



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 02:02 PM UTC

PDB ID : 8R55 / pdb_00008r55
EMDB ID : EMD-18901
Title : Bacillus subtilis MutS2-collided disome complex (collided 70S)
Authors : Park, E.; Mackens-Kiani, T.; Berhane, R.; Esser, H.; Erdenebat, C.; Burroughs, A.M.; Berninghausen, O.; Aravind, L.; Beckmann, R.; Green, R.; Buskirk, A.R.
Deposited on : 2023-11-16
Resolution : 3.57 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

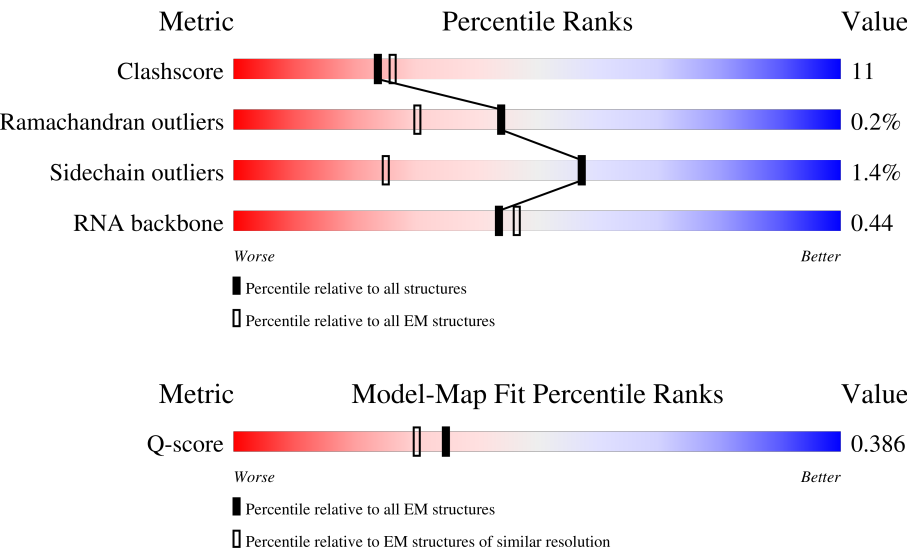
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.57 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	12682 (3.07 - 4.07)

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	59	12% 54% 36% 8%
2	1	48	54% 44%
3	2	44	89% 11%

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Mol	Chain	Length	Quality of chain
4	3	66	
5	4	37	
6	6	64	
7	7	73	
8	A	1533	
9	B	246	
10	C	218	
11	D	200	
12	E	166	
13	F	95	
14	G	156	
15	H	132	
16	I	130	
17	J	102	
18	K	131	
19	L	138	
20	M	121	
21	N	61	
22	O	89	
23	P	90	
24	Q	87	
25	R	79	
26	S	92	
27	T	88	
28	U	77	

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Mol	Chain	Length	Quality of chain
29	V	33	
30	Y	112	
31	Z	275	
32	a	207	
33	b	205	
34	c	178	
35	d	175	
36	e	142	
37	f	122	
38	i	146	
39	j	138	
40	k	119	
41	l	120	
42	m	115	
43	n	117	
44	o	101	
45	r	109	
46	s	93	
47	t	101	
48	u	82	
49	v	58	
50	w	65	
51	x	58	
52	X	2928	
53	z	785	

2 Entry composition [i](#)

There are 53 unique types of molecules in this entry. The entry contains 143867 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	54	Total	C	N	O	S	0	0
			426	262	86	71	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	48	Total	C	N	O	S	0	0
			402	244	80	74	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	44	Total	C	N	O	S	0	0
			368	222	89	55	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	48	SER	ALA	conflict	UNP A0A063XFQ7

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

- Molecule 6 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	63	Total	C	N	O	S	0	0
			499	312	91	91	5		

- Molecule 7 is a RNA chain called tRNA (73-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	73	Total	C	N	O	P	0	0
			1560	695	279	513	73		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	3	G	C	conflict	GB 1851743410
7	70	C	G	conflict	GB 1851743410

- Molecule 8 is a RNA chain called 16S rRNA (1533-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	1533	Total	C	N	O	P	0	0
			32891	14667	6034	10657	1533		

- Molecule 9 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	218	Total	C	N	O	S	0	0
			1757	1119	309	323	6		

- Molecule 10 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	206	Total	C	N	O	S	0	0
			1619	1011	304	301	3		

- Molecule 11 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	195	Total	C	N	O	S	0	0
			1569	991	291	285	2		

- Molecule 12 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	164	Total	C	N	O	S	0	0
			1219	767	225	225	2		

- Molecule 13 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	92	Total	C	N	O	S	0	0
			755	476	132	146	1		

- Molecule 14 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	149	Total	C	N	O	S	0	0
			1181	740	220	215	6		

- Molecule 15 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	131	Total	C	N	O	S	0	0
			1037	655	191	188	3		

- Molecule 16 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	125	Total	C	N	O	S	0	0
			966	599	191	175	1		

- Molecule 17 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	95	Total	C	N	O	S	0	0
			761	479	139	141	2		

- Molecule 18 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	114	Total	C	N	O	S	0	0
			839	516	164	157	2		

- Molecule 19 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	136	Total	C	N	O	S	0	0
			1052	653	211	186	2		

- Molecule 20 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	108	Total	C	N	O	S	0	0
			868	534	176	158			

- Molecule 21 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	60	Total	C	N	O	S	0	0
			498	317	98	78	5		

- Molecule 22 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	85	Total	C	N	O	S	0	0
			710	436	144	129	1		

- Molecule 23 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	88	Total	C	N	O	S	0	0
			695	441	128	124	2		

- Molecule 24 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	84	Total	C	N	O	S	0	0
			691	435	128	126	2		

- Molecule 25 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	64	Total	C	N	O	S	0	0
			518	332	96	88	2		

- Molecule 26 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	78	Total	C	N	O	S	0	0
			633	409	112	110	2		

- Molecule 27 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	83	Total	C	N	O	S	0	0
			637	390	130	116	1		

- Molecule 28 is a RNA chain called tRNA (77-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	77	Total	C	N	O	P	0	0
			1643	731	290	545	77		

- Molecule 29 is a RNA chain called mRNA (33-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	33	Total	C	N	O	P	0	0
			704	315	130	226	33		

- Molecule 30 is a RNA chain called 5S rRNA (112-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	112	Total	C	N	O	P	0	0
			2392	1068	435	778	111		

- Molecule 31 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	272	Total	C	N	O	S	0	0
			2083	1296	408	373	6		

- Molecule 32 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	206	Total	C	N	O	S	0	0
			1569	985	289	290	5		

- Molecule 33 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	205	Total	C	N	O	S	0	0
			1562	980	289	291	2		

- Molecule 34 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	176	Total	C	N	O	S	0	0
			1386	882	241	256	7		

- Molecule 35 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	175	Total	C	N	O	S	0	0
			1343	835	248	258	2		

- Molecule 36 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	142	Total	C	N	O	S	0	0
			1124	710	206	203	5		

- Molecule 37 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	122	Total	C	N	O	S	0	0
			921	571	173	173	4		

- Molecule 38 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	146	Total	C	N	O	S	0	0
			1082	671	207	202	2		

- Molecule 39 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	135	Total	C	N	O	S	0	0
			1076	690	205	176	5		

- Molecule 40 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	119	Total	C	N	O	S	0	0
			954	583	186	181	4		

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	120	Total	C	N	O	S	0	0
			913	564	176	172	1		

- Molecule 42 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	115	Total	C	N	O	S	0	0
			945	600	185	159	1		

- Molecule 43 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	n	117	Total	C	N	O	S	0	0
			941	591	189	157	4		

- Molecule 44 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	o	101	Total	C	N	O	S	0	0
			787	501	139	147			

- Molecule 45 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	r	109	Total	C	N	O	S	0	0
			843	525	164	151	3		

- Molecule 46 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	s	90	Total	C	N	O	S	0	0
			725	452	134	136	3		

- Molecule 47 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	t	101	Total	C	N	O	S	0	0
			763	478	142	139	4		

- Molecule 48 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	u	82	Total	C	N	O		0	0
			631	390	123	118			

- Molecule 49 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	v	58	Total	C	N	O	S	0	0
			445	275	92	76	2		

- Molecule 50 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	w	65	Total	C	N	O	S	0	0
			531	328	102	99	2		

- Molecule 51 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	58	Total	C	N	O	S	0	0
			456	281	89	85	1		

- Molecule 52 is a RNA chain called 23S RNA (2887-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
52	X	2887	Total	C	N	O	P	0	0
			62005	27661	11460	19998	2886		

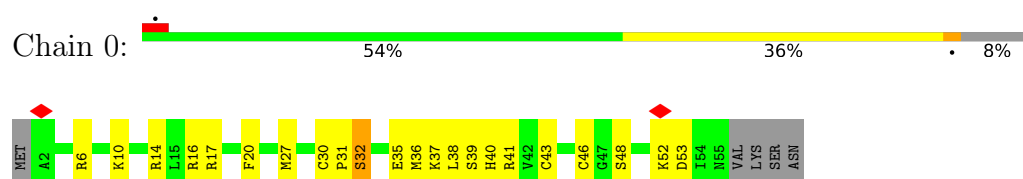
- Molecule 53 is a protein called Endonuclease MutS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	z	139	Total	C	N	O	S	0	0
			1083	683	195	204	1		

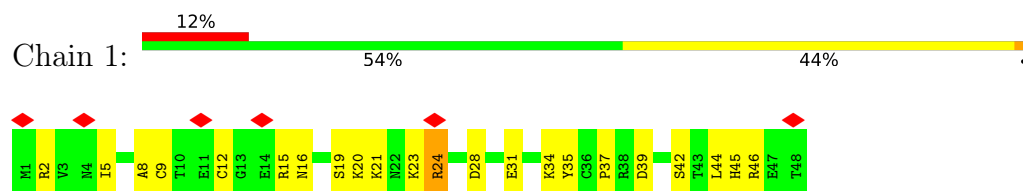
3 Residue-property plots [i](#)

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.

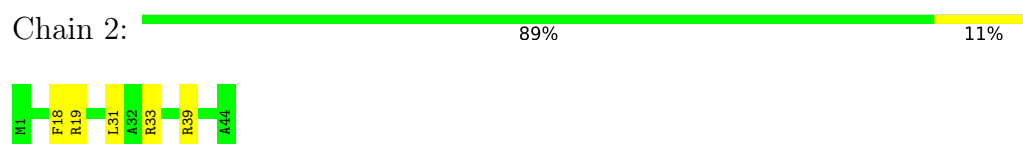
- Molecule 1: 50S ribosomal protein L32



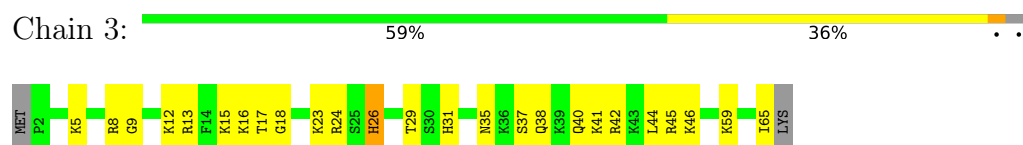
- Molecule 2: Large ribosomal subunit protein bL33



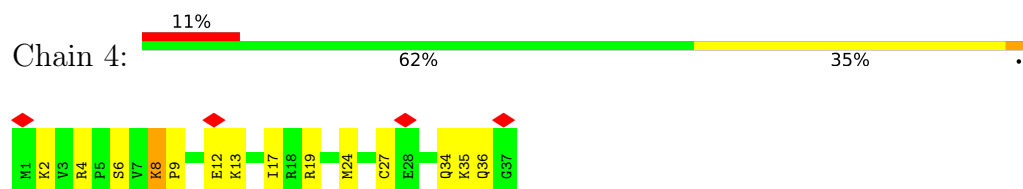
- Molecule 3: Large ribosomal subunit protein bL34



- Molecule 4: Large ribosomal subunit protein bL35



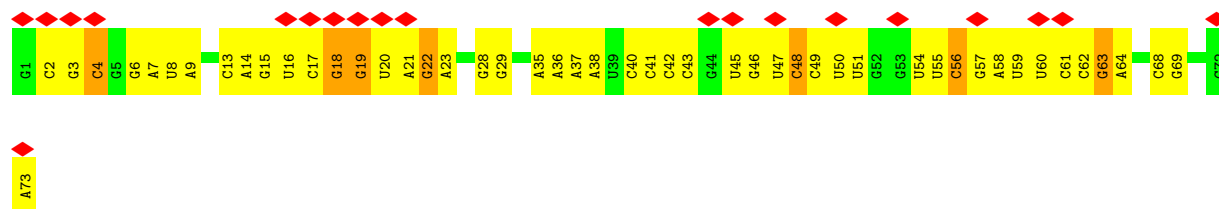
- Molecule 5: 50S ribosomal protein L36



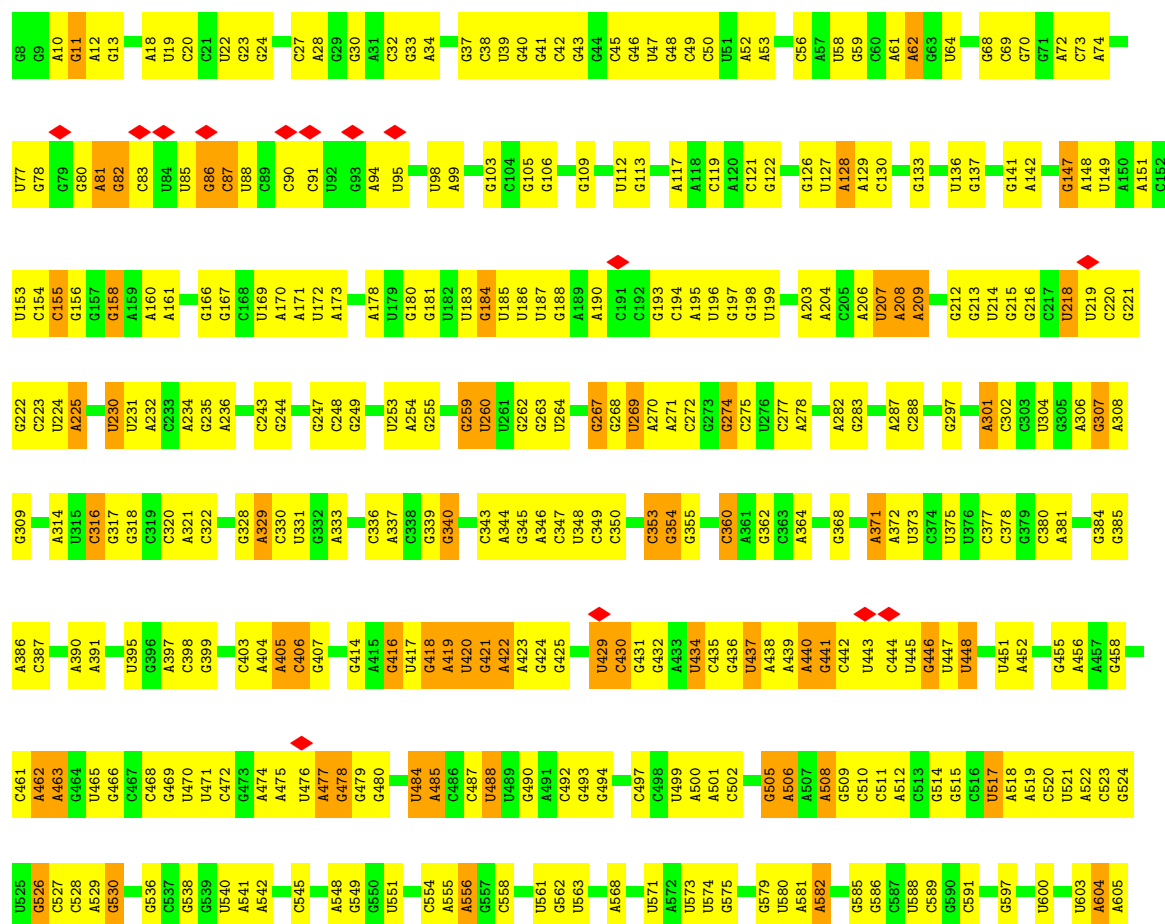
- Molecule 6: Large ribosomal subunit protein bL31

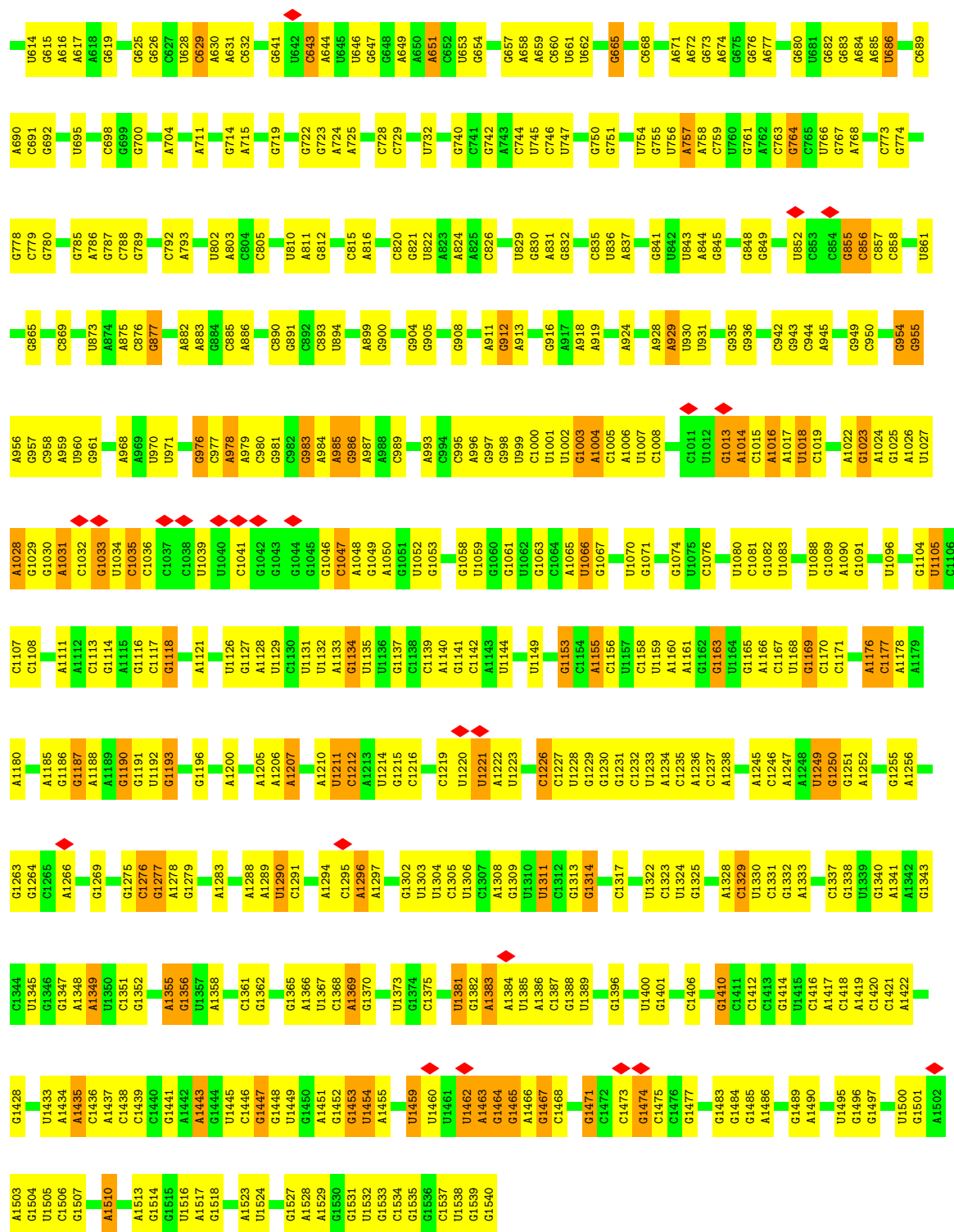


Chain 7: 27% 33% 58% 10%

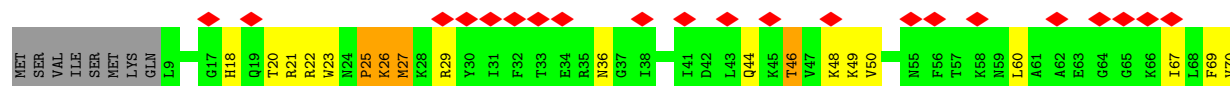


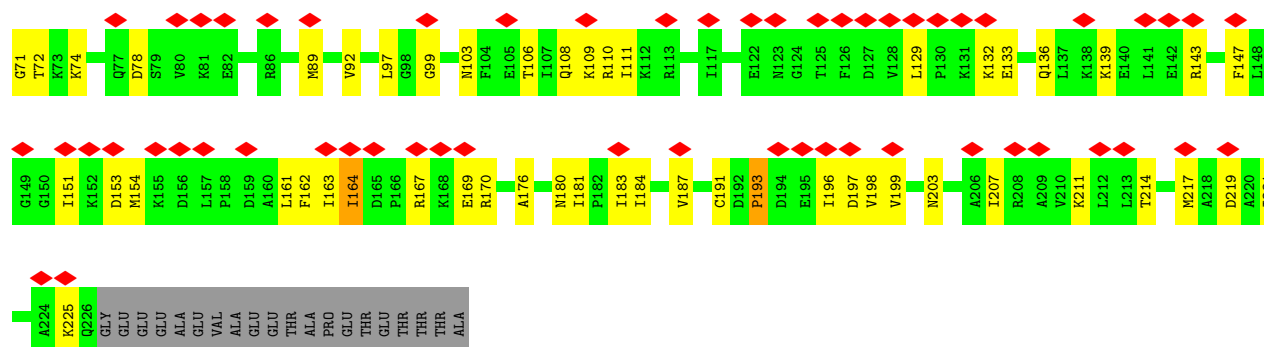
Chain A: 45% 46% 9%



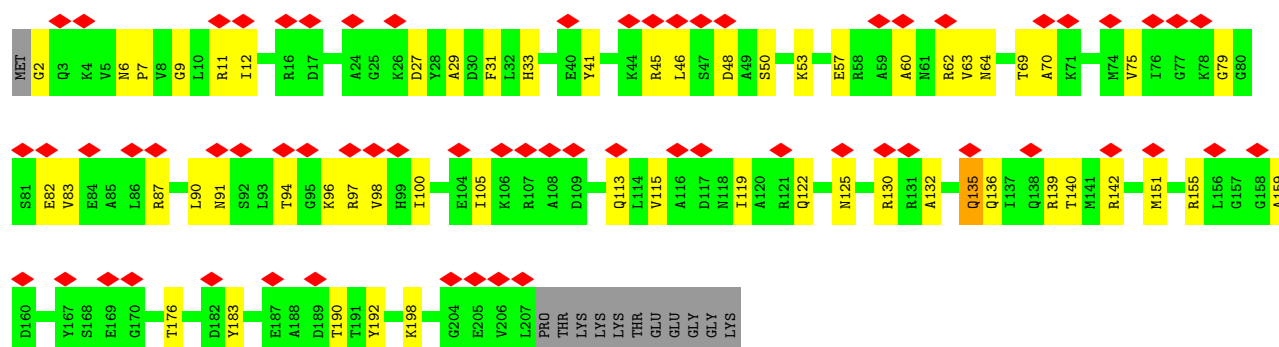


• Molecule 9: 30S ribosomal protein S2

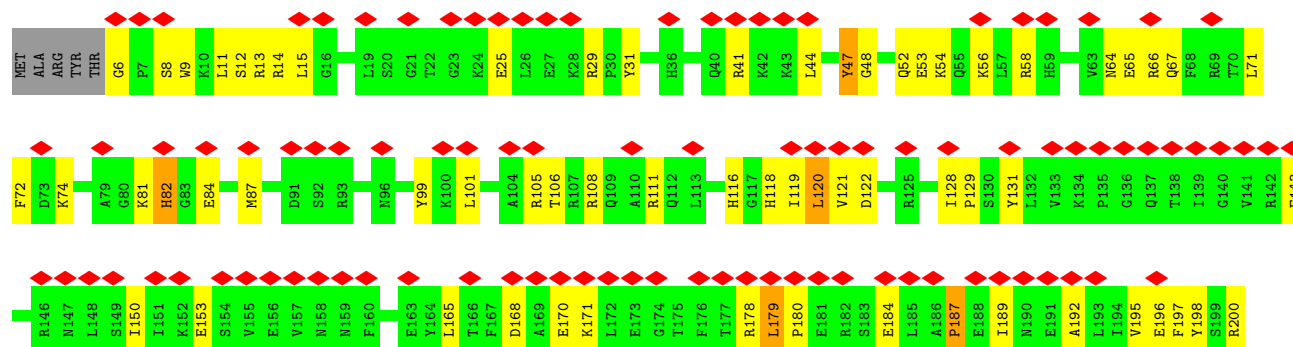




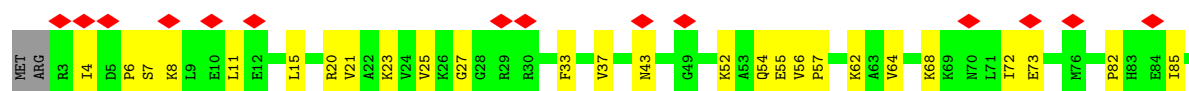
• Molecule 10: 30S ribosomal protein S3



• Molecule 11: 30S ribosomal protein S4

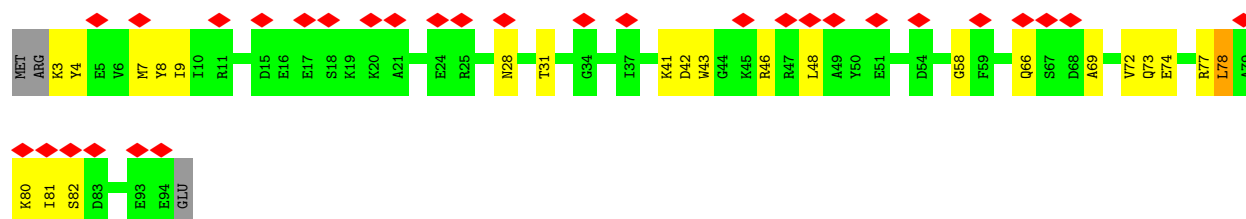
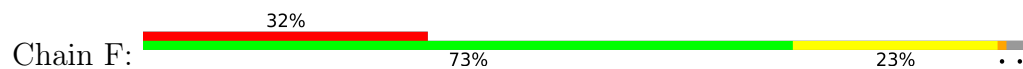


• Molecule 12: 30S ribosomal protein S5

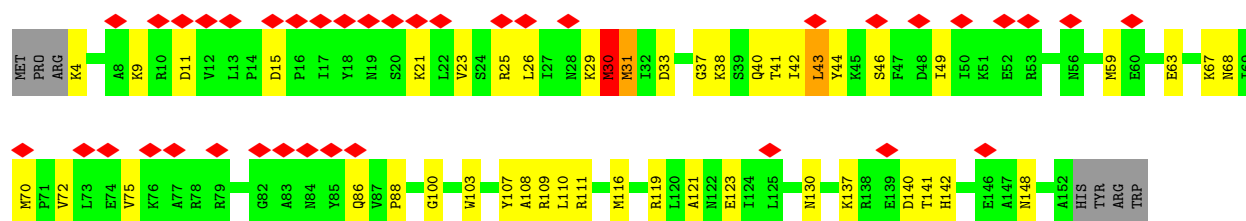




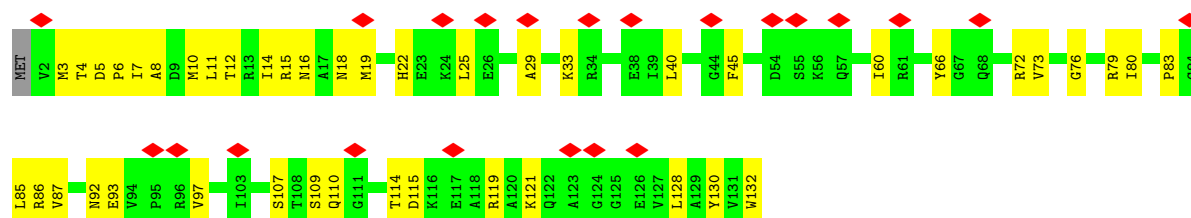
- Molecule 13: 30S ribosomal protein S6



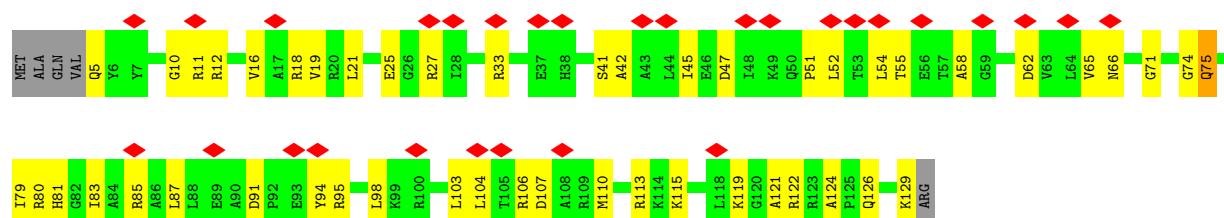
- Molecule 14: 30S ribosomal protein S7



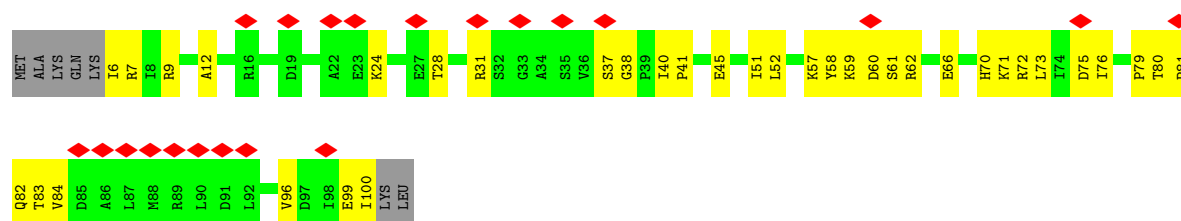
- Molecule 15: 30S ribosomal protein S8



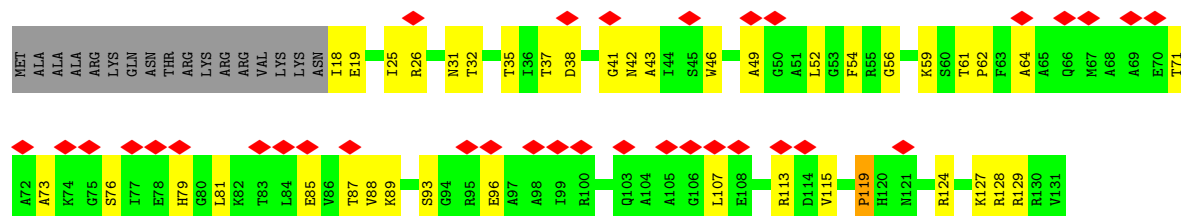
- Molecule 16: 30S ribosomal protein S9



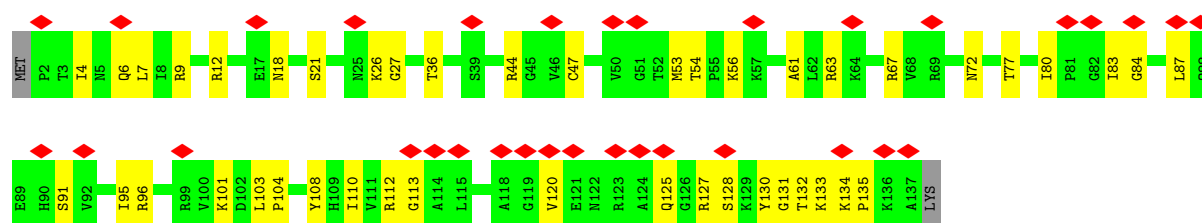
- Molecule 17: 30S ribosomal protein S10



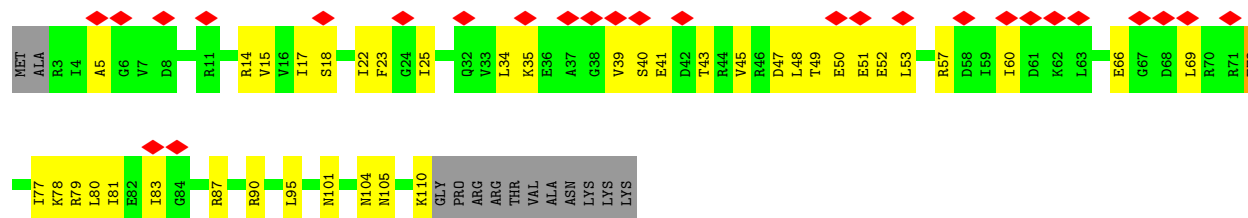
- Molecule 18: 30S ribosomal protein S11



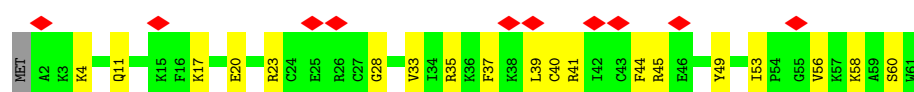
- Molecule 19: 30S ribosomal protein S12



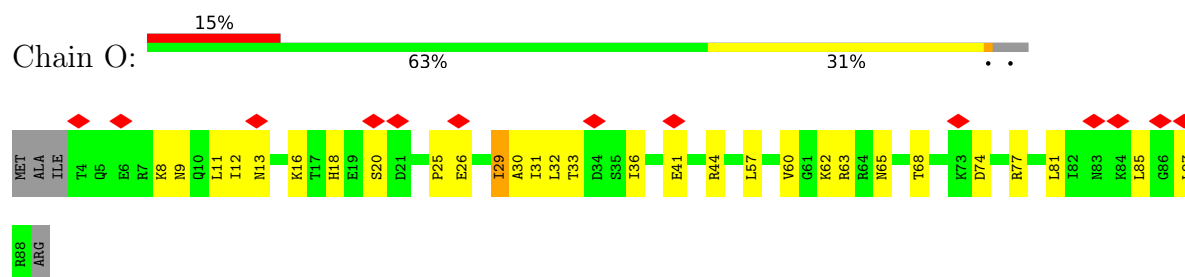
- Molecule 20: 30S ribosomal protein S13



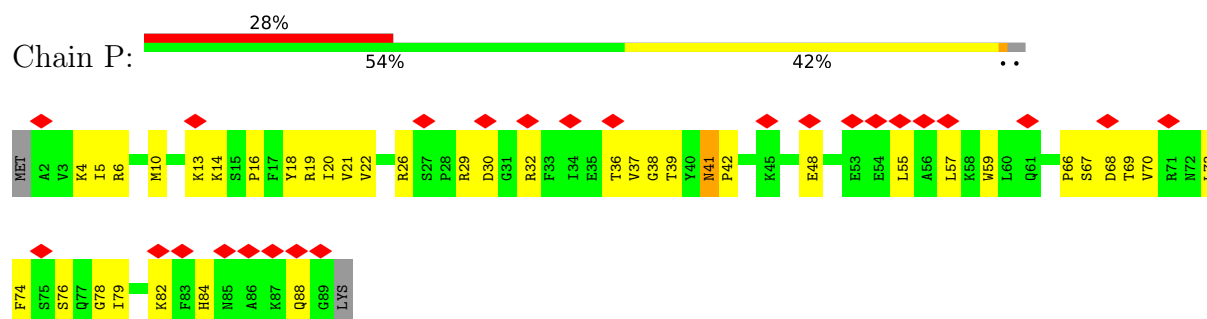
- Molecule 21: 30S ribosomal protein S14 type Z



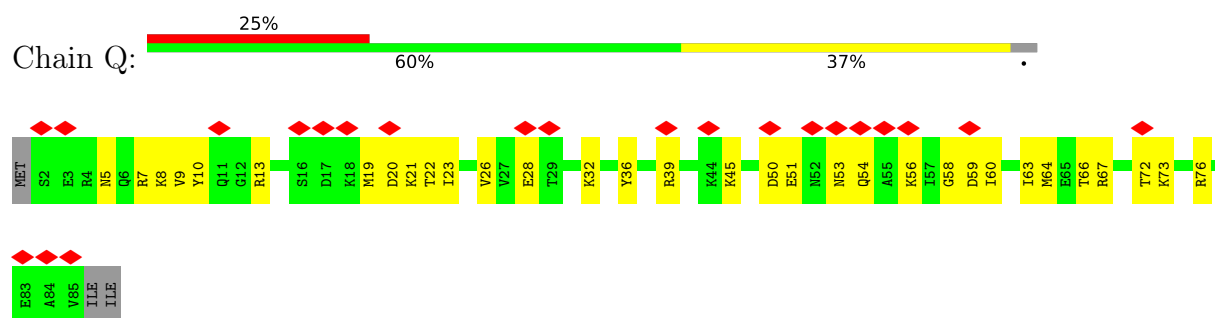
- Molecule 22: 30S ribosomal protein S15



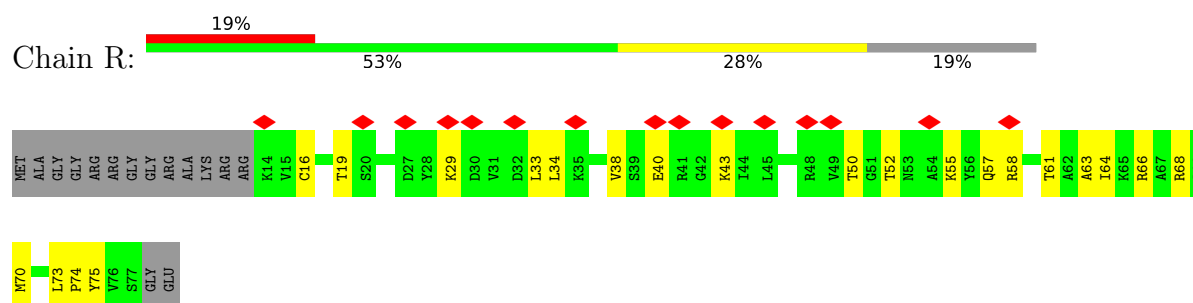
- Molecule 23: 30S ribosomal protein S16



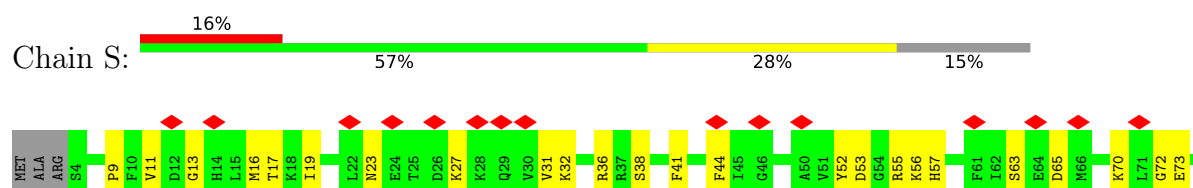
- Molecule 24: 30S ribosomal protein S17

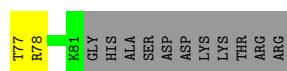


- Molecule 25: 30S ribosomal protein S18

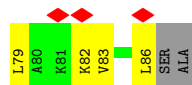
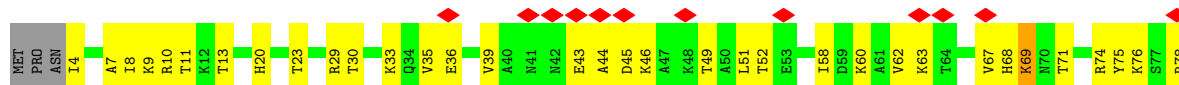


- Molecule 26: 30S ribosomal protein S19

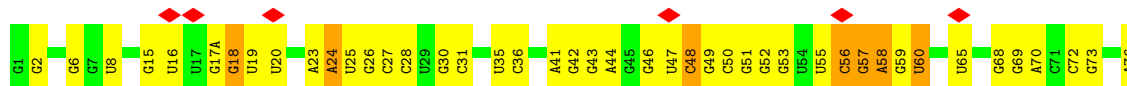
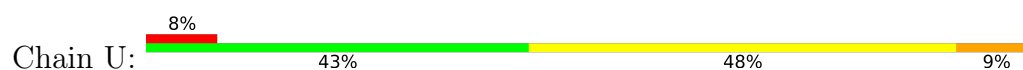




- Molecule 27: 30S ribosomal protein S20



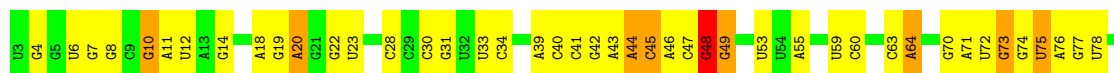
- Molecule 28: tRNA (77-MER)



- Molecule 29: mRNA (33-MER)



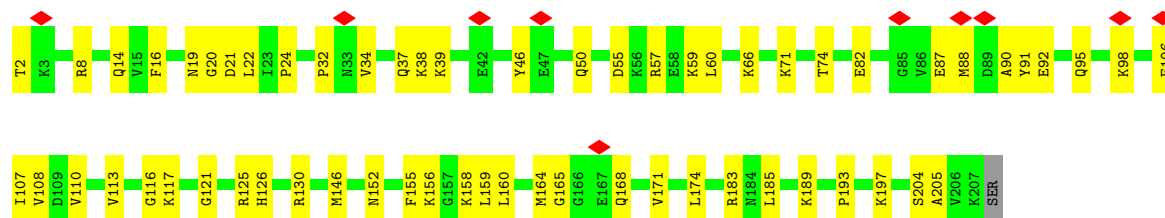
- Molecule 30: 5S rRNA (112-MER)



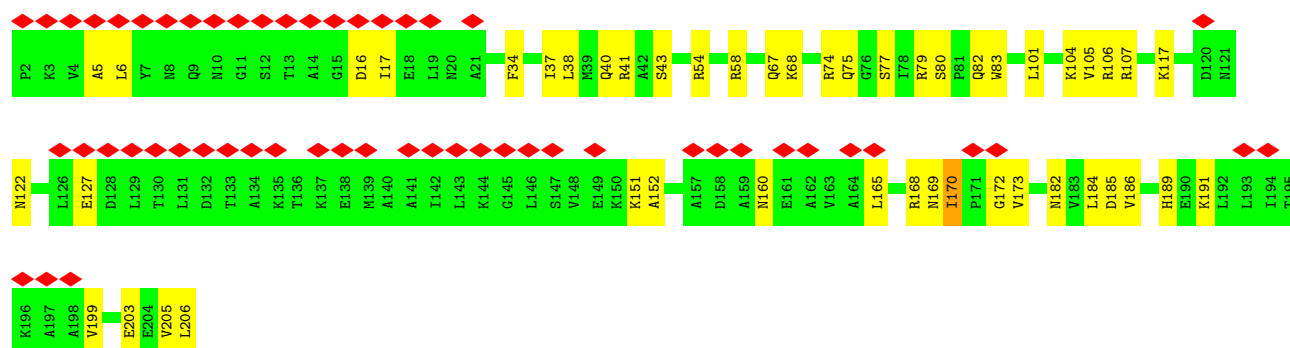
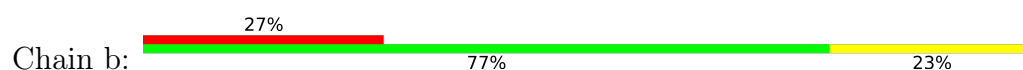
- Molecule 31: Large ribosomal subunit protein uL2



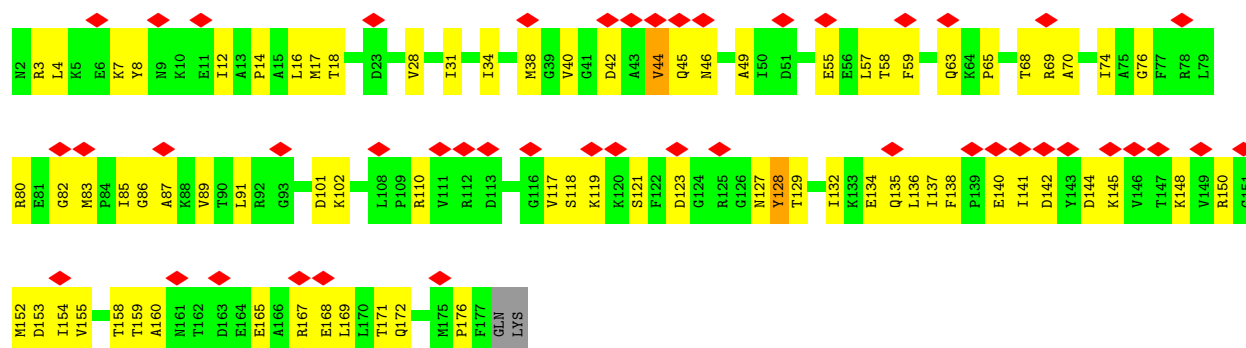
- Molecule 32: Large ribosomal subunit protein uL3



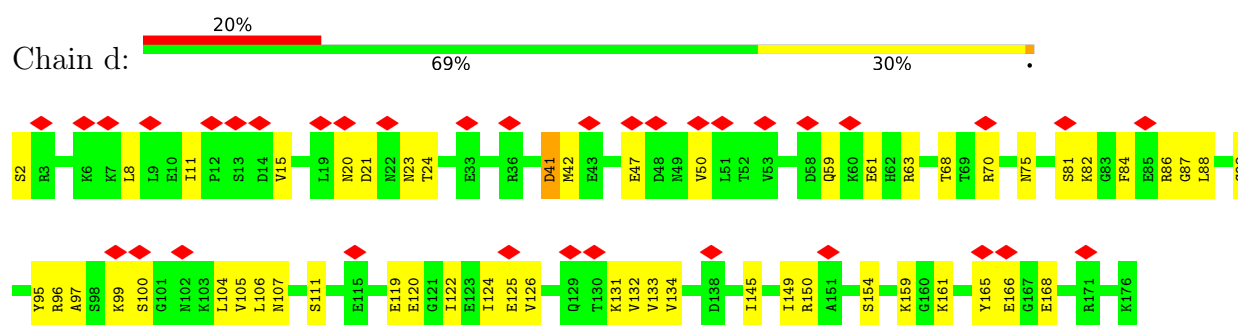
- Molecule 33: Large ribosomal subunit protein uL4



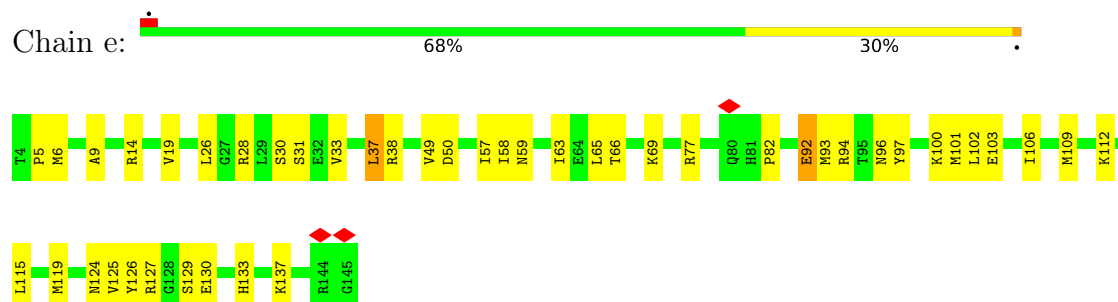
- Molecule 34: Large ribosomal subunit protein uL5



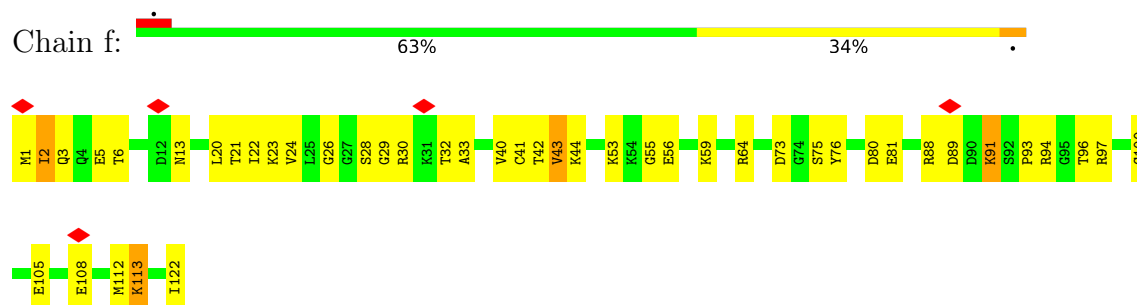
- Molecule 35: Large ribosomal subunit protein uL6



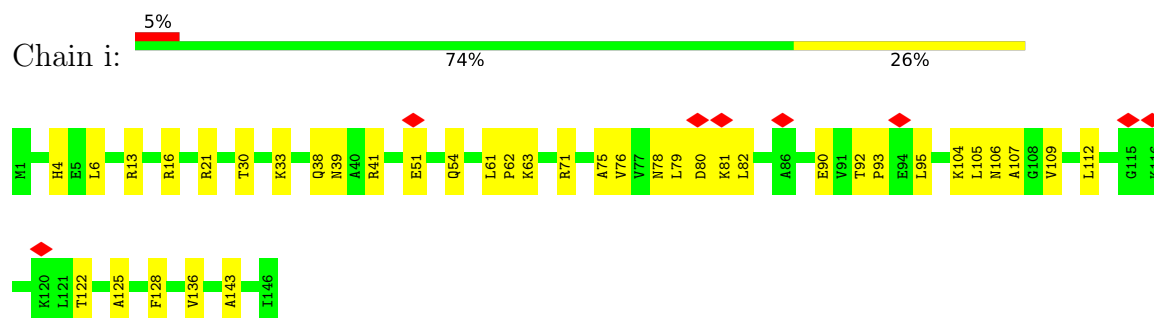
- Molecule 36: Large ribosomal subunit protein uL13



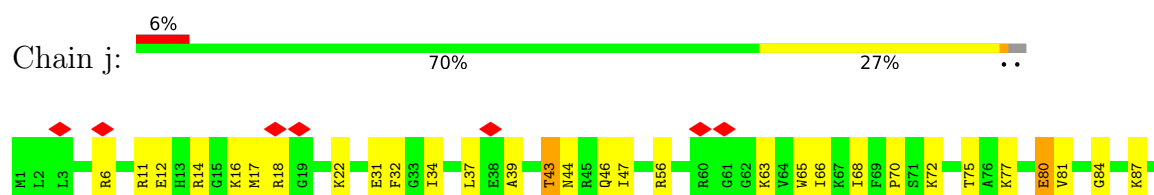
- Molecule 37: 50S ribosomal protein L14

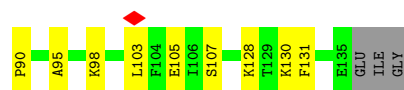


- Molecule 38: 50S ribosomal protein L15



- Molecule 39: Large ribosomal subunit protein uL16

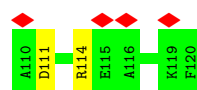
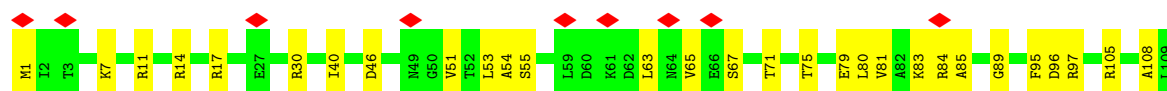
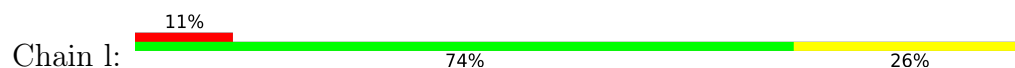




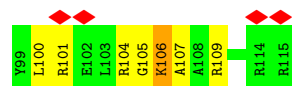
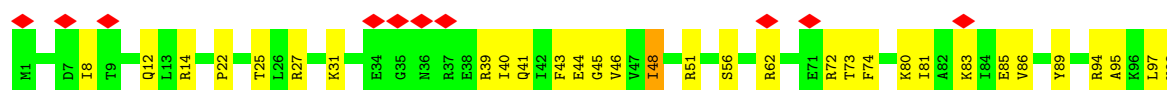
- Molecule 40: Large ribosomal subunit protein bL17



- Molecule 41: 50S ribosomal protein L18



- Molecule 42: 50S ribosomal protein L19

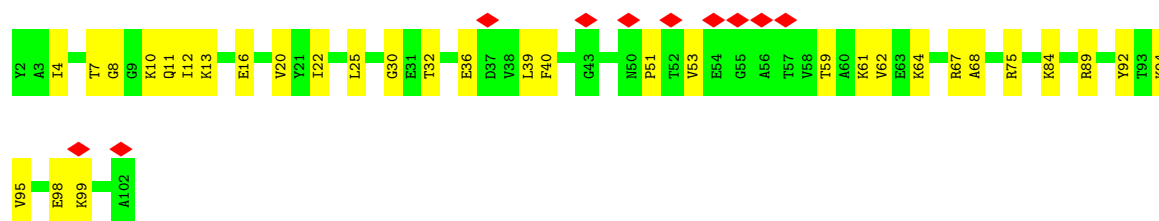


- Molecule 43: Large ribosomal subunit protein bL20

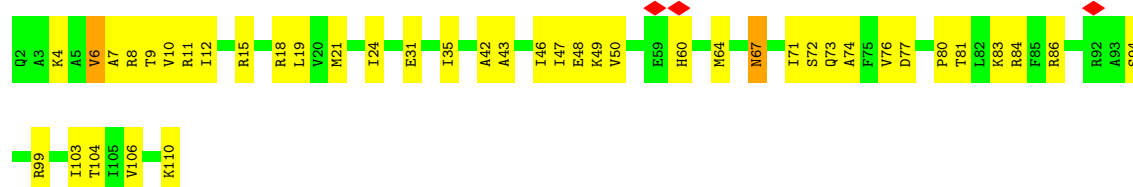


- Molecule 44: Large ribosomal subunit protein bL21

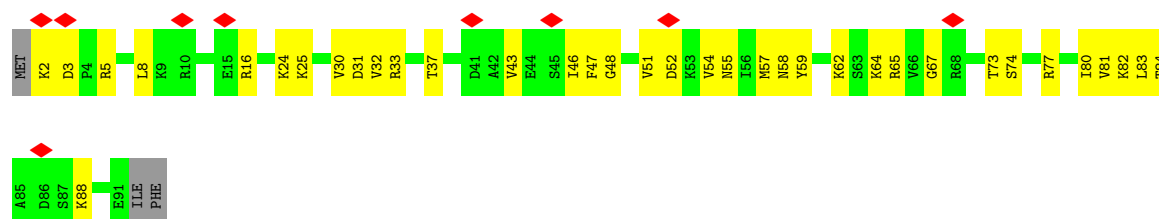




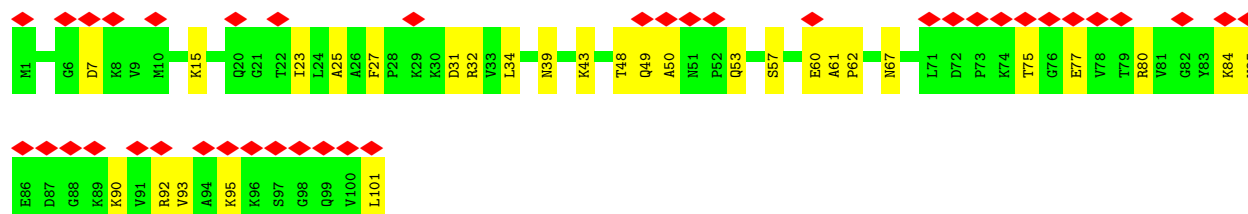
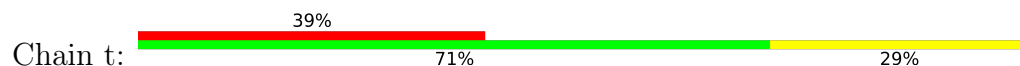
- Molecule 45: Large ribosomal subunit protein uL22



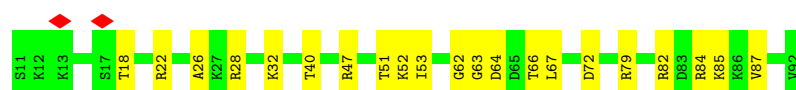
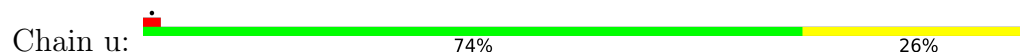
- Molecule 46: Large ribosomal subunit protein uL23



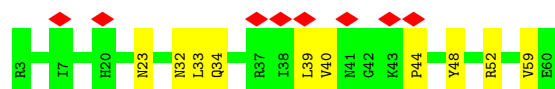
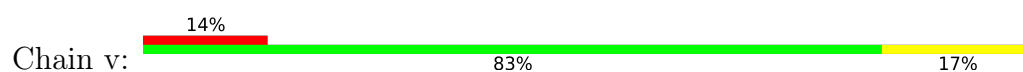
- Molecule 47: Large ribosomal subunit protein uL24



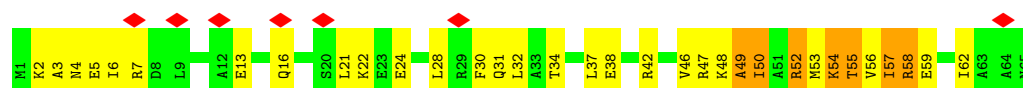
- Molecule 48: Large ribosomal subunit protein bL27



- Molecule 49: Large ribosomal subunit protein bL28



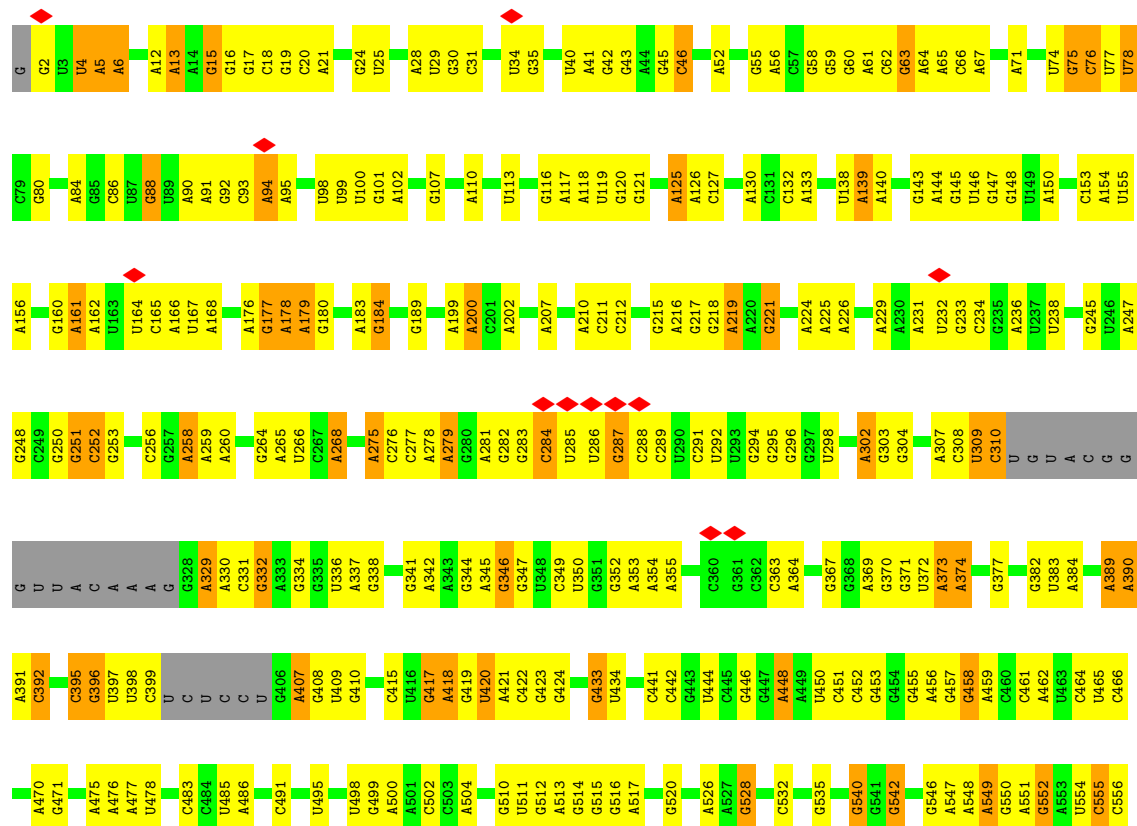
- Molecule 50: Large ribosomal subunit protein uL29



- Molecule 51: Large ribosomal subunit protein uL30



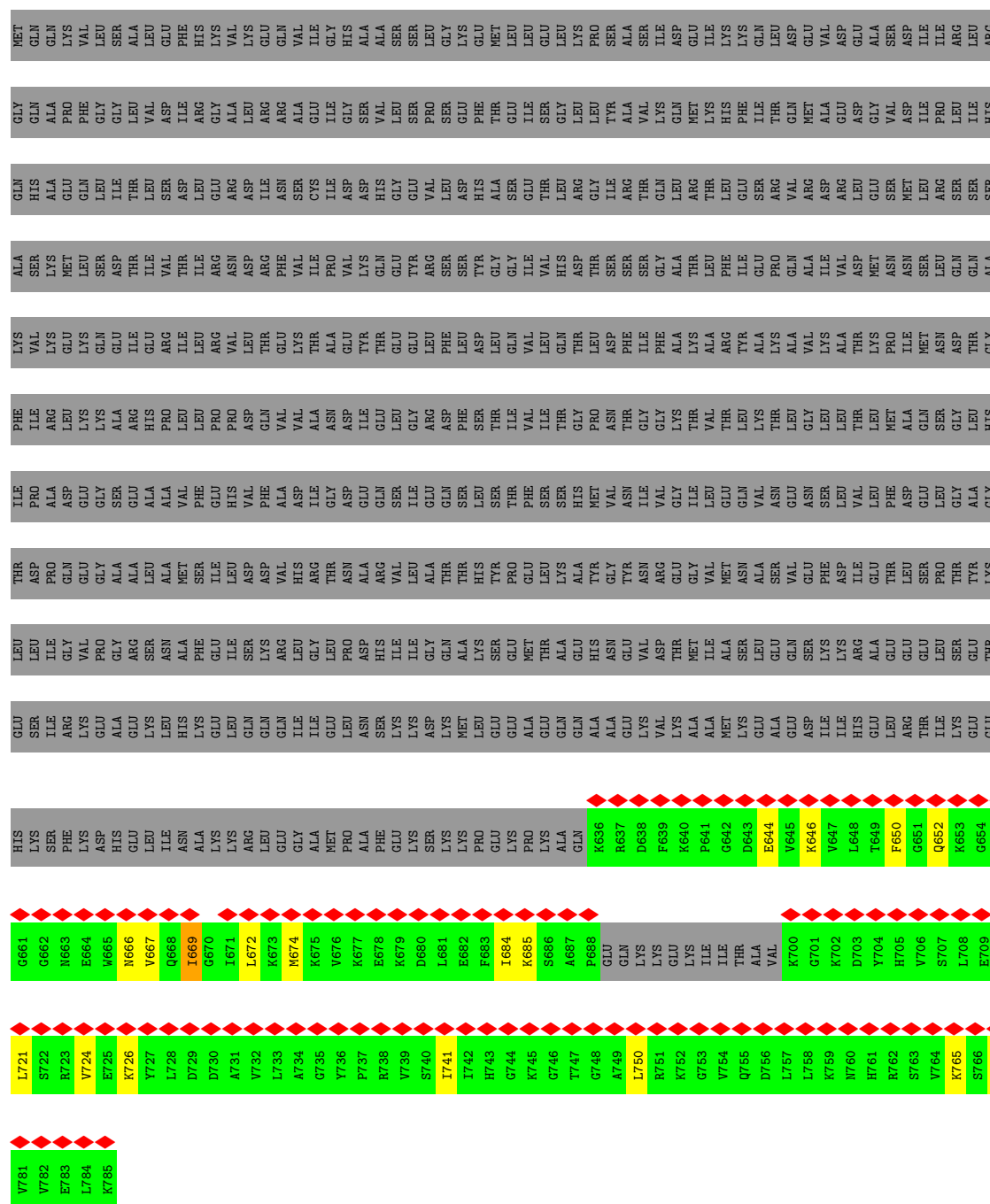
- Molecule 52: 23S RNA (2887-MER)





G2868	A2869	G2870	G2871	U2872	G2873	G2874	G2879	U2880	G2881	G2882	A2885	G2886	G2891	G2892	A2893	G2897	A2900	G2901	A2902	G2903	A2904	G2905	U2906	A2907	A2908	U2909	G2910	G2911	A2916	G2917	G2918	G2919	A2920	U2921	U2922	A2923	G2926	A	U																			
U2785	A2786	A2790	A2793	A2794	G2795	A2805	G2806	A2807	U2808	G2809	A2810	U2813	U2814	U2815	C2818	C2822	G2823	G2824	G2825	A2826	A2827	A2830	A2831	G2832	U2833	U2838	C2839	C2840	C2841	U2842	G2843	A2844	A2845	A2846	U2849	G2850	C2853	A2854	G2855	G2856	U2857	U2858	G2859	U2861	A2862	G2863	G2864											
C2896	G2899	A2900	G2903	U2904	A2905	A2906	A2907	U2908	U2909	U2910	U2911	U2912	U2913	U2914	U2915	U2916	U2917	U2918	U2919	U2920	U2921	U2922	U2923	U2924	U2925	U2926	U2927	U2928	U2929	U2930	U2931	U2932	U2933	U2934	U2935	U2936	U2937	U2938	U2939	U2940	U2941	U2942	U2943	U2944	U2945	U2946												
G2476	A2477	U2486	C2484	A2494	U2496	A2497	U2498	U2499	U2500	C2503	C2504	A2505	C2506	A2507	G2514	G2515	G2516	G2523	G2524	C2525	G2526	C2527	C2528	U2529	G2530	G2531	A2532	U2533	G2534	U2543	G2544	G2545	C2546	A2547	U2548	C2549	G2558	G2561	U2562	C2563	G2564	C2568	C2569	G2572	G2573	G2578	G2579	U2583	U2584									
A2590	A2595	G2596	A2601	G2605	C2608	G2611	G2612	U2613	U2614	C2615	C2620	G2621	G2628	A2629	C2630	A2631	G2632	G2637	U2638	C2639	U2642	U2648	C2655	G2656	G2657	A2658	G2659	U2665	A2670	G2671	G2674	C2675	G2684	U2685	A2686	G2688	A2689	G2690	A2691	G2692	G2693	A2694	C2695															
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A2100	G2101	C2102	U2103	U2104	U2105	U2106	G2107	U2108	U2118	A2119	U2120	U2121	G2122	A2123	A2124	U2125	G2126	U2127	U2128	G2129	U2130	U2131	A2132	C2133	A2134	G2135	C2136	U2137	U2138	G2139	U2140	A2141	C2142	A2143	G2144	C2145	A2146	U2147	A2148	G2149	U2151	A2152	G2153	G2154	A2155	G2156	C2157	U2158	U2159	U2160	G2161	G2162	A2163	A2164	A2165	C2166	C2167	
A2018	C2019	U2020	G2021	U2022	C2023	U2024	C2025	A2026	A2027	A2030	G2039	U2040	G2041	A2042	U2048	A2049	G2050	U2051	A2052	C2053	C2054	U2055	G2056	U2057	G2058	A2059	A2060	C2061	A2062	U2063	G2064	C2065	A2066	G2067	G2068	C2072	C2076	C2077	A2080	G2081	C2084	G2085	A2088	A2089	G2090	A2091	G2096	U2097	G2098	G2099								
U1899	A1900	A1901	G1902	U1905	C1910	G1911	A1912	A1913	A1914	U1915	C1922	G1935	G1936	A1942	U1943	U1944	U1945	U1946	U1952	C1953	G1958	G1959	U1960	A1965	U1966	A1967	C1971	U1972	G1983	U1984	U1985	G1986	C1987	A1988	A1989	A2000	G2001	A2006	A2009	G2090	A2091	G2096	U2097	G2098	G2099													
U1808	A1809	C1810	A1811	A1812	A1813	A1814	C1817	A1818	C1819	A1820	U1823	C1824	U1825	C1826	U1827	G1828	C1829	G1830	A1831	U1832	U1837	A1845	G1846	G1847	A1848	G1852	G1853	C1854	C1855	U1856	A1857	A1858	C1859	G1860	U1870	G1871	C1872	U1873	A1877	A1882	A1883	G1884	G1885	G1886	G1890	A1891	A1892	C1893	U1894	G1898								
U1733	A1734	A1735	U1738	A1739	G1740	G1741	G1742	A1744	A1746	G1747	G1748	G1749	G1750	U1754	C1755	U1756	A1757	U1758	U1759	A1760	G1761	G1762	G1763	U1764	G1765	C1766	A1767	C1771	G1772	A1773	A1774	G1775	A1776	G1777	G1778	G1779	C1783	A1784	G1785	U1786	G1792	G1793	A1797	C1800	A1801	A1802	C1803	U1804	G1805									

• Molecule 53: Endonuclease MutS2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11794	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 ($e^-/\text{\AA}^2$)	43.6	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.504	Depositor
Minimum map value	-1.281	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.132	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	522.5, 522.5, 522.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.37	0/433	0.84	1/574 (0.2%)
2	1	0.37	0/407	0.91	2/540 (0.4%)
3	2	0.34	0/371	0.67	0/483
4	3	0.33	0/519	0.74	0/680
5	4	0.37	0/300	0.77	1/393 (0.3%)
6	6	0.29	0/509	0.77	0/678
7	7	0.24	0/1743	0.42	0/2716
8	A	0.29	0/36826	0.40	0/57450
9	B	0.36	0/1782	0.94	7/2392 (0.3%)
10	C	0.30	0/1641	0.80	1/2208 (0.0%)
11	D	0.33	0/1599	0.86	3/2147 (0.1%)
12	E	0.31	0/1231	0.74	0/1655
13	F	0.32	0/766	0.76	0/1031
14	G	0.50	0/1196	0.87	1/1604 (0.1%)
15	H	0.35	0/1049	0.90	1/1407 (0.1%)
16	I	0.31	0/979	0.79	2/1315 (0.2%)
17	J	0.39	0/773	1.01	4/1044 (0.4%)
18	K	0.27	0/853	0.74	1/1153 (0.1%)
19	L	0.37	0/1069	0.77	0/1435
20	M	0.33	0/873	0.86	2/1166 (0.2%)
21	N	0.36	0/508	0.98	4/672 (0.6%)
22	O	0.35	0/718	0.88	0/960
23	P	0.44	1/708 (0.1%)	1.03	3/950 (0.3%)
24	Q	0.29	0/699	0.75	0/933
25	R	0.29	0/526	0.85	0/705
26	S	0.32	0/649	0.84	0/872
27	T	0.30	0/639	0.83	0/852
28	U	0.23	0/1834	0.36	0/2858
29	V	0.25	0/787	0.54	0/1224
30	Y	0.28	0/2675	0.43	1/4170 (0.0%)
31	Z	0.35	0/2120	0.71	0/2845
32	a	0.35	0/1591	0.71	0/2132
33	b	0.29	0/1581	0.66	0/2132
34	c	0.28	0/1405	0.73	1/1887 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	d	0.31	0/1361	0.64	0/1832
36	e	0.35	0/1147	0.76	4/1542 (0.3%)
37	f	0.44	0/928	0.92	4/1245 (0.3%)
38	i	0.31	0/1094	0.66	0/1457
39	j	0.33	0/1099	0.65	1/1468 (0.1%)
40	k	0.40	0/961	0.94	5/1284 (0.4%)
41	l	0.30	0/922	0.78	0/1236
42	m	0.38	0/958	0.84	1/1279 (0.1%)
43	n	0.35	0/953	0.74	0/1266
44	o	0.34	0/798	0.77	0/1070
45	r	0.39	0/852	0.86	2/1146 (0.2%)
46	s	0.36	0/731	0.94	0/974
47	t	0.26	0/773	0.62	0/1032
48	u	0.34	0/639	0.74	1/847 (0.1%)
49	v	0.38	0/449	0.83	1/596 (0.2%)
50	w	0.97	4/532 (0.8%)	1.27	0/707
51	x	0.37	0/458	0.95	3/613 (0.5%)
52	X	0.33	0/69451	0.40	3/108344 (0.0%)
53	z	0.19	0/1097	0.52	0/1462
All	All	0.33	5/156562 (0.0%)	0.53	60/234663 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	w	49	ALA	CA-C	-6.30	1.44	1.52
50	w	54	LYS	CA-C	-6.14	1.45	1.52
50	w	54	LYS	C-O	-5.39	1.18	1.24
23	P	76	SER	CA-C	-5.34	1.45	1.52
50	w	55	THR	CA-C	-5.24	1.46	1.52

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	X	138	U	OP1-P-O3'	-23.39	37.83	108.00
17	J	81	PRO	CA-N-CD	-12.13	95.02	112.00
23	P	42	PRO	CA-N-CD	-10.81	96.87	112.00
21	N	11	GLN	CA-CB-CG	10.12	134.35	114.10
2	1	37	PRO	CA-N-CD	-9.91	98.13	112.00

There are no chirality outliers.

There are no planarity outliers.

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	426	0	445	23	0
2	1	402	0	413	15	0
3	2	368	0	410	6	0
4	3	512	0	561	23	0
5	4	297	0	342	11	0
6	6	499	0	491	10	0
7	7	1560	0	788	31	0
8	A	32891	0	16559	561	0
9	B	1757	0	1830	49	0
10	C	1619	0	1658	38	0
11	D	1569	0	1604	60	0
12	E	1219	0	1300	40	0
13	F	755	0	746	17	0
14	G	1181	0	1235	39	0
15	H	1037	0	1095	28	0
16	I	966	0	1005	37	0
17	J	761	0	795	27	0
18	K	839	0	854	26	0
19	L	1052	0	1112	39	0
20	M	868	0	925	43	0
21	N	498	0	531	17	0
22	O	710	0	735	20	0
23	P	695	0	721	28	0
24	Q	691	0	728	26	0
25	R	518	0	555	18	0
26	S	633	0	649	21	0
27	T	637	0	696	30	0
28	U	1643	0	831	25	0
29	V	704	0	359	10	0
30	Y	2392	0	1213	37	0
31	Z	2083	0	2168	62	0
32	a	1569	0	1637	44	0
33	b	1562	0	1647	58	0
34	c	1386	0	1446	54	0
35	d	1343	0	1388	38	0
36	e	1124	0	1162	43	0
37	f	921	0	977	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	i	1082	0	1132	33	0
39	j	1076	0	1145	28	0
40	k	954	0	983	41	0
41	l	913	0	947	21	0
42	m	945	0	1020	26	0
43	n	941	0	1005	29	0
44	o	787	0	826	25	0
45	r	843	0	899	34	0
46	s	725	0	770	31	0
47	t	763	0	821	17	0
48	u	631	0	644	18	0
49	v	445	0	487	6	0
50	w	531	0	568	36	0
51	x	456	0	491	13	0
52	X	62005	0	31207	832	0
53	z	1083	0	1117	17	0
All	All	143867	0	95673	2515	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 11.

The worst 5 of 2515 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)
20:M:34:LEU:CD2	20:M:41:GLU:HG3	0.99	1.47
20:M:34:LEU:CD2	20:M:41:GLU:CG	1.95	1.40
20:M:34:LEU:HD23	20:M:41:GLU:CG	1.50	1.40
33:b:151:LYS:CE	33:b:172:GLY:HA3	1.55	1.35
33:b:151:LYS:HE2	33:b:172:GLY:CA	1.71	1.20

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	52/59 (88%)	52 (100%)	0	0	100	100
2	1	46/48 (96%)	44 (96%)	2 (4%)	0	100	100
3	2	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
4	3	62/66 (94%)	58 (94%)	4 (6%)	0	100	100
5	4	35/37 (95%)	35 (100%)	0	0	100	100
6	6	61/64 (95%)	53 (87%)	8 (13%)	0	100	100
9	B	216/246 (88%)	192 (89%)	23 (11%)	1 (0%)	24	57
10	C	204/218 (94%)	184 (90%)	19 (9%)	1 (0%)	24	57
11	D	193/200 (96%)	172 (89%)	19 (10%)	2 (1%)	12	44
12	E	162/166 (98%)	153 (94%)	9 (6%)	0	100	100
13	F	90/95 (95%)	84 (93%)	6 (7%)	0	100	100
14	G	147/156 (94%)	134 (91%)	11 (8%)	2 (1%)	9	38
15	H	129/132 (98%)	118 (92%)	11 (8%)	0	100	100
16	I	123/130 (95%)	112 (91%)	11 (9%)	0	100	100
17	J	93/102 (91%)	87 (94%)	6 (6%)	0	100	100
18	K	112/131 (86%)	108 (96%)	4 (4%)	0	100	100
19	L	134/138 (97%)	122 (91%)	12 (9%)	0	100	100
20	M	106/121 (88%)	97 (92%)	9 (8%)	0	100	100
21	N	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
22	O	83/89 (93%)	77 (93%)	6 (7%)	0	100	100
23	P	86/90 (96%)	80 (93%)	6 (7%)	0	100	100
24	Q	82/87 (94%)	80 (98%)	2 (2%)	0	100	100
25	R	62/79 (78%)	58 (94%)	4 (6%)	0	100	100
26	S	76/92 (83%)	73 (96%)	3 (4%)	0	100	100
27	T	81/88 (92%)	76 (94%)	4 (5%)	1 (1%)	10	41
31	Z	270/275 (98%)	252 (93%)	17 (6%)	1 (0%)	30	60
32	a	204/207 (99%)	194 (95%)	10 (5%)	0	100	100
33	b	203/205 (99%)	189 (93%)	14 (7%)	0	100	100
34	c	174/178 (98%)	166 (95%)	7 (4%)	1 (1%)	21	54
35	d	173/175 (99%)	159 (92%)	14 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	e	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
37	f	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
38	i	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
39	j	133/138 (96%)	124 (93%)	9 (7%)	0	100	100
40	k	117/119 (98%)	111 (95%)	5 (4%)	1 (1%)	14	46
41	l	118/120 (98%)	106 (90%)	12 (10%)	0	100	100
42	m	113/115 (98%)	102 (90%)	10 (9%)	1 (1%)	14	46
43	n	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
44	o	99/101 (98%)	85 (86%)	14 (14%)	0	100	100
45	r	107/109 (98%)	98 (92%)	9 (8%)	0	100	100
46	s	88/93 (95%)	85 (97%)	3 (3%)	0	100	100
47	t	99/101 (98%)	91 (92%)	8 (8%)	0	100	100
48	u	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
49	v	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
50	w	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
51	x	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
53	z	135/785 (17%)	130 (96%)	5 (4%)	0	100	100
All	All	5342/6250 (86%)	4963 (93%)	368 (7%)	11 (0%)	44	72

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	D	143	GLU
42	m	106	LYS
14	G	31	MET
10	C	50	SER
34	c	42	ASP

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	48/53 (91%)	48 (100%)	0	100	100
2	1	46/46 (100%)	46 (100%)	0	100	100
3	2	39/39 (100%)	38 (97%)	1 (3%)	40	62
4	3	54/57 (95%)	53 (98%)	1 (2%)	50	67
5	4	35/35 (100%)	35 (100%)	0	100	100
6	6	53/53 (100%)	53 (100%)	0	100	100
9	B	189/212 (89%)	187 (99%)	2 (1%)	65	74
10	C	168/178 (94%)	167 (99%)	1 (1%)	78	79
11	D	169/173 (98%)	165 (98%)	4 (2%)	43	63
12	E	128/130 (98%)	127 (99%)	1 (1%)	73	77
13	F	81/84 (96%)	80 (99%)	1 (1%)	63	73
14	G	125/132 (95%)	122 (98%)	3 (2%)	43	63
15	H	111/112 (99%)	111 (100%)	0	100	100
16	I	98/102 (96%)	97 (99%)	1 (1%)	68	75
17	J	86/92 (94%)	86 (100%)	0	100	100
18	K	86/100 (86%)	86 (100%)	0	100	100
19	L	114/116 (98%)	114 (100%)	0	100	100
20	M	94/104 (90%)	93 (99%)	1 (1%)	65	74
21	N	53/54 (98%)	53 (100%)	0	100	100
22	O	80/83 (96%)	78 (98%)	2 (2%)	42	63
23	P	74/76 (97%)	73 (99%)	1 (1%)	59	71
24	Q	77/80 (96%)	77 (100%)	0	100	100
25	R	56/64 (88%)	55 (98%)	1 (2%)	51	68
26	S	70/81 (86%)	69 (99%)	1 (1%)	59	71
27	T	66/70 (94%)	66 (100%)	0	100	100
31	Z	220/223 (99%)	216 (98%)	4 (2%)	51	68
32	a	167/168 (99%)	166 (99%)	1 (1%)	78	79
33	b	169/169 (100%)	168 (99%)	1 (1%)	78	79
34	c	151/153 (99%)	147 (97%)	4 (3%)	40	62
35	d	148/148 (100%)	145 (98%)	3 (2%)	48	66
36	e	120/120 (100%)	118 (98%)	2 (2%)	53	69
37	f	101/101 (100%)	99 (98%)	2 (2%)	48	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	i	110/110 (100%)	110 (100%)	0	100	100
39	j	109/111 (98%)	105 (96%)	4 (4%)	30	56
40	k	99/99 (100%)	96 (97%)	3 (3%)	36	60
41	l	93/93 (100%)	92 (99%)	1 (1%)	65	74
42	m	100/100 (100%)	98 (98%)	2 (2%)	48	66
43	n	96/96 (100%)	95 (99%)	1 (1%)	68	75
44	o	83/83 (100%)	83 (100%)	0	100	100
45	r	90/90 (100%)	87 (97%)	3 (3%)	33	58
46	s	81/84 (96%)	81 (100%)	0	100	100
47	t	85/85 (100%)	83 (98%)	2 (2%)	43	63
48	u	64/64 (100%)	64 (100%)	0	100	100
49	v	47/47 (100%)	45 (96%)	2 (4%)	26	52
50	w	56/56 (100%)	50 (89%)	6 (11%)	6	28
51	x	52/52 (100%)	52 (100%)	0	100	100
53	z	115/673 (17%)	113 (98%)	2 (2%)	53	69
All	All	4556/5251 (87%)	4492 (99%)	64 (1%)	57	71

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	w	50	ILE
50	w	54	LYS
31	Z	241	ILE
31	Z	201	GLU
50	w	57	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
34	c	172	GLN
41	l	8	ASN
35	d	23	ASN
40	k	72	ASN
42	m	41	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	U	76/77 (98%)	19 (25%)	0
29	V	32/33 (96%)	21 (65%)	0
30	Y	111/112 (99%)	35 (31%)	2 (1%)
52	X	2881/2928 (98%)	737 (25%)	23 (0%)
7	7	72/73 (98%)	25 (34%)	2 (2%)
8	A	1532/1533 (99%)	369 (24%)	14 (0%)
All	All	4704/4756 (98%)	1206 (25%)	41 (0%)

5 of 1206 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	7	4	C
7	7	6	G
7	7	7	A
7	7	8	U
7	7	9	A

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	X	1176	U
52	X	2133	C
52	X	1451	U
52	X	1567	U
52	X	2334	U

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

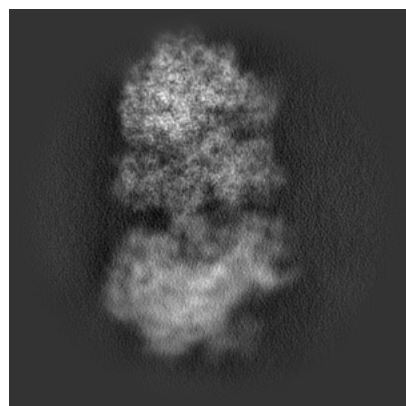
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18901. These allow visual inspection of the internal detail of the map and identification of artifacts.

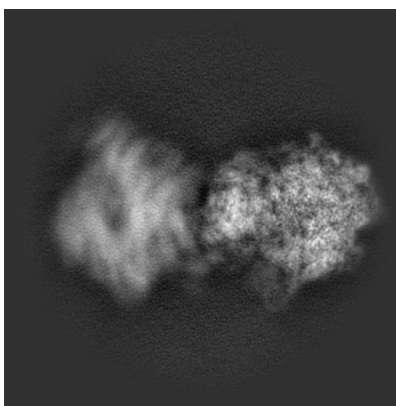
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

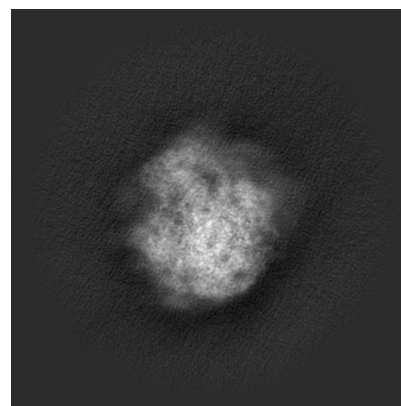
6.1.1 Primary map



X

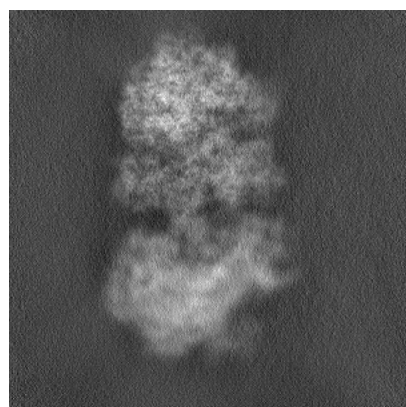


Y

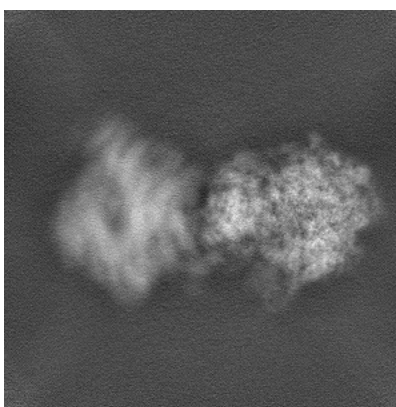


Z

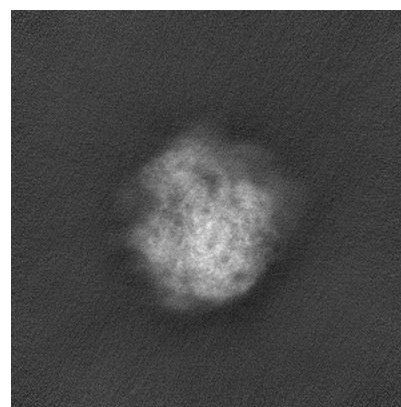
6.1.2 Raw map



X



Y

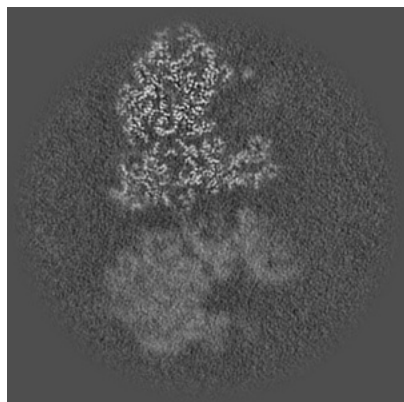


Z

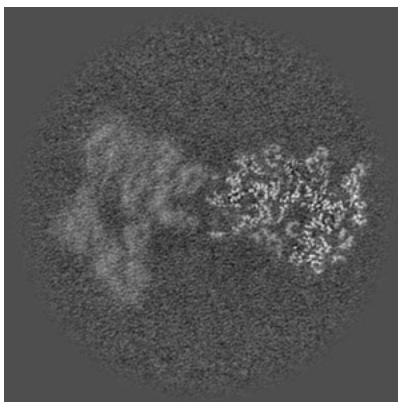
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

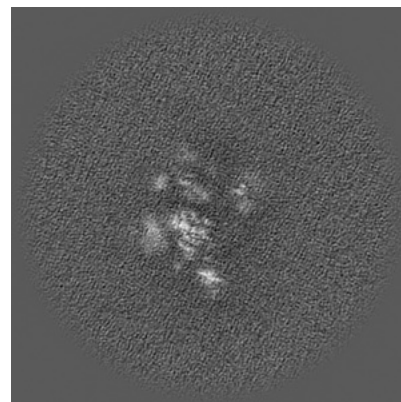
6.2.1 Primary map



X Index: 250

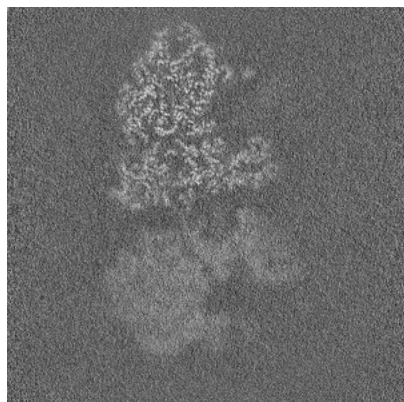


Y Index: 250

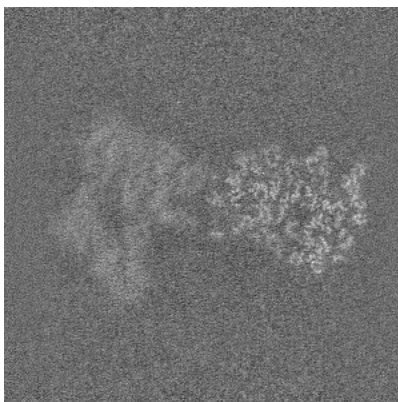


Z Index: 250

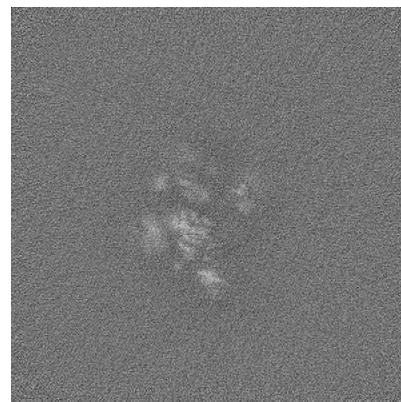
6.2.2 Raw map



X Index: 250



Y Index: 250

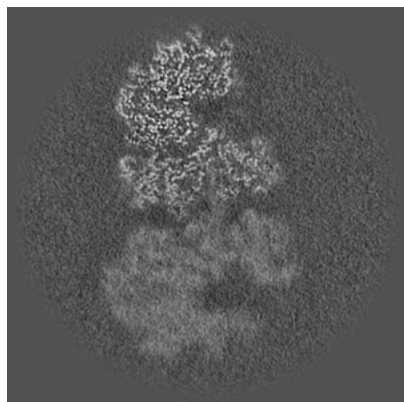


Z Index: 250

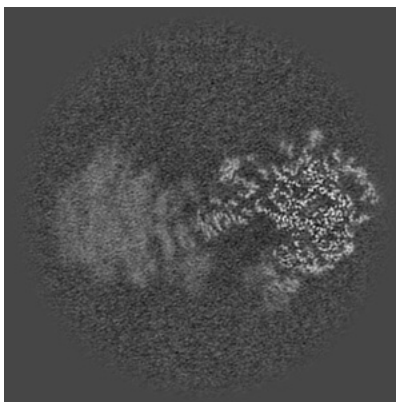
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

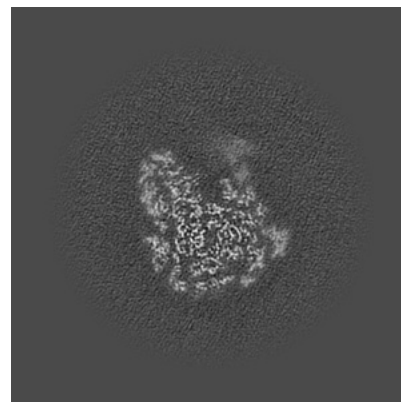
6.3.1 Primary map



X Index: 238

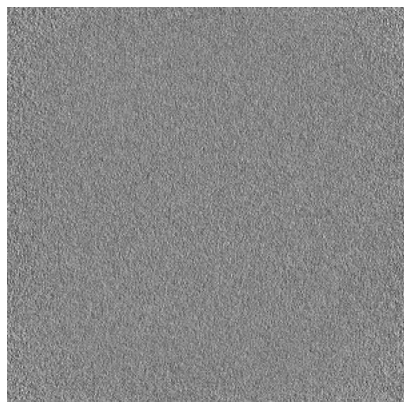


Y Index: 209

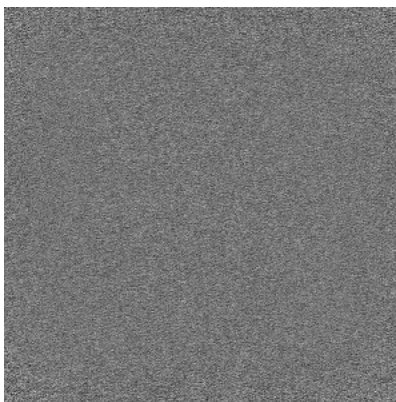


Z Index: 387

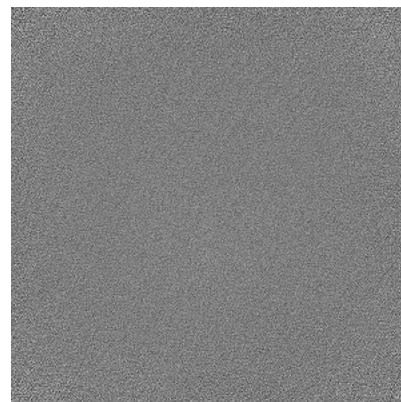
6.3.2 Raw map



X Index: 0



Y Index: 0

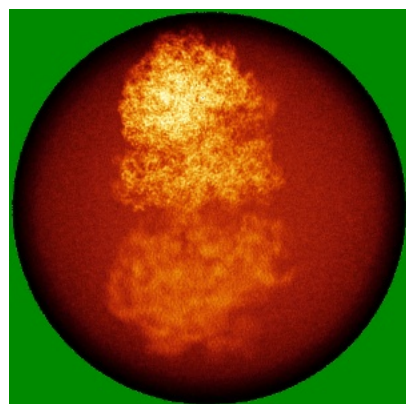


Z Index: 0

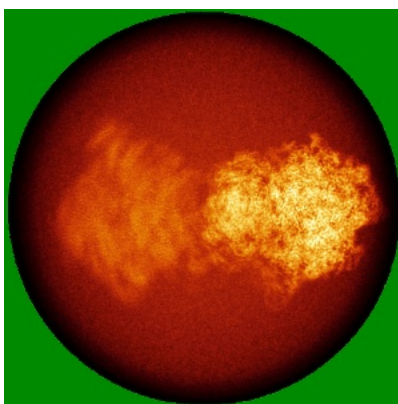
The images above show the largest variance slices of the map in three orthogonal directions.

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

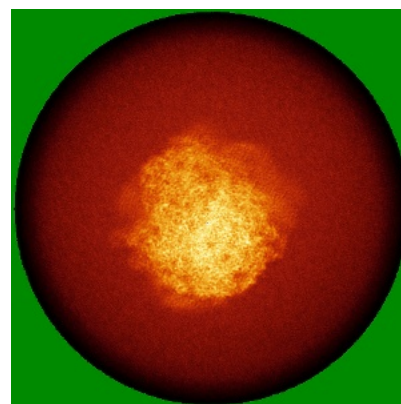
6.4.1 Primary map



X

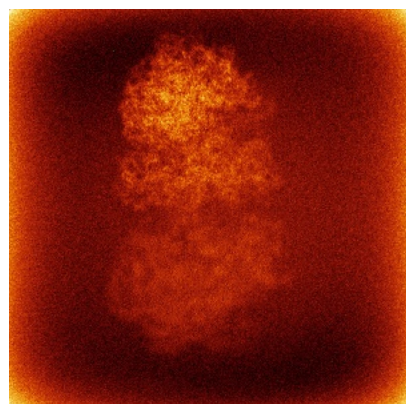


Y

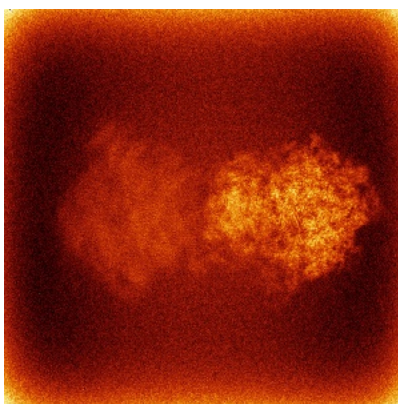


Z

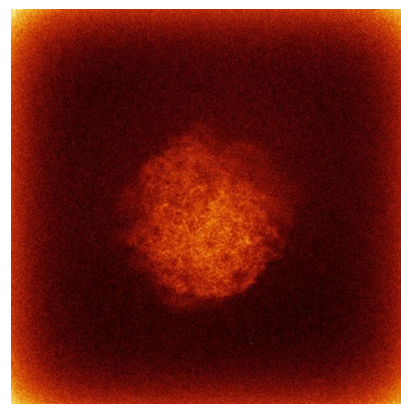
6.4.2 Raw map



X



Y

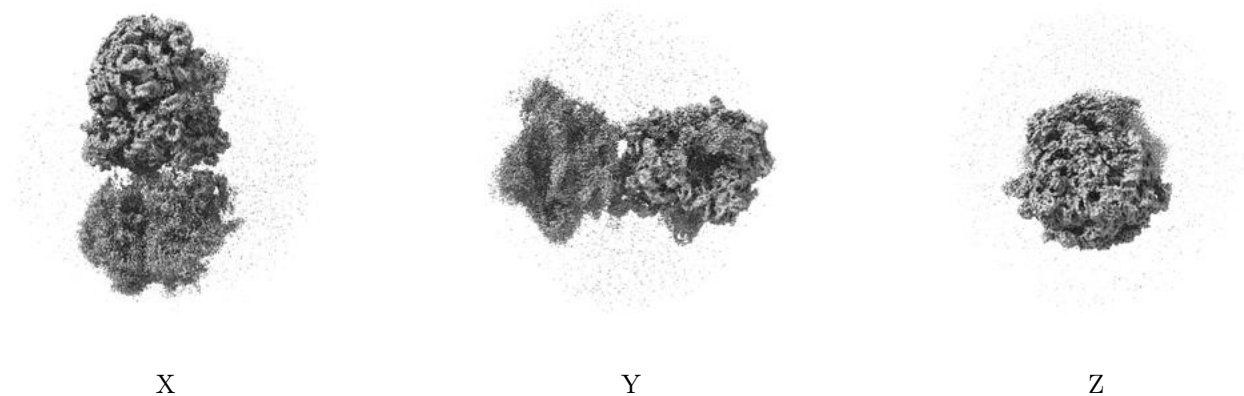


Z

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

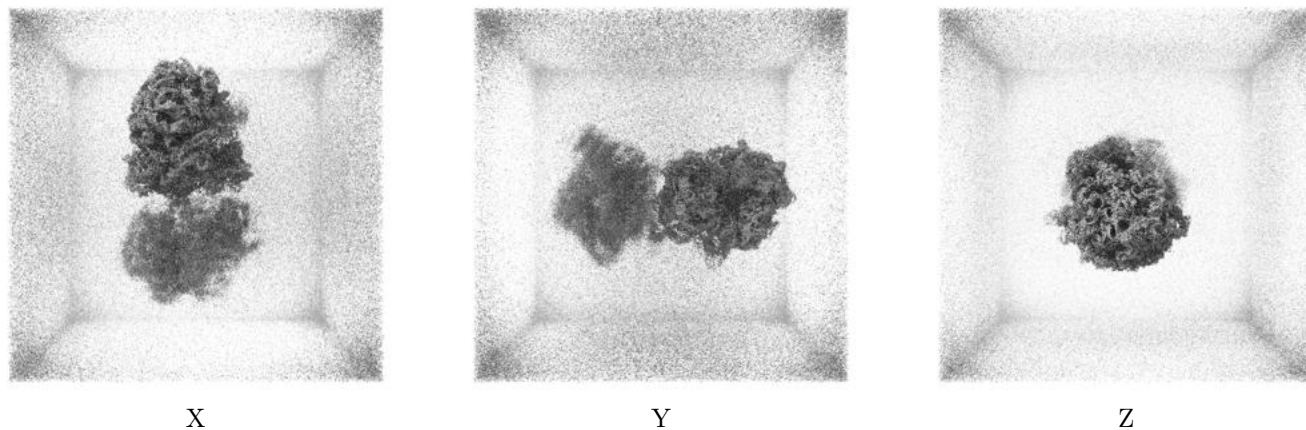
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

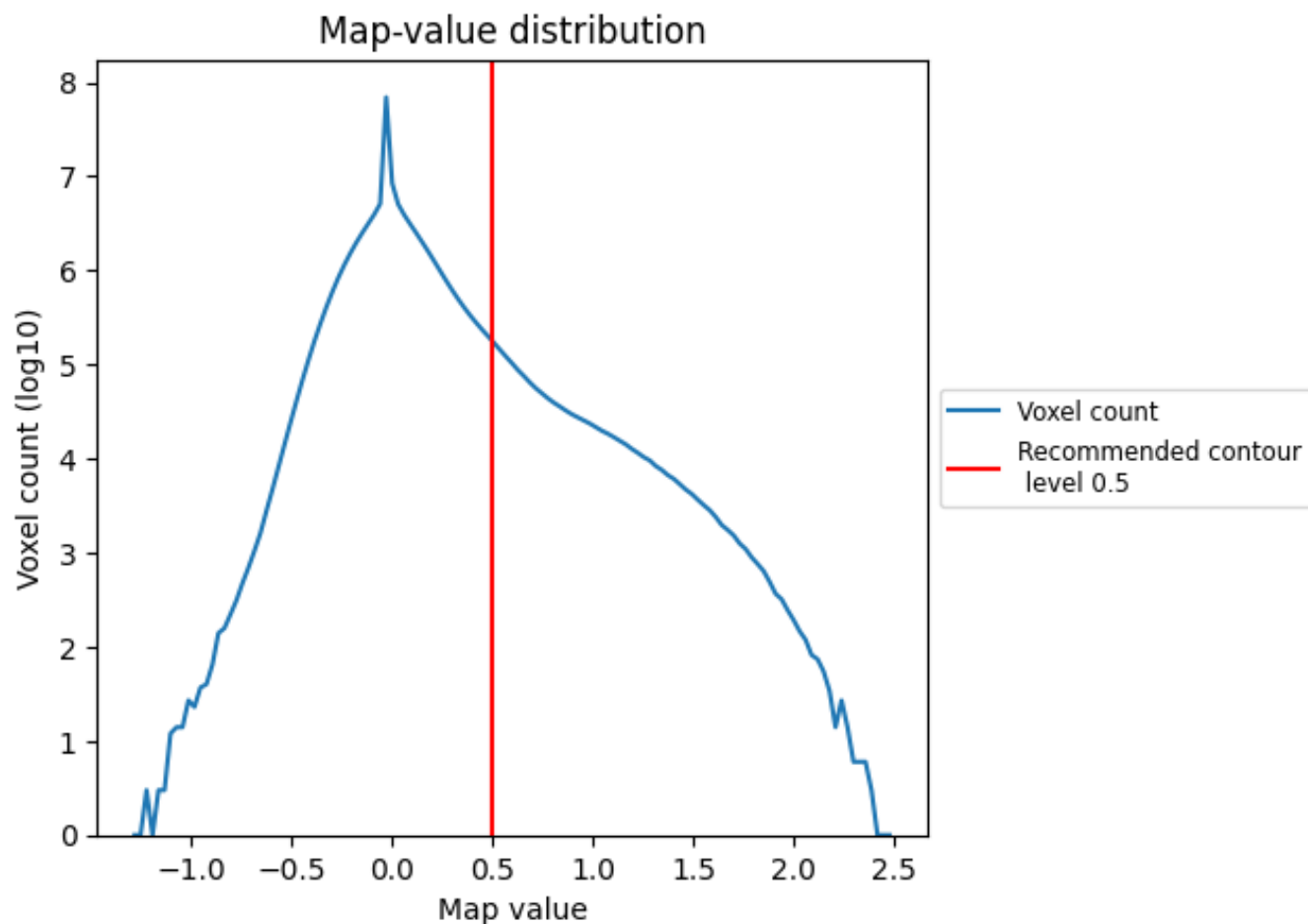
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

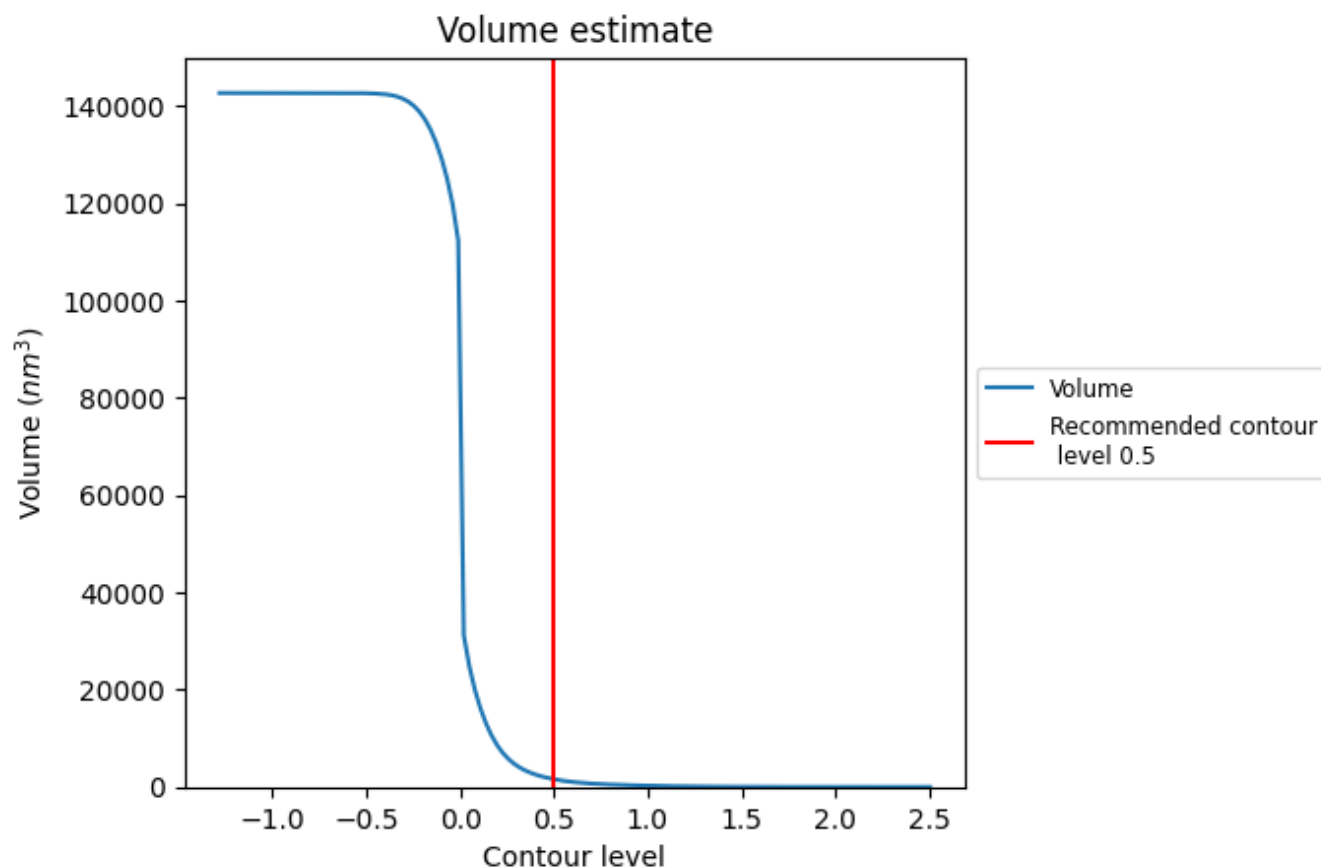
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

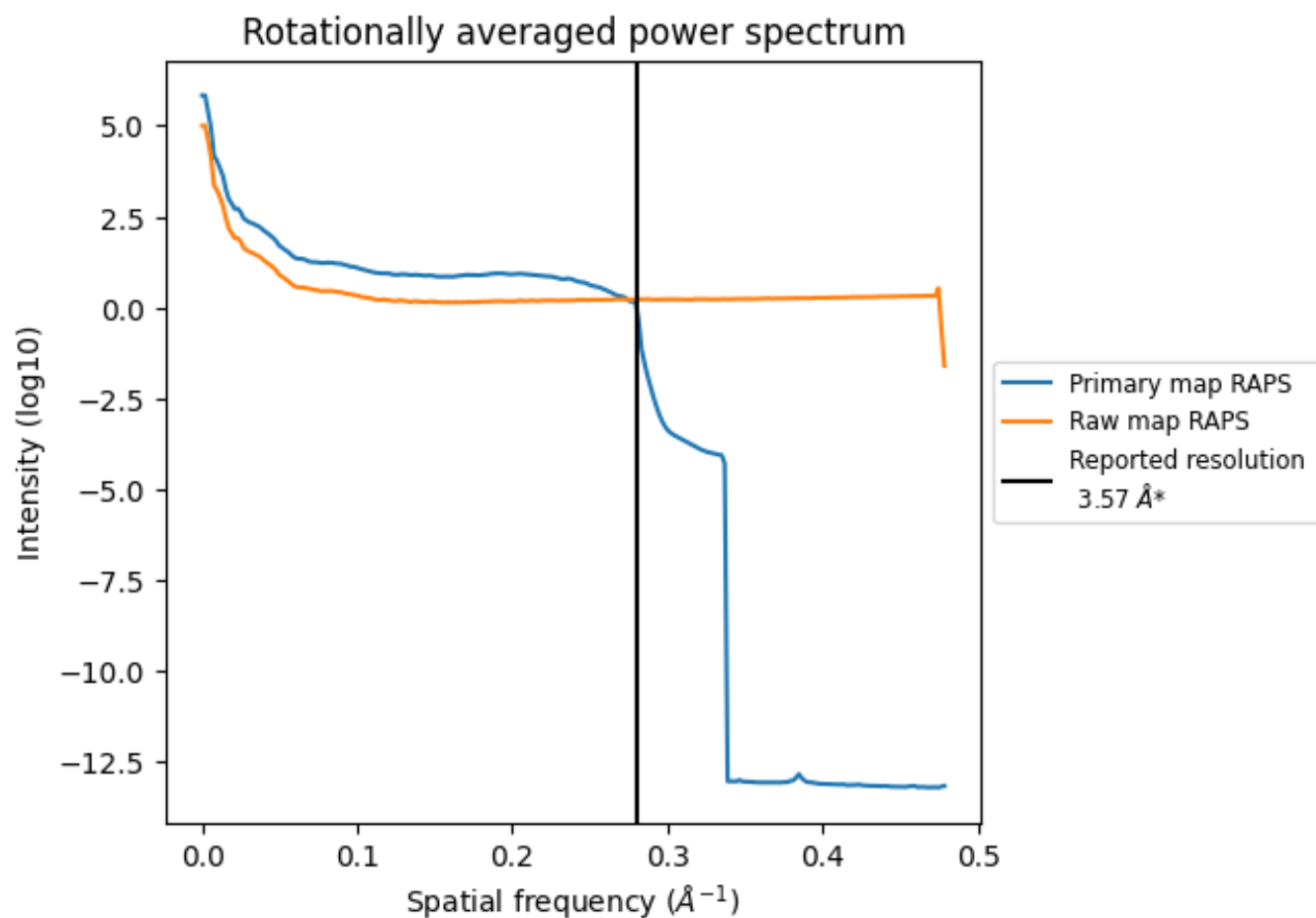
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1594 nm³; this corresponds to an approximate mass of 1440 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 ⓘ

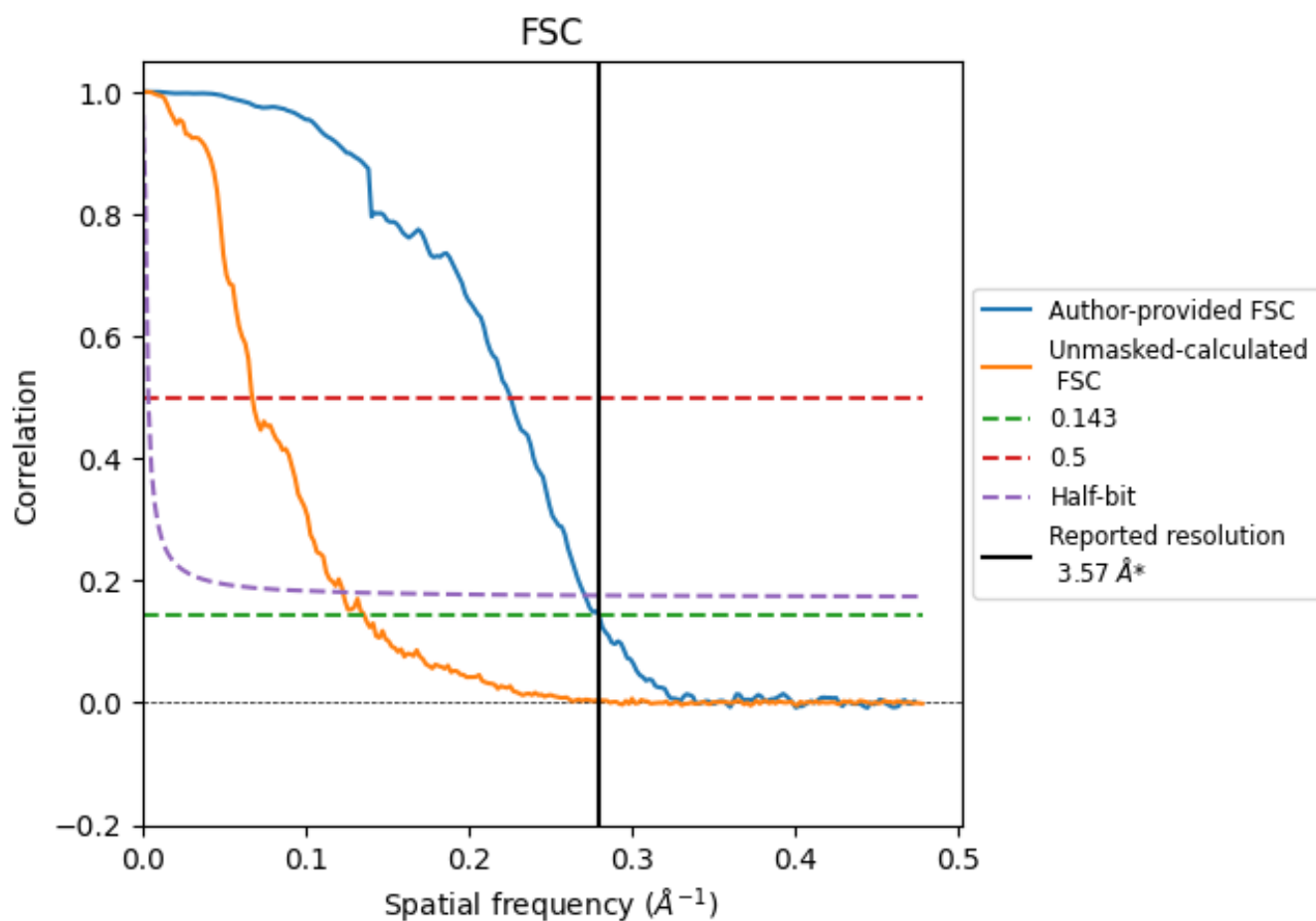


*Reported resolution corresponds to spatial frequency of 0.280 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.280 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

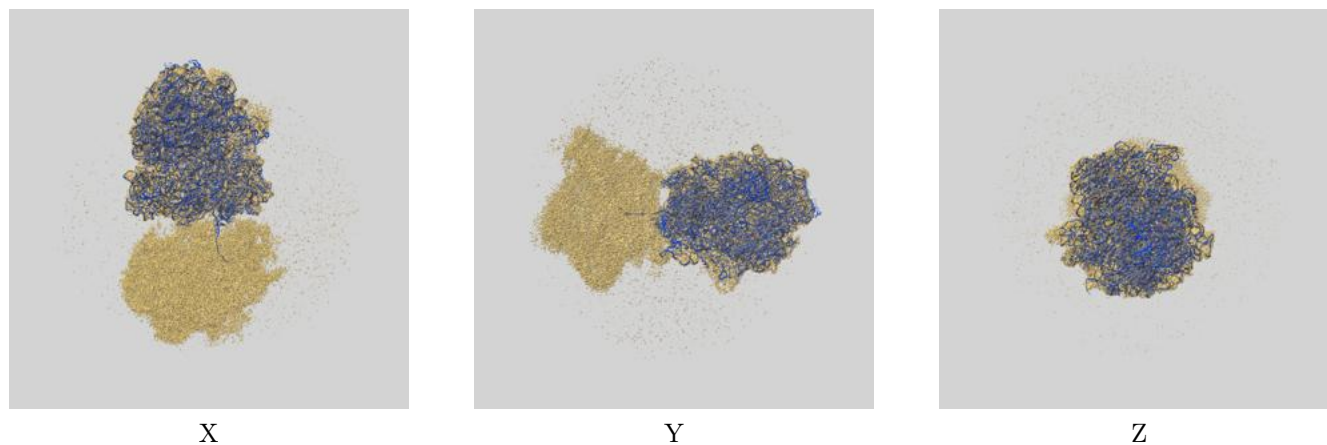
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.57	-	-
Author-provided FSC curve	3.57	4.43	3.68
Unmasked-calculated*	7.34	14.81	8.12

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.34 differs from the reported value 3.57 by more than 10 %

9 Map-model fit [i](#)

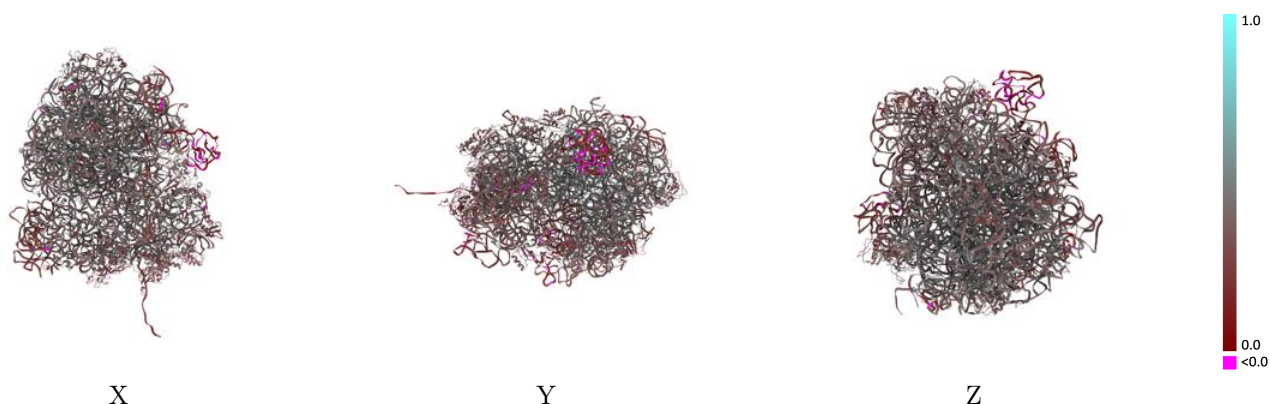
This section contains information regarding the fit between EMDB map EMD-18901 and PDB model 8R55. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



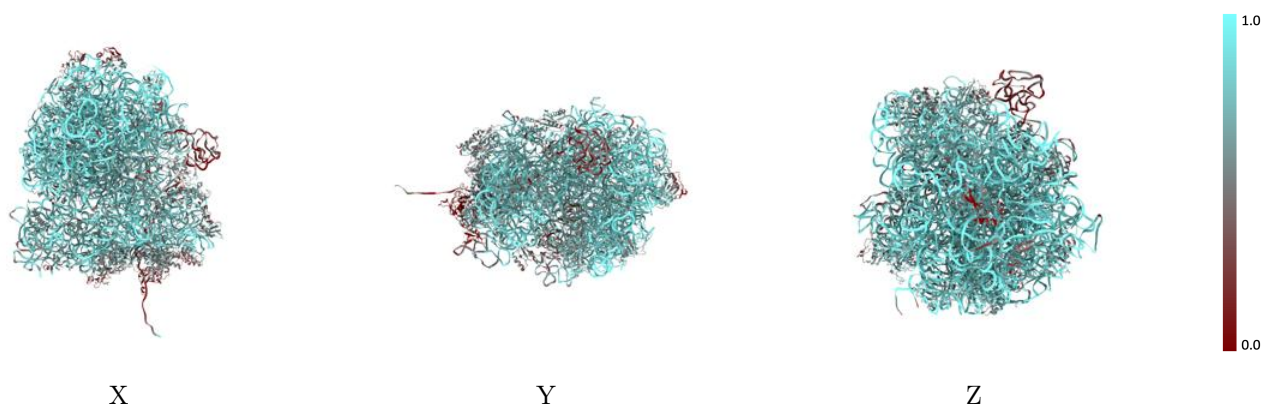
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



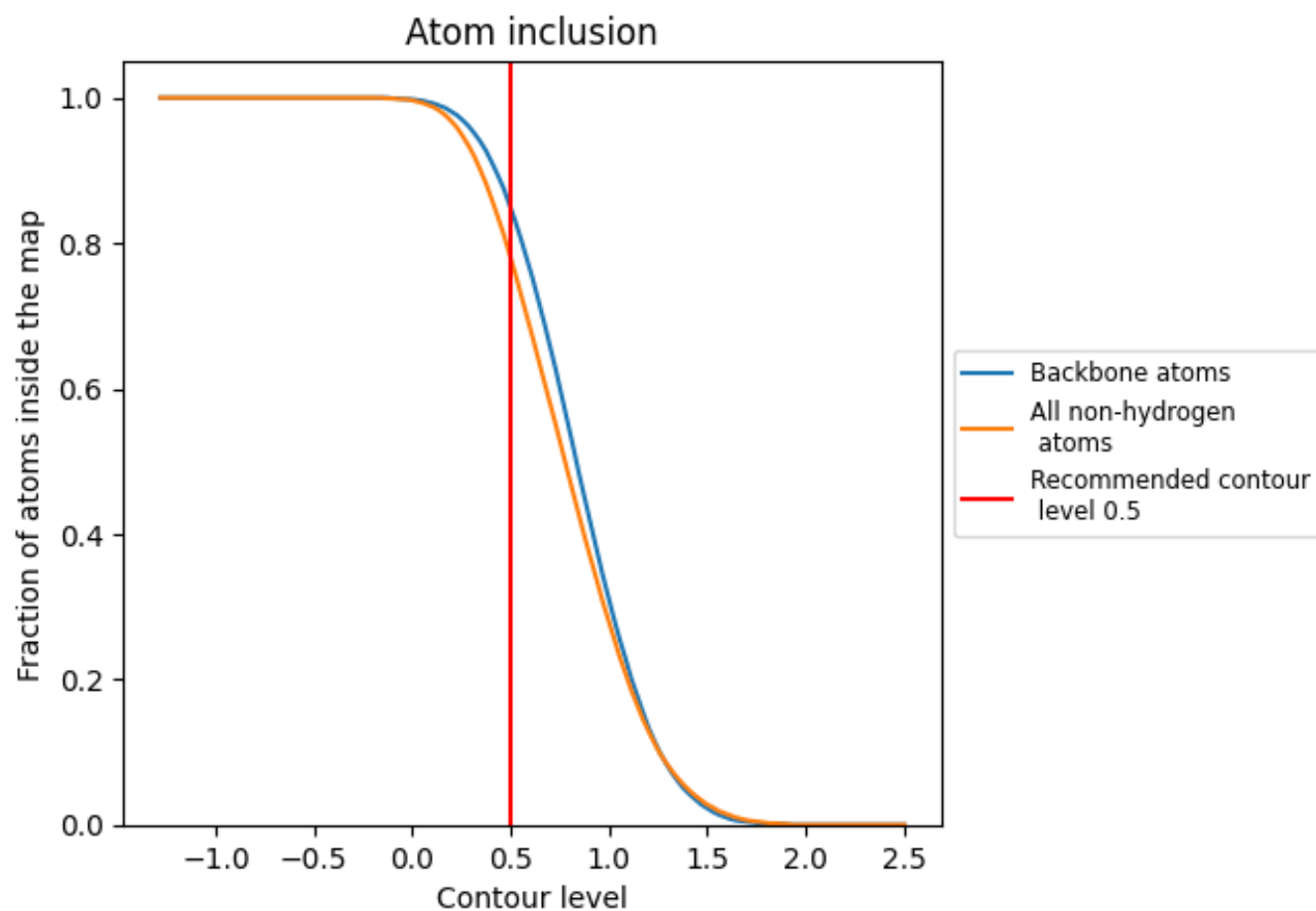
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 78% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7800	 0.3860
0	 0.7630	 0.4470
1	 0.6210	 0.3610
2	 0.8440	 0.4770
3	 0.7340	 0.4550
4	 0.7150	 0.4440
6	 0.4830	 0.2930
7	 0.5310	 0.2370
A	 0.8400	 0.3740
B	 0.4810	 0.3300
C	 0.5300	 0.3800
D	 0.3950	 0.2890
E	 0.5860	 0.4140
F	 0.5430	 0.3600
G	 0.5550	 0.3350
H	 0.6080	 0.3720
I	 0.6070	 0.3310
J	 0.5510	 0.3630
K	 0.5290	 0.3630
L	 0.5660	 0.3120
M	 0.5950	 0.3510
N	 0.6110	 0.3900
O	 0.6730	 0.3860
P	 0.5500	 0.3600
Q	 0.5330	 0.3590
R	 0.5900	 0.3860
S	 0.6030	 0.3610
T	 0.5950	 0.3280
U	 0.6660	 0.3450
V	 0.4060	 0.2580
X	 0.8740	 0.4040
Y	 0.9060	 0.3570
Z	 0.7300	 0.4600
a	 0.7200	 0.4480
b	 0.5750	 0.3930



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Chain	Atom inclusion	Q-score
c	 0.5550	 0.3110
d	 0.5580	 0.3380
e	 0.7250	 0.4280
f	 0.6950	 0.4530
i	 0.7250	 0.4150
j	 0.7110	 0.4360
k	 0.7360	 0.4200
l	 0.6700	 0.3460
m	 0.6720	 0.4190
n	 0.7650	 0.4150
o	 0.7070	 0.3990
r	 0.7460	 0.4350
s	 0.7100	 0.4230
t	 0.4380	 0.3690
u	 0.7510	 0.4340
v	 0.6280	 0.4350
w	 0.6620	 0.3590
x	 0.7330	 0.4250
z	 0.0480	 0.2260