



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jul 24, 2017 – 10:46 AM EDT

PDB ID : 5APO  
EMDB ID: : EMD-3151  
Title : Structure of the yeast 60S ribosomal subunit in complex with Arx1, Alb1 and C-terminally tagged Rei1  
Authors : Greber, B.J.; Gerhardy, S.; Leitner, A.; Leibundgut, M.; Salem, M.; Boehringer, D.; Leulliot, N.; Aebersold, R.; Panse, V.G.; Ban, N.  
Deposited on : unknown  
Resolution : 3.41 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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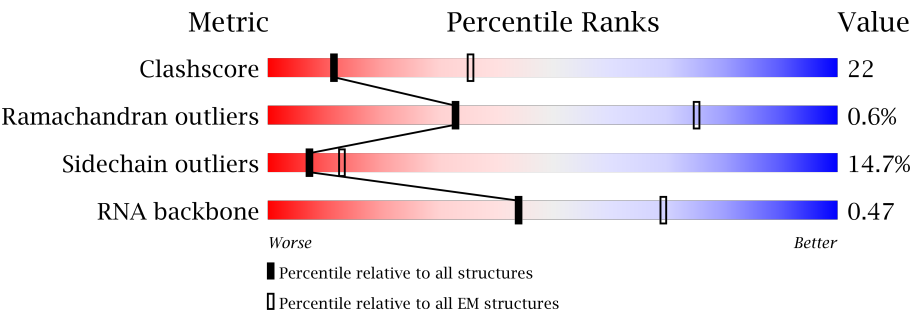
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.41 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	5	3396	<div><div>40%</div><div>38%</div><div>12%</div><div>•</div><div>8%</div></div>
2	7	121	<div><div>45%</div><div>49%</div><div>7%</div></div>
3	8	158	<div><div>47%</div><div>35%</div><div>16%</div><div>•</div></div>
4	A	254	<div><div>36%</div><div>38%</div><div>9%</div><div>17%</div></div>
5	B	387	<div><div>50%</div><div>40%</div><div>10%</div></div>
6	C	362	<div><div>49%</div><div>41%</div><div>10%</div><div>•</div></div>
7	D	297	<div><div>53%</div><div>38%</div><div>8%</div><div>•</div></div>
8	E	176	<div><div>55%</div><div>40%</div><div>5%</div><div>•</div></div>

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Mol	Chain	Length	Quality of chain
9	F	244	
10	G	256	
11	H	191	
12	I	221	
13	J	174	
14	L	199	
15	M	138	
16	N	204	
17	O	199	
18	P	184	
19	Q	186	
20	R	189	
21	S	172	
22	T	160	
23	U	121	
24	V	137	
25	W	155	
26	X	142	
27	Y	127	
28	Z	136	
29	a	149	
30	b	59	
31	c	105	
32	d	113	
33	e	130	

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Mol	Chain	Length	Quality of chain
34	f	107	 93% 6% .
35	g	121	 83% 10% 7% .
36	h	120	 83% 16% .
37	i	100	 76% 23% .
38	j	88	 86% 13% .
39	k	78	 88% 10% .
40	l	51	 78% 20% .
41	m	128	 35% 5% 59%
42	o	106	 82% 17% .
43	p	92	 80% 18% .
44	q	312	 33% 6% 62%
45	x	616	 87% 6% 6%
46	y	401	 50% . 46%
47	z	95	 89% 11%

## 2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 129386 atoms, of which 3 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	3112	Total	C	N	O	P	0	0
			66537	29736	11996	21694	3111		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	7	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	212	Total	C	N	O	S	0	0
			1630	1021	325	283	1		

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

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

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

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

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	294	Total	C	N	O	S	0	0
			2359	1489	412	456	2		

- Molecule 8 is a protein called 60S RIBOSOMAL PROTEIN EL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	175	Total	C	N	O	S	0	0
			1356	878	242	235	1		

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	223	Total	C	N	O	S	0	0
			1791	1155	325	310	1		

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	231	Total	C	N	O	S	0	0
			1763	1130	316	314	3		

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

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

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	213	Total	C	N	O	S	0	0
			1722	1094	325	297	6		

- Molecule 13 is a protein called 60S ribosomal protein L11-A.

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

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	L	194	Total	C	N	O	0	0
			1548	965	316	267		

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	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	O	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	P	183	Total	C	N	O	0	0
			1442	896	287	259		

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

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

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	156	Total	C	N	O	0	0
			1258	781	265	212		

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

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

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	102	Total	C	N	O	S	0	0
			808	524	132	152			

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

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

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	63	Total	C	N	O	S	0	0
			521	336	102	82	1		

- Molecule 26 is a protein called 60S ribosomal protein L25.

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

- Molecule 27 is a protein called 60S ribosomal protein L26-A.

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

- Molecule 28 is a protein called 60S ribosomal protein L27-A.



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

- Molecule 29 is a protein called 60S ribosomal protein L28.

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

- Molecule 30 is a protein called 60S ribosomal protein L29.

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

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	100	Total	C	N	O	S	0	0
			767	492	128	146	1		

- Molecule 32 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	109	Total	C	N	O	S	0	0
			883	559	167	156	1		

- Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	129	Total	C	N	O	S	0	0
			1034	655	207	171	1		

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 35 is a protein called 60S ribosomal protein L34-A.

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

- Molecule 36 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	119	Total	C	N	O	S	0	0
			965	612	185	167	1		

- Molecule 37 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	99	Total	C	N	O	S	0	0
			770	481	156	131	2		

- Molecule 38 is a protein called 60S ribosomal protein L37-A.

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

- Molecule 39 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	k	77	Total	C	N	O	0	0
			608	388	114	106		

- Molecule 40 is a protein called 60S ribosomal protein L39.

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

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 42 is a protein called 60S ribosomal protein L42-A.

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

- Molecule 43 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 44 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	q	120	Total	C	N	O	S	0	0
			962	618	169	172	3		

- Molecule 45 is a protein called Probable metalloprotease ARX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	579	Total	C	N	O	S	0	0
			4477	2823	772	867	15		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	-22	MET	-	initiating methionine	UNP Q03862
x	-21	GLY	-	expression tag	UNP Q03862
x	-20	SER	-	expression tag	UNP Q03862
x	-19	SER	-	expression tag	UNP Q03862
x	-18	HIS	-	expression tag	UNP Q03862
x	-17	HIS	-	expression tag	UNP Q03862
x	-16	HIS	-	expression tag	UNP Q03862
x	-15	HIS	-	expression tag	UNP Q03862
x	-14	HIS	-	expression tag	UNP Q03862
x	-13	HIS	-	expression tag	UNP Q03862
x	-12	SER	-	expression tag	UNP Q03862
x	-11	SER	-	expression tag	UNP Q03862
x	-10	GLY	-	expression tag	UNP Q03862
x	-9	LEU	-	expression tag	UNP Q03862
x	-8	VAL	-	expression tag	UNP Q03862
x	-7	PRO	-	expression tag	UNP Q03862
x	-6	ARG	-	expression tag	UNP Q03862
x	-5	GLY	-	expression tag	UNP Q03862
x	-4	SER	-	expression tag	UNP Q03862

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Chain	Residue	Modelled	Actual	Comment	Reference
x	-3	HIS	-	expression tag	UNP Q03862
x	-2	MET	-	expression tag	UNP Q03862
x	-1	LEU	-	expression tag	UNP Q03862
x	0	GLU	-	expression tag	UNP Q03862

- Molecule 46 is a protein called CYTOPLASMIC 60S SUBUNIT BIOGENESIS FACTOR REI1.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	y	217	Total	C	H	N	O	S	0	0
			1788	1131	3	324	322	8		

- Molecule 47 is a protein called ALB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	z	85	Total	C	N	O	0	0
			510	340	85	85		

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	P	1	Total	Mg	0
			1	1	
48	B	2	Total	Mg	0
			2	2	
48	C	1	Total	Mg	0
			1	1	
48	V	1	Total	Mg	0
			1	1	
48	7	6	Total	Mg	0
			6	6	
48	N	1	Total	Mg	0
			1	1	
48	5	259	Total	Mg	0
			259	259	
48	8	7	Total	Mg	0
			7	7	
48	R	1	Total	Mg	0
			1	1	
48	y	1	Total	Mg	0
			1	1	

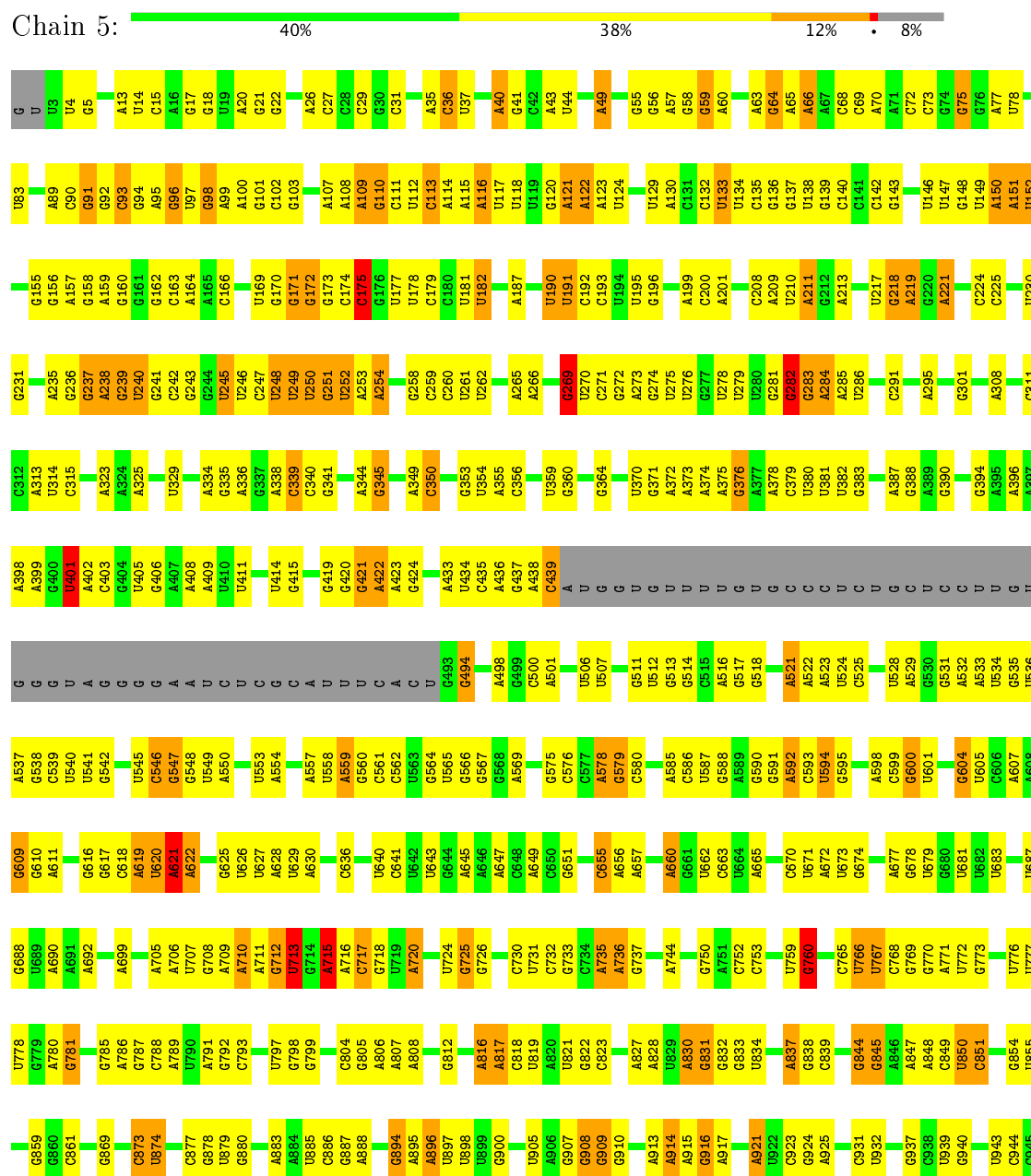
- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
49	p	1	Total 1	Zn 1	0
49	o	1	Total 1	Zn 1	0
49	j	1	Total 1	Zn 1	0
49	y	2	Total 2	Zn 2	0
49	m	1	Total 1	Zn 1	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

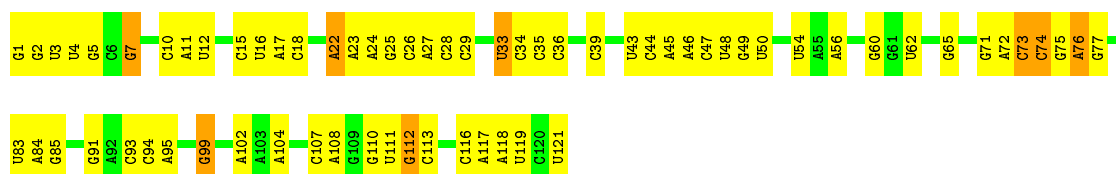
#### • Molecule 1: 25S ribosomal RNA





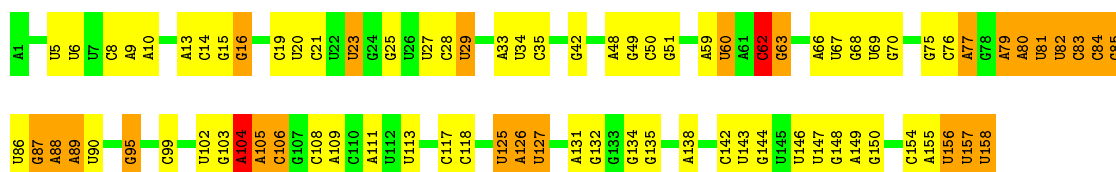

G3343	G3263	G3099	A3017	U2944	U2875	G2777	U2868	G2602	C2531	A2404	G2311	C2248
A3344	G3264	C3099	G3022	G2945	U2880	G2778	C2684	G2603	U2532	G2407	A2312	G2249
G3345	G3265	U3100	G3281	G2946	C2881	A2779	C2685	G2605	G2533	U2408	A2313	G
U3346	G	A3106	C3025	G2947	U2882	A2790	A2689	G2606	A2536	U2409	U2314	G
U3351	U3268	U3107	G3026	G2948	U2883	G2796	G2690	G2607	U2537	U2410	G2315	A
U3352	U3269	G3108	A3027	G2950	C2884	G2797	A2691	G2608	U2538	U2411	G2316	G
G3353	G3270	G3109	G3028	G2951	C2885	G2798	A2694	A2609	C2539	G	A2317	U
G3354	G3271	G3110	G3029	G2952	U2886	C2799	A2694	G2610	U2540	U2416	C2322	A
U3355	G3272	U3111	A3033	U2953	A2887	A2799	U2701	U2611	U2541	U2417	G2323	C
U3356	G3273	U3195	G3034	U2954	U2888	G2800	A2702	U2612	U2542	U2418	U	
G3357	A3273	U3196	A3035	U2955	C2889	A2801	A2703	U2613	U2543	A2419	A	
U3358	U3274	G3115	G3036	U2956	A2890	A2802	A2704	G2614	U2544	C2420	C2333	U
U3359	U3275	G3116	U3037	G2957	U2891	A2803	A2704	G2615	C2545	U2421	U2334	G
A3360	U3276	G3117	G3038	G2958	A2892	A2804		G2616	U2546	C2422	U2335	A
G3361	C3278	U3207	A3040	G2960	C2893	U2712	U2712	U2617	A2547	U2423	U2336	C
A3362	A3279	G3208	U3041	G2961	C2894	U2713	G2714	U2617	C2548	A2424	U2337	U
U3363	U3280	A3121	U3042	U2962	C2894	U2713	G2714	A2626	C2549	G2425	C2338	C
U3365	U3282	A3122	C3043	C2963	A2897	A2808		U2629	U2550	U2426	C2339	U
G3366	U3283	A3123	G3044	G2964	G2898	C2809	U2717	U2630	U2551	U2427	U2340	C2267
U3367	G3284	A3130	G3045	U2965	C2899	C2810	U2718	C2631	U2552	U2428	U2341	U2268
U3368	C3285	U3131	A3046	G2966	A2900	A2811	U2724	U2632	U2553	U2429	U2342	U2269
G3369	G3286	C3132	U3047	A2967	G2901	C2812	U2725	U2633	A2554	A2430	U2343	A2270
A3370	U3287	C3133	A3048	G2968	A2902	A2813	U2726	U2634	C2555	C2431	A2357	A2271
G3371	G3288	U3138	U3050	C2969	U2904	G2814	C2726	A2636	C2556	A2432	A2358	A2272
U3372	G3289	A3139	U3051	C2970	U2905	G2815	A2727	A2637	A2557	U2433	G2273	G2273
G3373	C3290	G3140	G3052	A2971	C2906	C2816	U2728	U2637	U2558	U2434	C2362	U2274
U3374	G3291	A3141	G3053	G2972	G2907	A2817	U2729	A2637	U2559	G2435	C2363	A2275
A3375	A3292	U3131	U3054	G2973	G2908	U2818	U2730	A2642	C2560	U2436	G2376	G2276
G3376	C3293	C3143	U3055	U2978	U2909	A2819	U2731	A2643	A2561	G2437	C2366	G2277
U3377	A3294	C3144	U3056	U2979	A2910	G2820	U2732	A2644	A2562	U2438	A2367	G2278
G3378	C3295	U3148	U3057	C2980	A2911	G2821	A2733	A2645	C2567	A2439	A2368	C2279
U3379	G3296	G3149	U3058	C2981	U2912	U2822	C2737	U2650	C2568	G	A2369	A2280
G3380	C3297	A3150	G3059	A2982	C2913	U2823	A2740	U2651	C2569	U	A2370	A2281
U3381	A3298	U3151	C3060	A2983	G2914	C2824	U2741	U2652	U2570	A	C2371	U2282
G3382	U3304	U3152	U3061	G2984	U2915	A2825	C2742	A2656	U2571	C	G2372	G2283
U3383	A3305	C	U3062	U2985	G2916	G2826		A2657	C2572	A	G2373	C2284
U3384	U3306	U	U3063	G2986	G2917	G2827		G2658	G2573	U	G2374	C2285
U3385	U3307	U	U3064	U2987	G2918	C2828		G2659	G2574	U	G2375	U2286
G3386	U3308	U	U3065	G2988	A2919	U2829		G2660	U2575	U	G2376	U2287
U3387	A3309	U	U3066	U2989	U2920	U2830		G2661	G2576	G	U2377	G2288
C3388	U3310	U	U3067	U2990	U2921	U2831		G2662	C2577	A	U2378	C2289
U3389	U3311	G1158	G3075	U2991	G2922	C2832		G2663	G2578	A	U2379	A2290
G3390	U3312	C3159	U3076	U2992	U2923	U2833		C2664	G2579	G	G2385	A2291
U3394	G3313	C3160	U3077	U2993	U2924	U2834		G2665	G2580	G	U2386	A2292
G3395	A3314	C3161	U3078	U2994	U2925	U2835		U2666	C2581	U	U2387	U2293
U3396	U3315	A3162	U3079	G2995	A2926	U2836		A2667	G2582	U	C2388	C2294
	G3316	C3163	G3083	U2996	C2927	C3001		U2668	G2583	U	A2389	A2295
	U3317	A3164	G3084	G2997	C2928	U2837		U2669	G2584	A	G2391	A2296
	U3318	C3165	G3085	U2998	C2929	U2838		G2670	G2585	G	C2392	U2297
	G3319	U3166	A3086	U2999	U2930	U2839		U2671	G2586	A	G2393	U2298
	C3320	A3167	A3087	U3000	C2931	U2840		A2672	A2589	A	U2394	A2299
	U3321	G3168	G3088	U3001	U2932	U2841		C2673	U2590	U	G2395	C2304
	G3322	U3169	C3089	U3002	U2933	U2842		C2674	A2591	U	A2397	C2305
	U3323	A3170	U3090	U3003	U2934	U2843		A2675	A2592	A	A2398	G2306
	G3324	U3171	C3092	A3012	A2935	U2844		A2676	C2593	G	G2399	C2307
	U3325	C3172	C3093	U3013	U2936	U2845		A2677	C2594	U	G2400	C2308
	G3326	A3173	G3094	U3014	U2937	U2846		A2678	U2599	G	A2401	A2309
	U3327	U3174	U3095	U3015	C2938	U2847		A2679	C2600	U	G2402	A2310
	G3328	C3175	G3096	A3016	U2939	U2848		A2680	U2599	G	G2403	
	U3329	A3176	U3097	A3017	C2940	U2849		C2682	A2601	G		
	G3330	U3177	U3098	A3018	C2941	U2850						
	U3331	C3178	U3099	A3019	C2942	U2851						
	G3332	A3179	U3100	A3020	C2943	U2852						
	U3333	U3180	U3101	A3021	C2944	U2853						
	G3334	C3181	U3102	A3022	C2945	U2854						
	U3335	A3182	U3103	A3023	C2946	U2855						
	G3336	U3183	U3104	A3024	C2947	U2856						
	U3337	C3184	U3105	A3025	C2948	U2857						
	G3338	A3185	U3106	A3026	C2949	U2858						
	U3339	U3186	U3107	A3027	C2950	U2859						
	G3340	C3187	U3108	A3028	C2951	U2860						
	U3341	A3188	U3109	A3029	C2952	U2861						
	G3342	U3189	U3110	A3030	C2953	U2862						
	U3343	C3190	U3111	A3031	C2954	U2863						
	G3344	A3191	U3112	A3032	C2955	U2864						
	U3345	U3192	U3113	A3033	C2956	U2865						
	G3346	C3193	U3114	A3034	C2957	U2866						
	U3347	A3194	U3115	A3035	C2958	U2867						
	G3348	U3195	U3116	A3036	C2959	U2868						
	U3349	C3196	U3117	A3037	C2960	U2869						
	G3350	A3197	U3118	A3038	C2961	U2870						
	U3351	U3198	U3119	A3039	C2962	U2871						
	G3352	C3199	U3120	A3040	C2963	U2872						
	U3353	A3200	U3121	A3041	C2964	U2873						
	G3354	U3201	U3122	A3042	C2965	U2874						
	U3355	C3202	A3123	C3043	C2966	U2875						
	G3356	U3203	A3124	G3044	C2967	U2876						
	U3357	A3204	A3212	G3045	C2968	U2877						
	G3358	U3205	A3213	G3046	C2969	U2878						
	U3359	C3206	A3214	G3047	C2970	U2879						
	G3360	U3207	A3215	G3048	C2971	U2880						
	U3361	A3208	A3216	G3049	C2972	U2881						
	G3362	C3209	A3217	G3050	C2973	U2882						
	U3363	U3210	A3218	G3051	C2974	U2883						
	G3364	A3211	A3219	G3052	C2975	U2884						
	U3365	C3212	A3220	G3053	C2976	U2885						
	G3366	U3213	A3221	G3054	C2977	U2886						
	U3367	A3214	A3222	G3055	C2978	U2887						
	G3368	C3215	A3223	G3056	C2979	U2888						
	U3369	U3216	A3224	G3057	C2980	U2889						
	G3370	A3217	A3225	G3058	C2981	U2890						
	U3371	C3218	A3226	G3059	C2982	U2891						
	G3372	U3219	A3227	G3060	C2983	U2892						
	U3373	A3220	A3228	G3061	C2984	U2893						
	G3374	C3221	A3229	G3062	C2985	U2894						
	U3375	U3222	A3230	G3063	C2986	U2895						
	G3376	A3223	A3231	G3064	C2987	U2896						
	U3377	C3224	A3232	G3065	C2988	U2897						
	G3378	U3225	A3233	G3066	C2989	U2898						
	U3379	A3226	A3234	G3067	C2990	U2899						
	G3380	C3227	A3235	G3068	C2991	U2900						
	U3381	U3228	A3236	G3069	C2992	U2901						
	G3382	A3229	A3237	G3070	C2993	U2902						
	U3383	C3230	A3238	G3071	C2994	U2903						
	G3384	U3231	A3239	G3072	C2995	U2904						
	U3385	A3232	A3240	G3073	C2996	U2905						
	G3386	C3233	A3241	G3074	C2997	U2906						





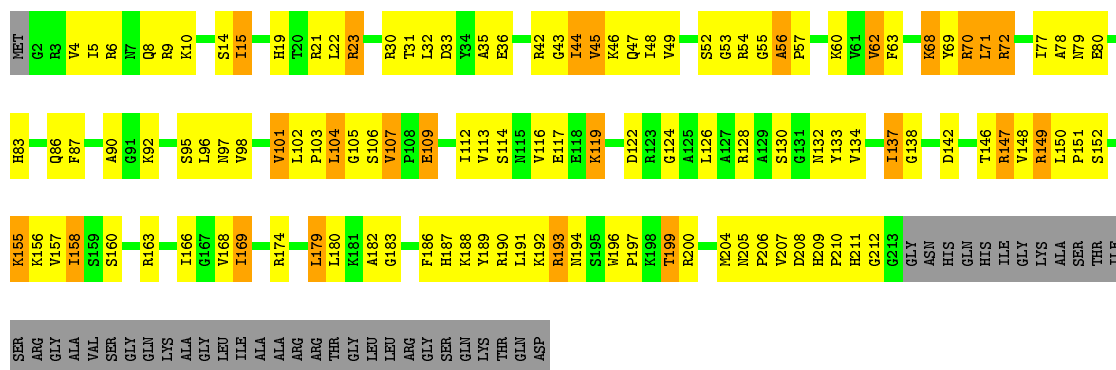
• Molecule 3: 5.8S ribosomal RNA

Chain 8: 47% 35% 16% .



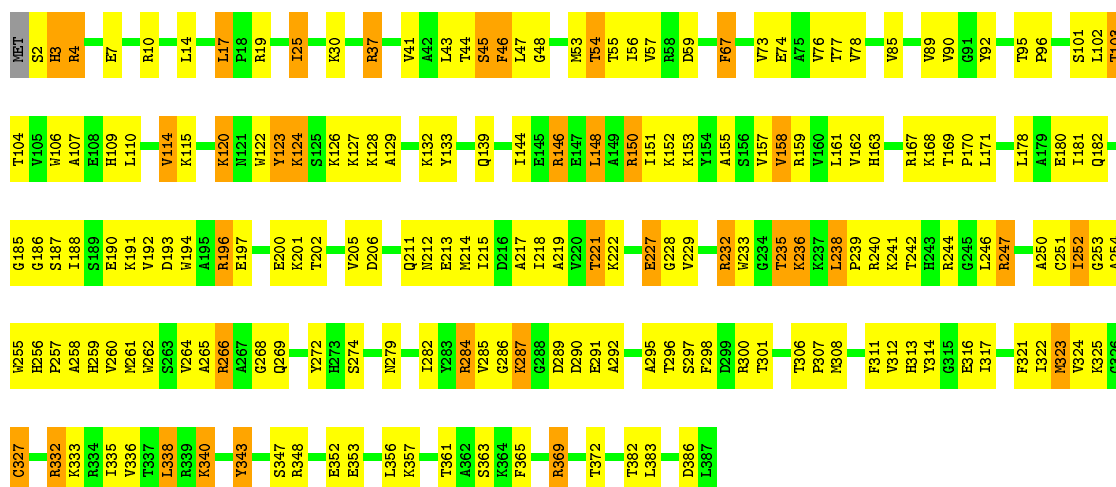
• Molecule 4: 60S ribosomal protein L2-A

Chain A: 36% 38% 9% 17%

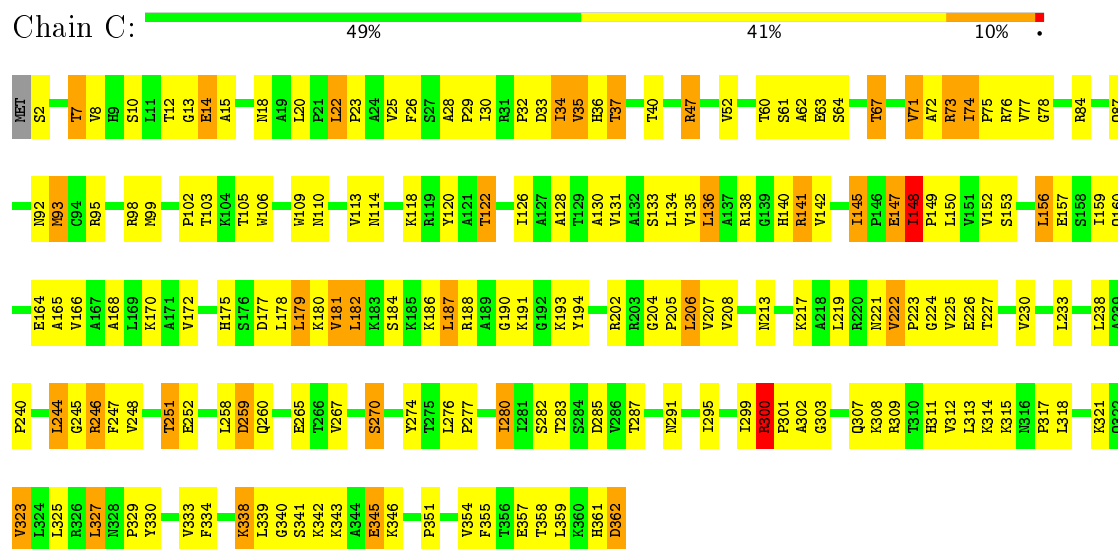


• Molecule 5: 60S ribosomal protein L3

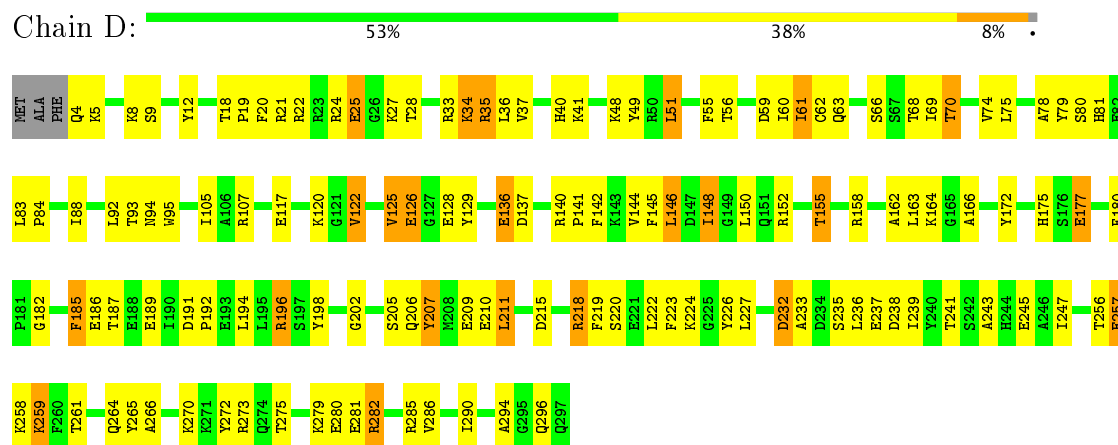
Chain B: 50% 40% 10%



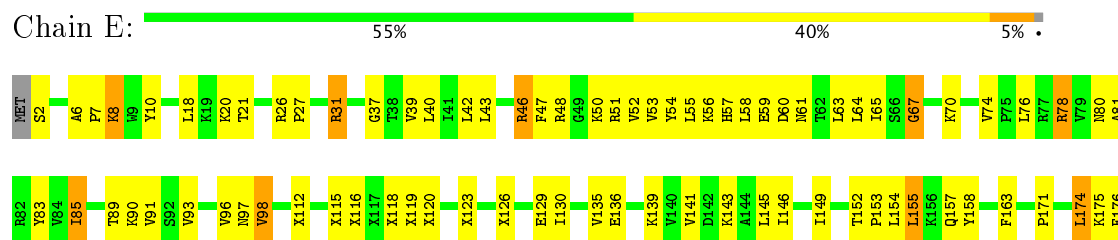
• Molecule 6: 60S ribosomal protein L4-A



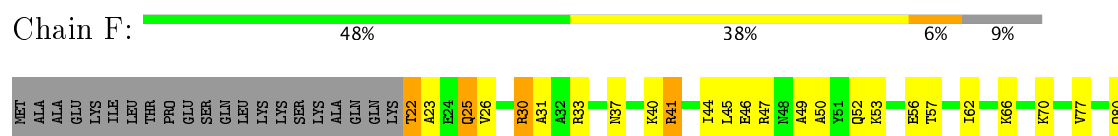
- Molecule 7: 60S ribosomal protein L5

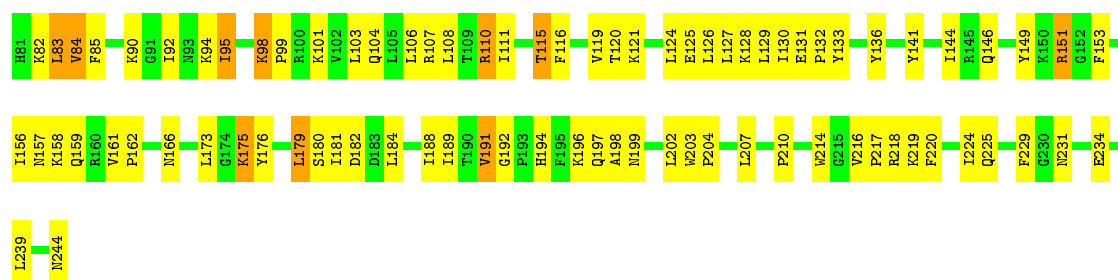


- Molecule 8: 60S RIBOSOMAL PROTEIN EL6

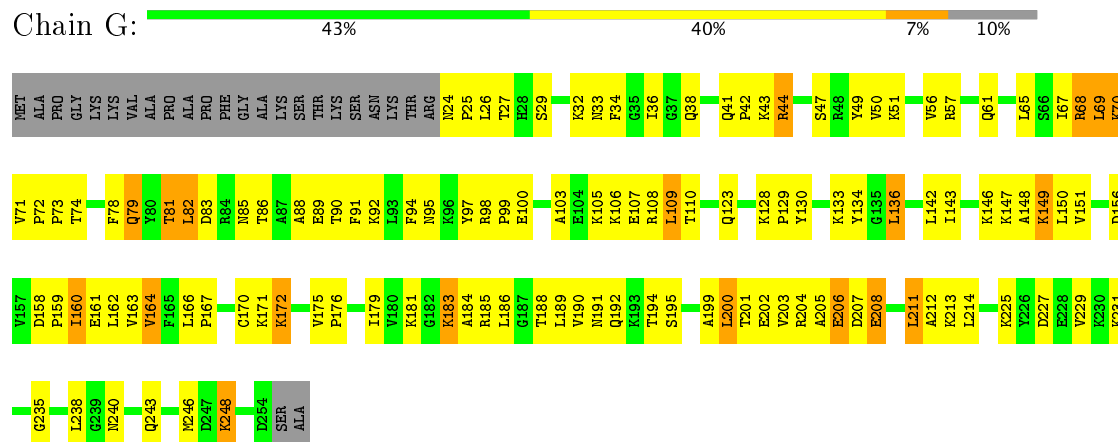


- Molecule 9: 60S ribosomal protein L7-A

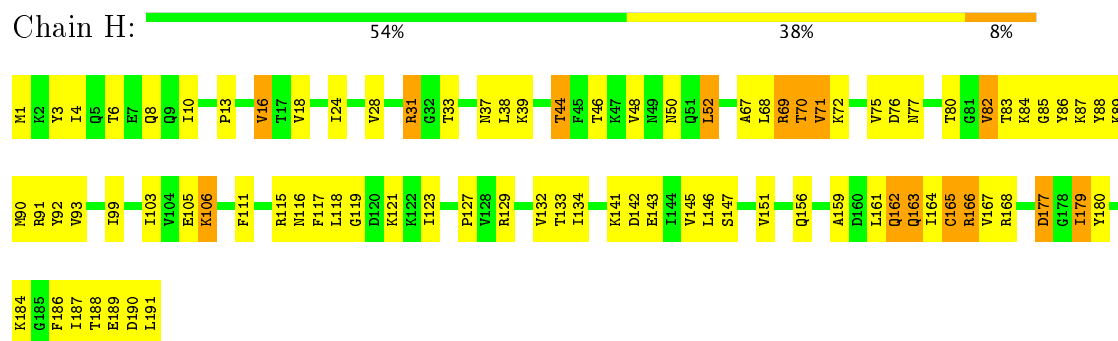




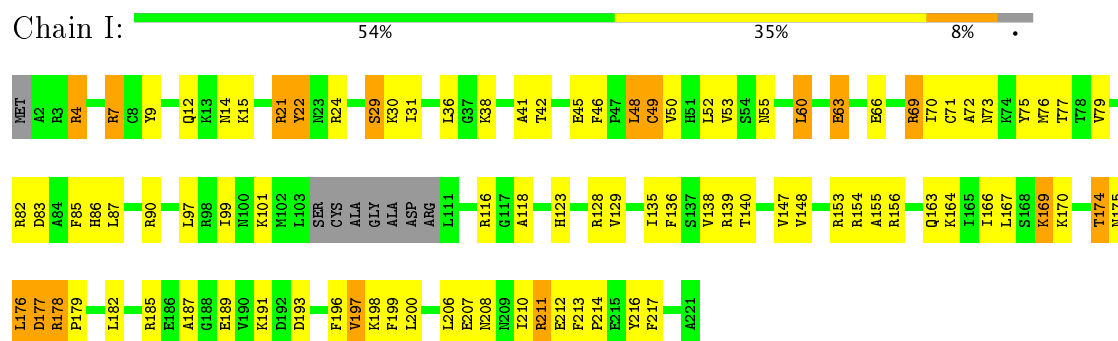
- Molecule 10: 60S ribosomal protein L8-A



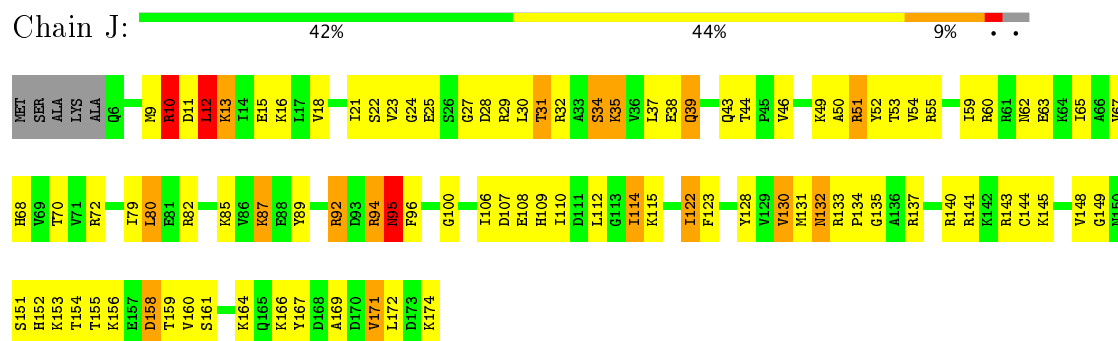
- Molecule 11: 60S ribosomal protein L9-A



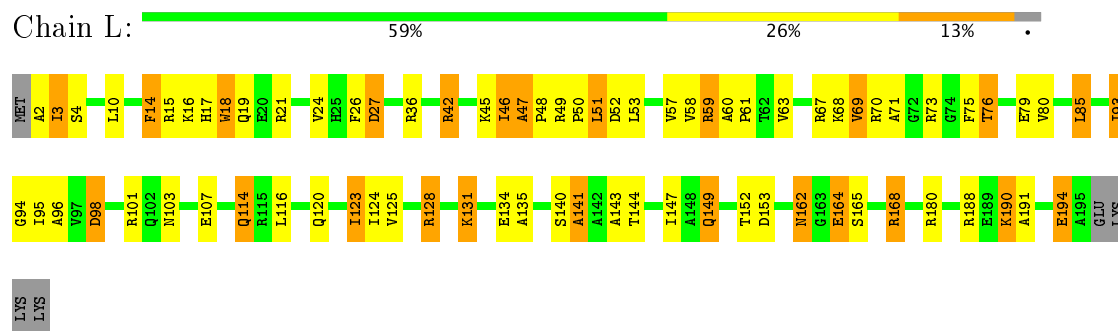
- Molecule 12: 60S ribosomal protein L10



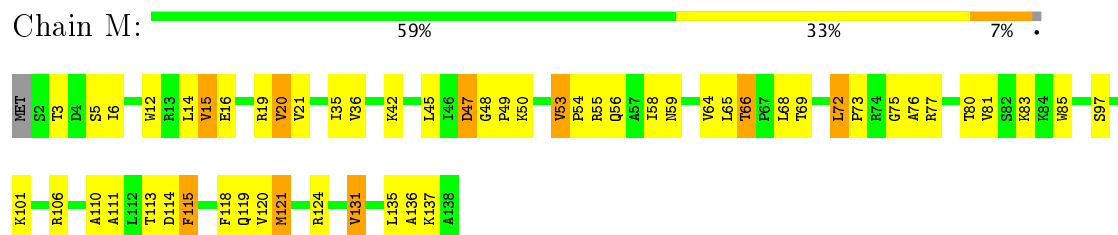
- Molecule 13: 60S ribosomal protein L11-A



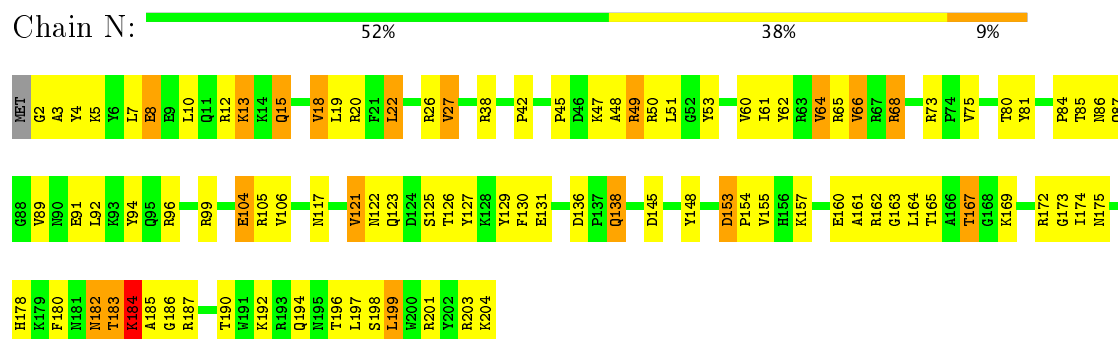
- Molecule 14: 60S ribosomal protein L13-A



- Molecule 15: 60S ribosomal protein L14-A

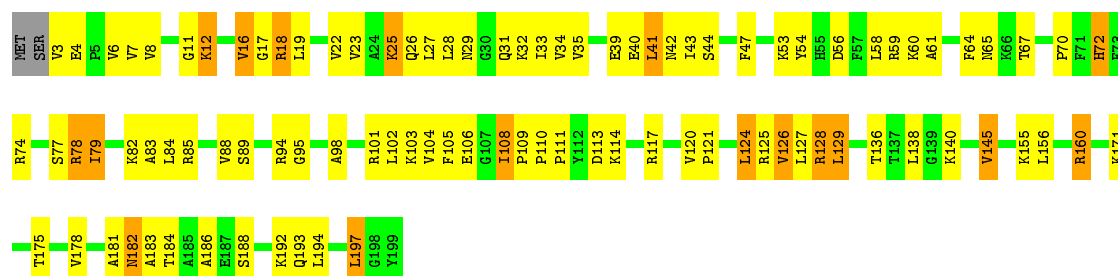


- Molecule 16: 60S ribosomal protein L15-A



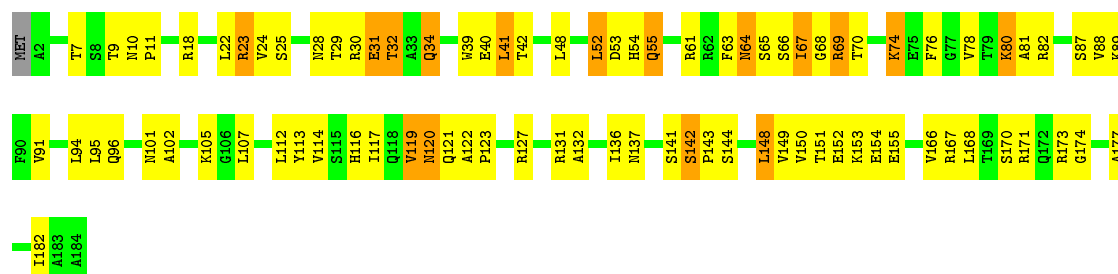
- Molecule 17: 60S ribosomal protein L16-A





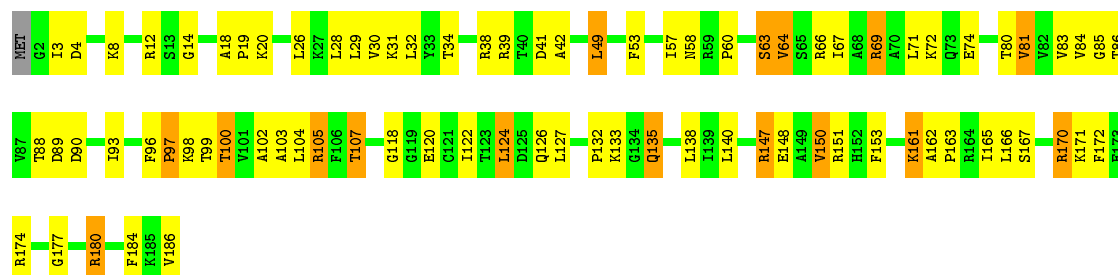
• Molecule 18: 60S ribosomal protein L17-A

Chain P: 53% 38% 9%



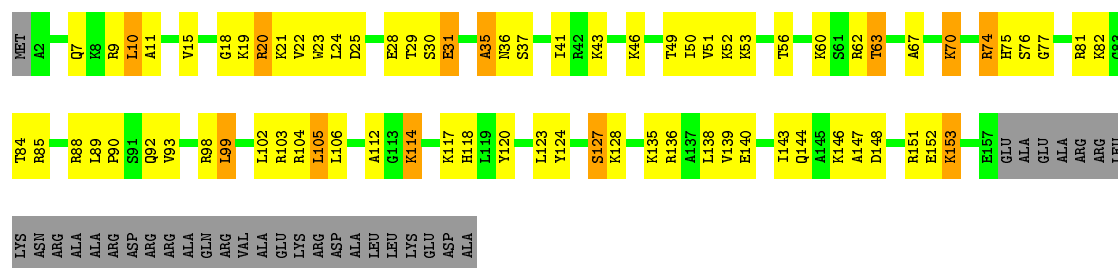
• Molecule 19: 60S ribosomal protein L18-A

Chain Q: 55% 35% 9%



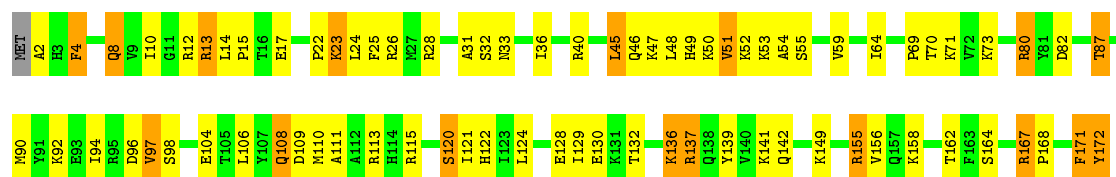
• Molecule 20: 60S ribosomal protein L19-A

Chain R: 42% 34% 6% 17%

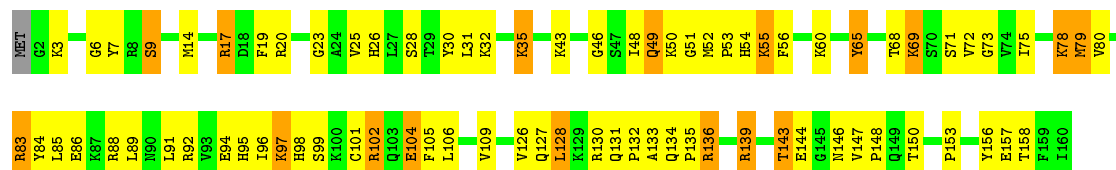


• Molecule 21: 60S ribosomal protein L20-A

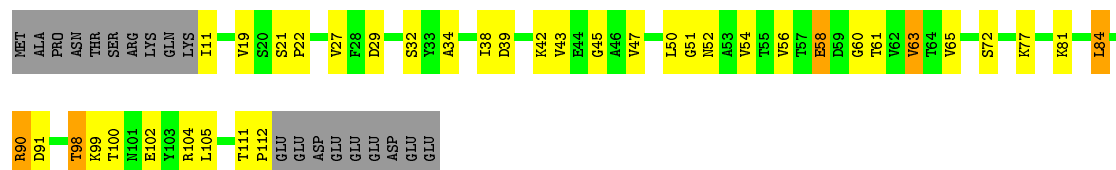
Chain S: 55% 35% 10%



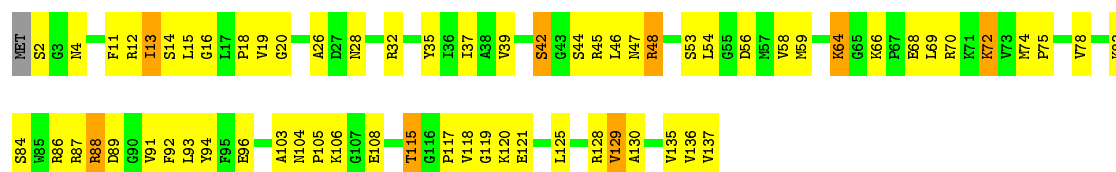
- Molecule 22: 60S ribosomal protein L21-A



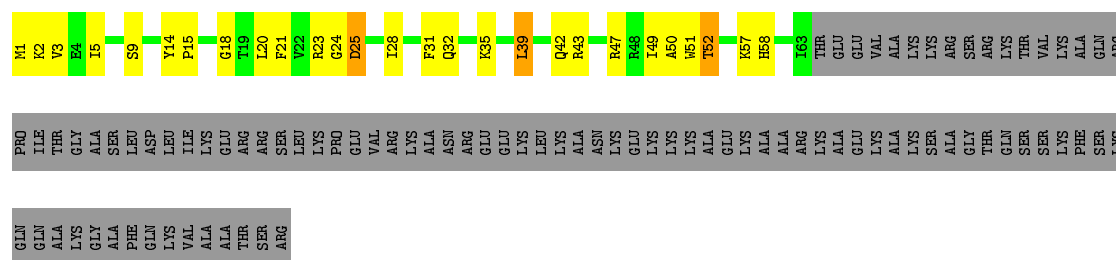
- Molecule 23: 60S ribosomal protein L22-A



- Molecule 24: 60S ribosomal protein L23-A

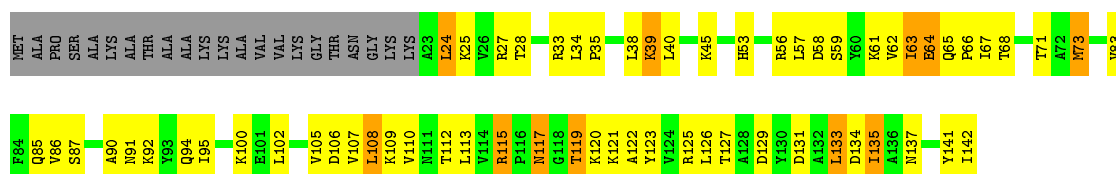


- Molecule 25: 60S ribosomal protein L24-A

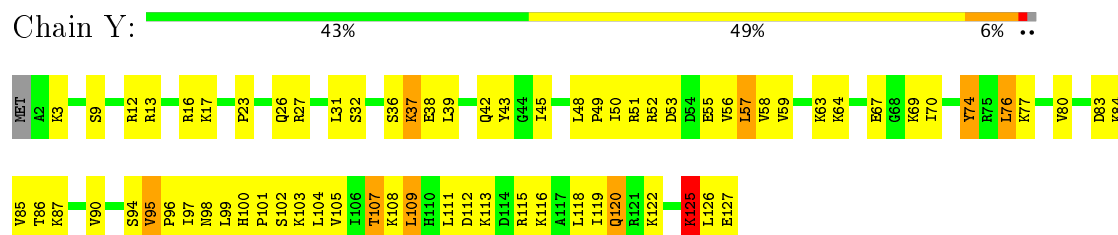


- Molecule 26: 60S ribosomal protein L25

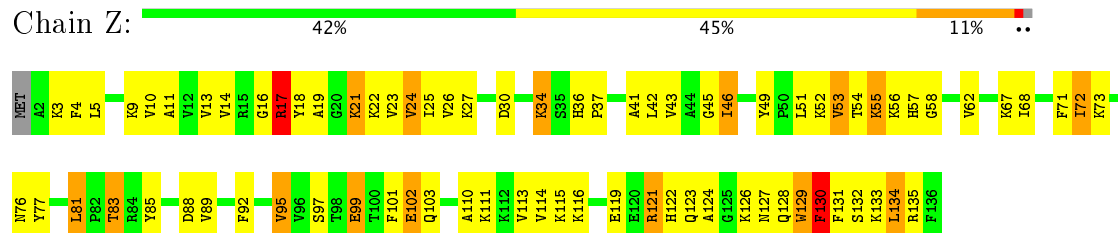




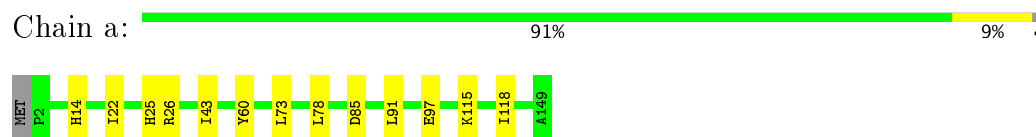
- Molecule 27: 60S ribosomal protein L26-A



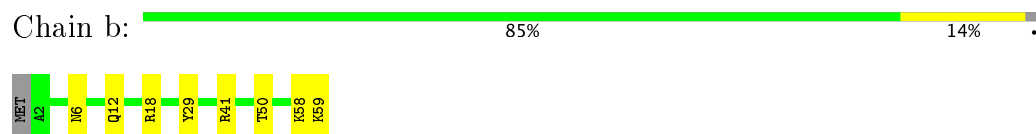
- Molecule 28: 60S ribosomal protein L27-A



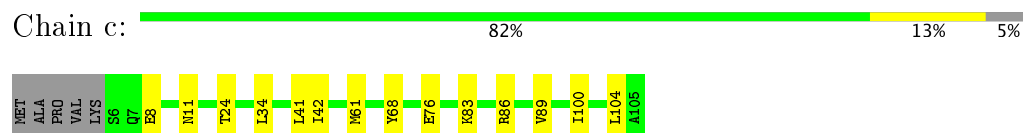
- Molecule 29: 60S ribosomal protein L28



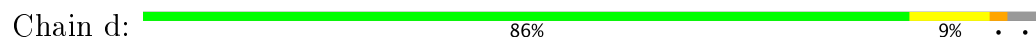
- Molecule 30: 60S ribosomal protein L29



- Molecule 31: 60S ribosomal protein L30



- Molecule 32: 60S ribosomal protein L31-A





- Molecule 33: 60S ribosomal protein L32

Chain e: 87% 12%



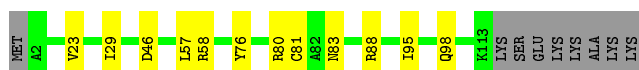
- Molecule 34: 60S ribosomal protein L33-A

Chain f: 93% 6%



- Molecule 35: 60S ribosomal protein L34-A

Chain g: 83% 10% 7%



- Molecule 36: 60S ribosomal protein L35-A

Chain h: 83% 16%



- Molecule 37: 60S ribosomal protein L36-A

Chain i: 76% 23%



- Molecule 38: 60S ribosomal protein L37-A

Chain j: 86% 13%



- Molecule 39: 60S ribosomal protein L38

Chain k: 88% 10%






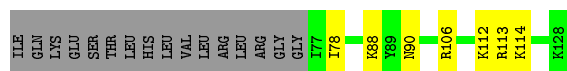
- Molecule 40: 60S ribosomal protein L39

Chain l:  78% 20%




- Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain m:  35% 5% 59%




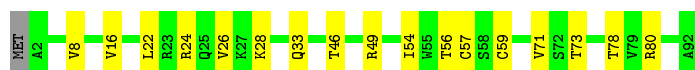
- Molecule 42: 60S ribosomal protein L42-A

Chain o:  82% 17%



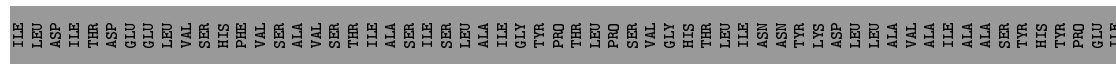
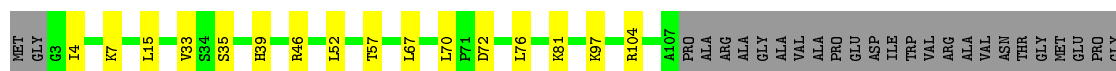
- Molecule 43: 60S ribosomal protein L43-A

Chain p:  80% 18%




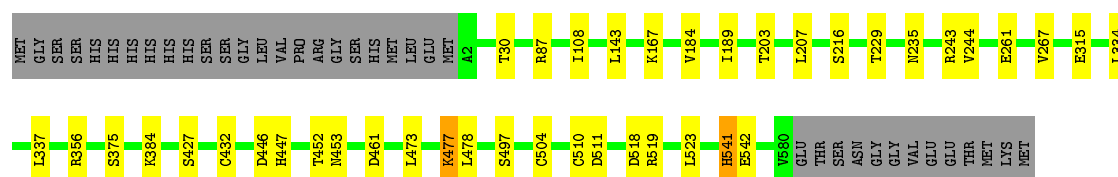
- Molecule 44: 60S acidic ribosomal protein P0

Chain q:  33% 6% 62%



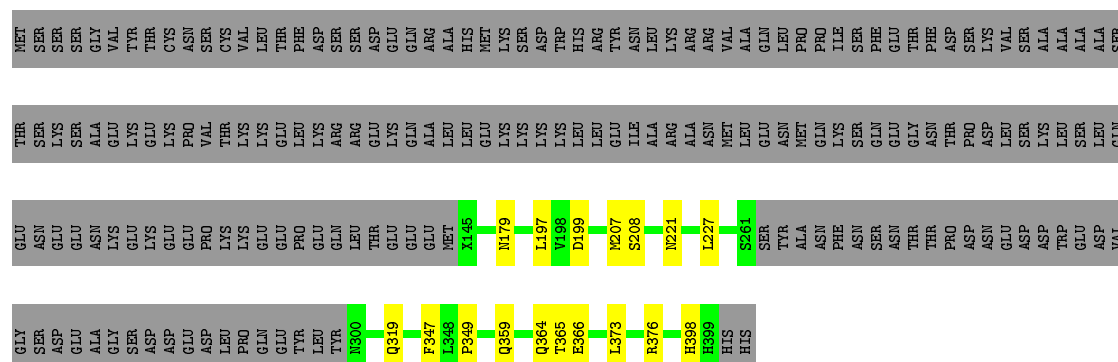
- Molecule 45: Probable metalloprotease ARX1

Chain x:  87% 6% 6%

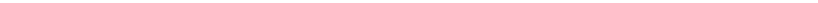


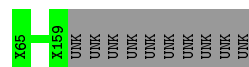
- Molecule 46: CYTOPLASMIC 60S SUBUNIT BIOGENESIS FACTOR REI1

Chain y:  50% 1% 46%



- Molecule 47: ALB1

Chain z:  89% 11%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	134701	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PER DETECTOR FRAME	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20	Depositor
Minimum defocus (nm)	800.00	Depositor
Maximum defocus (nm)	3000.00	Depositor
Magnification	100720	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: Y5P, ZN, P5P, MG

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  > 2$	RMSZ	# $ Z  > 2$
1	5	0.66	12/74039 (0.0%)	1.09	121/115426 (0.1%)
10	G	0.38	0/1795	0.58	0/2429
11	H	0.40	0/1539	0.54	0/2073
12	I	0.36	0/1758	0.57	0/2358
13	J	0.34	0/1374	0.55	0/1842
14	L	0.46	0/1573	0.61	0/2113
15	M	0.38	0/1074	0.55	0/1446
16	N	0.52	0/1757	0.65	0/2354
17	O	0.48	0/1585	0.63	1/2128 (0.0%)
18	P	0.50	0/1465	0.60	0/1968
19	Q	0.42	0/1465	0.61	0/1965
2	7	0.41	0/2883	0.90	1/4491 (0.0%)
20	R	0.39	0/1275	0.52	0/1702
21	S	0.45	0/1473	0.59	0/1980
22	T	0.42	0/1300	0.56	0/1743
23	U	0.36	0/825	0.56	0/1120
24	V	0.43	0/1018	0.60	0/1369
25	W	0.40	0/533	0.53	0/707
26	X	0.42	0/974	0.62	0/1314
27	Y	0.43	0/1004	0.62	0/1341
28	Z	0.38	0/1118	0.62	0/1497
29	a	0.47	0/1204	0.64	0/1612
3	8	0.69	0/3746	1.12	8/5832 (0.1%)
30	b	0.39	0/473	0.53	0/629
31	c	0.35	0/775	0.52	0/1040
32	d	0.46	0/897	0.62	0/1205
33	e	0.52	0/1055	0.63	0/1413
34	f	0.52	0/868	0.67	0/1168
35	g	0.43	0/890	0.63	0/1189
36	h	0.42	0/974	0.58	0/1297
37	i	0.35	0/777	0.55	0/1033
38	j	0.51	0/696	0.65	0/923

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	k	0.34	0/614	0.53	0/822
4	A	0.41	0/1662	0.60	0/2236
40	l	0.46	0/443	0.57	0/588
41	m	0.40	0/423	0.55	0/562
42	o	0.41	0/860	0.56	0/1136
43	p	0.46	0/701	0.62	0/934
44	q	0.58	0/977	0.61	0/1313
45	x	0.37	0/4557	0.57	0/6189
46	y	0.39	0/1746	0.54	0/2346
5	B	0.46	0/3146	0.59	0/4228
6	C	0.47	0/2800	0.67	1/3790 (0.0%)
7	D	0.34	0/2408	0.50	0/3248
8	E	0.39	0/1269	0.58	0/1705
9	F	0.46	0/1828	0.58	0/2461
All	All	0.57	12/137616 (0.0%)	0.93	132/202265 (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
14	L	0	1
16	N	0	1
27	Y	0	1
28	Z	0	1
32	d	0	3
37	i	0	1
45	x	0	3
46	y	0	1
6	C	0	3
8	E	0	1
All	All	0	16

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1152	G	N9-C4	-7.14	1.32	1.38
1	5	2368	A	N9-C4	-6.55	1.33	1.37
1	5	336	A	N9-C4	-6.44	1.33	1.37
1	5	2392	C	N1-C6	-6.25	1.33	1.37
1	5	1446	A	N9-C4	-6.19	1.34	1.37

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1152	G	N3-C4-C5	10.03	133.61	128.60
1	5	408	A	N1-C6-N6	-8.94	113.24	118.60
1	5	1232	C	O4'-C1'-N1	8.59	115.07	108.20
1	5	2193	U	N1-C2-N3	8.32	119.89	114.90
3	8	62	C	C6-N1-C2	8.32	123.63	120.30

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	C	145	ILE	Peptide
6	C	148	ILE	Peptide
6	C	300	ARG	Peptide
8	E	67	GLY	Peptide
14	L	141	ALA	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	5	66537	0	33466	1531	0
2	7	2579	0	1304	66	0
3	8	3353	0	1695	81	0
4	A	1630	0	1682	124	0
5	B	3075	0	3142	185	0
6	C	2748	0	2859	171	0
7	D	2359	0	2311	131	0
8	E	1356	0	1448	98	0
9	F	1791	0	1869	114	0
10	G	1763	0	1819	117	0
11	H	1518	0	1587	77	0
12	I	1722	0	1755	101	0
13	J	1353	0	1383	89	0
14	L	1548	0	1613	91	0
15	M	1059	0	1154	55	0
16	N	1720	0	1779	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	O	1555	0	1659	96	0
18	P	1442	0	1485	72	0
19	Q	1441	0	1543	77	0
20	R	1258	0	1342	70	0
21	S	1437	0	1475	77	0
22	T	1276	0	1323	87	0
23	U	808	0	822	24	0
24	V	1003	0	1048	71	0
25	W	521	0	551	26	0
26	X	959	0	1023	64	0
27	Y	993	0	1081	81	0
28	Z	1092	0	1155	73	0
29	a	1173	0	1215	0	0
30	b	462	0	491	0	0
31	c	767	0	816	0	0
32	d	883	0	918	0	0
33	e	1034	0	1101	0	0
34	f	850	0	880	0	0
35	g	880	0	945	0	0
36	h	965	0	1067	0	0
37	i	770	0	846	0	0
38	j	681	0	683	0	0
39	k	608	0	671	0	0
40	l	436	0	475	0	0
41	m	417	0	455	0	0
42	o	847	0	914	0	0
43	p	694	0	734	0	0
44	q	962	0	989	0	0
45	x	4477	0	4559	0	0
46	y	1785	3	1755	0	0
47	z	510	0	517	0	0
48	5	259	0	0	0	0
48	7	6	0	0	0	0
48	8	7	0	0	0	0
48	B	2	0	0	0	0
48	C	1	0	0	0	0
48	N	1	0	0	0	0
48	P	1	0	0	0	0
48	R	1	0	0	0	0
48	V	1	0	0	0	0
48	y	1	0	0	0	0
49	j	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	m	1	0	0	0	0
49	o	1	0	0	0	0
49	p	1	0	0	0	0
49	y	2	0	0	0	0
All	All	129383	3	95404	3548	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

The worst 5 of 3548 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:48:GLY:HA3	15:M:53:VAL:HG13	1.25	1.18
4:A:149:ARG:HH12	4:A:155:LYS:HE3	1.06	1.18
8:E:78:ARG:HG3	8:E:78:ARG:HH11	1.03	1.14
5:B:4:ARG:HG3	5:B:4:ARG:HH11	1.03	1.12
10:G:44:ARG:HH11	10:G:44:ARG:HG3	1.15	1.11

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	210/254 (83%)	195 (93%)	14 (7%)	1 (0%)	32	71
5	B	384/387 (99%)	367 (96%)	17 (4%)	0	100	100
6	C	359/362 (99%)	329 (92%)	28 (8%)	2 (1%)	28	68
7	D	292/297 (98%)	282 (97%)	8 (3%)	2 (1%)	25	66
8	E	155/176 (88%)	143 (92%)	9 (6%)	3 (2%)	9	45
9	F	221/244 (91%)	210 (95%)	10 (4%)	1 (0%)	32	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	G	229/256 (90%)	200 (87%)	28 (12%)	1 (0%)	38	75
11	H	189/191 (99%)	178 (94%)	10 (5%)	1 (0%)	32	71
12	I	209/221 (95%)	193 (92%)	16 (8%)	0	100	100
13	J	167/174 (96%)	143 (86%)	18 (11%)	6 (4%)	4	31
14	L	192/199 (96%)	170 (88%)	20 (10%)	2 (1%)	18	59
15	M	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
16	N	201/204 (98%)	187 (93%)	13 (6%)	1 (0%)	32	71
17	O	195/199 (98%)	193 (99%)	2 (1%)	0	100	100
18	P	181/184 (98%)	176 (97%)	5 (3%)	0	100	100
19	Q	183/186 (98%)	174 (95%)	8 (4%)	1 (0%)	32	71
20	R	154/189 (82%)	148 (96%)	5 (3%)	1 (1%)	28	68
21	S	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
22	T	157/160 (98%)	151 (96%)	4 (2%)	2 (1%)	14	53
23	U	100/121 (83%)	95 (95%)	5 (5%)	0	100	100
24	V	134/137 (98%)	130 (97%)	4 (3%)	0	100	100
25	W	61/155 (39%)	57 (93%)	3 (5%)	1 (2%)	11	49
26	X	118/142 (83%)	109 (92%)	9 (8%)	0	100	100
27	Y	124/127 (98%)	118 (95%)	5 (4%)	1 (1%)	22	63
28	Z	133/136 (98%)	112 (84%)	18 (14%)	3 (2%)	7	42
29	a	146/149 (98%)	132 (90%)	13 (9%)	1 (1%)	25	66
30	b	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
31	c	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
32	d	107/113 (95%)	97 (91%)	8 (8%)	2 (2%)	9	45
33	e	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
34	f	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
35	g	110/121 (91%)	104 (94%)	5 (4%)	1 (1%)	20	61
36	h	117/120 (98%)	109 (93%)	8 (7%)	0	100	100
37	i	97/100 (97%)	86 (89%)	8 (8%)	3 (3%)	5	35
38	j	85/88 (97%)	77 (91%)	8 (9%)	0	100	100
39	k	75/78 (96%)	70 (93%)	4 (5%)	1 (1%)	14	53
40	l	48/51 (94%)	47 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	m	50/128 (39%)	46 (92%)	3 (6%)	1 (2%)	9	44
42	o	103/106 (97%)	94 (91%)	9 (9%)	0	100	100
43	p	89/92 (97%)	82 (92%)	7 (8%)	0	100	100
44	q	116/312 (37%)	111 (96%)	4 (3%)	1 (1%)	20	61
45	x	577/616 (94%)	544 (94%)	32 (6%)	1 (0%)	51	84
46	y	201/401 (50%)	191 (95%)	10 (5%)	0	100	100
All	All	6958/7887 (88%)	6511 (94%)	407 (6%)	40 (1%)	33	68

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	E	98	VAL
13	J	10	ARG
13	J	95	ASN
16	N	184	LYS
25	W	25	ASP

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	166/196 (85%)	133 (80%)	33 (20%)	1	7
5	B	321/323 (99%)	260 (81%)	61 (19%)	2	8
6	C	288/289 (100%)	234 (81%)	54 (19%)	2	8
7	D	243/245 (99%)	209 (86%)	34 (14%)	4	21
8	E	135/136 (99%)	123 (91%)	12 (9%)	11	43
9	F	187/205 (91%)	168 (90%)	19 (10%)	8	36
10	G	177/208 (85%)	150 (85%)	27 (15%)	3	18
11	H	171/171 (100%)	148 (86%)	23 (14%)	4	23
12	I	179/187 (96%)	153 (86%)	26 (14%)	4	20
13	J	147/150 (98%)	122 (83%)	25 (17%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	L	154/159 (97%)	126 (82%)	28 (18%)	2	9
15	M	108/109 (99%)	95 (88%)	13 (12%)	6	28
16	N	175/176 (99%)	143 (82%)	32 (18%)	2	9
17	O	160/162 (99%)	129 (81%)	31 (19%)	1	7
18	P	145/146 (99%)	118 (81%)	27 (19%)	2	8
19	Q	150/151 (99%)	127 (85%)	23 (15%)	3	18
20	R	129/154 (84%)	106 (82%)	23 (18%)	2	10
21	S	155/156 (99%)	131 (84%)	24 (16%)	3	17
22	T	136/137 (99%)	113 (83%)	23 (17%)	2	13
23	U	89/107 (83%)	80 (90%)	9 (10%)	9	37
24	V	104/105 (99%)	93 (89%)	11 (11%)	8	34
25	W	55/129 (43%)	52 (94%)	3 (6%)	25	62
26	X	104/118 (88%)	86 (83%)	18 (17%)	2	12
27	Y	109/110 (99%)	96 (88%)	13 (12%)	6	28
28	Z	115/116 (99%)	92 (80%)	23 (20%)	1	7
29	a	118/119 (99%)	106 (90%)	12 (10%)	8	36
30	b	46/47 (98%)	38 (83%)	8 (17%)	2	12
31	c	84/88 (96%)	70 (83%)	14 (17%)	2	13
32	d	94/97 (97%)	85 (90%)	9 (10%)	10	39
33	e	110/111 (99%)	94 (86%)	16 (14%)	4	20
34	f	90/91 (99%)	84 (93%)	6 (7%)	19	57
35	g	95/103 (92%)	84 (88%)	11 (12%)	6	29
36	h	103/105 (98%)	84 (82%)	19 (18%)	2	9
37	i	80/82 (98%)	61 (76%)	19 (24%)	1	3
38	j	70/71 (99%)	59 (84%)	11 (16%)	3	17
39	k	67/69 (97%)	60 (90%)	7 (10%)	8	35
40	l	45/46 (98%)	35 (78%)	10 (22%)	1	4
41	m	47/116 (40%)	41 (87%)	6 (13%)	5	25
42	o	90/91 (99%)	72 (80%)	18 (20%)	1	7
43	p	71/72 (99%)	54 (76%)	17 (24%)	1	3
44	q	105/254 (41%)	88 (84%)	17 (16%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	x	508/540 (94%)	469 (92%)	39 (8%)	15	50
46	y	187/355 (53%)	171 (91%)	16 (9%)	12	45
All	All	5912/6602 (90%)	5042 (85%)	870 (15%)	7	19

5 of 870 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	O	41	LEU
20	R	114	LYS
44	q	52	LEU
17	O	108	ILE
18	P	127	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
17	O	122	GLN
22	T	77	ASN
45	x	377	GLN
18	P	55	GLN
20	R	58	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	5	3084/3396 (90%)	669 (21%)	73 (2%)
2	7	120/121 (99%)	14 (11%)	0
3	8	157/158 (99%)	36 (22%)	5 (3%)
All	All	3361/3675 (91%)	719 (21%)	78 (2%)

5 of 719 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	5	14	U
1	5	15	C
1	5	22	G
1	5	26	A
1	5	40	A

5 of 78 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	5	1816	A
1	5	2418	G
1	5	3357	U
1	5	1819	U
1	5	2204	C

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

20 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	Y5P	5	1986	1	15,19,20	2.53	2 (13%)	19,26,29	1.53	2 (10%)
1	Y5P	5	1987	1	15,19,20	2.54	2 (13%)	19,26,29	1.52	2 (10%)
1	Y5P	5	1988	1	15,19,20	2.54	2 (13%)	19,26,29	1.51	2 (10%)
1	Y5P	5	1989	1	15,19,20	2.54	2 (13%)	19,26,29	1.47	2 (10%)
1	Y5P	5	1990	1	15,19,20	2.53	2 (13%)	19,26,29	1.53	2 (10%)
1	Y5P	5	1991	1	15,19,20	2.57	2 (13%)	19,26,29	1.49	2 (10%)
1	Y5P	5	1992	1	15,19,20	2.50	2 (13%)	19,26,29	1.53	2 (10%)
1	Y5P	5	1993	1	15,19,20	2.58	2 (13%)	19,26,29	1.47	2 (10%)
1	Y5P	5	1994	1	15,19,20	2.55	2 (13%)	19,26,29	1.54	2 (10%)
1	Y5P	5	1995	1	15,19,20	2.53	2 (13%)	19,26,29	1.48	2 (10%)
1	P5P	5	2016	1	16,23,24	0.83	0	14,33,36	0.86	1 (7%)
1	P5P	5	2017	1	16,23,24	0.83	0	14,33,36	0.86	0
1	P5P	5	2018	1	16,23,24	0.83	0	14,33,36	0.87	0
1	P5P	5	2019	1	16,23,24	0.84	0	14,33,36	0.90	0
1	P5P	5	2020	1	16,23,24	0.83	0	14,33,36	0.87	0
1	P5P	5	2021	1	16,23,24	0.82	0	14,33,36	0.83	0
1	P5P	5	2022	1	16,23,24	0.83	0	14,33,36	0.89	0
1	P5P	5	2023	1	16,23,24	0.86	0	14,33,36	0.93	0
1	P5P	5	2024	1	16,23,24	0.82	0	14,33,36	0.87	0
1	P5P	5	2025	1	16,23,24	0.82	0	14,33,36	0.85	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	Y5P	5	1986	1	-	0/7/33/34	0/2/2/2
1	Y5P	5	1987	1	-	0/7/33/34	0/2/2/2
1	Y5P	5	1988	1	-	0/7/33/34	0/2/2/2
1	Y5P	5	1989	1	-	0/7/33/34	0/2/2/2
1	Y5P	5	1990	1	-	0/7/33/34	0/2/2/2
1	Y5P	5	1991	1	-	0/7/33/34	0/2/2/2
1	Y5P	5	1992	1	-	0/7/33/34	0/2/2/2
1	Y5P	5	1993	1	-	0/7/33/34	0/2/2/2
1	Y5P	5	1994	1	-	0/7/33/34	0/2/2/2
1	Y5P	5	1995	1	-	0/7/33/34	0/2/2/2
1	P5P	5	2016	1	-	0/3/25/26	0/3/3/3
1	P5P	5	2017	1	-	0/3/25/26	0/3/3/3
1	P5P	5	2018	1	-	0/3/25/26	0/3/3/3
1	P5P	5	2019	1	-	0/3/25/26	0/3/3/3
1	P5P	5	2020	1	-	0/3/25/26	0/3/3/3
1	P5P	5	2021	1	-	0/3/25/26	0/3/3/3
1	P5P	5	2022	1	-	0/3/25/26	0/3/3/3
1	P5P	5	2023	1	-	0/3/25/26	0/3/3/3
1	P5P	5	2024	1	-	0/3/25/26	0/3/3/3
1	P5P	5	2025	1	-	0/3/25/26	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	5	1991	Y5P	C4-N3	-8.82	1.38	1.46
1	5	1993	Y5P	C4-N3	-8.74	1.38	1.46
1	5	1987	Y5P	C4-N3	-8.71	1.38	1.46
1	5	1995	Y5P	C4-N3	-8.67	1.38	1.46
1	5	1989	Y5P	C4-N3	-8.66	1.38	1.46

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	1986	Y5P	N1-C2-N3	-3.98	114.34	125.46
1	5	1994	Y5P	N1-C2-N3	-3.97	114.37	125.46
1	5	1992	Y5P	N1-C2-N3	-3.92	114.50	125.46
1	5	1990	Y5P	N1-C2-N3	-3.91	114.53	125.46
1	5	1988	Y5P	N1-C2-N3	-3.88	114.61	125.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	5	1987	Y5P	1	0
1	5	1988	Y5P	1	0
1	5	1989	Y5P	2	0
1	5	1990	Y5P	2	0
1	5	1991	Y5P	1	0
1	5	1992	Y5P	1	0
1	5	1993	Y5P	1	0
1	5	1994	Y5P	1	0
1	5	2017	P5P	1	0
1	5	2018	P5P	1	0
1	5	2023	P5P	1	0
1	5	2024	P5P	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 286 ligands modelled in this entry, 286 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
47	<i>z</i>	2
1	<i>5</i>	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	<i>z</i>	107:UNK	C	115:UNK	N	20.22
1	<i>5</i>	1995:Y5P	O3'	2016:P5P	P	17.42
1	<i>z</i>	127:UNK	C	131:UNK	N	9.67