



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 06:29 AM UTC

PDB ID : 9HA6 / pdb_00009ha6
EMDB ID : EMD-51978
Title : mature 50S subunit supplemented with Api137
Authors : Lauer, S.; Nikolay, R.; Spahn, C.M.T.
Deposited on : 2024-11-01
Resolution : 3.08 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:

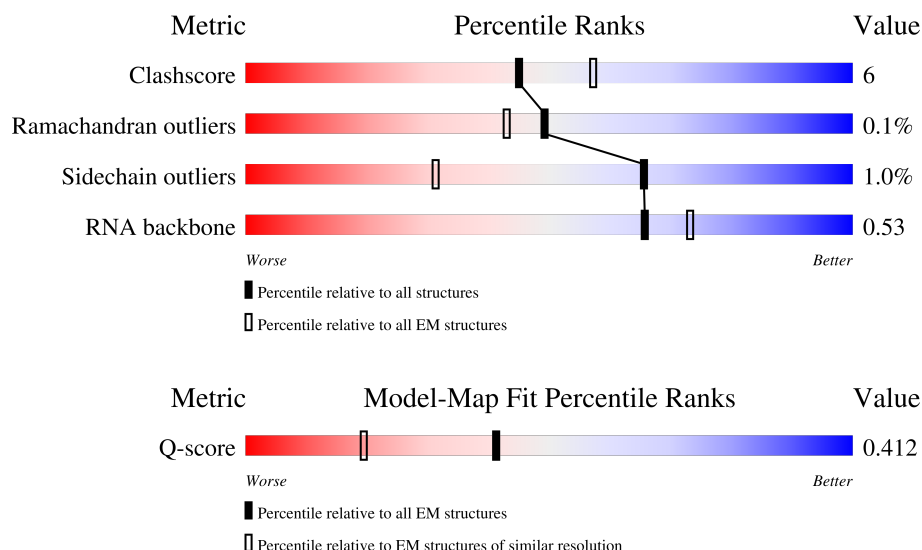
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.08 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.



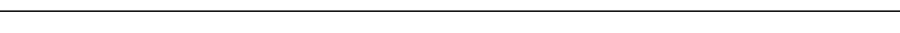
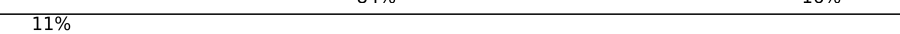
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14000 (2.58 - 3.58)

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

Mol	Chain	Length	Quality of chain
1	0	56	
2	1	50	
3	2	46	

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Mol	Chain	Length	Quality of chain
4	3	64	
5	4	38	
6	B	120	
7	C	271	
8	D	209	
9	E	201	
10	F	177	
11	G	176	
12	H	149	
13	J	142	
14	K	122	
15	L	143	
16	M	136	
17	N	120	
18	O	116	
19	P	114	
20	Q	117	
21	R	103	
22	S	110	
23	T	93	
24	U	102	
25	V	94	
26	W	75	
27	X	77	
28	Y	63	

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Mol	Chain	Length	Quality of chain
29	Z	58	 5% 81% 19%
30	A	2904	 5% 64% 31% 5%
31	y	17	 47% 47% 41% 12%
31	z	17	 47% 53% 47%

2 Entry composition [i](#)

There are 31 unique types of molecules in this entry. The entry contains 90242 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 Large ribosomal subunit protein bL32.

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

- Molecule 2 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 3 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 6 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 1402434313

- Molecule 7 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 8 is a protein called 50S ribosomal protein L3.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 11 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 12 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 13 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 14 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 15 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 16 is a protein called 50S ribosomal protein L16.

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

- Molecule 17 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 18 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 19 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 20 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 21 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 22 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	110	Total	C	N	O	S	1	0
			868	538	170	157	3		

- Molecule 23 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 24 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 25 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 26 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 27 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 28 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 29 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 30 is a RNA chain called 23S ribosomal rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	A	2900	Total	C	N	O	P	1	0
			62281	27783	11461	20136	2901		

- Molecule 31 is a protein called Apidaecins type 22.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	z	17	Total	C	N	O	0	0
			148	94	33	21		
31	y	17	Total	C	N	O	0	0
			148	94	33	21		

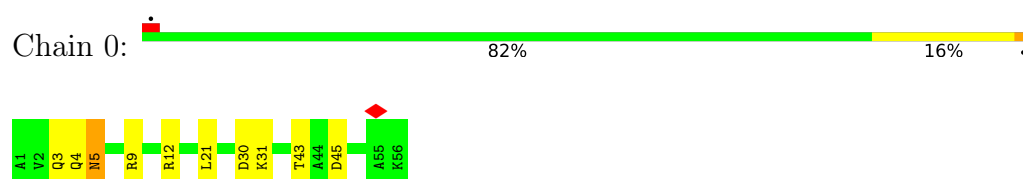
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	10	ARG	GLN	conflict	UNP P35581
y	10	ARG	GLN	conflict	UNP P35581

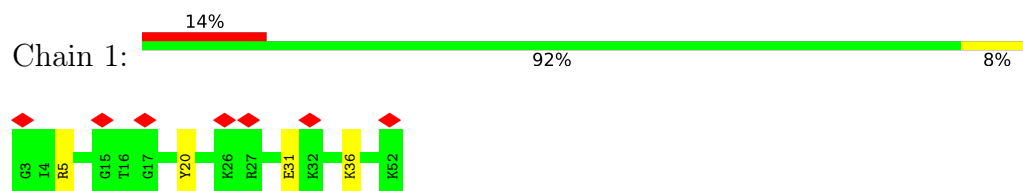
3 Residue-property plots [i](#)

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

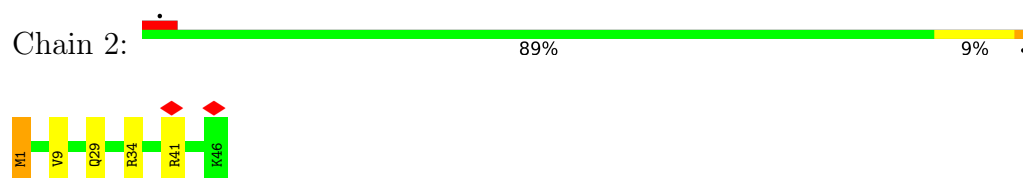
- Molecule 1: Large ribosomal subunit protein bL32



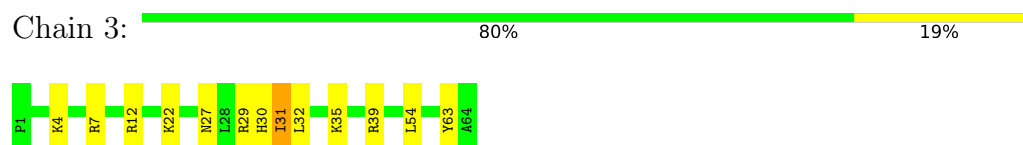
- Molecule 2: Large ribosomal subunit protein bL33



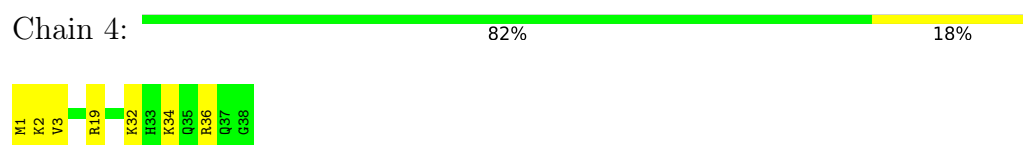
- Molecule 3: Large ribosomal subunit protein bL34



- Molecule 4: Large ribosomal subunit protein bL35

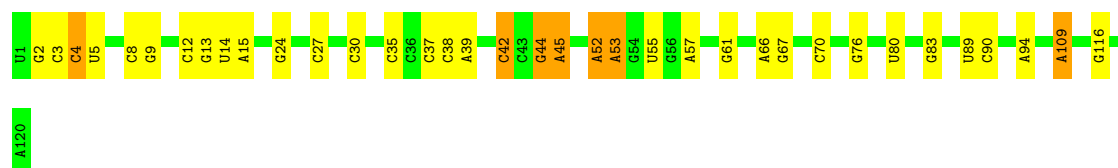


- Molecule 5: Large ribosomal subunit protein bL36A



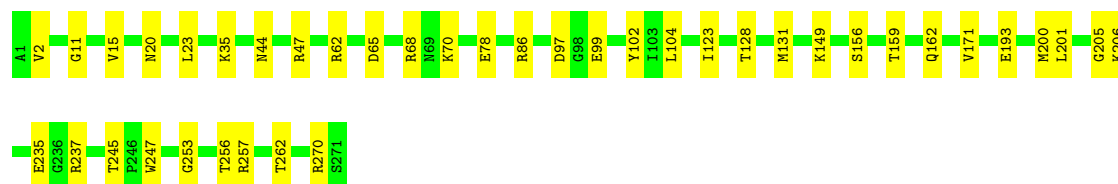
- Molecule 6: 5S ribosomal RNA

Chain B:  70% 24% 6%



- Molecule 7: Large ribosomal subunit protein uL2

Chain C:  85% 15%



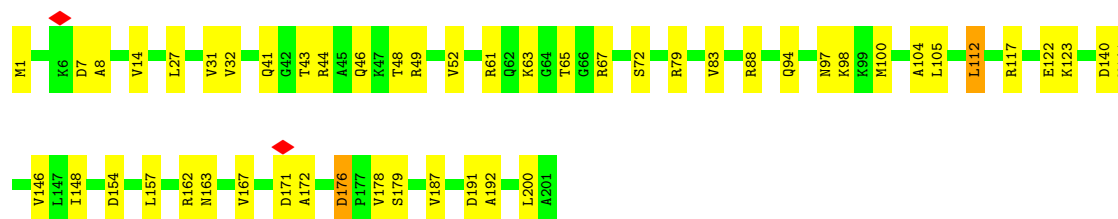
- Molecule 8: 50S ribosomal protein L3

Chain D:  85% 15%



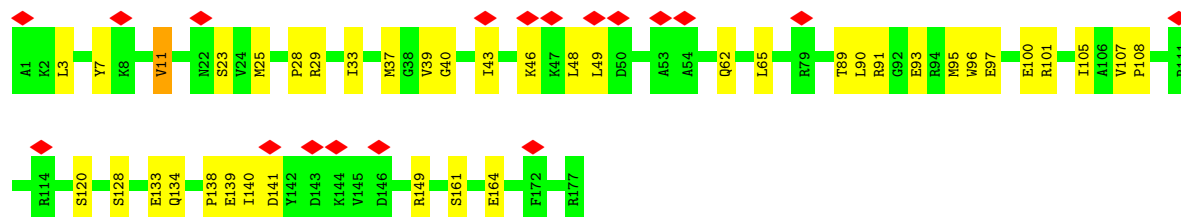
- Molecule 9: Large ribosomal subunit protein uL4

Chain E:  75% 24%

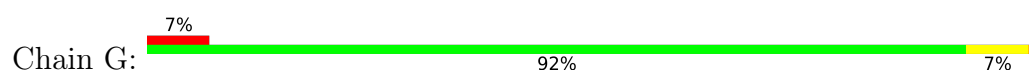


- Molecule 10: Large ribosomal subunit protein uL5

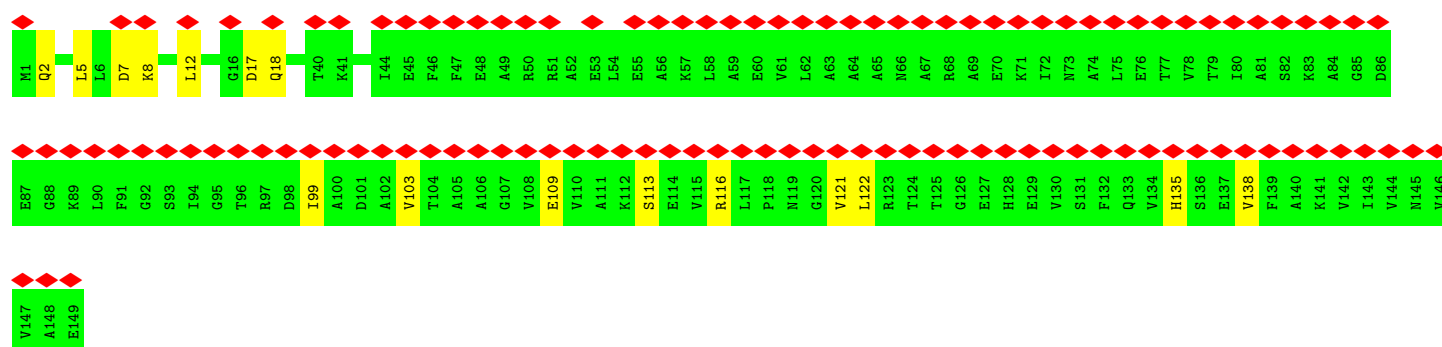
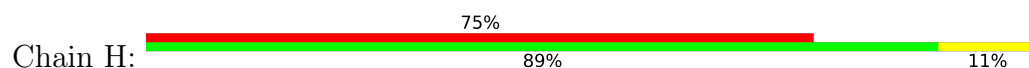
Chain F:  10% 77% 22%



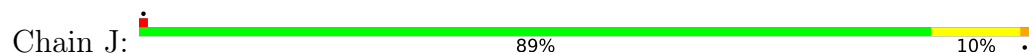
- Molecule 11: Large ribosomal subunit protein uL6



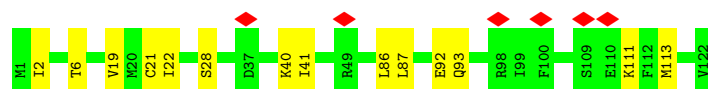
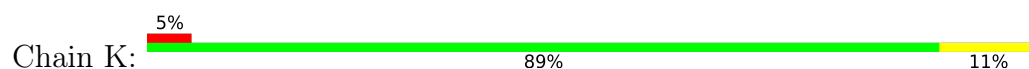
- Molecule 12: Large ribosomal subunit protein bL9



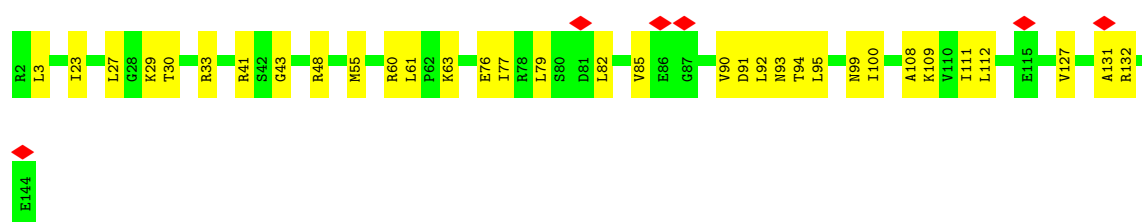
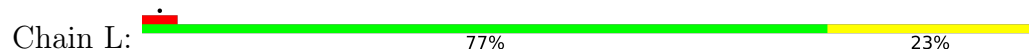
- Molecule 13: Large ribosomal subunit protein uL13



- Molecule 14: Large ribosomal subunit protein uL14

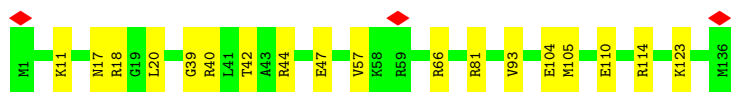


- Molecule 15: Large ribosomal subunit protein uL15

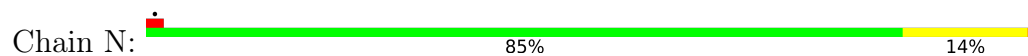


- Molecule 16: 50S ribosomal protein L16

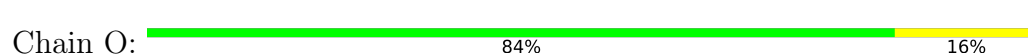




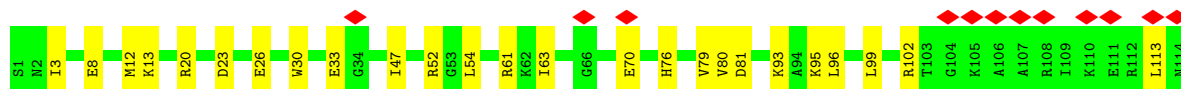
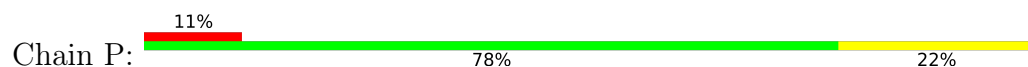
- Molecule 17: Large ribosomal subunit protein bL17



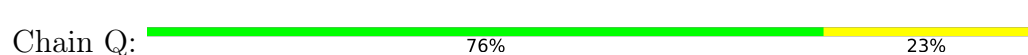
- Molecule 18: Large ribosomal subunit protein uL18



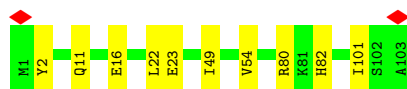
- Molecule 19: Large ribosomal subunit protein bL19



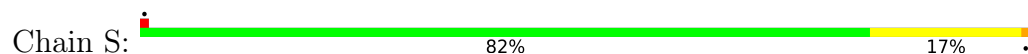
- Molecule 20: Large ribosomal subunit protein bL20



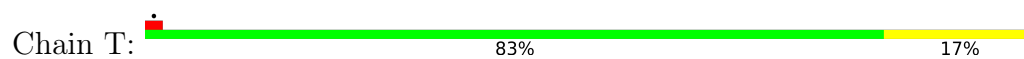
- Molecule 21: Large ribosomal subunit protein bL21



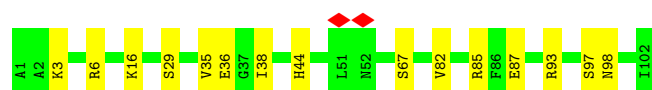
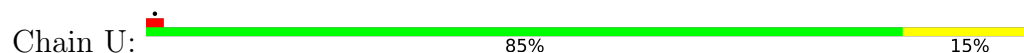
- Molecule 22: Large ribosomal subunit protein uL22



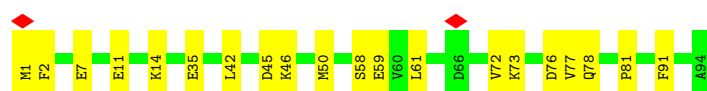
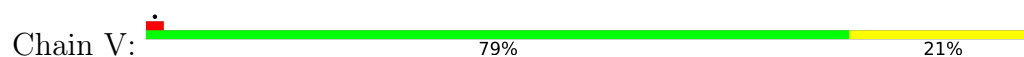
- Molecule 23: Large ribosomal subunit protein uL23



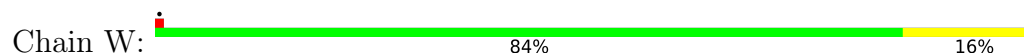
- Molecule 24: Large ribosomal subunit protein uL24



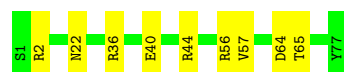
- Molecule 25: Large ribosomal subunit protein bL25



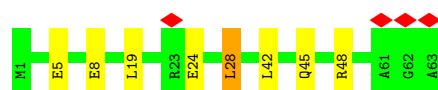
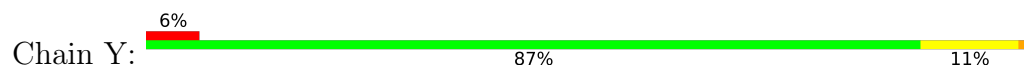
- Molecule 26: Large ribosomal subunit protein bL27



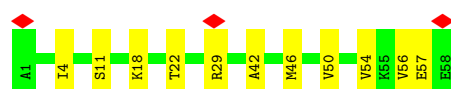
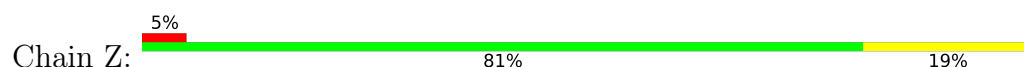
- Molecule 27: Large ribosomal subunit protein bL28



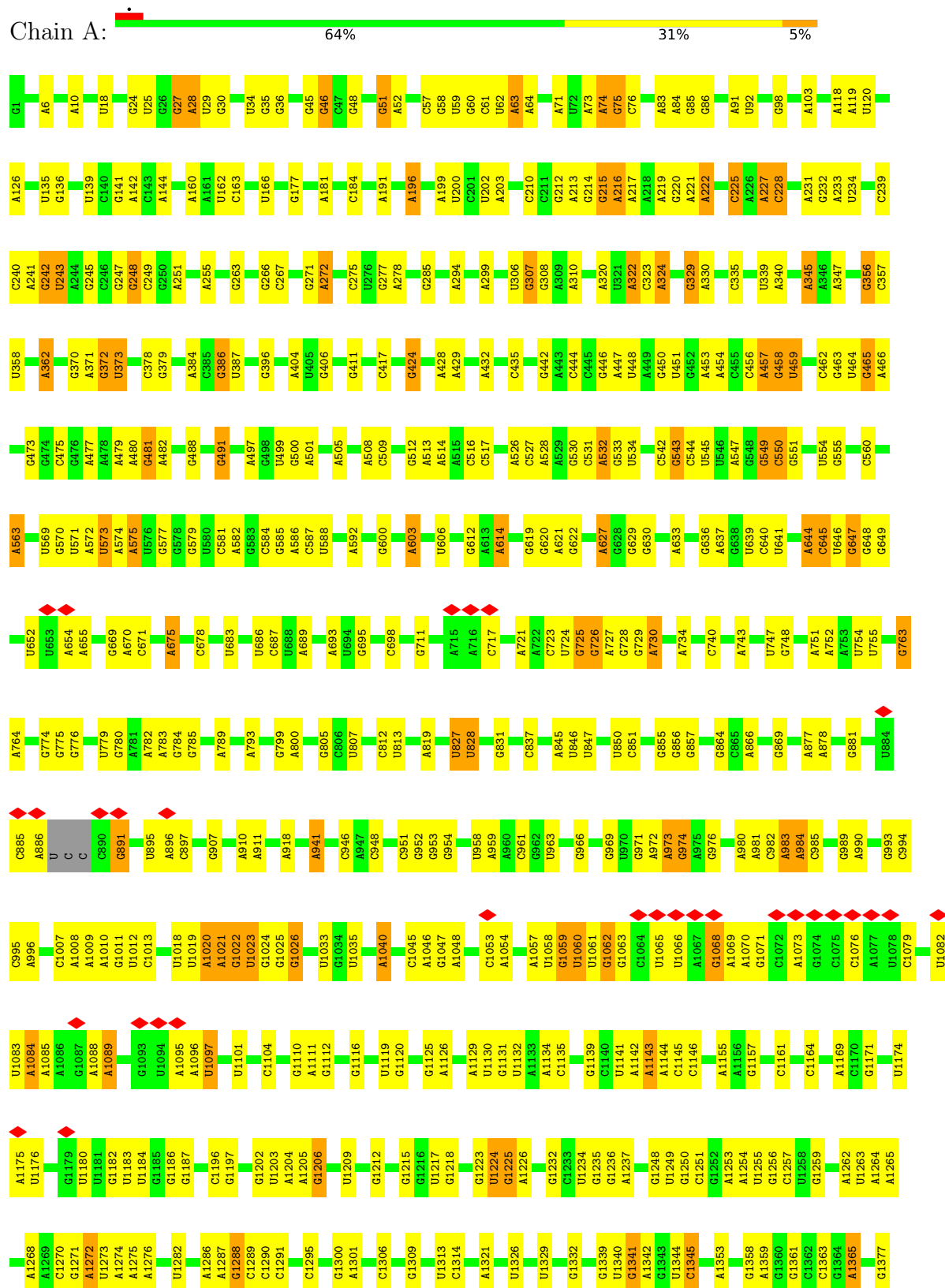
- Molecule 28: Large ribosomal subunit protein uL29



- Molecule 29: Large ribosomal subunit protein uL30



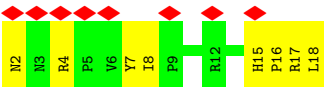
• Molecule 30: 23S ribosomal rRNA



G2743	A2635	G2527	G2444	C2362	G2239	U2151	C2089	A1858	C1764	G1663	A1378
G2744	G2636	U2528	G2445	G2363	U2243	G2152	A2090	U1864	U1769	A1664	A1379
G2745	G2637	G2529	G2446	G2364	G2243	C2153	G2093	U1865	G1770	G1666	G1380
G2746	G2638	A2530	G2447	G2365	G2250	A2154	G2096	A1866	A1771	A1528	A1383
G2747	G2645	G2535	A2448	A2369	G2251	U2155	C2096	G1869	A1772	A1535	C1386
A2748	C2646	A2547	A2451	U2372	C2258	G2157	U2099	A1988	A1773	C1536	A1387
A2749	U2647	A2547	C2452	G2373	A2266	G2158	G2100	A1989	G1776	A1537	
A2750	G2652	A2552	G2453	G2374	A2267	A2159	A2101	A1990	U1779	G1543	U1390
G2751	G2653	U2554	G2454	G2375	G2271	C2160	G2103	A1871	U1780	A1544	U1394
C2752	G2654	U2554	U2457	A2376	G2271	G2161	C2104	A1872	U1781	A1545	A1395
U2753	G2655	C2559	G2464	A2377	G2274	C2162	U2105	A1901	U1782	U1396	U1397
U2754	U2656	C2564	A2468	A2378	A2274	G2163	U2106	G1906	A1783	C1550	
U2755	U2657	A2564	A2469	G2380	A2279	A2164	U2107	G1884	A1784	G1563	G1416
U2756	A2661	A2565	A2474	G2381	G2279	C2165	U2108	C1686	A1785	U1559	A1419
A2757	A2662	G2567	U2475	G2382	G2283	U2166	G2109	C1687	U1787	G1560	A1420
G2758	G2573	C2573	A2476	U2383	A2284	U2167	A2110	U1688	C1788	C1565	G1425
G2759	G2576	A2577	A2481	U2384	C2285	U2168	G2111	A1913	A1789	A1566	G1426
G2760	A2577	G2578	G2484	U2385	A2287	A2169	U2112	A1914	G1696	G1567	A1427
G2761	G2579	G2582	A2487	U2386	U2291	A2170	G2113	A1915	A1790	G1568	C1428
G2762	U2680	U2585	G2488	U2387	U2296	A2171	U2114	A1916	A1791	A1569	
A2763	G2689	U2585	G2489	U2388	A2297	A2172	A2115	U1917	A1792	C1574	A1431
A2764	G2690	U2586	U2491	U2389	U2297	A2173	A2116	A1927	U1793	A1578	G1432
A2765	G2691	U2587	U2492	U2390	A2297	C2174	A2117	A1928	A1801	U1584	A1437
A2766	G2692	U2588	U2493	U2391	U2305	C2175	A2118	A1929	A1802	C1585	C1447
A2767	U2687	U2589	U2494	U2392	U2309	C2176	U2119	G1930	A1808	G1601	G1448
A2768	G2688	U2590	U2495	U2393	U2324	C2177	A2120	A1936	A1809	U1602	
A2769	U2689	U2591	U2496	U2394	G2325	C2178	G2121	A1937	U1812	A1603	C1454
A2770	G2690	U2592	U2497	U2395	U2326	C2179	U2122	U1940	U1813	A1604	U1458
A2771	G2691	U2593	U2498	U2396	A2327	C2180	G2123	C1941	G1814	A1608	C1461
A2772	U2692	U2594	U2499	U2397	U2330	U2181	G2124	C1942	A1815	A1610	U1466
A2773	U2693	U2595	U2500	U2398	G2337	U2182	G2125	U1951	G1816	G1622	G1475
A2774	U2694	U2596	U2501	U2399	U2343	A2183	G2126	A1952	G1817	U1477	U1476
A2775	U2695	U2597	U2502	U2400	U2344	A2184	G2127	U1953	G1734	A1634	A1477
A2776	U2696	U2598	U2503	U2401	U2345	U2189	G2128	G1954	A1735	C1638	G1482
A2777	U2697	U2599	U2504	U2402	G2346	U2190	G2129	U1955	U1736	G1645	A1490
A2778	U2698	U2600	U2505	U2403	U2347	U2191	G2130	U1956	G1737	C1646	G1491
A2779	U2699	U2601	U2506	U2404	U2348	U2192	U2131	C1962	A1738	U1647	U1497
A2780	U2700	U2602	U2507	U2405	U2349	U2193	U2132	G1964	A1739	C1649	C1498
A2781	U2701	U2603	U2508	U2406	U2350	U2194	G2133	C1967	A1744	A1654	A1508
A2782	U2702	U2604	U2509	U2407	U2351	U2195	G2134	U1970	A1754	G1514	A1515
A2783	U2703	U2605	U2510	U2408	G2357	U2196	G2135	U1971	G1756	G1659	
A2784	U2704	U2606	U2511	U2409	G2360	U2197	G2136	U1972	C1837	U1662	
A2785	U2705	U2607	U2512	U2410	G2361	U2198	G2137	A1977	C1843		
A2786	U2706	U2608	U2513	U2411		U2199	G2138	G1983	G1857		
A2787	U2707	U2609	U2514	U2412		U2200	G2139				
A2788	U2708	U2610	U2515	U2413		U2201	U2140				
A2789	U2709	U2611	U2516	U2414		U2202	G2141				
A2790	U2710	U2612	U2517	U2415		U2203	G2142				
A2791	U2711	U2613	U2518	U2416		U2204	G2143				
A2792	U2712	U2614	U2519	U2417		U2205	G2144				
A2793	U2713	U2615	U2520	U2418		U2206	G2145				
A2794	U2714	U2616	U2521	U2419		U2207	G2146				
A2795	U2715	U2617	U2522	U2420		U2208	G2147				
A2796	U2716	U2618	U2523	U2421		U2209	G2148				
A2797	U2717	U2619	U2524	U2422		U2210	G2149				
A2798	U2718	U2620	U2525	U2423		U2211	C2150				
A2799	U2719	U2621	U2526	U2424		U2212					
A2800	U2720	U2622	U2527	U2425		U2213					
A2801	U2721	U2623	U2528	U2426		U2214					
A2802	U2722	U2624	U2529	U2427		U2215					
A2803	U2723	U2625	U2530	U2428		U2216					
A2804	U2724	U2626	U2531	U2429		U2217					
A2805	U2725	U2627	U2532	U2430		U2218					
A2806	U2726	U2628	U2533	U2431		U2219					
A2807	U2727	U2629	U2534	U2432		U2220					
A2808	U2728	U2630	U2535	U2433		U2221					
A2809	U2729	U2631	U2536	U2434		U2222					
A2810	U2730	U2632	U2537	U2435		U2223					
A2811	U2731	U2633	U2538	U2436		U2224					
A2812	U2732	U2634	U2539	U2437		U2225					
A2813	U2733	U2635	U2540	U2438		U2226					
A2814	U2734	U2636	U2541	U2439		U2227					
A2815	U2735	U2637	U2542	U2440		U2228					
A2816	U2736	U2638	U2543	U2441		U2229					
A2817	U2737	U2639	U2544	U2442		U2230					
A2818	U2738	U2640	U2545	U2443		U2231					
A2819	U2739	U2641	U2546	U2444		U2232					
A2820	U2740	U2642	U2547	U2445		U2233					
A2821	U2741	U2643	U2548	U2446		U2234					
A2822	U2742	U2644	U2549	U2447		U2235					
A2823	U2743	U2645	U2550	U2448		U2236					
A2824	U2744	U2646	U2551	U2449		U2237					
A2825	U2745	U2647	U2552	U2450		U2238					
A2826	U2746	U2648	U2553	U2451		U2239					
A2827	U2747	U2649	U2554	U2452		U2240					
A2828	U2748	U2650	U2555	U2453		U2241					
A2829	U2749	U2651	U2556	U2454		U2242					
A2830	U2750	U2652	U2557	U2455		U2243					
A2831	U2751	U2653	U2558	U2456		U2244					
A2832	U2752	U2654	U2559	U2457		U2245					
A2833	U2753	U2655	U2560	U2458		U2246					
A2834	U2754	U2656	U2561	U2459		U2247					
A2835	U2755	U2657	U2562	U2460		U2248					
A2836	U2756	U2658	U2563	U2461		U2249					
A2837	U2757	U2659	U2564	U2462		U2250					
A2838	U2758	U2660	U2565	U2463		U2251					
A2839	U2759	U2661	U2566	U2464		U2252					
A2840	U2760	U2662	U2567	U2465		U2253					
A2841	U2761	U2663	U2568	U2466		U2254					
A2842	U2762	U2664	U2569	U2467		U2255					
A2843	U2763	U2665	U2570	U2468		U2256					
A2844	U2764	U2666	U2571	U2469		U2257					
A2845	U2765	U2667	U2572	U2470		U2258					
A2846	U2766	U2668	U2573	U2471		U2259					
A2847	U2767	U2669	U2574	U2472		U2260					
A2848	U2768	U2670	U2575	U2473		U2261					
A2849	U2769	U2671	U2576	U2474		U2262					
A2850	U2770	U2672	U2577	U2475		U2263					
A2851	U2771	U2673	U2578	U2476		U2264					
A2852	U2772	U2674	U2579	U2477		U2265					
A2853	U2773	U2675	U2580	U2478		U2266					
A2854	U2774	U2676	U2581	U2479		U2267					
A2855	U2775	U2677	U2582	U2480		U2268					
A2856	U2776	U2678	U2583	U2481		U2269					
A2857	U2777	U2679	U2584	U2482		U2270					
A2858	U2778	U2680	U2585	U2483		U2271					
A2859	U2779	U2681	U2586	U2484		U2272					
A2860	U2780	U2682	U2587	U2485		U2273					
A2861	U2781	U2683	U2588	U2486		U2274					
A2862	U2782	U2684	U2589	U2487		U2275					
A2863	U2783	U2685	U2590	U2488		U2276					
A2864	U2784	U2686	U2591	U2489		U2277					
A2865	U2785	U2687	U2592	U2490		U2278					
A2866	U2786	U2688	U2593	U2491		U2279					
A2867	U2787	U2689	U2594	U2492		U2280					
A2868	U2788	U2690	U2595	U2493		U2281					



● Molecule 31: Apidaecins type 22



● Molecule 31: Apidaecins type 22



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41476	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46.2	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.850	Depositor
Minimum map value	-0.385	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	399.6, 399.6, 399.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.332, 1.332, 1.332	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.12	0/450	0.25	0/599
2	1	0.07	0/416	0.19	0/554
3	2	0.11	0/380	0.18	0/498
4	3	0.07	0/513	0.19	0/676
5	4	0.12	0/303	0.18	0/397
6	B	0.07	0/2876	0.19	0/4483
7	C	0.09	0/2121	0.24	0/2852
8	D	0.09	0/1586	0.20	0/2134
9	E	0.10	0/1571	0.21	0/2113
10	F	0.10	0/1434	0.25	0/1926
11	G	0.09	0/1343	0.20	0/1816
12	H	0.10	0/1122	0.22	0/1515
13	J	0.09	0/1152	0.19	0/1551
14	K	0.09	0/947	0.22	0/1268
15	L	0.09	0/1054	0.27	0/1403
16	M	0.09	0/1093	0.20	0/1460
17	N	0.12	0/973	0.29	0/1301
18	O	0.07	0/902	0.20	0/1209
19	P	0.09	0/929	0.19	0/1242
20	Q	0.10	0/960	0.21	0/1278
21	R	0.10	0/829	0.22	0/1107
22	S	0.10	0/875	0.21	0/1170
23	T	0.28	0/744	0.41	0/994
24	U	0.10	0/787	0.24	0/1051
25	V	0.10	0/766	0.20	0/1025
26	W	0.07	0/582	0.20	0/769
27	X	0.10	0/635	0.19	0/848
28	Y	0.11	0/510	0.19	0/677
29	Z	0.11	0/453	0.19	0/605
30	A	0.07	0/69755	0.20	2/108820 (0.0%)
31	y	0.15	0/155	0.38	0/212
31	z	0.09	0/155	0.26	0/212
All	All	0.08	0/98371	0.21	2/147765 (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
23	T	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	1913	A	OP1-P-O3'	-8.77	81.70	108.00
30	A	1913	A	OP2-P-O3'	-8.31	83.07	108.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	T	73	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	444	0	461	7	0
2	1	409	0	440	5	0
3	2	377	0	418	4	0
4	3	504	0	574	11	0
5	4	302	0	343	6	0
6	B	2572	0	1302	22	0
7	C	2082	0	2157	33	0
8	D	1565	0	1616	22	0
9	E	1552	0	1619	39	0
10	F	1410	0	1447	31	0
11	G	1323	0	1374	10	0
12	H	1111	0	1148	12	0
13	J	1129	0	1162	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	K	938	0	1012	11	0
15	L	1045	0	1117	28	0
16	M	1074	0	1157	12	0
17	N	960	0	1000	13	0
18	O	892	0	923	14	0
19	P	917	0	965	17	0
20	Q	947	0	1022	24	0
21	R	816	0	839	8	0
22	S	868	0	934	15	0
23	T	738	0	807	11	0
24	U	779	0	834	12	0
25	V	753	0	780	16	0
26	W	575	0	592	10	0
27	X	625	0	655	8	0
28	Y	509	0	543	7	0
29	Z	449	0	491	10	0
30	A	62281	0	31323	620	0
31	y	148	0	152	40	0
31	z	148	0	150	57	0
All	All	90242	0	59357	904	0

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

The worst 5 of 904 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)
30:A:2505:G:N1	31:z:15:HIS:CD2	2.15	1.13
30:A:1321:A:H1'	31:y:15:HIS:O	1.49	1.13
30:A:2505:G:C6	31:z:15:HIS:CE1	2.34	1.12
30:A:508:A:C8	31:y:13:PRO:HB3	1.86	1.09
30:A:1321:A:C8	31:y:16:PRO:HA	1.92	1.04

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
2	1	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
3	2	44/46 (96%)	44 (100%)	0	0	100	100
4	3	62/64 (97%)	60 (97%)	1 (2%)	1 (2%)	7	28
5	4	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
7	C	269/271 (99%)	258 (96%)	11 (4%)	0	100	100
8	D	207/209 (99%)	196 (95%)	11 (5%)	0	100	100
9	E	199/201 (99%)	192 (96%)	6 (3%)	1 (0%)	24	54
10	F	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
11	G	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
12	H	147/149 (99%)	140 (95%)	7 (5%)	0	100	100
13	J	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
14	K	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
15	L	141/143 (99%)	132 (94%)	9 (6%)	0	100	100
16	M	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
17	N	118/120 (98%)	109 (92%)	9 (8%)	0	100	100
18	O	114/116 (98%)	113 (99%)	1 (1%)	0	100	100
19	P	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
20	Q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
21	R	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	12	39
22	S	109/110 (99%)	105 (96%)	4 (4%)	0	100	100
23	T	91/93 (98%)	88 (97%)	3 (3%)	0	100	100
24	U	100/102 (98%)	89 (89%)	11 (11%)	0	100	100
25	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
26	W	73/75 (97%)	69 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	X	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
28	Y	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
29	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
31	y	15/17 (88%)	12 (80%)	3 (20%)	0	100	100
31	z	15/17 (88%)	15 (100%)	0	0	100	100
All	All	3197/3256 (98%)	3076 (96%)	118 (4%)	3 (0%)	49	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	R	54	VAL
9	E	83	VAL
4	3	31	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/47 (100%)	45 (96%)	2 (4%)	26	55
2	1	45/45 (100%)	45 (100%)	0	100	100
3	2	38/38 (100%)	37 (97%)	1 (3%)	40	65
4	3	51/51 (100%)	50 (98%)	1 (2%)	48	69
5	4	34/34 (100%)	34 (100%)	0	100	100
7	C	216/216 (100%)	216 (100%)	0	100	100
8	D	164/164 (100%)	164 (100%)	0	100	100
9	E	165/165 (100%)	162 (98%)	3 (2%)	51	70
10	F	148/148 (100%)	146 (99%)	2 (1%)	59	73
11	G	137/137 (100%)	136 (99%)	1 (1%)	76	80
12	H	114/114 (100%)	114 (100%)	0	100	100
13	J	116/116 (100%)	115 (99%)	1 (1%)	70	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	K	103/103 (100%)	103 (100%)	0	100	100
15	L	102/102 (100%)	100 (98%)	2 (2%)	48	69
16	M	109/109 (100%)	108 (99%)	1 (1%)	70	78
17	N	100/100 (100%)	98 (98%)	2 (2%)	48	69
18	O	86/86 (100%)	85 (99%)	1 (1%)	63	75
19	P	99/99 (100%)	97 (98%)	2 (2%)	48	69
20	Q	89/89 (100%)	88 (99%)	1 (1%)	65	76
21	R	84/84 (100%)	84 (100%)	0	100	100
22	S	94/93 (101%)	93 (99%)	1 (1%)	65	76
23	T	80/80 (100%)	79 (99%)	1 (1%)	61	74
24	U	83/83 (100%)	83 (100%)	0	100	100
25	V	78/78 (100%)	77 (99%)	1 (1%)	61	74
26	W	57/57 (100%)	57 (100%)	0	100	100
27	X	67/67 (100%)	67 (100%)	0	100	100
28	Y	55/55 (100%)	54 (98%)	1 (2%)	51	70
29	Z	48/48 (100%)	48 (100%)	0	100	100
31	y	17/17 (100%)	15 (88%)	2 (12%)	5	20
31	z	17/17 (100%)	17 (100%)	0	100	100
All	All	2643/2642 (100%)	2617 (99%)	26 (1%)	65	77

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	N	20	MET
19	P	23	ASP
31	y	6	VAL
18	O	35	ILE
19	P	113	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
23	T	72	GLN
24	U	52	ASN
31	y	3	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	X	5	GLN
24	U	44	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	A	2897/2904 (99%)	462 (15%)	18 (0%)
6	B	119/120 (99%)	14 (11%)	2 (1%)
All	All	3016/3024 (99%)	476 (15%)	20 (0%)

5 of 476 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	B	4	C
6	B	9	G
6	B	12	C
6	B	13	G
6	B	24	G

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	A	1663	G
30	A	2326	C
30	A	2808	G
30	A	2655	G
30	A	549	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

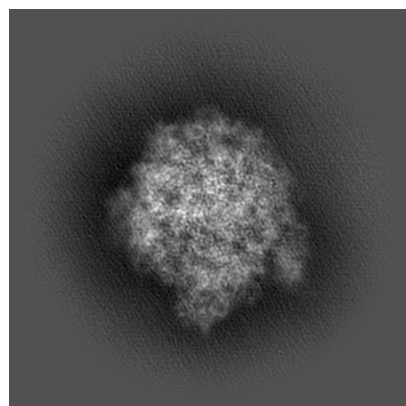
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51978. These allow visual inspection of the internal detail of the map and identification of artifacts.

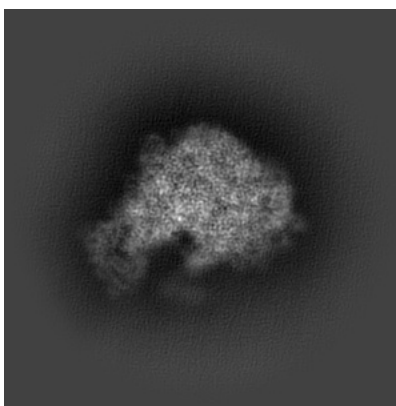
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

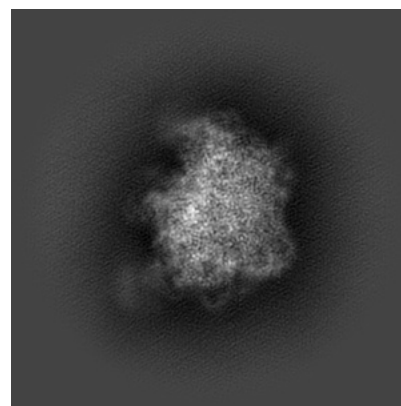
6.1.1 Primary map



X

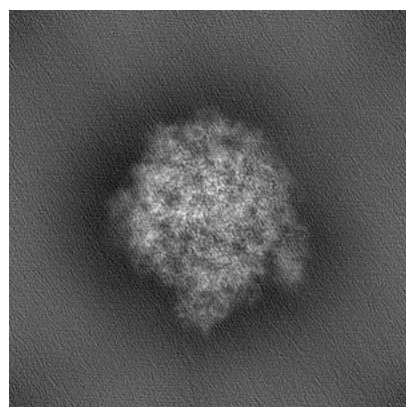


Y

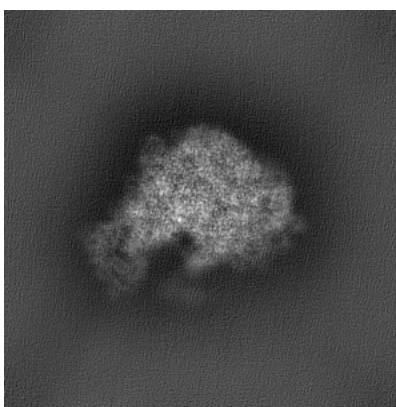


Z

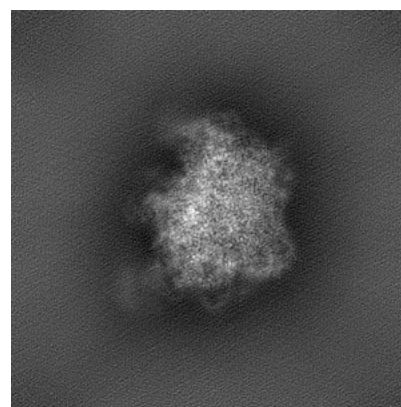
6.1.2 Raw map



X



Y

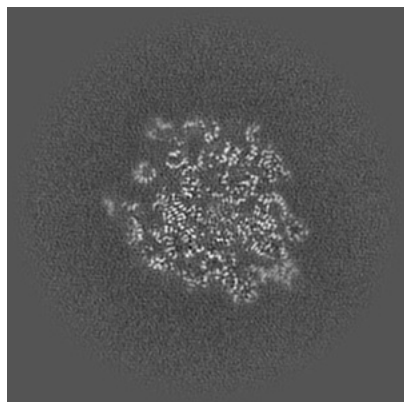


Z

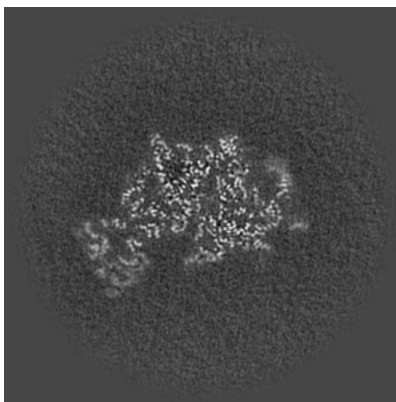
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

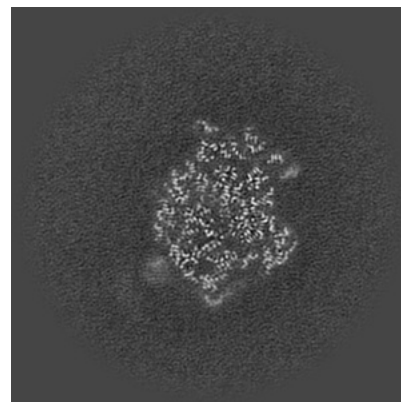
6.2.1 Primary map



X Index: 150

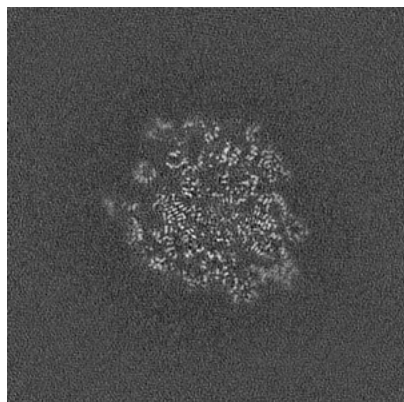


Y Index: 150

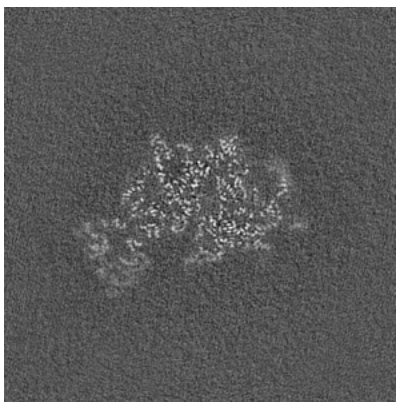


Z Index: 150

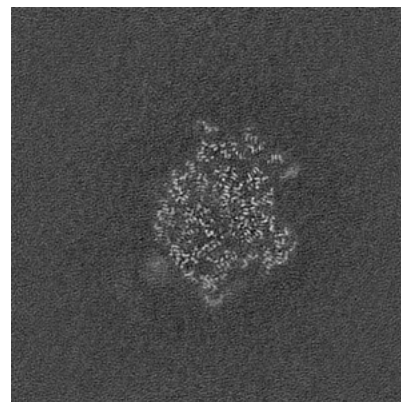
6.2.2 Raw map



X Index: 150



Y Index: 150

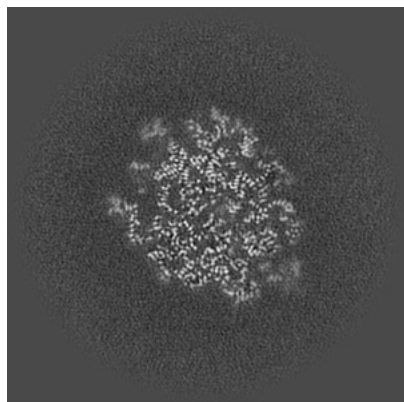


Z Index: 150

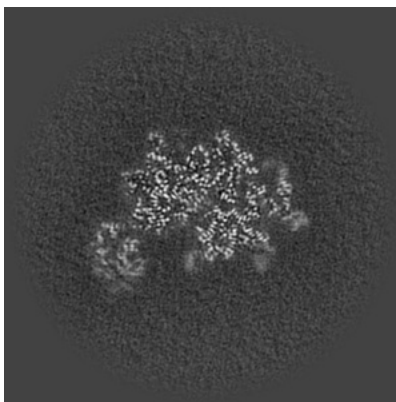
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

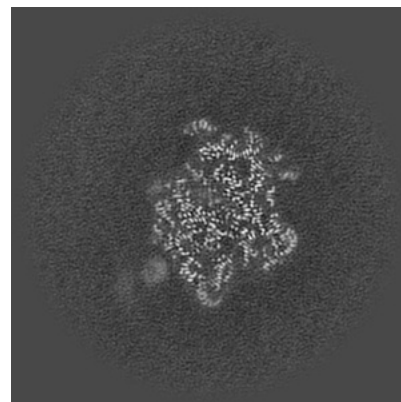
6.3.1 Primary map



X Index: 145

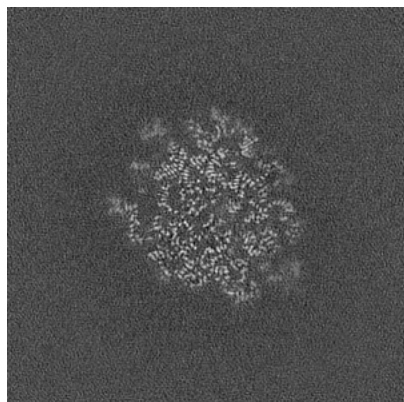


Y Index: 155

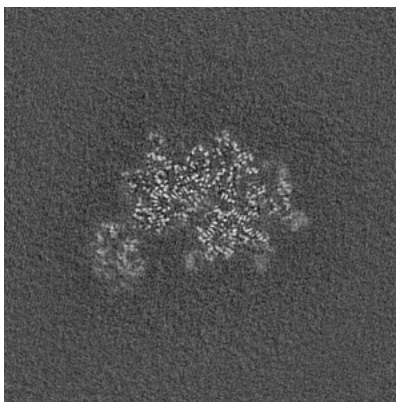


Z Index: 147

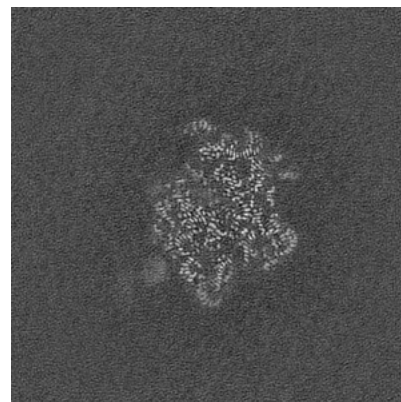
6.3.2 Raw map



X Index: 145



Y Index: 155

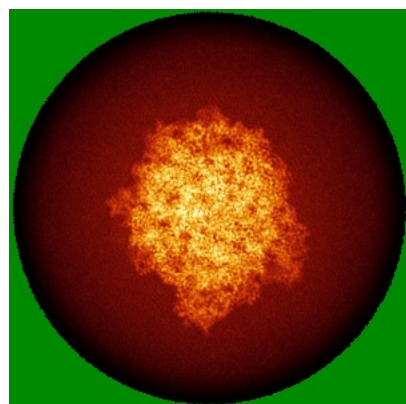


Z Index: 147

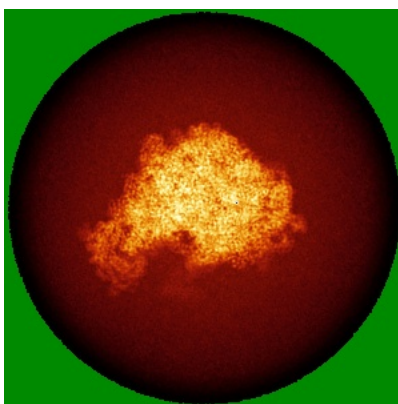
The images above show the largest variance slices of the map in three orthogonal directions.

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

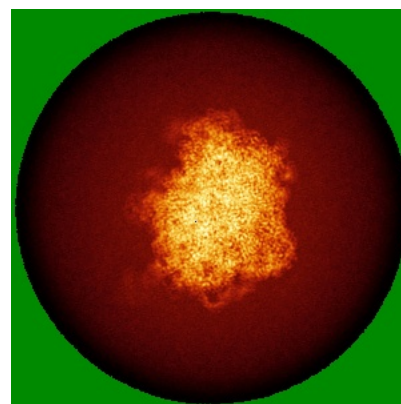
6.4.1 Primary map



X

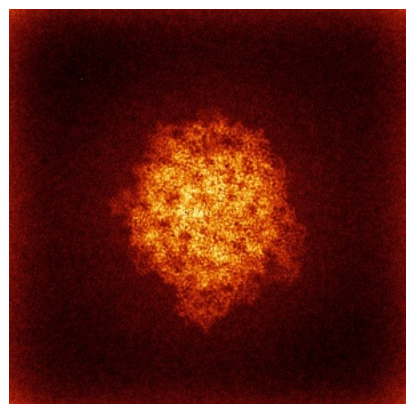


Y

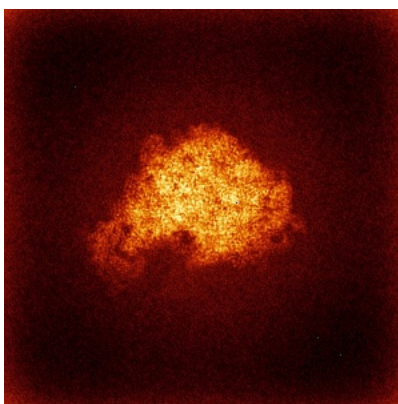


Z

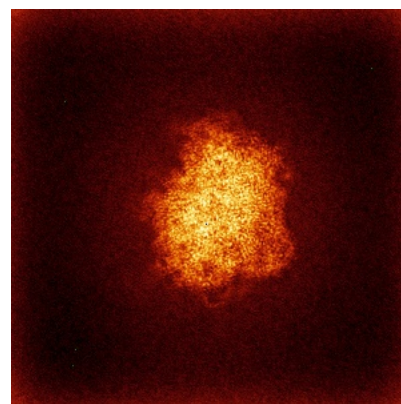
6.4.2 Raw map



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.

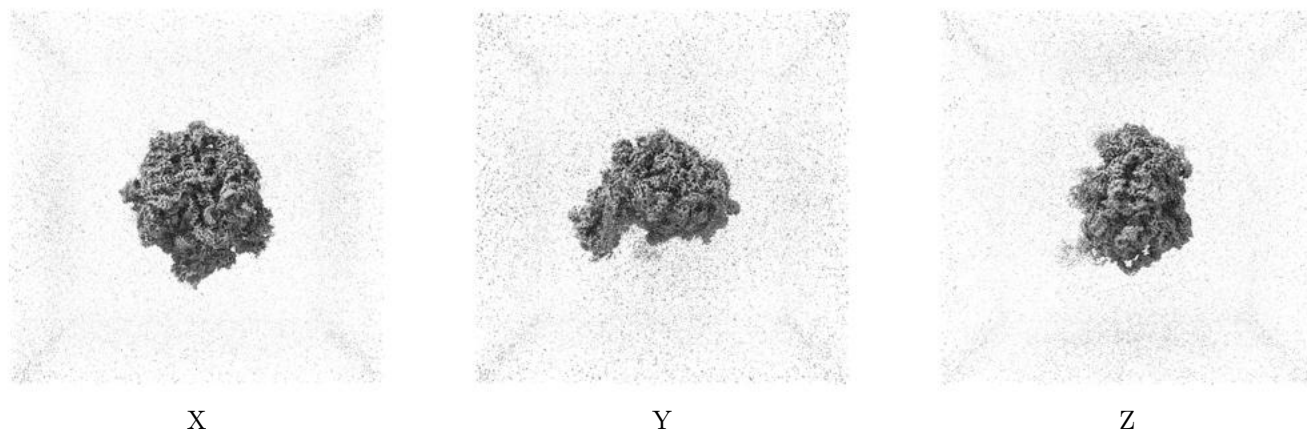
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

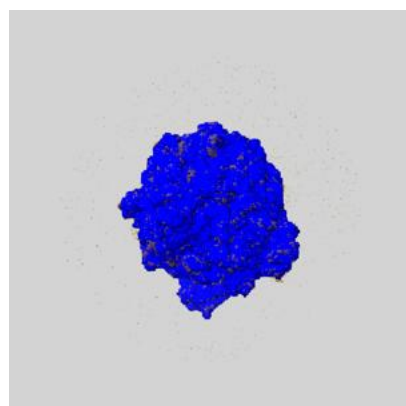
6.6 Mask visualisation [i](#)

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

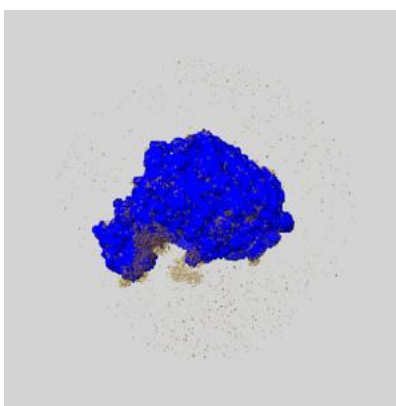
A mask typically either:

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

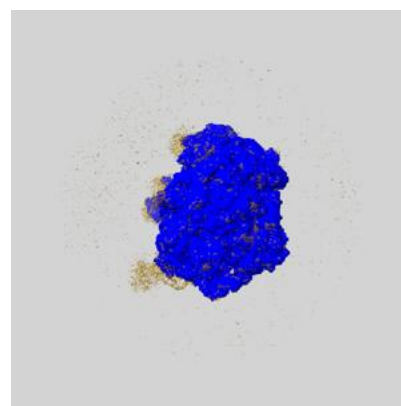
6.6.1 emd_51978_msk_1.map [i](#)



X



Y

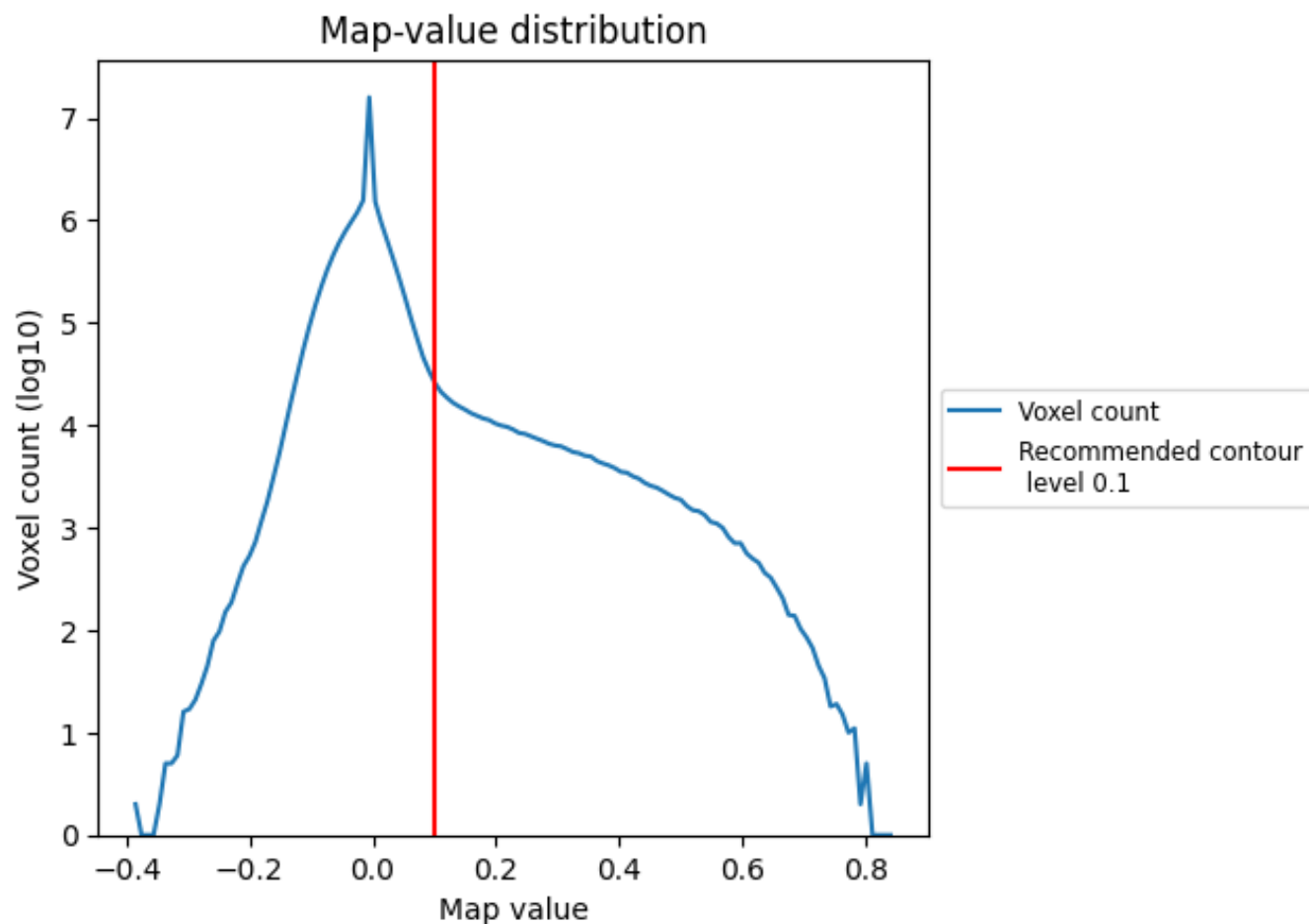


Z

7 Map analysis [i](#)

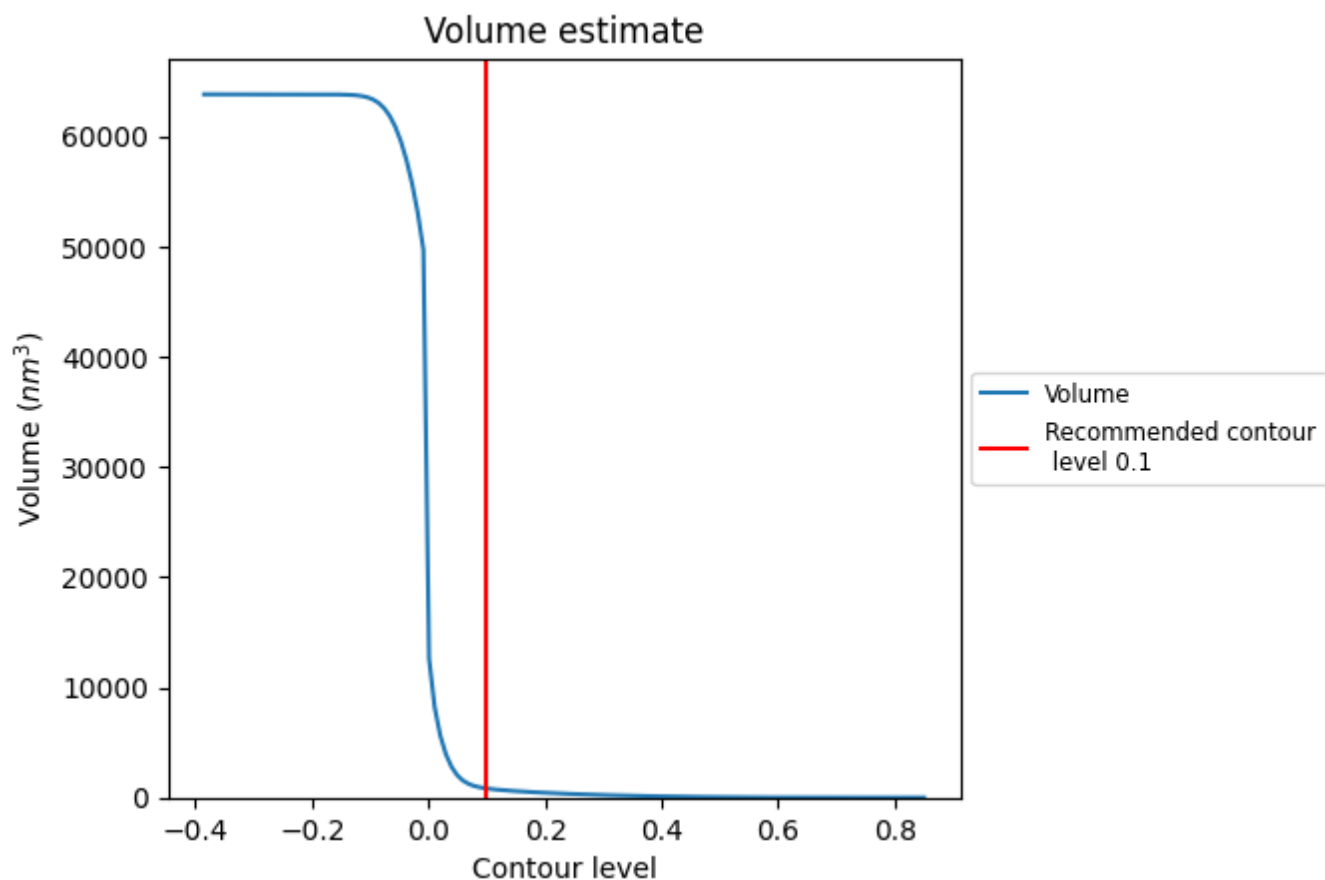
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

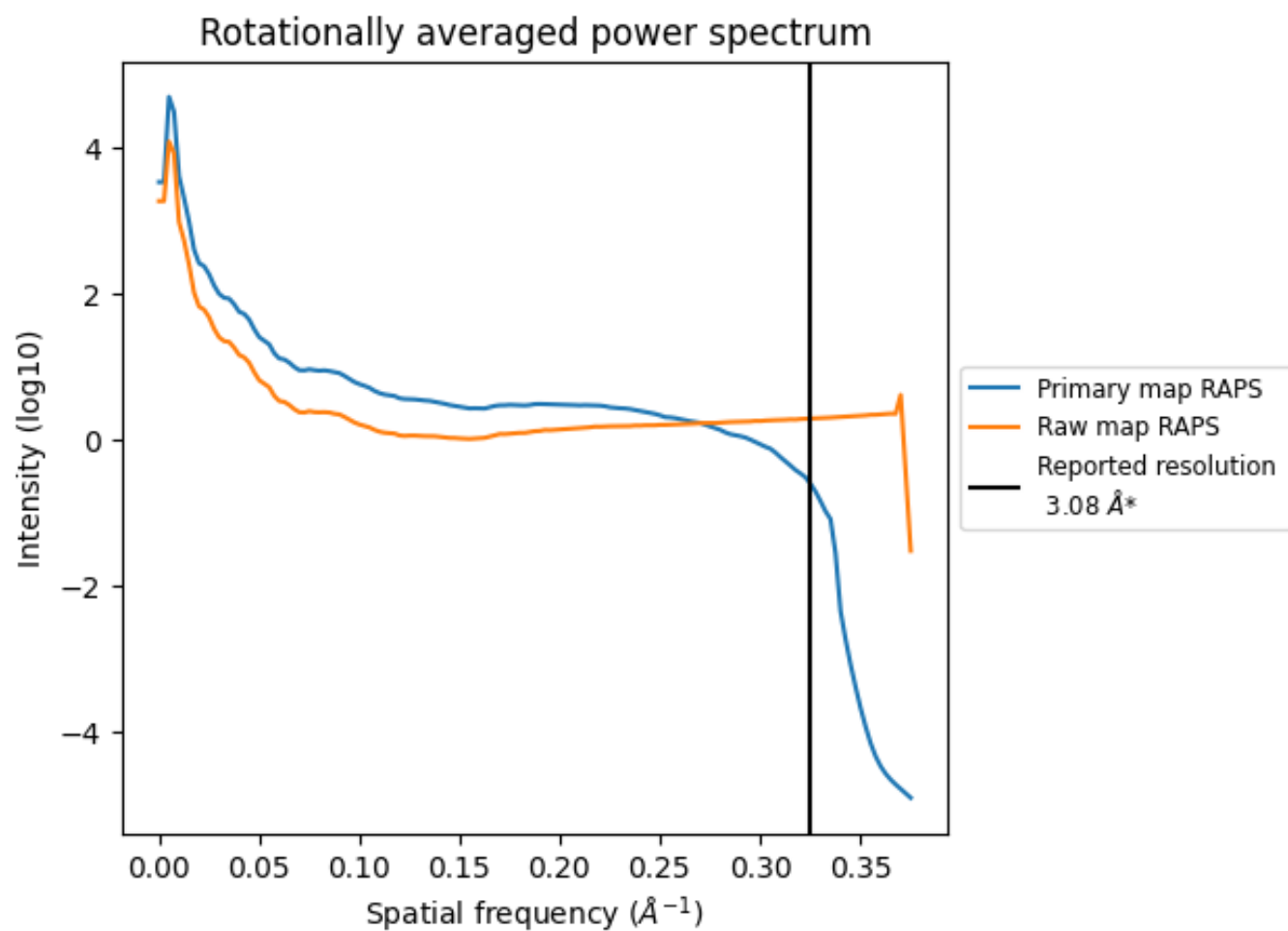
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 824 nm³; this corresponds to an approximate mass of 744 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 ⓘ

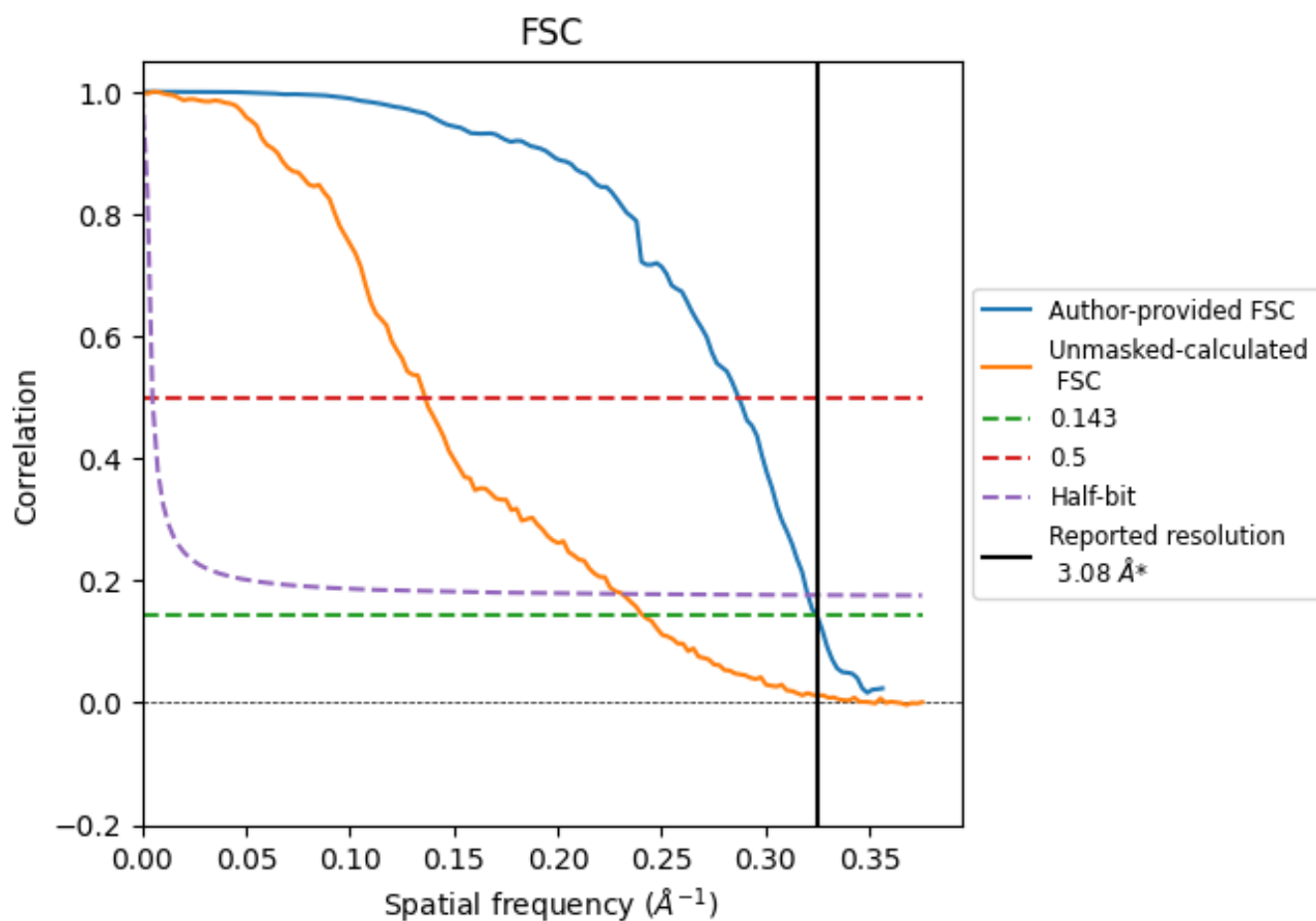


*Reported resolution corresponds to spatial frequency of 0.325 Å⁻¹

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 0.325 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

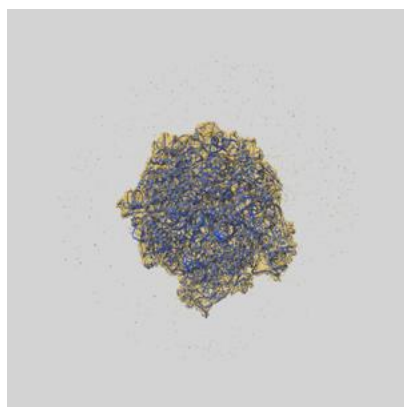
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	3.08	3.48	3.12
Unmasked-calculated*	4.15	7.34	4.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 3.08 by more than 10 %

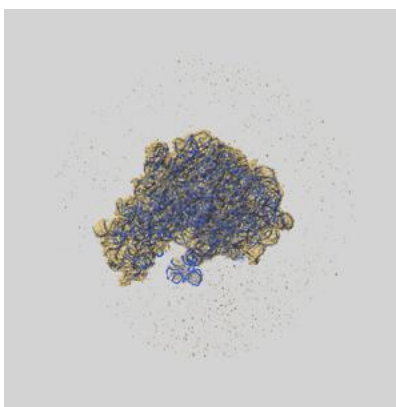
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51978 and PDB model 9HA6. Per-residue inclusion information can be found in section [3](#) on page [10](#).

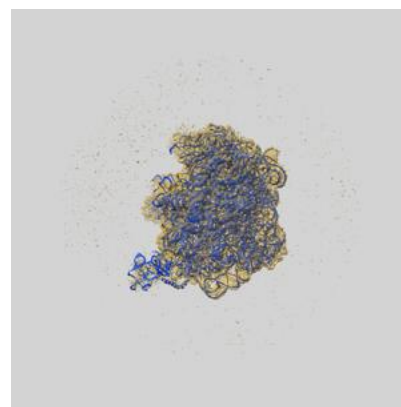
9.1 Map-model overlay [i](#)



X



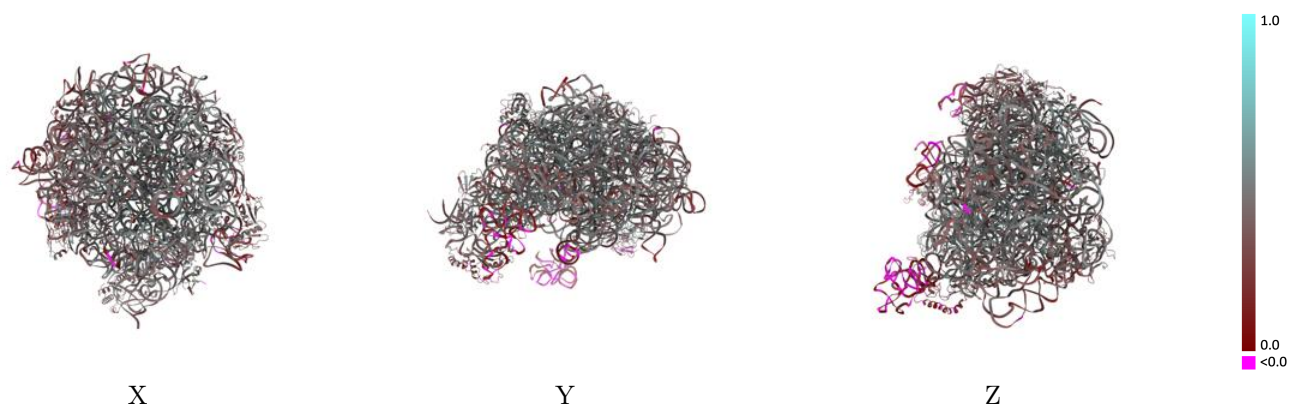
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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](#)

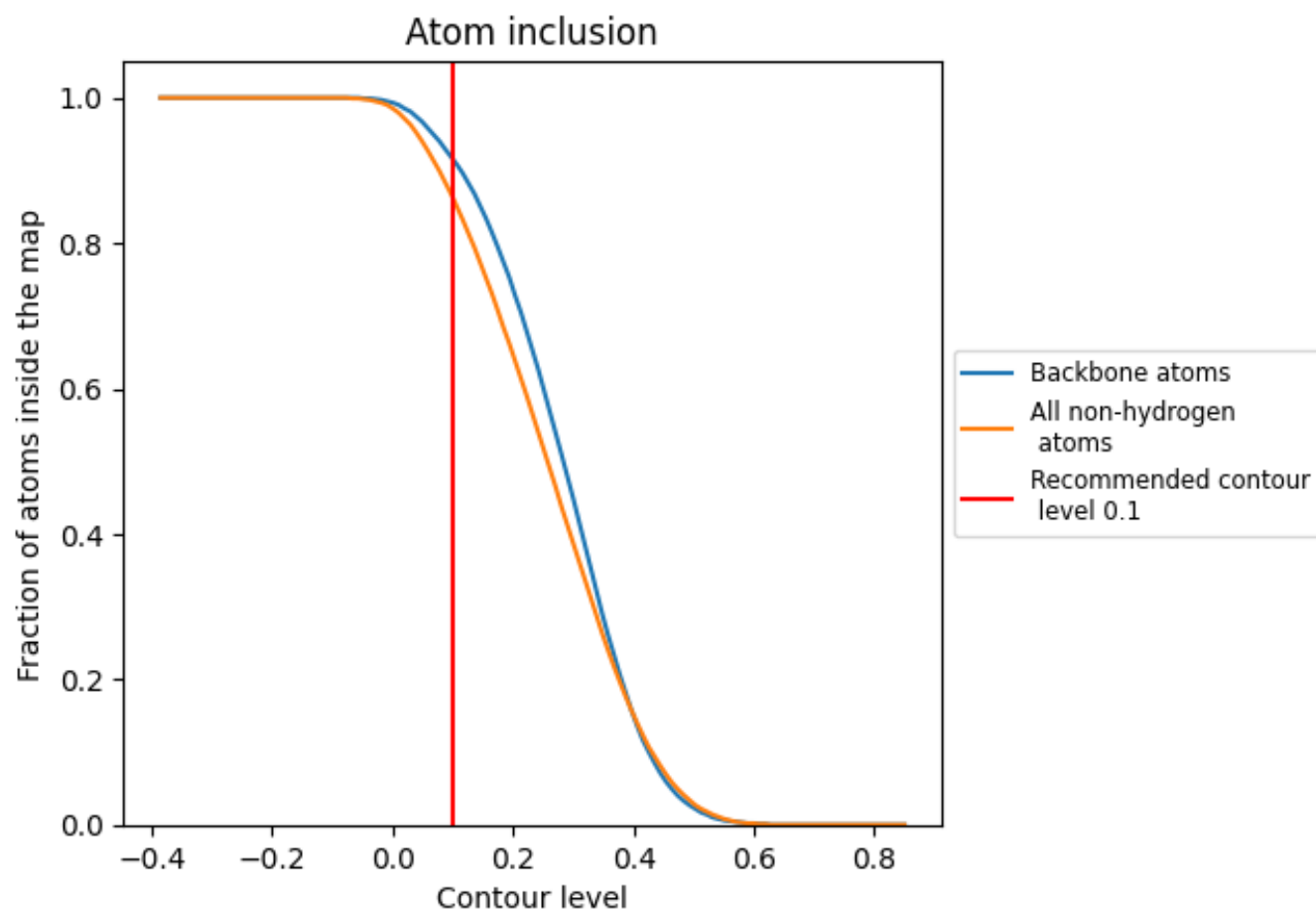


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 86% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8630	 0.4120
0	 0.8670	 0.4750
1	 0.6680	 0.4040
2	 0.8900	 0.4910
3	 0.8530	 0.4570
4	 0.7840	 0.4130
A	 0.8950	 0.4150
B	 0.9310	 0.4110
C	 0.8560	 0.4680
D	 0.8220	 0.4430
E	 0.7800	 0.3860
F	 0.6700	 0.2910
G	 0.7310	 0.3400
H	 0.2230	 0.1780
J	 0.8640	 0.4700
K	 0.7340	 0.3650
L	 0.8030	 0.4030
M	 0.8370	 0.4500
N	 0.8620	 0.4520
O	 0.7970	 0.3850
P	 0.7340	 0.3880
Q	 0.8810	 0.4770
R	 0.8180	 0.4260
S	 0.8460	 0.4630
T	 0.8100	 0.4360
U	 0.7900	 0.3910
V	 0.8280	 0.4170
W	 0.8610	 0.4820
X	 0.8550	 0.4540
Y	 0.7470	 0.3460
Z	 0.8120	 0.4540
y	 0.4100	 0.2240
z	 0.4460	 0.3410

