



wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 01:32 pm BST

PDB ID : 7BL3
EMDB ID : EMD-12216
Title : pre-50S-ObgE particle state 2
Authors : Hilal, T.; Nikolay, R.; Spahn, C.M.T.
Deposited on : 2021-01-18
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

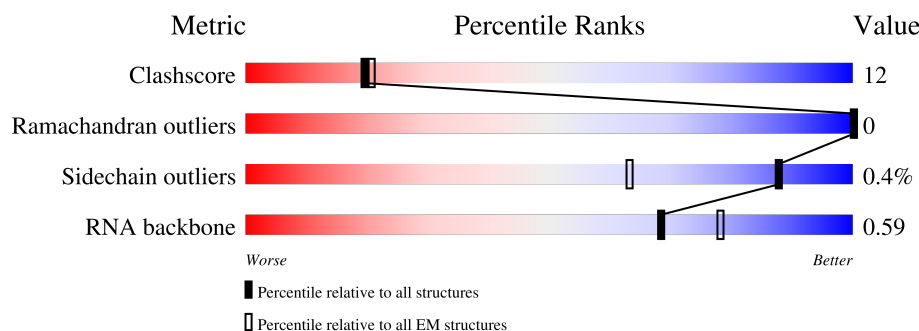
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	2919	
2	B	119	
3	9P	390	
4	b	70	
5	C	273	
6	D	209	
7	E	201	

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Mol	Chain	Length	Quality of chain
8	G	177	
9	J	142	
10	L	144	
11	N	127	
12	O	117	
13	Q	118	
14	R	103	
15	S	110	
16	T	100	
17	U	104	
18	V	94	
19	W	85	
20	X	78	
21	Y	63	
22	Z	59	
23	0	57	
24	1	55	
25	2	46	
26	I	142	
27	K	123	
28	P	115	
29	6	105	
30	H	149	
31	F	179	

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 92831 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2902	Total	C	N	O	P	0	0
			62301	27793	11465	20141	2902		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	119	Total	C	N	O	P	0	0
			2548	1135	466	829	118		

- Molecule 3 is a protein called GTPase ObgE/CgtA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	9P	338	Total	C	N	O	S	0	0
			2582	1626	453	490	13		

- Molecule 4 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	47	Total	C	N	O	S	0	0
			364	227	64	67	6		

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

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

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

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

- Molecule 7 is a protein called 50S ribosomal protein L4.

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

- Molecule 8 is a protein called 50S ribosomal protein L6.

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

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 11 is a protein called 50S ribosomal protein L17.

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

- Molecule 12 is a protein called 50S ribosomal protein L18.

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

- Molecule 13 is a protein called 50S ribosomal protein L20.

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

- Molecule 14 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 15 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 16 is a protein called 50S ribosomal protein L23.

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

- Molecule 17 is a protein called 50S ribosomal protein L24.

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

- Molecule 18 is a protein called 50S ribosomal protein L25.

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

- Molecule 19 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	76	Total	C	N	O	S	0	0
			575	356	117	101	1		

- Molecule 20 is a protein called 50S ribosomal protein L28.

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

- Molecule 21 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 22 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 23 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 24 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 26 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 27 is a protein called 50S ribosomal protein L14.

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

- Molecule 28 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	P	113	Total	C	N	O	S	0	0
			911	571	178	161	1		

- Molecule 29 is a protein called Ribosomal silencing factor RsfS.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	6	102	Total	C	N	O	S	0	0
			780	485	133	157	5		

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	H	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 31 is a protein called 50S ribosomal protein L5.

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

- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
32	b	1	Total	Zn	0
			1	1	

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	Q	1	Total	Mg	0
			1	1	

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		AltConf
34	A	21	Total	O	0
			21	21	
34	B	1	Total	O	0
			1	1	
34	C	2	Total	O	0
			2	2	

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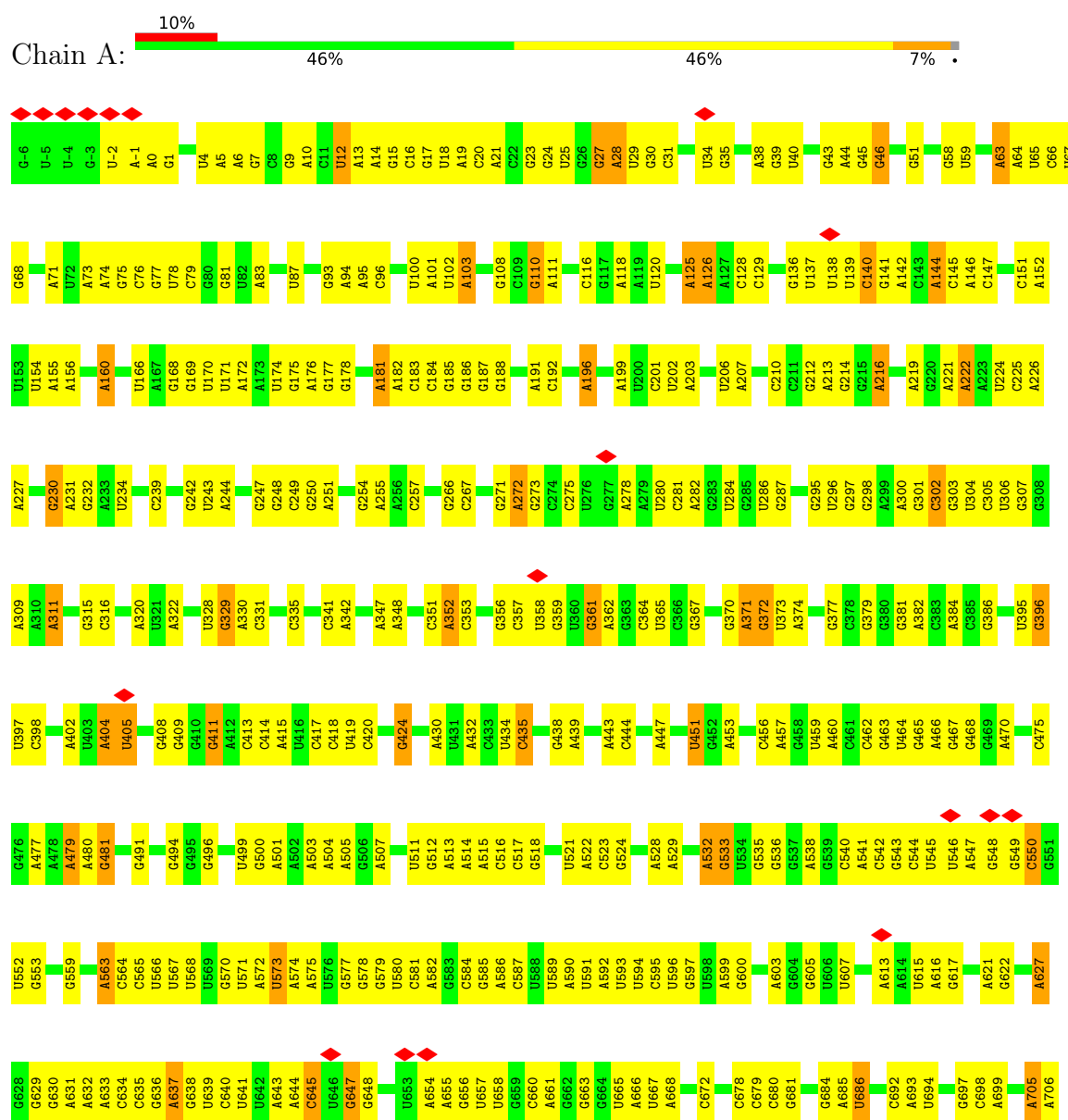
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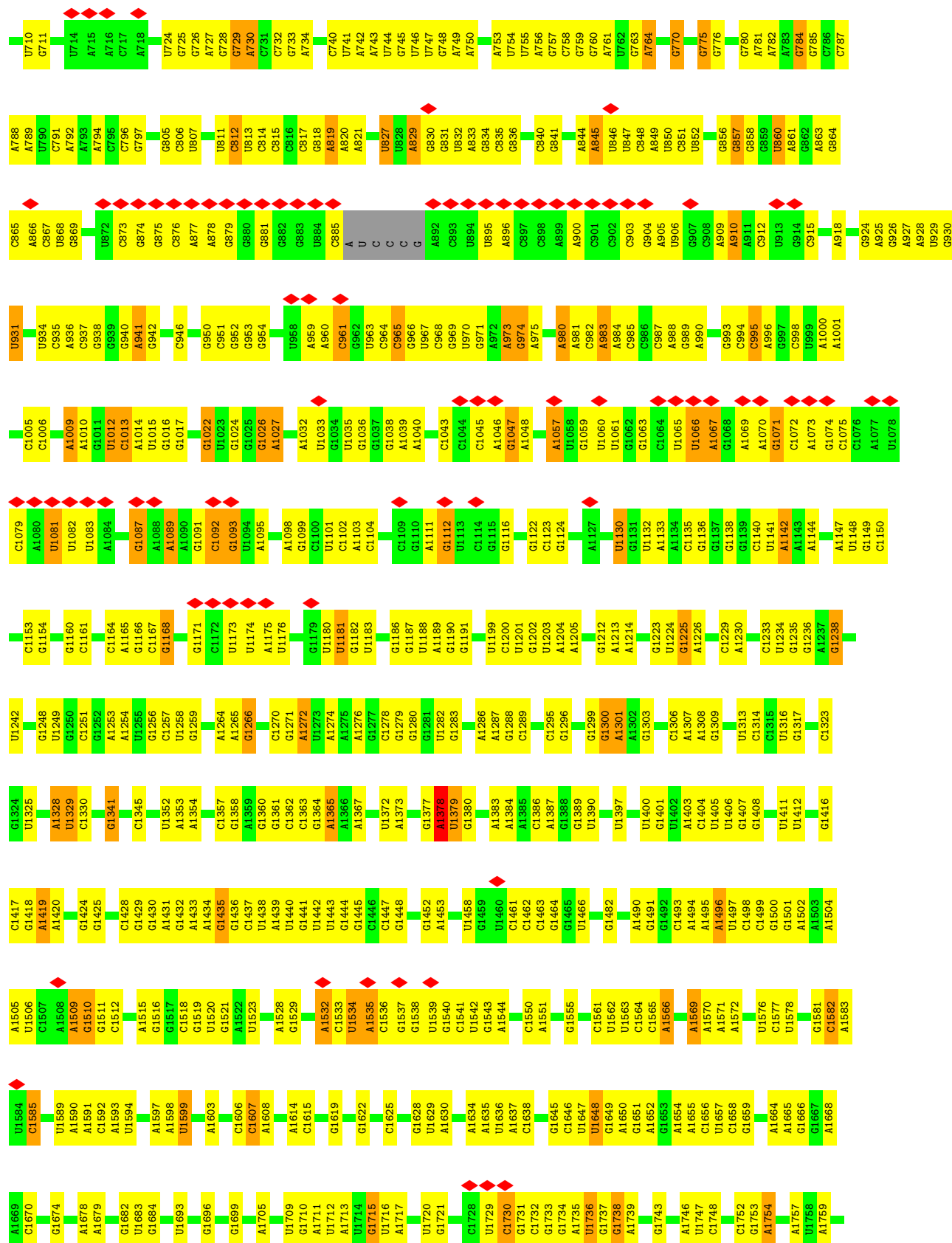
Mol	Chain	Residues	Atoms		AltConf
34	L	1	Total 1	O 1	0
34	N	1	Total 1	O 1	0
34	S	1	Total 1	O 1	0

3 Residue-property plots

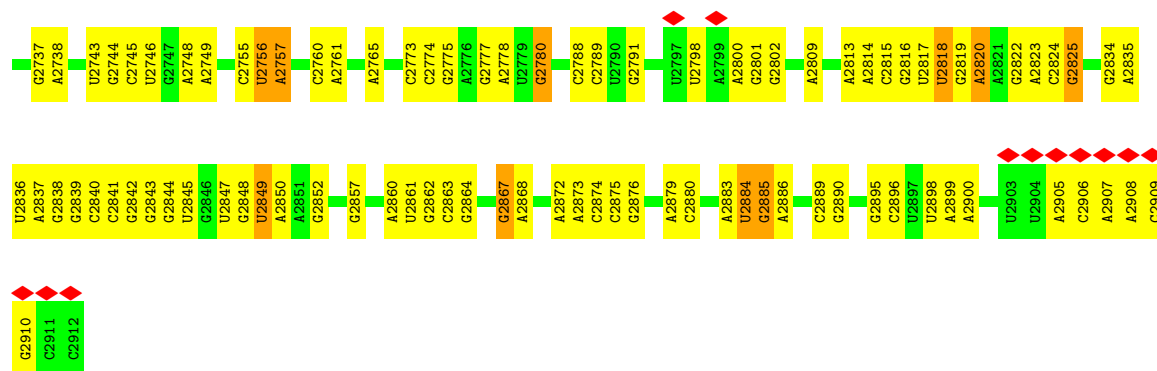
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 23S ribosomal RNA





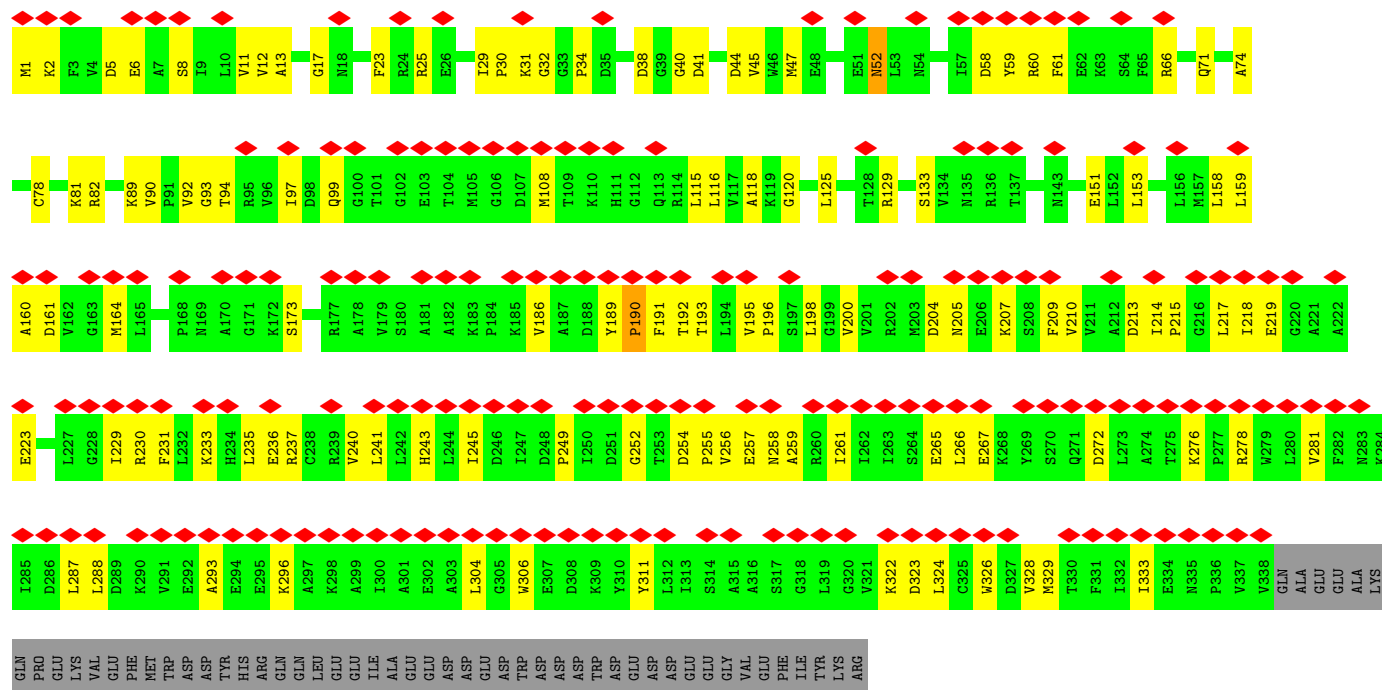
C2649	C2650	C2651	C2652	U2656	A2657	C2658	C2659	A2660	C2661	A2662	C2667	C2673	C2674	A2675	A2679	U2680	C2681	C2682	C2683	U2684	C2685	C2686	C2687	C2688	C2689	U2690	C2691	C2692	C2704	A2705	U2707	C2708	C2709	C2710	A2711	C2714	C2715	C2716	U2720	A2726	U2727	U2728	C2729	C2730	C2731	C2732	A2733													
G2576	A2577	G2578	C2579	U2580	G2581	C2582	G2583	C2584	U2585	A2586	A2587	G2592	U2593	C2594	G2595	A2598	A2602	G2603	G2608	U2609	C2610	C2611	C2612	U2613	C2614	C2615	C2616	U2617	C2618	G2621	G2625	C2626	G2627	C2628	U2629	G2630	G2631	A2632	C2636	U2637	C2638	A2639	G2640	U2641	C2642	G2643	G2644	C2645	C2646	C2647	G2648									
U	G2505	U2506	C2507	G2508	U2511	C2512	A2513	U2514	C2515	A2516	C2517	A2518	U2519	C2520	C2521	G2525	G2526	C2527	U2528	G2529	A2530	U2533	A2534	C2535	U2536	C2537	C2538	G2543	C2544	C2545	U2546	A2547	U2548	G2553	U2554	U2555	C2556	C2557	C2558	A2559	A2560	A2564	A2565	A2566	G2567	U2568	C2569	U2570	U2571	A2572	C2573	C2574	C2575	C2575						
G2444	G2445	U2446	G2447	A2448	U2449	A2450	A2451	C2452	A2453	G2454	C2455	C2456	U2457	G2458	A2459	U2460	A2461	C2462	C2463	G2464	C2465	C2466	C2467	A2468	A2469	G2470	A2471	C2472	U2473	U2474	C2475	A2476	U2477	A2478	U2479	C2480	G2481	A2482	C2483	G2484	C2485	C2486	G2487	G2488	U2489	G2490	U2491	U2492	U2493	G	G	C	A	C	C	U	U	C	C	A
U2372	G2373	C2374	G2375	A2376	G2379	C2380	U2383	C2384	C2385	A2386	G2391	A2392	U2393	C2394	C2395	G2396	C2397	U2398	C2399	U2402	C2403	U2404	G2405	A2406	A2407	U2408	G2409	C2410	A2411	A2412	G2413	G2414	C2415	C2416	C2417	A2418	C2422	U2423	C2424	A2425	A2426	C2427	G2428	C2429	A2430	A2434	A2435	U2439	C2440	U2441	C2442	C2443								
U2299	C2300	C2301	U2302	G2303	C2304	U2305	C2306	U2307	C2308	A2309	C2310	A2311	U2312	C2313	A2314	C2315	G2316	A2317	C2318	C2319	U2320	U2321	A2322	U2323	C2324	A2325	C2326	A2327	C2328	U2329	C2330	U2333	U2334	A2335	C2336	C2337	C2338	C2339	A2340	G2341	G2345	A2346	C2347	U2348	C2349	C2350	G2351	U2357	C2364	G2365	C2368	A2369	G2370	G2371						
A2225	C2226	A2227	G2228	U2229	G2230	U2231	C2232	G2233	G2234	C2238	U2239	A2241	G2242	U2245	G2246	A2247	C2248	U2249	G2250	C2251	C2252	G2256	U2257	C2258	C2261	U2262	C2263	C2264	U2265	A2266	A2267	G2271	U2272	A2273	A2274	C2275	C2283	A2284	C2285	U2286	A2287	C2288	U2289	C2290	U2291	U2292	G2293	C2294	C2295	U2296	A2297	A2298								
C2153	A2154	U2155	G2156	G2157	A2158	U2159	C2160	G2161	C2162	A2163	C2164	C2165	U2166	U2167	C2168	A2169	A2170	C2171	U2172	A2173	C2174	C2175	A2176	C2177	C2178	C2179	U2180	U2181	U2182	A2183	U2184	U2185	G2186	U2187	U2188	U2189	G2190	A2191	U2192	G2193	U2194	U2195	U2196	U2197	A2198	C2199	G2200	G2201	U2202	U2203	G2204	C2208	A2211	U2219	G2224					
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A2020	C2021	U2022	C2023	G2024	C2025	U2026	G2027	U2028	G2029	A2030	C2031	G2032	A2033	U2034	C2035	A2036	C2037	G2038	U2039	G2040	C2043	C2047	G2048	A2052	C2055	G2056	C2057	A2058	C2059	G2061	A2060	A2062	C2063	C2064	C2065	C2066	U2068	G2069	A2070	C2071	C2072	C2073	U2074	U2075	U2076	A2077	U2081	A2082	G2087	A2088	C2089	A2090								
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C2091	U2092	C2093	A2094	A2095	U2099	G2100	A2101	G2102	C2103	G2104	U2105	U2106	G2107	A2108	U2109	G2110	U2111	G2112	U2113	A2114	G2115	G2116	A2117	U2118	A2119	G2120	G2121	U2122	C2062	G2123	G2124	C2065	C2066	A2126	G2127	G2128	C2129	U2130	U2131	U2132	G2133	A2134	A2135	G2136	U2137	G2138	U2139	G2140	G2141	A2142	C2143	G2144	C2145	C2146	A2147	G2148	U2149	C2150	U2151	G2152
C2153	A2154	U2155	G2156	G2157	A2158	U2159	C2160	G2161	C2162	A2163	C2164	C2165	U2166	U2167	C2168	A2169	A2170	C2171	U2172	A2173	C2174	C2175	A2176	C2177	C2178	C2179	U2180	U2181	U2182	A2183	U2184	U2185	G2186	U2187	U2188	U2189	G2190	A2191	U2192	G2193	U2194	U2195	U2196	U2197	A2198	C2199	G2200	G2201	U2202	U2203	G2204	C2208	A2211	U2219	G2224					
A2225	C2226	A2227	G2228	U2229	G2230	U2231	C2232	G2233	G2234	C2238	U2239	A2241	G2242	U2245	G2246	A2247	C2248	U2249	G2250	C2251	C2252	G2256	U2257	C2258	C2261	U2262	C2263	C2264	U2265	A2266	A2267	G2271	U2272	A2273	A2274	C2275	C2283	A2284	C2285	U2286	A2287	C2288	U2289	C2290	U2291	U2292	G2293	C2294	C2295	U2296	A2297	A2298								
U2299	C2300	C2301	U2302	G2303	C2304	U2305	C2306	U2307	C2308	A2309	C2310	A2311	U2312	C2313	A2314	C2315	G2316	A2317	C2318	C2319	U2320	U2321	A2322	U2323	C2324	A2325	C2326	A2327	C2328	U2329	C2330	U2333	U2334	A2335	C2336	C2337	C2338	C2339	A2340	G2341	G2345	A2346	C2347	U2348	C2349	C2350	G2351	U2357	C2364	G2365	C2368	A2369	G2370	G2371						
A2225	C2226	A2227	G2228	U2229	G2230	U2231	C2232	G2233	G2234	C2238	U2239	A2241	G2242	U2245	G2246	A2247	C2248	U2249	G2250	C2251	C2252	G2256	U2257	C2258	C2261	U2262	C2263	C2264	U2265	A2266	A2267	G2271	U2272	A2273	A2274	C2275	C2283	A2284	C2285	U2286	A2287	C2288	U2289	C2290	U2291	U2292	G2293	C2294	C2295	U2296	A2297	A2298								
U2372	G2373	C2374	G2375	A2376	G2379	C2380	U2383	C2384	C2385	A2386	G2391	A2392	U2393	C2394	C2395	G2396	C2397																																											

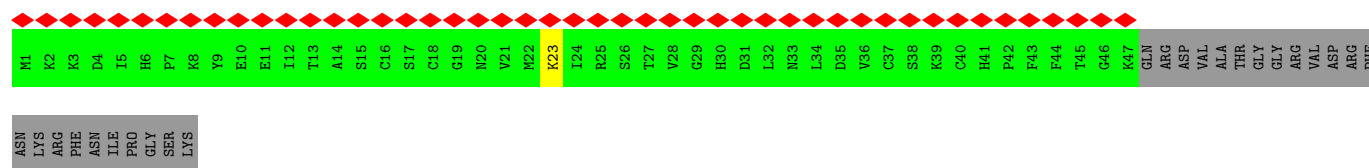


• Molecule 2: 5S ribosomal RNA

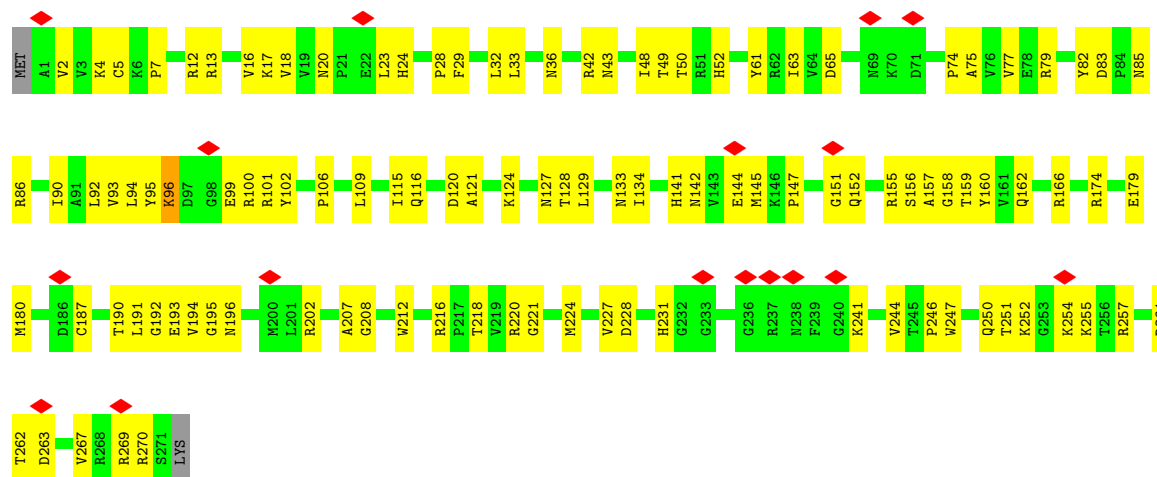


• Molecule 3: GTPase ObgE/CgtA

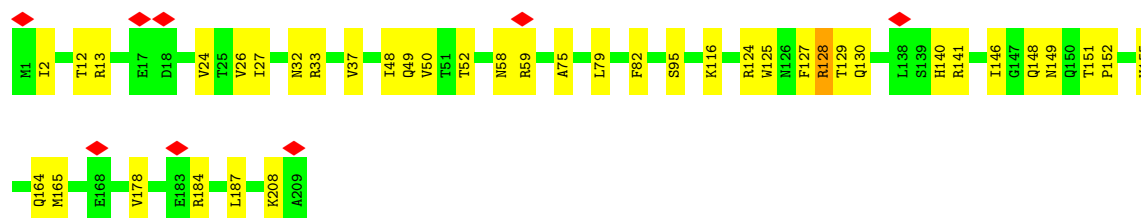
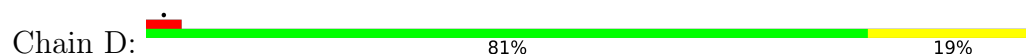




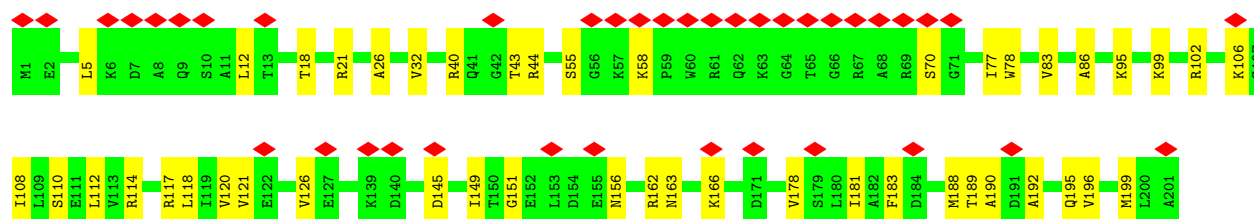
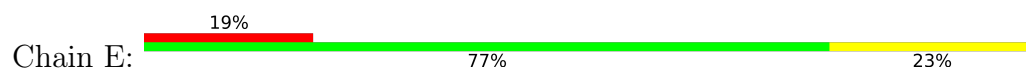
• Molecule 5: 50S ribosomal protein L2



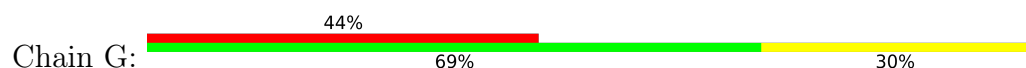
• Molecule 6: 50S ribosomal protein L3

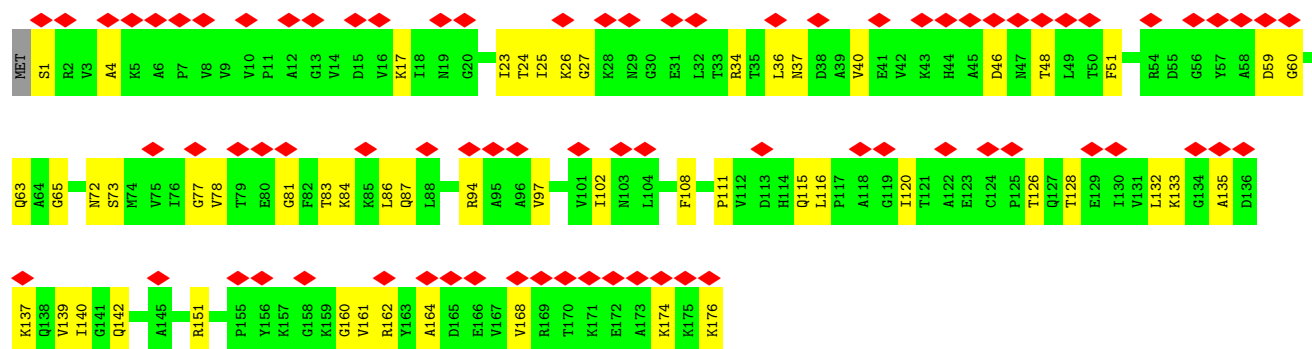


• Molecule 7: 50S ribosomal protein L4

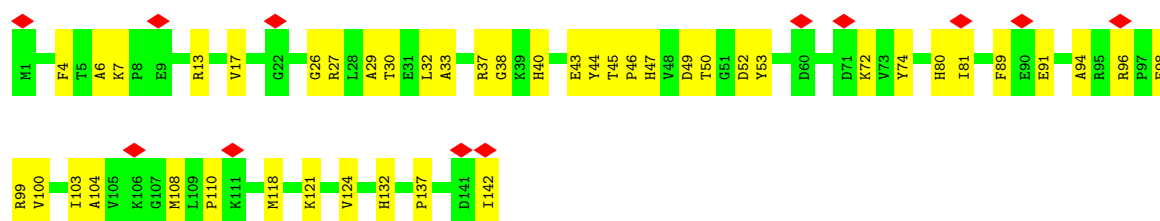


• Molecule 8: 50S ribosomal protein L6

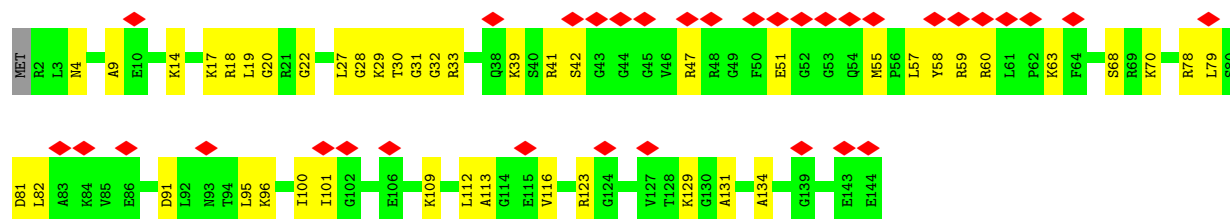




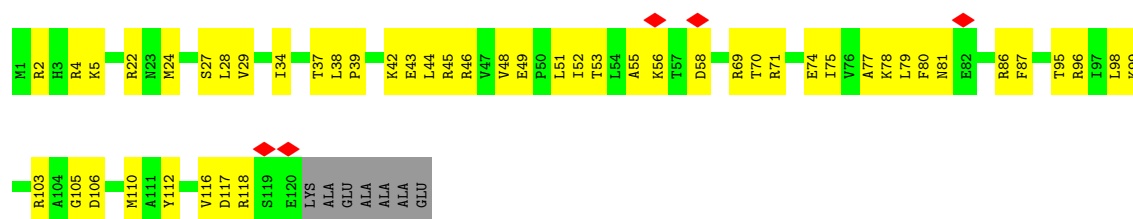
• Molecule 9: 50S ribosomal protein L13



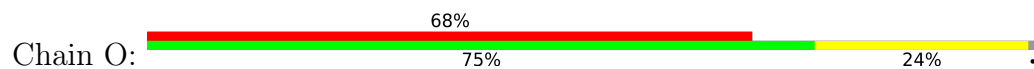
• Molecule 10: 50S ribosomal protein L15

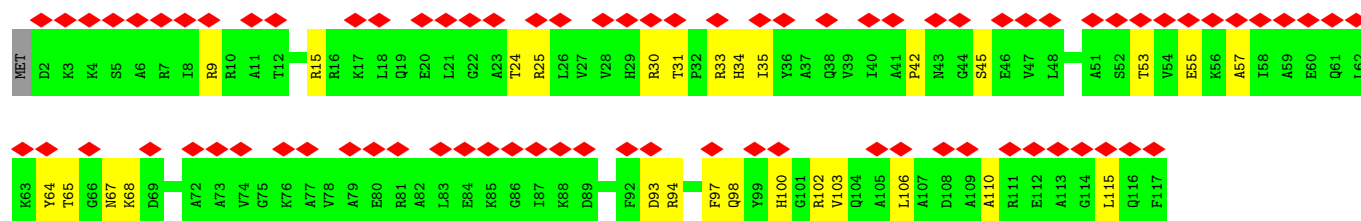


• Molecule 11: 50S ribosomal protein L17

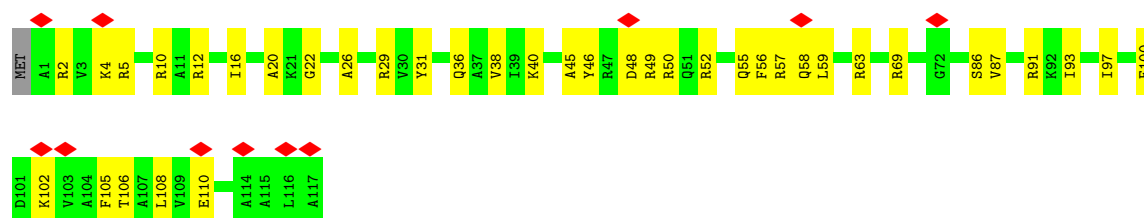


• Molecule 12: 50S ribosomal protein L18

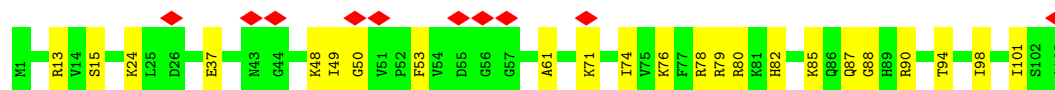
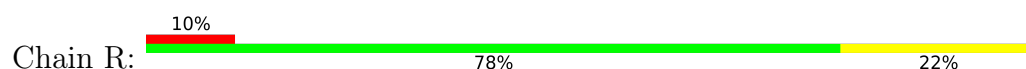




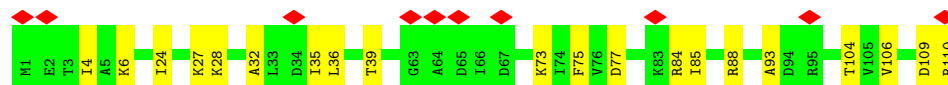
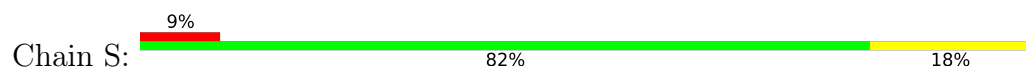
• Molecule 13: 50S ribosomal protein L20



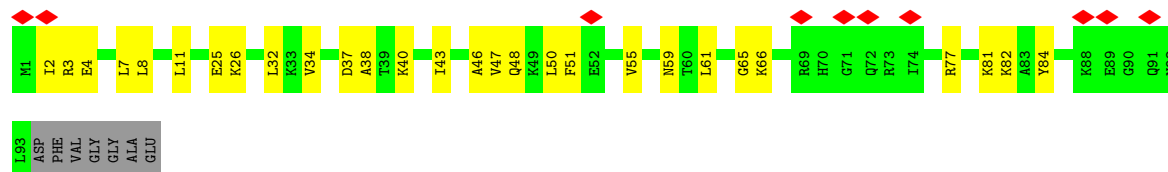
• Molecule 14: 50S ribosomal protein L21



• Molecule 15: 50S ribosomal protein L22

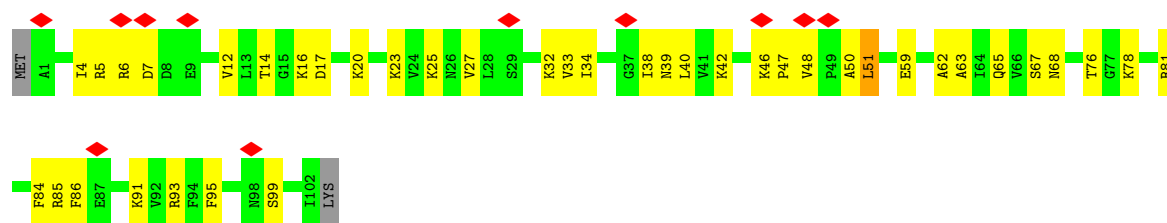


• Molecule 16: 50S ribosomal protein L23

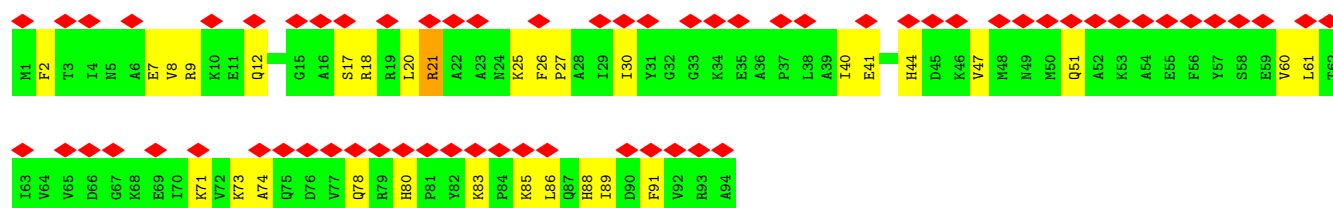


• Molecule 17: 50S ribosomal protein L24

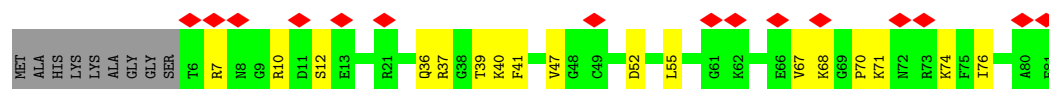




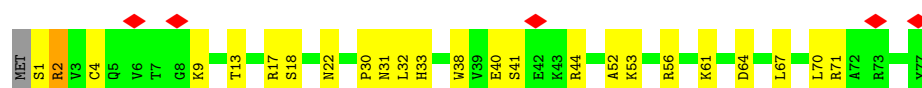
• Molecule 18: 50S ribosomal protein L25



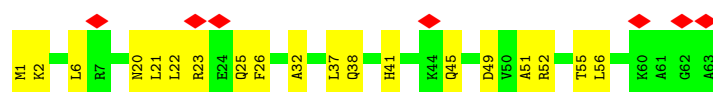
• Molecule 19: 50S ribosomal protein L27



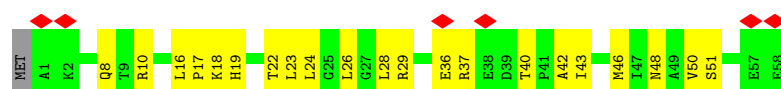
• Molecule 20: 50S ribosomal protein L28



• Molecule 21: 50S ribosomal protein L29



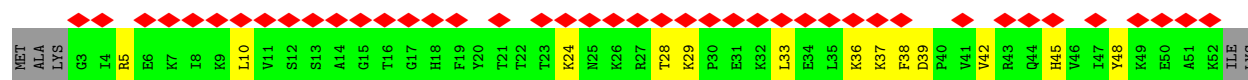
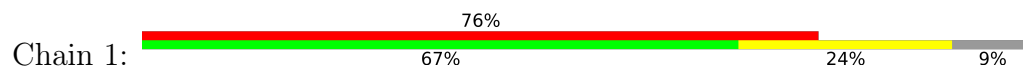
• Molecule 22: 50S ribosomal protein L30



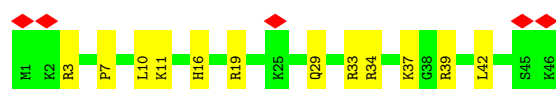
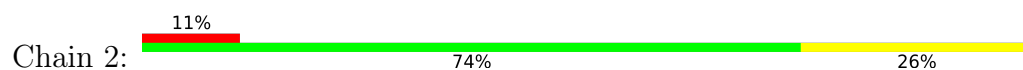
• Molecule 23: 50S ribosomal protein L32



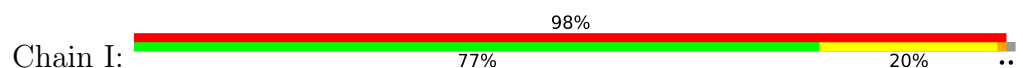
- Molecule 24: 50S ribosomal protein L33



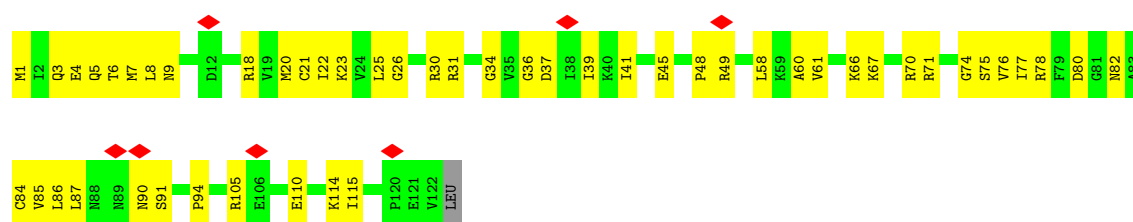
- Molecule 25: 50S ribosomal protein L34



- Molecule 26: 50S ribosomal protein L11

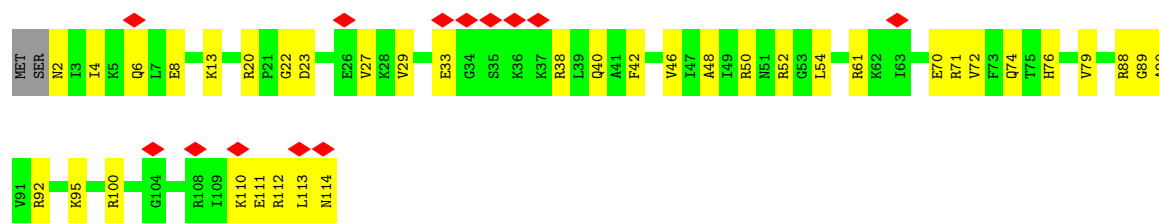


- Molecule 27: 50S ribosomal protein L14

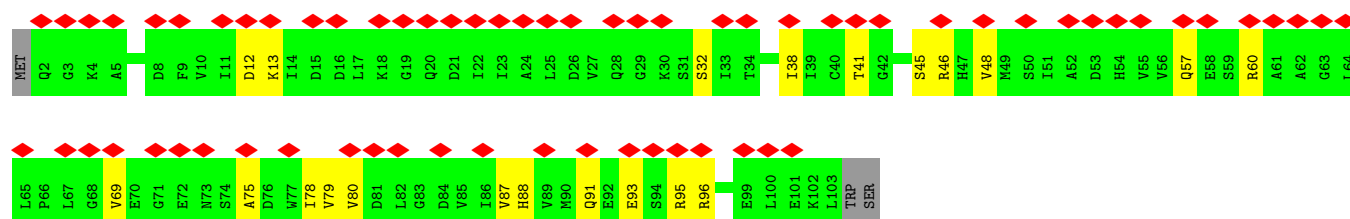
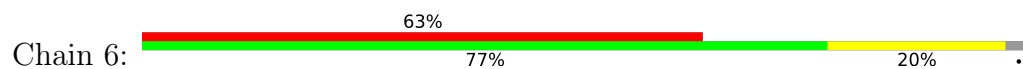


- Molecule 28: 50S ribosomal protein L19

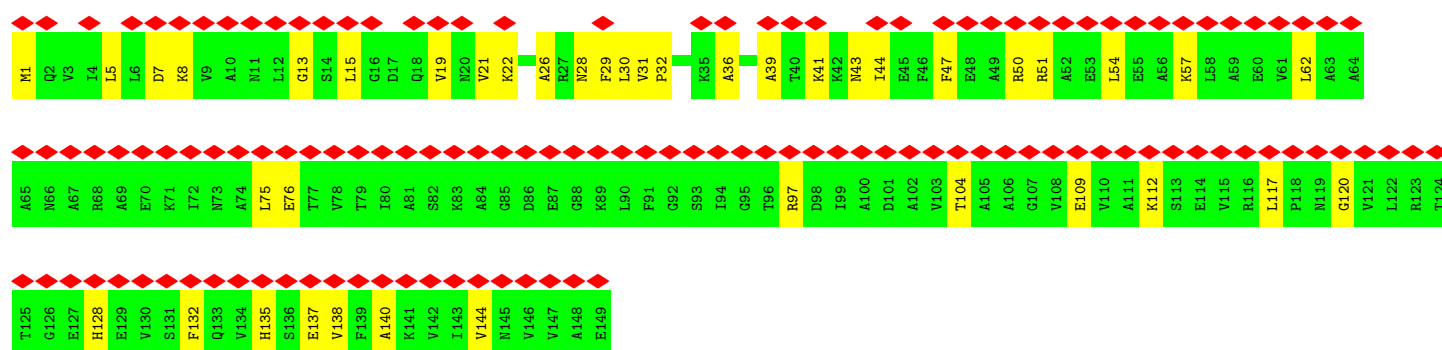
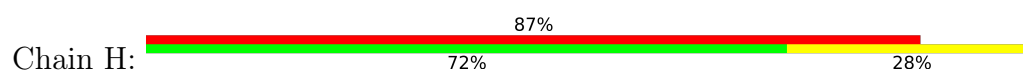




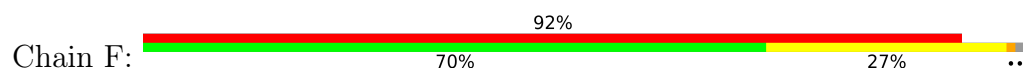
• Molecule 29: Ribosomal silencing factor RsfS



• Molecule 30: 50S ribosomal protein L9



• Molecule 31: 50S ribosomal protein L5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	23445	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	Not provided	
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	12.748	Depositor
Minimum map value	-6.150	Depositor
Average map value	0.034	Depositor
Map value standard deviation	0.805	Depositor
Recommended contour level	2.5	Depositor
Map size (\AA)	334.8, 334.8, 334.8	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.24, 1.24, 1.24	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.18	0/69777	0.74	14/108853 (0.0%)
2	B	0.16	0/2847	0.74	0/4440
3	9P	0.25	0/2626	0.47	0/3542
4	b	0.22	0/371	0.43	0/496
5	C	0.24	0/2121	0.44	0/2852
6	D	0.25	0/1586	0.47	0/2134
7	E	0.24	0/1571	0.43	0/2113
8	G	0.39	1/1343 (0.1%)	0.63	3/1816 (0.2%)
9	J	0.25	0/1152	0.44	0/1551
10	L	0.25	0/1054	0.52	0/1403
11	N	0.24	0/973	0.45	0/1301
12	O	0.24	0/902	0.43	0/1209
13	Q	0.24	0/960	0.38	0/1278
14	R	0.25	0/829	0.48	0/1107
15	S	0.23	0/864	0.41	0/1156
16	T	0.25	0/744	0.54	0/994
17	U	0.26	0/787	0.56	1/1051 (0.1%)
18	V	0.25	0/766	0.49	0/1025
19	W	0.26	0/582	0.46	0/769
20	X	0.24	0/635	0.47	0/848
21	Y	0.22	0/510	0.49	0/677
22	Z	0.24	0/453	0.52	0/605
23	0	0.25	0/450	0.51	0/599
24	1	0.24	0/416	0.45	0/554
25	2	0.25	0/380	0.44	0/498
26	I	0.25	0/1046	0.50	0/1410
27	K	0.25	0/947	0.48	0/1268
28	P	0.26	0/923	0.49	0/1234
29	6	0.24	0/787	0.44	0/1062
30	H	0.24	0/1121	0.46	0/1515
31	F	0.24	0/1434	0.47	0/1926
All	All	0.20	1/100957 (0.0%)	0.68	18/151286 (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
3	9P	0	1
26	I	0	1
31	F	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	111	PRO	CG-CD	-10.33	1.16	1.50

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	111	PRO	N-CD-CG	-13.03	83.65	103.20
8	G	111	PRO	CA-N-CD	-9.38	98.36	111.50
1	A	1625	C	N3-C2-O2	-7.62	116.57	121.90
1	A	1625	C	N1-C2-O2	7.62	123.47	118.90
8	G	111	PRO	CA-CB-CG	-7.30	90.12	104.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	9P	190	PRO	Peptide
31	F	175	PRO	Peptide
26	I	5	GLN	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	A	62301	0	31334	1158	0
2	B	2548	0	1292	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	9P	2582	0	2607	86	0
4	b	364	0	364	0	0
5	C	2082	0	2157	92	0
6	D	1565	0	1616	42	0
7	E	1552	0	1619	41	0
8	G	1323	0	1374	43	0
9	J	1129	0	1162	42	0
10	L	1045	0	1117	42	0
11	N	960	0	1000	34	0
12	O	892	0	923	24	0
13	Q	947	0	1022	42	0
14	R	816	0	839	23	0
15	S	857	0	922	17	0
16	T	738	0	807	27	0
17	U	779	0	834	31	0
18	V	753	0	780	23	0
19	W	575	0	589	21	0
20	X	625	0	655	19	0
21	Y	509	0	543	17	0
22	Z	449	0	491	20	0
23	0	444	0	461	21	0
24	1	409	0	440	10	0
25	2	377	0	418	13	0
26	I	1032	0	1088	23	0
27	K	938	0	1012	39	0
28	P	911	0	957	33	0
29	6	780	0	783	12	0
30	H	1110	0	1148	30	0
31	F	1410	0	1447	47	0
32	b	1	0	0	0	0
33	Q	1	0	0	0	0
34	A	21	0	0	0	0
34	B	1	0	0	0	0
34	C	2	0	0	0	0
34	L	1	0	0	0	0
34	N	1	0	0	0	0
34	S	1	0	0	0	0
All	All	92831	0	61801	1845	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 12.

The worst 5 of 1845 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)
1:A:1800:C:N4	1:A:1817:G:H22	1.58	1.01
1:A:1800:C:H42	1:A:1817:G:N2	1.57	1.01
2:B:78:A:H62	2:B:98:G:N2	1.58	1.00
1:A:950:G:H1	1:A:967:U:H3	1.09	0.98
1:A:377:G:H1	1:A:397:U:H3	1.01	0.98

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	9P	336/390 (86%)	313 (93%)	23 (7%)	0	100	100
4	b	45/70 (64%)	43 (96%)	2 (4%)	0	100	100
5	C	269/273 (98%)	250 (93%)	19 (7%)	0	100	100
6	D	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
7	E	199/201 (99%)	193 (97%)	6 (3%)	0	100	100
8	G	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
9	J	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
10	L	141/144 (98%)	121 (86%)	20 (14%)	0	100	100
11	N	118/127 (93%)	113 (96%)	5 (4%)	0	100	100
12	O	114/117 (97%)	105 (92%)	9 (8%)	0	100	100
13	Q	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
14	R	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
15	S	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
16	T	91/100 (91%)	80 (88%)	11 (12%)	0	100	100
17	U	100/104 (96%)	90 (90%)	10 (10%)	0	100	100
18	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	W	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
20	X	75/78 (96%)	75 (100%)	0	0	100	100
21	Y	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
22	Z	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
23	0	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
24	1	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
25	2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
26	I	139/142 (98%)	113 (81%)	26 (19%)	0	100	100
27	K	120/123 (98%)	114 (95%)	6 (5%)	0	100	100
28	P	111/115 (96%)	106 (96%)	5 (4%)	0	100	100
29	6	100/105 (95%)	97 (97%)	3 (3%)	0	100	100
30	H	147/149 (99%)	133 (90%)	14 (10%)	0	100	100
31	F	175/179 (98%)	162 (93%)	13 (7%)	0	100	100
All	All	3554/3735 (95%)	3325 (94%)	229 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	
3	9P	273/321 (85%)	272 (100%)	1 (0%)	89	95
4	b	43/62 (69%)	42 (98%)	1 (2%)	45	69
5	C	216/218 (99%)	214 (99%)	2 (1%)	75	86
6	D	164/164 (100%)	163 (99%)	1 (1%)	84	91
7	E	165/165 (100%)	165 (100%)	0	100	100
8	G	137/138 (99%)	136 (99%)	1 (1%)	81	89
9	J	116/116 (100%)	116 (100%)	0	100	100
10	L	102/103 (99%)	101 (99%)	1 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	N	100/103 (97%)	100 (100%)	0	100	100
12	O	86/87 (99%)	86 (100%)	0	100	100
13	Q	89/90 (99%)	89 (100%)	0	100	100
14	R	84/84 (100%)	84 (100%)	0	100	100
15	S	93/93 (100%)	93 (100%)	0	100	100
16	T	80/84 (95%)	80 (100%)	0	100	100
17	U	83/85 (98%)	83 (100%)	0	100	100
18	V	78/78 (100%)	77 (99%)	1 (1%)	65	81
19	W	56/63 (89%)	56 (100%)	0	100	100
20	X	67/68 (98%)	66 (98%)	1 (2%)	60	77
21	Y	55/55 (100%)	54 (98%)	1 (2%)	54	74
22	Z	48/49 (98%)	48 (100%)	0	100	100
23	0	47/48 (98%)	47 (100%)	0	100	100
24	1	45/49 (92%)	45 (100%)	0	100	100
25	2	38/38 (100%)	38 (100%)	0	100	100
26	I	109/110 (99%)	108 (99%)	1 (1%)	75	86
27	K	103/104 (99%)	103 (100%)	0	100	100
28	P	98/100 (98%)	98 (100%)	0	100	100
29	6	88/91 (97%)	88 (100%)	0	100	100
30	H	114/114 (100%)	114 (100%)	0	100	100
31	F	148/150 (99%)	147 (99%)	1 (1%)	81	89
All	All	2925/3030 (96%)	2913 (100%)	12 (0%)	88	95

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	V	21	ARG
20	X	2	ARG
31	F	32	LYS
21	Y	20	ASN
5	C	124	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
19	W	36	GLN
27	K	3	GLN
30	H	135	HIS
10	L	4	ASN
17	U	65	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2899/2919 (99%)	436 (15%)	14 (0%)
2	B	118/119 (99%)	18 (15%)	0
All	All	3017/3038 (99%)	454 (15%)	14 (0%)

5 of 454 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	14	A
1	A	27	G
1	A	28	A

5 of 14 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1606	C
1	A	2058	A
1	A	2756	U
1	A	2425	A
1	A	2573	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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

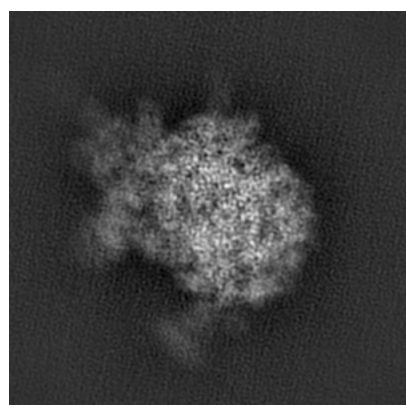
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12216. These allow visual inspection of the internal detail of the map and identification of artifacts.

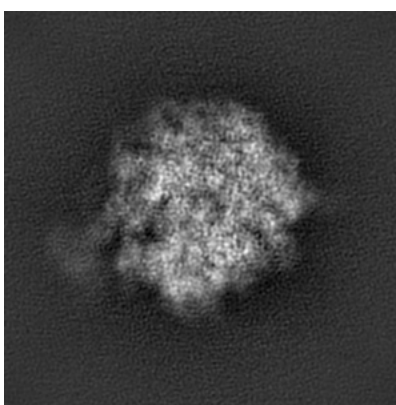
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

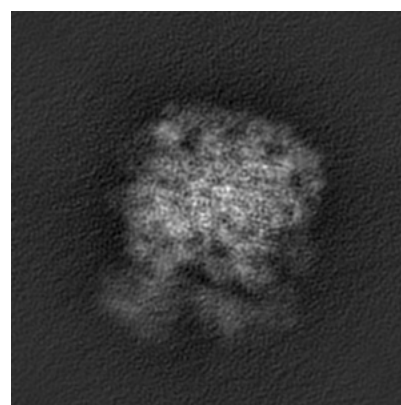
6.1.1 Primary map



X



Y

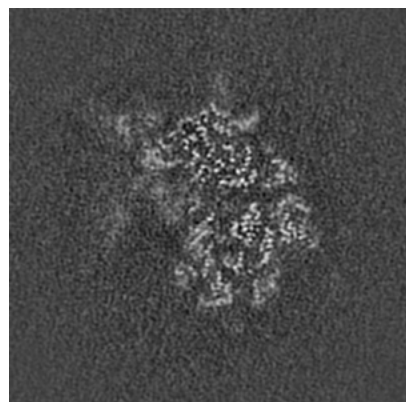


Z

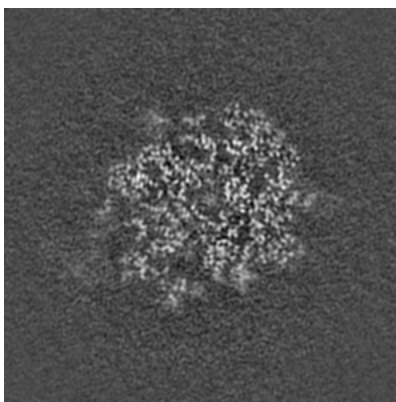
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

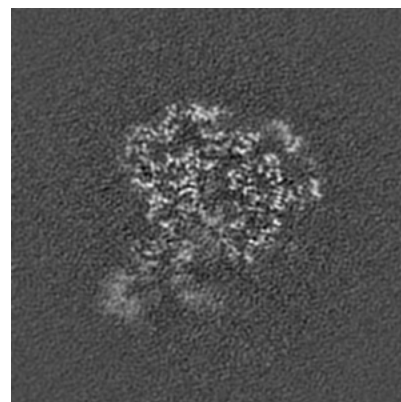
6.2.1 Primary map



X Index: 135



Y Index: 135

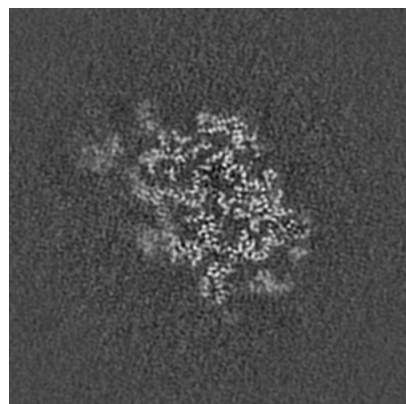


Z Index: 135

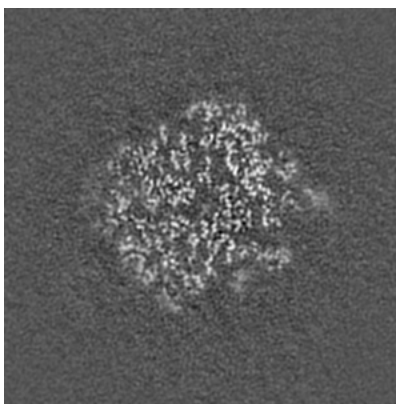
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

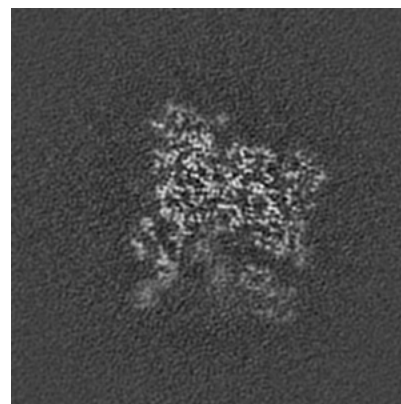
6.3.1 Primary map



X Index: 157



Y Index: 146

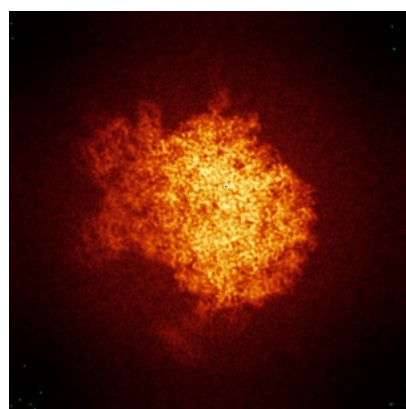


Z Index: 151

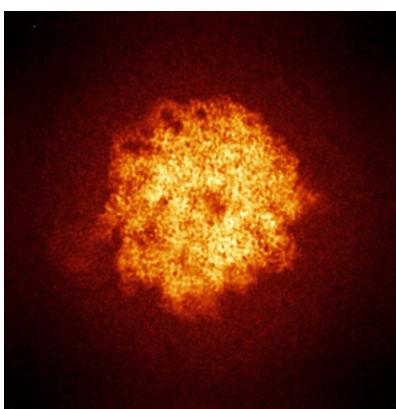
The images above show the largest variance slices of the map in three orthogonal directions.

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

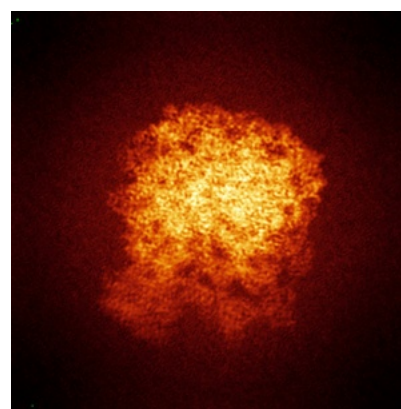
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

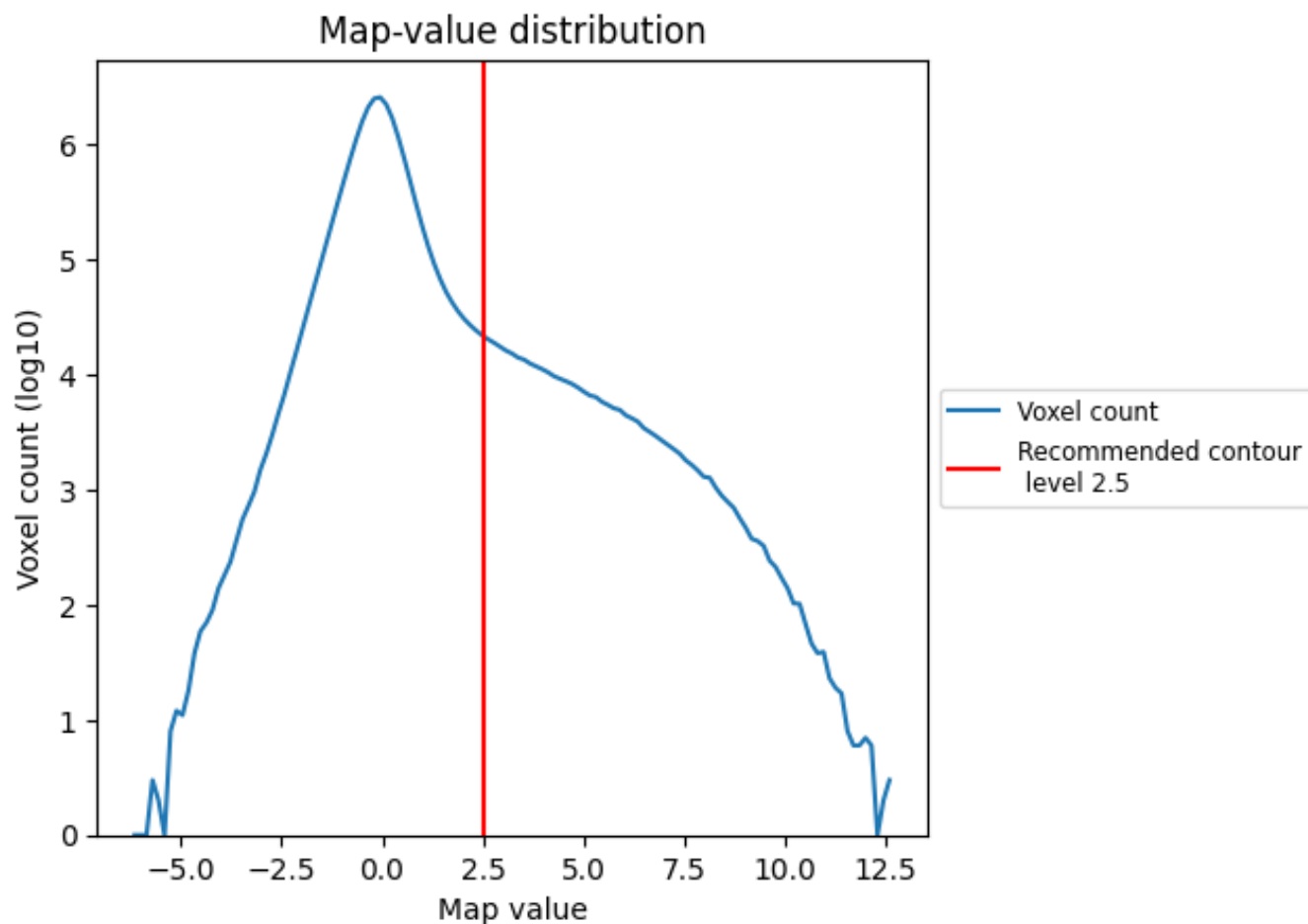
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

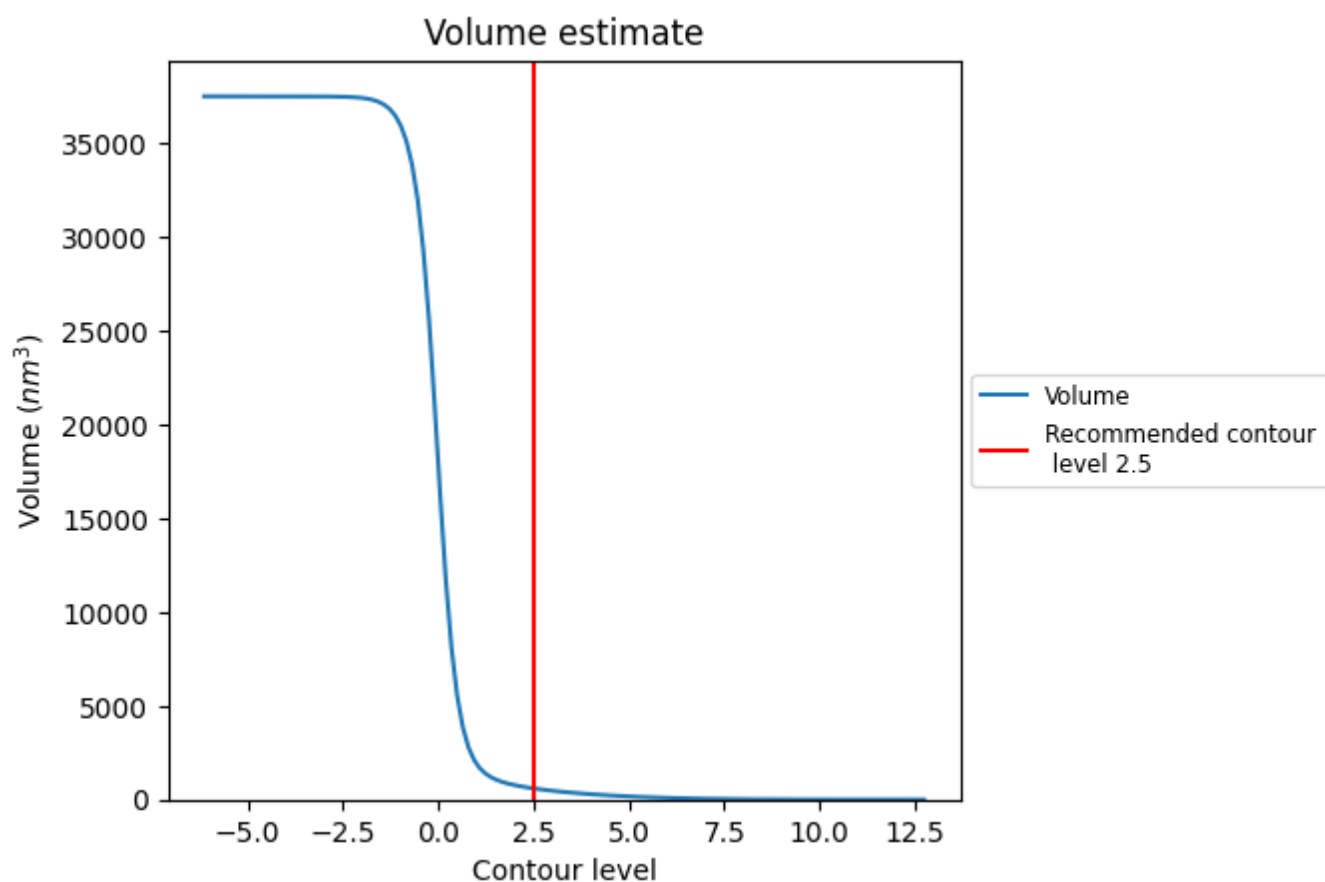
This section contains the results of statistical analysis of the map.

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.

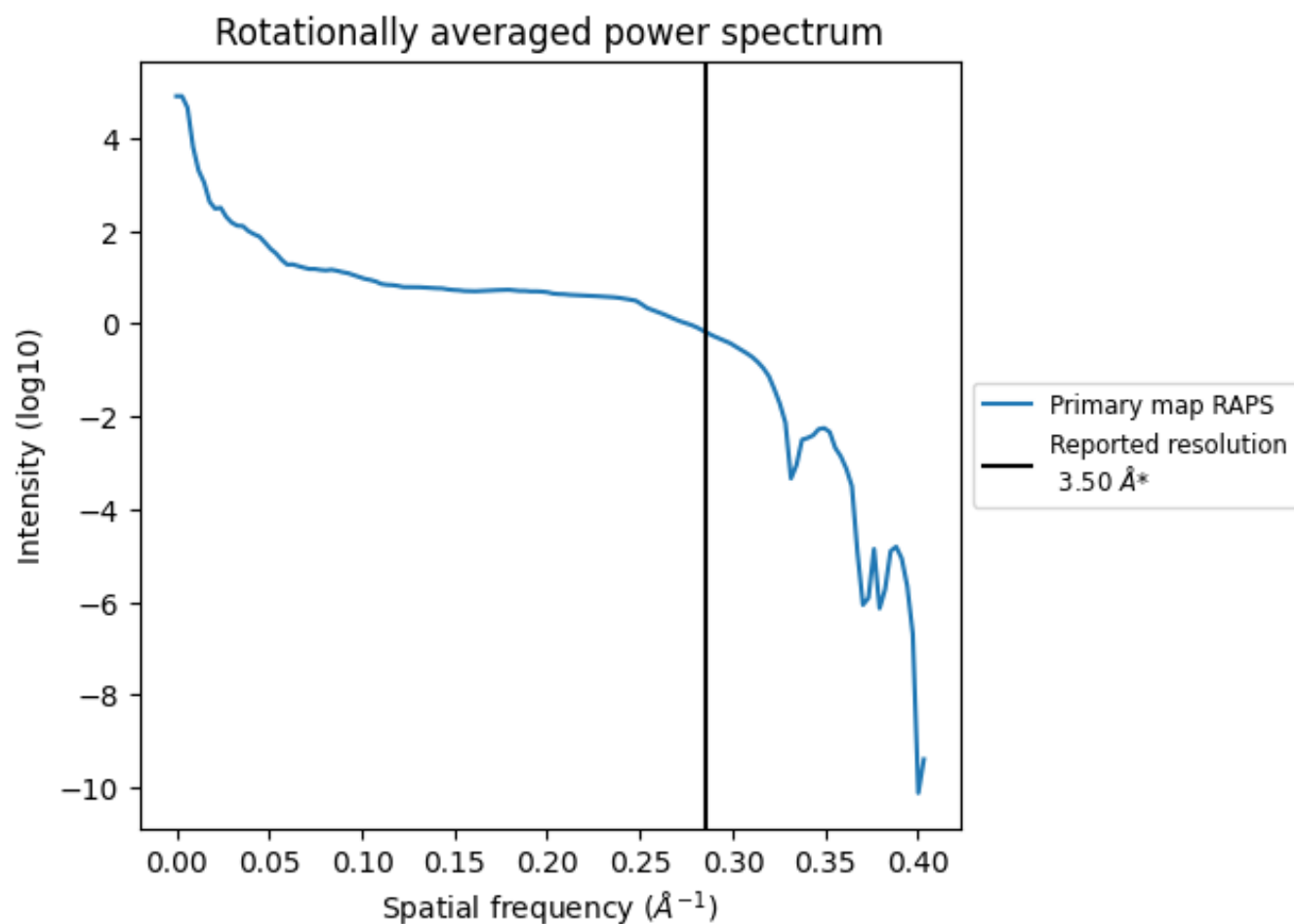
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 594 nm³; this corresponds to an approximate mass of 537 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 ⓘ

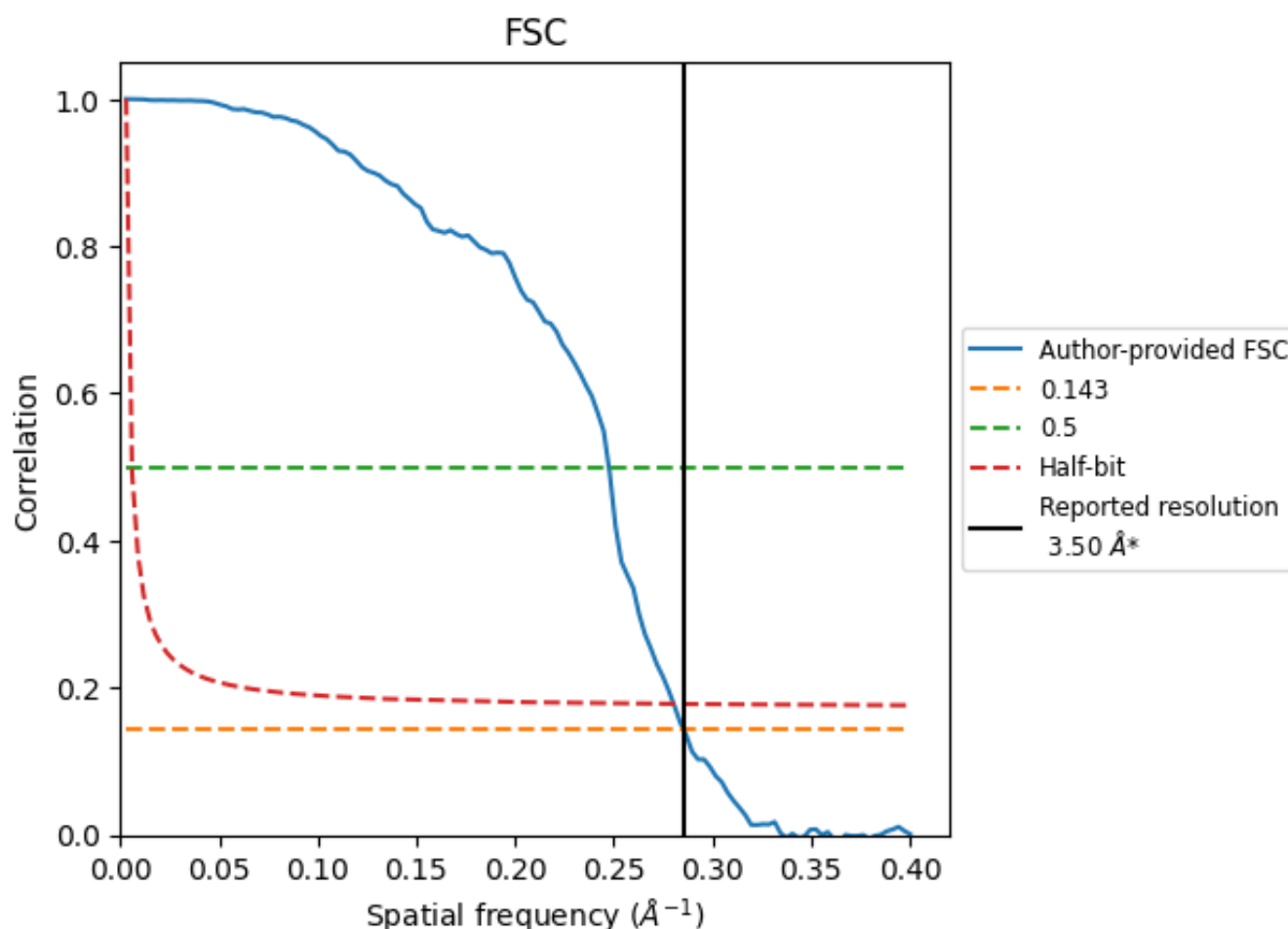


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

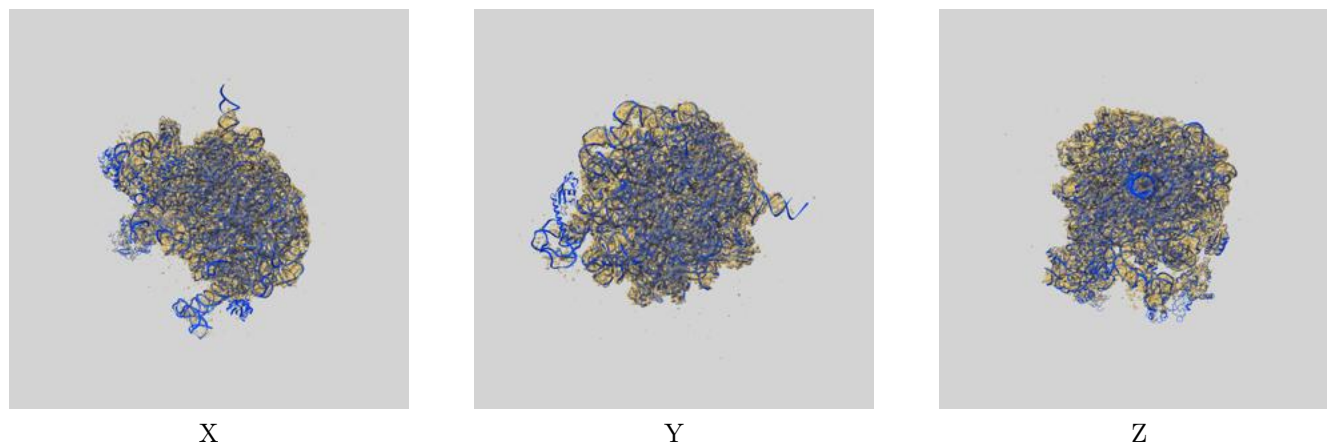
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.51	4.04	3.57
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

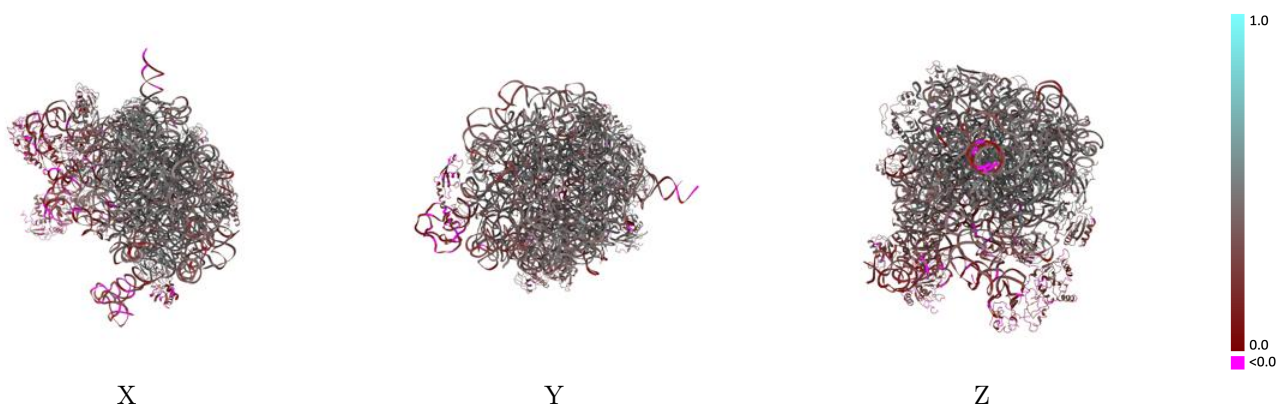
This section contains information regarding the fit between EMDB map EMD-12216 and PDB model 7BL3. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



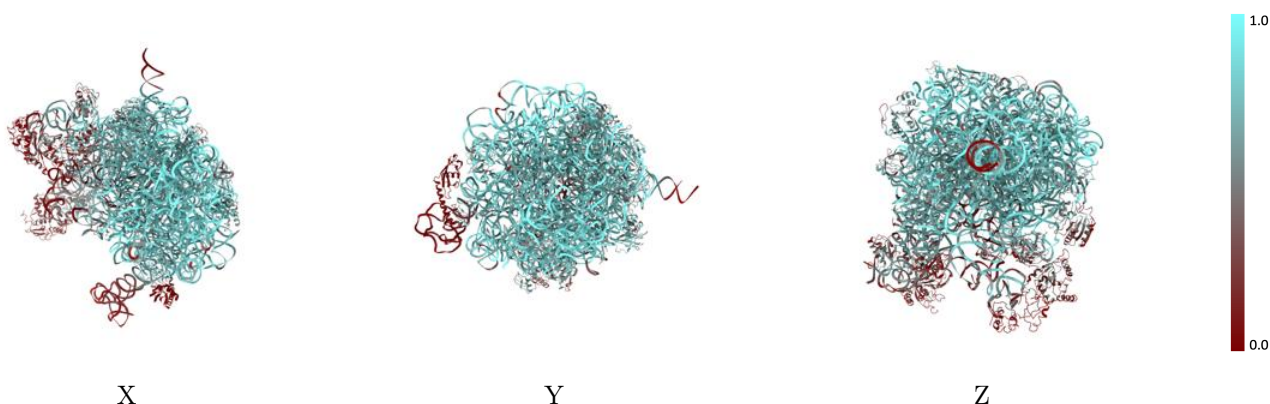
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



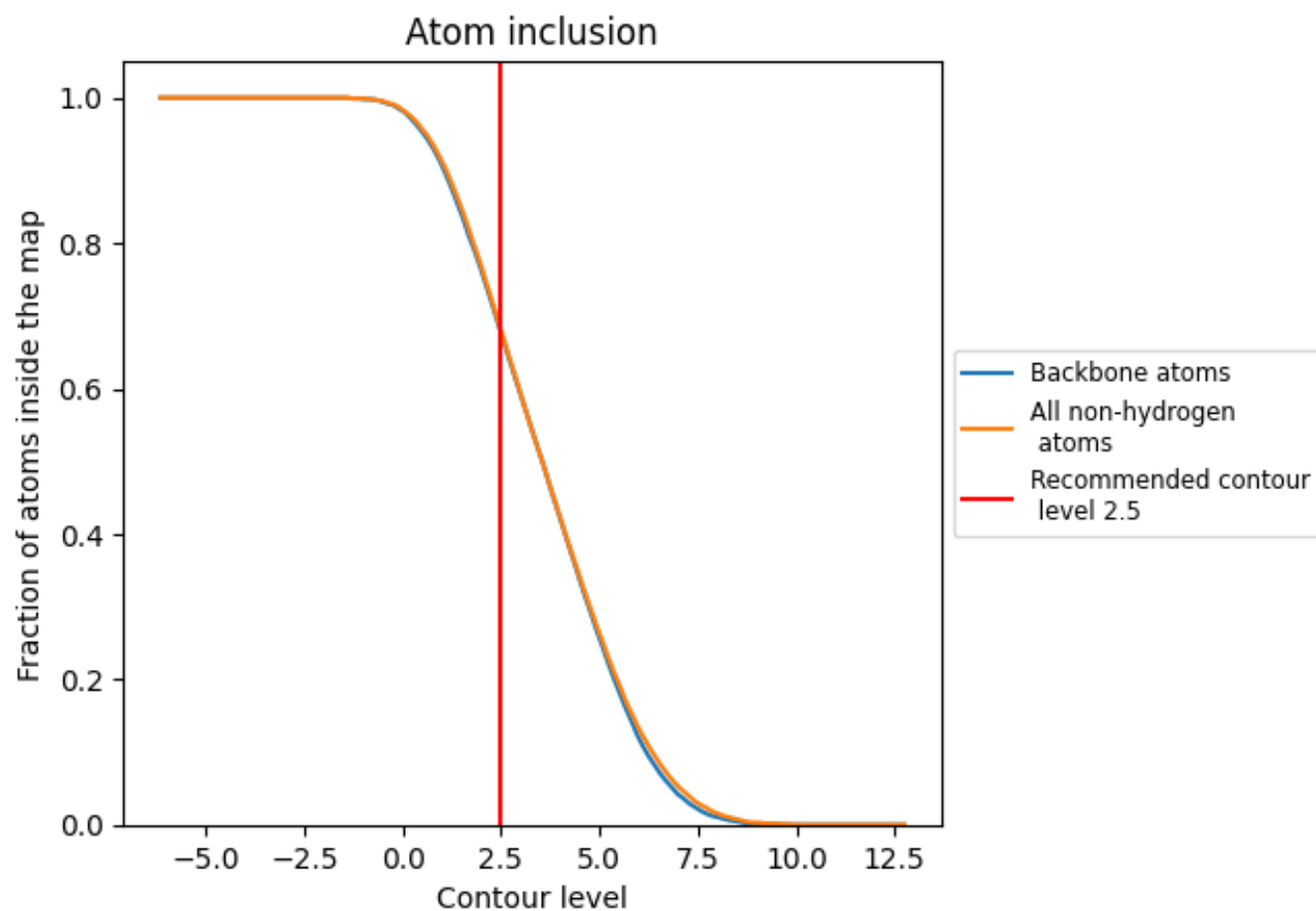
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.5).

































































9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 68% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6800	 0.3620
0	 0.6260	 0.4120
1	 0.2620	 0.2880
2	 0.6960	 0.4590
6	 0.3220	 0.3050
9P	 0.3630	 0.2690
A	 0.7660	 0.3710
B	 0.5230	 0.2230
C	 0.7100	 0.4430
D	 0.7020	 0.4530
E	 0.5930	 0.3910
F	 0.1240	 0.1670
G	 0.4420	 0.3140
H	 0.1320	 0.2030
I	 0.0320	 0.1490
J	 0.6840	 0.4460
K	 0.6540	 0.4260
L	 0.5380	 0.3650
N	 0.7260	 0.4500
O	 0.3050	 0.2340
P	 0.6540	 0.4220
Q	 0.7260	 0.4500
R	 0.6660	 0.4280
S	 0.6990	 0.4600
T	 0.6550	 0.4130
U	 0.6520	 0.4100
V	 0.3120	 0.2630
W	 0.5420	 0.3800
X	 0.6510	 0.4340
Y	 0.6300	 0.3870
Z	 0.6360	 0.4270
b	 0.0110	 0.1090

