



wwPDB EM Validation Summary Report ⓘ

Oct 29, 2024 – 11:05 PM EDT

PDB ID : 3J5L
EMDB ID : EMD-5771
Title : Structure of the E. coli 50S subunit with ErmBL nascent chain
Authors : Arenz, S.; Ramu, H.; Gupta, P.; Berninghausen, O.; Beckmann, R.; Vazquez-Laslop, N.; Mankin, A.S.; Wilson, D.N.
Deposited on : 2013-10-23
Resolution : 6.60 Å(reported)
Based on initial model : 3OFR

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

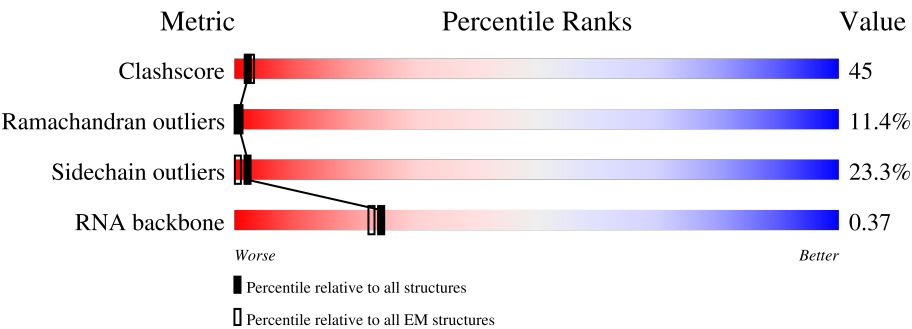
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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 6.60 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.



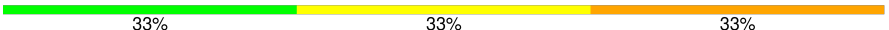

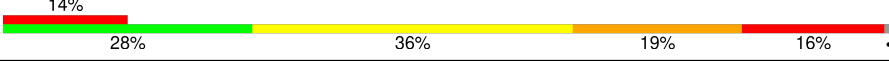
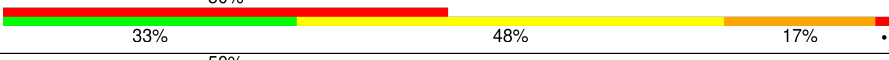
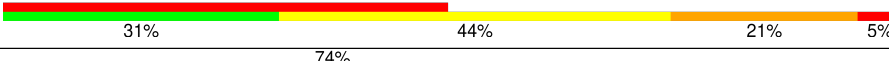
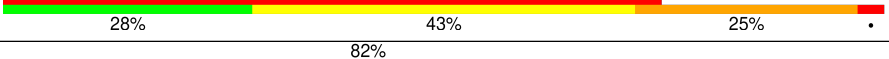

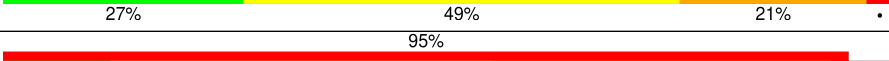
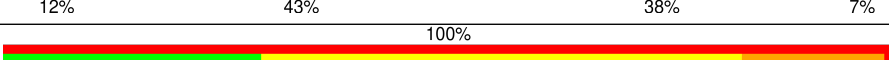
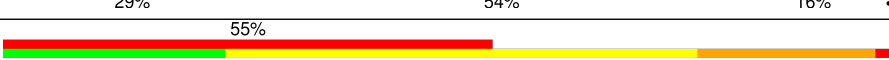
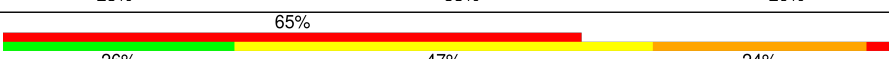

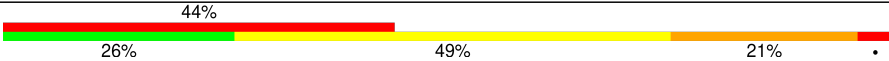

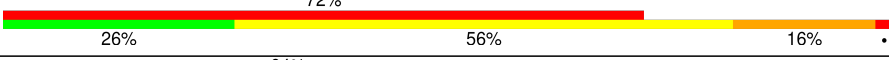


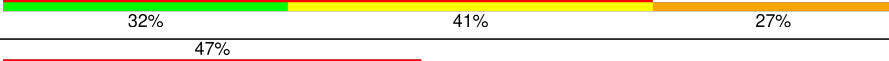


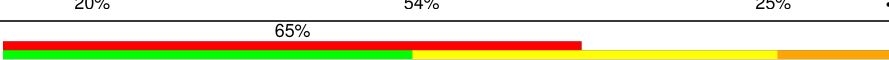

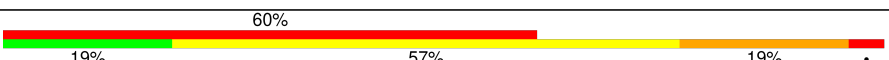


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	0	56	<div><div>62%</div><div><div>34%</div><div>48%</div><div>18%</div></div></div>
2	1	50	<div><div>62%</div><div><div>32%</div><div>48%</div><div>20%</div></div></div>
3	2	46	<div><div>43%</div><div><div>46%</div><div>33%</div><div>22%</div></div></div>
4	3	64	<div><div>58%</div><div><div>36%</div><div>45%</div><div>17%</div><div>.</div></div></div>
5	4	38	<div><div>58%</div><div><div>32%</div><div>53%</div><div>13%</div><div>.</div></div></div>
6	5	2	<div><div>50%</div><div><div>50%</div></div></div>
7	6	10	<div><div>30%</div><div><div>40%</div><div>40%</div><div>20%</div></div></div>

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Mol	Chain	Length	Quality of chain
8	7	3	
9	A	2904	
10	B	118	
11	C	271	
12	D	209	
13	E	201	
14	F	177	
15	G	176	
16	H	56	
17	I	141	
18	J	142	
19	K	122	
20	L	143	
21	M	136	
22	N	120	
23	O	116	
24	P	114	
25	Q	117	
26	R	103	
27	S	110	
28	T	93	
29	U	102	
30	V	94	
31	W	79	
32	X	77	

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Mol	Chain	Length	Quality of chain
33	Y	63	<div><div></div><div>70%</div><div>24%</div><div>48%</div><div>27%</div><div></div></div>
34	Z	58	<div><div></div><div>57%</div><div>41%</div><div>34%</div><div>22%</div><div></div></div>

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 89382 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 L32.

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 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 3 is a protein called 50S ribosomal protein L34.

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 50S ribosomal protein L35.

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 50S ribosomal protein L36.

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 5'-R(*CP*(MA6))-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	2	Total	C	N	O	P	0	0
			41	21	8	11	1		

- Molecule 7 is a protein called Erythromycin resistance leader peptide.

Mol	Chain	Residues	Atoms	AltConf	Trace
7	6	8	Total C 8 8	0	8

- Molecule 8 is a RNA chain called 5'-R(*CP*CP*A)-3'.

Mol	Chain	Residues	Atoms	AltConf	Trace
8	7	3	Total C N O P 59 28 11 18 2	0	0

- Molecule 9 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms	AltConf	Trace
9	A	2853	Total C N O P 61251 27324 11274 19800 2853	0	0

- Molecule 10 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms	AltConf	Trace
10	B	117	Total C N O P 2506 1116 459 814 117	0	0

- Molecule 11 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms	AltConf	Trace
11	C	271	Total C N O S 2083 1288 423 365 7	0	0

- Molecule 12 is a protein called 50S ribosomal protein L3.

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

- Molecule 13 is a protein called 50S ribosomal protein L4.

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

- Molecule 14 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 15 is a protein called 50S ribosomal protein L6.

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

- Molecule 16 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	56	Total	C	N	O	S	0	0
			431	275	77	78	1		

- Molecule 17 is a protein called 50S ribosomal protein L11.

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

- Molecule 18 is a protein called 50S ribosomal protein L13.

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

- Molecule 19 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 20 is a protein called 50S ribosomal protein L15.

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

- Molecule 21 is a protein called 50S ribosomal protein L16.

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

- Molecule 22 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 23 is a protein called 50S ribosomal protein L18.

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

- Molecule 24 is a protein called 50S ribosomal protein L19.

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

- Molecule 25 is a protein called 50S ribosomal protein L20.

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

- Molecule 26 is a protein called 50S ribosomal protein L21.

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

- Molecule 27 is a protein called 50S ribosomal protein L22.

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

- Molecule 28 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 29 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	102	Total	C	N	O	S	0	0
			780	492	146	142			

- Molecule 30 is a protein called 50S ribosomal protein L25.

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

- Molecule 31 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	79	Total	C	N	O	S	0	0
			596	367	120	108	1		

- Molecule 32 is a protein called 50S ribosomal protein L28.

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

- Molecule 33 is a protein called 50S ribosomal protein L29.

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

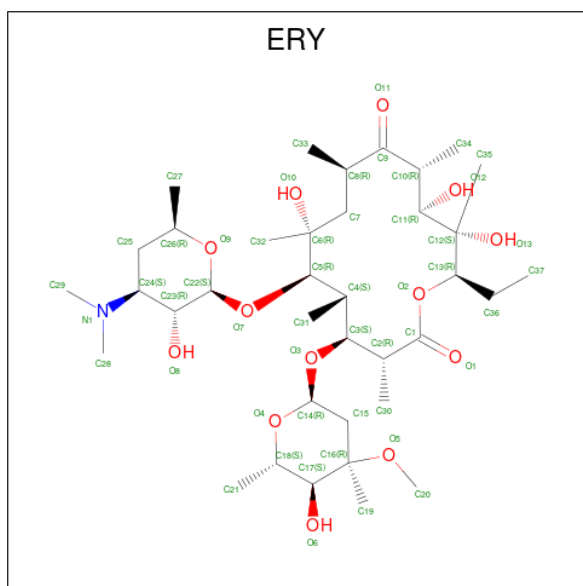
- Molecule 34 is a protein called 50S ribosomal protein L30.

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

- Molecule 35 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
35	5	1	4	2	1	1	0

- Molecule 36 is ERYTHROMYCIN A (three-letter code: ERY) (formula: $C_{37}H_{67}NO_{13}$).

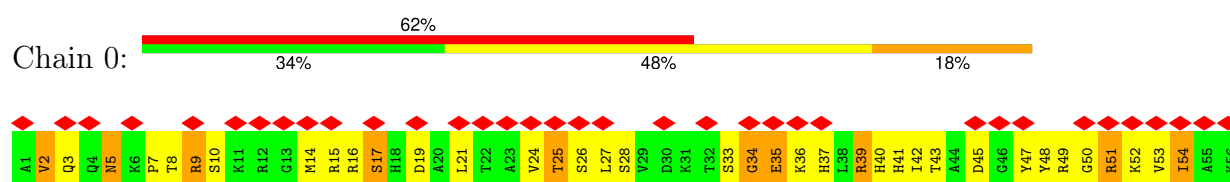


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
36	A	1	51	37	1	13	0

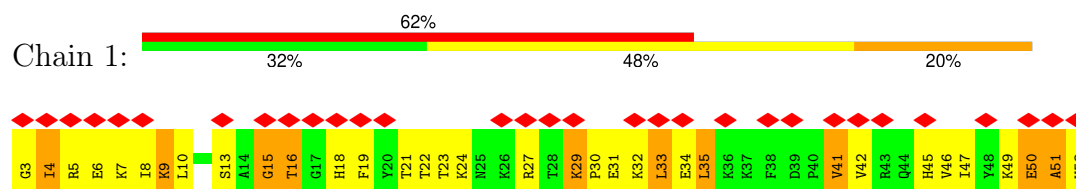
3 Residue-property plots [i](#)

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.

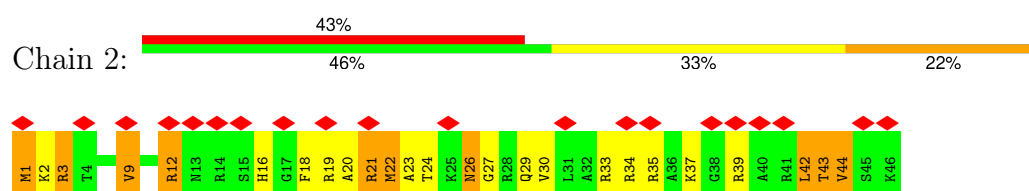
- Molecule 1: 50S ribosomal protein L32



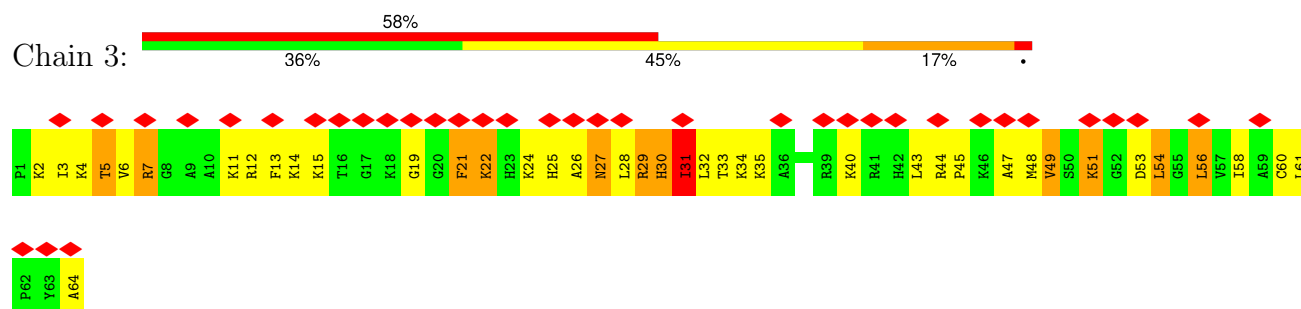
- Molecule 2: 50S ribosomal protein L33



- Molecule 3: 50S ribosomal protein L34



- Molecule 4: 50S ribosomal protein L35

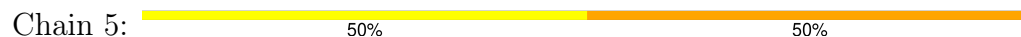


- Molecule 5: 50S ribosomal protein L36

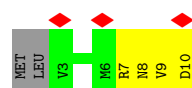
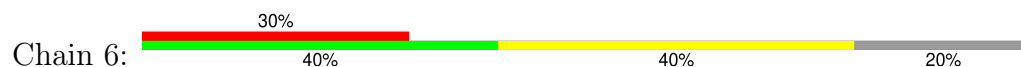




- Molecule 6: 5'-R(*CP*(MA6))-3'



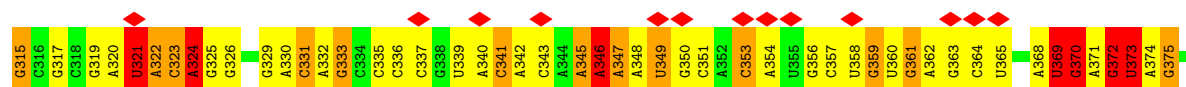
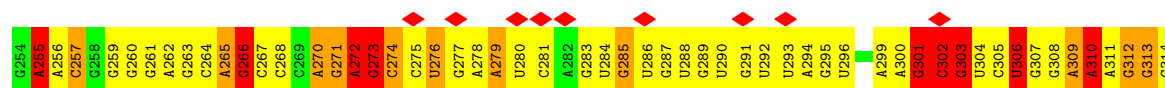
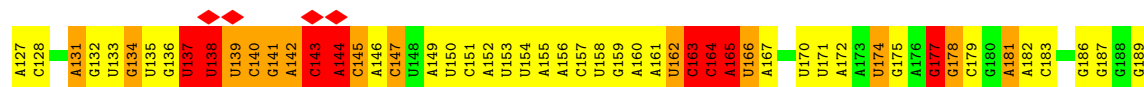
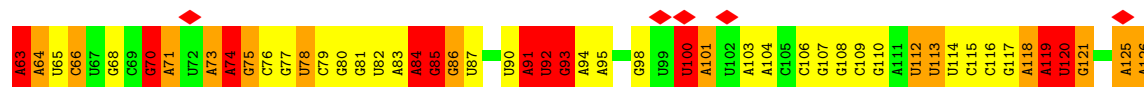
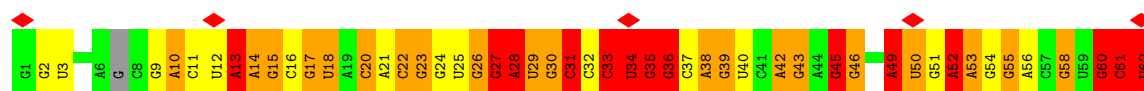
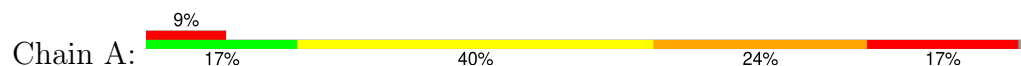
- Molecule 7: Erythromycin resistance leader peptide



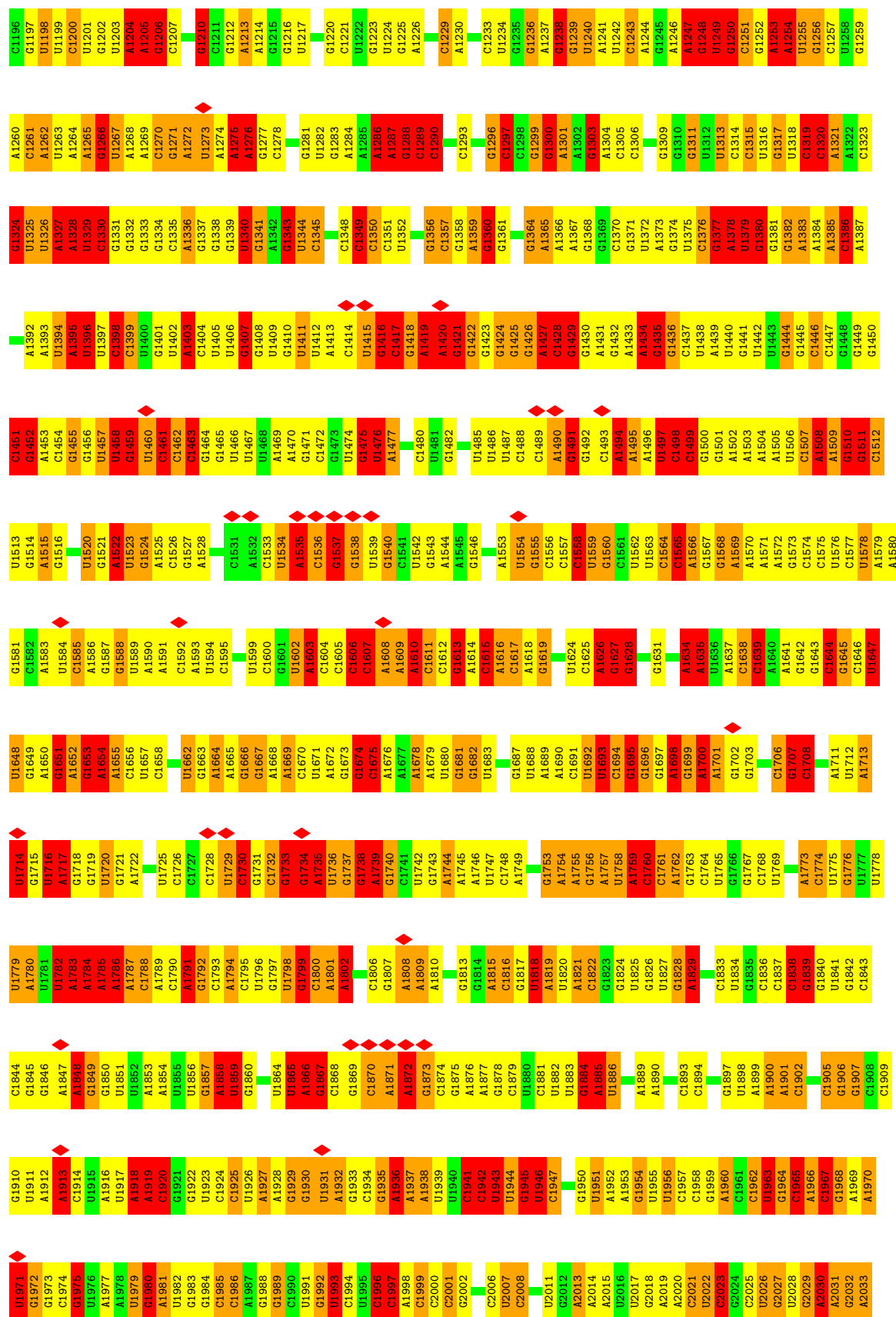
- Molecule 8: 5'-R(*CP*CP*A)-3'



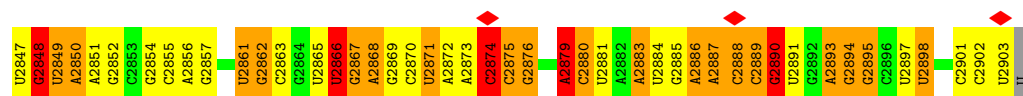
- Molecule 9: 23S ribosomal RNA



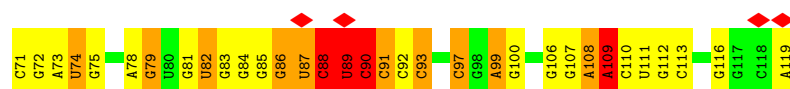
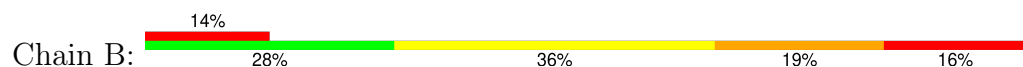




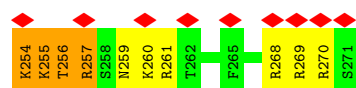
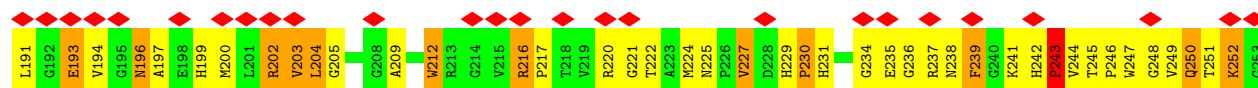
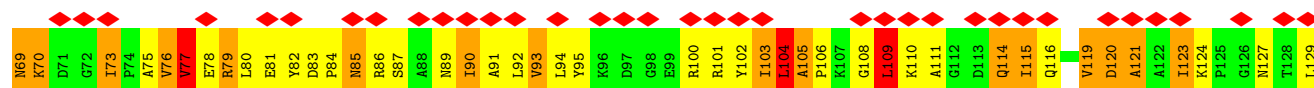
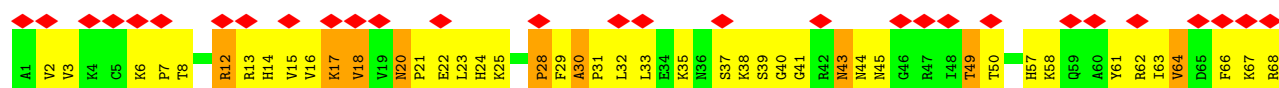
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U2786	G2723	G2659	G2532	A2411	U2344	A2284	G2221	C	A2101	C2036
C2787	U2724	A2660	G2594	A2412	G2345	C2285	C2222	G	G2102	A2037
C2788	A2725	G2661	G2595	G2413	A2346	G2286	G2223	A	C2103	G2038
C2789	A2726	A2662	G2596	G2414	C2347	G2287	G2224	C	U2039	U2039
U2790	G2727	G2663	U2537	G2415	U2348	A2288	A2225	C	A2042	A2042
G2791	U2728	G2664	C2538	G2416	G2349	G2289	C2226	U	C2043	C2043
A2792	G2729	A2665	C2539	C2417	U2477	G2290	A2227	U	C2044	C2044
C2793	G2730	G2666	C2540	A2418	G2351	G2291	U2228	G	U2105	U2105
C2794	G2731	C2667	A2541	U2419	A2352	U2292	U2229	A	U2106	U2106
C2795	G2732	G2668	A2542	G2420	G2353	G2293	G2230	A	G2107	G2107
G2796	A2733	G2669	G2543	G2421	C2354	G2294	U2231	A	A2108	A2108
U2797	A2734	A2670	G2544	G2422	G2355	G2295	C2232	U	U2109	U2109
U2797	G2735	G2671	G2545	U2423	U2356	U2296	U2233	A	G2110	G2110
U2798	A2736	U2672	U2546	G2424	G2357	A2297	G2234	C	U	U
A2799	G2737	G2673	A2547	A2425	A2358	A2298	G2235	C	G	G
A2800	A2740	C2674	U2548	A2426	G2361	U2299	U2236	A	U	U
G2801	G2741	G2675	G2549	G2427	C2362	C2300	G2237	C	A	A
G2802	U2742	U2676	C2550	A2428	G2363	U2301	G2238	C	G	G
G2803	G2743	C2612	U2551	G2429	G2364	G2302	G2239	C	G	G
U2804	G2744	U2680	U2552	A2430	G2365	G2303	U2243	A	A	A
C2805	G2745	C2681	U2553	U2431	G2366	G2304	U2244	A	A	A
C2806	U2746	A2682	U2554	A2432	A2367	U2305	U2245	G	G	G
U2807	G2747	G2683	U2555	A2433	G2368	G2306	G2246	A	A	A
U2807	A2748	U2684	C2556	A2434	G2369	G2307	A2247	U	U	U
G2808	U2749	G2685	G2557	A2435	G2370	G2308	U2248	G	G	G
A2809	A2750	G2686	C2558	U2436	G2373	A2309	U2249	G	G	G
G2810	G2751	U2687	U2559	G2437	C2374	C2310	G2250	G	G	G
G2811	U2752	G2688	G2611	U2438	C2375	A2311	G2251	A	A	A
A2812	A2753	U2689	G2612	A2439	G2380	U2312	G2252	G	G	G
C2813	U2754	U2690	G2613	U2440	A2381	C2313	G2253	C	C	C
A2814	G2755	G2691	A2564	U2441	G2382	A2314	G2254	U	U	U
C2815	U2756	G2692	A2565	C2442	C2383	G2315	G2255	C	U	U
G2816	A2757	U2693	U2566	G2443	G2384	U2316	U2257	U	U	U
U2817	G2758	G2694	G2567	C2444	C2385	A2317	G2258	U	U	U
A2820	U2759	U2695	U2568	G2445	A2386	G2318	U2259	G	G	G
A2821	A2761	G2696	G2569	U2446	U2387	U2319	U2260	U	U	U
G2822	U2762	G2697	U2570	A2447	A2388	G2320	C2261	A	A	A
A2823	A2763	C2698	U2571	U2448	U2389	U2321	U2262	A	A	A
G2824	U2764	U2700	A2572	A2449	U2390	A2322	G2263	A	A	A
G2825	A2765	G2699	C2573	U2450	U2391	G2323	U2264	A	A	A
A2826	G2766	U2701	G2574	A2451	A2392	U2324	A2265	A	A	A
C2827	C2702	G2702	C2575	C2452	A2393	G2325	A2266	A	A	A
G2828	G2703	C2703	A2576	A2453	U2394	G2326	A2267	A	A	A
A2829	U2704	G2641	G2577	G2454	C2395	G2327	G2268	A	A	A
C2830	A2705	A2578	U2578	A2455	G2396	A2328	U2269	A	A	A
G2831	G2706	C2579	C2579	U2457	G2397	U2329	A2270	A	A	A
U2832	U2707	U2580	A2581	G2458	U2398	G2330	G2271	A	A	A
G2833	G2708	U2519	C2582	A2459	G2399	U2331	U2272	A	A	A
G2834	A2711	C2520	U2583	U2460	U2401	C2332	A2273	A	A	A
A2835	G2712	G2521	U2584	A2461	U2402	G2333	A2274	A	A	A
U2836	U2713	U2522	U2585	C2462	C2403	U2334	C2275	A	A	A
G2837	G2714	G2523	G2586	G2463	G2404	A2335	G2276	A	A	A
A2838	U2715	G2524	U2587	A2464	C2405	A2336	A2277	A	A	A
G2839	C2716	U2525	G2588	C2465	G2406	G2337	A2278	A	A	A
C2840	G2717	A2526	A2589	C2466	A2407	C2338	G2279	A	A	A
G2841	U2783	U2527	U2590	A2468	A2408	G2339	G2280	A	A	A
G2842		G2528	C2591	A2469		A2341	A2281	A	A	A



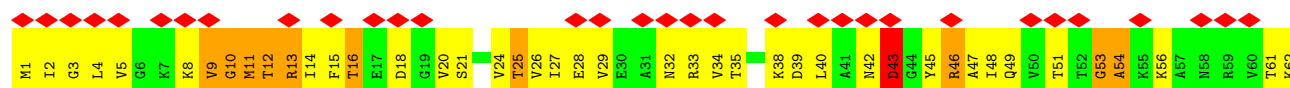
• Molecule 10: 5S ribosomal RNA

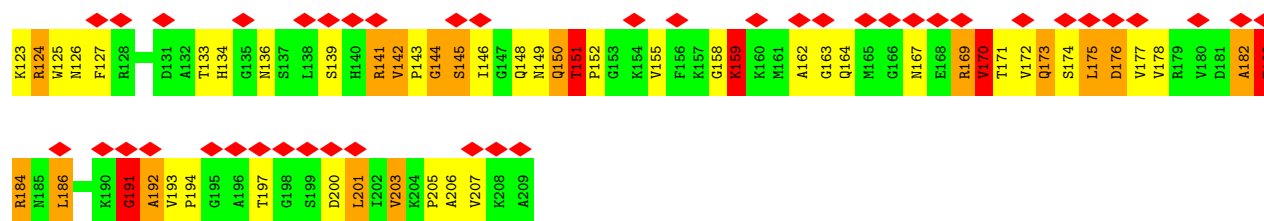


• Molecule 11: 50S ribosomal protein L2

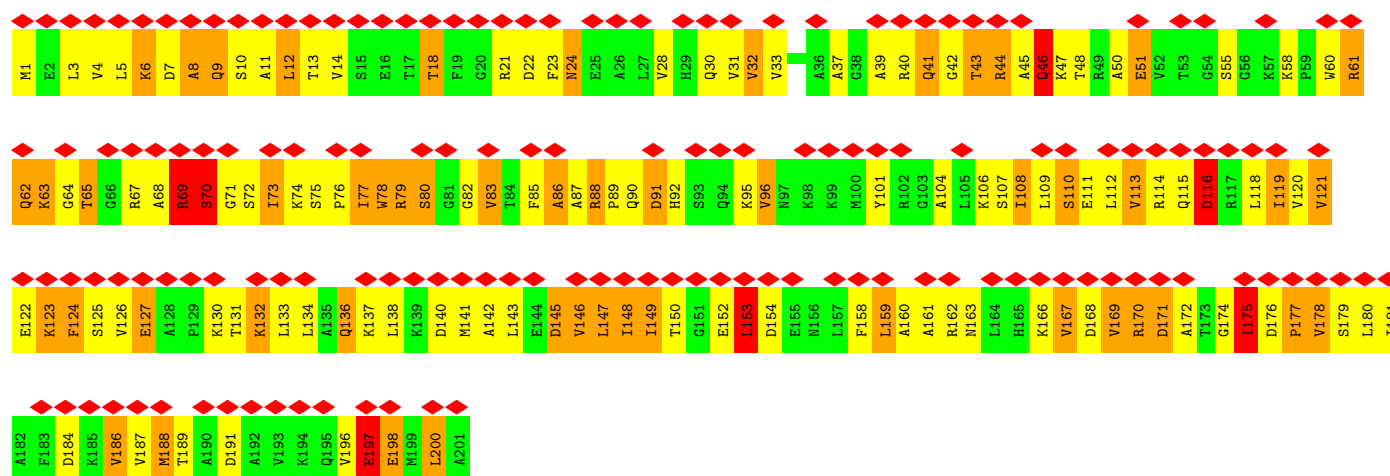
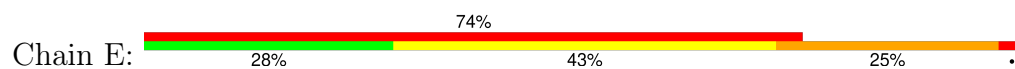


• Molecule 12: 50S ribosomal protein L3

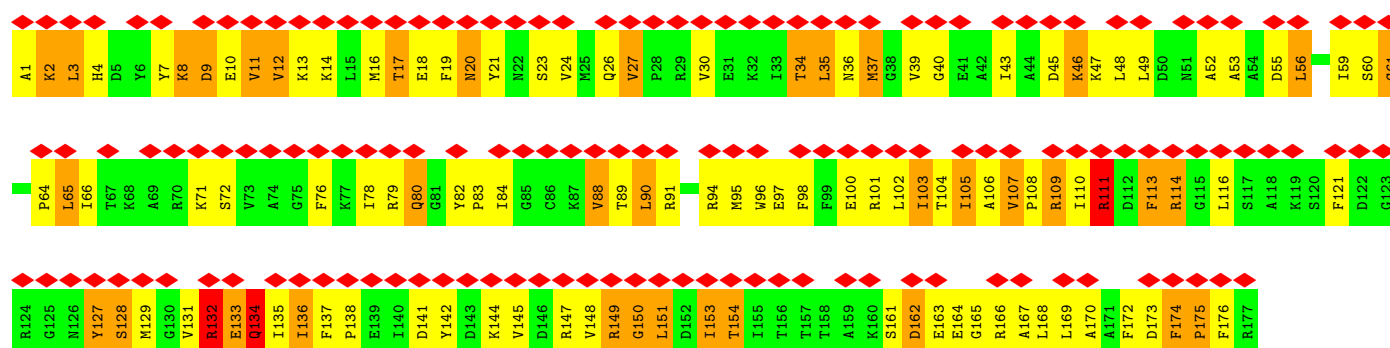
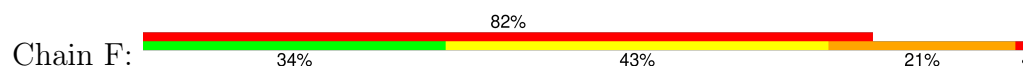




• Molecule 13: 50S ribosomal protein L4

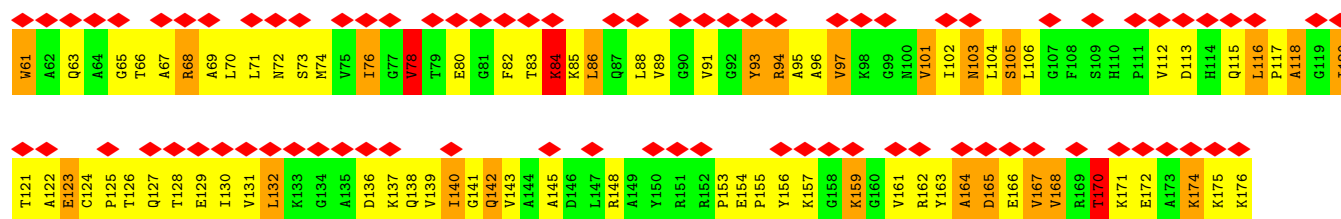


• Molecule 14: 50S ribosomal protein L5



• Molecule 15: 50S ribosomal protein L6

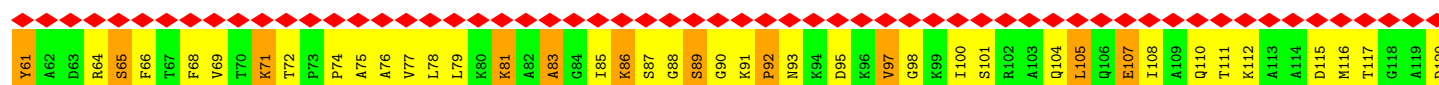
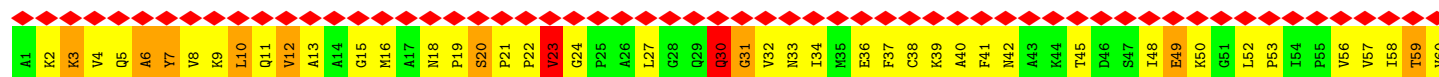




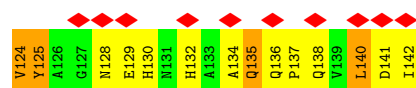
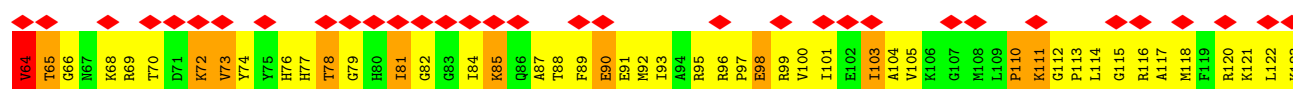
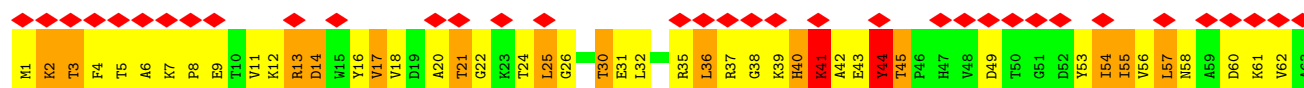
• Molecule 16: 50S ribosomal protein L9



• Molecule 17: 50S ribosomal protein L11



• Molecule 18: 50S ribosomal protein L13

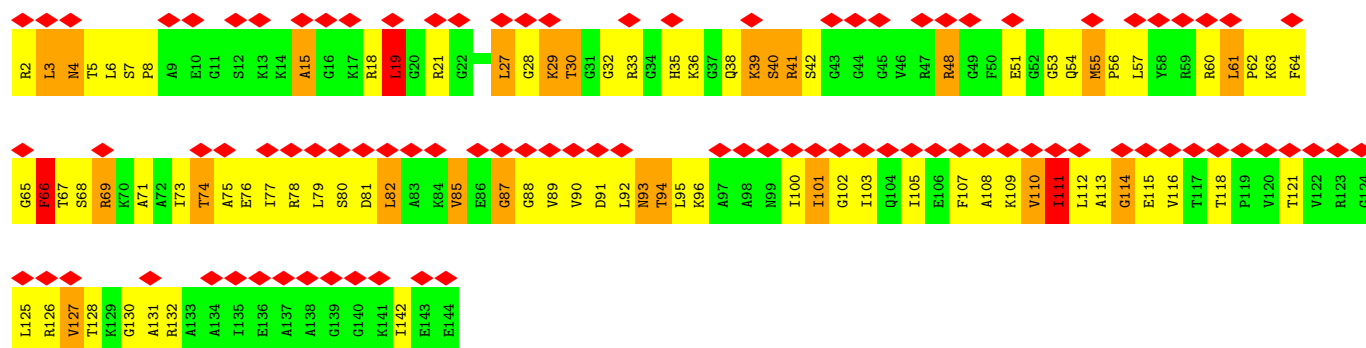
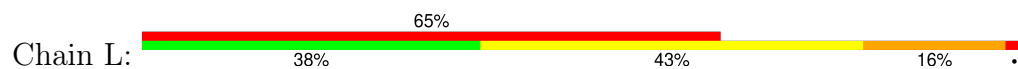


• Molecule 19: 50S ribosomal protein L14

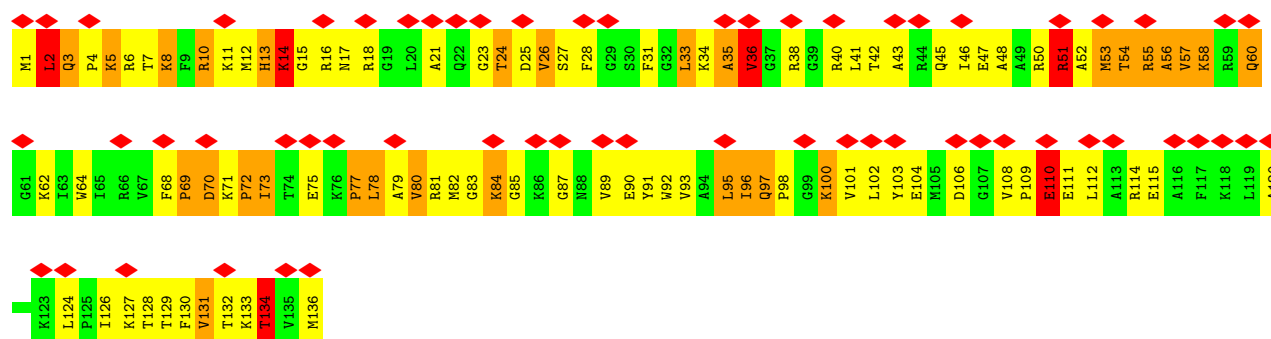




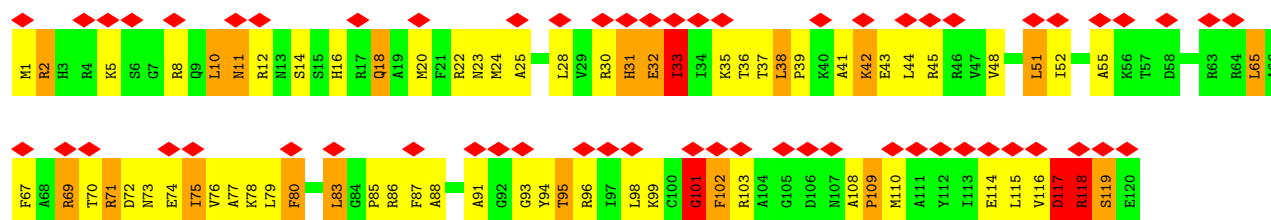
• Molecule 20: 50S ribosomal protein L15



• Molecule 21: 50S ribosomal protein L16

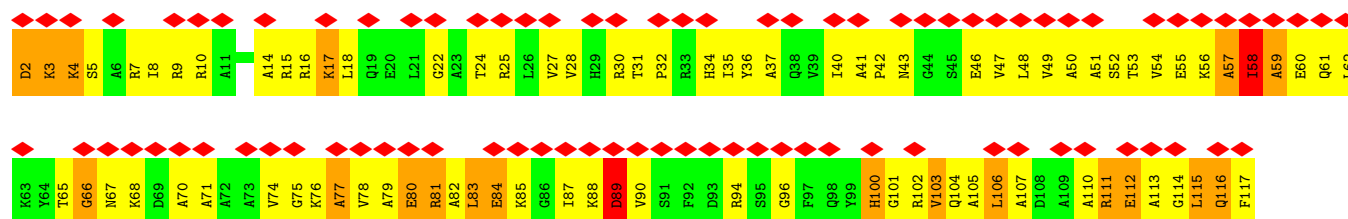


• Molecule 22: 50S ribosomal protein L17

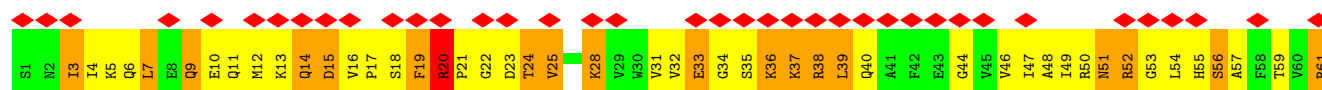
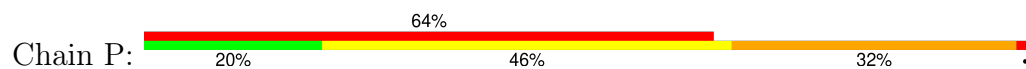


• Molecule 23: 50S ribosomal protein L18

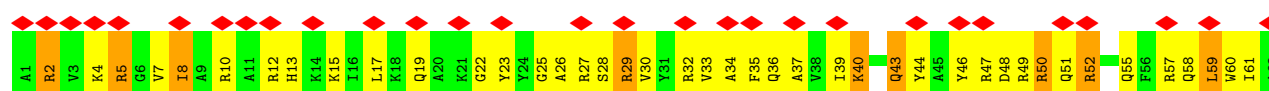




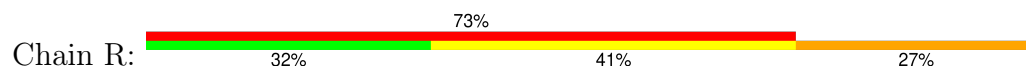
• Molecule 24: 50S ribosomal protein L19



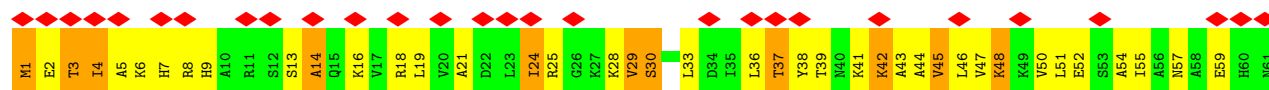
• Molecule 25: 50S ribosomal protein L20

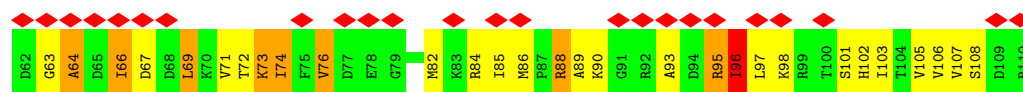


• Molecule 26: 50S ribosomal protein L21

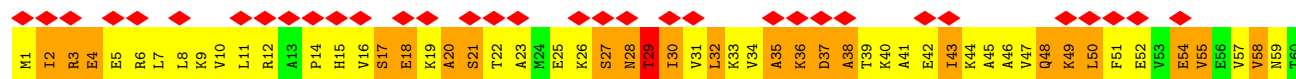
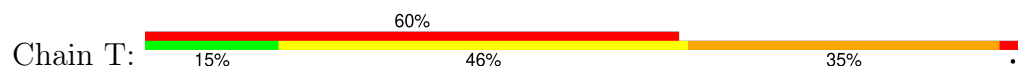


• Molecule 27: 50S ribosomal protein L22

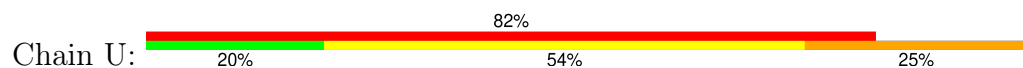




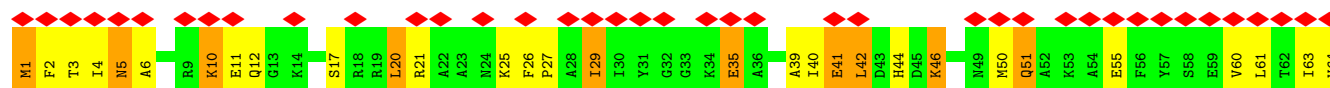
• Molecule 28: 50S ribosomal protein L23



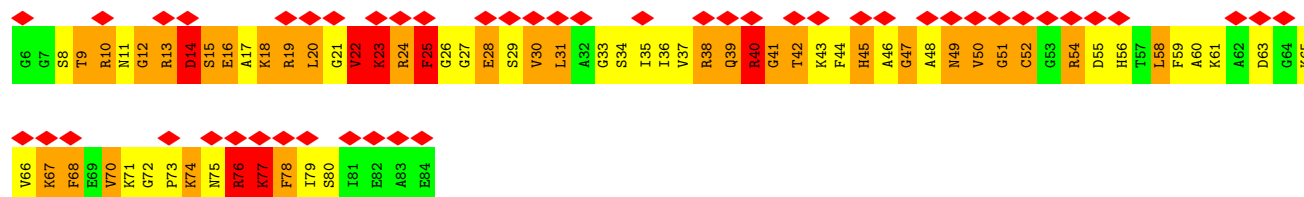
• Molecule 29: 50S ribosomal protein L24



• Molecule 30: 50S ribosomal protein L25

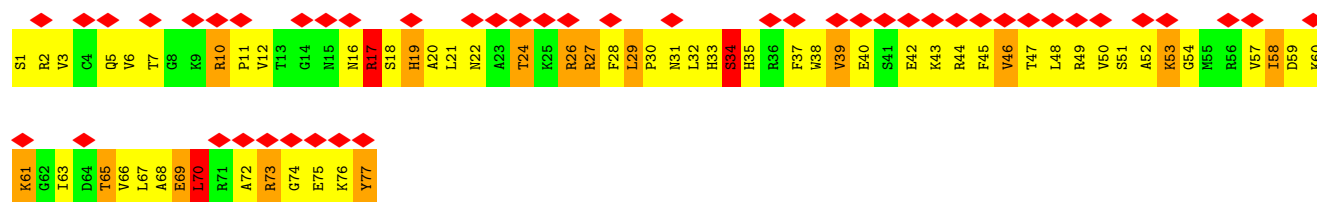


• Molecule 31: 50S ribosomal protein L27

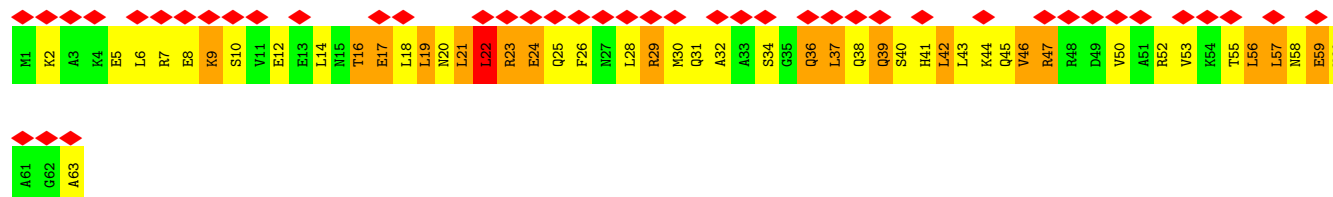


• Molecule 32: 50S ribosomal protein L28

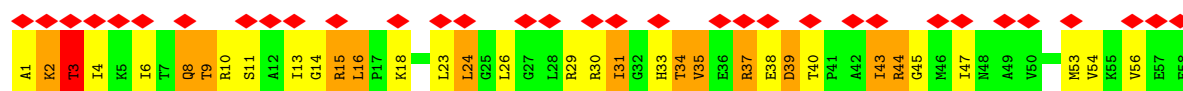




• Molecule 33: 50S ribosomal protein L29



• Molecule 34: 50S ribosomal protein L30



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	349744	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Defocus groups	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	148721	Depositor
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor
Maximum map value	0.004	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.0011	Depositor
Map size (\AA)	390.264, 390.264, 390.264	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0605, 1.0605, 1.0605	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, ERY, UNL

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	0.52	0/450	0.79	0/599
2	1	0.38	0/417	0.64	0/554
3	2	0.52	0/380	0.71	0/498
4	3	0.50	0/513	0.70	1/676 (0.1%)
5	4	0.41	0/303	0.64	0/397
6	5	0.31	0/18	0.53	0/26
8	7	0.44	0/65	0.95	1/99 (1.0%)
9	A	0.85	14/68599 (0.0%)	1.70	1689/107011 (1.6%)
10	B	0.75	0/2801	1.57	48/4365 (1.1%)
11	C	0.48	0/2122	0.74	1/2852 (0.0%)
12	D	0.61	0/1586	0.80	2/2134 (0.1%)
13	E	0.51	0/1571	0.73	0/2113
14	F	0.33	0/1435	0.55	0/1926
15	G	0.38	0/1343	0.61	0/1816
16	H	0.32	0/436	0.57	0/586
17	I	0.23	0/1046	0.47	0/1410
18	J	0.60	0/1152	0.84	1/1551 (0.1%)
19	K	0.61	1/948 (0.1%)	0.83	0/1268
20	L	0.50	0/1054	0.80	2/1403 (0.1%)
21	M	0.55	0/1093	0.78	0/1460
22	N	0.55	0/974	0.82	2/1301 (0.2%)
23	O	0.42	0/902	0.66	0/1209
24	P	0.52	0/929	0.72	0/1242
25	Q	0.73	0/960	0.89	1/1278 (0.1%)
26	R	0.68	2/829 (0.2%)	0.85	1/1107 (0.1%)
27	S	0.63	0/864	0.84	0/1156
28	T	0.51	0/745	0.80	0/994
29	U	0.45	0/788	0.75	0/1051
30	V	0.47	0/766	0.65	0/1025
31	W	0.67	0/603	0.93	1/797 (0.1%)
32	X	0.43	0/635	0.75	1/848 (0.1%)
33	Y	0.39	0/510	0.63	0/677

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
34	Z	0.58	0/453	0.93	2/605 (0.3%)
All	All	0.77	17/97290 (0.0%)	1.52	1753/146034 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	D	0	1
18	J	0	1
22	N	0	1
All	All	0	3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1142	A	N9-C4	-8.37	1.32	1.37
9	A	984	A	C5-C6	-7.42	1.34	1.41
26	R	86	GLN	CB-CG	7.24	1.72	1.52
9	A	1783	A	N7-C5	-6.73	1.35	1.39
9	A	2606	C	N1-C6	-5.88	1.33	1.37

The worst 5 of 1753 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	571	U	O4'-C1'-N1	17.58	122.26	108.20
9	A	2848	G	P-O3'-C3'	17.00	140.11	119.70
9	A	627	A	P-O3'-C3'	16.26	139.22	119.70
9	A	984	A	N1-C6-N6	16.12	128.27	118.60
9	A	1603	A	P-O3'-C3'	-15.82	100.71	119.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	D	191	GLY	Peptide
18	J	110	PRO	Peptide
22	N	101	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	444	0	461	53	0
2	1	410	0	440	69	0
3	2	377	0	418	27	0
4	3	504	0	574	68	0
5	4	302	0	341	48	0
6	5	41	0	27	3	0
7	6	8	0	0	3	0
8	7	59	0	35	3	0
9	A	61251	0	30809	3080	0
10	B	2506	0	1271	108	0
11	C	2083	0	2157	319	0
12	D	1565	0	1616	271	0
13	E	1552	0	1619	199	0
14	F	1411	0	1447	207	0
15	G	1323	0	1374	223	0
16	H	431	0	451	83	0
17	I	1032	0	1088	132	0
18	J	1129	0	1162	214	0
19	K	939	0	1012	153	0
20	L	1045	0	1117	169	0
21	M	1074	0	1157	149	0
22	N	961	0	1000	121	0
23	O	892	0	923	113	0
24	P	917	0	965	185	0
25	Q	947	0	1022	191	0
26	R	816	0	839	145	0
27	S	857	0	922	91	0
28	T	739	0	807	153	0
29	U	780	0	834	100	0
30	V	753	0	780	60	0
31	W	596	0	610	284	0
32	X	625	0	655	109	0
33	Y	509	0	543	72	0
34	Z	449	0	491	45	0
35	5	4	0	0	0	0
36	A	51	0	67	4	0
All	All	89382	0	59034	6679	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 45.

The worst 5 of 6679 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)
24:P:50:ARG:CG	24:P:57:ALA:H	1.24	1.48
24:P:50:ARG:HD2	24:P:51:ASN:N	1.27	1.41
24:P:50:ARG:HG2	24:P:57:ALA:N	1.13	1.40
25:Q:63:ARG:NH1	25:Q:96:ASP:HA	1.37	1.35
12:D:114:LYS:N	12:D:114:LYS:HE3	1.41	1.33

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	0	54/56 (96%)	41 (76%)	9 (17%)	4 (7%)	1	10
2	1	48/50 (96%)	37 (77%)	6 (12%)	5 (10%)	0	6
3	2	44/46 (96%)	37 (84%)	7 (16%)	0	100	100
4	3	62/64 (97%)	53 (86%)	5 (8%)	4 (6%)	1	12
5	4	36/38 (95%)	24 (67%)	9 (25%)	3 (8%)	0	9
11	C	269/271 (99%)	197 (73%)	47 (18%)	25 (9%)	0	8
12	D	207/209 (99%)	141 (68%)	32 (16%)	34 (16%)	0	2
13	E	199/201 (99%)	145 (73%)	34 (17%)	20 (10%)	0	7
14	F	175/177 (99%)	123 (70%)	36 (21%)	16 (9%)	0	8
15	G	174/176 (99%)	111 (64%)	38 (22%)	25 (14%)	0	3
16	H	54/56 (96%)	21 (39%)	13 (24%)	20 (37%)	0	0
17	I	139/141 (99%)	84 (60%)	41 (30%)	14 (10%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	J	140/142 (99%)	104 (74%)	24 (17%)	12 (9%)	0	9
19	K	120/122 (98%)	88 (73%)	18 (15%)	14 (12%)	0	4
20	L	141/143 (99%)	100 (71%)	30 (21%)	11 (8%)	1	10
21	M	134/136 (98%)	96 (72%)	18 (13%)	20 (15%)	0	3
22	N	118/120 (98%)	91 (77%)	16 (14%)	11 (9%)	0	8
23	O	114/116 (98%)	85 (75%)	18 (16%)	11 (10%)	0	7
24	P	112/114 (98%)	78 (70%)	20 (18%)	14 (12%)	0	4
25	Q	115/117 (98%)	100 (87%)	7 (6%)	8 (7%)	1	11
26	R	101/103 (98%)	76 (75%)	14 (14%)	11 (11%)	0	6
27	S	108/110 (98%)	89 (82%)	14 (13%)	5 (5%)	2	17
28	T	91/93 (98%)	49 (54%)	26 (29%)	16 (18%)	0	2
29	U	100/102 (98%)	66 (66%)	15 (15%)	19 (19%)	0	2
30	V	92/94 (98%)	75 (82%)	15 (16%)	2 (2%)	5	29
31	W	77/79 (98%)	31 (40%)	22 (29%)	24 (31%)	0	0
32	X	75/77 (97%)	58 (77%)	10 (13%)	7 (9%)	0	8
33	Y	61/63 (97%)	38 (62%)	15 (25%)	8 (13%)	0	4
34	Z	56/58 (97%)	47 (84%)	5 (9%)	4 (7%)	1	11
All	All	3216/3274 (98%)	2285 (71%)	564 (18%)	367 (11%)	1	5

5 of 367 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	51	ARG
1	0	54	ILE
2	1	16	THR
5	4	4	ARG
11	C	77	VAL

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%)	39 (83%)	8 (17%)	1	9
2	1	45/45 (100%)	37 (82%)	8 (18%)	1	8
3	2	38/38 (100%)	27 (71%)	11 (29%)	0	2
4	3	51/51 (100%)	42 (82%)	9 (18%)	1	8
5	4	34/34 (100%)	28 (82%)	6 (18%)	1	8
11	C	216/216 (100%)	170 (79%)	46 (21%)	1	5
12	D	164/164 (100%)	133 (81%)	31 (19%)	1	7
13	E	165/165 (100%)	110 (67%)	55 (33%)	0	1
14	F	148/148 (100%)	116 (78%)	32 (22%)	1	5
15	G	137/137 (100%)	106 (77%)	31 (23%)	1	5
16	H	44/44 (100%)	34 (77%)	10 (23%)	0	4
17	I	109/109 (100%)	91 (84%)	18 (16%)	2	9
18	J	116/116 (100%)	92 (79%)	24 (21%)	1	6
19	K	103/103 (100%)	77 (75%)	26 (25%)	0	3
20	L	102/102 (100%)	82 (80%)	20 (20%)	1	7
21	M	109/109 (100%)	81 (74%)	28 (26%)	0	3
22	N	100/100 (100%)	82 (82%)	18 (18%)	1	8
23	O	86/86 (100%)	67 (78%)	19 (22%)	1	5
24	P	99/99 (100%)	66 (67%)	33 (33%)	0	1
25	Q	89/89 (100%)	68 (76%)	21 (24%)	0	4
26	R	84/84 (100%)	66 (79%)	18 (21%)	1	5
27	S	93/93 (100%)	72 (77%)	21 (23%)	1	5
28	T	80/80 (100%)	53 (66%)	27 (34%)	0	1
29	U	83/83 (100%)	66 (80%)	17 (20%)	1	6
30	V	78/78 (100%)	62 (80%)	16 (20%)	1	6
31	W	59/59 (100%)	38 (64%)	21 (36%)	0	1
32	X	67/67 (100%)	51 (76%)	16 (24%)	0	3
33	Y	55/55 (100%)	42 (76%)	13 (24%)	0	4
34	Z	48/48 (100%)	35 (73%)	13 (27%)	0	3
All	All	2649/2649 (100%)	2033 (77%)	616 (23%)	2	4

5 of 616 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	R	51	VAL
31	W	77	LYS
27	S	29	VAL
26	R	48	LYS
29	U	4	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 111 such sidechains are listed below:

Mol	Chain	Res	Type
19	K	3	GLN
33	Y	58	ASN
22	N	73	ASN
33	Y	41	HIS
30	V	44	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B	115/118 (97%)	34 (29%)	17 (14%)
6	5	0/2	-	-
8	7	2/3 (66%)	0	0
9	A	2848/2904 (98%)	908 (31%)	423 (14%)
All	All	2965/3027 (97%)	942 (31%)	440 (14%)

5 of 942 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A	10	A
9	A	13	A
9	A	14	A
9	A	15	G
9	A	23	G

5 of 440 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	1497	U
9	A	1865	U
10	B	108	A
9	A	2728	U
9	A	1554	U

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

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
6	MA6	5	76	35,6,9	19,26,27	0.94	1 (5%)	18,38,41	1.24	1 (5%)

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
6	MA6	5	76	35,6,9	-	0/7/29/30	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	76	MA6	C6-N1	2.15	1.35	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	76	MA6	C2-N1-C6	2.14	118.94	116.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	5	76	MA6	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is unknown - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
36	ERY	A	9000	-	53,53,53	0.82	1 (1%)	82,82,82	1.69	18 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ERY	A	9000	-	-	9/72/107/107	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A	9000	ERY	C6-C5	2.43	1.59	1.55

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A	9000	ERY	C25-C24-C23	-5.06	102.75	110.02
36	A	9000	ERY	O7-C5-C6	-4.99	100.45	106.40
36	A	9000	ERY	O2-C1-O1	-3.68	117.30	123.95
36	A	9000	ERY	C3-C2-C1	-3.45	102.96	109.93
36	A	9000	ERY	C27-C26-C25	-3.17	108.47	113.27

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

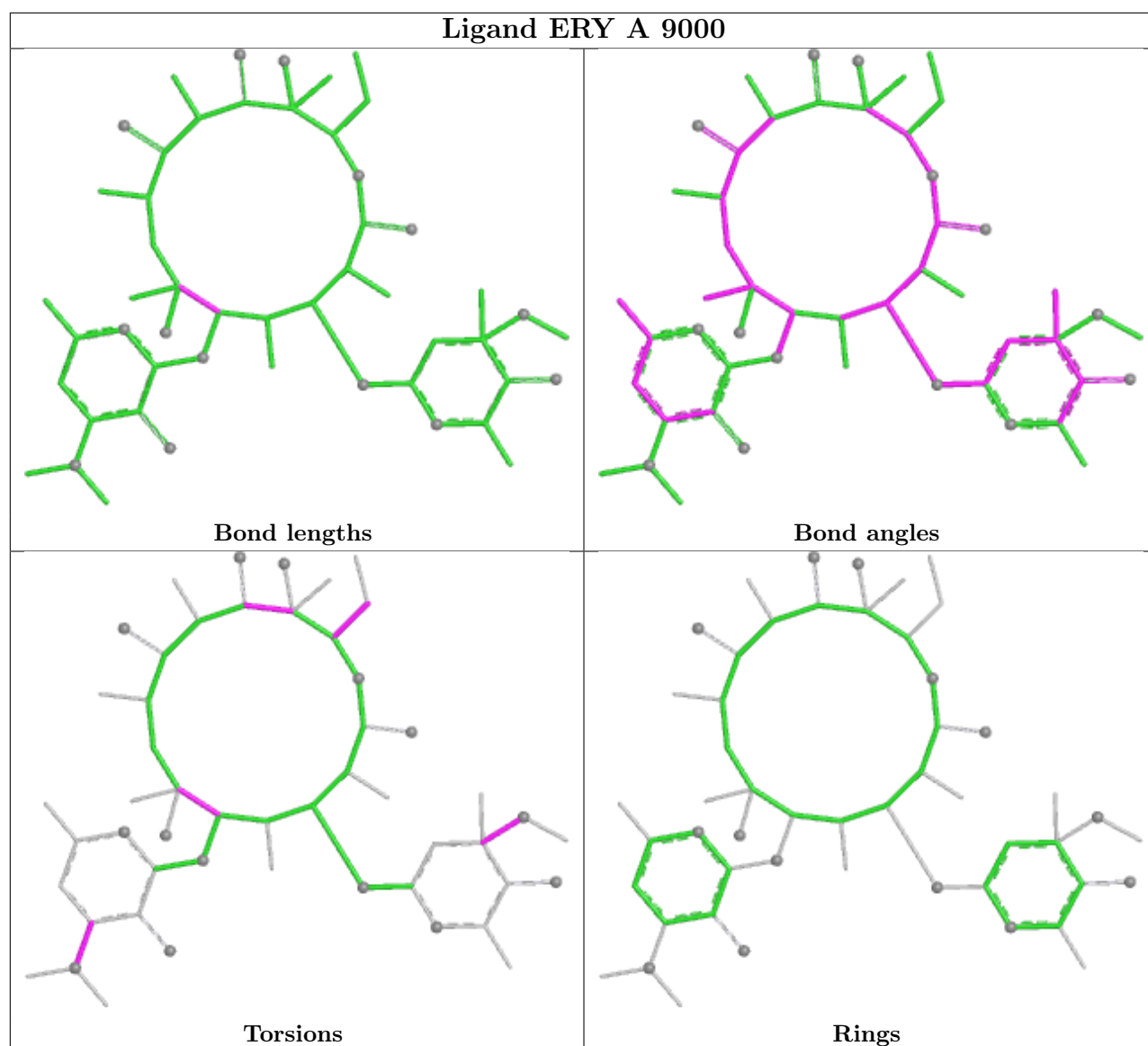
Mol	Chain	Res	Type	Atoms
36	A	9000	ERY	C15-C16-O5-C20
36	A	9000	ERY	C19-C16-O5-C20
36	A	9000	ERY	C10-C11-C12-O13
36	A	9000	ERY	C25-C24-N1-C28
36	A	9000	ERY	C4-C5-C6-C32

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	A	9000	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.

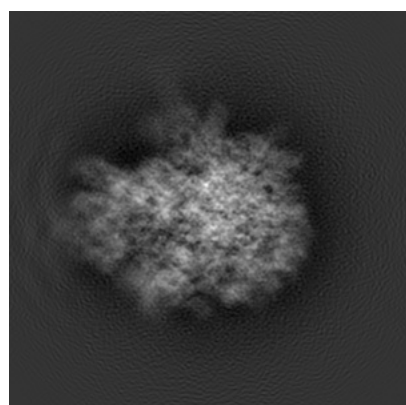
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5771. These allow visual inspection of the internal detail of the map and identification of artifacts.

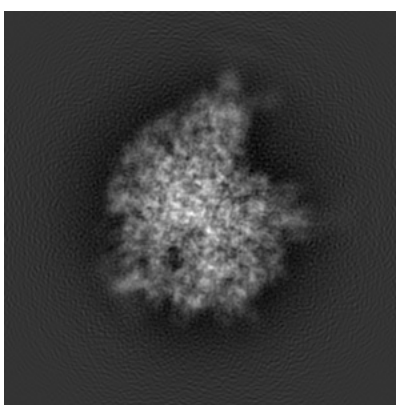
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

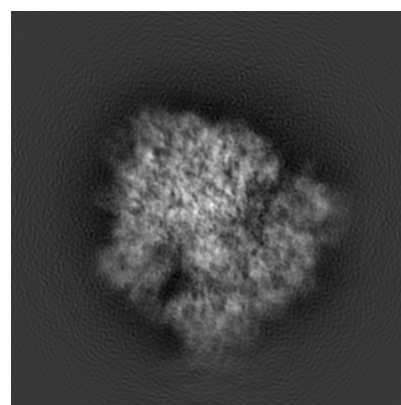
6.1.1 Primary map



X



Y

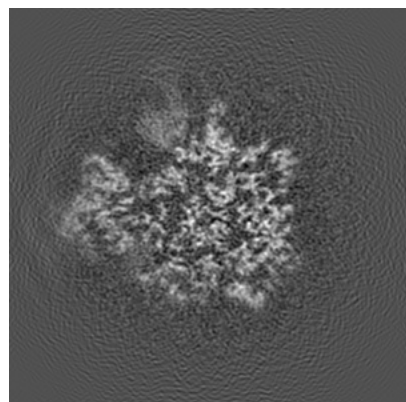


Z

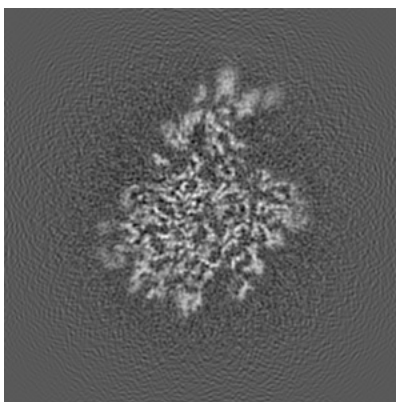
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

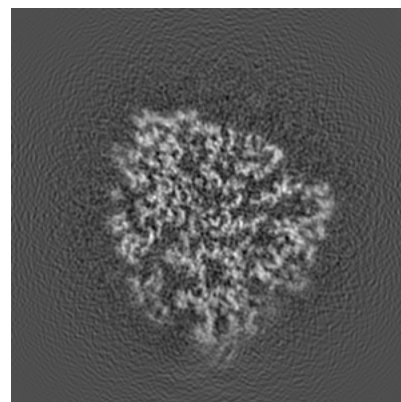
6.2.1 Primary map



X Index: 184



Y Index: 184

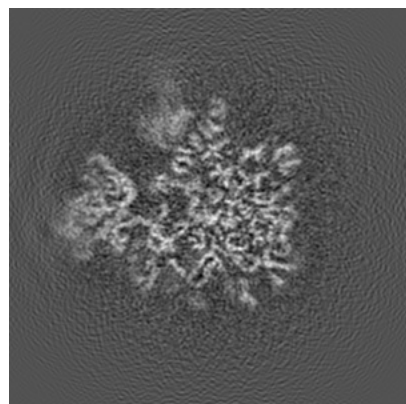


Z Index: 184

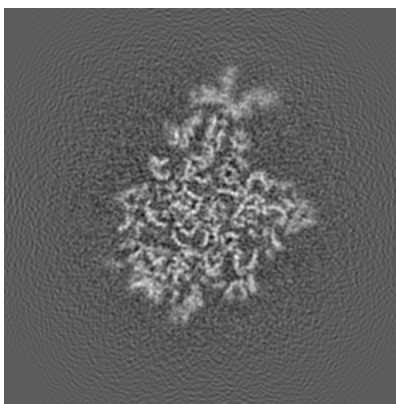
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

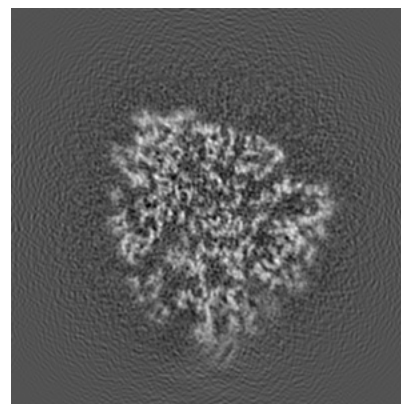
6.3.1 Primary map



X Index: 180



Y Index: 189

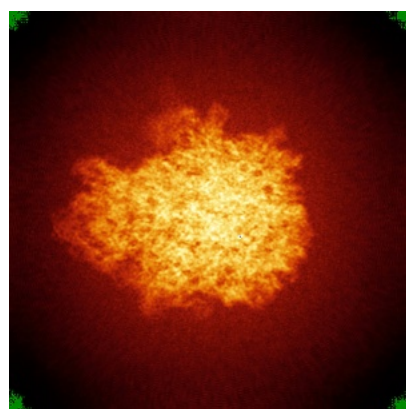


Z Index: 183

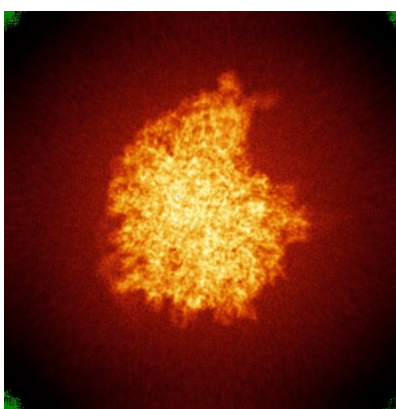
The images above show the largest variance slices of the map in three orthogonal directions.

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

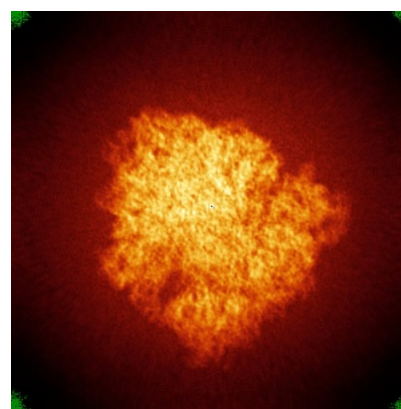
6.4.1 Primary map



X



Y

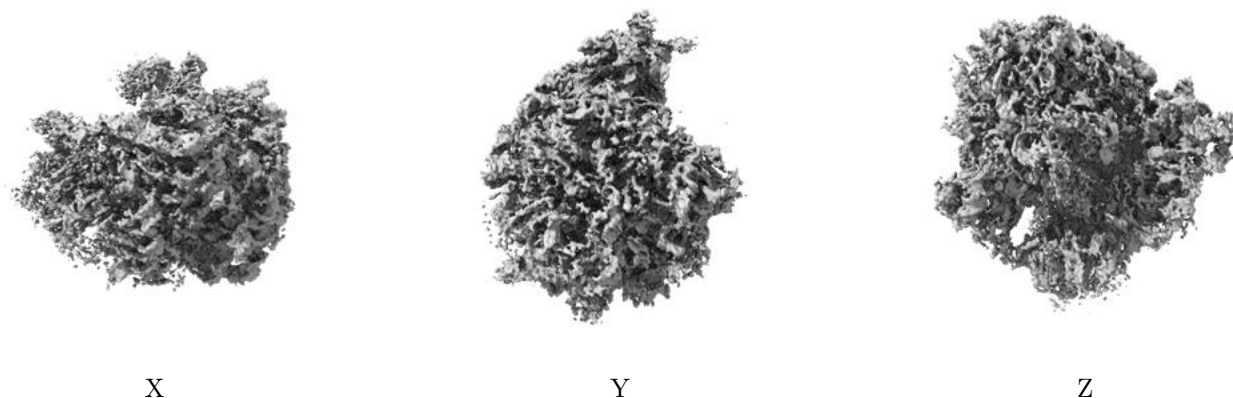


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

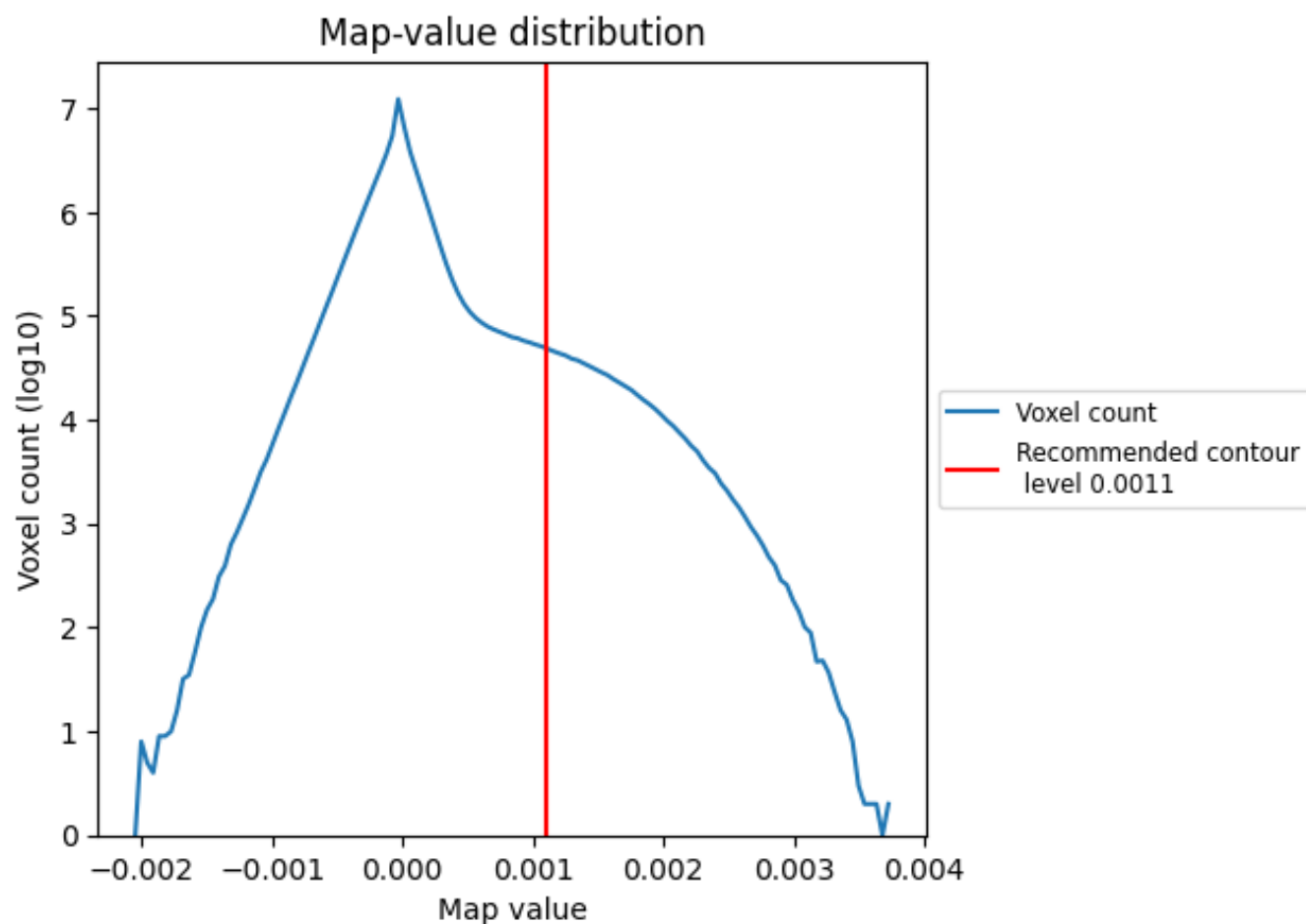
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

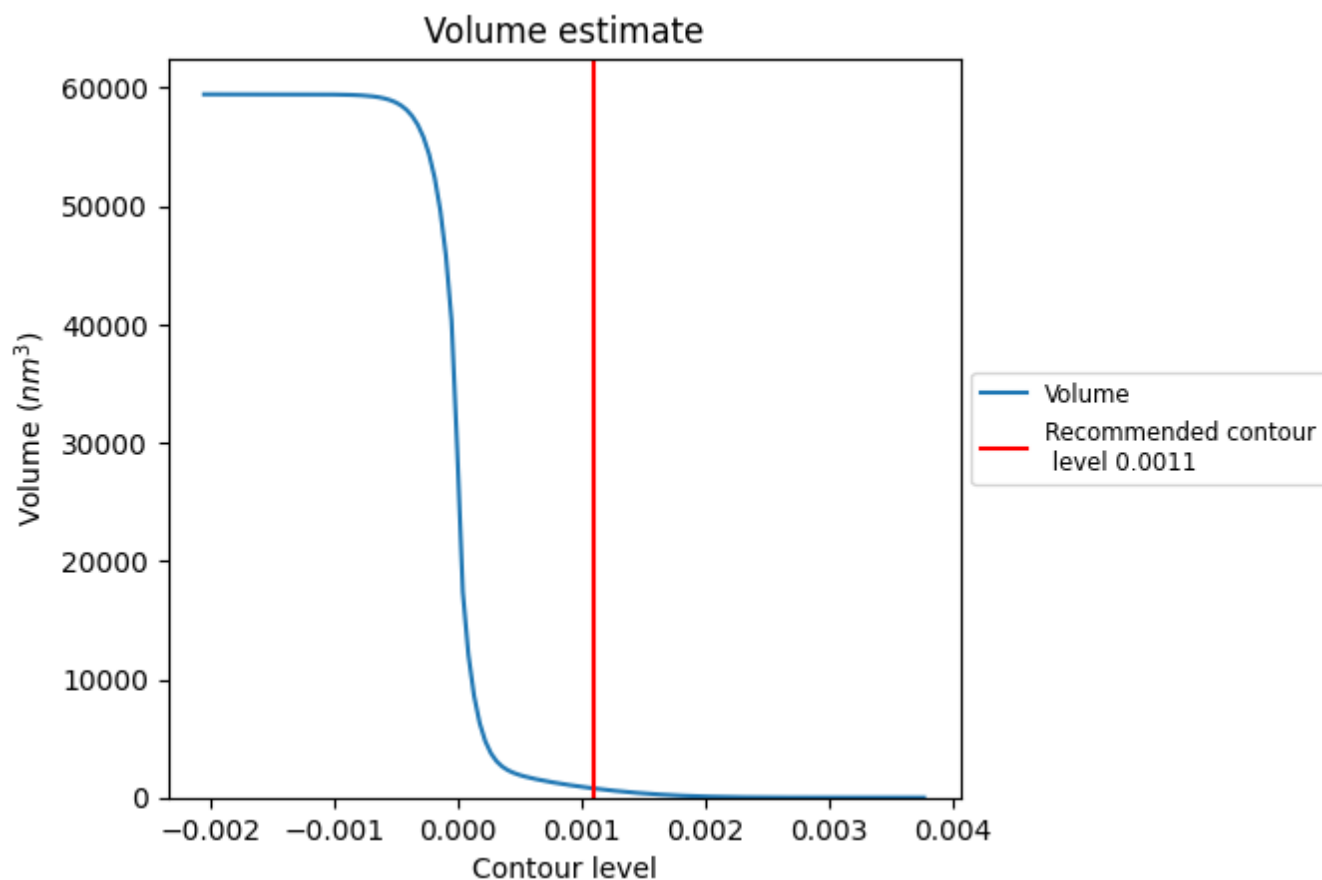
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

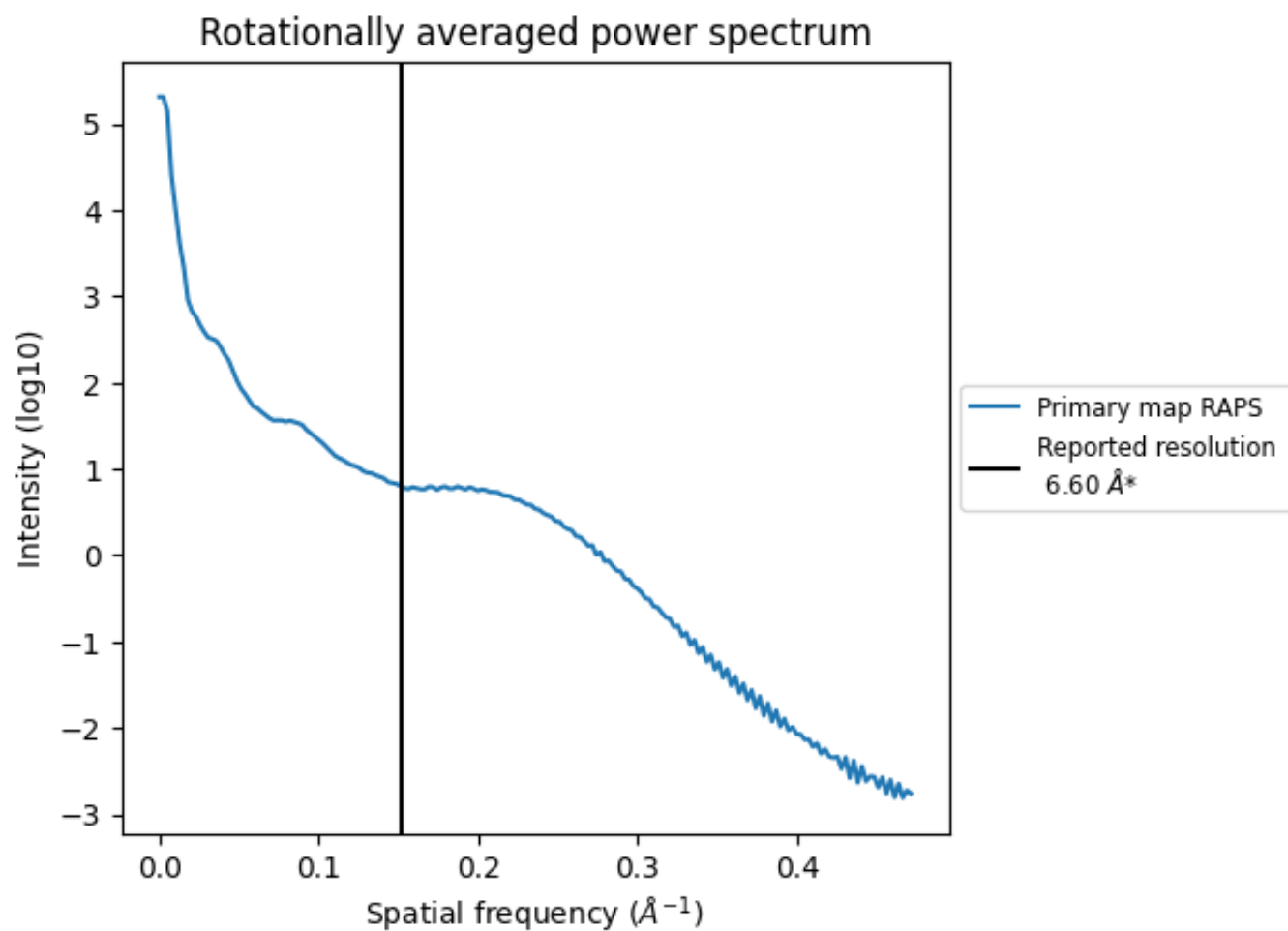
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 776 nm³; this corresponds to an approximate mass of 701 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 0.152 Å⁻¹

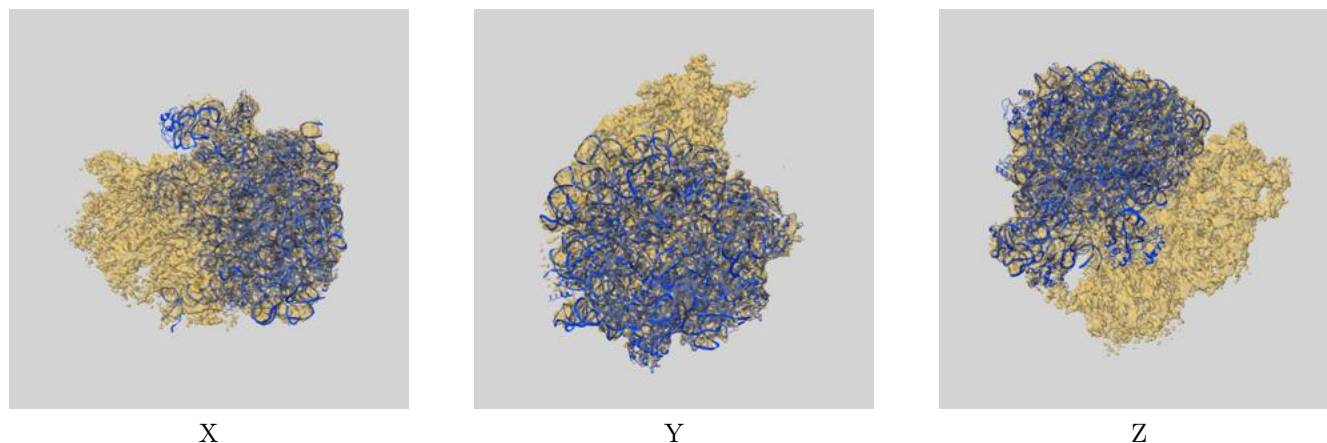
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

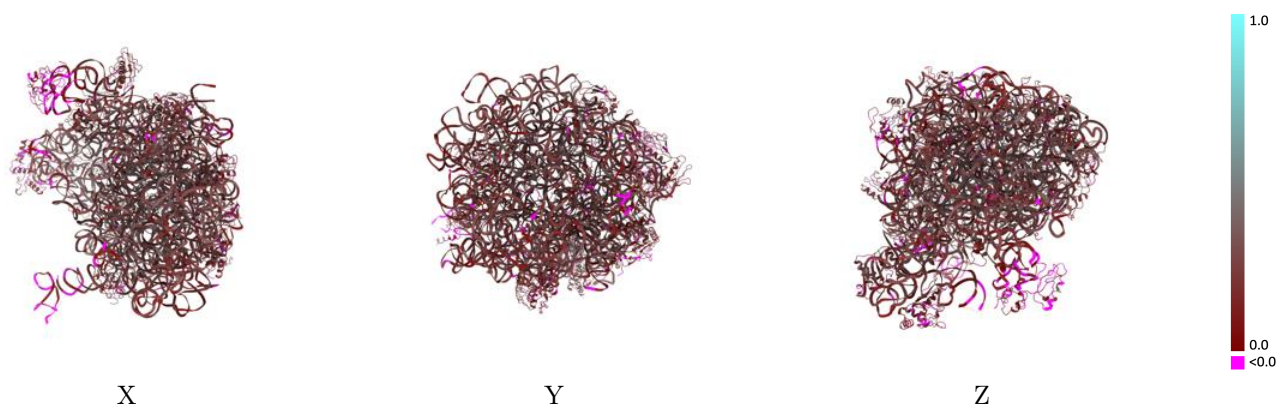
This section contains information regarding the fit between EMDB map EMD-5771 and PDB model 3J5L. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



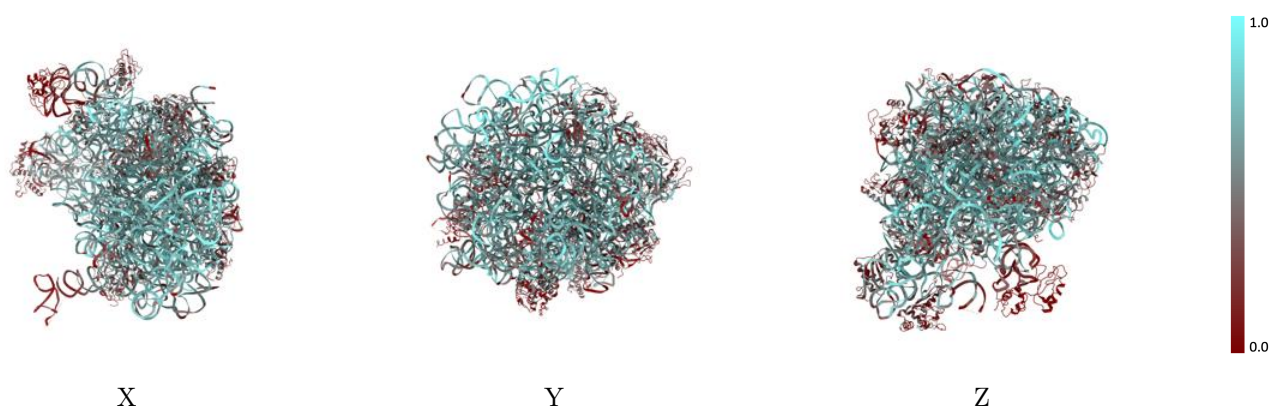
The images above show the 3D surface view of the map at the recommended contour level 0.0011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



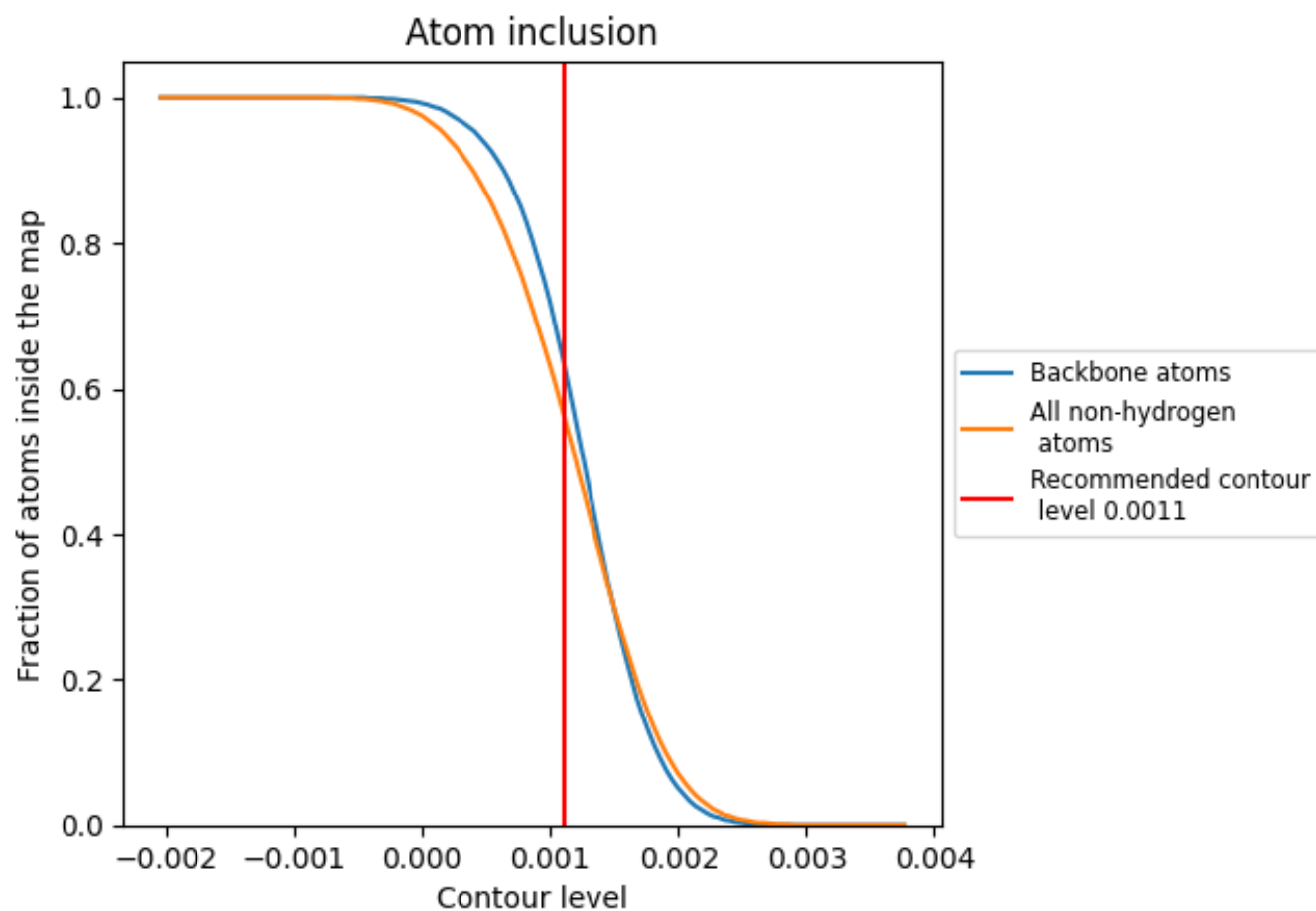
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0011).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 57% 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 (0.0011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5670	 0.2470
0	 0.3640	 0.2200
1	 0.3260	 0.1940
2	 0.4250	 0.2620
3	 0.3690	 0.2420
4	 0.4250	 0.2410
5	 0.4440	 0.2410
6	 0.6250	 0.3380
7	 0.6100	 0.3120
A	 0.6650	 0.2640
B	 0.6360	 0.2360
C	 0.3950	 0.2600
D	 0.3820	 0.2500
E	 0.2490	 0.1960
F	 0.1990	 0.1110
G	 0.2820	 0.1940
H	 0.0900	 0.1270
I	 0.0040	 0.0030
J	 0.3740	 0.2450
K	 0.3490	 0.2320
L	 0.3120	 0.2380
M	 0.4200	 0.2470
N	 0.3990	 0.2410
O	 0.2720	 0.1930
P	 0.3450	 0.2360
Q	 0.3940	 0.2070
R	 0.2660	 0.2300
S	 0.4040	 0.2150
T	 0.3150	 0.2000
U	 0.2130	 0.1780
V	 0.3280	 0.2110
W	 0.3450	 0.2220
X	 0.3790	 0.2340
Y	 0.2940	 0.2020
Z	 0.3390	 0.2070

