



wwPDB EM Validation Summary Report ⓘ

Dec 16, 2024 – 02:42 PM EST

PDB ID : 9BS0
EMDB ID : EMD-44849
Title : YphC-treated 45SYphC particle. Class 5
Authors : Arpin, D.; Ortega, J.
Deposited on : 2024-05-12
Resolution : 3.30 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

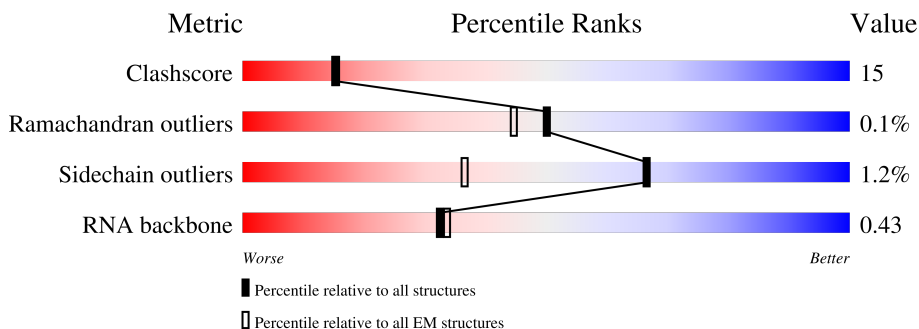
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 Å.

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





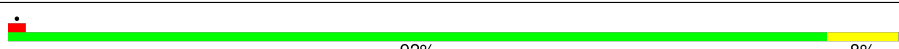
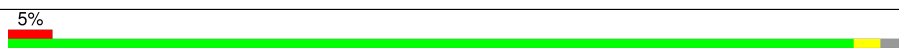
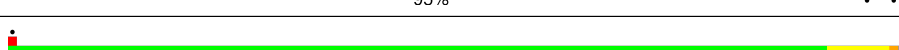
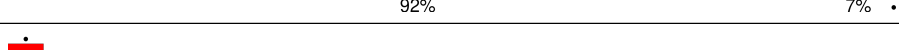
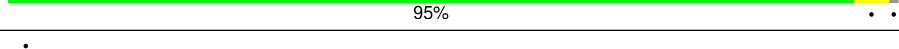

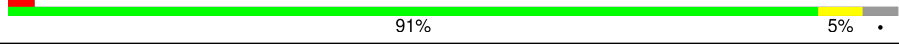



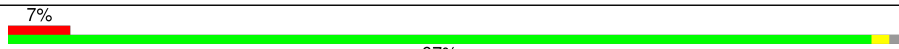
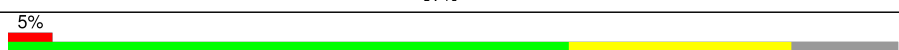

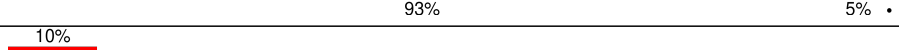


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	2927	
2	B	119	
3	C	277	
4	D	209	
5	E	207	
6	F	179	
7	G	145	

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Mol	Chain	Length	Quality of chain
8	H	122	 90% 9%
9	I	146	 75% 5% 20% 7%
10	J	120	 92% 8%
11	K	115	 95%
12	L	118	 92% 7%
13	M	102	 95%
14	N	113	 88% 8%
15	O	95	 91% 5%
16	P	103	 87% 10%
17	Q	94	 57% 9% 34%
18	R	66	 92% 6%
19	S	59	 97% 7%
20	T	59	 63% 25% 12%
21	U	44	 93% 5%
22	V	120	 82% 7% 12% 10%
23	W	436	 84% 10% 6% 21%
24	Z	49	 76% 20%
25	Y	232	 54% 19% 23% 58%

2 Entry composition [i](#)

There are 26 unique types of molecules in this entry. The entry contains 81446 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2678	57517	25661	10633	18545	2678	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	267	C	U	conflict	GB 1775206404
A	640	U	C	conflict	GB 1775206404
A	1558	C	G	conflict	GB 1775206404

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	111	2375	1059	433	772	111	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	266	1977	1231	381	361	4	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	184	1351	852	238	257	4	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	205	1499	938	275	285	1	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	65	468	288	87	91	2	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	144	1121	709	206	202	4	0	0

- Molecule 8 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	121	880	546	164	167	3	0	0

- Molecule 9 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	117	854	532	161	160	1	0	0

- Molecule 10 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	119	933	572	185	172	4	0	0

- Molecule 11 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	K	112	869	553	168	148	0	0

- Molecule 12 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	117	904	566	182	153	3	0	0

- Molecule 13 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	101	Total	C	N	O	0	0
			770	491	134	145		

- Molecule 14 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	109	Total	C	N	O	S	0	0
			824	514	158	150	2		

- Molecule 15 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	91	Total	C	N	O	S	0	0
			725	452	133	137	3		

- Molecule 16 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	93	Total	C	N	O	S	0	0
			686	433	127	124	2		

- Molecule 17 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	62	Total	C	N	O	0	0
			398	244	77	77		

- Molecule 18 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	65	Total	C	N	O	S	0	0
			500	305	97	96	2		

- Molecule 19 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	58	Total	C	N	O	S	0	0
			447	275	87	84	1		

- Molecule 20 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	52	Total	C	N	O	S	0	0
			402	246	81	68	7		

- Molecule 21 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	44	Total	C	N	O	S	0	0
			363	219	88	54	2		

- Molecule 22 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace	
22	V	106	Total	C	N	O		0	0
			739	455	142	142			

- Molecule 23 is a protein called GTPase Der.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	411	Total	C	N	O	S	0	0
			3064	1942	526	590	6		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	70	THR	ALA	conflict	UNP P50743
W	98	SER	ALA	conflict	UNP P50743
W	159	CYS	VAL	conflict	UNP P50743
W	217	ALA	SER	conflict	UNP P50743
W	262	GLY	ALA	conflict	UNP P50743
W	269	ASN	GLU	conflict	UNP P50743
W	292	ILE	VAL	conflict	UNP P50743
W	311	GLN	GLU	conflict	UNP P50743
W	315	GLU	ASP	conflict	UNP P50743
W	325	VAL	ILE	conflict	UNP P50743

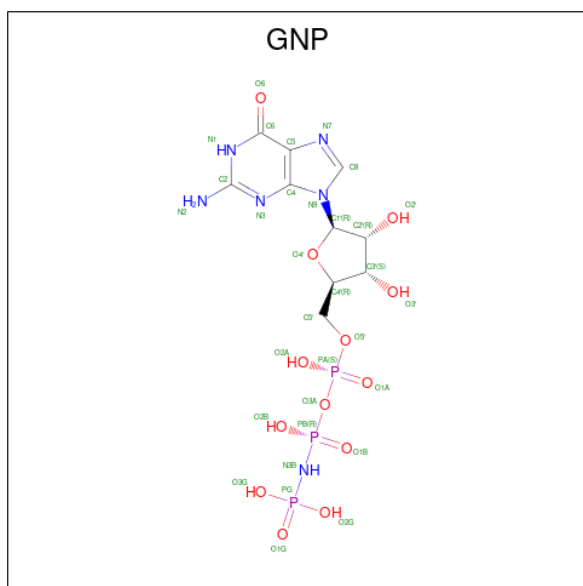
- Molecule 24 is a protein called Large ribosomal subunit protein bL33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	47	Total	C	N	O	S	0	0
			373	227	71	72	3		

- Molecule 25 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Y	178	1343	857	227	255	4	0	0

- Molecule 26 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).

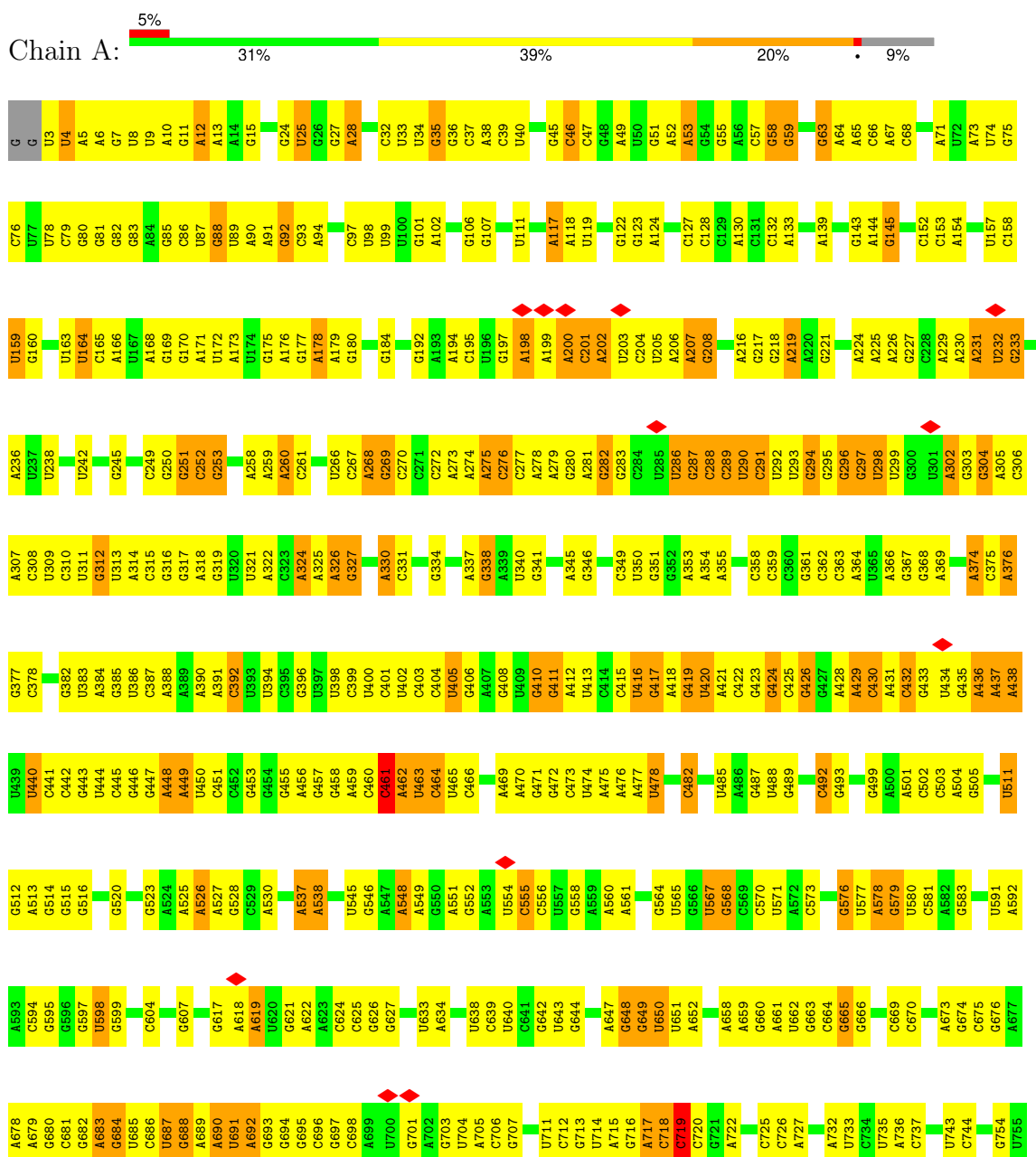


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
26	W	1	32	10	6	13	3	0
26	W	1	32	10	6	13	3	0

3 Residue-property plots [i](#)

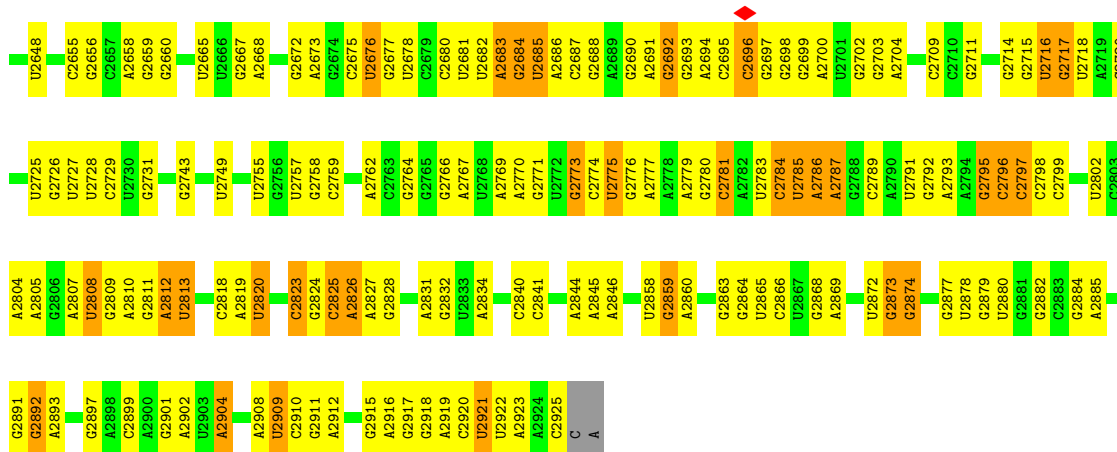
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 23S rRNA

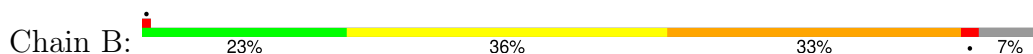


U1716	C1623	A1490	G1414	A1326	U1163	G1030	C961	U900	G824	U756
G1719	U1624	A1491	C1416	U1327	C1164	C1031	C962	U901	G825	C757
A1722	C1625	C1492	G1417	C1328	U1165	C1037	G963	G902	A758	A758
A1723	U1626	C1493	A1418	C1329	G1166	C1037	A964	G903	G827	G760
A1724	C1629	G1494	G1419	C1331	C1167	A1042	A965	A904	A829	U761
U1725	G1630	C1495	G1420	U1332	U1248	A1044	G966	G905	G829	A762
U1726	A1631	G1496	A1424	C1333	G1260	A1046	G967	G906	A830	A762
A1727	C1632	U1497	G1425	G1337	U1251	A1047	C968	A908	A763	C764
C1728	U1633	U1498	A1426	C1338	G1252	A1047	C969	A909	A765	A765
C1731	U1634	U1499	G1427	A1339	A1172	C1053	A970	A910	A835	A766
C1732	G1635	U1500	A1428	A1340	A1173	C1053	A971	A911	A836	C766
U1733	U1636	U1501	G1429	U1341	A1174	C1054	U972	G912	U837	U767
U1734	C1651	G1502	U1430	U1342	A1175	A1055	G973	C912	C838	G768
A1735	U1652	U1503	U1431	G1342	U1176	A1056	A974	A913	G769	A769
C1736	A1653	U1504	A1432	C1343	U1177	G1057	C975	C914	A770	A770
C1737	U1654	U1505	U1433	U1344	U1178	U1060	A978	U915	G772	G772
A1738	G1655	A1506	A1434	C1344	A1179	A1059	C981	A916	G773	G773
C1739	C1656	U1507	U1435	U1345	C1180	A1061	U982	G917	G774	G774
A1743	U1657	C1508	U1436	A1346	C1082	C1062	U983	A918	A774	A774
G1744	C1657	U1509	U1437	A1347	C1181	U1063	G984	U919	G775	G775
A1745	U1658	G1510	C1438	U1352	C1182	U1064	U985	G920	G776	G776
A1746	G1574	C1511	U1439	C1353	G1185	U1065	U986	A921	C777	C777
G1747	U1579	U1512	G1440	C1354	C1186	A1066	U987	A922	C778	C778
A1661	A1580	U1513	U1441	U1355	U1187	A1067	U988	C	C783	C783
G1664	U1581	C1514	A1442	U1356	A1188	G1068	U989	A	C784	C784
G1665	A1582	C1515	G1443	G1357	G1188	U1069	U990	G	C785	C785
G1666	U1583	A1516	U1444	U1358	G1192	C1279	C990	G	C786	C786
G1667	A1584	A1517	A1445	G1359	U1193	U1070	A991	G	C787	C787
G1668	U1585	G1518	U1446	A1360	U1193	A1071	C992	G	C788	C788
C1669	A1586	G1519	U1447	A1361	A1194	A1072	C	C	C789	C789
C1670	U1587	A1520	C1449	G1362	G1285	A1073	U995	C	C790	C790
A1671	U1588	U1521	C1455	C1363	U1289	A1074	A999	C	C791	C791
A1672	A1588	U1522	U1456	C1364	G1292	A1075	G1000	C	C792	C792
G1673	A1592	A1523	A1457	U1373	A1201	A1076	U1001	C	U869	U869
G1674	U1592	U1524	U1458	C1374	G1293	A1077	G1001	C	U870	U870
A1675	G1593	G1525	U1459	A1375	A1293	U1078	U1002	C	A871	A871
A1676	U1594	U1526	U1460	G1376	G1296	U1079	G1003	C	C872	C872
U1681	U1595	C1527	G1461	U1379	A1302	U1080	U1004	G	U873	U873
C1682	U1596	C1527	G1462	U1380	U1211	U1081	U1005	G	U874	U874
A1685	C1597	U1528	A1463	U1381	G1213	G1083	A1006	G	U875	U875
A1686	U1598	G1529	A1464	U1382	U1214	U1084	U1007	G	U876	U876
A1691	G1600	U1530	A1465	C1384	U1215	G1085	U1008	A	A877	A877
U1692	U1603	A1533	G1471	G1385	U1216	U1087	U1009	C	G877	G877
C1693	C1604	U1534	U1472	U1386	U1217	C1087	C1010	C	G878	G878
A1695	G1605	U1535	A1473	C1387	U1218	U1088	C1011	C	G879	G879
G1696	U1606	A1536	C1474	A1388	C1219	G1089	A948	C	C880	C880
C1697	C1607	G1537	G1475	C1389	G1220	U1090	U949	C	G881	G881
A1698	U1608	U1538	U1476	U1390	A1221	U1091	U950	C	A808	A808
U1699	U1610	A1540	A1477	A1392	U1222	A1092	U951	C	U809	U809
G1706	A1614	U1541	G1478	G1400	C1223	G1093	A888	C	G810	G810
A1709	G1615	A1542	U1479	A1401	G1225	C1095	A889	C	A811	A811
G1712	U1616	C1545	G1480	U1404	G1226	U1096	G891	C	G812	G812
A1788	G1617	U1546	U1481	A1404	U1227	A1097	C955	C	G813	G813
A1789	A1618	U1547	A1482	U1411	G1228	C1098	A856	C	G818	G818
U1790	U1619	U1548	U1483	A1412	U1229	C	A957	C	G822	G822
A1791	C1715	U1549	A1484	A1412	A1230	A	A958	C	G822	G822
		C1550	U1485	A1485	G1231	G	C1028	C	U899	U899
		C1551	A1485	G1413	G1231	G	A1029	C	C999	C999

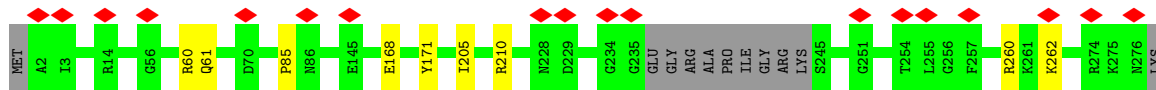
G1792	C1866	G1826	C	G2076	C2142	A2902	C2969	A3239	A2389	G2450	G	G2572
G1793	C1867	U1927	C	G2077	A2143	C2203	A2270	A2330	A2390	C2451	A	U2573
G1798	C1868	A1928	G	A2083	G2144	U2204	G2271	U2331	G2391	U2452	C2512	U2574
G1799	G1869	A1929	A	A2084	G2145	A2205	U2272	G2332	G2392	C2453	G2513	U2575
A1802	G1870	A	C	C2084	A2146	C2206	U2273	G2333	C2393	A2454	G2514	U2576
A1803	C1871	C	C	C2085	U2147	C2207	U	U	A2455	C2456	G2515	G2577
U1804	C1872	C	C	G2086	A2148	U2209	G	G	A2456	C2457	G2516	C2580
G1875	U1873	C	C	G2087	G2149	G2210	A	G	C2458	U2457	A2517	U2581
U1808	G1874	C	C	A2088	G2150	G2211	U	A	G2459	G2458	G2519	U2582
A1809	A1876	C	C	A2089	U2151	C2212	U	A	G2460	U2460	U2520	U2583
G1810	A1877	C	C	G2090	A2152	U2213	G	A	A2461	A2461	U2521	U2584
C1811	A1878	C	C	A2091	G2153	G2214	C	C2342	A2462	A2462	U2522	C2585
A1813	G1879	C	C	G2092	A2154	U2215	G	U2343	G2463	A2463	G2523	C2586
A1814	U1880	C	C	C2093	G2155	U2216	G	U2344	A2406	A2464	G2524	C2587
A1815	U1881	C	C	G2094	A2156	U2217	C	U2345	A2407	G2465	G2525	C2588
A1816	U1882	C	C	C2095	C2157	G2218	U	U2346	A2408	C2466	A2526	U2591
C1817	A1883	C	C	G2096	U2159	A2220	C	G2347	G2408	U2467	C	U2592
A1818	G1884	C	C	U2097	U2160	C2221	G	C2348	U2409	U2468	C	U2593
C1819	A1885	U	U	G2098	G2161	G2222	C2289	A2349	C2410	A2469	U	U2594
A1820	G1886	A	A	A2100	G2162	U2223	C2290	G2350	G2411	C2468	C	A2595
U1823	A1887	A	A	G2101	A2163	U2224	U2291	A2351	C2412	C2469	C	A2596
C1824	G1888	C	C	C2102	A2164	C2225	C2292	G2352	G2413	C2470	G	U2597
U1825	U1889	G	G	U2103	A2165	U2226	U2293	U2353	C2414	C2471	A	C2598
C1826	C1890	U	U	U2104	C2166	A2227	U2294	G2354	U2415	C2472	U	U2599
U1827	G	C	C	U2105	C2167	A2228	C2295	U2355	U2416	G	C	U2600
G1828	C	C	C	U2106	G2168	G2231	C2296	A2296	U2416	G	C	A
C1829	U	U	U	C2023	A2169	C2232	C2297	A2297	A2317	G	C	C
G1830	U	U	U	U2107	A2170	U2233	C2298	A2298	A2318	G	C	C
A1831	A	A	A	U2108	G2171	U2234	U2299	G2359	G2319	A	C	C
A1832	C	C	C	G2109	C2172	C2235	G2299	G2360	G2320	U	C	C
G1833	C	C	C	A2026	G2173	U2236	G2300	C2361	G2420	U	C	C
C1834	G	G	G	G2029	C2174	U2237	U2301	A2362	A2421	A	C	C
A1838	C	C	C	A2030	C2175	U2238	A2302	A2363	U2422	C	C	C
A1839	C	C	C	G2031	A2176	U2240	A2303	A2364	C2423	A	C	C
G1840	C	C	C	C2112	G2177	A2241	C2304	A2365	G2424	G	C	C
G1841	C	C	C	G2113	C2178	U2242	G2305	G2366	G2425	G	C	C
C1842	C	C	C	C2114	U2179	U2243	G2306	G2367	U2426	U	C	C
A1845	C	C	C	U2115	U2180	G2244	A2307	G2368	U2427	U	C	C
U1848	C	C	C	G2116	C2181	G2248	G2308	A2369	G2428	U	C	C
U1849	C	C	C	A2119	G2182	G2249	G2309	G2370	G2429	U	C	C
A1850	C	C	C	U2120	U2183	G2249	G2310	G2371	U2430	U	C	C
G1851	C	C	C	U2121	G2184	G2249	G2311	U2372	U2431	U	C	C
G1854	C	C	C	G2122	G2185	G2249	C2312	U2373	C2432	U	C	C
C1855	C	C	C	A2049	G2186	G2249	C2313	G2374	G2433	U	C	C
A1858	C	C	C	G2050	A2187	U2249	C2314	A2375	G2434	U	C	C
U1915	C	C	C	U2051	G2188	U2249	A2315	C2376	C2435	U	C	C
G1917	C	C	C	A2052	G2189	U2249	A2316	U2377	A2436	U	C	C
A1918	C	C	C	A2060	C2190	G2249	A2317	U2378	U2437	U	C	C
A1919	C	C	C	G2061	A2191	G2249	G2318	C2379	G2438	U	C	C
C1920	C	C	C	G2062	U2192	U2260	G2319	G2380	G2439	U	C	C
C1922	C	C	C	U2063	C2193	C2261	U2320	A2381	A2440	U	C	C
C1923	C	C	C	G2064	G2194	A2262	U2321	G2382	A2441	U	C	C
C1924	C	C	C	A2066	G2195	G2263	C2322	A2383	G2442	U	C	C
A1925	C	C	C	G2067	U2196	U2265	C2323	C2384	U2443	U	C	C
	C	C	C	U2070	G2197	U2266	U2324	C2385	G2444	U	C	C
	C	C	C	A2071	U2137	G2266	U2325	U2386	C2445	U	C	C
	C	C	C	U2072	U2138	G2267	U2326	C2446	C2446	U	C	C
	C	C	C		U2140	G2268	G2328	C2388	C2449	U	C	C
	C	C	C		A2141					U	C	C



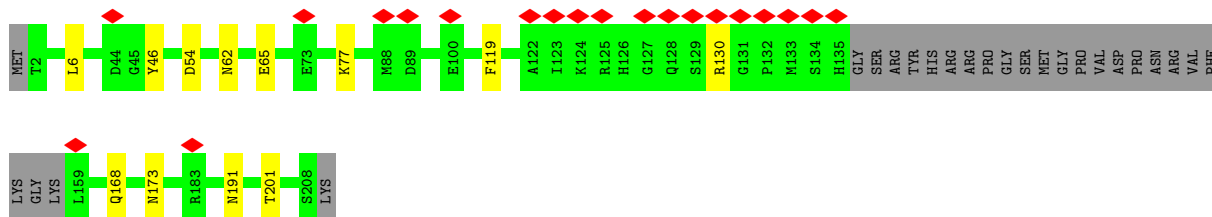
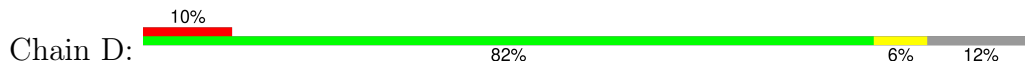
• Molecule 2: 5S rRNA



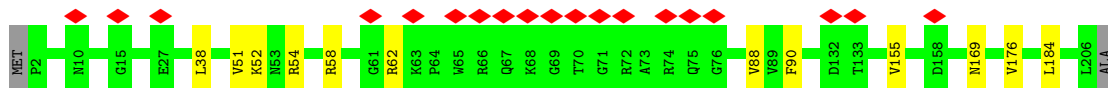
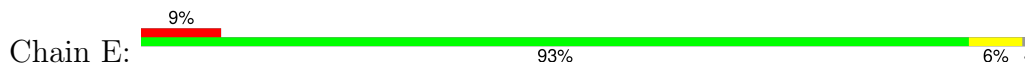
• Molecule 3: Large ribosomal subunit protein uL2




• Molecule 4: Large ribosomal subunit protein uL3

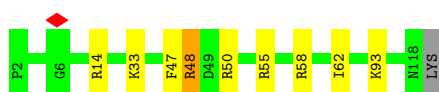


• Molecule 5: Large ribosomal subunit protein uL4



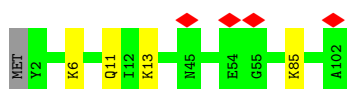
- Molecule 12: Large ribosomal subunit protein bL20

Chain L:  92% 7% ..




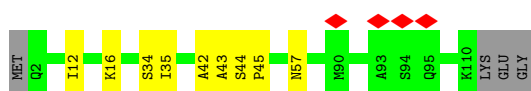
- Molecule 13: Large ribosomal subunit protein bL21

Chain M:  95% ..



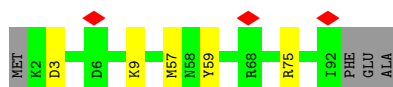
- Molecule 14: Large ribosomal subunit protein uL22

Chain N:  88% 8% .




- Molecule 15: Large ribosomal subunit protein uL23

Chain O:  91% 5% .



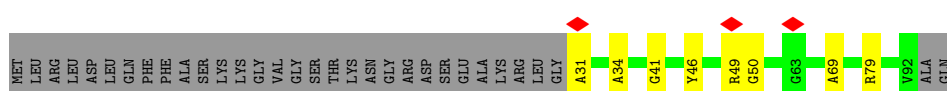
- Molecule 16: Large ribosomal subunit protein uL24

Chain P:  87% 10% .

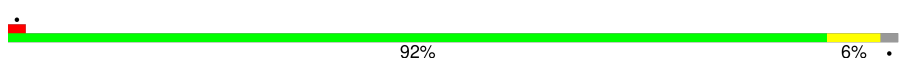


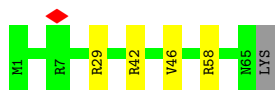
- Molecule 17: Large ribosomal subunit protein bL27

Chain Q:  57% 9% 34%

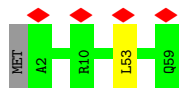


- Molecule 18: Large ribosomal subunit protein uL29

Chain R:  92% 6% .



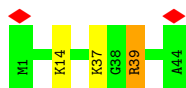
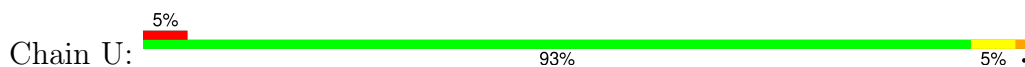
• Molecule 19: Large ribosomal subunit protein uL30



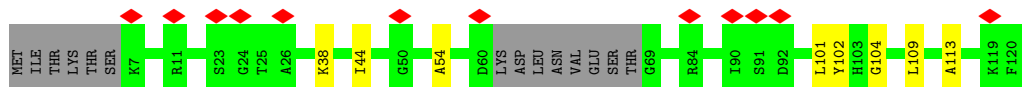
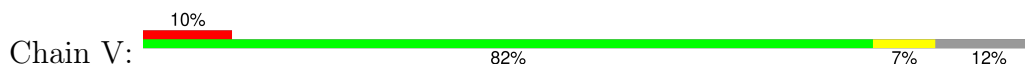
• Molecule 20: Large ribosomal subunit protein bL32



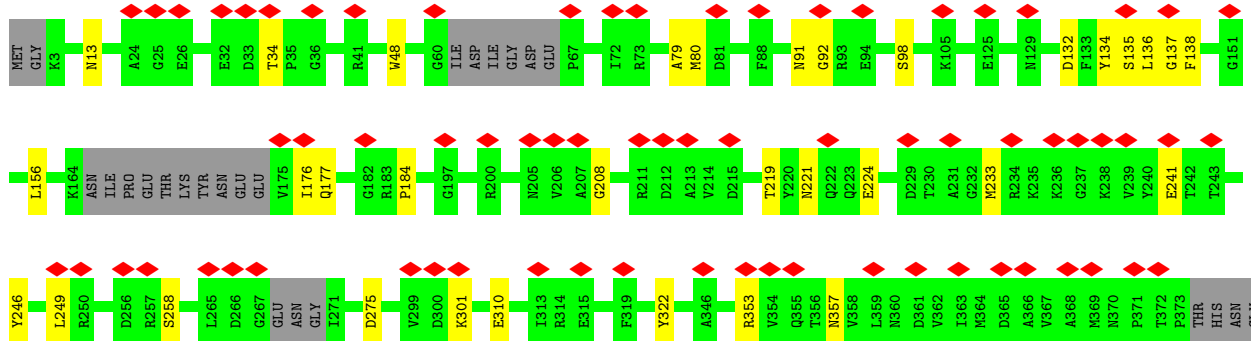
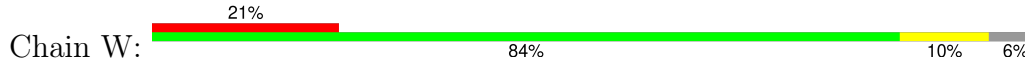
• Molecule 21: Large ribosomal subunit protein bL34

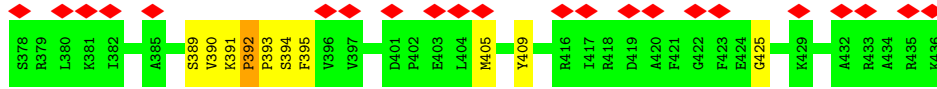


• Molecule 22: Large ribosomal subunit protein uL18

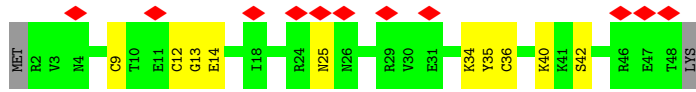
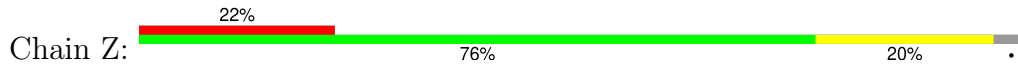


• Molecule 23: GTPase Der

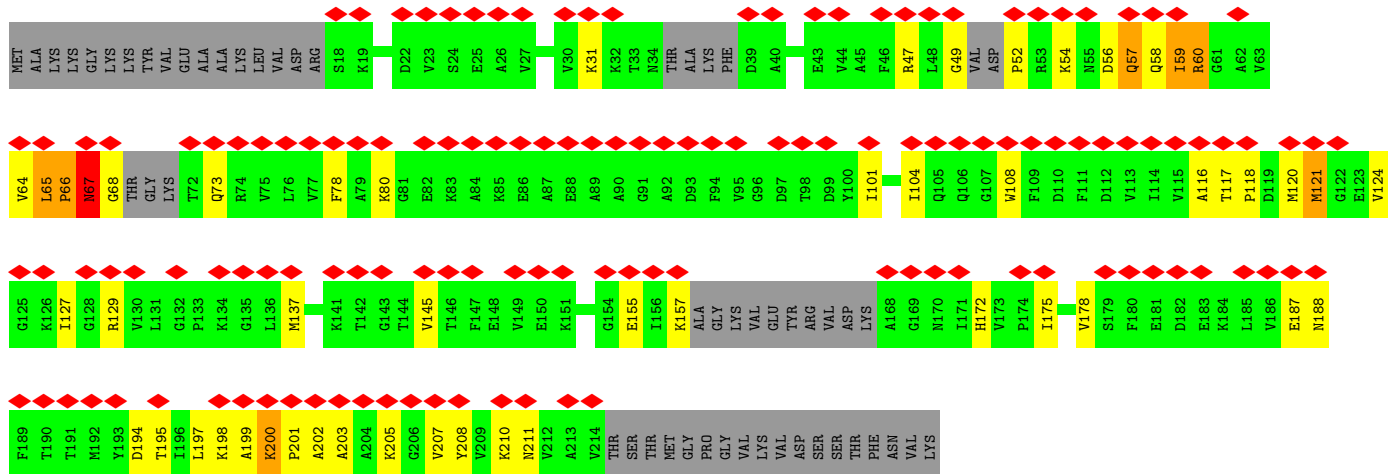




• Molecule 24: Large ribosomal subunit protein bL33A



• Molecule 25: Large ribosomal subunit protein uL1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18086	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2750	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.941	Depositor
Minimum map value	-0.280	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.255	Depositor
Map size (\AA)	362.52002, 362.52002, 362.52002	wwPDB
Map dimensions	424, 424, 424	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.855, 0.855, 0.855	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: GNP

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	0.54	0/64420	0.88	47/100477 (0.0%)
2	B	0.36	0/2655	0.85	3/4136 (0.1%)
3	C	0.32	0/2011	0.57	0/2710
4	D	0.31	0/1365	0.59	0/1834
5	E	0.33	0/1516	0.55	0/2057
6	F	0.28	0/472	0.57	0/634
7	G	0.32	0/1144	0.57	0/1543
8	H	0.36	0/887	0.66	1/1200 (0.1%)
9	I	0.32	0/860	0.62	0/1146
10	J	0.33	0/940	0.68	0/1260
11	K	0.37	0/882	0.65	0/1189
12	L	0.40	0/916	0.60	0/1224
13	M	0.35	0/781	0.60	0/1051
14	N	0.33	0/833	0.62	0/1125
15	O	0.40	0/731	0.78	1/977 (0.1%)
16	P	0.34	0/694	0.62	0/928
17	Q	0.35	0/404	0.66	0/549
18	R	0.30	0/501	0.61	0/674
19	S	0.34	0/449	0.71	0/605
20	T	0.34	0/409	0.65	0/544
21	U	0.32	0/366	0.72	0/479
22	V	0.27	0/745	0.60	0/1006
23	W	0.31	0/3115	0.58	0/4237
24	Z	0.35	0/378	0.68	0/508
25	Y	0.34	0/1361	0.69	1/1833 (0.1%)
All	All	0.49	0/88835	0.83	53/133926 (0.0%)

There are no bond length outliers.

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1433	U	C2-N1-C1'	7.30	126.46	117.70
1	A	461	C	C2-N1-C1'	7.06	126.57	118.80
1	A	1921	C	N3-C2-O2	-6.89	117.08	121.90
1	A	461	C	N1-C2-O2	6.85	123.01	118.90
25	Y	54	LYS	N-CA-CB	-6.75	98.45	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	57517	0	28951	1602	0
2	B	2375	0	1203	78	0
3	C	1977	0	1995	6	0
4	D	1351	0	1384	12	0
5	E	1499	0	1523	9	0
6	F	468	0	460	12	0
7	G	1121	0	1145	11	0
8	H	880	0	895	6	0
9	I	854	0	886	13	0
10	J	933	0	956	8	0
11	K	869	0	883	3	0
12	L	904	0	921	16	0
13	M	770	0	791	2	0
14	N	824	0	861	7	0
15	O	725	0	759	4	0
16	P	686	0	724	2	0
17	Q	398	0	311	12	0
18	R	500	0	491	4	0
19	S	447	0	469	1	0
20	T	402	0	403	12	0
21	U	363	0	399	3	0
22	V	739	0	700	5	0
23	W	3064	0	2926	66	0
24	Z	373	0	355	9	0
25	Y	1343	0	1366	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	W	64	0	26	1	0
All	All	81446	0	51783	1886	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 15.

The worst 5 of 1886 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)
23:W:132:ASP:HA	25:Y:137:MET:CE	1.33	1.55
23:W:132:ASP:CA	25:Y:137:MET:HE1	1.35	1.52
23:W:389:SER:OG	23:W:394:SER:HB2	1.21	1.36
23:W:134:TYR:O	25:Y:129:ARG:CD	1.83	1.26
1:A:2351:A:H2	1:A:2361:C:N4	1.31	1.26

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	
3	C	262/277 (95%)	238 (91%)	24 (9%)	0	100	100
4	D	180/209 (86%)	170 (94%)	10 (6%)	0	100	100
5	E	203/207 (98%)	189 (93%)	14 (7%)	0	100	100
6	F	61/179 (34%)	59 (97%)	2 (3%)	0	100	100
7	G	142/145 (98%)	130 (92%)	12 (8%)	0	100	100
8	H	119/122 (98%)	106 (89%)	13 (11%)	0	100	100
9	I	111/146 (76%)	105 (95%)	6 (5%)	0	100	100
10	J	117/120 (98%)	108 (92%)	9 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	110/115 (96%)	103 (94%)	7 (6%)	0	100	100
12	L	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
13	M	99/102 (97%)	89 (90%)	10 (10%)	0	100	100
14	N	107/113 (95%)	100 (94%)	7 (6%)	0	100	100
15	O	89/95 (94%)	81 (91%)	8 (9%)	0	100	100
16	P	89/103 (86%)	80 (90%)	9 (10%)	0	100	100
17	Q	60/94 (64%)	56 (93%)	4 (7%)	0	100	100
18	R	63/66 (96%)	58 (92%)	5 (8%)	0	100	100
19	S	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
20	T	50/59 (85%)	46 (92%)	4 (8%)	0	100	100
21	U	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
22	V	102/120 (85%)	94 (92%)	8 (8%)	0	100	100
23	W	401/436 (92%)	367 (92%)	33 (8%)	1 (0%)	44	71
24	Z	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
25	Y	168/232 (72%)	148 (88%)	18 (11%)	2 (1%)	11	38
All	All	2791/3210 (87%)	2572 (92%)	216 (8%)	3 (0%)	50	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	Y	66	PRO
25	Y	67	ASN
23	W	392	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	202/225 (90%)	202 (100%)	0	100	100
4	D	139/170 (82%)	138 (99%)	1 (1%)	81	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	155/170 (91%)	154 (99%)	1 (1%)	84	90
6	F	48/151 (32%)	47 (98%)	1 (2%)	48	70
7	G	117/123 (95%)	117 (100%)	0	100	100
8	H	92/101 (91%)	92 (100%)	0	100	100
9	I	85/110 (77%)	85 (100%)	0	100	100
10	J	94/100 (94%)	94 (100%)	0	100	100
11	K	85/100 (85%)	85 (100%)	0	100	100
12	L	86/97 (89%)	85 (99%)	1 (1%)	67	80
13	M	79/84 (94%)	78 (99%)	1 (1%)	65	79
14	N	86/93 (92%)	85 (99%)	1 (1%)	67	80
15	O	80/85 (94%)	79 (99%)	1 (1%)	65	79
16	P	74/87 (85%)	74 (100%)	0	100	100
17	Q	27/74 (36%)	27 (100%)	0	100	100
18	R	48/57 (84%)	48 (100%)	0	100	100
19	S	50/53 (94%)	50 (100%)	0	100	100
20	T	44/53 (83%)	43 (98%)	1 (2%)	45	68
21	U	38/39 (97%)	37 (97%)	1 (3%)	41	66
22	V	64/93 (69%)	63 (98%)	1 (2%)	58	76
23	W	309/372 (83%)	302 (98%)	7 (2%)	45	68
24	Z	41/47 (87%)	41 (100%)	0	100	100
25	Y	140/185 (76%)	130 (93%)	10 (7%)	12	37
All	All	2183/2669 (82%)	2156 (99%)	27 (1%)	66	80

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	W	395	PHE
25	Y	56	ASP
25	Y	200	LYS
23	W	409	TYR
25	Y	57	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
25	Y	188	ASN
25	Y	106	GLN
23	W	13	ASN
25	Y	67	ASN
21	U	6	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2666/2927 (91%)	919 (34%)	75 (2%)
2	B	109/119 (91%)	55 (50%)	5 (4%)
All	All	2775/3046 (91%)	974 (35%)	80 (2%)

5 of 974 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	12	A
1	A	13	A
1	A	15	G
1	A	25	U

5 of 80 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2374	G
1	A	2784	C
1	A	2400	G
1	A	2450	G
2	B	13	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	GNP	W	502	-	29,34,34	1.58	6 (20%)	33,54,54	2.22	5 (15%)
26	GNP	W	501	-	29,34,34	1.52	7 (24%)	33,54,54	2.18	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	GNP	W	502	-	-	5/14/38/38	0/3/3/3
26	GNP	W	501	-	-	6/14/38/38	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	W	502	GNP	PB-O3A	4.36	1.64	1.59
26	W	501	GNP	PB-O3A	3.24	1.63	1.59
26	W	501	GNP	C6-N1	3.11	1.38	1.33
26	W	501	GNP	PB-O1B	3.10	1.50	1.46
26	W	502	GNP	C6-N1	2.98	1.38	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	W	502	GNP	C5-C6-N1	-8.64	111.87	123.42
26	W	501	GNP	C5-C6-N1	-8.64	111.87	123.42
26	W	501	GNP	C2-N1-C6	6.65	125.21	115.96
26	W	502	GNP	C2-N1-C6	6.62	125.16	115.96
26	W	501	GNP	N3-C2-N1	-2.87	123.56	127.21

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

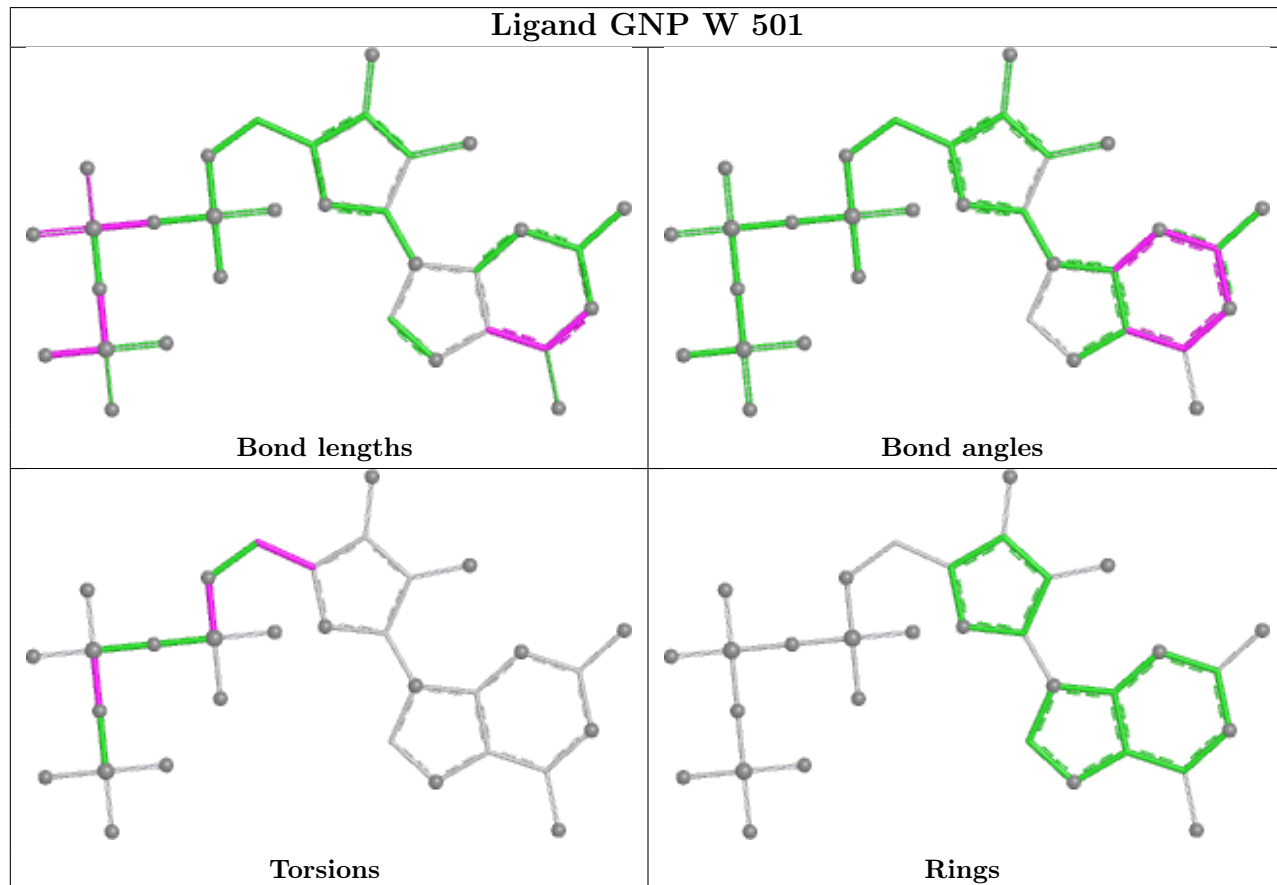
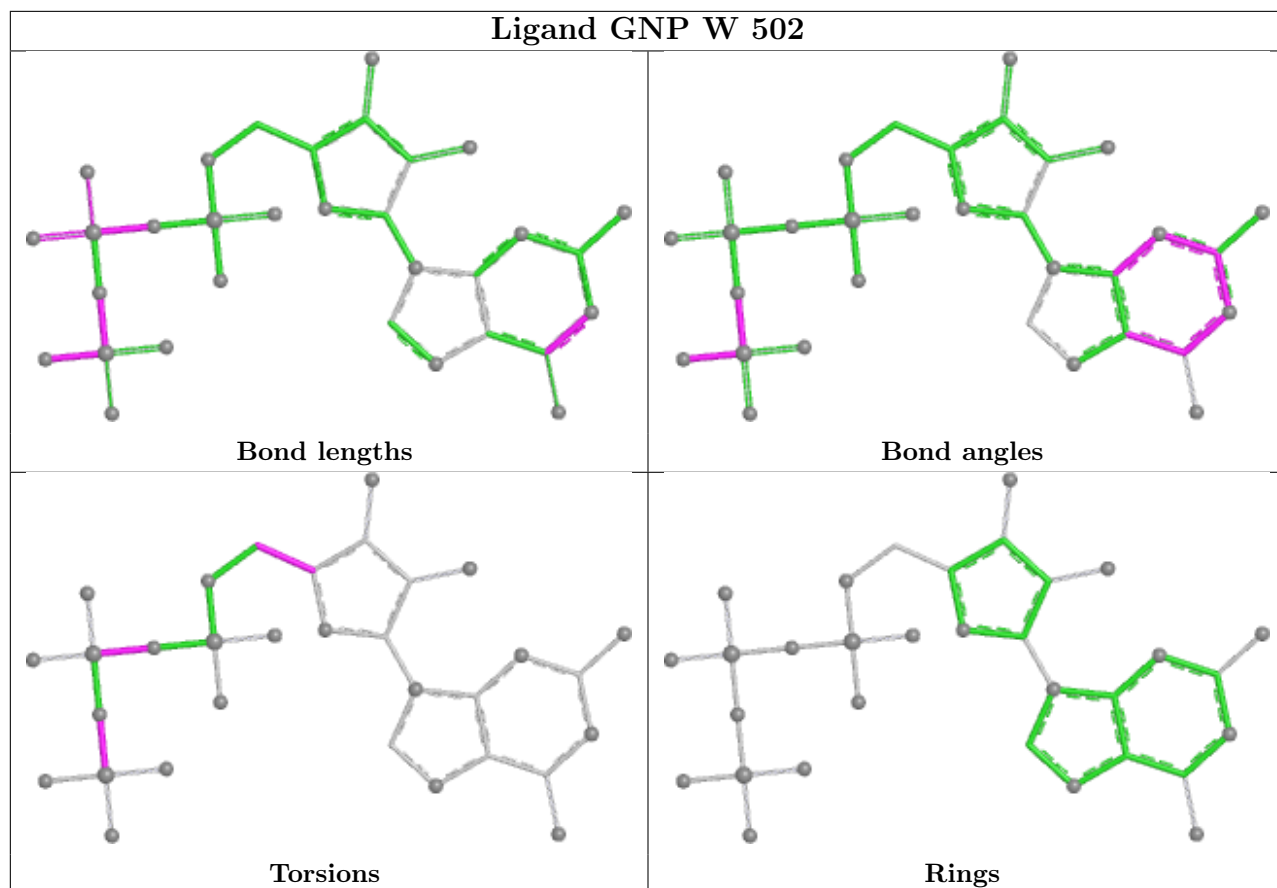
Mol	Chain	Res	Type	Atoms
26	W	501	GNP	PG-N3B-PB-O1B
26	W	501	GNP	C5'-O5'-PA-O3A
26	W	501	GNP	C5'-O5'-PA-O2A
26	W	501	GNP	O4'-C4'-C5'-O5'
26	W	502	GNP	PB-N3B-PG-O1G

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	W	502	GNP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

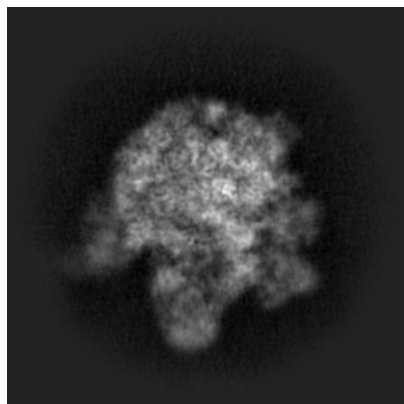
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44849. These allow visual inspection of the internal detail of the map and identification of artifacts.

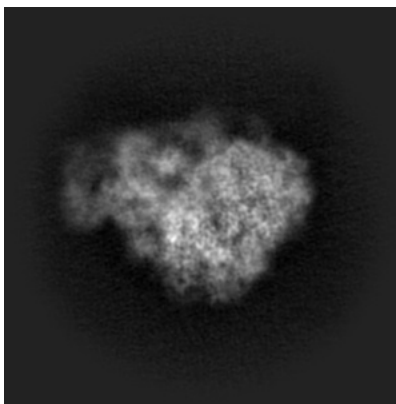
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

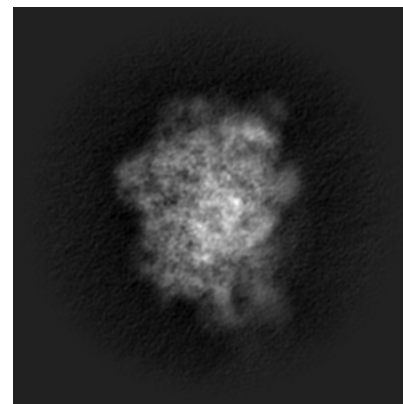
6.1.1 Primary map



X

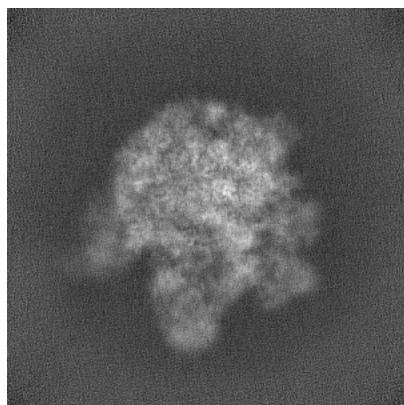


Y

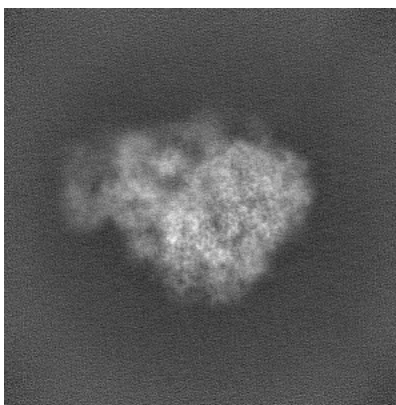


Z

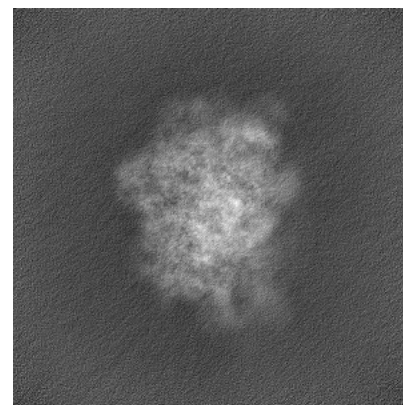
6.1.2 Raw map



X



Y

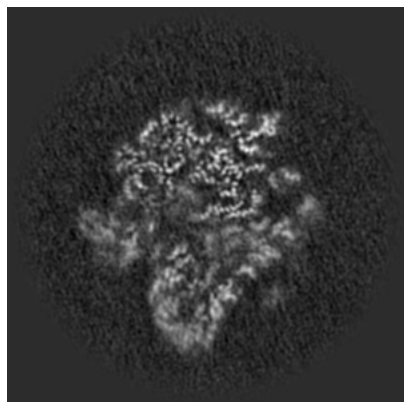


Z

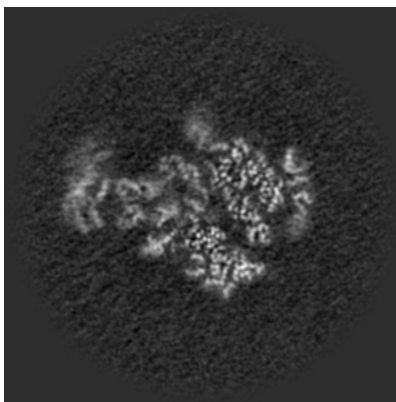
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

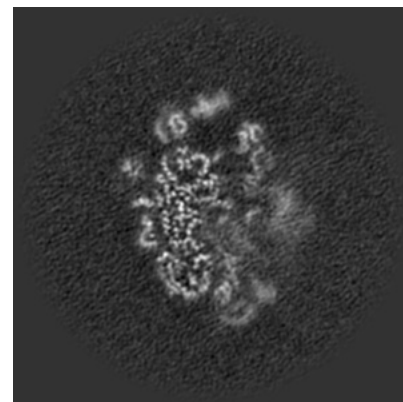
6.2.1 Primary map



X Index: 212

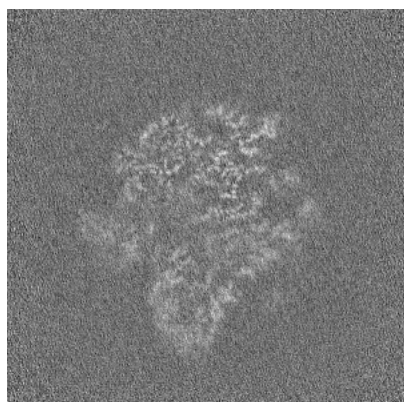


Y Index: 212

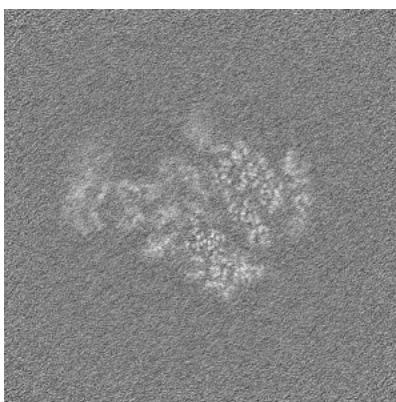


Z Index: 212

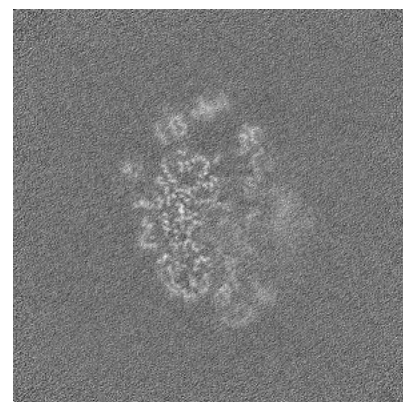
6.2.2 Raw map



X Index: 212



Y Index: 212

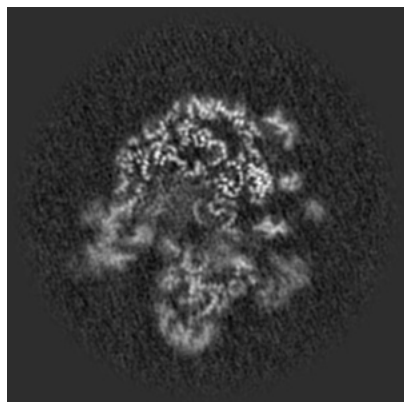


Z Index: 212

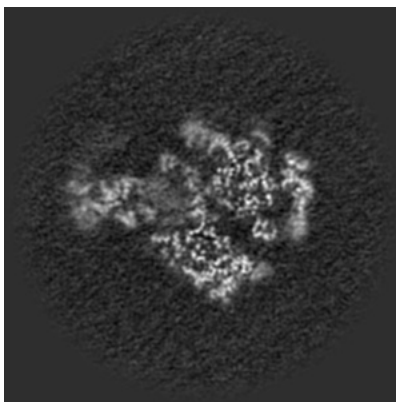
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

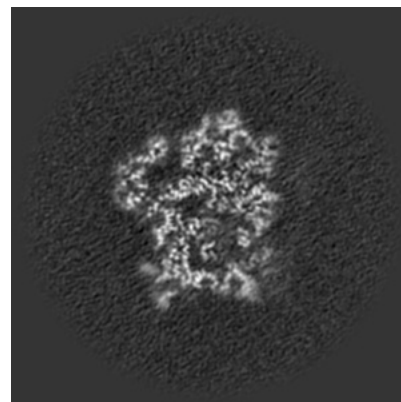
6.3.1 Primary map



X Index: 224

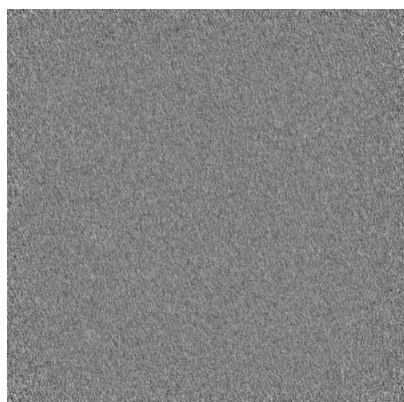


Y Index: 219

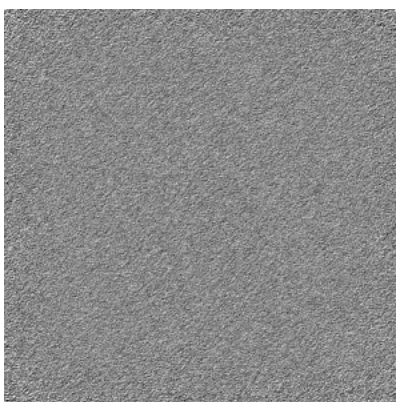


Z Index: 238

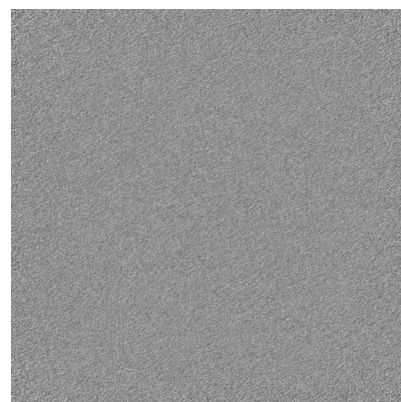
6.3.2 Raw map



X Index: 0



Y Index: 0

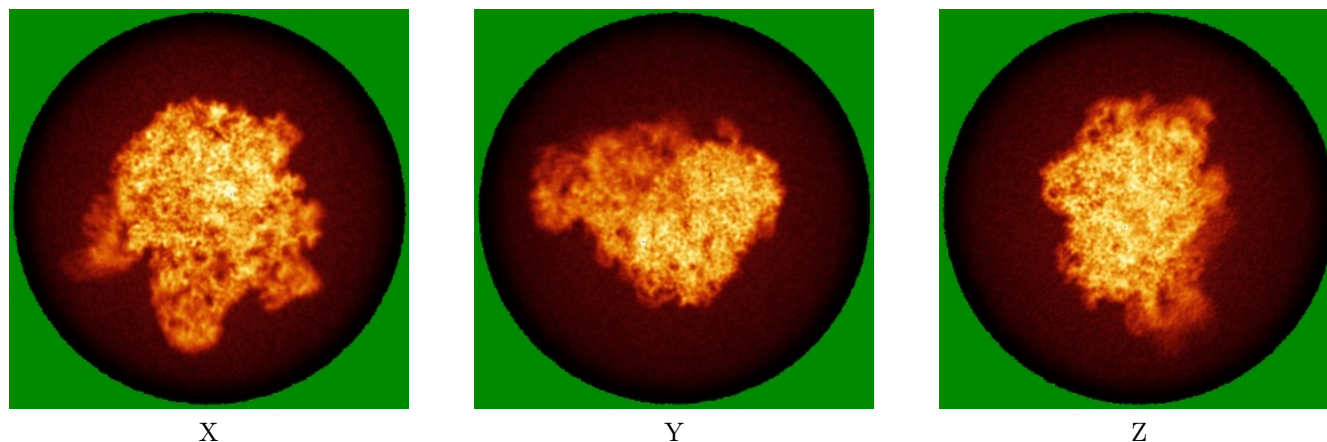


Z Index: 0

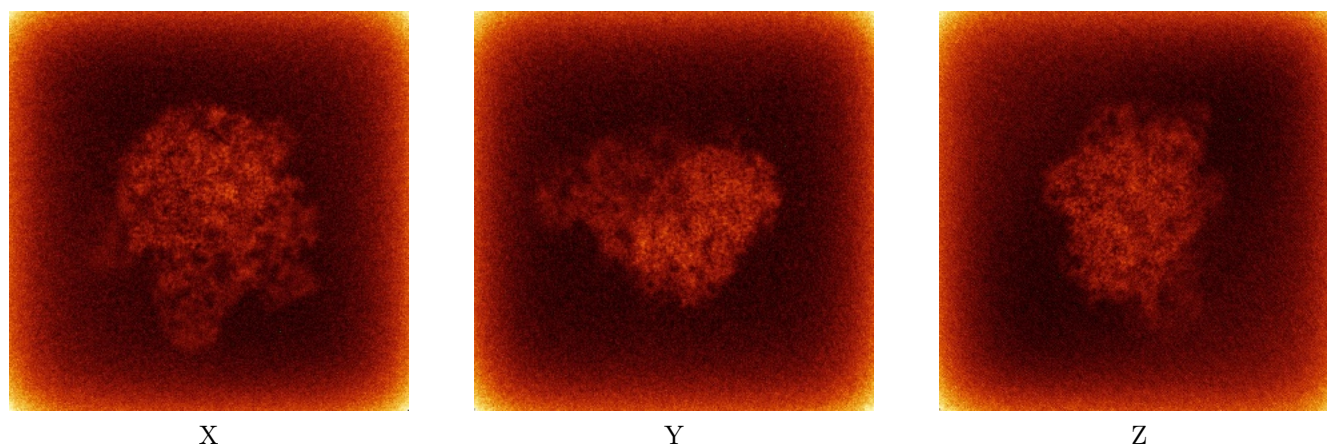
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



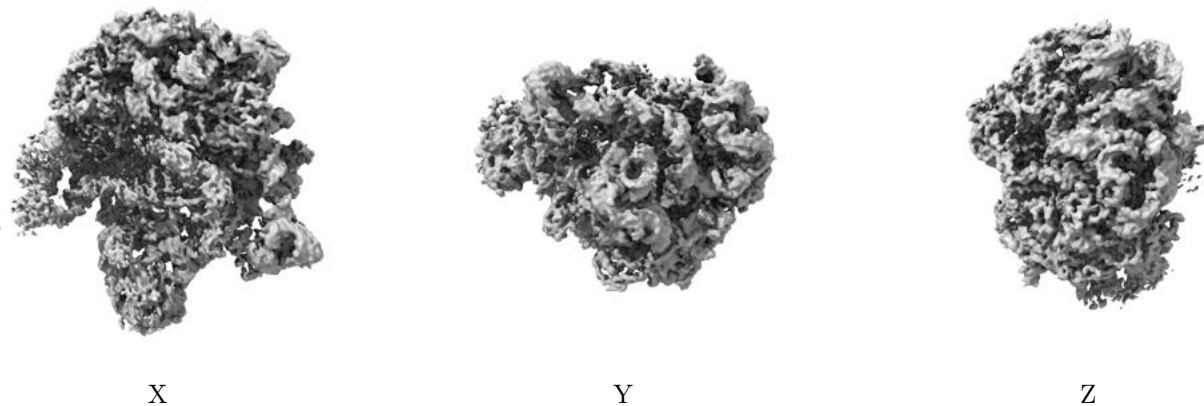
6.4.2 Raw map



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

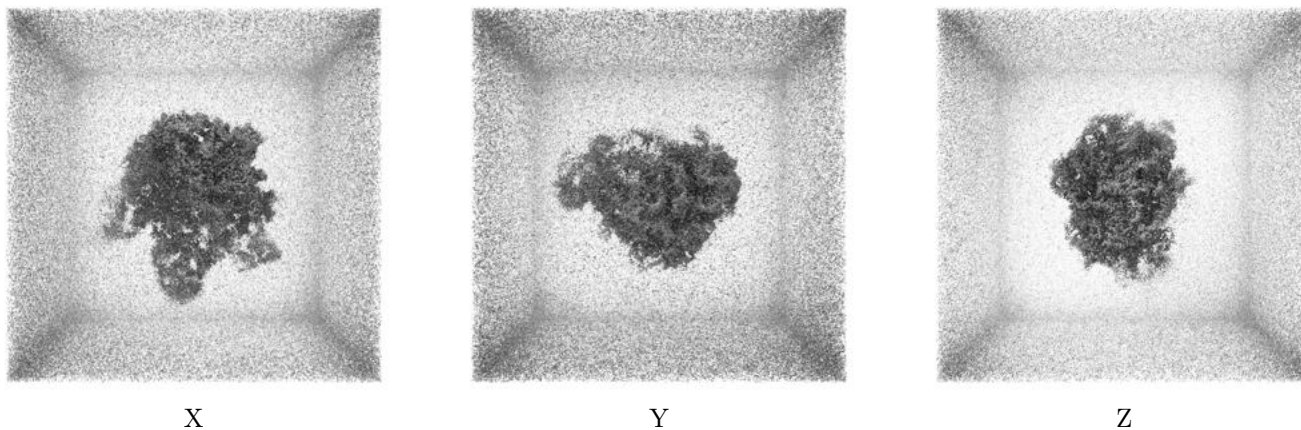
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.255. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

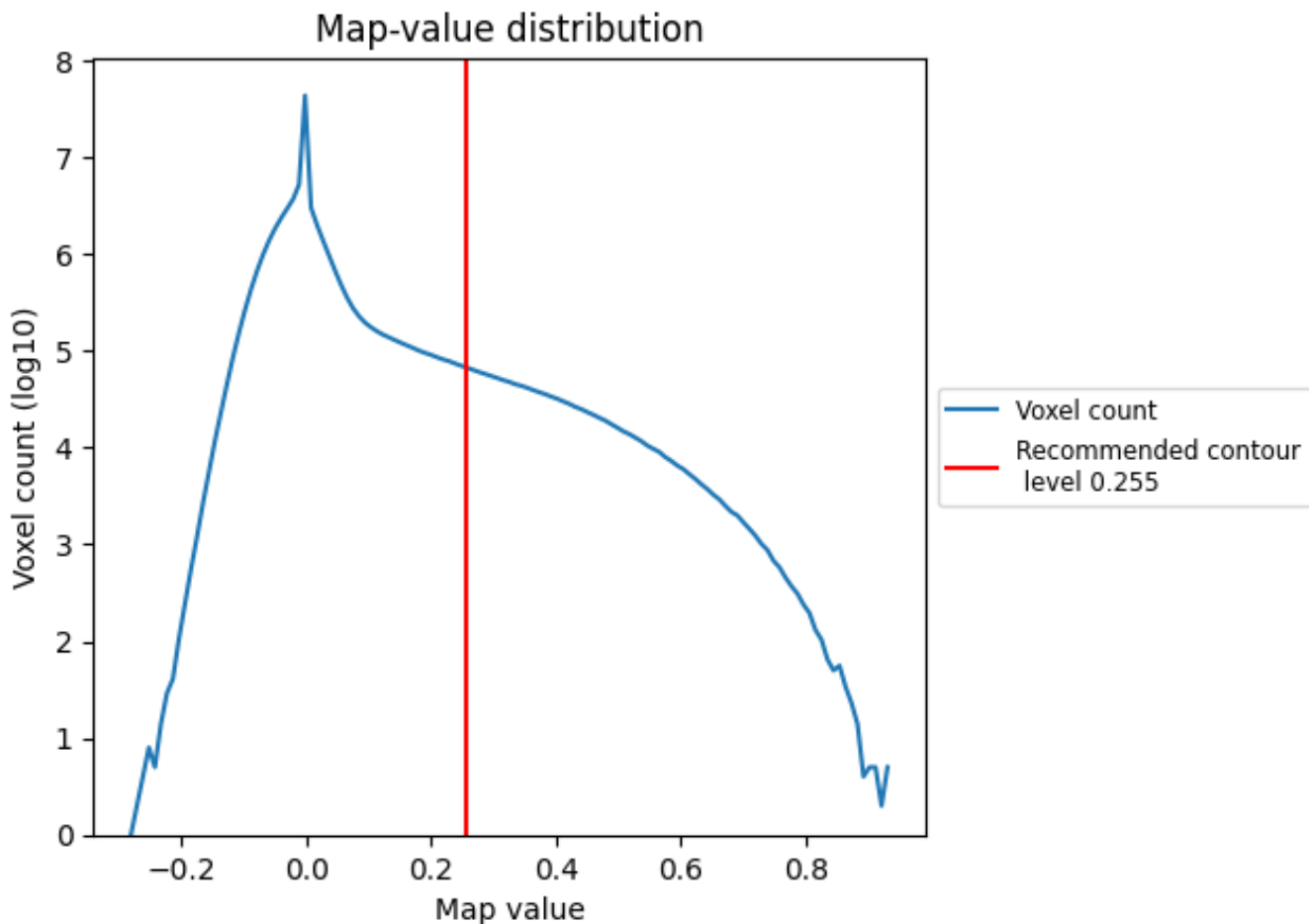
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

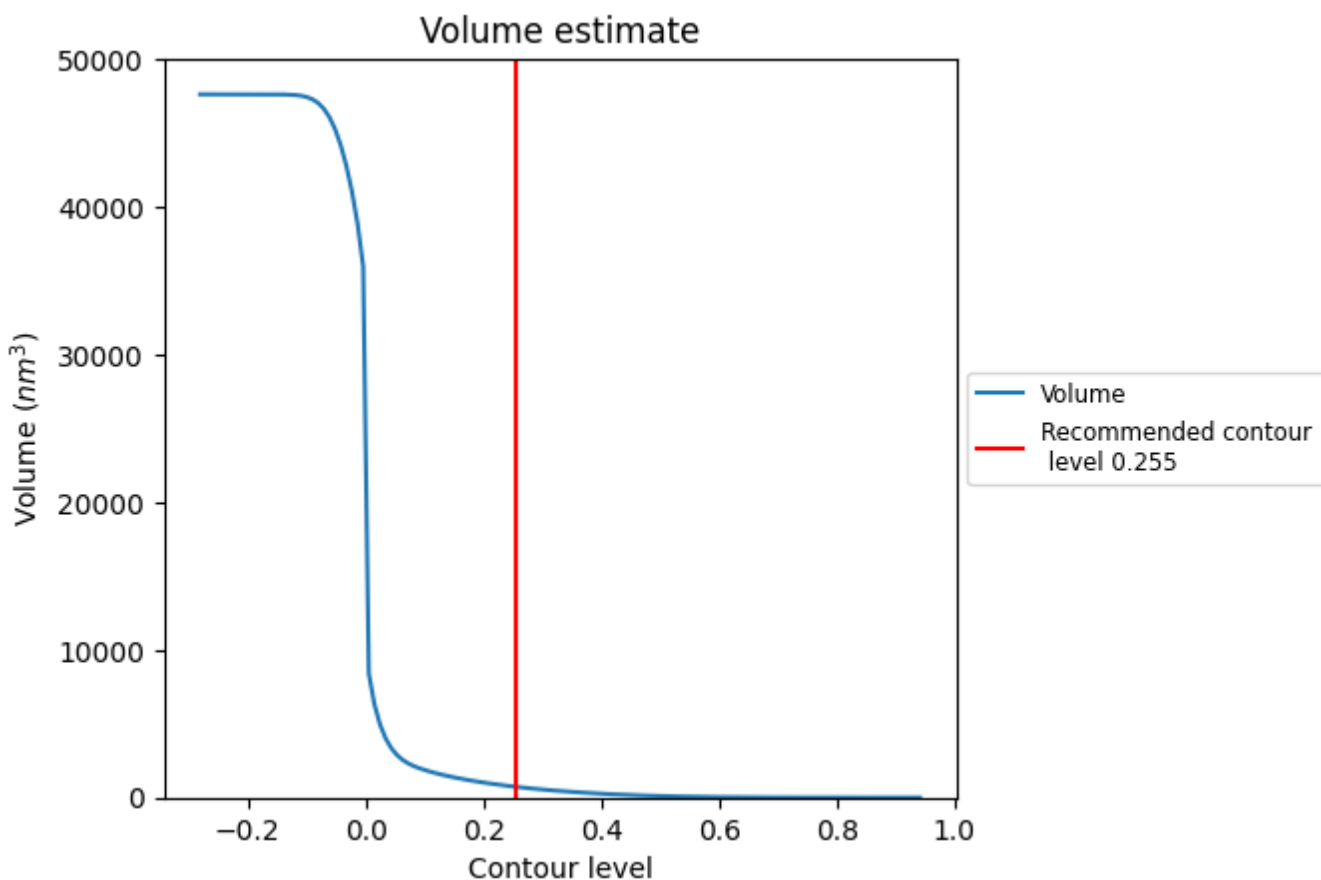
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

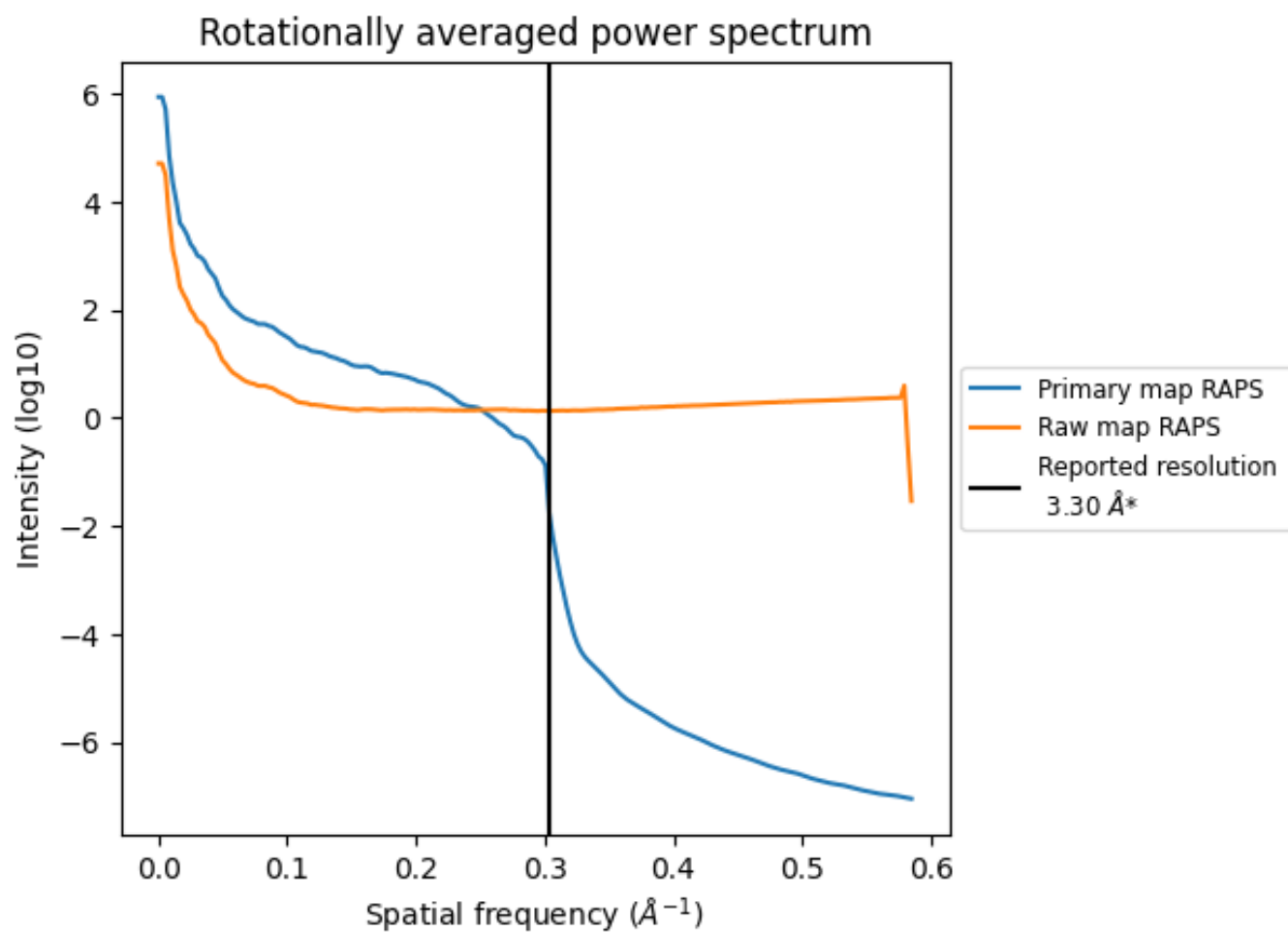
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 729 nm³; this corresponds to an approximate mass of 658 kDa.

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

7.3 Rotationally averaged power spectrum i

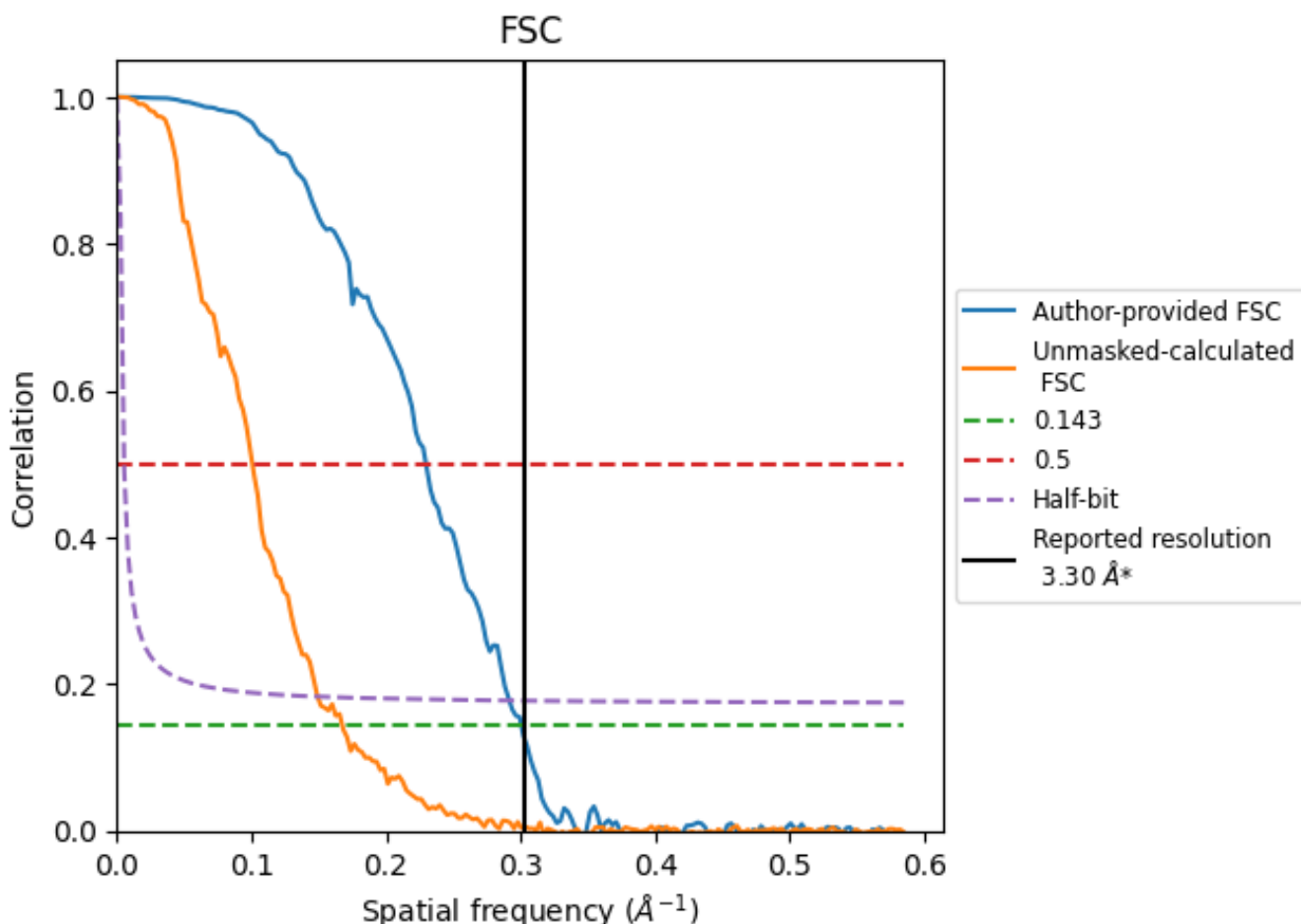


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

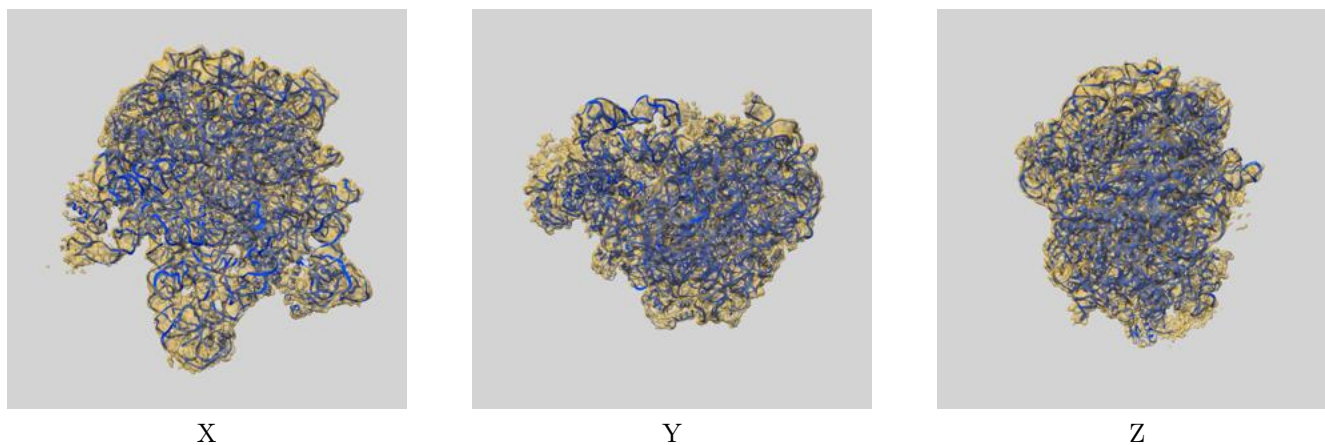
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.33	4.35	3.43
Unmasked-calculated*	5.97	9.93	6.70

*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 5.97 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

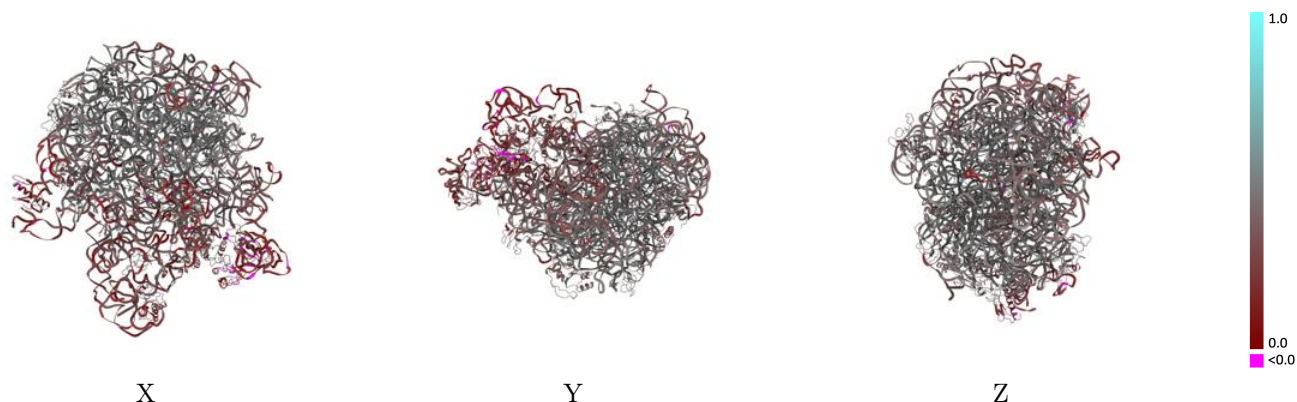
This section contains information regarding the fit between EMDB map EMD-44849 and PDB model 9BS0. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



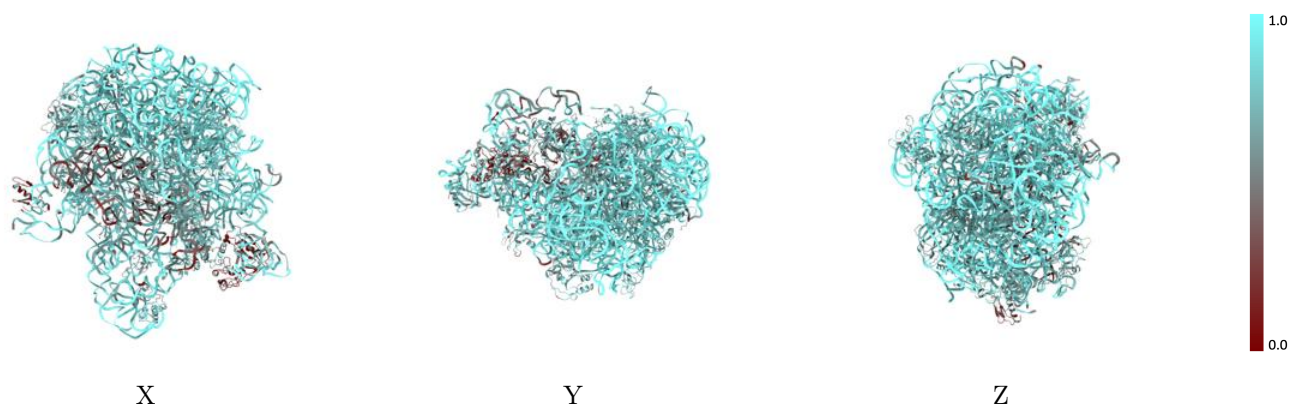
The images above show the 3D surface view of the map at the recommended contour level 0.255 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



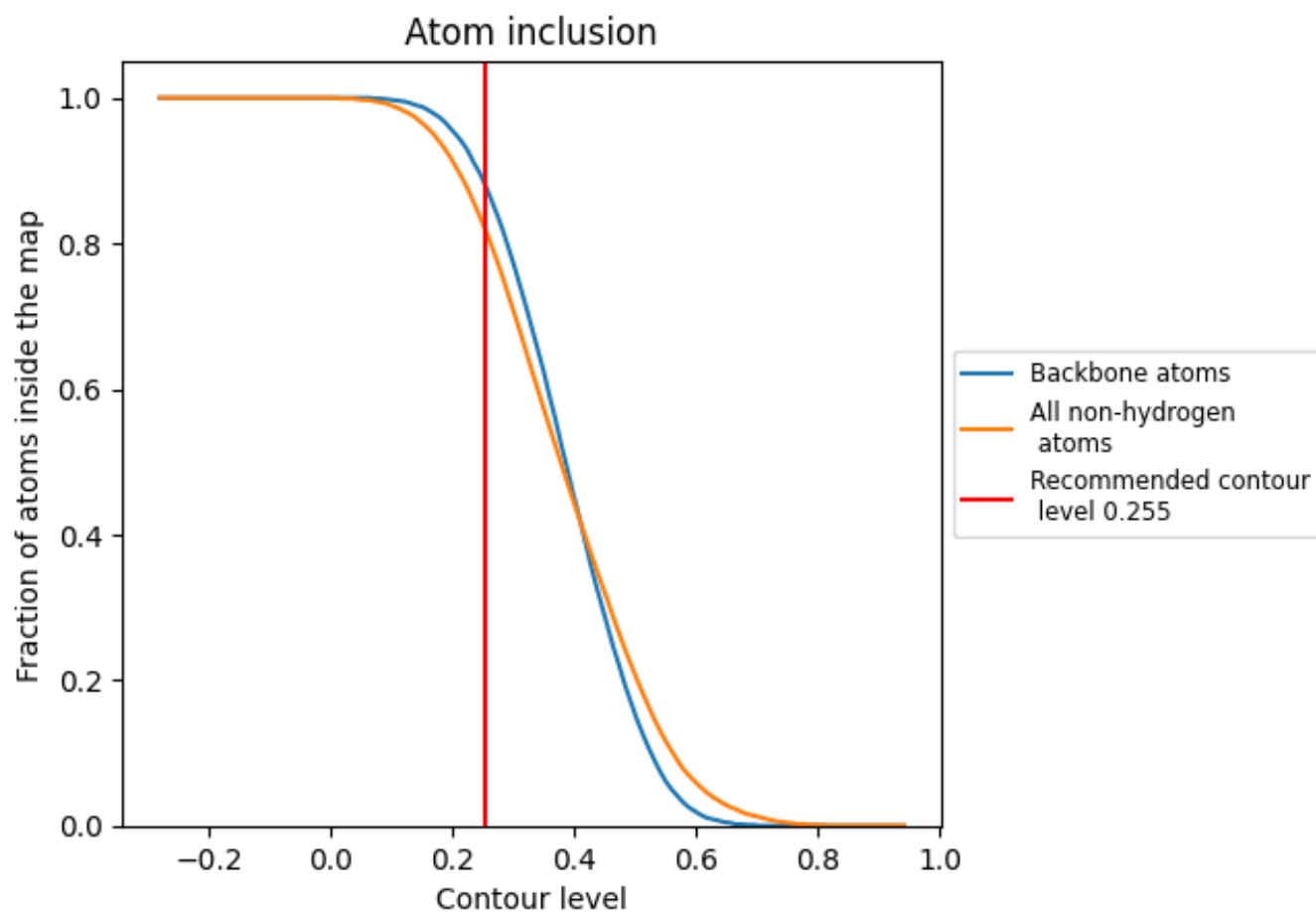
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.255).





















































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 82% 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 (0.255) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8170	 0.3900
A	 0.8760	 0.3950
B	 0.8790	 0.2760
C	 0.7050	 0.4410
D	 0.6730	 0.4380
E	 0.7060	 0.4210
F	 0.3720	 0.2340
G	 0.7180	 0.4260
H	 0.6880	 0.4240
I	 0.6780	 0.3970
J	 0.7370	 0.4270
K	 0.7280	 0.4280
L	 0.7680	 0.4470
M	 0.7280	 0.4420
N	 0.7180	 0.4530
O	 0.7090	 0.4390
P	 0.7550	 0.4150
Q	 0.6910	 0.4120
R	 0.7090	 0.3410
S	 0.6730	 0.3920
T	 0.7280	 0.4430
U	 0.7570	 0.4790
V	 0.6720	 0.2970
W	 0.5640	 0.3520
Y	 0.2440	 0.1470
Z	 0.5950	 0.3740

