



wwPDB EM Validation Summary Report ⓘ

Apr 22, 2025 – 07:33 AM EDT

PDB ID : 8VK0 / pdb_00008vk0
EMDB ID : EMD-43294
Title : Structure of Mycobacterium smegmatis 50S ribosomal subunit bound to HflX:50S-HflX-A
Authors : Majumdar, S.; Koripella, R.K.; Sharma, M.R.; Manjari, S.R.; Banavali, N.K.; Agrawal, R.K.
Deposited on : 2024-01-08
Resolution : 3.14 Å (reported)
Based on initial models : 5O61, 6DZI

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.dev117
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) : 2.42

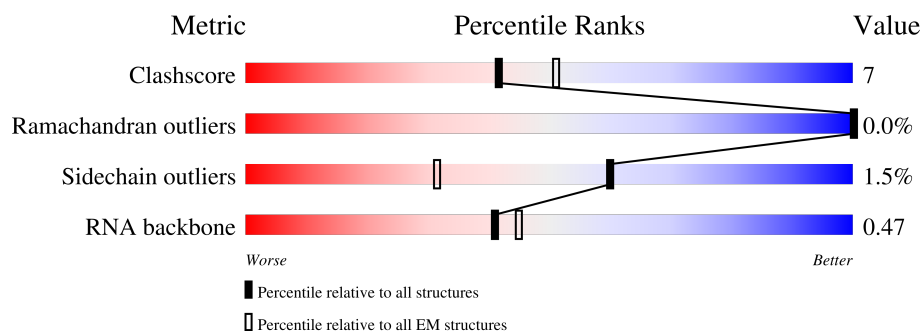
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.14 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	2	61	92% 5% .
2	3	24	83% 12% .
3	4	470	14% 24% 61% 6% 9%
4	A	3120	5% 65% 27% 7% .
5	B	118	50% 37% 9% .
6	C	278	85% 14% .
7	D	217	91% 8% .

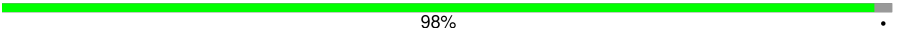
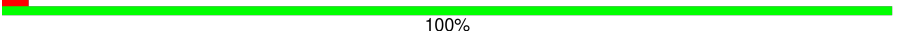

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Mol	Chain	Length	Quality of chain
8	E	215	
9	F	187	
10	G	179	
11	H	151	
12	I	175	
13	J	142	
14	K	147	
15	L	122	
16	M	147	
17	N	138	
18	O	199	
19	P	127	
20	Q	113	
21	R	129	
22	S	103	
23	T	153	
24	U	100	
25	V	105	
26	W	215	
27	X	88	
28	Y	64	
29	Z	77	
30	b	57	
31	c	55	
32	d	47	

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Mol	Chain	Length	Quality of chain
33	e	64	 98%
34	f	37	 100%
35	g	75	 41% 64% 36%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	GCP	4	501	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 100928 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 L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	2	59	Total	C	N	O	0	0
			474	292	95	87		

- Molecule 2 is a protein called 50S Ribosomal Protein L37.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	3	23	Total	C	N	O	0	0
			189	111	50	28		

- Molecule 3 is a protein called GTPase HflX.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	426	Total	C	N	O	S	0	0
			3228	1997	599	625	7		

- Molecule 4 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	3119	Total	C	N	O	P	0	0
			66981	29854	12313	21695	3119		

- Molecule 5 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	118	Total	C	N	O	P	0	0
			2522	1126	468	810	118		

- Molecule 6 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	275	Total	C	N	O	S	0	0
			2110	1298	438	370	4		

- Molecule 7 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	214	Total	C	N	O	S	0	0
			1587	982	310	290	5		

- Molecule 8 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	209	Total	C	N	O	S	0	0
			1569	969	295	303	2		

- Molecule 9 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	182	Total	C	N	O	S	0	0
			1445	907	271	261	6		

- Molecule 10 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	176	Total	C	N	O	S	0	0
			1348	845	249	253	1		

- Molecule 11 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	151	Total	C	N	O	S	0	0
			1018	635	188	194	1		

- Molecule 12 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	126	Total	C	N	O	S	0	0
			918	580	156	180	2		

- Molecule 13 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	133	Total	C	N	O	S	0	0
			990	625	175	187	3		

- Molecule 14 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	146	Total	C	N	O	S	0	0
			1130	722	207	200	1		

- Molecule 15 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	122	Total	C	N	O	S	0	0
			938	586	179	170	3		

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	145	Total	C	N	O	S	0	0
			1078	676	205	194	3		

- Molecule 17 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	136	Total	C	N	O	S	0	0
			1092	690	213	187	2		

- Molecule 18 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	118	Total	C	N	O	S	0	0
			928	583	180	163	2		

- Molecule 19 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	126	Total	C	N	O	S	0	0
			956	586	199	171			

- Molecule 20 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	113	Total	C	N	O	S	0	0
			907	570	171	165	1		

- Molecule 21 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	R	124	Total	C	N	O	0	0
			988	613	203	172		

- Molecule 22 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	S	100	Total	C	N	O	0	0
			754	478	137	139		

- Molecule 23 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	T	114	Total	C	N	O	0	0
			873	543	171	159		

- Molecule 24 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	U	97	Total	C	N	O	0	0
			756	479	138	139		

- Molecule 25 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	97	Total	C	N	O	S	0	0
			732	456	137	137	2		

- Molecule 26 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	W	192	Total	C	N	O	0	0
			1428	881	255	292		

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	X	79	Total	C	N	O	0	0
			586	361	123	102		

- Molecule 28 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	63	Total	C	N	O	S	0	0
			470	283	103	80	4		

- Molecule 29 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	64	Total	C	N	O	S	0	0
			531	324	103	103	1		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	54	Total	C	N	O	S	0	0
			423	260	93	69	1		

- Molecule 31 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	49	Total	C	N	O	S	0	0
			405	248	82	71	4		

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	46	Total	C	N	O	S	0	0
			377	225	97	54	1		

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	e	63	Total	C	N	O	0	0
			502	302	115	85		

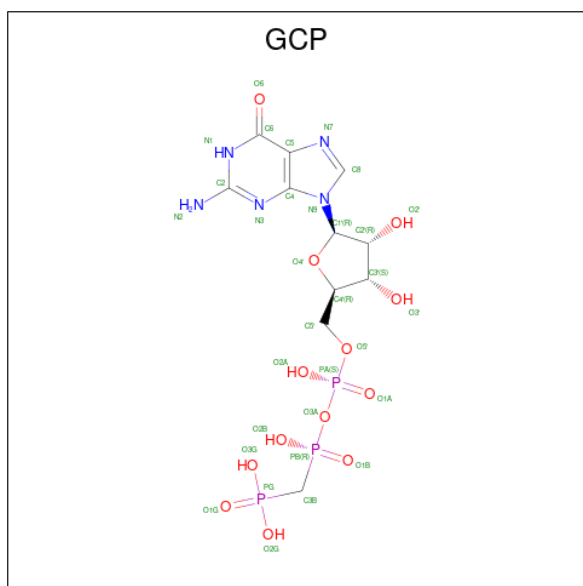
- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	37	Total	C	N	O	S	0	0
			299	181	66	47	5		

- Molecule 35 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	48	Total	C	N	O	S	0	0
			364	225	63	71	5		

- Molecule 36 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



3 Residue-property plots


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

- Molecule 1: 50S ribosomal protein L30

Chain 2: 



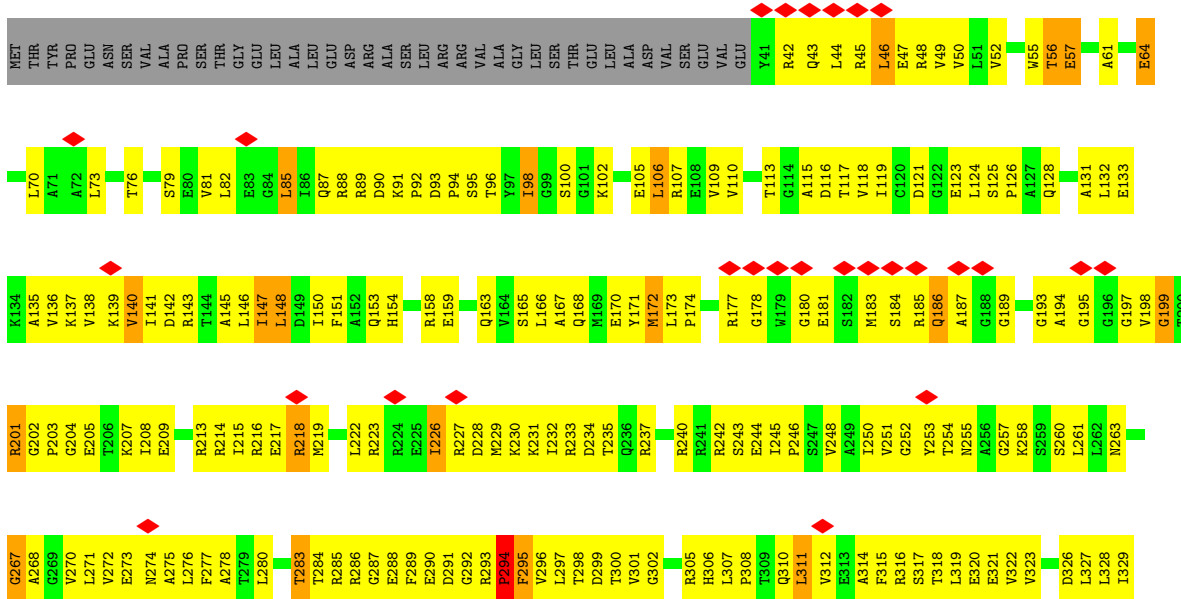
- Molecule 2: 50S Ribosomal Protein L37

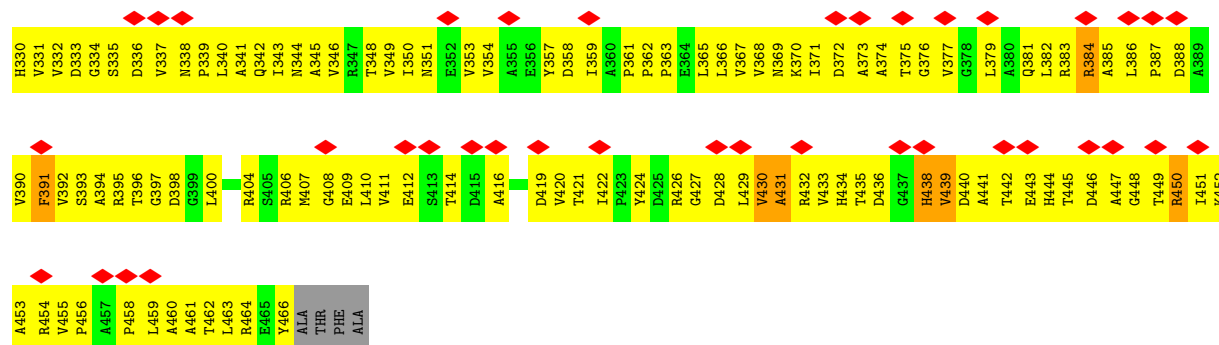
Chain 3: 



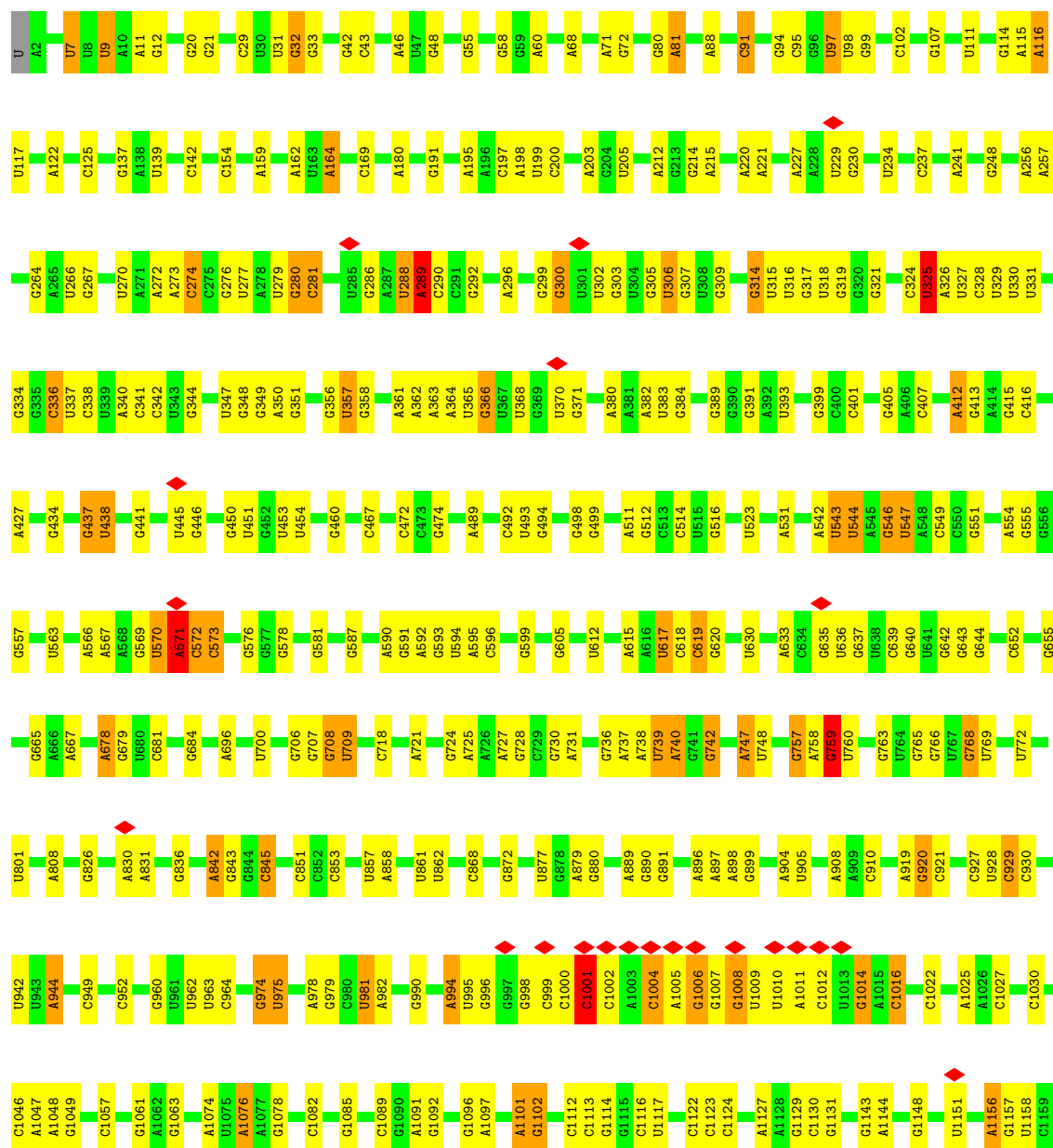
- Molecule 3: GTPase HflX

Chain 4: 





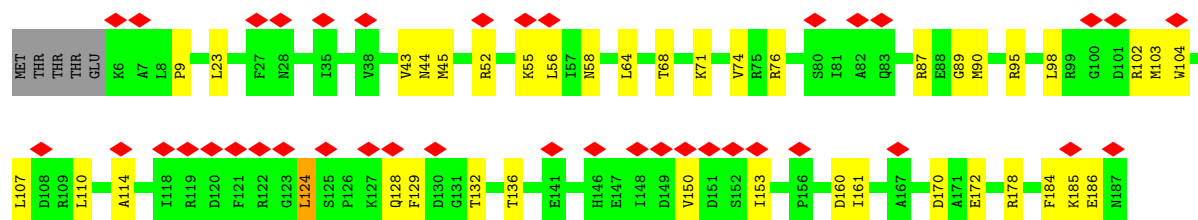
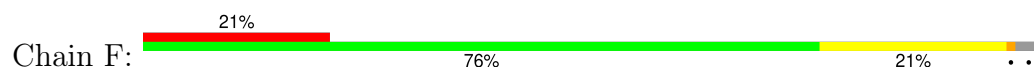
• Molecule 4: 23S ribosomal RNA



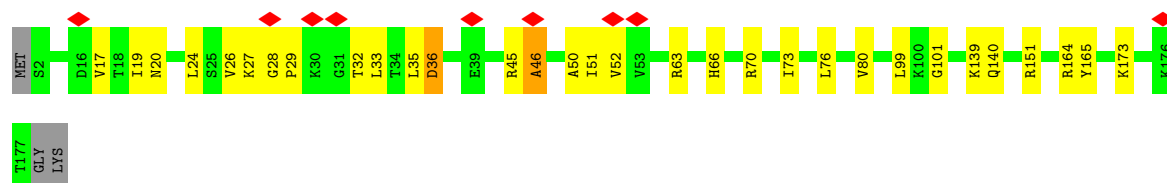
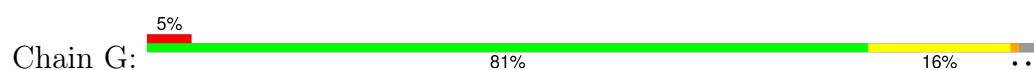
U2401	G1160	A1221	G1353	C1478	G1574	A1640	A1755	C1893	G2017	U2141	G2249	U2341	U2402
C2402	C1161	A1222	G1363	G1479	A1575	A1648	G1756	C1900	G2018	A2142	A2250	A2341	C2403
U2403	A1163	U1223	A1362	A1480	C1576	C1649	G1757	C1901	U2022	C2143	G2251	G2342	G2404
G2405	G1164	G1225	G1364	A1493	C1577	G1650	G1758	C1902	C2025	C2145	A2254	G2343	U2406
U2407	G1165	U1226	U1364	A1494	C1578	G1651	A1759	C1903	A2026	C2146	A2255	U2345	G2408
C2407	A1166	C1227	G1365	A1499	C1579	C1651	A1764	C1904	U2026	U2147	G2256	G2346	U2409
U2408	C1167	U1228	G1371	A1508	A1580	G1668	U1767	C1909	U2033	C2148	C2260	G2347	A2410
U2409	C1170	A1229	A1377	U1508	C1581	G1669	C1767	U1910	G2034	A2151	G2261	G2348	U2411
A2410	U1172	G1230	U1509	A1510	C1582	U1670	C1768	U1911	U2035	A2152	G2262	A2349	U2412
U2411	G1173	G1231	A1380	C1513	U1583	G1672	G1769	C1912	U2036	G2153	G2263	G2350	G2413
U2412	G1174	U1232	G1381	C1514	U1584	G1673	A1778	A1916	C2043	G2154	C2267	C2351	U2414
G2413	G1175	U1235	U1382	A1518	U1585	G1674	U1777	C1917	U2044	U2155	G2268	C2352	G2415
G2414	A1176	U1236	G1386	A1519	C1586	U1675	A1778	C1918	A2045	A2160	G2269	U2353	U2416
U2418	G1177	U1237	A1387	C1521	G1587	G1676	G1786	A1931	A2046	A2161	G2270	U2354	U2417
A2421	G1178	U1238	U1388	C1522	U1588	U1677	A1787	U1932	A2070	A2162	G2271	U2355	U2418
A2422	U1179	G1239	U1389	G1530	G1589	U1678	A1788	U1933	A2071	U2163	G2272	G2356	U2419
C2423	U1180	U1240	U1390	U1591	C1590	U1681	A1789	U1934	G2075	U2164	G2273	A2357	C2424
C2430	G1181	A1246	G1398	U1592	U1591	G1688	U1798	A1940	A2076	C2165	A2284	A2358	U2420
C2431	U1182	U1247	A1399	U1593	U1591	U1689	A1941	A1941	C2077	A2176	G2285	G2359	U2421
U2434	U1183	U1248	G1400	U1533	U1592	U1690	G1802	G1942	U2077	U2179	A2286	C2360	U2422
U2435	U1184	U1249	A1401	C1534	U1593	A1690	A1803	C1943	A2083	U2180	A2287	U2361	U2423
U2438	A1185	U1250	A1402	C1535	G1594	A1691	C1813	U1945	A2084	U2181	G2288	C2362	U2430
G2446	A1186	U1251	C1403	A1536	G1595	U1946	C1814	U1946	U2085	U2182	C2289	A2363	U2431
A2449	A1187	G1252	C1404	U1537	C1596	A1948	C1815	U1947	U2086	U2183	G2290	C2364	U2432
C2455	A1188	G1253	C1409	U1538	G1597	U1697	C1816	A1949	C2089	A2190	G2291	A2365	U2433
G2462	U1189	C1254	C1415	U1540	U1598	U1698	C1817	C1949	U2090	C2191	G2292	C2366	U2434
G2463	A1191	A1261	A1416	G1541	U1599	G1703	A1825	A1955	U2091	A2194	G2293	C2367	U2435
U2467	G1192	C1269	C1421	A1546	U1601	U1704	A1826	G1961	U2092	U2195	G2294	C2368	U2436
A2470	C1193	G1270	C1428	G1547	G1602	G1707	A1847	U1972	G2093	C2199	G2295	C2369	U2437
A2471	C1194	G1271	C1429	C1548	G1603	A1708	A1848	A1973	G2094	U2200	G2296	C2370	U2438
G2472	A1195	C1272	C1436	G1549	G1606	U1709	U1847	C1974	G2095	U2201	G2297	U2372	U2439
G2474	C1196	G1273	C1436	U1551	U1607	A1710	A1848	A1975	G2096	U2202	G2298	U2373	U2440
G2475	C1197	A1274	C1441	A1552	C1610	U1713	U1849	U1976	G2099	U2203	G2299	U2374	U2441
G2476	G1198	G1276	C1441	C1553	A1611	A1716	A1851	U1981	A2113	U2204	G2300	G2375	U2442
G2477	U1199	U1292	U1444	U1554	G1615	U1717	A1852	A1982	C2116	C2224	C2301	G2376	U2443
U2483	G1201	G1293	C1448	A1555	A1616	C1718	A1853	A1990	C2117	C2225	G2302	U2377	U2444
A2490	A1202	C1298	U1455	C1556	C1617	U1723	U1863	C1991	G2128	A2227	G2303	U2378	U2445
A2491	A1203	G1302	U1456	C1557	C1618	A1729	U1864	U1992	C2129	C2228	G2304	U2379	U2446
A2492	A1204	U1303	G1456	C1558	C1619	U1730	U1865	G1993	G2130	A2229	G2305	U2380	U2447
G2503	G1205	C1314	A1457	C1559	U1619	A1731	C1866	U1996	G2131	C2230	G2306	U2381	U2448
G2506	U1208	C1314	G1458	C1560	U1620	A1737	G1871	U1999	U2132	U2231	G2307	U2382	U2449
C2507	G1209	C1330	C1465	C1561	C1621	A1744	A1872	C2005	G2133	C2232	G2308	U2383	U2450
	A1210	G1332	U1467	C1562	G1622	U1745	A1873	A2008	U2134	C2233	G2309	U2384	U2451
	G1211	C1333	A1468	A1563	U1623	U1746	C1874	G2014	U2135	C2234	G2310	U2385	U2452
	A1214	G1337	A1468	A1564	U1624	G1746	U1877	U2015	A2136	C2245	G2311	U2386	U2453
	U1215	A1344	C1477	C1565	U1625	U1746	A1887	G2016	U2137	C2246	G2312	U2387	U2454
	U1216				A1628				U2138	U2247	G2313	U2388	U2455
	G1217				G1629				U2139	C2248	G2314	U2389	U2456
	C1218				A1631						G2315	U2390	U2457
	U1219				G1632						G2316	G2391	U2458
					A1636						G2317	A2392	U2459
					C1637						G2318	A2393	U2460
					C1638						G2319	A2394	U2461
					G1639						G2320	U2395	U2462
											G2321	A2396	U2463
											G2322	U2397	U2464
											G2323	A2398	U2465
											G2324	U2399	U2466
											G2325	G2400	U2467



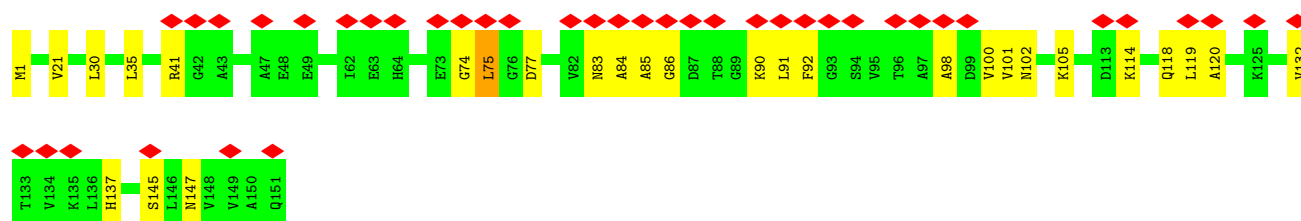
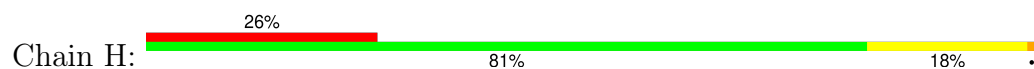
• Molecule 9: 50S Ribosomal Protein L5



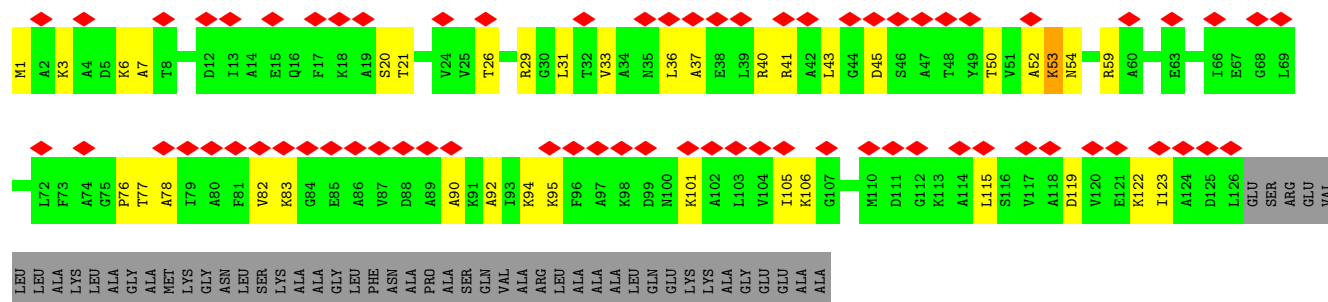
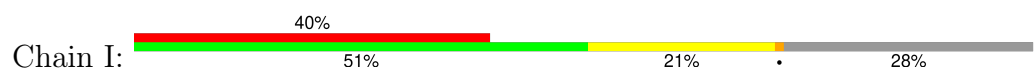
• Molecule 10: 50S ribosomal protein L6



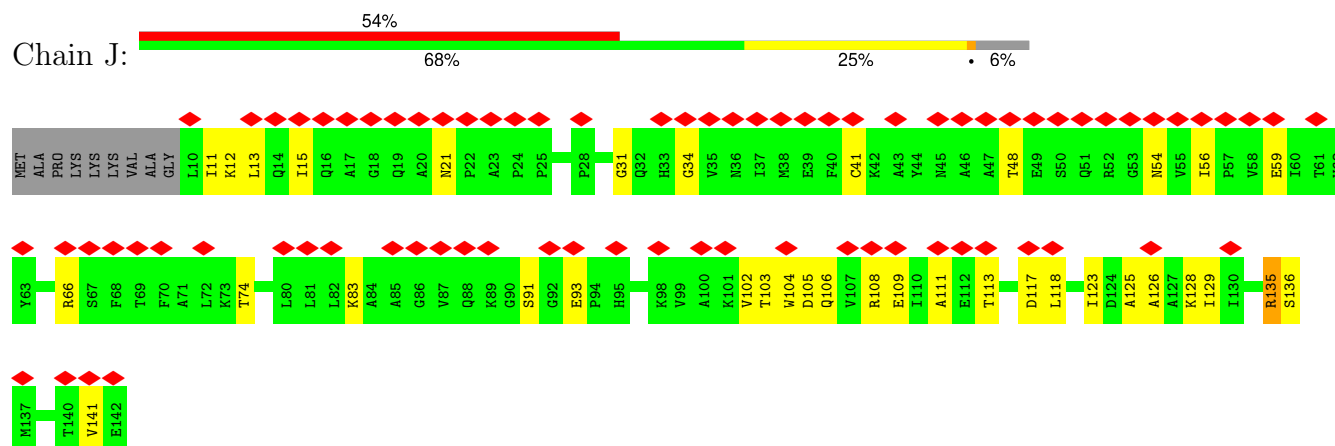
• Molecule 11: 50S ribosomal protein L9



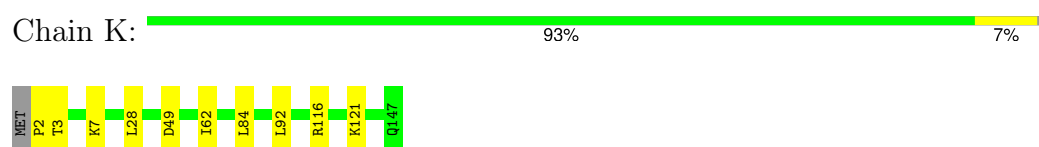
• Molecule 12: 50S ribosomal protein L10



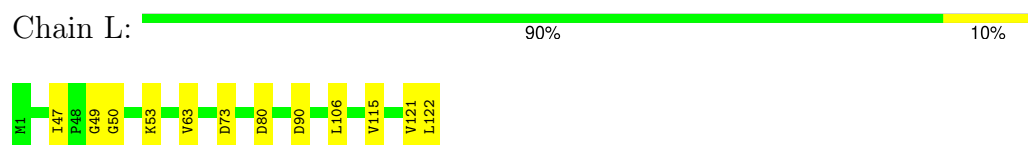
- Molecule 13: 50S ribosomal protein L11



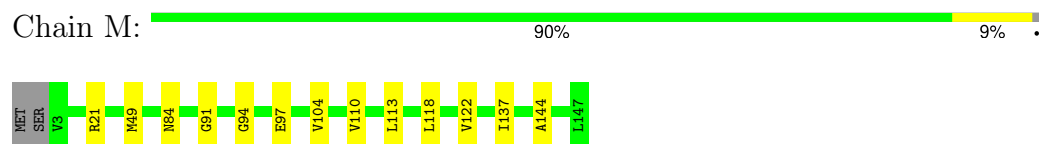
- Molecule 14: 50S Ribosomal Protein L13



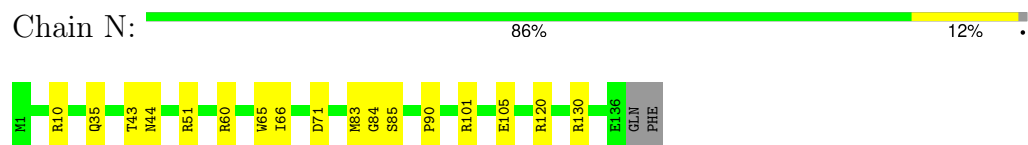
- Molecule 15: 50S ribosomal protein L14



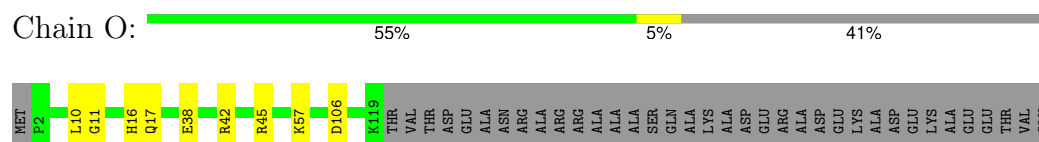
- Molecule 16: 50S ribosomal protein L15



- Molecule 17: Large ribosomal subunit protein uL16



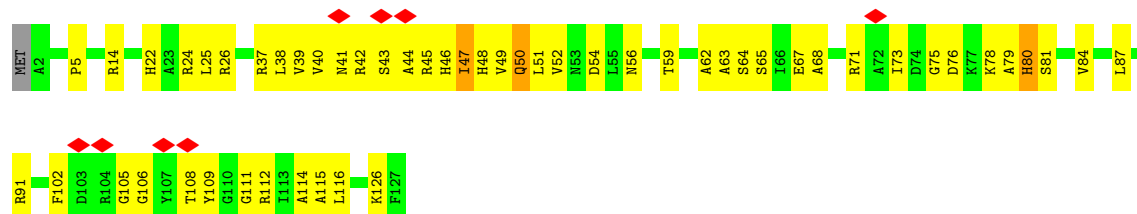
- Molecule 18: 50S ribosomal protein L17




ALA PRO ALA ALA GLU GLU SER SER THR GLU GLU ALA ALA ALA ALA GLU GLU THR THR VAL VAL GLU GLU THR THR THR GLU ALA ALA PRO PRO ALA GLU GLU SER SER THR THR ALA ALA LYS ASP ASP THR LYS

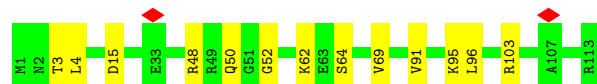
• Molecule 19: 50S Ribosomal Protein L18

Chain P: 



• Molecule 20: 50S ribosomal protein L19

Chain Q: 




• Molecule 21: 50S Ribosomal Protein L20

Chain R: 



• Molecule 22: 50S Ribosomal Protein L21

Chain S: 



• Molecule 23: 50S Ribosomal Protein L22

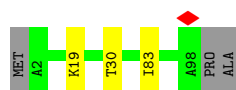
Chain T: 



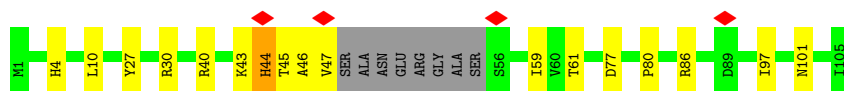
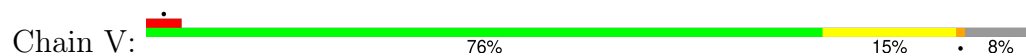
• Molecule 24: 50S Ribosomal Protein L23

Chain U: 

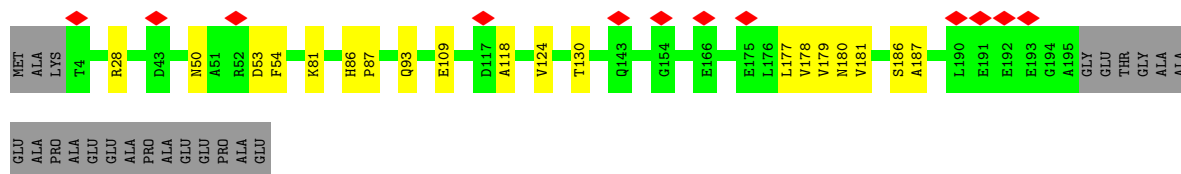
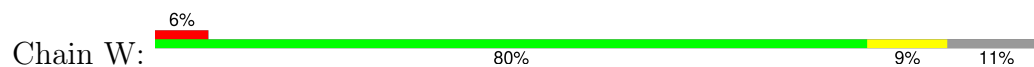




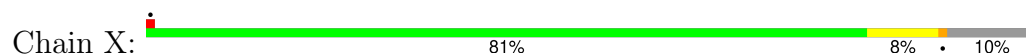
- Molecule 25: 50S ribosomal protein L24



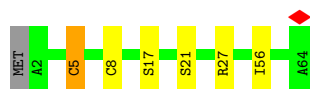
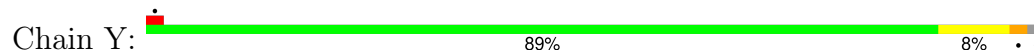
- Molecule 26: 50S ribosomal protein L25



- Molecule 27: 50S ribosomal protein L27



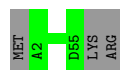
- Molecule 28: 50S Ribosomal Protein L28



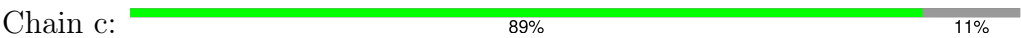
- Molecule 29: 50S ribosomal protein L29



- Molecule 30: 50S ribosomal protein L32



• Molecule 31: 50S Ribosomal Protein L33



• Molecule 32: 50S ribosomal protein L34



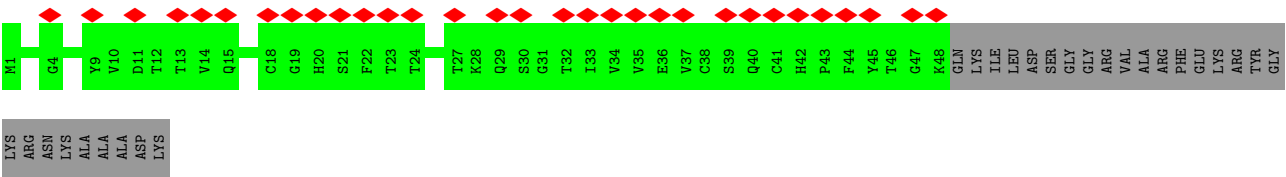
• Molecule 33: 50S ribosomal protein L35



• Molecule 34: 50S ribosomal protein L36



• Molecule 35: 50S Ribosomal Protein L31



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57434	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 ($e^-/\text{\AA}^2$)	51.22	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.771	Depositor
Minimum map value	-0.951	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	433.19998, 433.19998, 433.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.083, 1.083, 1.083	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GCP

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	2	0.47	0/477	0.56	0/640
2	3	0.36	0/191	0.49	0/247
3	4	0.51	0/3268	0.67	3/4428 (0.1%)
4	A	0.90	1/75001 (0.0%)	1.18	566/117027 (0.5%)
5	B	0.72	0/2821	1.38	57/4396 (1.3%)
6	C	0.50	0/2153	0.58	0/2895
7	D	0.51	0/1609	0.60	0/2165
8	E	0.47	0/1592	0.61	2/2153 (0.1%)
9	F	0.32	0/1467	0.64	2/1973 (0.1%)
10	G	0.35	0/1369	0.64	0/1848
11	H	0.32	0/1027	0.68	1/1398 (0.1%)
12	I	0.31	0/925	0.64	0/1246
13	J	0.31	0/1006	0.64	0/1364
14	K	0.48	0/1157	0.54	0/1567
15	L	0.51	0/946	0.56	0/1268
16	M	0.44	0/1091	0.56	0/1457
17	N	0.43	0/1118	0.57	0/1506
18	O	0.53	0/945	0.60	0/1267
19	P	0.41	0/966	0.75	1/1298 (0.1%)
20	Q	0.49	0/921	0.62	1/1236 (0.1%)
21	R	0.54	0/1000	0.56	0/1341
22	S	0.47	0/764	0.58	0/1030
23	T	0.50	0/887	0.59	0/1204
24	U	0.50	0/766	0.56	0/1030
25	V	0.44	0/738	0.64	0/987
26	W	0.33	0/1443	0.60	0/1970
27	X	0.47	0/595	0.59	0/798
28	Y	0.47	0/478	0.55	0/641
29	Z	0.44	0/534	0.53	0/713
30	b	0.48	0/427	0.63	0/572
31	c	0.40	0/413	0.48	0/553
32	d	0.49	0/380	0.52	0/500

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.41	0/507	0.51	0/672
34	f	0.46	0/303	0.54	0/401
35	g	0.34	0/372	0.61	0/503
All	All	0.79	1/109657 (0.0%)	1.07	633/164294 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	F	0	1
10	G	0	2
11	H	0	1
12	I	0	2
13	J	0	1
18	O	0	1
19	P	0	4
26	W	0	1
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	571	A	N9-C4	6.05	1.41	1.37

The worst 5 of 633 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2402	C	N1-C2-O2	14.25	127.45	118.90
4	A	2402	C	N3-C2-O2	-13.03	112.78	121.90
4	A	617	U	C2-N1-C1'	11.10	131.02	117.70
4	A	1567	C	N3-C2-O2	-10.84	114.32	121.90
4	A	1220	C	C2-N1-C1'	10.53	130.38	118.80

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	F	68	THR	Peptide
10	G	46	ALA	Peptide

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Mol	Chain	Res	Type	Group
10	G	52	VAL	Peptide
11	H	137	HIS	Peptide
12	I	52	ALA	Peptide

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	2	474	0	500	2	0
2	3	189	0	205	3	0
3	4	3228	0	3284	515	0
4	A	66981	0	33700	293	0
5	B	2522	0	1285	20	0
6	C	2110	0	2165	28	0
7	D	1587	0	1630	12	0
8	E	1569	0	1607	13	0
9	F	1445	0	1476	23	0
10	G	1348	0	1399	20	0
11	H	1018	0	988	19	0
12	I	918	0	959	29	0
13	J	990	0	1021	26	0
14	K	1130	0	1167	8	0
15	L	938	0	1000	7	0
16	M	1078	0	1151	8	0
17	N	1092	0	1128	9	0
18	O	928	0	972	5	0
19	P	956	0	991	42	0
20	Q	907	0	938	8	0
21	R	988	0	1038	11	0
22	S	754	0	802	7	0
23	T	873	0	909	8	0
24	U	756	0	802	2	0
25	V	732	0	782	13	0
26	W	1428	0	1443	11	0
27	X	586	0	601	7	0
28	Y	470	0	482	4	0
29	Z	531	0	541	3	0
30	b	423	0	463	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	c	405	0	411	0	0
32	d	377	0	411	0	0
33	e	502	0	541	0	0
34	f	299	0	324	0	0
35	g	364	0	352	0	0
36	4	32	0	14	15	0
All	All	100928	0	67482	1038	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 7.

The worst 5 of 1038 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)
3:4:445:THR:CG2	3:4:450:ARG:HB2	1.86	1.06
3:4:202:GLY:HA3	4:A:2676:C:C4'	1.86	1.05
3:4:354:VAL:HG11	3:4:361:PRO:HG3	1.38	1.04
3:4:426:ARG:HG3	3:4:429:LEU:HB2	1.38	1.04
3:4:85:LEU:HD11	3:4:106:LEU:HD21	1.40	1.02

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	2	57/61 (93%)	56 (98%)	1 (2%)	0	100	100
2	3	21/24 (88%)	20 (95%)	1 (5%)	0	100	100
3	4	424/470 (90%)	343 (81%)	79 (19%)	2 (0%)	25	55
6	C	273/278 (98%)	258 (94%)	15 (6%)	0	100	100
7	D	212/217 (98%)	196 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	E	207/215 (96%)	192 (93%)	15 (7%)	0	100	100
9	F	180/187 (96%)	146 (81%)	34 (19%)	0	100	100
10	G	174/179 (97%)	151 (87%)	23 (13%)	0	100	100
11	H	149/151 (99%)	110 (74%)	39 (26%)	0	100	100
12	I	124/175 (71%)	108 (87%)	16 (13%)	0	100	100
13	J	131/142 (92%)	100 (76%)	31 (24%)	0	100	100
14	K	144/147 (98%)	137 (95%)	7 (5%)	0	100	100
15	L	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
16	M	143/147 (97%)	130 (91%)	13 (9%)	0	100	100
17	N	134/138 (97%)	124 (92%)	10 (8%)	0	100	100
18	O	116/199 (58%)	107 (92%)	9 (8%)	0	100	100
19	P	124/127 (98%)	88 (71%)	36 (29%)	0	100	100
20	Q	111/113 (98%)	95 (86%)	16 (14%)	0	100	100
21	R	122/129 (95%)	118 (97%)	4 (3%)	0	100	100
22	S	98/103 (95%)	92 (94%)	6 (6%)	0	100	100
23	T	112/153 (73%)	110 (98%)	2 (2%)	0	100	100
24	U	95/100 (95%)	90 (95%)	5 (5%)	0	100	100
25	V	93/105 (89%)	82 (88%)	11 (12%)	0	100	100
26	W	190/215 (88%)	170 (90%)	20 (10%)	0	100	100
27	X	77/88 (88%)	71 (92%)	6 (8%)	0	100	100
28	Y	61/64 (95%)	55 (90%)	6 (10%)	0	100	100
29	Z	62/77 (80%)	62 (100%)	0	0	100	100
30	b	52/57 (91%)	52 (100%)	0	0	100	100
31	c	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
32	d	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
33	e	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
34	f	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
35	g	46/75 (61%)	41 (89%)	5 (11%)	0	100	100
All	All	4039/4461 (90%)	3594 (89%)	443 (11%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	4	294	PRO
3	4	431	ALA

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	2	52/54 (96%)	52 (100%)	0	100	100
2	3	18/19 (95%)	18 (100%)	0	100	100
3	4	337/372 (91%)	310 (92%)	27 (8%)	10	31
6	C	215/218 (99%)	214 (100%)	1 (0%)	86	92
7	D	160/163 (98%)	160 (100%)	0	100	100
8	E	169/173 (98%)	169 (100%)	0	100	100
9	F	151/156 (97%)	149 (99%)	2 (1%)	65	80
10	G	148/150 (99%)	145 (98%)	3 (2%)	50	71
11	H	90/116 (78%)	90 (100%)	0	100	100
12	I	89/120 (74%)	89 (100%)	0	100	100
13	J	102/108 (94%)	100 (98%)	2 (2%)	50	71
14	K	119/120 (99%)	119 (100%)	0	100	100
15	L	100/100 (100%)	99 (99%)	1 (1%)	73	85
16	M	112/114 (98%)	111 (99%)	1 (1%)	75	86
17	N	114/116 (98%)	112 (98%)	2 (2%)	54	74
18	O	97/158 (61%)	97 (100%)	0	100	100
19	P	93/94 (99%)	88 (95%)	5 (5%)	18	44
20	Q	100/100 (100%)	100 (100%)	0	100	100
21	R	97/99 (98%)	97 (100%)	0	100	100
22	S	81/83 (98%)	81 (100%)	0	100	100
23	T	90/117 (77%)	89 (99%)	1 (1%)	70	83
24	U	83/85 (98%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	V	81/86 (94%)	80 (99%)	1 (1%)	67	81
26	W	155/168 (92%)	155 (100%)	0	100	100
27	X	58/63 (92%)	57 (98%)	1 (2%)	56	75
28	Y	50/51 (98%)	49 (98%)	1 (2%)	50	71
29	Z	58/66 (88%)	57 (98%)	1 (2%)	56	75
30	b	43/46 (94%)	43 (100%)	0	100	100
31	c	47/52 (90%)	47 (100%)	0	100	100
32	d	35/36 (97%)	35 (100%)	0	100	100
33	e	53/54 (98%)	53 (100%)	0	100	100
34	f	35/35 (100%)	35 (100%)	0	100	100
35	g	43/63 (68%)	43 (100%)	0	100	100
All	All	3275/3555 (92%)	3226 (98%)	49 (2%)	60	78

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	F	52	ARG
15	L	73	ASP
9	F	74	VAL
10	G	66	HIS
17	N	60	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
23	T	67	ASN
27	X	50	ASN
23	T	109	HIS
26	W	14	ASN
35	g	42	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	A	3118/3120 (99%)	760 (24%)	22 (0%)
5	B	117/118 (99%)	37 (31%)	2 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	3235/3238 (99%)	797 (24%)	24 (0%)

5 of 797 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	A	7	U
4	A	9	U
4	A	11	A
4	A	12	G
4	A	20	G

5 of 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	A	2135	U
4	A	2328	G
4	A	2320	C
4	A	2345	U
4	A	974	G

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](#)

1 ligand is 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
36	GCP	4	501	-	27,34,34	1.36	3 (11%)	35,54,54	1.93	7 (20%)

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
36	GCP	4	501	-	-	5/15/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	4	501	GCP	C5-C6	3.99	1.48	1.41
36	4	501	GCP	PG-O2G	2.85	1.61	1.55
36	4	501	GCP	PG-O3G	2.61	1.60	1.55

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	4	501	GCP	C2-N3-C4	4.84	120.70	115.48
36	4	501	GCP	PB-O3A-PA	-4.58	117.42	132.37
36	4	501	GCP	C2-N1-C6	4.23	121.85	115.96
36	4	501	GCP	C5-C6-N1	-3.91	118.19	123.42
36	4	501	GCP	N3-C2-N1	-3.17	123.18	127.21

There are no chirality outliers.

All (5) torsion outliers are listed below:

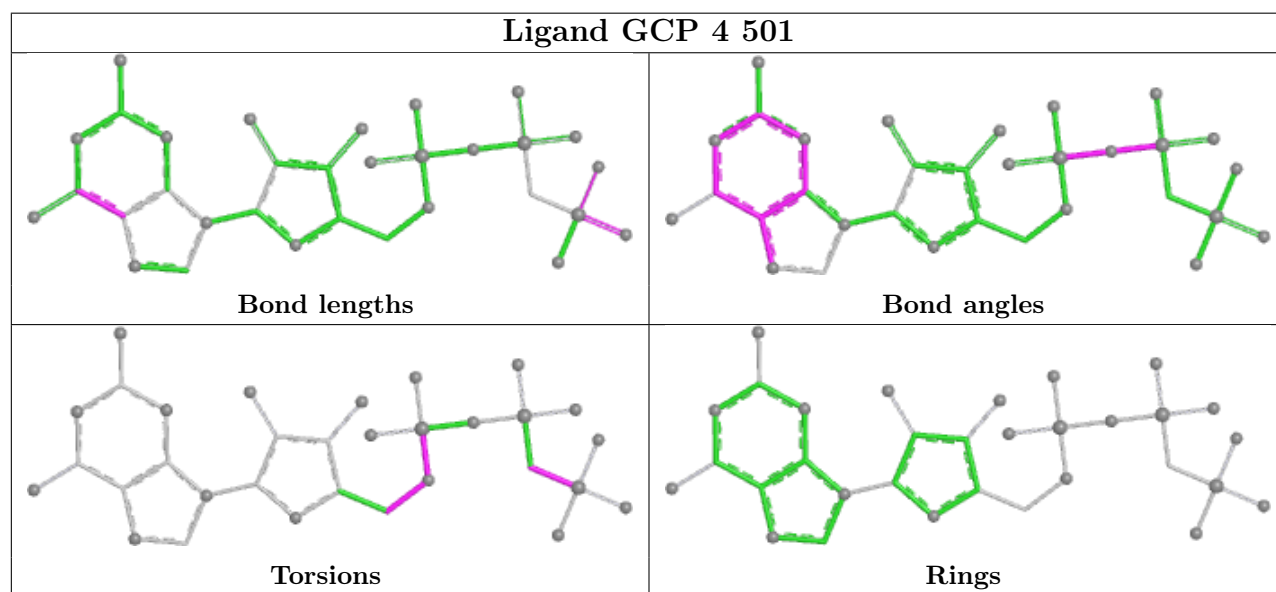
Mol	Chain	Res	Type	Atoms
36	4	501	GCP	PB-C3B-PG-O1G
36	4	501	GCP	PB-C3B-PG-O2G
36	4	501	GCP	PB-C3B-PG-O3G
36	4	501	GCP	C5'-O5'-PA-O1A
36	4	501	GCP	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	4	501	GCP	15	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.

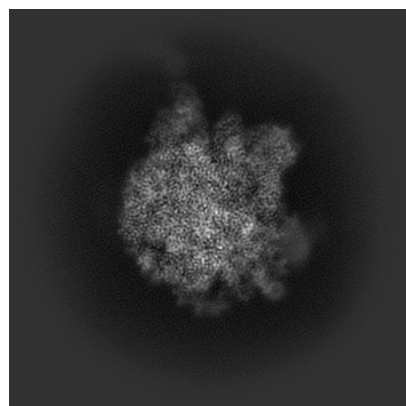
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43294. These allow visual inspection of the internal detail of the map and identification of artifacts.

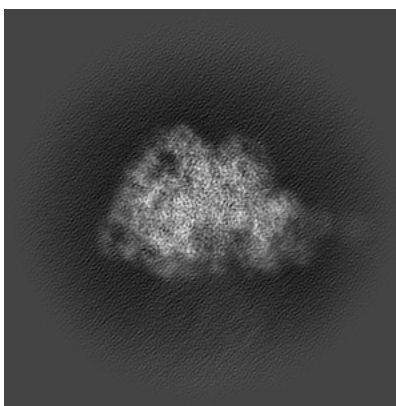
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

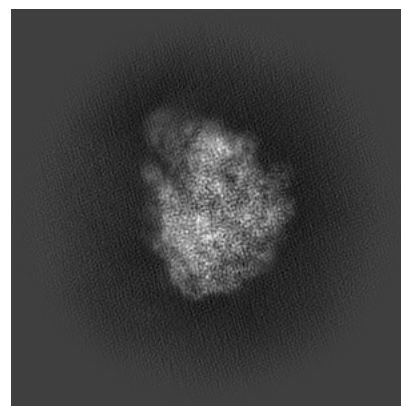
6.1.1 Primary map



X

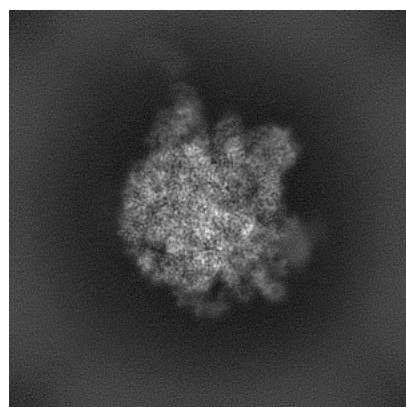


Y

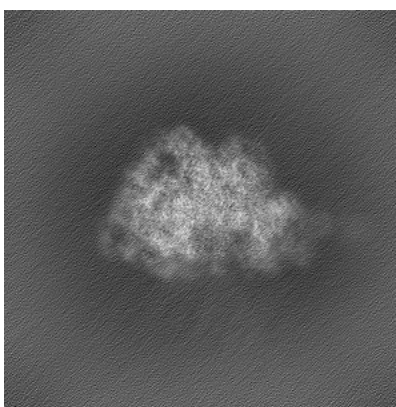


Z

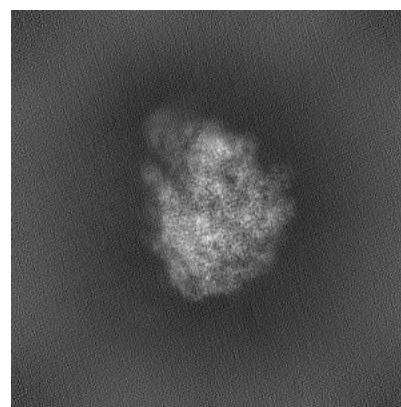
6.1.2 Raw map



X



Y

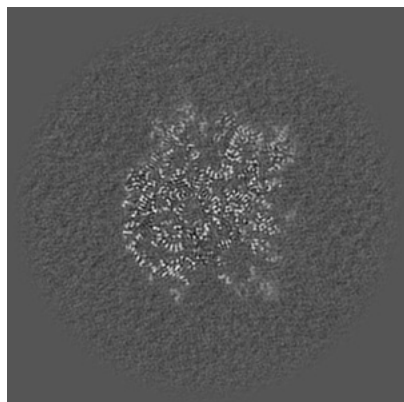


Z

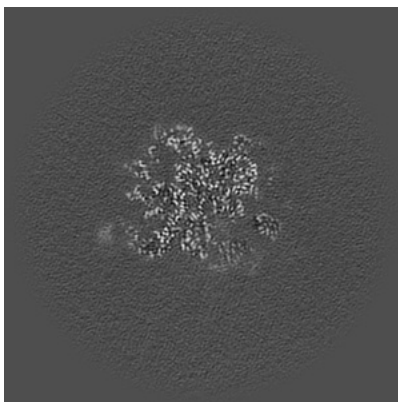
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

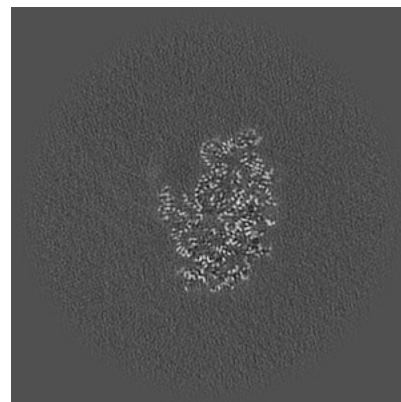
6.2.1 Primary map



X Index: 200

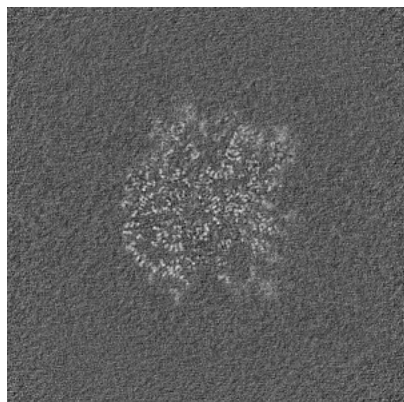


Y Index: 200

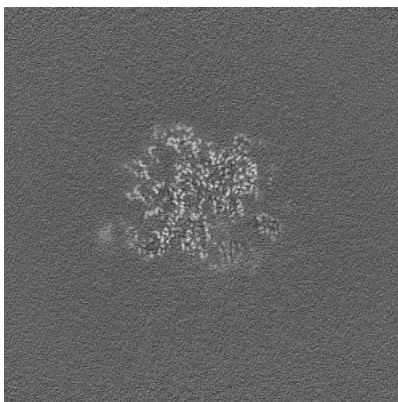


Z Index: 200

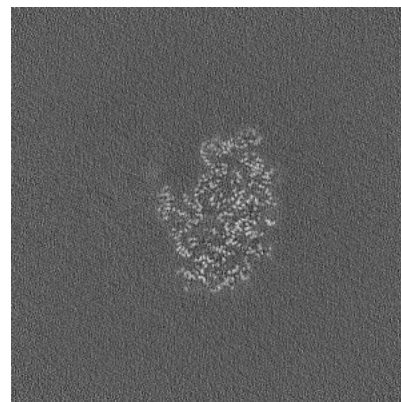
6.2.2 Raw map



X Index: 200



Y Index: 200

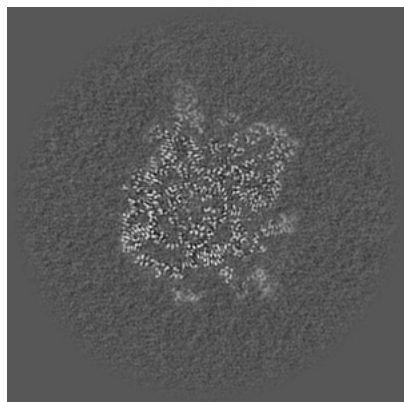


Z Index: 200

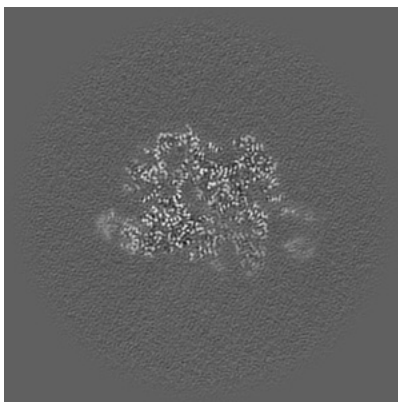
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

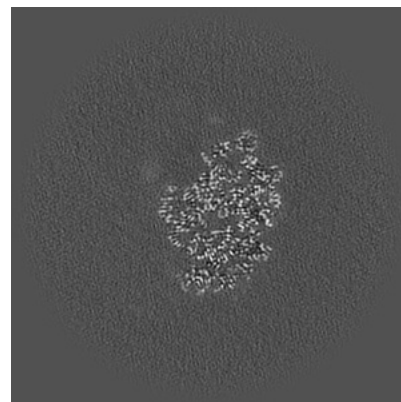
6.3.1 Primary map



X Index: 194

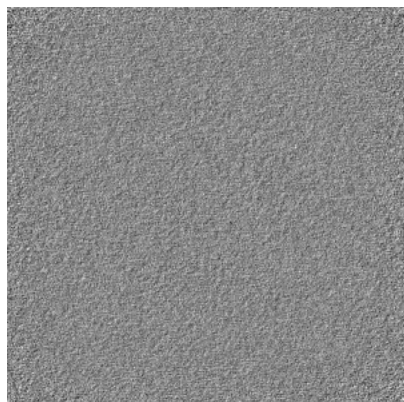


Y Index: 190

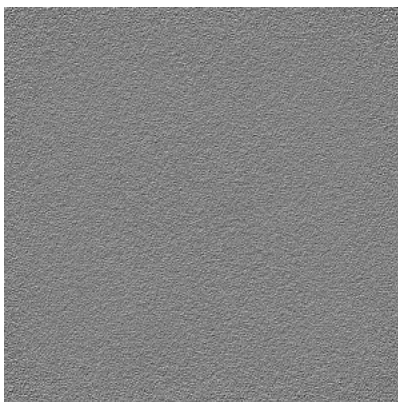


Z Index: 196

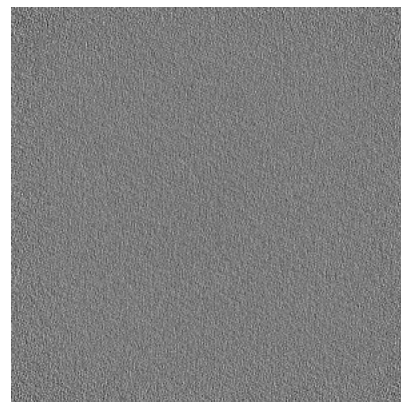
6.3.2 Raw map



X Index: 0



Y Index: 0

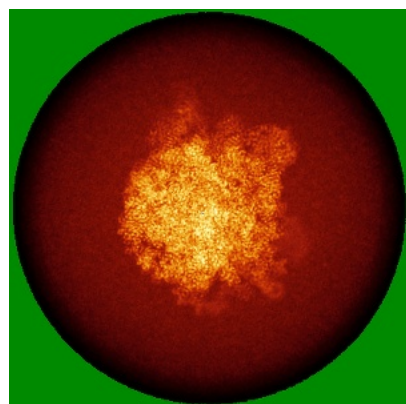


Z Index: 0

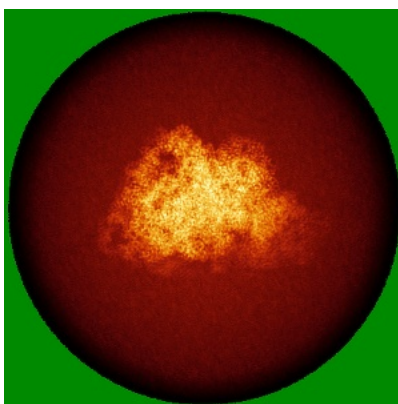
The images above show the largest variance slices of the map in three orthogonal directions.

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

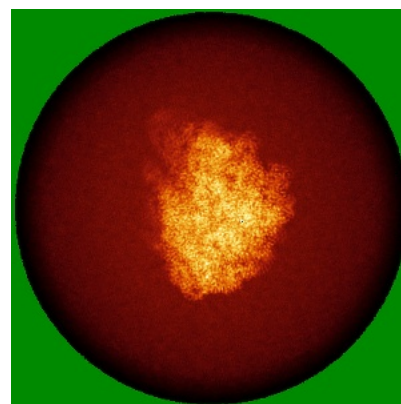
6.4.1 Primary map



X

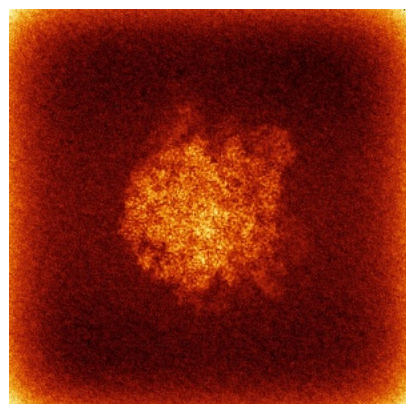


Y

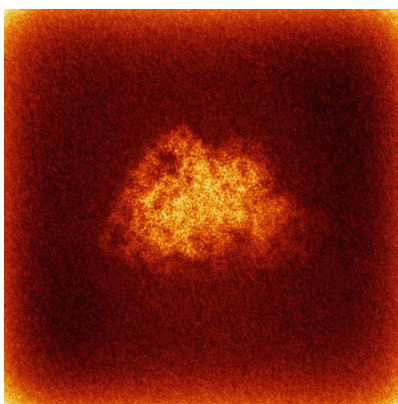


Z

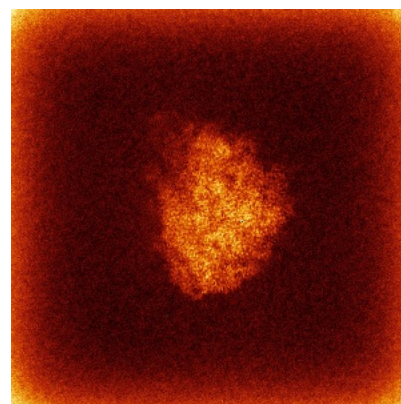
6.4.2 Raw map



X



Y

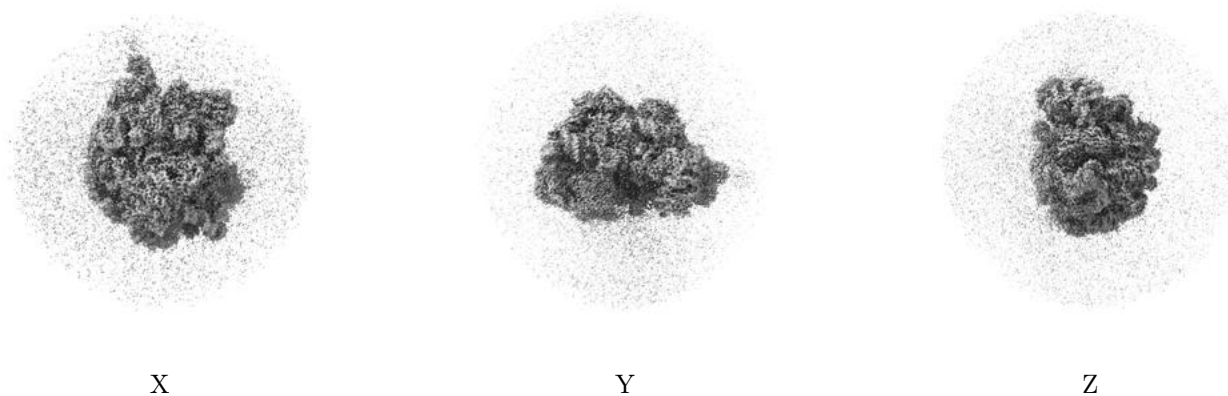


Z

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.

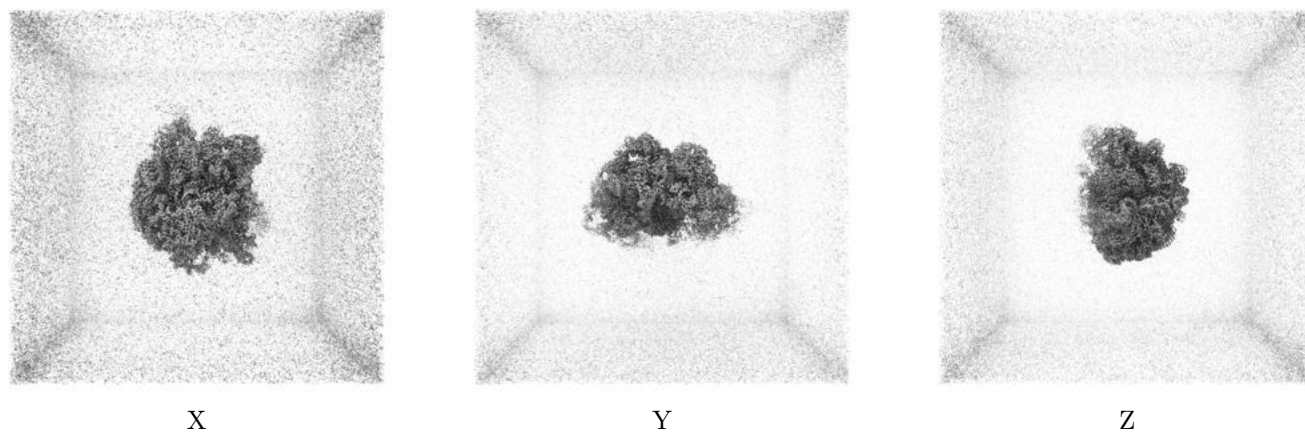
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.19. 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.

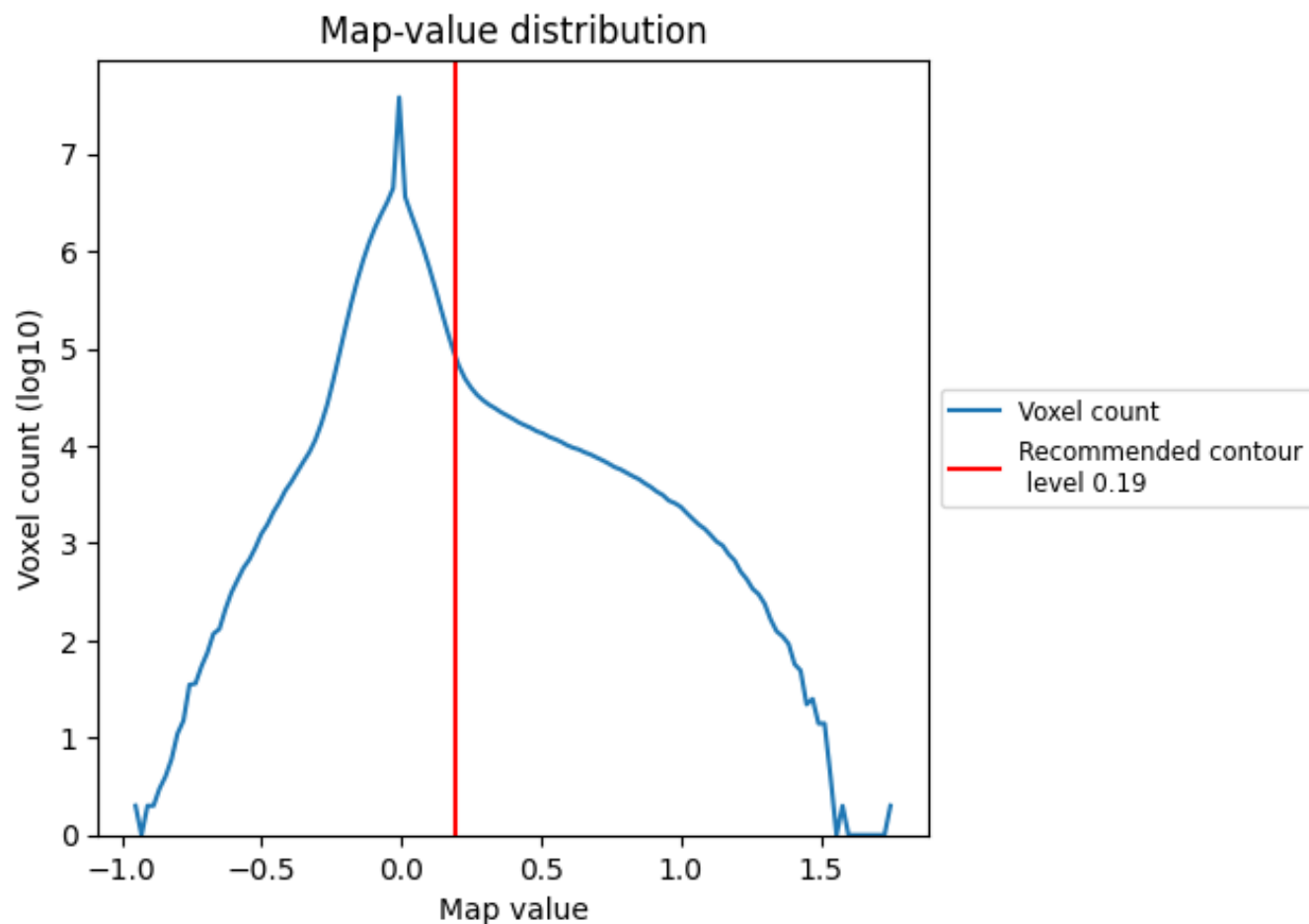
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

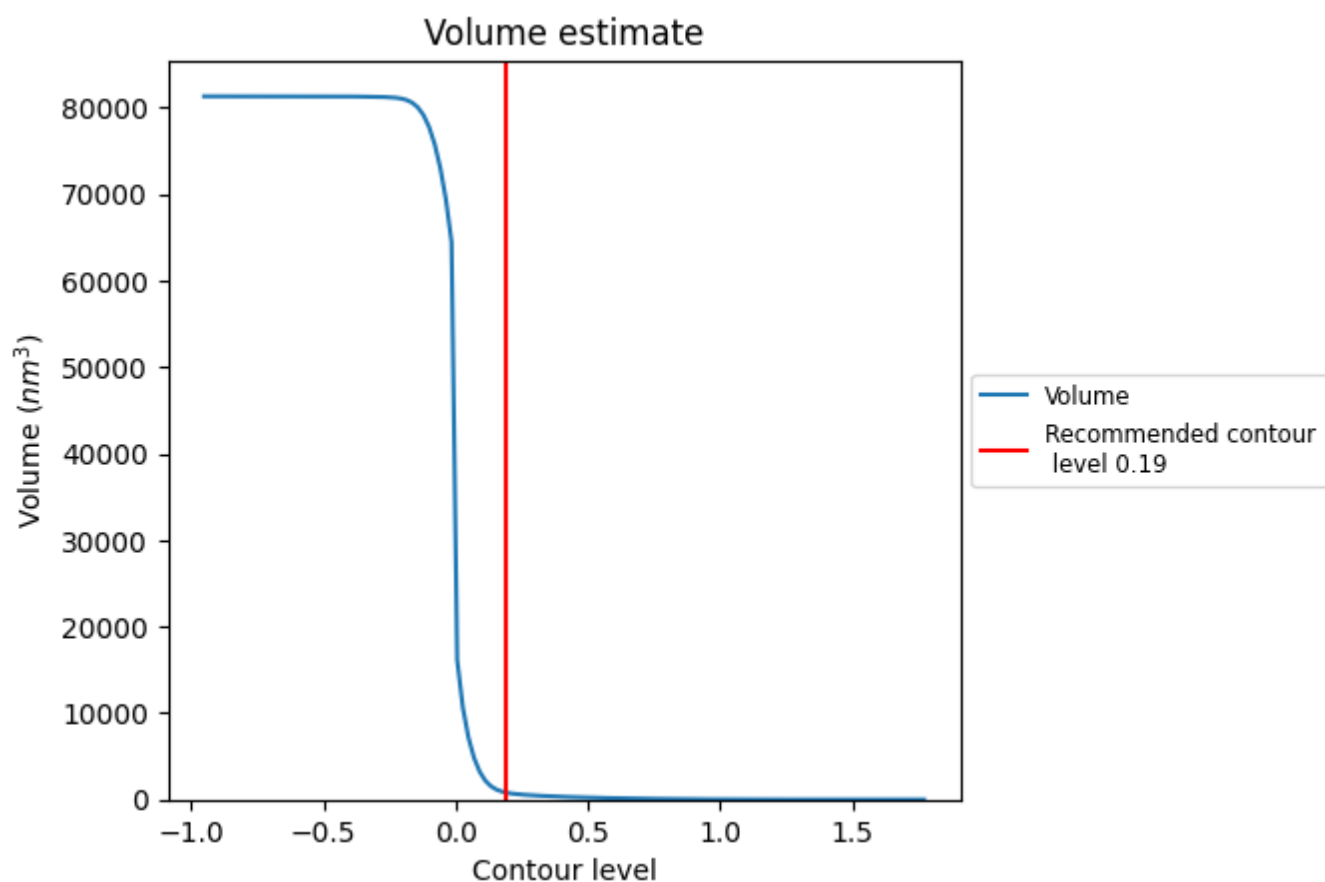
This section contains the results of statistical analysis of the map.

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.

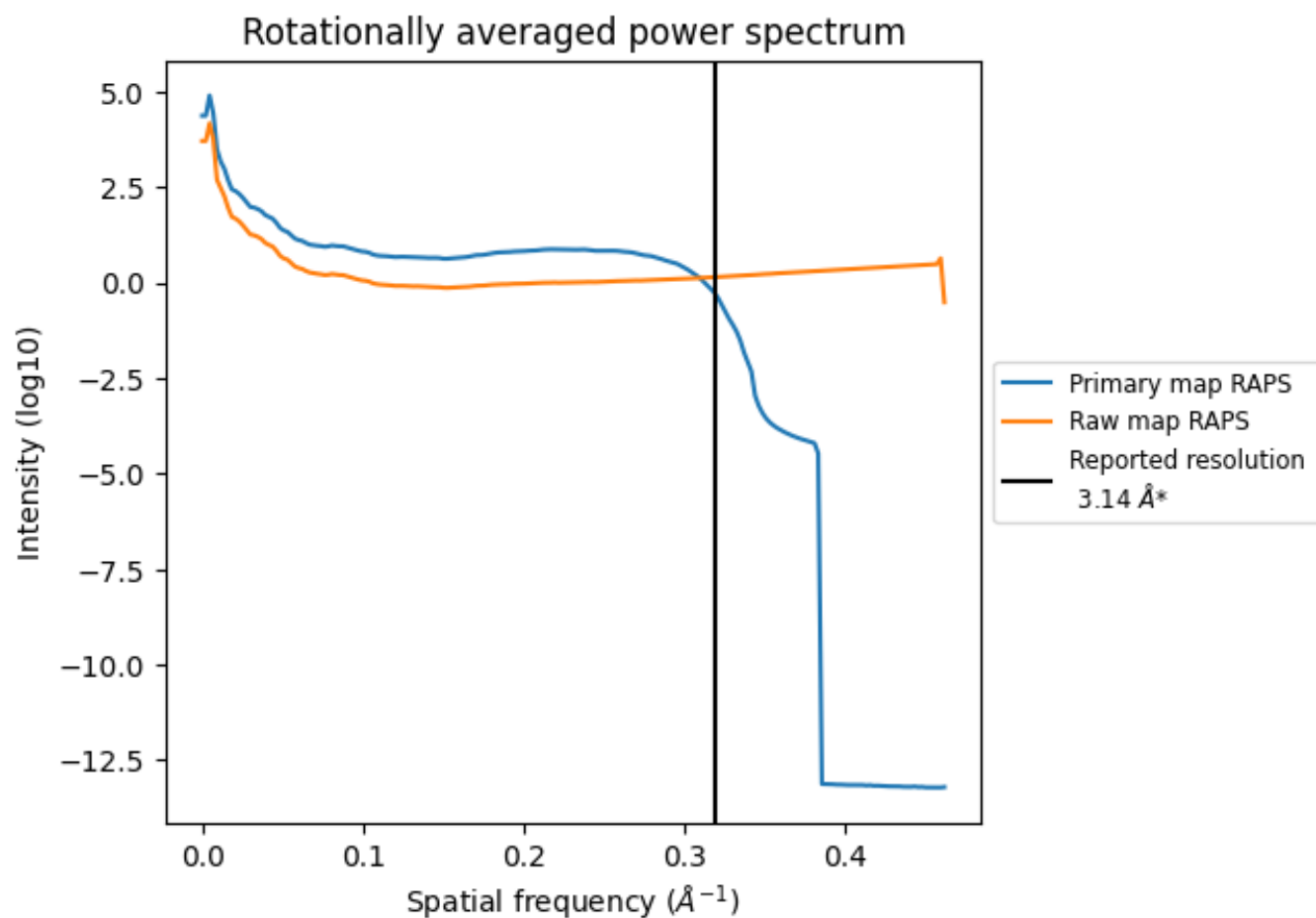
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 817 nm³; this corresponds to an approximate mass of 738 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 ⓘ

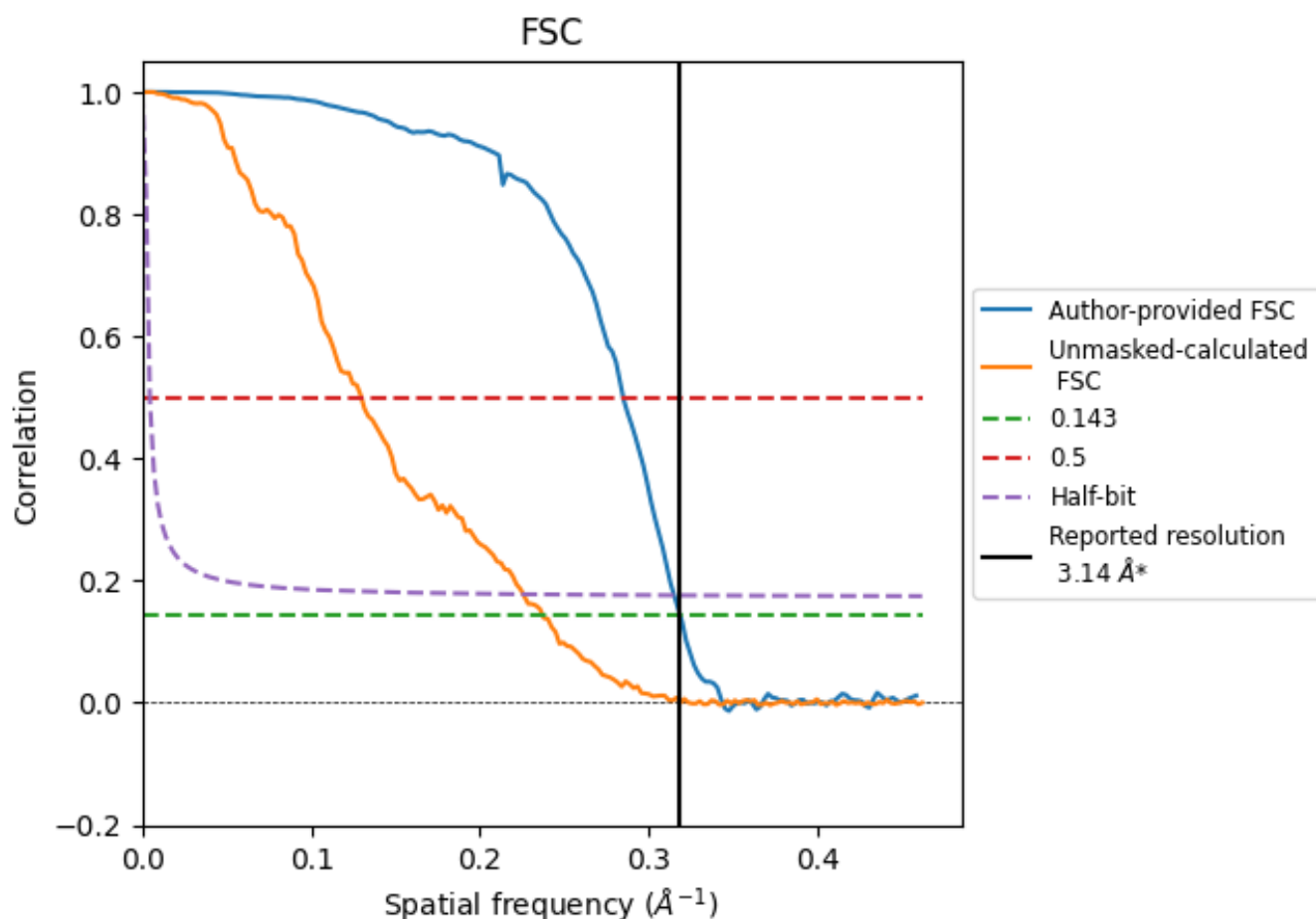


*Reported resolution corresponds to spatial frequency of 0.318 Å⁻¹

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 0.318 \AA^{-1}

8.2 Resolution estimates [i](#)

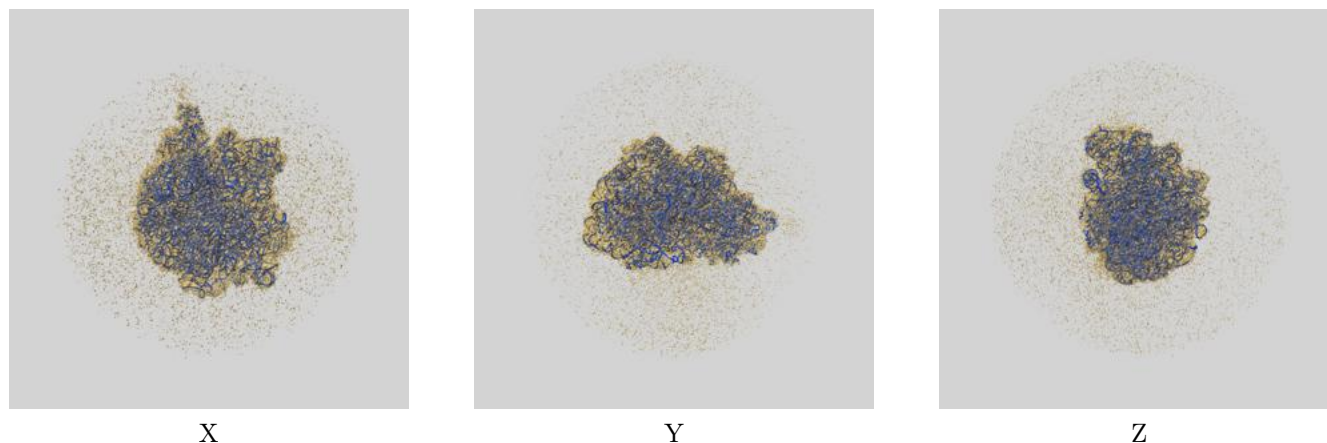
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	3.14	3.51	3.18
Unmasked-calculated*	4.22	7.72	4.43

*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 4.22 differs from the reported value 3.14 by more than 10 %

9 Map-model fit [i](#)

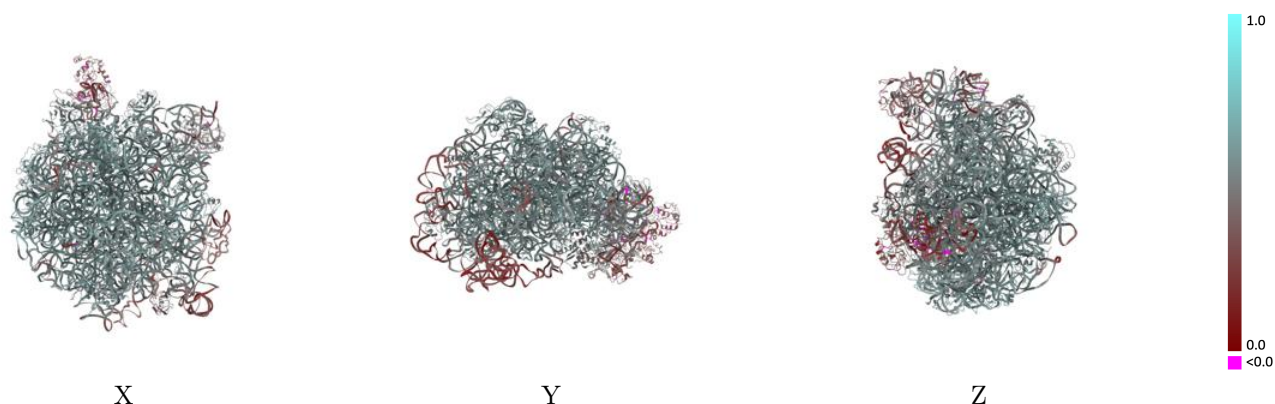
This section contains information regarding the fit between EMDB map EMD-43294 and PDB model 8VK0. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



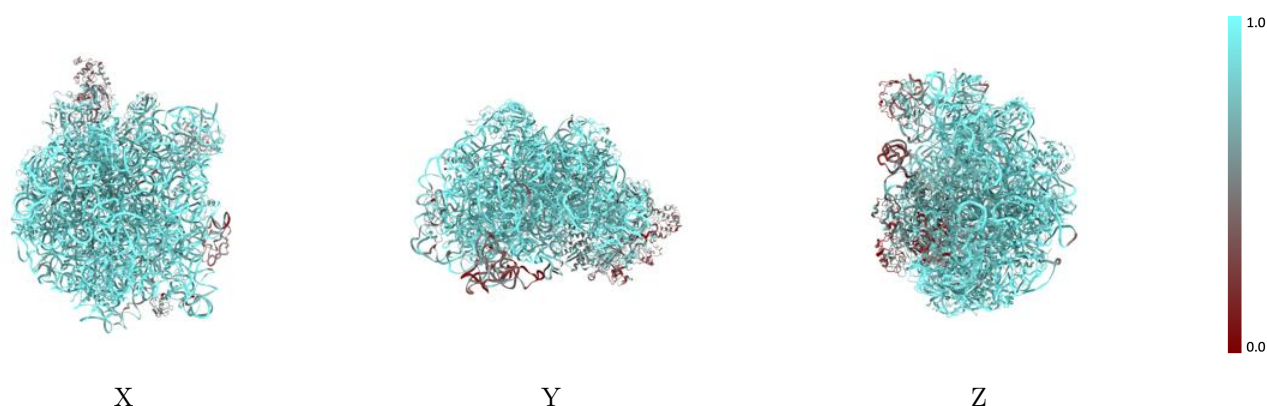
The images above show the 3D surface view of the map at the recommended contour level 0.19 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



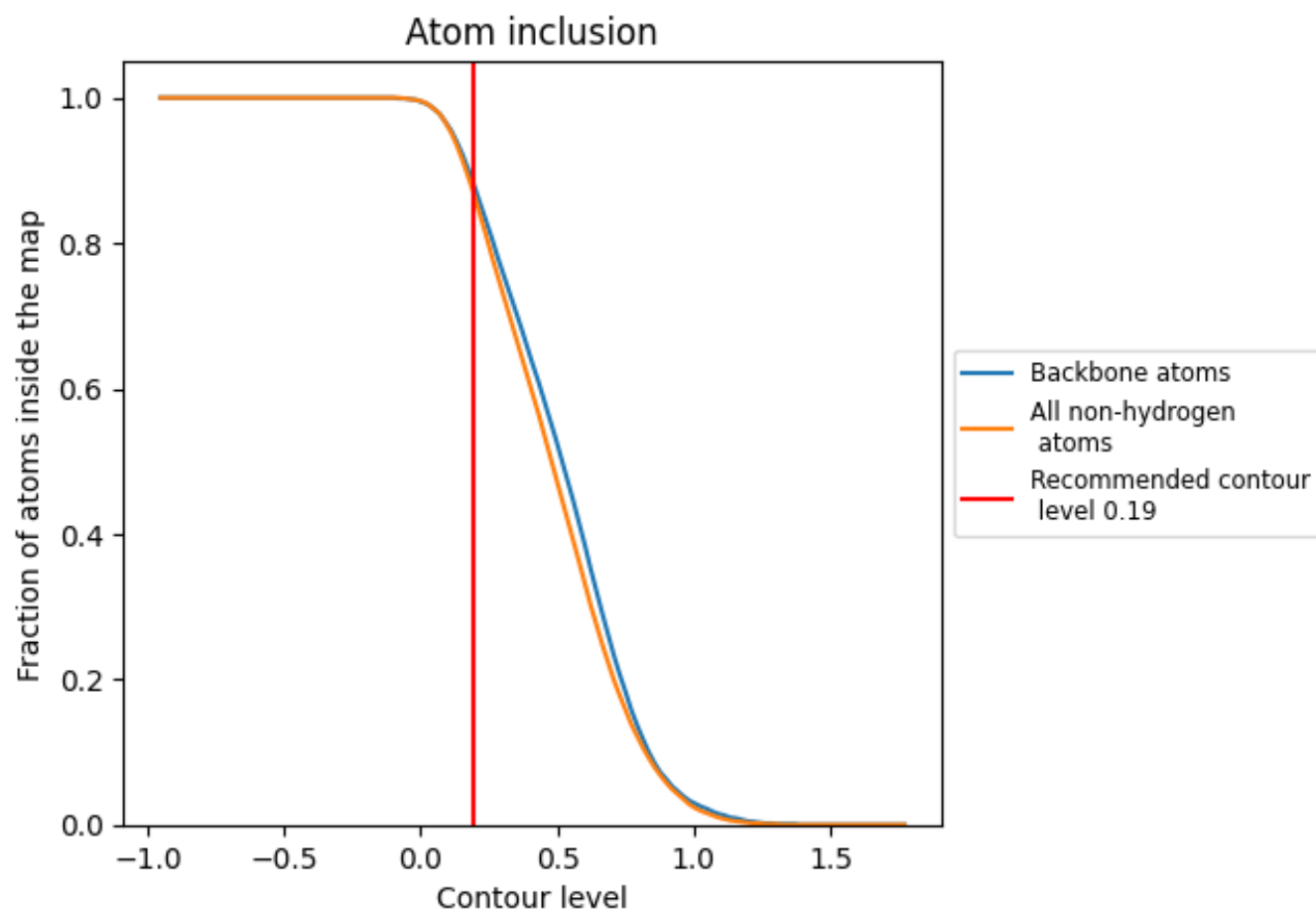
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.19).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8740	 0.5190
2	 0.9410	 0.5870
3	 0.8660	 0.5910
4	 0.6210	 0.4740
A	 0.9060	 0.5190
B	 0.9180	 0.4820
C	 0.9240	 0.5820
D	 0.9270	 0.5810
E	 0.9000	 0.5690
F	 0.6140	 0.3960
G	 0.7870	 0.4960
H	 0.5930	 0.4280
I	 0.3830	 0.2960
J	 0.3570	 0.2730
K	 0.9350	 0.5860
L	 0.8990	 0.5700
M	 0.9170	 0.5720
N	 0.8540	 0.5740
O	 0.9300	 0.5840
P	 0.7640	 0.4290
Q	 0.8660	 0.5520
R	 0.9370	 0.5890
S	 0.9310	 0.5870
T	 0.9240	 0.5810
U	 0.9120	 0.5700
V	 0.8560	 0.5250
W	 0.7330	 0.5330
X	 0.9190	 0.5790
Y	 0.9230	 0.5720
Z	 0.8900	 0.5520
b	 0.9030	 0.5800
c	 0.9090	 0.5780
d	 0.9230	 0.5910
e	 0.9190	 0.5970
f	 0.8570	 0.5790
g	 0.3360	 0.3560

