Full wwPDB EM Validation Report (i)

Nov 7, 2022 – 05:20 AM EST

PDB ID : 6N8L
EMDB ID : EMD-0371
Title : Cryo-EM structure of early cytoplasmic-late (ECL) pre-60S ribosomal subunit
Authors : Zhou, Y.; Musalgaonkar, S.; Johnson, A.W.; Taylor, D.W.
Deposited on : 2018-11-29
Resolution : 3.60 Å(reported)
Based on initial model : 3JCT

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

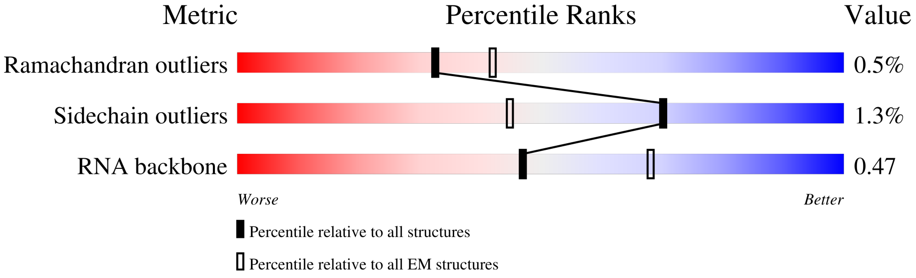
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance ⓘ

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

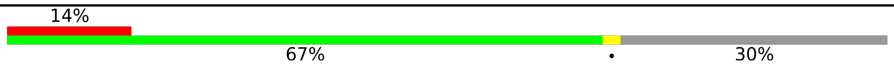
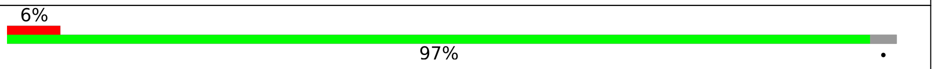
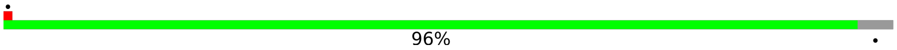
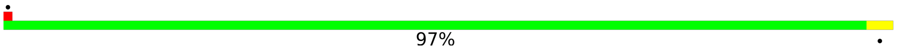
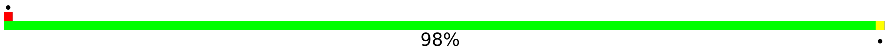
The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	v	518	
2	s	217	
3	A	254	
4	a	149	
5	B	387	
6	b	647	
7	C	362	
8	c	105	

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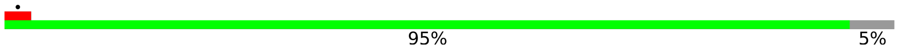
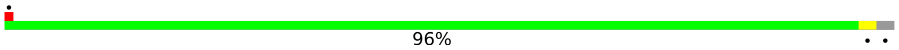
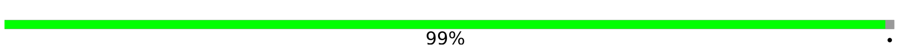
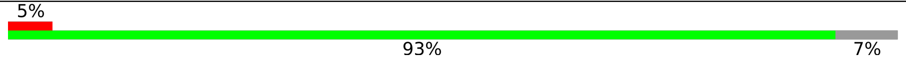
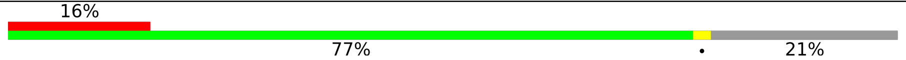
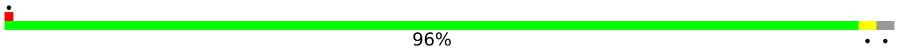
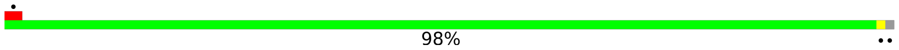
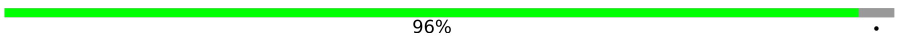
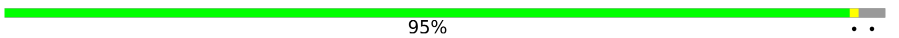
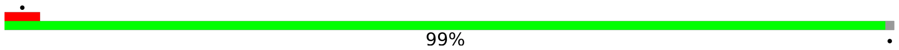
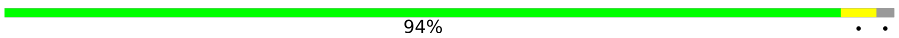
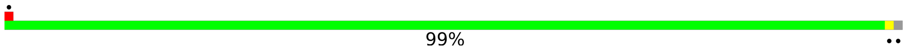
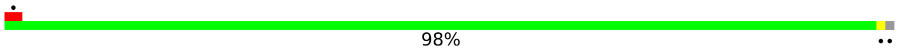
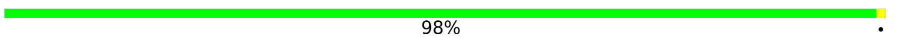
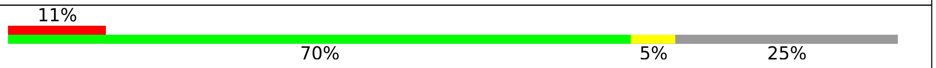
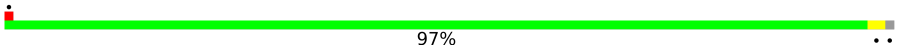
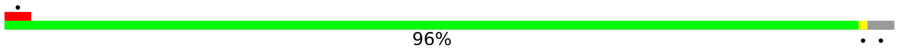
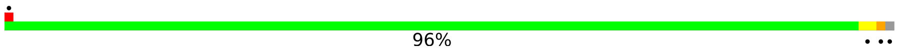
Mol	Chain	Length	Quality of chain
9	d	113	
10	E	176	
11	e	130	
12	F	244	
13	f	107	
14	G	256	
15	g	121	
16	I	166	
17	H	191	
18	h	120	
19	i	100	
20	j	88	
21	k	78	
22	L	199	
23	l	51	
24	M	138	
25	p	92	
26	N	204	
27	u	199	
28	O	199	
29	P	184	
30	Q	186	
31	R	189	
32	S	172	
33	T	160	

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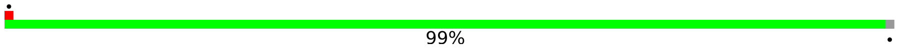
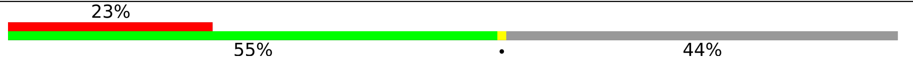
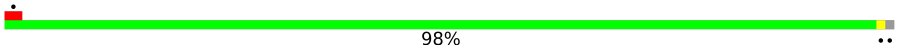
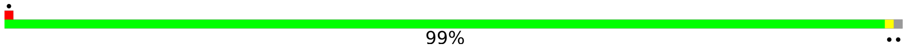
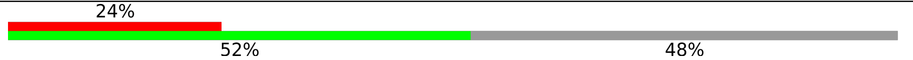
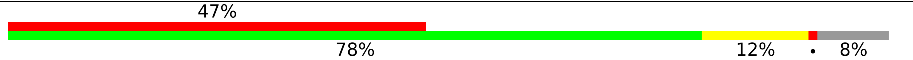
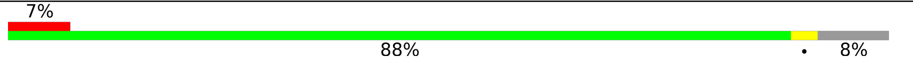
Mol	Chain	Length	Quality of chain
34	U	121	
35	V	137	
36	W	236	
37	X	142	
38	Y	127	
39	y	245	
40	Z	136	
41	z	106	
42	D	297	
43	J	174	
44	q	106	
45	o	59	
46	1	3396	
47	2	121	
48	3	158	

2 Entry composition (i)

There are 48 unique types of molecules in this entry. The entry contains 129926 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 60S ribosomal export protein NMD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	v	362	2783	1770	472	522	19	0	0

- Molecule 2 is a protein called Ribosomal Protein uL1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	s	210	1050	630	210	210	0	0

- Molecule 3 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	245	1863	1162	376	324	1	0	0

- Molecule 4 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	a	94	742	484	131	126	1	0	0

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	386	3081	1956	584	533	8	0	0

- Molecule 6 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	b	248	1989	1222	372	387	8	0	0

- Molecule 7 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	361	2749	1730	522	494	3	0	0

- Molecule 8 is a protein called 60S ribosomal protein L30.

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

- Molecule 9 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	d	107	873	553	165	154	1	0	0

- Molecule 10 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	E	160	1270	818	229	222	1	0	0

- Molecule 11 is a protein called 60S ribosomal protein L32.

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

- Molecule 12 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 13 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 14 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	230	Total 1798	C 1149	N 323	O 323	S 3	0	0

- Molecule 15 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	112	Total 881	C 546	N 179	O 152	S 4	0	0

- Molecule 16 is a protein called Bud site selection protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	131	Total 1056	C 660	N 195	O 198	S 3	0	0

- Molecule 17 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	188	Total 1493	C 948	N 271	O 270	S 4	0	0

- Molecule 18 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 19 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	i	96	Total 743	C 465	N 148	O 128	S 2	0	0

- Molecule 20 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	j	85	Total 670	C 408	N 146	O 111	S 5	0	0

- Molecule 21 is a protein called 60S ribosomal protein L38.

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

- Molecule 22 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	L	187	1491	929	306	256	0	0

- Molecule 23 is a protein called 60S ribosomal protein L39.

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

- Molecule 24 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	M	137	1059	678	200	179	2	0	0

- Molecule 25 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 26 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 27 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	u	149	1256	788	252	207	9	0	0

- Molecule 28 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 29 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	P	178	1409	876	281	252	0	0

- Molecule 30 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Q	154	1191	753	231	205	2	0	0

- Molecule 31 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	R	154	1241	772	262	207	0	0

- Molecule 32 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	S	170	1425	916	265	241	3	0	0

- Molecule 33 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	T	61	476	295	95	85	1	0	0

- Molecule 34 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	U	104	826	535	136	155	0	0

- Molecule 35 is a protein called 60S ribosomal protein L23-A.

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

- Molecule 36 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	W	133	1053	660	177	214	2	0	0

- Molecule 37 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	X	120	959	617	168	172	2	0	0

- Molecule 38 is a protein called 60S ribosomal protein L26-A.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	y	225	1698	1054	295	343	6	0	0

- Molecule 40 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 41 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
41	z	55	444	273	88	83	0	0

- Molecule 42 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	D	251	1983	1253	353	375	2	0	0

- Molecule 43 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	J	164	1304	816	243	242	3	0	0

- Molecule 44 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	q	97	783	493	158	127	5	0	0

- Molecule 45 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
45	o	54	433	271	94	68	0	0

- Molecule 46 is a RNA chain called Saccharomyces cerevisiae S288C 35S pre-ribosomal RNA (RDN37-1), miscRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
46	1	3201	68471	30584	12345	22341	3201	0	0

- Molecule 47 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
47	2	121	2579	1152	461	845	121	0	0

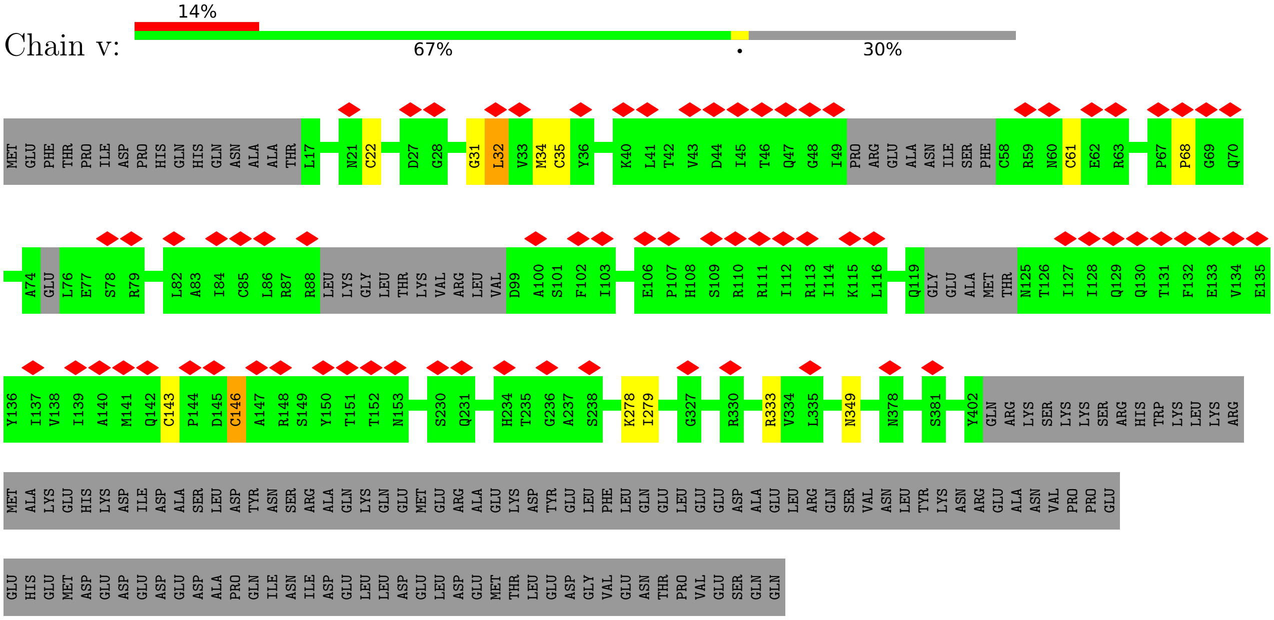
- Molecule 48 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
48	3	157	3333	1491	584	1101	157	0	0

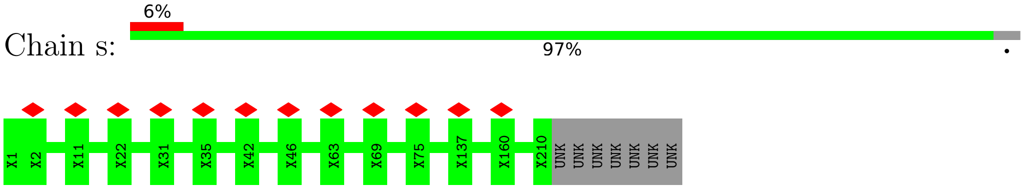
3 Residue-property plots ⓘ

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

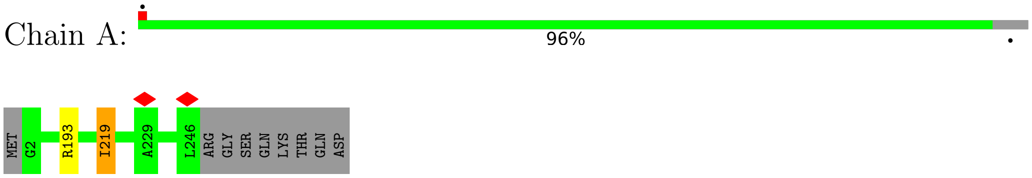
- Molecule 1: 60S ribosomal export protein NMD3



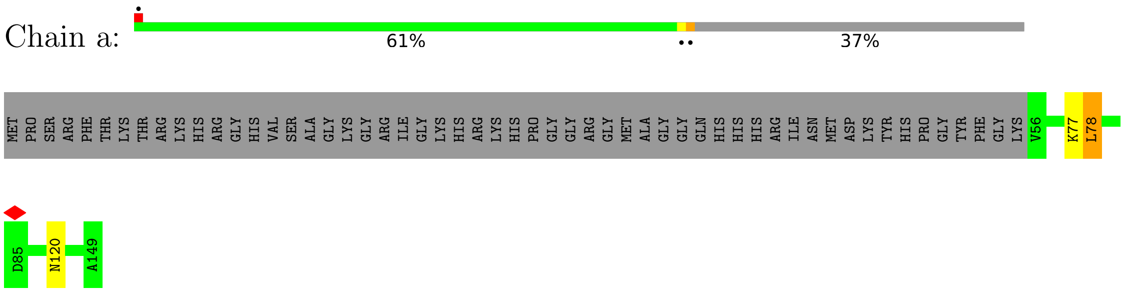
- Molecule 2: Ribosomal Protein uL1



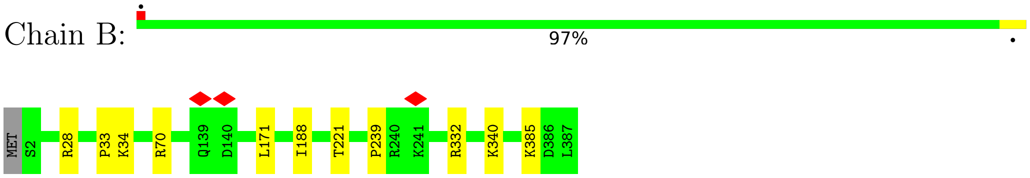
- Molecule 3: 60S ribosomal protein L2-A



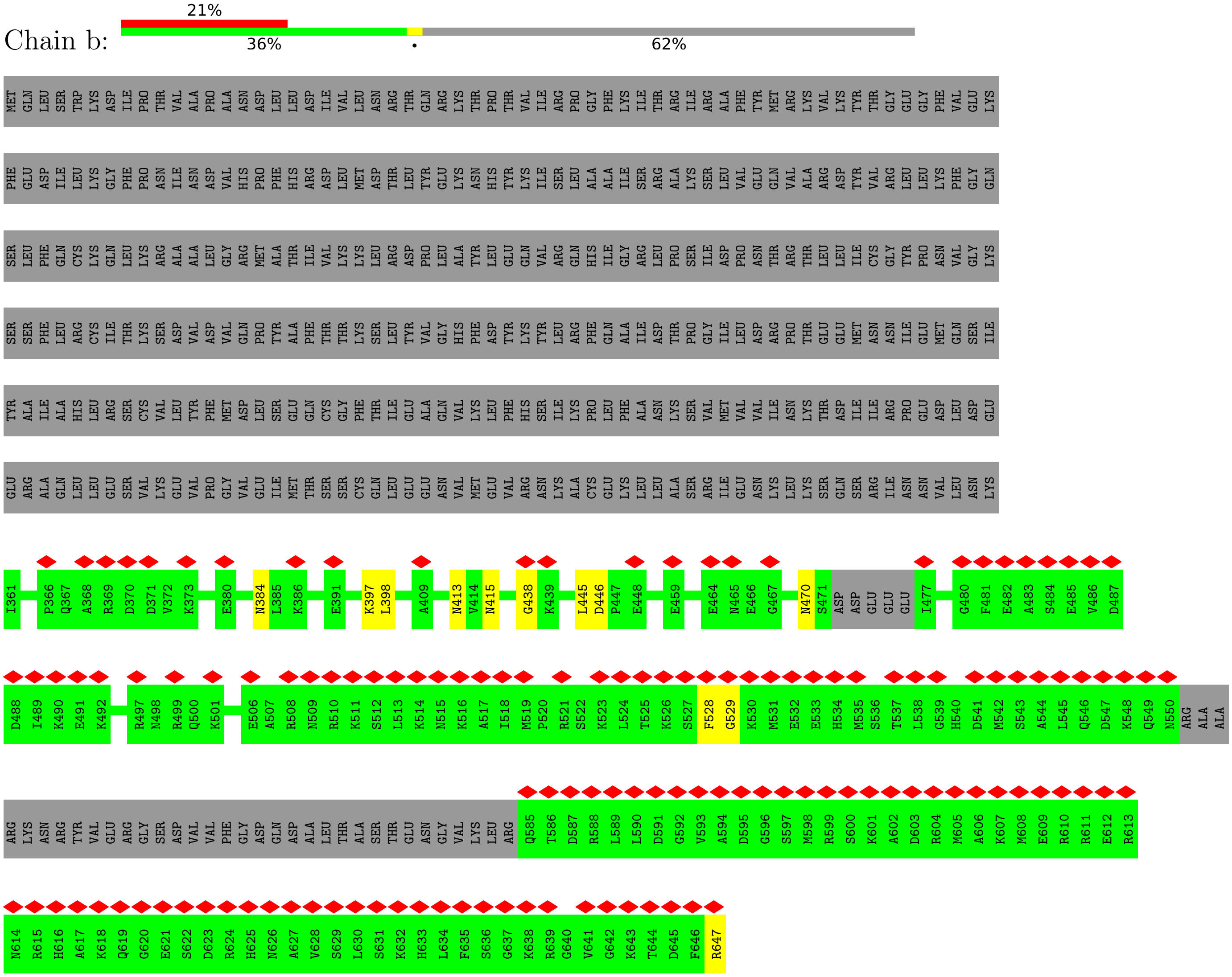
- Molecule 4: 60S ribosomal protein L28



- Molecule 5: 60S ribosomal protein L3

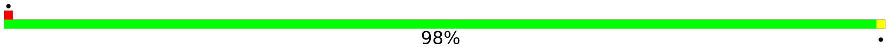


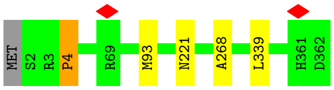
- Molecule 6: Nucleolar GTP-binding protein 1



- Molecule 7: 60S ribosomal protein L4-A

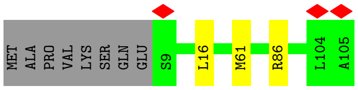
Chain C:





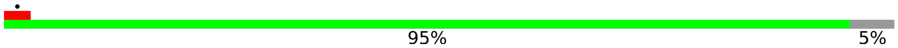
- Molecule 8: 60S ribosomal protein L30

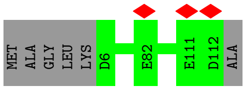
Chain c:



- Molecule 9: 60S ribosomal protein L31-A

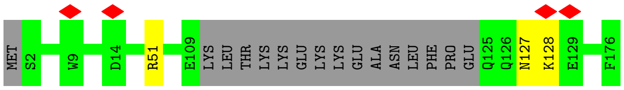
Chain d:





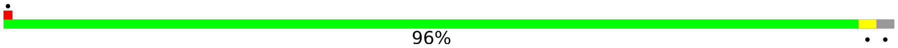
- Molecule 10: 60S ribosomal protein L6-A

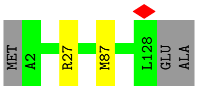
Chain E:



- Molecule 11: 60S ribosomal protein L32

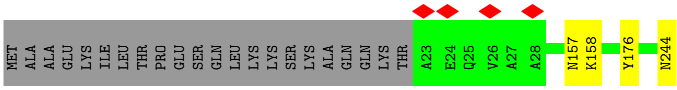
Chain e:





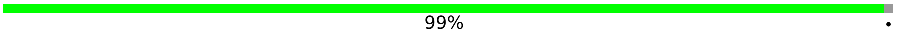
- Molecule 12: 60S ribosomal protein L7-A

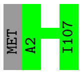
Chain F:



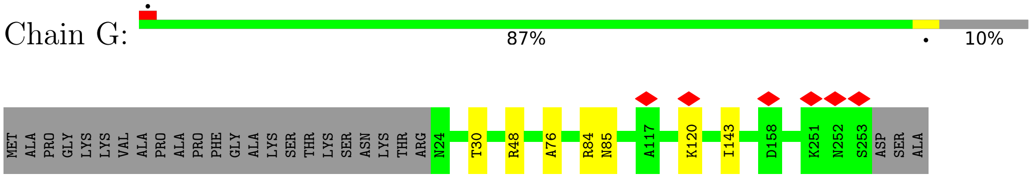
- Molecule 13: 60S ribosomal protein L33-A

Chain f:

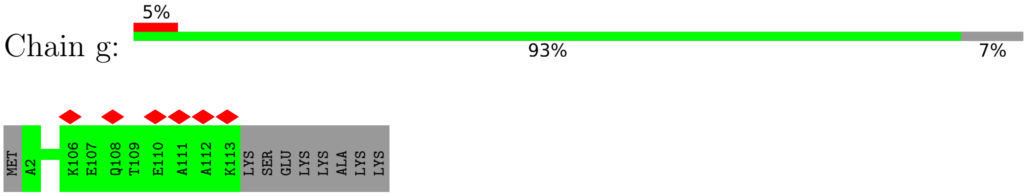




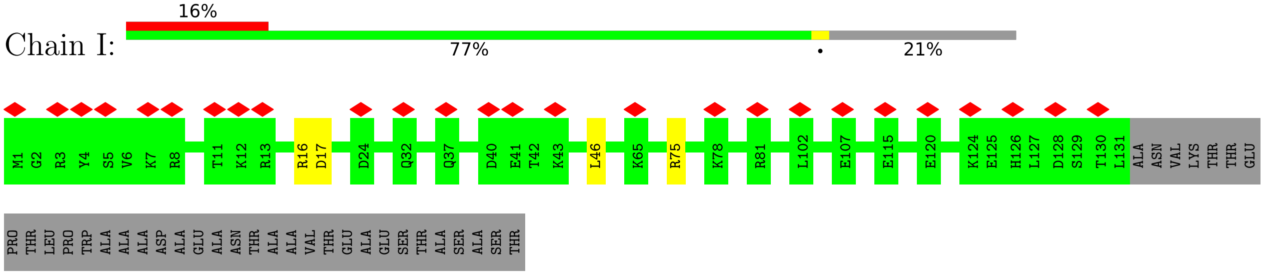
- Molecule 14: 60S ribosomal protein L8-A



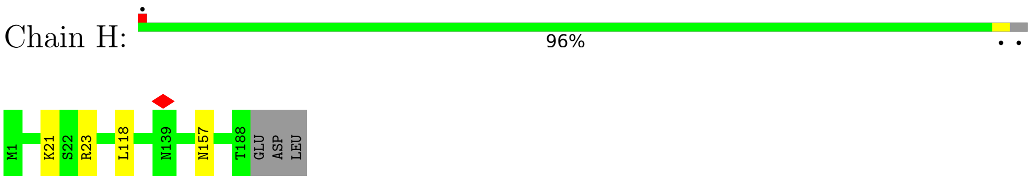
- Molecule 15: 60S ribosomal protein L34-A



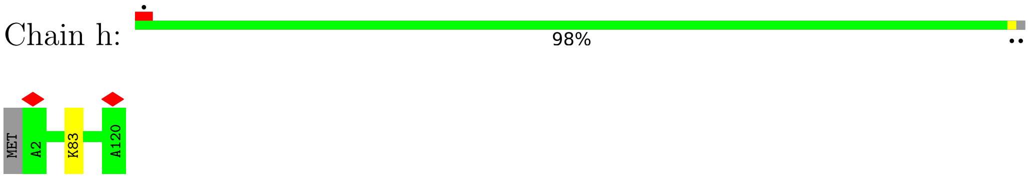
- Molecule 16: Bud site selection protein 20



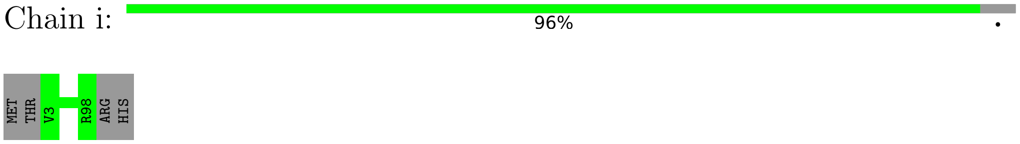
- Molecule 17: 60S ribosomal protein L9-A



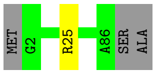
- Molecule 18: 60S ribosomal protein L35-A



- Molecule 19: 60S ribosomal protein L36-A

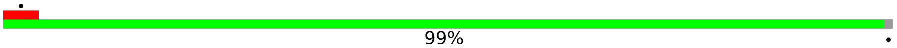


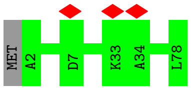
- Molecule 20: 60S ribosomal protein L37-A



- Molecule 21: 60S ribosomal protein L38

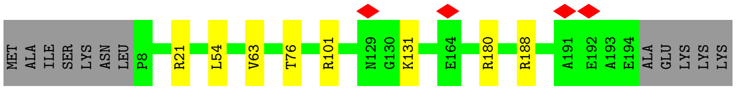
Chain k:





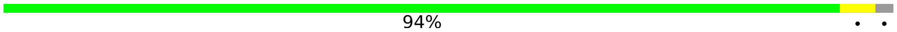
- Molecule 22: 60S ribosomal protein L13-A

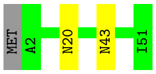
Chain L:



- Molecule 23: 60S ribosomal protein L39

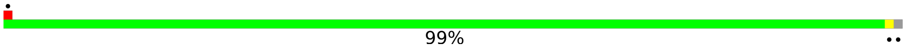
Chain l:

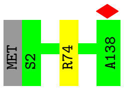




- Molecule 24: 60S ribosomal protein L14-A

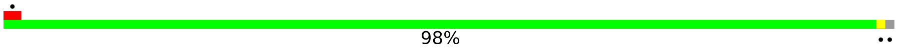
Chain M:

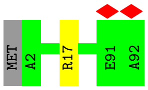




- Molecule 25: 60S ribosomal protein L43-A

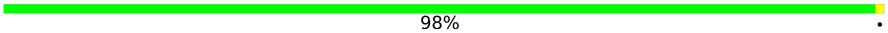
Chain p:

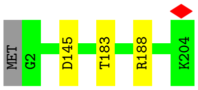




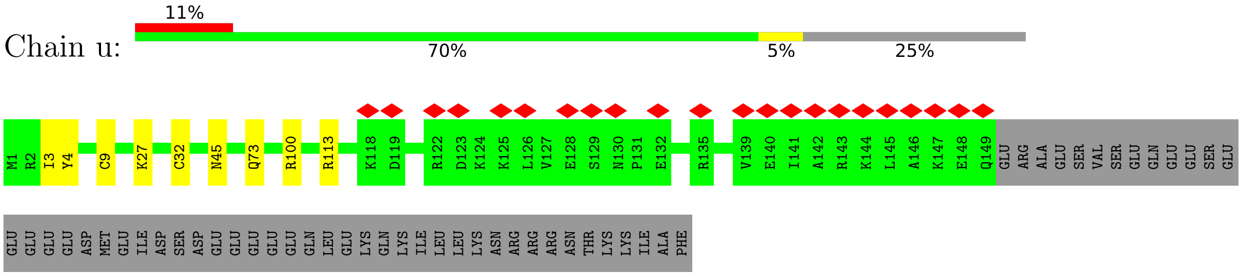
- Molecule 26: 60S ribosomal protein L15-A

Chain N:

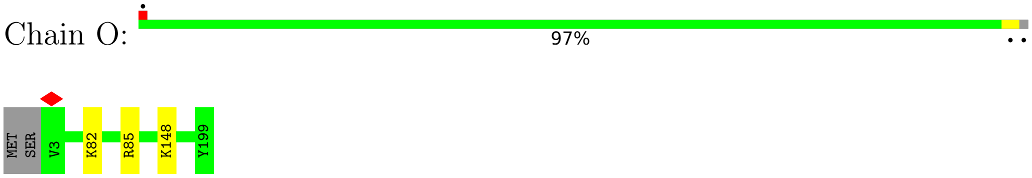




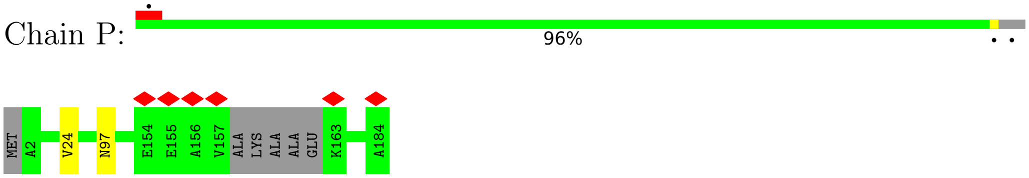
- Molecule 27: Ribosome biogenesis protein RLP24



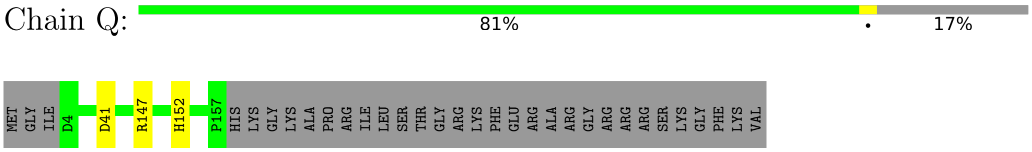
- Molecule 28: 60S ribosomal protein L16-A



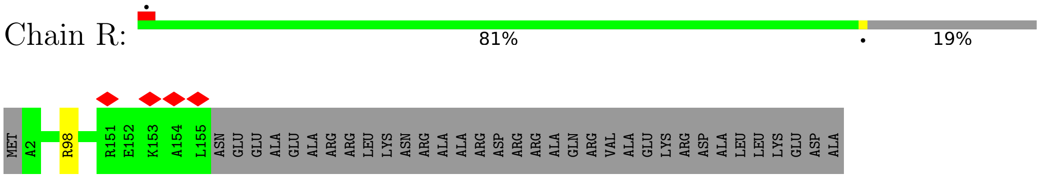
- Molecule 29: 60S ribosomal protein L17-A



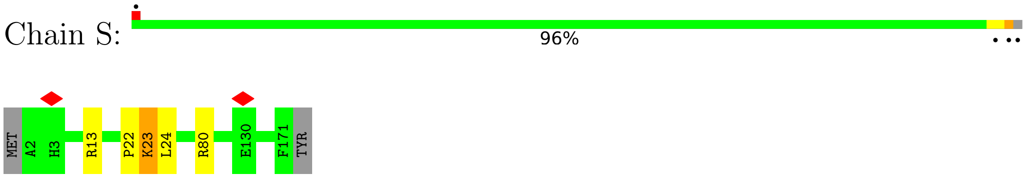
- Molecule 30: 60S ribosomal protein L18-A



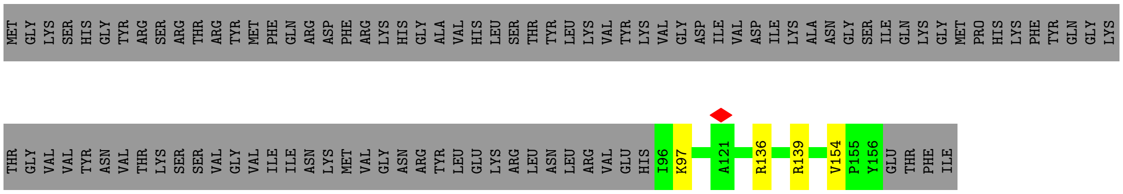
- Molecule 31: 60S ribosomal protein L19-A



- Molecule 32: 60S ribosomal protein L20-A

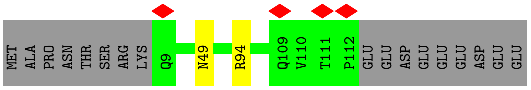


- Molecule 33: 60S ribosomal protein L21-A



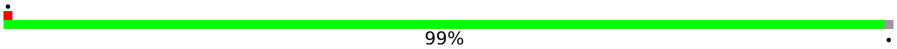
- Molecule 34: 60S ribosomal protein L22-A

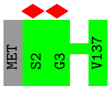
Chain U:



- Molecule 35: 60S ribosomal protein L23-A

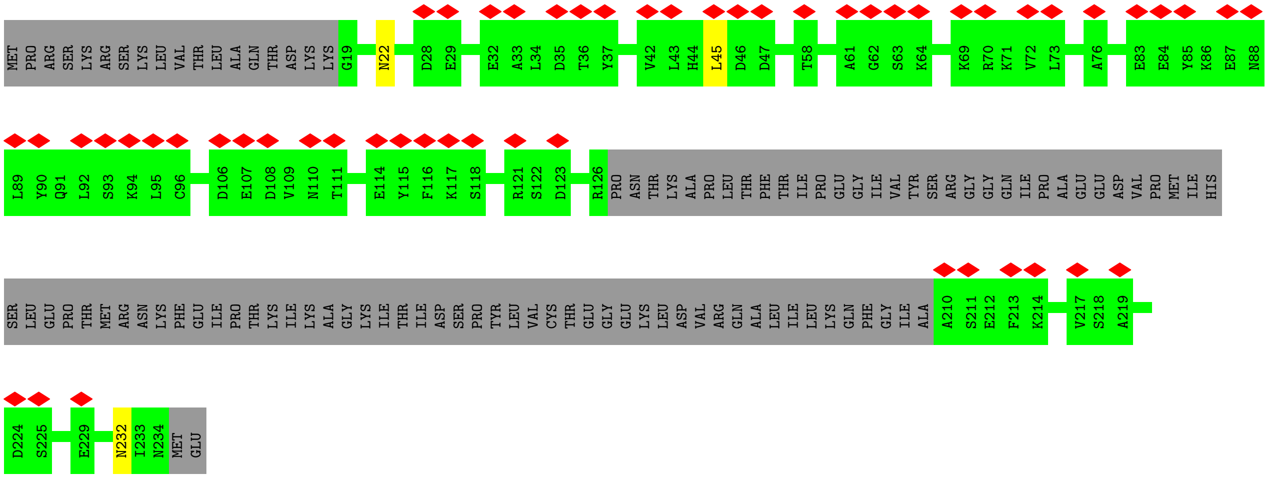
Chain V:





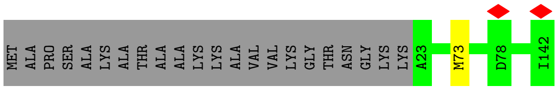
- Molecule 36: Ribosome assembly factor MRT4

Chain W:



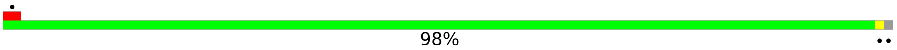
- Molecule 37: 60S ribosomal protein L25

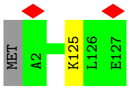
Chain X:



- Molecule 38: 60S ribosomal protein L26-A

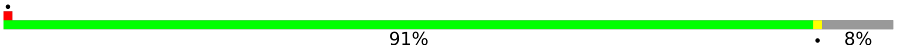
Chain Y:

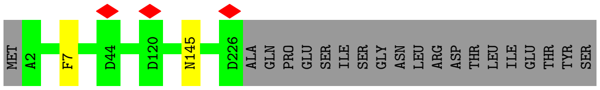




- Molecule 39: Eukaryotic translation initiation factor 6

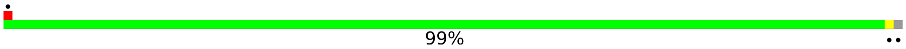
Chain y:

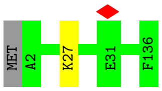




- Molecule 40: 60S ribosomal protein L27-A

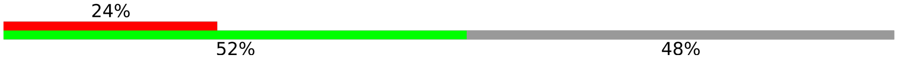
Chain Z:

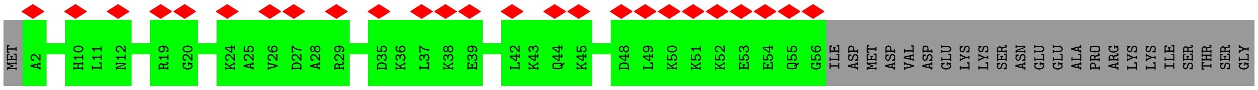




- Molecule 41: UPF0642 protein YBL028C

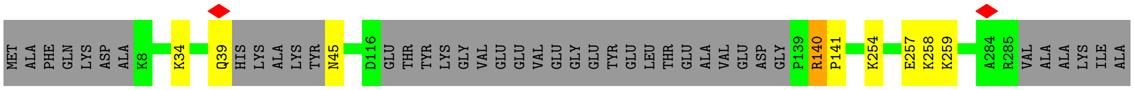
Chain z:

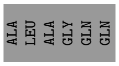




- Molecule 42: 60S ribosomal protein L5

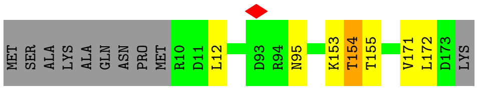
Chain D:





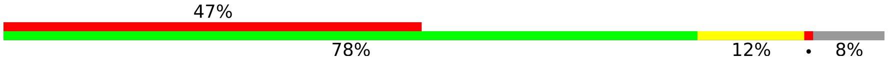
- Molecule 43: 60S ribosomal protein L11-A

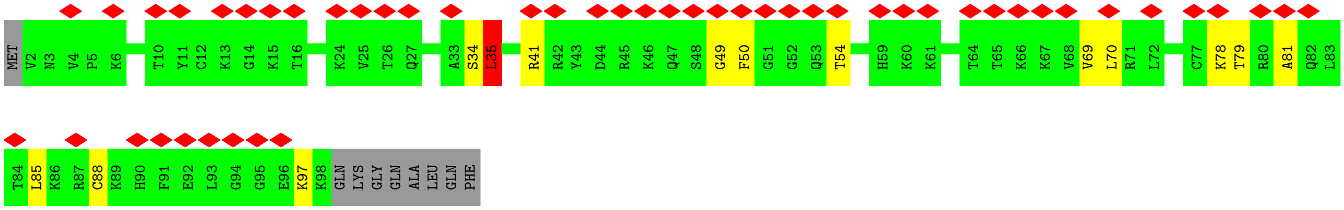
Chain J:



- Molecule 44: 60S ribosomal protein L42-A

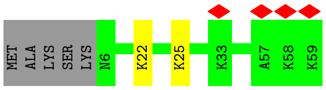
Chain q:





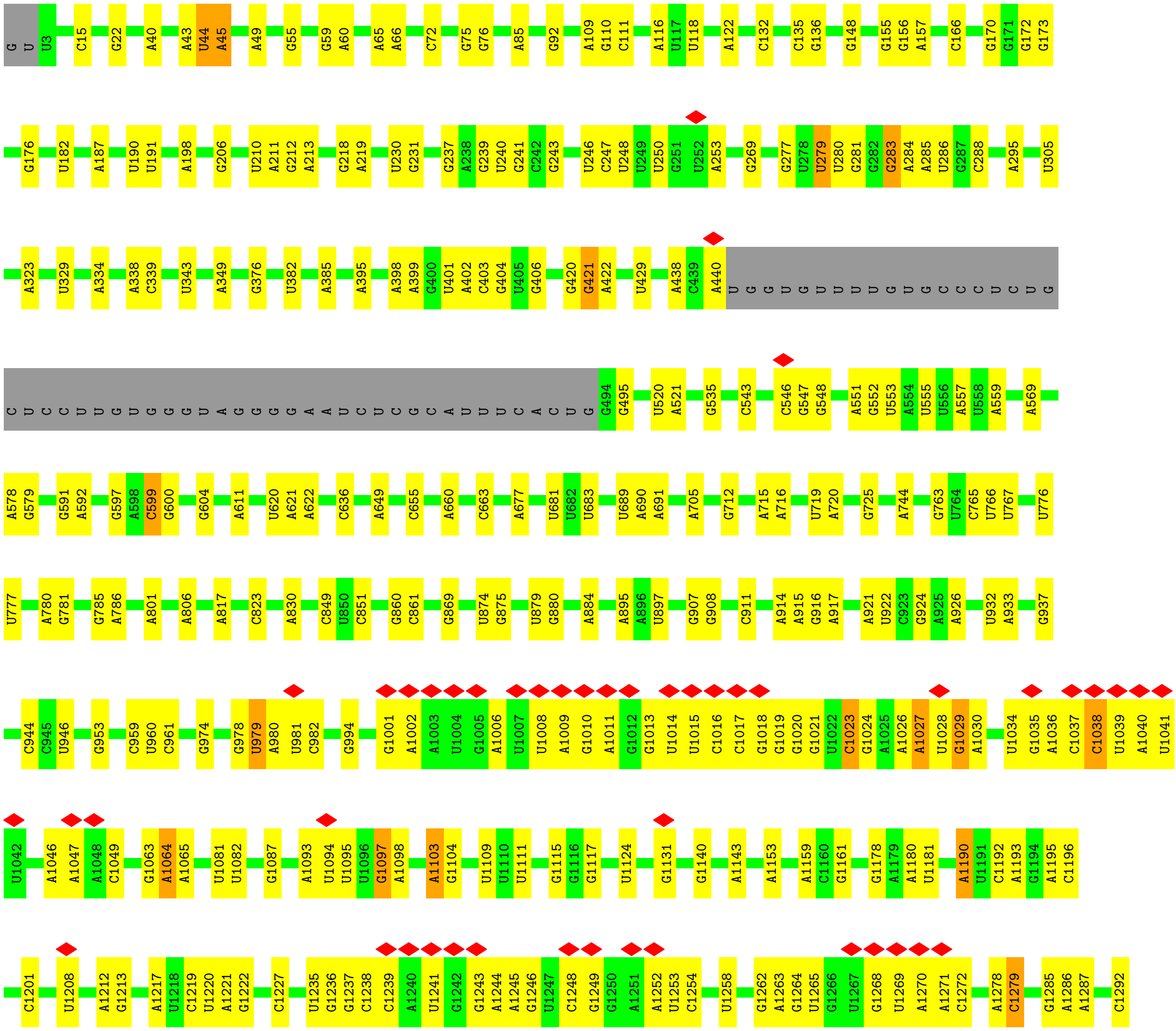
- Molecule 45: 60S ribosomal protein L29

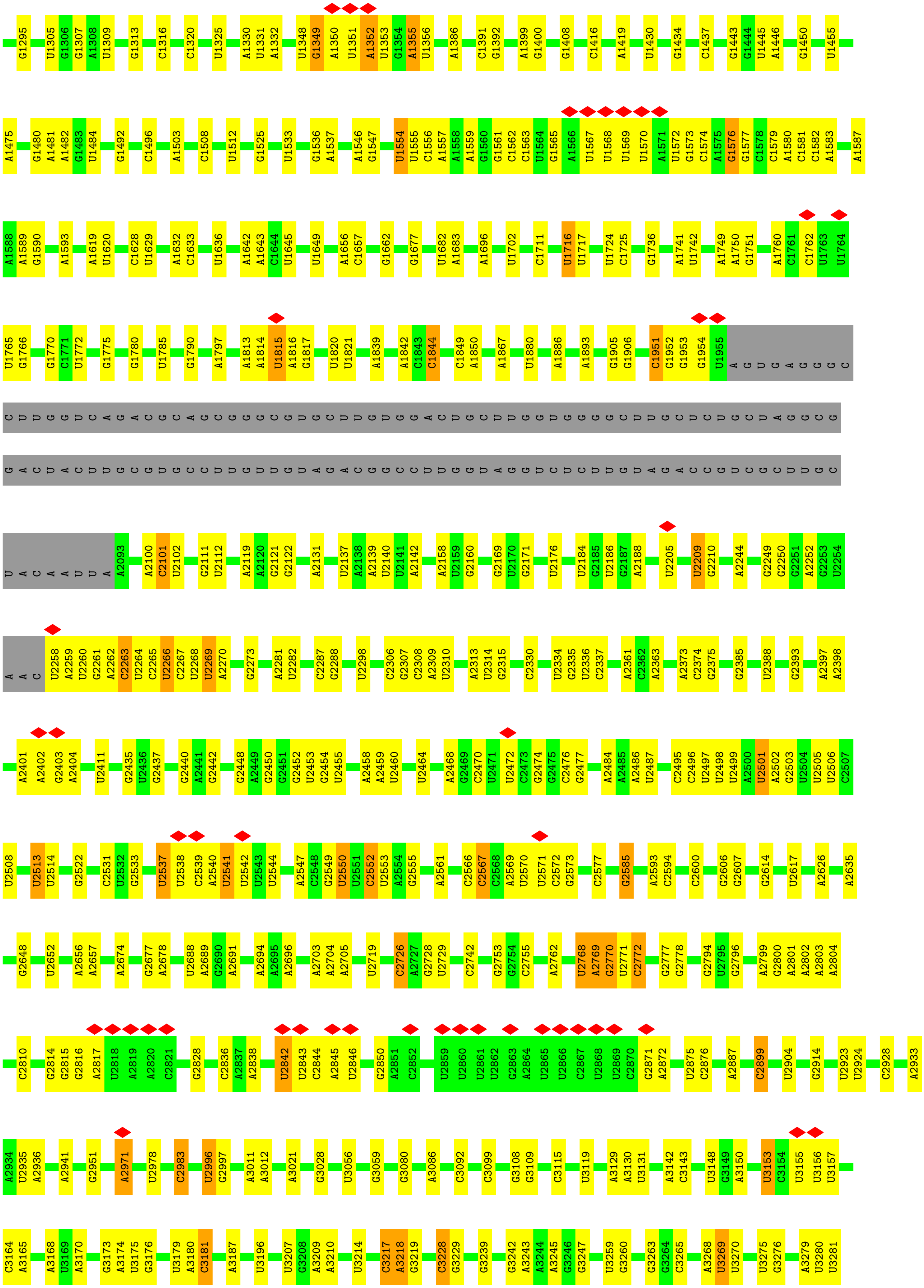
Chain o:



- Molecule 46: Saccharomyces cerevisiae S288C 35S pre-ribosomal RNA (RDN37-1), miscRNA

Chain 1:

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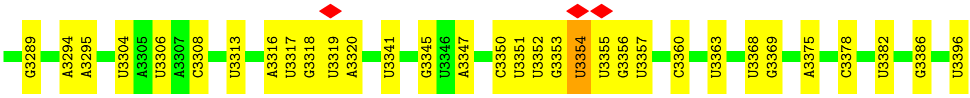
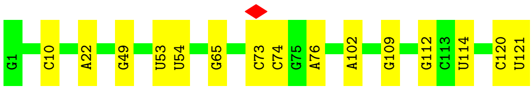
G A C U A C U U G C G U G C C U U G U U G U A G A C G G C C U U G G U A G G U C U C U U G U A G A C C G U C G C U U G C
U A C A A U U A A2093 A2100 C2101 U2102 G2111 U2112 A2119 A2120 G2121 G2122 A2131 U2137 A2138 A2139 U2140 U2141 A2142 A2158 U2159 G2160 G2169 U2170 G2171 U2176 U2184 G2185 U2186 G2187 A2188 U2205 U2209 G2210 A2244 G2249 G2250 G2251 A2252 G2253 U2254
A A C U2258 A2259 U2260 G2261 A2262 C2263 U2264 C2265 U2266 C2267 U2268 U2269 A2270 G2273 A2281 U2282 C2287 G2288 U2298 C2306 G2307 C2308 A2309 U2310 A2313 U2314 G2315 C2330 U2334 G2335 U2336 C2337 A2361 C2362 A2363 A2373 C2374 G2375 G2385 U2388 G2393 A2397 A2398
A2401 A2402 G2403 A2404 U2411 G2435 U2436 G2437 G2440 A2441 G2442 G2448 A2449 G2450 G2451 C2452 U2453 G2454 U2455 A2458 A2459 U2460 U2464 A2468 G2469 C2470 U2471 U2472 C2473 G2474 G2475 C2476 G2477 A2484 A2485 A2486 U2487 C2495 C2496 U2497 U2498 U2499 A2500 U2501 A2502 G2503 U2504 U2505 U2506 C2507
U2508 U2513 U2514 G2522 C2531 U2532 G2533 U2537 U2538 C2539 A2540 U2541 U2542 U2543 U2544 A2547 C2548 G2549 U2550 U2551 C2552 U2553 A2554 G2555 A2561 C2566 C2567 C2568 A2569 U2570 U2571 C2572 G2573 C2577 G2585 A2593 C2594 C2600 G2606 G2607 G2614 U2617 A2626 A2635
G2648 U2652 A2656 G2657 A2674 G2677 A2678 U2688 A2689 G2690 U2691 A2694 A2695 A2696 A2703 A2704 A2705 U2719 C2726 A2727 G2728 U2729 C2742 G2753 G2754 C2755 A2762 U2768 A2769 G2770 U2771 C2772 G2777 G2778 G2794 U2795 G2796 A2799 G2800 A2801 A2802 A2803 A2804
C2810 G2814 G2815 G2816 A2817 U2818 A2819 A2820 C2821 G2828 C2836 A2837 A2838 U2842 U2843 C2844 A2845 U2846 G2850 A2851 C2852 U2859 U2860 U2861 U2862 G2863 A2864 U2865 U2866 C2867 U2868 U2869 C2870 G2871 A2872 U2875 C2876 A2887 C2899 U2904 G2914 U2923 U2924 C2928 A2933
A2934 U2935 A2936 A2941 G2951 A2971 U2978 C2983 U2996 G2997 A3011 A3012 A3021 G3028 U3056 G3059 G3080 A3086 C3092 C3099 G3108 G3109 C3115 U3119 A3129 A3130 U3131 A3142 C3143 U3148 G3149 A3150 U3153 C3154 U3155 U3156 U3157
C3164 A3165 A3168 U3169 A3170 G3173 A3174 U3175 G3176 U3179 A3180 C3181 A3187 U3196 U3207 G3208 A3209 A3210 U3214 C3217 A3218 G3219 C3228 G3229 G3239 G3242 A3243 A3244 A3245 G3246 G3247 U3259 G3260 G3263 G3264 C3265 A3268 U3269 U3270 U3275 G3276 A3279 U3280 U3281



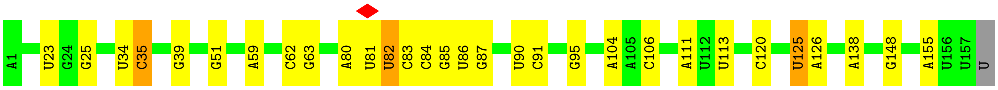
- Molecule 47: 5S rRNA

Chain 2:



- Molecule 48: 5.8S rRNA

Chain 3:



4 Experimental information

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	42030	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.145	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	v	0.40	0/2831	0.68	4/3847 (0.1%)
3	A	0.46	0/1897	0.65	0/2550
4	a	0.43	0/758	0.53	0/1023
5	B	0.47	0/3152	0.66	1/4239 (0.0%)
6	b	0.30	0/2016	0.59	0/2692
7	C	0.41	0/2801	0.60	0/3792
8	c	0.41	0/751	0.56	0/1008
9	d	0.44	0/887	0.58	0/1191
10	E	0.37	0/1291	0.57	0/1735
11	e	0.39	0/1041	0.55	0/1394
12	F	0.42	0/1821	0.60	2/2451 (0.1%)
13	f	0.48	0/868	0.53	0/1168
14	G	0.41	0/1830	0.64	1/2469 (0.0%)
15	g	0.44	0/891	0.59	0/1191
16	I	0.31	0/1072	0.58	1/1440 (0.1%)
17	H	0.38	0/1514	0.57	1/2039 (0.0%)
18	h	0.36	0/978	0.56	0/1301
19	i	0.36	0/749	0.58	0/995
20	j	0.45	0/685	0.62	0/908
21	k	0.37	0/618	0.56	0/826
22	L	0.41	0/1516	0.62	0/2037
23	l	0.40	0/443	0.60	0/588
24	M	0.38	0/1074	0.53	0/1446
25	p	0.43	0/701	0.58	0/934
26	N	0.49	0/1757	0.60	1/2354 (0.0%)
27	u	0.39	0/1278	0.62	2/1699 (0.1%)
28	O	0.42	0/1585	0.54	0/2128
29	P	0.43	0/1431	0.56	0/1921
30	Q	0.40	0/1211	0.65	1/1633 (0.1%)
31	R	0.41	0/1258	0.59	0/1679
32	S	0.42	0/1460	0.58	0/1962
33	T	0.33	0/483	0.55	0/650
34	U	0.34	0/843	0.58	0/1143
35	V	0.43	0/1018	0.60	0/1369

Mol	**Chain**	**Bond lengths**		**Bond angles**	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
36	W	0.28	0/1068	0.55	1/1442 (0.1%)
37	X	0.42	0/974	0.57	0/1314
38	Y	0.38	0/1004	0.57	0/1341
39	y	0.34	0/1719	0.57	0/2340
40	Z	0.42	0/1118	0.58	0/1497
41	z	0.25	0/445	0.43	0/585
42	D	0.38	0/2023	0.58	0/2729
43	J	0.31	0/1324	0.60	0/1778
44	q	0.50	1/795 (0.1%)	0.93	4/1050 (0.4%)
45	o	0.38	0/444	0.55	0/592
46	1	0.76	1/76644 (0.0%)	0.97	150/119495 (0.1%)
47	2	0.64	0/2883	0.88	0/4491
48	3	0.80	0/3724	0.94	5/5798 (0.1%)
All	All	0.64	2/138674 (0.0%)	0.85	174/204254 (0.1%)

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**
1	v	0	3
3	A	0	1
5	B	0	3
6	b	0	3
7	C	0	1
12	F	0	1
14	G	0	2
16	I	0	1
17	H	0	1
18	h	0	1
22	L	0	1
30	Q	0	1
32	S	0	2
33	T	0	1
38	Y	0	1
39	y	0	2
42	D	0	3
43	J	0	3
44	q	0	9
45	o	0	1
All	All	0	41

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	1	2971	A	N9-C4	5.09	1.41	1.37
44	q	69	VAL	CB-CG1	-5.04	1.42	1.52

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	1	3217	C	N1-C2-O2	11.81	125.99	118.90
30	Q	41	ASP	CB-CG-OD1	9.70	127.03	118.30
46	1	3217	C	C2-N1-C1'	9.70	129.47	118.80
46	1	3217	C	N3-C2-O2	-9.02	115.59	121.90
1	v	146	CYS	CA-CB-SG	8.84	129.91	114.00
46	1	2768	U	C5-C6-N1	8.58	126.99	122.70
46	1	2770	G	C8-N9-C4	-8.40	103.04	106.40
46	1	1013	G	N3-C4-C5	-8.39	124.41	128.60
46	1	922	U	C2-N1-C1'	8.31	127.67	117.70
46	1	2770	G	N7-C8-N9	8.27	117.23	113.10
46	1	2137	U	C2-N1-C1'	8.13	127.46	117.70
46	1	1034	U	N1-C2-O2	7.94	128.35	122.80
46	1	1034	U	C2-N1-C1'	7.64	126.87	117.70
46	1	1034	U	N3-C2-O2	-7.57	116.90	122.20
46	1	279	U	O5'-P-OP1	-7.51	98.94	105.70
46	1	2541	U	P-O3'-C3'	7.48	128.67	119.70
46	1	1576	G	P-O3'-C3'	7.32	128.48	119.70
46	1	2770	G	O4'-C1'-N9	7.27	114.02	108.20
46	1	1013	G	N3-C4-N9	7.25	130.35	126.00
46	1	1013	G	C2-N3-C4	7.22	115.51	111.90
46	1	1027	A	P-O3'-C3'	7.21	128.35	119.70
46	1	1815	U	P-O3'-C3'	7.17	128.30	119.70
46	1	283	G	N3-C4-N9	7.15	130.29	126.00
46	1	283	G	C4-N9-C1'	7.15	135.79	126.50
46	1	1038	C	P-O3'-C3'	7.13	128.26	119.70
46	1	2263	C	C2-N1-C1'	7.09	126.59	118.80
46	1	1013	G	C4-N9-C1'	7.07	135.69	126.50
46	1	1029	G	P-O3'-C3'	7.04	128.15	119.70
46	1	979	U	P-O3'-C3'	6.99	128.09	119.70
1	v	35	CYS	CA-CB-SG	6.97	126.55	114.00
46	1	3181	C	C2-N1-C1'	6.97	126.47	118.80
46	1	2996	U	N1-C2-O2	6.97	127.68	122.80
46	1	283	G	O5'-P-OP1	-6.96	99.44	105.70
46	1	1279	C	C5-C6-N1	6.91	124.45	121.00
26	N	145	ASP	CB-CG-OD1	6.91	124.52	118.30
46	1	1951	C	N1-C2-O2	6.90	123.04	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	1	3217	C	C6-N1-C1'	-6.90	112.52	120.80
5	B	171	LEU	CA-CB-CG	6.87	131.09	115.30
46	1	2137	U	N1-C2-O2	6.86	127.60	122.80
46	1	283	G	OP1-P-O3'	6.82	120.20	105.20
46	1	2513	U	OP1-P-O3'	6.81	120.18	105.20
46	1	3181	C	N1-C2-O2	6.73	122.94	118.90
46	1	2768	U	C6-N1-C2	-6.71	116.97	121.00
46	1	2101	C	P-O3'-C3'	6.64	127.67	119.70
46	1	1349	G	N3-C4-C5	-6.60	125.30	128.60
46	1	1064	A	P-O3'-C3'	6.56	127.57	119.70
46	1	2836	C	C2-N1-C1'	6.56	126.01	118.80
1	v	34	MET	CA-CB-CG	6.53	124.39	113.30
46	1	2537	U	P-O3'-C3'	6.48	127.48	119.70
16	I	46	LEU	CA-CB-CG	6.45	130.12	115.30
46	1	1349	G	N3-C4-N9	6.45	129.87	126.00
46	1	288	C	C6-N1-C2	-6.42	117.73	120.30
44	q	85	LEU	CA-CB-CG	6.40	130.02	115.30
46	1	2513	U	P-O3'-C3'	6.37	127.34	119.70
46	1	1103	A	P-O3'-C3'	6.32	127.29	119.70
46	1	2585	G	N3-C4-C5	-6.32	125.44	128.60
46	1	1115	G	C4-N9-C1'	6.31	134.71	126.50
46	1	1352	A	P-O3'-C3'	6.30	127.26	119.70
46	1	3228	C	P-O3'-C3'	6.29	127.25	119.70
46	1	2550	U	C2-N1-C1'	6.28	125.24	117.70
46	1	283	G	C8-N9-C1'	-6.28	118.84	127.00
46	1	283	G	N3-C4-C5	-6.27	125.46	128.60
46	1	2726	C	C2-N1-C1'	6.26	125.69	118.80
46	1	1716	U	P-O3'-C3'	6.23	127.17	119.70
46	1	2836	C	N1-C2-O2	6.22	122.63	118.90
27	u	32	CYS	CA-CB-SG	-6.22	102.81	114.00
46	1	3153	U	N3-C2-O2	-6.21	117.85	122.20
46	1	2585	G	N3-C4-N9	6.21	129.72	126.00
46	1	2137	U	N3-C2-O2	-6.20	117.86	122.20
46	1	1023	C	N1-C2-O2	6.20	122.62	118.90
46	1	2770	G	C5'-C4'-O4'	6.16	116.50	109.10
46	1	1279	C	C6-N1-C2	-6.16	117.84	120.30
46	1	2541	U	C2-N1-C1'	6.14	125.07	117.70
17	H	118	LEU	CA-CB-CG	6.13	129.39	115.30
46	1	3217	C	C6-N1-C2	-6.11	117.86	120.30
46	1	1349	G	C4-N9-C1'	6.10	134.44	126.50
46	1	3217	C	C5-C6-N1	6.10	124.05	121.00
46	1	1097	G	P-O3'-C3'	6.08	127.00	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	1	15	C	C6-N1-C2	-6.06	117.88	120.30
48	3	82	U	P-O3'-C3'	6.03	126.94	119.70
46	1	2842	U	C2-N1-C1'	6.00	124.90	117.70
46	1	2550	U	N3-C2-O2	-6.00	118.00	122.20
46	1	3153	U	N1-C2-O2	5.99	126.99	122.80
46	1	2137	U	C6-N1-C1'	-5.98	112.83	121.20
36	W	45	LEU	CA-CB-CG	5.95	128.98	115.30
46	1	1525	G	C4-N9-C1'	5.92	134.20	126.50
46	1	3306	U	C2-N1-C1'	5.89	124.77	117.70
46	1	2899	C	N1-C2-O2	5.89	122.43	118.90
46	1	3218	A	P-O3'-C3'	5.87	126.75	119.70
46	1	1190	A	C4-N9-C1'	5.87	136.86	126.30
46	1	1355	A	P-O3'-C3'	5.86	126.73	119.70
46	1	922	U	C6-N1-C1'	-5.83	113.04	121.20
46	1	2899	C	C2-N1-C1'	5.82	125.20	118.80
46	1	1951	C	N3-C2-O2	-5.78	117.85	121.90
46	1	2552	C	C2-N1-C1'	5.77	125.14	118.80
44	q	54	THR	C-N-CA	-5.76	107.29	121.70
46	1	2263	C	N1-C2-O2	5.75	122.35	118.90
46	1	915	A	C4-N9-C1'	5.73	136.61	126.30
46	1	2996	U	N3-C2-O2	-5.72	118.19	122.20
46	1	599	C	P-O3'-C3'	5.71	126.55	119.70
46	1	3214	U	C2-N1-C1'	5.69	124.53	117.70
46	1	1115	G	C8-N9-C1'	-5.68	119.62	127.00
46	1	2209	U	P-O3'-C3'	5.65	126.48	119.70
48	3	125	U	C2-N1-C1'	5.64	124.47	117.70
46	1	1190	A	C2-N3-C4	5.62	113.41	110.60
46	1	2842	U	N1-C2-O2	5.62	126.73	122.80
46	1	979	U	N3-C2-O2	-5.61	118.27	122.20
46	1	1115	G	N3-C4-N9	5.60	129.36	126.00
46	1	915	A	C2-N3-C4	5.59	113.40	110.60
46	1	1021	G	O4'-C1'-N9	5.59	112.67	108.20
46	1	3269	U	P-O3'-C3'	5.53	126.34	119.70
46	1	1554	U	P-O3'-C3'	5.53	126.34	119.70
46	1	2550	U	N1-C2-O2	5.53	126.67	122.80
46	1	979	U	C6-N1-C2	-5.52	117.69	121.00
46	1	3181	C	N3-C2-O2	-5.51	118.04	121.90
46	1	2552	C	N1-C2-O2	5.51	122.21	118.90
46	1	1573	G	N3-C4-N9	5.50	129.30	126.00
46	1	1269	U	C2-N1-C1'	5.50	124.30	117.70
46	1	2836	C	N3-C2-O2	-5.46	118.08	121.90
27	u	9	CYS	CA-CB-SG	-5.45	104.18	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	3	35	C	N1-C2-O2	5.45	122.17	118.90
46	1	2769	A	P-O3'-C3'	5.43	126.22	119.70
44	q	35	LEU	CA-CB-CG	5.43	127.78	115.30
46	1	1525	G	C8-N9-C1'	-5.40	119.98	127.00
46	1	2553	U	N1-C2-O2	5.39	126.57	122.80
46	1	1013	G	C8-N9-C1'	-5.38	120.01	127.00
46	1	922	U	N1-C2-O2	5.38	126.56	122.80
46	1	3354	U	C2-N1-C1'	5.37	124.14	117.70
12	F	157	ASN	C-N-CA	5.36	135.09	121.70
46	1	280	U	C5-C6-N1	5.35	125.37	122.70
46	1	1320	C	C6-N1-C2	-5.34	118.16	120.30
46	1	44	U	N1-C2-O2	5.34	126.54	122.80
48	3	120	C	C6-N1-C2	-5.33	118.17	120.30
46	1	915	A	N3-C4-N9	5.32	131.66	127.40
46	1	2971	A	C2-N3-C4	5.30	113.25	110.60
46	1	1573	G	N3-C4-C5	-5.30	125.95	128.60
46	1	283	G	P-O3'-C3'	5.29	126.05	119.70
48	3	35	C	C6-N1-C2	-5.29	118.18	120.30
46	1	3265	C	N1-C2-O2	5.29	122.08	118.90
46	1	1013	G	C8-N9-C4	-5.28	104.29	106.40
46	1	2585	G	C4-N9-C1'	5.28	133.37	126.50
46	1	1573	G	C4-N9-C1'	5.28	133.36	126.50
46	1	2996	U	C2-N1-C1'	5.28	124.03	117.70
46	1	2983	C	C2-N1-C1'	5.26	124.59	118.80
46	1	663	C	C6-N1-C2	-5.26	118.20	120.30
46	1	1023	C	N3-C2-O2	-5.25	118.22	121.90
46	1	2846	U	C2-N1-C1'	5.25	124.00	117.70
46	1	280	U	C6-N1-C1'	5.24	128.53	121.20
46	1	2567	C	N1-C2-O2	5.24	122.04	118.90
46	1	1349	G	C2-N3-C4	5.23	114.51	111.90
46	1	44	U	N3-C2-O2	-5.22	118.54	122.20
46	1	1844	C	C6-N1-C2	-5.22	118.21	120.30
46	1	860	G	N3-C4-N9	5.21	129.13	126.00
12	F	176	TYR	C-N-CA	-5.21	111.37	122.30
46	1	3306	U	N3-C2-O2	-5.18	118.57	122.20
46	1	2726	C	N3-C2-O2	-5.17	118.28	121.90
46	1	2501	U	P-O3'-C3'	5.16	125.89	119.70
46	1	2553	U	N3-C2-O2	-5.16	118.59	122.20
46	1	45	A	OP1-P-OP2	5.15	127.32	119.60
46	1	280	U	C6-N1-C2	-5.14	117.91	121.00
46	1	2269	U	N1-C2-O2	5.14	126.40	122.80
46	1	1190	A	N3-C4-N9	5.14	131.51	127.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	1	2772	C	C2-N1-C1'	5.13	124.44	118.80
46	1	922	U	N3-C2-O2	-5.13	118.61	122.20
46	1	1349	G	C8-N9-C1'	-5.10	120.36	127.00
46	1	421	G	C4-N9-C1'	5.10	133.13	126.50
46	1	2266	U	P-O3'-C3'	5.09	125.81	119.70
46	1	2617	U	N1-C2-O2	5.09	126.36	122.80
46	1	2770	G	O5'-C5'-C4'	5.07	121.33	111.70
14	G	143	ILE	CG1-CB-CG2	-5.06	100.28	111.40
44	q	70	LEU	CA-CB-CG	5.05	126.92	115.30
1	v	61	CYS	CA-CB-SG	5.04	123.07	114.00
46	1	3269	U	OP2-P-O3'	5.02	116.25	105.20
46	1	3181	C	C6-N1-C1'	-5.01	114.78	120.80

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	219	ILE	Peptide
5	B	221	THR	Peptide
5	B	33	PRO	Peptide
5	B	340	LYS	Peptide
7	C	4	PRO	Peptide
42	D	140	ARG	Peptide
42	D	257	GLU	Peptide
42	D	259	LYS	Peptide
12	F	158	LYS	Peptide
14	G	30	THR	Peptide
14	G	76	ALA	Peptide
17	H	21	LYS	Peptide
16	I	16	ARG	Peptide
43	J	153	LYS	Peptide
43	J	154	THR	Peptide
43	J	171	VAL	Peptide
22	L	131	LYS	Peptide
30	Q	152	HIS	Peptide
32	S	22	PRO	Peptide
32	S	23	LYS	Peptide
33	T	154	VAL	Peptide
38	Y	125	LYS	Peptide
6	b	438	GLY	Peptide
6	b	446	ASP	Peptide
6	b	528	PHE	Peptide

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Mol	Chain	Res	Type	Group
18	h	83	LYS	Peptide
45	o	25	LYS	Peptide
44	q	34	SER	Peptide
44	q	35	LEU	Peptide
44	q	41	ARG	Peptide
44	q	49	GLY	Peptide
44	q	50	PHE	Peptide
44	q	78	LYS	Peptide
44	q	79	THR	Peptide
44	q	81	ALA	Peptide
44	q	97	LYS	Peptide
1	v	278	LYS	Peptide
1	v	31	GLY	Peptide
1	v	32	LEU	Peptide
39	y	145	ASN	Peptide
39	y	7	PHE	Peptide

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	v	352/518 (68%)	305 (87%)	44 (12%)	3 (1%)	17	57
3	A	243/254 (96%)	217 (89%)	25 (10%)	1 (0%)	34	71
4	a	92/149 (62%)	84 (91%)	6 (6%)	2 (2%)	6	39
5	B	384/387 (99%)	343 (89%)	38 (10%)	3 (1%)	19	59
6	b	242/647 (37%)	226 (93%)	13 (5%)	3 (1%)	13	51
7	C	359/362 (99%)	325 (90%)	31 (9%)	3 (1%)	19	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	c	95/105 (90%)	91 (96%)	4 (4%)	0	100	100
9	d	105/113 (93%)	100 (95%)	5 (5%)	0	100	100
10	E	156/176 (89%)	148 (95%)	8 (5%)	0	100	100
11	e	125/130 (96%)	118 (94%)	7 (6%)	0	100	100
12	F	220/244 (90%)	197 (90%)	23 (10%)	0	100	100
13	f	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
14	G	228/256 (89%)	209 (92%)	19 (8%)	0	100	100
15	g	110/121 (91%)	106 (96%)	4 (4%)	0	100	100
16	I	129/166 (78%)	116 (90%)	12 (9%)	1 (1%)	19	59
17	H	186/191 (97%)	168 (90%)	18 (10%)	0	100	100
18	h	117/120 (98%)	114 (97%)	3 (3%)	0	100	100
19	i	94/100 (94%)	87 (93%)	7 (7%)	0	100	100
20	j	83/88 (94%)	76 (92%)	7 (8%)	0	100	100
21	k	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
22	L	185/199 (93%)	163 (88%)	21 (11%)	1 (0%)	29	68
23	l	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
24	M	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
25	p	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
26	N	201/204 (98%)	186 (92%)	15 (8%)	0	100	100
27	u	147/199 (74%)	137 (93%)	7 (5%)	3 (2%)	7	41
28	O	195/199 (98%)	190 (97%)	5 (3%)	0	100	100
29	P	174/184 (95%)	169 (97%)	5 (3%)	0	100	100
30	Q	152/186 (82%)	141 (93%)	11 (7%)	0	100	100
31	R	152/189 (80%)	145 (95%)	7 (5%)	0	100	100
32	S	168/172 (98%)	149 (89%)	16 (10%)	3 (2%)	8	43
33	T	59/160 (37%)	54 (92%)	5 (8%)	0	100	100
34	U	102/121 (84%)	94 (92%)	8 (8%)	0	100	100
35	V	134/137 (98%)	129 (96%)	5 (4%)	0	100	100
36	W	129/236 (55%)	126 (98%)	3 (2%)	0	100	100
37	X	118/142 (83%)	114 (97%)	4 (3%)	0	100	100
38	Y	124/127 (98%)	122 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	y	223/245 (91%)	211 (95%)	12 (5%)	0	100	100
40	Z	133/136 (98%)	117 (88%)	16 (12%)	0	100	100
41	z	53/106 (50%)	53 (100%)	0	0	100	100
42	D	245/297 (82%)	225 (92%)	17 (7%)	3 (1%)	13	51
43	J	162/174 (93%)	141 (87%)	17 (10%)	4 (2%)	5	36
44	q	95/106 (90%)	76 (80%)	18 (19%)	1 (1%)	14	53
45	o	52/59 (88%)	48 (92%)	4 (8%)	0	100	100
All	All	6774/8171 (83%)	6248 (92%)	495 (7%)	31 (0%)	32	68

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	C	339	LEU
27	u	3	ILE
43	J	95	ASN
16	I	17	ASP
22	L	63	VAL
42	D	140	ARG
43	J	154	THR
43	J	155	THR
3	A	219	ILE
4	a	78	LEU
5	B	34	LYS
6	b	398	LEU
7	C	4	PRO
27	u	73	GLN
43	J	172	LEU
4	a	77	LYS
27	u	4	TYR
32	S	13	ARG
32	S	24	LEU
1	v	32	LEU
1	v	279	ILE
6	b	397	LYS
6	b	529	GLY
42	D	258	LYS
44	q	35	LEU
7	C	268	ALA
32	S	23	LYS
1	v	68	PRO

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Mol	Chain	Res	Type
5	B	188	ILE
5	B	239	PRO
42	D	141	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	v	309/467 (66%)	304 (98%)	5 (2%)	62	83
3	A	188/196 (96%)	187 (100%)	1 (0%)	88	95
4	a	77/119 (65%)	75 (97%)	2 (3%)	46	74
5	B	322/323 (100%)	318 (99%)	4 (1%)	71	87
6	b	211/573 (37%)	205 (97%)	6 (3%)	43	72
7	C	288/289 (100%)	286 (99%)	2 (1%)	84	93
8	c	81/88 (92%)	78 (96%)	3 (4%)	34	66
9	d	94/97 (97%)	94 (100%)	0	100	100
10	E	137/153 (90%)	134 (98%)	3 (2%)	52	77
11	e	109/111 (98%)	107 (98%)	2 (2%)	59	81
12	F	186/205 (91%)	185 (100%)	1 (0%)	88	95
13	f	90/91 (99%)	90 (100%)	0	100	100
14	G	189/208 (91%)	185 (98%)	4 (2%)	53	78
15	g	95/103 (92%)	95 (100%)	0	100	100
16	I	116/141 (82%)	115 (99%)	1 (1%)	78	90
17	H	168/171 (98%)	166 (99%)	2 (1%)	71	87
18	h	104/105 (99%)	104 (100%)	0	100	100
19	i	78/82 (95%)	78 (100%)	0	100	100
20	j	69/71 (97%)	68 (99%)	1 (1%)	67	85
21	k	68/69 (99%)	68 (100%)	0	100	100
22	L	147/159 (92%)	141 (96%)	6 (4%)	30	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	l	45/46 (98%)	43 (96%)	2 (4%)	28	63
24	M	108/109 (99%)	107 (99%)	1 (1%)	78	90
25	p	71/72 (99%)	70 (99%)	1 (1%)	67	85
26	N	175/176 (99%)	173 (99%)	2 (1%)	73	88
27	u	132/180 (73%)	128 (97%)	4 (3%)	41	71
28	O	160/162 (99%)	157 (98%)	3 (2%)	57	80
29	P	143/146 (98%)	141 (99%)	2 (1%)	67	85
30	Q	126/151 (83%)	125 (99%)	1 (1%)	81	91
31	R	127/154 (82%)	126 (99%)	1 (1%)	81	91
32	S	154/156 (99%)	153 (99%)	1 (1%)	86	94
33	T	50/137 (36%)	47 (94%)	3 (6%)	19	54
34	U	91/107 (85%)	89 (98%)	2 (2%)	52	77
35	V	104/105 (99%)	104 (100%)	0	100	100
36	W	113/213 (53%)	111 (98%)	2 (2%)	59	81
37	X	104/118 (88%)	103 (99%)	1 (1%)	76	88
38	Y	109/110 (99%)	109 (100%)	0	100	100
39	y	192/211 (91%)	192 (100%)	0	100	100
40	Z	115/116 (99%)	114 (99%)	1 (1%)	78	90
41	z	48/95 (50%)	48 (100%)	0	100	100
42	D	203/245 (83%)	199 (98%)	4 (2%)	55	79
43	J	140/150 (93%)	139 (99%)	1 (1%)	84	93
44	q	84/91 (92%)	83 (99%)	1 (1%)	71	87
45	o	43/47 (92%)	42 (98%)	1 (2%)	50	76
All	All	5763/6918 (83%)	5686 (99%)	77 (1%)	70	86

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	v	22	CYS
1	v	143	CYS
1	v	146	CYS
1	v	333	ARG
1	v	349	ASN
3	A	193	ARG

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Mol	Chain	Res	Type
4	a	78	LEU
4	a	120	ASN
5	B	28	ARG
5	B	70	ARG
5	B	332	ARG
5	B	385	LYS
6	b	384	ASN
6	b	413	ASN
6	b	415	ASN
6	b	445	LEU
6	b	470	ASN
6	b	647	ARG
7	C	93	MET
7	C	221	ASN
8	c	16	LEU
8	c	61	MET
8	c	86	ARG
10	E	51	ARG
10	E	127	ASN
10	E	128	LYS
11	e	27	ARG
11	e	87	MET
12	F	244	ASN
14	G	48	ARG
14	G	84	ARG
14	G	85	ASN
14	G	120	LYS
16	I	75	ARG
17	H	23	ARG
17	H	157	ASN
20	j	25	ARG
22	L	21	ARG
22	L	54	LEU
22	L	76	THR
22	L	101	ARG
22	L	180	ARG
22	L	188	ARG
23	l	20	ASN
23	l	43	ASN
24	M	74	ARG
25	p	17	ARG
26	N	183	THR

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Mol	Chain	Res	Type
26	N	188	ARG
27	u	27	LYS
27	u	45	ASN
27	u	100	ARG
27	u	113	ARG
28	O	82	LYS
28	O	85	ARG
28	O	148	LYS
29	P	24	VAL
29	P	97	ASN
30	Q	147	ARG
31	R	98	ARG
32	S	80	ARG
33	T	97	LYS
33	T	136	ARG
33	T	139	ARG
34	U	49	ASN
34	U	94	ARG
36	W	22	ASN
36	W	232	ASN
37	X	73	MET
40	Z	27	LYS
42	D	34	LYS
42	D	39	GLN
42	D	45	ASN
42	D	254	LYS
43	J	12	LEU
44	q	88	CYS
45	o	22	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	v	349	ASN
4	a	120	ASN
5	B	371	GLN
6	b	384	ASN
6	b	413	ASN
6	b	415	ASN
6	b	470	ASN
6	b	509	ASN
7	C	110	ASN

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Mol	Chain	Res	Type
7	C	221	ASN
9	d	57	GLN
10	E	125	GLN
12	F	244	ASN
14	G	85	ASN
16	I	99	ASN
18	h	59	ASN
23	l	11	GLN
23	l	20	ASN
26	N	37	HIS
27	u	24	ASN
27	u	45	ASN
29	P	97	ASN
29	P	118	GLN
30	Q	10	HIS
32	S	108	GLN
32	S	122	HIS
32	S	157	GLN
33	T	103	GLN
34	U	49	ASN
35	V	98	ASN
36	W	22	ASN
36	W	232	ASN
39	y	106	ASN
40	Z	57	HIS
42	D	45	ASN
43	J	95	ASN
43	J	109	HIS
44	q	82	GLN
44	q	90	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	1	3198/3396 (94%)	722 (22%)	39 (1%)
47	2	120/121 (99%)	15 (12%)	0
48	3	156/158 (98%)	28 (17%)	2 (1%)
All	All	3474/3675 (94%)	765 (22%)	41 (1%)

All (765) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	1	22	G
46	1	40	A
46	1	43	A
46	1	44	U
46	1	45	A
46	1	49	A
46	1	55	G
46	1	59	G
46	1	60	A
46	1	65	A
46	1	66	A
46	1	72	C
46	1	75	G
46	1	76	G
46	1	85	A
46	1	92	G
46	1	109	A
46	1	110	G
46	1	111	C
46	1	116	A
46	1	118	U
46	1	122	A
46	1	132	C
46	1	135	C
46	1	136	G
46	1	148	G
46	1	155	G
46	1	156	G
46	1	157	A
46	1	166	C
46	1	170	G
46	1	172	G
46	1	173	G
46	1	176	G
46	1	182	U
46	1	187	A
46	1	190	U
46	1	191	U
46	1	198	A
46	1	206	G
46	1	210	U
46	1	211	A
46	1	212	G

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Mol	Chain	Res	Type
46	1	213	A
46	1	218	G
46	1	219	A
46	1	230	U
46	1	231	G
46	1	237	G
46	1	240	U
46	1	241	G
46	1	243	G
46	1	246	U
46	1	247	C
46	1	248	U
46	1	250	U
46	1	253	A
46	1	269	G
46	1	277	G
46	1	279	U
46	1	281	G
46	1	283	G
46	1	284	A
46	1	285	A
46	1	286	U
46	1	295	A
46	1	305	U
46	1	323	A
46	1	329	U
46	1	334	A
46	1	338	A
46	1	339	C
46	1	343	U
46	1	349	A
46	1	376	G
46	1	382	U
46	1	385	A
46	1	395	A
46	1	398	A
46	1	399	A
46	1	401	U
46	1	402	A
46	1	403	C
46	1	404	G
46	1	406	G

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Mol	Chain	Res	Type
46	1	420	G
46	1	421	G
46	1	422	A
46	1	429	U
46	1	438	A
46	1	440	A
46	1	495	G
46	1	520	U
46	1	521	A
46	1	535	G
46	1	543	C
46	1	546	C
46	1	547	G
46	1	548	G
46	1	551	A
46	1	552	G
46	1	553	U
46	1	555	U
46	1	557	A
46	1	559	A
46	1	569	A
46	1	578	A
46	1	579	G
46	1	591	G
46	1	592	A
46	1	597	G
46	1	600	G
46	1	604	G
46	1	611	A
46	1	620	U
46	1	621	A
46	1	622	A
46	1	636	C
46	1	649	A
46	1	655	C
46	1	660	A
46	1	677	A
46	1	681	U
46	1	683	U
46	1	689	U
46	1	690	A
46	1	691	A

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Mol	Chain	Res	Type
46	1	705	A
46	1	712	G
46	1	715	A
46	1	716	A
46	1	719	U
46	1	720	A
46	1	725	G
46	1	744	A
46	1	763	G
46	1	765	C
46	1	766	U
46	1	767	U
46	1	776	U
46	1	777	U
46	1	780	A
46	1	781	G
46	1	785	G
46	1	786	A
46	1	801	A
46	1	806	A
46	1	817	A
46	1	823	C
46	1	830	A
46	1	849	C
46	1	851	C
46	1	861	C
46	1	869	G
46	1	874	U
46	1	875	G
46	1	879	U
46	1	880	G
46	1	884	A
46	1	895	A
46	1	897	U
46	1	907	G
46	1	908	G
46	1	911	C
46	1	914	A
46	1	916	G
46	1	917	A
46	1	921	A
46	1	924	G

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Mol	Chain	Res	Type
46	1	926	A
46	1	932	U
46	1	933	A
46	1	937	G
46	1	944	C
46	1	946	U
46	1	953	G
46	1	959	C
46	1	960	U
46	1	961	C
46	1	974	G
46	1	978	G
46	1	979	U
46	1	980	A
46	1	981	U
46	1	982	C
46	1	994	G
46	1	1001	G
46	1	1002	A
46	1	1006	A
46	1	1008	U
46	1	1009	A
46	1	1010	G
46	1	1011	A
46	1	1014	U
46	1	1015	U
46	1	1016	C
46	1	1017	C
46	1	1018	G
46	1	1019	G
46	1	1020	G
46	1	1023	C
46	1	1024	G
46	1	1026	A
46	1	1027	A
46	1	1028	U
46	1	1029	G
46	1	1030	A
46	1	1035	G
46	1	1036	A
46	1	1037	C
46	1	1038	C

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Mol	Chain	Res	Type
46	1	1039	U
46	1	1040	A
46	1	1041	U
46	1	1046	A
46	1	1047	A
46	1	1049	C
46	1	1063	G
46	1	1064	A
46	1	1065	A
46	1	1081	U
46	1	1082	U
46	1	1087	G
46	1	1093	A
46	1	1094	U
46	1	1095	U
46	1	1097	G
46	1	1098	A
46	1	1103	A
46	1	1104	G
46	1	1109	U
46	1	1111	U
46	1	1117	G
46	1	1124	U
46	1	1131	G
46	1	1140	G
46	1	1143	A
46	1	1153	A
46	1	1159	A
46	1	1161	G
46	1	1178	G
46	1	1180	A
46	1	1181	U
46	1	1190	A
46	1	1192	C
46	1	1193	A
46	1	1195	A
46	1	1196	C
46	1	1201	C
46	1	1208	U
46	1	1212	A
46	1	1213	G
46	1	1217	A

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Mol	Chain	Res	Type
46	1	1219	C
46	1	1220	U
46	1	1221	A
46	1	1222	G
46	1	1227	C
46	1	1235	U
46	1	1236	G
46	1	1237	G
46	1	1238	C
46	1	1239	C
46	1	1241	U
46	1	1243	G
46	1	1244	A
46	1	1245	A
46	1	1246	G
46	1	1248	C
46	1	1249	G
46	1	1252	A
46	1	1253	U
46	1	1254	C
46	1	1258	U
46	1	1262	G
46	1	1263	A
46	1	1264	G
46	1	1265	U
46	1	1268	G
46	1	1270	A
46	1	1271	A
46	1	1272	C
46	1	1278	A
46	1	1279	C
46	1	1285	G
46	1	1286	A
46	1	1287	A
46	1	1292	C
46	1	1295	G
46	1	1305	U
46	1	1307	G
46	1	1309	U
46	1	1313	G
46	1	1316	C
46	1	1325	U

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Mol	Chain	Res	Type
46	1	1330	A
46	1	1331	U
46	1	1332	A
46	1	1348	U
46	1	1349	G
46	1	1350	A
46	1	1351	U
46	1	1352	A
46	1	1353	U
46	1	1356	U
46	1	1386	A
46	1	1391	C
46	1	1392	G
46	1	1399	A
46	1	1400	G
46	1	1408	G
46	1	1416	C
46	1	1419	A
46	1	1430	U
46	1	1434	G
46	1	1437	C
46	1	1443	G
46	1	1445	U
46	1	1446	A
46	1	1450	G
46	1	1455	U
46	1	1475	A
46	1	1480	G
46	1	1481	A
46	1	1482	A
46	1	1484	U
46	1	1492	G
46	1	1496	C
46	1	1503	A
46	1	1508	C
46	1	1512	U
46	1	1533	U
46	1	1536	G
46	1	1537	A
46	1	1546	A
46	1	1547	G
46	1	1555	U

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Mol	Chain	Res	Type
46	1	1556	C
46	1	1557	A
46	1	1559	A
46	1	1561	G
46	1	1562	C
46	1	1563	C
46	1	1565	G
46	1	1567	U
46	1	1568	U
46	1	1569	U
46	1	1570	U
46	1	1572	U
46	1	1574	C
46	1	1576	G
46	1	1577	G
46	1	1579	C
46	1	1580	A
46	1	1581	C
46	1	1582	C
46	1	1583	A
46	1	1587	A
46	1	1589	A
46	1	1590	G
46	1	1593	A
46	1	1619	A
46	1	1620	U
46	1	1628	C
46	1	1629	U
46	1	1632	A
46	1	1633	C
46	1	1636	U
46	1	1642	A
46	1	1643	A
46	1	1645	U
46	1	1649	U
46	1	1656	A
46	1	1657	C
46	1	1662	G
46	1	1677	G
46	1	1682	U
46	1	1683	A
46	1	1696	A

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Mol	Chain	Res	Type
46	1	1702	U
46	1	1711	C
46	1	1716	U
46	1	1717	U
46	1	1724	U
46	1	1725	C
46	1	1736	G
46	1	1741	A
46	1	1742	U
46	1	1749	A
46	1	1750	A
46	1	1751	G
46	1	1760	A
46	1	1762	C
46	1	1765	U
46	1	1766	G
46	1	1770	G
46	1	1772	U
46	1	1775	G
46	1	1780	G
46	1	1785	U
46	1	1790	G
46	1	1797	A
46	1	1813	A
46	1	1814	A
46	1	1816	A
46	1	1817	G
46	1	1820	U
46	1	1821	U
46	1	1839	A
46	1	1842	A
46	1	1844	C
46	1	1849	C
46	1	1850	A
46	1	1867	A
46	1	1880	U
46	1	1886	A
46	1	1893	A
46	1	1905	G
46	1	1906	G
46	1	1951	C
46	1	1952	G

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Mol	Chain	Res	Type
46	1	1953	G
46	1	1954	G
46	1	2100	A
46	1	2101	C
46	1	2102	U
46	1	2111	G
46	1	2112	U
46	1	2119	A
46	1	2121	G
46	1	2122	G
46	1	2131	A
46	1	2139	A
46	1	2140	U
46	1	2142	A
46	1	2158	A
46	1	2160	G
46	1	2169	G
46	1	2171	G
46	1	2176	U
46	1	2184	U
46	1	2186	U
46	1	2188	A
46	1	2205	U
46	1	2209	U
46	1	2210	G
46	1	2244	A
46	1	2249	G
46	1	2250	G
46	1	2252	A
46	1	2259	A
46	1	2260	U
46	1	2261	G
46	1	2262	A
46	1	2263	C
46	1	2265	C
46	1	2267	C
46	1	2268	U
46	1	2269	U
46	1	2270	A
46	1	2273	G
46	1	2281	A
46	1	2282	U

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Mol	Chain	Res	Type
46	1	2287	C
46	1	2288	G
46	1	2298	U
46	1	2306	C
46	1	2307	G
46	1	2308	C
46	1	2309	A
46	1	2310	U
46	1	2313	A
46	1	2314	U
46	1	2315	G
46	1	2330	C
46	1	2334	U
46	1	2335	G
46	1	2336	U
46	1	2337	C
46	1	2361	A
46	1	2363	A
46	1	2373	A
46	1	2374	C
46	1	2375	G
46	1	2385	G
46	1	2388	U
46	1	2393	G
46	1	2397	A
46	1	2398	A
46	1	2401	A
46	1	2402	A
46	1	2403	G
46	1	2404	A
46	1	2411	U
46	1	2435	G
46	1	2437	G
46	1	2440	G
46	1	2442	G
46	1	2448	G
46	1	2450	G
46	1	2452	G
46	1	2453	U
46	1	2454	G
46	1	2455	U
46	1	2458	A

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Mol	Chain	Res	Type
46	1	2459	A
46	1	2460	U
46	1	2464	U
46	1	2468	A
46	1	2470	C
46	1	2472	U
46	1	2474	G
46	1	2476	C
46	1	2477	G
46	1	2484	A
46	1	2486	A
46	1	2487	U
46	1	2495	C
46	1	2496	C
46	1	2497	U
46	1	2498	U
46	1	2499	U
46	1	2501	U
46	1	2502	A
46	1	2503	G
46	1	2505	U
46	1	2506	U
46	1	2508	U
46	1	2514	U
46	1	2522	G
46	1	2531	C
46	1	2533	G
46	1	2537	U
46	1	2538	U
46	1	2539	C
46	1	2540	A
46	1	2541	U
46	1	2542	U
46	1	2544	U
46	1	2547	A
46	1	2549	G
46	1	2550	U
46	1	2552	C
46	1	2555	G
46	1	2561	A
46	1	2566	C
46	1	2567	C

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Mol	Chain	Res	Type
46	1	2569	A
46	1	2570	U
46	1	2571	U
46	1	2572	C
46	1	2573	G
46	1	2577	C
46	1	2585	G
46	1	2593	A
46	1	2594	C
46	1	2600	C
46	1	2606	G
46	1	2607	G
46	1	2614	G
46	1	2626	A
46	1	2635	A
46	1	2648	G
46	1	2652	U
46	1	2656	A
46	1	2657	A
46	1	2674	A
46	1	2677	G
46	1	2678	A
46	1	2688	U
46	1	2689	A
46	1	2691	A
46	1	2694	A
46	1	2696	A
46	1	2703	A
46	1	2704	A
46	1	2705	A
46	1	2719	U
46	1	2726	C
46	1	2728	G
46	1	2729	U
46	1	2742	C
46	1	2753	G
46	1	2755	C
46	1	2762	A
46	1	2768	U
46	1	2769	A
46	1	2770	G
46	1	2771	U

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Mol	Chain	Res	Type
46	1	2772	C
46	1	2777	G
46	1	2778	G
46	1	2794	G
46	1	2796	G
46	1	2799	A
46	1	2800	G
46	1	2801	A
46	1	2802	A
46	1	2803	A
46	1	2804	A
46	1	2810	C
46	1	2814	G
46	1	2816	G
46	1	2817	A
46	1	2828	G
46	1	2838	A
46	1	2842	U
46	1	2843	U
46	1	2844	C
46	1	2845	A
46	1	2850	G
46	1	2871	G
46	1	2872	A
46	1	2875	U
46	1	2876	C
46	1	2887	A
46	1	2899	C
46	1	2904	U
46	1	2914	G
46	1	2923	U
46	1	2924	U
46	1	2928	C
46	1	2933	A
46	1	2935	U
46	1	2936	A
46	1	2941	A
46	1	2951	G
46	1	2971	A
46	1	2978	U
46	1	2983	C
46	1	2996	U

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Mol	Chain	Res	Type
46	1	2997	G
46	1	3011	A
46	1	3012	A
46	1	3021	A
46	1	3028	G
46	1	3056	U
46	1	3059	G
46	1	3080	G
46	1	3086	A
46	1	3092	C
46	1	3099	C
46	1	3108	G
46	1	3109	G
46	1	3115	C
46	1	3119	U
46	1	3129	A
46	1	3130	A
46	1	3131	U
46	1	3142	A
46	1	3143	C
46	1	3148	U
46	1	3150	A
46	1	3153	U
46	1	3155	U
46	1	3156	U
46	1	3157	U
46	1	3164	C
46	1	3165	A
46	1	3168	A
46	1	3170	A
46	1	3173	G
46	1	3174	A
46	1	3175	U
46	1	3176	G
46	1	3179	U
46	1	3180	A
46	1	3181	C
46	1	3187	A
46	1	3196	U
46	1	3207	U
46	1	3209	A
46	1	3210	A

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Mol	Chain	Res	Type
46	1	3217	C
46	1	3218	A
46	1	3219	G
46	1	3229	G
46	1	3239	G
46	1	3242	G
46	1	3243	A
46	1	3245	A
46	1	3247	G
46	1	3259	U
46	1	3260	G
46	1	3263	G
46	1	3268	A
46	1	3270	U
46	1	3275	U
46	1	3276	G
46	1	3279	A
46	1	3280	U
46	1	3281	U
46	1	3289	G
46	1	3294	A
46	1	3295	A
46	1	3304	U
46	1	3308	C
46	1	3313	U
46	1	3316	A
46	1	3317	U
46	1	3318	G
46	1	3319	U
46	1	3320	A
46	1	3341	U
46	1	3345	G
46	1	3347	A
46	1	3350	C
46	1	3351	U
46	1	3352	U
46	1	3354	U
46	1	3355	U
46	1	3356	G
46	1	3357	U
46	1	3360	C
46	1	3363	U

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Mol	Chain	Res	Type
46	1	3368	U
46	1	3369	G
46	1	3375	A
46	1	3378	C
46	1	3382	U
46	1	3386	G
46	1	3396	U
47	2	10	C
47	2	22	A
47	2	49	G
47	2	53	U
47	2	54	U
47	2	65	G
47	2	73	C
47	2	74	C
47	2	76	A
47	2	102	A
47	2	109	G
47	2	112	G
47	2	114	U
47	2	120	C
47	2	121	U
48	3	23	U
48	3	25	G
48	3	34	U
48	3	35	C
48	3	39	G
48	3	51	G
48	3	59	A
48	3	62	C
48	3	63	G
48	3	80	A
48	3	81	U
48	3	82	U
48	3	83	C
48	3	84	C
48	3	86	U
48	3	87	G
48	3	90	U
48	3	91	C
48	3	95	G
48	3	104	A

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Mol	Chain	Res	Type
48	3	106	C
48	3	111	A
48	3	113	U
48	3	125	U
48	3	126	A
48	3	138	A
48	3	148	G
48	3	155	A

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
46	1	239	G
46	1	283	G
46	1	285	A
46	1	547	G
46	1	599	C
46	1	916	G
46	1	979	U
46	1	1027	A
46	1	1029	G
46	1	1038	C
46	1	1064	A
46	1	1097	G
46	1	1103	A
46	1	1352	A
46	1	1355	A
46	1	1554	U
46	1	1576	G
46	1	1716	U
46	1	1815	U
46	1	1816	A
46	1	2101	C
46	1	2209	U
46	1	2249	G
46	1	2258	U
46	1	2264	U
46	1	2266	U
46	1	2454	G
46	1	2501	U
46	1	2513	U
46	1	2537	U

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Mol	Chain	Res	Type
46	1	2541	U
46	1	2593	A
46	1	2769	A
46	1	2770	G
46	1	2815	G
46	1	3218	A
46	1	3228	C
46	1	3269	U
46	1	3353	G
48	3	82	U
48	3	85	G

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

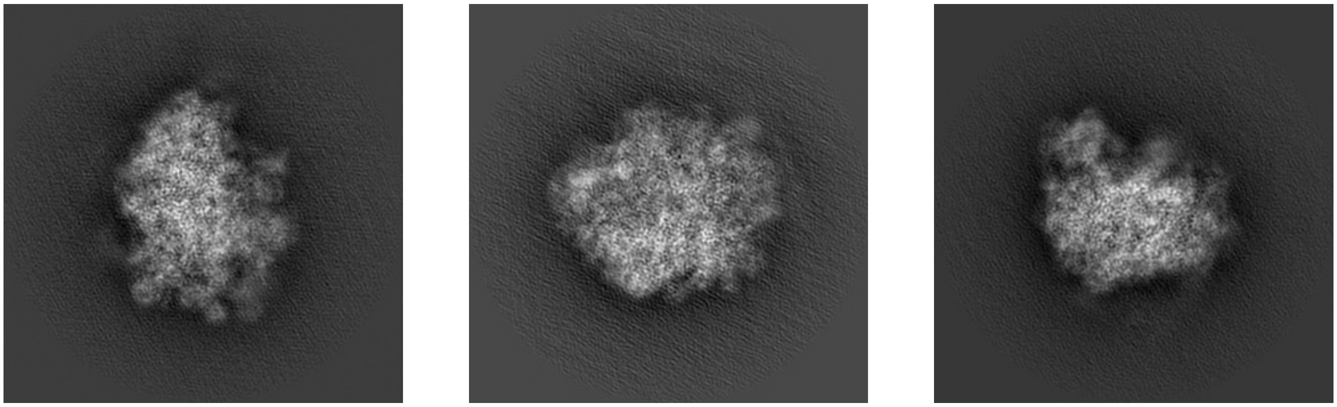
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0371. 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

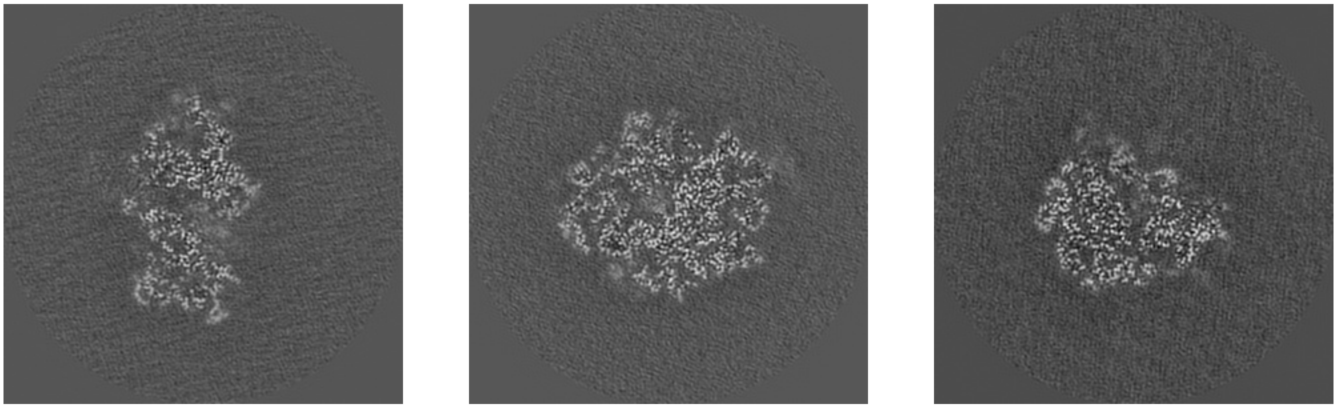


X Y Z

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

6.2 Central slices

6.2.1 Primary map

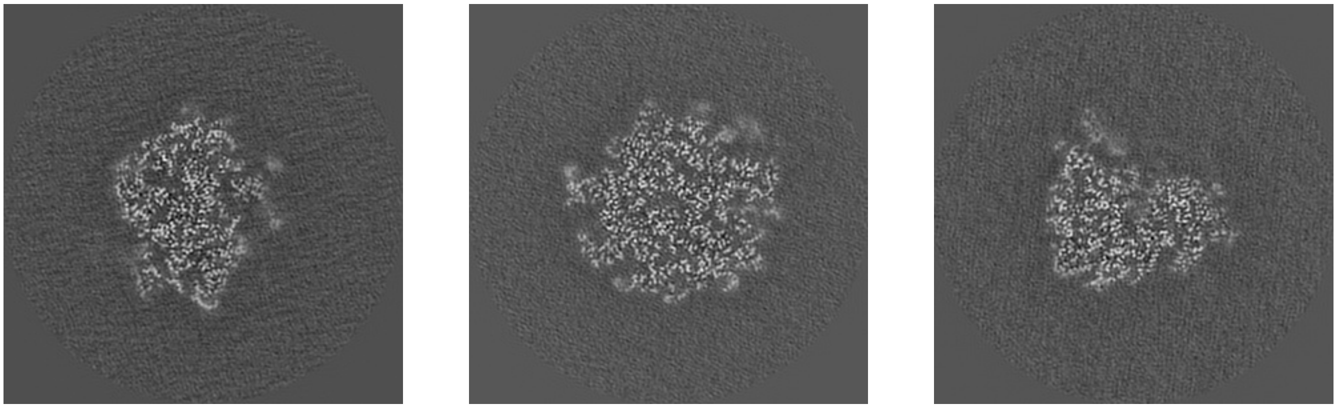


X Index: 192 Y Index: 192 Z Index: 192

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

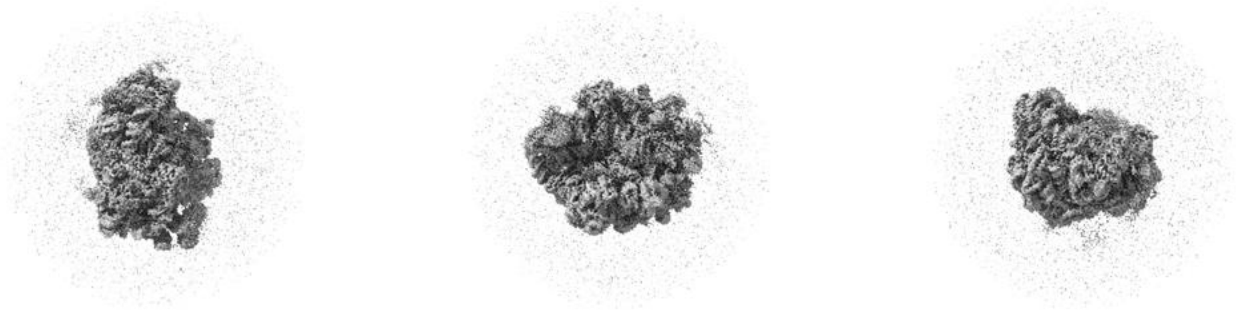


X Index: 166 Y Index: 173 Z Index: 184

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

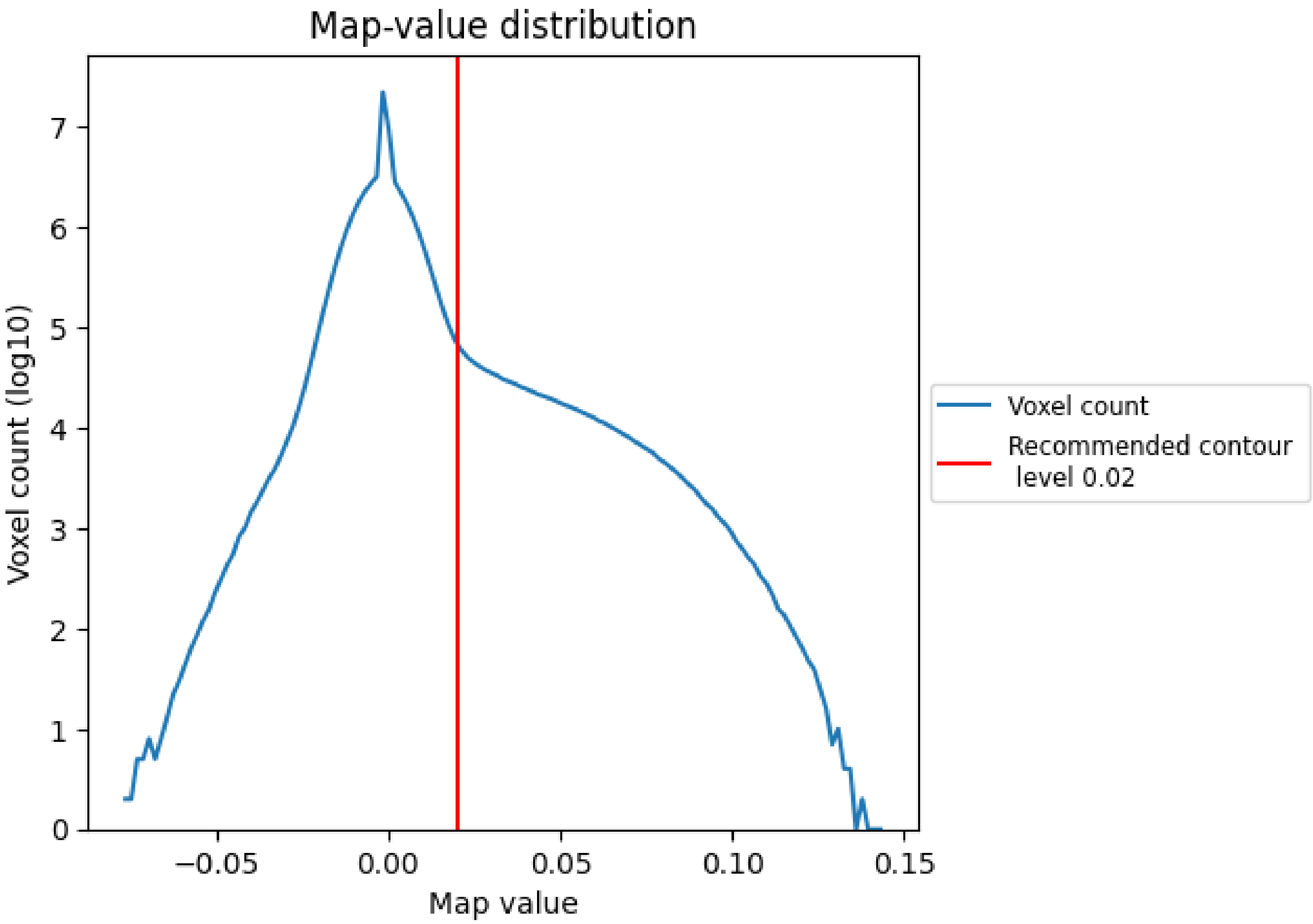
6.5 Mask visualisation (i)

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

7 Map analysis ⓘ

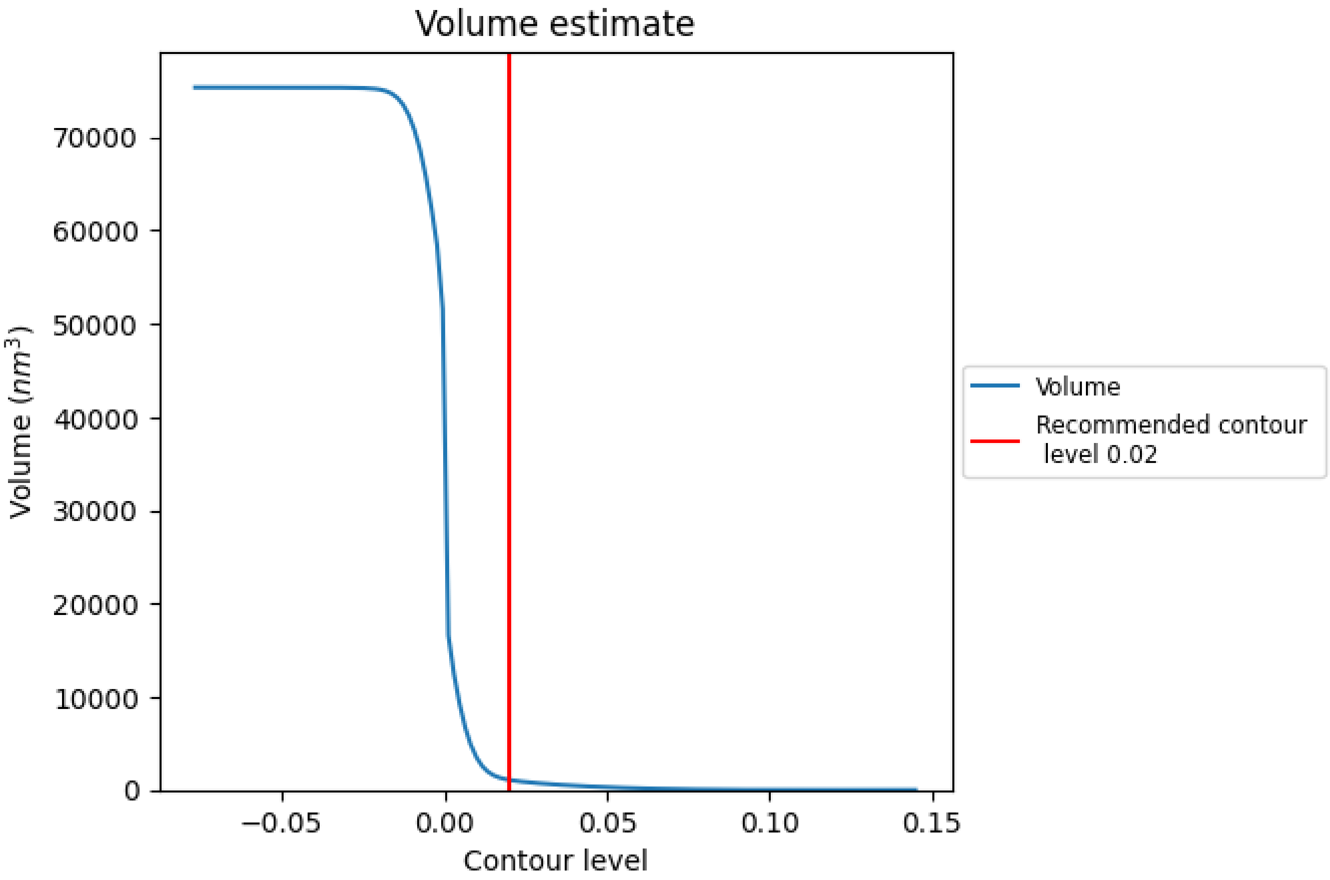
This section contains the results of statistical analysis of the map.

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.

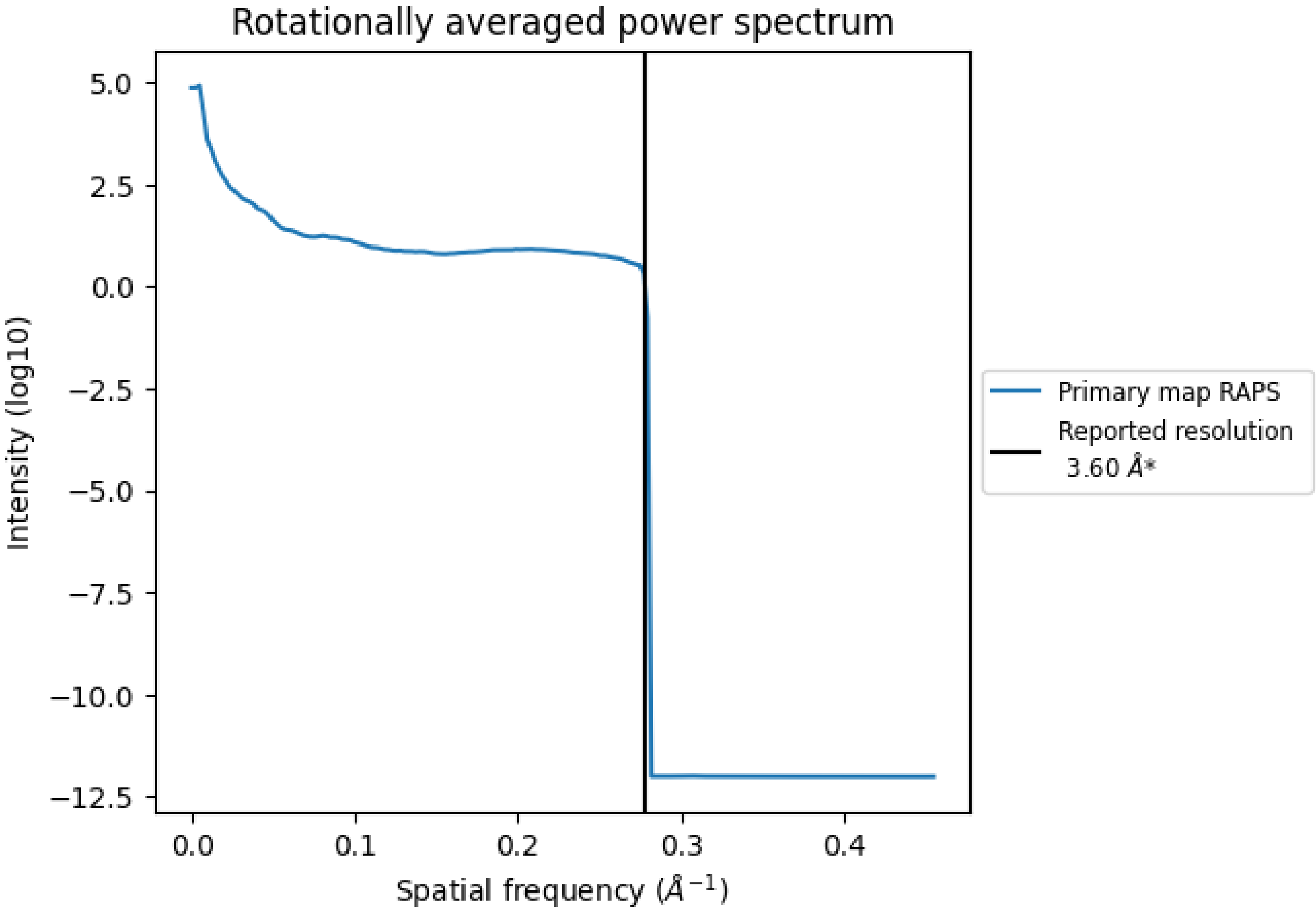
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 1076 nm^3; this corresponds to an approximate mass of 972 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

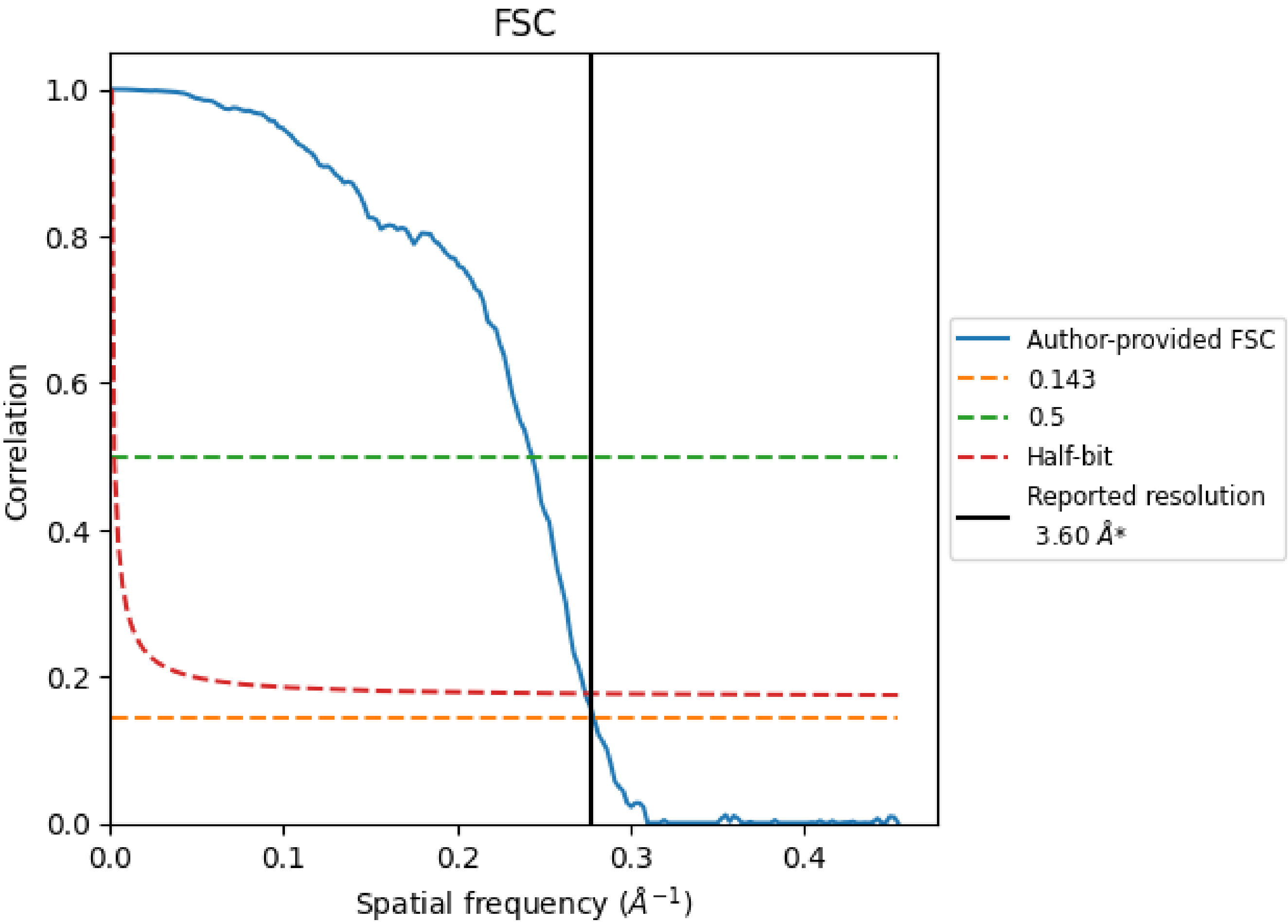


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



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

8.2 Resolution estimates

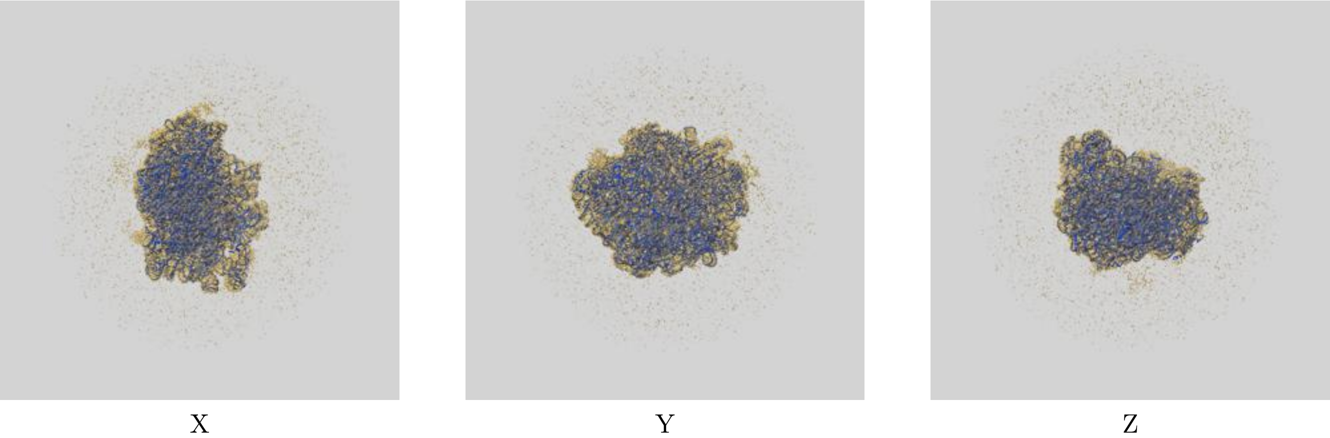
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	4.11	3.65
Unmasked-calculated*	-	-	-

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

9 Map-model fit ⓘ

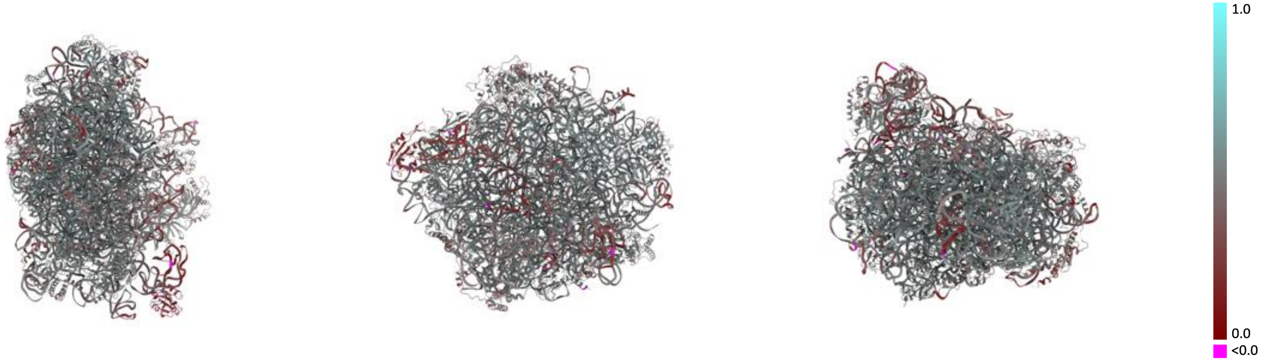
This section contains information regarding the fit between EMDB map EMD-0371 and PDB model 6N8L. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay ⓘ



The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

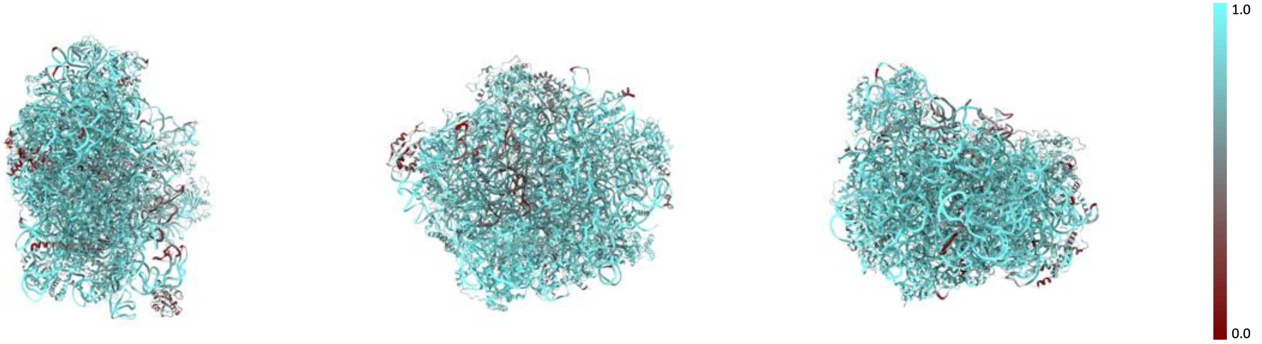
9.2 Q-score mapped to coordinate model



X Y Z

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

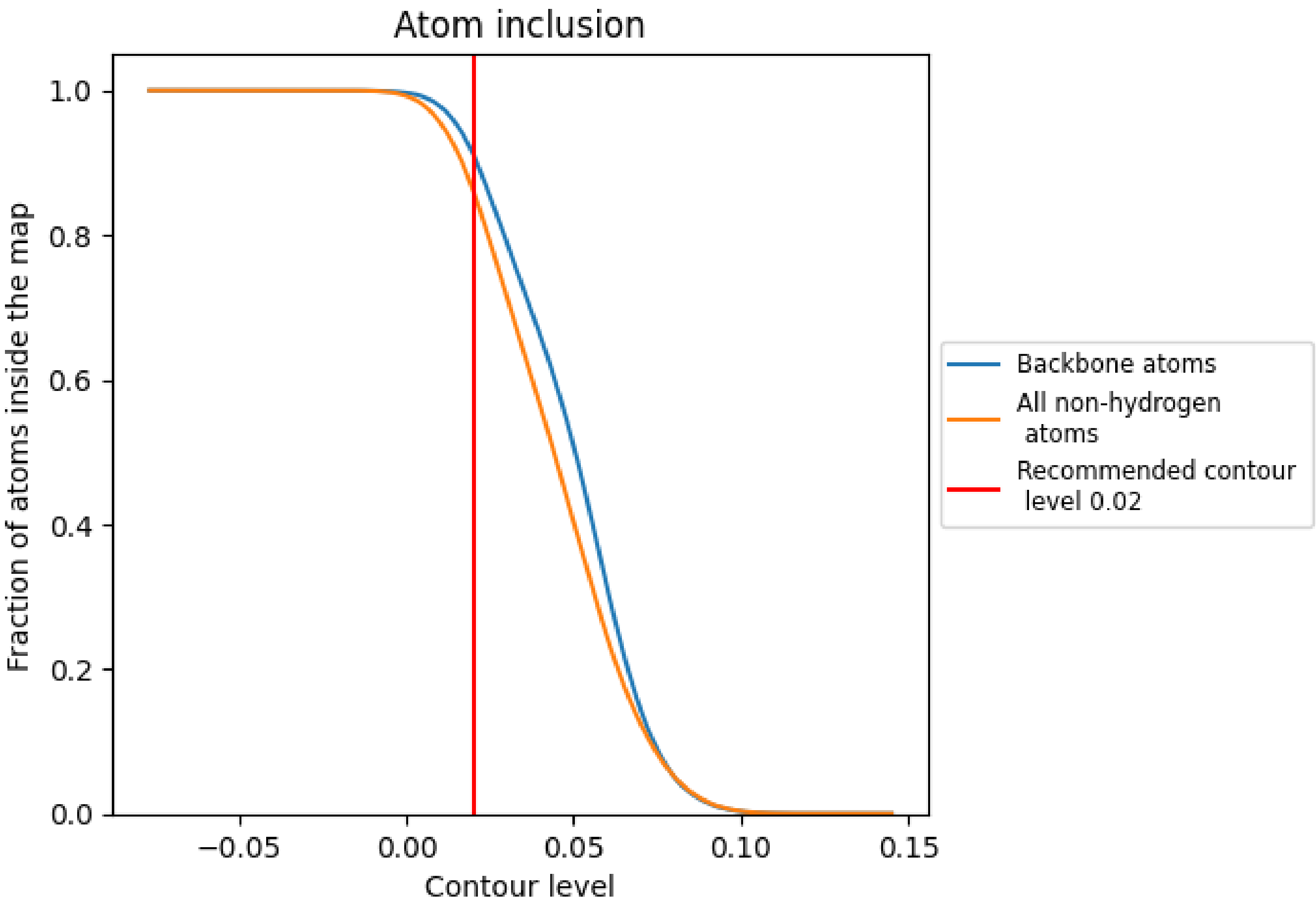
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 86% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8616	0.4720
1	0.9177	0.4740
2	0.9620	0.4790
3	0.9550	0.4970
A	0.8593	0.5240
B	0.8508	0.5050
C	0.8374	0.5050
D	0.8248	0.4450
E	0.7982	0.4730
F	0.8381	0.4930
G	0.8296	0.4780
H	0.8314	0.4790
I	0.5742	0.4450
J	0.7512	0.4120
L	0.8502	0.4950
M	0.8372	0.4800
N	0.8687	0.5260
O	0.8534	0.5110
P	0.8239	0.5010
Q	0.8533	0.5040
R	0.8385	0.4980
S	0.8214	0.4960
T	0.7754	0.4230
U	0.7796	0.4170
V	0.7957	0.5020
W	0.4713	0.2330
X	0.8356	0.5020
Y	0.8447	0.5010
Z	0.8273	0.4950
a	0.8418	0.4950
b	0.3886	0.3710
c	0.8249	0.4680
d	0.8276	0.5000
e	0.8260	0.5170
f	0.8538	0.5260

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Chain	Atom inclusion	Q-score
g	0.7969	0.5000
h	0.8324	0.4920
i	0.8428	0.4850
j	0.8866	0.5350
k	0.7596	0.4660
l	0.8530	0.5220
o	0.7991	0.4720
p	0.8191	0.5090
q	0.4149	0.1540
s	0.8419	0.4070
u	0.6984	0.4340
v	0.6307	0.4180
y	0.7813	0.4540
z	0.4171	0.3790