



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:21 PM BST

PDB ID : 4V7C  
EMDB ID: : EMD-5799  
Title : Structure of the Ribosome with Elongation Factor G Trapped in the Pre-Translocation State (pre-translocation 70S\*tRNA structure)  
Authors : Brilot, A.F.; Korostelev, A.A.; Ermolenko, D.N.; Grigorieff, N.  
Deposited on : 2013-11-20  
Resolution : 7.60 Å(reported)  
Based on PDB ID : 4GD1

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
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>

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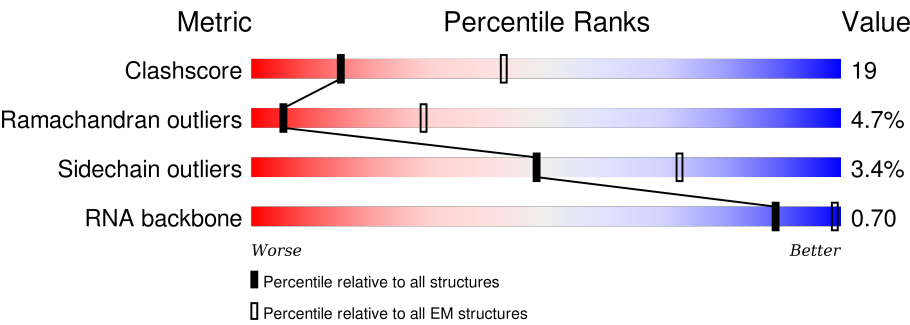
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

# 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 7.60 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.




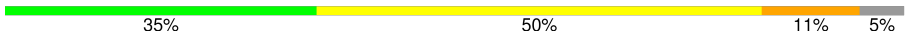
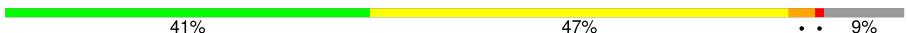


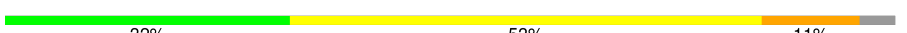
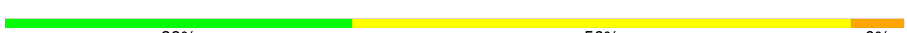




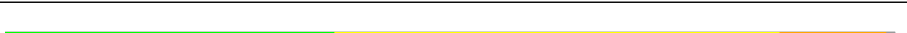













Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	AA	1542	<div><div>54%</div><div>41%</div><div>5%</div></div>
2	AB	240	<div><div>21%</div><div>58%</div><div>11%</div><div>9%</div></div>
3	AC	232	<div><div>38%</div><div>47%</div><div>•</div><div>11%</div></div>
4	AD	205	<div><div>36%</div><div>53%</div><div>11%</div></div>
5	AE	166	<div><div>46%</div><div>40%</div><div>•</div><div>10%</div></div>
6	AF	131	<div><div>28%</div><div>43%</div><div>5%</div><div>24%</div></div>
7	AG	178	<div><div>40%</div><div>42%</div><div>•</div><div>15%</div></div>
8	AH	129	<div><div>49%</div><div>48%</div><div>•</div></div>


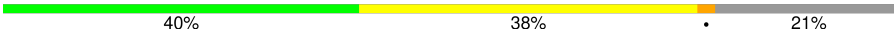






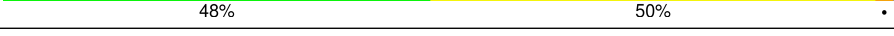

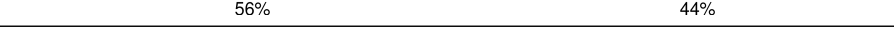
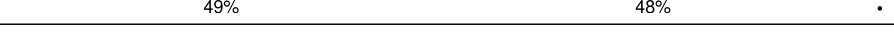

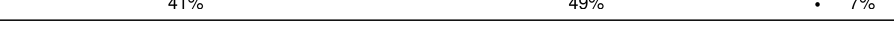


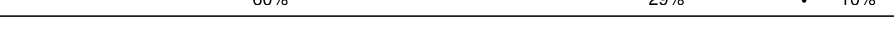

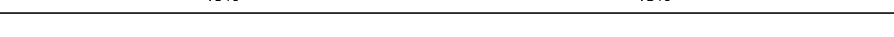






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Mol	Chain	Length	Quality of chain
9	AI	129	
10	AJ	103	
11	AK	128	
12	AL	123	
13	AM	117	
14	AN	100	
15	AO	88	
16	AP	82	
17	AQ	83	
18	AR	74	
19	AS	91	
20	AT	86	
21	AU	70	
22	AV	76	
22	AW	76	
23	AX	18	
24	AY	6	
25	BA	2903	
26	BB	119	
27	BC	233	
28	BD	272	
29	BE	209	
30	BF	201	
31	BG	178	
32	BH	176	

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Mol	Chain	Length	Quality of chain
33	BI	149	
34	BJ	165	
35	BK	141	
36	BL	142	
37	BM	123	
38	BN	144	
39	BO	136	
40	BP	127	
41	BQ	117	
42	BR	114	
43	BS	117	
44	BT	103	
45	BU	110	
46	BV	100	
47	BW	103	
48	BX	94	
49	BY	84	
50	BZ	77	
51	B1	63	
52	B2	58	
53	B3	56	
54	B4	54	
55	B5	46	
56	B6	64	
57	B7	38	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	5OH	AY	6	-	-	X	-

## 2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 148028 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1538	Total	C	N	O	P	0	0
			32995	14716	6050	10691	1538		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.



Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 22 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		
22	AW	76	Total	C	N	O	P	0	0
			1622	723	290	533	76		

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AX	18	Total	C	N	O	P	0	0
			386	173	71	124	18		

- Molecule 24 is a protein called viomycin.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	AY	6	Total	C	N	O	0	0
			48	25	13	10		

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BA	2897	Total	C	N	O	P	0	0
			62192	27744	11444	20107	2897		

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BB	119	Total	C	N	O	P	0	0
			2548	1135	466	829	118		

- Molecule 27 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BC	225	Total	C	N	O	S	0	0
			1675	1047	305	317	6		

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BD	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BE	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BF	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BG	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BH	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BI	53	Total	C	N	O	S	0	0
			409	261	74	73	1		

- Molecule 34 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BJ	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 35 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BK	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 36 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BL	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BM	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BN	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BO	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 40 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BP	120	Total	C	N	O	S	0	0
			959	592	196	166	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
41	BQ	116	Total	C	N	O	0	0
			892	552	178	162		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BR	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 43 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BS	117	Total	C	N	O	S	0	0
			947	604	192	151			

- Molecule 44 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BT	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 45 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BU	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 46 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BV	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 47 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BW	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 48 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BX	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 49 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BY	76	Total	C	N	O	S	0	0
			575	356	117	101	1		

- Molecule 50 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BZ	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 51 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B1	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 52 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B2	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B3	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 54 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	B4	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 55 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B5	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 56 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	B6	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 57 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	B7	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

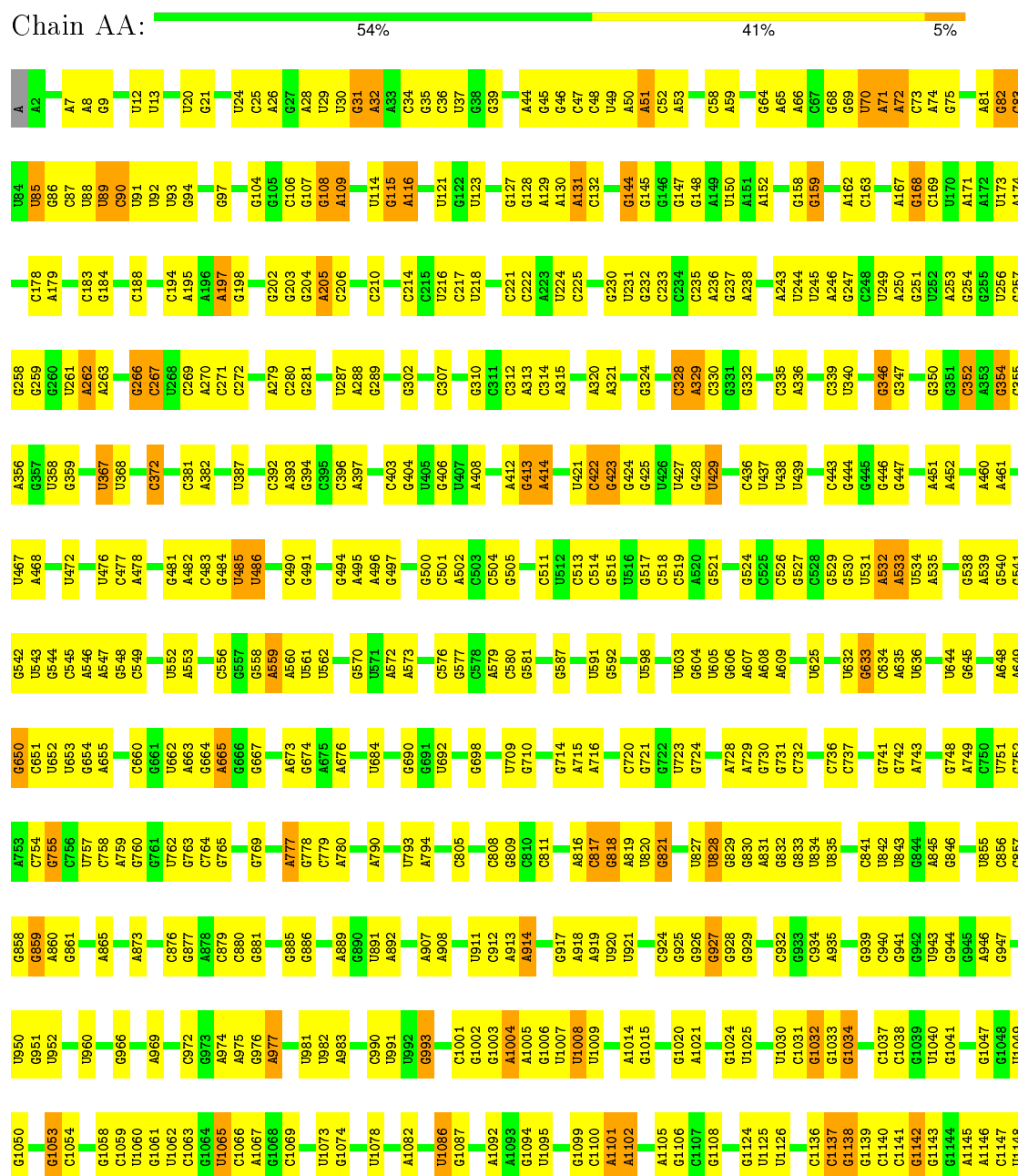
- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

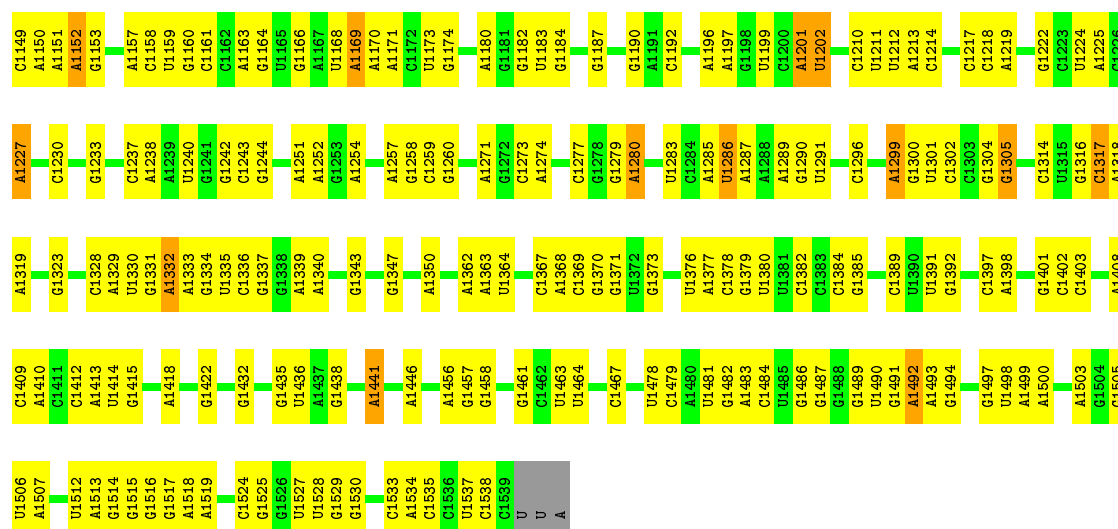
Mol	Chain	Residues	Atoms		AltConf
58	B7	1	Total	Zn	0
			1	1	

### 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 errors 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.

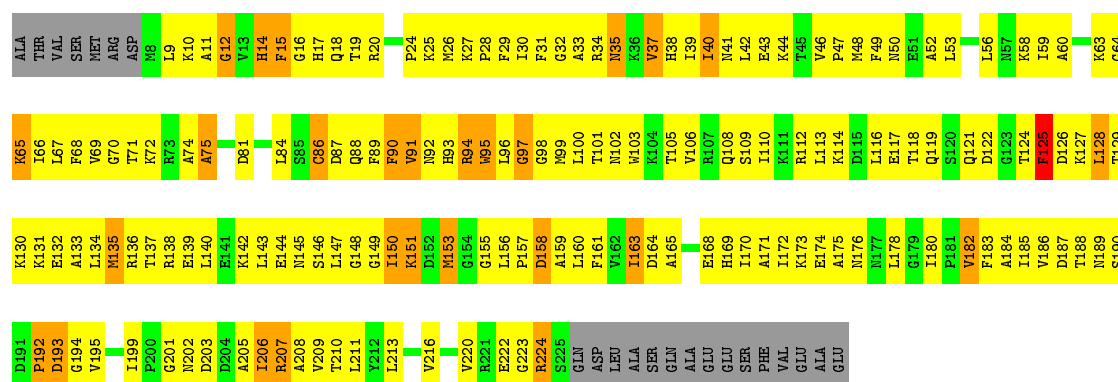
#### • Molecule 1: 16S ribosomal RNA





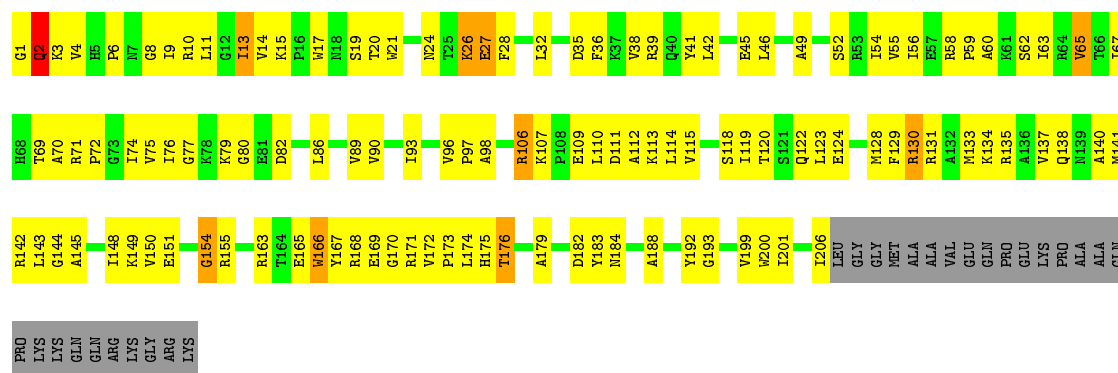
• Molecule 2: 30S ribosomal protein S2

Chain AB: 21% 58% 11% 9%



• Molecule 3: 30S ribosomal protein S3

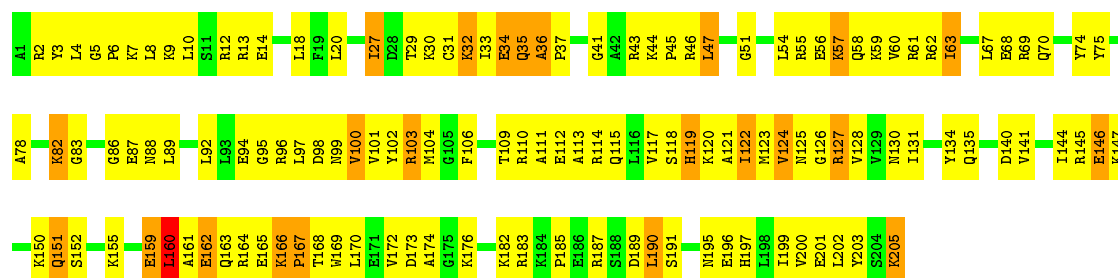
Chain AC: 38% 47% 11%



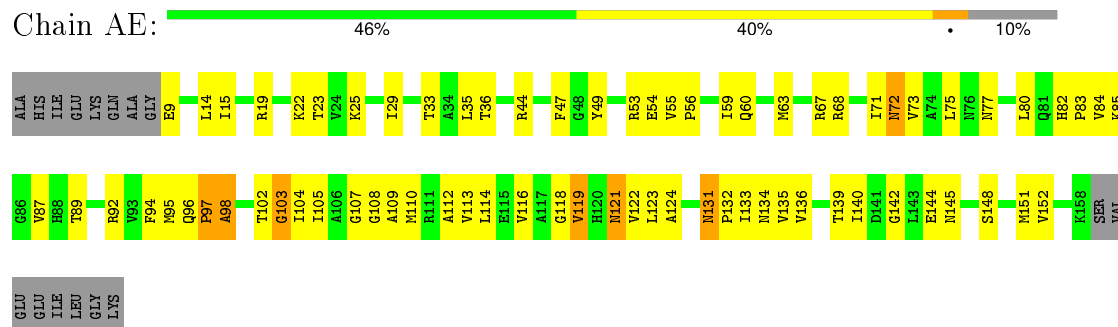
• Molecule 4: 30S ribosomal protein S4

Chain AD: 36% 53% 11%

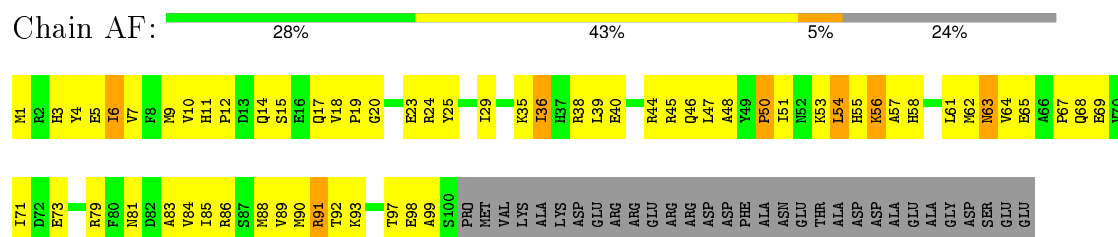




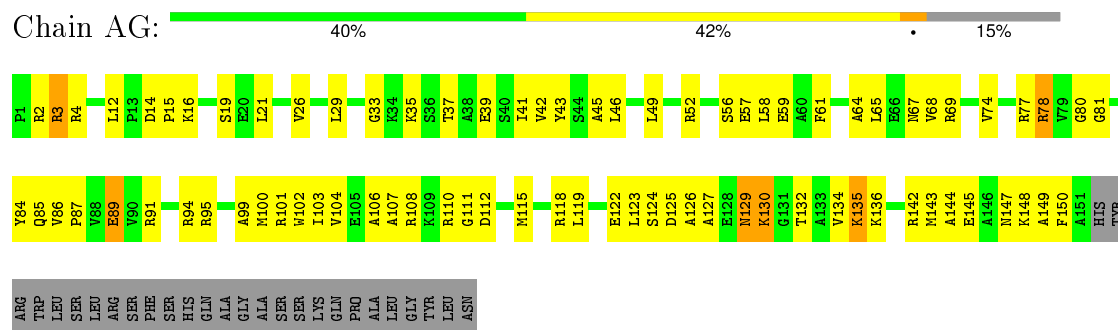
• Molecule 5: 30S ribosomal protein S5



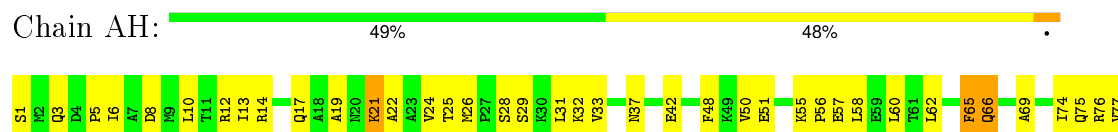
• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7



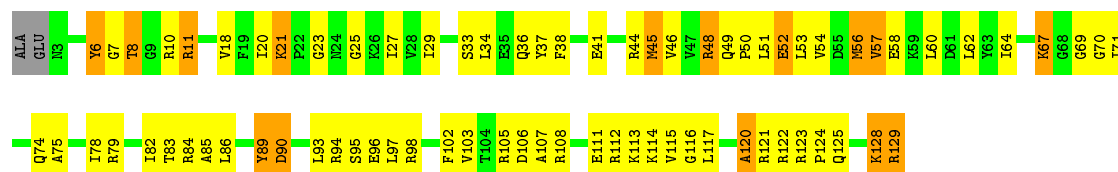
• Molecule 8: 30S ribosomal protein S8





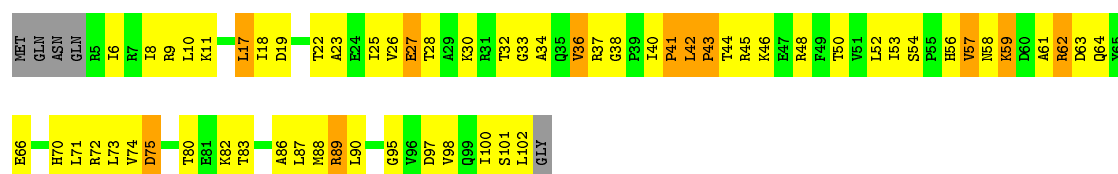
• Molecule 9: 30S ribosomal protein S9

Chain AI: 40% 47% 12%



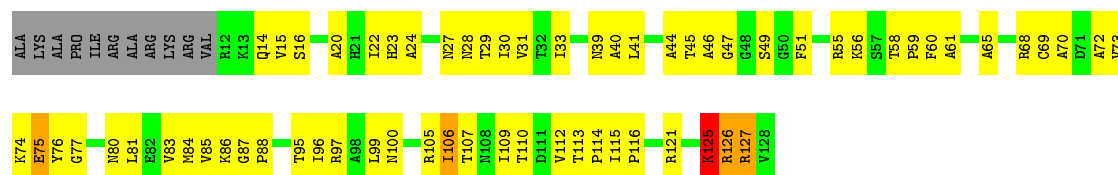
• Molecule 10: 30S ribosomal protein S10

Chain AJ: 35% 50% 11% 5%



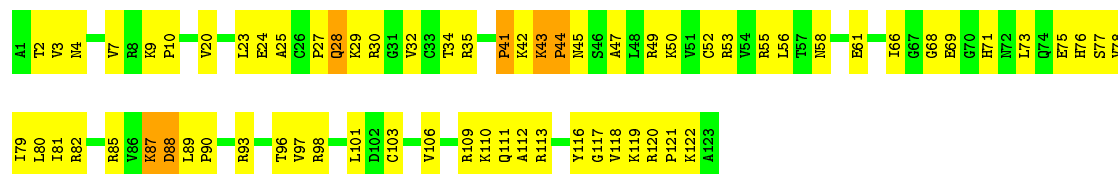
• Molecule 11: 30S ribosomal protein S11

Chain AK: 41% 47% 9%



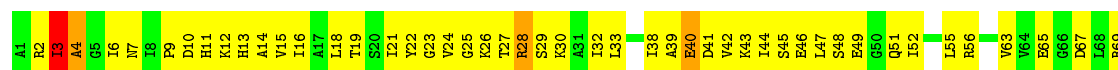
• Molecule 12: 30S ribosomal protein S12

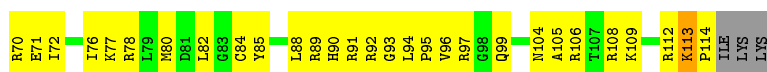
Chain AL: 45% 50% 5%



• Molecule 13: 30S ribosomal protein S13

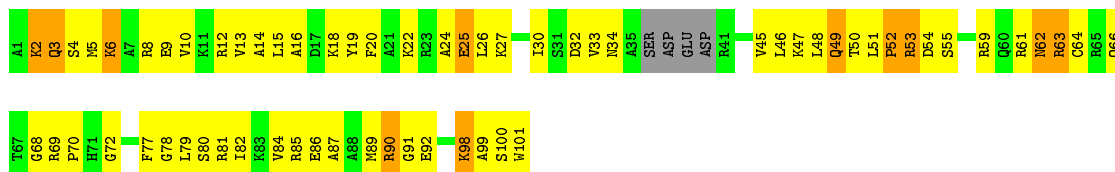
Chain AM: 32% 61% 7%





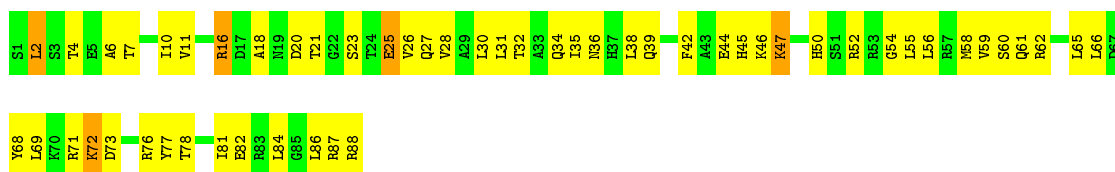
- Molecule 14: 30S ribosomal protein S14

Chain AN: 



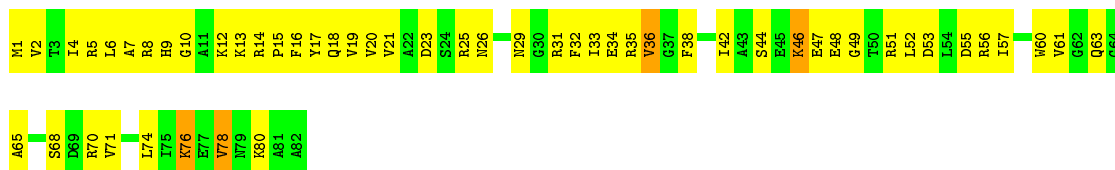
- Molecule 15: 30S ribosomal protein S15

Chain AO: 



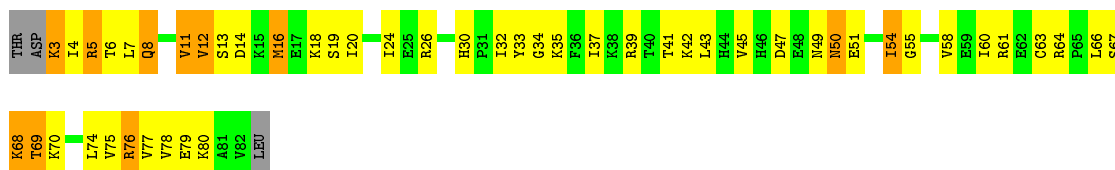
- Molecule 16: 30S ribosomal protein S16

Chain AP:  35% 60% 5%



- Molecule 17: 30S ribosomal protein S17

Chain AQ: 

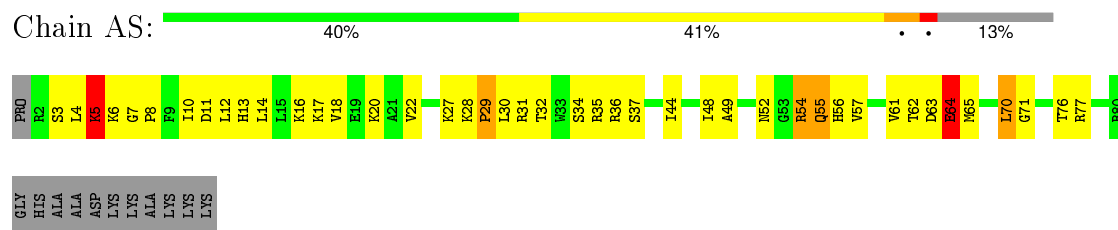


- Molecule 18: 30S ribosomal protein S18

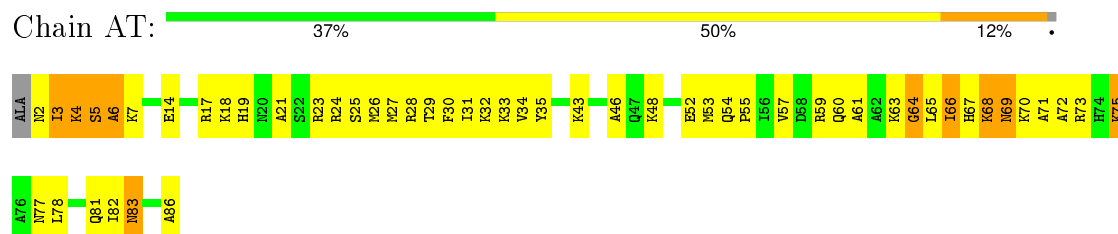
Chain AR: 



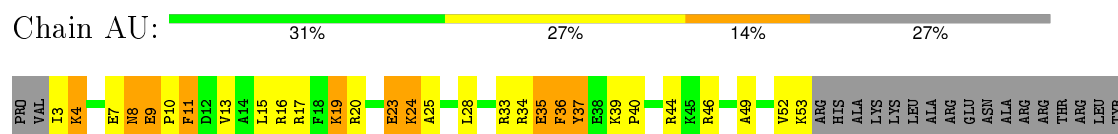
- Molecule 19: 30S ribosomal protein S19



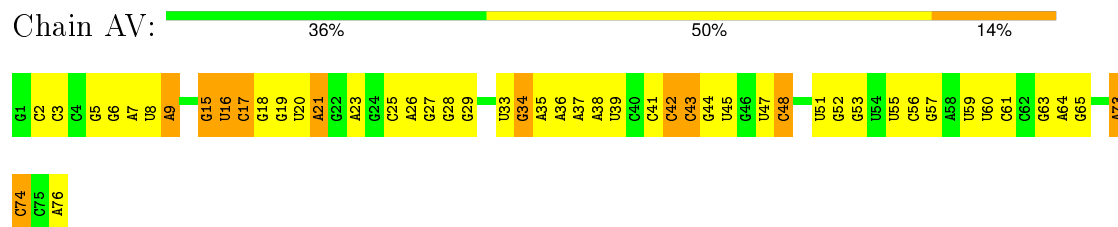
- Molecule 20: 30S ribosomal protein S20



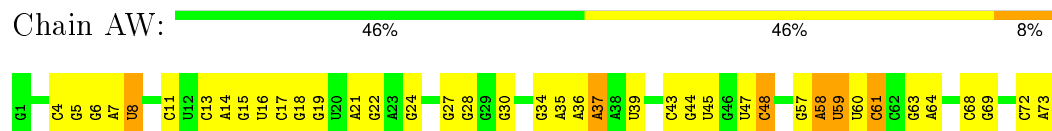
- Molecule 21: 30S ribosomal protein S21



- Molecule 22: tRNA



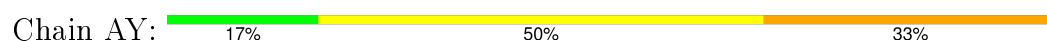
- Molecule 22: tRNA



- Molecule 23: mRNA



- Molecule 24: viomycin

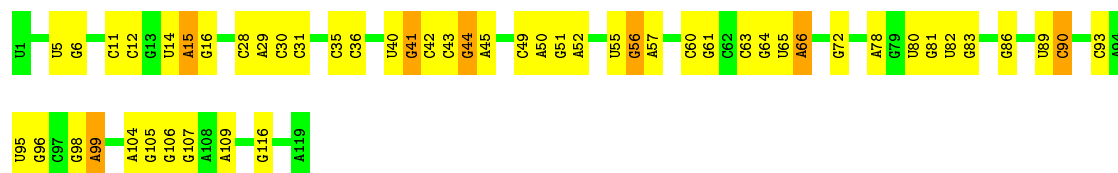




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A2826	A2726	U2629	C2551	C2462	C2368	G2279	U2188	G2093	G2010	U1929	A1821	G1721	A1598	A1509	A1419
C2830	A2727	G2633	U2552	C2463	A2376	G2280	U2189	G2097	G2011	G1930	G1822	U1729	C1600	A1510	A1421
G2831	G2728	C2636	U2553	C2465	A2377	A2281	U2192	U2098	G2012	U1931	G1826	C1730	A1515	G1516	G1425
G2834	G2732	U2637	U2554	C2466	G2379	G2283	G2193	U2099	A2013	G1933	U1827	G1738	C1607	U1523	G1426
U2849	A2733	G2638	U2555	A2469	C2380	A2284	G2198	G2110	A2014	G1934	G1828	A1739	A1608	G1524	A1427
U2845	A2741	G2641	A2564	G2470	A2381	C2285	A2198	G2111	U2016	G1936	G1829	G1740	A1609	A1525	G1428
G2846	G2742	U2642	U2565	C2471	G2382	G2286	A2199	U2112	U2017	A1937	U1834	A1744	A1610	G1526	G1429
G2847	U2743	G2643	A2566	G2472	C2383	A2287	C2200	G2113	G2018	A1938	U1837	A1745	A1616	G1527	A1434
G2848	G2744	U2644	U2567	C2475	U2384	G2288	U2203	A2114	A2019	U1939	G1837	C1762	A1628	U1528	A1435
U2849	C2745	G2645	U2568	A2476	A2386	G2290	G2204	G2115	A2020	U1943	C1836	C1762	G1628	G1529	G1436
C2853	U2746	U2646	G2569	U2390	U2390	U2291	A2211	A2117	C2021	U1944	G1839	G1763	G1628	G1530	U1437
G2854	G2747	G2647	G2570	G2481	U2391	U2292	A2212	U2118	U2022	G1945	U1855	A1754	A1641	U1535	U1438
G2855	A2748	U2648	U2571	C2480	C2394	C2295	U2213	U2130	G2023	U1946	U1856	G1756	A1641	C1536	U1439
A2856	G2751	G2661	C2573	U2489	C2395	U2296	U2214	A2119	G2024	C1947	G1857	A1757	C1642	G1537	U1440
U2860	A2758	G2663	G2574	G2490	C2396	A2297	C2215	A2122	C2025	G1948	A1858	U1764	C1645	U1539	U1441
U2861	A2765	U2664	U2576	U2491	G2399	U2305	G2216	G2128	G2029	A1952	G1869	C1764	C1646	G1540	U1442
G2867	U2768	G2668	G2578	C2496	U2402	C2313	U2220	U2130	A2030	G1953	G1870	A1772	C1647	U1541	U1443
A2868	U2769	G2669	U2579	U2497	U2403	G2314	G2221	U2131	A2031	U1955	A1871	A1773	U1647	U1542	G1444
G2869	U2770	U2670	U2580	C2498	A2406	U2321	G2224	U2132	G2032	U1956	A1872	C1776	A1652	G1543	C1447
C2870	C2774	U2680	G2581	C2499	A2407	A2322	A2225	G2133	G2038	G1959	G1875	G1776	G1653	G1546	G1448
U2875	G2775	G2681	U2582	U2500	U2408	G2323	C2226	A2134	U2039	A1960	G1874	U1777	A1654	C1547	G1449
G2876	A2776	A2682	G2583	C2501	G2409	G2325	G2226	G2135	G2040	U1970	G1875	U1778	A1655	G1450	G1450
U2877	G2777	G2683	U2584	G2502	G2410	G2326	U2233	G2136	U2041	A1969	U1880	C1788	C1665	C1461	C1451
A2878	A2778	U2684	U2585	A2503	A2411	A2327	G2234	G2137	A2042	U1971	G1881	U1781	G1666	C1462	C1462
U2879	U2779	G2685	U2586	U2504	A2412	A2328	G2235	U2138	C2043	G1972	U1882	U1782	A1667	G1463	G1463
G2880	G2780	U2686	A2587	U2505	U2413	G2329	G2236	G2140	C2044	U1973	U1883	U1783	A1668	G1464	G1464
U2881	A2781	U2687	G2588	G2506	U2414	G2330	G2237	G2141	C2045	C1974	U1884	G1792	A1669	U1465	U1466
A2882	U2782	G2688	U2589	U2511	A2425	G2331	U2244	G2142	G2049	U1979	G1903	U1796	C1674	A1570	A1470
A2883	U2783	U2689	A2590	U2512	A2426	C2332	U2245	C2145	C2050	G1980	U1904	U1797	A1675	A1571	A1471
U2884	G2784	G2690	U2591	U2513	C2427	C2333	U2246	A2147	A2051	G1983	U1912	U1798	A1676	A1572	U1472
G2889	U2791	G2691	G2592	C2515	G2428	U2334	G2247	G2148	G2052	U1987	A1913	G1799	U1683	G1579	G1475
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A2893	U2793	U2693	G2594	A2517	A2430	G2336	U2249	G2150	C2054	G1989	C1914	G1807	G1699	G1582	G1479
G2894	A2794	G2694	U2595	U2518	A2431	C2337	G2251	A2158	C2055	U1990	U1915	A1808	U1584	U1583	G1482
U2903	G2795	U2695	G2596	C2520	A2432	U2338	G2252	G2162	G2056	C1990	U1916	A1809	C1704	U1584	G1483
U2904	U2796	G2696	U2597	U2521	U2441	U2344	G2255	A2163	A2059	G1991	A1917	A1810	C1705	G1492	G1492
G2905	A2797	U2697	A2602	G2522	C2442	G2345	G2256	C2164	A2060	U1992	U1918	G1811	A1705	C1493	C1493
U2906	U2798	G2698	U2603	U2523	C2443	U2346	U2257	C2165	G2061	A1987	A1919	G1707	G1587	A1494	A1494
A2810	G2804	G2708	G2607	U2533	G2444	U2347	C2258	C2166	A2062	G1988	C1914	A1807	U1588	G1592	G1501
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U2812	U2810	U2711	U2613	U2537	G2446	G2349	G2260	A2171	G2066	C1990	U1916	A1809	C1704	U1594	U1506
A2813	A2810	G2712	A2614	C2538	A2447	U2344	G2261	A2172	U2068	C1991	A1917	A1810	C1705	C1595	U1507
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G2815	A2812	G2714	C2616	C2452	C2452	U2358	U2265	C2175	A2070	U1993	A1919	G1812	G1707	G1597	G1508
U2816	C2813	U2715	U2617	A2542	G2455	G2359	U2266	C2176	A2071	C1994	A1919	G1813	A1713	G1598	G1509
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G2818	U2717	U2619	U2619	G2544	U2457	G2361	A2268	C2178	U2086	C1996	U1923	G1815	G1715	C1599	U1511
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A2820	A2816	U2719	U2624	U2546	G2459	G2363	G2270	U2182	G2088	G2003	U1925	A1820	G1717	U1599	U1513
A2821	U2724	U2625	G2625	G2547	G2460	A2366	A2270	U2183	G2089	G2004	U1926	A1821	G1718	U1599	U1514

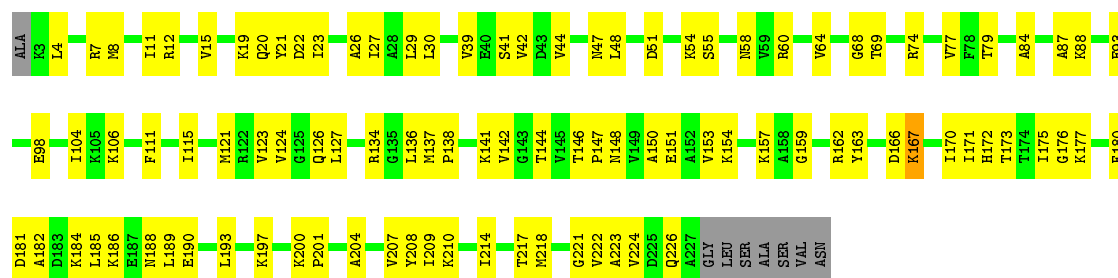
- Molecule 26: 5S ribosomal RNA

Chain BB: 



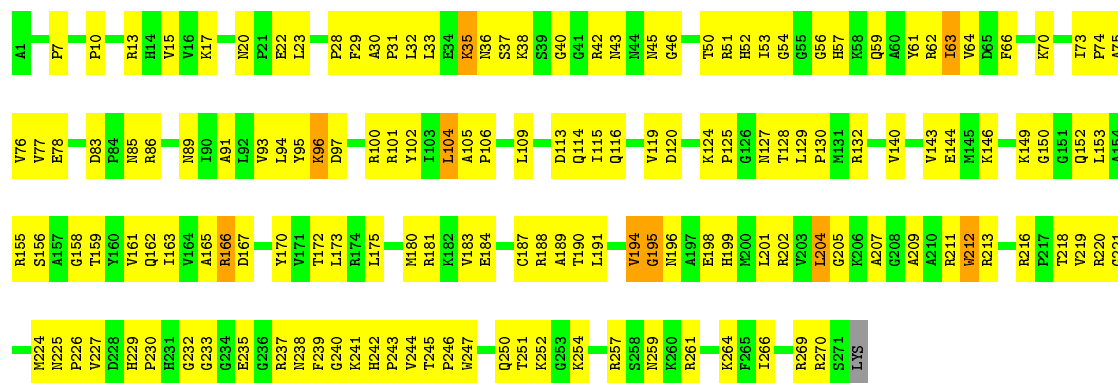
- Molecule 27: 50S ribosomal protein L1

Chain BC: 



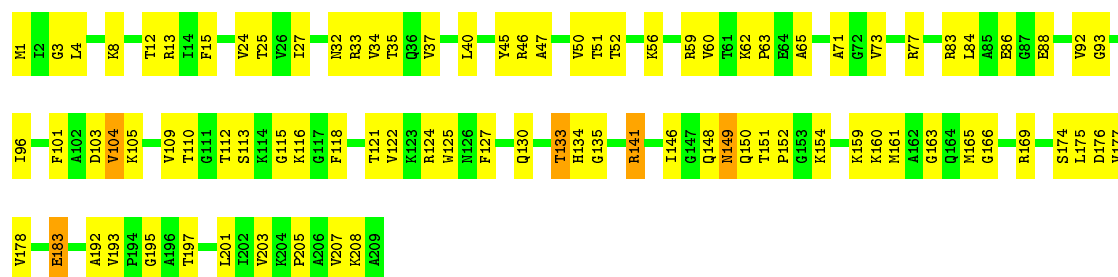
- Molecule 28: 50S ribosomal protein L2

Chain BD: 

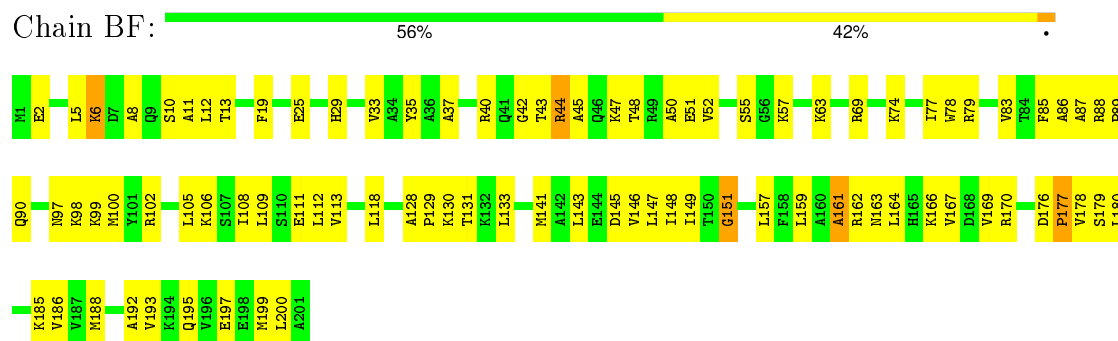


- Molecule 29: 50S ribosomal protein L3

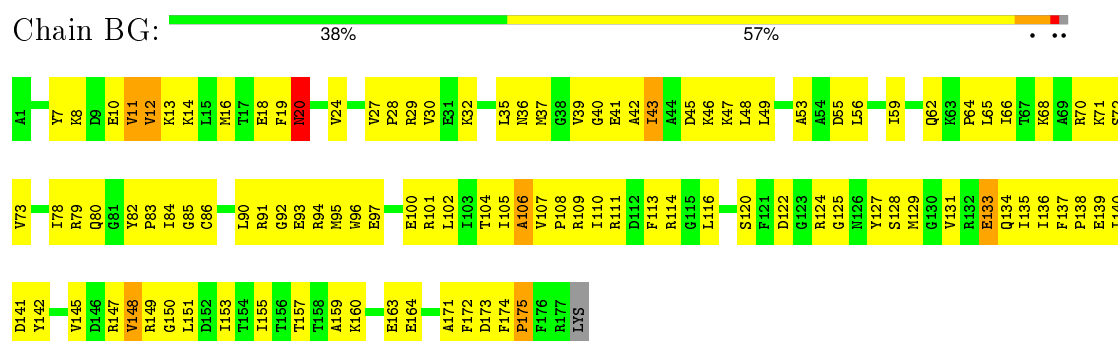
Chain BE: 



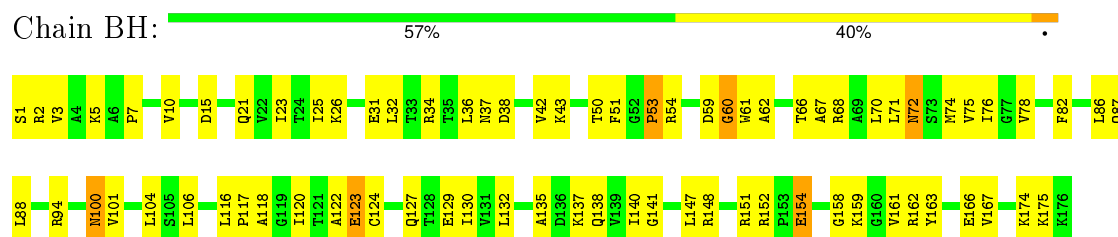
- Molecule 30: 50S ribosomal protein L4



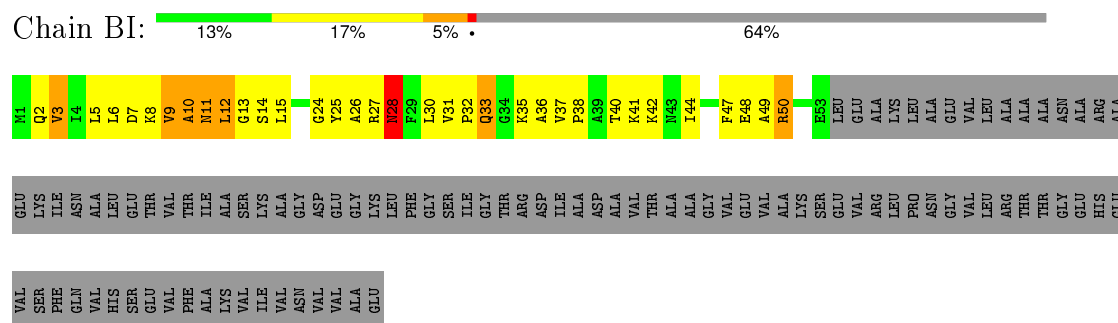
- Molecule 31: 50S ribosomal protein L5



- Molecule 32: 50S ribosomal protein L6



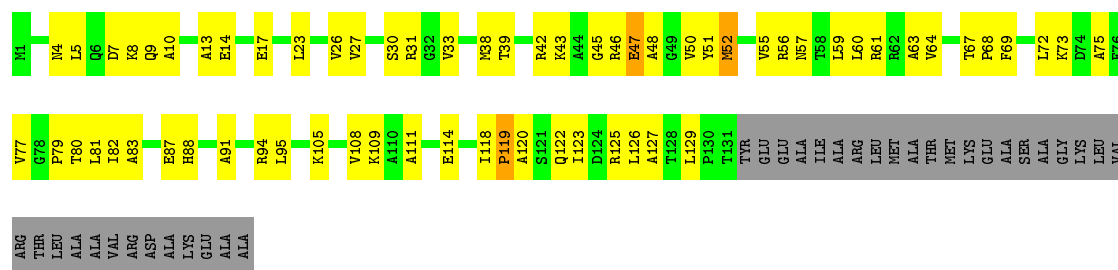
- Molecule 33: 50S ribosomal protein L9



- Molecule 34: 50S ribosomal protein L10

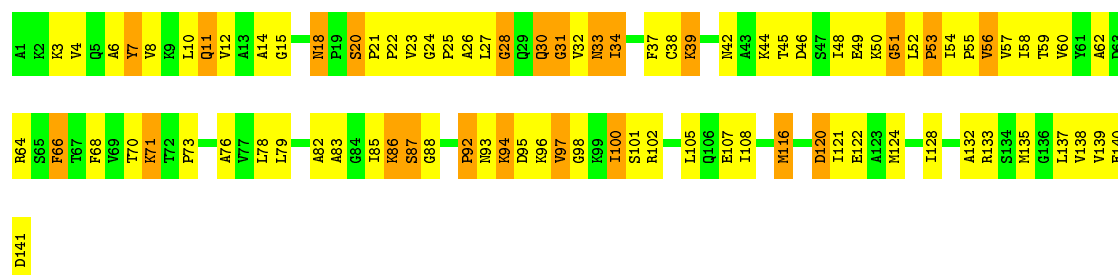






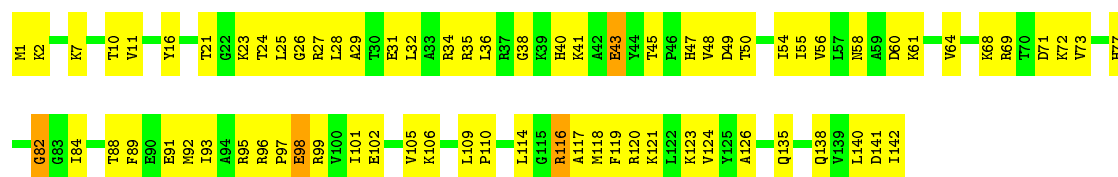
• Molecule 35: 50S ribosomal protein L11

Chain BK: 38% 46% 16%



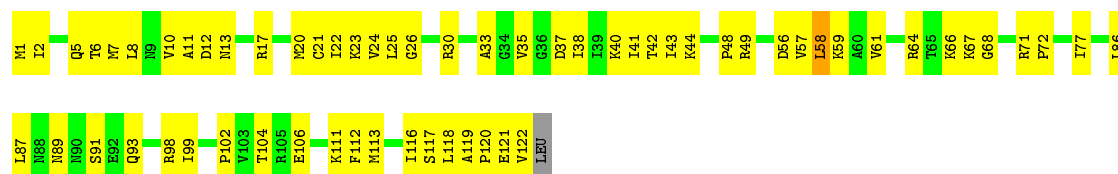
• Molecule 36: 50S ribosomal protein L13

Chain BL: 48% 49%



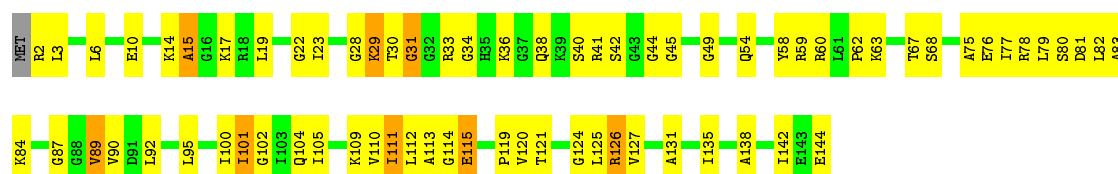
• Molecule 37: 50S ribosomal protein L14

Chain BM: 49% 50%

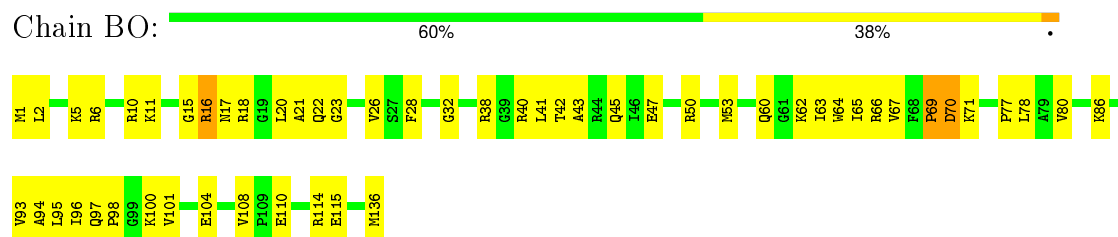


• Molecule 38: 50S ribosomal protein L15

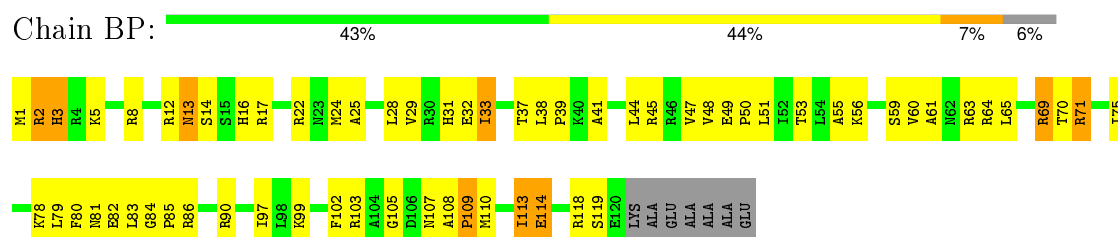
Chain BN: 50% 44% 6%



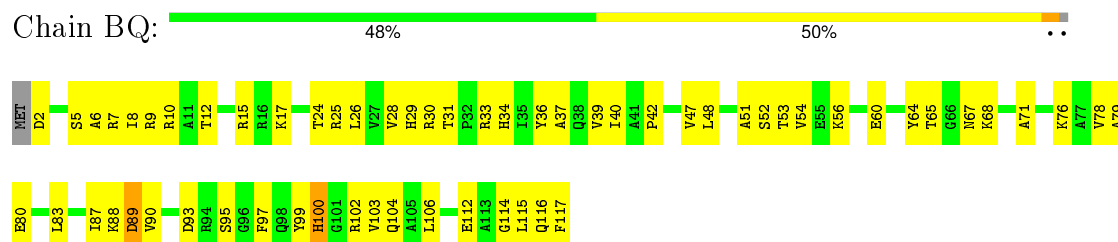
- Molecule 39: 50S ribosomal protein L16



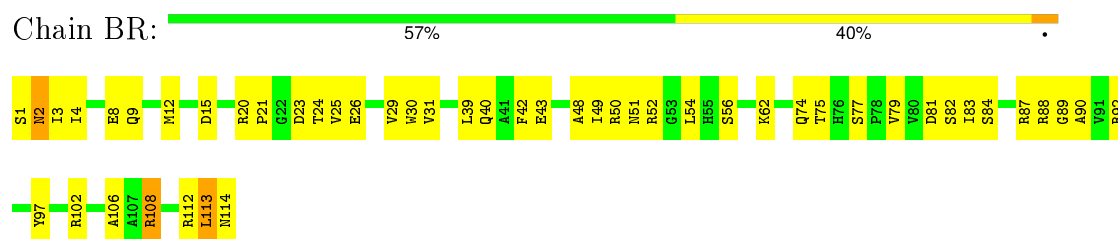
- Molecule 40: 50S ribosomal protein L17



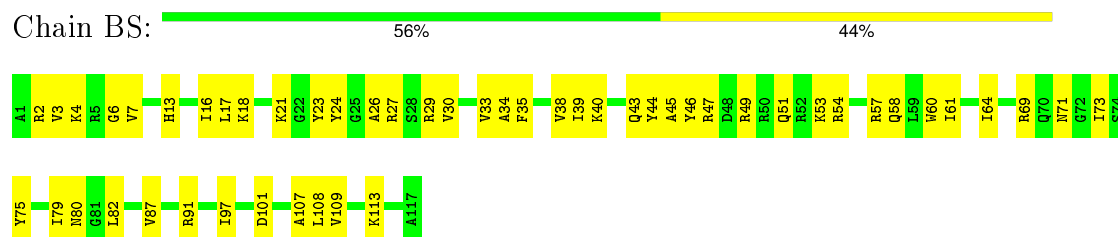
- Molecule 41: 50S ribosomal protein L18



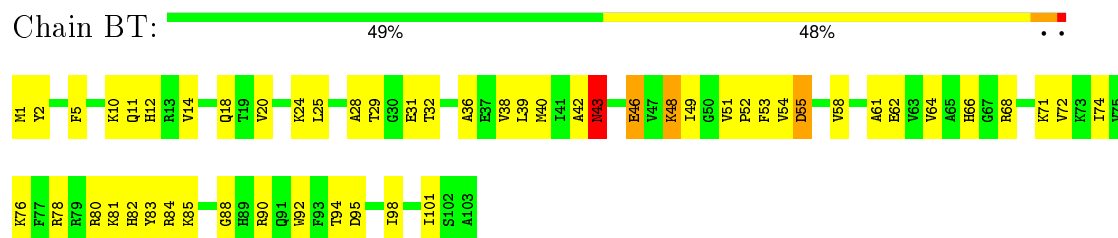
- Molecule 42: 50S ribosomal protein L19



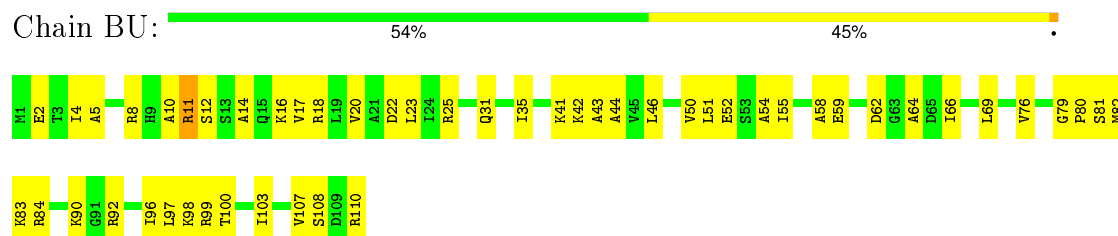
- Molecule 43: 50S ribosomal protein L20



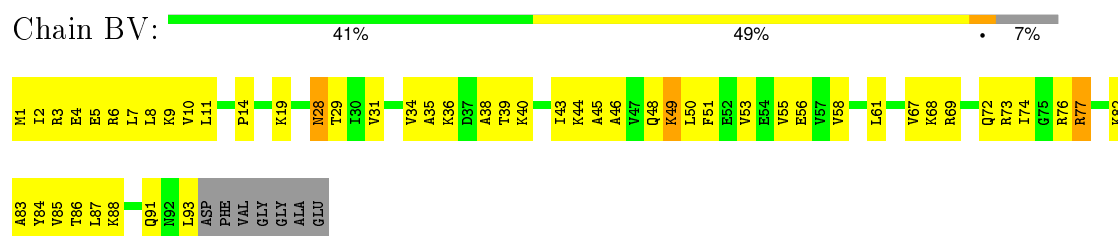
- Molecule 44: 50S ribosomal protein L21



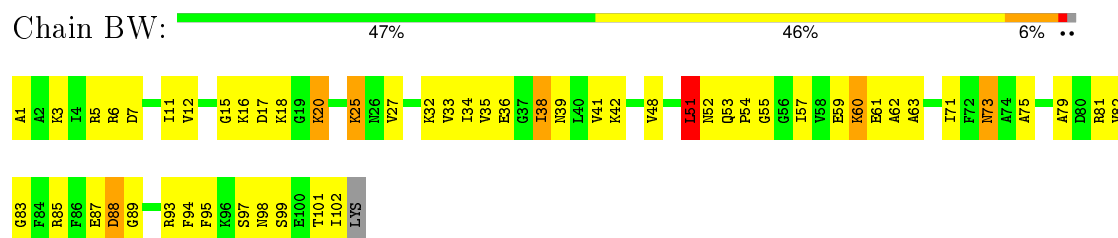
- Molecule 45: 50S ribosomal protein L22



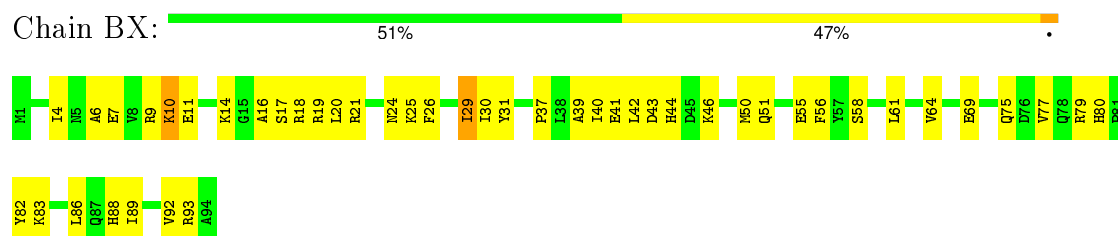
- Molecule 46: 50S ribosomal protein L23



- Molecule 47: 50S ribosomal protein L24

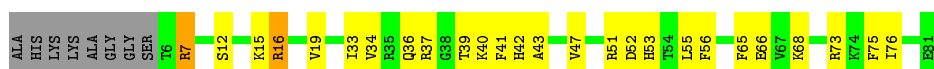


- Molecule 48: 50S ribosomal protein L25



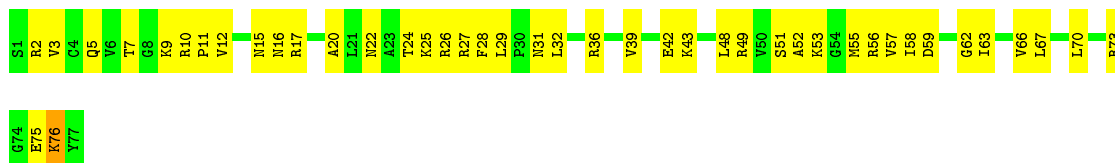
- Molecule 49: 50S ribosomal protein L27





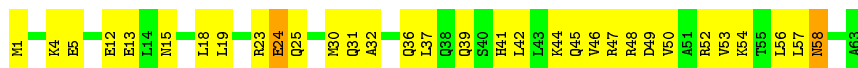
- Molecule 50: 50S ribosomal protein L28

Chain BZ: 44% 55%



- Molecule 51: 50S ribosomal protein L29

Chain B1: 49% 48%



- Molecule 52: 50S ribosomal protein L30

Chain B2: 57% 41%



- Molecule 53: 50S ribosomal protein L32

Chain B3: 55% 41%



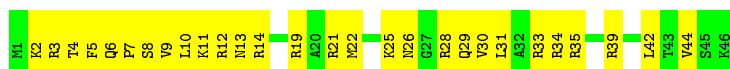
- Molecule 54: 50S ribosomal protein L33

Chain B4: 52% 39% 7%



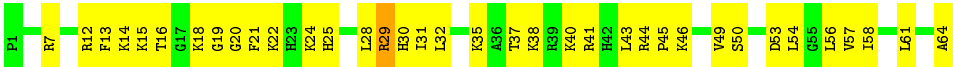
- Molecule 55: 50S ribosomal protein L34

Chain B5: 39% 61%



- Molecule 56: 50S ribosomal protein L35

Chain B6: 44% 55%



- Molecule 57: 50S ribosomal protein L36



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	85115	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	CTFFIND3, FREALIGN per micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	1150	Depositor
Maximum defocus (nm)	6950	Depositor
Magnification	133333	Depositor
Image detector	FEI FALCON I (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: ZN, 5OH, DPP, UAL, KBE

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	AA	0.21	0/36944	0.62	0/57632
10	AJ	0.22	0/796	0.45	0/1077
11	AK	0.24	0/893	0.41	0/1205
12	AL	0.22	0/969	0.42	0/1300
13	AM	0.21	0/892	0.42	0/1193
14	AN	0.24	0/785	0.38	0/1043
15	AO	0.23	0/722	0.40	0/964
16	AP	0.25	0/659	0.39	0/884
17	AQ	0.23	0/657	0.43	0/881
18	AR	0.23	0/462	0.41	0/621
19	AS	0.25	0/652	0.42	0/877
2	AB	0.25	0/1735	0.42	0/2338
20	AT	0.24	0/671	0.41	0/888
21	AU	0.26	0/430	0.42	0/570
22	AV	0.30	0/1809	0.67	0/2819
22	AW	0.24	0/1812	0.62	0/2823
23	AX	0.32	0/432	0.65	0/671
24	AY	2.44	2/11 (18.2%)	0.74	0/13
25	BA	0.26	1/69653 (0.0%)	0.62	3/108657 (0.0%)
26	BB	0.21	0/2847	0.61	0/4440
27	BC	0.21	0/1690	0.40	0/2278
28	BD	0.21	0/2121	0.41	0/2852
29	BE	0.24	0/1586	0.41	0/2134
3	AC	0.23	0/1651	0.41	0/2225
30	BF	0.23	0/1571	0.40	0/2113
31	BG	0.25	0/1434	0.40	0/1926
32	BH	0.22	0/1343	0.41	0/1816
33	BI	0.27	0/414	0.42	0/556
34	BJ	0.24	0/1001	0.41	0/1350
35	BK	0.24	0/1046	0.43	0/1410
36	BL	0.23	0/1152	0.40	0/1551
37	BM	0.22	0/947	0.42	0/1268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
38	BN	0.23	0/1054	0.42	0/1403
39	BO	0.25	0/1093	0.41	0/1460
4	AD	0.22	0/1665	0.40	0/2227
40	BP	0.24	0/970	0.38	0/1295
41	BQ	0.22	0/902	0.38	0/1209
42	BR	0.23	0/929	0.40	0/1242
43	BS	0.24	0/960	0.36	0/1278
44	BT	0.25	0/829	0.43	0/1107
45	BU	0.21	0/864	0.41	0/1156
46	BV	0.22	0/744	0.41	0/994
47	BW	0.24	0/787	0.40	0/1051
48	BX	0.24	0/766	0.38	0/1025
49	BY	0.26	0/582	0.37	0/769
5	AE	0.23	0/1118	0.42	0/1504
50	BZ	0.24	0/635	0.39	0/848
51	B1	0.23	0/510	0.41	0/677
52	B2	0.23	0/453	0.42	0/605
53	B3	0.22	0/450	0.40	0/599
54	B4	0.26	0/416	0.41	0/554
55	B5	0.25	0/380	0.39	0/498
56	B6	0.24	0/513	0.41	0/676
57	B7	0.22	0/303	0.39	0/397
6	AF	0.24	0/835	0.43	0/1128
7	AG	0.22	0/1195	0.42	0/1602
8	AH	0.23	0/989	0.41	0/1326
9	AI	0.23	0/1034	0.42	0/1375
All	All	0.24	3/160763 (0.0%)	0.57	3/240380 (0.0%)

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
25	BA	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1911	U	O3'-P	-40.57	1.12	1.61
24	AY	3	SER	CA-C	-5.17	1.39	1.52
24	AY	4	SER	CA-C	-5.17	1.39	1.52



All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	1911	U	P-O3'-C3'	-14.37	102.45	119.70
25	BA	1911	U	OP1-P-O3'	-9.93	83.36	105.20
25	BA	1911	U	OP2-P-O3'	9.58	126.28	105.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	BA	1915	U	Sidechain

## 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	AA	32995	0	16607	584	0
2	AB	1704	0	1732	189	0
3	AC	1624	0	1699	125	0
4	AD	1643	0	1710	168	0
5	AE	1105	0	1148	78	0
6	AF	817	0	808	67	0
7	AG	1181	0	1240	93	0
8	AH	979	0	1034	86	0
9	AI	1022	0	1070	109	0
10	AJ	786	0	828	79	0
11	AK	877	0	887	72	0
12	AL	955	0	1019	84	0
13	AM	883	0	944	79	0
14	AN	774	0	827	84	0
15	AO	714	0	737	53	0
16	AP	649	0	666	57	0
17	AQ	648	0	691	56	0
18	AR	455	0	478	32	0
19	AS	637	0	665	43	0
20	AT	665	0	714	63	0
21	AU	425	0	449	32	0
22	AV	1619	0	822	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	AW	1622	0	821	39	0
23	AX	386	0	194	8	0
24	AY	48	0	40	13	0
25	BA	62192	0	31283	1057	0
26	BB	2548	0	1292	44	0
27	BC	1675	0	1763	92	0
28	BD	2082	0	2157	170	0
29	BE	1565	0	1616	92	0
30	BF	1552	0	1619	99	0
31	BG	1410	0	1447	115	0
32	BH	1323	0	1374	67	0
33	BI	409	0	429	34	0
34	BJ	988	0	1025	53	0
35	BK	1032	0	1088	92	0
36	BL	1129	0	1162	71	0
37	BM	938	0	1012	51	0
38	BN	1045	0	1117	92	0
39	BO	1074	0	1157	48	0
40	BP	959	0	998	73	0
41	BQ	892	0	923	51	0
42	BR	917	0	965	54	0
43	BS	947	0	1022	61	0
44	BT	816	0	839	54	0
45	BU	857	0	922	48	0
46	BV	738	0	807	49	0
47	BW	779	0	834	49	0
48	BX	753	0	780	42	0
49	BY	575	0	589	33	0
50	BZ	625	0	655	39	0
51	B1	509	0	543	37	0
52	B2	449	0	491	27	0
53	B3	444	0	461	31	0
54	B4	409	0	440	22	0
55	B5	377	0	418	37	0
56	B6	504	0	574	49	0
57	B7	302	0	343	22	0
58	B7	1	0	0	0	0
All	All	148028	0	99975	4831	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 19.

The worst 5 of 4831 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)
25:BA:45:G:H5'	25:BA:46:G:H5'	1.24	1.16
25:BA:1912:A:C2	25:BA:1919:A:C5	2.33	1.16
1:AA:1033:G:H2'	1:AA:1034:G:H5''	1.31	1.10
48:BX:10:LYS:H	48:BX:10:LYS:HE2	1.16	1.09
27:BC:201:PRO:HG2	27:BC:204:ALA:HB2	1.39	1.02

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	
2	AB	216/240 (90%)	140 (65%)	51 (24%)	25 (12%)	0	9
3	AC	204/232 (88%)	169 (83%)	28 (14%)	7 (3%)	5	40
4	AD	203/205 (99%)	161 (79%)	26 (13%)	16 (8%)	1	19
5	AE	148/166 (89%)	111 (75%)	28 (19%)	9 (6%)	2	26
6	AF	98/131 (75%)	72 (74%)	19 (19%)	7 (7%)	1	22
7	AG	149/178 (84%)	120 (80%)	25 (17%)	4 (3%)	6	45
8	AH	127/129 (98%)	113 (89%)	10 (8%)	4 (3%)	5	42
9	AI	125/129 (97%)	94 (75%)	25 (20%)	6 (5%)	3	32
10	AJ	96/103 (93%)	66 (69%)	18 (19%)	12 (12%)	0	8
11	AK	115/128 (90%)	88 (76%)	22 (19%)	5 (4%)	3	34
12	AL	121/123 (98%)	96 (79%)	17 (14%)	8 (7%)	1	24
13	AM	112/117 (96%)	94 (84%)	12 (11%)	6 (5%)	2	29
14	AN	92/100 (92%)	66 (72%)	19 (21%)	7 (8%)	1	20
15	AO	86/88 (98%)	72 (84%)	12 (14%)	2 (2%)	8	48
16	AP	80/82 (98%)	60 (75%)	15 (19%)	5 (6%)	2	25
17	AQ	78/83 (94%)	57 (73%)	13 (17%)	8 (10%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	53/74 (72%)	48 (91%)	5 (9%)	0	100	100
19	AS	77/91 (85%)	59 (77%)	11 (14%)	7 (9%)	1	17
20	AT	83/86 (96%)	70 (84%)	6 (7%)	7 (8%)	1	18
21	AU	49/70 (70%)	29 (59%)	13 (26%)	7 (14%)	0	6
24	AY	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
27	BC	223/233 (96%)	204 (92%)	18 (8%)	1 (0%)	39	80
28	BD	269/272 (99%)	220 (82%)	41 (15%)	8 (3%)	5	42
29	BE	207/209 (99%)	180 (87%)	22 (11%)	5 (2%)	7	47
30	BF	199/201 (99%)	170 (85%)	23 (12%)	6 (3%)	5	42
31	BG	175/178 (98%)	147 (84%)	19 (11%)	9 (5%)	2	30
32	BH	174/176 (99%)	144 (83%)	24 (14%)	6 (3%)	5	40
33	BI	51/149 (34%)	29 (57%)	14 (28%)	8 (16%)	0	5
34	BJ	129/165 (78%)	111 (86%)	14 (11%)	4 (3%)	5	42
35	BK	139/141 (99%)	77 (55%)	40 (29%)	22 (16%)	0	5
36	BL	140/142 (99%)	117 (84%)	22 (16%)	1 (1%)	26	71
37	BM	120/123 (98%)	101 (84%)	14 (12%)	5 (4%)	3	34
38	BN	141/144 (98%)	107 (76%)	24 (17%)	10 (7%)	1	22
39	BO	134/136 (98%)	116 (87%)	14 (10%)	4 (3%)	5	42
40	BP	116/127 (91%)	96 (83%)	14 (12%)	6 (5%)	2	30
41	BQ	114/117 (97%)	94 (82%)	16 (14%)	4 (4%)	4	39
42	BR	112/114 (98%)	94 (84%)	15 (13%)	3 (3%)	6	45
43	BS	115/117 (98%)	102 (89%)	13 (11%)	0	100	100
44	BT	101/103 (98%)	82 (81%)	15 (15%)	4 (4%)	4	35
45	BU	108/110 (98%)	87 (81%)	19 (18%)	2 (2%)	10	52
46	BV	91/100 (91%)	79 (87%)	11 (12%)	1 (1%)	17	63
47	BW	100/103 (97%)	78 (78%)	15 (15%)	7 (7%)	1	22
48	BX	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
49	BY	74/84 (88%)	63 (85%)	10 (14%)	1 (1%)	14	58
50	BZ	75/77 (97%)	65 (87%)	10 (13%)	0	100	100
51	B1	61/63 (97%)	51 (84%)	8 (13%)	2 (3%)	5	40
52	B2	56/58 (97%)	53 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	B3	54/56 (96%)	46 (85%)	8 (15%)	0	100	100
54	B4	48/54 (89%)	38 (79%)	9 (19%)	1 (2%)	9	50
55	B5	44/46 (96%)	39 (89%)	5 (11%)	0	100	100
56	B6	62/64 (97%)	53 (86%)	8 (13%)	1 (2%)	12	56
57	B7	36/38 (95%)	28 (78%)	7 (19%)	1 (3%)	6	44
All	All	5874/6355 (92%)	4742 (81%)	858 (15%)	274 (5%)	5	32

5 of 274 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	PHE
2	AB	33	ALA
2	AB	86	CYS
2	AB	94	ARG
2	AB	163	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/198 (91%)	169 (94%)	11 (6%)	23	60
3	AC	170/189 (90%)	162 (95%)	8 (5%)	32	68
4	AD	172/172 (100%)	160 (93%)	12 (7%)	19	56
5	AE	113/125 (90%)	109 (96%)	4 (4%)	43	74
6	AF	87/112 (78%)	84 (97%)	3 (3%)	44	75
7	AG	124/146 (85%)	120 (97%)	4 (3%)	46	76
8	AH	104/104 (100%)	102 (98%)	2 (2%)	65	86
9	AI	105/106 (99%)	95 (90%)	10 (10%)	11	41
10	AJ	86/90 (96%)	83 (96%)	3 (4%)	43	74
11	AK	90/98 (92%)	84 (93%)	6 (7%)	20	57
12	AL	103/103 (100%)	101 (98%)	2 (2%)	65	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	AM	92/95 (97%)	89 (97%)	3 (3%)	45	76
14	AN	79/83 (95%)	72 (91%)	7 (9%)	12	44
15	AO	76/76 (100%)	73 (96%)	3 (4%)	39	72
16	AP	65/65 (100%)	62 (95%)	3 (5%)	33	68
17	AQ	74/77 (96%)	69 (93%)	5 (7%)	20	57
18	AR	48/64 (75%)	47 (98%)	1 (2%)	61	84
19	AS	70/78 (90%)	66 (94%)	4 (6%)	25	62
20	AT	65/65 (100%)	62 (95%)	3 (5%)	33	68
21	AU	44/60 (73%)	40 (91%)	4 (9%)	12	43
24	AY	2/2 (100%)	2 (100%)	0	100	100
27	BC	175/180 (97%)	173 (99%)	2 (1%)	80	91
28	BD	216/217 (100%)	213 (99%)	3 (1%)	74	89
29	BE	164/164 (100%)	162 (99%)	2 (1%)	78	90
30	BF	165/165 (100%)	165 (100%)	0	100	100
31	BG	148/149 (99%)	145 (98%)	3 (2%)	63	85
32	BH	137/137 (100%)	132 (96%)	5 (4%)	42	74
33	BI	42/114 (37%)	39 (93%)	3 (7%)	18	55
34	BJ	100/123 (81%)	99 (99%)	1 (1%)	82	92
35	BK	109/109 (100%)	98 (90%)	11 (10%)	9	38
36	BL	116/116 (100%)	113 (97%)	3 (3%)	54	80
37	BM	103/104 (99%)	102 (99%)	1 (1%)	82	92
38	BN	102/103 (99%)	100 (98%)	2 (2%)	63	85
39	BO	109/109 (100%)	106 (97%)	3 (3%)	51	78
40	BP	100/103 (97%)	96 (96%)	4 (4%)	38	71
41	BQ	86/87 (99%)	85 (99%)	1 (1%)	78	90
42	BR	99/99 (100%)	97 (98%)	2 (2%)	63	85
43	BS	89/89 (100%)	89 (100%)	0	100	100
44	BT	84/84 (100%)	82 (98%)	2 (2%)	57	82
45	BU	93/93 (100%)	93 (100%)	0	100	100
46	BV	80/84 (95%)	77 (96%)	3 (4%)	40	73
47	BW	83/84 (99%)	78 (94%)	5 (6%)	24	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	BX	78/78 (100%)	76 (97%)	2 (3%)	54	80
49	BY	56/62 (90%)	55 (98%)	1 (2%)	66	87
50	BZ	67/67 (100%)	66 (98%)	1 (2%)	72	88
51	B1	55/55 (100%)	54 (98%)	1 (2%)	66	87
52	B2	48/48 (100%)	47 (98%)	1 (2%)	61	84
53	B3	47/47 (100%)	44 (94%)	3 (6%)	22	58
54	B4	45/48 (94%)	45 (100%)	0	100	100
55	B5	38/38 (100%)	38 (100%)	0	100	100
56	B6	51/51 (100%)	50 (98%)	1 (2%)	63	85
57	B7	34/34 (100%)	34 (100%)	0	100	100
All	All	4868/5149 (94%)	4704 (97%)	164 (3%)	48	75

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	AN	63	ARG
20	AT	4	LYS
47	BW	51	LEU
15	AO	25	GLU
17	AQ	51	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 152 such sidechains are listed below:

Mol	Chain	Res	Type
28	BD	114	GLN
33	BI	28	ASN
51	B1	15	ASN
28	BD	162	GLN
30	BF	30	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1542 (99%)	163 (10%)	3 (0%)
22	AV	75/76 (98%)	20 (26%)	2 (2%)
22	AW	75/76 (98%)	12 (16%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	AX	17/18 (94%)	3 (17%)	0
25	BA	2894/2903 (99%)	293 (10%)	6 (0%)
26	BB	118/119 (99%)	11 (9%)	0
All	All	4716/4734 (99%)	502 (10%)	11 (0%)

5 of 502 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	47	C

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	AV	73	A
25	BA	1052	C
25	BA	1911	U
22	AV	15	G
25	BA	1645	G

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

4 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	$\# Z  > 2$
24	KBE	AY	1	24	8,8,9	0.52	0	7,8,10	0.99	1 (14%)
24	DPP	AY	2	24	2,5,6	0.63	0	1,5,7	1.91	0
24	UAL	AY	5	24	7,8,9	2.07	3 (42%)	4,9,11	1.56	1 (25%)
24	5OH	AY	6	24	8,12,13	0.53	0	6,16,18	1.68	1 (16%)



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
24	KBE	AY	1	24	-	0/7/7/8	0/0/0/0
24	DPP	AY	2	24	-	0/2/4/6	0/0/0/0
24	UAL	AY	5	24	-	0/3/7/9	0/0/0/0
24	5OH	AY	6	24	-	0/1/18/20	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	5	UAL	C-CA	-3.51	1.39	1.45
24	AY	5	UAL	C1-N1	-3.45	1.34	1.40
24	AY	5	UAL	CA-N	2.23	1.40	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	6	5OH	CR-CB-CA	-3.46	109.24	112.77
24	AY	5	UAL	O-C-CA	-2.80	121.68	125.59
24	AY	1	KBE	CD-CG-CB	-2.10	108.84	115.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AY	1	KBE	2	0
24	AY	5	UAL	2	0
24	AY	6	5OH	8	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	BA	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	1916:A	O3'	1917:U	P	2.60
1	BA	1911:U	O3'	1912:A	P	1.12