



## wwPDB EM Validation Summary Report ⓘ

Feb 10, 2025 – 10:34 AM EST

PDB ID : 8VKI  
EMDB ID : EMD-43317  
Title : Structure of Mycobacterium smegmatis 50S ribosomal subunit bound to HflX:50S-HflX-C  
Authors : Majumdar, S.; Koripella, R.K.; Sharma, M.R.; Manjari, S.R.; Banavali, N.K.; Agrawal, R.K.  
Deposited on : 2024-01-09  
Resolution : 2.96 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](mailto: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>.

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

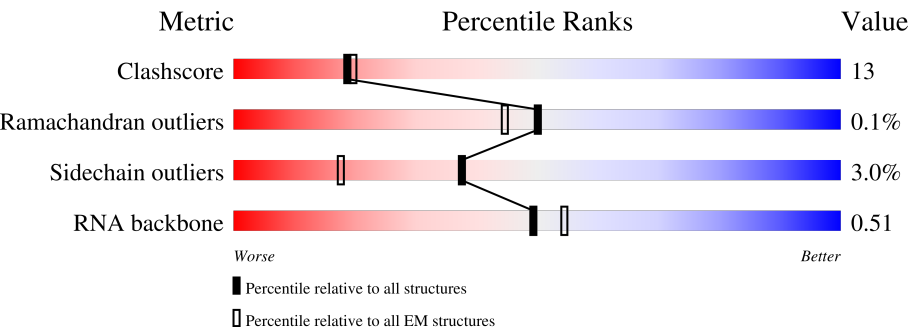
EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal 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 2.96 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.



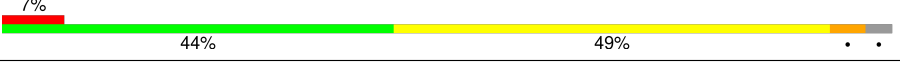

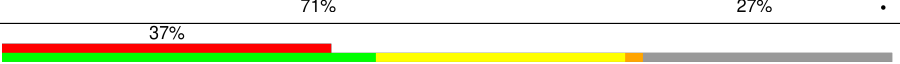
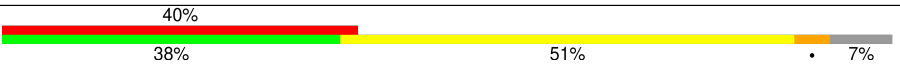


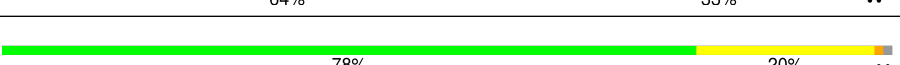
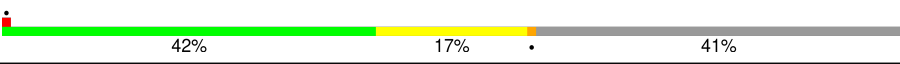
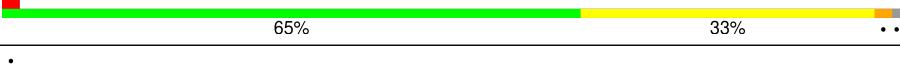




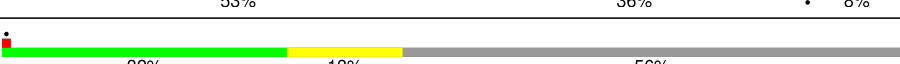

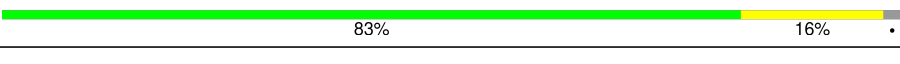

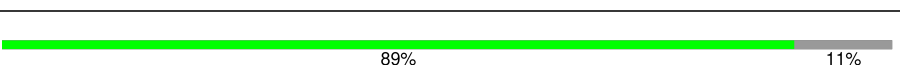
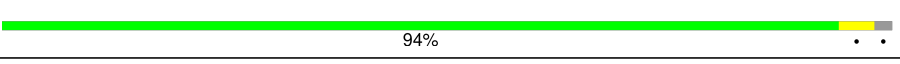
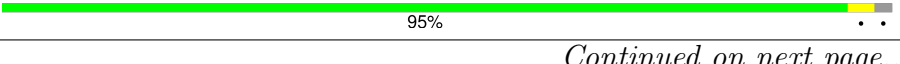



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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	<div><div></div><div>66%30%..</div></div>
2	3	24	<div><div>79%17%. .</div></div>
3	4	470	<div><div>8%55%43%..</div></div>
4	B	118	<div><div>47%43%10%</div></div>
5	C	278	<div><div>78%21%. .</div></div>
6	D	217	<div><div>67%30%..</div></div>
7	E	215	<div><div>75%20%..</div></div>

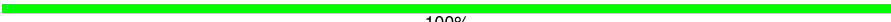

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Mol	Chain	Length	Quality of chain
8	F	187	
9	G	179	
10	H	151	
11	I	175	
12	J	142	
13	K	147	
14	L	122	
15	M	147	
16	N	138	
17	O	199	
18	P	127	
19	Q	113	
20	R	129	
21	S	103	
22	T	153	
23	U	100	
24	V	105	
25	W	215	
26	X	88	
27	Y	64	
28	Z	77	
29	b	57	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

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Mol	Chain	Length	Quality of chain
33	f	37	 100%
34	A	3120	 49% 35% 10% 5%

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
35	GCP	4	501	-	-	X	-

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 96565 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	466	Total	C	N	O	S	0	0
			3516	2171	649	689	7		

- Molecule 4 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 5 is a protein called 50S ribosomal protein L2.

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

- Molecule 6 is a protein called 50S ribosomal protein L3.

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

- Molecule 7 is a protein called 50S Ribosomal Protein L4.

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

- Molecule 8 is a protein called 50S Ribosomal Protein L5.

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

- Molecule 9 is a protein called 50S ribosomal protein L6.

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

- Molecule 10 is a protein called 50S ribosomal protein L9.

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

- Molecule 11 is a protein called 50S ribosomal protein L10.

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

- Molecule 12 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	132	Total	C	N	O	S	0	0
			958	602	172	181	3		

- Molecule 13 is a protein called 50S Ribosomal Protein L13.

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

- Molecule 14 is a protein called 50S ribosomal protein L14.

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

- Molecule 15 is a protein called 50S ribosomal protein L15.

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

- Molecule 16 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 17 is a protein called 50S ribosomal protein L17.

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

- Molecule 18 is a protein called 50S Ribosomal Protein L18.

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

- Molecule 19 is a protein called 50S ribosomal protein L19.

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

- Molecule 20 is a protein called 50S Ribosomal Protein L20.

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

- Molecule 21 is a protein called 50S Ribosomal Protein L21.

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

- Molecule 22 is a protein called 50S Ribosomal Protein L22.

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

- Molecule 23 is a protein called 50S Ribosomal Protein L23.

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

- Molecule 24 is a protein called 50S ribosomal protein L24.

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

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	W	95	Total	C	N	O	0	0
			735	452	149	134		

- Molecule 26 is a protein called 50S ribosomal protein L27.

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

- Molecule 27 is a protein called 50S Ribosomal Protein L28.

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

- Molecule 28 is a protein called 50S ribosomal protein L29.



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

- Molecule 29 is a protein called 50S ribosomal protein L32.

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

- Molecule 30 is a protein called 50S Ribosomal Protein L33.

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

- Molecule 31 is a protein called 50S ribosomal protein L34.

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

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

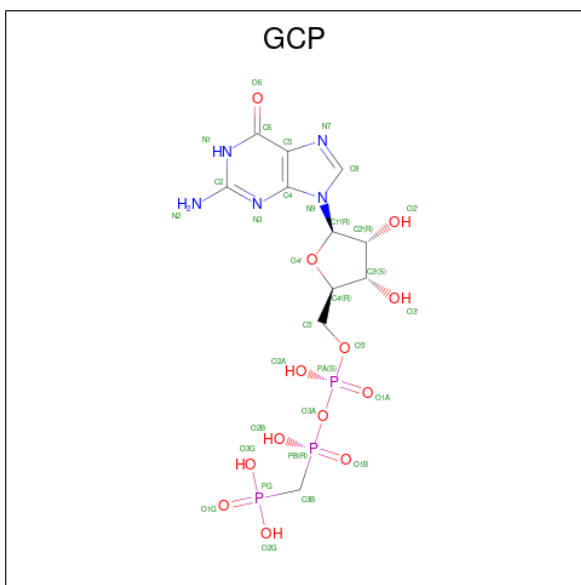
- Molecule 33 is a protein called 50S ribosomal protein L36.

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

- Molecule 34 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	A	2952	Total	C	N	O	P	0	0
			63419	28264	11675	20528	2952		

- Molecule 35 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
35	4	1	Total	C	N	O	P	0
			32	11	5	13	3	

### 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.

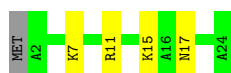
- Molecule 1: 50S ribosomal protein L30

Chain 2: 



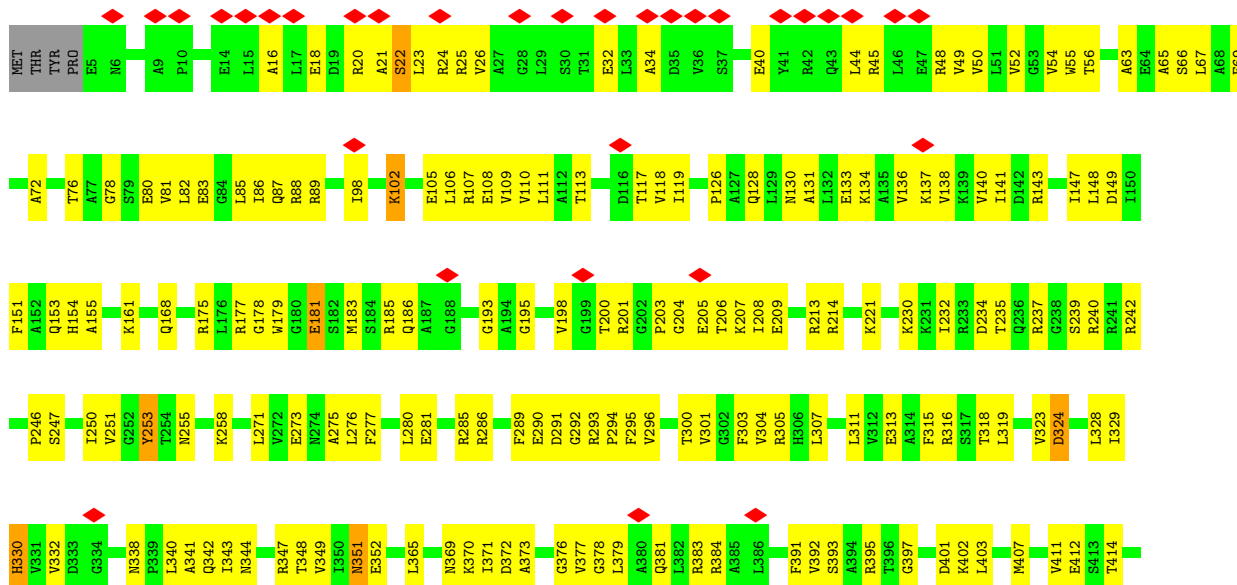
- Molecule 2: 50S Ribosomal Protein L37

Chain 3: 



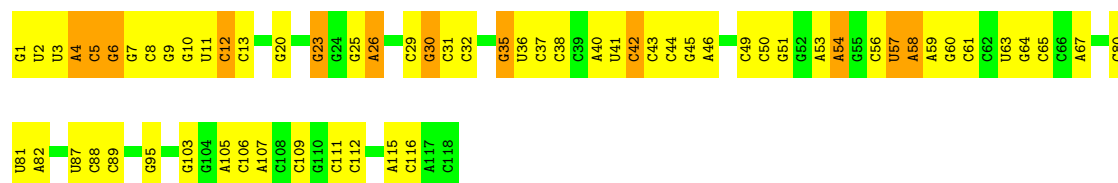
- Molecule 3: GTPase HflX

Chain 4: 

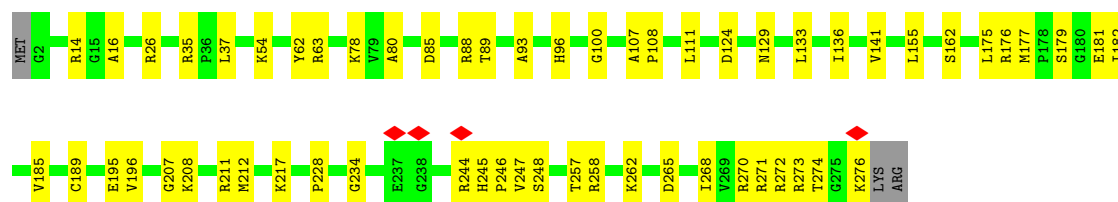
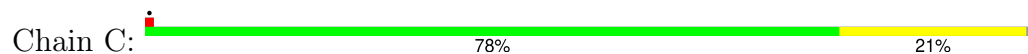




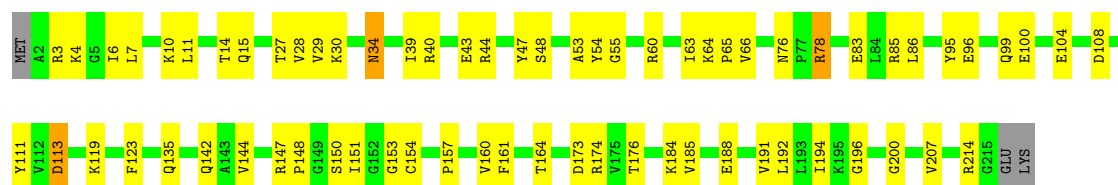
- Molecule 4: 5S ribosomal RNA



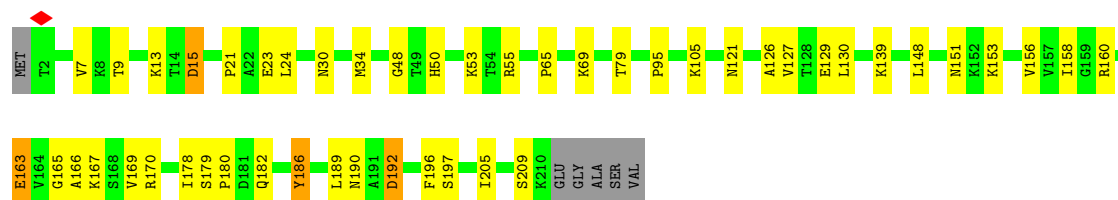
- Molecule 5: 50S ribosomal protein L2



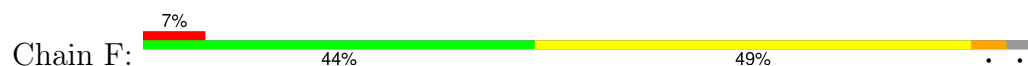
- Molecule 6: 50S ribosomal protein L3

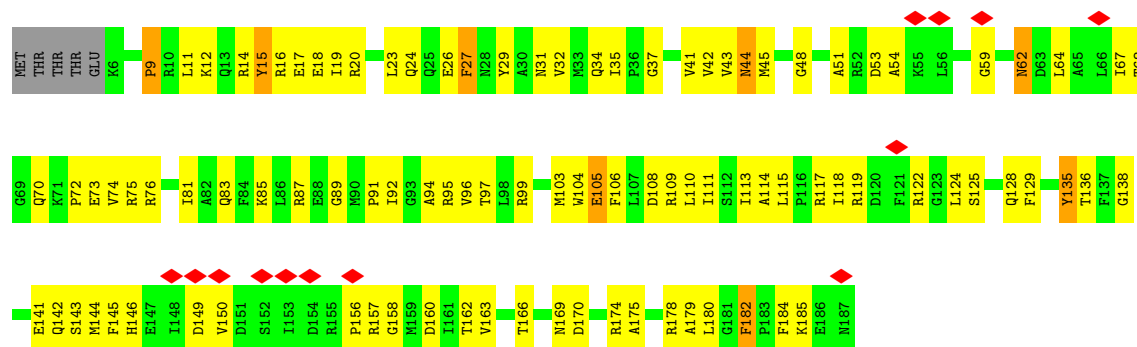


- Molecule 7: 50S Ribosomal Protein L4



- Molecule 8: 50S Ribosomal Protein L5

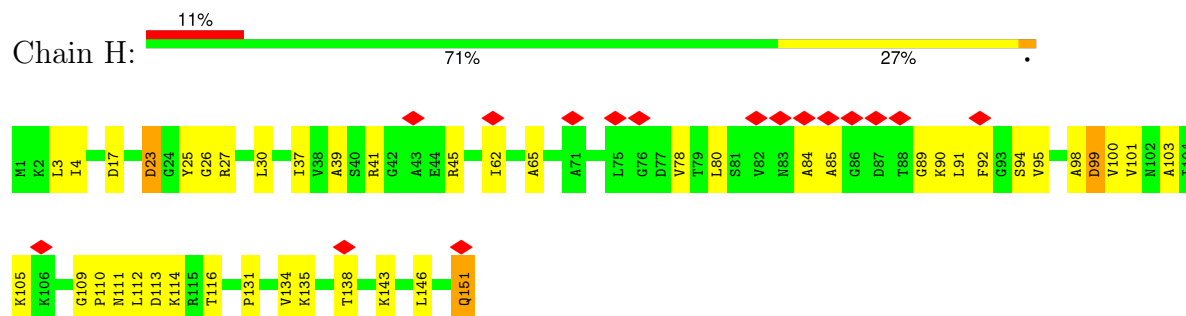




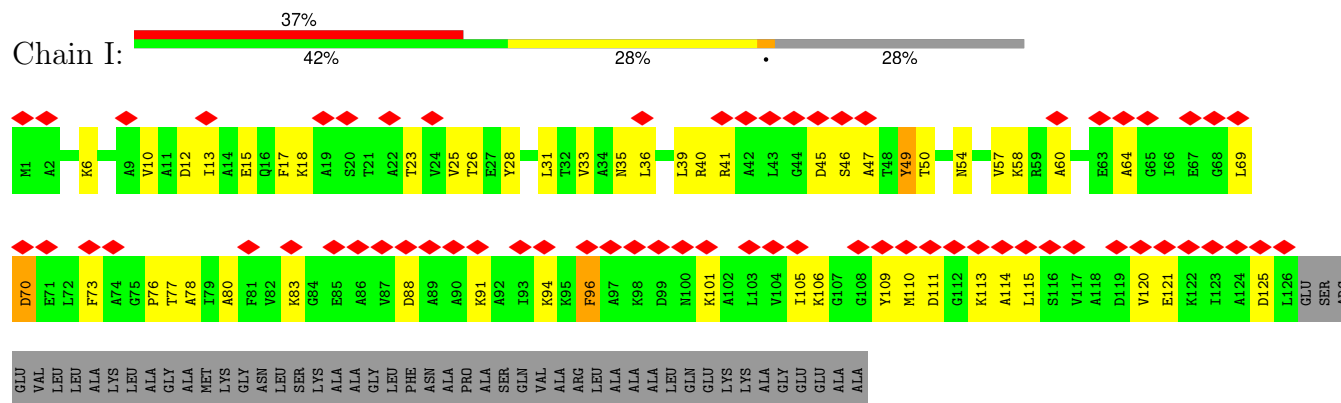
• Molecule 9: 50S ribosomal protein L6



• Molecule 10: 50S ribosomal protein L9



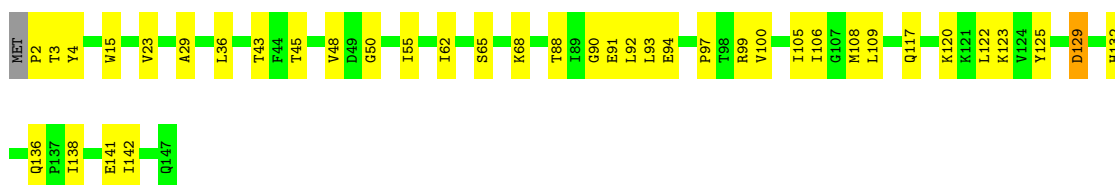
• Molecule 11: 50S ribosomal protein L10



• Molecule 12: 50S ribosomal protein L11

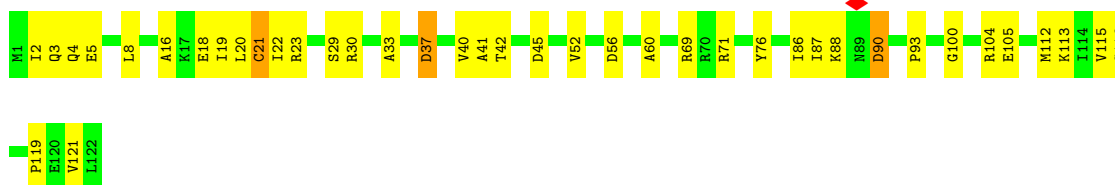
- Molecule 13: 50S Ribosomal Protein L13

Chain K:  73% 26%



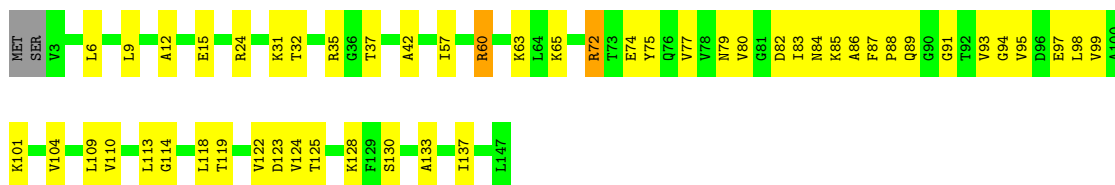
- Molecule 14: 50S ribosomal protein L14

Chain L:  67% 30%



- Molecule 15: 50S ribosomal protein L15

Chain M:  64% 33% ..

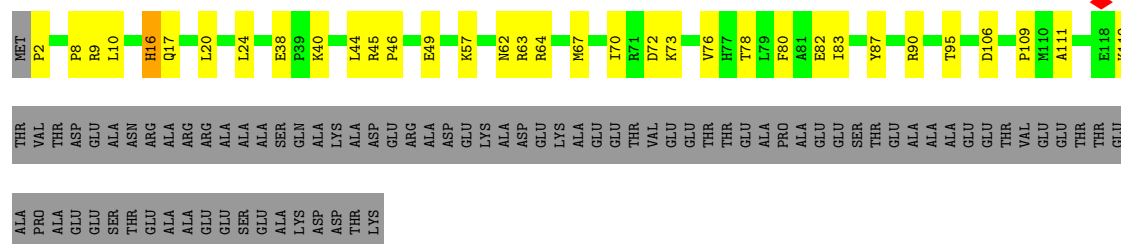


- Molecule 16: Large ribosomal subunit protein uL16

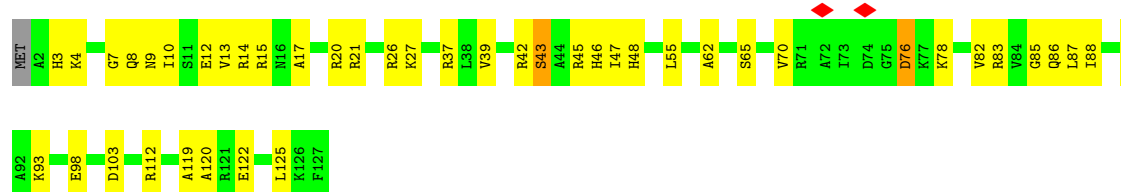
Chain N:  78% 20%



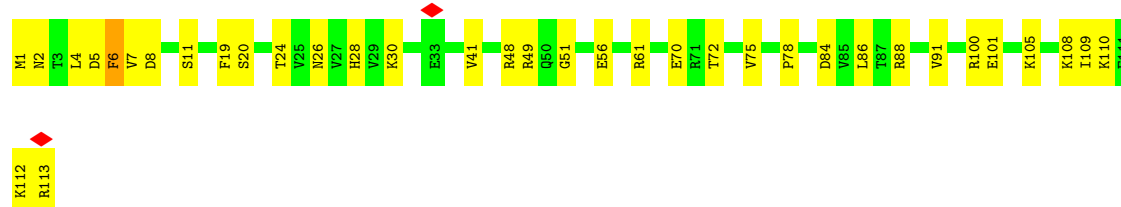
- Molecule 17: 50S ribosomal protein L17



• Molecule 18: 50S Ribosomal Protein L18



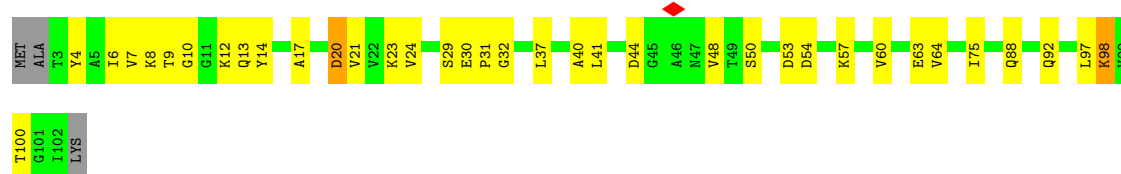
• Molecule 19: 50S ribosomal protein L19



• Molecule 20: 50S Ribosomal Protein L20

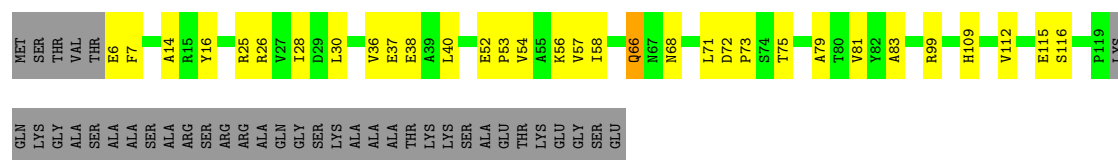


• Molecule 21: 50S Ribosomal Protein L21



• Molecule 22: 50S Ribosomal Protein L22

Chain T: 



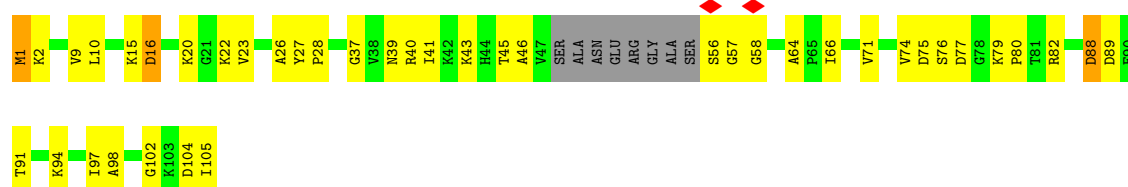
• Molecule 23: 50S Ribosomal Protein L23

Chain U: 




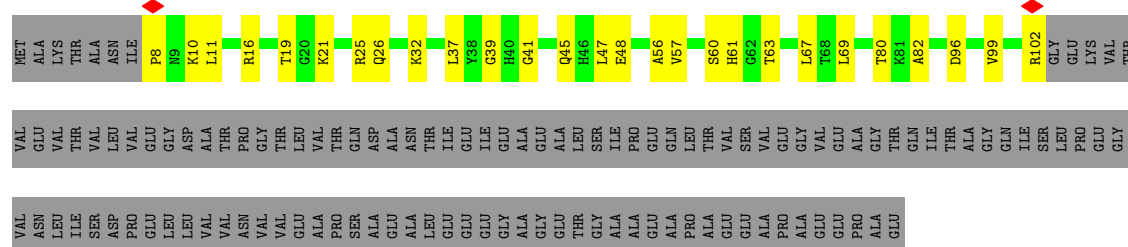
• Molecule 24: 50S ribosomal protein L24

Chain V: 



• Molecule 25: 50S ribosomal protein L25

Chain W: 




• Molecule 26: 50S ribosomal protein L27

Chain X: 



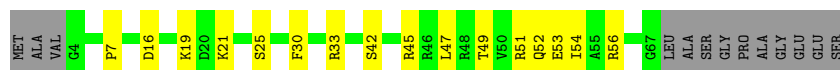
• Molecule 27: 50S Ribosomal Protein L28

Chain Y: 

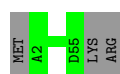




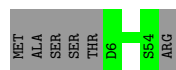
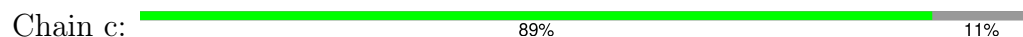
- Molecule 28: 50S ribosomal protein L29



- Molecule 29: 50S ribosomal protein L32



- Molecule 30: 50S Ribosomal Protein L33



- Molecule 31: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L35

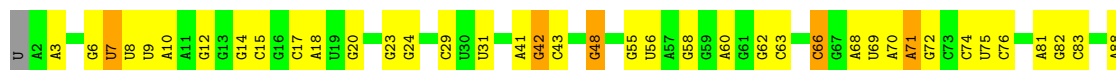


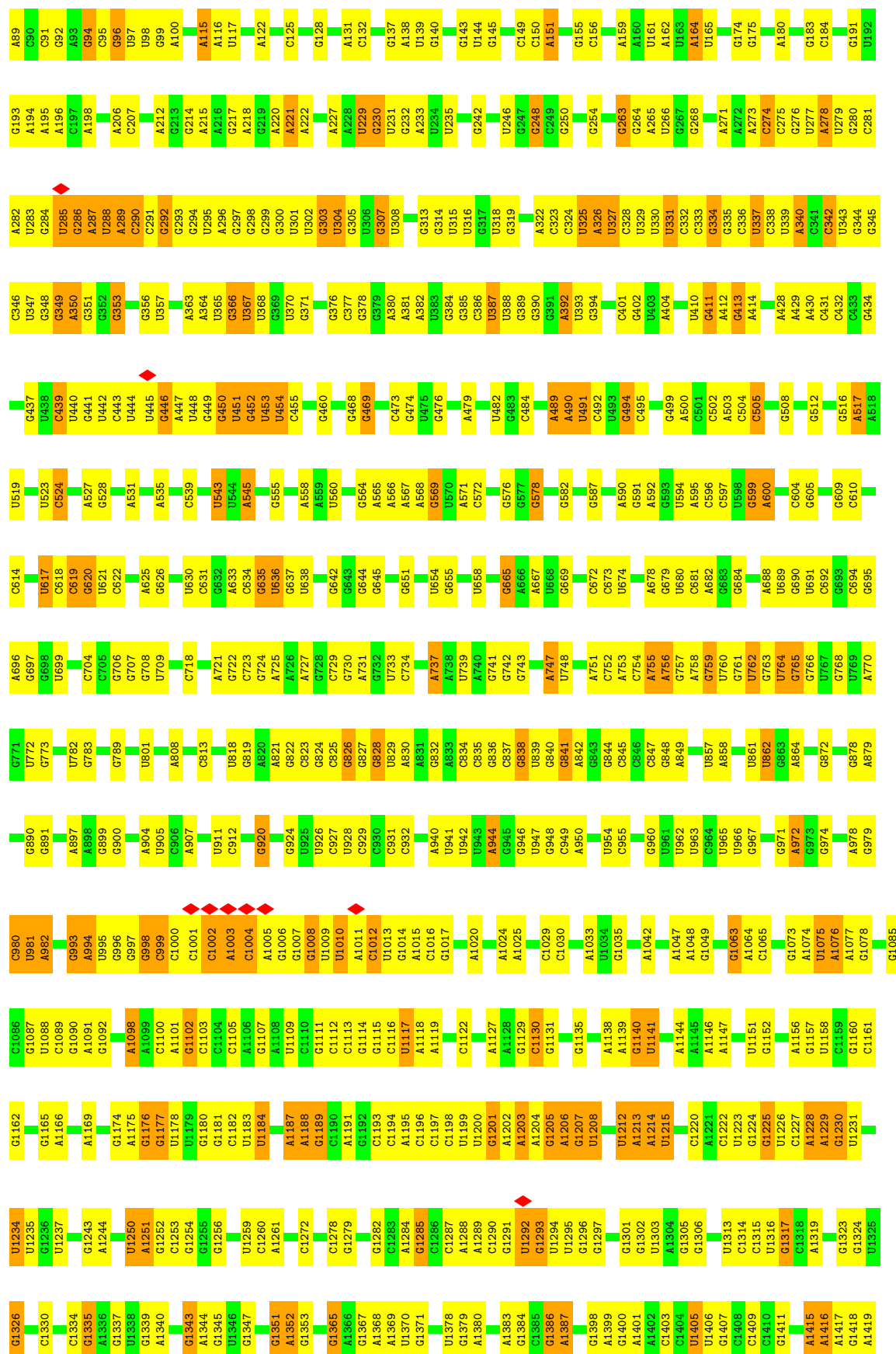
- Molecule 33: 50S ribosomal protein L36



There are no outlier residues recorded for this chain.

- Molecule 34: 23S ribosomal RNA





A2405	U2345	G2276	A	C	G2056	G1951	C1843	G1756	C1651	G	U1529	G1425
U2406	G2346	G2277	A	C	G2057	C1952	A1844	U1757	A1652	U	G1530	G1426
C2407	A2278	G2279	U	C	U2058	A1955	A1852	G1758	G1653	U	G1531	U1427
G2408	G2347	G2280	U	C	G2059	A1956	A1853	A1759	G1654	G	G1532	U1428
U2409	G2348	G2281	U	C	G2060	G1959	A1854	G1760	C	G	U1533	C1429
A2410	A2282	A2283	C	C	U2061	U1960	A1855	G1761	C	C	U1534	C1430
U2411	G2350	G2284	C	G	G2062	G1961	C1856	G1762	U	U	C1535	U1431
U2412	A2351	U2285	A	A	G2063	G1962	U1864	A1763	G	G	A1536	G1434
G2413	C2352	G2286	C	C	A	A1963	A1865	U1767	U	U	G1541	G1435
G2414	U2353	U2287	U	U	G	U1964	G1866	G1768	G	G	A1542	C1436
G2415	G2354	G2288	U	A	G	G1977	G1867	G1769	U	U	A1543	U1444
C2416	G2355	C2289	C	A	G	U1981	A1868	G1770	G	G	U1544	C1445
U2417	U2356	C2290	C	A	G	U1982	G1869	A1778	U	U	C1545	C1449
U2418	G2357	C2291	A	A	G	U1983	U1870	U1779	G	G	A	G1456
C2419	A2358	G2292	C	A	G	A1985	G1871	G1780	C	C	G	A1457
U2420	G2359	U2293	A	A	G	A1990	U1872	U1781	U	U	C	G1465
A2421	C2360	C2294	A	A	G	U1996	U1877	C1784	G	G	C	C1466
G2422	U2361	A2295	A	A	G	U1997	A1883	C1785	C	C	C	U1467
C2431	C2362	G2195	G	G	G	U1998	G1884	G1786	A	A	U	A1468
A2436	A2363	G2196	A	A	A	U1999	G1885	A1787	U	U	C	G1473
G2447	C2364	G2197	C	C	C	A2000	U1889	G1788	G	G	A	G1475
G2448	A2365	G2198	C	C	C	A2001	C1890	A1789	U	U	C	G1476
G2449	C2366	G2199	C	C	C	A2002	G1891	A1790	G	G	C	U1477
A2449	C2367	G2200	C	C	C	C2007	G1892	A1791	C	C	A	C1477
G2462	C2368	U2215	U	U	U	A2008	G1893	U1798	C	C	C	G1478
G2463	C2369	G2216	A	A	A	A2009	G1894	U1799	U	U	C	G1479
G2466	A2370	U2217	A	A	A	G2014	U1898	A1803	U	U	C	A1480
U2467	G2371	G2218	A	A	A	U2015	G1899	G1804	U	U	C	C1481
U2468	U2372	C2219	C	C	C	G2016	C1900	G1805	U	U	C	A1482
U2469	G2373	C2220	C	C	C	C2017	C1901	A1806	U	U	C	U1487
A2470	C2374	G2221	C	C	C	G2018	C1902	C1807	U	U	C	A1488
A2471	G2375	U2222	C	C	C	G2019	C1903	U1808	U	U	C	A1493
C2472	C2376	G2223	C	C	C	A2020	A1907	U1809	U	U	C	U1494
U2473	G2377	U2224	C	C	C	G2025	A1908	A1810	U	U	C	A1499
G2474	U2378	C2225	U	U	U	A2026	A1909	C1811	U	U	C	C1500
G2479	C2379	A2244	A	A	G	G2027	U1911	A1812	U	U	C	G1502
G2480	G2380	U2245	G	G	G	G2028	G1917	G1815	U	U	C	U1509
U2481	C2381	C2246	U	U	U	G2031	C1928	C1816	U	U	C	A1510
U2482	A2382	A2247	G	G	G	A2032	A1931	C1822	U	U	C	U1511
U2486	U2383	G2248	A	A	A	U2033	G1932	C1823	U	U	C	U1512
C2487	C2384	G2249	A	A	A	G2038	G1933	C1824	U	U	C	C1514
A2490	G2385	A2255	G	G	G	G2039	G1934	C1825	U	U	C	G1524
A2491	U2386	G2256	C	C	C	G2040	G1935	A1826	U	U	C	U1525
G2495	G2387	A2257	G	G	G	U2044	G1936	A1827	U	U	C	G1528
U2496	U2388	G2258	A	A	A	G2045	U1937	A1828	U	U	C	
A2497	C2389	U2261	G	G	G	A2046	G1938	A1832	U	U	C	
A2498	G2390	C2262	A	A	A	U2051	C1944	C1833	U	U	C	
G2503	U2391	U2263	A	A	A	G2052	U1945	A1834	U	U	C	
C2507	A2392	C2267	U	U	U	C2053	U1946	C1835	U	U	C	
	U2393	G2274	C	C	C	C2054	U1947	G1840	U	U	C	
	A2394	A2275	U	U	U	C2055			U	U	C	
	U2395		U	U	U				U	U	C	
	C2396		C	C	C				U	U	C	
	C2397		G	G	G				U	U	C	
	C2398		U	U	U				U	U	C	
	A2399		U	U	U				U	U	C	
	C2400		C	C	C				U	U	C	
	U2401		U	U	U				U	U	C	
	C2402		U	U	U				U	U	C	
	U2403		U	U	U				U	U	C	
	U2404		U	U	U				U	U	C	



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	132147	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 ( $e^-/\text{\AA}^2$ )	51.85	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.399	Depositor
Minimum map value	-1.560	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.111	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	430.4, 430.4, 430.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.076, 1.076, 1.076	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	0.39	0/477	0.59	0/640
2	3	0.37	0/191	0.66	0/247
3	4	0.40	2/3558 (0.1%)	0.75	4/4822 (0.1%)
4	B	0.70	0/2821	0.85	0/4396
5	C	0.43	0/2153	0.59	0/2895
6	D	0.45	0/1609	0.61	1/2165 (0.0%)
7	E	0.40	0/1592	0.55	0/2153
8	F	0.43	2/1467 (0.1%)	0.76	2/1973 (0.1%)
9	G	0.34	0/1369	0.60	0/1848
10	H	0.33	0/1027	0.60	0/1398
11	I	0.27	0/925	0.52	0/1246
12	J	0.36	0/971	0.79	1/1315 (0.1%)
13	K	0.42	0/1157	0.54	0/1567
14	L	0.42	0/946	0.65	1/1268 (0.1%)
15	M	0.44	1/1091 (0.1%)	0.56	0/1457
16	N	0.42	0/1118	0.57	0/1506
17	O	0.42	0/945	0.57	0/1267
18	P	0.37	0/966	0.61	0/1298
19	Q	0.42	0/921	0.58	0/1236
20	R	0.48	0/1000	0.60	0/1341
21	S	0.45	1/764 (0.1%)	0.56	0/1030
22	T	0.41	0/887	0.57	0/1204
23	U	0.41	0/766	0.54	0/1030
24	V	0.36	0/738	0.58	0/987
25	W	0.33	0/745	0.57	0/1008
26	X	0.41	0/595	0.61	0/798
27	Y	0.46	0/478	0.57	0/641
28	Z	0.35	0/534	0.60	0/713
29	b	0.40	0/427	0.64	0/572
30	c	0.40	0/413	0.55	0/553
31	d	0.44	0/380	0.71	0/500
32	e	0.40	0/507	0.63	0/672

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	f	0.42	0/303	0.61	0/401
34	A	0.91	0/71013	0.87	49/110798 (0.0%)
All	All	0.79	6/104854 (0.0%)	0.81	58/156945 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	J	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	458	PRO	CG-CD	-11.45	1.12	1.50
3	4	458	PRO	CB-CG	-6.40	1.18	1.50
15	M	60	ARG	C-N	-5.80	1.20	1.34
8	F	9	PRO	CG-CD	-5.67	1.31	1.50
21	S	29	SER	C-N	-5.35	1.21	1.34

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	458	PRO	N-CD-CG	-21.18	71.43	103.20
3	4	458	PRO	CA-CB-CG	-15.62	74.33	104.00
8	F	9	PRO	CA-N-CD	-12.34	94.22	111.50
8	F	9	PRO	N-CD-CG	-9.26	89.31	103.20
34	A	2245	C	C2-N1-C1'	8.52	128.17	118.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	J	72	LEU	Mainchain

## 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	16	0
2	3	189	0	205	4	0
3	4	3516	0	3564	198	0
4	B	2522	0	1285	45	0
5	C	2110	0	2165	43	0
6	D	1587	0	1630	58	0
7	E	1569	0	1607	36	0
8	F	1445	0	1476	94	0
9	G	1348	0	1399	58	0
10	H	1018	0	988	34	0
11	I	918	0	959	47	0
12	J	958	0	961	138	0
13	K	1130	0	1167	26	0
14	L	938	0	1000	25	0
15	M	1078	0	1151	36	0
16	N	1092	0	1128	22	0
17	O	928	0	972	25	0
18	P	956	0	991	39	0
19	Q	907	0	938	25	0
20	R	988	0	1038	24	0
21	S	754	0	801	24	0
22	T	873	0	909	22	0
23	U	756	0	802	22	0
24	V	732	0	782	33	0
25	W	735	0	756	18	0
26	X	586	0	601	14	0
27	Y	470	0	484	5	0
28	Z	531	0	541	15	0
29	b	423	0	463	0	0
30	c	405	0	411	0	0
31	d	377	0	411	0	0
32	e	502	0	541	0	0
33	f	299	0	324	0	0
34	A	63419	0	31905	1007	0
35	4	32	0	14	11	0
All	All	96565	0	64869	1959	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 13.

The worst 5 of 1959 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)
12:J:56:ILE:CD1	12:J:74:THR:HG22	1.48	1.39
12:J:56:ILE:HD13	12:J:74:THR:CG2	1.49	1.39
12:J:56:ILE:HD12	12:J:74:THR:CA	1.52	1.37
12:J:56:ILE:CD1	12:J:74:THR:HA	1.58	1.31
12:J:24:PRO:HG2	12:J:25:PRO:CD	1.58	1.30

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%)	54 (95%)	3 (5%)	0	100	100
2	3	21/24 (88%)	21 (100%)	0	0	100	100
3	4	464/470 (99%)	396 (85%)	67 (14%)	1 (0%)	44	67
5	C	273/278 (98%)	256 (94%)	17 (6%)	0	100	100
6	D	212/217 (98%)	197 (93%)	15 (7%)	0	100	100
7	E	207/215 (96%)	192 (93%)	15 (7%)	0	100	100
8	F	180/187 (96%)	162 (90%)	18 (10%)	0	100	100
9	G	174/179 (97%)	153 (88%)	21 (12%)	0	100	100
10	H	149/151 (99%)	117 (78%)	32 (22%)	0	100	100
11	I	124/175 (71%)	103 (83%)	21 (17%)	0	100	100
12	J	130/142 (92%)	113 (87%)	16 (12%)	1 (1%)	16	39
13	K	144/147 (98%)	133 (92%)	11 (8%)	0	100	100
14	L	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
15	M	143/147 (97%)	128 (90%)	15 (10%)	0	100	100
16	N	134/138 (97%)	125 (93%)	9 (7%)	0	100	100
17	O	116/199 (58%)	111 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	P	124/127 (98%)	112 (90%)	12 (10%)	0	100	100
19	Q	111/113 (98%)	97 (87%)	14 (13%)	0	100	100
20	R	122/129 (95%)	119 (98%)	3 (2%)	0	100	100
21	S	98/103 (95%)	90 (92%)	8 (8%)	0	100	100
22	T	112/153 (73%)	101 (90%)	11 (10%)	0	100	100
23	U	95/100 (95%)	88 (93%)	7 (7%)	0	100	100
24	V	93/105 (89%)	80 (86%)	13 (14%)	0	100	100
25	W	93/215 (43%)	85 (91%)	8 (9%)	0	100	100
26	X	77/88 (88%)	75 (97%)	2 (3%)	0	100	100
27	Y	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
28	Z	62/77 (80%)	60 (97%)	2 (3%)	0	100	100
29	b	52/57 (91%)	49 (94%)	3 (6%)	0	100	100
30	c	47/55 (86%)	45 (96%)	2 (4%)	0	100	100
31	d	44/47 (94%)	39 (89%)	5 (11%)	0	100	100
32	e	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
33	f	35/37 (95%)	35 (100%)	0	0	100	100
All	All	3935/4386 (90%)	3566 (91%)	367 (9%)	2 (0%)	50	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	J	75	PRO
3	4	22	SER

### 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%)	51 (98%)	1 (2%)	52	73
2	3	18/19 (95%)	18 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	4	367/372 (99%)	351 (96%)	16 (4%)	24	49
5	C	215/218 (99%)	211 (98%)	4 (2%)	52	73
6	D	160/163 (98%)	156 (98%)	4 (2%)	42	66
7	E	169/173 (98%)	162 (96%)	7 (4%)	26	51
8	F	151/156 (97%)	144 (95%)	7 (5%)	23	47
9	G	148/150 (99%)	141 (95%)	7 (5%)	22	46
10	H	90/116 (78%)	86 (96%)	4 (4%)	24	49
11	I	89/120 (74%)	86 (97%)	3 (3%)	32	57
12	J	93/108 (86%)	89 (96%)	4 (4%)	25	49
13	K	119/120 (99%)	116 (98%)	3 (2%)	42	66
14	L	100/100 (100%)	97 (97%)	3 (3%)	36	60
15	M	112/114 (98%)	109 (97%)	3 (3%)	40	64
16	N	114/116 (98%)	113 (99%)	1 (1%)	75	86
17	O	97/158 (61%)	95 (98%)	2 (2%)	48	70
18	P	93/94 (99%)	90 (97%)	3 (3%)	34	59
19	Q	100/100 (100%)	95 (95%)	5 (5%)	20	44
20	R	97/99 (98%)	96 (99%)	1 (1%)	73	85
21	S	81/83 (98%)	77 (95%)	4 (5%)	21	45
22	T	90/117 (77%)	89 (99%)	1 (1%)	70	83
23	U	83/85 (98%)	83 (100%)	0	100	100
24	V	81/86 (94%)	76 (94%)	5 (6%)	15	36
25	W	77/168 (46%)	76 (99%)	1 (1%)	65	80
26	X	58/63 (92%)	58 (100%)	0	100	100
27	Y	50/51 (98%)	49 (98%)	1 (2%)	50	72
28	Z	58/66 (88%)	56 (97%)	2 (3%)	32	57
29	b	43/46 (94%)	43 (100%)	0	100	100
30	c	47/52 (90%)	47 (100%)	0	100	100
31	d	35/36 (97%)	33 (94%)	2 (6%)	17	39
32	e	53/54 (98%)	51 (96%)	2 (4%)	28	53
33	f	35/35 (100%)	35 (100%)	0	100	100
All	All	3175/3492 (91%)	3079 (97%)	96 (3%)	37	60

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	K	4	TYR
18	P	86	GLN
13	K	129	ASP
15	M	128	LYS
19	Q	20	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
19	Q	79	ASN
30	c	44	ASN
8	F	44	ASN
8	F	142	GLN
11	I	100	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	A	2946/3120 (94%)	662 (22%)	23 (0%)
4	B	117/118 (99%)	29 (24%)	0
All	All	3063/3238 (94%)	691 (22%)	23 (0%)

5 of 691 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	B	4	A
4	B	5	C
4	B	6	G
4	B	8	C
4	B	9	G

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	A	2122	U
34	A	2125	A
34	A	2124	A
34	A	2336	U
34	A	1002	C

## 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	$\# Z  > 2$
35	GCP	4	501	-	27,34,34	1.34	3 (11%)	35,54,54	2.10	9 (25%)

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
35	GCP	4	501	-	-	7/15/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	4	501	GCP	C5-C6	4.06	1.48	1.41
35	4	501	GCP	PG-O2G	2.82	1.61	1.55
35	4	501	GCP	PG-O3G	2.75	1.61	1.55

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	4	501	GCP	PB-O3A-PA	-5.08	115.78	132.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	4	501	GCP	C2-N3-C4	4.89	120.76	115.48
35	4	501	GCP	C2-N1-C6	4.65	122.43	115.96
35	4	501	GCP	C5-C6-N1	-4.16	117.85	123.42
35	4	501	GCP	C4'-O4'-C1'	-3.64	106.60	109.92

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

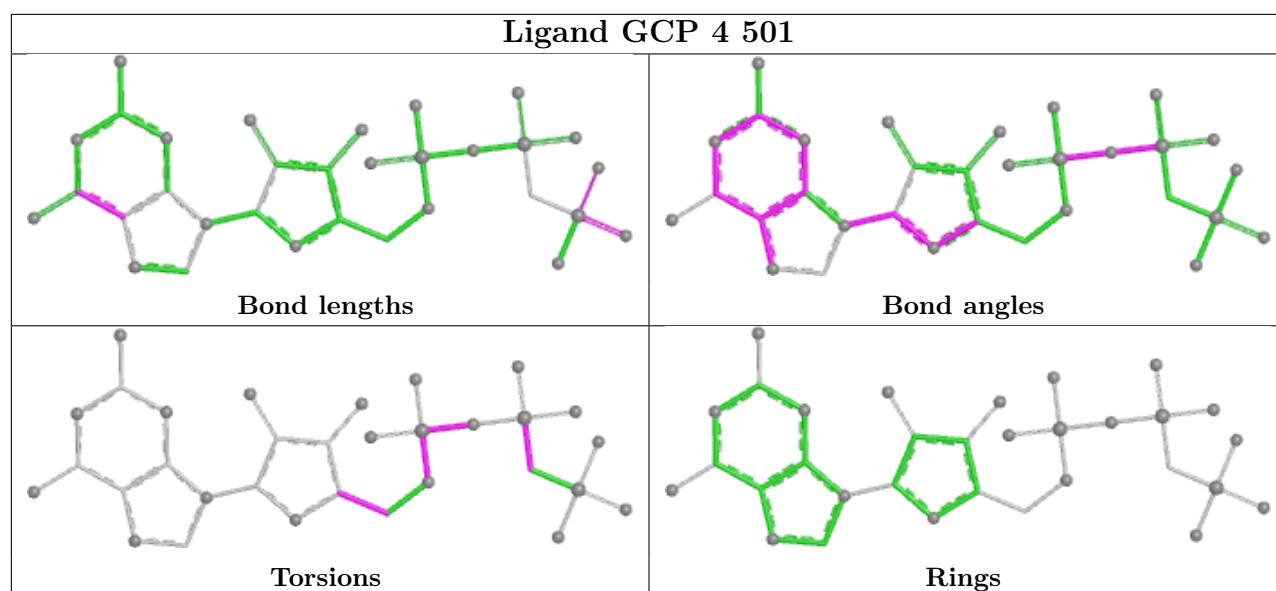
Mol	Chain	Res	Type	Atoms
35	4	501	GCP	C5'-O5'-PA-O3A
35	4	501	GCP	C5'-O5'-PA-O1A
35	4	501	GCP	C5'-O5'-PA-O2A
35	4	501	GCP	O4'-C4'-C5'-O5'
35	4	501	GCP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	4	501	GCP	11	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.

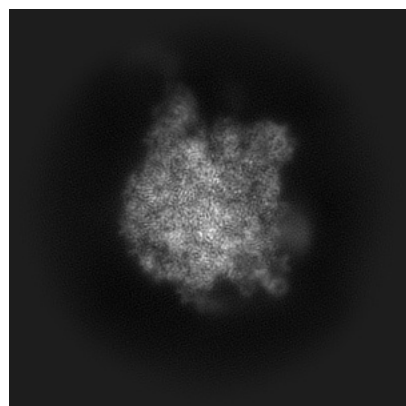
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43317. These allow visual inspection of the internal detail of the map and identification of artifacts.

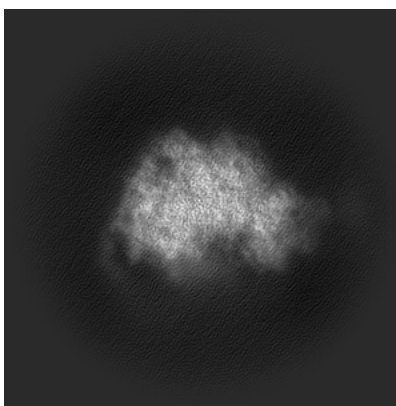
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

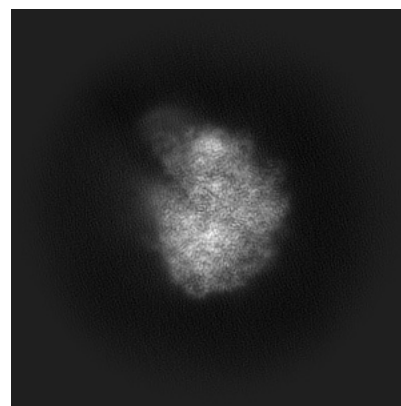
#### 6.1.1 Primary map



X

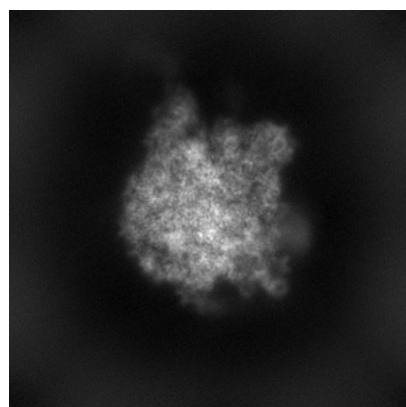


Y

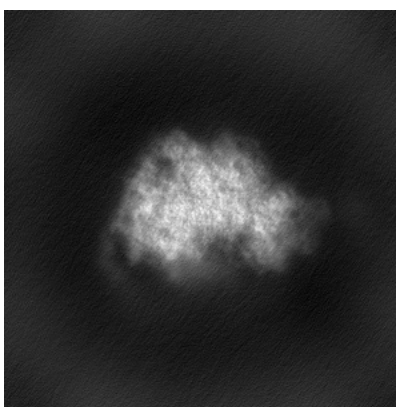


Z

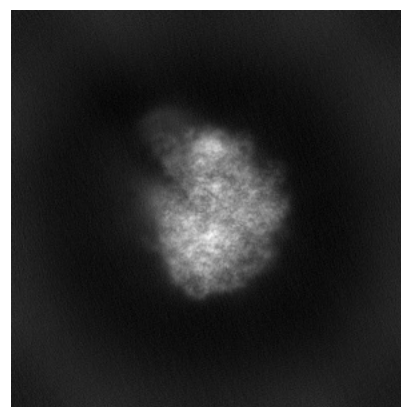
#### 6.1.2 Raw map



X



Y



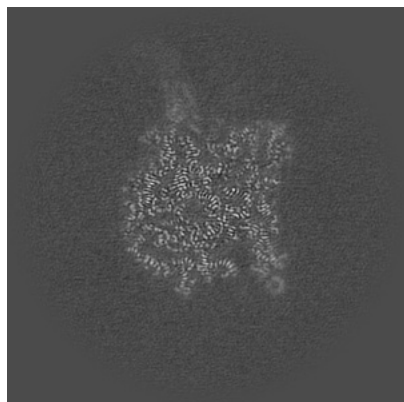
Z

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

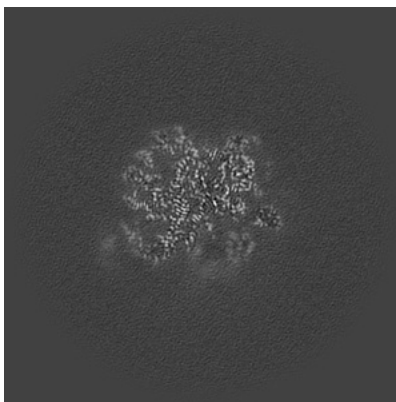


## 6.2 Central slices [i](#)

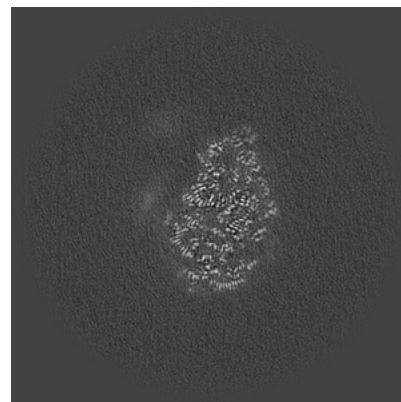
### 6.2.1 Primary map



X Index: 200

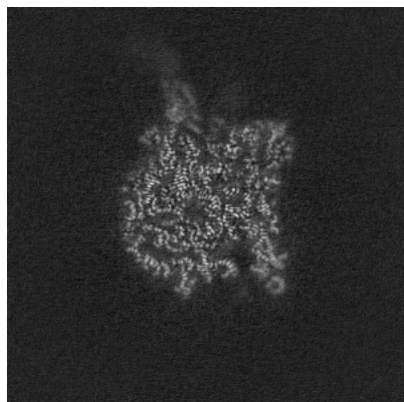


Y Index: 200

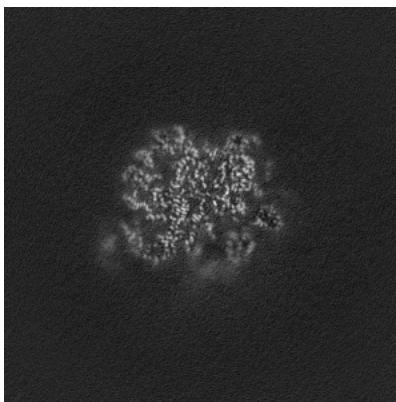


Z Index: 200

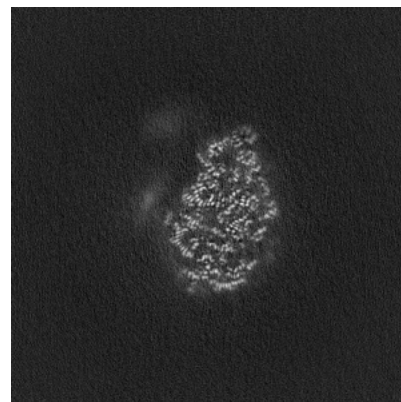
### 6.2.2 Raw map



X Index: 200



Y Index: 200

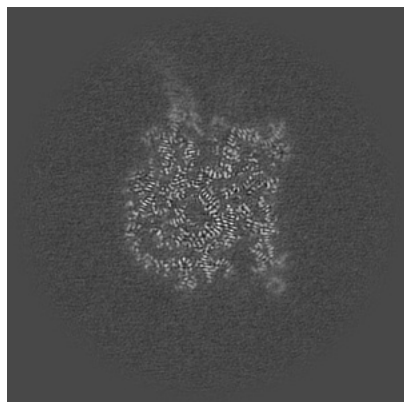


Z Index: 200

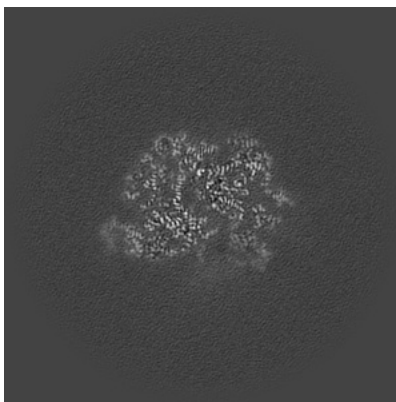
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

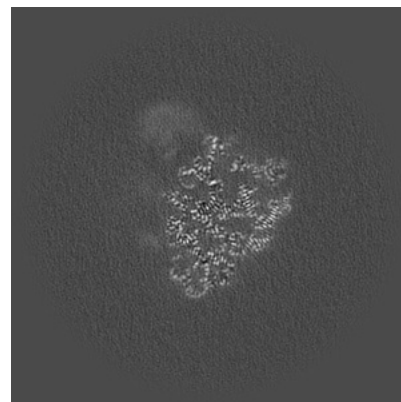
### 6.3.1 Primary map



X Index: 202

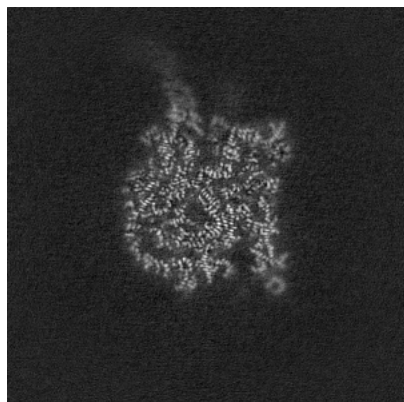


Y Index: 192

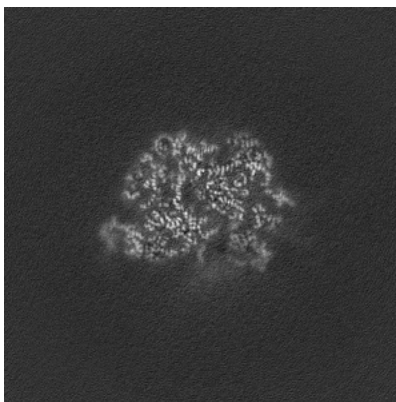


Z Index: 176

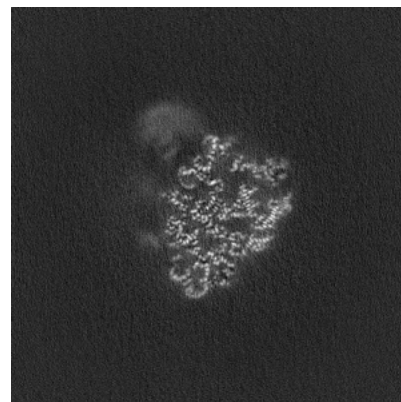
### 6.3.2 Raw map



X Index: 202



Y Index: 192

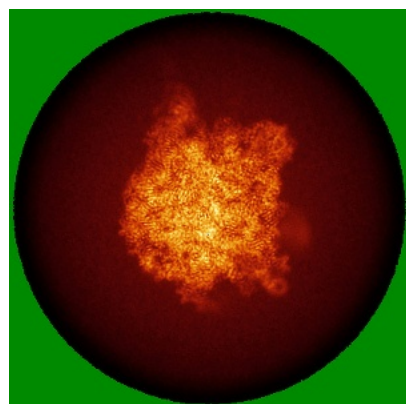


Z Index: 176

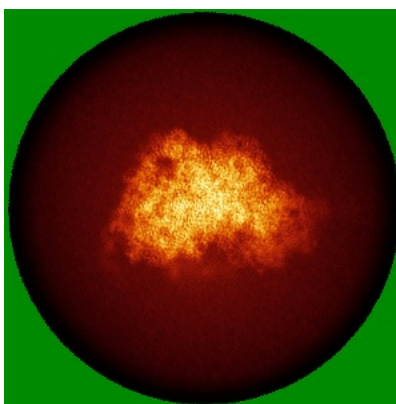
The images above show the largest variance slices of the map in three orthogonal directions.

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

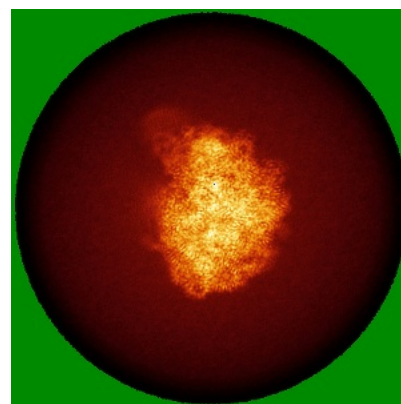
### 6.4.1 Primary map



X

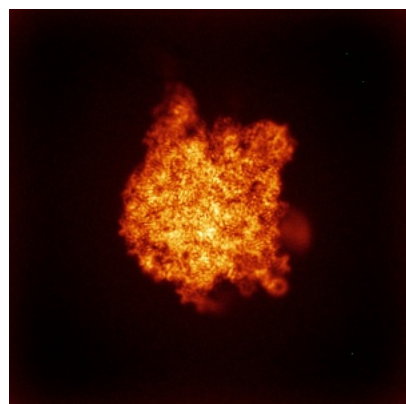


Y

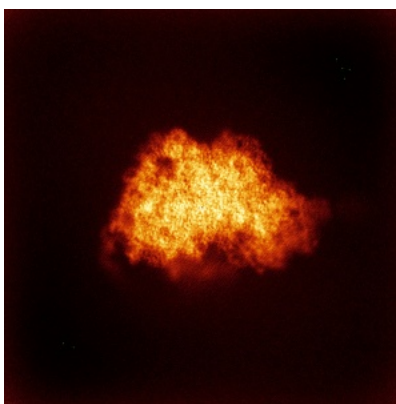


Z

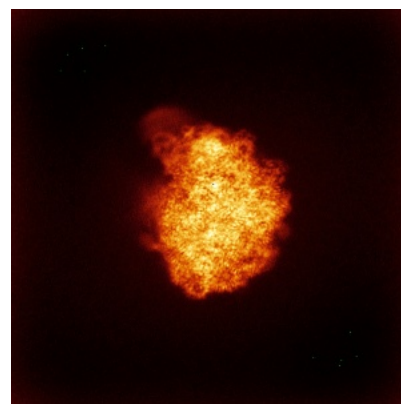
### 6.4.2 Raw map



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.

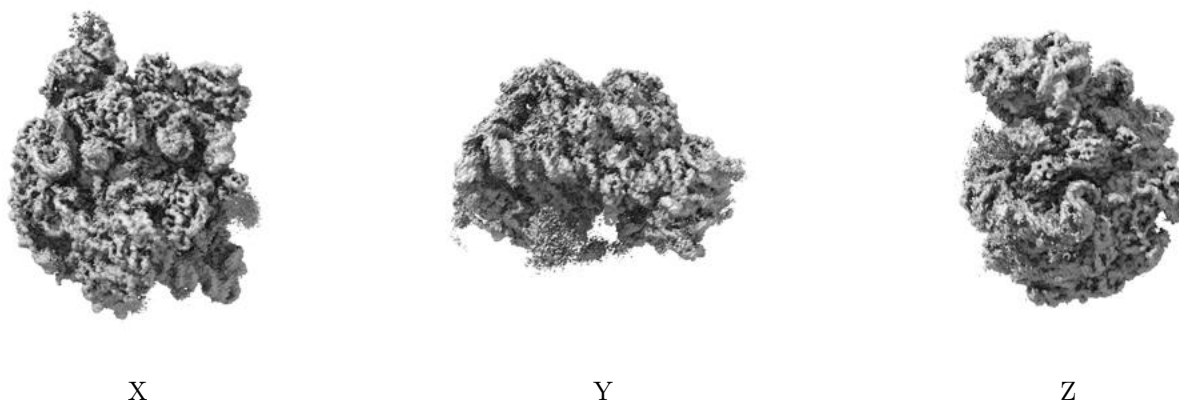
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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.

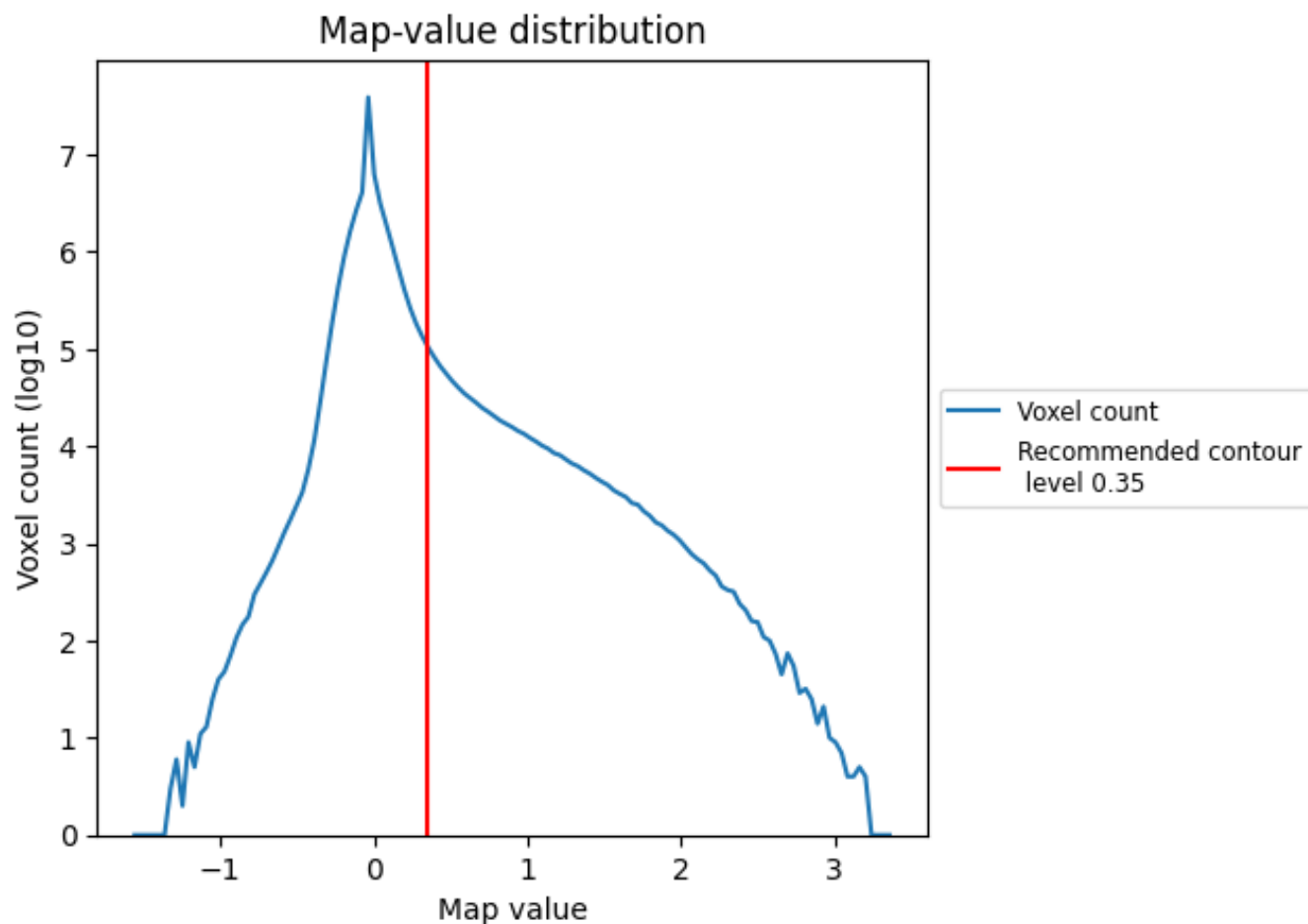
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

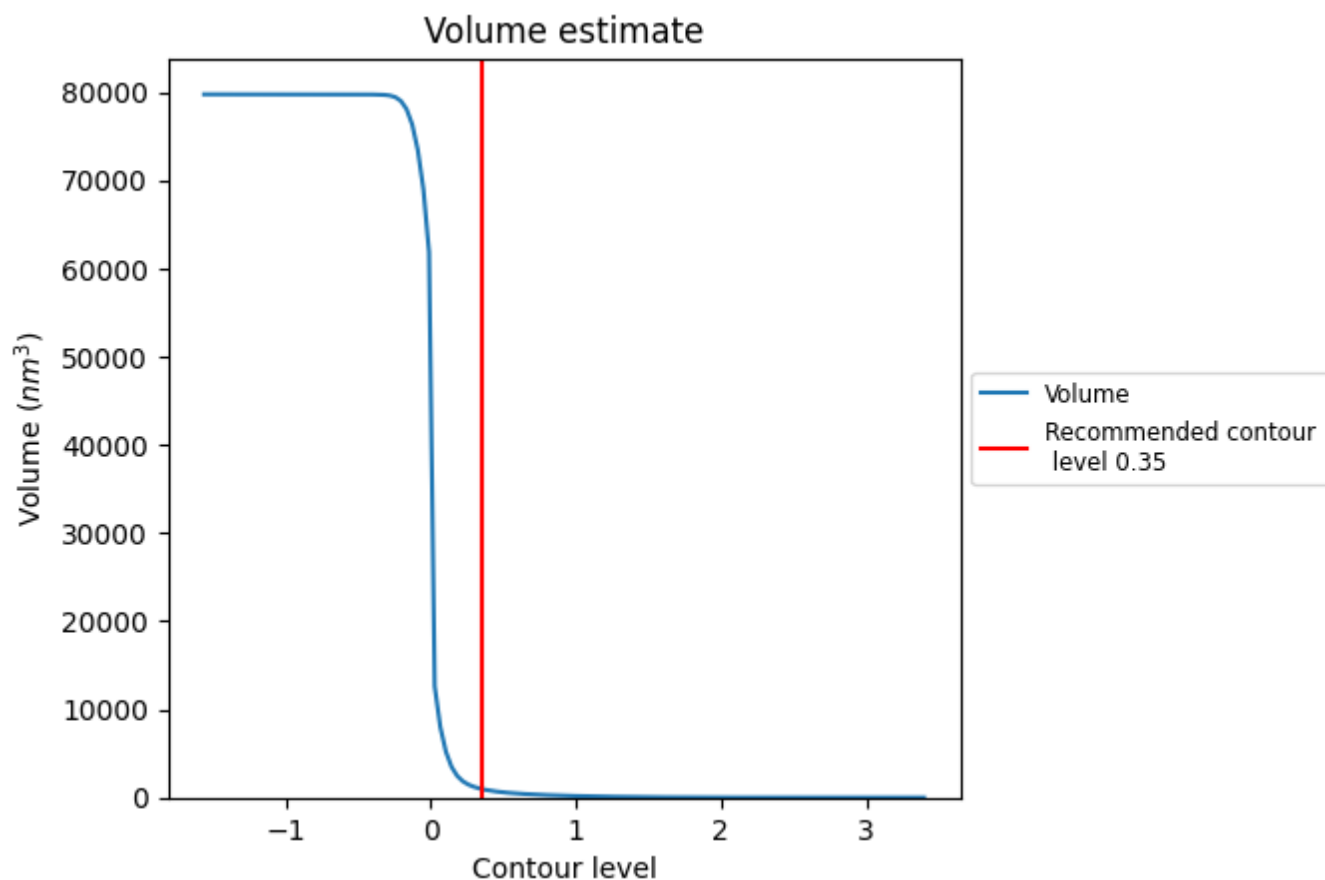
This section contains the results of statistical analysis of the map.

### 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](#)

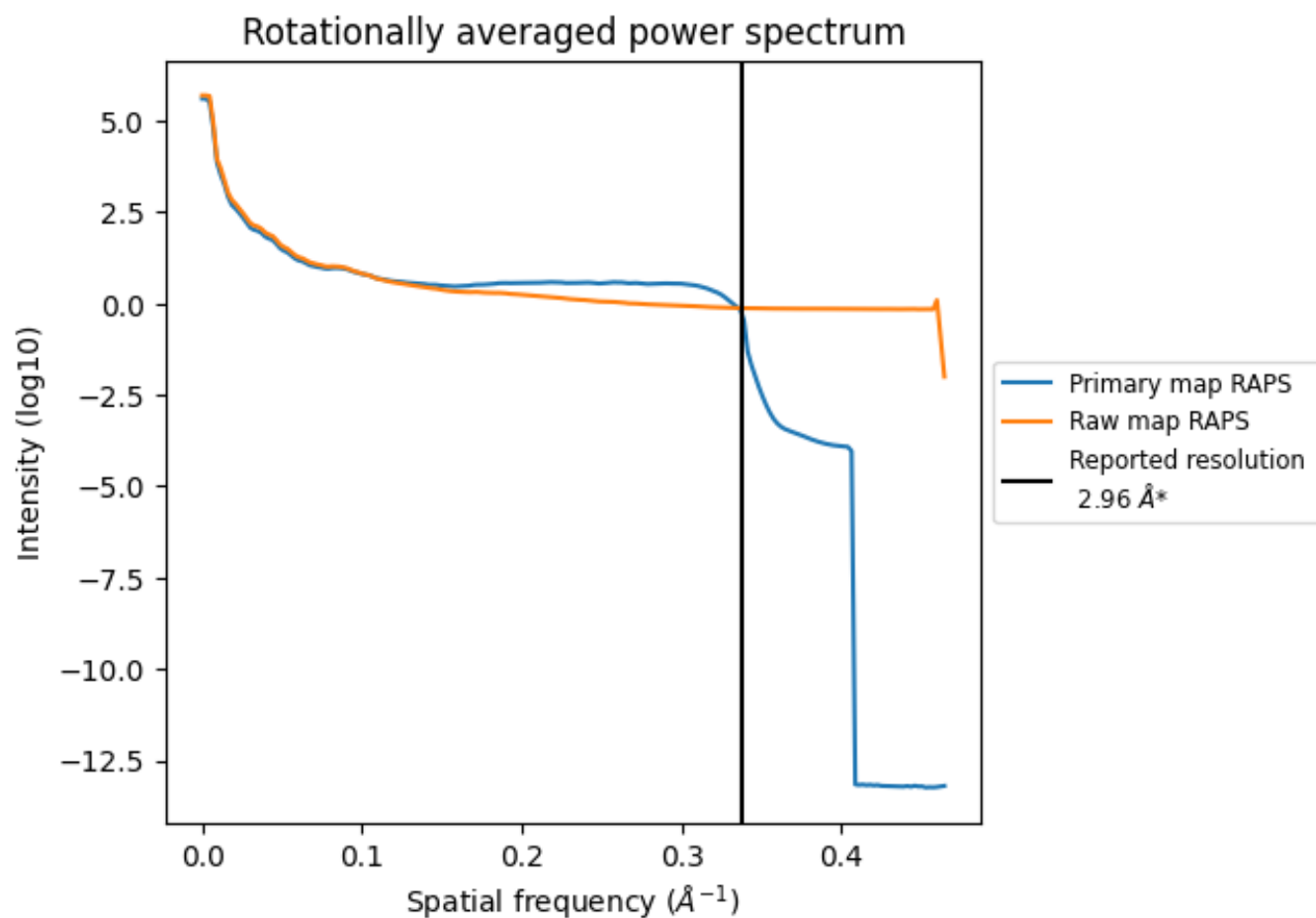


The volume at the recommended contour level is 982  $\text{nm}^3$ ; this corresponds to an approximate mass of 887 kDa.

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 ⓘ

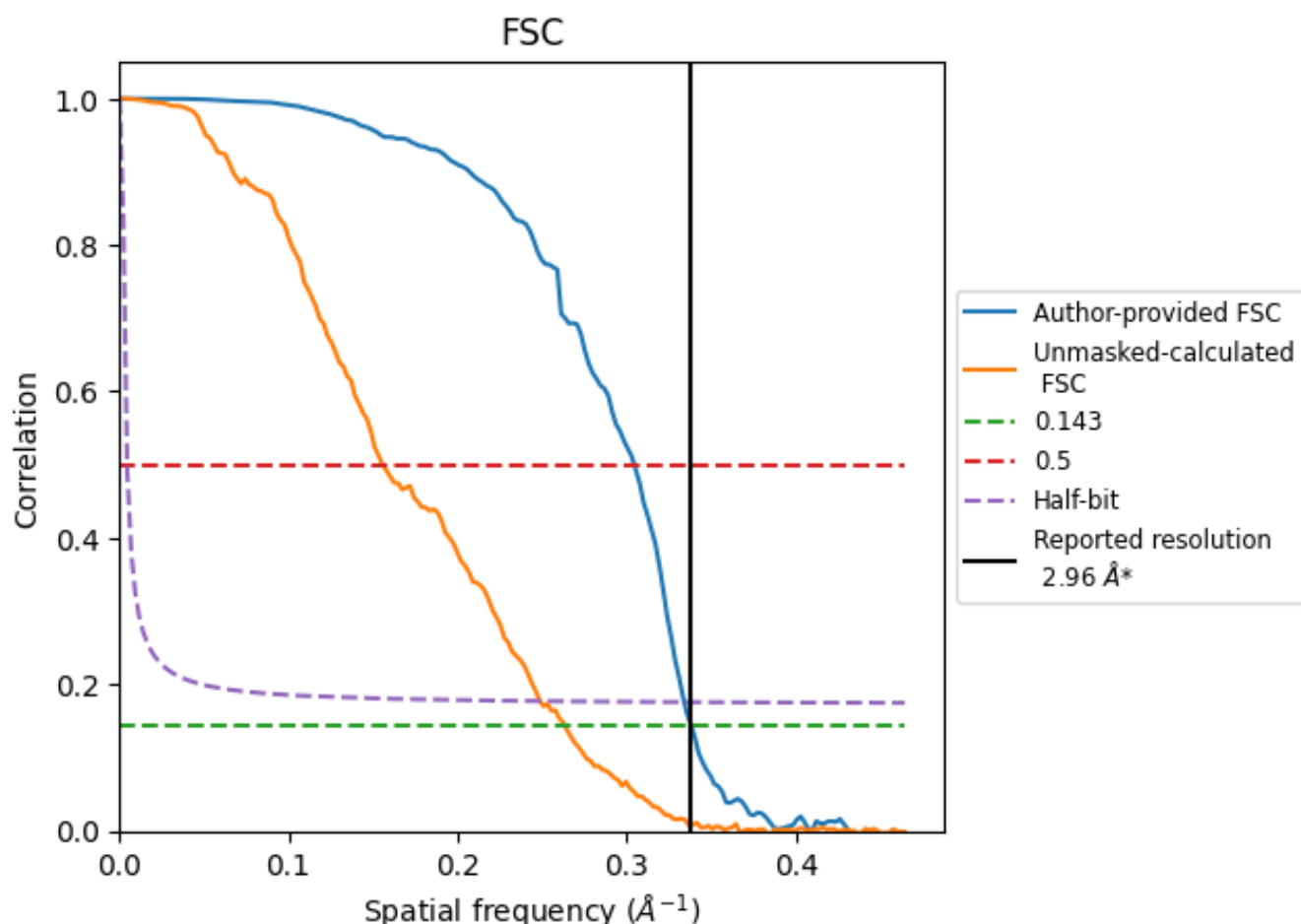


\*Reported resolution corresponds to spatial frequency of 0.338  $\text{\AA}^{-1}$

## 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 0.338  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

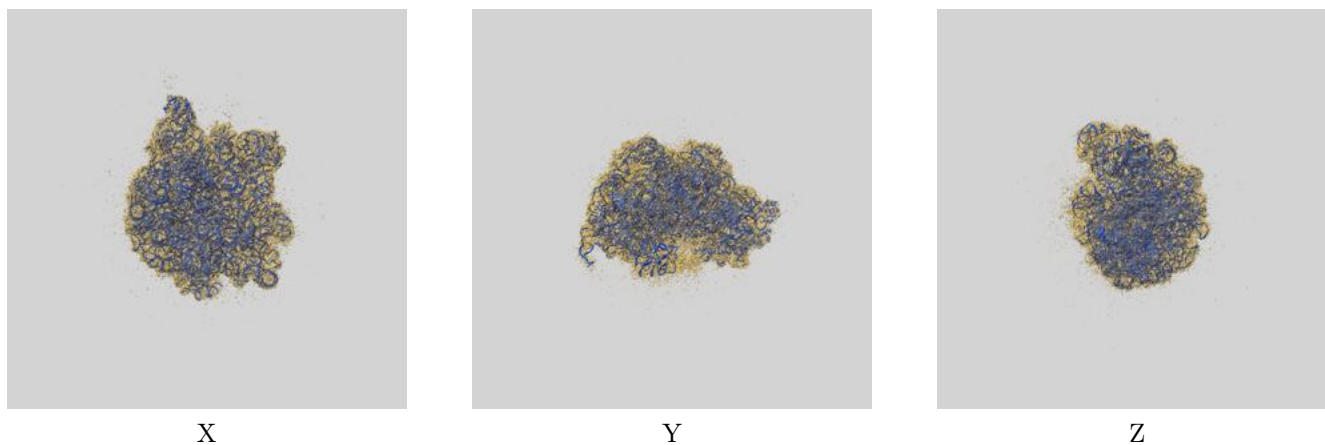
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.28	2.99
Unmasked-calculated*	3.79	6.43	4.02

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.79 differs from the reported value 2.96 by more than 10 %

## 9 Map-model fit [i](#)

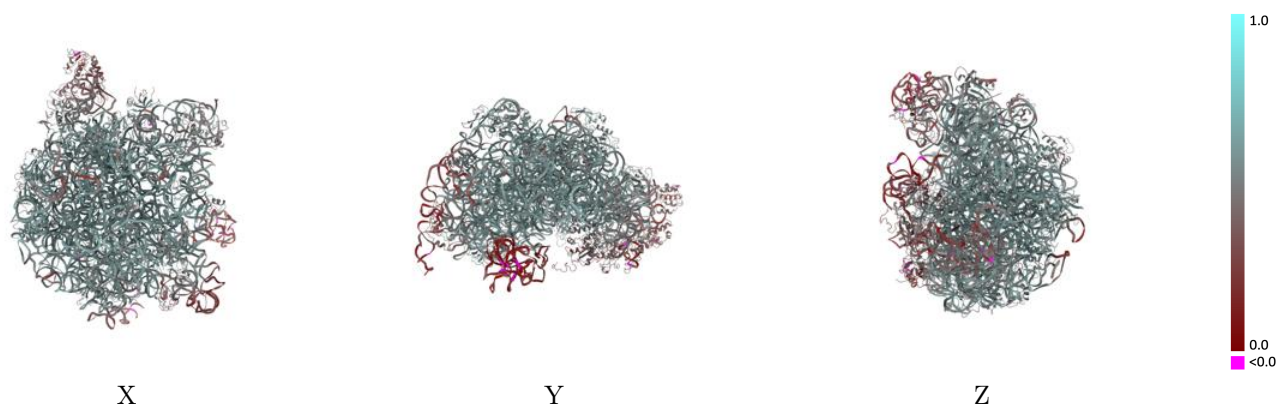
This section contains information regarding the fit between EMDB map EMD-43317 and PDB model 8VKI. Per-residue inclusion information can be found in section [3](#) on page [11](#).

### 9.1 Map-model overlay [i](#)



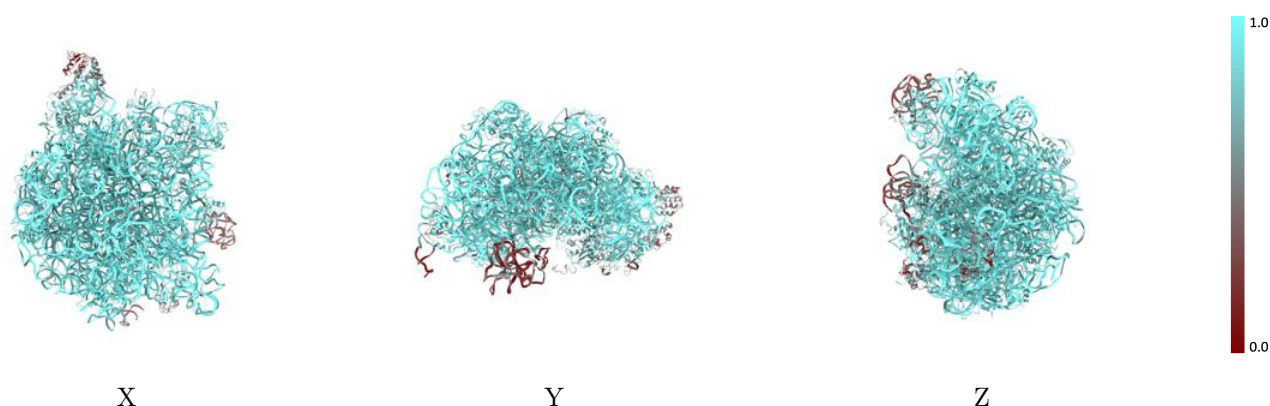
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



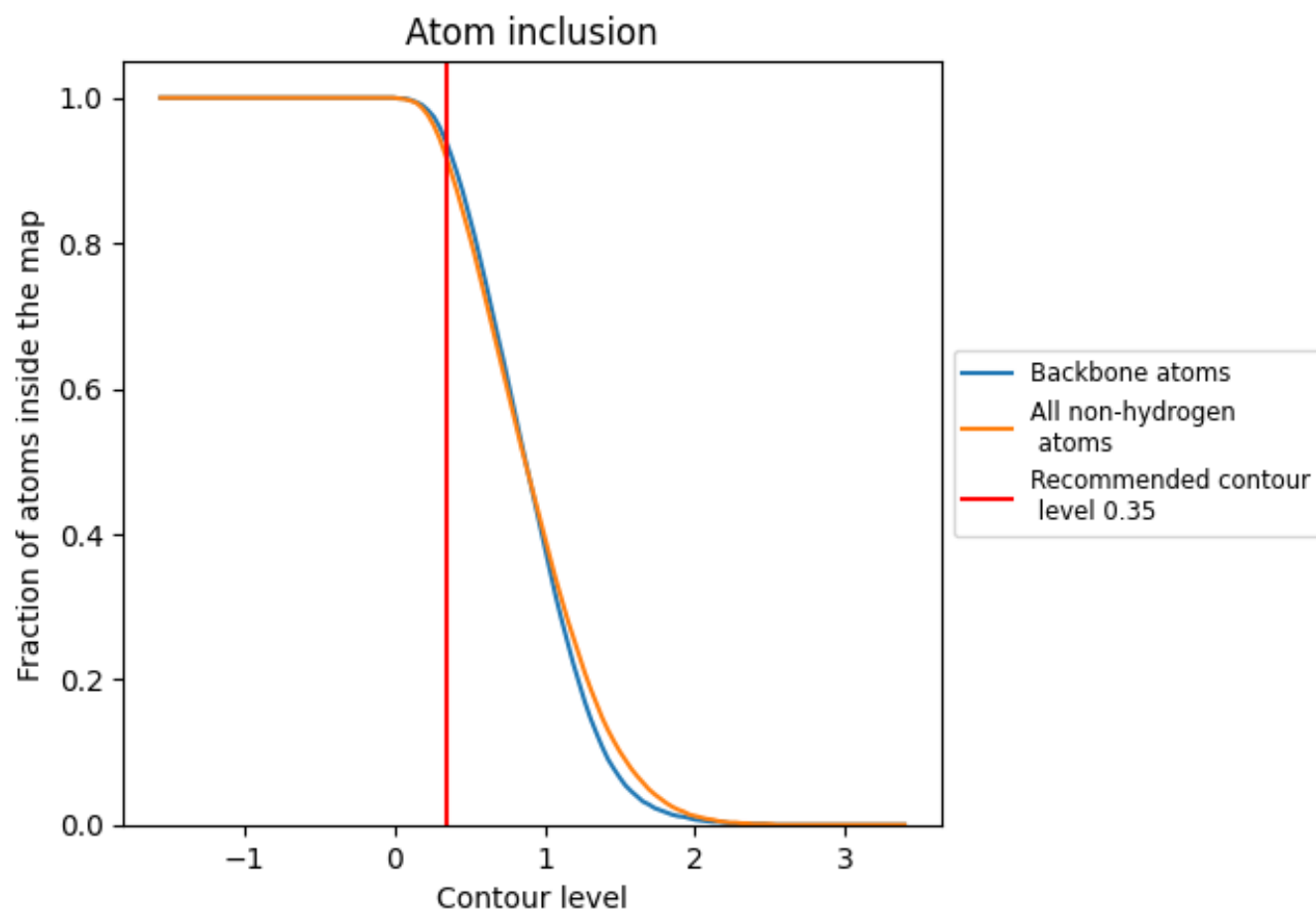
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9150	 0.5200
2	 0.9350	 0.5680
3	 0.9550	 0.6090
4	 0.7710	 0.4150
A	 0.9370	 0.5250
B	 0.9700	 0.5110
C	 0.9330	 0.5660
D	 0.9530	 0.5670
E	 0.9240	 0.5470
F	 0.7600	 0.3950
G	 0.8260	 0.4740
H	 0.7230	 0.4480
I	 0.4020	 0.3090
J	 0.4590	 0.3130
K	 0.9520	 0.5700
L	 0.9310	 0.5560
M	 0.9350	 0.5590
N	 0.9280	 0.5670
O	 0.9500	 0.5720
P	 0.9050	 0.4960
Q	 0.8870	 0.5250
R	 0.9570	 0.5700
S	 0.9100	 0.5550
T	 0.9490	 0.5720
U	 0.9430	 0.5490
V	 0.8940	 0.5020
W	 0.8450	 0.5210
X	 0.9400	 0.5810
Y	 0.9690	 0.5700
Z	 0.9250	 0.5290
b	 0.9680	 0.5820
c	 0.9570	 0.5620
d	 0.9600	 0.5930
e	 0.9750	 0.5890
f	 0.9650	 0.5780

