wwPDB EM Validation Summary 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)

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

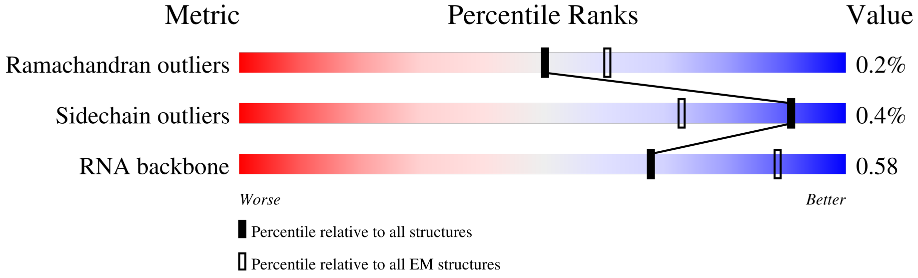
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance (i)

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

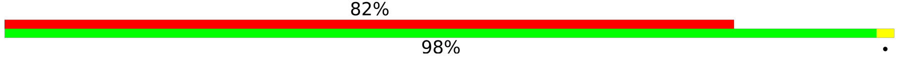
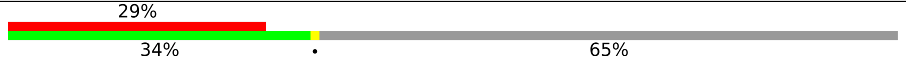
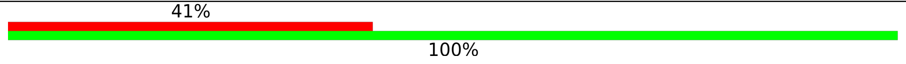
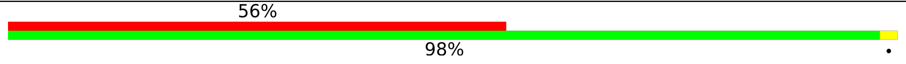
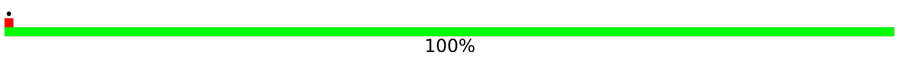
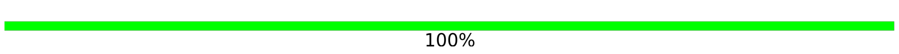
The reported resolution of this entry is 3.80 Å.

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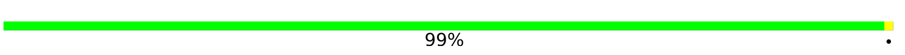
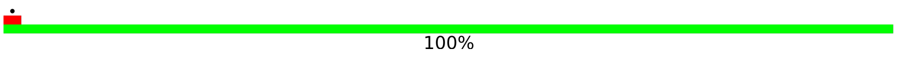
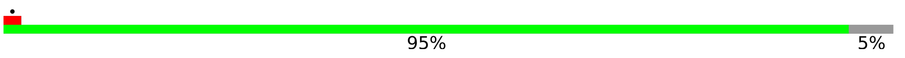
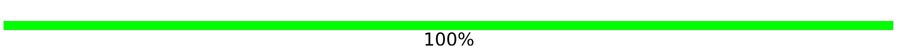
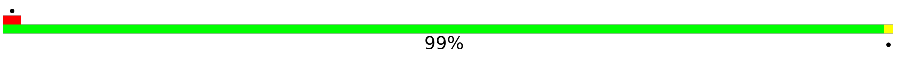
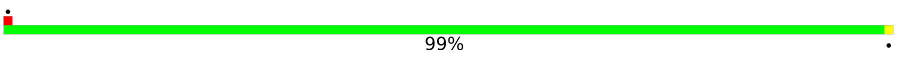
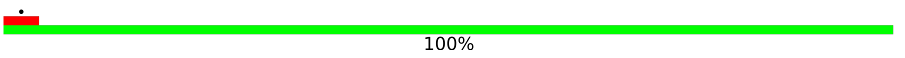
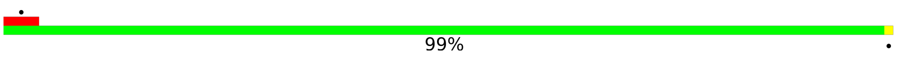
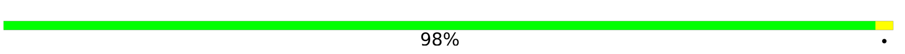
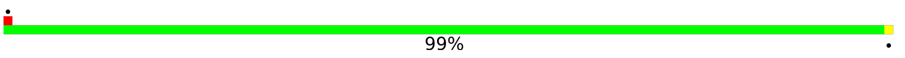
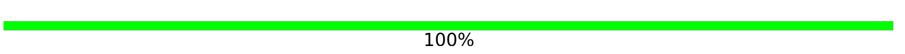
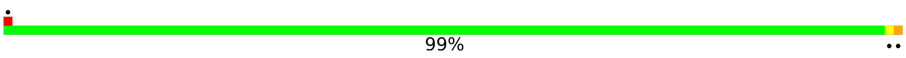
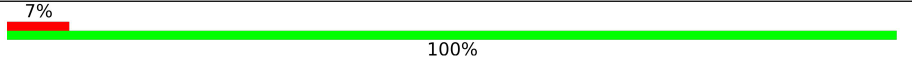
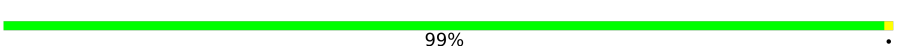
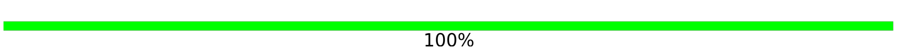
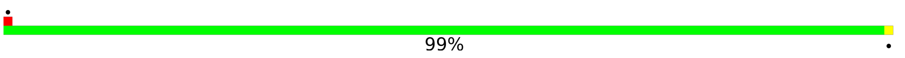
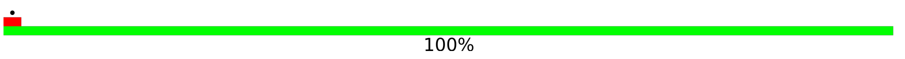
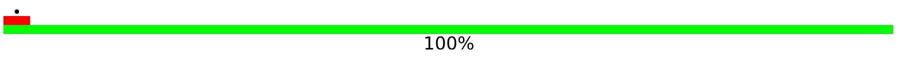
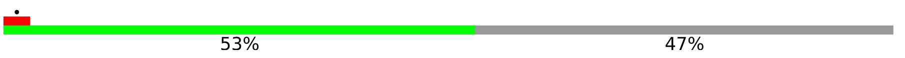
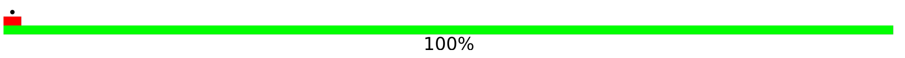
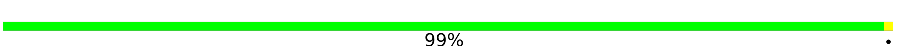
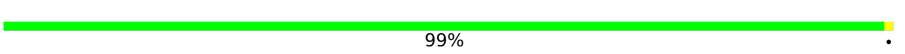
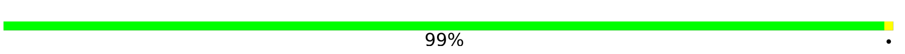
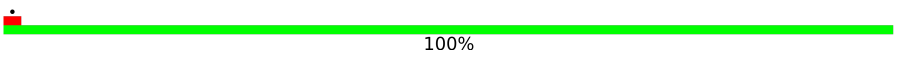
Mol	Chain	Length	Quality of chain
7	LC	361	
8	LD	294	
9	LE	175	
10	LF	222	
11	LG	233	
12	LH	191	
13	LI	218	
14	LJ	169	
15	LL	193	
16	LM	136	
17	LN	203	
18	LO	197	
19	LP	183	
20	LQ	185	
21	LR	188	
22	LS	171	
23	LT	159	
24	LU	100	
25	LV	136	
26	LW	126	
27	LX	121	
28	LY	125	
29	LZ	135	
30	La	148	
31	Lb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

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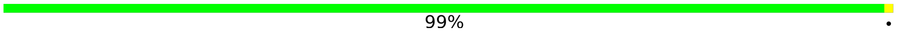
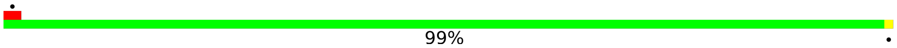
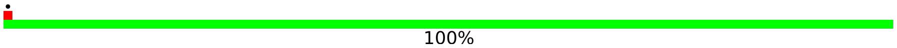
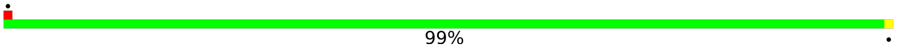
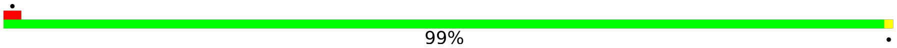
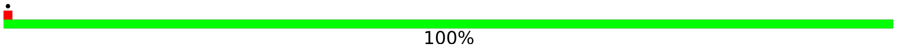
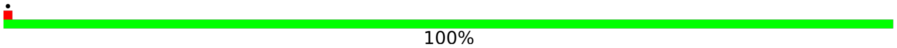
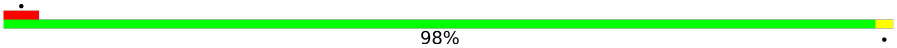
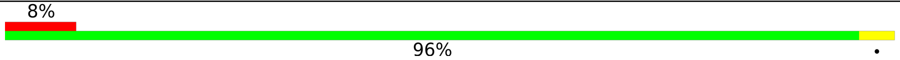
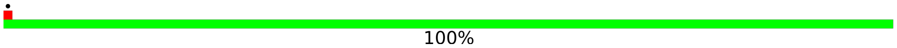
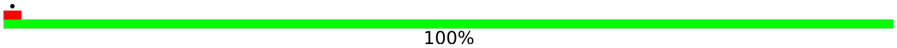
Mol	Chain	Length	Quality of chain
32	Lc	96	
33	Ld	109	
34	Le	127	
35	Lf	106	
36	Lg	112	
37	Lh	119	
38	Li	99	
39	Lj	85	
40	Lk	77	
41	Ll	50	
42	Lm	52	
43	Ln	25	
44	Lo	103	
45	Lp	91	
46	1	3395	

2 Entry composition ⓘ

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	1612	1030	273	297	12	0	0
			Total	C	N	O	S		
1	C	68	571	378	81	107	5	0	0

- 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	6536	4195	1080	1231	30	0	0
			Total	C	N	O	S		
2	D	796	6536	4195	1080	1231	30	0	0

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

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

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

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

- 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	1899	1182	385	331	1	0	0

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

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

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

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

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

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

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

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

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
10	LF	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LV	136	Total 1003	C 628	N 189	O 179	S 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
			Total	C	N	O	S		
32	Lc	96	737	476	123	137	1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

- 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	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
46	1	3301	Total C N O P 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 Mg 1 1	0
47	C3	1	Total Mg 1 1	0
47	LA	2	Total Mg 2 2	0
47	LB	1	Total Mg 1 1	0
47	LN	1	Total Mg 1 1	0
47	LP	1	Total Mg 1 1	0
47	LR	1	Total Mg 1 1	0
47	LV	1	Total Mg 1 1	0
47	La	1	Total Mg 1 1	0
47	Le	1	Total Mg 1 1	0
47	1	195	Total Mg 195 195	0

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

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

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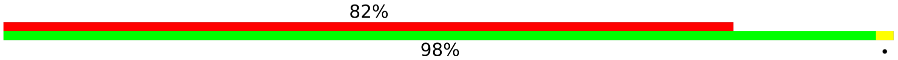
Mol	Chain	Residues	Atoms	AltConf
48	Lm	1	Total Zn 1 1	0
48	Lo	1	Total Zn 1 1	0
48	Lp	1	Total Zn 1 1	0

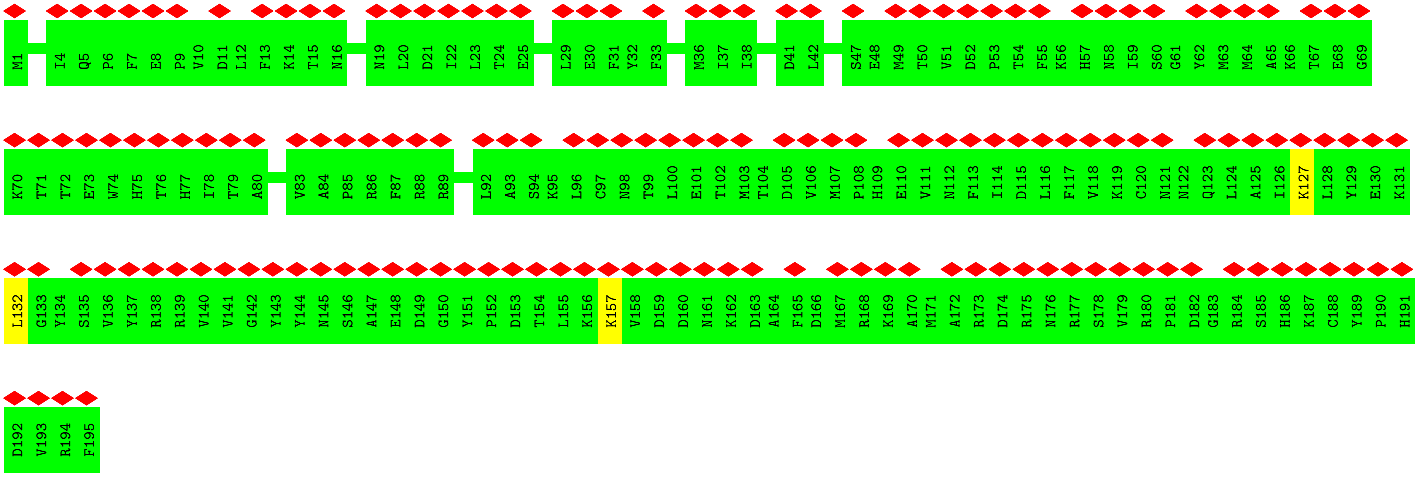
3 Residue-property plots ⓘ

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

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

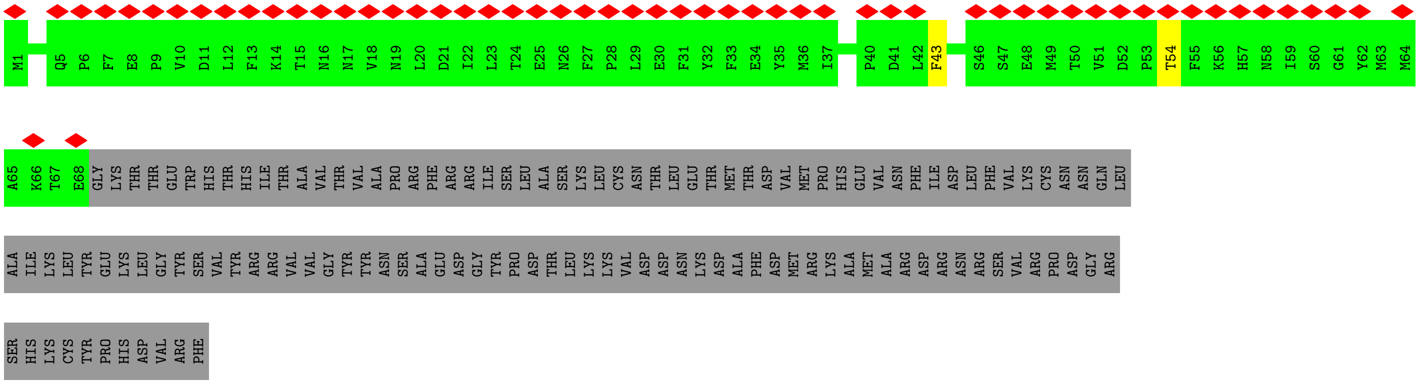
Chain A:





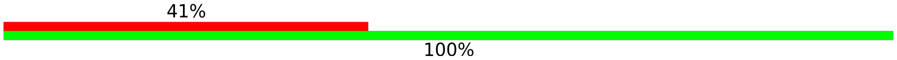
- Molecule 1: N-terminal acetyltransferase B complex catalytic subunit NAT3

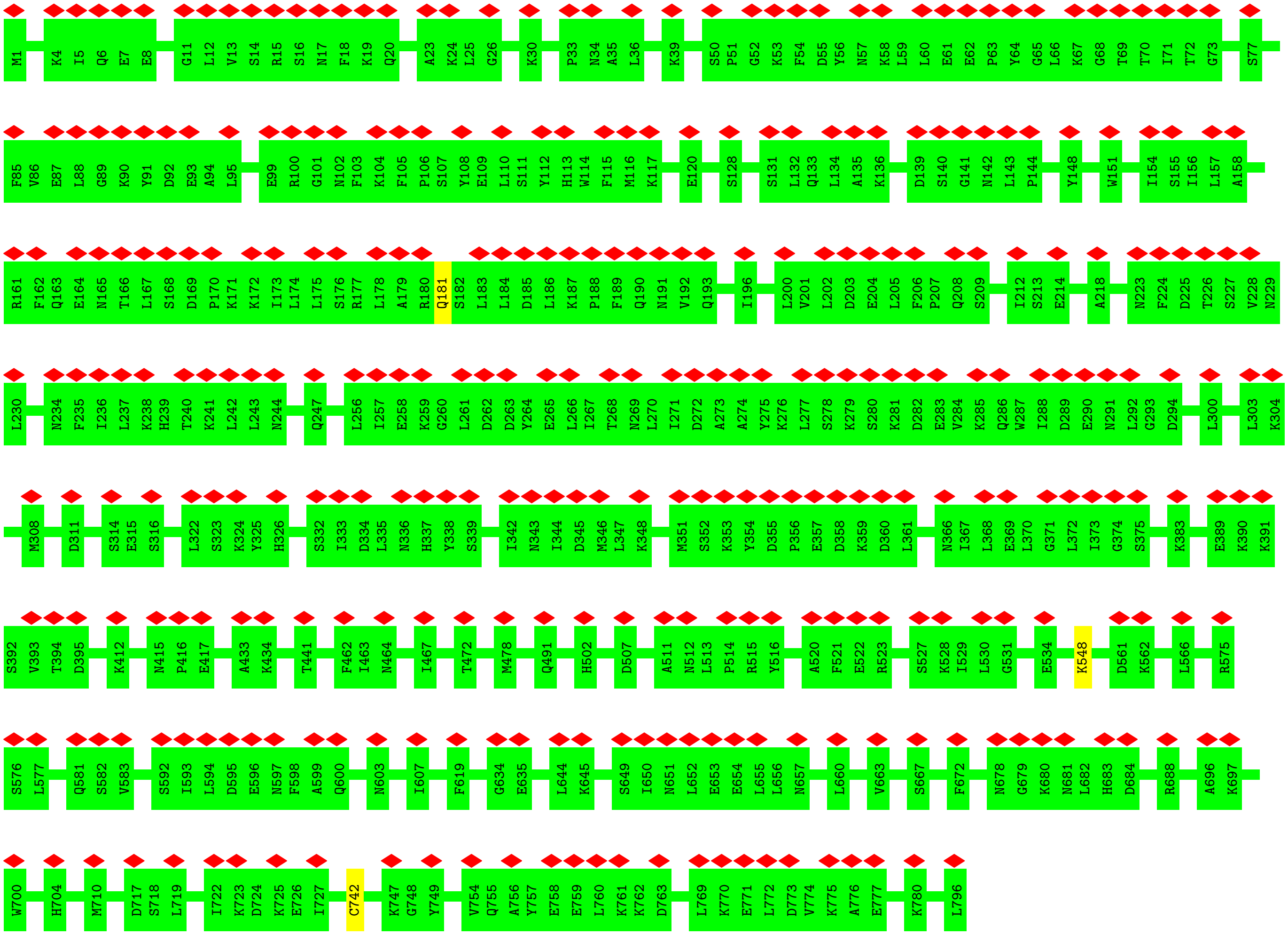
Chain C:



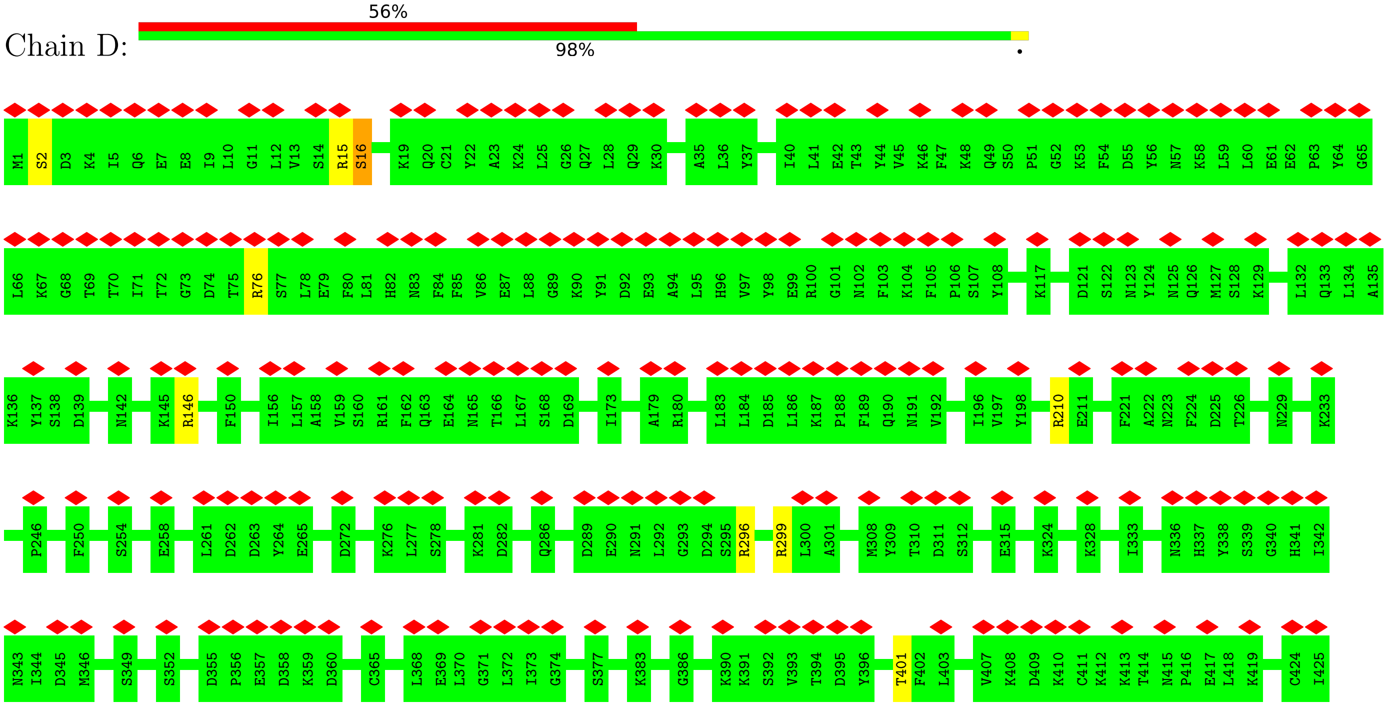
- Molecule 2: N-terminal acetyltransferase B complex subunit MDM20

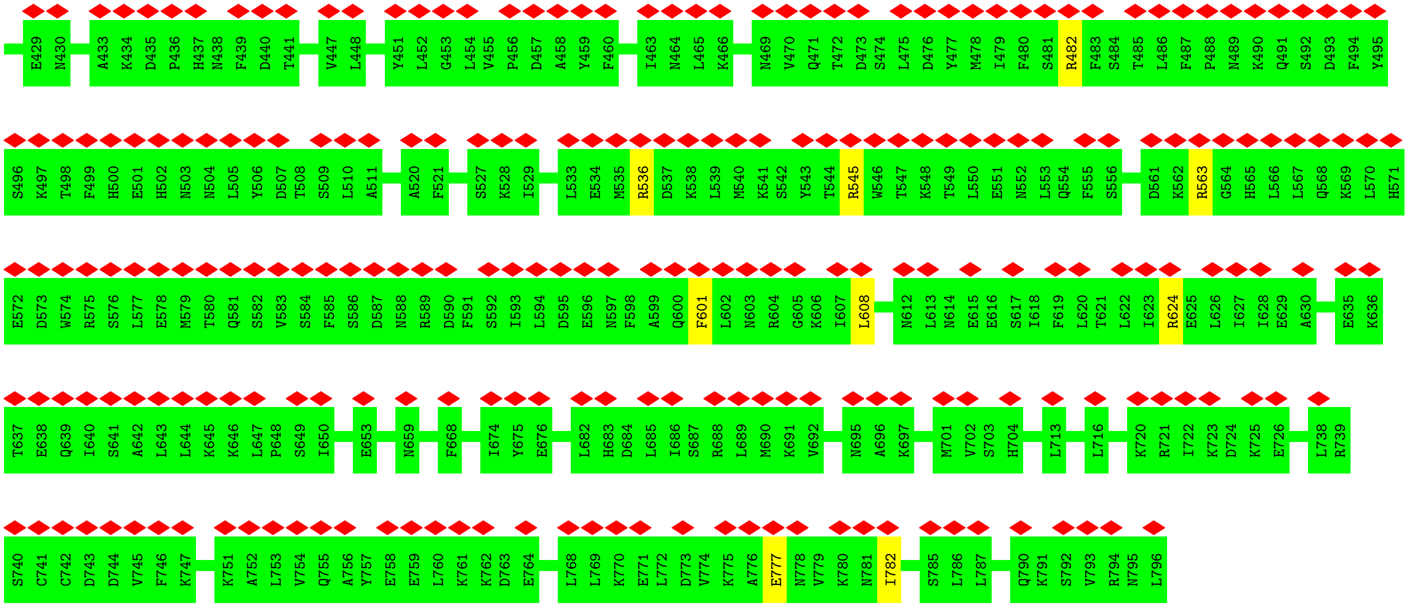
Chain B:





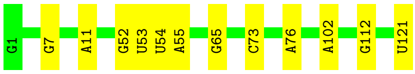
- Molecule 2: N-terminal acetyltransferase B complex subunit MDM20





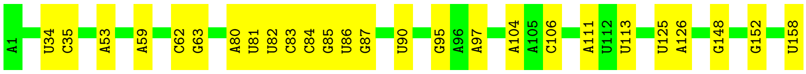
- Molecule 3: 5S rRNA

Chain C4:



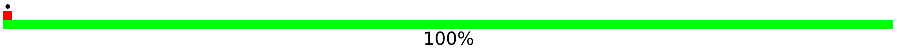
- Molecule 4: 5.8S rRNA

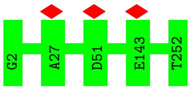
Chain C3:



- Molecule 5: 60S ribosomal protein L2-A

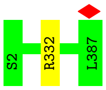
Chain LA:





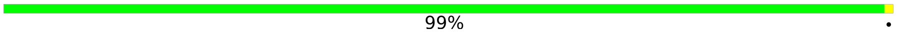
- Molecule 6: 60S ribosomal protein L3

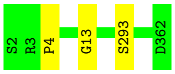
Chain LB:



- Molecule 7: 60S ribosomal protein L4-A

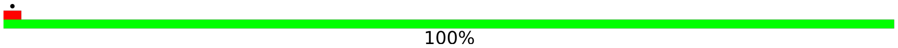
Chain LC:

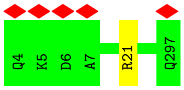




- Molecule 8: 60S ribosomal protein L5

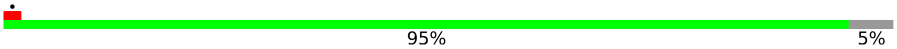
Chain LD:

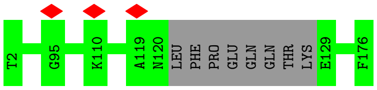




- Molecule 9: 60S ribosomal protein L6-B

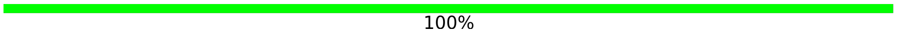
Chain LE:





- Molecule 10: 60S ribosomal protein L7-A

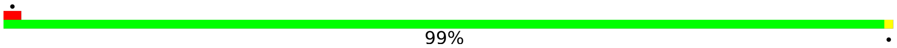
Chain LF:

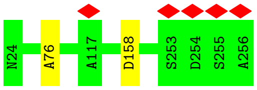


There are no outlier residues recorded for this chain.

- Molecule 11: 60S ribosomal protein L8-A

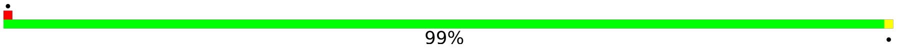
Chain LG:

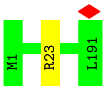




- Molecule 12: 60S ribosomal protein L9-A

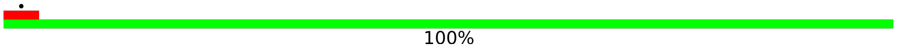
Chain LH:

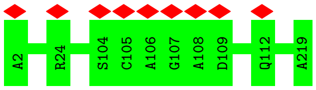




- Molecule 13: 60S ribosomal protein L10

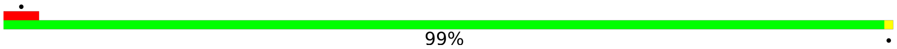
Chain LI:

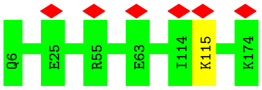




- Molecule 14: 60S ribosomal protein L11-B

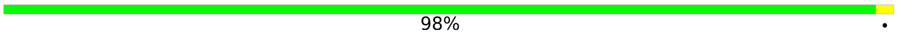
Chain LJ:





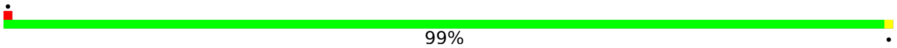
- Molecule 15: 60S ribosomal protein L13-A

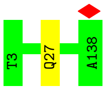
Chain LL:



- Molecule 16: 60S ribosomal protein L14-A

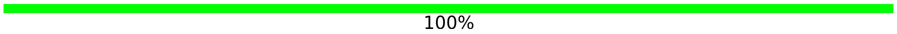
Chain LM:

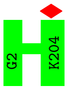




- Molecule 17: 60S ribosomal protein L15-A

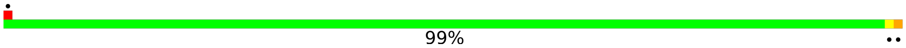
Chain LN:

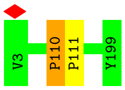




- Molecule 18: 60S ribosomal protein L16-A

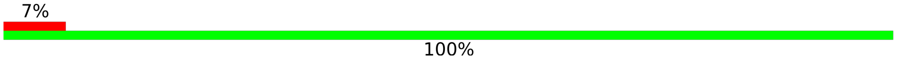
Chain LO:

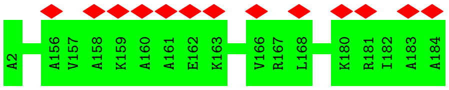




- Molecule 19: 60S ribosomal protein L17-A

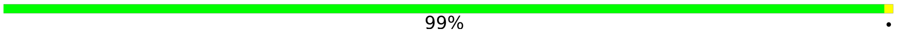
Chain LP:

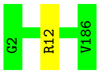




- Molecule 20: 60S ribosomal protein L18-A

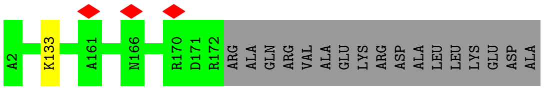
Chain LQ:





- Molecule 21: 60S ribosomal protein L19-A

Chain LR:



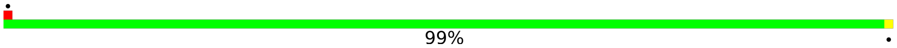
- Molecule 22: 60S ribosomal protein L20-A

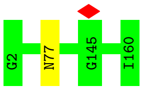
Chain LS:

There are no outlier residues recorded for this chain.

- Molecule 23: 60S ribosomal protein L21-A

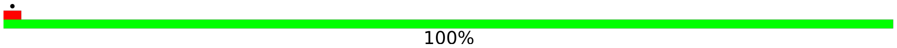
Chain LT:

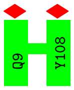




- Molecule 24: 60S ribosomal protein L22-A

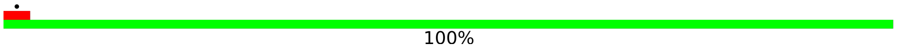
Chain LU:

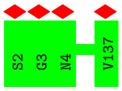




- Molecule 25: 60S ribosomal protein L23-A

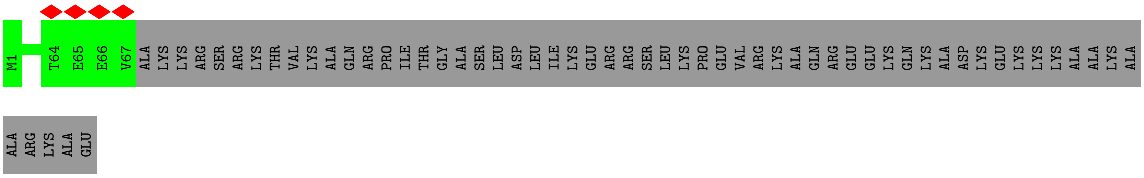
Chain LV:





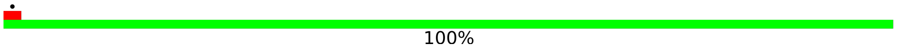
- Molecule 26: 60S ribosomal protein L24-A

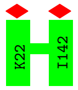
Chain LW:



- Molecule 27: 60S ribosomal protein L25

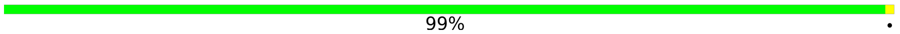
Chain LX:

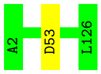




- Molecule 28: 60S ribosomal protein L26-A

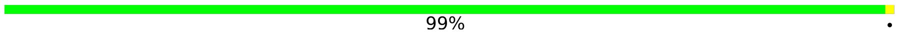
Chain LY:

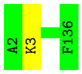




- Molecule 29: 60S ribosomal protein L27-A

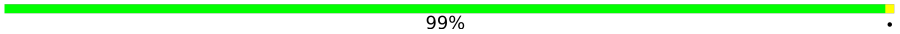
Chain LZ:

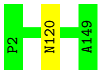




- Molecule 30: 60S ribosomal protein L28

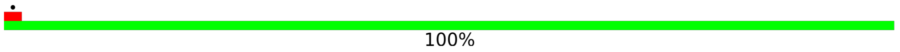
Chain La:

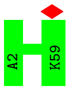




- Molecule 31: 60S ribosomal protein L29

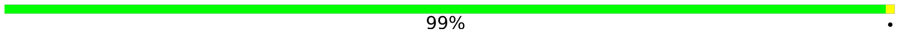
Chain Lb:

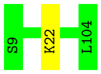




- Molecule 32: 60S ribosomal protein L30

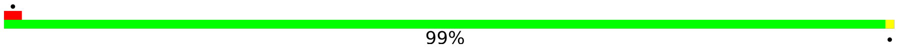
Chain Lc:

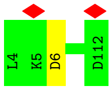




- Molecule 33: 60S ribosomal protein L31-A

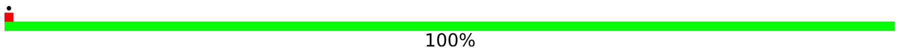
Chain Ld:

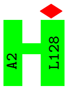




- Molecule 34: 60S ribosomal protein L32

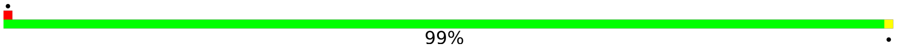
Chain Le:

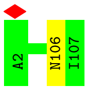




- Molecule 35: 60S ribosomal protein L33-A

Chain Lf:





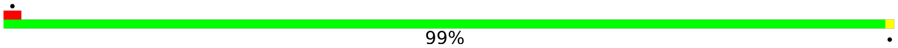
- Molecule 36: 60S ribosomal protein L34-A

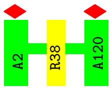
Chain Lg:

There are no outlier residues recorded for this chain.

- Molecule 37: 60S ribosomal protein L35-A

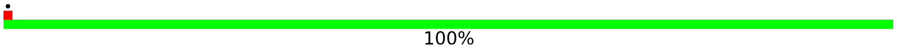
Chain Lh:

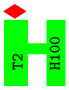




- Molecule 38: 60S ribosomal protein L36-A

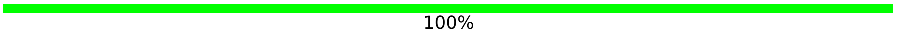
Chain Li:





- Molecule 39: 60S ribosomal protein L37-A

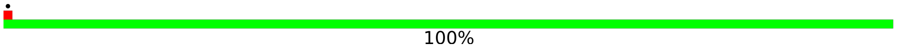
Chain Lj:

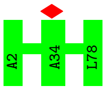


There are no outlier residues recorded for this chain.

- Molecule 40: 60S ribosomal protein L38

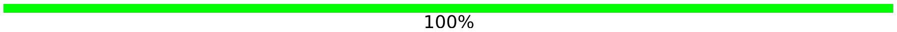
Chain Lk:





- Molecule 41: 60S ribosomal protein L39

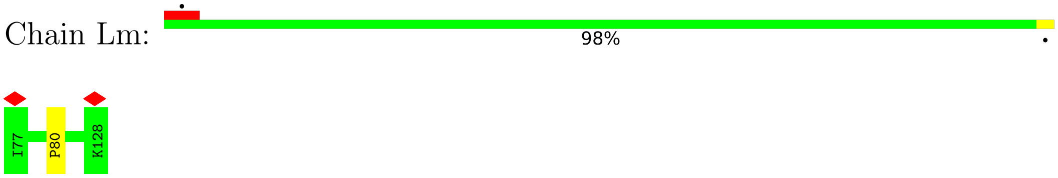
Chain Ll:



There are no outlier residues recorded for this chain.

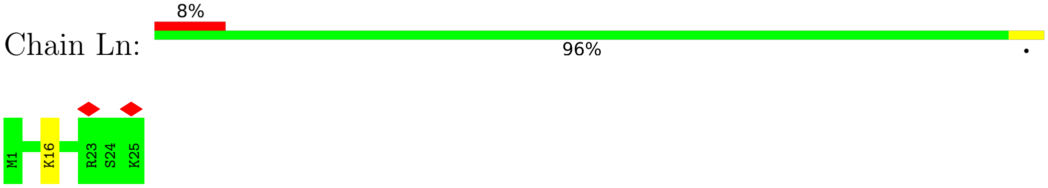
- Molecule 42: 60S ribosomal protein L40-A

Chain Lm:



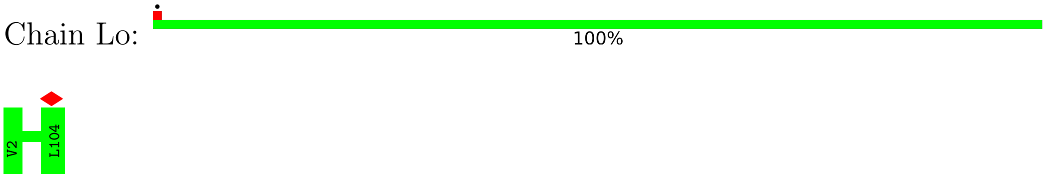
- Molecule 43: 60S ribosomal protein L41-A

Chain Ln:



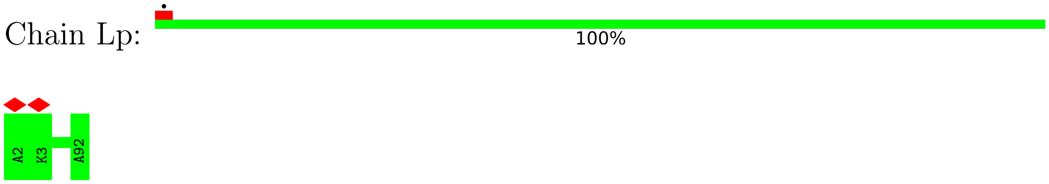
- Molecule 44: 60S ribosomal protein L42-A

Chain Lo:



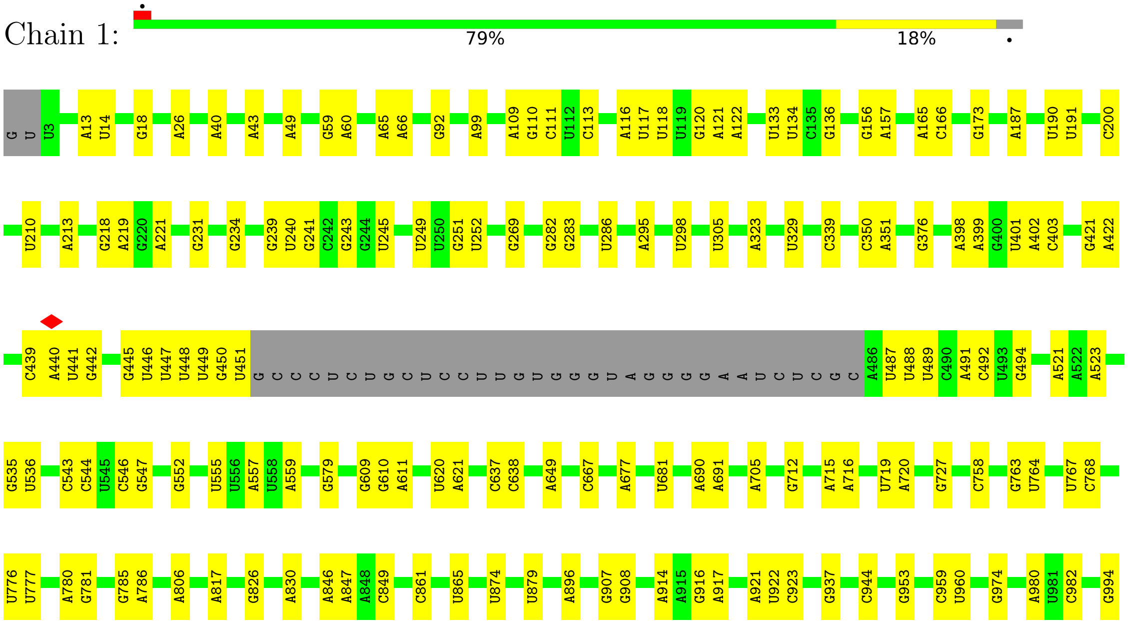
- Molecule 45: 60S ribosomal protein L43-A

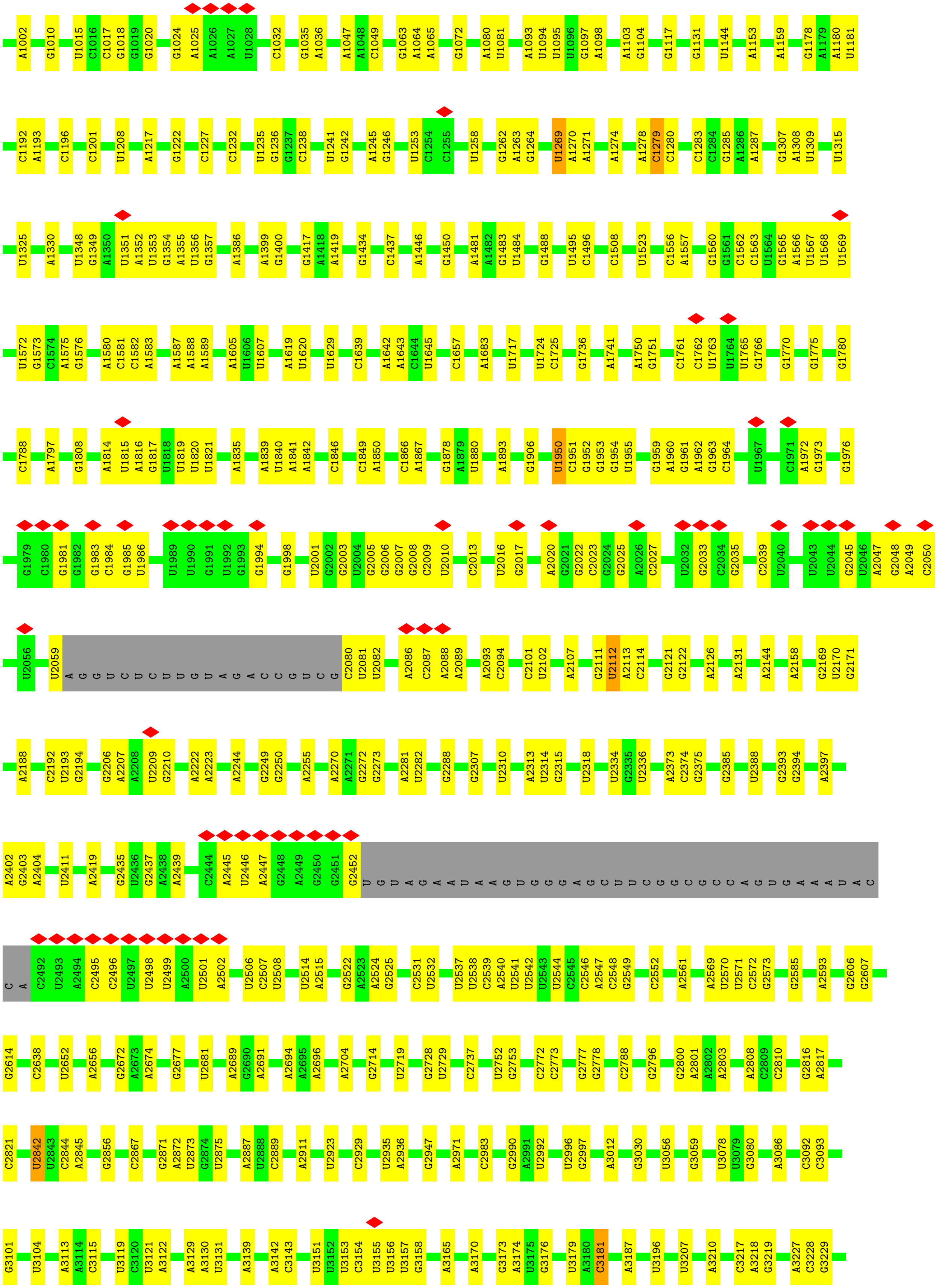
Chain Lp:

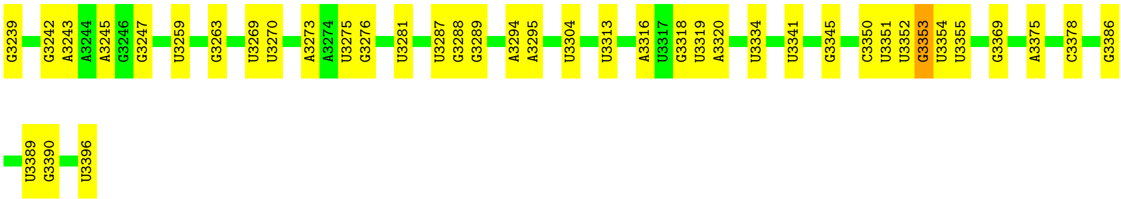


- Molecule 46: 25S rRNA

Chain 1:




A1002 G1010 U1015 C1016 C1017 G1018 G1019 G1020 G1024 A1025 A1026 A1027 U1028 C1032 G1035 A1036 A1047 A1048 C1049 G1063 A1064 A1065 G1072 A1080 U1081 A1093 U1094 U1095 U1096 G1097 A1098 A1103 G1104 G1117 G1131 U1144 A1153 A1159 G1178 A1179 A1180 U1181
C1192 A1193 C1196 C1201 U1208 A1217 G1222 C1227 C1232 U1235 G1236 G1237 C1238 U1241 G1242 A1245 G1246 U1253 C1254 C1255 U1258 G1262 A1263 G1264 U1269 A1270 A1271 A1274 A1278 C1279 C1280 C1283 C1284 G1285 A1286 A1287 G1307 A1308 U1309 U1315
U1325 A1330 U1348 G1349 A1350 U1351 A1352 U1353 G1354 A1355 U1356 G1357 A1386 A1399 G1400 G1417 A1418 A1419 G1434 C1437 A1446 G1450 A1481 A1482 G1483 U1484 G1488 U1495 C1496 C1508 U1523 C1556 A1557 G1560 G1561 C1562 C1563 U1564 G1565 A1566 U1567 U1568 U1569
U1572 G1573 C1574 A1575 G1576 A1580 C1581 C1582 A1583 A1587 A1588 A1589 A1605 U1606 U1607 A1619 U1620 U1629 C1639 A1642 A1643 C1644 U1645 C1657 A1683 U1717 U1724 C1725 G1736 A1741 A1750 G1751 C1761 C1762 U1763 U1764 U1765 G1766 G1770 G1775 G1780
C1788 A1797 G1808 A1814 U1815 A1816 G1817 U1818 U1819 U1820 U1821 A1835 A1839 U1840 A1841 A1842 C1846 C1849 A1850 C1866 A1867 G1878 A1879 U1880 A1893 G1906 U1950 C1951 G1952 G1953 G1954 U1955 G1959 A1960 G1961 A1962 G1963 C1964 U1967 C1971 A1972 G1973 G1976
G1979 C1980 G1981 G1982 G1983 C1984 G1985 U1986 U1989 U1990 G1991 U1992 G1993 G1994 G1998 U2001 G2002 G2003 U2004 G2005 G2006 G2007 G2008 C2009 U2010 C2013 U2016 G2017 A2020 G2021 G2022 C2023 G2024 G2025 A2026 C2027 U2032 G2033 C2034 G2035 C2039 U2040 U2043 U2044 G2045 U2046 A2047 G2048 A2049 C2050
U2056 U2059 A G G U C U C U U G U A G A C C G U C G C2080 U2081 U2082 A2086 C2087 A2088 A2089 A2093 C2094 C2101 U2102 A2107 G2111 U2112 A2113 C2114 G2121 G2122 A2126 A2131 A2144 A2158 G2169 U2170 G2171
A2188 C2192 U2193 G2194 G2206 A2207 A2208 U2209 G2210 A2222 A2223 A2244 G2249 G2250 A2255 A2270 A2271 G2272 G2273 A2281 U2282 G2288 G2307 U2310 A2313 U2314 G2315 U2318 U2334 G2335 U2336 A2373 C2374 G2375 G2385 U2388 G2393 G2394 A2397
A2402 G2403 A2404 U2411 A2419 G2435 U2436 G2437 A2438 A2439 C2444 A2445 U2446 A2447 G2448 A2449 G2450 G2451 G2452 U G U A G A A U A A G U G G G A G C U U C G G C G C C A G U G A A U A C
C A C2492 U2493 A2494 C2495 G2496 U2497 U2498 U2499 A2500 U2501 A2502 U2506 C2507 U2508 U2514 A2515 G2522 A2523 A2524 G2525 C2531 U2532 U2537 U2538 C2539 A2540 G2541 U2542 U2543 U2544 C2545 C2546 A2547 C2548 G2549 C2552 A2561 A2569 U2570 U2571 C2572 G2573 G2585 A2593 G2606 G2607
G2614 C2638 U2652 A2656 G2672 A2673 A2674 G2677 U2681 A2689 G2690 A2691 A2694 A2695 A2696 A2704 G2714 U2719 G2728 U2729 C2737 U2752 G2753 C2772 C2773 G2777 G2778 C2788 G2796 G2800 A2801 A2802 A2803 A2808 C2809 C2810 G2816 A2817
C2821 U2842 U2843 C2844 A2845 G2856 C2867 G2871 A2872 U2873 G2874 U2875 A2887 U2888 C2889 A2911 U2923 C2929 U2935 A2936 G2947 A2971 C2983 G2990 A2991 U2992 U2996 G2997 A3012 G3030 U3056 G3059 U3078 U3079 G3080 A3086 C3092 C3093
G3101 U3104 A3113 A3114 C3115 U3119 C3120 U3121 A3122 A3129 A3130 U3131 A3139 A3142 C3143 U3151 U3152 U3153 C3154 U3155 U3156 U3157 G3158 A3165 A3170 G3173 A3174 U3175 G3176 U3179 A3180 C3181 A3187 U3196 U3207 A3210 C3217 A3218 G3219 A3227 C3228 G3229


G3239
G3242
A3243
A3244
A3245
G3246
G3247
U3259
G3263
U3269
U3270
A3273
A3274
U3275
G3276
U3281
U3287
G3288
G3289
A3294
A3295
U3304
U3313
A3316
U3317
G3318
U3319
A3320
U3334
U3341
G3345
C3350
U3351
U3352
G3353
U3354
U3355
G3369
A3375
C3378
G3386
U3389
G3390
U3396

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 ($e^-/\AA^2$)	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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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

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 ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

5 of 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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	Lc	22	LYS
43	Ln	16	LYS
2	D	782	ILE
37	Lh	38	ARG
1	C	43	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
22	LS	8	GLN
30	La	62	HIS
25	LV	98	ASN
30	La	64	GLN
2	B	469	ASN

5.3.3 RNA ⓘ

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%)

5 of 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

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
46	1	2537	U
46	1	3228	C
46	1	2541	U
46	1	3154	C
46	1	3275	U

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

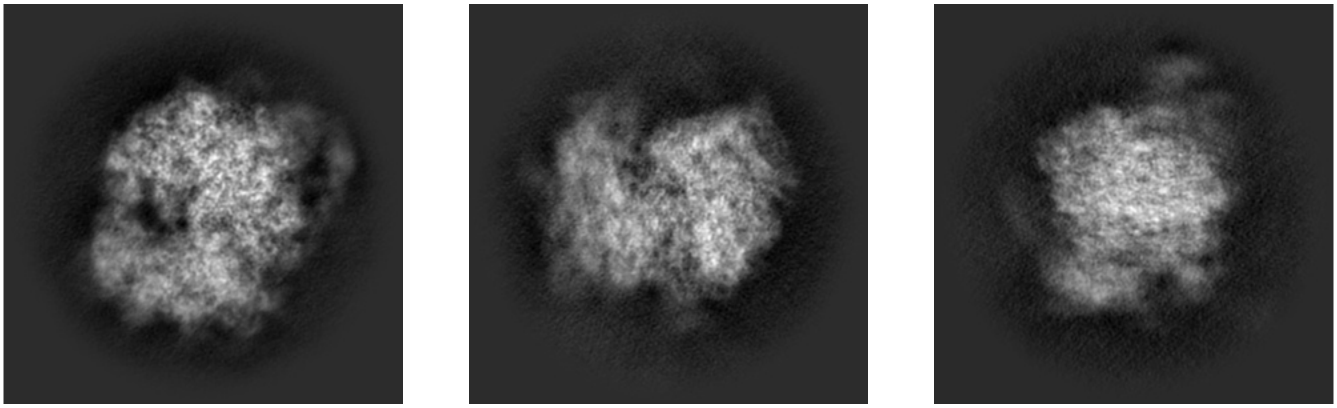
6 Map visualisation ⓘ

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.

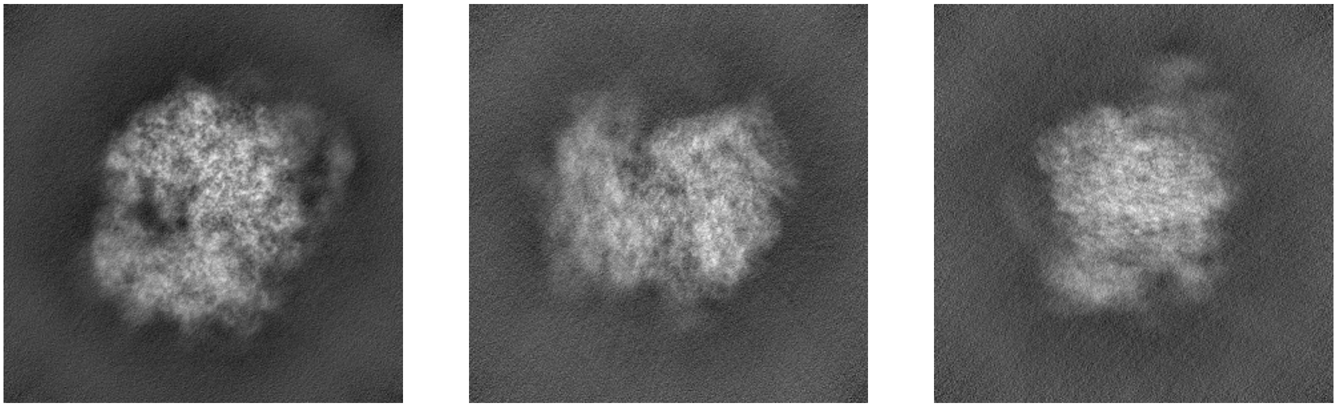
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

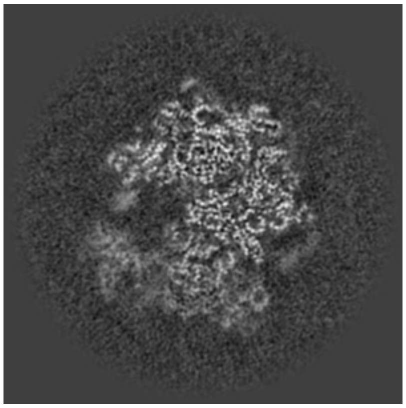


X Y Z

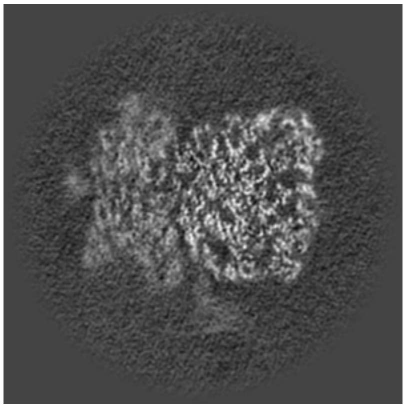
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

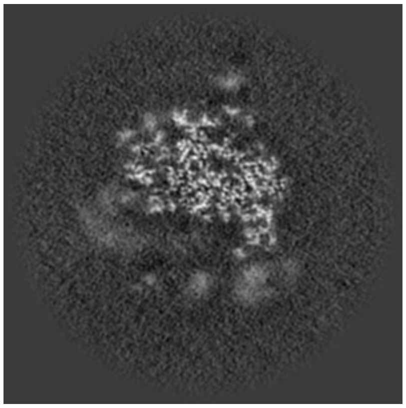
6.2.1 Primary map



X Index: 200

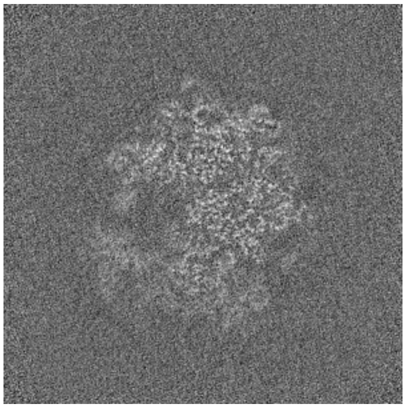


Y Index: 200

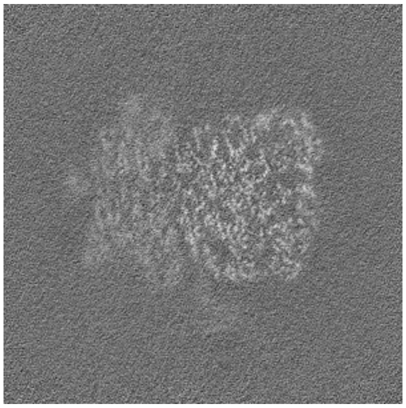


Z Index: 200

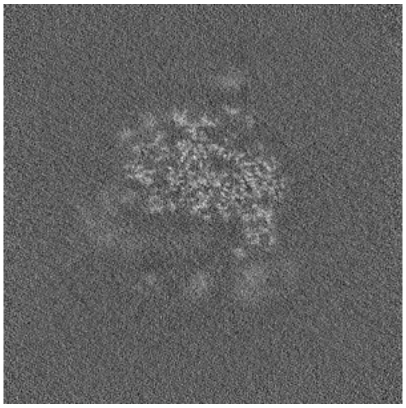
6.2.2 Raw map



X Index: 200



Y Index: 200

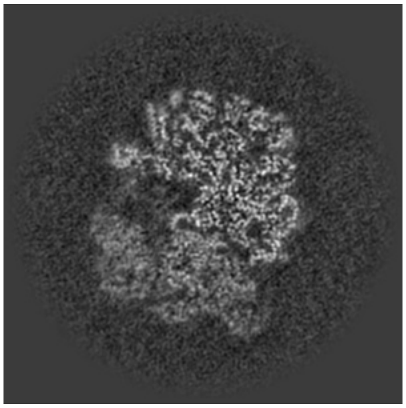


Z Index: 200

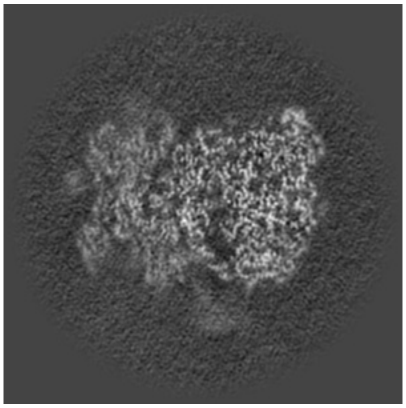
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

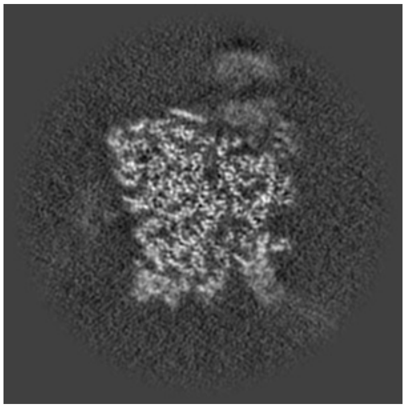
6.3.1 Primary map



X Index: 182

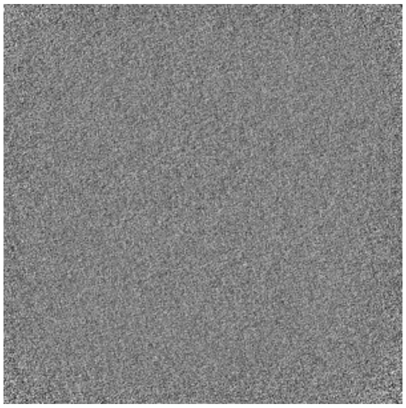


Y Index: 194

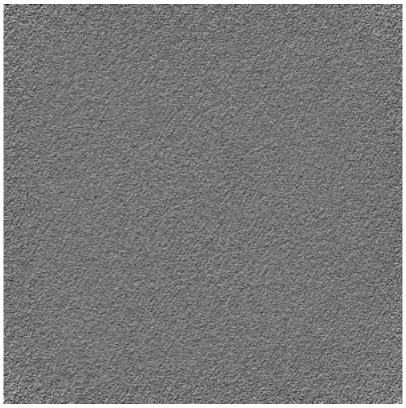


Z Index: 237

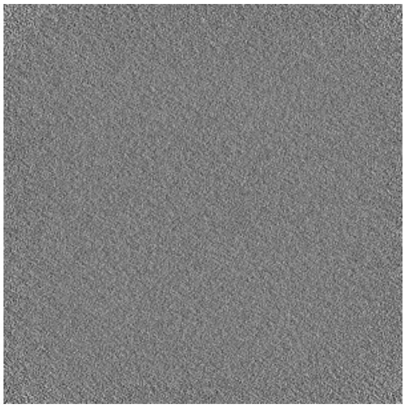
6.3.2 Raw map



X Index: 0



Y Index: 0

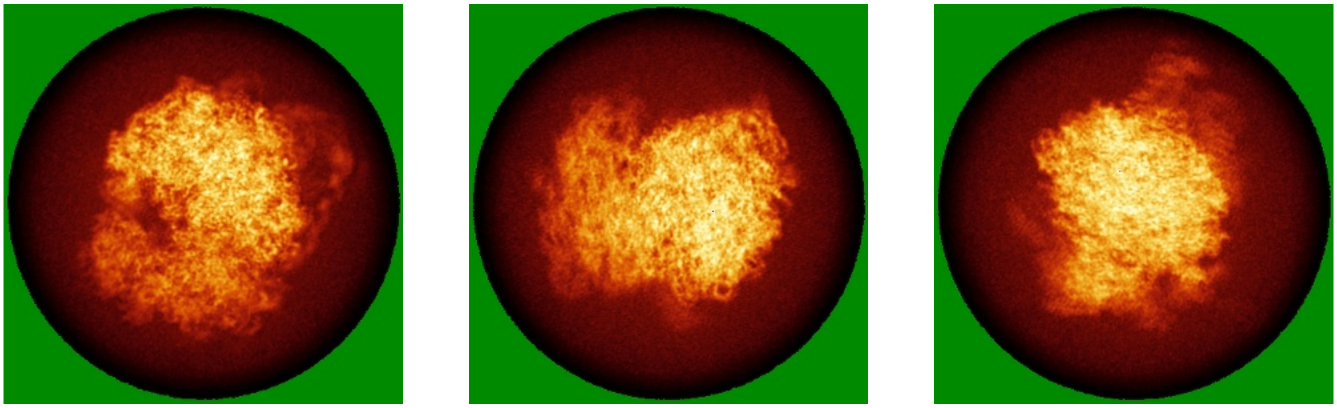


Z Index: 0

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

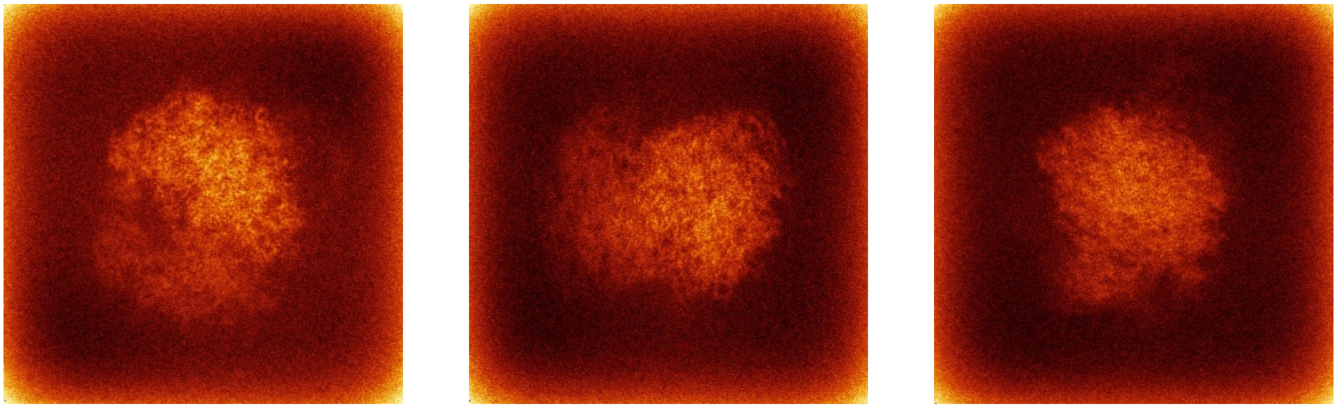
6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

6.5.1 Primary map

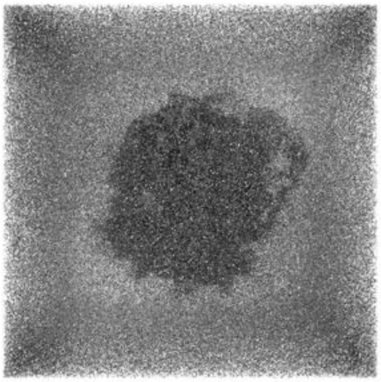
X

Y

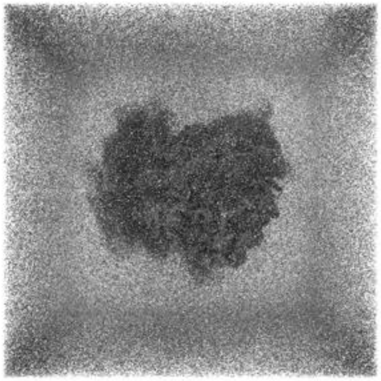
Z

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.

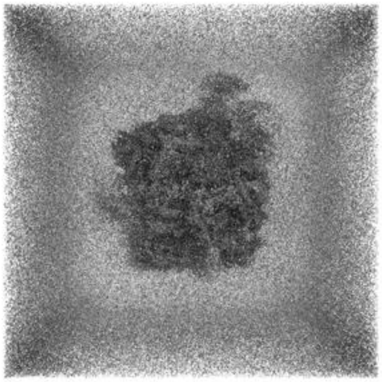
6.5.2 Raw map



X



Y



Z

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.

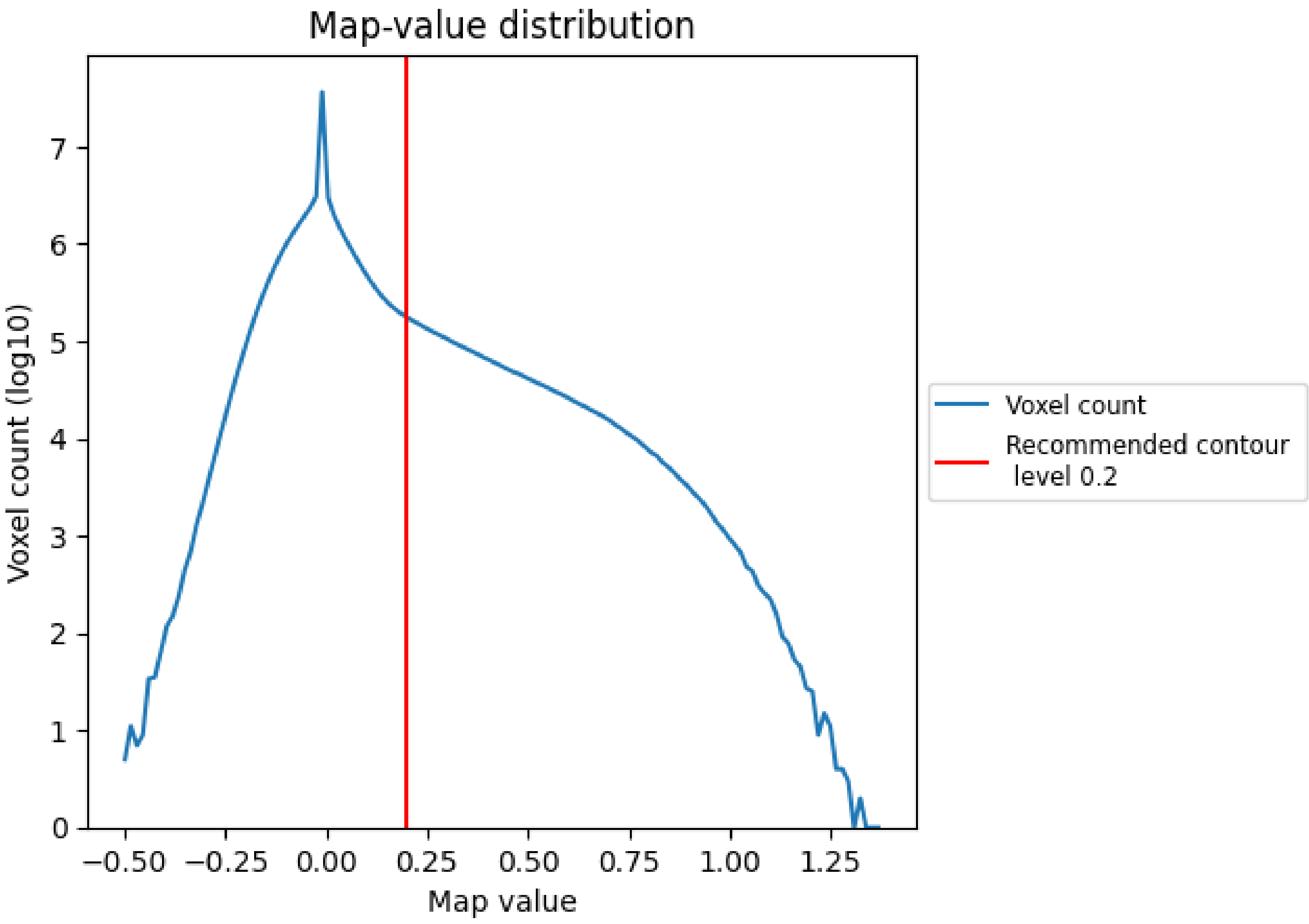
6.6 Mask visualisation

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

7 Map analysis (i)

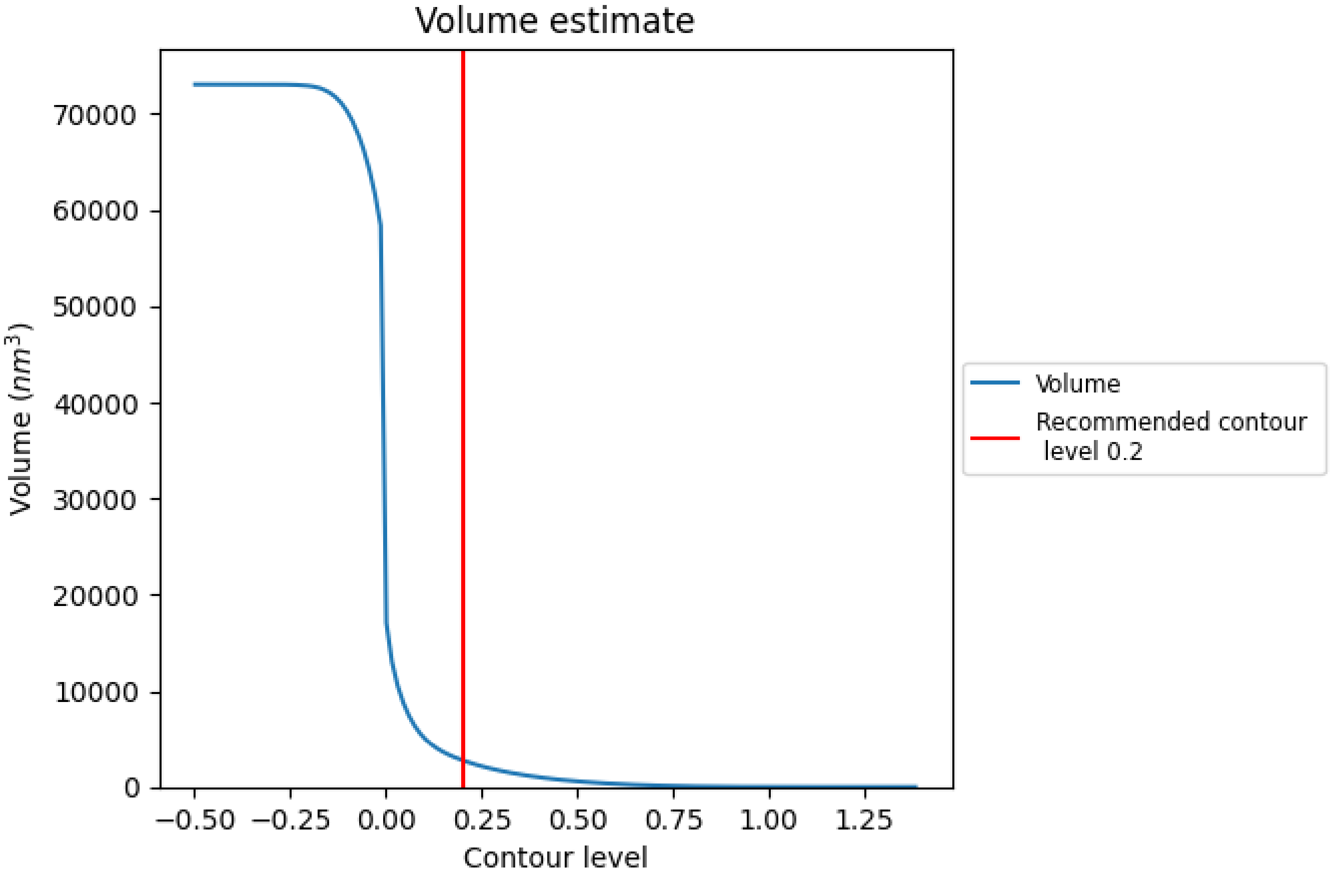
This section contains the results of statistical analysis of the map.

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.

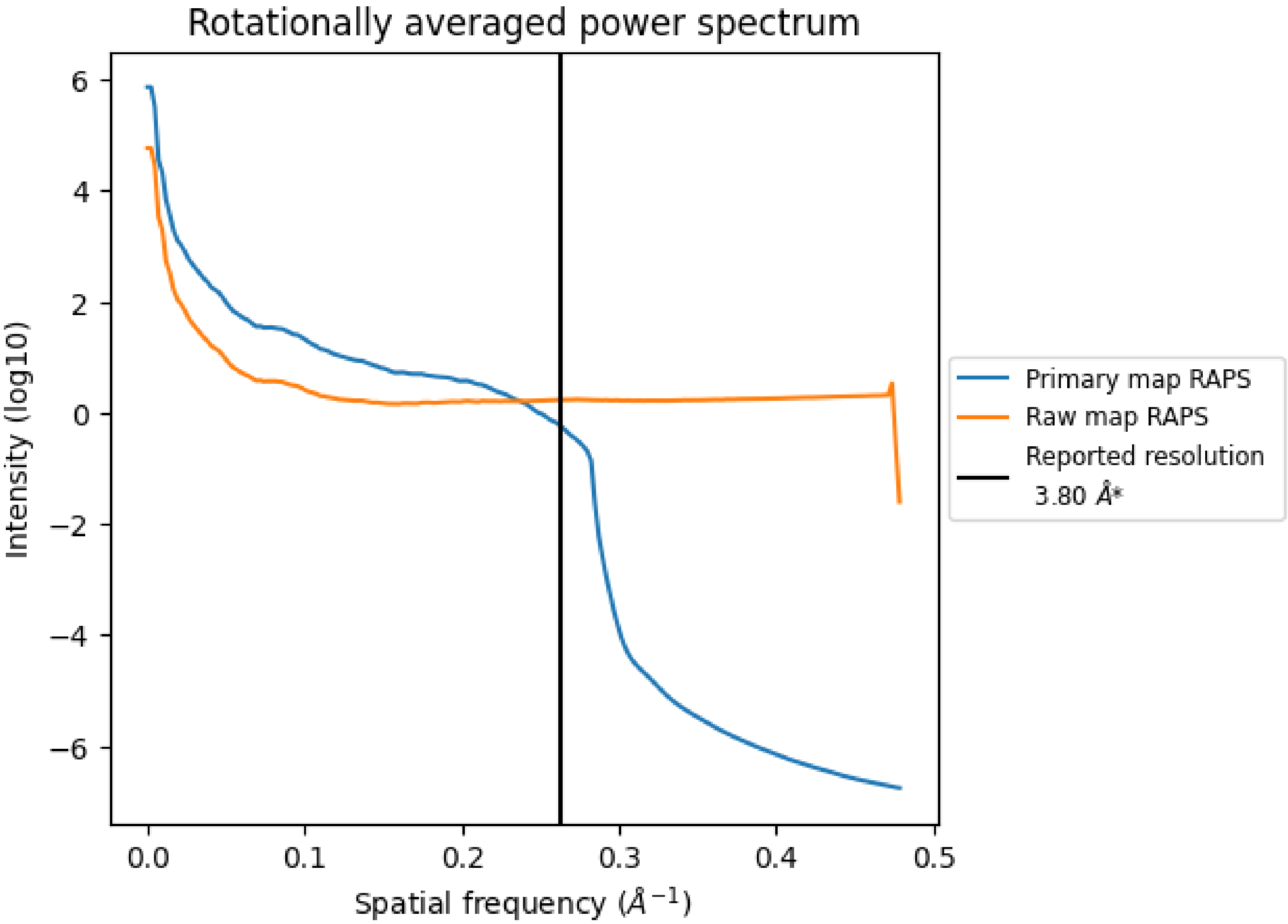
7.2 Volume estimate ⓘ



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 ⓘ

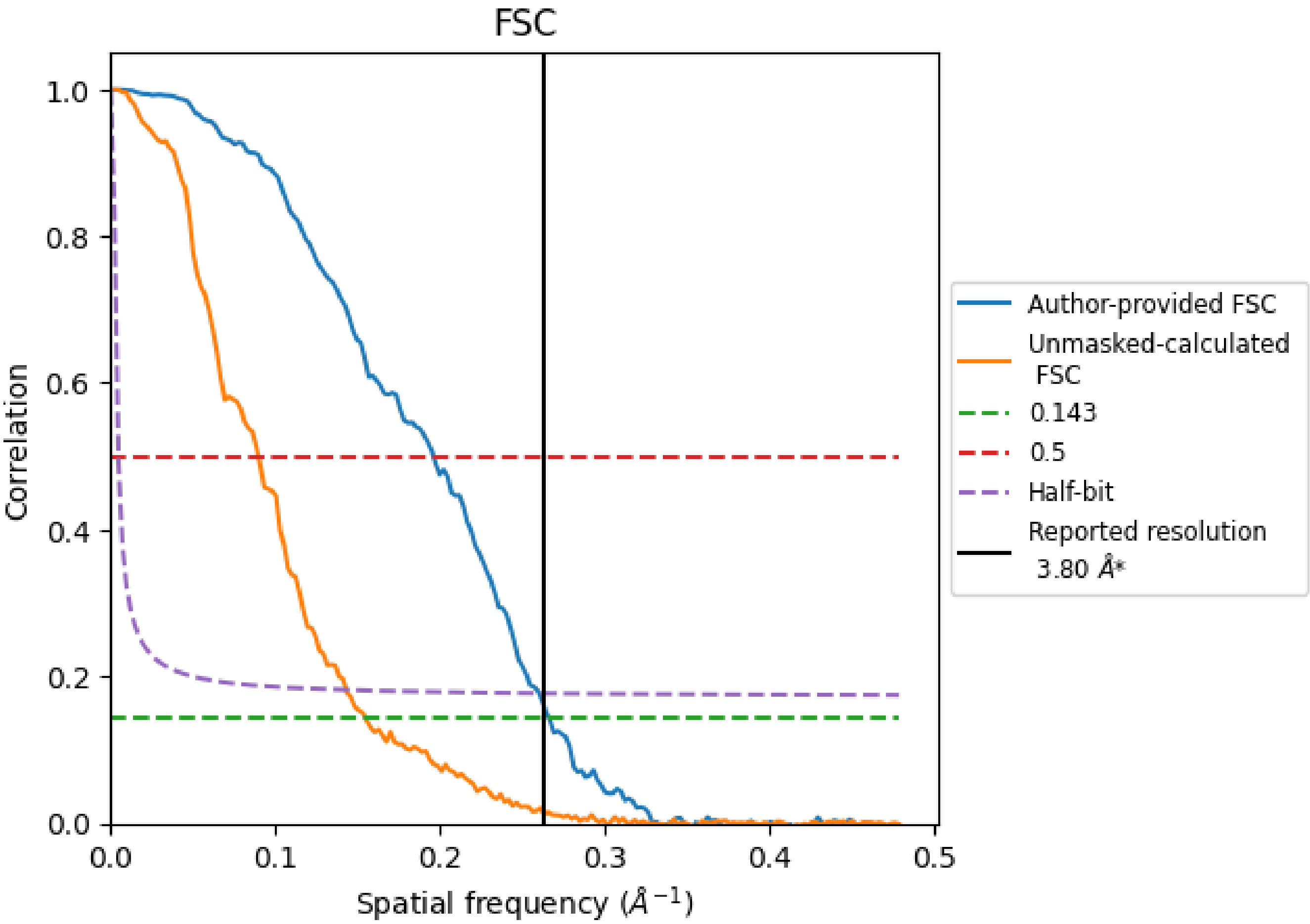


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.263 $\AA^{-1}$

8.2 Resolution estimates

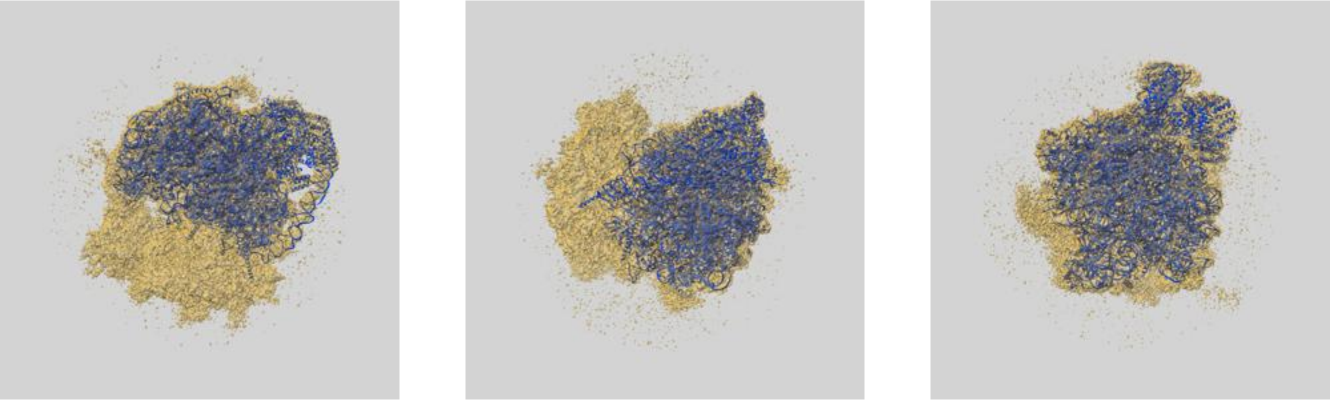
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.76	5.10	3.85
Unmasked-calculated*	6.46	11.15	6.99

*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

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.

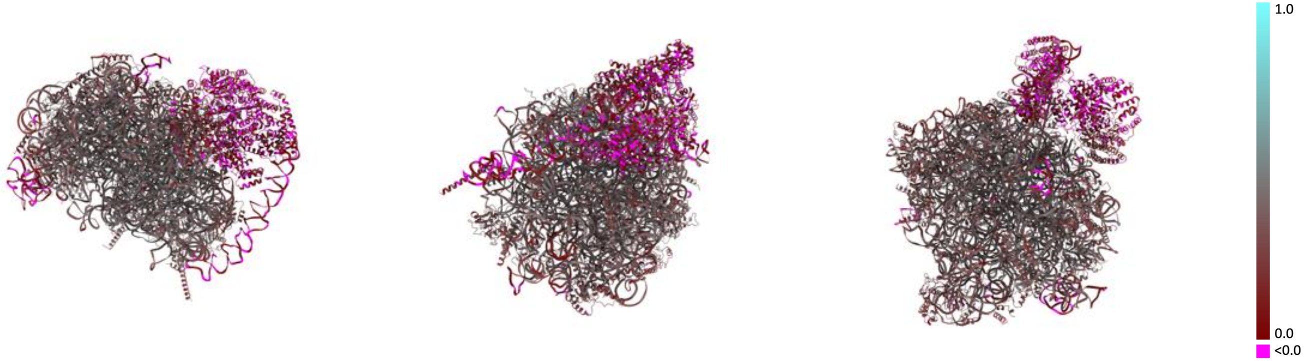
9.1 Map-model overlay



X Y Z

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.

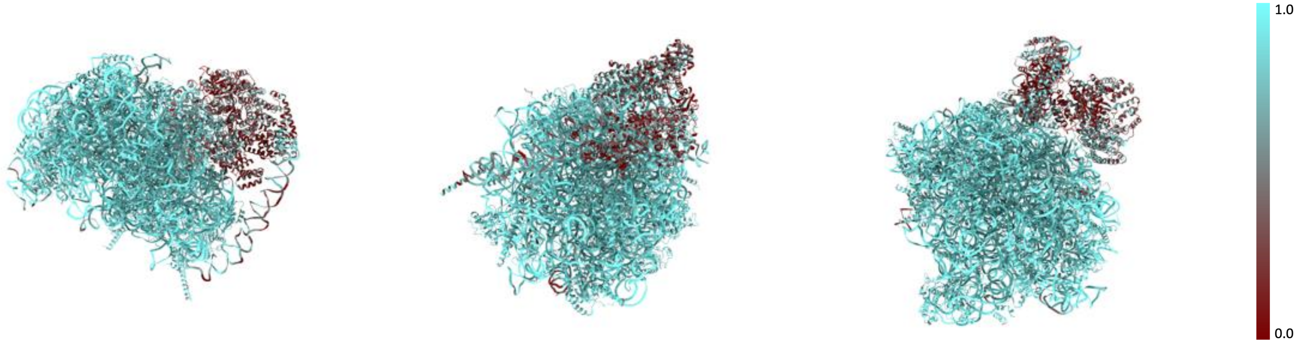
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

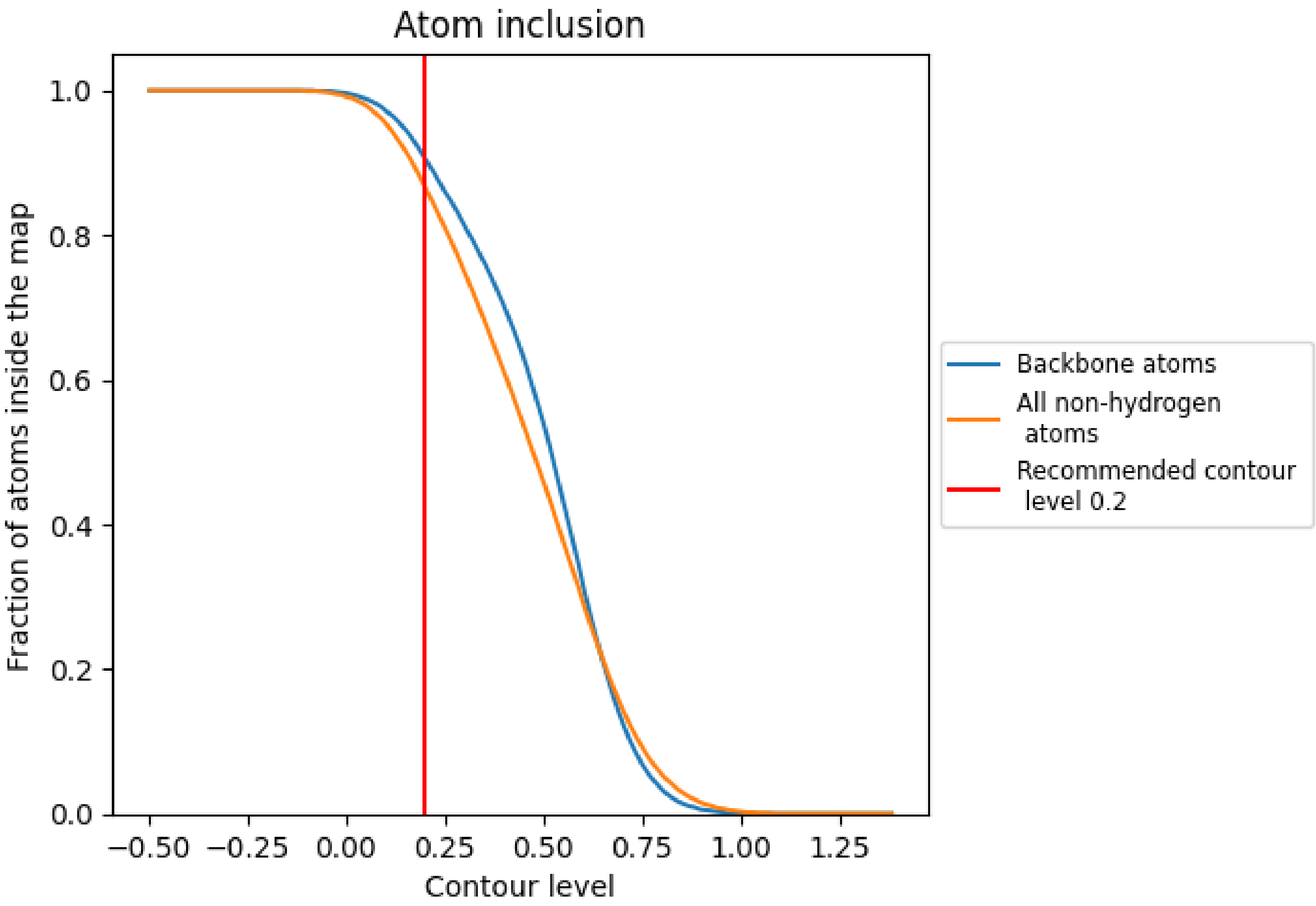
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

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 ⓘ



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