Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 12:00 pm GMT

PDB ID	:	6QIK
EMDB ID	:	EMD-4560
Title	:	Cryo-EM structures of Lsg1-TAP pre-60S ribosomal particles
Authors	:	Kargas, V.; Warren, A.J.
Deposited on	:	2019-01-20
Resolution	:	3.10 Å(reported)
Based on initial model	:	4V88

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

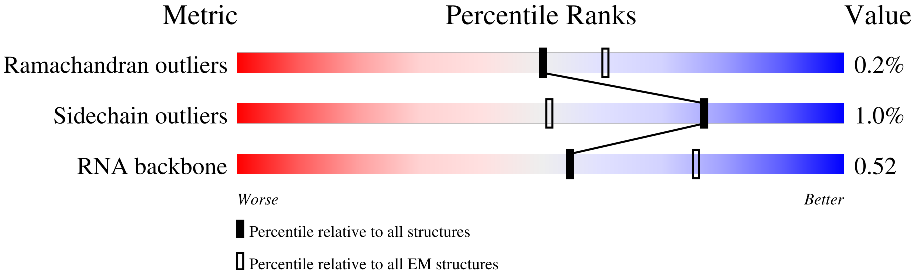
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance ⓘ

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

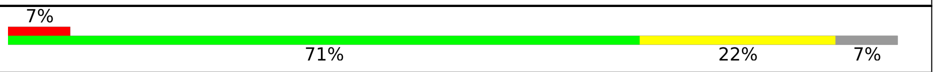
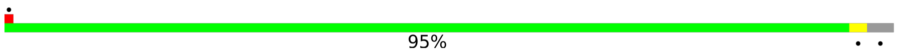
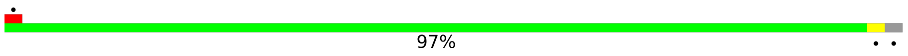
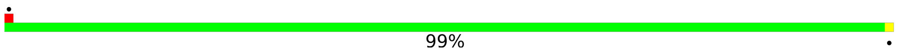
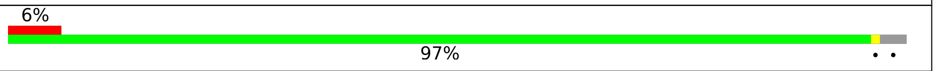
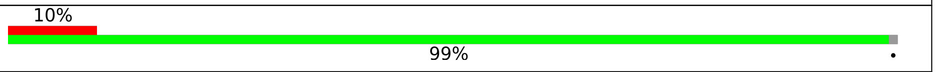
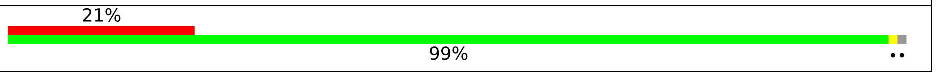
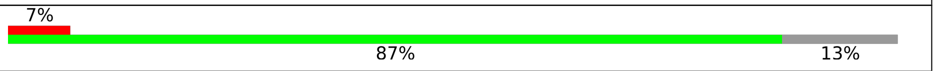
The reported resolution of this entry is 3.10 Å.

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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	3396	
2	B	254	
3	C	387	
4	D	362	
5	E	174	
6	F	191	
7	G	176	
8	H	256	

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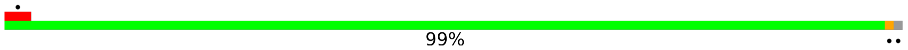
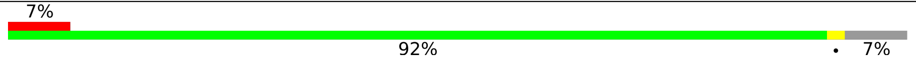
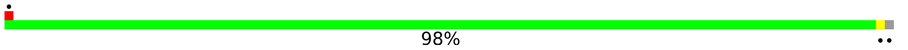
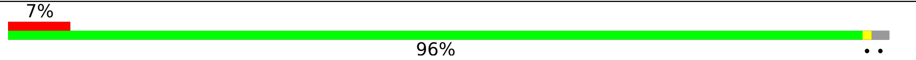
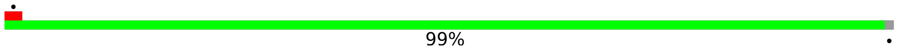
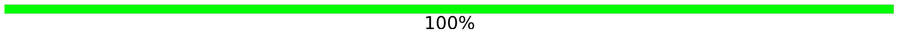
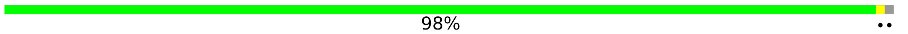
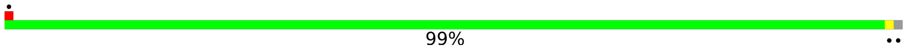
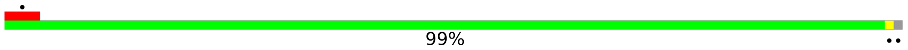
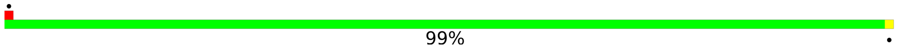
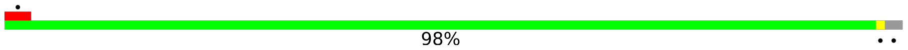
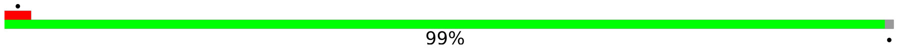
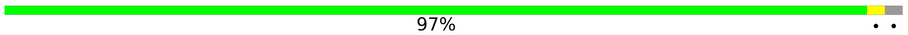
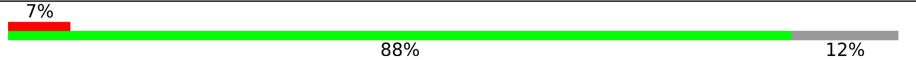
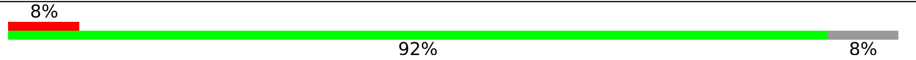
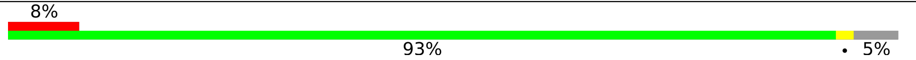
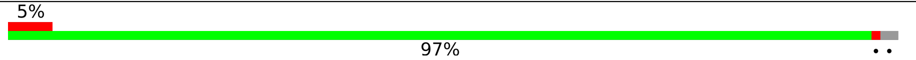
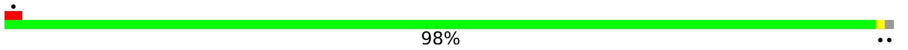
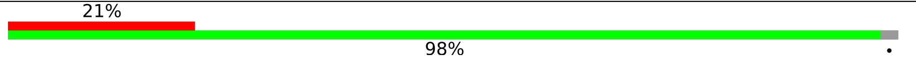
Mol	Chain	Length	Quality of chain
9	J	198	
10	K	199	
11	L	137	
12	M	138	
13	N	149	
14	O	204	
15	P	297	
16	Q	186	
17	R	189	
18	S	172	
19	T	160	
20	U	154	
21	V	121	
22	W	142	
23	X	127	
24	Y	136	
25	Z	120	
26	a	59	
27	b	244	
28	c	105	
29	d	113	
30	e	130	
31	f	107	
32	g	121	
33	h	100	

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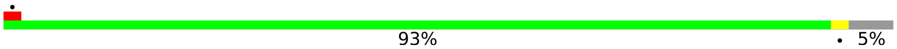
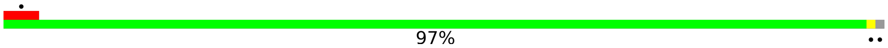
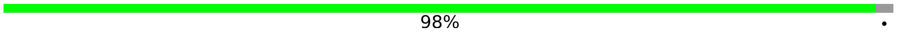
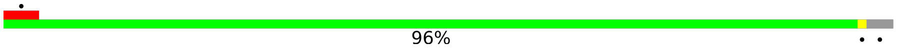
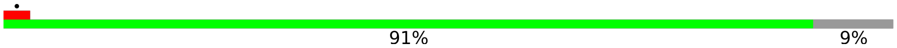
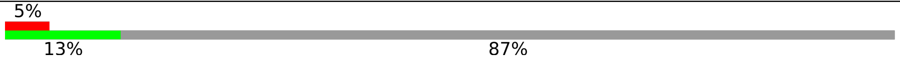
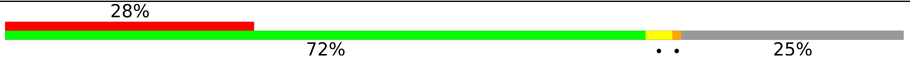
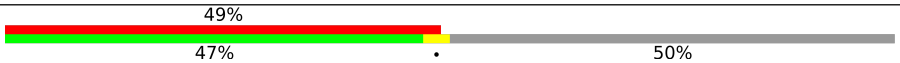
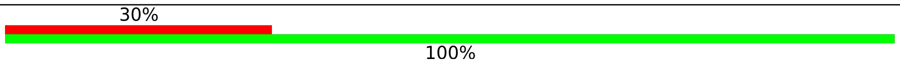
Mol	Chain	Length	Quality of chain
34	i	88	
35	j	78	
36	k	51	
37	l	106	
38	m	92	
39	n	245	
40	z	432	
41	w	518	
42	v	155	
43	o	640	
44	p	210	
45	t	128	
46	x	121	
47	y	158	

2 Entry composition ⓘ

There are 48 unique types of molecules in this entry. The entry contains 128569 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	3146	67292	30062	12142	21944	3144	0	0

- Molecule 2 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	247	1878	1170	381	326	1	0	0

- Molecule 3 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	381	3039	1928	577	526	8	0	0

- Molecule 4 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	361	2748	1730	522	493	3	0	0

- Molecule 5 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	169	1352	847	253	248	4	0	0

- Molecule 6 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	189	1502	953	272	273	4	0	0

- Molecule 7 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	175	Total 1399	C 902	N 251	O 245	S 1	0	0

- Molecule 8 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	223	Total 1742	C 1117	N 309	O 313	S 3	0	0

- Molecule 9 is a protein called 60S ribosomal protein L16-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	197	Total 1563	C 1005	N 292	O 265	S 1	0	0

- Molecule 10 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	186	Total 1486	C 929	N 304	O 253	0	0

- Molecule 11 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	136	Total 1002	C 628	N 189	O 178	S 7	0	0

- Molecule 12 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	135	Total 1045	C 669	N 197	O 177	S 2	0	0

- Molecule 13 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	148	Total 1172	C 749	N 231	O 189	S 3	0	0

- Molecule 14 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	203	1719	1077	361	280	1	0	0

- Molecule 15 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	P	269	2176	1378	375	421	2	0	0

- Molecule 16 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	185	1440	908	290	240	2	0	0

- Molecule 17 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	R	150	1209	752	257	200	0	0

- Molecule 18 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	S	171	1436	925	266	242	3	0	0

- Molecule 19 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	T	159	1275	805	246	220	4	0	0

- Molecule 20 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	U	154	1222	761	237	224	0	0

- Molecule 21 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	V	99	Total	C	N	O	0	0
			786	510	129	147		

- Molecule 22 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	120	Total	C	N	O	S	0	0
			958	617	168	171	2		

- Molecule 23 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	X	125	Total	C	N	O	0	0
			984	620	191	173		

- Molecule 24 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Y	135	Total	C	N	O	0	0
			1091	710	202	179		

- Molecule 25 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	118	Total	C	N	O	S	0	0
			963	612	185	165	1		

- Molecule 26 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	a	52	Total	C	N	O	0	0
			415	259	90	66		

- Molecule 27 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	219	Total	C	N	O	S	0	0
			1760	1138	320	301	1		

- Molecule 28 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	97	Total 741	C 479	N 124	O 137	S 1	0	0

- Molecule 29 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	107	Total 872	C 553	N 165	O 153	S 1	0	0

- Molecule 30 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	127	Total 1020	C 646	N 205	O 167	S 2	0	0

- Molecule 31 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	106	Total 849	C 540	N 165	O 143	S 1	0	0

- Molecule 32 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	103	Total 812	C 504	N 167	O 137	S 4	0	0

- Molecule 33 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	98	Total 763	C 477	N 155	O 129	S 2	0	0

- Molecule 34 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	84	Total 665	C 405	N 145	O 110	S 5	0	0

- Molecule 35 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	j	77	Total 611	C 391	N 115	O 105	0	0

- Molecule 36 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	50	Total 435	C 272	N 97	O 64	S 2	0	0

- Molecule 37 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	94	Total 756	C 476	N 153	O 122	S 5	0	0

- Molecule 38 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	89	Total 680	C 421	N 136	O 117	S 6	0	0

- Molecule 39 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	224	Total 1691	C 1051	N 293	O 340	S 7	0	0

- Molecule 40 is a protein called Cytoplasmic 60S subunit biogenesis factor REH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	z	58	Total 491	C 301	N 100	O 87	S 3	0	0

- Molecule 41 is a protein called 60S ribosomal export protein NMD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	w	389	Total 3076	C 1955	N 530	O 571	S 20	0	0

- Molecule 42 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms	AltConf	Trace
42	v	60	Total C N O S 500 322 98 79 1	0	0

- Molecule 43 is a protein called Large subunit GTPase 1.

Mol	Chain	Residues	Atoms	AltConf	Trace
43	o	322	Total C N O S 2593 1660 449 477 7	0	0

- Molecule 44 is a protein called uL1.

Mol	Chain	Residues	Atoms	AltConf	Trace
44	p	210	Total C N O 1050 630 210 210	0	0

- Molecule 45 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms	AltConf	Trace
45	t	52	Total C N O S 417 259 86 67 5	0	0

- Molecule 46 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms	AltConf	Trace
46	x	121	Total C N O P 2576 1152 461 843 120	0	0

- Molecule 47 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms	AltConf	Trace
47	y	156	Total C N O P 3310 1482 582 1091 155	0	0

- Molecule 48 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
48	g	1	Total Zn 1 1	0
48	i	1	Total Zn 1 1	0
48	l	1	Total Zn 1 1	0

Continued on next page...

Continued from previous page...

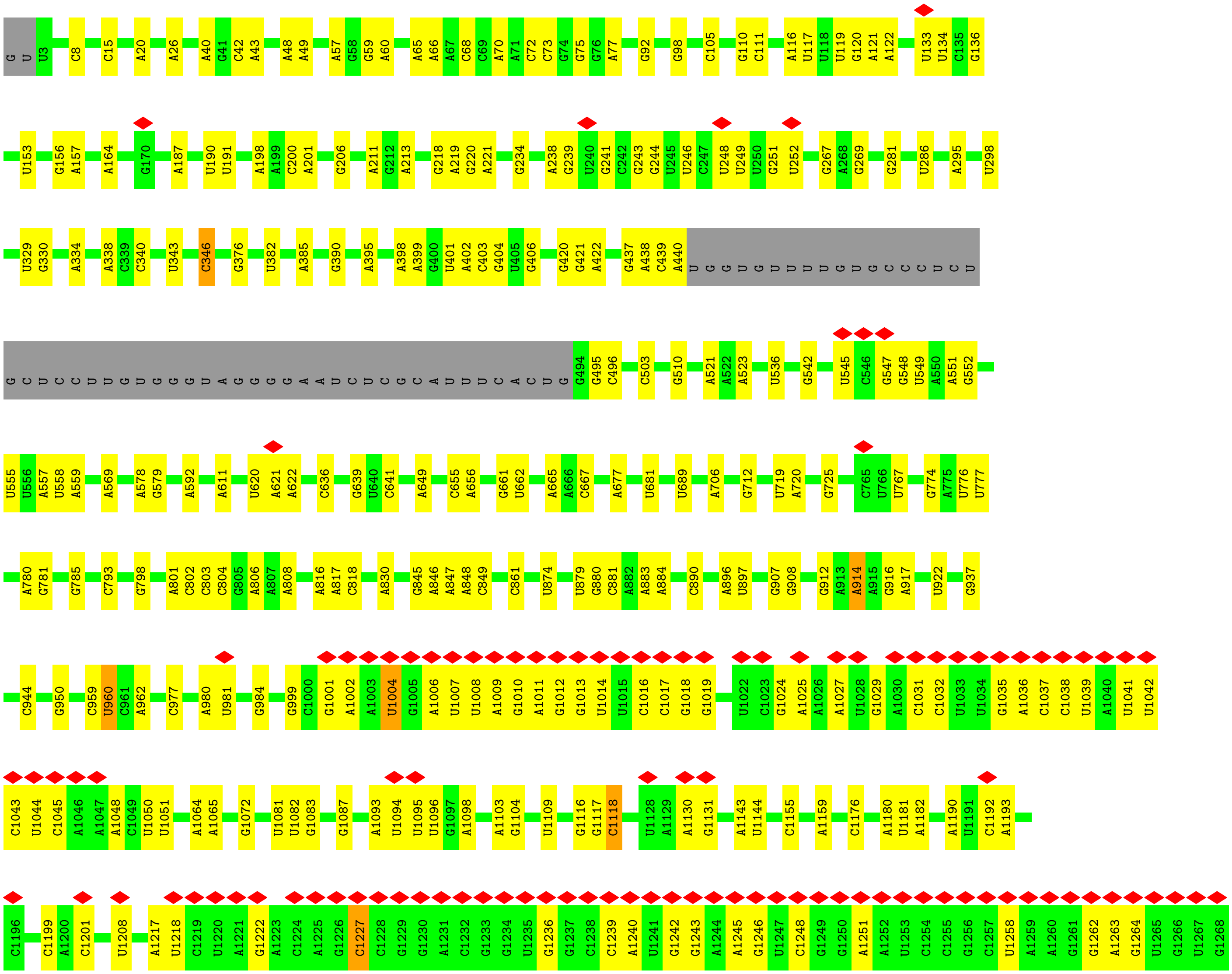
Mol	Chain	Residues	Atoms	AltConf
48	m	1	Total Zn 1 1	0
48	w	2	Total Zn 2 2	0
48	t	1	Total Zn 1 1	0

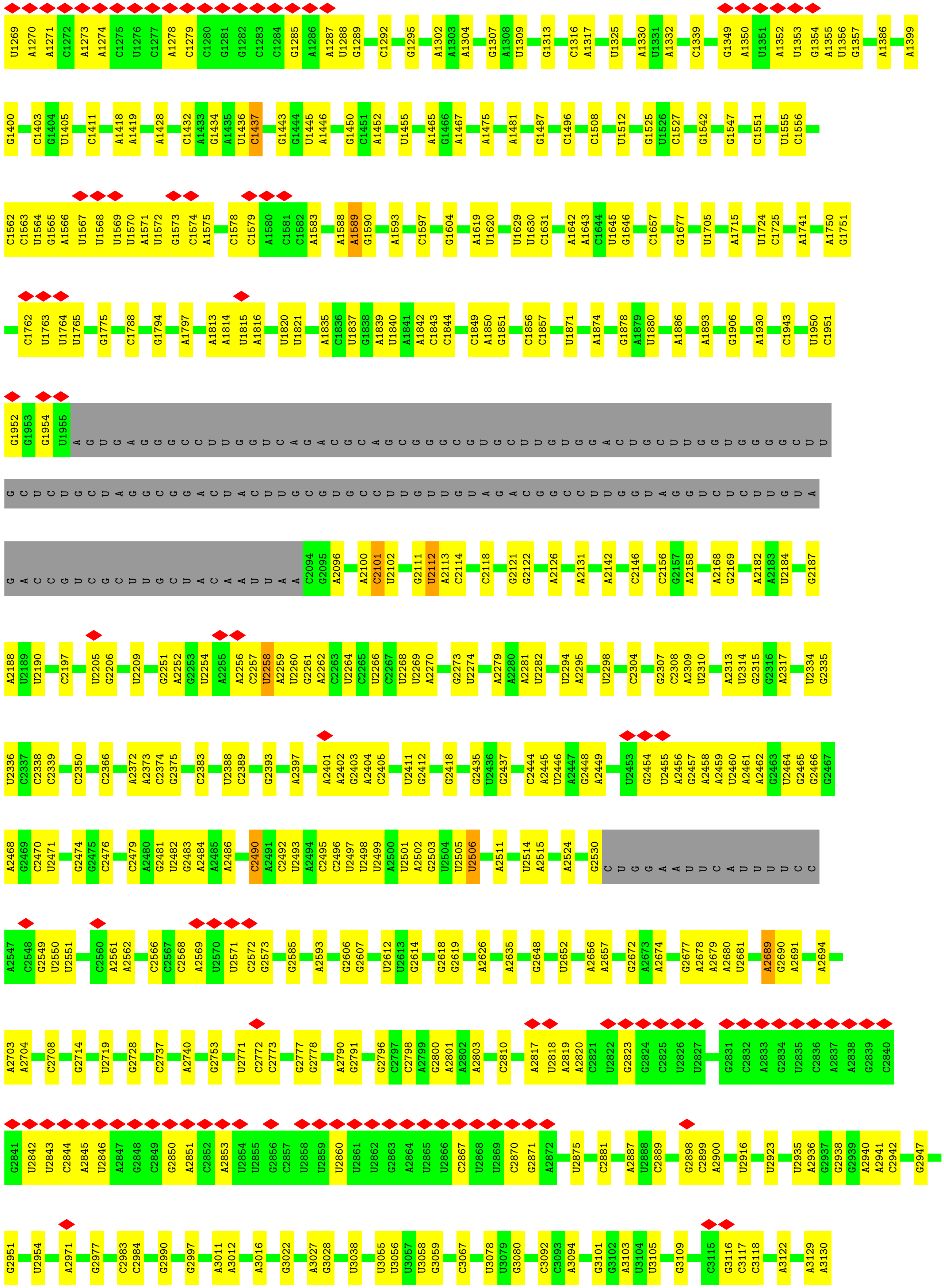
3 Residue-property plots

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

- Molecule 1: 25S ribosomal RNA

Chain A:

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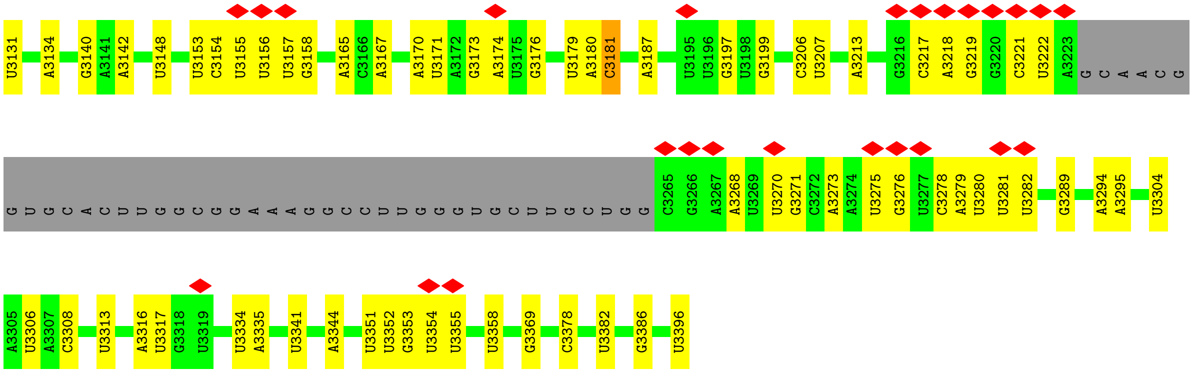
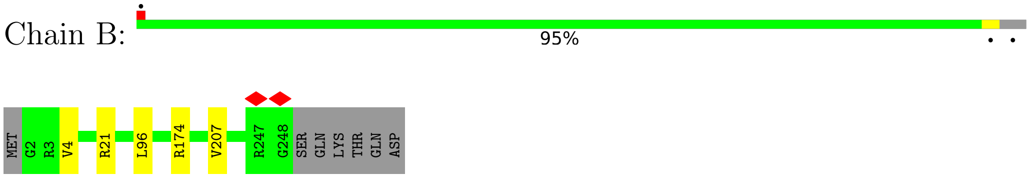
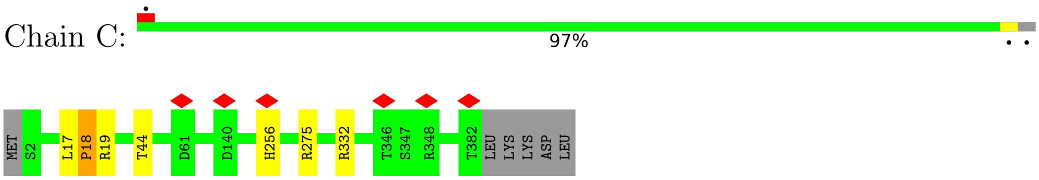
G1400 C1403 G1404 U1405 C1411 A1418 A1419 A1428 C1432 A1433 G1434 A1435 U1436 C1437 G1443 G1444 U1445 A1446 G1450 C1451 A1452 U1455 A1465 G1466 A1467 A1475 A1481 G1487 C1496 C1508 U1512 G1525 U1526 C1527 G1542 G1547 C1551 U1555 C1556
C1562 C1563 U1564 G1565 A1566 U1567 U1568 U1569 U1570 A1571 U1572 G1573 C1574 A1575 C1578 C1579 A1580 C1581 C1582 A1583 A1588 A1589 G1590 A1593 C1597 G1604 A1619 U1620 U1629 U1630 C1631 A1642 A1643 C1644 U1645 G1646 C1657 G1677 U1705 A1715 U1724 C1725 A1741 A1750 G1751
C1762 U1763 U1764 U1765 G1775 C1788 G1794 A1797 A1813 A1814 U1815 A1816 U1820 U1821 A1835 C1836 U1837 G1838 A1839 U1840 A1841 A1842 C1843 C1844 C1849 A1850 G1851 C1856 C1857 U1871 A1874 G1878 A1879 U1880 A1886 A1893 G1906 A1930 C1943 U1950 C1951
G1952 G1953 G1954 U1955 A G U G A G G G C C U U G G U C A G A C G C A G C G G G C G U G C U U G U G G A C U G C U U G G U G G G C U U
G C U C U G C U A G G C G G A C U A C U U G C G U G C C U U G U U G U A G A C G G C C U U G G U A G G U C U C U U G U A
G A C C G U C G C U U G C U A C A A U U A A C2094 G2095 A2096 A2100 C2101 U2102 G2111 U2112 A2113 C2114 C2118 G2121 G2122 A2126 A2131 A2142 C2146 C2156 G2157 A2158 A2168 G2169 A2182 A2183 U2184 G2187
A2188 U2189 U2190 C2197 U2205 G2206 U2209 G2251 A2252 G2253 U2254 A2255 A2256 C2257 U2258 A2259 U2260 G2261 A2262 C2263 U2264 C2265 U2266 C2267 U2268 U2269 A2270 G2273 U2274 A2279 A2280 U2281 U2282 U2294 A2295 U2298 C2304 G2307 C2308 A2309 U2310 A2313 U2314 G2315 G2316 A2317 U2334 G2335
U2336 C2337 C2338 C2339 C2350 C2366 A2372 A2373 C2374 G2375 C2383 U2388 C2389 G2393 A2397 A2401 A2402 G2403 A2404 C2405 U2411 G2412 G2418 G2435 U2436 G2437 C2444 A2445 U2446 A2447 G2448 A2449 U2453 G2454 U2455 A2456 G2457 A2458 A2459 U2460 A2461 A2462 G2463 U2464 G2465 G2466 G2467
A2468 G2469 C2470 U2471 G2474 G2475 C2476 C2479 A2480 G2481 U2482 G2483 A2484 A2485 A2486 C2490 A2491 C2492 U2493 A2494 C2495 C2496 U2497 U2498 U2499 A2500 U2501 A2502 G2503 U2504 U2505 U2506 A2511 U2514 A2515 A2524 G2530 C U G G A A U U C A U U U U C C
A2547 C2548 G2549 U2550 U2551 C2560 A2561 A2562 C2566 C2567 C2568 A2569 U2570 U2571 C2572 G2573 G2585 A2593 G2606 G2607 U2612 U2613 G2614 G2618 G2619 A2626 A2635 G2648 U2652 A2656 A2657 G2672 A2673 A2674 G2677 A2678 A2679 A2680 U2681 A2689 G2690 A2691 A2694
A2703 A2704 C2708 G2714 U2719 G2728 C2737 A2740 G2753 U2771 C2772 C2773 G2777 G2778 A2790 G2791 G2796 C2797 C2798 A2799 G2800 A2801 A2802 A2803 C2810 A2817 U2818 A2819 A2820 C2821 U2822 G2823 G2824 C2825 U2826 U2827 G2831 C2832 A2833 G2834 U2835 C2836 A2837 A2838 G2839 C2840
G2841 U2842 U2843 C2844 A2845 U2846 A2847 G2848 C2849 G2850 A2851 C2852 A2853 U2854 U2855 G2856 C2857 U2858 U2859 U2860 U2861 U2862 G2863 A2864 U2865 U2866 C2867 U2868 U2869 C2870 G2871 A2872 U2875 C2881 A2887 U2888 C2889 G2898 C2899 A2900 U2916 U2923 U2935 A2936 G2937 G2938 G2939 A2940 A2941 C2942 G2947
G2951 U2954 A2971 G2977 C2983 C2984 G2990 G2997 A3011 A3012 A3016 G3022 A3027 G3028 U3038 U3055 U3056 U3057 U3058 G3059 C3067 U3078 U3079 G3080 C3092 C3093 A3094 G3101 G3102 A3103 U3104 U3105 G3109 C3115 G3116 C3117 C3118 A3122 A3129 A3130



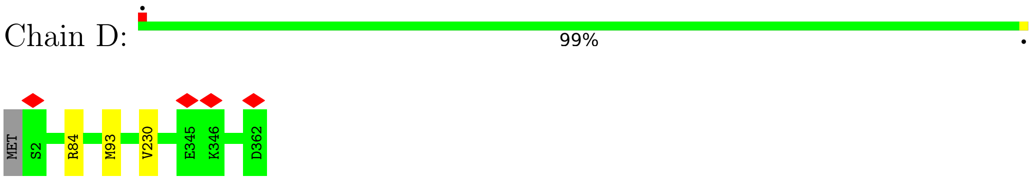
- Molecule 2: 60S ribosomal protein L2-A



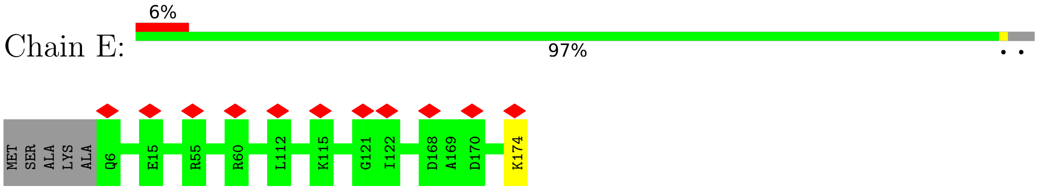
- Molecule 3: 60S ribosomal protein L3



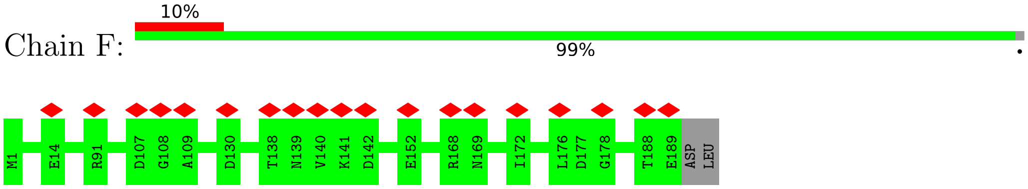
- Molecule 4: 60S ribosomal protein L4-A



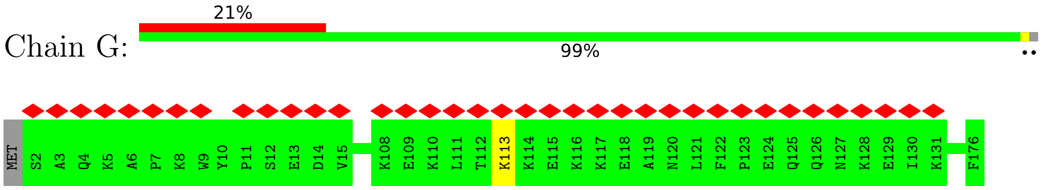
- Molecule 5: 60S ribosomal protein L11-A



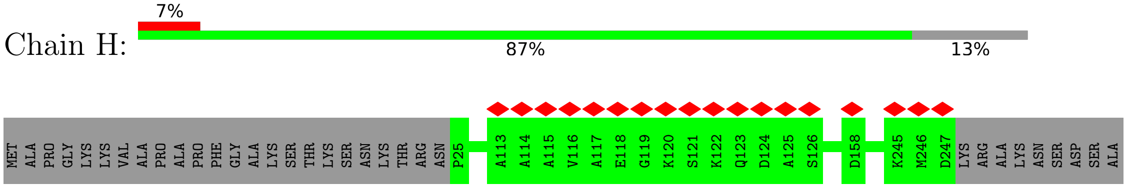
- Molecule 6: 60S ribosomal protein L9-A



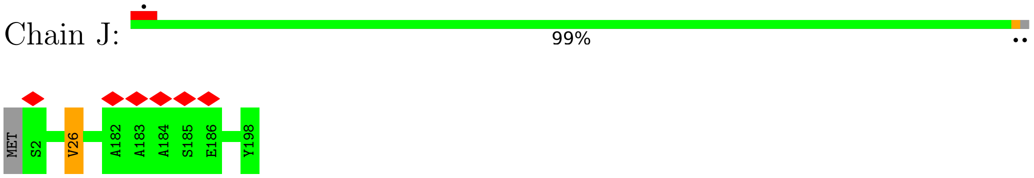
- Molecule 7: 60S ribosomal protein L6-A



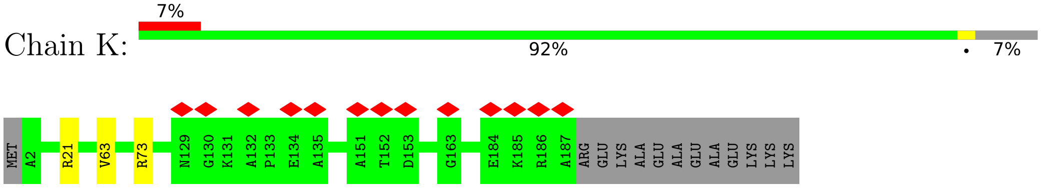
- Molecule 8: 60S ribosomal protein L8-A



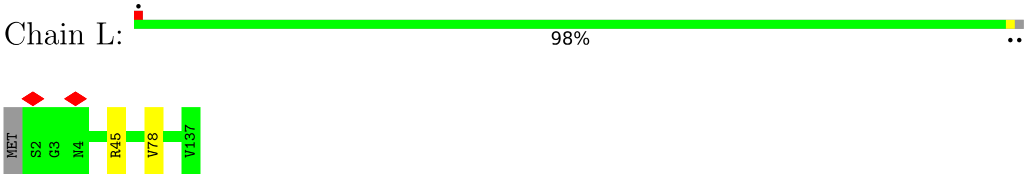
- Molecule 9: 60S ribosomal protein L16-B



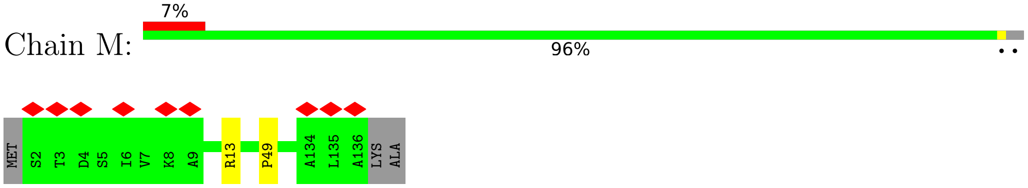
- Molecule 10: 60S ribosomal protein L13-A



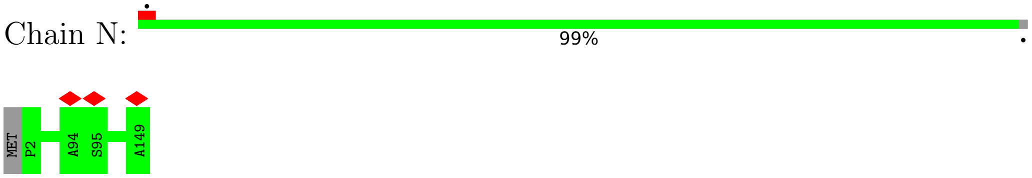
- Molecule 11: 60S ribosomal protein L23-A



- Molecule 12: 60S ribosomal protein L14-A

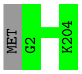


- Molecule 13: 60S ribosomal protein L28



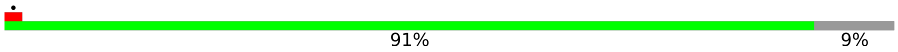
- Molecule 14: 60S ribosomal protein L15-A

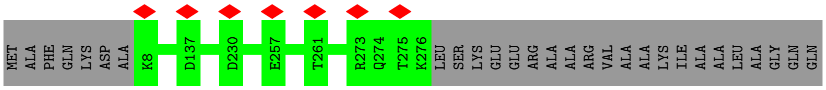
Chain O:



- Molecule 15: 60S ribosomal protein L5

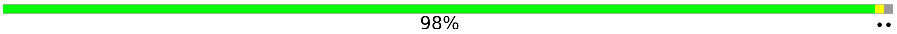
Chain P:

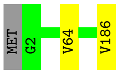




- Molecule 16: 60S ribosomal protein L18-A

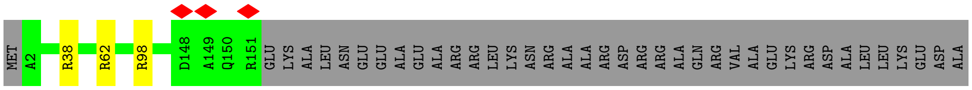
Chain Q:





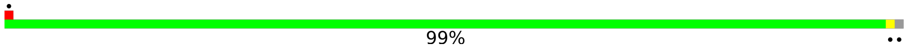
- Molecule 17: 60S ribosomal protein L19-A

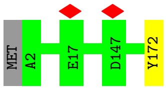
Chain R:



- Molecule 18: 60S ribosomal protein L20-A

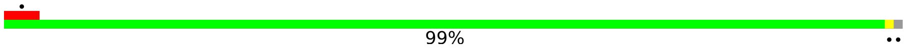
Chain S:

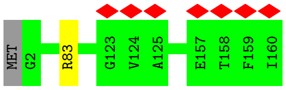




- Molecule 19: 60S ribosomal protein L21-A

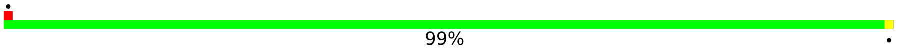
Chain T:

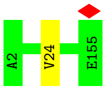




- Molecule 20: 60S ribosomal protein L17-A

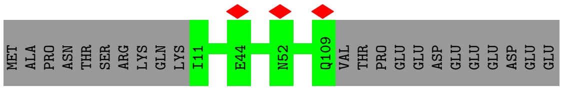
Chain U:





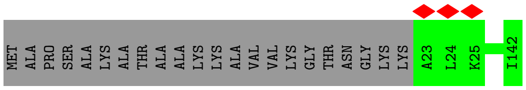
- Molecule 21: 60S ribosomal protein L22-A

Chain V:



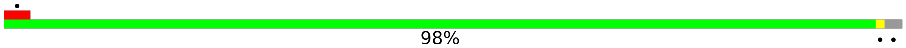
- Molecule 22: 60S ribosomal protein L25

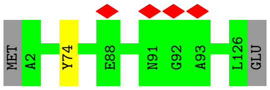
Chain W:



- Molecule 23: 60S ribosomal protein L26-A

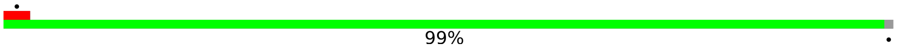
Chain X:

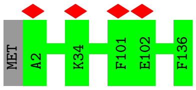




- Molecule 24: 60S ribosomal protein L27-A

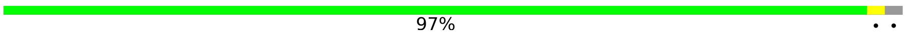
Chain Y:

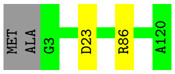




- Molecule 25: 60S ribosomal protein L35-A

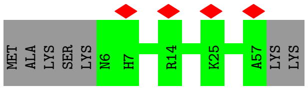
Chain Z:





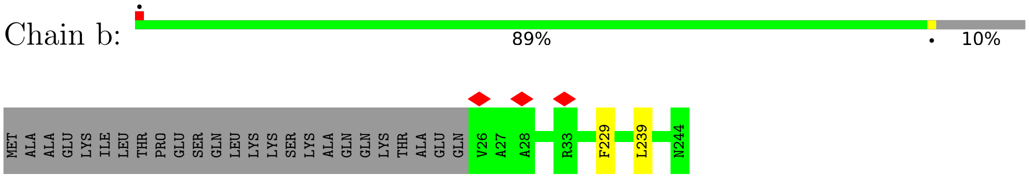
- Molecule 26: 60S ribosomal protein L29

Chain a:



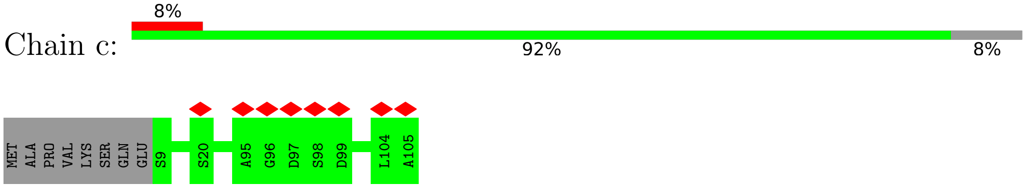
- Molecule 27: 60S ribosomal protein L7-A

Chain b:



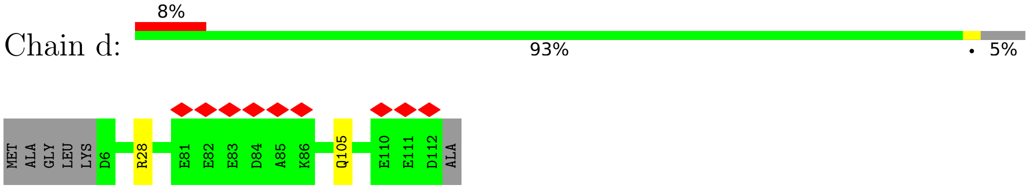
- Molecule 28: 60S ribosomal protein L30

Chain c:



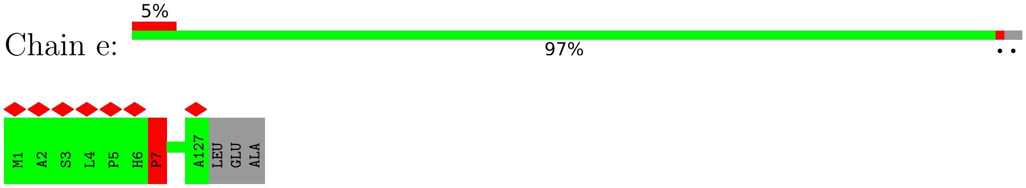
- Molecule 29: 60S ribosomal protein L31-A

Chain d:



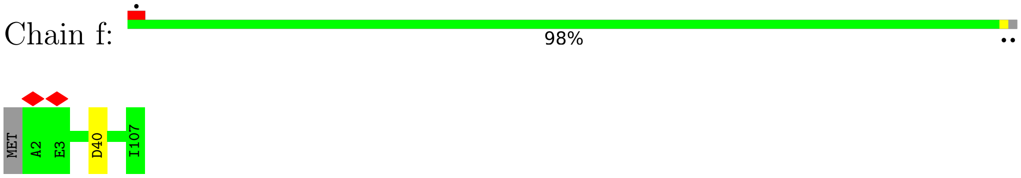
- Molecule 30: 60S ribosomal protein L32

Chain e:



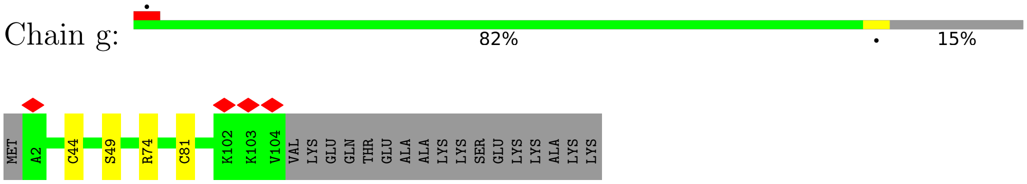
- Molecule 31: 60S ribosomal protein L33-A

Chain f:



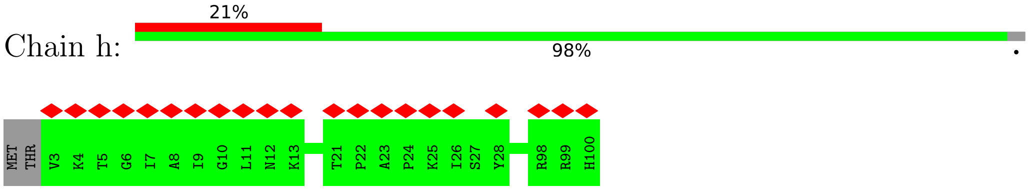
- Molecule 32: 60S ribosomal protein L34-A

Chain g:



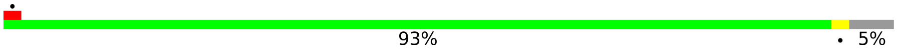
- Molecule 33: 60S ribosomal protein L36-A

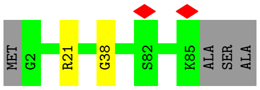
Chain h:



- Molecule 34: 60S ribosomal protein L37-A

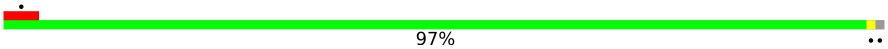
Chain i:

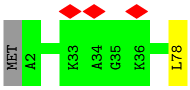




- Molecule 35: 60S ribosomal protein L38

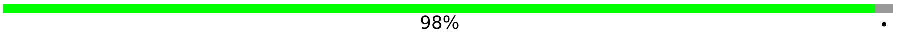
Chain j:

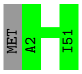




- Molecule 36: 60S ribosomal protein L39

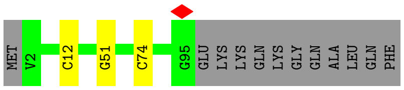
Chain k:





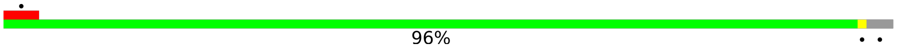
- Molecule 37: 60S ribosomal protein L42-A

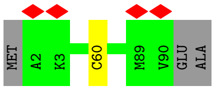
Chain l:



- Molecule 38: 60S ribosomal protein L43-A

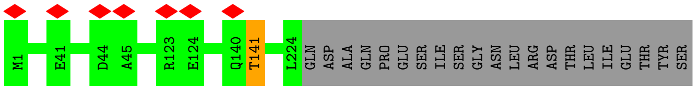
Chain m:





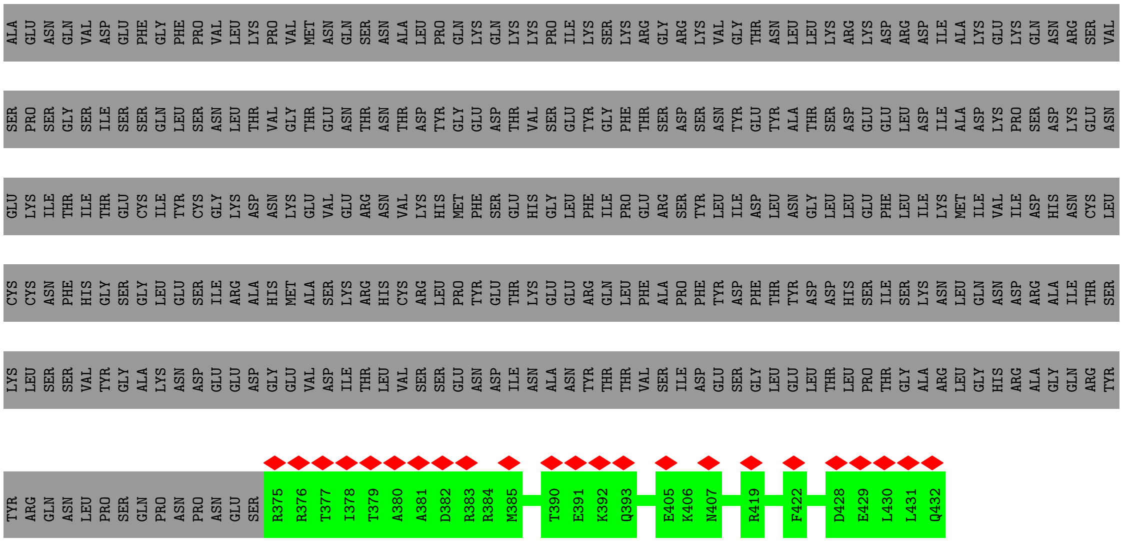
- Molecule 39: Eukaryotic translation initiation factor 6

Chain n:



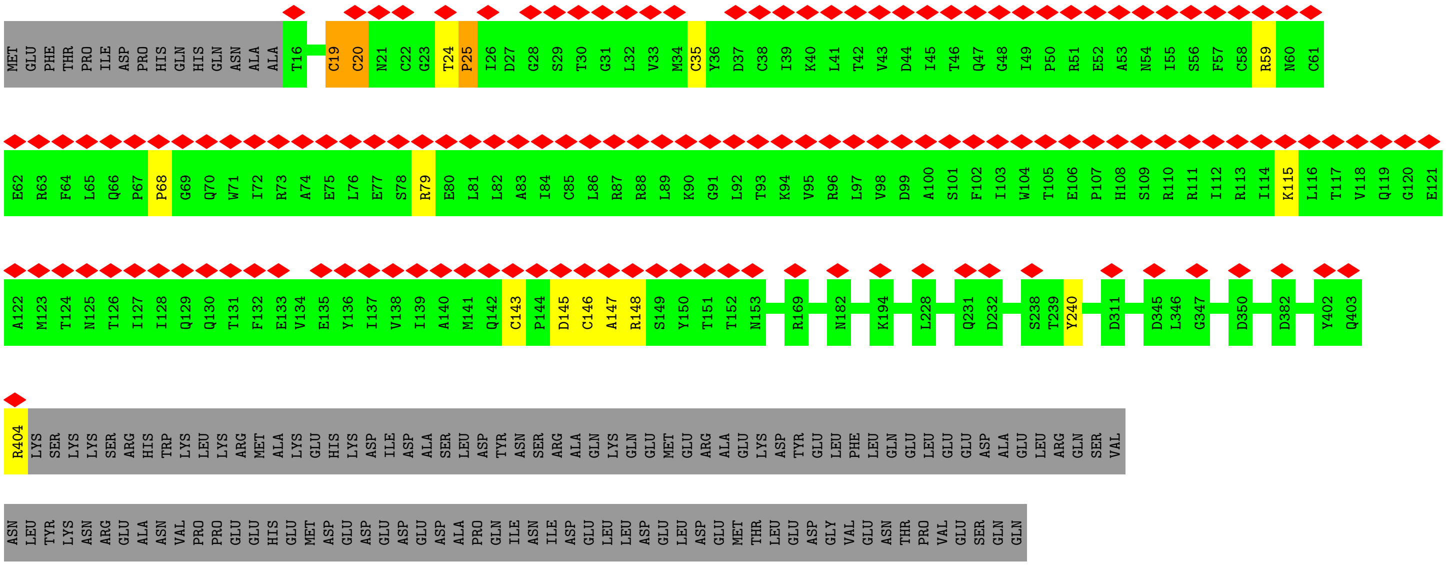
- Molecule 40: Cytoplasmic 60S subunit biogenesis factor REH1

Chain z:



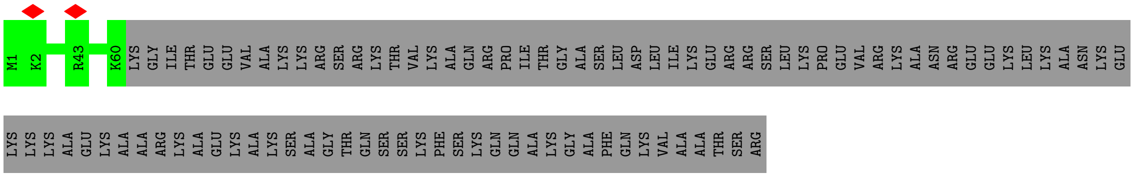
- Molecule 41: 60S ribosomal export protein NMD3

Chain w:



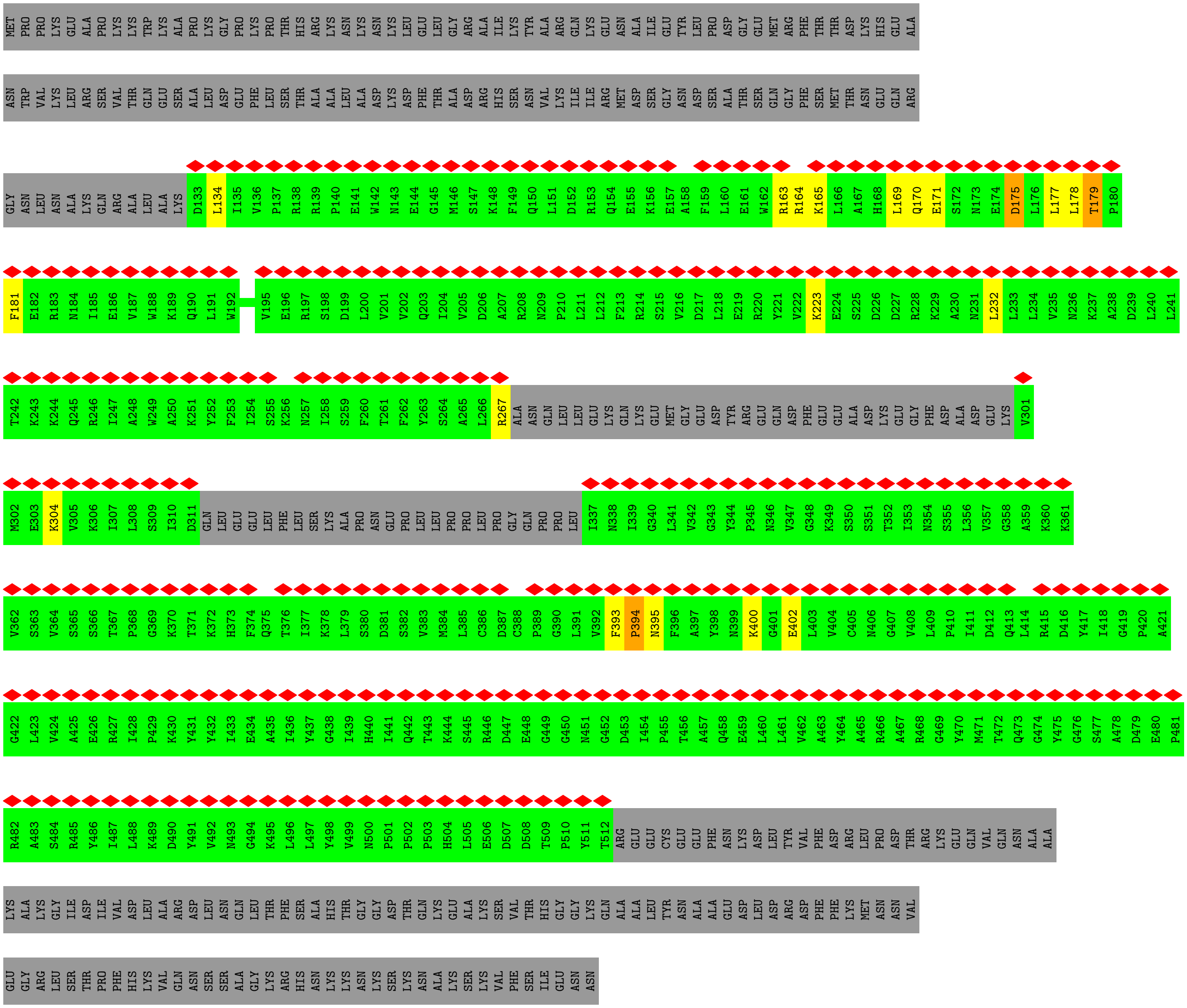
- Molecule 42: 60S ribosomal protein L24-A

Chain v:

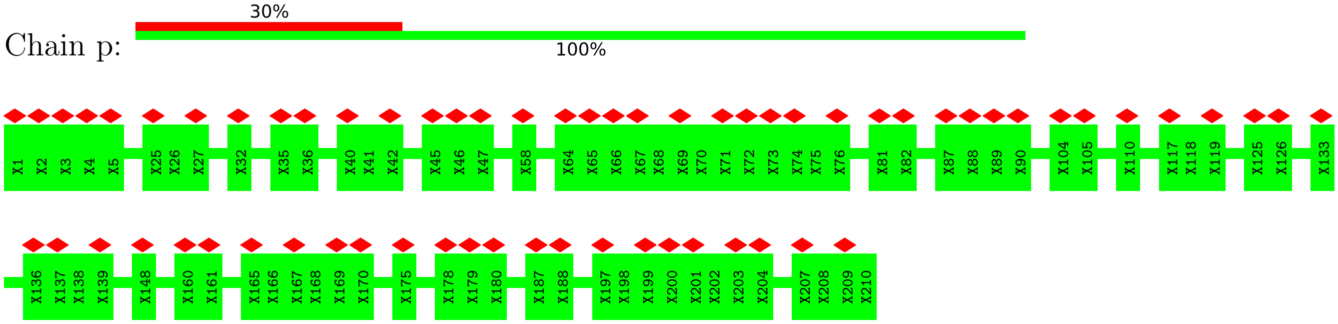


- Molecule 43: Large subunit GTPase 1

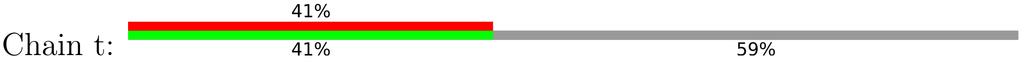
Chain o:

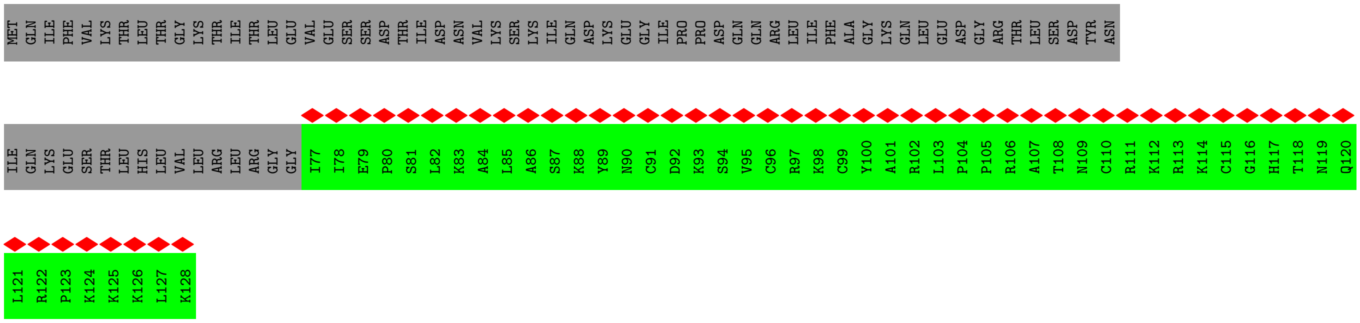


- Molecule 44: uL1

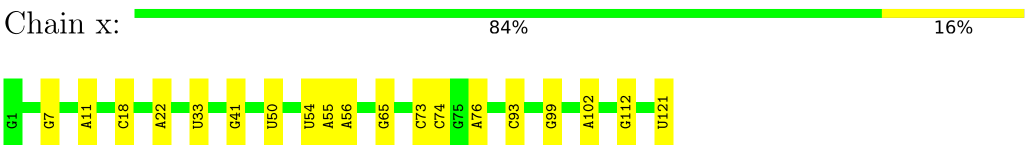


- Molecule 45: Ubiquitin-60S ribosomal protein L40

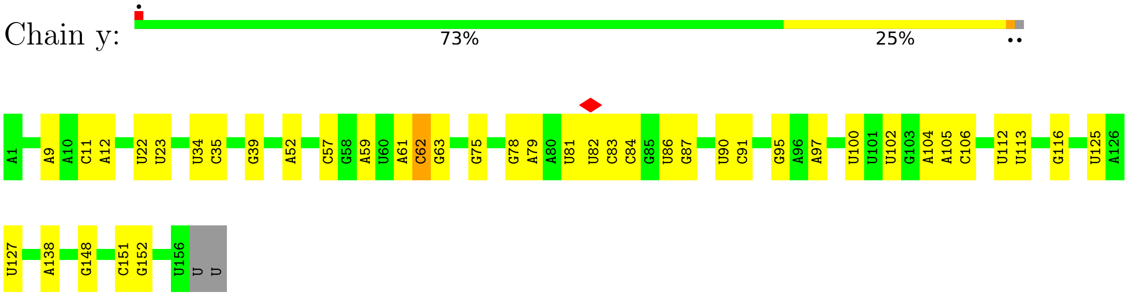




- Molecule 46: 5S ribosomal RNA



- Molecule 47: 5.8S ribosomal RNA



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	260853	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	63	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.560	Depositor
Minimum map value	-0.287	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	383.40002, 383.40002, 383.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	1.25	40/75327 (0.1%)	1.14	104/117440 (0.1%)
2	B	0.89	2/1912 (0.1%)	0.78	3/2569 (0.1%)
3	C	0.87	0/3110	0.80	3/4184 (0.1%)
4	D	0.86	1/2800 (0.0%)	0.68	1/3791 (0.0%)
5	E	0.45	0/1373	0.63	0/1841
6	F	0.44	0/1523	0.61	0/2051
7	G	0.57	0/1423	0.63	0/1911
8	H	0.68	0/1774	0.62	0/2395
9	J	0.86	1/1593 (0.1%)	0.69	0/2137
10	K	0.79	0/1511	0.77	1/2031 (0.0%)
11	L	0.81	1/1017 (0.1%)	0.74	1/1368 (0.1%)
12	M	0.62	0/1060	0.66	0/1428
13	N	0.89	0/1203	0.70	0/1611
14	O	1.00	0/1756	0.79	0/2353
15	P	0.65	0/2225	0.61	0/3004
16	Q	0.86	1/1464 (0.1%)	0.74	0/1964
17	R	0.83	0/1226	0.75	4/1637 (0.2%)
18	S	0.76	0/1472	0.63	0/1979
19	T	0.78	0/1299	0.66	0/1742
20	U	0.94	1/1245 (0.1%)	0.71	0/1676
21	V	0.60	0/802	0.60	0/1087
22	W	0.80	0/973	0.65	0/1313
23	X	0.77	0/995	0.73	0/1329
24	Y	0.59	0/1117	0.65	0/1496
25	Z	0.72	0/972	0.71	2/1293 (0.2%)
26	a	0.62	0/426	0.61	0/570
27	b	0.87	0/1797	0.67	0/2419
28	c	0.68	0/749	0.63	0/1007
29	d	0.80	0/886	0.75	1/1190 (0.1%)
30	e	0.81	0/1041	0.70	1/1393 (0.1%)
31	f	0.91	0/867	0.79	1/1167 (0.1%)
32	g	0.87	0/822	0.77	1/1099 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	h	0.56	0/770	0.67	0/1023
34	i	0.90	0/680	0.81	0/901
35	j	0.58	0/617	0.63	0/825
36	k	0.86	0/442	0.73	0/587
37	l	0.79	0/768	0.77	0/1016
38	m	0.85	0/687	0.76	0/915
39	n	0.48	0/1712	0.60	0/2330
40	z	0.41	0/494	0.67	0/654
41	w	0.59	3/3135 (0.1%)	0.63	1/4255 (0.0%)
42	v	0.57	0/512	0.61	0/680
43	o	0.49	3/2647 (0.1%)	0.67	2/3582 (0.1%)
45	t	0.29	0/423	0.56	0/562
46	x	1.08	0/2880	1.08	0/4487
47	y	1.40	5/3699 (0.1%)	1.19	7/5760 (0.1%)
All	All	1.07	58/137226 (0.0%)	1.00	133/202052 (0.1%)

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	w	25	PRO	N-CA	14.19	1.71	1.47
43	o	394	PRO	N-CA	13.54	1.70	1.47
43	o	179	THR	C-N	8.59	1.50	1.34
1	A	42	C	C4-C5	-6.82	1.37	1.43
1	A	346	C	N1-C6	-6.18	1.33	1.37
1	A	639	G	N9-C8	-6.08	1.33	1.37
47	y	12	A	N9-C4	-6.06	1.34	1.37
1	A	3067	C	N1-C6	-6.03	1.33	1.37
43	o	393	PHE	C-N	5.97	1.45	1.34
1	A	2258	U	C1'-N1	5.94	1.57	1.48
41	w	24	THR	C-N	5.92	1.45	1.34
20	U	24	VAL	CB-CG1	-5.92	1.40	1.52
1	A	914	A	N9-C4	-5.85	1.34	1.37
1	A	655	C	N1-C6	-5.79	1.33	1.37
1	A	1597	C	C4-C5	-5.70	1.38	1.43
1	A	1844	C	N1-C6	-5.69	1.33	1.37
1	A	340	C	N1-C6	-5.65	1.33	1.37
4	D	230	VAL	CB-CG1	-5.64	1.41	1.52
1	A	2366	C	C4-C5	-5.60	1.38	1.43
47	y	57	C	N1-C6	-5.46	1.33	1.37
1	A	803	C	N1-C6	-5.44	1.33	1.37
1	A	665	A	N9-C4	-5.43	1.34	1.37
1	A	1857	C	N1-C6	-5.43	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	y	11	C	N1-C6	-5.41	1.33	1.37
1	A	2338	C	N1-C6	-5.39	1.33	1.37
1	A	98	G	N7-C5	-5.38	1.36	1.39
1	A	2389	C	C4-C5	-5.36	1.38	1.43
11	L	78	VAL	CB-CG2	-5.35	1.41	1.52
1	A	962	A	C5-C6	-5.31	1.36	1.41
1	A	1496	C	C4-C5	-5.29	1.38	1.43
2	B	207	VAL	CB-CG1	-5.29	1.41	1.52
9	J	26	VAL	CB-CG2	-5.27	1.41	1.52
47	y	62	C	N1-C6	-5.26	1.33	1.37
1	A	2156	C	N1-C6	-5.25	1.34	1.37
1	A	1437	C	C4-C5	-5.24	1.38	1.43
1	A	802	C	N1-C6	-5.24	1.34	1.37
1	A	1843	C	C4-C5	-5.22	1.38	1.43
41	w	19	CYS	C-O	-5.22	1.13	1.23
16	Q	64	VAL	CB-CG2	-5.20	1.42	1.52
1	A	2881	C	N1-C6	-5.20	1.34	1.37
1	A	68	C	C4-C5	-5.14	1.38	1.43
1	A	1176	C	N1-C6	-5.12	1.34	1.37
2	B	4	VAL	CB-CG2	-5.12	1.42	1.52
1	A	804	C	N1-C6	-5.11	1.34	1.37
1	A	2798	C	N1-C6	-5.10	1.34	1.37
1	A	883	A	N9-C4	-5.07	1.34	1.37
1	A	1403	C	N1-C6	-5.07	1.34	1.37
1	A	655	C	C4-C5	-5.07	1.38	1.43
1	A	3344	A	N9-C4	-5.05	1.34	1.37
1	A	1432	C	N1-C6	-5.05	1.34	1.37
47	y	61	A	N9-C4	-5.05	1.34	1.37
1	A	2339	C	N1-C6	-5.04	1.34	1.37
1	A	1411	C	N1-C6	-5.03	1.34	1.37
1	A	2383	C	N1-C6	-5.03	1.34	1.37
1	A	2182	A	N9-C4	-5.02	1.34	1.37
1	A	2146	C	C4-C5	-5.01	1.39	1.43
1	A	641	C	N1-C6	-5.01	1.34	1.37
1	A	3308	C	C4-C5	-5.01	1.39	1.43

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	18	PRO	CA-N-CD	-15.99	89.11	111.50
1	A	962	A	N1-C6-N6	8.65	123.79	118.60
43	o	394	PRO	CA-N-CD	-8.28	99.91	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	962	A	C5-C6-N6	-7.93	117.36	123.70
1	A	406	G	O4'-C1'-N9	7.53	114.22	108.20
1	A	922	U	C2-N1-C1'	7.52	126.73	117.70
41	w	25	PRO	CA-N-CD	-7.17	101.46	111.50
1	A	1496	C	C6-N1-C2	-7.13	117.45	120.30
1	A	962	A	C4-C5-N7	6.99	114.19	110.70
43	o	232	LEU	CA-CB-CG	6.82	130.99	115.30
1	A	1857	C	N1-C2-O2	6.75	122.95	118.90
1	A	2790	A	C5-C6-N6	-6.63	118.39	123.70
1	A	2101	C	C6-N1-C2	-6.41	117.74	120.30
1	A	2790	A	N1-C6-N6	6.41	122.44	118.60
1	A	1496	C	C2-N1-C1'	6.38	125.82	118.80
1	A	2366	C	N1-C2-O2	6.36	122.72	118.90
1	A	1496	C	N1-C2-O2	6.30	122.68	118.90
1	A	8	C	N1-C2-O2	6.16	122.59	118.90
1	A	1118	C	C6-N1-C2	-6.16	117.84	120.30
1	A	3344	A	N1-C6-N6	6.07	122.24	118.60
1	A	2190	U	C5-C4-O4	-6.01	122.29	125.90
1	A	42	C	N3-C4-N4	5.99	122.19	118.00
47	y	39	G	C2-N3-C4	-5.99	108.91	111.90
1	A	42	C	C5-C4-N4	-5.96	116.03	120.20
1	A	2418	G	C4-N9-C1'	5.96	134.25	126.50
1	A	1004	U	C2-N1-C1'	5.95	124.84	117.70
1	A	2118	C	C5-C4-N4	-5.95	116.03	120.20
1	A	2984	C	C6-N1-C2	-5.94	117.93	120.30
1	A	2190	U	N3-C4-O4	5.93	123.55	119.40
47	y	9	A	C5-C6-N6	-5.92	118.97	123.70
47	y	62	C	C5-C4-N4	-5.90	116.07	120.20
1	A	3181	C	C2-N1-C1'	5.85	125.23	118.80
4	D	84	ARG	NE-CZ-NH1	5.84	123.22	120.30
47	y	9	A	N1-C6-N6	5.83	122.09	118.60
1	A	793	C	C5-C4-N4	-5.82	116.13	120.20
1	A	798	G	N1-C2-N2	-5.79	110.99	116.20
1	A	912	G	C2-N3-C4	-5.78	109.01	111.90
1	A	3181	C	N1-C2-O2	5.78	122.37	118.90
1	A	3058	U	C2-N1-C1'	5.77	124.62	117.70
1	A	960	U	C2-N1-C1'	5.75	124.60	117.70
1	A	2490	C	C2-N1-C1'	5.75	125.12	118.80
3	C	275	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	A	343	U	C6-N1-C2	-5.72	117.57	121.00
1	A	1118	C	C5-C6-N1	5.71	123.86	121.00
1	A	706	A	N9-C4-C5	-5.71	103.52	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	962	A	N9-C4-C5	-5.71	103.52	105.80
1	A	1432	C	C5-C4-N4	-5.70	116.21	120.20
47	y	9	A	N9-C4-C5	-5.68	103.53	105.80
1	A	42	C	N1-C2-O2	5.67	122.30	118.90
1	A	340	C	C2-N1-C1’	5.66	125.02	118.80
1	A	1525	G	C4-N9-C1’	5.64	133.84	126.50
1	A	2304	C	N1-C2-O2	5.63	122.28	118.90
29	d	28	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	1144	U	C5-C4-O4	-5.60	122.54	125.90
1	A	1837	U	N3-C4-O4	5.59	123.31	119.40
47	y	9	A	C4-C5-N7	5.55	113.48	110.70
1	A	3308	C	C5-C4-N4	-5.54	116.32	120.20
1	A	1597	C	C5-C4-N4	-5.53	116.33	120.20
1	A	3308	C	N3-C4-N4	5.50	121.85	118.00
1	A	665	A	C5-N7-C8	-5.49	101.16	103.90
1	A	2418	G	C8-N9-C1’	-5.49	119.86	127.00
1	A	962	A	C5-N7-C8	-5.48	101.16	103.90
1	A	98	G	C2-N3-C4	-5.47	109.17	111.90
1	A	1339	C	C5-C4-N4	-5.46	116.38	120.20
1	A	2490	C	N1-C2-O2	5.40	122.14	118.90
31	f	40	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	2506	U	N3-C2-O2	-5.39	118.42	122.20
1	A	1837	U	C5-C4-O4	-5.39	122.67	125.90
1	A	922	U	C5-C6-N1	5.38	125.39	122.70
1	A	818	C	C5-C4-N4	-5.38	116.44	120.20
17	R	98	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	881	C	C5-C4-N4	-5.36	116.45	120.20
1	A	1292	C	N1-C2-O2	5.34	122.11	118.90
1	A	1109	U	C5-C6-N1	5.34	125.37	122.70
1	A	2612	U	N3-C4-O4	5.33	123.14	119.40
1	A	3306	U	C2-N1-C1’	5.33	124.10	117.70
1	A	2870	C	C6-N1-C2	-5.32	118.17	120.30
1	A	1109	U	N3-C4-O4	5.30	123.11	119.40
1	A	1155	C	C6-N1-C2	-5.29	118.18	120.30
1	A	1227	C	C6-N1-C2	-5.28	118.19	120.30
1	A	3317	U	C2-N1-C1’	5.27	124.02	117.70
1	A	1109	U	C5-C4-O4	-5.26	122.74	125.90
25	Z	86	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	1525	G	C8-N9-C1’	-5.24	120.19	127.00
17	R	62	ARG	NE-CZ-NH1	5.23	122.91	120.30
10	K	73	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	1527	C	N1-C2-O2	5.22	122.03	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2689	A	C5-C6-N6	-5.22	119.52	123.70
1	A	2689	A	N1-C6-N6	5.22	121.73	118.60
1	A	950	G	N1-C2-N2	-5.20	111.52	116.20
30	e	7	PRO	N-CA-CB	-5.19	96.89	102.60
1	A	2304	C	N3-C2-O2	-5.18	118.27	121.90
2	B	21	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	A	3344	A	C5-N7-C8	-5.17	101.32	103.90
1	A	2317	A	C5-C6-N6	-5.16	119.57	123.70
1	A	3181	C	N3-C2-O2	-5.16	118.29	121.90
3	C	18	PRO	CB-CA-C	5.16	124.89	112.00
11	L	45	ARG	NE-CZ-NH1	5.16	122.88	120.30
17	R	62	ARG	NE-CZ-NH2	-5.15	117.72	120.30
2	B	96	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	1851	G	C4-C5-N7	5.14	112.86	110.80
1	A	798	G	N3-C2-N2	5.14	123.50	119.90
1	A	1857	C	N3-C2-O2	-5.14	118.30	121.90
1	A	2112	U	P-O3'-C3'	5.13	125.86	119.70
1	A	2118	C	N3-C4-N4	5.12	121.59	118.00
25	Z	23	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	1589	A	C5-C6-N1	5.12	120.26	117.70
1	A	2954	U	C2-N1-C1'	5.12	123.84	117.70
1	A	57	A	C5-C6-N6	-5.12	119.61	123.70
1	A	1604	G	C4-N9-C1'	5.11	133.15	126.50
1	A	1851	G	C6-C5-N7	-5.11	127.33	130.40
2	B	174	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	656	A	C5-N7-C8	-5.10	101.35	103.90
1	A	950	G	C2-N3-C4	-5.08	109.36	111.90
17	R	38	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	20	A	N9-C4-C5	-5.08	103.77	105.80
1	A	2366	C	C5-C4-N4	-5.08	116.64	120.20
1	A	340	C	C6-N1-C2	-5.08	118.27	120.30
1	A	201	A	C4-C5-N7	5.07	113.23	110.70
1	A	1590	G	C4-C5-N7	5.07	112.83	110.80
1	A	1856	C	N1-C2-O2	5.07	121.94	118.90
32	g	74	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	656	A	N9-C4-C5	-5.06	103.78	105.80
1	A	1190	A	C4-N9-C1'	5.06	135.40	126.30
1	A	656	A	N1-C6-N6	5.05	121.63	118.60
1	A	2954	U	N1-C2-O2	5.05	126.33	122.80
47	y	100	U	N3-C4-O4	5.04	122.93	119.40
1	A	656	A	C4-C5-N7	5.04	113.22	110.70
1	A	382	U	C5-C4-O4	-5.01	122.89	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3140	G	C2-N3-C4	-5.00	109.40	111.90
1	A	922	U	C6-N1-C1’	-5.00	114.20	121.20
1	A	1512	U	N3-C4-O4	5.00	122.90	119.40
1	A	1551	C	N1-C2-O2	5.00	121.90	118.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	245/254 (96%)	221 (90%)	24 (10%)	0	100	100
3	C	379/387 (98%)	347 (92%)	31 (8%)	1 (0%)	41	73
4	D	359/362 (99%)	332 (92%)	27 (8%)	0	100	100
5	E	167/174 (96%)	158 (95%)	9 (5%)	0	100	100
6	F	187/191 (98%)	175 (94%)	12 (6%)	0	100	100
7	G	173/176 (98%)	156 (90%)	17 (10%)	0	100	100
8	H	221/256 (86%)	204 (92%)	17 (8%)	0	100	100
9	J	195/198 (98%)	187 (96%)	8 (4%)	0	100	100
10	K	184/199 (92%)	173 (94%)	11 (6%)	0	100	100
11	L	134/137 (98%)	126 (94%)	8 (6%)	0	100	100
12	M	133/138 (96%)	123 (92%)	9 (7%)	1 (1%)	19	54
13	N	146/149 (98%)	123 (84%)	23 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	O	201/204 (98%)	184 (92%)	17 (8%)	0	100	100
15	P	267/297 (90%)	253 (95%)	14 (5%)	0	100	100
16	Q	183/186 (98%)	173 (94%)	10 (6%)	0	100	100
17	R	148/189 (78%)	146 (99%)	2 (1%)	0	100	100
18	S	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
19	T	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
20	U	152/154 (99%)	142 (93%)	10 (7%)	0	100	100
21	V	97/121 (80%)	88 (91%)	9 (9%)	0	100	100
22	W	118/142 (83%)	108 (92%)	10 (8%)	0	100	100
23	X	123/127 (97%)	114 (93%)	9 (7%)	0	100	100
24	Y	133/136 (98%)	121 (91%)	12 (9%)	0	100	100
25	Z	116/120 (97%)	113 (97%)	3 (3%)	0	100	100
26	a	50/59 (85%)	43 (86%)	7 (14%)	0	100	100
27	b	217/244 (89%)	200 (92%)	17 (8%)	0	100	100
28	c	95/105 (90%)	90 (95%)	5 (5%)	0	100	100
29	d	105/113 (93%)	91 (87%)	14 (13%)	0	100	100
30	e	125/130 (96%)	110 (88%)	14 (11%)	1 (1%)	19	54
31	f	104/107 (97%)	96 (92%)	8 (8%)	0	100	100
32	g	101/121 (84%)	88 (87%)	13 (13%)	0	100	100
33	h	96/100 (96%)	88 (92%)	8 (8%)	0	100	100
34	i	82/88 (93%)	70 (85%)	11 (13%)	1 (1%)	13	44
35	j	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
36	k	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
37	l	92/106 (87%)	85 (92%)	6 (6%)	1 (1%)	14	46
38	m	87/92 (95%)	81 (93%)	6 (7%)	0	100	100
39	n	222/245 (91%)	199 (90%)	22 (10%)	1 (0%)	29	64
40	z	56/432 (13%)	48 (86%)	8 (14%)	0	100	100
41	w	387/518 (75%)	340 (88%)	41 (11%)	6 (2%)	9	37
42	v	58/155 (37%)	57 (98%)	1 (2%)	0	100	100
43	o	316/640 (49%)	246 (78%)	68 (22%)	2 (1%)	25	59
45	t	50/128 (39%)	47 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	6753/8141 (83%)	6178 (92%)	561 (8%)	14 (0%)	50	79

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	18	PRO
41	w	148	ARG
41	w	20	CYS
41	w	68	PRO
30	e	7	PRO
39	n	141	THR
34	i	38	GLY
41	w	147	ALA
43	o	175	ASP
41	w	25	PRO
43	o	394	PRO
41	w	143	CYS
37	l	51	GLY
12	M	49	PRO

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	
2	B	189/196 (96%)	189 (100%)	0	100	100
3	C	317/323 (98%)	312 (98%)	5 (2%)	62	84
4	D	288/289 (100%)	287 (100%)	1 (0%)	92	96
5	E	147/150 (98%)	146 (99%)	1 (1%)	84	93
6	F	169/171 (99%)	169 (100%)	0	100	100
7	G	152/153 (99%)	151 (99%)	1 (1%)	84	93
8	H	183/208 (88%)	183 (100%)	0	100	100
9	J	163/164 (99%)	162 (99%)	1 (1%)	86	94
10	K	149/159 (94%)	147 (99%)	2 (1%)	69	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L	104/105 (99%)	104 (100%)	0	100	100
12	M	107/109 (98%)	106 (99%)	1 (1%)	78	91
13	N	118/119 (99%)	118 (100%)	0	100	100
14	O	175/176 (99%)	175 (100%)	0	100	100
15	P	227/245 (93%)	227 (100%)	0	100	100
16	Q	150/151 (99%)	149 (99%)	1 (1%)	84	93
17	R	124/154 (80%)	124 (100%)	0	100	100
18	S	155/156 (99%)	154 (99%)	1 (1%)	86	94
19	T	136/137 (99%)	135 (99%)	1 (1%)	84	93
20	U	125/125 (100%)	125 (100%)	0	100	100
21	V	86/107 (80%)	86 (100%)	0	100	100
22	W	104/118 (88%)	104 (100%)	0	100	100
23	X	108/110 (98%)	107 (99%)	1 (1%)	78	91
24	Y	115/116 (99%)	115 (100%)	0	100	100
25	Z	104/105 (99%)	104 (100%)	0	100	100
26	a	41/47 (87%)	41 (100%)	0	100	100
27	b	184/205 (90%)	182 (99%)	2 (1%)	73	89
28	c	81/88 (92%)	81 (100%)	0	100	100
29	d	94/97 (97%)	93 (99%)	1 (1%)	73	89
30	e	109/111 (98%)	108 (99%)	1 (1%)	78	91
31	f	90/91 (99%)	90 (100%)	0	100	100
32	g	88/103 (85%)	85 (97%)	3 (3%)	37	69
33	h	80/82 (98%)	80 (100%)	0	100	100
34	i	69/71 (97%)	68 (99%)	1 (1%)	67	86
35	j	68/69 (99%)	67 (98%)	1 (2%)	65	85
36	k	45/46 (98%)	45 (100%)	0	100	100
37	l	81/91 (89%)	79 (98%)	2 (2%)	47	75
38	m	70/72 (97%)	69 (99%)	1 (1%)	67	86
39	n	192/211 (91%)	191 (100%)	1 (0%)	88	94
40	z	53/392 (14%)	53 (100%)	0	100	100
41	w	348/467 (74%)	338 (97%)	10 (3%)	42	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	v	53/129 (41%)	53 (100%)	0	100	100
43	o	284/555 (51%)	266 (94%)	18 (6%)	18	48
45	t	47/116 (40%)	47 (100%)	0	100	100
All	All	5772/6889 (84%)	5715 (99%)	57 (1%)	77	90

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	17	LEU
3	C	19	ARG
3	C	44	THR
3	C	256	HIS
3	C	332	ARG
4	D	93	MET
5	E	174	LYS
7	G	113	LYS
9	J	26	VAL
10	K	21	ARG
10	K	63	VAL
12	M	13	ARG
16	Q	186	VAL
18	S	172	TYR
19	T	83	ARG
23	X	74	TYR
27	b	229	PHE
27	b	239	LEU
29	d	105	GLN
30	e	7	PRO
32	g	44	CYS
32	g	49	SER
32	g	81	CYS
34	i	21	ARG
35	j	78	LEU
37	l	12	CYS
37	l	74	CYS
38	m	60	CYS
39	n	141	THR
41	w	19	CYS
41	w	20	CYS
41	w	35	CYS
41	w	59	ARG

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Mol	Chain	Res	Type
41	w	79	ARG
41	w	115	LYS
41	w	145	ASP
41	w	146	CYS
41	w	240	TYR
41	w	404	ARG
43	o	134	LEU
43	o	163	ARG
43	o	164	ARG
43	o	165	LYS
43	o	169	LEU
43	o	170	GLN
43	o	171	GLU
43	o	175	ASP
43	o	177	LEU
43	o	178	LEU
43	o	179	THR
43	o	181	PHE
43	o	223	LYS
43	o	267	ARG
43	o	304	LYS
43	o	395	ASN
43	o	400	LYS
43	o	402	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
43	o	395	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3141/3396 (92%)	664 (21%)	22 (0%)
46	x	120/121 (99%)	19 (15%)	0
47	y	155/158 (98%)	34 (21%)	0
All	All	3416/3675 (92%)	717 (20%)	22 (0%)

All (717) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	15	C
1	A	26	A
1	A	40	A
1	A	43	A
1	A	48	A
1	A	49	A
1	A	59	G
1	A	60	A
1	A	65	A
1	A	66	A
1	A	70	A
1	A	72	C
1	A	73	C
1	A	75	G
1	A	77	A
1	A	92	G
1	A	105	C
1	A	110	G
1	A	111	C
1	A	116	A
1	A	117	U
1	A	119	U
1	A	120	G
1	A	121	A
1	A	122	A
1	A	133	U
1	A	134	U
1	A	136	G
1	A	153	U
1	A	156	G
1	A	157	A
1	A	164	A
1	A	187	A
1	A	190	U
1	A	191	U
1	A	198	A
1	A	200	C
1	A	206	G
1	A	211	A
1	A	213	A
1	A	218	G
1	A	219	A
1	A	220	G

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Mol	Chain	Res	Type
1	A	221	A
1	A	234	G
1	A	238	A
1	A	239	G
1	A	241	G
1	A	243	G
1	A	244	G
1	A	246	U
1	A	248	U
1	A	249	U
1	A	251	G
1	A	252	U
1	A	267	G
1	A	269	G
1	A	281	G
1	A	286	U
1	A	295	A
1	A	298	U
1	A	329	U
1	A	330	G
1	A	334	A
1	A	338	A
1	A	346	C
1	A	376	G
1	A	385	A
1	A	390	G
1	A	395	A
1	A	398	A
1	A	399	A
1	A	401	U
1	A	402	A
1	A	403	C
1	A	404	G
1	A	420	G
1	A	421	G
1	A	422	A
1	A	437	G
1	A	438	A
1	A	439	C
1	A	440	A
1	A	495	G
1	A	496	C

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Mol	Chain	Res	Type
1	A	503	C
1	A	510	G
1	A	521	A
1	A	523	A
1	A	536	U
1	A	542	G
1	A	545	U
1	A	547	G
1	A	548	G
1	A	549	U
1	A	551	A
1	A	552	G
1	A	555	U
1	A	557	A
1	A	558	U
1	A	559	A
1	A	569	A
1	A	578	A
1	A	579	G
1	A	592	A
1	A	611	A
1	A	620	U
1	A	621	A
1	A	622	A
1	A	636	C
1	A	649	A
1	A	661	G
1	A	662	U
1	A	667	C
1	A	677	A
1	A	681	U
1	A	689	U
1	A	712	G
1	A	719	U
1	A	720	A
1	A	725	G
1	A	767	U
1	A	774	G
1	A	776	U
1	A	777	U
1	A	780	A
1	A	781	G

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Mol	Chain	Res	Type
1	A	785	G
1	A	801	A
1	A	806	A
1	A	808	A
1	A	816	A
1	A	817	A
1	A	830	A
1	A	845	G
1	A	846	A
1	A	847	A
1	A	848	A
1	A	849	C
1	A	861	C
1	A	874	U
1	A	879	U
1	A	880	G
1	A	884	A
1	A	890	C
1	A	896	A
1	A	897	U
1	A	907	G
1	A	908	G
1	A	914	A
1	A	916	G
1	A	917	A
1	A	937	G
1	A	944	C
1	A	959	C
1	A	960	U
1	A	977	C
1	A	980	A
1	A	981	U
1	A	984	G
1	A	999	G
1	A	1001	G
1	A	1002	A
1	A	1004	U
1	A	1006	A
1	A	1007	U
1	A	1008	U
1	A	1009	A
1	A	1010	G

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Mol	Chain	Res	Type
1	A	1011	A
1	A	1012	G
1	A	1013	G
1	A	1014	U
1	A	1016	C
1	A	1017	C
1	A	1018	G
1	A	1019	G
1	A	1024	G
1	A	1025	A
1	A	1027	A
1	A	1029	G
1	A	1031	C
1	A	1032	C
1	A	1035	G
1	A	1036	A
1	A	1037	C
1	A	1038	C
1	A	1039	U
1	A	1041	U
1	A	1042	U
1	A	1043	C
1	A	1044	U
1	A	1045	C
1	A	1048	A
1	A	1050	U
1	A	1051	U
1	A	1064	A
1	A	1065	A
1	A	1072	G
1	A	1081	U
1	A	1082	U
1	A	1083	G
1	A	1087	G
1	A	1093	A
1	A	1094	U
1	A	1095	U
1	A	1096	U
1	A	1098	A
1	A	1103	A
1	A	1104	G
1	A	1116	G

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Mol	Chain	Res	Type
1	A	1117	G
1	A	1118	C
1	A	1130	A
1	A	1131	G
1	A	1143	A
1	A	1159	A
1	A	1180	A
1	A	1181	U
1	A	1182	A
1	A	1192	C
1	A	1193	A
1	A	1199	C
1	A	1201	C
1	A	1208	U
1	A	1217	A
1	A	1218	U
1	A	1222	G
1	A	1227	C
1	A	1236	G
1	A	1239	C
1	A	1240	A
1	A	1242	G
1	A	1243	G
1	A	1245	A
1	A	1246	G
1	A	1248	C
1	A	1251	A
1	A	1258	U
1	A	1262	G
1	A	1263	A
1	A	1264	G
1	A	1269	U
1	A	1270	A
1	A	1271	A
1	A	1274	A
1	A	1278	A
1	A	1279	C
1	A	1285	G
1	A	1287	A
1	A	1288	U
1	A	1289	G
1	A	1295	G

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Mol	Chain	Res	Type
1	A	1302	A
1	A	1304	A
1	A	1307	G
1	A	1309	U
1	A	1313	G
1	A	1316	C
1	A	1317	A
1	A	1325	U
1	A	1330	A
1	A	1332	A
1	A	1349	G
1	A	1350	A
1	A	1352	A
1	A	1353	U
1	A	1354	G
1	A	1355	A
1	A	1356	U
1	A	1357	G
1	A	1386	A
1	A	1399	A
1	A	1400	G
1	A	1405	U
1	A	1418	A
1	A	1419	A
1	A	1428	A
1	A	1434	G
1	A	1436	U
1	A	1437	C
1	A	1443	G
1	A	1445	U
1	A	1446	A
1	A	1450	G
1	A	1452	A
1	A	1455	U
1	A	1465	A
1	A	1467	A
1	A	1475	A
1	A	1481	A
1	A	1487	G
1	A	1508	C
1	A	1542	G
1	A	1547	G

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Mol	Chain	Res	Type
1	A	1555	U
1	A	1556	C
1	A	1562	C
1	A	1563	C
1	A	1564	U
1	A	1565	G
1	A	1566	A
1	A	1567	U
1	A	1568	U
1	A	1569	U
1	A	1570	U
1	A	1571	A
1	A	1572	U
1	A	1573	G
1	A	1574	C
1	A	1575	A
1	A	1578	C
1	A	1579	C
1	A	1583	A
1	A	1588	A
1	A	1589	A
1	A	1593	A
1	A	1619	A
1	A	1620	U
1	A	1629	U
1	A	1630	U
1	A	1631	C
1	A	1642	A
1	A	1643	A
1	A	1645	U
1	A	1646	G
1	A	1657	C
1	A	1677	G
1	A	1705	U
1	A	1715	A
1	A	1724	U
1	A	1725	C
1	A	1741	A
1	A	1750	A
1	A	1751	G
1	A	1762	C
1	A	1763	U

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Mol	Chain	Res	Type
1	A	1764	U
1	A	1765	U
1	A	1775	G
1	A	1788	C
1	A	1794	G
1	A	1797	A
1	A	1813	A
1	A	1814	A
1	A	1815	U
1	A	1816	A
1	A	1820	U
1	A	1821	U
1	A	1835	A
1	A	1839	A
1	A	1840	U
1	A	1842	A
1	A	1849	C
1	A	1850	A
1	A	1871	U
1	A	1874	A
1	A	1878	G
1	A	1880	U
1	A	1886	A
1	A	1893	A
1	A	1906	G
1	A	1930	A
1	A	1943	C
1	A	1950	U
1	A	1951	C
1	A	1952	G
1	A	1954	G
1	A	2096	A
1	A	2100	A
1	A	2101	C
1	A	2102	U
1	A	2111	G
1	A	2112	U
1	A	2113	A
1	A	2114	C
1	A	2121	G
1	A	2122	G
1	A	2126	A

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Mol	Chain	Res	Type
1	A	2131	A
1	A	2142	A
1	A	2158	A
1	A	2168	A
1	A	2169	G
1	A	2184	U
1	A	2187	G
1	A	2188	A
1	A	2197	C
1	A	2205	U
1	A	2206	G
1	A	2209	U
1	A	2251	G
1	A	2252	A
1	A	2254	U
1	A	2256	A
1	A	2257	C
1	A	2258	U
1	A	2259	A
1	A	2260	U
1	A	2261	G
1	A	2262	A
1	A	2264	U
1	A	2266	U
1	A	2268	U
1	A	2269	U
1	A	2270	A
1	A	2273	G
1	A	2274	U
1	A	2279	A
1	A	2281	A
1	A	2282	U
1	A	2294	U
1	A	2295	A
1	A	2298	U
1	A	2307	G
1	A	2308	C
1	A	2309	A
1	A	2310	U
1	A	2313	A
1	A	2314	U
1	A	2315	G

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Mol	Chain	Res	Type
1	A	2334	U
1	A	2335	G
1	A	2336	U
1	A	2350	C
1	A	2372	A
1	A	2373	A
1	A	2374	C
1	A	2375	G
1	A	2388	U
1	A	2393	G
1	A	2397	A
1	A	2401	A
1	A	2402	A
1	A	2403	G
1	A	2404	A
1	A	2405	C
1	A	2411	U
1	A	2412	G
1	A	2435	G
1	A	2437	G
1	A	2444	C
1	A	2445	A
1	A	2446	U
1	A	2448	G
1	A	2449	A
1	A	2454	G
1	A	2455	U
1	A	2456	A
1	A	2457	G
1	A	2458	A
1	A	2459	A
1	A	2460	U
1	A	2461	A
1	A	2462	A
1	A	2464	U
1	A	2465	G
1	A	2466	G
1	A	2468	A
1	A	2470	C
1	A	2471	U
1	A	2474	G
1	A	2476	C

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Mol	Chain	Res	Type
1	A	2479	C
1	A	2481	G
1	A	2482	U
1	A	2483	G
1	A	2484	A
1	A	2486	A
1	A	2490	C
1	A	2492	C
1	A	2493	U
1	A	2495	C
1	A	2496	C
1	A	2497	U
1	A	2498	U
1	A	2499	U
1	A	2501	U
1	A	2502	A
1	A	2503	G
1	A	2505	U
1	A	2506	U
1	A	2511	A
1	A	2514	U
1	A	2515	A
1	A	2524	A
1	A	2530	G
1	A	2549	G
1	A	2550	U
1	A	2551	U
1	A	2561	A
1	A	2562	A
1	A	2566	C
1	A	2568	C
1	A	2569	A
1	A	2571	U
1	A	2572	C
1	A	2573	G
1	A	2585	G
1	A	2593	A
1	A	2606	G
1	A	2607	G
1	A	2614	G
1	A	2618	G
1	A	2619	G

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Mol	Chain	Res	Type
1	A	2626	A
1	A	2635	A
1	A	2648	G
1	A	2652	U
1	A	2656	A
1	A	2657	A
1	A	2672	G
1	A	2674	A
1	A	2677	G
1	A	2678	A
1	A	2679	A
1	A	2680	A
1	A	2681	U
1	A	2689	A
1	A	2690	G
1	A	2691	A
1	A	2694	A
1	A	2703	A
1	A	2704	A
1	A	2708	C
1	A	2714	G
1	A	2719	U
1	A	2728	G
1	A	2737	C
1	A	2740	A
1	A	2753	G
1	A	2771	U
1	A	2772	C
1	A	2773	C
1	A	2777	G
1	A	2778	G
1	A	2791	G
1	A	2796	G
1	A	2800	G
1	A	2801	A
1	A	2803	A
1	A	2810	C
1	A	2817	A
1	A	2818	U
1	A	2819	A
1	A	2820	A
1	A	2823	G

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Mol	Chain	Res	Type
1	A	2842	U
1	A	2843	U
1	A	2844	C
1	A	2845	A
1	A	2846	U
1	A	2850	G
1	A	2851	A
1	A	2853	A
1	A	2860	U
1	A	2867	C
1	A	2871	G
1	A	2875	U
1	A	2887	A
1	A	2889	C
1	A	2898	G
1	A	2899	C
1	A	2900	A
1	A	2916	U
1	A	2923	U
1	A	2935	U
1	A	2936	A
1	A	2938	G
1	A	2940	A
1	A	2941	A
1	A	2942	C
1	A	2947	G
1	A	2951	G
1	A	2971	A
1	A	2977	G
1	A	2983	C
1	A	2990	G
1	A	2997	G
1	A	3011	A
1	A	3012	A
1	A	3016	A
1	A	3022	G
1	A	3027	A
1	A	3028	G
1	A	3038	U
1	A	3056	U
1	A	3059	G
1	A	3078	U

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Mol	Chain	Res	Type
1	A	3080	G
1	A	3092	C
1	A	3094	A
1	A	3101	G
1	A	3103	A
1	A	3105	U
1	A	3109	G
1	A	3116	G
1	A	3117	C
1	A	3118	C
1	A	3122	A
1	A	3129	A
1	A	3130	A
1	A	3131	U
1	A	3134	A
1	A	3142	A
1	A	3148	U
1	A	3153	U
1	A	3154	C
1	A	3155	U
1	A	3156	U
1	A	3157	U
1	A	3158	G
1	A	3165	A
1	A	3167	A
1	A	3170	A
1	A	3171	U
1	A	3173	G
1	A	3174	A
1	A	3176	G
1	A	3179	U
1	A	3180	A
1	A	3181	C
1	A	3187	A
1	A	3197	G
1	A	3199	G
1	A	3206	C
1	A	3207	U
1	A	3213	A
1	A	3217	C
1	A	3218	A
1	A	3219	G

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Mol	Chain	Res	Type
1	A	3221	C
1	A	3222	U
1	A	3268	A
1	A	3270	U
1	A	3271	G
1	A	3273	A
1	A	3275	U
1	A	3276	G
1	A	3278	C
1	A	3279	A
1	A	3280	U
1	A	3281	U
1	A	3282	U
1	A	3289	G
1	A	3294	A
1	A	3295	A
1	A	3304	U
1	A	3313	U
1	A	3316	A
1	A	3334	U
1	A	3335	A
1	A	3341	U
1	A	3351	U
1	A	3352	U
1	A	3353	G
1	A	3354	U
1	A	3355	U
1	A	3358	U
1	A	3369	G
1	A	3378	C
1	A	3382	U
1	A	3386	G
1	A	3396	U
46	x	7	G
46	x	11	A
46	x	18	C
46	x	22	A
46	x	33	U
46	x	41	G
46	x	50	U
46	x	54	U
46	x	55	A

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Mol	Chain	Res	Type
46	x	56	A
46	x	65	G
46	x	73	C
46	x	74	C
46	x	76	A
46	x	93	C
46	x	99	G
46	x	102	A
46	x	112	G
46	x	121	U
47	y	22	U
47	y	23	U
47	y	34	U
47	y	35	C
47	y	52	A
47	y	59	A
47	y	62	C
47	y	63	G
47	y	75	G
47	y	78	G
47	y	79	A
47	y	81	U
47	y	82	U
47	y	83	C
47	y	84	C
47	y	86	U
47	y	87	G
47	y	90	U
47	y	91	C
47	y	95	G
47	y	97	A
47	y	102	U
47	y	104	A
47	y	105	A
47	y	106	C
47	y	112	U
47	y	113	U
47	y	116	G
47	y	125	U
47	y	127	U
47	y	138	A
47	y	148	G

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Mol	Chain	Res	Type
47	y	151	C
47	y	152	G

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	621	A
1	A	916	G
1	A	1010	G
1	A	1064	A
1	A	1217	A
1	A	1273	A
1	A	1287	A
1	A	1288	U
1	A	1355	A
1	A	1629	U
1	A	1815	U
1	A	2101	C
1	A	2112	U
1	A	2261	G
1	A	2404	A
1	A	2458	A
1	A	2459	A
1	A	2497	U
1	A	3027	A
1	A	3055	U
1	A	3206	C
1	A	3353	G

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

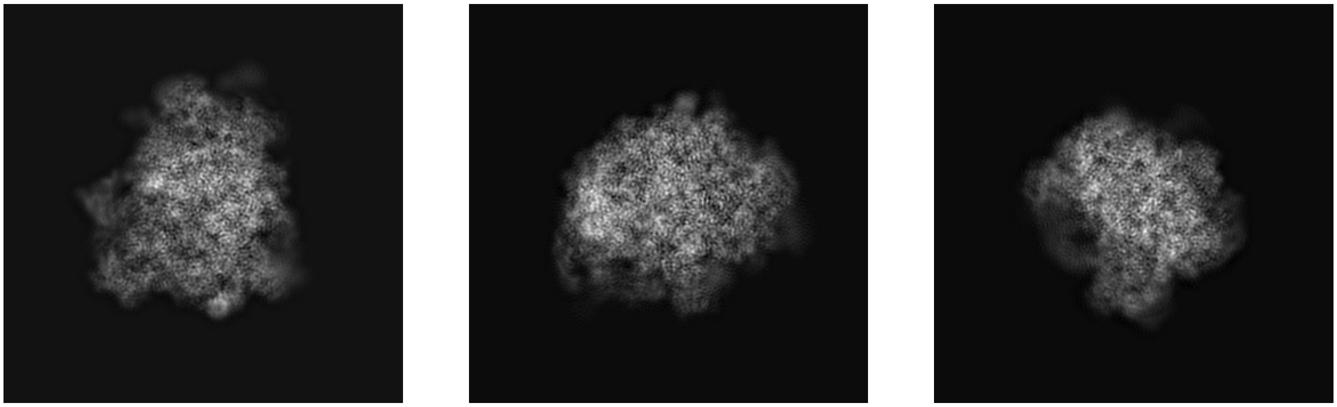
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-4560. 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 ⓘ

6.1.1 Primary map

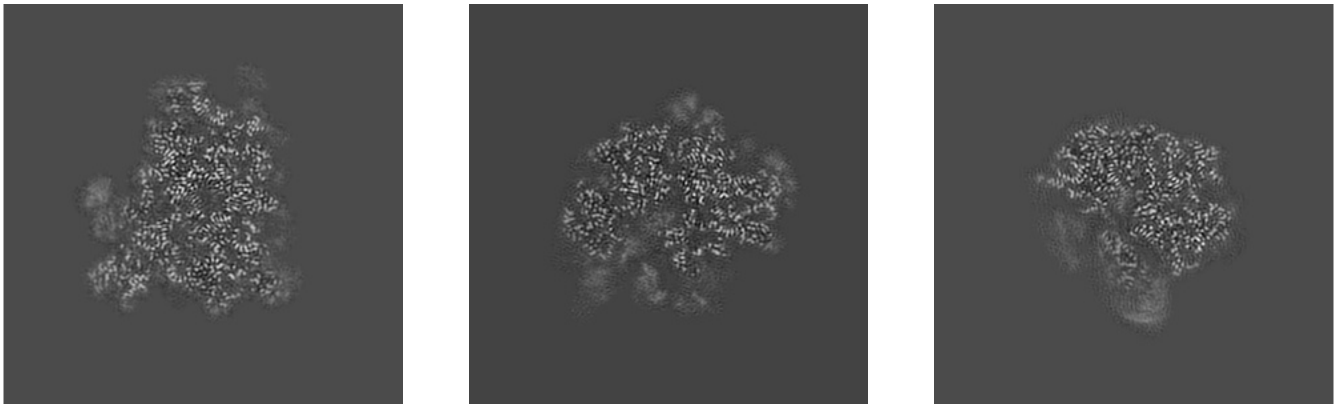


X Y Z

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

6.2 Central slices ⓘ

6.2.1 Primary map

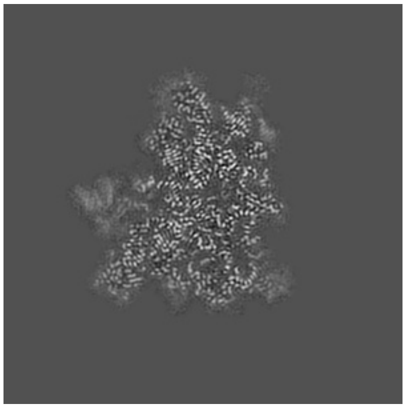


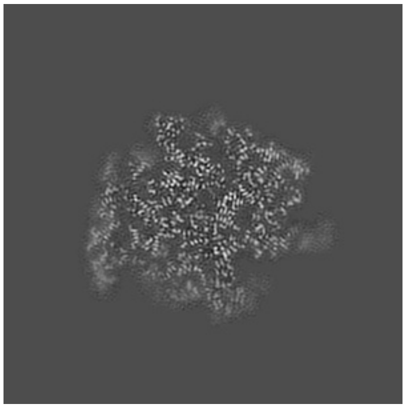
X Index: 180 Y Index: 180 Z Index: 180

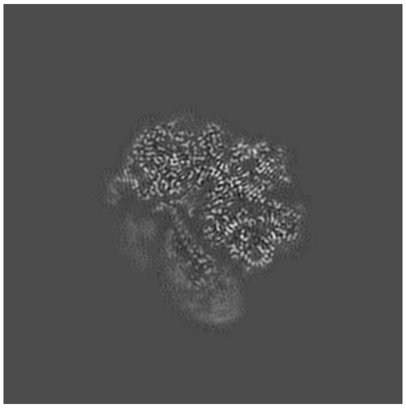
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

6.3.1 Primary map


X Index: 189

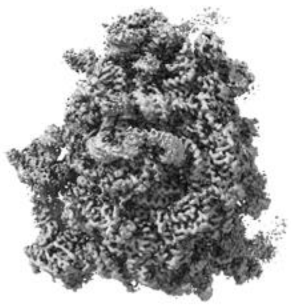

Y Index: 196


Z Index: 177

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

6.4 Orthogonal surface views

6.4.1 Primary map


X


Y


Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

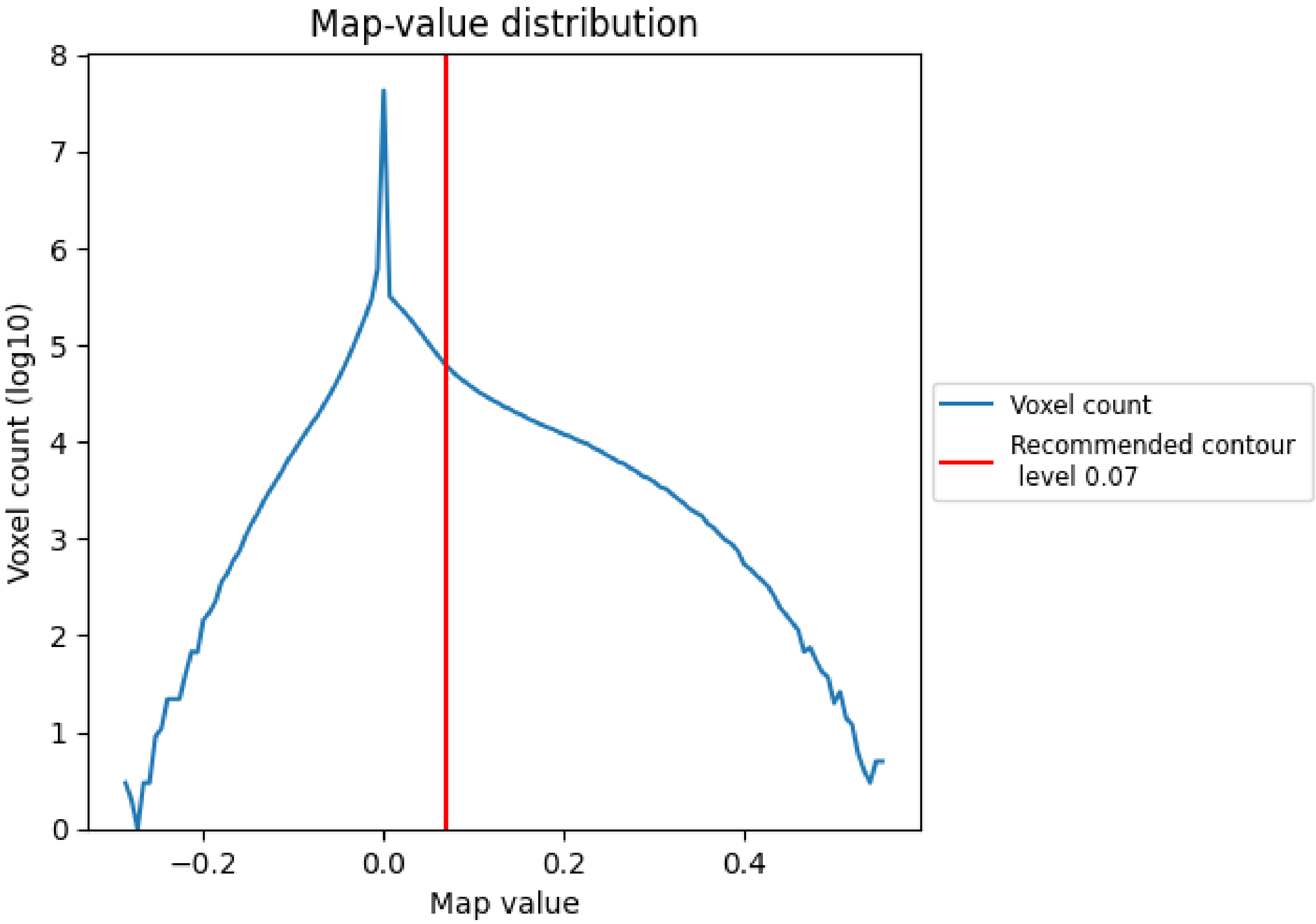
6.5 Mask visualisation (i)

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

7 Map analysis ⓘ

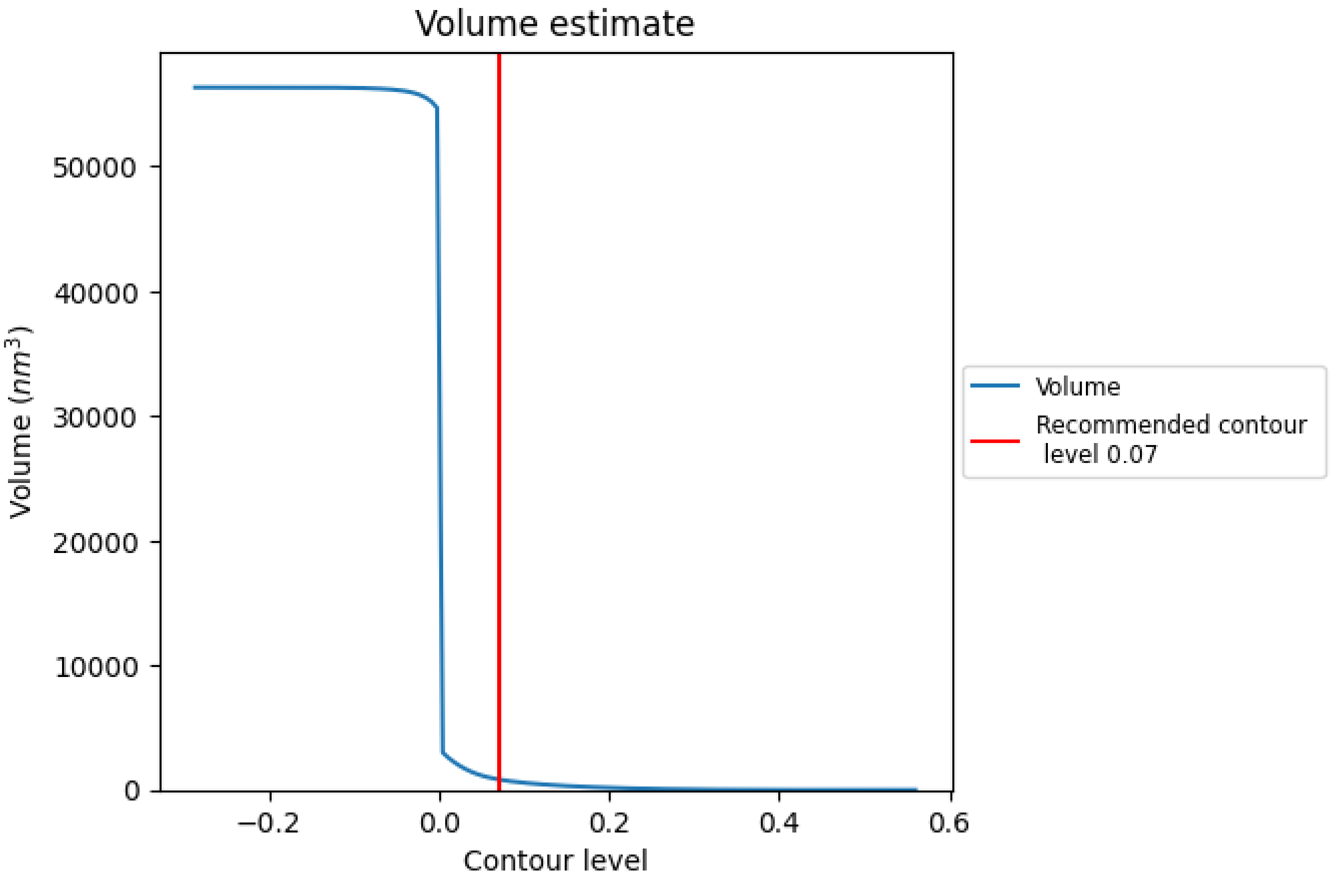
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

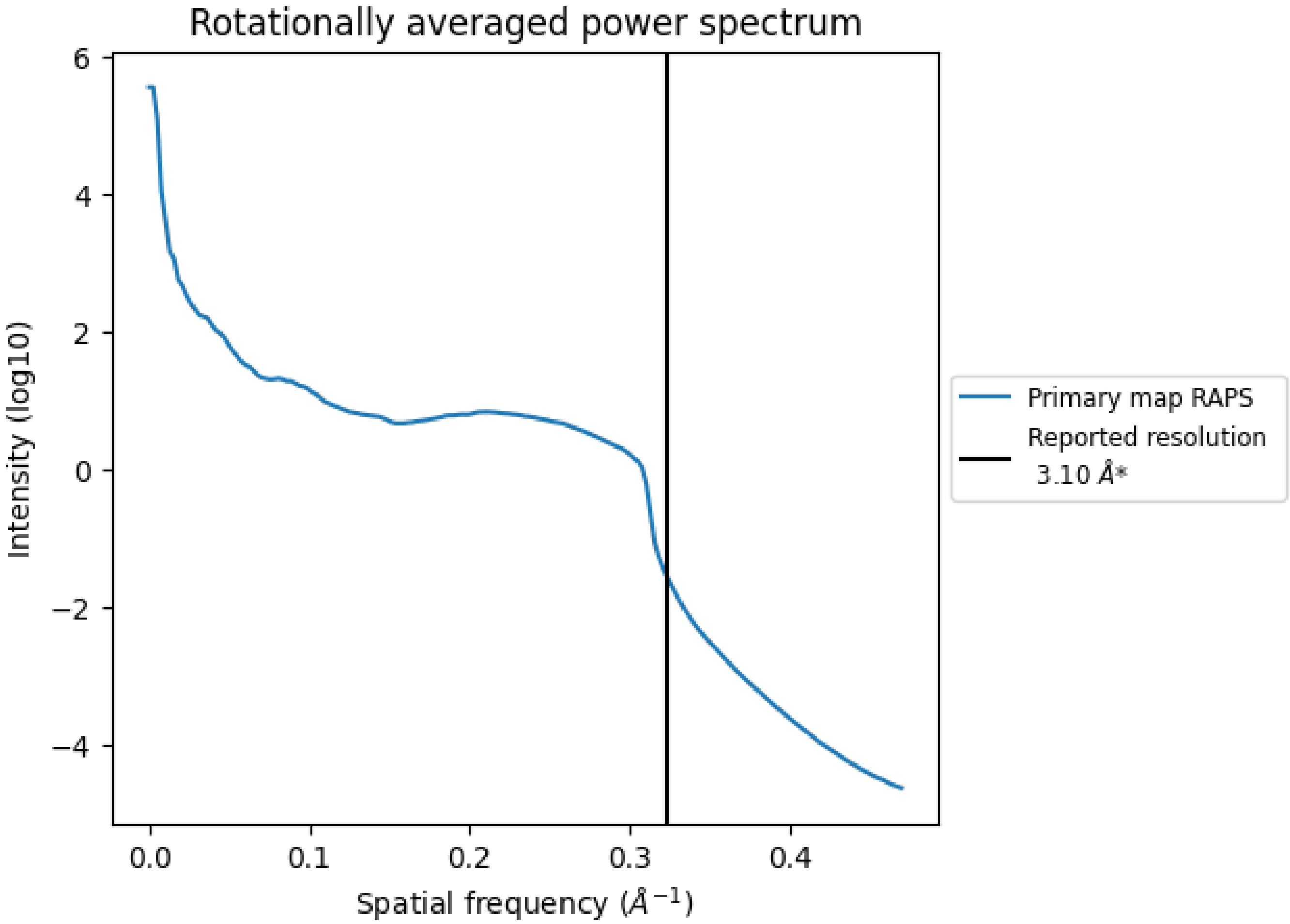
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 838 nm^3; this corresponds to an approximate mass of 757 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 0.323 Å^{-1}

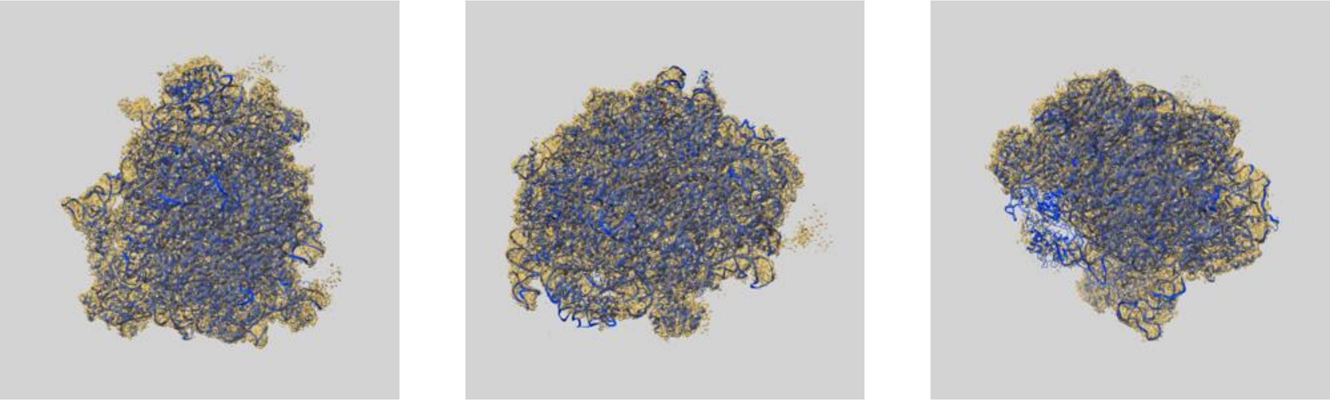
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4560 and PDB model 6QIK. Per-residue inclusion information can be found in section 3 on page 13.

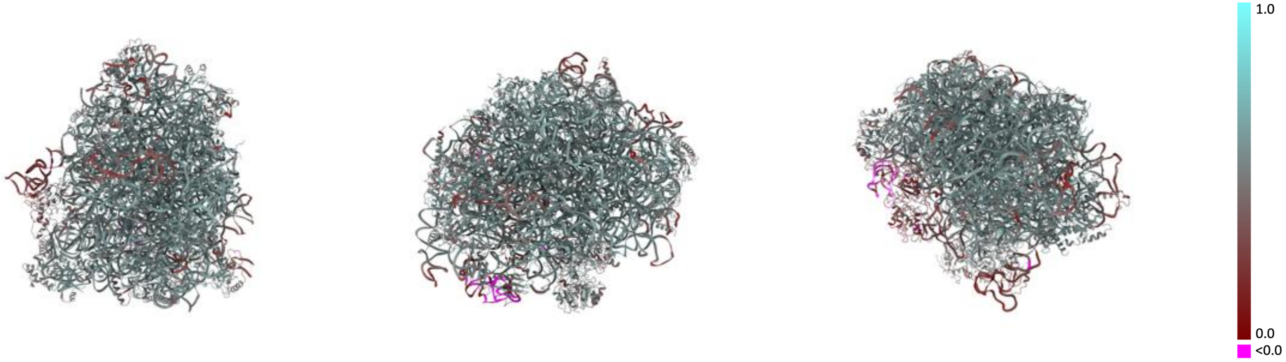
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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.

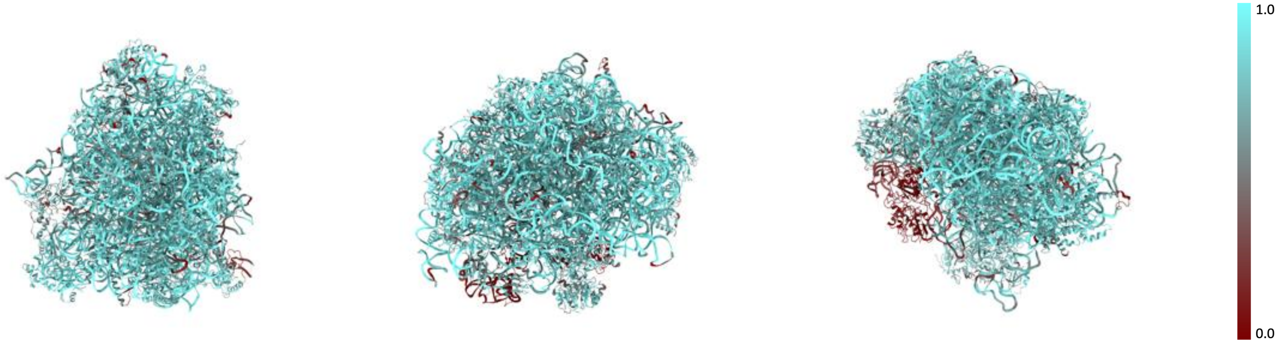
9.2 Q-score mapped to coordinate model



X Y Z

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

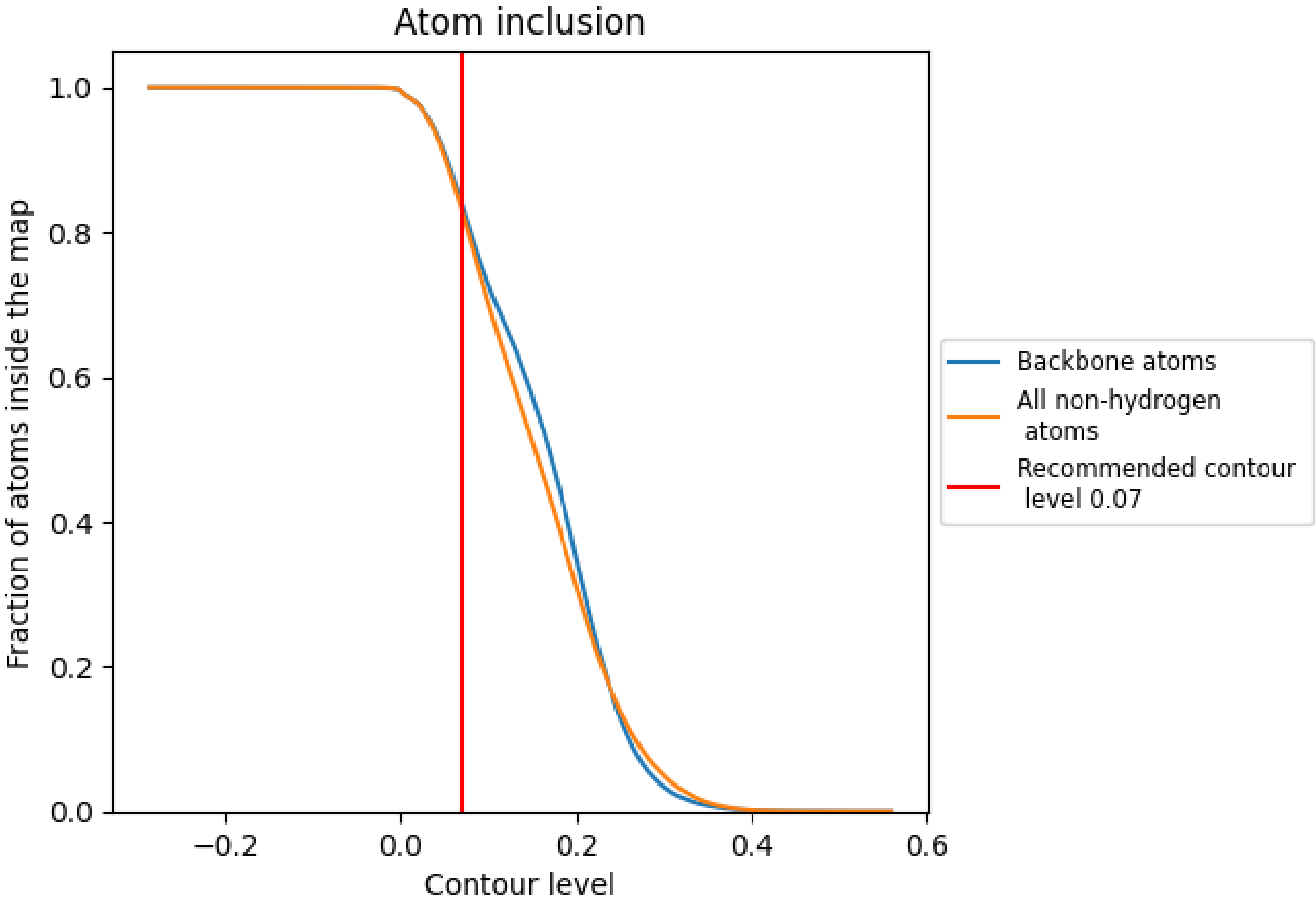
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.07).

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 83% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8278	0.5190
A	0.8778	0.5150
B	0.8614	0.5770
C	0.8639	0.5630
D	0.8518	0.5690
E	0.7489	0.4610
F	0.6791	0.4980
G	0.6781	0.4830
H	0.7845	0.5170
J	0.8336	0.5540
K	0.8031	0.5460
L	0.8292	0.5690
M	0.7967	0.5290
N	0.8764	0.5670
O	0.8796	0.5860
P	0.8356	0.5290
Q	0.8716	0.5780
R	0.8349	0.5530
S	0.8435	0.5580
T	0.8039	0.5440
U	0.8592	0.5720
V	0.8070	0.5060
W	0.8333	0.5540
X	0.8433	0.5640
Y	0.8159	0.5130
Z	0.8335	0.5500
a	0.7802	0.5470
b	0.8527	0.5570
c	0.7805	0.5000
d	0.7920	0.5430
e	0.8119	0.5700
f	0.8451	0.5750
g	0.8431	0.5660
h	0.6472	0.5110
i	0.8688	0.5840

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Chain	Atom inclusion	Q-score
j	0.7977	0.5120
k	0.8502	0.5830
l	0.8550	0.5810
m	0.8201	0.5570
n	0.7449	0.4860
o	0.0668	0.2950
p	0.6143	0.3640
t	0.0025	0.3180
v	0.7335	0.5290
w	0.4819	0.4100
x	0.9686	0.5410
y	0.9677	0.5680
z	0.4609	0.5160