



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 07:47 AM UTC

PDB ID : 8XZ3 / pdb_00008xz3
EMDB ID : EMD-38788
Title : Mycobacterium smegmatis 50S ribosomal subunit with Erythromycin
Authors : Srinivasan, K.; Banerjee, A.; Sengupta, J.
Deposited on : 2024-01-20
Resolution : 3.60 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:

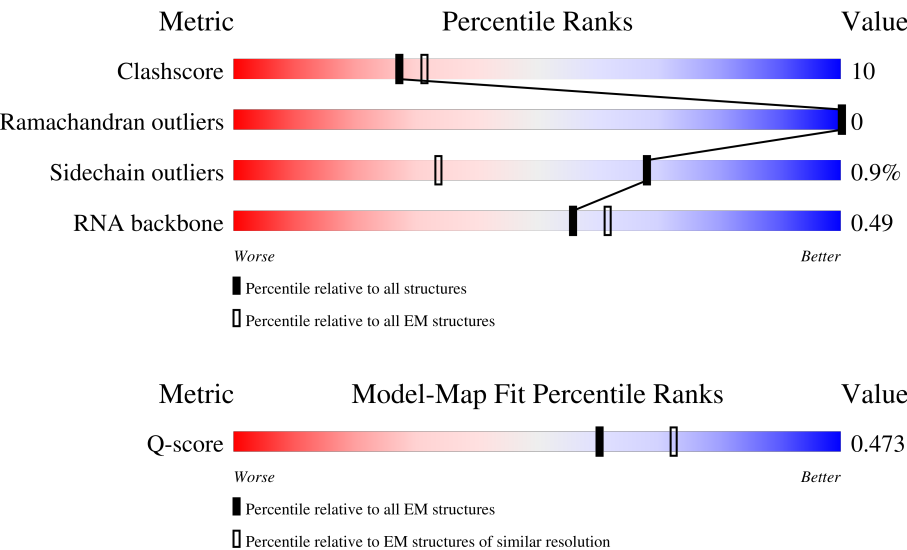
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	3	23	65%35%
2	A	3119	5% 51%40%9%
3	B	118	54%40%6%

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Mol	Chain	Length	Quality of chain
4	C	275	
5	D	214	
6	E	209	
7	F	182	
8	G	176	
9	H	151	
10	I	126	
11	J	133	
12	K	146	
13	L	122	
14	M	145	
15	N	136	
16	O	118	
17	P	126	
18	Q	113	
19	R	124	
20	S	100	
21	T	114	
22	U	97	
23	V	105	
24	W	192	
25	X	79	
26	Y	63	
27	Z	64	
28	a	59	

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Mol	Chain	Length	Quality of chain
29	b	54	 85% 15%
30	c	49	 88% 12%
31	d	46	 70% 30%
32	e	63	 5% 71% 29%
33	f	37	 81% 19%
34	g	48	 25% 63% 38%

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 97741 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein bL37.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	3	23	Total	C	N	O	0	0
			189	111	50	28		

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	3119	Total	C	N	O	P	1	0
			67003	29864	12318	21701	3120		

- Molecule 3 is a RNA chain called 5S rRNA.

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

- Molecule 4 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 6 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 8 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 9 is a protein called 50S ribosomal protein L9.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL10.

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

- Molecule 11 is a protein called Large ribosomal subunit protein uL11.

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

- Molecule 12 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 13 is a protein called 50S ribosomal protein L14.

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

- Molecule 14 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 15 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 16 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 17 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 18 is a protein called 50S ribosomal protein L19.

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

- Molecule 19 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 20 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 21 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 22 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 23 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 24 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 25 is a protein called Large ribosomal subunit protein bL27.

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

- Molecule 26 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 27 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 28 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 29 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 30 is a protein called Large ribosomal subunit protein bL33A.

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

- Molecule 31 is a protein called Large ribosomal subunit protein bL34.

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

- Molecule 32 is a protein called Large ribosomal subunit protein bL35.

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

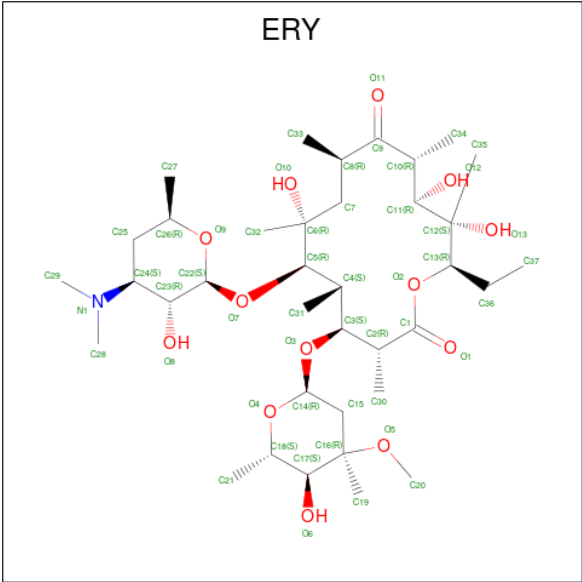
- Molecule 33 is a protein called 50S ribosomal protein L36.

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

- Molecule 34 is a protein called Large ribosomal subunit protein bL31.

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

- Molecule 35 is ERYTHROMYCIN A (CCD ID: ERY) (formula: $C_{37}H_{67}NO_{13}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
35	A	1	51	37	1	13	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.

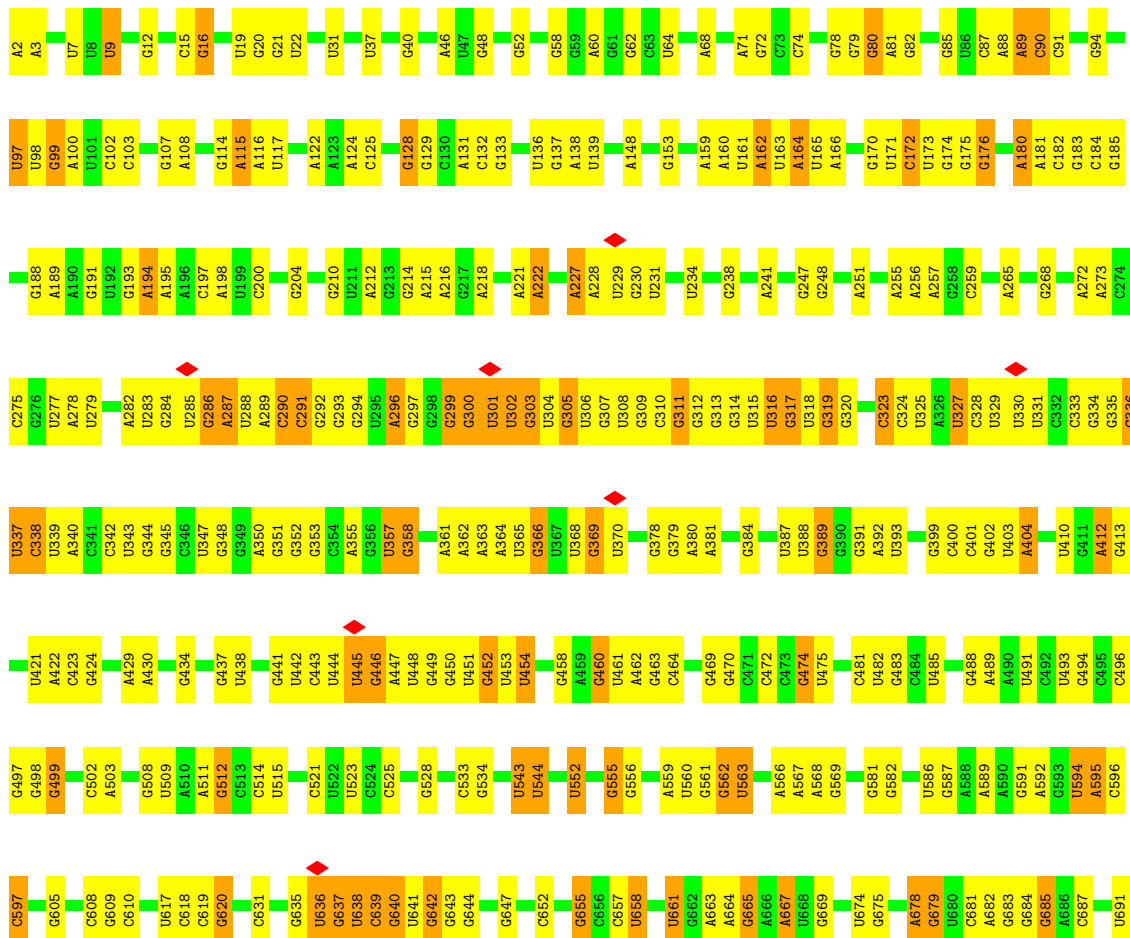
- Molecule 1: 50S ribosomal protein bL37

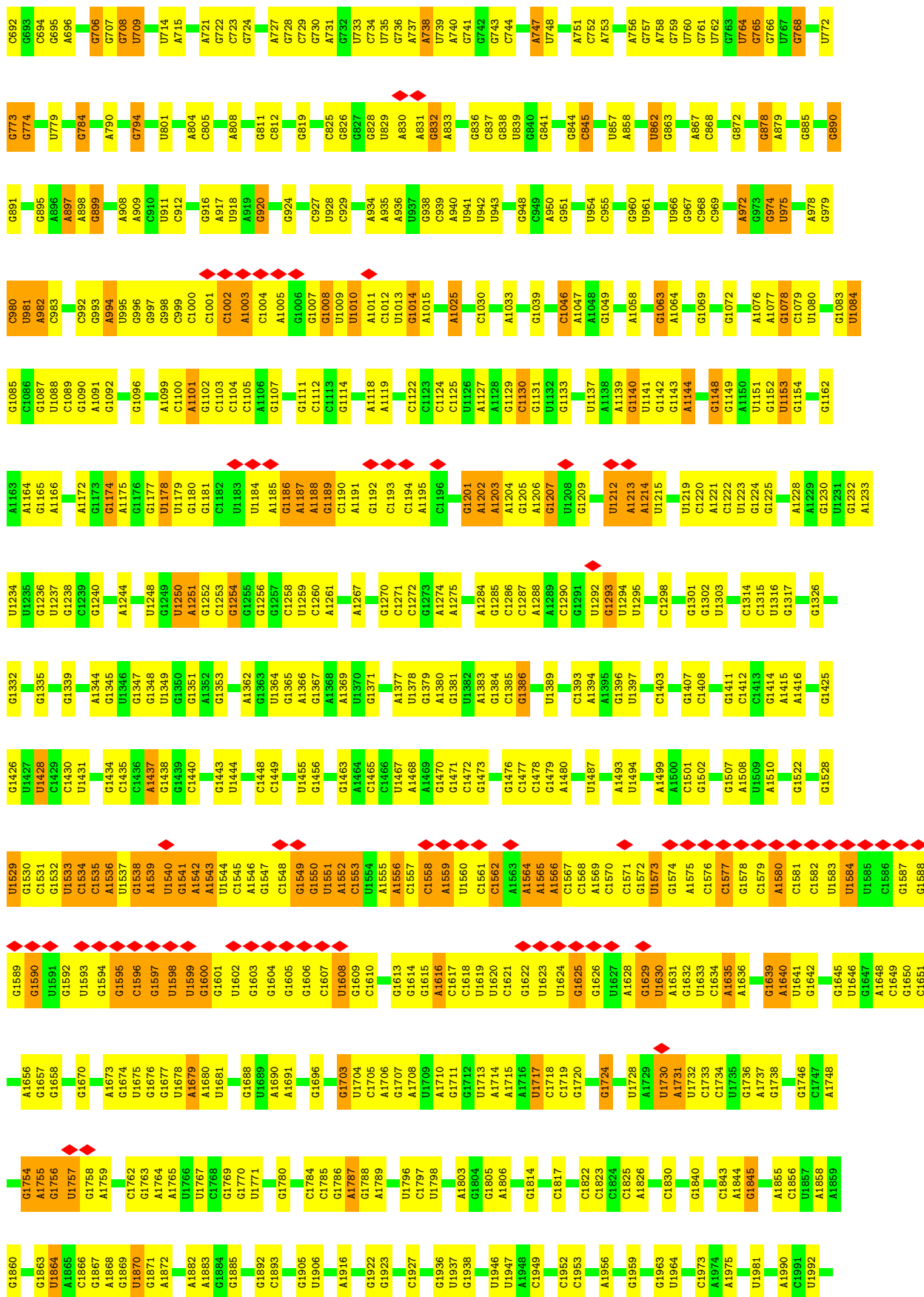
Chain 3: 



- Molecule 2: 23S rRNA

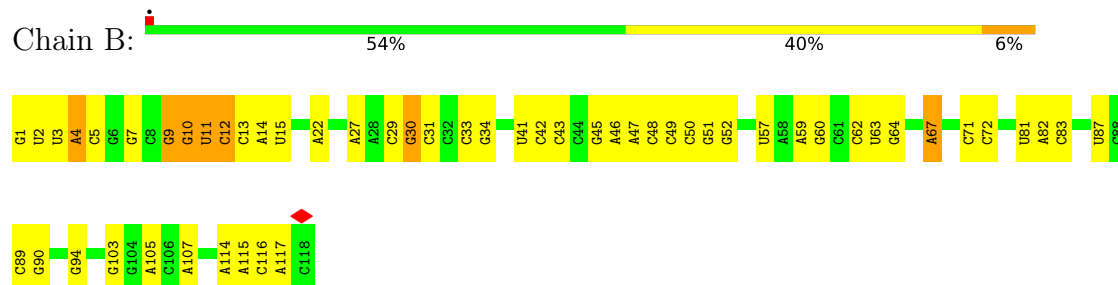
Chain A: 



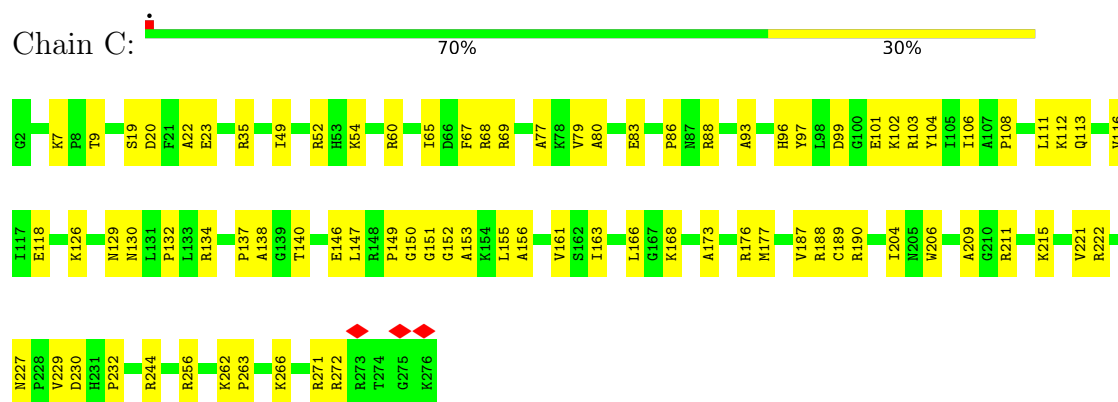


C3105	C3106	G3107	G3111	A3112	A3115	C3116	U3117	U3118	A3119	C3120	U3018	C3019	U3020	A3021	G3022	G3023	A3024	U3029	A3030	A3031	G3032	G3033	C3034	C3035	C3038	A3042	C3046	A3047	A3052	U3053	U3054	G3055	A3056	G3059	A3060	C3066	C3067	U3068	G3069	G3070	A3071	C3074	C3075	A3080	A3081	U3082	G3087	C3088	A3089	A3093	U3096	G3097	G3098	C3013	A3014	C3015	C3016	C3017	A3104
G2827	U2922	C2923	G2830	A2926	G2930	G2933	C2936	G2937	G2938	C2948	A2949	C2950	G2951	G2952	U2953	G2956	A2957	G2961	A2962	U2963	A2964	G2968	C2969	U2970	A2971	G2972	C2973	A2974	U2980	A2981	G2985	G2986	G2987	A2988	C2989	C2997	C2998	A3002	A3005	C3008	U3009	G3010	A3011	C3012	A3013	C3014	C3015	C3016	C3017	A3104									
G2737	U2738	C2739	G2740	A2741	G2742	U2743	C2744	G2747	G2753	G2754	A2755	G2756	C2757	G2758	U2759	G2760	U2761	C2762	C2763	C2764	U2778	G2781	C2782	U2796	U2797	A2798	G2799	U2800	A2801	C2802	C2803	U2804	U2810	A2813	A2814	G2815	G2816	U2817	U2818	G2819	U2820	G2821	A2822	A2826															
G2852	G2853	A2854	U2855	A2856	G2857	U2858	A2859	G2862	U2863	A2864	U2865	G2866	U2867	G2868	C2869	U2870	U2871	A2872	G2873	G2874	U2878	U2886	U2887	G2888	C2889	U2890	G2891	G2894	C2898	C2899	U2900	A2901	A2902	C2903	C2904	C2905	U2908	U2909	G2910	U2911	U2912	U2913	A2914	C2915															
G2831	C2832	U2833	U2837	A2838	U2839	G2842	C2843	C2850	G2851	U2852	C2853	C2859	G2862	A2863	G2864	U2865	A2866	G2867	C2868	G2869	U2870	U2871	A2872	U2873	A2878	G2879	C2883	A2886	G2887	C2888	A2889	C2890	C2891	A2902	C2903	C2904	C2905	U2908	U2909	G2910	U2911	U2912	U2913	A2914	C2915														
U3018	C3019	U3020	A3021	G3022	G3023	A3024	U3029	A3030	A3031	G3032	G3033	C3034	C3035	C3038	A3042	C3046	A3047	A3052	U3053	U3054	G3055	A3056	G3059	A3060	C3066	C3067	U3068	G3069	G3070	A3071	C3074	C3075	A3080	A3081	U3082	G3087	C3088	A3089	A3093	U3096	G3097	G3098	C3013	A3014	C3015	C3016	C3017	A3104											
U1996	A1997	C1998	U1999	A2000	A2001	A2002	A2003	A2004	C2005	A2006	C2007	U2011	C2012	G2013	G2014	U2015	G2016	C2017	G2018	A2019	C2025	A2026	A2029	C2030	G2031	U2032	U2033	U2034	U2035	A2036	G2040	G2041	U2044	G2045	A2046	C2047	G2048	C2049	C2054	C2055	G2056	G2057	U2061	A2064	A2065	G2066	G2067	U2068	U2069	A2070	A2071								
A2151	A2152	G2153	G2154	U2081	U2082	A2083	A2084	C2085	U2086	C2087	C2088	C2089	U2090	U2091	C2092	G2093	G2094	G2095	G2096	C2097	U2098	G2099	A2106	G2107	U2110	U2111	U2112	A2113	A2114	U2115	C2117	A2123	G2128	C2129	G2130	G2131	U2132	G2133	G2134	A2136	A2137	C2138	U2139	A2140	U2141	A2142	A2143	C2144	C2145	A2146	C2148								
A2247	C2248	G2249	G2251	U2252	A2253	A2254	A2255	A2256	A2257	C2262	G2263	U2264	C2265	C2267	G2276	C2279	G2280	A2281	A2282	U2283	A2284	G2285	C2288	C2289	C2290	A2294	C2295	C2296	U2297	U2298	C2299	U2315	G2316	C2320	G2323	A2324	U2325	A2326	C2327	G2328	C2329	U2330	U2331	U2332	G2333	U2334	G2335	U2336	A2337										
G2338	G2339	A2340	U2341	A2342	G2343	U2345	G2346	G2347	G2348	A2349	G2350	A2351	C2352	U2353	G2354	U2355	G2356	A2357	A2358	G2359	C2360	U2361	C2362	A2363	C2364	A2365	C2366	G2367	C2368	C2369	A2370	G2371	U2372	U2373	U2374	G2375	G2376	G2377	U2378	G2379	C2380	A2381	C2382	U2383	C2384	U2385	U2386	U2387	G2388	U2389	U2390	G2391	A2392	A2393	A2394	U2395	A2396	C2397	
C2398	A2399	U2400	U2401	C2402	U2403	G2404	C2407	G2408	U2409	U2410	A2411	U2412	G2413	C2419	U2420	A2421	C2423	C2424	U2425	C2426	G2427	C2431	U2432	U2433	A2434	U2435	A2436	U2443	C2444	G2447	G2448	A2449	G2454	G2462	G2463	U2467	A2470	A2471	C2472	U2473	G2474	G2475	U2482	G2483	C2484	C2485	C2488												
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G2652	G2653	A2654	U2655	A2659	A2663	C2664	C2665	C2667	G2668	A2672	G2677	U2678	G2679	C2680	U2681	U2686	U2687	G2688	C2689	U2690	A2691	G2694	C2698	C2699	U2700	A2701	A2702	G2705	G2709	U2715	G2718	G2719	C2720	A2721	C2722	C2723	U2724	G2725	G2726	A2727	U2728	G2729	U2730	G2731	G2732	C2736													
G2737	U2738	C2739	G2740	A2741	G2742	U2743	C2744	G2747	G2753	G2754	A2755	G2756	C2757	G2758	U2759	G2760	U2761	C2762	C2763	C2764	U2778	G2781	C2782	U2796	U2797	A2798	G2799	U2800	A2801	C2802	C2803	U2804	U2810	A2813	A2814	G2815	G2816	U2817	U2818	G2819	U2820	G2821	A2822	A2826															
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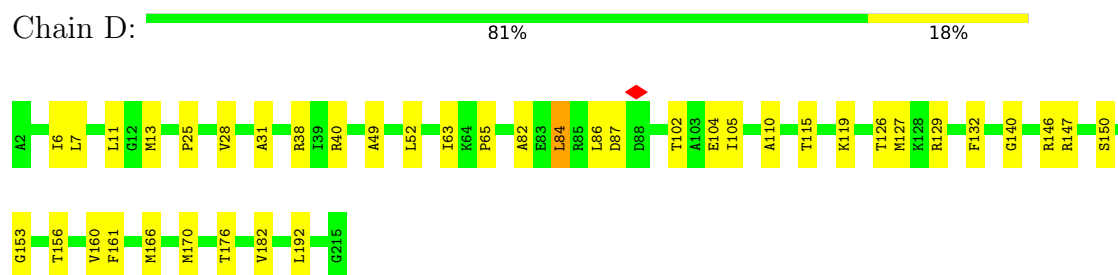
- Molecule 3: 5S rRNA



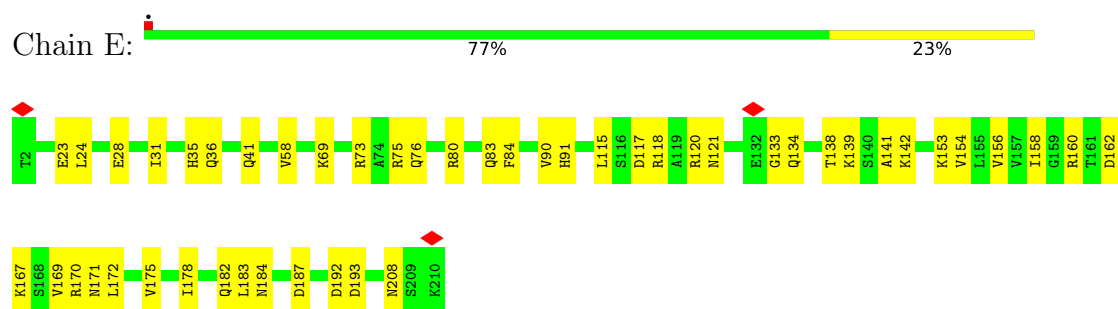
- Molecule 4: Large ribosomal subunit protein uL2



- Molecule 5: Large ribosomal subunit protein uL3

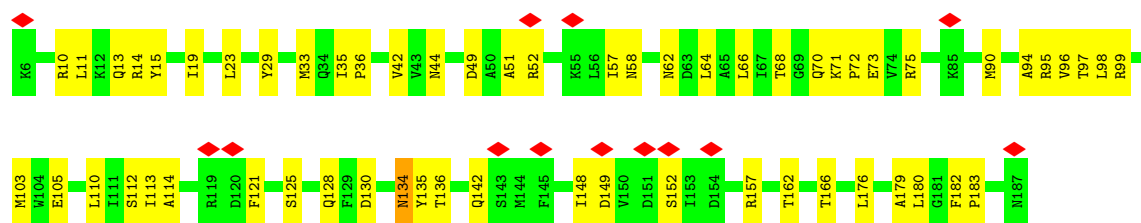


- Molecule 6: Large ribosomal subunit protein uL4

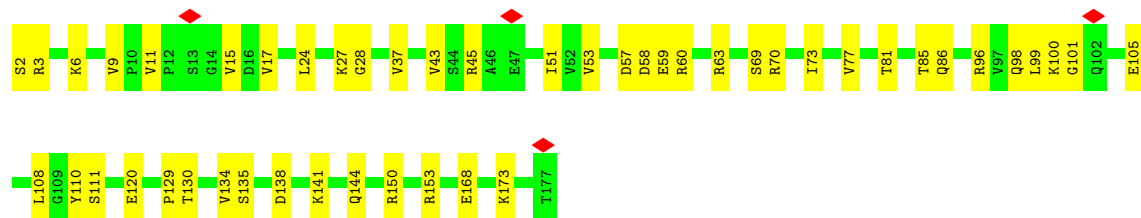
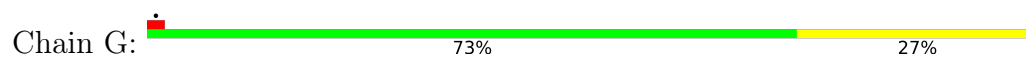


- Molecule 7: Large ribosomal subunit protein uL5

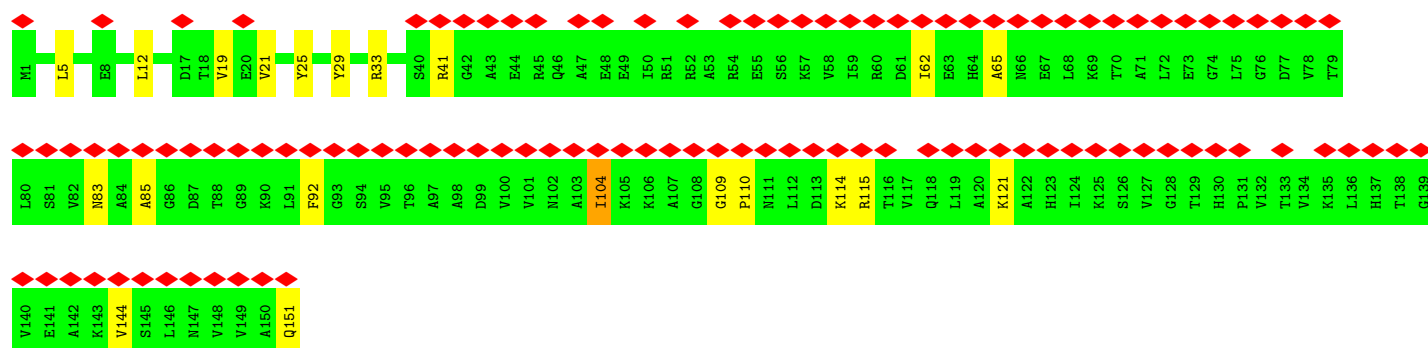
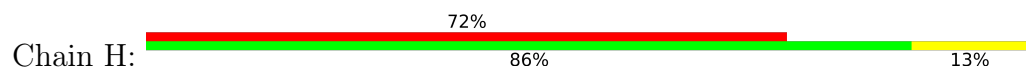




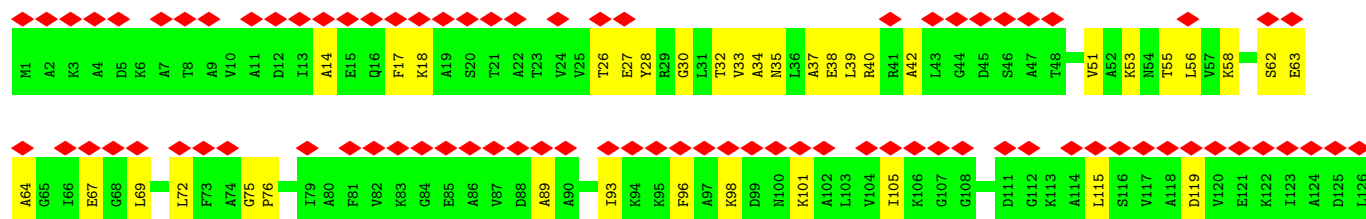
- Molecule 8: Large ribosomal subunit protein uL6



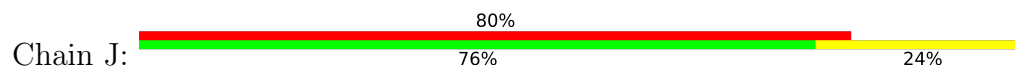
- Molecule 9: 50S ribosomal protein L9

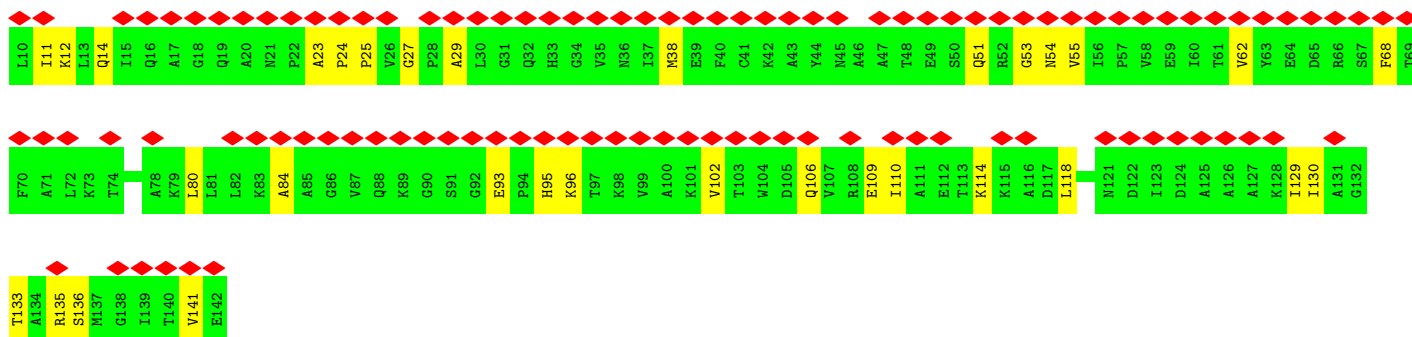


- Molecule 10: Large ribosomal subunit protein uL10



- Molecule 11: Large ribosomal subunit protein uL11





- Molecule 12: Large ribosomal subunit protein uL13

Chain K: 79% 21%



- Molecule 13: 50S ribosomal protein L14

Chain L: 73% 27%



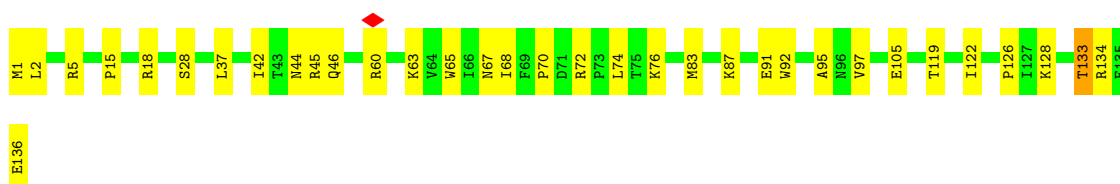
- Molecule 14: Large ribosomal subunit protein uL15

Chain M: 79% 20%



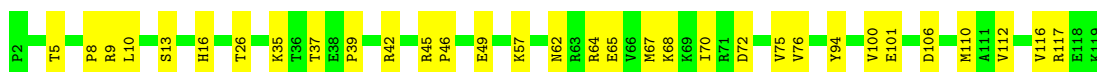
- Molecule 15: Large ribosomal subunit protein uL16

Chain N: 75% 24%

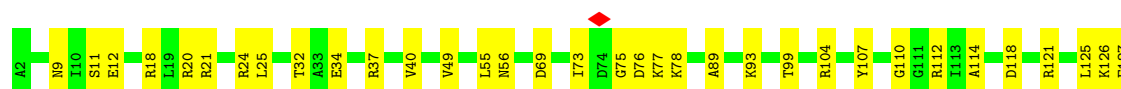
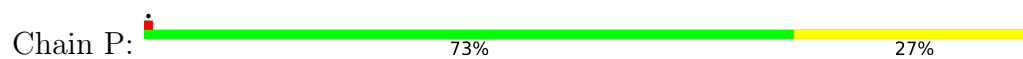


- Molecule 16: Large ribosomal subunit protein bL17

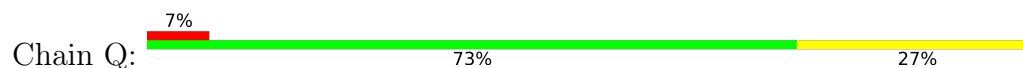
Chain O: 73% 27%



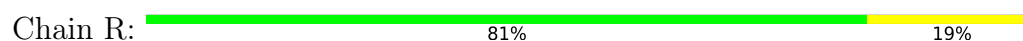
- Molecule 17: Large ribosomal subunit protein uL18



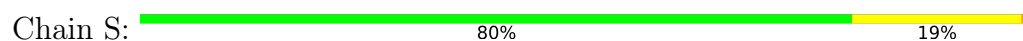
- Molecule 18: 50S ribosomal protein L19



- Molecule 19: Large ribosomal subunit protein bL20



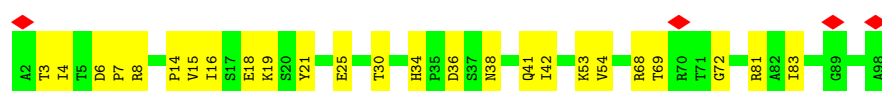
- Molecule 20: Large ribosomal subunit protein bL21



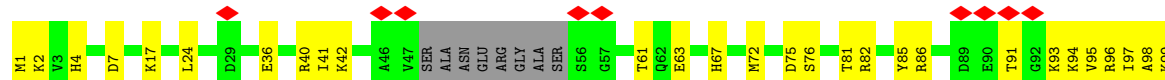
- Molecule 21: Large ribosomal subunit protein uL22

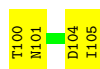


- Molecule 22: Large ribosomal subunit protein uL23

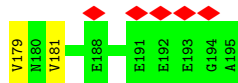
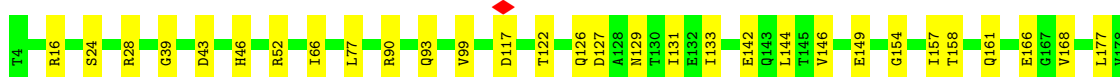
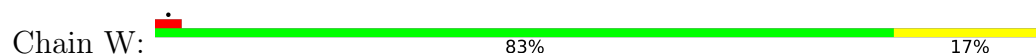


- Molecule 23: Large ribosomal subunit protein uL24

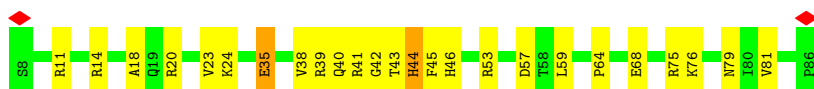




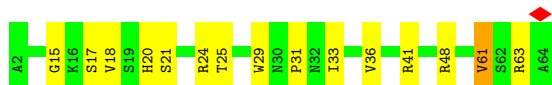
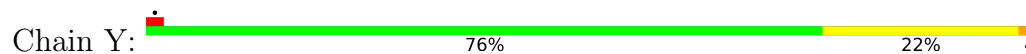
- Molecule 24: Large ribosomal subunit protein bL25



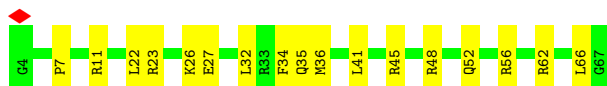
- Molecule 25: Large ribosomal subunit protein bL27



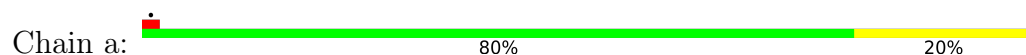
- Molecule 26: Large ribosomal subunit protein bL28



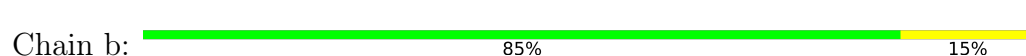
- Molecule 27: Large ribosomal subunit protein uL29



- Molecule 28: Large ribosomal subunit protein uL30

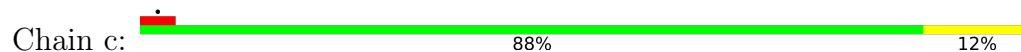


- Molecule 29: Large ribosomal subunit protein bL32

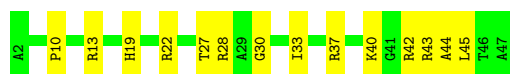




- Molecule 30: Large ribosomal subunit protein bL33A



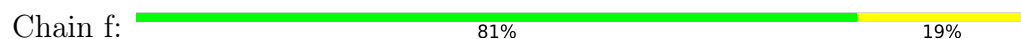
- Molecule 31: Large ribosomal subunit protein bL34



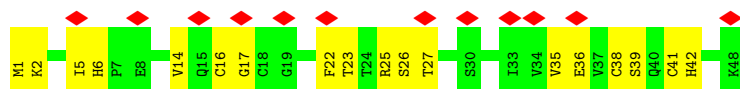
- Molecule 32: Large ribosomal subunit protein bL35



- Molecule 33: 50S ribosomal protein L36



- Molecule 34: Large ribosomal subunit protein bL31



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43558	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28.75	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	30.405	Depositor
Minimum map value	-14.822	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.6	Depositor
Map size (Å)	449.40002, 449.40002, 449.40002	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	3	0.30	0/191	0.38	0/247
2	A	0.33	0/75026	0.34	0/117066
3	B	0.26	0/2821	0.29	0/4396
4	C	0.35	0/2153	0.40	0/2895
5	D	0.35	0/1609	0.40	0/2165
6	E	0.31	0/1592	0.35	0/2153
7	F	0.20	0/1467	0.37	0/1973
8	G	0.24	0/1369	0.37	0/1848
9	H	0.15	0/1027	0.31	0/1398
10	I	0.13	0/925	0.34	0/1246
11	J	0.12	0/1006	0.35	0/1364
12	K	0.36	0/1157	0.38	0/1567
13	L	0.34	0/946	0.41	0/1268
14	M	0.32	0/1091	0.42	0/1457
15	N	0.32	0/1118	0.39	0/1506
16	O	0.34	0/945	0.40	0/1267
17	P	0.24	0/966	0.35	0/1298
18	Q	0.30	0/921	0.38	0/1236
19	R	0.37	0/1000	0.38	0/1341
20	S	0.32	0/764	0.32	0/1030
21	T	0.35	0/887	0.37	0/1204
22	U	0.30	0/766	0.35	0/1030
23	V	0.27	0/738	0.39	0/987
24	W	0.24	0/1443	0.33	0/1970
25	X	0.34	0/595	0.44	1/798 (0.1%)
26	Y	0.34	0/478	0.34	0/641
27	Z	0.28	0/534	0.38	0/713
28	a	0.35	0/477	0.40	0/640
29	b	0.32	0/427	0.33	0/572
30	c	0.23	0/413	0.42	0/553
31	d	0.34	0/380	0.33	0/500
32	e	0.21	0/507	0.33	0/672

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	f	0.31	0/303	0.33	0/401
34	g	0.18	0/372	0.40	0/503
All	All	0.32	0/106414	0.35	1/159905 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	X	44	HIS	N-CA-C	-5.84	104.83	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	189	0	205	8	0
2	A	67003	0	33711	1016	0
3	B	2522	0	1285	40	0
4	C	2110	0	2165	63	0
5	D	1587	0	1630	31	0
6	E	1569	0	1607	40	0
7	F	1445	0	1476	54	0
8	G	1348	0	1399	40	0
9	H	1018	0	988	15	0
10	I	918	0	959	30	0
11	J	990	0	1021	23	0
12	K	1130	0	1167	29	0
13	L	938	0	1000	23	0
14	M	1078	0	1151	30	0
15	N	1092	0	1128	25	0
16	O	928	0	972	25	0
17	P	956	0	991	27	0
18	Q	907	0	938	19	0
19	R	988	0	1038	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	S	754	0	802	14	0
21	T	873	0	909	17	0
22	U	756	0	802	20	0
23	V	732	0	782	25	0
24	W	1428	0	1443	22	0
25	X	586	0	601	18	0
26	Y	470	0	484	11	0
27	Z	531	0	541	11	0
28	a	474	0	500	8	0
29	b	423	0	463	7	0
30	c	405	0	411	5	0
31	d	377	0	411	12	0
32	e	502	0	541	17	0
33	f	299	0	324	5	0
34	g	364	0	352	21	0
35	A	51	0	67	4	0
All	All	97741	0	64264	1558	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 10.

The worst 5 of 1558 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)
2:A:279:U:H3	2:A:307:G:H1	0.95	0.93
2:A:1547:G:H1	2:A:1623:U:H3	1.11	0.93
2:A:2131:G:H1	2:A:2147:U:H3	1.14	0.89
2:A:1367:G:N7	19:R:36:LYS:NZ	2.24	0.86
22:U:8:ARG:NE	27:Z:27:GLU:OE2	2.09	0.86

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	3	21/23 (91%)	21 (100%)	0	0	100	100
4	C	273/275 (99%)	257 (94%)	16 (6%)	0	100	100
5	D	212/214 (99%)	196 (92%)	16 (8%)	0	100	100
6	E	207/209 (99%)	199 (96%)	8 (4%)	0	100	100
7	F	180/182 (99%)	172 (96%)	8 (4%)	0	100	100
8	G	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
9	H	149/151 (99%)	142 (95%)	7 (5%)	0	100	100
10	I	124/126 (98%)	117 (94%)	7 (6%)	0	100	100
11	J	131/133 (98%)	127 (97%)	4 (3%)	0	100	100
12	K	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
13	L	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
14	M	143/145 (99%)	127 (89%)	16 (11%)	0	100	100
15	N	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
16	O	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
17	P	124/126 (98%)	122 (98%)	2 (2%)	0	100	100
18	Q	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
19	R	122/124 (98%)	116 (95%)	6 (5%)	0	100	100
20	S	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
21	T	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
22	U	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
23	V	93/105 (89%)	90 (97%)	3 (3%)	0	100	100
24	W	190/192 (99%)	184 (97%)	6 (3%)	0	100	100
25	X	77/79 (98%)	71 (92%)	6 (8%)	0	100	100
26	Y	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
27	Z	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
28	a	57/59 (97%)	52 (91%)	5 (9%)	0	100	100
29	b	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
30	c	47/49 (96%)	43 (92%)	4 (8%)	0	100	100
31	d	44/46 (96%)	44 (100%)	0	0	100	100
32	e	61/63 (97%)	60 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	f	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
34	g	46/48 (96%)	43 (94%)	3 (6%)	0	100	100
All	All	3615/3689 (98%)	3442 (95%)	173 (5%)	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	
1	3	18/18 (100%)	18 (100%)	0	100	100
4	C	215/215 (100%)	215 (100%)	0	100	100
5	D	160/160 (100%)	159 (99%)	1 (1%)	78	79
6	E	169/169 (100%)	169 (100%)	0	100	100
7	F	151/151 (100%)	150 (99%)	1 (1%)	76	78
8	G	148/148 (100%)	147 (99%)	1 (1%)	76	78
9	H	90/116 (78%)	89 (99%)	1 (1%)	65	74
10	I	89/89 (100%)	89 (100%)	0	100	100
11	J	102/102 (100%)	102 (100%)	0	100	100
12	K	119/119 (100%)	119 (100%)	0	100	100
13	L	100/100 (100%)	100 (100%)	0	100	100
14	M	112/112 (100%)	109 (97%)	3 (3%)	39	61
15	N	114/114 (100%)	112 (98%)	2 (2%)	51	68
16	O	97/97 (100%)	96 (99%)	1 (1%)	68	75
17	P	93/93 (100%)	93 (100%)	0	100	100
18	Q	100/100 (100%)	98 (98%)	2 (2%)	48	66
19	R	97/97 (100%)	96 (99%)	1 (1%)	68	75
20	S	81/81 (100%)	79 (98%)	2 (2%)	42	63
21	T	90/90 (100%)	87 (97%)	3 (3%)	33	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	U	83/83 (100%)	82 (99%)	1 (1%)	63	73
23	V	81/86 (94%)	81 (100%)	0	100	100
24	W	155/155 (100%)	155 (100%)	0	100	100
25	X	58/58 (100%)	55 (95%)	3 (5%)	21	48
26	Y	50/50 (100%)	49 (98%)	1 (2%)	48	66
27	Z	58/58 (100%)	56 (97%)	2 (3%)	32	57
28	a	52/52 (100%)	52 (100%)	0	100	100
29	b	43/43 (100%)	43 (100%)	0	100	100
30	c	47/47 (100%)	47 (100%)	0	100	100
31	d	35/35 (100%)	35 (100%)	0	100	100
32	e	53/53 (100%)	53 (100%)	0	100	100
33	f	35/35 (100%)	35 (100%)	0	100	100
34	g	43/43 (100%)	43 (100%)	0	100	100
All	All	2938/2969 (99%)	2913 (99%)	25 (1%)	68	76

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	S	100	THR
21	T	84	ASP
27	Z	66	LEU
21	T	80	THR
22	U	3	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
16	O	17	GLN
31	d	9	GLN
19	R	39	GLN
25	X	12	ASN
17	P	9	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	3117/3119 (99%)	637 (20%)	24 (0%)
3	B	117/118 (99%)	18 (15%)	1 (0%)
All	All	3234/3237 (99%)	655 (20%)	25 (0%)

5 of 655 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	7	U
2	A	9	U
2	A	12	G
2	A	16	G
2	A	19	U

5 of 25 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	1084	U
2	A	1597	G
3	B	10	G
2	A	1535	C
2	A	1730	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	ERY	A	3201	-	53,53,53	1.26	3 (5%)	82,82,82	1.88	28 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ERY	A	3201	-	-	21/72/107/107	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	3201	ERY	C6-C5	3.14	1.61	1.55
35	A	3201	ERY	O10-C6	-2.77	1.40	1.44
35	A	3201	ERY	C22-C23	2.67	1.60	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	3201	ERY	O3-C3-C4	5.51	114.72	108.23
35	A	3201	ERY	O7-C5-C6	4.72	112.02	106.40
35	A	3201	ERY	O6-C17-C16	-4.41	103.08	111.08
35	A	3201	ERY	O7-C5-C4	-3.36	106.72	111.58
35	A	3201	ERY	C13-C12-C11	3.09	114.14	108.21

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

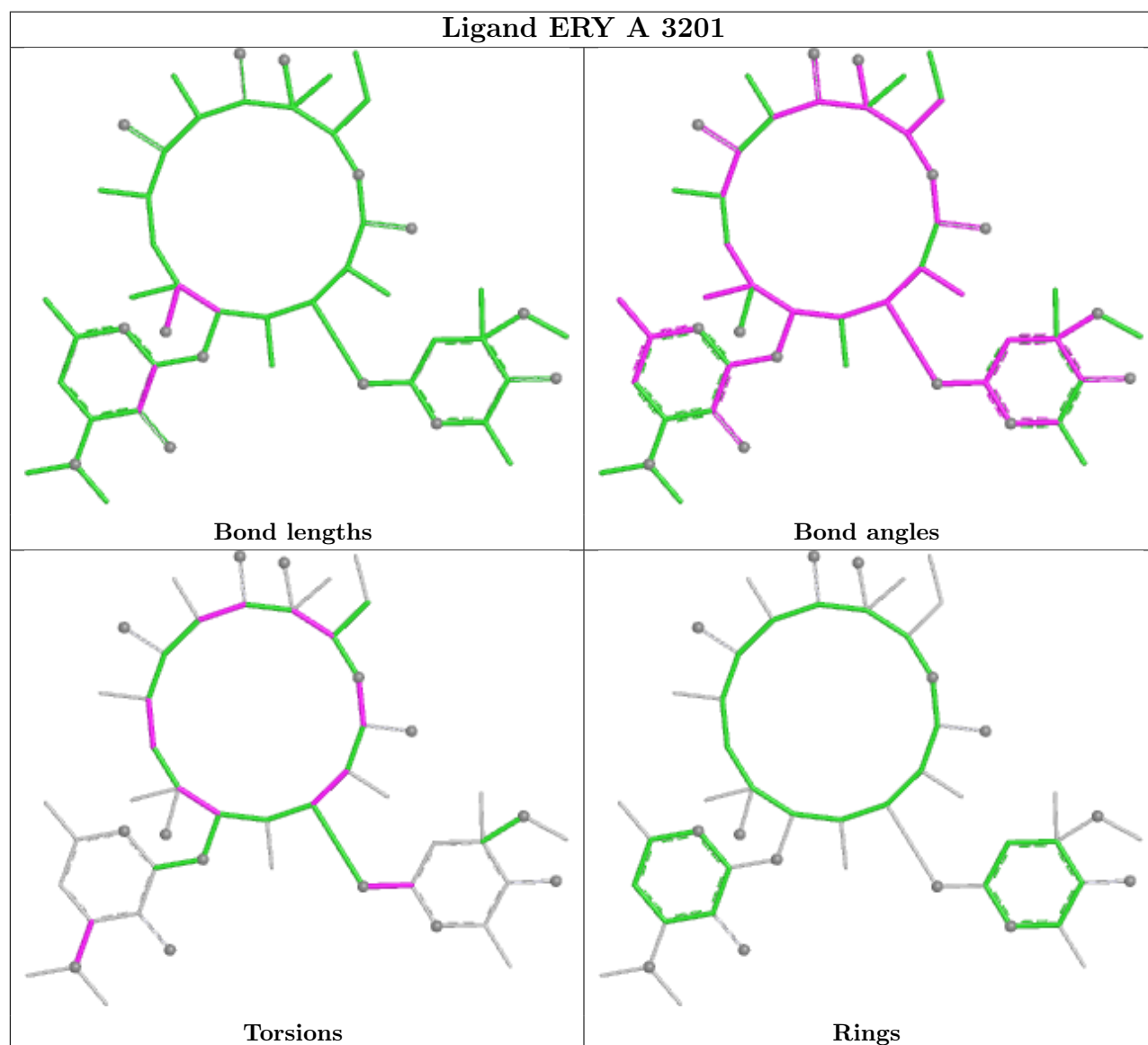
Mol	Chain	Res	Type	Atoms
35	A	3201	ERY	C9-C10-C11-C12
35	A	3201	ERY	C9-C10-C11-O12
35	A	3201	ERY	C34-C10-C11-C12
35	A	3201	ERY	C34-C10-C11-O12
35	A	3201	ERY	C11-C12-C13-O2

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	3201	ERY	4	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

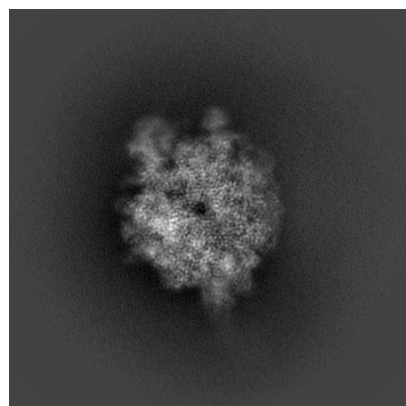
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38788. These allow visual inspection of the internal detail of the map and identification of artifacts.

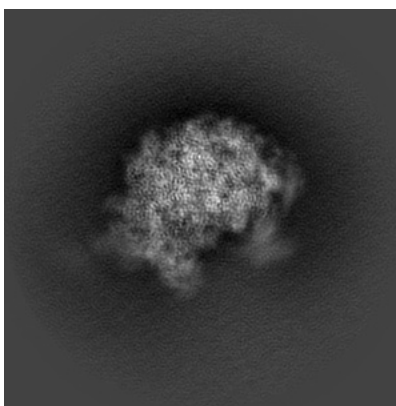
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

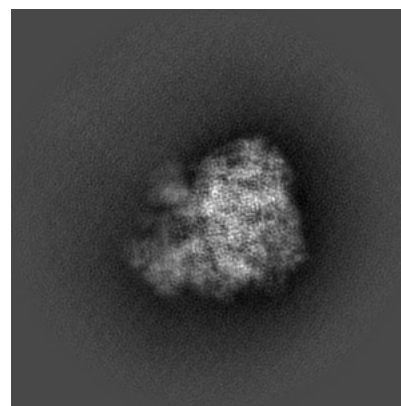
6.1.1 Primary map



X

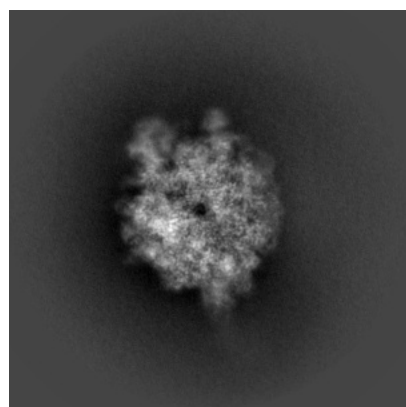


Y

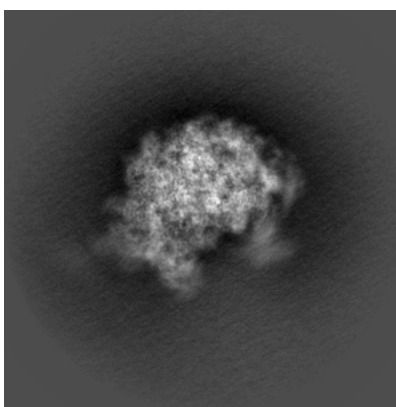


Z

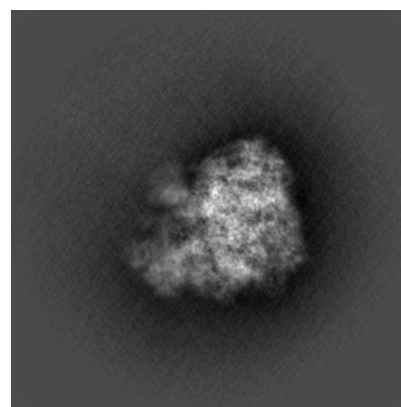
6.1.2 Raw map



X



Y

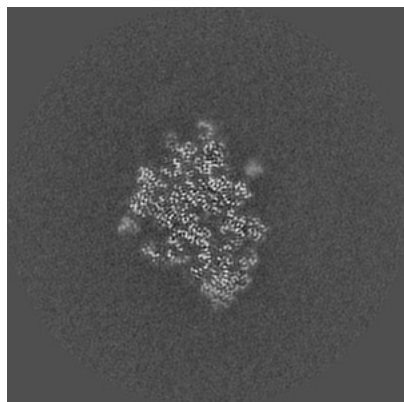


Z

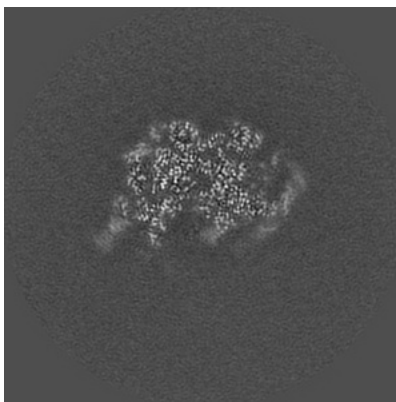
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

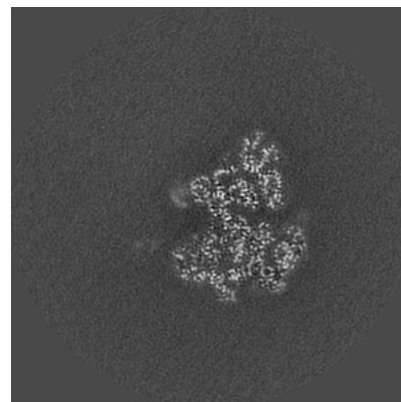
6.2.1 Primary map



X Index: 210

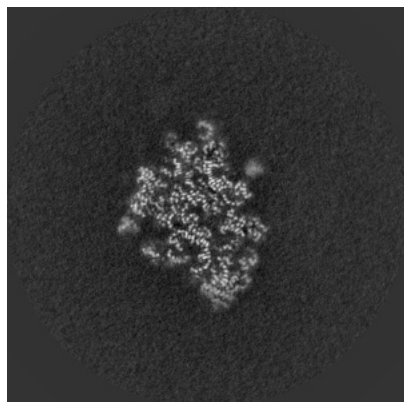


Y Index: 210

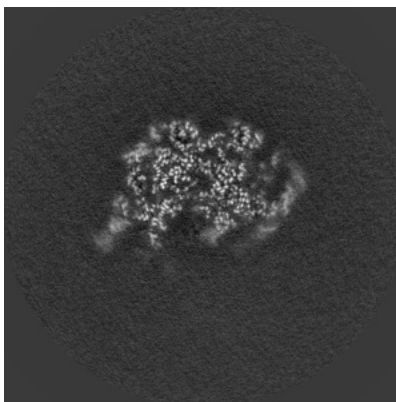


Z Index: 210

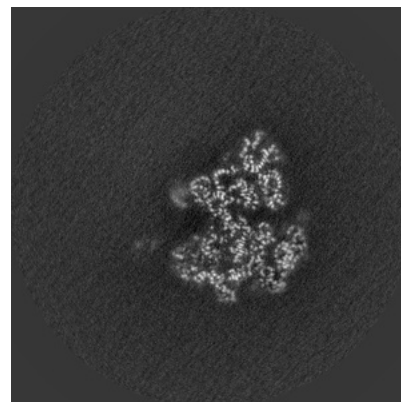
6.2.2 Raw map



X Index: 210



Y Index: 210

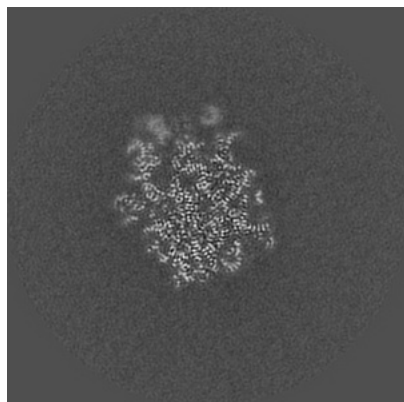


Z Index: 210

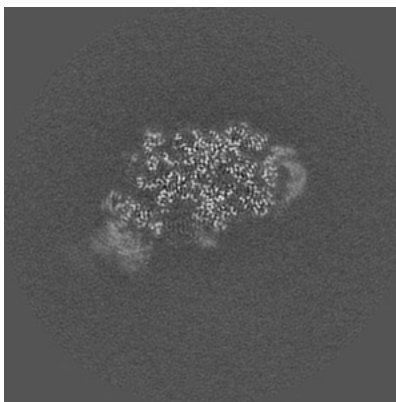
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

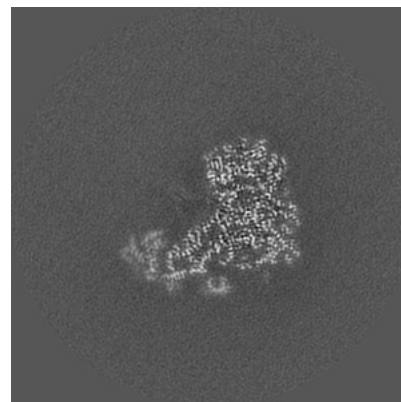
6.3.1 Primary map



X Index: 230

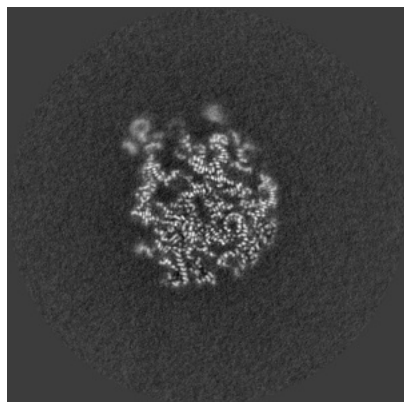


Y Index: 219

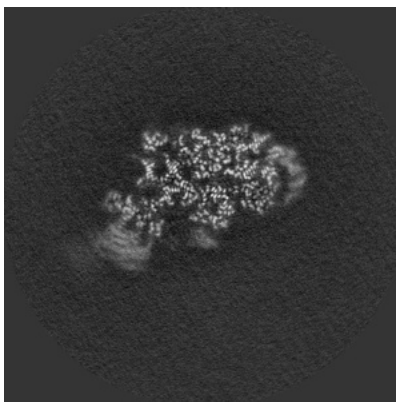


Z Index: 191

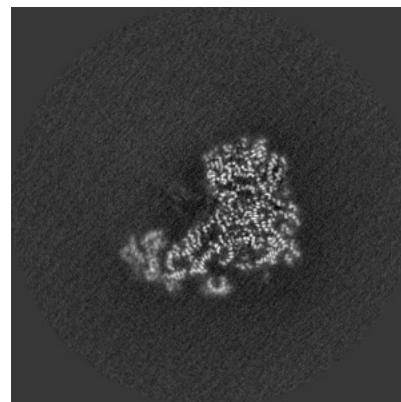
6.3.2 Raw map



X Index: 245



Y Index: 222

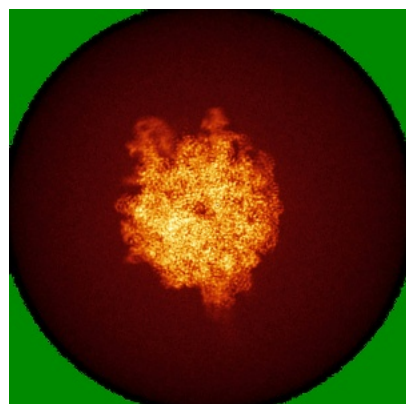


Z Index: 191

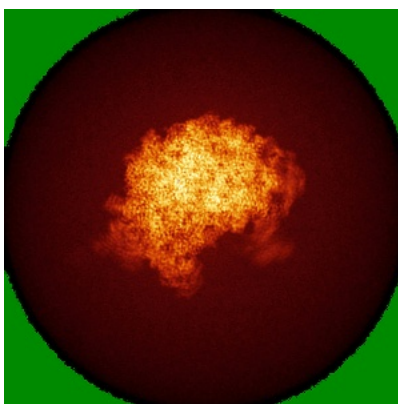
The images above show the largest variance slices of the map in three orthogonal directions.

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

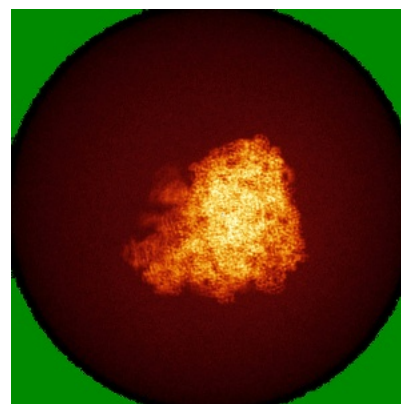
6.4.1 Primary map



X

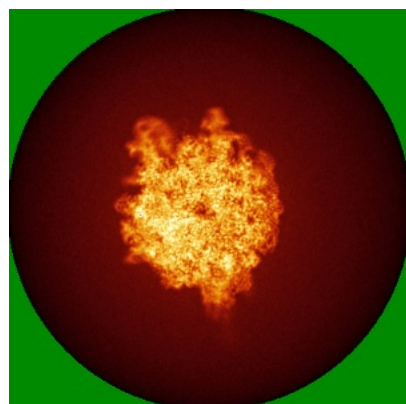


Y

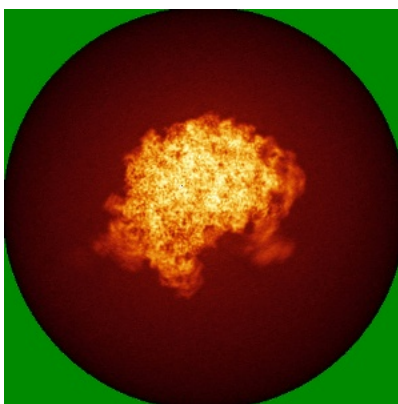


Z

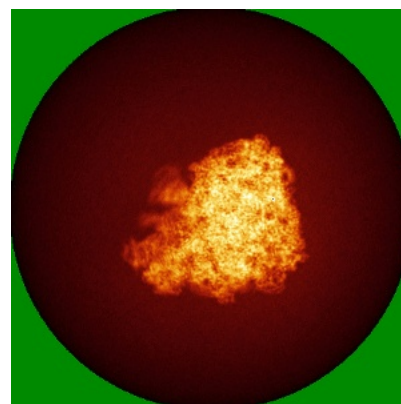
6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.6. 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



X



Y



Z

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

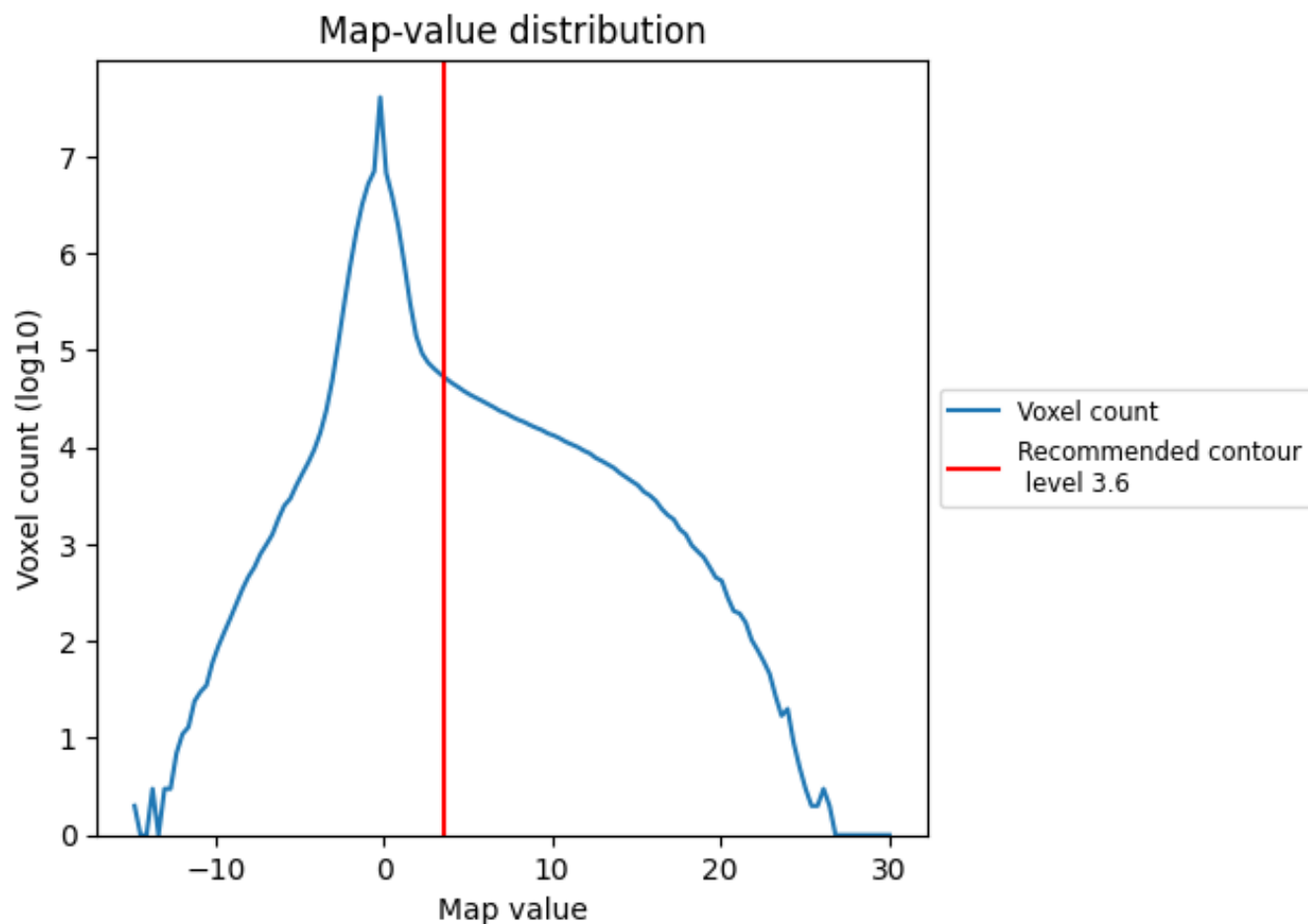
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

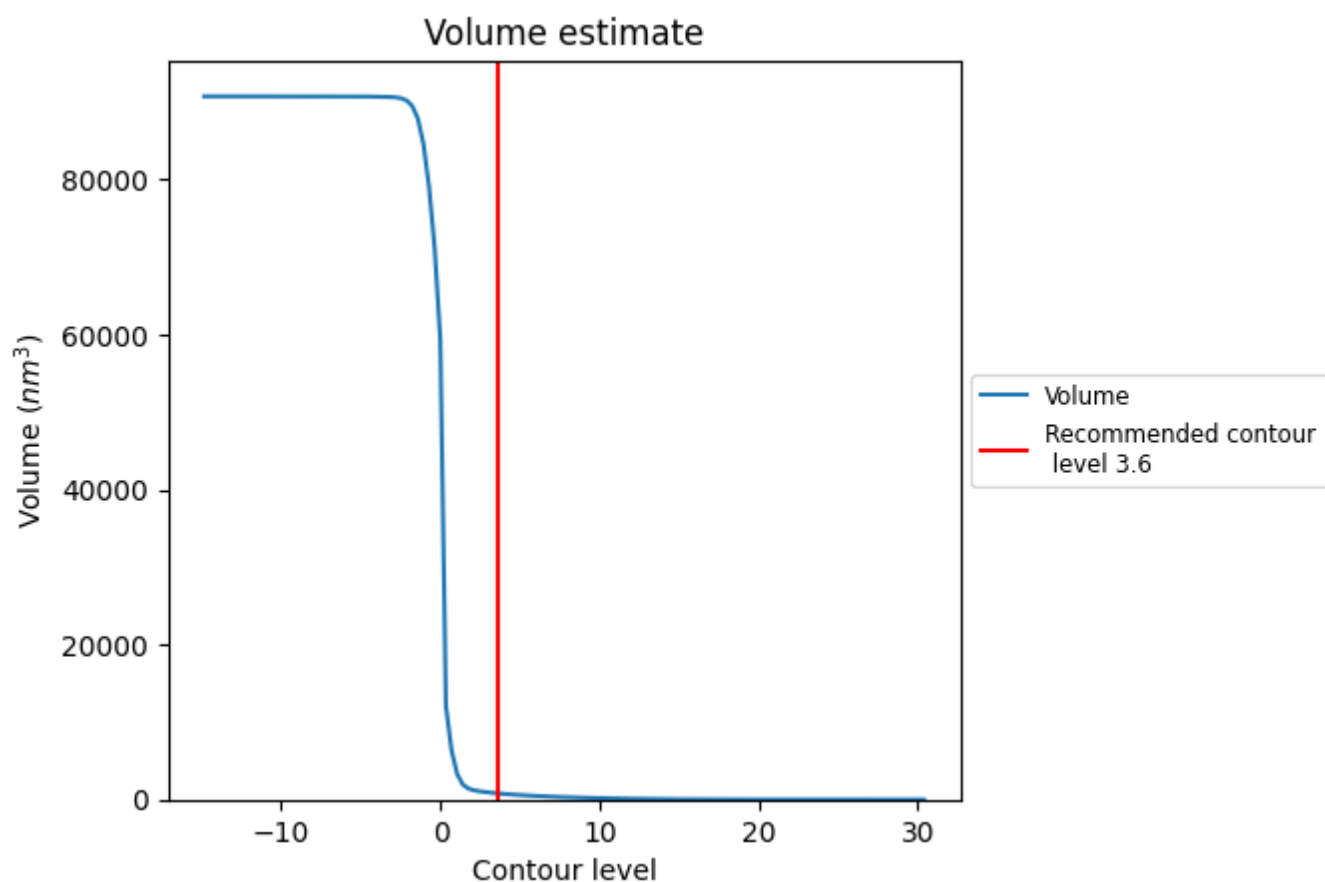
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

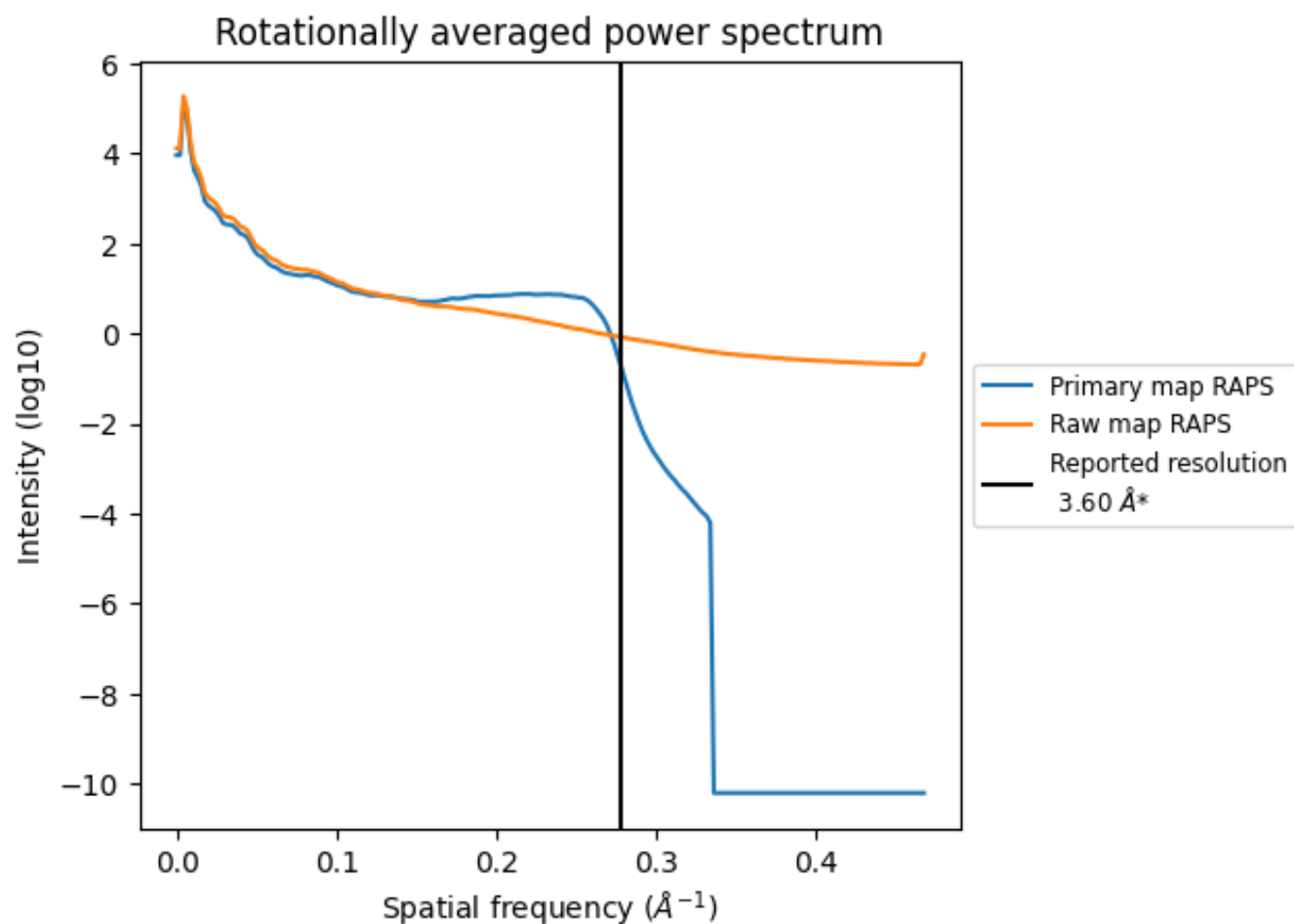
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 803 nm^3 ; this corresponds to an approximate mass of 725 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 ⓘ

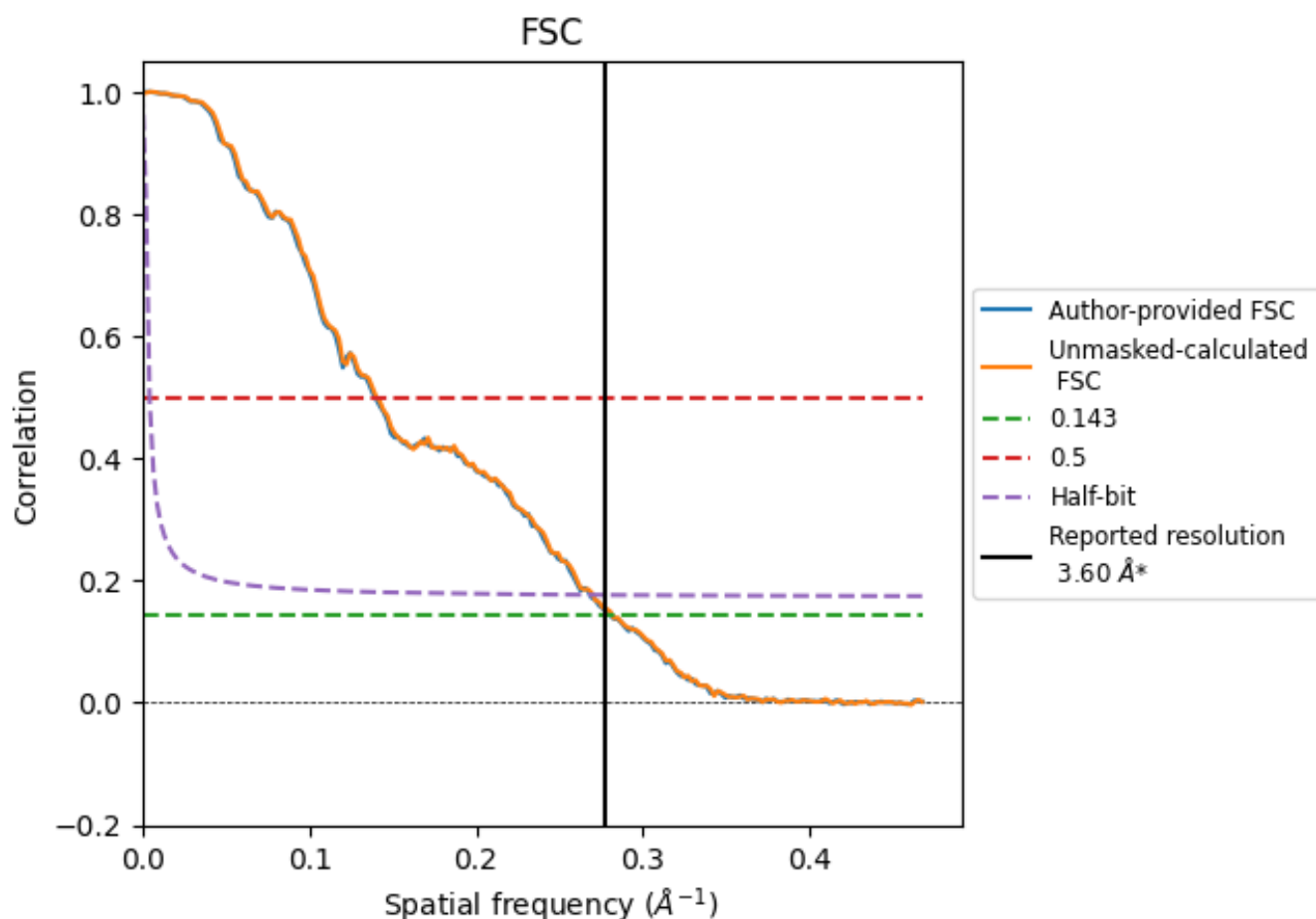


*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.278 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

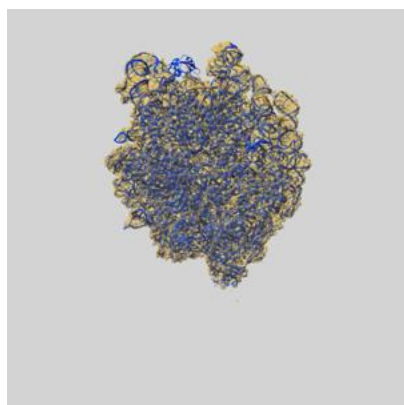
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.56	7.17	3.73
Unmasked-calculated*	3.55	7.13	3.71

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

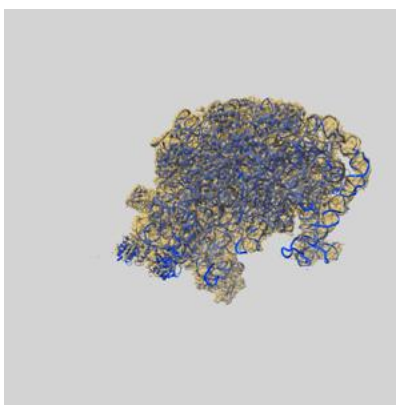
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38788 and PDB model 8XZ3. Per-residue inclusion information can be found in section [3](#) on page [11](#).

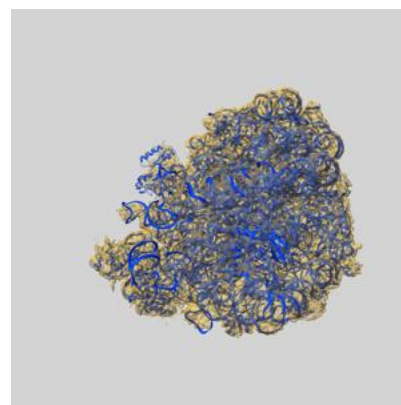
9.1 Map-model overlay [i](#)



X



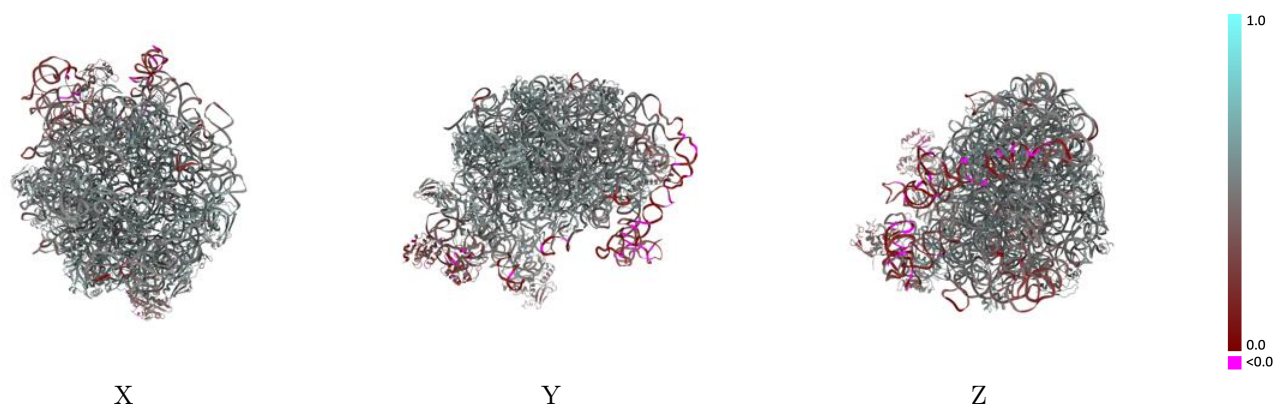
Y



Z

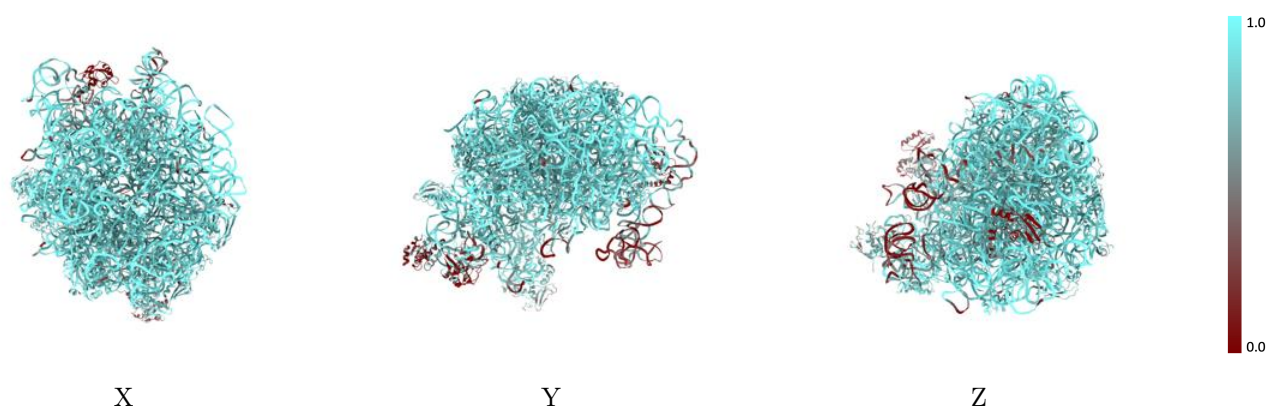
The images above show the 3D surface view of the map at the recommended contour level 3.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



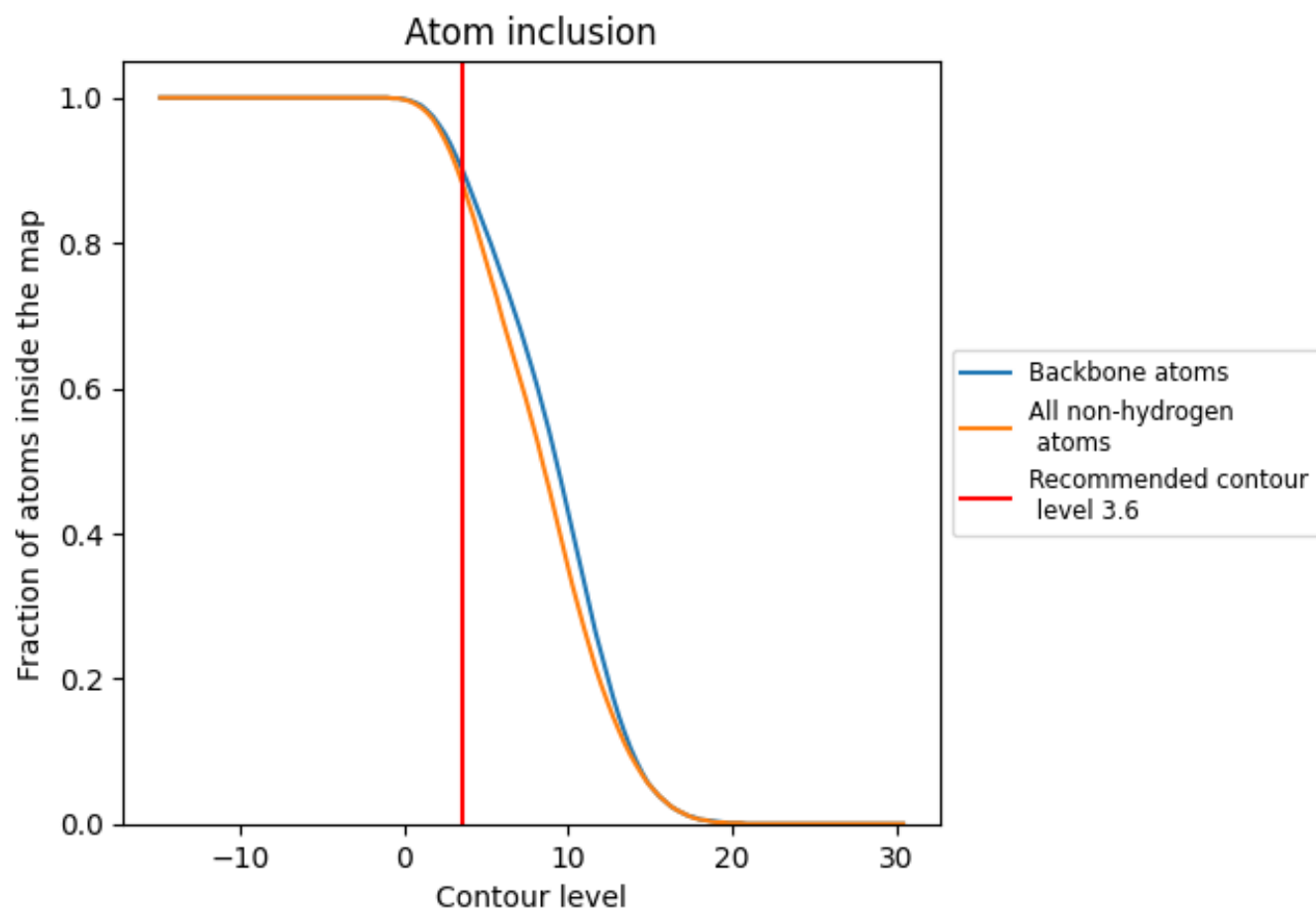
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 88% 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 (3.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8800	 0.4730
3	 0.8440	 0.5460
A	 0.9100	 0.4610
B	 0.9600	 0.4680
C	 0.9030	 0.5450
D	 0.9100	 0.5490
E	 0.8730	 0.5280
F	 0.7480	 0.4200
G	 0.8430	 0.4760
H	 0.2490	 0.4160
I	 0.3230	 0.2700
J	 0.2280	 0.2490
K	 0.9150	 0.5500
L	 0.8770	 0.5380
M	 0.8870	 0.5330
N	 0.8650	 0.5440
O	 0.8990	 0.5460
P	 0.8970	 0.5020
Q	 0.8160	 0.5270
R	 0.9310	 0.5420
S	 0.9070	 0.5540
T	 0.9040	 0.5510
U	 0.8450	 0.5220
V	 0.8000	 0.4990
W	 0.8050	 0.5100
X	 0.8900	 0.5390
Y	 0.8850	 0.5290
Z	 0.8750	 0.5130
a	 0.9150	 0.5410
b	 0.9000	 0.5490
c	 0.8120	 0.5400
d	 0.9170	 0.5610
e	 0.7060	 0.5440
f	 0.9060	 0.5600
g	 0.5750	 0.3330

