Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 10:44 pm GMT

PDB ID	:	6R86
EMDB ID	:	EMD-4752
Title	:	Yeast Vms1-60S ribosomal subunit complex (post-state)
Authors	:	Su, T.; Izawa, T.; Cheng, J.; Yamashita, Y.; Berninghausen, O.; Inada, T.; Neupert, W.; Beckmann, R.
Deposited on	:	2019-03-31
Resolution	:	3.40 Å(reported)

This is a Full wwPDB EM Validation 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:

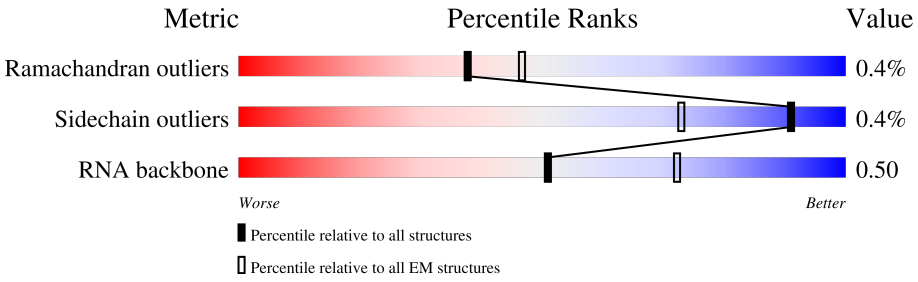
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.40 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	R	475	23% 74% · 25%
2	X	224	100%
3	i	112	· 100%
4	J	222	98% ·
5	j	119	97% · ·
6	K	233	· 98% ·
7	k	99	99% ·
8	7	191	· 98% ·

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Mol	Chain	Length	Quality of chain
9	l	87	100%
10	M	169	99%
11	m	77	96%
12	N	193	96%
13	n	50	100%
14	O	136	99%
15	o	52	48% 100%
16	p	203	98%
17	Q	197	99%
18	5	183	99%
19	S	185	99%
20	s	220	96%
21	T	152	99%
22	U	172	99%
23	V	159	99%
24	W	100	100%
25	P	155	63% 97%
26	r	197	19% 61% 39%
27	x	136	100%
28	3	121	74% 23%
29	Y	62	100%
30	4	158	72% 27%
31	Z	121	99%
32	a	126	100%
33	b	135	99%

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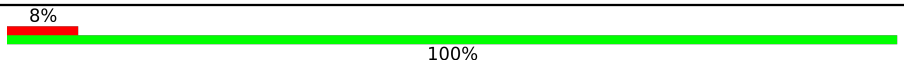
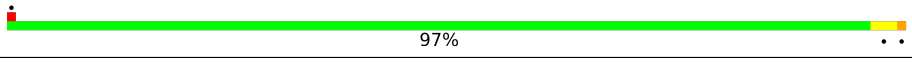
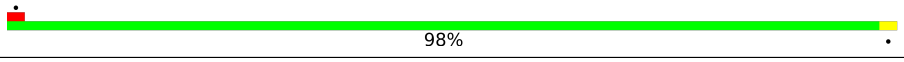
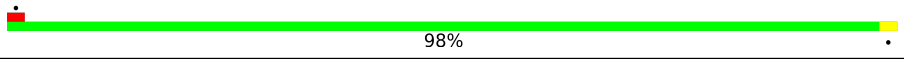
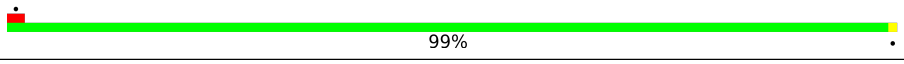
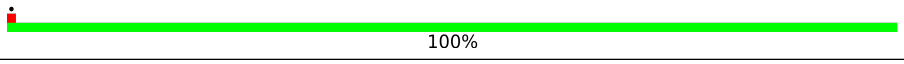
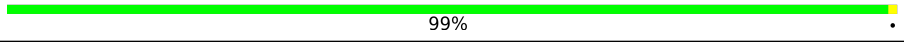
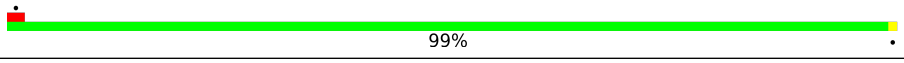
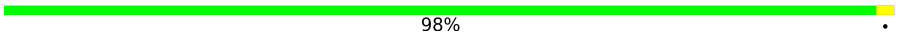
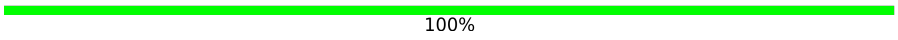
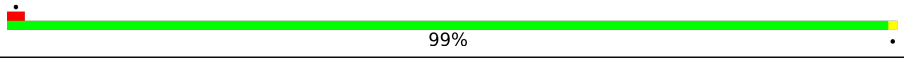
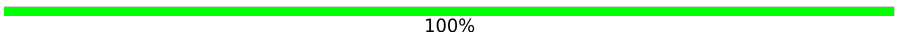
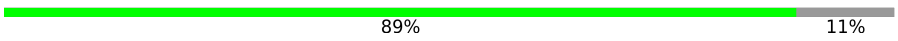
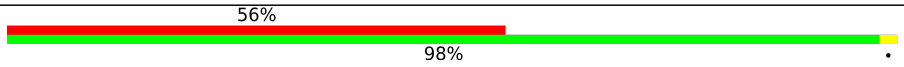
Mol	Chain	Length	Quality of chain
34	C	105	
35	c	148	
36	D	91	
37	d	58	
38	E	252	
39	e	97	
40	F	386	
41	f	109	
42	G	361	
43	g	127	
44	H	296	
45	h	106	
46	I	175	
47	L	204	
48	1	3260	

2 Entry composition (i)

There are 49 unique types of molecules in this entry. The entry contains 132446 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 Protein VMS1,Protein VMS1,Protein VMS1,Protein VMS1,Protein VMS1,Protein VMS1,Protein VMS1,Protein VMS1,Protein VMS1,Protein VMS1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	R	356	Total	C	N	O	S	Se	0	0
			2784	1776	495	500	12	1		

- Molecule 2 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	224	Total	C	N	O	S	0	0
			1633	1019	279	328	7		

- Molecule 3 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	i	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 4 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 5 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	j	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 6 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 7 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	k	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 8 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 9 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	l	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 10 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 11 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	m	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 12 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	N	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 13 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	n	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 14 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 15 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	5	183	Total	C	N	O	0	0
			1420	882	281	257		

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 20 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	s	220	Total	C	N	O	S	0	0
			1770	1121	335	307	7		

- Molecule 21 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	T	152	Total 1228	C 763	N 260	O 205	0	0

- Molecule 22 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	172	Total 1445	C 930	N 267	O 244	S 4	0	0

- Molecule 23 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	159	Total 1276	C 805	N 246	O 221	S 4	0	0

- Molecule 24 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	W	100	Total 796	C 516	N 131	O 149	0	0

- Molecule 25 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	P	150	Total 737	C 437	N 150	O 150	0	0

- Molecule 26 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	r	121	Total 967	C 621	N 170	O 173	S 3	0	0

- Molecule 27 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	x	136	Total 1003	C 628	N 189	O 179	S 7	0	0

- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 29 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	62	Total	C	N	O	S	0	0
			513	330	101	81	1		

- Molecule 30 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 31 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 32 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	a	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 33 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	b	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 34 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	C	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 35 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 36 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	D	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 37 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	d	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 38 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	E	252	Total	C	N	O	S	0	0
			1914	1191	388	334	1		

- Molecule 39 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 40 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	F	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 41 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	f	109	Total	C	N	O	S	0	0
			876	556	167	152	1		

- Molecule 42 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	G	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 43 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	g	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 44 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	H	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 45 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	h	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 46 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	I	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 47 is a protein called 60S ribosomal protein L1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	L	204	Total	C	N	O	S	0	0
			1609	1031	279	290	9		

- Molecule 48 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	1	3260	Total	C	N	O	P	0	0
			69730	31146	12569	22755	3260		

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

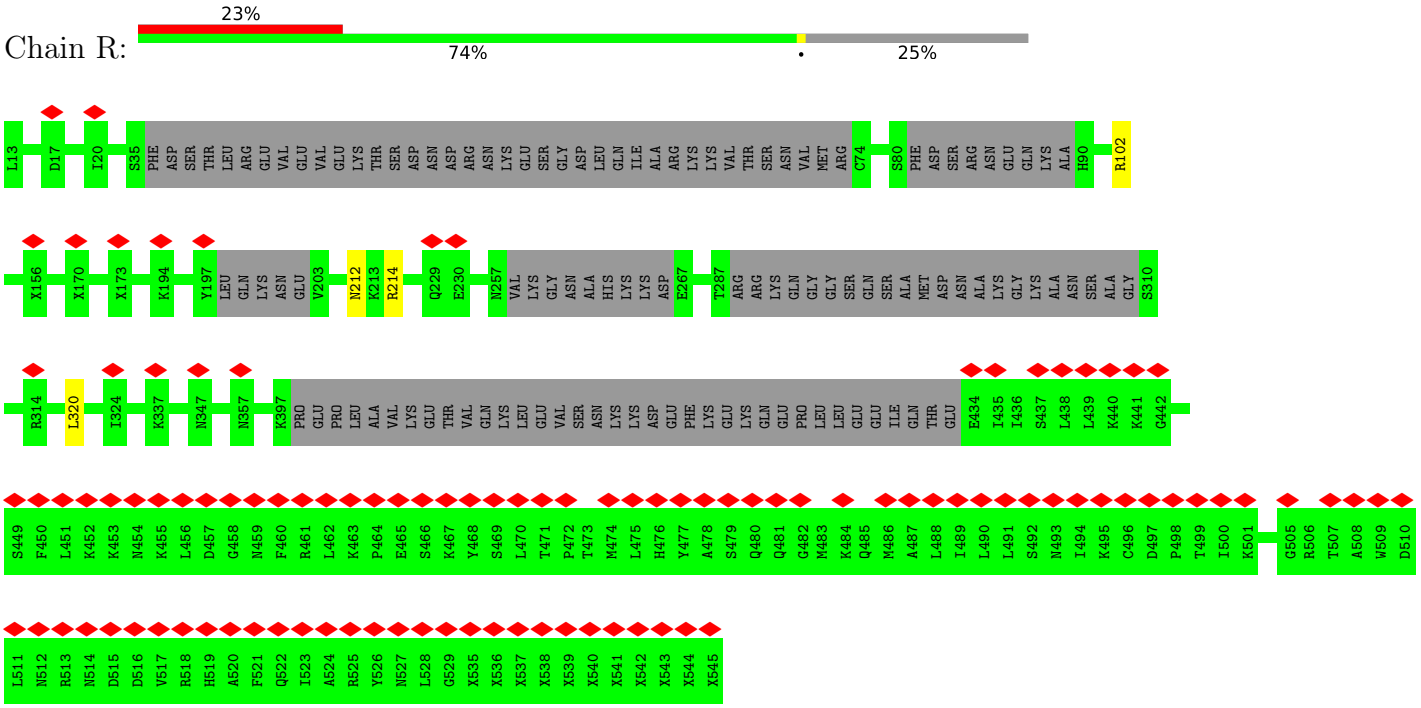
Mol	Chain	Residues	Atoms		AltConf
49	R	1	Total	Zn	0
			1	1	

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.

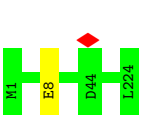
• Molecule 1: Protein VMS1,Protein VMS1,Protein VMS1,Protein VMS1,Protein VMS1,Protein VMS1,Protein VMS1,Protein VMS1,Protein VMS1,Protein VMS1

Chain R:



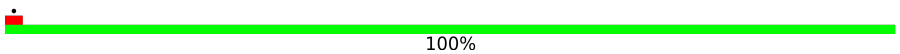
• Molecule 2: Eukaryotic translation initiation factor 6

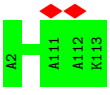
Chain X:



• Molecule 3: 60S ribosomal protein L34-A

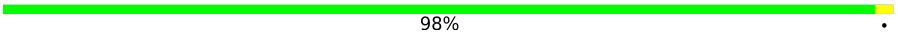
Chain i:

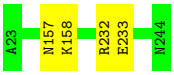




• Molecule 4: 60S ribosomal protein L7-A

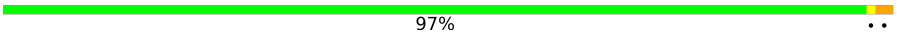
Chain J:

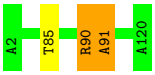




• Molecule 5: 60S ribosomal protein L35-A

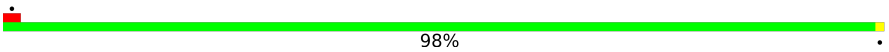
Chain j:

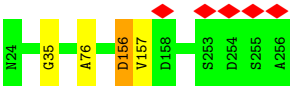




• Molecule 6: 60S ribosomal protein L8-A

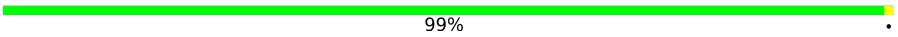
Chain K:





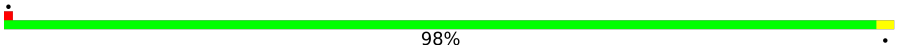
• Molecule 7: 60S ribosomal protein L36-A

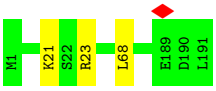
Chain k:



• Molecule 8: 60S ribosomal protein L9-A

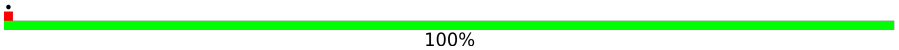
Chain 7:





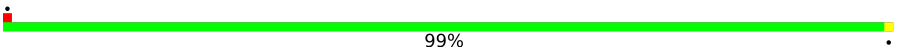
• Molecule 9: 60S ribosomal protein L37-A

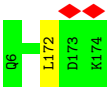
Chain l:



• Molecule 10: 60S ribosomal protein L11-B

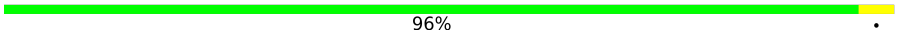
Chain M:

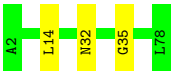




• Molecule 11: 60S ribosomal protein L38

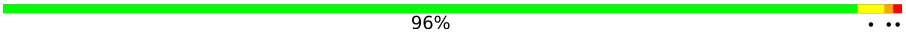
Chain m:





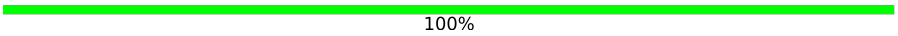
• Molecule 12: 60S ribosomal protein L13-A

Chain N:



• Molecule 13: 60S ribosomal protein L39

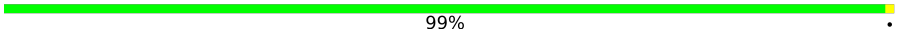
Chain n:



There are no outlier residues recorded for this chain.

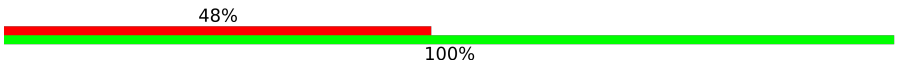
• Molecule 14: 60S ribosomal protein L14-A

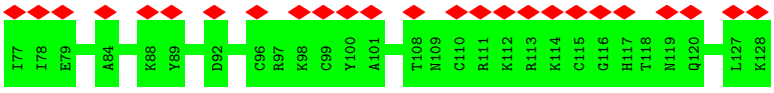
Chain O:



• Molecule 15: Ubiquitin-60S ribosomal protein L40

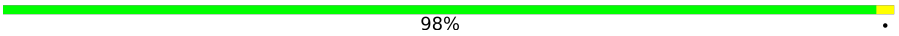
Chain o:





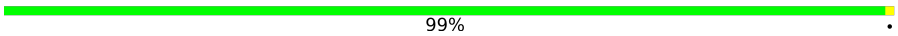
• Molecule 16: 60S ribosomal protein L15-A

Chain p:



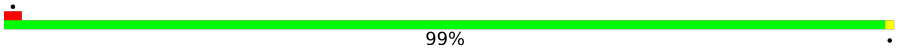
• Molecule 17: 60S ribosomal protein L16-A

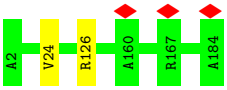
Chain Q:



• Molecule 18: 60S ribosomal protein L17-A

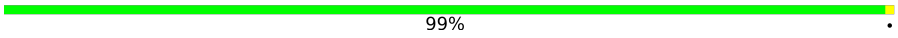
Chain 5:





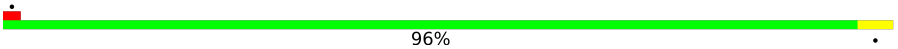
• Molecule 19: 60S ribosomal protein L18-A

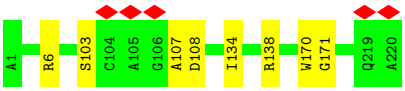
Chain S:



• Molecule 20: 60S ribosomal protein L10

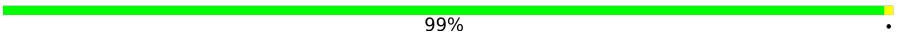
Chain s:





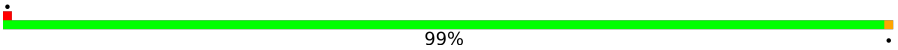
• Molecule 21: 60S ribosomal protein L19-A

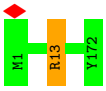
Chain T:



• Molecule 22: 60S ribosomal protein L20-A

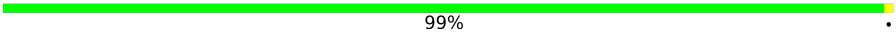
Chain U:

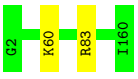




• Molecule 23: 60S ribosomal protein L21-A

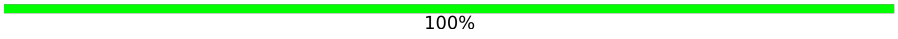
Chain V:





• Molecule 24: 60S ribosomal protein L22-A

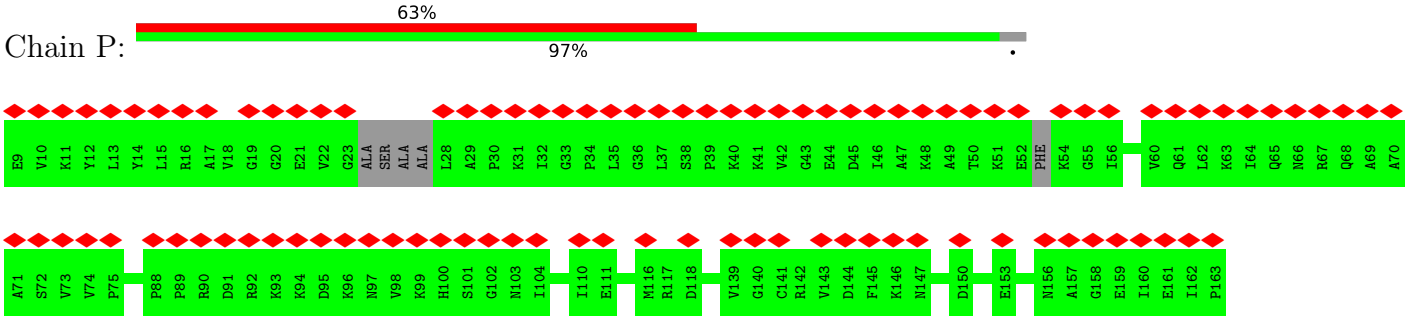
Chain W:



There are no outlier residues recorded for this chain.

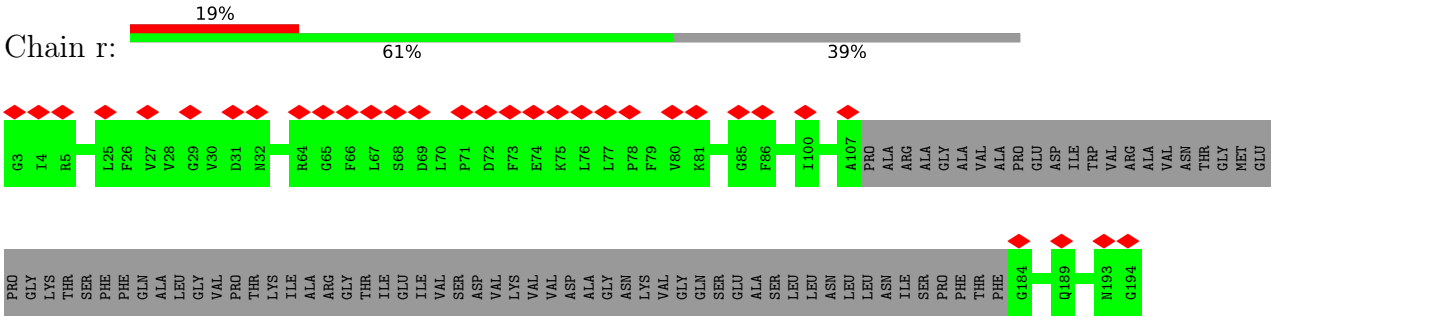
• Molecule 25: 60S ribosomal protein L12-A

Chain P:



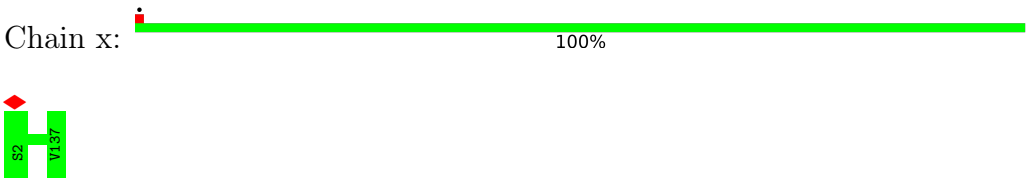
• Molecule 26: 60S acidic ribosomal protein P0

Chain r:



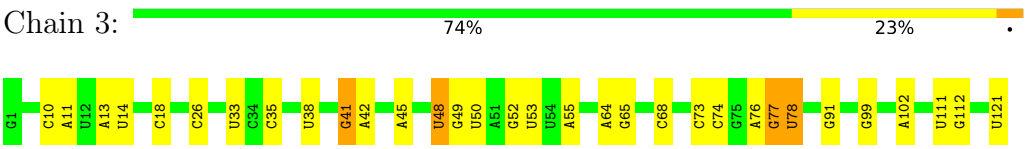
• Molecule 27: 60S ribosomal protein L23-A

Chain x:



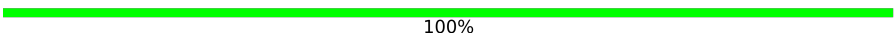
• Molecule 28: 5S ribosomal RNA

Chain 3:



• Molecule 29: 60S ribosomal protein L24-A

Chain Y:

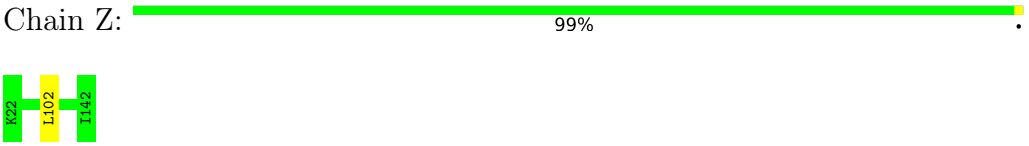


There are no outlier residues recorded for this chain.

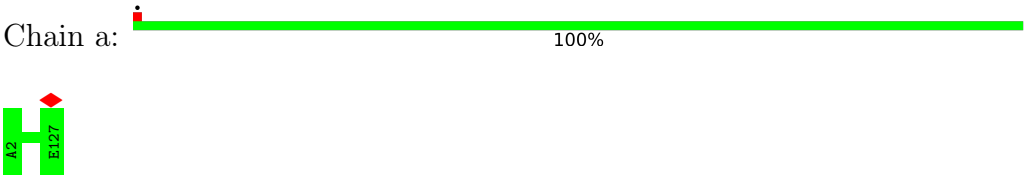
• Molecule 30: 5.8S ribosomal RNA

Chain 4:

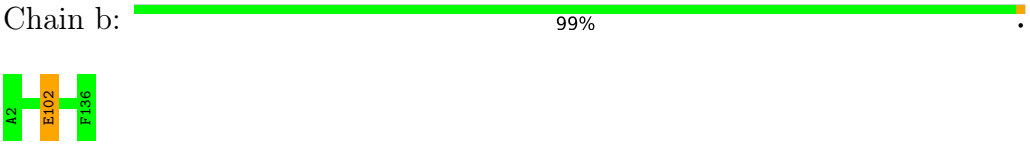
• Molecule 31: 60S ribosomal protein L25



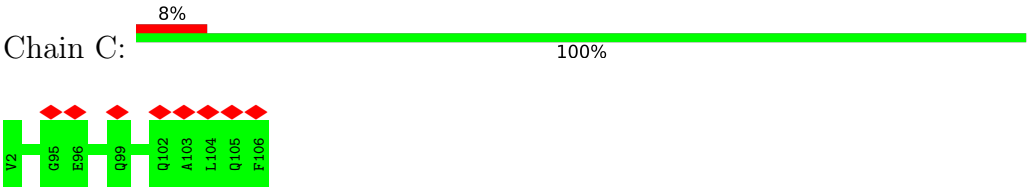
• Molecule 32: 60S ribosomal protein L26-A



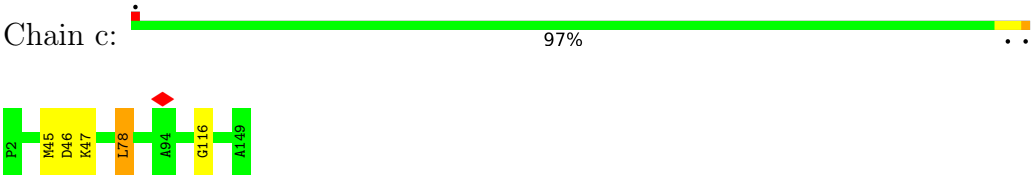
• Molecule 33: 60S ribosomal protein L27-A



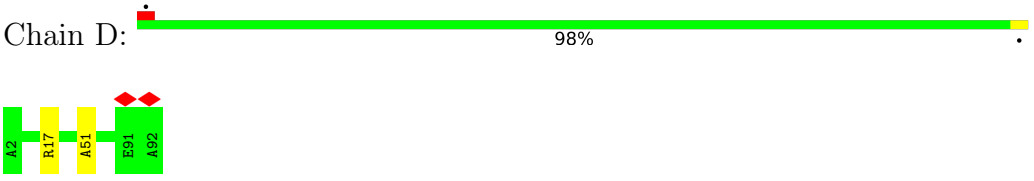
• Molecule 34: 60S ribosomal protein L42-A



• Molecule 35: 60S ribosomal protein L28

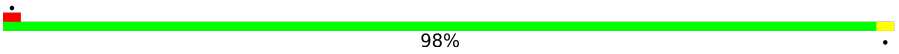


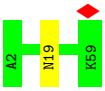
• Molecule 36: 60S ribosomal protein L43-A



• Molecule 37: 60S ribosomal protein L29

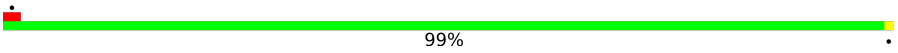
Chain d:

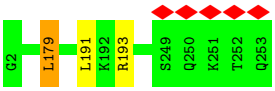




• Molecule 38: 60S ribosomal protein L2-A

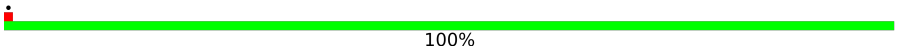
Chain E:





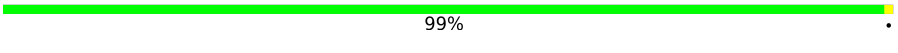
• Molecule 39: 60S ribosomal protein L30

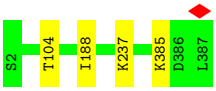
Chain e:



• Molecule 40: 60S ribosomal protein L3

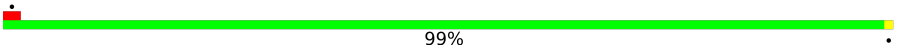
Chain F:

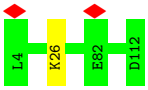




• Molecule 41: 60S ribosomal protein L31-A

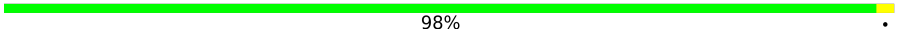
Chain f:

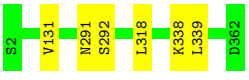




• Molecule 42: 60S ribosomal protein L4-A

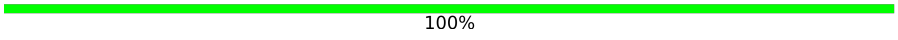
Chain G:





• Molecule 43: 60S ribosomal protein L32

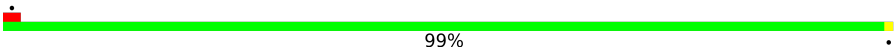
Chain g:

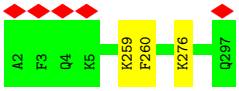


There are no outlier residues recorded for this chain.

• Molecule 44: 60S ribosomal protein L5

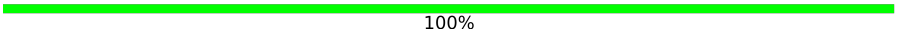
Chain H:





• Molecule 45: 60S ribosomal protein L33-A

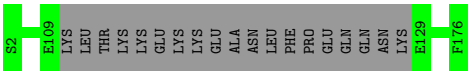
Chain h:



There are no outlier residues recorded for this chain.

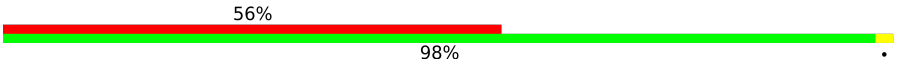
• Molecule 46: 60S ribosomal protein L6-A

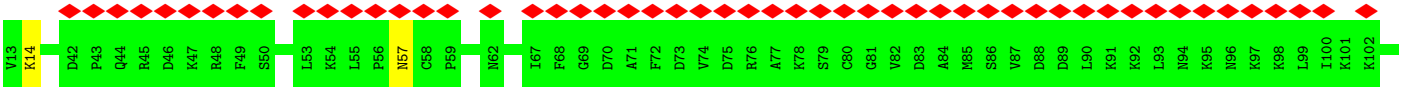
Chain I:

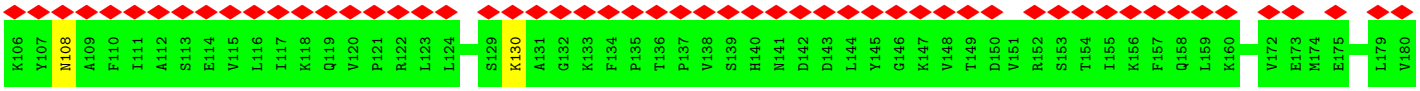


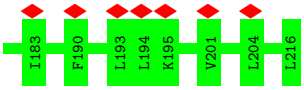
• Molecule 47: 60S ribosomal protein L1-A

Chain L:



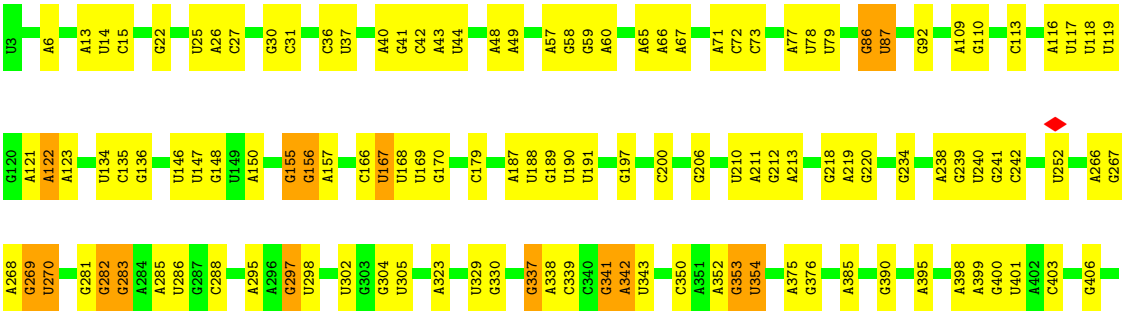


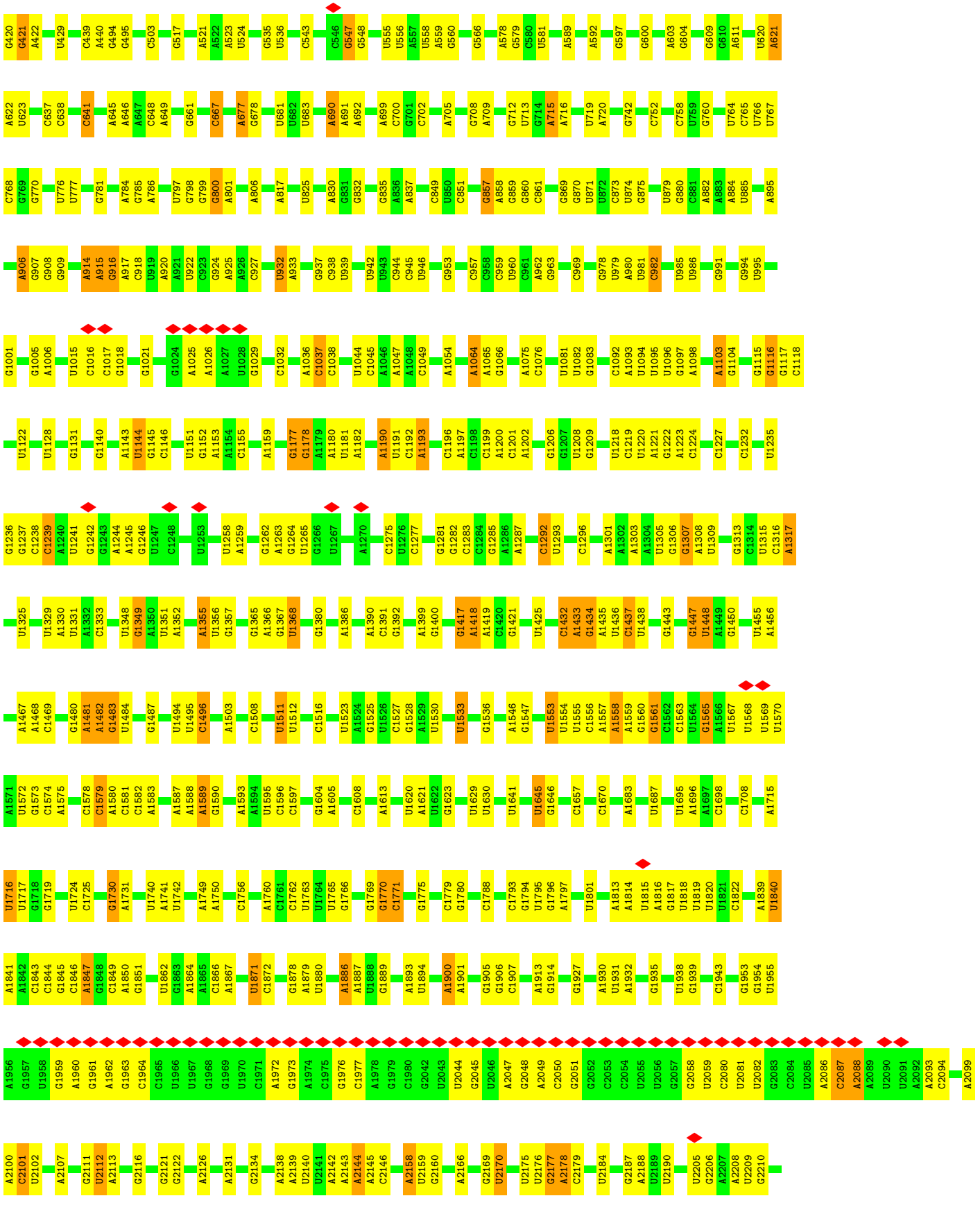


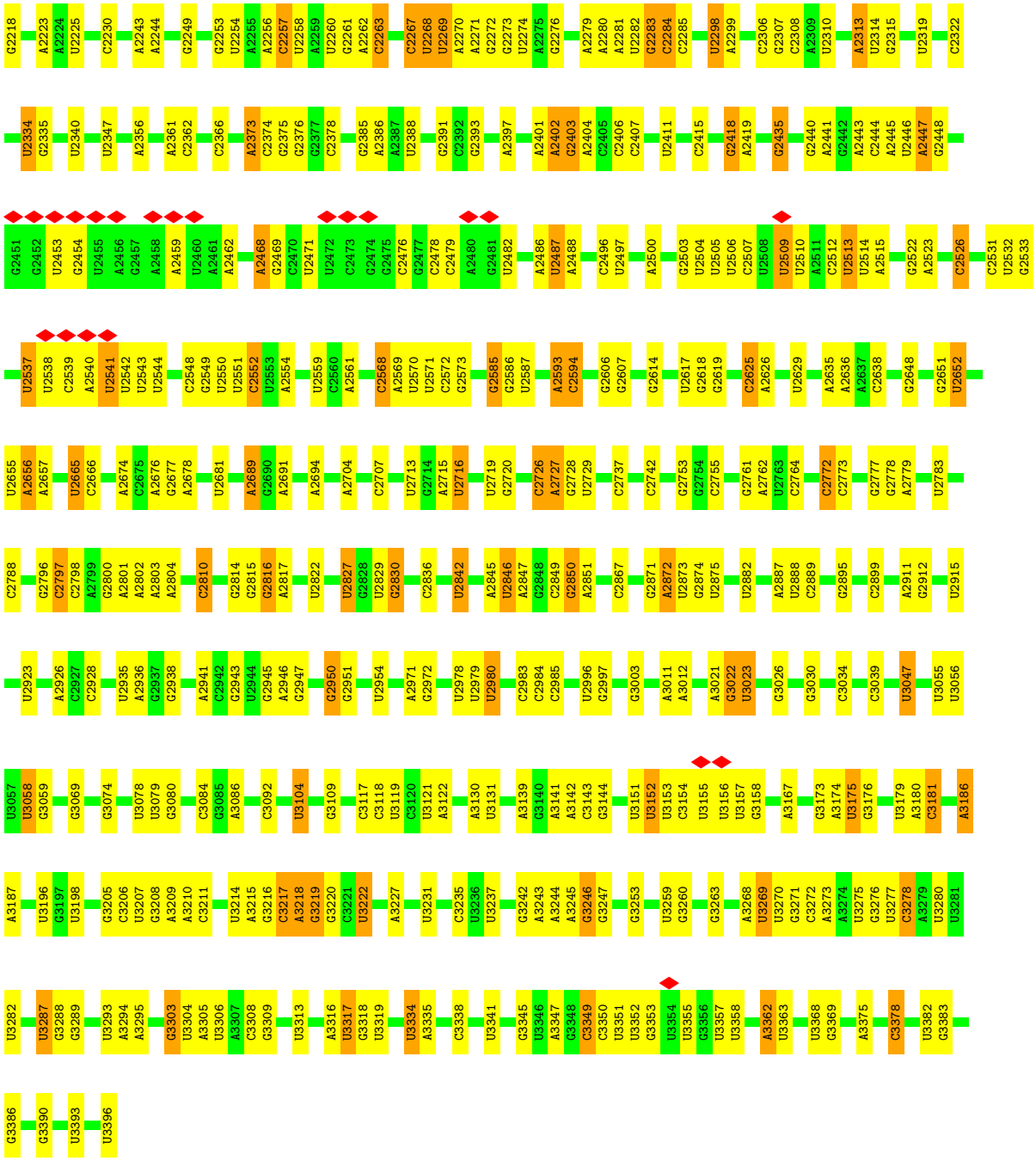


• Molecule 48: 25S ribosomal RNA

Chain 1:






G2218 A2223 A2224 U2225 C2230 A2243 A2244 G2249 G2253 U2254 A2255 A2256 C2257 U2258 A2259 U2260 G2261 A2262 C2263 C2267 U2268 U2269 A2270 A2271 G2272 G2273 U2274 A2275 G2276 A2279 A2280 A2281 U2282 G2283 C2284 C2285 U2298 A2299 C2306 G2307 C2308 A2309 U2310 A2313 U2314 G2315 U2319 C2322
U2334 G2335 U2340 U2347 A2356 A2361 C2362 C2366 A2373 C2374 G2375 G2376 G2377 C2378 G2385 A2386 A2387 U2388 G2391 C2392 G2393 A2397 A2401 A2402 G2403 A2404 C2405 C2406 C2407 U2411 C2415 G2418 A2419 G2435 G2440 A2441 G2442 A2443 C2444 A2445 U2446 A2447 G2448
G2451 G2452 U2453 G2454 U2455 A2456 G2457 A2458 A2459 U2460 A2461 A2462 A2468 G2469 C2470 U2471 U2472 C2473 G2474 G2475 C2476 G2477 C2478 C2479 A2480 G2481 U2482 A2486 U2487 A2488 C2496 U2497 A2500 G2503 U2504 U2505 U2506 C2507 U2508 U2509 U2510 A2511 C2512 U2513 U2514 A2515 G2522 A2523 C2526 C2531 U2532 G2533
U2537 U2538 C2539 A2540 U2541 U2542 U2543 U2544 C2548 G2549 U2550 U2551 C2552 U2553 A2554 U2559 C2560 A2561 C2568 A2569 U2570 U2571 C2572 G2573 G2585 G2586 U2587 A2593 C2594 G2606 G2607 G2614 U2617 G2618 G2619 C2625 A2626 U2629 A2635 A2636 A2637 C2638 G2648 G2651 U2652
U2655 A2656 A2657 U2665 C2666 A2674 C2675 A2676 G2677 A2678 U2681 A2689 G2690 A2691 A2694 A2704 C2707 U2713 G2714 A2715 U2716 U2719 G2720 C2726 A2727 G2728 U2729 C2737 C2742 G2753 G2754 C2755 G2761 A2762 U2763 C2764 C2772 C2773 G2777 G2778 A2779 U2783
C2788 G2796 C2797 C2798 A2799 G2800 A2801 A2802 A2803 A2804 C2810 G2814 G2815 G2816 A2817 U2822 U2827 G2828 U2829 G2830 C2836 U2842 A2845 U2846 A2847 G2848 C2849 G2850 A2851 C2867 G2871 A2872 U2873 G2874 U2875 U2882 A2887 U2888 C2889 G2895 C2899 A2911 G2912 U2915
U2923 A2926 C2927 C2928 U2935 A2936 G2937 G2938 A2941 C2942 G2943 U2944 G2945 A2946 G2947 G2950 G2951 U2954 A2971 G2972 U2978 U2979 U2980 C2983 C2984 C2985 U2996 G2997 G3003 A3011 A3012 A3021 G3022 U3023 G3026 G3030 C3034 C3039 U3047 U3055 U3056
U3057 U3058 G3059 G3069 G3074 U3078 U3079 G3080 C3084 G3085 A3086 C3092 U3104 G3109 C3117 C3118 U3119 C3120 U3121 A3122 A3130 U3131 A3139 G3140 A3141 A3142 C3143 G3144 U3151 U3152 U3153 C3154 U3155 U3156 U3157 G3158 A3167 G3173 A3174 U3175 G3176 U3179 A3180 C3181 A3186
A3187 U3196 G3197 U3198 G3205 C3206 U3207 G3208 A3209 A3210 C3211 U3214 A3215 G3216 C3217 A3218 G3219 G3220 C3221 U3222 A3227 U3231 C3235 U3236 U3237 G3242 A3243 A3244 A3245 G3246 G3247 G3253 U3259 G3260 G3263 A3268 U3269 U3270 G3271 C3272 A3273 A3274 U3275 G3276 U3277 C3278 A3279 U3280 U3281
U3282 U3287 G3288 G3289 U3293 A3294 A3295 G3303 U3304 A3305 U3306 A3307 C3308 G3309 U3313 A3316 U3317 G3318 U3319 U3334 A3335 C3338 U3341 G3345 U3346 A3347 G3348 C3349 C3350 U3351 U3352 G3353 U3354 U3355 G3356 U3357 U3358 A3362 U3363 U3368 G3369 A3375 C3378 U3382 G3383
G3386 G3390 U3393 U3396

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	115812	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 ($e^-/Å^2$)	2.8	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	0.812	Depositor
Minimum map value	-0.588	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	429.264, 429.264, 429.264	wwPDB
Map dimensions	396, 396, 396	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	R	0.27	0/2631	0.51	1/3532 (0.0%)
2	X	0.30	0/1653	0.54	0/2255
3	i	0.43	0/890	0.59	0/1189
4	J	0.44	0/1821	0.61	0/2451
5	j	0.34	0/978	0.62	0/1301
6	K	0.38	0/1836	0.63	0/2481
7	k	0.36	0/778	0.62	0/1034
8	7	0.34	0/1539	0.55	0/2073
9	l	0.47	0/696	0.64	0/923
10	M	0.30	0/1374	0.59	0/1842
11	m	0.34	0/618	0.62	1/826 (0.1%)
12	N	0.42	0/1568	0.68	4/2106 (0.2%)
13	n	0.42	0/443	0.65	0/588
14	O	0.37	0/1068	0.58	0/1438
15	o	0.28	0/423	0.57	0/562
16	p	0.52	0/1757	0.67	1/2354 (0.0%)
17	Q	0.42	0/1585	0.57	1/2128 (0.0%)
18	5	0.39	0/1443	0.62	0/1944
19	S	0.38	0/1465	0.65	1/1965 (0.1%)
20	s	0.36	0/1807	0.66	1/2425 (0.0%)
21	T	0.37	0/1245	0.61	0/1661
22	U	0.43	0/1481	0.60	0/1990
23	V	0.42	0/1300	0.58	0/1743
24	W	0.35	0/812	0.55	0/1099
25	P	0.25	0/734	0.53	0/1015
26	r	0.27	0/982	0.57	0/1320
27	x	0.42	0/1018	0.62	0/1369
28	3	0.57	0/2883	1.11	18/4491 (0.4%)
29	Y	0.38	0/525	0.55	0/696
30	4	0.69	0/3746	1.09	13/5832 (0.2%)
31	Z	0.42	0/979	0.61	1/1321 (0.1%)
32	a	0.35	0/1004	0.58	0/1341

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	b	0.35	0/1118	0.54	0/1497
34	C	0.35	0/860	0.61	0/1136
35	c	0.45	0/1204	0.66	0/1612
36	D	0.46	0/701	0.65	0/934
37	d	0.34	0/473	0.51	0/629
38	E	0.48	0/1948	0.66	2/2617 (0.1%)
39	e	0.33	0/751	0.53	0/1008
40	F	0.47	1/3146 (0.0%)	0.63	0/4228
41	f	0.44	0/890	0.59	0/1196
42	G	0.41	0/2800	0.62	0/3790
43	g	0.38	0/1041	0.57	0/1394
44	H	0.36	0/2425	0.56	0/3271
45	h	0.46	0/868	0.58	0/1168
46	I	0.33	0/1260	0.54	0/1694
47	L	0.28	0/1634	0.58	0/2195
48	1	0.70	2/78052 (0.0%)	1.16	494/121690 (0.4%)
All	All	0.59	3/142253 (0.0%)	0.99	538/209354 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	X	0	1
4	J	0	2
5	j	0	2
6	K	0	3
7	k	0	1
8	7	0	1
10	M	0	1
11	m	0	2
12	N	0	3
14	O	0	1
20	s	0	4
33	b	0	1
35	c	0	3
36	D	0	1
37	d	0	1
38	E	0	1
40	F	0	1
42	G	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
44	H	0	1
All	All	0	34

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	F	237	LYS	C-N	-7.03	1.17	1.34
48	1	3047	U	N3-C4	-5.82	1.33	1.38
48	1	3186	A	N9-C4	-5.00	1.34	1.37

All (538) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	1	2080	C	N1-C2-O2	13.81	127.19	118.90
48	1	3278	C	C2-N1-C1'	13.74	133.91	118.80
48	1	3278	C	N1-C2-O2	13.45	126.97	118.90
48	1	2080	C	N3-C2-O2	-12.68	113.02	121.90
48	1	2080	C	C2-N1-C1'	10.80	130.68	118.80
48	1	3047	U	N3-C2-O2	-10.46	114.88	122.20
48	1	3217	C	N1-C2-O2	10.39	125.14	118.90
48	1	3278	C	N3-C2-O2	-10.24	114.73	121.90
48	1	3217	C	C2-N1-C1'	10.01	129.81	118.80
48	1	3278	C	C6-N1-C1'	-9.95	108.86	120.80
48	1	1496	C	N1-C2-O2	9.49	124.59	118.90
48	1	922	U	C2-N1-C1'	9.42	129.00	117.70
48	1	3047	U	C5-C4-O4	9.28	131.47	125.90
48	1	1530	U	N1-C2-O2	9.27	129.29	122.80
48	1	3152	U	C2-N1-C1'	9.11	128.63	117.70
48	1	3152	U	N1-C2-O2	9.10	129.17	122.80
48	1	2080	C	C6-N1-C2	-9.10	116.66	120.30
48	1	2551	U	C2-N1-C1'	9.09	128.61	117.70
48	1	1530	U	N3-C2-O2	-9.04	115.87	122.20
48	1	2551	U	N1-C2-O2	9.00	129.10	122.80
48	1	3047	U	N1-C2-N3	8.80	120.18	114.90
28	3	26	C	N1-C2-O2	8.66	124.09	118.90
48	1	2298	U	N3-C2-O2	-8.64	116.15	122.20
48	1	1437	C	C2-N1-C1'	8.48	128.13	118.80
48	1	3152	U	N3-C2-O2	-8.38	116.33	122.20
48	1	1448	U	C5-C6-N1	8.33	126.86	122.70
48	1	908	G	C4-N9-C1'	8.31	137.30	126.50
48	1	2298	U	N1-C2-O2	8.19	128.54	122.80
48	1	2652	U	N3-C2-O2	-8.18	116.48	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	1	2551	U	N3-C2-O2	-8.17	116.48	122.20
48	1	1037	C	C2-N1-C1'	8.16	127.78	118.80
48	1	1208	U	C2-N1-C1'	7.97	127.27	117.70
48	1	2875	U	N1-C2-O2	7.96	128.37	122.80
48	1	42	C	C5-C6-N1	7.93	124.97	121.00
48	1	3181	C	N1-C2-O2	7.93	123.66	118.90
48	1	2479	C	N1-C2-O2	7.92	123.65	118.90
48	1	1977	C	N1-C2-O2	7.92	123.65	118.90
48	1	908	G	C8-N9-C1'	-7.85	116.79	127.00
48	1	3278	C	C6-N1-C2	-7.83	117.17	120.30
48	1	2478	C	N1-C2-O2	7.78	123.57	118.90
48	1	1208	U	N1-C2-O2	7.73	128.21	122.80
48	1	2638	C	N1-C2-O2	7.64	123.49	118.90
48	1	1645	U	N3-C2-O2	-7.64	116.85	122.20
48	1	1448	U	C2-N1-C1'	7.63	126.86	117.70
48	1	3217	C	N3-C2-O2	-7.62	116.57	121.90
48	1	2652	U	N1-C2-O2	7.54	128.08	122.80
48	1	36	C	N1-C2-O2	7.43	123.36	118.90
48	1	1483	G	O4'-C1'-N9	7.42	114.14	108.20
48	1	3217	C	C6-N1-C1'	-7.42	111.89	120.80
48	1	1349	G	N3-C4-C5	-7.41	124.90	128.60
48	1	2984	C	C2-N1-C1'	7.38	126.92	118.80
48	1	1579	C	N3-C2-O2	-7.38	116.73	121.90
48	1	1118	C	C5-C6-N1	7.37	124.68	121.00
30	4	64	U	N3-C2-O2	-7.36	117.05	122.20
48	1	922	U	N1-C2-O2	7.36	127.95	122.80
48	1	1779	C	C6-N1-C2	-7.35	117.36	120.30
48	1	3047	U	N3-C4-O4	-7.35	114.25	119.40
48	1	3306	U	N3-C2-O2	-7.34	117.06	122.20
48	1	3034	C	N1-C2-O2	7.33	123.30	118.90
48	1	1208	U	N3-C2-O2	-7.32	117.08	122.20
48	1	2984	C	N1-C2-O2	7.31	123.28	118.90
48	1	1579	C	C6-N1-C2	-7.30	117.38	120.30
48	1	638	C	C5-C6-N1	7.29	124.64	121.00
48	1	2541	U	P-O3'-C3'	7.26	128.41	119.70
48	1	156	G	P-O3'-C3'	7.26	128.41	119.70
48	1	167	U	N3-C2-O2	-7.25	117.12	122.20
48	1	1645	U	N1-C2-O2	7.24	127.87	122.80
48	1	2366	C	C5-C6-N1	7.22	124.61	121.00
48	1	1218	U	C5-C6-N1	7.21	126.31	122.70
1	R	320	LEU	CA-CB-CG	7.20	131.86	115.30
48	1	3058	U	N1-C2-O2	7.18	127.82	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	1	1118	C	C6-N1-C2	-7.17	117.43	120.30
48	1	2468	A	P-O3'-C3'	7.15	128.28	119.70
48	1	1645	U	C2-N1-C1'	7.14	126.27	117.70
48	1	1349	G	N3-C4-N9	7.12	130.27	126.00
48	1	927	C	C5-C6-N1	7.11	124.55	121.00
48	1	1496	C	N3-C2-O2	-7.10	116.93	121.90
48	1	857	G	N3-C4-N9	-7.10	121.74	126.00
48	1	2094	C	C5-C6-N1	7.08	124.54	121.00
48	1	3181	C	C2-N1-C1'	7.08	126.59	118.80
48	1	946	U	C5-C6-N1	7.08	126.24	122.70
48	1	2842	U	N1-C2-O2	7.08	127.75	122.80
48	1	908	G	N3-C4-N9	7.05	130.23	126.00
48	1	2415	C	C5-C6-N1	7.03	124.51	121.00
48	1	1604	G	C2-N3-C4	7.03	115.41	111.90
48	1	2447	A	P-O3'-C3'	7.01	128.11	119.70
48	1	2509	U	P-O3'-C3'	7.01	128.11	119.70
48	1	354	U	C5-C6-N1	7.00	126.20	122.70
48	1	2727	A	P-O3'-C3'	7.00	128.10	119.70
48	1	524	U	N3-C2-O2	-6.97	117.32	122.20
48	1	3181	C	N3-C2-O2	-6.92	117.06	121.90
48	1	1437	C	C6-N1-C2	-6.91	117.54	120.30
48	1	3278	C	C5-C6-N1	6.89	124.45	121.00
48	1	1496	C	C2-N1-C1'	6.89	126.38	118.80
48	1	2418	G	C4-N9-C1'	6.88	135.45	126.50
48	1	524	U	N1-C2-O2	6.88	127.61	122.80
28	3	26	C	N3-C2-O2	-6.87	117.09	121.90
48	1	2146	C	C6-N1-C2	-6.85	117.56	120.30
48	1	942	U	C5-C6-N1	6.85	126.12	122.70
48	1	3023	U	N3-C2-O2	-6.85	117.41	122.20
48	1	2415	C	C6-N1-C2	-6.84	117.56	120.30
48	1	1432	C	N1-C2-O2	6.84	123.00	118.90
48	1	1307	G	P-O3'-C3'	6.83	127.89	119.70
48	1	1533	U	N3-C2-O2	-6.83	117.42	122.20
48	1	1597	C	C5-C6-N1	6.82	124.41	121.00
48	1	2418	G	N3-C4-N9	6.81	130.09	126.00
48	1	2080	C	C6-N1-C1'	-6.80	112.64	120.80
19	S	41	ASP	CB-CG-OD1	6.80	124.42	118.30
48	1	2407	C	C5-C6-N1	6.79	124.39	121.00
48	1	1349	G	C4-N9-C1'	6.78	135.31	126.50
48	1	113	C	C2-N1-C1'	6.76	126.23	118.80
48	1	2298	U	O4'-C1'-N1	6.75	113.60	108.20
48	1	2585	G	N3-C4-C5	-6.73	125.23	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	1	2842	U	N3-C2-O2	-6.73	117.49	122.20
48	1	1779	C	N1-C2-O2	6.72	122.93	118.90
48	1	2267	C	P-O3'-C3'	6.72	127.77	119.70
48	1	2875	U	N3-C2-O2	-6.72	117.50	122.20
48	1	2764	C	N1-C2-O2	6.70	122.92	118.90
48	1	2268	U	C5-C6-N1	6.70	126.05	122.70
48	1	1900	A	P-O3'-C3'	6.69	127.72	119.70
48	1	922	U	N3-C2-O2	-6.68	117.52	122.20
48	1	122	A	C2-N3-C4	6.66	113.93	110.60
48	1	857	G	P-O3'-C3'	6.64	127.67	119.70
28	3	48	U	C2-N1-C1'	6.64	125.67	117.70
48	1	1565	G	N3-C4-N9	6.62	129.97	126.00
48	1	1553	U	P-O3'-C3'	6.59	127.61	119.70
48	1	1448	U	N1-C2-O2	6.59	127.42	122.80
48	1	3058	U	C2-N1-C1'	6.59	125.61	117.70
48	1	1511	U	P-O3'-C3'	6.59	127.61	119.70
48	1	3349	C	C2-N1-C1'	6.58	126.04	118.80
48	1	922	U	C6-N1-C1'	-6.57	112.00	121.20
48	1	3023	U	N1-C2-O2	6.56	127.39	122.80
48	1	167	U	N1-C2-O2	6.55	127.39	122.80
48	1	2362	C	C5-C6-N1	6.54	124.27	121.00
48	1	36	C	N3-C2-O2	-6.54	117.32	121.90
48	1	641	C	C6-N1-C2	-6.54	117.69	120.30
48	1	1604	G	N3-C4-C5	-6.53	125.34	128.60
48	1	1432	C	C2-N1-C1'	6.51	125.96	118.80
48	1	3047	U	C6-N1-C2	-6.51	117.09	121.00
48	1	1530	U	C2-N1-C1'	6.51	125.51	117.70
48	1	1558	A	P-O3'-C3'	6.51	127.51	119.70
48	1	2177	G	P-O3'-C3'	6.50	127.50	119.70
48	1	1670	C	N3-C2-O2	-6.50	117.35	121.90
48	1	677	A	P-O3'-C3'	6.50	127.50	119.70
48	1	1283	C	N3-C2-O2	-6.49	117.36	121.90
48	1	2638	C	N3-C2-O2	-6.48	117.36	121.90
48	1	957	C	C5-C6-N1	6.48	124.24	121.00
48	1	1604	G	C4-N9-C1'	6.47	134.92	126.50
48	1	908	G	C6-C5-N7	-6.47	126.52	130.40
48	1	2593	A	P-O3'-C3'	6.46	127.46	119.70
28	3	48	U	N1-C2-O2	6.46	127.32	122.80
48	1	1977	C	C2-N1-C1'	6.46	125.90	118.80
48	1	1309	U	N3-C2-O2	-6.44	117.69	122.20
48	1	857	G	N3-C4-C5	6.43	131.82	128.60
48	1	155	G	P-O3'-C3'	6.43	127.41	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	1	2146	C	C5-C6-N1	6.43	124.21	121.00
48	1	3047	U	C2-N1-C1'	6.42	125.41	117.70
48	1	713	U	N3-C2-O2	-6.42	117.70	122.20
48	1	1977	C	N3-C2-O2	-6.42	117.41	121.90
48	1	3058	U	N3-C2-O2	-6.41	117.71	122.20
48	1	3104	U	N3-C2-O2	-6.41	117.71	122.20
48	1	1425	U	N3-C2-O2	-6.41	117.71	122.20
48	1	2479	C	N3-C2-O2	-6.41	117.42	121.90
48	1	353	G	P-O3'-C3'	6.40	127.38	119.70
48	1	2112	U	OP2-P-O3'	6.40	119.27	105.20
48	1	3350	C	C2-N1-C1'	6.39	125.83	118.80
48	1	3350	C	C6-N1-C2	-6.39	117.74	120.30
16	p	75	VAL	CA-CB-CG2	6.39	120.49	110.90
28	3	26	C	C2-N1-C1'	6.39	125.83	118.80
48	1	1844	C	C6-N1-C2	-6.38	117.75	120.30
48	1	1037	C	C6-N1-C2	-6.36	117.75	120.30
48	1	1418	A	OP1-P-O3'	6.35	119.17	105.20
48	1	2551	U	C6-N1-C1'	-6.35	112.31	121.20
48	1	3349	C	C6-N1-C2	-6.33	117.77	120.30
48	1	2087	C	C6-N1-C2	-6.32	117.77	120.30
48	1	78	U	N3-C2-O2	-6.30	117.79	122.20
48	1	543	C	N1-C2-O2	6.30	122.68	118.90
48	1	2487	U	P-O3'-C3'	6.30	127.26	119.70
48	1	2144	A	O4'-C1'-N9	6.30	113.24	108.20
48	1	2298	U	C2-N1-C1'	6.29	125.25	117.70
48	1	87	U	C5-C6-N1	6.29	125.84	122.70
48	1	1670	C	N1-C2-O2	6.28	122.67	118.90
48	1	2788	C	N1-C2-O2	6.27	122.66	118.90
48	1	2849	C	N3-C2-O2	-6.27	117.51	121.90
48	1	2313	A	P-O3'-C3'	6.27	127.22	119.70
48	1	354	U	N1-C2-O2	6.27	127.19	122.80
48	1	927	C	C6-N1-C2	-6.27	117.79	120.30
48	1	2112	U	P-O3'-C3'	6.26	127.21	119.70
48	1	1292	C	N1-C2-O2	6.24	122.65	118.90
48	1	2846	U	C2-N1-C1'	6.24	125.19	117.70
48	1	1604	G	N3-C4-N9	6.24	129.74	126.00
48	1	2836	C	N1-C2-O2	6.24	122.64	118.90
48	1	2849	C	N1-C2-O2	6.24	122.64	118.90
48	1	2415	C	C2-N1-C1'	6.23	125.65	118.80
28	3	48	U	N3-C2-O2	-6.23	117.84	122.20
48	1	2537	U	P-O3'-C3'	6.23	127.17	119.70
48	1	857	G	C4-N9-C1'	-6.22	118.42	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	4	64	U	N1-C2-O2	6.22	127.15	122.80
48	1	543	C	C2-N1-C1'	6.21	125.64	118.80
48	1	86	G	P-O3'-C3'	6.21	127.15	119.70
48	1	3152	U	C6-N1-C1'	-6.21	112.51	121.20
48	1	2816	G	O4'-C1'-N9	6.20	113.16	108.20
48	1	2836	C	C2-N1-C1'	6.20	125.62	118.80
48	1	1433	A	P-O3'-C3'	6.19	127.13	119.70
48	1	2875	U	C2-N1-C1'	6.18	125.12	117.70
48	1	1037	C	N1-C2-O2	6.18	122.61	118.90
48	1	79	U	N3-C2-O2	-6.17	117.88	122.20
48	1	1103	A	O4'-C1'-N9	6.17	113.14	108.20
48	1	1496	C	C6-N1-C2	-6.17	117.83	120.30
48	1	2478	C	N3-C2-O2	-6.17	117.58	121.90
48	1	1525	G	C4-N9-C1'	6.15	134.50	126.50
48	1	3306	U	C2-N1-C1'	6.15	125.08	117.70
48	1	915	A	C2-N3-C4	6.15	113.68	110.60
30	4	35	C	N1-C2-O2	6.15	122.59	118.90
48	1	269	G	P-O3'-C3'	6.15	127.08	119.70
48	1	2094	C	C6-N1-C2	-6.14	117.84	120.30
48	1	915	A	O5'-P-OP2	-6.14	100.17	105.70
48	1	3317	U	N3-C2-O2	-6.14	117.90	122.20
48	1	2928	C	C6-N1-C2	-6.14	117.84	120.30
48	1	297	G	O4'-C1'-N9	6.12	113.09	108.20
48	1	1596	C	C6-N1-C2	-6.12	117.85	120.30
48	1	918	C	C6-N1-C2	-6.11	117.86	120.30
48	1	1730	G	P-O3'-C3'	6.11	127.03	119.70
48	1	3104	U	N1-C2-O2	6.10	127.07	122.80
48	1	2283	G	P-O3'-C3'	6.09	127.01	119.70
48	1	1309	U	N1-C2-O2	6.09	127.06	122.80
48	1	2418	G	C8-N9-C1'	-6.08	119.10	127.00
38	E	179	LEU	CA-CB-CG	6.08	129.28	115.30
48	1	3175	U	OP2-P-O3'	6.08	118.57	105.20
48	1	3047	U	C4-C5-C6	6.08	123.34	119.70
48	1	2815	G	N1-C6-O6	-6.07	116.26	119.90
48	1	3219	G	P-O3'-C3'	6.07	126.98	119.70
48	1	969	C	C6-N1-C2	-6.06	117.88	120.30
17	Q	41	LEU	CA-CB-CG	6.06	129.24	115.30
48	1	969	C	C5-C6-N1	6.04	124.02	121.00
48	1	3317	U	N1-C2-O2	6.04	127.03	122.80
48	1	3350	C	C5-C6-N1	6.04	124.02	121.00
48	1	2479	C	C2-N1-C1'	6.03	125.44	118.80
28	3	26	C	C6-N1-C2	-6.03	117.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	1	2418	G	N3-C4-C5	-6.03	125.59	128.60
48	1	2284	C	N1-C2-O2	6.00	122.50	118.90
48	1	2726	C	C2-N1-C1'	6.00	125.40	118.80
48	1	1283	C	N1-C2-O2	5.99	122.49	118.90
48	1	2178	A	P-O3'-C3'	5.99	126.88	119.70
48	1	3235	C	C2-N1-C1'	5.98	125.37	118.80
28	3	77	G	P-O3'-C3'	5.97	126.87	119.70
48	1	1481	A	O4'-C1'-N9	5.97	112.98	108.20
48	1	1779	C	C5-C6-N1	5.97	123.99	121.00
48	1	1177	G	P-O3'-C3'	5.96	126.85	119.70
48	1	2550	U	N3-C2-O2	-5.96	118.03	122.20
48	1	2899	C	C2-N1-C1'	5.95	125.34	118.80
48	1	3022	G	P-O3'-C3'	5.94	126.82	119.70
48	1	2435	G	N3-C4-N9	5.93	129.56	126.00
48	1	1565	G	C4-N9-C1'	5.93	134.20	126.50
48	1	1292	C	N3-C2-O2	-5.92	117.75	121.90
48	1	1561	G	N3-C4-N9	-5.92	122.44	126.00
30	4	59	A	O5'-P-OP2	-5.92	100.38	105.70
48	1	31	C	C6-N1-C2	-5.91	117.94	120.30
48	1	2190	U	C2-N1-C1'	5.91	124.79	117.70
48	1	1977	C	C6-N1-C2	-5.91	117.94	120.30
48	1	1418	A	P-O3'-C3'	5.91	126.79	119.70
48	1	800	G	N3-C4-C5	-5.91	125.65	128.60
48	1	3269	U	P-O3'-C3'	5.90	126.78	119.70
48	1	800	G	C4-N9-C1'	5.90	134.17	126.50
48	1	1116	G	P-O3'-C3'	5.89	126.77	119.70
48	1	2830	G	N3-C4-C5	-5.89	125.65	128.60
48	1	690	A	P-O3'-C3'	5.89	126.77	119.70
28	3	18	C	N1-C2-O2	5.88	122.43	118.90
48	1	156	G	OP1-P-O3'	5.88	118.13	105.20
30	4	100	U	N1-C2-O2	5.87	126.91	122.80
12	N	61	PRO	C-N-CA	5.86	136.36	121.70
48	1	2656	A	P-O3'-C3'	5.86	126.73	119.70
48	1	270	U	N3-C2-O2	-5.86	118.10	122.20
48	1	690	A	OP1-P-O3'	5.86	118.09	105.20
48	1	916	G	P-O3'-C3'	5.86	126.73	119.70
48	1	1496	C	C5-C6-N1	5.86	123.93	121.00
48	1	1574	C	C5-C6-N1	5.85	123.93	121.00
48	1	1064	A	P-O3'-C3'	5.85	126.72	119.70
48	1	1115	G	C4-N9-C1'	5.85	134.10	126.50
48	1	2080	C	C5-C6-N1	5.85	123.92	121.00
48	1	857	G	C8-N9-C1'	5.84	134.59	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	1	2513	U	P-O3'-C3'	5.83	126.70	119.70
48	1	1770	G	C4-N9-C1'	5.83	134.08	126.50
48	1	1333	C	C5-C6-N1	5.83	123.91	121.00
48	1	283	G	C8-N9-C1'	-5.82	119.43	127.00
48	1	2402	A	O4'-C1'-N9	5.82	112.86	108.20
28	3	18	C	C2-N1-C1'	5.82	125.20	118.80
48	1	1872	C	N1-C2-O2	5.81	122.39	118.90
48	1	2980	U	N1-C2-O2	5.81	126.87	122.80
48	1	283	G	C4-N9-C1'	5.81	134.05	126.50
48	1	945	C	C5-C6-N1	5.80	123.90	121.00
48	1	2846	U	N3-C2-O2	-5.80	118.14	122.20
48	1	2263	C	C6-N1-C2	-5.80	117.98	120.30
48	1	2716	U	N3-C2-O2	-5.80	118.14	122.20
48	1	1840	U	N3-C2-O2	-5.79	118.15	122.20
48	1	1533	U	N1-C2-O2	5.78	126.84	122.80
48	1	1437	C	C5-C6-N1	5.77	123.89	121.00
48	1	1227	C	N1-C2-O2	5.76	122.36	118.90
48	1	1317	A	O4'-C1'-N9	5.76	112.81	108.20
48	1	3034	C	N3-C2-O2	-5.75	117.87	121.90
48	1	2594	C	C5-C6-N1	5.75	123.88	121.00
48	1	1368	U	N1-C2-O2	5.74	126.82	122.80
12	N	48	PRO	C-N-CA	5.74	136.04	121.70
48	1	1771	C	C2-N1-C1'	5.74	125.11	118.80
48	1	3349	C	C5-C6-N1	5.73	123.87	121.00
48	1	2170	U	N1-C2-O2	5.73	126.81	122.80
48	1	1779	C	N3-C2-O2	-5.73	117.89	121.90
48	1	1483	G	P-O3'-C3'	5.72	126.57	119.70
48	1	2403	G	P-O3'-C3'	5.72	126.57	119.70
48	1	1208	U	C5-C6-N1	5.72	125.56	122.70
48	1	503	C	C6-N1-C2	-5.71	118.02	120.30
48	1	667	C	C6-N1-C2	-5.71	118.02	120.30
48	1	2407	C	C6-N1-C2	-5.70	118.02	120.30
48	1	37	U	N3-C2-O2	-5.69	118.22	122.20
48	1	3306	U	N1-C2-O2	5.69	126.78	122.80
48	1	2170	U	N3-C2-O2	-5.69	118.22	122.20
48	1	2366	C	C6-N1-C2	-5.69	118.02	120.30
48	1	1296	C	C6-N1-C2	-5.69	118.03	120.30
48	1	2366	C	C2-N1-C1'	5.69	125.05	118.80
48	1	1447	G	O4'-C1'-N9	5.68	112.74	108.20
48	1	1604	G	C8-N9-C1'	-5.68	119.62	127.00
48	1	1597	C	C6-N1-C2	-5.67	118.03	120.30
48	1	2822	U	N3-C2-O2	-5.67	118.23	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	1	1565	G	N3-C4-C5	-5.67	125.76	128.60
48	1	2625	C	P-O3'-C3'	5.67	126.50	119.70
30	4	100	U	C2-N1-C1'	5.66	124.50	117.70
48	1	1770	G	C8-N9-C1'	-5.66	119.64	127.00
48	1	908	G	C4-C5-N7	5.66	113.06	110.80
48	1	702	C	C6-N1-C2	-5.65	118.04	120.30
48	1	2846	U	N1-C2-O2	5.65	126.76	122.80
48	1	270	U	N1-C2-O2	5.64	126.75	122.80
48	1	1889	G	C4-N9-C1'	5.64	133.83	126.50
48	1	1482	A	C4-N9-C1'	5.64	136.45	126.30
48	1	700	C	C6-N1-C2	-5.63	118.05	120.30
48	1	986	U	N3-C2-O2	-5.63	118.26	122.20
48	1	1788	C	N1-C2-O2	5.63	122.28	118.90
48	1	2378	C	C2-N1-C1'	5.63	124.99	118.80
48	1	2269	U	N3-C2-O2	-5.62	118.26	122.20
48	1	3039	C	C6-N1-C2	-5.62	118.05	120.30
48	1	1333	C	C6-N1-C2	-5.62	118.05	120.30
48	1	113	C	C6-N1-C2	-5.61	118.06	120.30
48	1	2476	C	N1-C2-O2	5.60	122.26	118.90
48	1	1390	A	O4'-C1'-N9	5.60	112.68	108.20
48	1	2257	C	N1-C2-O2	5.60	122.26	118.90
48	1	915	A	C4-N9-C1'	5.59	136.37	126.30
48	1	3303	G	OP1-P-O3'	5.59	117.51	105.20
30	4	58	G	OP1-P-O3'	5.59	117.50	105.20
11	m	14	LEU	CB-CG-CD1	-5.58	101.51	111.00
48	1	3334	U	P-O3'-C3'	5.58	126.39	119.70
12	N	54	LEU	CB-CG-CD1	-5.58	101.52	111.00
48	1	2842	U	C2-N1-C1'	5.57	124.39	117.70
30	4	30	C	C6-N1-C2	-5.57	118.07	120.30
48	1	2479	C	C6-N1-C2	-5.57	118.07	120.30
48	1	2689	A	O4'-C1'-N9	5.55	112.64	108.20
48	1	2403	G	OP1-P-O3'	5.55	117.42	105.20
48	1	1771	C	N1-C2-O2	5.54	122.22	118.90
48	1	914	A	P-O3'-C3'	5.54	126.34	119.70
48	1	2478	C	C2-N1-C1'	5.53	124.89	118.80
48	1	3246	G	P-O3'-C3'	5.53	126.34	119.70
30	4	102	U	N3-C2-O2	-5.53	118.33	122.20
48	1	179	C	C6-N1-C2	-5.52	118.09	120.30
48	1	1448	U	N3-C2-O2	-5.51	118.34	122.20
48	1	27	C	C6-N1-C2	-5.51	118.09	120.30
48	1	1871	U	N1-C2-O2	5.51	126.65	122.80
48	1	1525	G	C8-N9-C1'	-5.50	119.85	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	1	1146	C	C6-N1-C2	-5.50	118.10	120.30
48	1	3350	C	N1-C2-O2	5.50	122.20	118.90
48	1	1437	C	C6-N1-C1'	-5.49	114.21	120.80
48	1	2263	C	C5-C6-N1	5.49	123.75	121.00
48	1	3231	U	N1-C2-O2	5.49	126.64	122.80
48	1	3047	U	C2-N3-C4	-5.48	123.71	127.00
28	3	68	C	C6-N1-C2	-5.48	118.11	120.30
48	1	1349	G	C8-N9-C1'	-5.46	119.90	127.00
28	3	41	G	C4-N9-C1'	-5.46	119.41	126.50
48	1	982	C	C2-N1-C1'	5.46	124.80	118.80
48	1	2585	G	C2-N3-C4	5.46	114.63	111.90
48	1	2980	U	N3-C2-O2	-5.45	118.38	122.20
48	1	906	A	P-O3'-C3'	5.44	126.23	119.70
48	1	932	U	P-O3'-C3'	5.44	126.22	119.70
48	1	1437	C	N1-C2-O2	5.43	122.16	118.90
48	1	3218	A	P-O3'-C3'	5.43	126.22	119.70
28	3	41	G	C8-N9-C1'	5.42	134.05	127.00
48	1	2665	U	P-O3'-C3'	5.42	126.20	119.70
48	1	1349	G	C2-N3-C4	5.42	114.61	111.90
48	1	1239	C	O5'-P-OP1	5.42	117.20	110.70
48	1	1144	U	N3-C4-O4	5.42	123.19	119.40
48	1	2850	G	P-O3'-C3'	5.42	126.20	119.70
48	1	1770	G	N3-C4-N9	5.41	129.25	126.00
48	1	1178	G	O5'-P-OP2	-5.41	100.83	105.70
48	1	2727	A	OP1-P-O3'	5.41	117.10	105.20
48	1	2836	C	N3-C2-O2	-5.41	118.11	121.90
48	1	2827	U	N3-C2-O2	-5.40	118.42	122.20
48	1	1281	G	N3-C4-N9	5.39	129.23	126.00
48	1	353	G	OP2-P-O3'	5.39	117.06	105.20
48	1	1218	U	C2-N1-C1'	5.39	124.17	117.70
48	1	37	U	N1-C2-O2	5.39	126.57	122.80
48	1	2810	C	N1-C2-O2	5.38	122.13	118.90
48	1	3287	U	N1-C2-O2	5.38	126.57	122.80
48	1	1218	U	C6-N1-C2	-5.38	117.77	121.00
48	1	945	C	C6-N1-C2	-5.37	118.15	120.30
48	1	1698	C	C6-N1-C2	-5.37	118.15	120.30
48	1	1144	U	P-O3'-C3'	5.37	126.14	119.70
48	1	167	U	C2-N1-C1'	5.37	124.14	117.70
48	1	3235	C	C6-N1-C2	-5.37	118.15	120.30
48	1	1355	A	P-O3'-C3'	5.36	126.14	119.70
48	1	283	G	N3-C4-N9	5.36	129.22	126.00
48	1	1037	C	C6-N1-C1'	-5.36	114.37	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	3	35	C	N1-C2-O2	5.35	122.11	118.90
48	1	2872	A	O4'-C1'-N9	5.35	112.48	108.20
48	1	2526	C	C6-N1-C2	-5.35	118.16	120.30
48	1	2665	U	OP1-P-O3'	5.34	116.96	105.20
48	1	1756	C	C6-N1-C2	-5.34	118.16	120.30
48	1	1886	A	O5'-P-OP1	-5.34	100.89	105.70
28	3	35	C	C6-N1-C2	-5.33	118.17	120.30
48	1	421	G	N3-C4-N9	5.33	129.20	126.00
48	1	1482	A	C8-N9-C1'	-5.33	118.10	127.70
48	1	3231	U	N3-C2-O2	-5.33	118.47	122.20
48	1	2526	C	C2-N1-C1'	5.33	124.66	118.80
48	1	2594	C	C6-N1-C2	-5.32	118.17	120.30
48	1	1325	U	N3-C2-O2	-5.31	118.48	122.20
48	1	547	G	P-O3'-C3'	5.31	126.07	119.70
48	1	1037	C	C5-C6-N1	5.31	123.66	121.00
48	1	342	A	O4'-C1'-N9	5.31	112.44	108.20
48	1	908	G	C5-C6-O6	-5.30	125.42	128.60
48	1	3214	U	C2-N1-C1'	5.30	124.06	117.70
48	1	2928	C	C5-C6-N1	5.30	123.65	121.00
48	1	1608	C	N1-C2-O2	5.29	122.08	118.90
48	1	1115	G	C8-N9-C1'	-5.29	120.13	127.00
48	1	957	C	C6-N1-C2	-5.28	118.19	120.30
48	1	2797	C	OP2-P-O3'	5.28	116.81	105.20
48	1	3362	A	O4'-C1'-N9	5.28	112.42	108.20
48	1	2594	C	N1-C2-O2	5.28	122.06	118.90
48	1	1417	G	P-O3'-C3'	5.27	126.02	119.70
48	1	2366	C	N1-C2-O2	5.26	122.06	118.90
48	1	2373	A	O4'-C1'-N9	5.26	112.41	108.20
48	1	2478	C	C6-N1-C2	-5.26	118.20	120.30
48	1	2783	U	N3-C2-O2	-5.25	118.53	122.20
48	1	337	G	P-O3'-C3'	5.24	125.99	119.70
48	1	2984	C	C6-N1-C1'	-5.24	114.51	120.80
30	4	102	U	N1-C2-O2	5.24	126.47	122.80
48	1	1801	U	C5-C6-N1	5.23	125.32	122.70
48	1	2158	A	P-O3'-C3'	5.23	125.98	119.70
48	1	1708	C	C6-N1-C2	-5.23	118.21	120.30
12	N	46	ILE	CG1-CB-CG2	-5.23	99.90	111.40
48	1	1716	U	P-O3'-C3'	5.22	125.96	119.70
48	1	1756	C	C5-C6-N1	5.22	123.61	121.00
48	1	1516	C	N1-C2-O2	5.22	122.03	118.90
48	1	2984	C	C5-C6-N1	5.21	123.61	121.00
48	1	2726	C	C6-N1-C1'	-5.21	114.55	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	1	2585	G	N3-C4-N9	5.21	129.12	126.00
48	1	1368	U	C5-C6-N1	5.20	125.30	122.70
48	1	2088	A	C4-N9-C1'	5.20	135.66	126.30
48	1	1448	U	C6-N1-C2	-5.20	117.88	121.00
28	3	78	U	N1-C2-O2	5.20	126.44	122.80
48	1	752	C	C6-N1-C2	-5.20	118.22	120.30
48	1	3378	C	N1-C2-O2	5.19	122.02	118.90
48	1	58	G	N1-C6-O6	-5.19	116.79	119.90
30	4	11	C	N1-C2-O2	5.19	122.01	118.90
48	1	2101	C	P-O3'-C3'	5.18	125.92	119.70
48	1	2652	U	C2-N1-C1'	5.18	123.92	117.70
48	1	2764	C	N3-C2-O2	-5.18	118.28	121.90
31	Z	102	LEU	CB-CG-CD2	-5.17	102.21	111.00
48	1	3222	U	N1-C2-O2	5.17	126.42	122.80
48	1	42	C	C4-C5-C6	-5.17	114.82	117.40
48	1	354	U	N3-C2-O2	-5.17	118.58	122.20
48	1	621	A	P-O3'-C3'	5.17	125.90	119.70
48	1	1227	C	N3-C2-O2	-5.17	118.28	121.90
38	E	191	LEU	CB-CG-CD2	-5.16	102.22	111.00
48	1	1483	G	OP1-P-O3'	5.16	116.55	105.20
48	1	1565	G	C8-N9-C1'	-5.16	120.29	127.00
48	1	2552	C	C2-N1-C1'	5.16	124.47	118.80
48	1	3287	U	C2-N1-C1'	5.15	123.89	117.70
48	1	267	G	O4'-C1'-N9	-5.15	104.08	108.20
48	1	1275	C	N1-C2-O2	5.15	121.99	118.90
48	1	1698	C	C5-C6-N1	5.14	123.57	121.00
48	1	1190	A	C4-N9-C1'	5.14	135.55	126.30
48	1	715	A	P-O3'-C3'	5.13	125.86	119.70
48	1	1847	A	O4'-C1'-N9	5.13	112.31	108.20
48	1	942	U	C6-N1-C2	-5.13	117.92	121.00
48	1	1368	U	C2-N1-C1'	5.13	123.86	117.70
48	1	2810	C	N3-C2-O2	-5.13	118.31	121.90
48	1	1425	U	N1-C2-O2	5.13	126.39	122.80
30	4	28	C	C6-N1-C2	-5.13	118.25	120.30
48	1	421	G	C4-N9-C1'	5.13	133.17	126.50
48	1	2568	C	O4'-C1'-N1	5.12	112.30	108.20
48	1	638	C	C6-N1-C2	-5.12	118.25	120.30
48	1	3084	C	C6-N1-C2	-5.12	118.25	120.30
48	1	982	C	C6-N1-C2	-5.12	118.25	120.30
48	1	2284	C	C2-N1-C1'	5.12	124.43	118.80
20	s	138	ARG	CA-CB-CG	5.12	124.66	113.40
48	1	1862	U	C5-C6-N1	5.12	125.26	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	1	341	G	P-O3'-C3'	5.12	125.84	119.70
48	1	1218	U	N1-C2-O2	5.12	126.38	122.80
48	1	302	U	C5-C6-N1	5.11	125.25	122.70
48	1	2707	C	C5-C6-N1	5.11	123.55	121.00
48	1	2950	G	P-O3'-C3'	5.11	125.83	119.70
48	1	3217	C	C5-C6-N1	5.10	123.55	121.00
48	1	1589	A	O4'-C1'-N9	5.09	112.28	108.20
48	1	2269	U	C6-N1-C2	-5.09	117.94	121.00
28	3	26	C	C5-C6-N1	5.09	123.54	121.00
48	1	2362	C	N1-C2-O2	5.09	121.95	118.90
48	1	3338	C	C5-C6-N1	5.08	123.54	121.00
48	1	1432	C	N3-C2-O2	-5.08	118.34	121.90
48	1	2943	G	C4-N9-C1'	5.08	133.10	126.50
48	1	2830	G	C4-N9-C1'	5.07	133.09	126.50
48	1	873	C	P-O3'-C3'	5.07	125.78	119.70
48	1	938	C	C6-N1-C2	-5.06	118.28	120.30
48	1	2447	A	OP1-P-O3'	5.05	116.32	105.20
48	1	1788	C	N3-C2-O2	-5.05	118.37	121.90
48	1	543	C	C6-N1-C2	-5.05	118.28	120.30
48	1	3034	C	C2-N1-C1'	5.05	124.35	118.80
28	3	35	C	N3-C2-O2	-5.04	118.37	121.90
48	1	1481	A	P-O3'-C3'	5.04	125.75	119.70
48	1	1177	G	OP1-P-O3'	5.04	116.29	105.20
48	1	2406	C	C6-N1-C2	-5.04	118.28	120.30
48	1	2677	G	C4-N9-C1'	5.04	133.05	126.50
48	1	2497	U	N1-C2-O2	5.03	126.32	122.80
48	1	2585	G	C4-N9-C1'	5.03	133.04	126.50
48	1	3181	C	C6-N1-C1'	-5.03	114.76	120.80
30	4	11	C	C5-C6-N1	5.03	123.52	121.00
48	1	543	C	N3-C2-O2	-5.03	118.38	121.90
48	1	1871	U	N3-C2-O2	-5.03	118.68	122.20
48	1	1193	A	O5'-P-OP1	-5.03	101.18	105.70
48	1	2177	G	OP2-P-O3'	5.03	116.26	105.20
48	1	242	C	N1-C2-O2	5.02	121.91	118.90
48	1	859	G	P-O3'-C3'	5.02	125.73	119.70
48	1	282	G	P-O3'-C3'	5.02	125.72	119.70
48	1	2322	C	C6-N1-C2	-5.02	118.29	120.30
48	1	1277	C	C6-N1-C2	-5.01	118.30	120.30
48	1	2772	C	C2-N1-C1'	5.01	124.31	118.80
48	1	939	U	N3-C2-O2	-5.01	118.69	122.20
48	1	3023	U	C2-N1-C1'	5.01	123.71	117.70
48	1	288	C	C6-N1-C2	-5.00	118.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	1	1433	A	OP1-P-O3'	5.00	116.21	105.20
48	1	2334	U	N1-C2-O2	5.00	126.30	122.80
48	1	1434	G	C4-N9-C1'	-5.00	120.00	126.50
48	1	797	U	C5-C6-N1	5.00	125.20	122.70
48	1	1432	C	C6-N1-C1'	-5.00	114.80	120.80

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	7	21	LYS	Peptide
36	D	51	ALA	Peptide
38	E	179	LEU	Peptide
40	F	385	LYS	Peptide
42	G	131	VAL	Peptide
42	G	291	ASN	Peptide
42	G	318	LEU	Peptide
42	G	338	LYS	Peptide
44	H	259	LYS	Peptide
4	J	157	ASN	Peptide
4	J	232	ARG	Peptide
6	K	156	ASP	Peptide
6	K	35	GLY	Peptide
6	K	76	ALA	Peptide
10	M	172	LEU	Peptide
12	N	4	SER	Peptide
12	N	47	ALA	Peptide
12	N	61	PRO	Peptide
14	O	48	GLY	Peptide
2	X	8	GLU	Peptide
33	b	102	GLU	Peptide
35	c	116	GLY	Peptide
35	c	45	MET	Peptide
35	c	46	ASP	Peptide
37	d	19	ASN	Peptide
5	j	90	ARG	Peptide
5	j	91	ALA	Peptide
7	k	27	SER	Peptide
11	m	32	ASN	Peptide
11	m	35	GLY	Peptide
20	s	103	SER	Peptide
20	s	107	ALA	Peptide

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Mol	Chain	Res	Type	Group
20	s	134	ILE	Peptide
20	s	170	TRP	Peptide

5.2 Too-close contacts (i)

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

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	R	300/475 (63%)	284 (95%)	16 (5%)	0	100	100
2	X	222/224 (99%)	211 (95%)	11 (5%)	0	100	100
3	i	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
4	J	220/222 (99%)	202 (92%)	16 (7%)	2 (1%)	17	49
5	j	117/119 (98%)	109 (93%)	5 (4%)	3 (3%)	5	26
6	K	231/233 (99%)	215 (93%)	14 (6%)	2 (1%)	17	49
7	k	97/99 (98%)	89 (92%)	8 (8%)	0	100	100
8	7	189/191 (99%)	176 (93%)	13 (7%)	0	100	100
9	l	85/87 (98%)	75 (88%)	10 (12%)	0	100	100
10	M	167/169 (99%)	145 (87%)	22 (13%)	0	100	100
11	m	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
12	N	191/193 (99%)	173 (91%)	14 (7%)	4 (2%)	7	30
13	n	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
14	O	134/136 (98%)	123 (92%)	11 (8%)	0	100	100
15	o	50/52 (96%)	47 (94%)	3 (6%)	0	100	100
16	p	201/203 (99%)	182 (90%)	16 (8%)	3 (2%)	10	36
17	Q	195/197 (99%)	187 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	5	181/183 (99%)	163 (90%)	18 (10%)	0	100	100
19	S	183/185 (99%)	171 (93%)	12 (7%)	0	100	100
20	s	218/220 (99%)	194 (89%)	22 (10%)	2 (1%)	17	49
21	T	150/152 (99%)	141 (94%)	8 (5%)	1 (1%)	22	55
22	U	170/172 (99%)	158 (93%)	11 (6%)	1 (1%)	25	57
23	V	157/159 (99%)	145 (92%)	12 (8%)	0	100	100
24	W	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
25	P	144/155 (93%)	124 (86%)	20 (14%)	0	100	100
26	r	117/197 (59%)	108 (92%)	9 (8%)	0	100	100
27	x	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
29	Y	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
31	Z	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
32	a	124/126 (98%)	118 (95%)	6 (5%)	0	100	100
33	b	133/135 (98%)	123 (92%)	9 (7%)	1 (1%)	19	51
34	C	103/105 (98%)	89 (86%)	14 (14%)	0	100	100
35	c	146/148 (99%)	128 (88%)	16 (11%)	2 (1%)	11	37
36	D	89/91 (98%)	82 (92%)	7 (8%)	0	100	100
37	d	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
38	E	250/252 (99%)	229 (92%)	21 (8%)	0	100	100
39	e	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
40	F	384/386 (100%)	354 (92%)	29 (8%)	1 (0%)	41	72
41	f	107/109 (98%)	96 (90%)	11 (10%)	0	100	100
42	G	359/361 (99%)	325 (90%)	32 (9%)	2 (1%)	25	57
43	g	125/127 (98%)	122 (98%)	3 (2%)	0	100	100
44	H	294/296 (99%)	274 (93%)	18 (6%)	2 (1%)	22	55
45	h	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
46	I	152/175 (87%)	147 (97%)	5 (3%)	0	100	100
47	L	202/204 (99%)	165 (82%)	37 (18%)	0	100	100
All	All	7086/7457 (95%)	6532 (92%)	528 (8%)	26 (0%)	38	67

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	s	108	ASP
35	c	47	LYS
35	c	78	LEU
42	G	339	LEU
4	J	158	LYS
4	J	233	GLU
6	K	157	VAL
12	N	62	THR
16	p	74	PRO
21	T	131	ALA
5	j	85	THR
5	j	91	ALA
12	N	48	PRO
5	j	90	ARG
6	K	156	ASP
22	U	13	ARG
12	N	61	PRO
42	G	292	SER
44	H	276	LYS
12	N	47	ALA
16	p	146	ALA
33	b	102	GLU
44	H	260	PHE
16	p	75	VAL
40	F	188	ILE
20	s	171	GLY

5.3.2 Protein sidechains (i)

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	R	288/392 (74%)	285 (99%)	3 (1%)	76 88
2	X	177/192 (92%)	177 (100%)	0	100 100
3	i	95/95 (100%)	95 (100%)	0	100 100
4	J	186/186 (100%)	186 (100%)	0	100 100
5	j	104/104 (100%)	104 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	K	187/191 (98%)	187 (100%)	0	100	100
7	k	81/81 (100%)	81 (100%)	0	100	100
8	7	171/171 (100%)	169 (99%)	2 (1%)	71	85
9	l	70/70 (100%)	70 (100%)	0	100	100
10	M	147/147 (100%)	147 (100%)	0	100	100
11	m	68/68 (100%)	68 (100%)	0	100	100
12	N	154/154 (100%)	153 (99%)	1 (1%)	86	94
13	n	45/45 (100%)	45 (100%)	0	100	100
14	O	107/107 (100%)	107 (100%)	0	100	100
15	o	47/47 (100%)	47 (100%)	0	100	100
16	p	175/175 (100%)	173 (99%)	2 (1%)	73	86
17	Q	160/160 (100%)	160 (100%)	0	100	100
18	5	140/145 (97%)	138 (99%)	2 (1%)	67	83
19	S	150/150 (100%)	150 (100%)	0	100	100
20	s	184/186 (99%)	183 (100%)	1 (0%)	88	94
21	T	126/126 (100%)	126 (100%)	0	100	100
22	U	156/156 (100%)	155 (99%)	1 (1%)	86	94
23	V	136/136 (100%)	134 (98%)	2 (2%)	65	82
24	W	87/87 (100%)	87 (100%)	0	100	100
26	r	105/166 (63%)	105 (100%)	0	100	100
27	x	104/104 (100%)	104 (100%)	0	100	100
29	Y	54/54 (100%)	54 (100%)	0	100	100
31	Z	104/105 (99%)	104 (100%)	0	100	100
32	a	109/109 (100%)	109 (100%)	0	100	100
33	b	115/115 (100%)	115 (100%)	0	100	100
34	C	90/90 (100%)	90 (100%)	0	100	100
35	c	118/118 (100%)	117 (99%)	1 (1%)	81	91
36	D	71/71 (100%)	70 (99%)	1 (1%)	67	83
37	d	46/46 (100%)	46 (100%)	0	100	100
38	E	193/194 (100%)	192 (100%)	1 (0%)	88	94
39	e	81/81 (100%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	F	319/322 (99%)	318 (100%)	1 (0%)	92 97
41	f	92/96 (96%)	91 (99%)	1 (1%)	73 86
42	G	288/288 (100%)	288 (100%)	0	100 100
43	g	109/109 (100%)	109 (100%)	0	100 100
44	H	244/244 (100%)	244 (100%)	0	100 100
45	h	90/90 (100%)	90 (100%)	0	100 100
46	I	134/152 (88%)	134 (100%)	0	100 100
47	L	185/185 (100%)	181 (98%)	4 (2%)	52 75
All	All	5892/6110 (96%)	5869 (100%)	23 (0%)	91 95

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	102	ARG
1	R	212	ASN
1	R	214	ARG
8	7	23	ARG
8	7	68	LEU
12	N	58	VAL
16	p	183	THR
16	p	193	ARG
18	5	24	VAL
18	5	126	ARG
20	s	6	ARG
22	U	13	ARG
23	V	60	LYS
23	V	83	ARG
35	c	78	LEU
36	D	17	ARG
38	E	193	ARG
40	F	104	THR
41	f	26	LYS
47	L	14	LYS
47	L	57	ASN
47	L	108	ASN
47	L	130	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	212	ASN
2	X	11	ASN
2	X	106	ASN
3	i	52	GLN
5	j	59	ASN
6	K	240	ASN
16	p	37	HIS
16	p	181	ASN
19	S	73	GLN
21	T	130	ASN
22	U	122	HIS
26	r	56	ASN
27	x	98	ASN
29	Y	32	GLN
33	b	57	HIS
34	C	22	GLN
35	c	64	GLN
37	d	12	GLN
38	E	79	ASN
38	E	132	ASN
38	E	209	HIS
40	F	109	HIS
41	f	57	GLN
42	G	48	GLN
42	G	110	ASN
42	G	114	ASN
43	g	52	GLN
45	h	42	GLN
47	L	44	GLN
47	L	57	ASN
47	L	108	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	3	120/121 (99%)	28 (23%)	1 (0%)
30	4	157/158 (99%)	36 (22%)	5 (3%)
48	1	3257/3260 (99%)	906 (27%)	158 (4%)
All	All	3534/3539 (99%)	970 (27%)	164 (4%)

All (970) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
28	3	10	C
28	3	11	A
28	3	13	A
28	3	14	U
28	3	33	U
28	3	38	U
28	3	41	G
28	3	42	A
28	3	45	A
28	3	48	U
28	3	49	G
28	3	50	U
28	3	52	G
28	3	53	U
28	3	55	A
28	3	64	A
28	3	65	G
28	3	73	C
28	3	74	C
28	3	76	A
28	3	77	G
28	3	78	U
28	3	91	G
28	3	99	G
28	3	102	A
28	3	111	U
28	3	112	G
28	3	121	U
30	4	13	A
30	4	16	G
30	4	22	U
30	4	23	U
30	4	24	G
30	4	34	U
30	4	35	C
30	4	39	G
30	4	40	A
30	4	49	G
30	4	51	G
30	4	52	A
30	4	59	A
30	4	60	U
30	4	63	G

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Mol	Chain	Res	Type
30	4	80	A
30	4	81	U
30	4	82	U
30	4	83	C
30	4	85	G
30	4	86	U
30	4	87	G
30	4	90	U
30	4	95	G
30	4	104	A
30	4	106	C
30	4	111	A
30	4	112	U
30	4	113	U
30	4	116	G
30	4	125	U
30	4	126	A
30	4	129	C
30	4	138	A
30	4	147	U
30	4	152	G
48	1	6	A
48	1	13	A
48	1	14	U
48	1	15	C
48	1	22	G
48	1	25	U
48	1	26	A
48	1	30	G
48	1	40	A
48	1	41	G
48	1	43	A
48	1	44	U
48	1	48	A
48	1	49	A
48	1	57	A
48	1	59	G
48	1	60	A
48	1	65	A
48	1	66	A
48	1	67	A
48	1	72	C

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Mol	Chain	Res	Type
48	1	73	C
48	1	77	A
48	1	86	G
48	1	87	U
48	1	92	G
48	1	109	A
48	1	110	G
48	1	116	A
48	1	117	U
48	1	118	U
48	1	119	U
48	1	121	A
48	1	122	A
48	1	123	A
48	1	134	U
48	1	135	C
48	1	136	G
48	1	146	U
48	1	147	U
48	1	148	G
48	1	150	A
48	1	155	G
48	1	156	G
48	1	157	A
48	1	166	C
48	1	167	U
48	1	168	U
48	1	169	U
48	1	170	G
48	1	187	A
48	1	188	U
48	1	189	G
48	1	190	U
48	1	191	U
48	1	197	G
48	1	200	C
48	1	206	G
48	1	210	U
48	1	211	A
48	1	212	G
48	1	213	A
48	1	218	G

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Mol	Chain	Res	Type
48	1	219	A
48	1	220	G
48	1	234	G
48	1	238	A
48	1	240	U
48	1	241	G
48	1	252	U
48	1	266	A
48	1	269	G
48	1	270	U
48	1	281	G
48	1	283	G
48	1	285	A
48	1	286	U
48	1	295	A
48	1	297	G
48	1	298	U
48	1	304	G
48	1	305	U
48	1	323	A
48	1	329	U
48	1	330	G
48	1	337	G
48	1	338	A
48	1	339	C
48	1	342	A
48	1	343	U
48	1	350	C
48	1	352	A
48	1	353	G
48	1	354	U
48	1	375	A
48	1	376	G
48	1	385	A
48	1	390	G
48	1	395	A
48	1	398	A
48	1	399	A
48	1	401	U
48	1	403	C
48	1	406	G
48	1	420	G

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Mol	Chain	Res	Type
48	1	421	G
48	1	422	A
48	1	429	U
48	1	439	C
48	1	440	A
48	1	495	G
48	1	517	G
48	1	521	A
48	1	523	A
48	1	535	G
48	1	536	U
48	1	547	G
48	1	548	G
48	1	555	U
48	1	556	U
48	1	558	U
48	1	559	A
48	1	560	G
48	1	566	G
48	1	578	A
48	1	579	G
48	1	581	U
48	1	589	A
48	1	592	A
48	1	597	G
48	1	600	G
48	1	603	A
48	1	604	G
48	1	609	G
48	1	611	A
48	1	620	U
48	1	621	A
48	1	622	A
48	1	623	U
48	1	637	C
48	1	641	C
48	1	645	A
48	1	646	A
48	1	648	C
48	1	649	A
48	1	661	G
48	1	667	C

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Mol	Chain	Res	Type
48	1	677	A
48	1	678	G
48	1	681	U
48	1	683	U
48	1	690	A
48	1	691	A
48	1	692	A
48	1	699	A
48	1	705	A
48	1	708	G
48	1	709	A
48	1	712	G
48	1	715	A
48	1	716	A
48	1	719	U
48	1	720	A
48	1	742	G
48	1	758	C
48	1	760	G
48	1	764	U
48	1	765	C
48	1	766	U
48	1	767	U
48	1	768	C
48	1	770	G
48	1	776	U
48	1	777	U
48	1	781	G
48	1	784	A
48	1	785	G
48	1	786	A
48	1	798	G
48	1	799	G
48	1	800	G
48	1	801	A
48	1	806	A
48	1	817	A
48	1	825	U
48	1	830	A
48	1	832	G
48	1	835	G
48	1	837	A

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Mol	Chain	Res	Type
48	1	849	C
48	1	851	C
48	1	857	G
48	1	858	A
48	1	860	G
48	1	861	C
48	1	869	G
48	1	871	U
48	1	874	U
48	1	875	G
48	1	879	U
48	1	880	G
48	1	882	A
48	1	884	A
48	1	885	U
48	1	895	A
48	1	907	G
48	1	909	G
48	1	914	A
48	1	915	A
48	1	916	G
48	1	917	A
48	1	920	A
48	1	925	A
48	1	932	U
48	1	933	A
48	1	937	G
48	1	944	C
48	1	953	G
48	1	959	C
48	1	960	U
48	1	962	A
48	1	963	G
48	1	978	G
48	1	980	A
48	1	981	U
48	1	982	C
48	1	985	U
48	1	991	G
48	1	995	U
48	1	1001	G
48	1	1005	G

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Mol	Chain	Res	Type
48	1	1006	A
48	1	1015	U
48	1	1016	C
48	1	1017	C
48	1	1018	G
48	1	1021	G
48	1	1025	A
48	1	1026	A
48	1	1029	G
48	1	1032	C
48	1	1036	A
48	1	1037	C
48	1	1038	C
48	1	1044	U
48	1	1045	C
48	1	1047	A
48	1	1049	C
48	1	1054	A
48	1	1065	A
48	1	1066	G
48	1	1075	A
48	1	1076	C
48	1	1081	U
48	1	1082	U
48	1	1083	G
48	1	1092	C
48	1	1093	A
48	1	1094	U
48	1	1095	U
48	1	1096	U
48	1	1097	G
48	1	1098	A
48	1	1103	A
48	1	1104	G
48	1	1117	G
48	1	1122	U
48	1	1128	U
48	1	1131	G
48	1	1140	G
48	1	1143	A
48	1	1144	U
48	1	1145	G

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Mol	Chain	Res	Type
48	1	1151	U
48	1	1153	A
48	1	1155	C
48	1	1159	A
48	1	1177	G
48	1	1178	G
48	1	1180	A
48	1	1181	U
48	1	1182	A
48	1	1190	A
48	1	1191	U
48	1	1192	C
48	1	1193	A
48	1	1196	C
48	1	1197	A
48	1	1199	C
48	1	1200	A
48	1	1201	C
48	1	1202	A
48	1	1206	G
48	1	1209	G
48	1	1219	C
48	1	1220	U
48	1	1221	A
48	1	1222	G
48	1	1223	A
48	1	1224	C
48	1	1232	C
48	1	1235	U
48	1	1236	G
48	1	1237	G
48	1	1238	C
48	1	1239	C
48	1	1241	U
48	1	1242	G
48	1	1244	A
48	1	1245	A
48	1	1246	G
48	1	1258	U
48	1	1259	A
48	1	1262	G
48	1	1263	A

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Mol	Chain	Res	Type
48	1	1264	G
48	1	1265	U
48	1	1282	G
48	1	1285	G
48	1	1287	A
48	1	1292	C
48	1	1293	U
48	1	1301	A
48	1	1303	A
48	1	1305	U
48	1	1306	G
48	1	1307	G
48	1	1308	A
48	1	1313	G
48	1	1315	U
48	1	1316	C
48	1	1317	A
48	1	1329	U
48	1	1330	A
48	1	1331	U
48	1	1349	G
48	1	1351	U
48	1	1352	A
48	1	1355	A
48	1	1356	U
48	1	1357	G
48	1	1366	A
48	1	1367	G
48	1	1368	U
48	1	1380	G
48	1	1386	A
48	1	1391	C
48	1	1392	G
48	1	1399	A
48	1	1400	G
48	1	1418	A
48	1	1419	A
48	1	1421	G
48	1	1432	C
48	1	1434	G
48	1	1435	A
48	1	1436	U

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Mol	Chain	Res	Type
48	1	1437	C
48	1	1438	U
48	1	1443	G
48	1	1447	G
48	1	1448	U
48	1	1450	G
48	1	1456	A
48	1	1467	A
48	1	1468	A
48	1	1469	C
48	1	1480	G
48	1	1482	A
48	1	1483	G
48	1	1484	U
48	1	1487	G
48	1	1494	U
48	1	1495	U
48	1	1496	C
48	1	1503	A
48	1	1508	C
48	1	1511	U
48	1	1512	U
48	1	1523	U
48	1	1527	C
48	1	1528	G
48	1	1533	U
48	1	1536	G
48	1	1546	A
48	1	1547	G
48	1	1554	U
48	1	1555	U
48	1	1556	C
48	1	1558	A
48	1	1559	A
48	1	1560	G
48	1	1561	G
48	1	1563	C
48	1	1565	G
48	1	1567	U
48	1	1568	U
48	1	1569	U
48	1	1570	U

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Mol	Chain	Res	Type
48	1	1572	U
48	1	1573	G
48	1	1575	A
48	1	1578	C
48	1	1579	C
48	1	1580	A
48	1	1581	C
48	1	1582	C
48	1	1583	A
48	1	1587	A
48	1	1588	A
48	1	1589	A
48	1	1590	G
48	1	1593	A
48	1	1595	U
48	1	1605	A
48	1	1613	A
48	1	1620	U
48	1	1621	A
48	1	1623	G
48	1	1629	U
48	1	1630	U
48	1	1641	U
48	1	1645	U
48	1	1646	G
48	1	1657	C
48	1	1683	A
48	1	1687	U
48	1	1696	A
48	1	1715	A
48	1	1717	U
48	1	1719	G
48	1	1724	U
48	1	1725	C
48	1	1730	G
48	1	1731	A
48	1	1741	A
48	1	1742	U
48	1	1749	A
48	1	1750	A
48	1	1760	A
48	1	1762	C

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Mol	Chain	Res	Type
48	1	1763	U
48	1	1765	U
48	1	1766	G
48	1	1769	G
48	1	1770	G
48	1	1771	C
48	1	1775	G
48	1	1780	G
48	1	1794	G
48	1	1795	U
48	1	1796	G
48	1	1797	A
48	1	1813	A
48	1	1814	A
48	1	1815	U
48	1	1816	A
48	1	1817	G
48	1	1818	U
48	1	1819	U
48	1	1820	U
48	1	1822	C
48	1	1839	A
48	1	1840	U
48	1	1841	A
48	1	1843	C
48	1	1845	G
48	1	1846	C
48	1	1847	A
48	1	1849	C
48	1	1850	A
48	1	1851	G
48	1	1864	A
48	1	1866	C
48	1	1867	A
48	1	1871	U
48	1	1878	G
48	1	1879	A
48	1	1880	U
48	1	1886	A
48	1	1887	A
48	1	1893	A
48	1	1894	U

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Mol	Chain	Res	Type
48	1	1901	A
48	1	1905	G
48	1	1906	G
48	1	1907	C
48	1	1913	A
48	1	1914	G
48	1	1927	G
48	1	1930	A
48	1	1931	U
48	1	1932	A
48	1	1935	G
48	1	1939	G
48	1	1943	C
48	1	1953	G
48	1	1954	G
48	1	1955	U
48	1	1959	G
48	1	1960	A
48	1	1961	G
48	1	1962	A
48	1	1963	G
48	1	1964	C
48	1	1972	A
48	1	1973	G
48	1	1976	G
48	1	2044	U
48	1	2045	G
48	1	2047	A
48	1	2048	G
48	1	2049	A
48	1	2050	C
48	1	2051	G
48	1	2058	G
48	1	2059	U
48	1	2081	U
48	1	2082	U
48	1	2087	C
48	1	2088	A
48	1	2093	A
48	1	2099	A
48	1	2100	A
48	1	2101	C

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Mol	Chain	Res	Type
48	1	2102	U
48	1	2107	A
48	1	2111	G
48	1	2112	U
48	1	2113	A
48	1	2116	G
48	1	2121	G
48	1	2122	G
48	1	2126	A
48	1	2131	A
48	1	2134	G
48	1	2138	A
48	1	2139	A
48	1	2140	U
48	1	2142	A
48	1	2143	A
48	1	2144	A
48	1	2145	A
48	1	2159	U
48	1	2160	G
48	1	2166	A
48	1	2169	G
48	1	2170	U
48	1	2175	U
48	1	2176	U
48	1	2178	A
48	1	2179	C
48	1	2184	U
48	1	2187	G
48	1	2188	A
48	1	2205	U
48	1	2206	G
48	1	2209	U
48	1	2210	G
48	1	2218	G
48	1	2223	A
48	1	2225	U
48	1	2230	C
48	1	2243	A
48	1	2244	A
48	1	2249	G
48	1	2253	G

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Mol	Chain	Res	Type
48	1	2254	U
48	1	2256	A
48	1	2257	C
48	1	2258	U
48	1	2260	U
48	1	2261	G
48	1	2262	A
48	1	2263	C
48	1	2267	C
48	1	2268	U
48	1	2269	U
48	1	2270	A
48	1	2272	G
48	1	2273	G
48	1	2274	U
48	1	2276	G
48	1	2279	A
48	1	2280	A
48	1	2281	A
48	1	2282	U
48	1	2283	G
48	1	2284	C
48	1	2285	C
48	1	2298	U
48	1	2299	A
48	1	2306	C
48	1	2307	G
48	1	2308	C
48	1	2310	U
48	1	2313	A
48	1	2314	U
48	1	2315	G
48	1	2319	U
48	1	2334	U
48	1	2335	G
48	1	2340	U
48	1	2347	U
48	1	2356	A
48	1	2361	A
48	1	2373	A
48	1	2374	C
48	1	2375	G

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Mol	Chain	Res	Type
48	1	2376	G
48	1	2386	A
48	1	2388	U
48	1	2391	G
48	1	2393	G
48	1	2397	A
48	1	2401	A
48	1	2402	A
48	1	2403	G
48	1	2404	A
48	1	2411	U
48	1	2418	G
48	1	2419	A
48	1	2435	G
48	1	2440	G
48	1	2441	A
48	1	2443	A
48	1	2444	C
48	1	2445	A
48	1	2446	U
48	1	2447	A
48	1	2448	G
48	1	2453	U
48	1	2454	G
48	1	2459	A
48	1	2462	A
48	1	2469	G
48	1	2471	U
48	1	2482	U
48	1	2486	A
48	1	2487	U
48	1	2488	A
48	1	2496	C
48	1	2500	A
48	1	2503	G
48	1	2504	U
48	1	2505	U
48	1	2506	U
48	1	2507	C
48	1	2509	U
48	1	2510	U
48	1	2512	C

Continued on next page...

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Mol	Chain	Res	Type
48	1	2513	U
48	1	2514	U
48	1	2515	A
48	1	2522	G
48	1	2523	A
48	1	2526	C
48	1	2531	C
48	1	2532	U
48	1	2533	G
48	1	2537	U
48	1	2538	U
48	1	2539	C
48	1	2540	A
48	1	2541	U
48	1	2542	U
48	1	2543	U
48	1	2544	U
48	1	2548	C
48	1	2549	G
48	1	2552	C
48	1	2554	A
48	1	2559	U
48	1	2561	A
48	1	2568	C
48	1	2569	A
48	1	2570	U
48	1	2571	U
48	1	2572	C
48	1	2573	G
48	1	2585	G
48	1	2587	U
48	1	2593	A
48	1	2594	C
48	1	2606	G
48	1	2607	G
48	1	2614	G
48	1	2618	G
48	1	2619	G
48	1	2626	A
48	1	2629	U
48	1	2635	A
48	1	2636	A

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Mol	Chain	Res	Type
48	1	2648	G
48	1	2651	G
48	1	2652	U
48	1	2655	U
48	1	2657	A
48	1	2666	C
48	1	2674	A
48	1	2676	A
48	1	2678	A
48	1	2681	U
48	1	2689	A
48	1	2691	A
48	1	2694	A
48	1	2704	A
48	1	2713	U
48	1	2716	U
48	1	2719	U
48	1	2720	G
48	1	2726	C
48	1	2727	A
48	1	2728	G
48	1	2729	U
48	1	2737	C
48	1	2742	C
48	1	2753	G
48	1	2755	C
48	1	2761	G
48	1	2762	A
48	1	2772	C
48	1	2773	C
48	1	2777	G
48	1	2778	G
48	1	2779	A
48	1	2796	G
48	1	2797	C
48	1	2798	C
48	1	2800	G
48	1	2801	A
48	1	2802	A
48	1	2804	A
48	1	2810	C
48	1	2814	G

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Mol	Chain	Res	Type
48	1	2816	G
48	1	2817	A
48	1	2827	U
48	1	2829	U
48	1	2830	G
48	1	2842	U
48	1	2845	A
48	1	2846	U
48	1	2847	A
48	1	2850	G
48	1	2851	A
48	1	2867	C
48	1	2871	G
48	1	2872	A
48	1	2873	U
48	1	2874	G
48	1	2882	U
48	1	2887	A
48	1	2888	U
48	1	2889	C
48	1	2895	G
48	1	2912	G
48	1	2915	U
48	1	2923	U
48	1	2926	A
48	1	2935	U
48	1	2936	A
48	1	2938	G
48	1	2941	A
48	1	2945	G
48	1	2946	A
48	1	2947	G
48	1	2951	G
48	1	2954	U
48	1	2971	A
48	1	2972	G
48	1	2978	U
48	1	2979	U
48	1	2980	U
48	1	2983	C
48	1	2985	C
48	1	2996	U

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Mol	Chain	Res	Type
48	1	2997	G
48	1	3003	G
48	1	3011	A
48	1	3012	A
48	1	3021	A
48	1	3022	G
48	1	3023	U
48	1	3026	G
48	1	3030	G
48	1	3047	U
48	1	3056	U
48	1	3058	U
48	1	3059	G
48	1	3069	G
48	1	3074	G
48	1	3078	U
48	1	3079	U
48	1	3080	G
48	1	3086	A
48	1	3092	C
48	1	3104	U
48	1	3109	G
48	1	3117	C
48	1	3118	C
48	1	3119	U
48	1	3122	A
48	1	3130	A
48	1	3131	U
48	1	3139	A
48	1	3141	A
48	1	3142	A
48	1	3143	C
48	1	3144	G
48	1	3151	U
48	1	3152	U
48	1	3153	U
48	1	3154	C
48	1	3155	U
48	1	3156	U
48	1	3157	U
48	1	3158	G
48	1	3167	A

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Mol	Chain	Res	Type
48	1	3173	G
48	1	3174	A
48	1	3175	U
48	1	3176	G
48	1	3179	U
48	1	3180	A
48	1	3181	C
48	1	3186	A
48	1	3187	A
48	1	3196	U
48	1	3198	U
48	1	3205	G
48	1	3206	C
48	1	3207	U
48	1	3208	G
48	1	3209	A
48	1	3210	A
48	1	3211	C
48	1	3215	A
48	1	3217	C
48	1	3218	A
48	1	3219	G
48	1	3220	G
48	1	3222	U
48	1	3227	A
48	1	3237	U
48	1	3242	G
48	1	3243	A
48	1	3244	A
48	1	3245	A
48	1	3246	G
48	1	3247	G
48	1	3253	G
48	1	3259	U
48	1	3260	G
48	1	3263	G
48	1	3268	A
48	1	3269	U
48	1	3270	U
48	1	3271	G
48	1	3272	C
48	1	3273	A

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Mol	Chain	Res	Type
48	1	3275	U
48	1	3276	G
48	1	3277	U
48	1	3278	C
48	1	3280	U
48	1	3282	U
48	1	3287	U
48	1	3288	G
48	1	3289	G
48	1	3293	U
48	1	3294	A
48	1	3295	A
48	1	3303	G
48	1	3304	U
48	1	3305	A
48	1	3308	C
48	1	3309	G
48	1	3313	U
48	1	3316	A
48	1	3317	U
48	1	3318	G
48	1	3319	U
48	1	3335	A
48	1	3341	U
48	1	3345	G
48	1	3347	A
48	1	3349	C
48	1	3351	U
48	1	3352	U
48	1	3353	G
48	1	3355	U
48	1	3357	U
48	1	3358	U
48	1	3362	A
48	1	3363	U
48	1	3368	U
48	1	3369	G
48	1	3375	A
48	1	3378	C
48	1	3382	U
48	1	3383	G
48	1	3386	G

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Mol	Chain	Res	Type
48	1	3390	G
48	1	3393	U
48	1	3396	U

All (164) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
28	3	77	G
30	4	22	U
30	4	38	U
30	4	48	A
30	4	51	G
30	4	58	G
48	1	14	U
48	1	43	A
48	1	66	A
48	1	71	A
48	1	86	G
48	1	116	A
48	1	122	A
48	1	147	U
48	1	155	G
48	1	156	G
48	1	189	G
48	1	211	A
48	1	218	G
48	1	219	A
48	1	239	G
48	1	268	A
48	1	269	G
48	1	282	G
48	1	337	G
48	1	341	G
48	1	342	A
48	1	352	A
48	1	353	G
48	1	400	G
48	1	494	G
48	1	547	G
48	1	558	U
48	1	621	A
48	1	645	A

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Mol	Chain	Res	Type
48	1	648	C
48	1	661	G
48	1	677	A
48	1	715	A
48	1	764	U
48	1	857	G
48	1	870	G
48	1	884	A
48	1	906	A
48	1	914	A
48	1	916	G
48	1	920	A
48	1	924	G
48	1	932	U
48	1	962	A
48	1	979	U
48	1	994	G
48	1	1064	A
48	1	1075	A
48	1	1097	G
48	1	1116	G
48	1	1144	U
48	1	1152	G
48	1	1177	G
48	1	1192	C
48	1	1199	C
48	1	1241	U
48	1	1305	U
48	1	1307	G
48	1	1329	U
48	1	1348	U
48	1	1355	A
48	1	1365	G
48	1	1391	C
48	1	1417	G
48	1	1418	A
48	1	1433	A
48	1	1434	G
48	1	1455	U
48	1	1481	A
48	1	1483	G
48	1	1511	U

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Mol	Chain	Res	Type
48	1	1553	U
48	1	1554	U
48	1	1557	A
48	1	1558	A
48	1	1580	A
48	1	1588	A
48	1	1589	A
48	1	1695	U
48	1	1716	U
48	1	1730	G
48	1	1740	U
48	1	1793	C
48	1	1795	U
48	1	1815	U
48	1	1816	A
48	1	1840	U
48	1	1849	C
48	1	1850	A
48	1	1866	C
48	1	1900	A
48	1	1906	G
48	1	1913	A
48	1	1938	U
48	1	1959	G
48	1	2086	A
48	1	2101	C
48	1	2111	G
48	1	2112	U
48	1	2139	A
48	1	2158	A
48	1	2175	U
48	1	2177	G
48	1	2178	A
48	1	2187	G
48	1	2208	A
48	1	2262	A
48	1	2267	C
48	1	2271	A
48	1	2282	U
48	1	2283	G
48	1	2298	U
48	1	2313	A

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Mol	Chain	Res	Type
48	1	2385	G
48	1	2403	G
48	1	2447	A
48	1	2468	A
48	1	2487	U
48	1	2509	U
48	1	2513	U
48	1	2537	U
48	1	2541	U
48	1	2586	G
48	1	2593	A
48	1	2617	U
48	1	2625	C
48	1	2635	A
48	1	2656	A
48	1	2665	U
48	1	2715	A
48	1	2727	A
48	1	2796	G
48	1	2797	C
48	1	2803	A
48	1	2816	G
48	1	2850	G
48	1	2872	A
48	1	2911	A
48	1	2950	G
48	1	3022	G
48	1	3055	U
48	1	3078	U
48	1	3121	U
48	1	3154	C
48	1	3156	U
48	1	3175	U
48	1	3179	U
48	1	3208	G
48	1	3216	G
48	1	3218	A
48	1	3219	G
48	1	3246	G
48	1	3269	U
48	1	3293	U
48	1	3303	G

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Mol	Chain	Res	Type
48	1	3334	U
48	1	3368	U
48	1	3375	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	R	4
48	1	3
40	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	173:UNK	C	188:SER	N	30.28
1	R	105:ARG	C	113:UNK	N	19.44
1	1	1980:C	O3'	2042:G	P	19.07
1	R	529:GLY	C	535:UNK	N	17.02
1	R	123:UNK	C	156:UNK	N	12.97
1	1	440:A	O3'	494:G	P	12.88
1	1	2059:U	O3'	2080:C	P	12.20
1	F	237:LYS	C	238:LEU	N	1.17

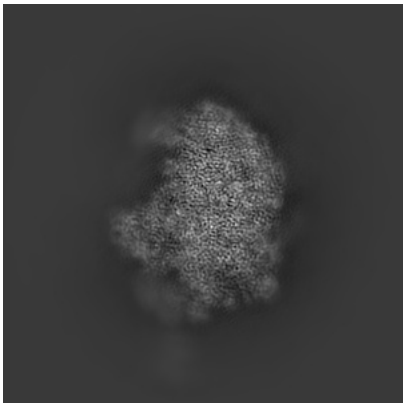
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4752. These allow visual inspection of the internal detail of the map and identification of artifacts.

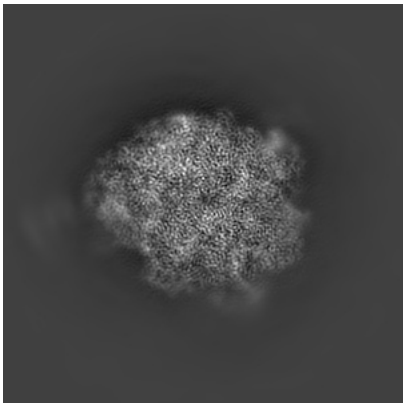
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

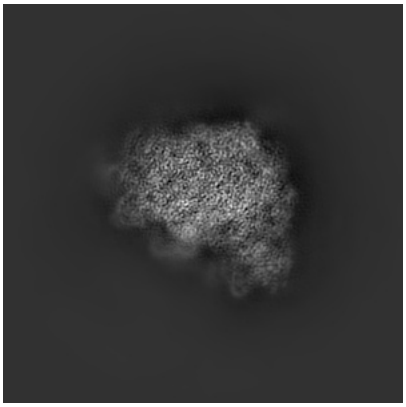
6.1.1 Primary map



X



Y

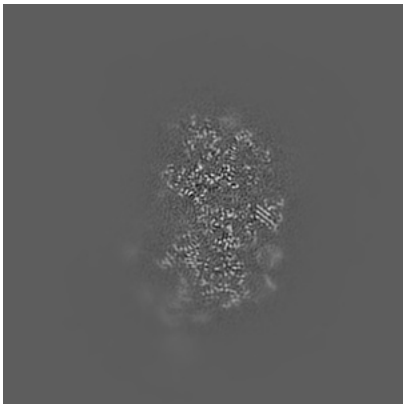


Z

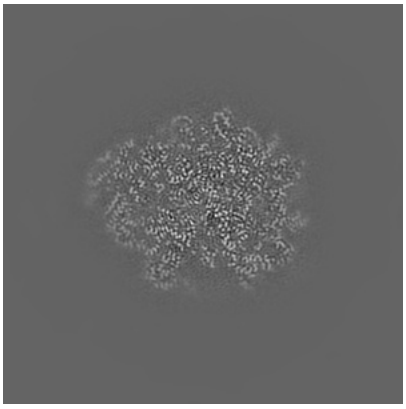
The images above show the map projected in three orthogonal directions.

6.2 Central slices

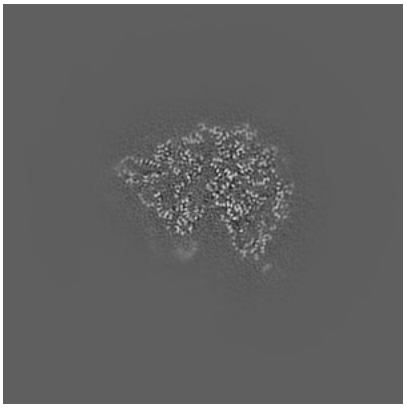
6.2.1 Primary map



X Index: 198



Y Index: 198

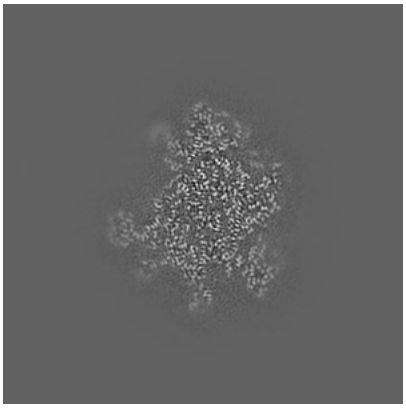


Z Index: 198

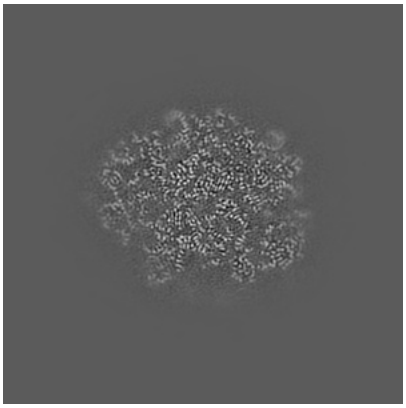
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

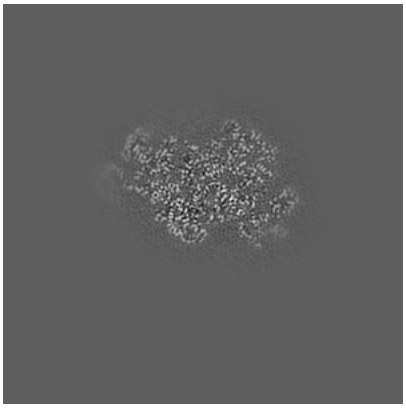
6.3.1 Primary map



X Index: 235



Y Index: 206



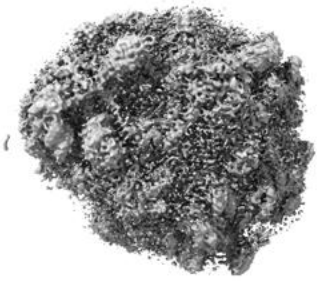
Z Index: 217

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

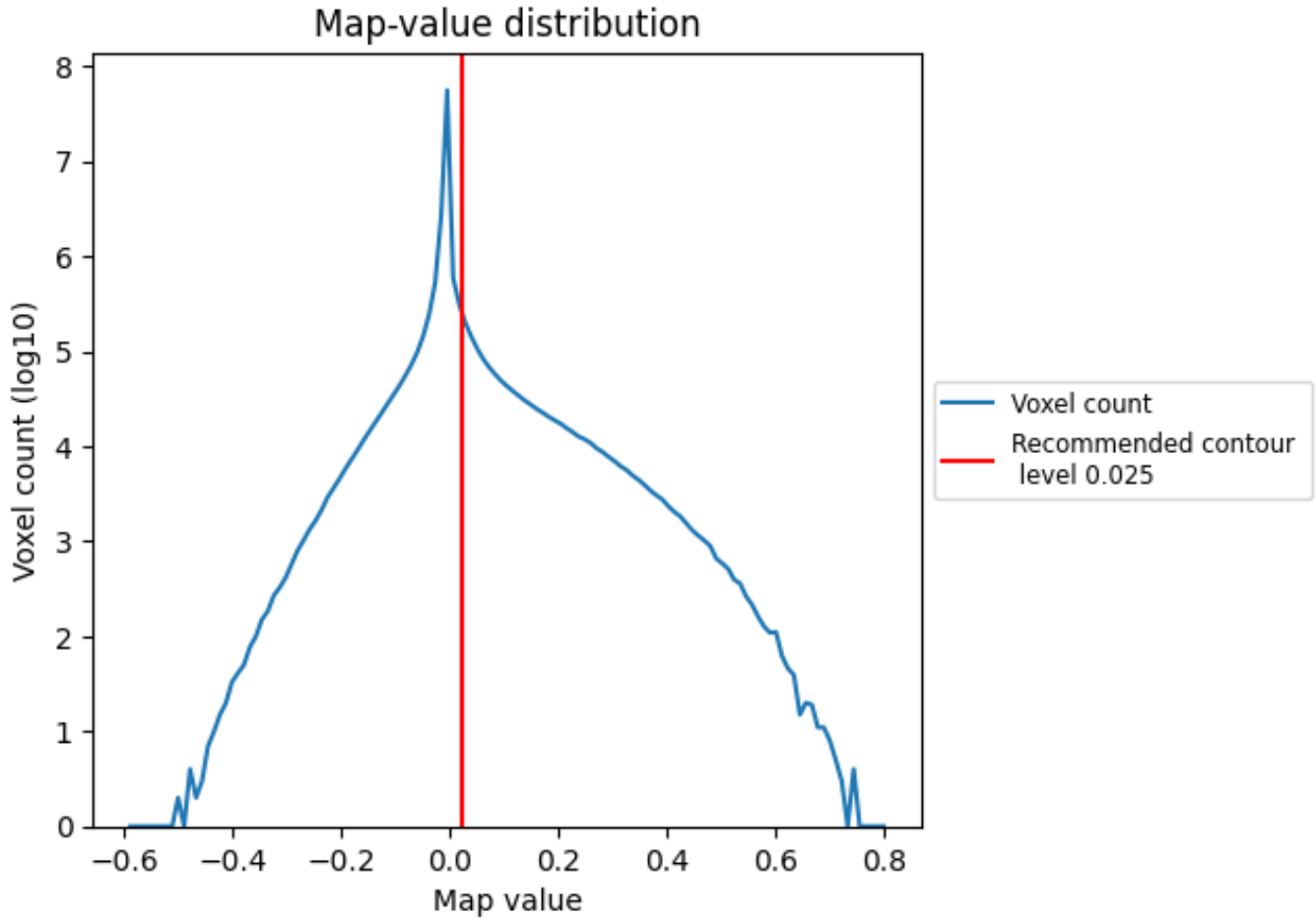
6.5 Mask visualisation (i)

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

7 Map analysis

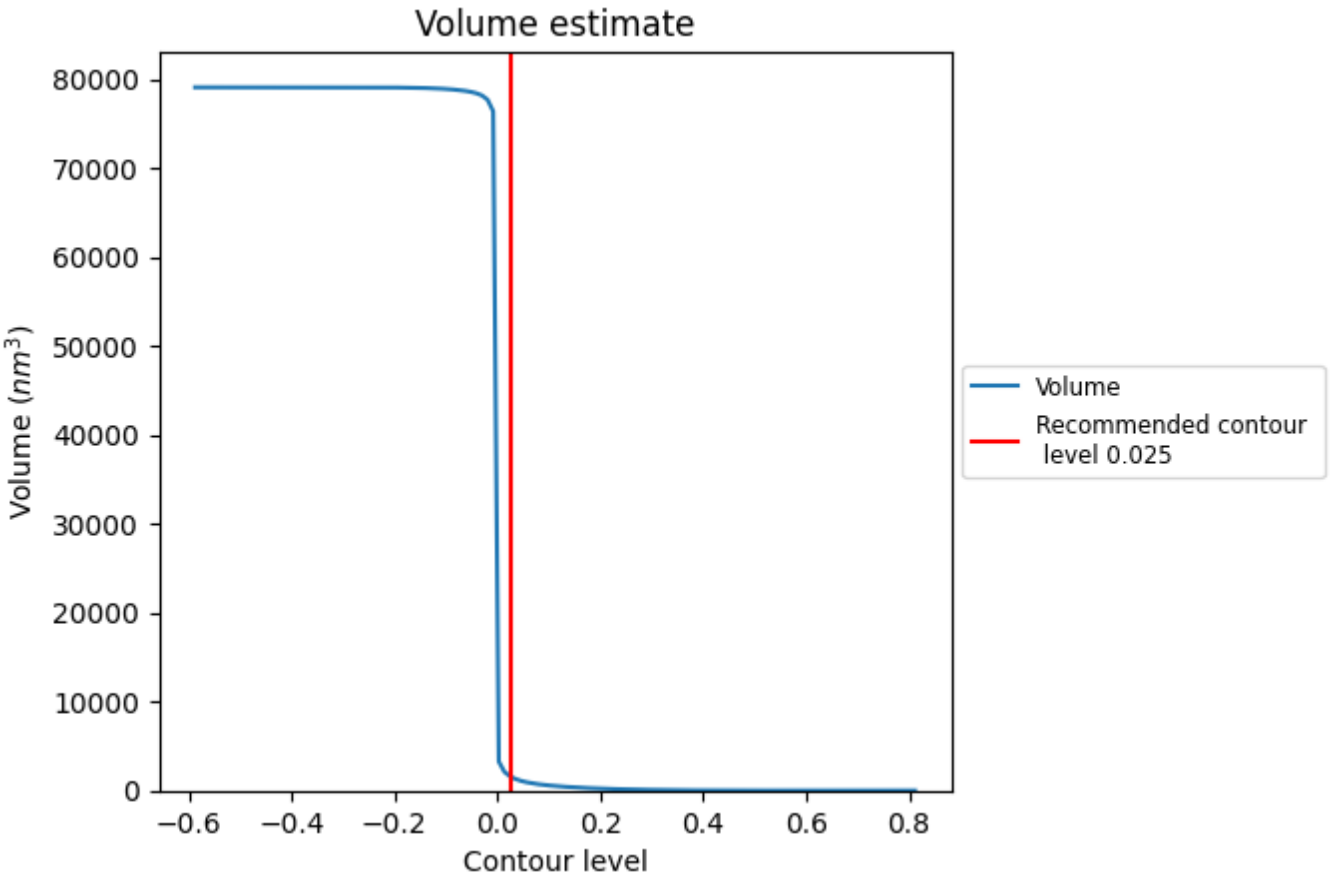
This section contains the results of statistical analysis of the map.

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.

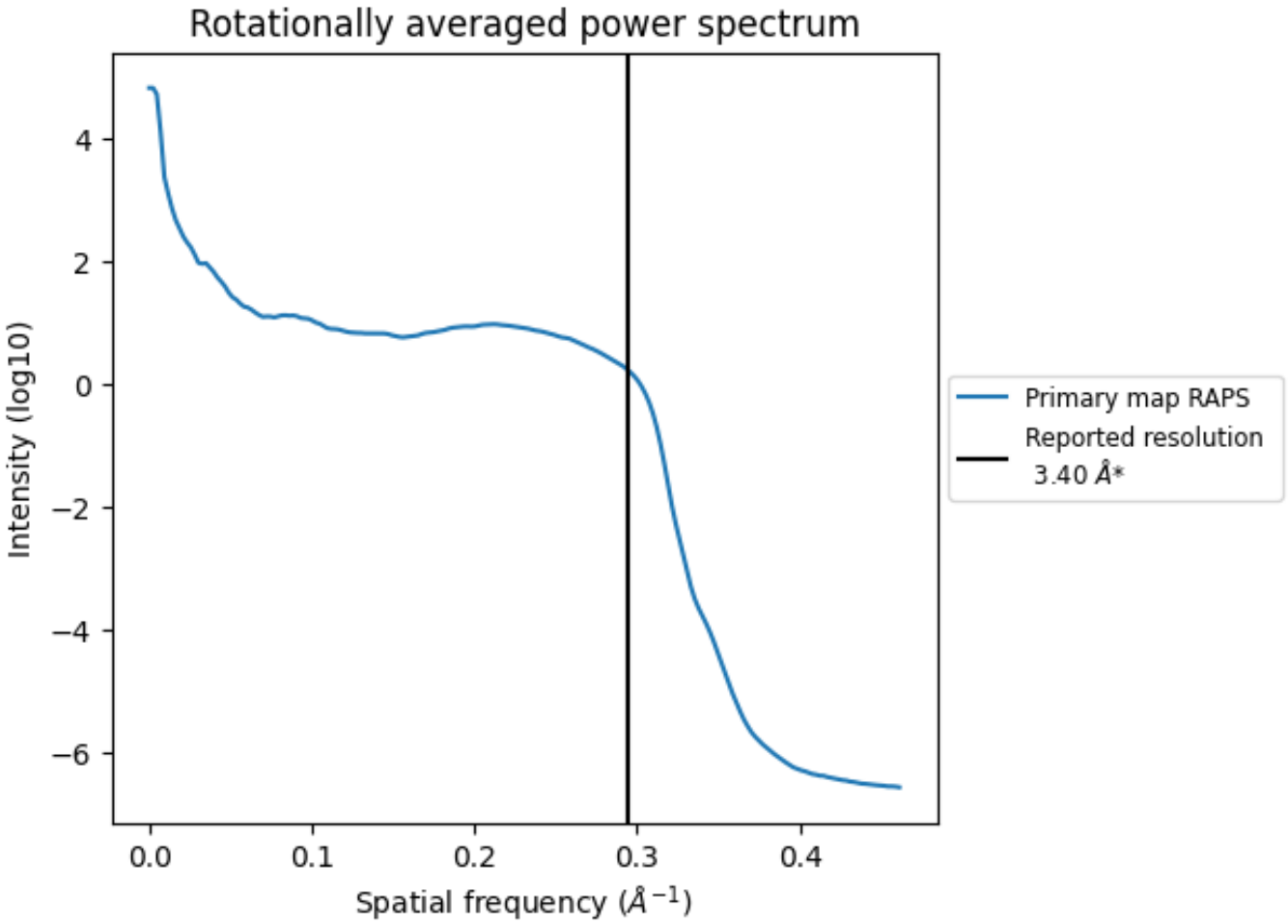
7.2 Volume estimate



The volume at the recommended contour level is 1583 nm^3; this corresponds to an approximate mass of 1430 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 (i)



*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

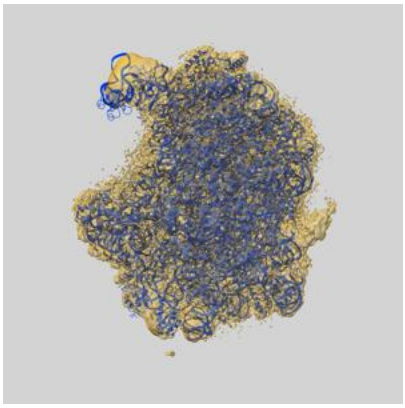
8 Fourier-Shell correlation (i)

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

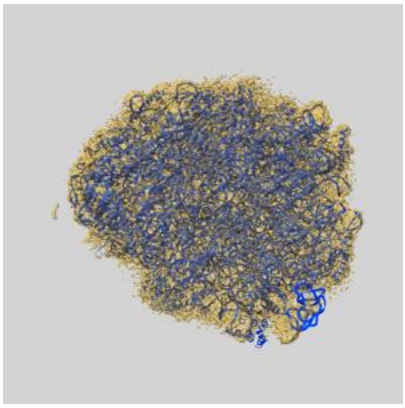
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4752 and PDB model 6R86. Per-residue inclusion information can be found in section 3 on page 13.

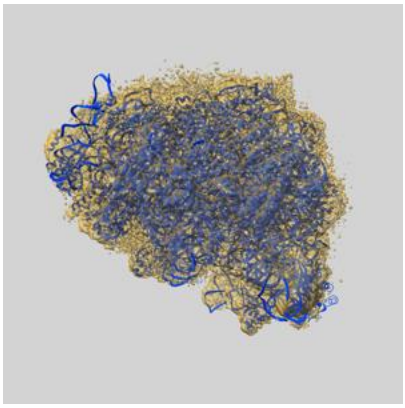
9.1 Map-model overlay



X



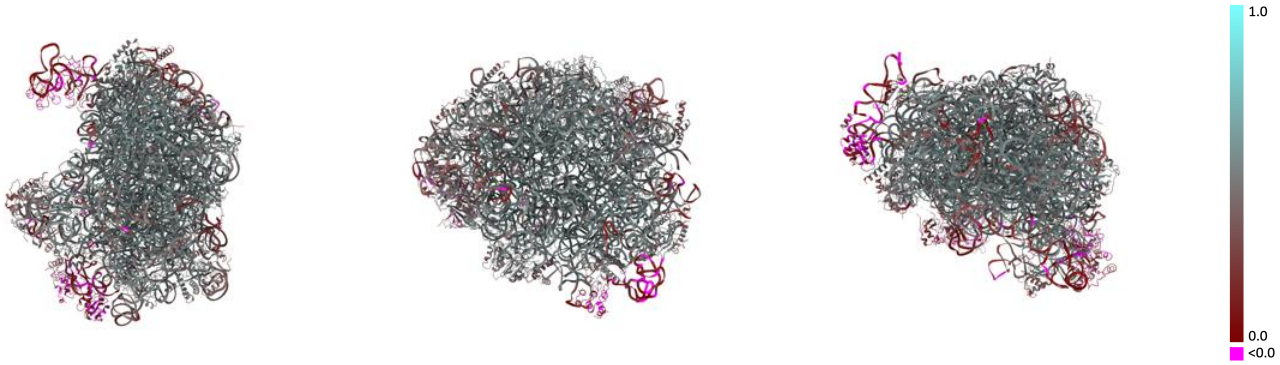
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

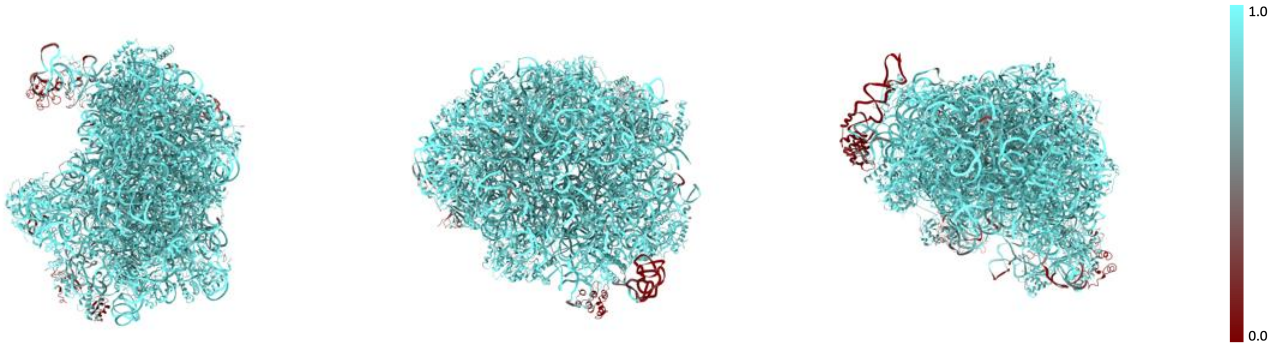
9.2 Q-score mapped to coordinate model (i)



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.

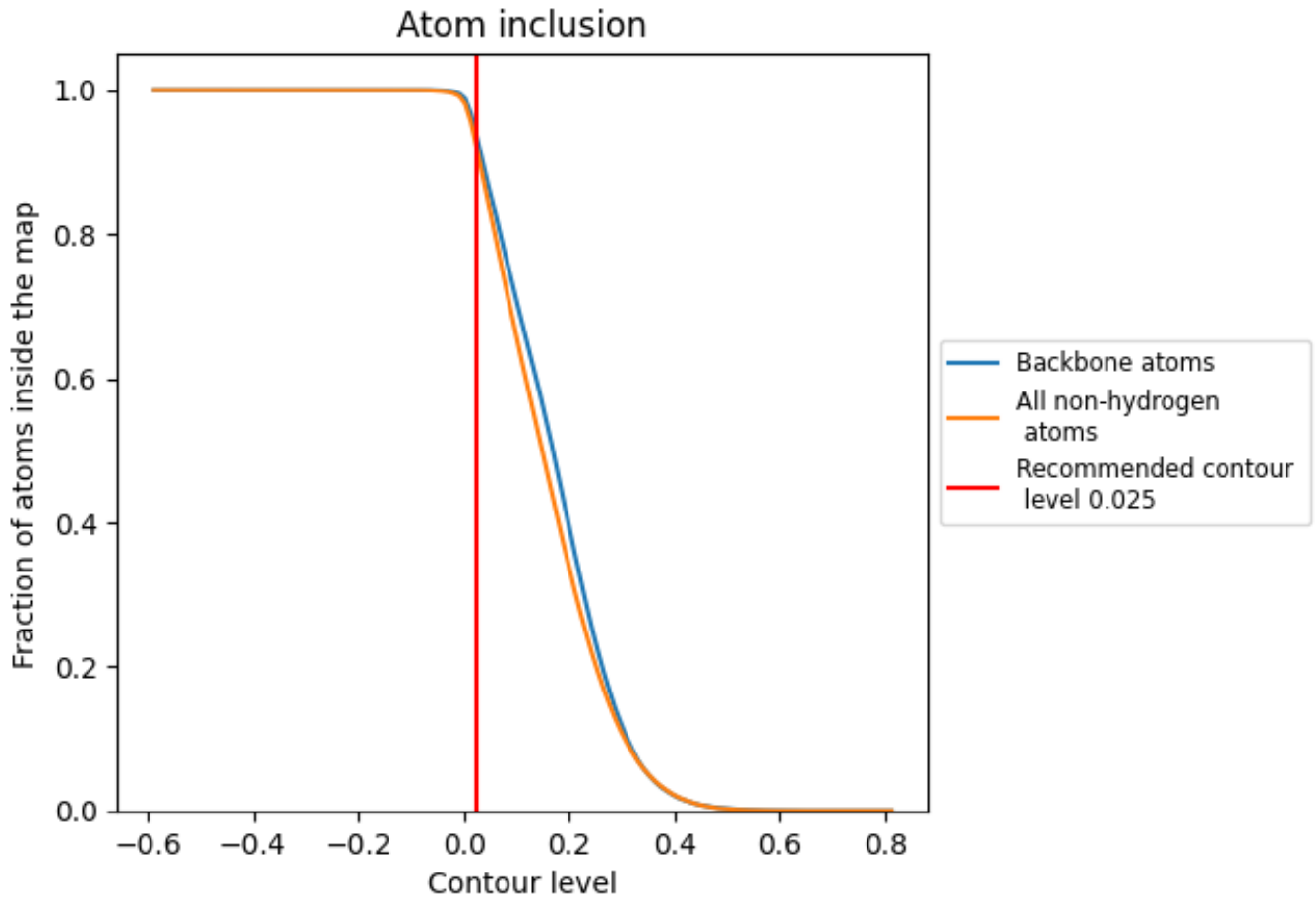
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9177	0.4620
1	0.9431	0.4680
3	0.9845	0.4910
4	0.9746	0.5130
5	0.9208	0.4980
7	0.9154	0.4580
C	0.8563	0.4840
D	0.9223	0.5110
E	0.9326	0.5330
F	0.9438	0.5170
G	0.9404	0.5110
H	0.9066	0.4360
I	0.9110	0.4590
J	0.9403	0.5070
K	0.9182	0.4680
L	0.3866	0.0560
M	0.8700	0.3790
N	0.9361	0.5050
O	0.9230	0.4740
P	0.3664	0.0790
Q	0.9511	0.5190
R	0.6071	0.1760
S	0.9341	0.5090
T	0.9298	0.5060
U	0.9180	0.4900
V	0.9427	0.5100
W	0.9054	0.4440
X	0.9224	0.4450
Y	0.9396	0.5090
Z	0.9437	0.5110
a	0.9255	0.5030
b	0.9244	0.4710
c	0.9562	0.5330
d	0.9181	0.4880
e	0.9042	0.4580

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Chain	Atom inclusion	Q-score
f	0.9071	0.4930
g	0.9437	0.5280
h	0.9464	0.5350
i	0.9166	0.5070
j	0.9236	0.4930
k	0.9235	0.4740
l	0.9588	0.5480
m	0.9098	0.4610
n	0.9590	0.5320
o	0.4268	0.1660
p	0.9572	0.5540
r	0.6381	0.0610
s	0.8921	0.4590
x	0.9408	0.5320