.
Deposited on : 2022-11-05
Resolution : 3.80 Å(reported)

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

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

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.dev50
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

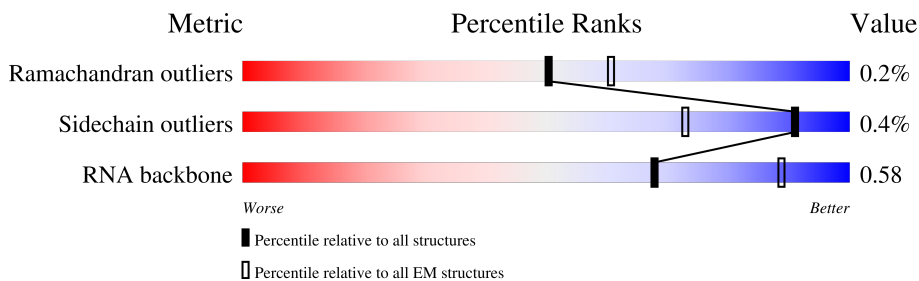
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



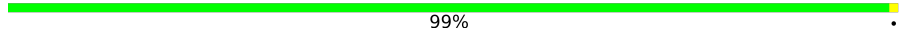
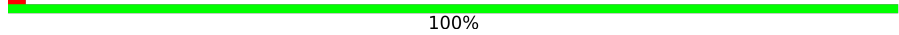
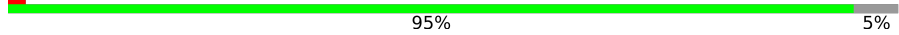
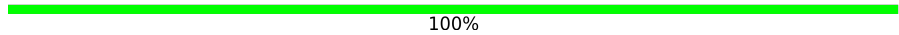
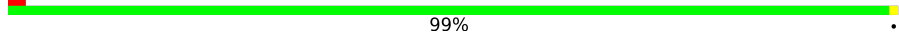
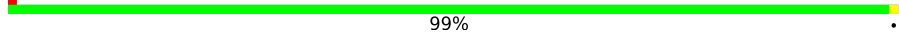
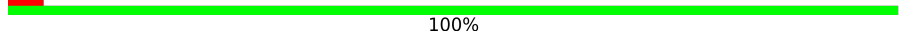
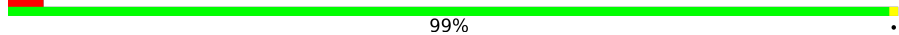
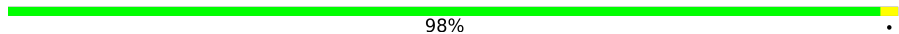
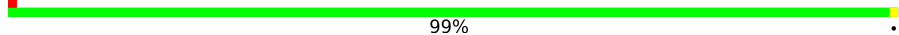
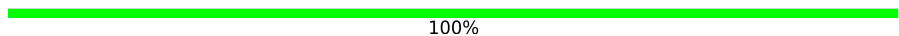
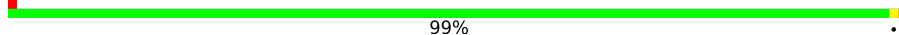
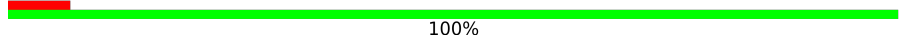
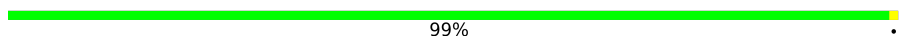

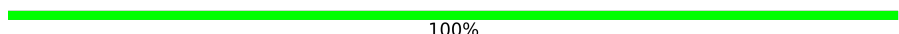
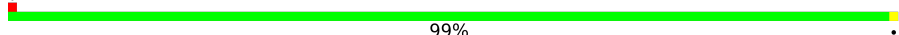
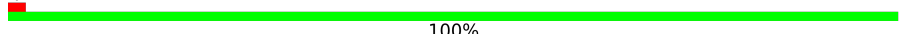
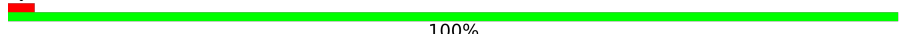

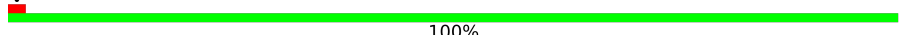
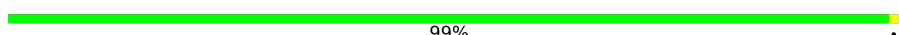
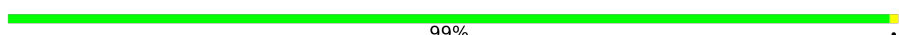
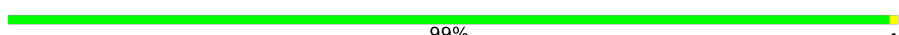
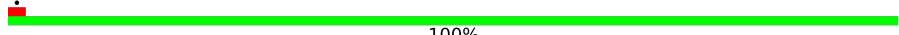
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	195	
1	C	195	
2	B	796	
2	D	796	
3	C4	121	
4	C3	158	
5	LA	251	
6	LB	386	

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Mol	Chain	Length	Quality of chain
7	LC	361	 99%
8	LD	294	 100%
9	LE	175	 95% 5%
10	LF	222	 100%
11	LG	233	 99%
12	LH	191	 99%
13	LI	218	 100%
14	LJ	169	 99%
15	LL	193	 98%
16	LM	136	 99%
17	LN	203	 100%
18	LO	197	 99%
19	LP	183	 7% 100%
20	LQ	185	 99%
21	LR	188	 90% 9%
22	LS	171	 100%
23	LT	159	 99%
24	LU	100	 100%
25	LV	136	 100%
26	LW	126	 53% 47%
27	LX	121	 100%
28	LY	125	 99%
29	LZ	135	 99%
30	La	148	 99%
31	Lb	58	 100%

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Mol	Chain	Length	Quality of chain
32	Lc	96	 99%
33	Ld	109	 99%
34	Le	127	 100%
35	Lf	106	 99%
36	Lg	112	 100%
37	Lh	119	 99%
38	Li	99	 100%
39	Lj	85	 100%
40	Lk	77	 100%
41	Ll	50	 100%
42	Lm	52	 98%
43	Ln	25	 8% 96%
44	Lo	103	 100%
45	Lp	91	 100%
46	1	3395	 79% 18%

2 Entry composition [i](#)

There are 48 unique types of molecules in this entry. The entry contains 141384 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 N-terminal acetyltransferase B complex catalytic subunit NAT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	195	Total	C	N	O	S	0	0
			1612	1030	273	297	12		
1	C	68	Total	C	N	O	S	0	0
			571	378	81	107	5		

- Molecule 2 is a protein called N-terminal acetyltransferase B complex subunit MDM20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	796	Total	C	N	O	S	0	0
			6536	4195	1080	1231	30		
2	D	796	Total	C	N	O	S	0	0
			6536	4195	1080	1231	30		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C4	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 4 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	C3	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 5 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	LA	251	Total	C	N	O	S	0	0
			1899	1182	385	331	1		

- Molecule 6 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	LB	386	3075	1950	584	533	8	0	0

- Molecule 7 is a protein called 60S ribosomal protein L4-A.

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

- Molecule 8 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	LD	294	2351	1484	410	455	2	0	0

- Molecule 9 is a protein called 60S ribosomal protein L6-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	LE	167	1305	841	234	229	1	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LE	132	ALA	THR	conflict	UNP P05739
LE	146	ILE	LEU	conflict	UNP P05739
LE	173	MET	LEU	conflict	UNP P05739

- Molecule 10 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 11 is a protein called 60S ribosomal protein L8-A.

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

- Molecule 12 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LH	191	Total	C	N	O	S	0	0
			1508	957	274	273	4		

- Molecule 13 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LI	218	Total	C	N	O	S	0	0
			1764	1117	334	306	7		

- Molecule 14 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LJ	169	Total	C	N	O	S	0	0
			1350	846	253	247	4		

- Molecule 15 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	LL	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 16 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LM	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 17 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 18 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 19 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	LP	183	1416	879	284	253	0	0

- Molecule 20 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 21 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
21	LR	171	1378	850	294	234	0	0

- Molecule 22 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	LS	171	1437	925	266	243	3	0	0

- Molecule 23 is a protein called 60S ribosomal protein L21-A.

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

- Molecule 24 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	LU	100	796	516	131	149	0	0

- Molecule 25 is a protein called 60S ribosomal protein L23-A.

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

- Molecule 26 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	LW	67	538	345	106	86	1	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LW	104	GLN	ASN	conflict	UNP P04449
LW	109	GLN	LEU	conflict	UNP P04449
LW	112	ASP	ASN	conflict	UNP P04449
LW	119	ALA	GLU	conflict	UNP P04449

- Molecule 27 is a protein called 60S ribosomal protein L25.

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

- Molecule 28 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	LY	125	984	620	191	173	0	0

- Molecule 29 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 30 is a protein called 60S ribosomal protein L28.

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

- Molecule 31 is a protein called 60S ribosomal protein L29.

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

- Molecule 32 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Lc	96	Total	C	N	O	S	0	0
			737	476	123	137	1		

- Molecule 33 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ld	109	Total	C	N	O	S	0	0
			880	559	168	152	1		

- Molecule 34 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Le	127	Total	C	N	O	S	0	0
			1017	644	205	167	1		

- Molecule 35 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 36 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lg	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 37 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 38 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Li	99	Total	C	N	O	S	0	0
			766	478	154	132	2		

- Molecule 39 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lj	85	Total	C	N	O	S	0	0
			670	408	146	111	5		

- Molecule 40 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lk	77	Total	C	N	O	S	0	0
			612	391	115	106			

- Molecule 41 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Ll	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 42 is a protein called 60S ribosomal protein L40-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lm	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 43 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Ln	25	Total	C	N	O	S	0	0
			229	139	62	27	1		

- Molecule 44 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lo	103	Total	C	N	O	S	0	0
			824	517	167	135	5		

- Molecule 45 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 46 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
46	1	3301	70586	31525	12690	23070	3301	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	?	-	G	deletion	GB 1262303
1	1962	A	G	conflict	GB 1262303

- Molecule 47 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
47	C4	1	Total 1	Mg 1	0
47	C3	1	Total 1	Mg 1	0
47	LA	2	Total 2	Mg 2	0
47	LB	1	Total 1	Mg 1	0
47	LN	1	Total 1	Mg 1	0
47	LP	1	Total 1	Mg 1	0
47	LR	1	Total 1	Mg 1	0
47	LV	1	Total 1	Mg 1	0
47	La	1	Total 1	Mg 1	0
47	Le	1	Total 1	Mg 1	0
47	1	195	Total 195	Mg 195	0

- Molecule 48 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
48	Lg	1	Total 1	Zn 1	0
48	Lj	1	Total 1	Zn 1	0

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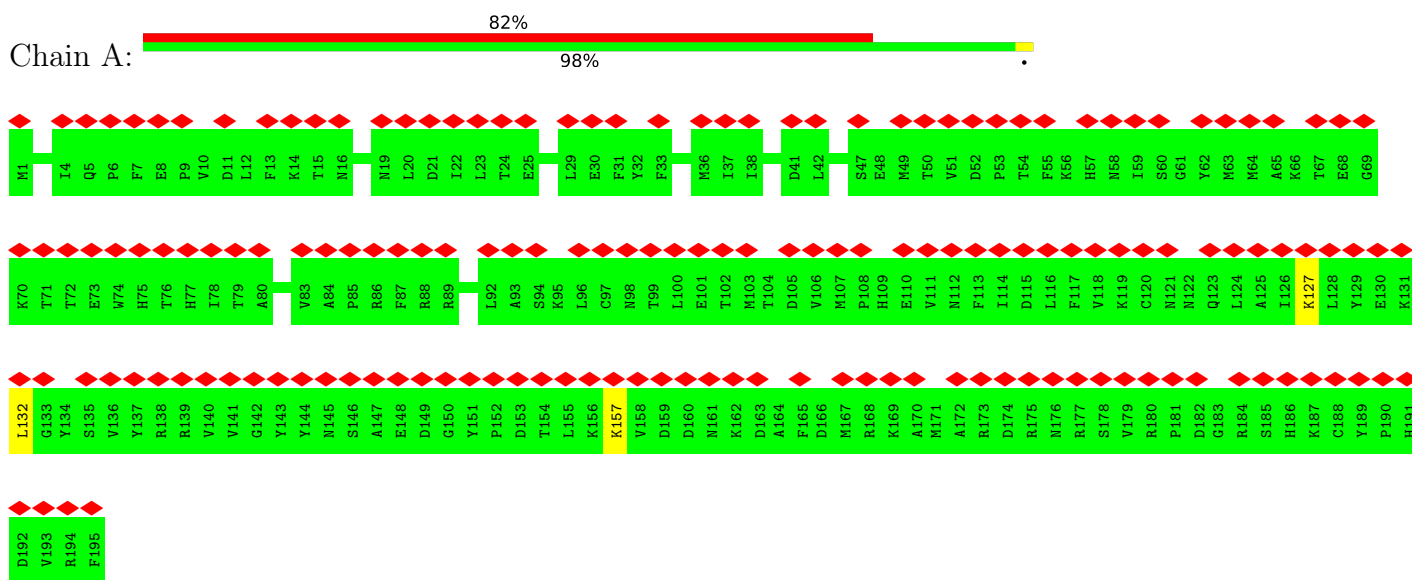
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Mol	Chain	Residues	Atoms		AltConf
48	Lm	1	Total 1	Zn 1	0
48	Lo	1	Total 1	Zn 1	0
48	Lp	1	Total 1	Zn 1	0

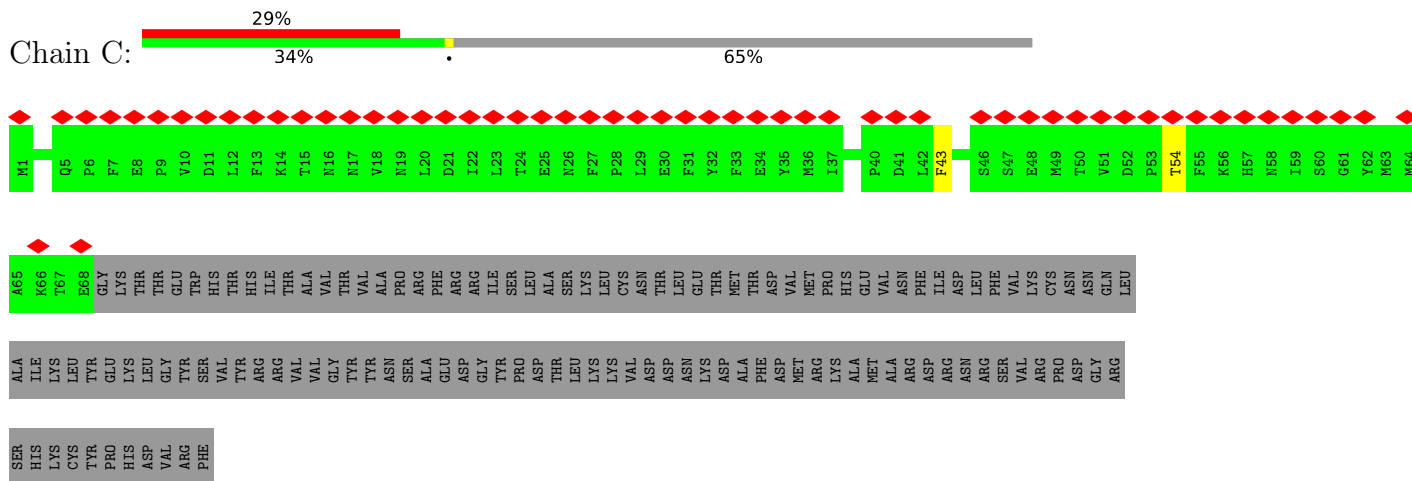
3 Residue-property plots [i](#)

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.

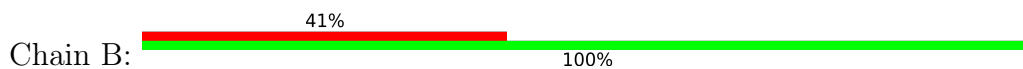
- Molecule 1: N-terminal acetyltransferase B complex catalytic subunit NAT3

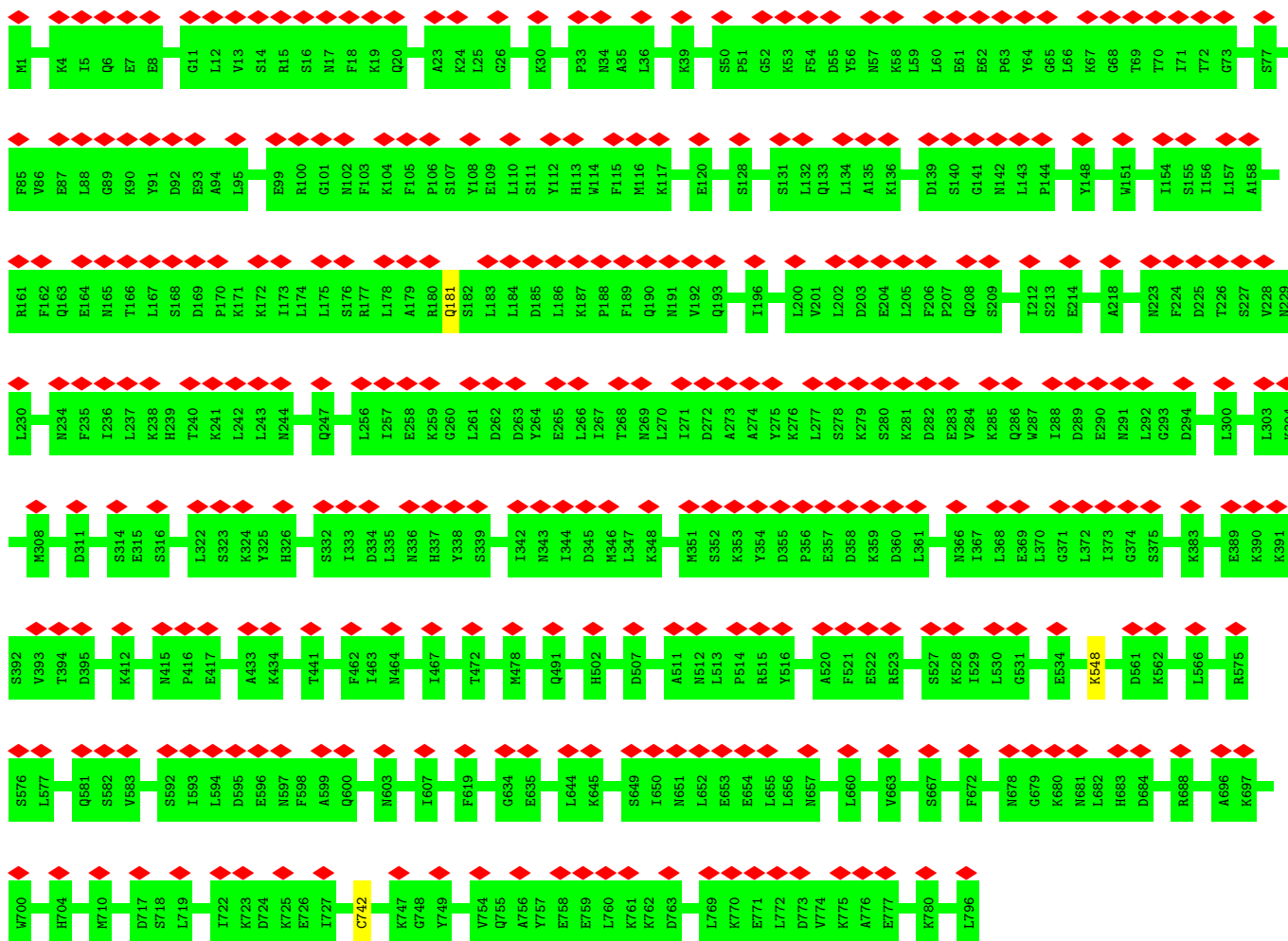


- Molecule 1: N-terminal acetyltransferase B complex catalytic subunit NAT3

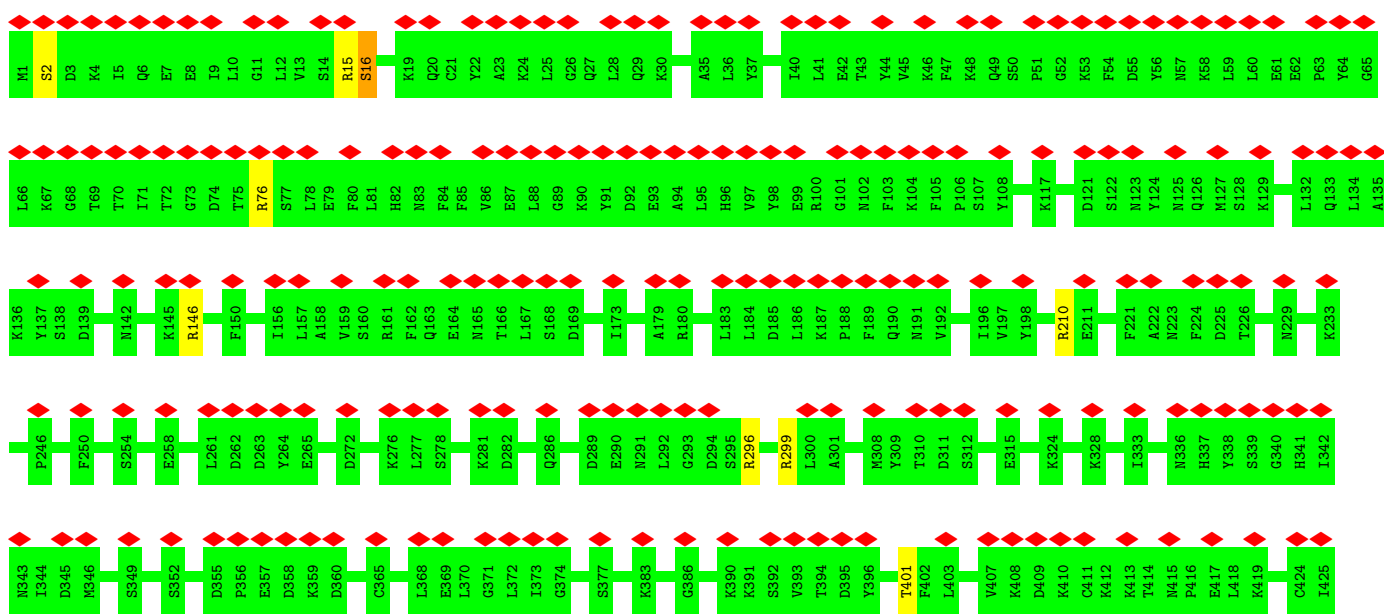


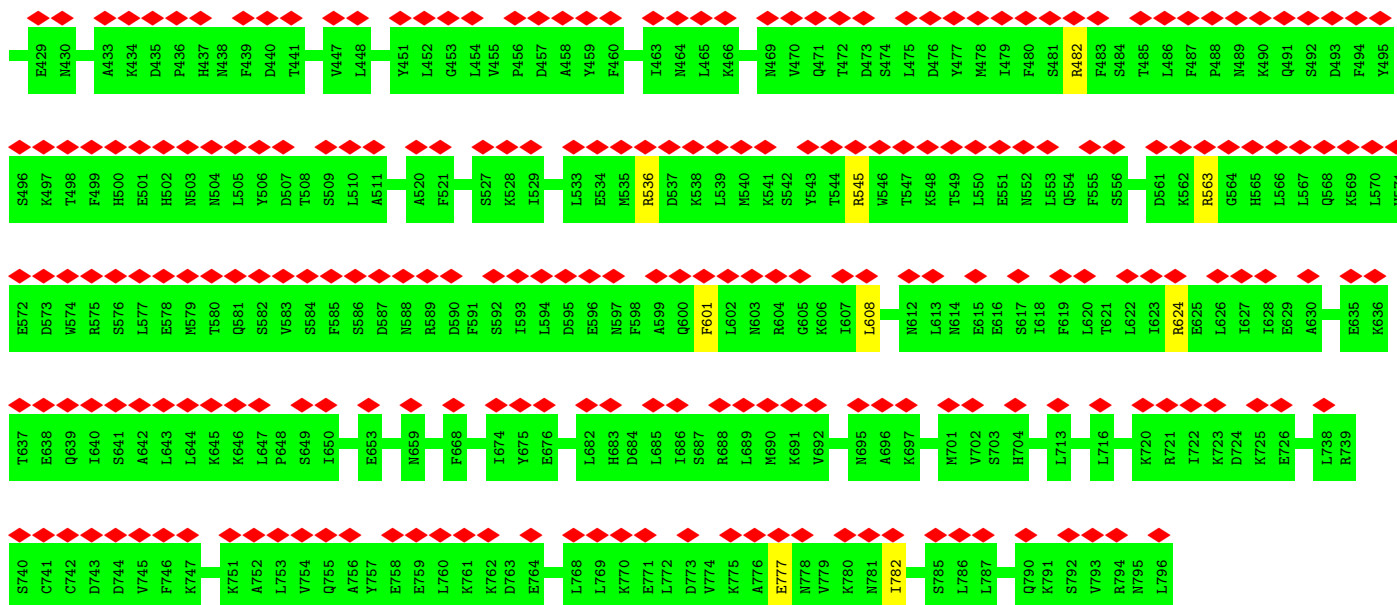
- Molecule 2: N-terminal acetyltransferase B complex subunit MDM20





• Molecule 2: N-terminal acetyltransferase B complex subunit MDM20

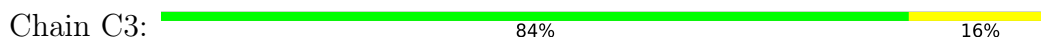




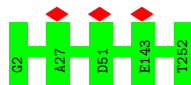
• Molecule 3: 5S rRNA



• Molecule 4: 5.8S rRNA



• Molecule 5: 60S ribosomal protein L2-A



• Molecule 6: 60S ribosomal protein L3

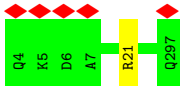


• Molecule 7: 60S ribosomal protein L4-A

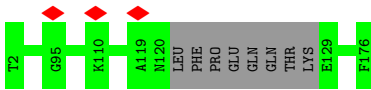




- Molecule 8: 60S ribosomal protein L5



- Molecule 9: 60S ribosomal protein L6-B

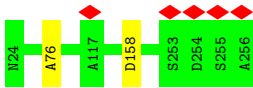


- Molecule 10: 60S ribosomal protein L7-A

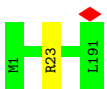


There are no outlier residues recorded for this chain.

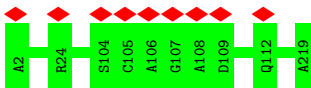
- Molecule 11: 60S ribosomal protein L8-A



- Molecule 12: 60S ribosomal protein L9-A

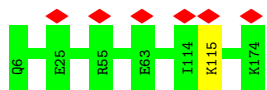


- Molecule 13: 60S ribosomal protein L10



- Molecule 14: 60S ribosomal protein L11-B





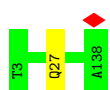
- Molecule 15: 60S ribosomal protein L13-A

Chain LL: 98%



- Molecule 16: 60S ribosomal protein L14-A

Chain LM: 99%



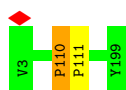
- Molecule 17: 60S ribosomal protein L15-A

Chain LN: 100%



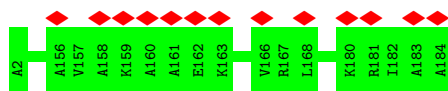
- Molecule 18: 60S ribosomal protein L16-A

Chain LO: 99%



- Molecule 19: 60S ribosomal protein L17-A

Chain LP: 7% 100%

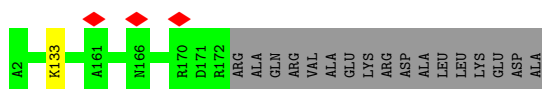
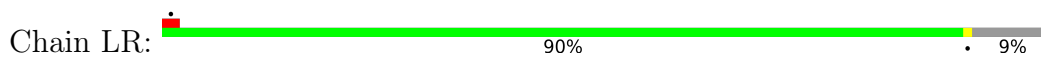


- Molecule 20: 60S ribosomal protein L18-A

Chain LQ: 99%



- Molecule 21: 60S ribosomal protein L19-A



- Molecule 22: 60S ribosomal protein L20-A



There are no outlier residues recorded for this chain.

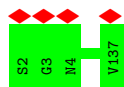
- Molecule 23: 60S ribosomal protein L21-A



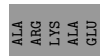
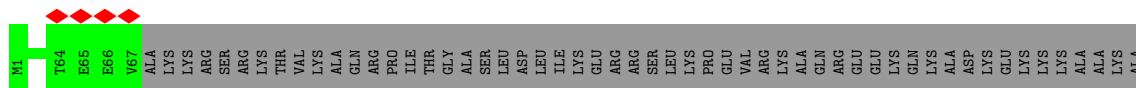
- Molecule 24: 60S ribosomal protein L22-A



- Molecule 25: 60S ribosomal protein L23-A



- Molecule 26: 60S ribosomal protein L24-A



- Molecule 27: 60S ribosomal protein L25





- Molecule 28: 60S ribosomal protein L26-A

Chain LY:  99%



- Molecule 29: 60S ribosomal protein L27-A

Chain LZ:  99%



- Molecule 30: 60S ribosomal protein L28

Chain La:  99%



- Molecule 31: 60S ribosomal protein L29

Chain Lb:  100%



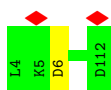
- Molecule 32: 60S ribosomal protein L30

Chain Lc:  99%



- Molecule 33: 60S ribosomal protein L31-A

Chain Ld:  99%



- Molecule 34: 60S ribosomal protein L32

Chain Le:  100%



- Molecule 35: 60S ribosomal protein L33-A

Chain Lf:  99%



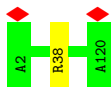
- Molecule 36: 60S ribosomal protein L34-A

Chain Lg:  100%

There are no outlier residues recorded for this chain.

- Molecule 37: 60S ribosomal protein L35-A

Chain Lh:  99%



- Molecule 38: 60S ribosomal protein L36-A

Chain Li:  100%



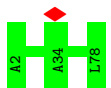
- Molecule 39: 60S ribosomal protein L37-A

Chain Lj:  100%

There are no outlier residues recorded for this chain.

- Molecule 40: 60S ribosomal protein L38

Chain Lk:  100%

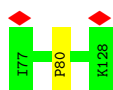


- Molecule 41: 60S ribosomal protein L39

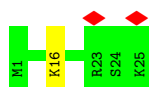
Chain Ll:  100%

There are no outlier residues recorded for this chain.

- Molecule 42: 60S ribosomal protein L40-A



- Molecule 43: 60S ribosomal protein L41-A



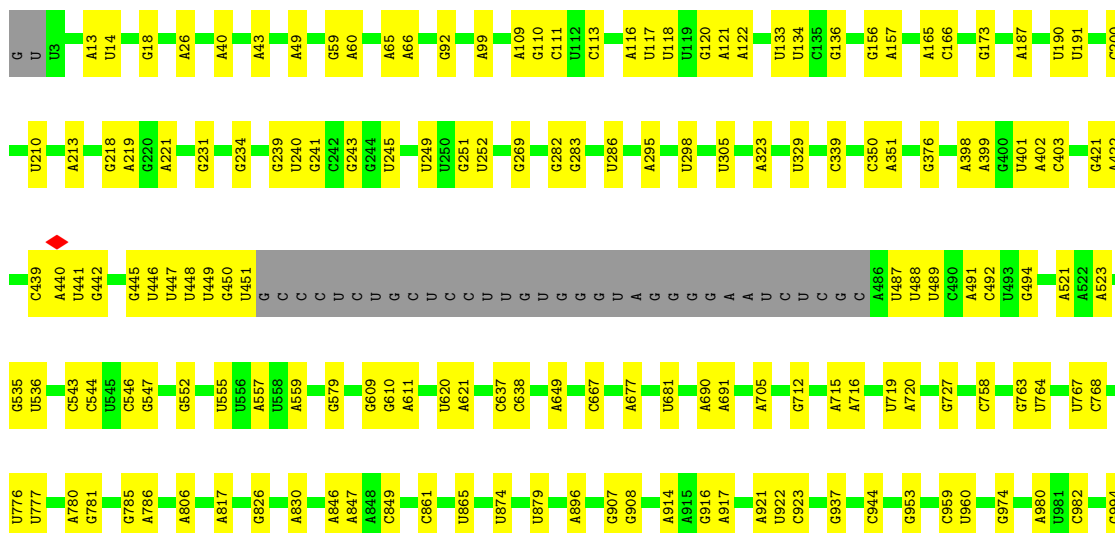
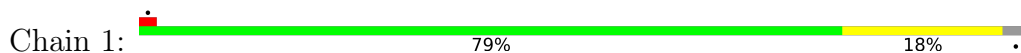
- Molecule 44: 60S ribosomal protein L42-A

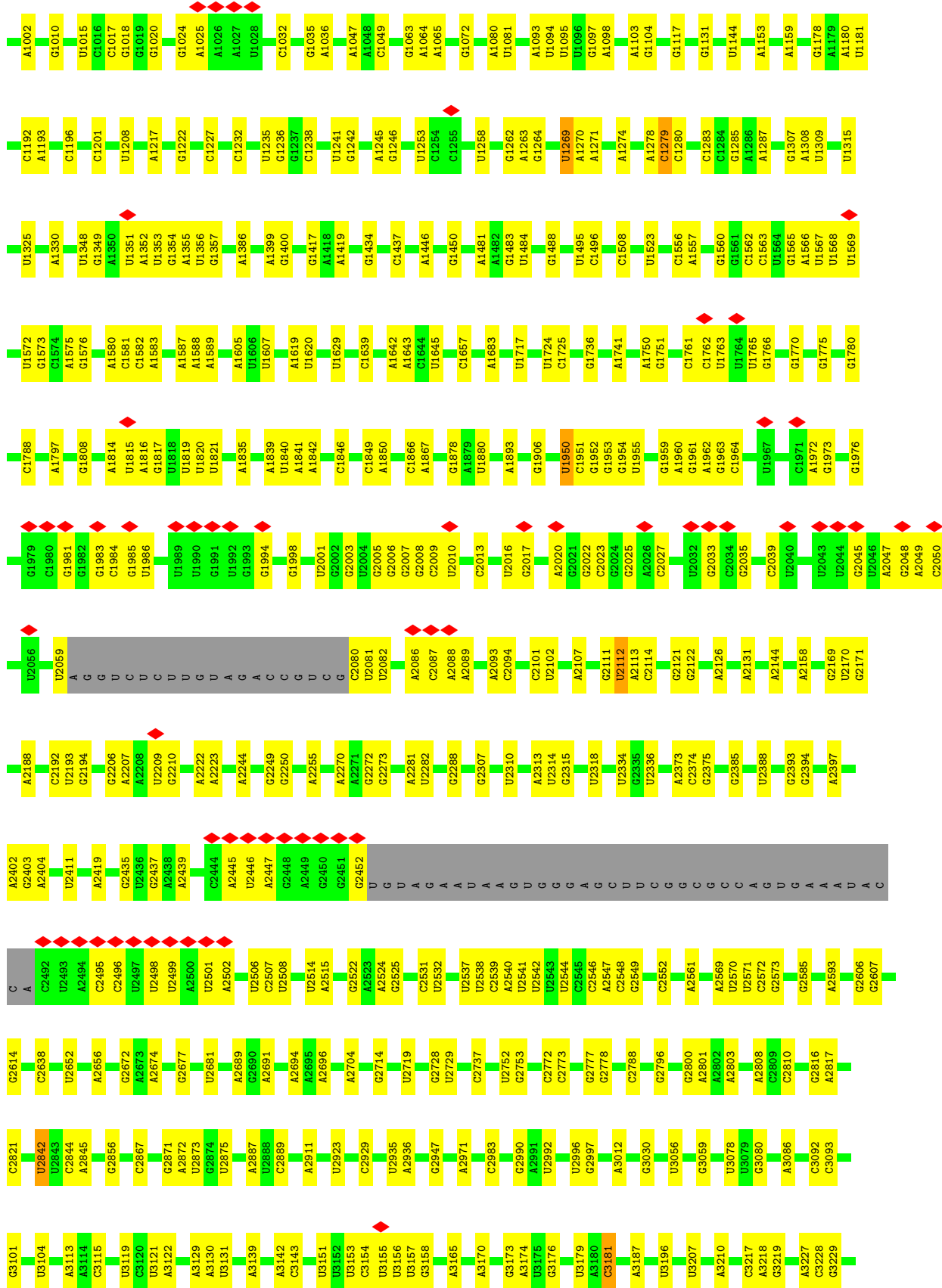


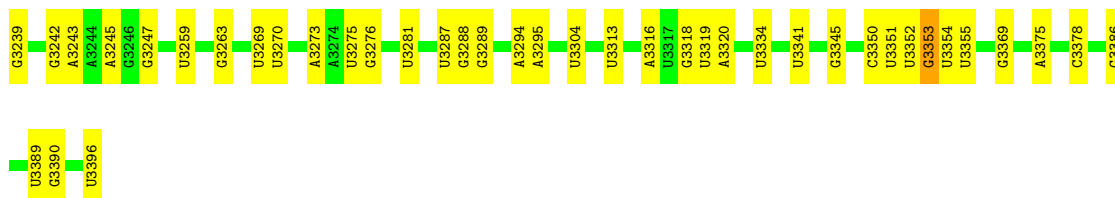
- Molecule 45: 60S ribosomal protein L43-A



- Molecule 46: 25S rRNA







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9645	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 ($e^-/\text{\AA}^2$)	45.2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.382	Depositor
Minimum map value	-0.498	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.093	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	417.99997, 417.99997, 417.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	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: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/1654	0.56	1/2237 (0.0%)
1	C	0.67	0/589	0.82	0/800
2	B	0.25	0/6665	0.47	0/8979
2	D	0.64	0/6665	0.86	14/8979 (0.2%)
3	C4	0.37	0/2883	0.74	0/4491
4	C3	0.43	0/3746	0.77	0/5832
5	LA	0.31	0/1933	0.58	0/2598
6	LB	0.30	0/3146	0.53	0/4228
7	LC	0.30	0/2800	0.53	0/3790
8	LD	0.28	0/2400	0.52	0/3239
9	LE	0.29	0/1327	0.51	0/1790
10	LF	0.31	0/1821	0.50	0/2451
11	LG	0.29	0/1836	0.51	0/2481
12	LH	0.30	0/1529	0.55	0/2060
13	LI	0.29	0/1801	0.54	0/2416
14	LJ	0.28	0/1371	0.60	0/1838
15	LL	0.30	0/1568	0.62	0/2106
16	LM	0.29	0/1068	0.54	0/1438
17	LN	0.31	0/1757	0.59	0/2354
18	LO	0.31	0/1585	0.52	0/2128
19	LP	0.30	0/1439	0.56	0/1938
20	LQ	0.29	0/1465	0.56	0/1965
21	LR	0.29	0/1395	0.57	0/1861
22	LS	0.33	0/1473	0.60	0/1980
23	LT	0.31	0/1300	0.55	0/1743
24	LU	0.30	0/812	0.53	0/1099
25	LV	0.31	0/1018	0.57	0/1369
26	LW	0.31	0/550	0.58	0/731
27	LX	0.31	0/979	0.51	0/1321
28	LY	0.31	0/995	0.62	1/1329 (0.1%)
29	LZ	0.32	0/1118	0.55	0/1497
30	La	0.30	0/1204	0.54	0/1612

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	Lb	0.28	0/473	0.54	0/629
32	Lc	0.32	0/745	0.51	0/1001
33	Ld	0.31	0/894	0.58	0/1200
34	Le	0.29	0/1038	0.54	0/1390
35	Lf	0.33	0/868	0.57	0/1168
36	Lg	0.31	0/890	0.59	0/1189
37	Lh	0.29	0/978	0.54	0/1301
38	Li	0.28	0/772	0.56	0/1026
39	Lj	0.31	0/685	0.59	0/908
40	Lk	0.29	0/618	0.56	0/826
41	Ll	0.30	0/443	0.66	0/588
42	Lm	0.30	0/423	0.63	0/562
43	Ln	0.26	0/230	0.82	0/296
44	Lo	0.30	0/836	0.57	0/1104
45	Lp	0.33	0/701	0.64	0/934
46	1	0.42	2/79000 (0.0%)	0.80	26/123166 (0.0%)
All	All	0.39	2/151486 (0.0%)	0.72	42/221968 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	LC	0	1
11	LG	0	2
15	LL	0	1
18	LO	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	1	2094	C	O3'-P	-16.91	1.40	1.61
46	1	1950	U	O3'-P	-14.84	1.43	1.61

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	1	1950	U	O3'-P-O5'	27.53	156.31	104.00
46	1	1950	U	OP2-P-O3'	-12.81	77.02	105.20
46	1	1950	U	P-O3'-C3'	-11.39	106.03	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	1	1950	U	OP1-P-O3'	-7.96	87.69	105.20
28	LY	53	ASP	CB-CG-OD1	7.33	124.90	118.30
2	D	545	ARG	NE-CZ-NH1	7.08	123.84	120.30
2	D	146	ARG	NE-CZ-NH1	6.85	123.72	120.30
2	D	482	ARG	NE-CZ-NH1	6.74	123.67	120.30
2	D	296	ARG	NE-CZ-NH1	6.69	123.65	120.30
2	D	210	ARG	NE-CZ-NH2	-6.65	116.97	120.30
46	1	922	U	C2-N1-C1'	6.63	125.66	117.70
46	1	1269	U	C2-N1-C1'	6.58	125.59	117.70
46	1	3353	G	N3-C4-N9	-6.38	122.17	126.00
2	D	210	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	132	LEU	CA-CB-CG	6.31	129.81	115.30
46	1	1269	U	N1-C2-O2	6.17	127.12	122.80
46	1	758	C	C2-N1-C1'	6.01	125.41	118.80
2	D	299	ARG	NE-CZ-NH1	5.95	123.28	120.30
46	1	1283	C	N3-C2-O2	-5.80	117.84	121.90
46	1	1269	U	N3-C2-O2	-5.79	118.14	122.20
2	D	563	ARG	NE-CZ-NH1	5.70	123.15	120.30
2	D	536	ARG	NE-CZ-NH1	5.67	123.14	120.30
46	1	3353	G	N3-C4-C5	5.66	131.43	128.60
2	D	15	ARG	C-N-CA	5.59	135.67	121.70
2	D	299	ARG	CD-NE-CZ	5.54	131.35	123.60
46	1	2842	U	N1-C2-O2	5.52	126.66	122.80
46	1	2080	C	N1-C2-O2	5.43	122.16	118.90
46	1	1280	C	N3-C2-O2	-5.42	118.10	121.90
46	1	2112	U	OP2-P-O3'	5.42	117.11	105.20
2	D	76	ARG	NE-CZ-NH1	5.34	122.97	120.30
46	1	922	U	N1-C2-O2	5.33	126.53	122.80
46	1	2842	U	C2-N1-C1'	5.28	124.04	117.70
2	D	624	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	D	16	SER	N-CA-CB	5.26	118.39	110.50
46	1	3353	G	C4-N9-C1'	-5.25	119.68	126.50
46	1	2027	C	N1-C2-O2	5.23	122.04	118.90
46	1	2080	C	N3-C2-O2	-5.14	118.30	121.90
46	1	1279	C	N1-C2-O2	5.12	121.97	118.90
46	1	2027	C	N3-C2-O2	-5.12	118.31	121.90
46	1	1496	C	C2-N1-C1'	5.07	124.38	118.80
46	1	3181	C	C2-N1-C1'	5.03	124.33	118.80
46	1	2112	U	P-O3'-C3'	5.01	125.71	119.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	LC	13	GLY	Peptide
11	LG	158	ASP	Peptide
11	LG	76	ALA	Peptide
15	LL	75	PHE	Peptide
18	LO	110[A]	PRO	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	193/195 (99%)	192 (100%)	1 (0%)	0	100	100
1	C	66/195 (34%)	66 (100%)	0	0	100	100
2	B	794/796 (100%)	790 (100%)	3 (0%)	1 (0%)	51	83
2	D	794/796 (100%)	770 (97%)	22 (3%)	2 (0%)	41	74
5	LA	249/251 (99%)	234 (94%)	15 (6%)	0	100	100
6	LB	384/386 (100%)	358 (93%)	26 (7%)	0	100	100
7	LC	359/361 (99%)	329 (92%)	28 (8%)	2 (1%)	25	62
8	LD	292/294 (99%)	274 (94%)	17 (6%)	1 (0%)	41	74
9	LE	163/175 (93%)	155 (95%)	8 (5%)	0	100	100
10	LF	220/222 (99%)	205 (93%)	15 (7%)	0	100	100
11	LG	231/233 (99%)	221 (96%)	10 (4%)	0	100	100
12	LH	189/191 (99%)	176 (93%)	13 (7%)	0	100	100
13	LI	216/218 (99%)	208 (96%)	8 (4%)	0	100	100
14	LJ	167/169 (99%)	152 (91%)	15 (9%)	0	100	100
15	LL	191/193 (99%)	174 (91%)	15 (8%)	2 (1%)	15	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	LM	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
17	LN	201/203 (99%)	191 (95%)	10 (5%)	0	100	100
18	LO	195/197 (99%)	185 (95%)	8 (4%)	2 (1%)	15	52
19	LP	181/183 (99%)	171 (94%)	10 (6%)	0	100	100
20	LQ	183/185 (99%)	176 (96%)	7 (4%)	0	100	100
21	LR	169/188 (90%)	163 (96%)	6 (4%)	0	100	100
22	LS	169/171 (99%)	157 (93%)	12 (7%)	0	100	100
23	LT	157/159 (99%)	148 (94%)	9 (6%)	0	100	100
24	LU	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
25	LV	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
26	LW	65/126 (52%)	61 (94%)	4 (6%)	0	100	100
27	LX	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
28	LY	123/125 (98%)	117 (95%)	6 (5%)	0	100	100
29	LZ	133/135 (98%)	123 (92%)	10 (8%)	0	100	100
30	La	146/148 (99%)	133 (91%)	13 (9%)	0	100	100
31	Lb	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
32	Lc	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
33	Ld	107/109 (98%)	99 (92%)	7 (6%)	1 (1%)	17	54
34	Le	125/127 (98%)	120 (96%)	5 (4%)	0	100	100
35	Lf	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
36	Lg	110/112 (98%)	106 (96%)	4 (4%)	0	100	100
37	Lh	117/119 (98%)	110 (94%)	7 (6%)	0	100	100
38	Li	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
39	Lj	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
40	Lk	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
41	Ll	48/50 (96%)	48 (100%)	0	0	100	100
42	Lm	50/52 (96%)	47 (94%)	2 (4%)	1 (2%)	7	41
43	Ln	23/25 (92%)	23 (100%)	0	0	100	100
44	Lo	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
45	Lp	89/91 (98%)	88 (99%)	1 (1%)	0	100	100
All	All	7994/8297 (96%)	7629 (95%)	353 (4%)	12 (0%)	50	79

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	742	CYS
7	LC	293	SER
33	Ld	6	ASP
2	D	16	SER
2	D	777	GLU
8	LD	21	ARG
18	LO	111[A]	PRO
15	LL	63	VAL
7	LC	4	PRO
18	LO	110[A]	PRO
15	LL	77	LEU
42	Lm	80	PRO

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	
1	A	180/180 (100%)	178 (99%)	2 (1%)	73	85
1	C	66/180 (37%)	64 (97%)	2 (3%)	41	66
2	B	743/743 (100%)	741 (100%)	2 (0%)	92	96
2	D	743/743 (100%)	738 (99%)	5 (1%)	84	91
5	LA	190/193 (98%)	190 (100%)	0	100	100
6	LB	318/322 (99%)	317 (100%)	1 (0%)	92	96
7	LC	288/288 (100%)	288 (100%)	0	100	100
8	LD	241/243 (99%)	241 (100%)	0	100	100
9	LE	138/153 (90%)	138 (100%)	0	100	100
10	LF	186/186 (100%)	186 (100%)	0	100	100
11	LG	187/191 (98%)	187 (100%)	0	100	100
12	LH	168/171 (98%)	167 (99%)	1 (1%)	86	92
13	LI	185/185 (100%)	185 (100%)	0	100	100
14	LJ	146/147 (99%)	145 (99%)	1 (1%)	84	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	LL	154/154 (100%)	153 (99%)	1 (1%)	86	92
16	LM	107/107 (100%)	106 (99%)	1 (1%)	78	88
17	LN	175/175 (100%)	175 (100%)	0	100	100
18	LO	160/160 (100%)	160 (100%)	0	100	100
19	LP	138/145 (95%)	138 (100%)	0	100	100
20	LQ	150/150 (100%)	149 (99%)	1 (1%)	84	91
21	LR	139/153 (91%)	138 (99%)	1 (1%)	84	91
22	LS	155/155 (100%)	155 (100%)	0	100	100
23	LT	136/136 (100%)	135 (99%)	1 (1%)	84	91
24	LU	87/87 (100%)	87 (100%)	0	100	100
25	LV	104/104 (100%)	104 (100%)	0	100	100
26	LW	54/107 (50%)	54 (100%)	0	100	100
27	LX	104/105 (99%)	104 (100%)	0	100	100
28	LY	108/108 (100%)	108 (100%)	0	100	100
29	LZ	115/115 (100%)	114 (99%)	1 (1%)	78	88
30	La	118/118 (100%)	117 (99%)	1 (1%)	81	89
31	Lb	46/46 (100%)	46 (100%)	0	100	100
32	Lc	81/81 (100%)	80 (99%)	1 (1%)	71	84
33	Ld	93/96 (97%)	93 (100%)	0	100	100
34	Le	108/109 (99%)	108 (100%)	0	100	100
35	Lf	90/90 (100%)	89 (99%)	1 (1%)	73	85
36	Lg	95/95 (100%)	95 (100%)	0	100	100
37	Lh	104/104 (100%)	103 (99%)	1 (1%)	76	86
38	Li	80/81 (99%)	80 (100%)	0	100	100
39	Lj	69/69 (100%)	69 (100%)	0	100	100
40	Lk	68/68 (100%)	68 (100%)	0	100	100
41	Ll	45/45 (100%)	45 (100%)	0	100	100
42	Lm	47/47 (100%)	47 (100%)	0	100	100
43	Ln	22/23 (96%)	21 (96%)	1 (4%)	27	57
44	Lo	87/88 (99%)	87 (100%)	0	100	100
45	Lp	71/71 (100%)	71 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6889/7117 (97%)	6864 (100%)	25 (0%)	91 95

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	LYS
1	A	157	LYS
2	B	181	GLN
2	B	548	LYS
6	LB	332	ARG
12	LH	23	ARG
14	LJ	115	LYS
15	LL	104	ARG
16	LM	27	GLN
20	LQ	12	ARG
21	LR	133	LYS
23	LT	77	ASN
29	LZ	3	LYS
30	La	120	ASN
32	Lc	22	LYS
35	Lf	106	ASN
37	Lh	38	ARG
43	Ln	16	LYS
1	C	43	PHE
1	C	54	THR
2	D	2	SER
2	D	401	THR
2	D	601	PHE
2	D	608	LEU
2	D	782	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	109	HIS
2	B	20	GLN
2	B	29	GLN
2	B	181	GLN
2	B	430	ASN
2	B	469	ASN

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Mol	Chain	Res	Type
2	B	491	GLN
2	B	755	GLN
5	LA	83	HIS
9	LE	167	ASN
12	LH	9	GLN
20	LQ	5	HIS
21	LR	134	HIS
22	LS	8	GLN
23	LT	58	GLN
25	LV	98	ASN
30	La	62	HIS
30	La	64	GLN
30	La	67	HIS
36	Lg	34	HIS
2	D	17	ASN
2	D	34	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C4	120/121 (99%)	11 (9%)	1 (0%)
4	C3	157/158 (99%)	26 (16%)	1 (0%)
46	1	3297/3395 (97%)	609 (18%)	39 (1%)
All	All	3574/3674 (97%)	646 (18%)	41 (1%)

All (646) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C4	7	G
3	C4	11	A
3	C4	53	U
3	C4	54	U
3	C4	55	A
3	C4	65	G
3	C4	73	C
3	C4	76	A
3	C4	102	A
3	C4	112	G
3	C4	121	U
4	C3	34	U
4	C3	35	C

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Mol	Chain	Res	Type
4	C3	53	A
4	C3	59	A
4	C3	62	C
4	C3	63	G
4	C3	80	A
4	C3	81	U
4	C3	82	U
4	C3	83	C
4	C3	84	C
4	C3	85	G
4	C3	86	U
4	C3	87	G
4	C3	90	U
4	C3	95	G
4	C3	97	A
4	C3	104	A
4	C3	106	C
4	C3	111	A
4	C3	113	U
4	C3	125	U
4	C3	126	A
4	C3	148	G
4	C3	152	G
4	C3	158	U
46	1	13	A
46	1	14	U
46	1	18	G
46	1	26	A
46	1	40	A
46	1	43	A
46	1	49	A
46	1	59	G
46	1	60	A
46	1	65	A
46	1	66	A
46	1	92	G
46	1	99	A
46	1	109	A
46	1	110	G
46	1	111	C
46	1	113	C
46	1	116	A

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Mol	Chain	Res	Type
46	1	117	U
46	1	118	U
46	1	120	G
46	1	121	A
46	1	122	A
46	1	133	U
46	1	134	U
46	1	136	G
46	1	156	G
46	1	157	A
46	1	165	A
46	1	166	C
46	1	173	G
46	1	187	A
46	1	190	U
46	1	191	U
46	1	200	C
46	1	210	U
46	1	213	A
46	1	218	G
46	1	219	A
46	1	221	A
46	1	231	G
46	1	234	G
46	1	240	U
46	1	241	G
46	1	243	G
46	1	245	U
46	1	249	U
46	1	251	G
46	1	252	U
46	1	269	G
46	1	283	G
46	1	286	U
46	1	295	A
46	1	298	U
46	1	305	U
46	1	323	A
46	1	329	U
46	1	339	C
46	1	350	C
46	1	351	A

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Mol	Chain	Res	Type
46	1	376	G
46	1	398	A
46	1	399	A
46	1	401	U
46	1	402	A
46	1	403	C
46	1	421	G
46	1	422	A
46	1	439	C
46	1	440	A
46	1	441	U
46	1	442	G
46	1	445	G
46	1	446	U
46	1	447	U
46	1	448	U
46	1	449	U
46	1	450	G
46	1	451	U
46	1	487	U
46	1	488	U
46	1	489	U
46	1	491	A
46	1	492	C
46	1	494	G
46	1	521	A
46	1	523	A
46	1	535	G
46	1	536	U
46	1	543	C
46	1	544	C
46	1	546	C
46	1	547	G
46	1	552	G
46	1	555	U
46	1	557	A
46	1	559	A
46	1	579	G
46	1	609	G
46	1	610	G
46	1	611	A
46	1	620	U

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Mol	Chain	Res	Type
46	1	621	A
46	1	637	C
46	1	638	C
46	1	649	A
46	1	667	C
46	1	677	A
46	1	681	U
46	1	690	A
46	1	691	A
46	1	705	A
46	1	712	G
46	1	715	A
46	1	716	A
46	1	719	U
46	1	720	A
46	1	727	G
46	1	764	U
46	1	767	U
46	1	768	C
46	1	776	U
46	1	777	U
46	1	780	A
46	1	781	G
46	1	785	G
46	1	786	A
46	1	806	A
46	1	817	A
46	1	826	G
46	1	830	A
46	1	846	A
46	1	847	A
46	1	849	C
46	1	861	C
46	1	865	U
46	1	874	U
46	1	879	U
46	1	896	A
46	1	907	G
46	1	908	G
46	1	914	A
46	1	916	G
46	1	917	A

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Mol	Chain	Res	Type
46	1	921	A
46	1	923	C
46	1	937	G
46	1	944	C
46	1	953	G
46	1	959	C
46	1	960	U
46	1	974	G
46	1	980	A
46	1	982	C
46	1	994	G
46	1	1002	A
46	1	1010	G
46	1	1015	U
46	1	1017	C
46	1	1018	G
46	1	1020	G
46	1	1024	G
46	1	1025	A
46	1	1032	C
46	1	1035	G
46	1	1036	A
46	1	1047	A
46	1	1049	C
46	1	1063	G
46	1	1064	A
46	1	1065	A
46	1	1072	G
46	1	1080	A
46	1	1081	U
46	1	1093	A
46	1	1094	U
46	1	1095	U
46	1	1097	G
46	1	1098	A
46	1	1103	A
46	1	1104	G
46	1	1117	G
46	1	1131	G
46	1	1144	U
46	1	1153	A
46	1	1159	A

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Mol	Chain	Res	Type
46	1	1178	G
46	1	1180	A
46	1	1181	U
46	1	1192	C
46	1	1193	A
46	1	1196	C
46	1	1201	C
46	1	1208	U
46	1	1217	A
46	1	1222	G
46	1	1227	C
46	1	1232	C
46	1	1235	U
46	1	1236	G
46	1	1238	C
46	1	1241	U
46	1	1242	G
46	1	1245	A
46	1	1246	G
46	1	1253	U
46	1	1258	U
46	1	1262	G
46	1	1263	A
46	1	1264	G
46	1	1269	U
46	1	1270	A
46	1	1271	A
46	1	1274	A
46	1	1278	A
46	1	1279	C
46	1	1285	G
46	1	1287	A
46	1	1307	G
46	1	1308	A
46	1	1309	U
46	1	1315	U
46	1	1325	U
46	1	1330	A
46	1	1348	U
46	1	1349	G
46	1	1351	U
46	1	1352	A

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Mol	Chain	Res	Type
46	1	1353	U
46	1	1354	G
46	1	1355	A
46	1	1356	U
46	1	1357	G
46	1	1386	A
46	1	1399	A
46	1	1400	G
46	1	1417	G
46	1	1419	A
46	1	1434	G
46	1	1437	C
46	1	1446	A
46	1	1450	G
46	1	1481	A
46	1	1483	G
46	1	1484	U
46	1	1488	G
46	1	1495	U
46	1	1508	C
46	1	1523	U
46	1	1556	C
46	1	1557	A
46	1	1560	G
46	1	1562	C
46	1	1563	C
46	1	1565	G
46	1	1566	A
46	1	1567	U
46	1	1568	U
46	1	1569	U
46	1	1572	U
46	1	1573	G
46	1	1575	A
46	1	1576	G
46	1	1580	A
46	1	1581	C
46	1	1582	C
46	1	1583	A
46	1	1587	A
46	1	1588	A
46	1	1589	A

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Mol	Chain	Res	Type
46	1	1605	A
46	1	1607	U
46	1	1619	A
46	1	1620	U
46	1	1629	U
46	1	1639	C
46	1	1642	A
46	1	1643	A
46	1	1645	U
46	1	1657	C
46	1	1683	A
46	1	1717	U
46	1	1724	U
46	1	1725	C
46	1	1736	G
46	1	1741	A
46	1	1750	A
46	1	1751	G
46	1	1761	C
46	1	1762	C
46	1	1763	U
46	1	1765	U
46	1	1766	G
46	1	1770	G
46	1	1775	G
46	1	1780	G
46	1	1788	C
46	1	1797	A
46	1	1808	G
46	1	1814	A
46	1	1816	A
46	1	1817	G
46	1	1819	U
46	1	1820	U
46	1	1821	U
46	1	1835	A
46	1	1839	A
46	1	1840	U
46	1	1841	A
46	1	1842	A
46	1	1846	C
46	1	1849	C

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Mol	Chain	Res	Type
46	1	1850	A
46	1	1866	C
46	1	1867	A
46	1	1878	G
46	1	1880	U
46	1	1893	A
46	1	1906	G
46	1	1951	C
46	1	1952	G
46	1	1953	G
46	1	1954	G
46	1	1955	U
46	1	1960	A
46	1	1961	G
46	1	1962	A
46	1	1963	G
46	1	1964	C
46	1	1972	A
46	1	1973	G
46	1	1976	G
46	1	1981	G
46	1	1983	G
46	1	1984	C
46	1	1985	G
46	1	1986	U
46	1	1994	G
46	1	1998	G
46	1	2001	U
46	1	2003	G
46	1	2005	G
46	1	2006	G
46	1	2007	G
46	1	2008	G
46	1	2009	C
46	1	2010	U
46	1	2013	C
46	1	2016	U
46	1	2017	G
46	1	2020	A
46	1	2022	G
46	1	2023	C
46	1	2025	G

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Mol	Chain	Res	Type
46	1	2033	G
46	1	2035	G
46	1	2039	C
46	1	2045	G
46	1	2047	A
46	1	2048	G
46	1	2049	A
46	1	2050	C
46	1	2059	U
46	1	2081	U
46	1	2082	U
46	1	2087	C
46	1	2088	A
46	1	2089	A
46	1	2093	A
46	1	2101	C
46	1	2102	U
46	1	2107	A
46	1	2111	G
46	1	2112	U
46	1	2113	A
46	1	2114	C
46	1	2121	G
46	1	2122	G
46	1	2126	A
46	1	2131	A
46	1	2144	A
46	1	2158	A
46	1	2169	G
46	1	2170	U
46	1	2171	G
46	1	2188	A
46	1	2192	C
46	1	2193	U
46	1	2194	G
46	1	2206	G
46	1	2207	A
46	1	2209	U
46	1	2210	G
46	1	2222	A
46	1	2223	A
46	1	2244	A

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Mol	Chain	Res	Type
46	1	2249	G
46	1	2250	G
46	1	2255	A
46	1	2270	A
46	1	2272	G
46	1	2273	G
46	1	2281	A
46	1	2282	U
46	1	2288	G
46	1	2307	G
46	1	2310	U
46	1	2313	A
46	1	2314	U
46	1	2315	G
46	1	2318	U
46	1	2334	U
46	1	2336	U
46	1	2373	A
46	1	2374	C
46	1	2375	G
46	1	2385	G
46	1	2388	U
46	1	2393	G
46	1	2394	G
46	1	2397	A
46	1	2402	A
46	1	2403	G
46	1	2404	A
46	1	2411	U
46	1	2419	A
46	1	2435	G
46	1	2437	G
46	1	2439	A
46	1	2445	A
46	1	2446	U
46	1	2447	A
46	1	2452	G
46	1	2496	C
46	1	2498	U
46	1	2499	U
46	1	2501	U
46	1	2502	A

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Mol	Chain	Res	Type
46	1	2506	U
46	1	2507	C
46	1	2508	U
46	1	2514	U
46	1	2515	A
46	1	2522	G
46	1	2524	A
46	1	2525	G
46	1	2531	C
46	1	2532	U
46	1	2537	U
46	1	2538	U
46	1	2539	C
46	1	2540	A
46	1	2541	U
46	1	2542	U
46	1	2544	U
46	1	2546	C
46	1	2547	A
46	1	2548	C
46	1	2549	G
46	1	2552	C
46	1	2561	A
46	1	2569	A
46	1	2570	U
46	1	2571	U
46	1	2572	C
46	1	2573	G
46	1	2585	G
46	1	2593	A
46	1	2606	G
46	1	2607	G
46	1	2614	G
46	1	2638	C
46	1	2652	U
46	1	2656	A
46	1	2672	G
46	1	2674	A
46	1	2677	G
46	1	2681	U
46	1	2689	A
46	1	2691	A

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Mol	Chain	Res	Type
46	1	2694	A
46	1	2696	A
46	1	2704	A
46	1	2714	G
46	1	2719	U
46	1	2728	G
46	1	2729	U
46	1	2737	C
46	1	2752	U
46	1	2753	G
46	1	2772	C
46	1	2773	C
46	1	2777	G
46	1	2778	G
46	1	2788	C
46	1	2796	G
46	1	2800	G
46	1	2801	A
46	1	2803	A
46	1	2808	A
46	1	2810	C
46	1	2816	G
46	1	2817	A
46	1	2821	C
46	1	2842	U
46	1	2844	C
46	1	2845	A
46	1	2856	G
46	1	2867	C
46	1	2871	G
46	1	2872	A
46	1	2873	U
46	1	2875	U
46	1	2887	A
46	1	2889	C
46	1	2911	A
46	1	2923	U
46	1	2929	C
46	1	2935	U
46	1	2936	A
46	1	2947	G
46	1	2971	A

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Mol	Chain	Res	Type
46	1	2983	C
46	1	2990	G
46	1	2992	U
46	1	2996	U
46	1	2997	G
46	1	3012	A
46	1	3030	G
46	1	3056	U
46	1	3059	G
46	1	3078	U
46	1	3080	G
46	1	3086	A
46	1	3092	C
46	1	3093	C
46	1	3101	G
46	1	3104	U
46	1	3113	A
46	1	3115	C
46	1	3119	U
46	1	3122	A
46	1	3129	A
46	1	3130	A
46	1	3131	U
46	1	3139	A
46	1	3142	A
46	1	3143	C
46	1	3151	U
46	1	3153	U
46	1	3154	C
46	1	3155	U
46	1	3156	U
46	1	3157	U
46	1	3158	G
46	1	3165	A
46	1	3170	A
46	1	3173	G
46	1	3174	A
46	1	3176	G
46	1	3179	U
46	1	3181	C
46	1	3187	A
46	1	3196	U

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Mol	Chain	Res	Type
46	1	3207	U
46	1	3210	A
46	1	3217	C
46	1	3218	A
46	1	3219	G
46	1	3227	A
46	1	3229	G
46	1	3239	G
46	1	3242	G
46	1	3243	A
46	1	3245	A
46	1	3247	G
46	1	3259	U
46	1	3263	G
46	1	3269	U
46	1	3270	U
46	1	3273	A
46	1	3276	G
46	1	3281	U
46	1	3287	U
46	1	3288	G
46	1	3289	G
46	1	3294	A
46	1	3295	A
46	1	3304	U
46	1	3313	U
46	1	3316	A
46	1	3318	G
46	1	3319	U
46	1	3320	A
46	1	3334	U
46	1	3341	U
46	1	3345	G
46	1	3351	U
46	1	3352	U
46	1	3353	G
46	1	3354	U
46	1	3355	U
46	1	3369	G
46	1	3375	A
46	1	3378	C
46	1	3386	G

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Mol	Chain	Res	Type
46	1	3389	U
46	1	3390	G
46	1	3396	U

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	C4	52	G
4	C3	85	G
46	1	13	A
46	1	239	G
46	1	282	G
46	1	637	C
46	1	715	A
46	1	763	G
46	1	916	G
46	1	1064	A
46	1	1097	G
46	1	1307	G
46	1	1348	U
46	1	1355	A
46	1	1562	C
46	1	1762	C
46	1	1815	U
46	1	1820	U
46	1	1950	U
46	1	1959	G
46	1	1983	G
46	1	2016	U
46	1	2086	A
46	1	2101	C
46	1	2112	U
46	1	2249	G
46	1	2495	C
46	1	2501	U
46	1	2537	U
46	1	2541	U
46	1	2547	A
46	1	3121	U
46	1	3154	C
46	1	3157	U
46	1	3218	A

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Mol	Chain	Res	Type
46	1	3228	C
46	1	3269	U
46	1	3275	U
46	1	3319	U
46	1	3350	C
46	1	3351	U

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 211 ligands modelled in this entry, 211 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

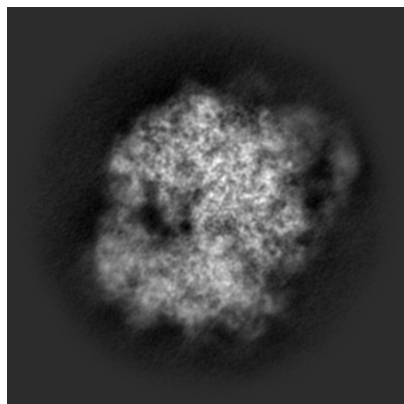
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16090. These allow visual inspection of the internal detail of the map and identification of artifacts.

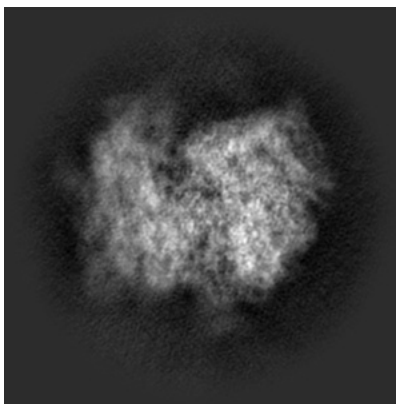
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

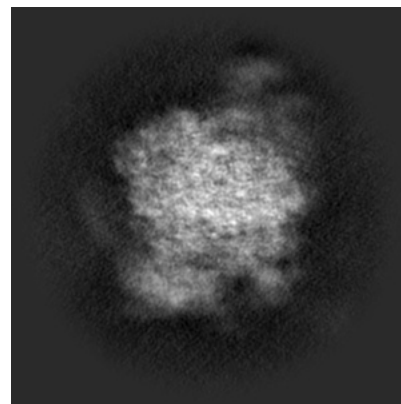
6.1.1 Primary map



X

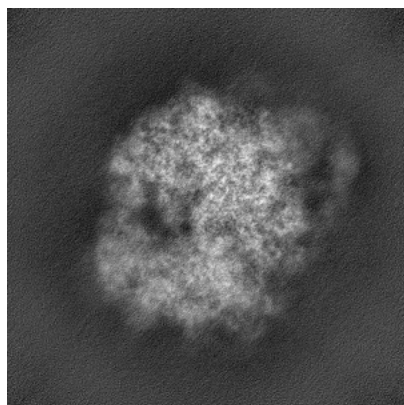


Y

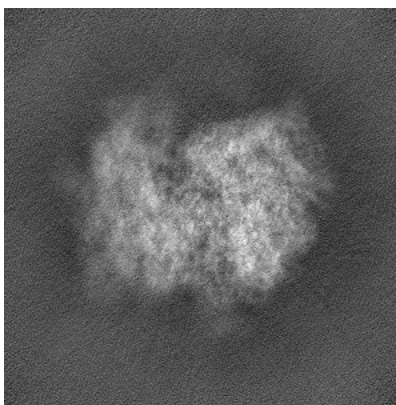


Z

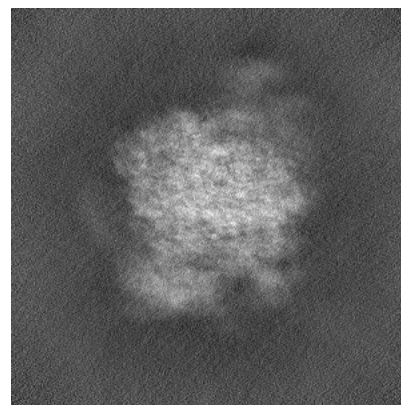
6.1.2 Raw map



X



Y

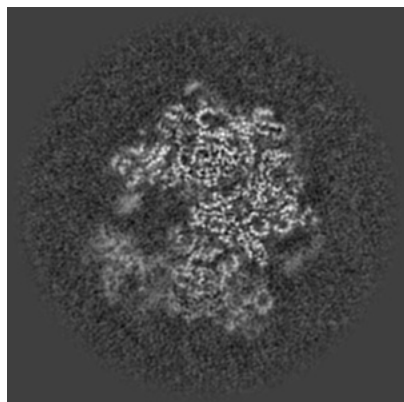


Z

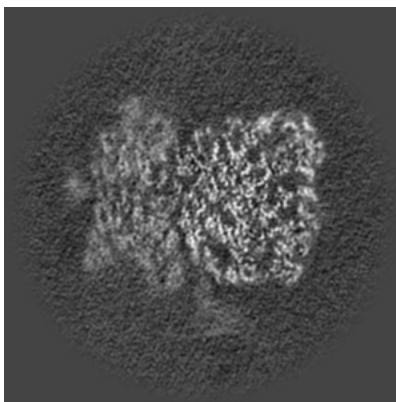
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

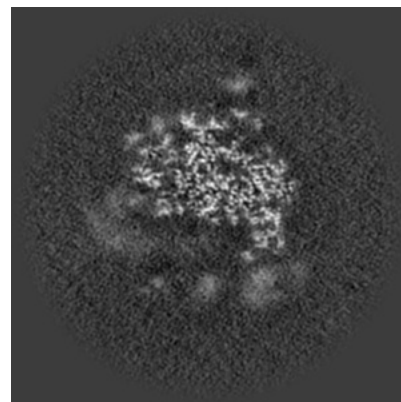
6.2.1 Primary map



X Index: 200

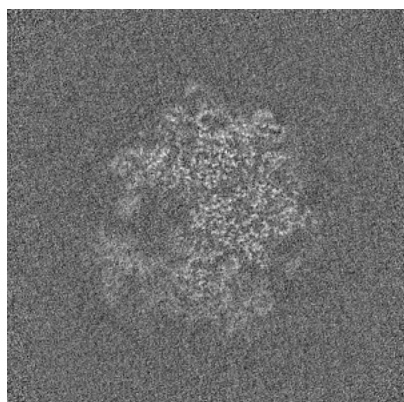


Y Index: 200

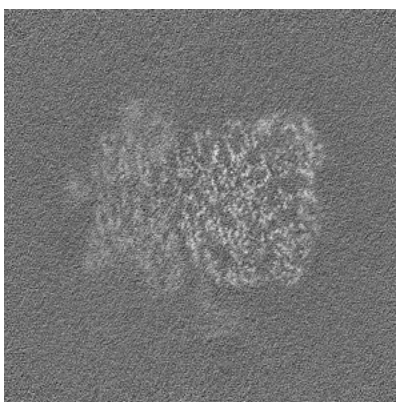


Z Index: 200

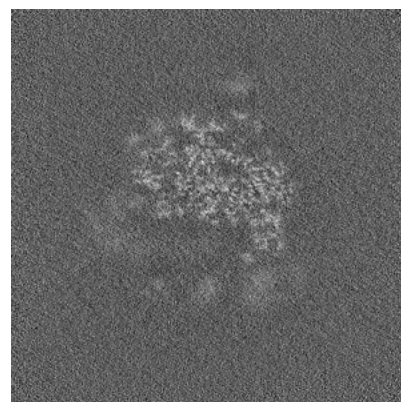
6.2.2 Raw map



X Index: 200



Y Index: 200

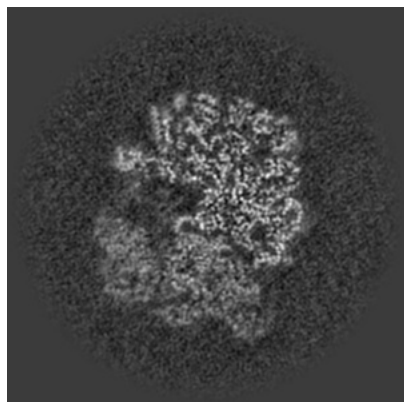


Z Index: 200

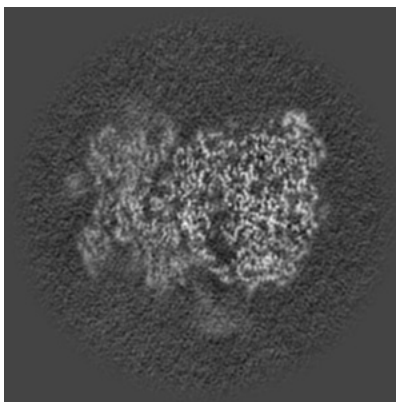
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

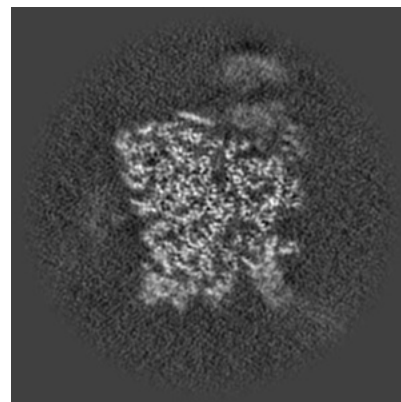
6.3.1 Primary map



X Index: 182

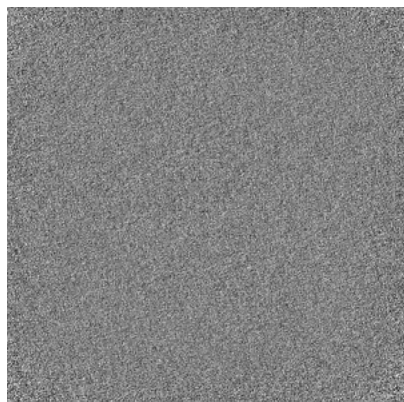


Y Index: 194

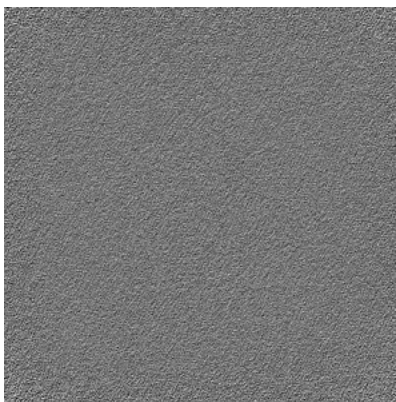


Z Index: 237

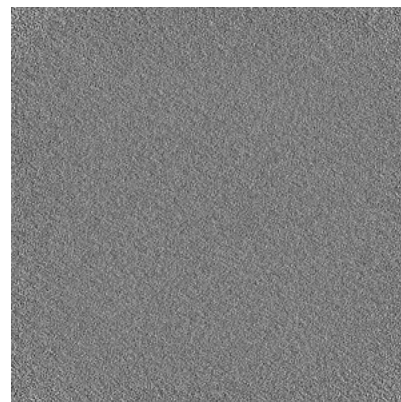
6.3.2 Raw map



X Index: 0



Y Index: 0

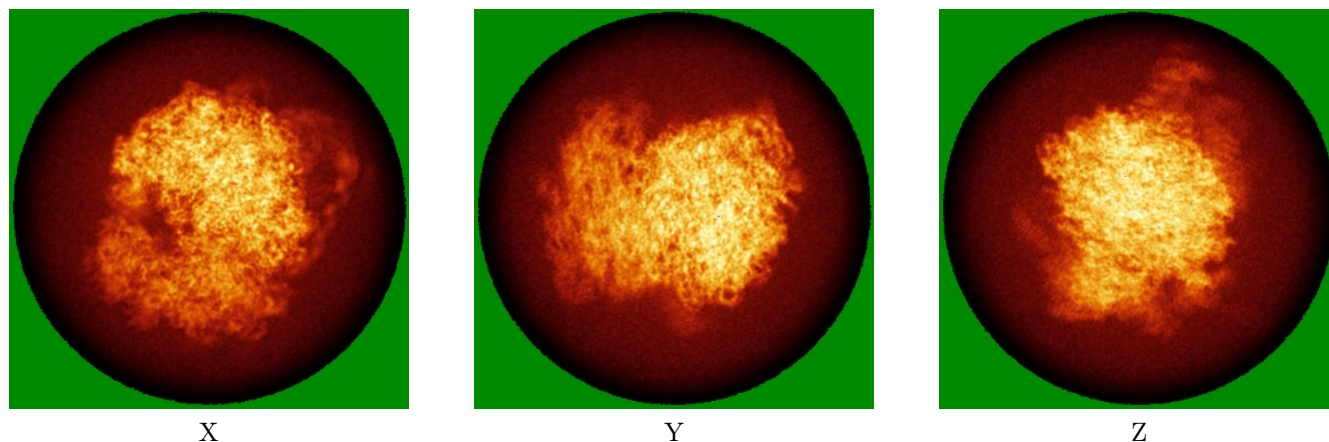


Z Index: 0

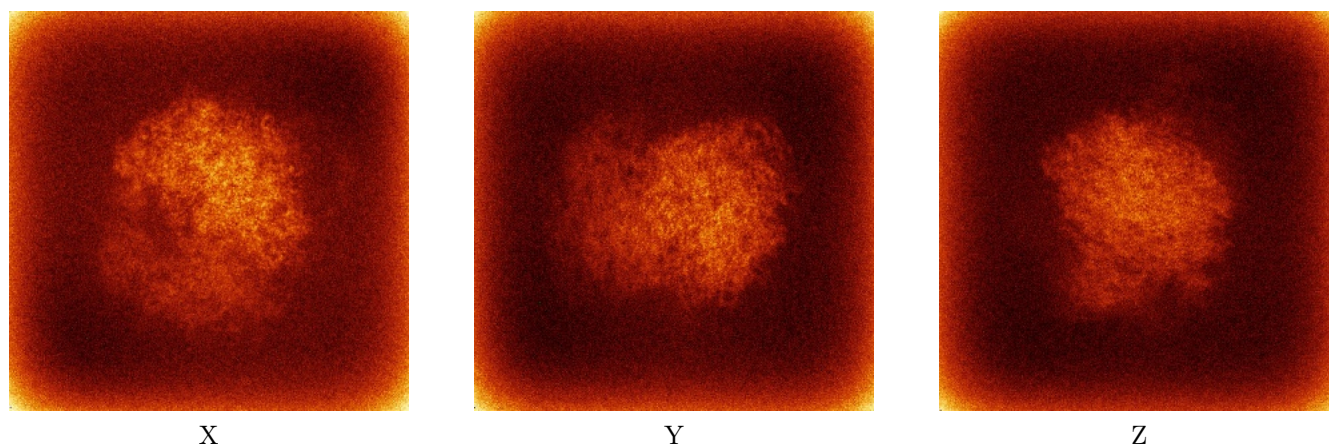
The images above show the largest variance slices of the map in three orthogonal directions.

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.

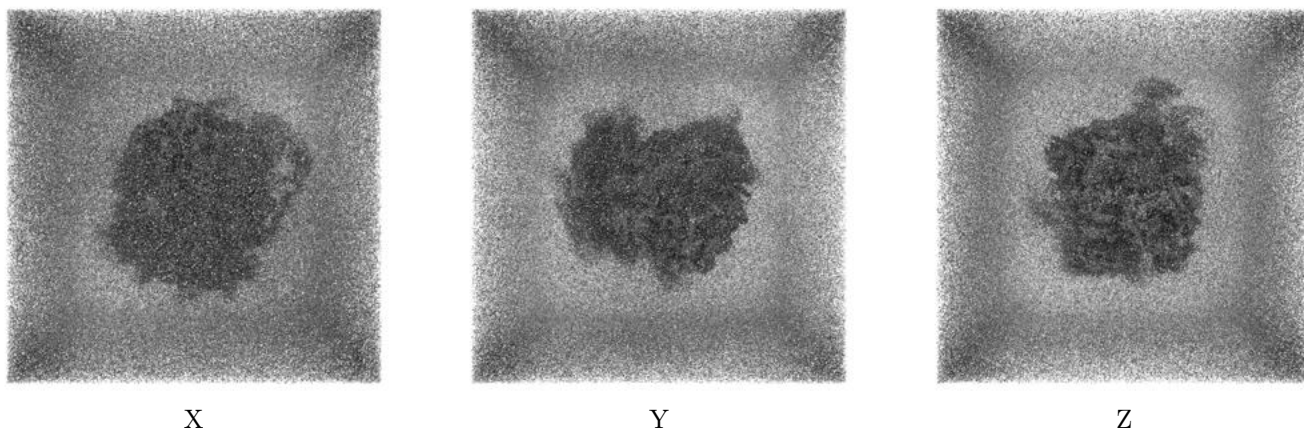
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

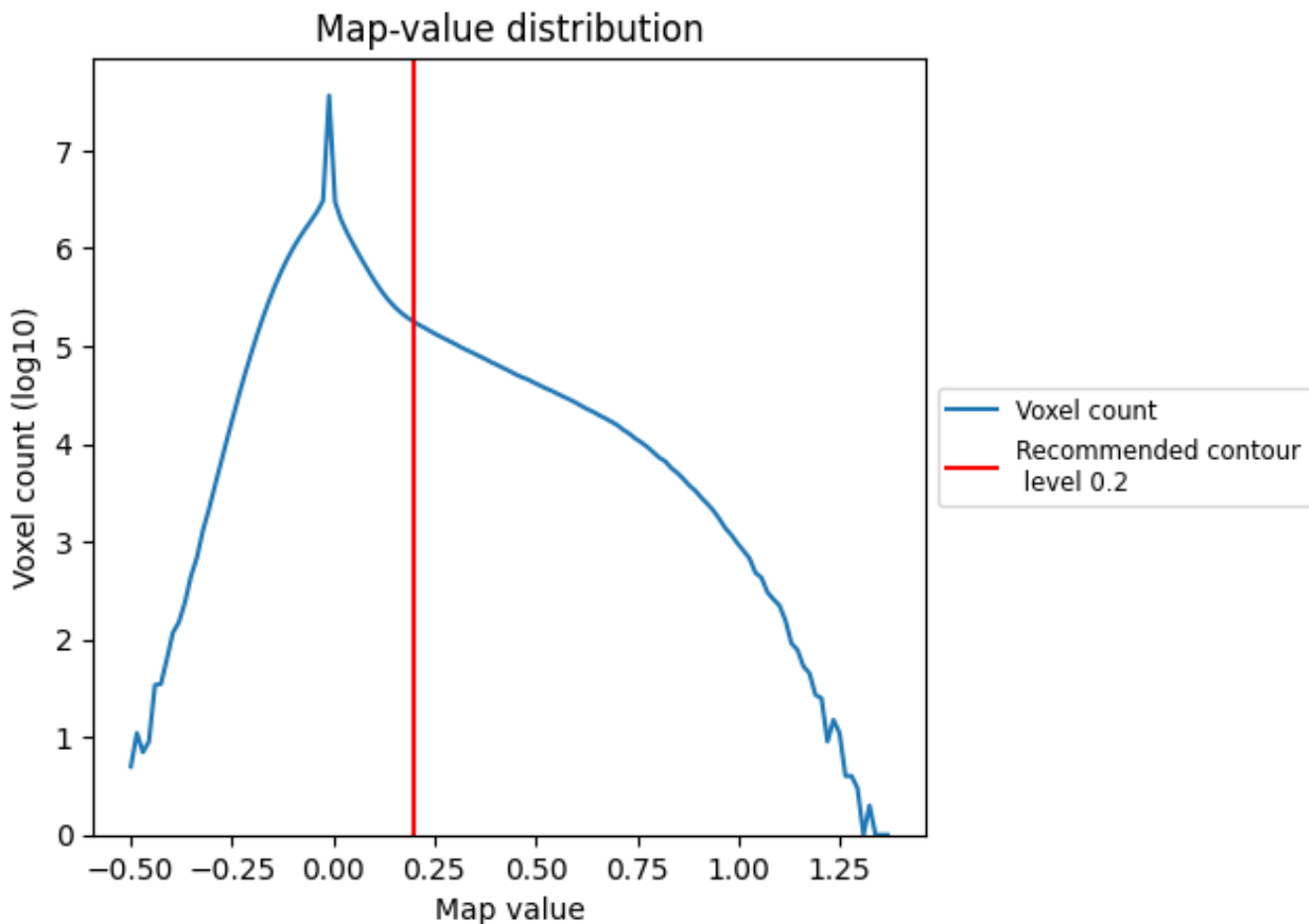
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

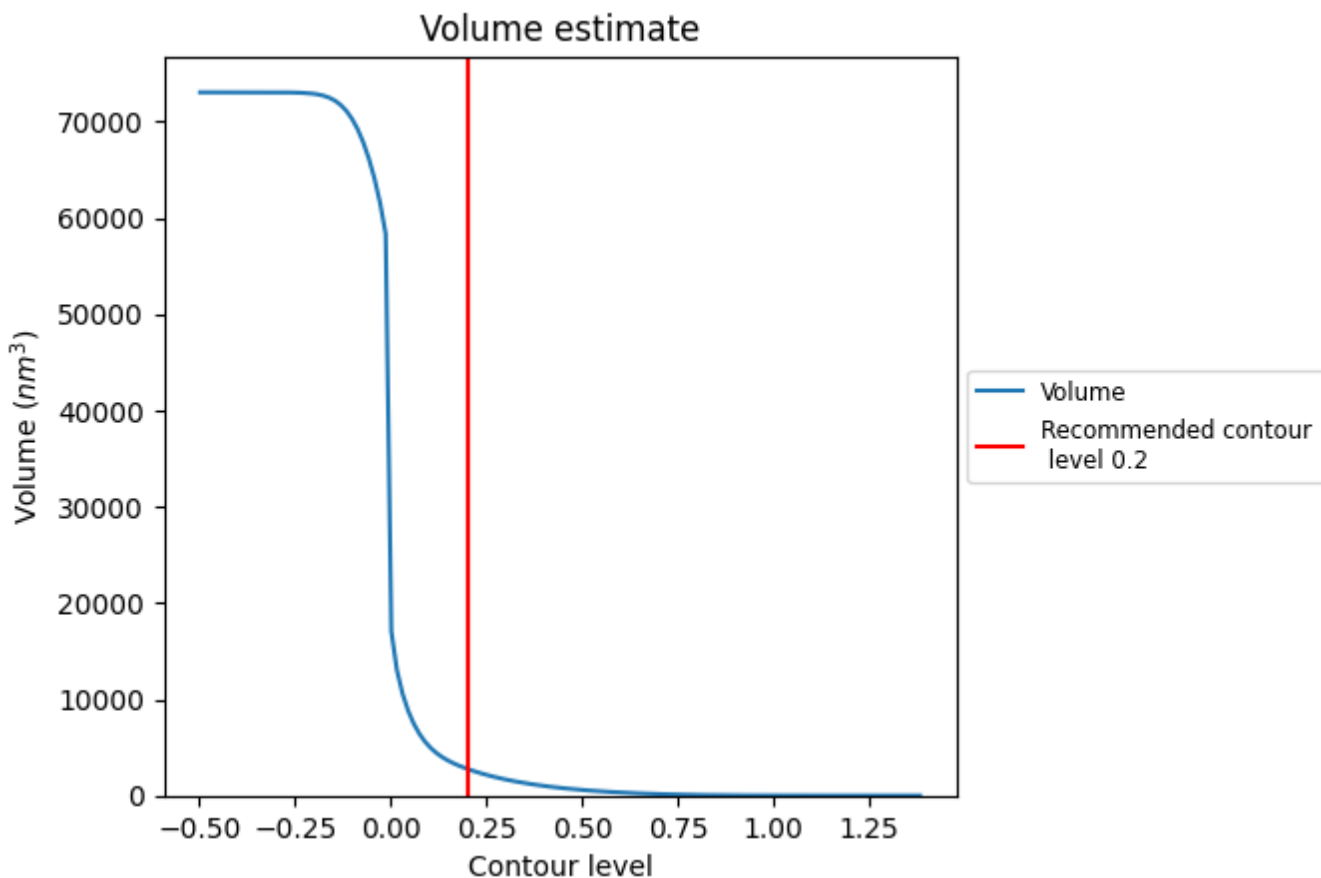
This section contains the results of statistical analysis of the map.

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.

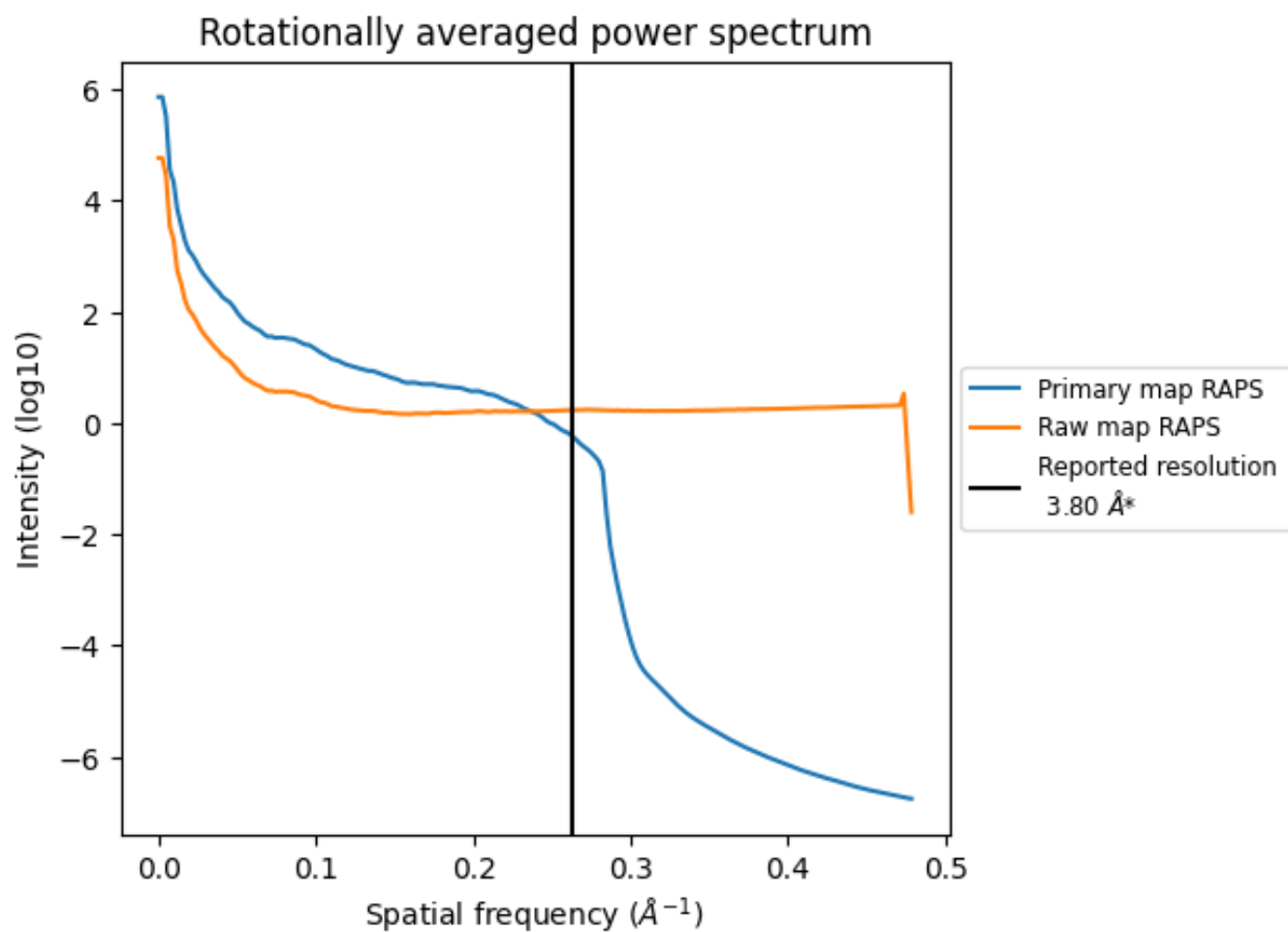
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2769 nm^3 ; this corresponds to an approximate mass of 2501 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

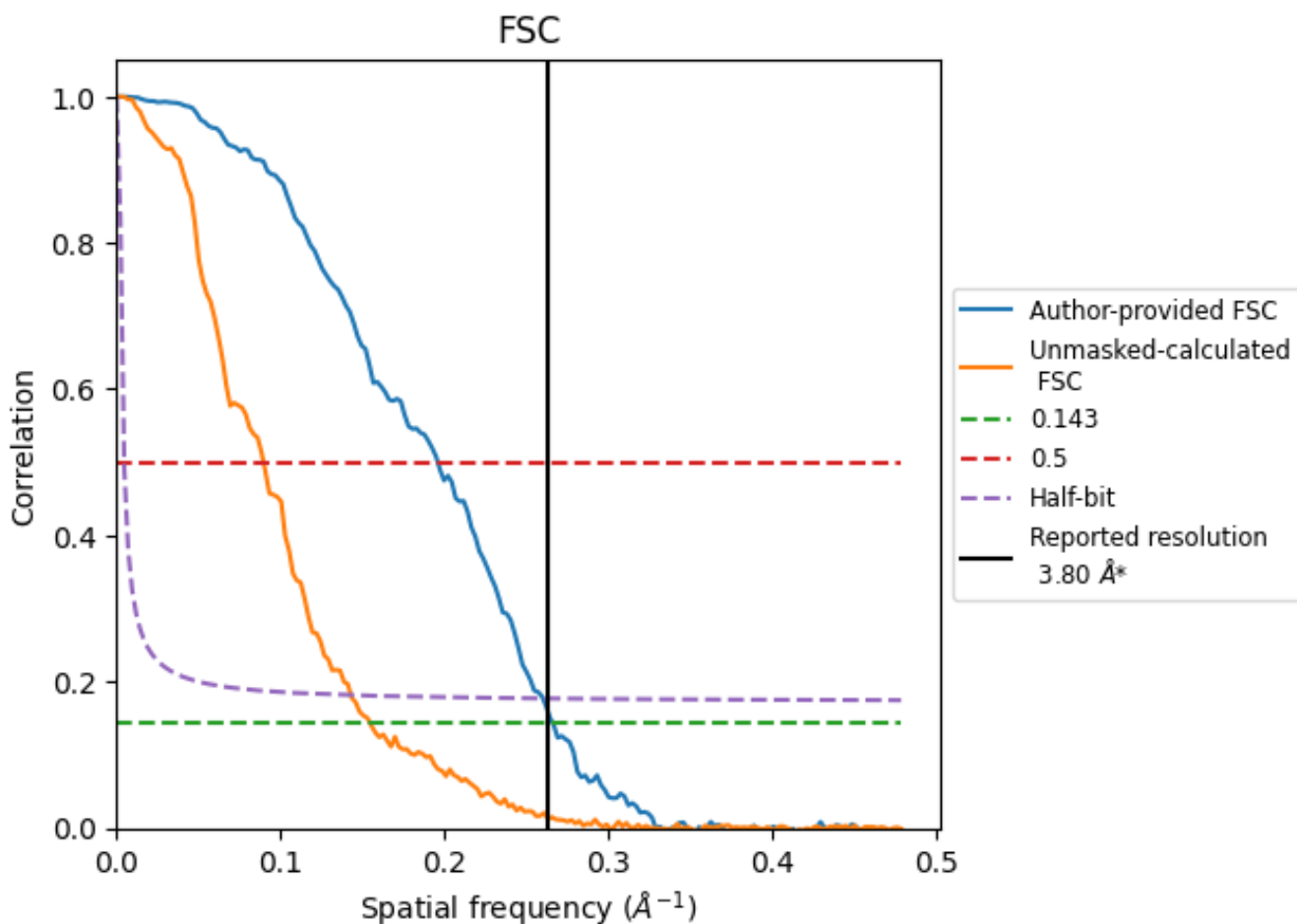


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

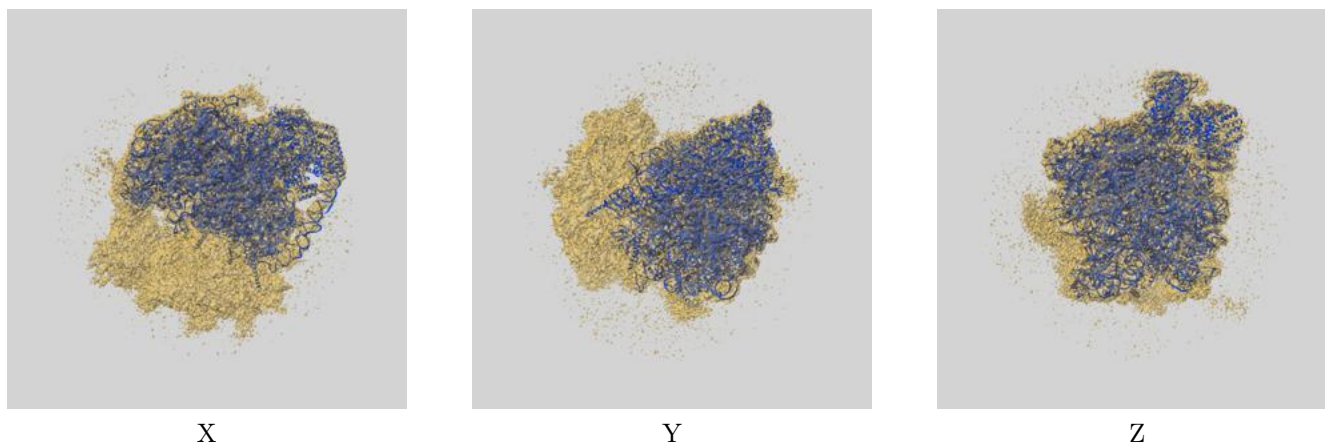
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.76	5.10	3.85
Unmasked-calculated*	6.46	11.15	6.99

*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 6.46 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

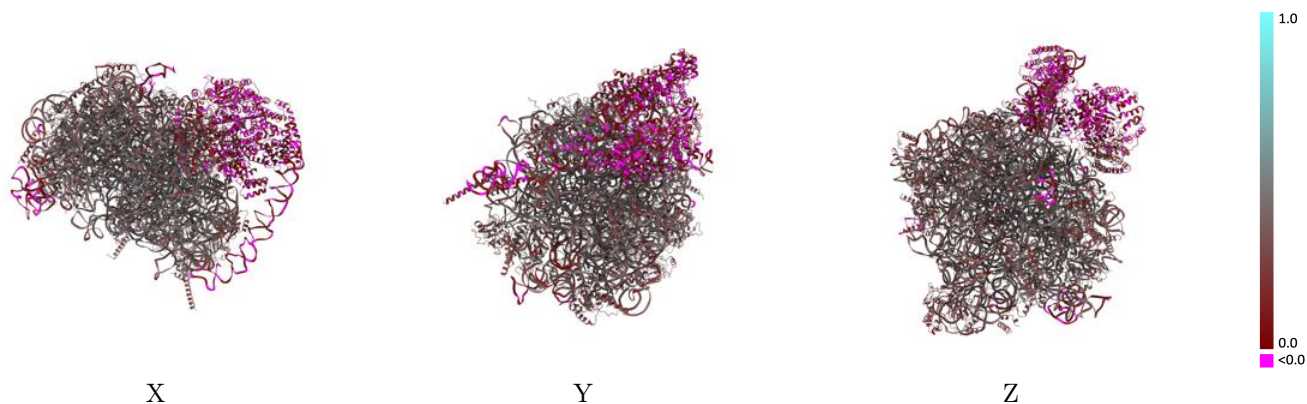
This section contains information regarding the fit between EMDB map EMD-16090 and PDB model 8BJQ. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



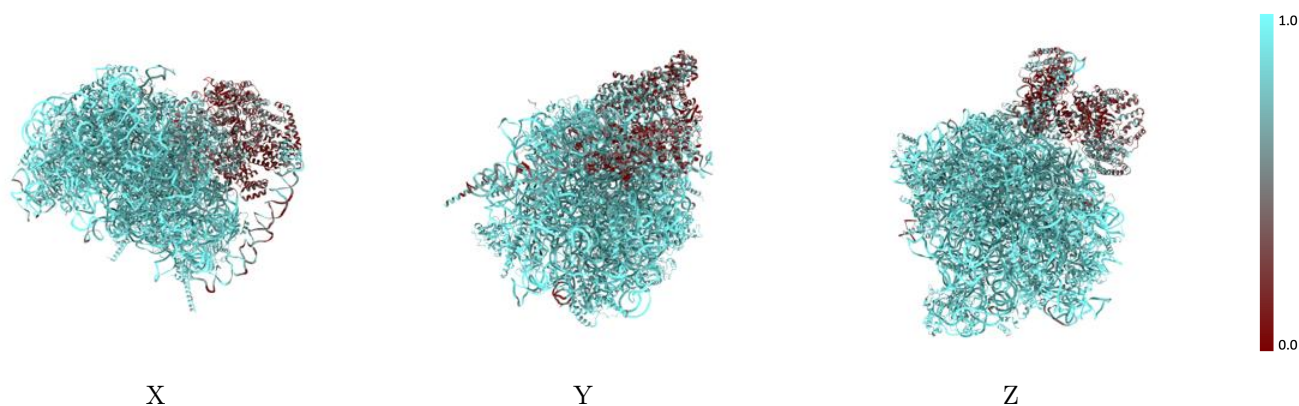
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



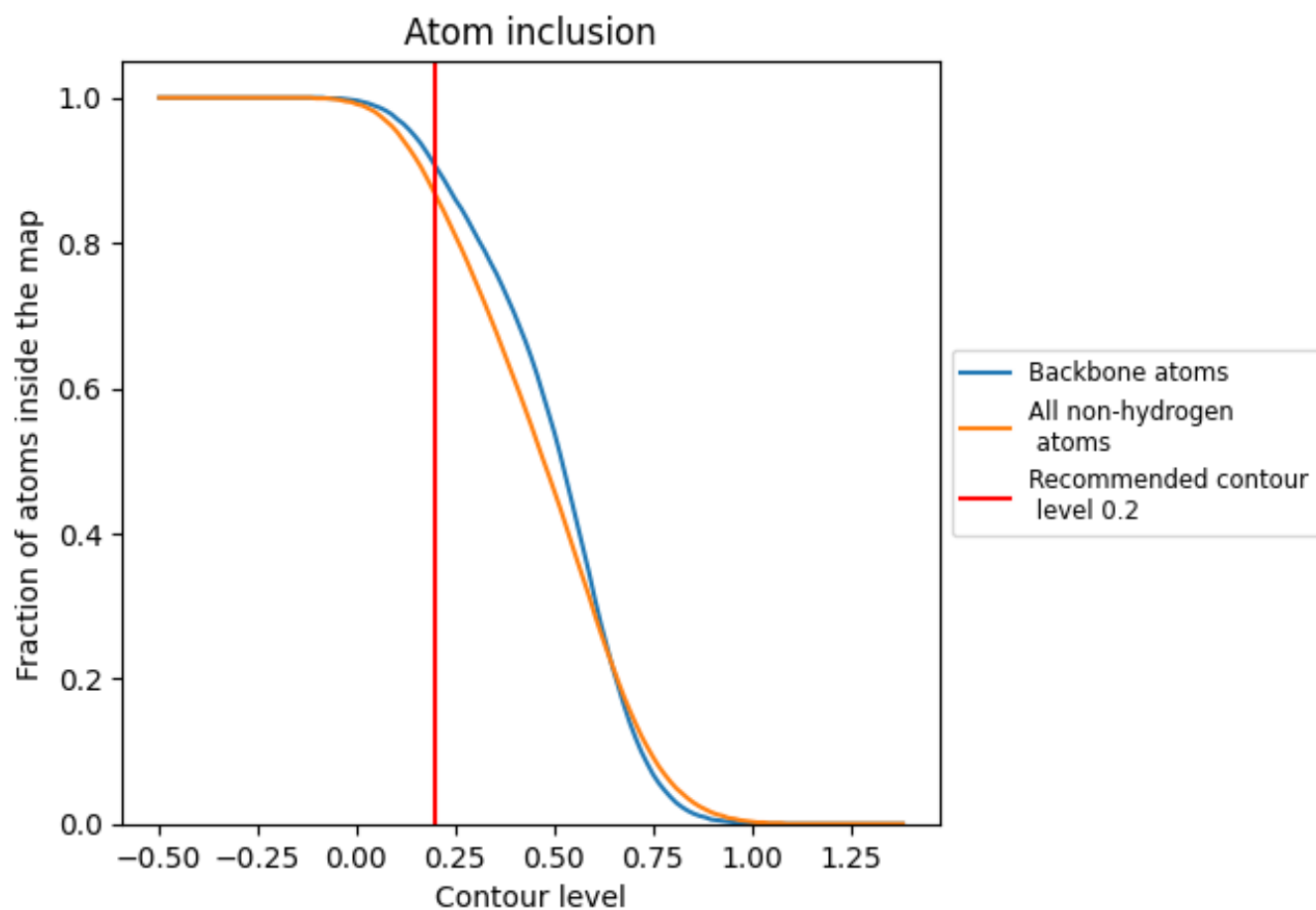
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 87% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8660	 0.3370
1	 0.9560	 0.3660
A	 0.1720	 0.0460
B	 0.4710	 0.1120
C	 0.1710	 0.0690
C3	 0.9890	 0.3810
C4	 0.9940	 0.3620
D	 0.3710	 0.0800
LA	 0.8480	 0.4090
LB	 0.9000	 0.4110
LC	 0.8880	 0.3830
LD	 0.8750	 0.2840
LE	 0.8540	 0.2940
LF	 0.8850	 0.3770
LG	 0.8540	 0.3350
LH	 0.8950	 0.3730
LI	 0.8570	 0.3560
LJ	 0.8060	 0.2790
LL	 0.8630	 0.3360
LM	 0.8920	 0.3610
LN	 0.8650	 0.3780
LO	 0.8940	 0.4090
LP	 0.8370	 0.3760
LQ	 0.8890	 0.3760
LR	 0.8480	 0.3690
LS	 0.8840	 0.3990
LT	 0.8800	 0.3910
LU	 0.8340	 0.3000
LV	 0.8140	 0.4190
LW	 0.8200	 0.3950
LX	 0.8710	 0.3860
LY	 0.8640	 0.3510
LZ	 0.8950	 0.3510
La	 0.8760	 0.3470
Lb	 0.8430	 0.3460



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Chain	Atom inclusion	Q-score
Lc	 0.8880	 0.3450
Ld	 0.8760	 0.4000
Le	 0.8780	 0.4100
Lf	 0.8990	 0.4200
Lg	 0.8770	 0.3860
Lh	 0.8810	 0.3370
Li	 0.8260	 0.3310
Lj	 0.9180	 0.4140
Lk	 0.8330	 0.3420
Ll	 0.8580	 0.3570
Lm	 0.8740	 0.3840
Ln	 0.8120	 0.3120
Lo	 0.8610	 0.3750
Lp	 0.8390	 0.3730