



wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 08:47 pm BST

PDB ID : 6YS3
EMDB ID : EMD-10891
Title : Cryo-EM structure of the 50S ribosomal subunit at 2.58 Angstroms with modeled GBC SecM peptide
Authors : Schulte, L.; Reitz, J.; Kudlinzki, D.; Hodirnau, V.V.; Frangakis, A.; Schwalbe, H.
Deposited on : 2020-04-20
Resolution : 2.58 Å (reported)
Based on initial model : 3JBU

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

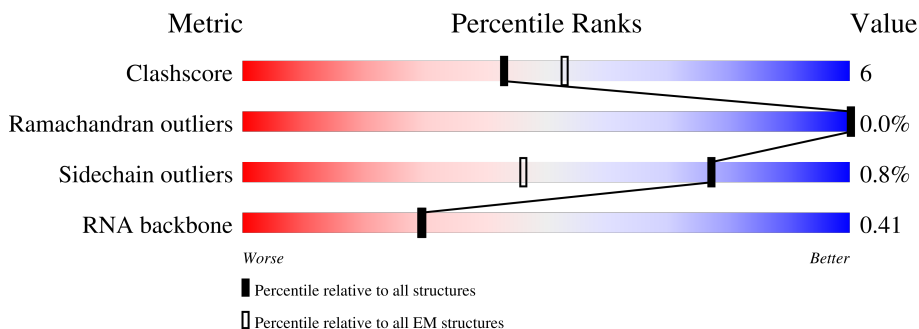
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.58 Å.

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



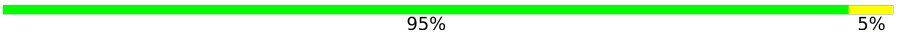


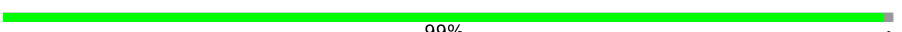
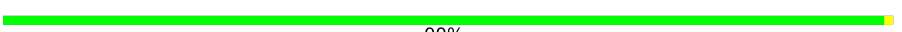
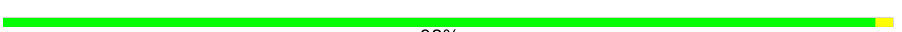






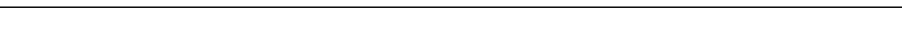

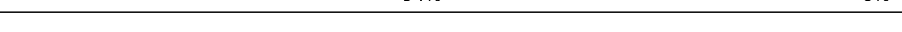
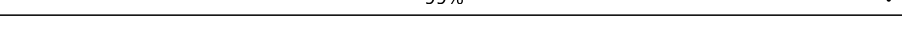
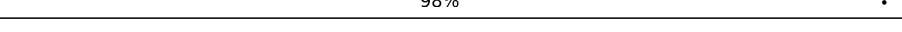
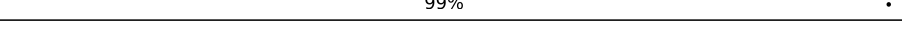
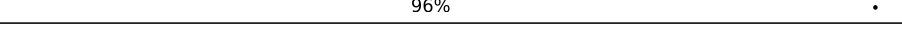
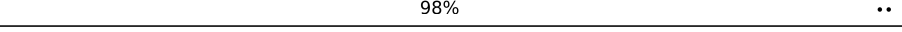

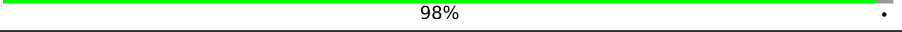

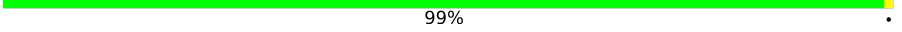

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	0	78	92% 6% .
2	1	63	83% 14% .
3	2	59	93% . .
4	3	57	84% 12% .
5	4	55	84% 7% 9%
6	6	46	96% .
7	7	65	92% . . .

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Mol	Chain	Length	Quality of chain
8	8	38	
9	a	120	
10	b	2906	
11	c	273	
12	d	209	
13	e	201	
14	f	179	
15	g	177	
16	h	149	
17	j	142	
18	k	123	
19	l	144	
20	m	136	
21	n	127	
22	o	117	
23	p	115	
24	q	118	
25	r	103	
26	s	110	
27	t	100	
28	u	104	
29	v	75	
30	w	94	
31	y	85	
32	z	61	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 90553 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	57	Total	C	N	O	S	0	0
			439	276	86	75	2		

- Molecule 4 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 5 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	4	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 6 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 7 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 8 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 9 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	118	Total	C	N	O	P	0	0
			2528	1126	464	821	117		

- Molecule 10 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	2888	Total	C	N	O	P	0	0
			62008	27660	11413	20047	2888		

- Molecule 11 is a protein called 50S ribosomal protein L2.

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

- Molecule 12 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 13 is a protein called 50S ribosomal protein L4.

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

- Molecule 14 is a protein called 50S ribosomal protein L5.

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

- Molecule 15 is a protein called 50S ribosomal protein L6.

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

- Molecule 16 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	39	Total	C	N	O	S	0	0
			287	184	51	51	1		

- Molecule 17 is a protein called 50S ribosomal protein L13.

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

- Molecule 18 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	k	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	l	143	Total	C	N	O	S	0	0
			1042	648	206	186	2		

- Molecule 20 is a protein called 50S ribosomal protein L16.

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

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	n	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 22 is a protein called 50S ribosomal protein L18.

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

- Molecule 23 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	p	113	Total	C	N	O	S	0	0
			908	570	177	160	1		

- Molecule 24 is a protein called 50S ribosomal protein L20.

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

- Molecule 25 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	r	99	Total	C	N	O	S	0	0
			791	500	149	140	2		

- Molecule 26 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	s	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 27 is a protein called 50S ribosomal protein L23.

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

- Molecule 28 is a protein called 50S ribosomal protein L24.

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

- Molecule 29 is a RNA chain called glycine-tRNA glyT.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	v	75	Total	C	N	O	P	0	0
			1583	707	270	531	75		

- Molecule 30 is a protein called 50S ribosomal protein L25.

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

- Molecule 31 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	y	74	Total	C	N	O	S	0	0
			559	348	112	98	1		

- Molecule 32 is a protein called Gamma-crystallin B.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	z	35	Total	C	N	O	S	0	0
			275	172	48	51	4		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	-12	MET	-	initiating methionine	UNP P02526
z	-11	GLY	-	expression tag	UNP P02526
z	-10	HIS	-	expression tag	UNP P02526
z	-9	HIS	-	expression tag	UNP P02526
z	-8	HIS	-	expression tag	UNP P02526
z	-7	HIS	-	expression tag	UNP P02526
z	-6	HIS	-	expression tag	UNP P02526
z	-5	HIS	-	expression tag	UNP P02526
z	-4	HIS	-	expression tag	UNP P02526
z	-3	HIS	-	expression tag	UNP P02526
z	-2	HIS	-	expression tag	UNP P02526
z	-1	HIS	-	expression tag	UNP P02526

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Chain	Residue	Modelled	Actual	Comment	Reference
z	150	PHE	ASN	conflict	UNP P02526
z	152	THR	ILE	conflict	UNP P02526
z	153	PRO	ARG	conflict	UNP P02526
z	155	TRP	-	expression tag	UNP P02526
z	156	ILE	-	expression tag	UNP P02526
z	157	SER	-	expression tag	UNP P02526
z	158	GLN	-	expression tag	UNP P02526
z	159	ALA	-	expression tag	UNP P02526
z	160	GLN	-	expression tag	UNP P02526
z	161	GLY	-	expression tag	UNP P02526
z	162	ILE	-	expression tag	UNP P02526
z	163	ARG	-	expression tag	UNP P02526
z	164	ALA	-	expression tag	UNP P02526
z	165	GLY	-	expression tag	UNP P02526

3 Residue-property plots [i](#)


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

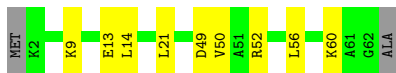
- Molecule 1: 50S ribosomal protein L28

Chain 0:  92% 6% .



- Molecule 2: 50S ribosomal protein L29

Chain 1:  83% 14% .




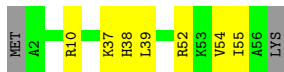
- Molecule 3: 50S ribosomal protein L30

Chain 2:  93% . .




- Molecule 4: 50S ribosomal protein L32

Chain 3:  84% 12% .



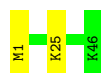
- Molecule 5: 50S ribosomal protein L33

Chain 4:  84% 7% 9%



- Molecule 6: 50S ribosomal protein L34

Chain 6:  96%



- Molecule 7: 50S ribosomal protein L35

Chain 7:  92%



- Molecule 8: 50S ribosomal protein L36

Chain 8:  95%



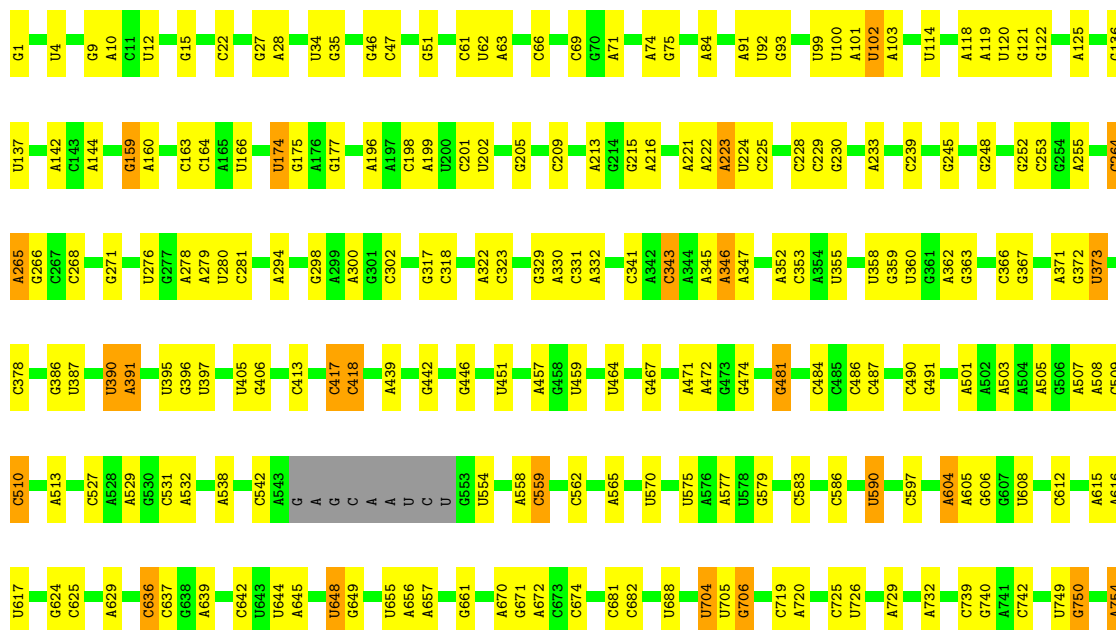
- Molecule 9: 5S rRNA

Chain a:  70%

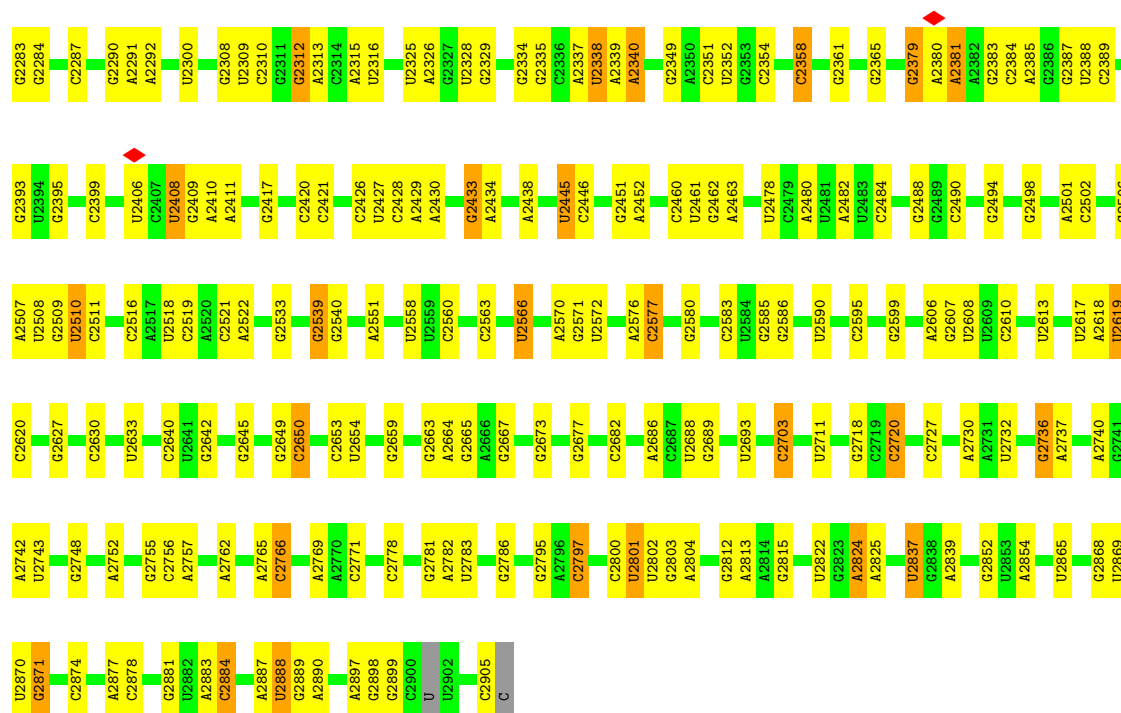


- Molecule 10: 23S rRNA

Chain b:  67%

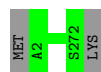


C2168	C2169	U2170	U2171	G2172	A2173	A2174	U2175	U2176	A2177	C2178	C2179	A2180	C2181	C2182	C2183	U2184	U2185	U2186	U2189	U2190	U2191	U2192	U2196	A2202	A2203	U2207	G2208	C2215	A2216	U2217	C2218	U2224	A2229	U2233	C2236	G2242	G2243	U2244	U2247	G2254	C2265	A2272	G2275											
G2104	A2105	G2106	C2107	C2108	U2109	U2110	G2111	A2112	U2113	G2114	U2115	G2116	G2119	G2120	A2121	U2122	A2123	G2124	G2125	U2126	G2127	G2128	G2129	A2130	G2131	G2132	C2133	U2134	U2135	U2136	A2139	G2140	U2141	G2142	U2143	A2146	C2149	C2150	A2151	G2152	U2153	C2154	U2155	G2156	C2157	A2158	U2159	G2160	A2161	G2163	C2164	G2165	G2166	G2167
C1989	U1995	U1996	U1997	C1998	C2001	A2002	C2003	C2004	C2010	U2011	C2012	A2024	C2027	A2034	A2035	G2036	A2037	U2038	C2039	C2040	A2046	C2047	C2048	A1931	A1932	G1933	G1934	U1935	C2059	G2060	A2064	G2065	A2066	C2067	C2068	C2069	C2070	U1960	G1968	C1971	C2077	A2081	U2155	A2084	C2093	G2097	U2102	U2103						
C1883	U1886	U1887	U1888	G1889	G1892	C1896	C1897	C1898	C1899	G1910	G1911	C1912	C1913	G1914	A1917	C1918	A1922	A1923	C1924	C1928	C1929	A1931	A1932	G1933	G1934	U1935	A1941	A1942	U1943	U1944	U1947	U1959	U1960	G1968	C1971	C1974	U1975	G1976	G1977	U1978	G1979	A1985	U1986											
U1760	A1764	G1765	C1766	U1771	A1775	U1777	G1778	U1781	A1782	U1783	U1784	A1785	A1786	A1787	A1788	A1793	C1797	C1802	A1803	A1810	G1813	C1818	U1829	G1830	A1831	C1832	C1835	C1839	G1844	G1851	G1859	G1864	C1870	G1871	G	U	A	C	G1877															
C1611	A1612	C1613	U1620	G1621	C1641	C1646	U1649	U1650	G1651	G1662	U1670	A1671	C1672	G1676	C1677	A1680	C1693	A1697	G1699	G1701	G1705	C1706	A1707	C1708	G1709	G1717	U1718	A1719	G1720	G1723	A1724	C1730	U1731	G1732	G1733	G1734	G1735	G1736	G1740	C1750	G1758	A1759												
A1511	C1514	U1525	G1526	A1527	C1528	G1531	A1534	C1535	C1538	G1539	G1540	U1541	G1542	C1543	U1544	G1545	C1549	A1554	U1555	U1556	C1557	U1561	G1562	C1563	C1566	C1567	A1568	G1569	A1570	A1571	C1577	U1580	G1583	C1584	U1586	C1587	A1597	A1598	U1601	C1602	C1609	A1610												
A1397	U1398	U1399	C1400	C1401	U1402	G1412	U1413	C1416	U1417	G1418	A1421	A1422	G1423	A1429	C1430	C1439	U1444	C1453	G1454	A1455	C1456	G1457	U1461	U1462	C1463	U1469	U1470	A1471	A1472	G1473	G1477	U1478	A1479	G1480	G1484	C1495	A1496	A1497	A1498	U1499	C1500	A1505	A1506	A1507	A1510									
A1289	G1290	C1291	C1292	C1293	U1296	C1297	G1301	A1302	A1303	A1304	C1308	G1313	U1314	U1315	C1316	U1320	C1321	C1322	A1323	U1328	U1329	U1331	U1336	U1342	G1345	U1346	C1347	U1354	C1359	G1360	A1361	C1365	G1366	A1367	G1370	A1380	U1381	G1382	G1383	G1384	A1385	C1388	U1396											
G1188	G1189	U1190	G1197	C1202	A1206	A1207	G1208	C1209	G1212	U1213	G1214	U1226	G1229	G1234	C1235	U1237	G1238	A1249	G1250	U1251	G1252	A1255	A1256	U1257	G1258	G1268	U1269	G1273	A1274	U1275	A1276	A1277	G1278	G1279	C1280	G1281	A1286																	
U1085	A1086	A1087	A1088	G1089	A1090	A1091	A1092	G1093	C1094	A1097	U1099	A1100	C1102	U1103	C1104	A1105	C1106	U1107	G1108	C1111	G1112	A1113	G1114	C1119	C1120	U1121	U1132	G1133	U1134	A1135	A1136	C1137	G1138	A1144	C1154	C1155	C1166	G1170	A1171	C1172	G1173	C1174	U1175	U1176	A1177	U1178	G1179	G1187						
C1007	C1008	A1012	G1013	U1014	C1015	U1021	G1024	G1028	C1032	U1035	G1036	U1037	G	U1039	C1040	U1044	C1046	C1047	A1048	G1049	C1055	A1056	G1057	G1058	A1059	C948	G1061	U1062	U1063	G1064	G1065	C1066	U1067	U1068	A1069	G1070	A1071	A1072	G1073	C1074	A1075	G1076	C1077	C1078	G1079	U1080	C1081	A1082	U1083	U1084				
G882	G883	G884	G885	U886	U889	C890	U891	U896	U897	A898	C899	A902	U903	G909	A912	A913	C914	C917	U921	U933	C939	A943	A947	C948	C953	U960	C963	C967	A975	G976	C984	A985	G991	A992	A998	G999	C1000	U1001	U1005	G1006														
G759	U764	G765	A766	C767	G777	G778	A784	A785	G786	G787	U896	U897	A898	C899	A902	U903	G909	A912	A913	C914	C917	U921	U933	C939	A943	A947	C948	C953	U960	C963	C967	A975	G976	C984	A985	G991	A992	A998	G999	C1000	U1001	U1005	G1006											



• Molecule 11: 50S ribosomal protein L2

Chain c: 99%



• Molecule 12: 50S ribosomal protein L3

Chain d: 99%



• Molecule 13: 50S ribosomal protein L4

Chain e: 98%



• Molecule 14: 50S ribosomal protein L5

Chain f: 98%



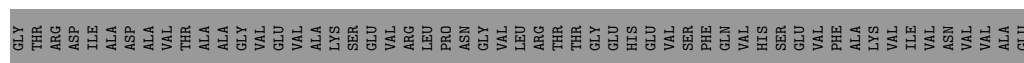
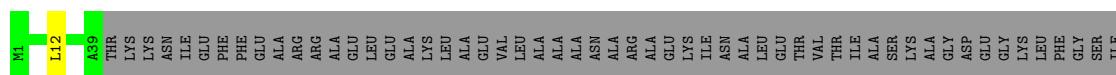
- Molecule 15: 50S ribosomal protein L6

Chain g:  98% ..



- Molecule 16: 50S ribosomal protein L9

Chain h:  26%  74%



- Molecule 17: 50S ribosomal protein L13

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 18: 50S ribosomal protein L14

Chain k:  98% ..



- Molecule 19: 50S ribosomal protein L15

Chain l:  99% .



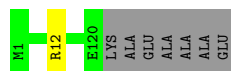
- Molecule 20: 50S ribosomal protein L16

Chain m:  99% .



- Molecule 21: 50S ribosomal protein L17

Chain n:  94%  6%



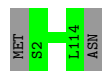
- Molecule 22: 50S ribosomal protein L18

Chain o:  99% .



- Molecule 23: 50S ribosomal protein L19

Chain p:  98% .



- Molecule 24: 50S ribosomal protein L20

Chain q:  99% .



- Molecule 25: 50S ribosomal protein L21

Chain r:  96% .



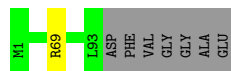
- Molecule 26: 50S ribosomal protein L22

Chain s:  98% ..



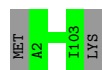
- Molecule 27: 50S ribosomal protein L23

Chain t:  92% . 7%

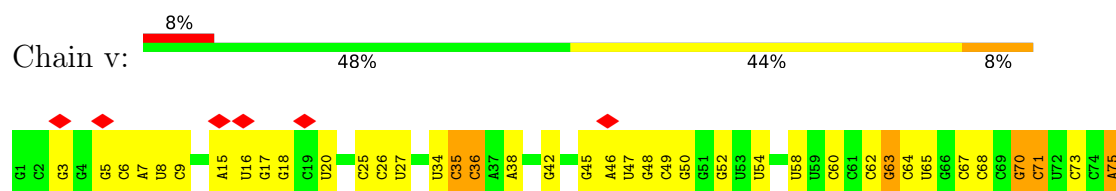


- Molecule 28: 50S ribosomal protein L24

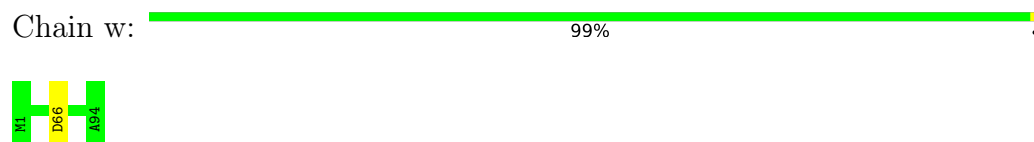
Chain u:  98% .



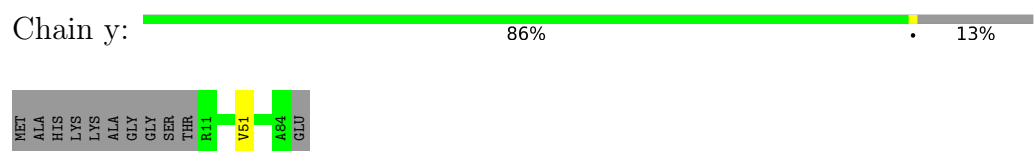
- Molecule 29: glycine-tRNA glyT



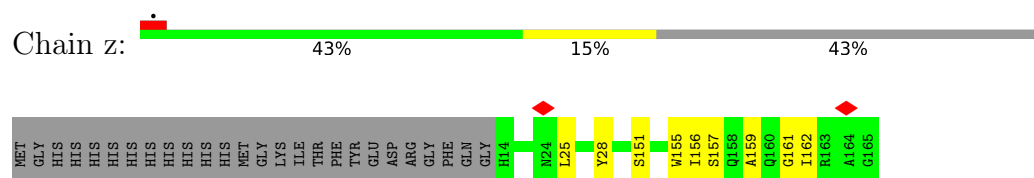
- Molecule 30: 50S ribosomal protein L25



- Molecule 31: 50S ribosomal protein L27



- Molecule 32: Gamma-crystallin B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	196254	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.109	Depositor
Minimum map value	-0.034	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.00741	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.57	0/635	0.58	0/848
2	1	0.45	0/496	0.55	0/660
3	2	0.53	0/443	0.62	0/593
4	3	0.69	0/440	0.62	0/588
5	4	0.47	0/416	0.62	0/554
6	6	0.69	0/380	0.56	0/498
7	7	0.61	0/513	0.57	0/676
8	8	0.67	0/303	0.68	0/397
9	a	0.97	0/2824	1.07	3/4402 (0.1%)
10	b	1.42	1/69446 (0.0%)	1.22	537/108330 (0.5%)
11	c	0.66	0/2121	0.64	0/2852
12	d	0.65	0/1586	0.62	0/2134
13	e	0.59	0/1571	0.68	1/2113 (0.0%)
14	f	0.40	0/1434	0.63	0/1926
15	g	0.43	0/1343	0.74	2/1816 (0.1%)
16	h	0.44	0/290	0.74	0/392
17	j	0.63	0/1152	0.58	0/1551
18	k	0.62	0/947	0.64	0/1268
19	l	0.61	0/1051	0.65	0/1400
20	m	0.63	0/1093	0.58	0/1460
21	n	0.63	0/973	0.65	0/1301
22	o	0.44	0/902	0.62	0/1209
23	p	0.58	0/920	0.57	0/1231
24	q	0.76	0/960	0.63	0/1278
25	r	0.64	0/803	0.61	0/1070
26	s	0.60	0/852	0.58	0/1142
27	t	0.54	0/744	0.60	0/994
28	u	0.50	0/787	0.65	0/1051
29	v	0.64	0/1764	1.29	17/2744 (0.6%)
30	w	0.50	0/766	0.61	1/1025 (0.1%)
31	y	0.63	0/566	0.61	0/750
32	z	0.35	0/284	1.39	9/386 (2.3%)
All	All	1.24	1/98805 (0.0%)	1.11	570/148639 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	b	1	G	OP3-P	-10.15	1.49	1.61

The worst 5 of 570 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	g	45	HIS	N-CA-C	-12.39	77.55	111.00
32	z	159	ALA	N-CA-C	-11.50	79.94	111.00
10	b	2888	U	N3-C2-O2	-10.24	115.03	122.20
10	b	2027	C	N1-C2-O2	10.23	125.04	118.90
10	b	819	C	C6-N1-C2	-10.12	116.25	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	625	0	652	2	0
2	1	495	0	526	6	0
3	2	439	0	482	1	0
4	3	434	0	445	4	0
5	4	409	0	440	2	0
6	6	377	0	418	2	0
7	7	504	0	572	5	0
8	8	302	0	341	1	0
9	a	2528	0	1283	0	0
10	b	62008	0	31185	0	0
11	c	2082	0	2154	0	0
12	d	1565	0	1616	0	0
13	e	1552	0	1619	0	0
14	f	1410	0	1444	0	0
15	g	1323	0	1371	0	0
16	h	287	0	307	0	0
17	j	1129	0	1162	0	0
18	k	938	0	1012	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	l	1042	0	1121	0	0
20	m	1074	0	1157	0	0
21	n	960	0	1000	0	0
22	o	892	0	923	0	0
23	p	908	0	956	0	0
24	q	947	0	1019	0	0
25	r	791	0	811	0	0
26	s	845	0	908	0	0
27	t	738	0	807	0	0
28	u	779	0	831	0	0
29	v	1583	0	807	0	0
30	w	753	0	780	0	0
31	y	559	0	575	0	0
32	z	275	0	247	0	0
All	All	90553	0	58971	23	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 23 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:12:SER:HB3	3:2:32:ILE:HD11	1.88	0.56
2:1:14:LEU:HD11	2:1:56:LEU:HD23	1.90	0.53
2:1:9:LYS:HE3	2:1:13:GLU:HG2	1.90	0.52
6:6:1:MET:SD	6:6:1:MET:N	2.74	0.51
2:1:49:ASP:OD1	2:1:52:ARG:NH2	2.43	0.51

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
2	1	59/63 (94%)	53 (90%)	6 (10%)	0	100	100
3	2	55/59 (93%)	51 (93%)	4 (7%)	0	100	100
4	3	53/57 (93%)	51 (96%)	2 (4%)	0	100	100
5	4	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
6	6	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
7	7	62/65 (95%)	56 (90%)	6 (10%)	0	100	100
8	8	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	c	269/273 (98%)	257 (96%)	12 (4%)	0	100	100
12	d	207/209 (99%)	190 (92%)	17 (8%)	0	100	100
13	e	199/201 (99%)	188 (94%)	11 (6%)	0	100	100
14	f	175/179 (98%)	155 (89%)	20 (11%)	0	100	100
15	g	174/177 (98%)	160 (92%)	13 (8%)	1 (1%)	22	41
16	h	37/149 (25%)	33 (89%)	4 (11%)	0	100	100
17	j	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
18	k	120/123 (98%)	112 (93%)	8 (7%)	0	100	100
19	l	141/144 (98%)	129 (92%)	12 (8%)	0	100	100
20	m	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
21	n	118/127 (93%)	104 (88%)	14 (12%)	0	100	100
22	o	114/117 (97%)	104 (91%)	10 (9%)	0	100	100
23	p	111/115 (96%)	106 (96%)	5 (4%)	0	100	100
24	q	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
25	r	95/103 (92%)	85 (90%)	10 (10%)	0	100	100
26	s	107/110 (97%)	103 (96%)	4 (4%)	0	100	100
27	t	91/100 (91%)	84 (92%)	7 (8%)	0	100	100
28	u	100/104 (96%)	80 (80%)	20 (20%)	0	100	100
30	w	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
31	y	72/85 (85%)	67 (93%)	5 (7%)	0	100	100
32	z	33/61 (54%)	25 (76%)	8 (24%)	0	100	100
All	All	3076/3328 (92%)	2855 (93%)	220 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	g	47	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	67/68 (98%)	66 (98%)	1 (2%)	60	80
2	1	54/55 (98%)	54 (100%)	0	100	100
3	2	47/49 (96%)	47 (100%)	0	100	100
4	3	46/48 (96%)	45 (98%)	1 (2%)	47	70
5	4	45/49 (92%)	45 (100%)	0	100	100
6	6	38/38 (100%)	38 (100%)	0	100	100
7	7	51/52 (98%)	49 (96%)	2 (4%)	27	51
8	8	34/34 (100%)	34 (100%)	0	100	100
11	c	216/218 (99%)	216 (100%)	0	100	100
12	d	164/164 (100%)	162 (99%)	2 (1%)	67	84
13	e	165/165 (100%)	162 (98%)	3 (2%)	54	75
14	f	148/150 (99%)	146 (99%)	2 (1%)	62	81
15	g	137/138 (99%)	137 (100%)	0	100	100
16	h	30/114 (26%)	29 (97%)	1 (3%)	33	57
17	j	116/116 (100%)	116 (100%)	0	100	100
18	k	103/104 (99%)	102 (99%)	1 (1%)	73	87
19	l	102/103 (99%)	102 (100%)	0	100	100
20	m	109/109 (100%)	108 (99%)	1 (1%)	75	89
21	n	100/103 (97%)	99 (99%)	1 (1%)	73	87
22	o	86/87 (99%)	86 (100%)	0	100	100
23	p	98/100 (98%)	98 (100%)	0	100	100
24	q	89/90 (99%)	89 (100%)	0	100	100
25	r	82/84 (98%)	82 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	s	92/93 (99%)	91 (99%)	1 (1%)	70	86
27	t	80/84 (95%)	79 (99%)	1 (1%)	65	83
28	u	83/85 (98%)	83 (100%)	0	100	100
30	w	78/78 (100%)	78 (100%)	0	100	100
31	y	55/63 (87%)	54 (98%)	1 (2%)	54	75
32	z	31/53 (58%)	29 (94%)	2 (6%)	14	29
All	All	2546/2694 (94%)	2526 (99%)	20 (1%)	77	91

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	n	12	ARG
31	y	51	VAL
32	z	157	SER
32	z	25	LEU
13	e	134	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
5	4	26	ASN
14	f	27	GLN
14	f	135	GLN
15	g	73	ASN
32	z	24	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	b	2882/2906 (99%)	765 (26%)	0
29	v	74/75 (98%)	37 (50%)	0
9	a	116/120 (96%)	33 (28%)	0
All	All	3072/3101 (99%)	835 (27%)	0

5 of 835 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	a	4	C

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Mol	Chain	Res	Type
9	a	5	U
9	a	7	G
9	a	9	G
9	a	13	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

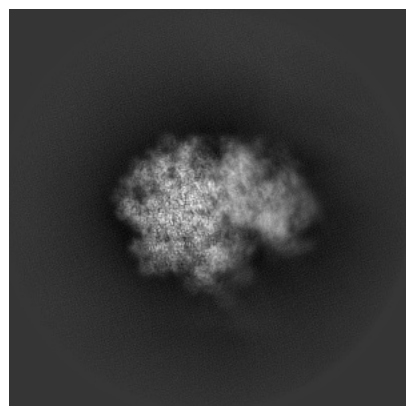
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10891. These allow visual inspection of the internal detail of the map and identification of artifacts.

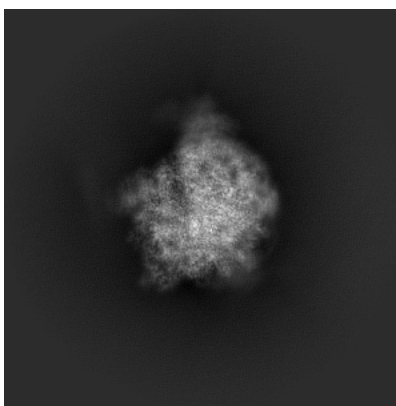
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

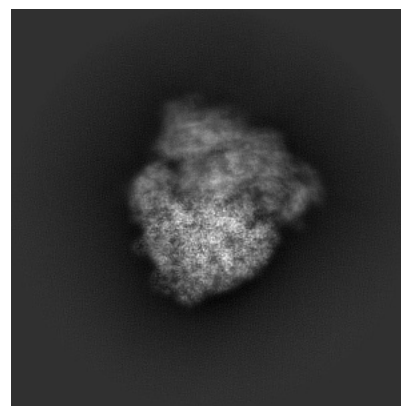
6.1.1 Primary map



X

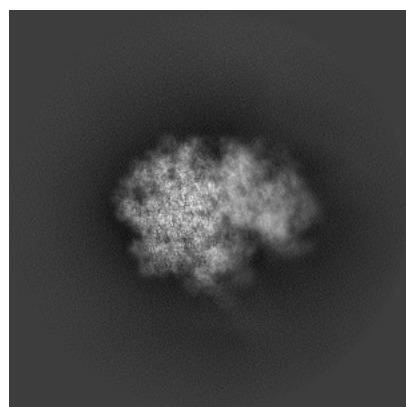


Y

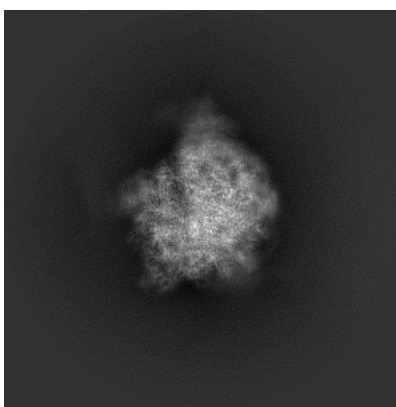


Z

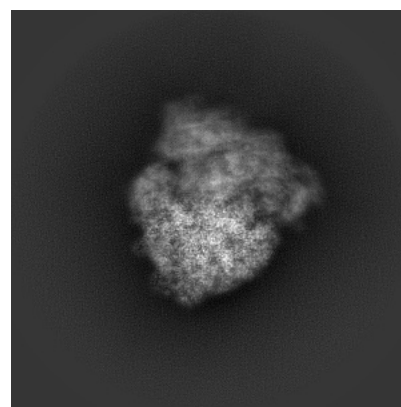
6.1.2 Raw map



X



Y

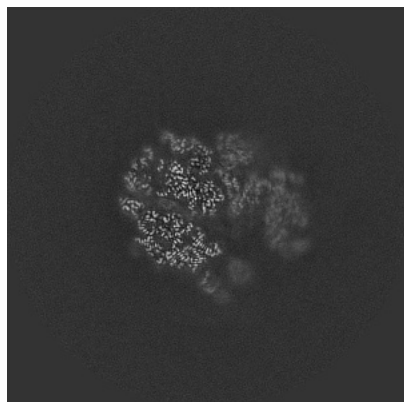


Z

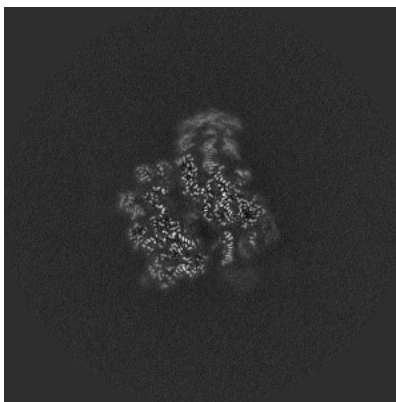
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

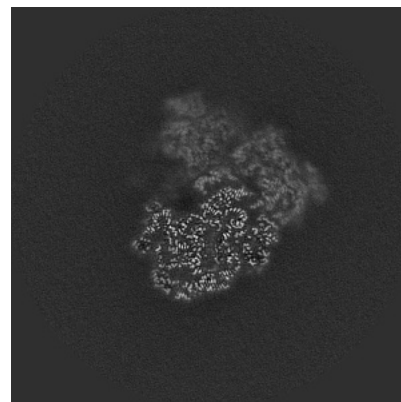
6.2.1 Primary map



X Index: 240

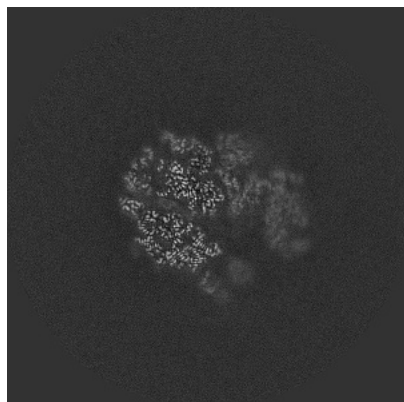


Y Index: 240

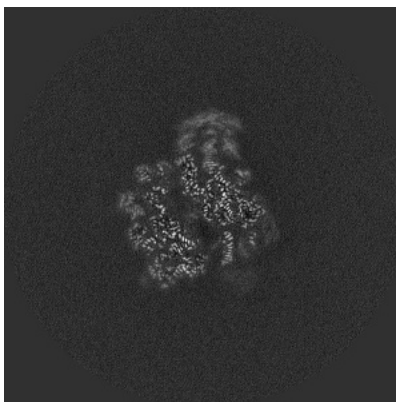


Z Index: 240

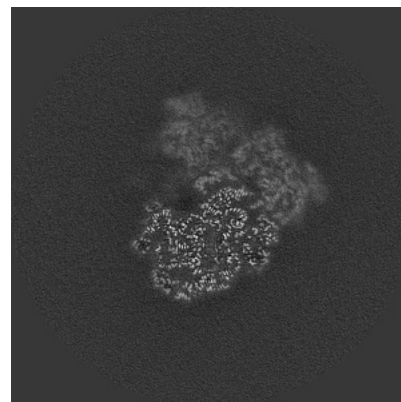
6.2.2 Raw map



X Index: 240



Y Index: 240

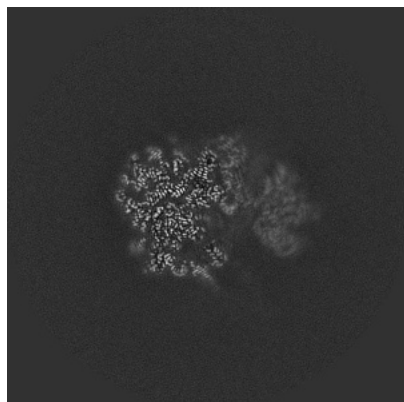


Z Index: 240

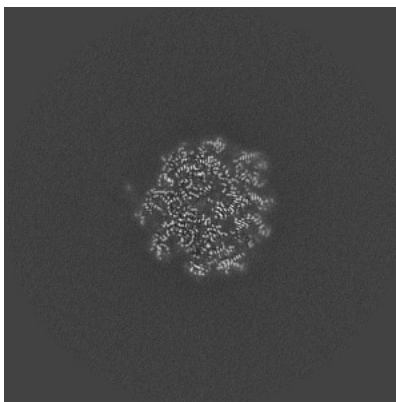
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

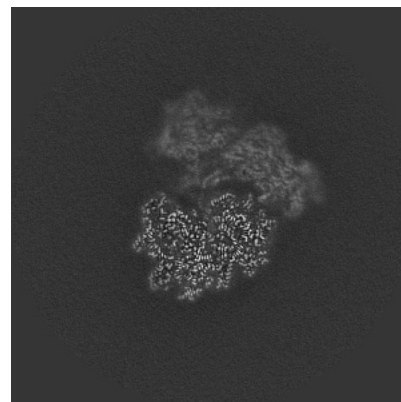
6.3.1 Primary map



X Index: 230

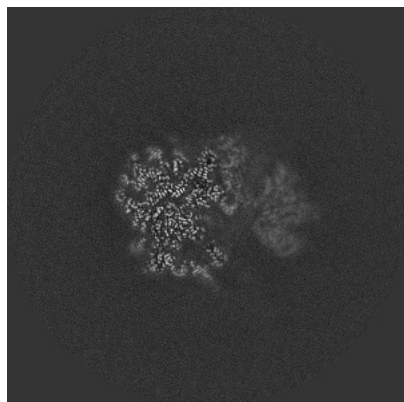


Y Index: 208

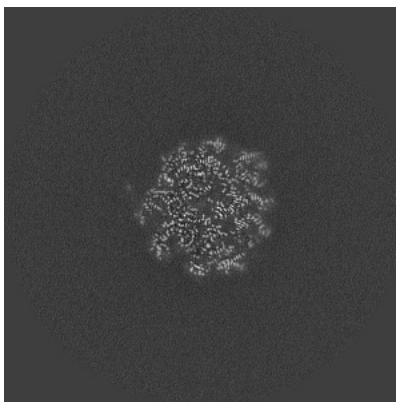


Z Index: 231

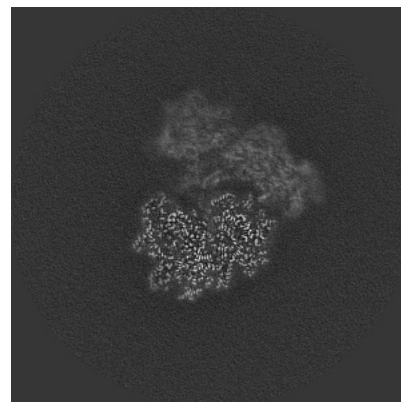
6.3.2 Raw map



X Index: 230



Y Index: 208

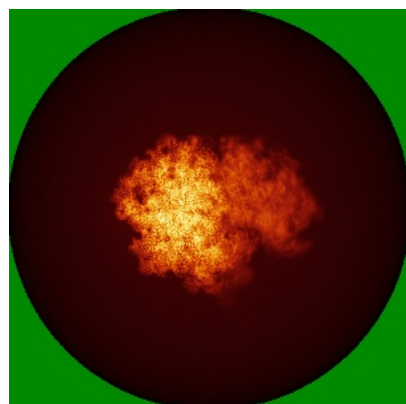


Z Index: 231

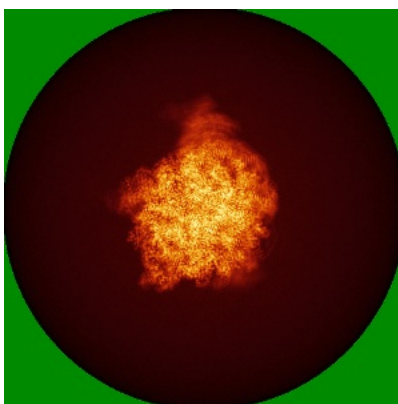
The images above show the largest variance slices of the map in three orthogonal directions.

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

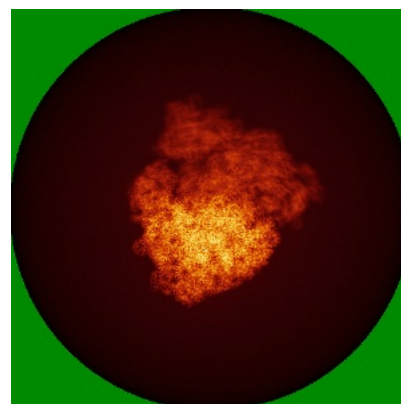
6.4.1 Primary map



X

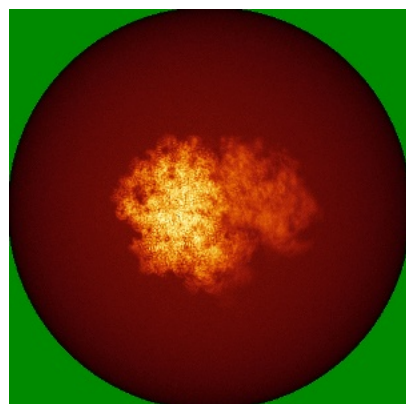


Y

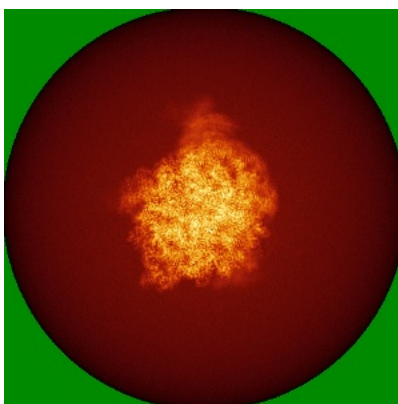


Z

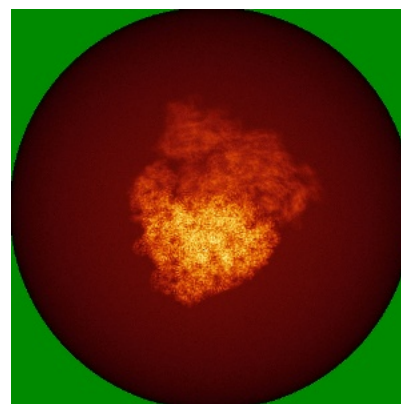
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



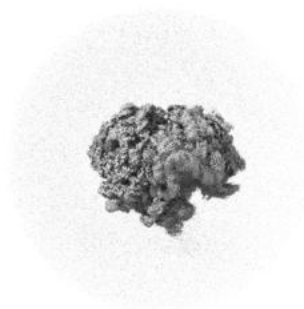
Y



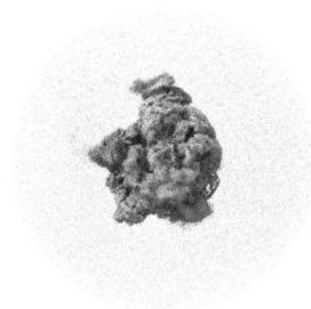
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00741. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

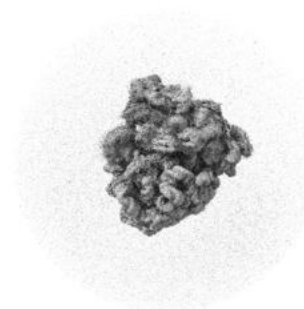
6.5.2 Raw map



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.

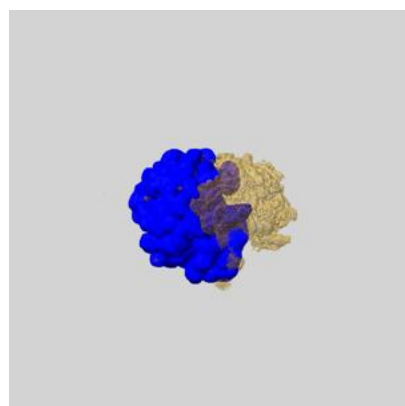
6.6 Mask visualisation [i](#)

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

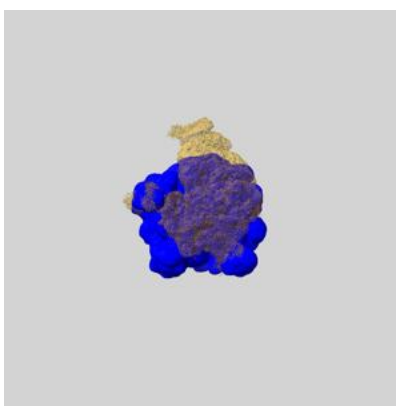
A mask typically either:

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

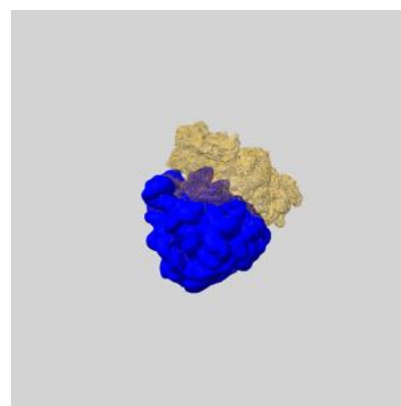
6.6.1 emd_10891_msk_1.map [i](#)



X



Y

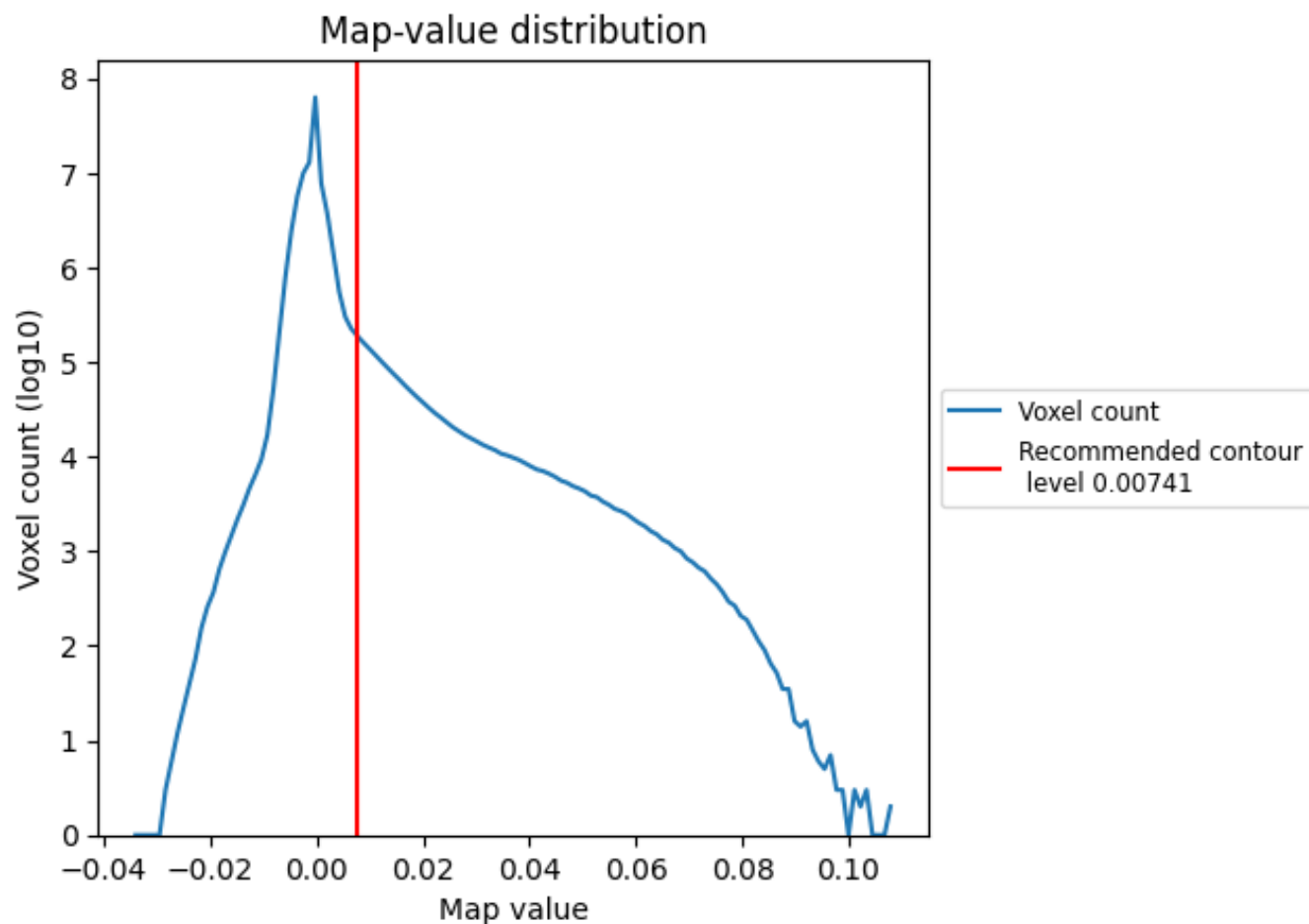


Z

7 Map analysis [i](#)

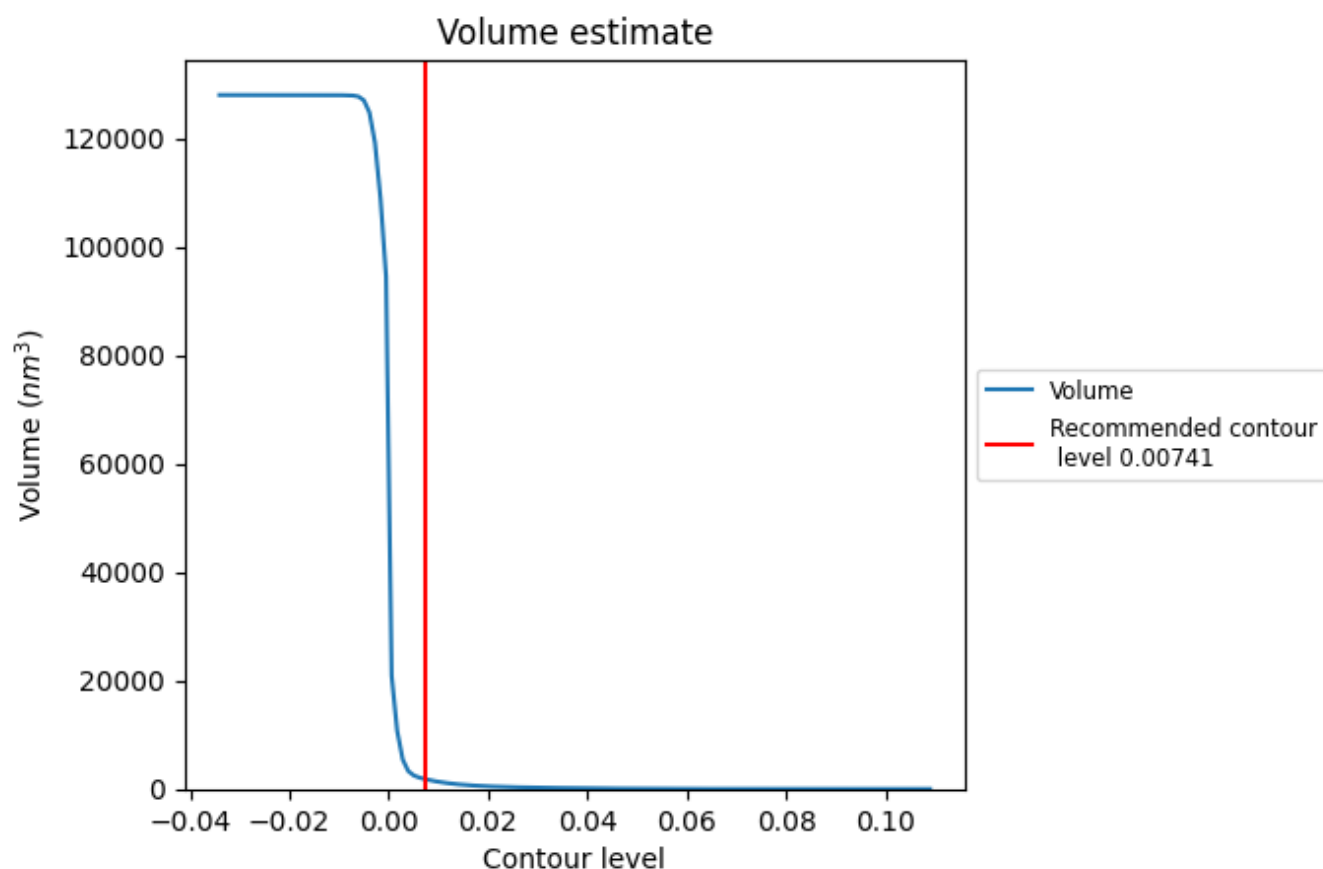
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

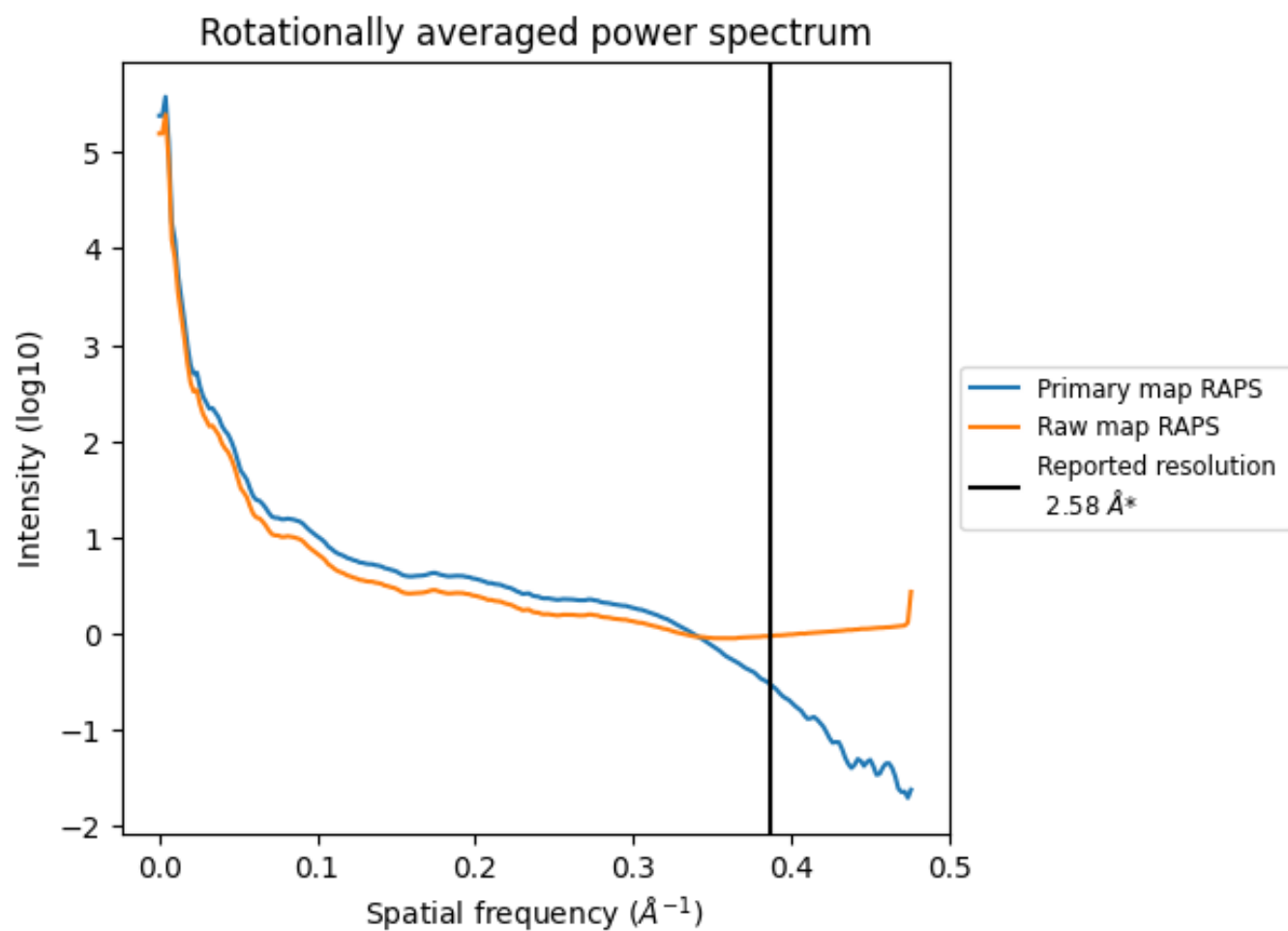
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1796 nm^3 ; this corresponds to an approximate mass of 1623 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 ⓘ

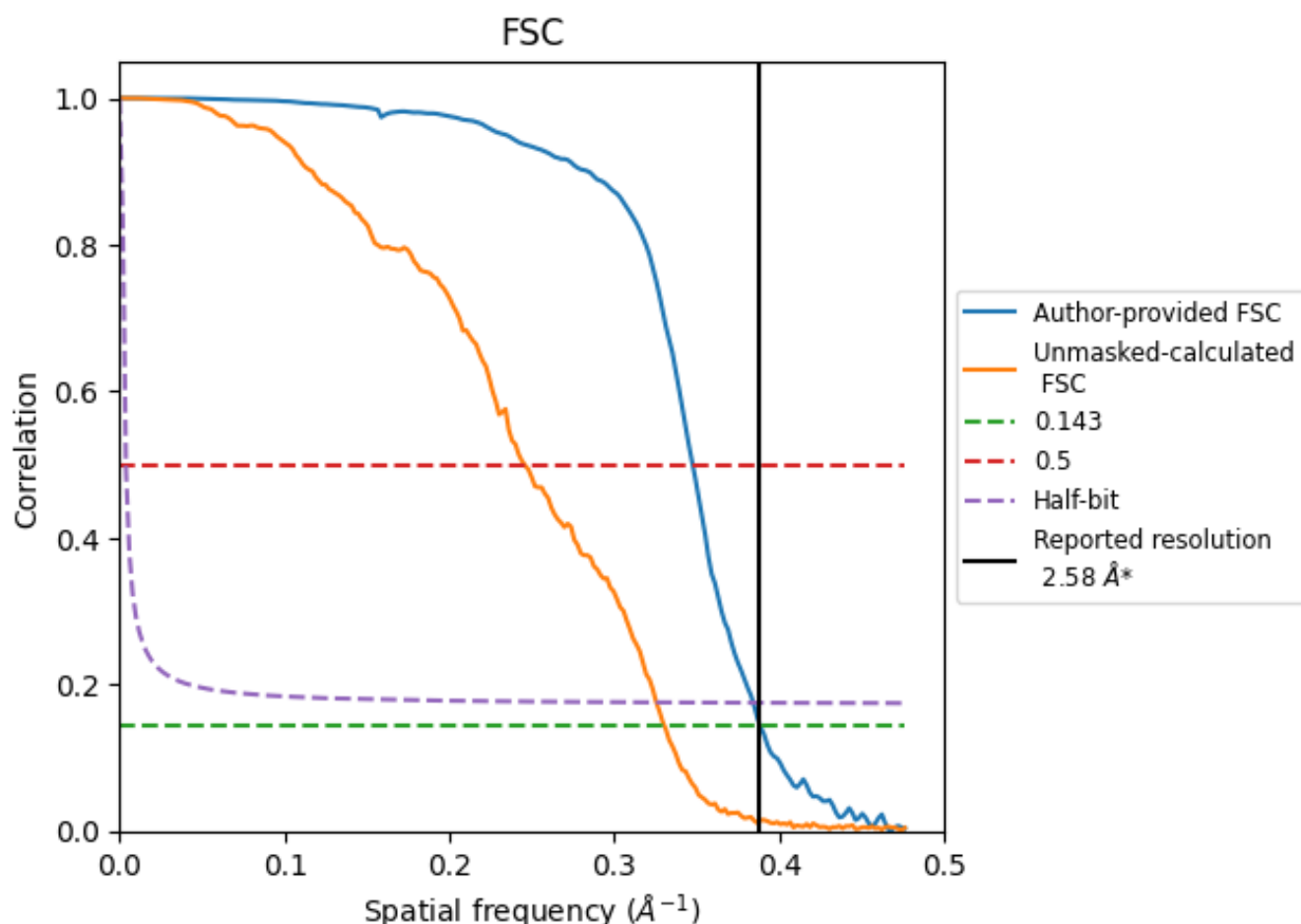


*Reported resolution corresponds to spatial frequency of 0.388 Å⁻¹

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 0.388 \AA^{-1}

8.2 Resolution estimates [i](#)

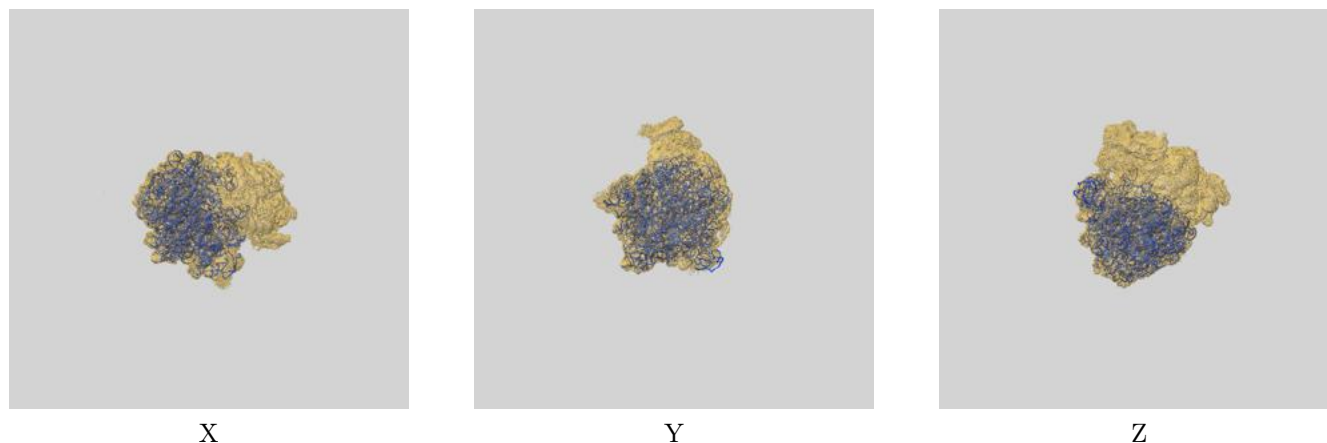
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	2.57	2.88	2.60
Unmasked-calculated*	3.03	4.07	3.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.03 differs from the reported value 2.58 by more than 10 %

9 Map-model fit [i](#)

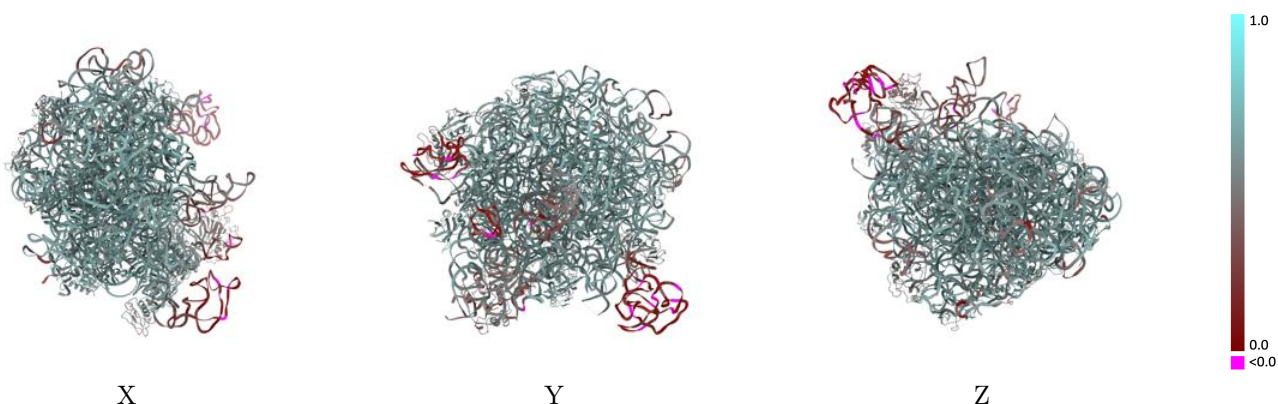
This section contains information regarding the fit between EMDB map EMD-10891 and PDB model 6YS3. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



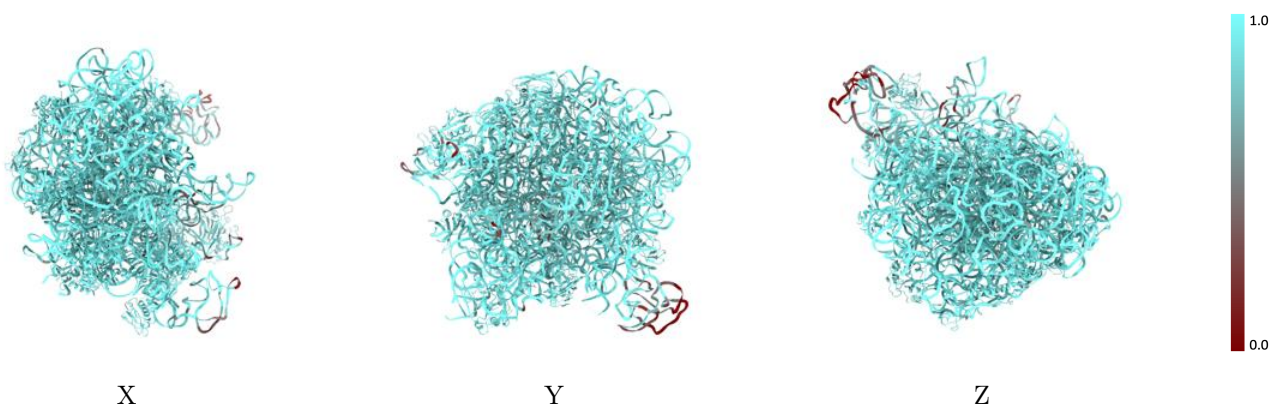
The images above show the 3D surface view of the map at the recommended contour level 0.00741 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



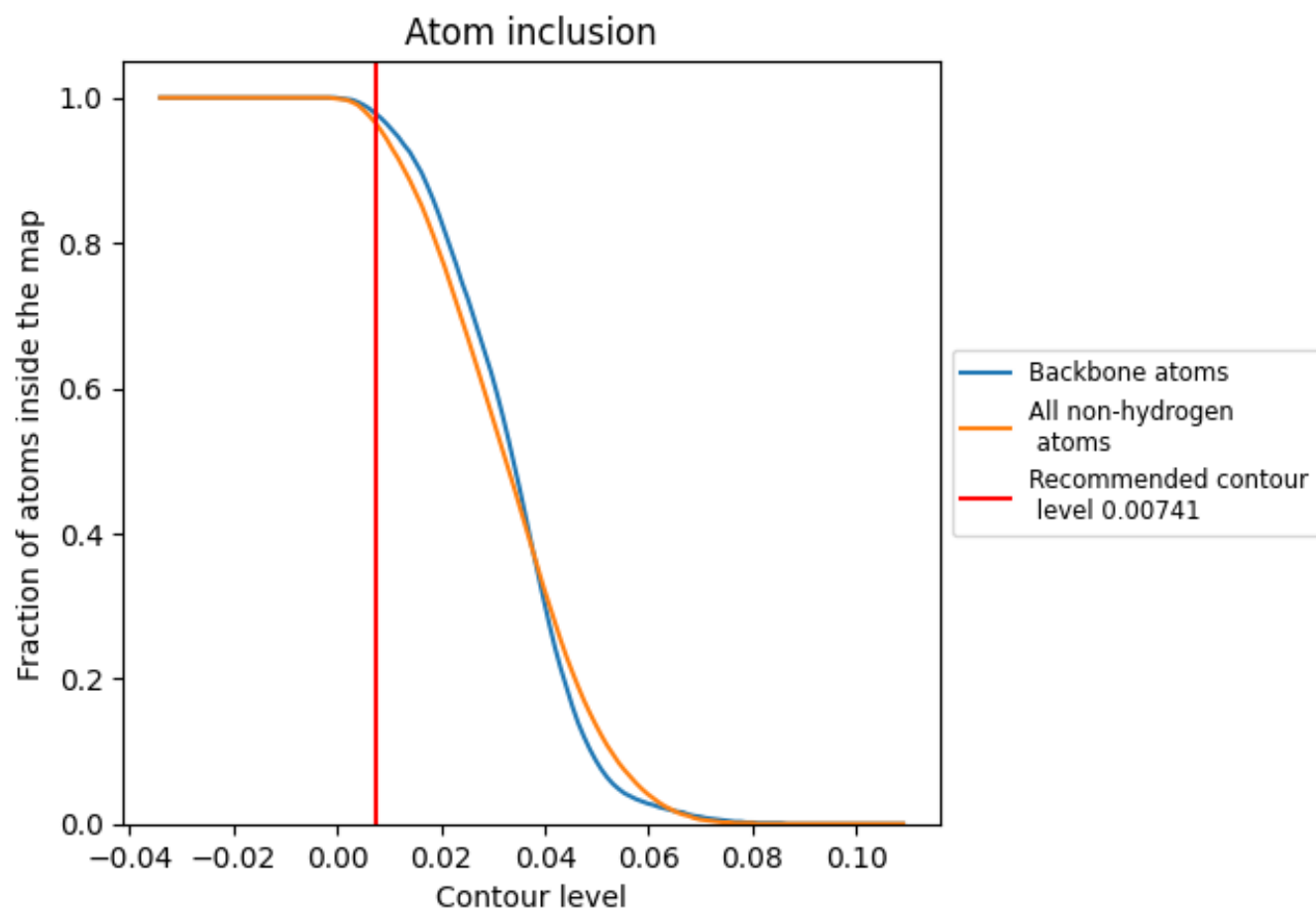
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00741).



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.00741) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9650	 0.5680
0	 0.9680	 0.5890
1	 0.9250	 0.5280
2	 0.9630	 0.5880
3	 0.9830	 0.6010
4	 0.9280	 0.5590
6	 0.9800	 0.6240
7	 0.9800	 0.6330
8	 0.9690	 0.5930
a	 0.9870	 0.5370
b	 0.9750	 0.5750
c	 0.9720	 0.6040
d	 0.9630	 0.6020
e	 0.9400	 0.5640
f	 0.8810	 0.3830
g	 0.9220	 0.4980
h	 0.8870	 0.4860
j	 0.9660	 0.6040
k	 0.9560	 0.5900
l	 0.9610	 0.5910
m	 0.9660	 0.6000
n	 0.9860	 0.6090
o	 0.9470	 0.4960
p	 0.9410	 0.5770
q	 0.9770	 0.6140
r	 0.9560	 0.5860
s	 0.9610	 0.6020
t	 0.9430	 0.5570
u	 0.9450	 0.5310
v	 0.7420	 0.3480
w	 0.9420	 0.5670
y	 0.9730	 0.6070
z	 0.7430	 0.3460

