



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2024 – 09:11 PM EST

PDB ID : 4V4R  
Title : Crystal structure of the whole ribosomal complex.  
Authors : Petry, S.; Brodersen, D.E.; Murphy IV, F.V.; Dunham, C.M.; Selmer, M.;  
Tarry, M.J.; Kelley, A.C.; Ramakrishnan, V.  
Deposited on : 2005-09-30  
Resolution : 5.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

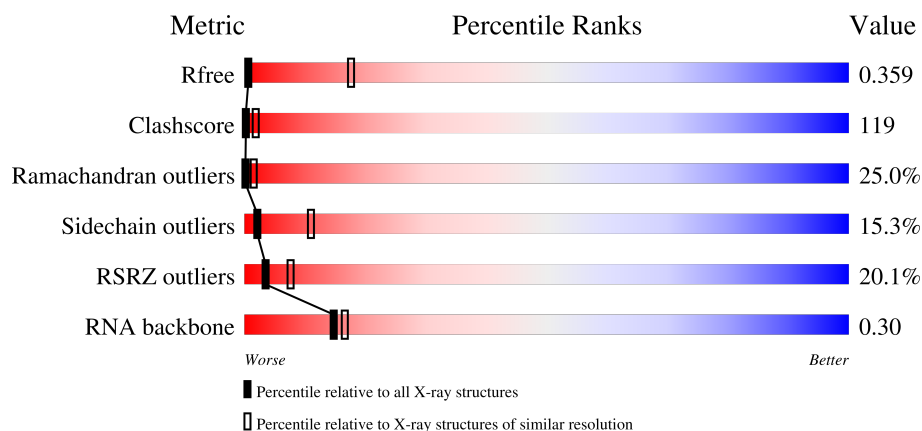
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.90 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1075 (7.80-4.00)
Clashscore	180529	1115 (7.80-4.00)
Ramachandran outliers	177936	1008 (7.82-3.98)
Sidechain outliers	177891	1013 (7.82-3.96)
RSRZ outliers	164620	1070 (7.80-4.00)
RNA backbone	3690	1173 (8.50-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1522	<div> <div>5%</div> <div>25% 42% 24% 9%</div> </div>
2	AV	76	<div> <div>7%</div> <div>17% 57% 22%</div> </div>
3	AW	76	<div> <div>7%</div> <div>29% 43% 18% 9%</div> </div>
4	AX	18	<div> <div>67%</div> <div>61% 33% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
5	AB	256	
6	AC	239	
7	AD	209	
8	AE	162	
9	AF	101	
10	AG	156	
11	AH	138	
12	AI	128	
13	AJ	105	
14	AK	129	
15	AL	135	
16	AM	126	
17	AN	61	
18	AO	89	
19	AP	88	
20	AQ	105	
21	AR	88	
22	AS	93	
23	AT	106	
24	AU	27	
25	AY	354	
26	BB	123	
27	BA	2916	
28	BD	173	
29	BE	338	

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Mol	Chain	Length	Quality of chain
30	BF	246	
31	BG	176	
32	BH	177	
33	BI	149	
34	BN	145	
35	BO	122	
36	BP	164	
37	BQ	138	
38	BS	186	
39	BT	66	
40	BW	113	
41	BX	84	
42	BY	119	
43	BZ	253	
44	BR	118	
45	BU	118	
46	BV	100	
47	B2	70	
48	B3	60	
49	B0	91	
50	B4	73	
51	B5	60	
52	B6	82	
53	B7	47	
54	B8	64	

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Mol	Chain	Length	Quality of chain
55	B9	36	
56	BK	141	

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
3	YYG	AW	37	X	-	X	-

## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 142780 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
1	AA	1515	Total	C	N	O	P	0	0	0
			32551	14490	6022	10525	1514			

- Molecule 2 is a RNA chain called P-site tRNA (Phe).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AV	76	Total	C	N	O	P	0	0	0
			1622	725	293	529	75			

- Molecule 3 is a RNA chain called E-site tRNA (Phe).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AW	76	Total	C	N	O	P	0	0	0
			1638	736	294	533	75			

- Molecule 4 is a RNA chain called 5'-R(\*AP\*UP\*GP\*UP\*UP\*CP\*UP\*AP\*GP\*UP\*AP\*C  
P\*AP\*AP\*UP\*AP\*AP\*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AX	17	Total	C	N	O	P	0	0	11
			136	56	19	44	17			

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AB	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 7 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 8 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AE	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 9 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 10 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 11 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AI	127	Total	C	N	O		0	0	0
			1011	639	198	174				

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AJ	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AL	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 17 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 19 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 20 is a protein called 30S ribosomal protein S17.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AQ	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 21 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AR	73	Total	C	N	O		0	0	0
			597	380	118	99				

- Molecule 22 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AS	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

- Molecule 23 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 24 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AU	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 25 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
25	AY	333	Total	C	0	0	333
			333	333			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BB	123	Total	C	N	O	P	0	0	0
			2637	1175	488	852	122			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	-1	A	-	insertion	GB 48271

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BA	2814	Total	C	N	O	P	0	0	0
			60600	26974	11331	19482	2813			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	493	G	-	insertion	GB 48268

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BD	173	Total	C	N	O	S	0	0	0
			1308	820	246	236	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BE	191	Total	C	N	O	S	0	0	0
			1507	940	290	273	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BF	189	Total	C	N	O	S	0	0	0
			1430	872	255	302	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BG	122	Total	C	N	O	S	0	0	0
			957	597	176	180	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	164	Total	C	N	O	S	0	0	0
			1251	787	225	237	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BI	148	Total	C	N	O	S	0	0	0
			1145	727	205	212	1			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BN	117	Total	C	N	O	S	0	0	0
			917	570	164	180	3			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BO	122	Total	C	N	O	S	0	0	0
			937	585	180	169	3			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BP	84	Total	C	N	O	0	0	0
			639	391	109	139			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BQ	138	Total	C	N	O	S	0	0	0
			1081	678	208	192	3			

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BS	113	Total	C	N	O	S	0	0	0
			866	536	165	164	1			

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BT	52	Total	C	N	O	S	0	0	0
			406	242	74	85	5			

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	BW	108	Total	C	N	O	0	0	0
			860	542	169	149			

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BX	76	Total	C	N	O	S	0	0	0
			602	366	102	131	3			

- Molecule 42 is a protein called 50S ribosomal protein 24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	BY	110	Total	C	N	O	0	0	0
			879	531	166	182			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BZ	177	Total	C	N	O	S	0	0	0
			1360	859	238	257	6			

- Molecule 44 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BR	105	Total	C	N	O	0	0	0
			855	536	174	145			

- Molecule 45 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BU	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 46 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BV	100	Total	C	N	O	S	0	0	0
			787	495	146	145	1			

- Molecule 47 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B2	64	Total	C	N	O	S	0	0	0
			494	301	93	99	1			

- Molecule 48 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B3	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B0	86	Total	C	N	O	S	0	0	0
			641	402	124	114	1			

- Molecule 50 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B4	73	Total	C	N	O	S	0	0	0
			604	382	110	108	4			

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B5	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B6	53	Total	C	N	O	S	0	0	0
			431	274	80	76	1			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B7	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B8	63	Total	C	N	O	S	0	0	0
			496	312	101	78	5			

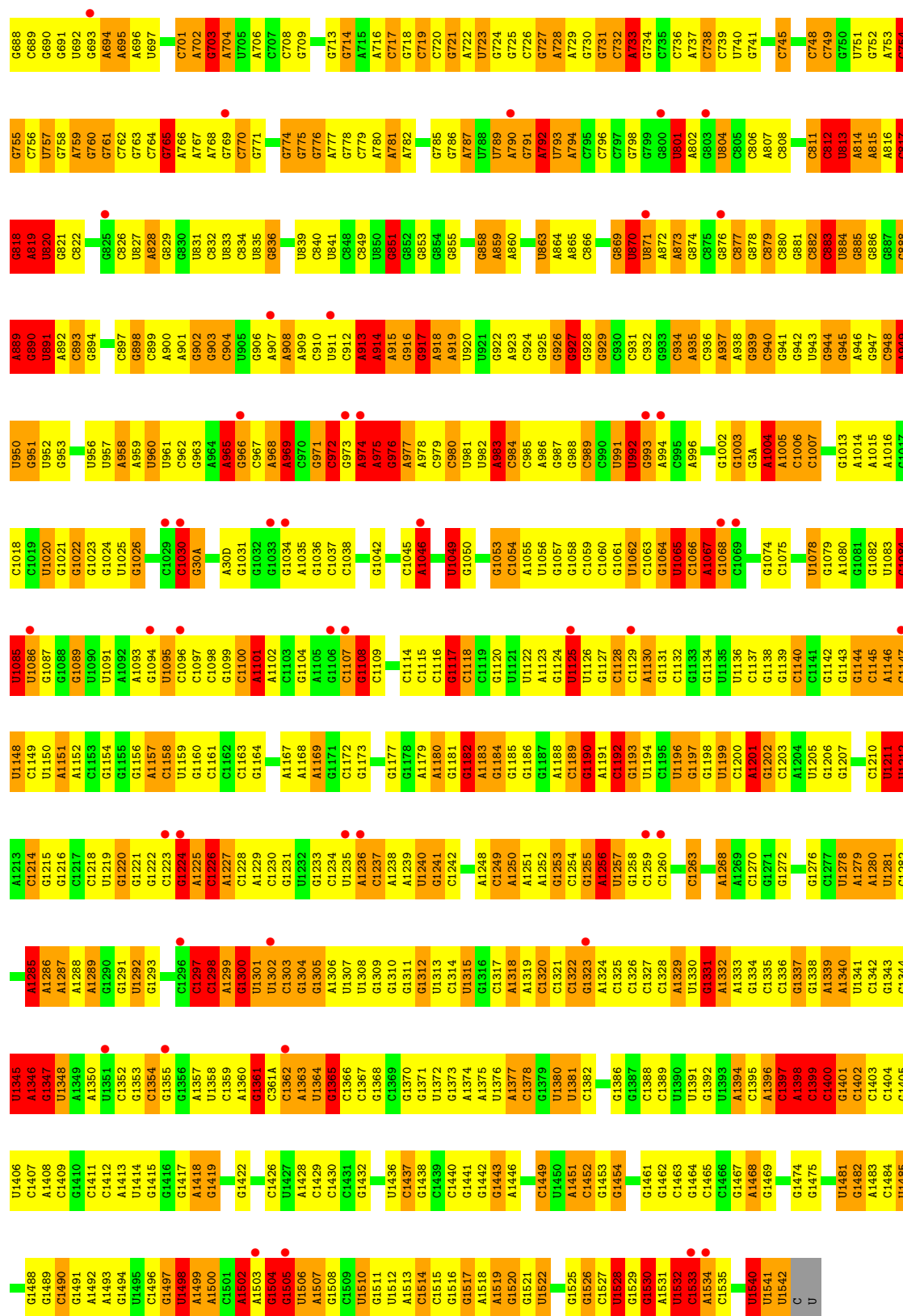
- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B9	35	Total	C	N	O	S	0	0	0
			285	172	64	45	4			

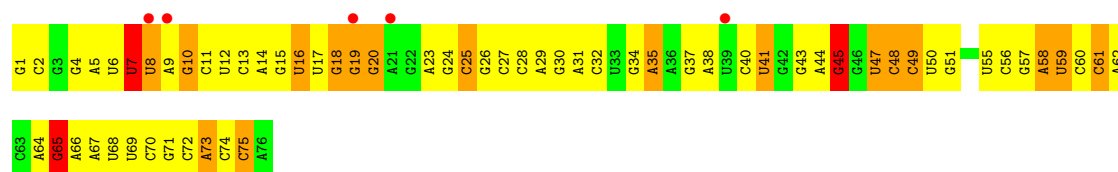
- Molecule 56 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BK	133	Total	C	N	O	S	0	0	0
			999	642	169	182	6			

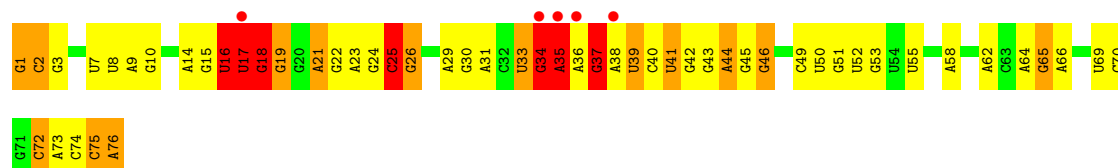




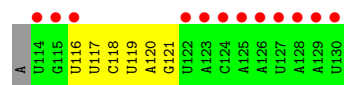




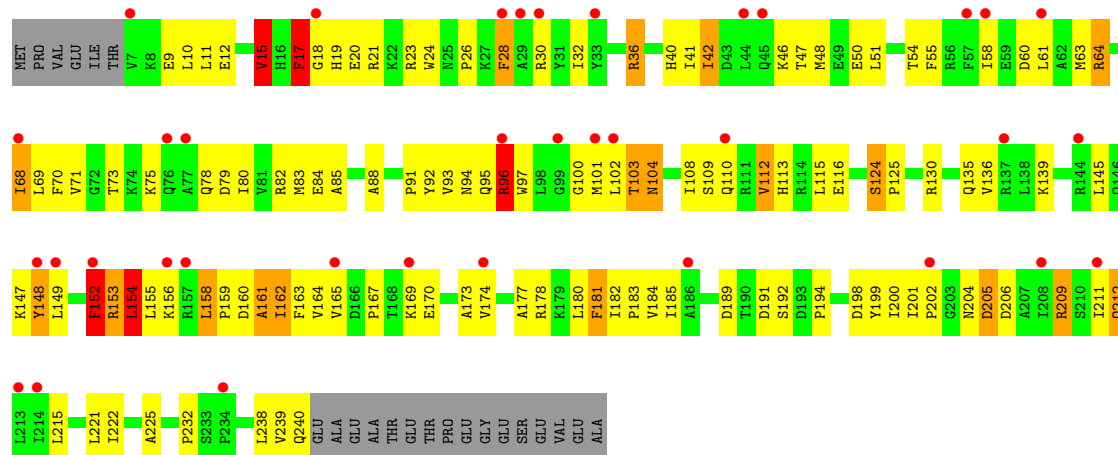
• Molecule 3: E-site tRNA (Phe)



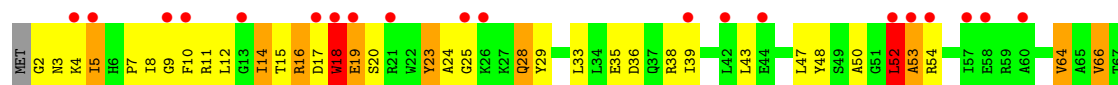
• Molecule 4: 5'-R(\*AP\*UP\*GP\*UP\*UP\*CP\*UP\*AP\*GP\*UP\*AP\*CP\*AP\*AP\*UP\*AP\*AP\*U)-3'

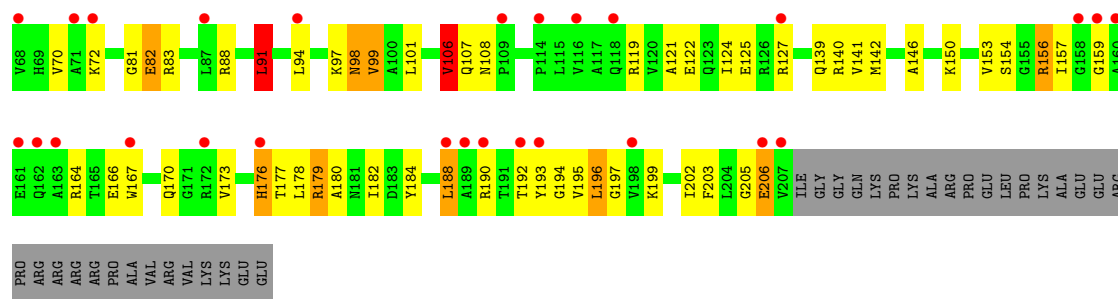


• Molecule 5: 30S ribosomal protein S2

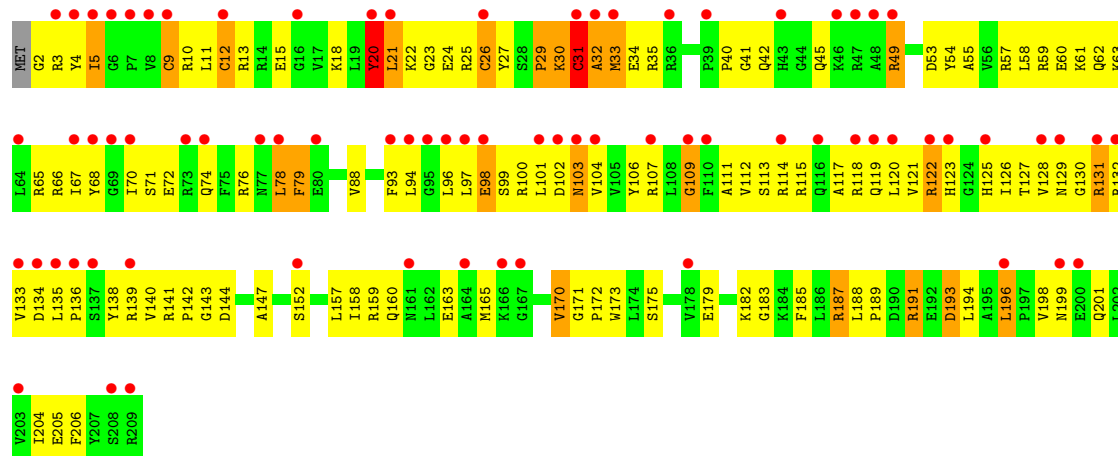


• Molecule 6: 30S ribosomal protein S3

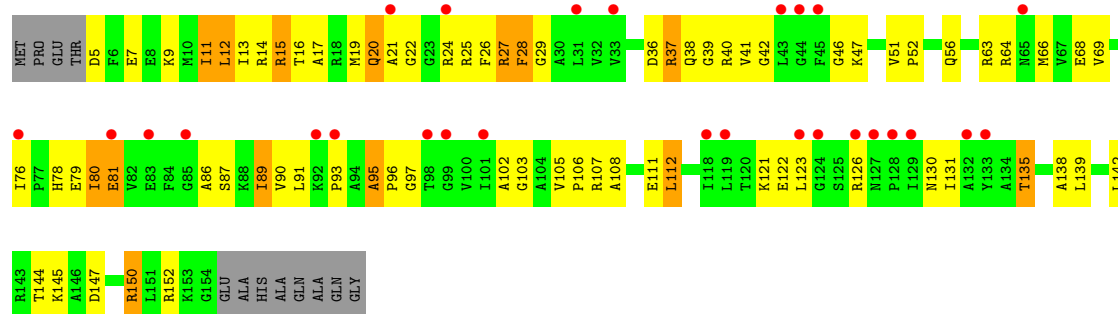




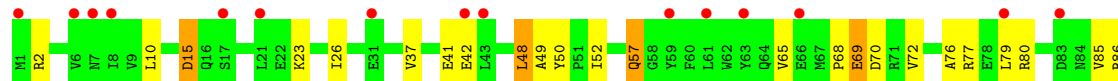
• Molecule 7: 30S ribosomal protein S4



• Molecule 8: 30S ribosomal protein S5

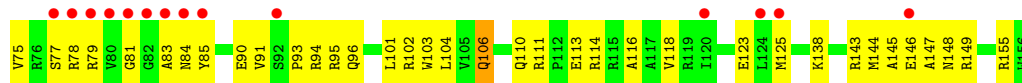
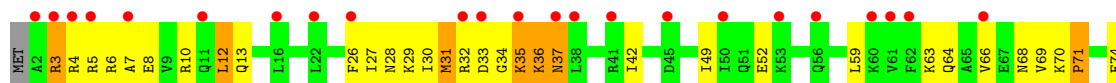


• Molecule 9: 30S ribosomal protein S6

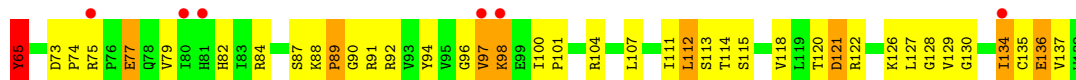
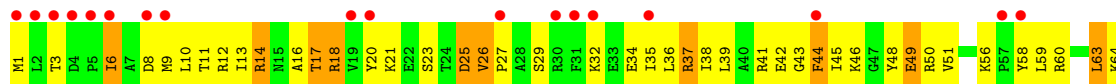




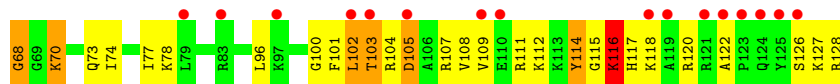
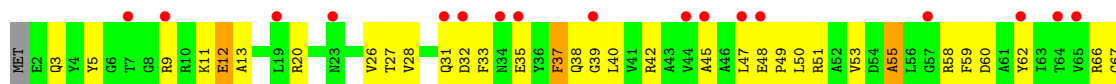
• Molecule 10: 30S ribosomal protein S7



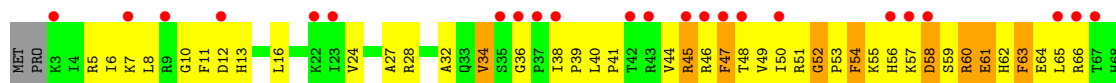
• Molecule 11: 30S ribosomal protein S8



• Molecule 12: 30S ribosomal protein S9

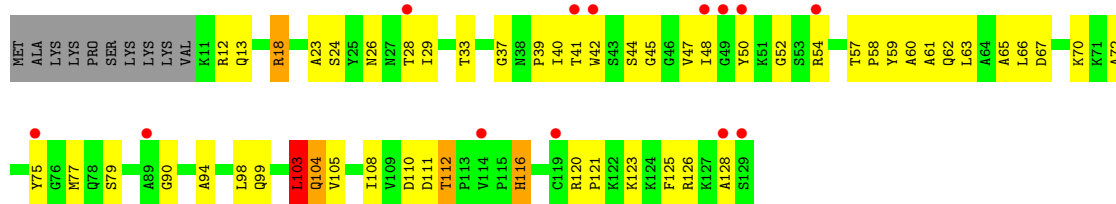


• Molecule 13: 30S ribosomal protein S10

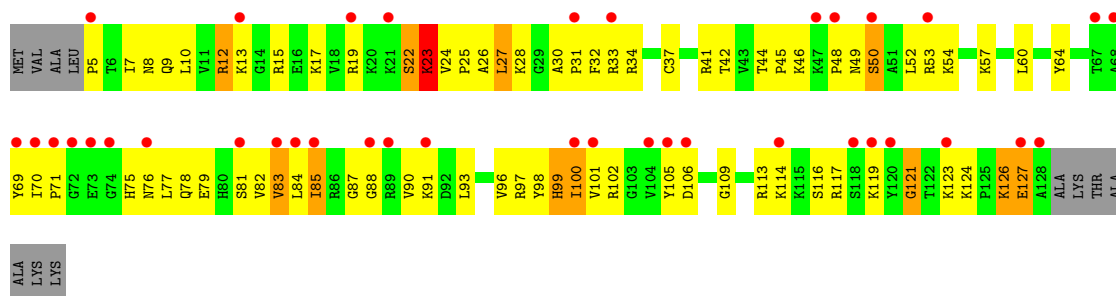


• Molecule 14: 30S ribosomal protein S11

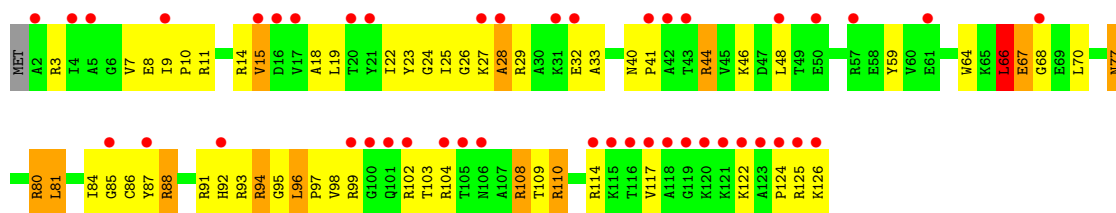




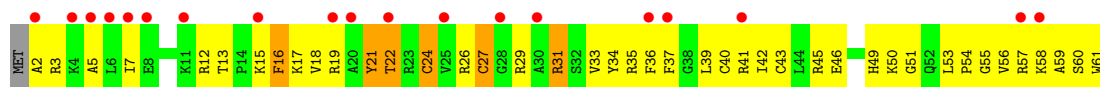
• Molecule 15: 30S ribosomal protein S12



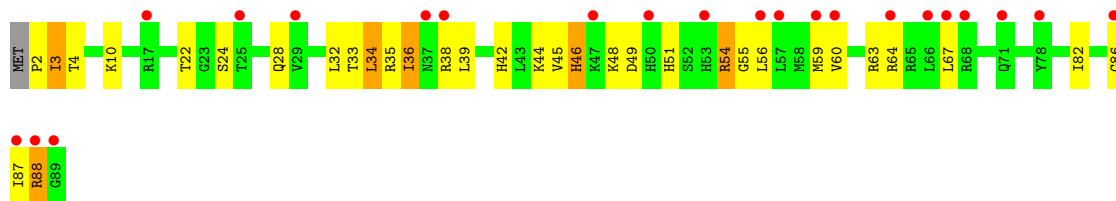
• Molecule 16: 30S ribosomal protein S13



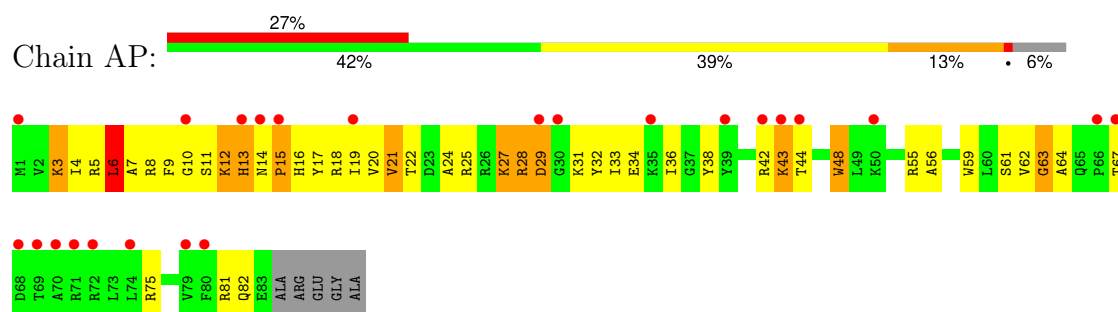
• Molecule 17: 30S ribosomal protein S14



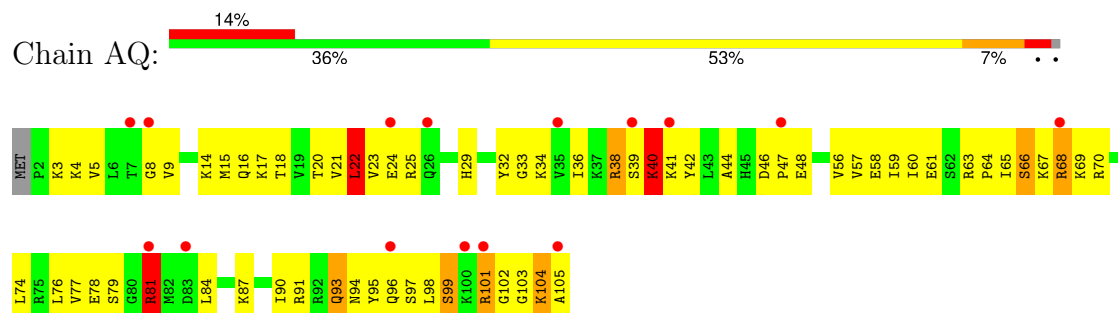
• Molecule 18: 30S ribosomal protein S15



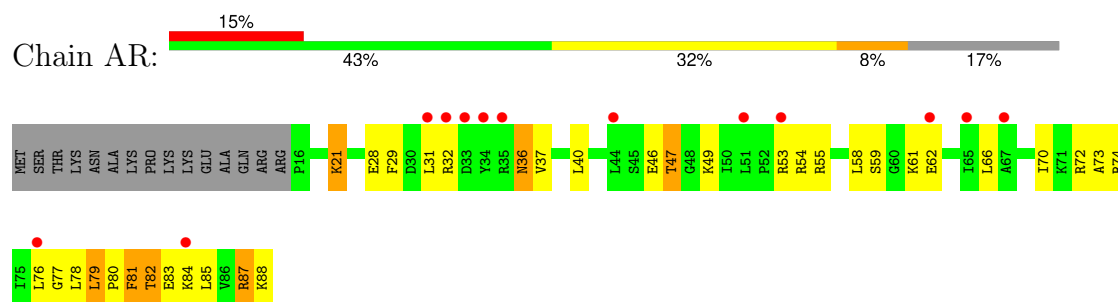
• Molecule 19: 30S ribosomal protein S16



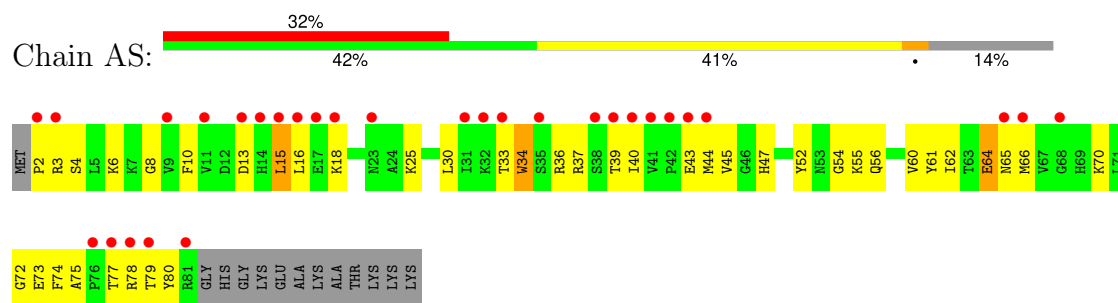
- Molecule 20: 30S ribosomal protein S17



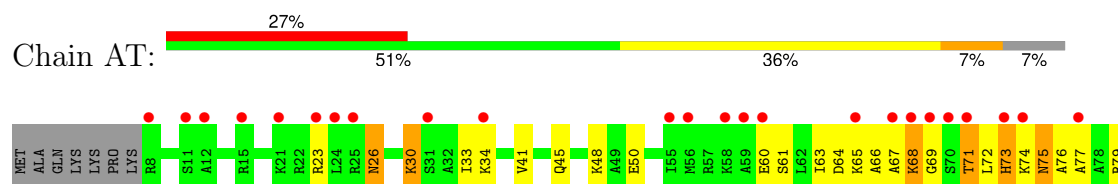
- Molecule 21: 30S ribosomal protein S18

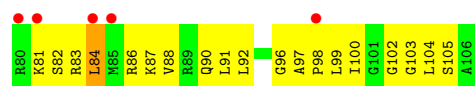


- Molecule 22: 30S ribosomal protein S19

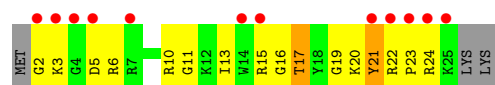


- Molecule 23: 30S ribosomal protein S20

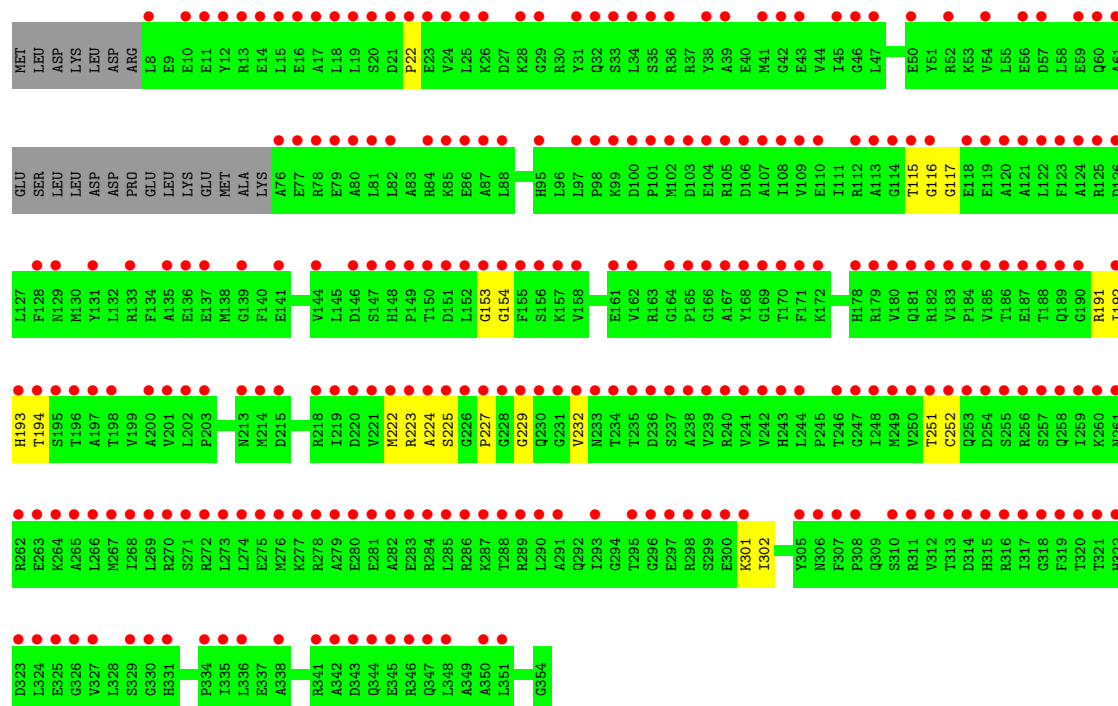
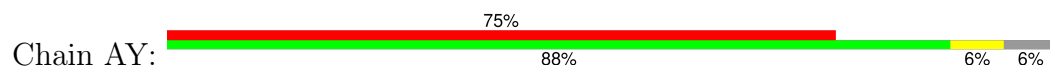




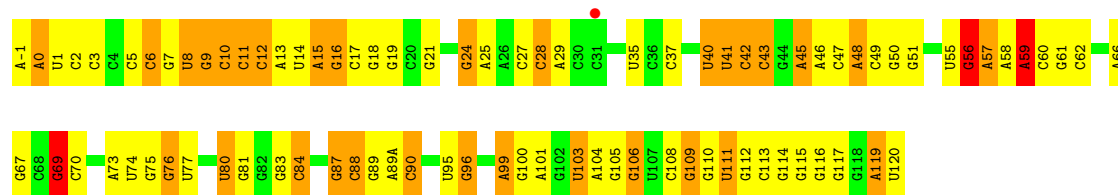
- Molecule 24: 30S ribosomal protein Thx



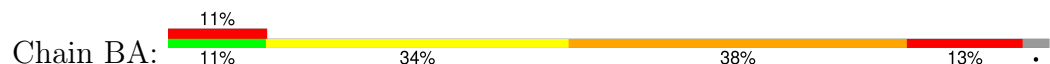
- Molecule 25: Peptide chain release factor 1



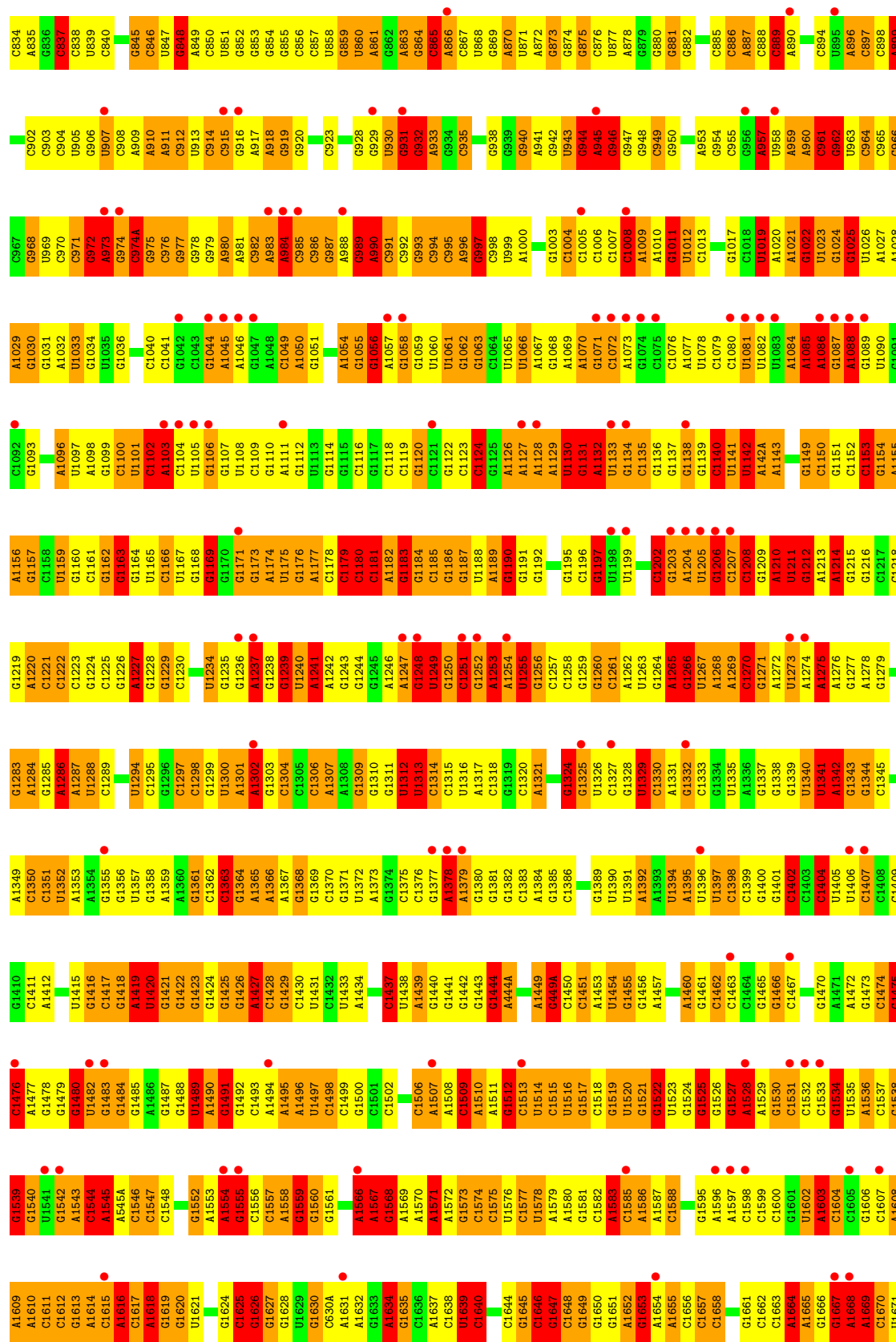
- Molecule 26: 5S ribosomal RNA



- Molecule 27: 23S ribosomal RNA

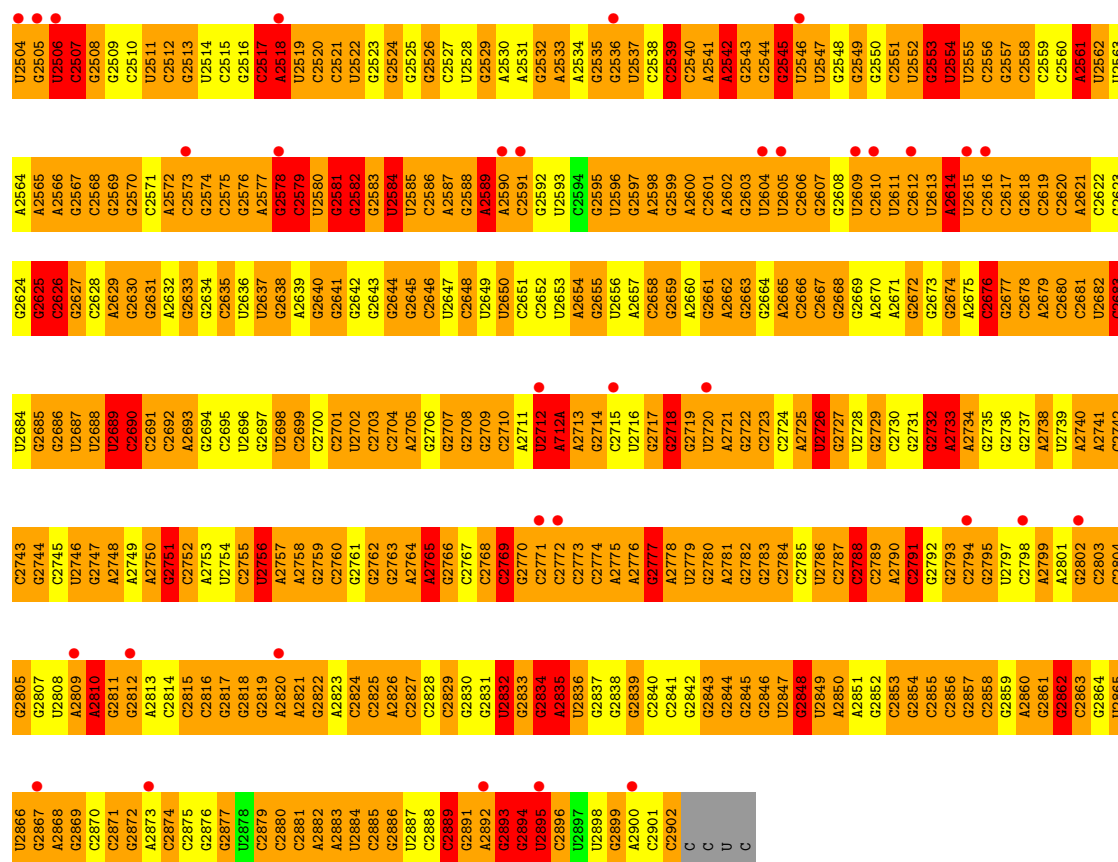




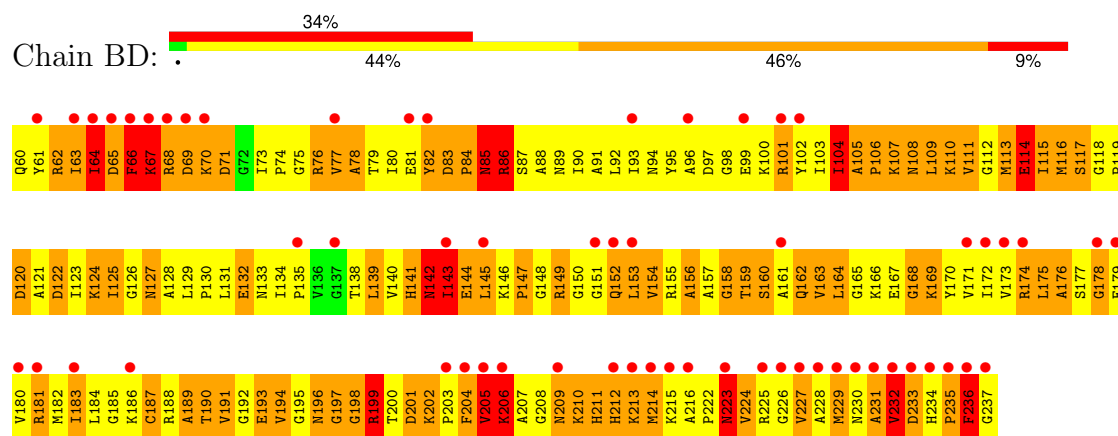




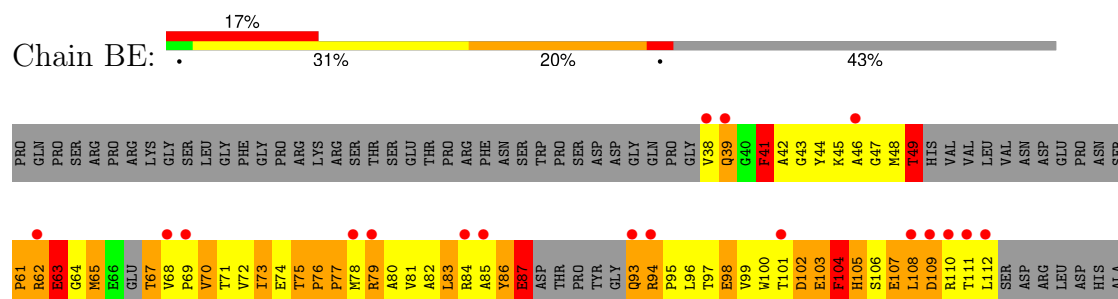
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G2445	C2385	G2325	U2265	C2195	U2075	A2015	A1952	A1869	G1816	A1755	U1673
G2446	C2386	C2326	A2266	U2196	U2076	U2016	A1953	A1890	G1817	G1756	G1674
G2447	C2387	A2327	A2267	U2197	A2077	U2017	G1954	G1891	U1818	U1757	C1675
A2448	A2388	A2328	A2268	A2198	U1955	G2018	U1956	C1896	A1819	G1758	A1676
U2449	G2389	G2329	A2269	A2199	C2078	A2019	C1957	G1896	U1820	A1759	A1677
A2450	U2390	G2330	G2270	C2205	G2080	A2020	C1958	C1899	A1821	A1760	G1678
A2451	G2391	G2331	G2271	C2206	C2081	C2021	C1959	G1899	G1822	G1761	U1679
A2452	A2392	U2332	U2272	C2207	U2082	U2022	G1960	G1899	G1823	A1762	U1680
A2453	A2393	A2333	A2273	U2208	C2083	G2023	A1960	A1900	G1824	G1763	G1681
G2454	G2394	G2334	A2274	U2209	C2084	G2024	C1961	A1901	A1825	G1764	G1682
G2455	G2395	A2335	C2275	C2210	C2085	C2025	U1962	C1902	G1826	G1765	G1683
G2456	G2396	A2336	G2276	G2211	U2086	C2026	U1963	G1903	C1827	U1766	C1684
U2457	G2397	G2337	G2277	A2212	G2087	G2027	G1964	G1904	G1828	C1767	C1685
G2458	U2398	G2338	A2278	U2213	G2088	U2028	C1965	C1905	A1829	U1768	C1686
A2459	G2399	G2339	G2279	G2215	A1966	U2029	A1967	G1906	C1830	G1769	G1687
U2460	G2400	G2340	G2280	G2216	C2089	A2030	C1968	G1907	G1831	G1770	U1688
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U2462	C2402	C2342	G2282	G2218	U2092	G2032	A1969	C1909	U1833	G1772	A1690
C2463	C2403	C2343	C2283	G2219	G2093	A2033	A1970	G1910	U1834	A1773	U1693
C2464	U2404	U2344	G2224	G2220	G2094	U2034	A1971	G1911	G1835	C1774	G1694
G2465	G2405	G2345	A2225	A2221	C2095	G2035	A1972	U1912	C1836	U1775	G1695
C2466	U2406	A2346	C2286	G2226	U2096	G2036	G1973	A1913	G1837	G1776	G1696
G2467	G2407	G2347	A2287	A2227	C2097	G2037	C1974	U1915	C1838	U1777	G1697
A2468	U2408	U2348	A2288	G2228	U2098	G2038	G1975	A1916	G1839	U1778	G1698
G2469	G2409	G2349	G2289	C2229	U2099	C2039	U1976	A1917	G1840	U1779	A1699
G2470	A2410	G2350	G2290	G2230	G2100	C2040	A1977	U1917	U1841	A1780	G1699
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G2472	A2412	A2352	C2292	U2232	U2102	A2042	C1979	A1919	C1843	C1782	A1701
U2473	G2413	G2353	C2293	U2233	C2103	C2043	G1980	C1920	A1783	G1783	G1702
G2474	G2414	G2354	G2294	G2234	G2104	C2044	A1981	G1921	A1784	A1784	G1703
G2475	G2415	C2355	C2295	G2235	C2105	C2045	C1982	G1922	A1847	G1785	G1704
A2476	U2416	G2356	U2296	G2236	G	G2046	C1983	U1923	A1848	A1786	G1705
C2477	G2417	U2357	G2297	G2237	U	U2047	G1984	C1924	U1851	A1787	U1706
A2478	A2418	G2358	A2298	G2238	C	G2048	C1988	C1925	C1852	C1788	G1707
G2479	U2419	G2359	G2299	G2239	U	G2049	G1989	U1926	A1853	A1789	C1708
C2480	A2420	A2360	G2300	G2240	A	C2050	C1990	A1927	A1854	C1790	U1709
G2481	G2421	A2361	C2301	A2241	A	A2051	G1991	A1928	G1855	A1791	C1710
G2482	A2422	G2362	G2302	G2242	U	G2052	U1991	G1929	G1856	G1792	G1718
U2423	G2423	C2363	G2303	U2243	A	G2053	G1992	G1930	C1795	G1795	G1725
G2484	A2424	C2364	G2304	U2244	C	A2054	U1993	U1931	U1796	U1796	G1726
A2425	A2425	G2365	A2305	U2245	C	G2055	C1994	A1932	G1857	C1797	U1727
A2426	A2426	A2366	C2306	G2246	A	G2056	U1995	G1933	A1859	U1798	G1728
G2487	C2427	G2367	G2307	A2247	C	A2057	C1996	C1934	G1860	G1799	A1729
A2488	G2428	C2368	G2308	C2248	U	A2058	G1997	G1935	G1861	G1799	A1730
G2489	U2429	A2369	A2309	U2249	C	A2059	C1998	A1936	G1862	C1800	G1731
G2490	A2430	G2370	A2310	G2250	A	A2060	C1999	A1937	C1870	A1801	A1732
U2491	U2431	G2371	G2311	G2251	U	G2061	G2000	A1938	A1871	A1802	G1733
U2492	A2432	G2372	U2312	G2252	G	A2062	A2001	U1939	A1872	A1803	G1734
U2493	A2433	G2373	C2313	G2253	G	C2063	G2002	U1940	G1873	C1804	C1735
G2494	A2434	C2374	C2314	G2254	G	C2064	G2003	C1941	U1865	U1805	C1741
G2495	A2435	G2375	G2315	G2255	G	C2065	G2004	C1942	C1878	C1806	G1742
G2496	G2436	A2376	G2316	G2256	A	G2066	C2005	U1943	C1880	G1807	G1743
A2497	U2437	A2377	G2317	G2257	G	G2067	C2006	U1944	C1881	U1808	G1744
C2498	U2438	A2378	G2318	G2258	C	U2068	C2007	C1945	C1882	A1809	G1746
U2499	A2439	G2379	G2319	G2259	U	G2069	C2008	U1946	G1883	A1810	G1747
U2500	C2440	C2380	A2320	C2260	U	G2070	G2009	C1947	A1884	G1811	C1751
C2501	U2441	C2381	G2321	U2261	G	A2071	G2010	U1948	A1885	A1812	G1752
G2502	G2442	G2382	A2322	U2262	U	G2072	G2012	G1949	C1886	G1813	C1753
A2503	G2443	G2383	C2323	C2263	G	G2073	A2013	G1950	C1887	G1814	G1754

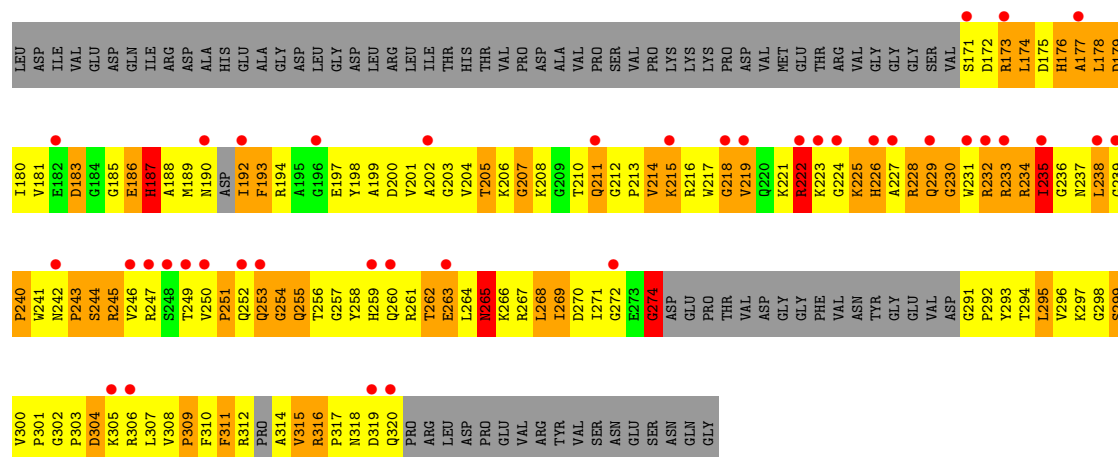


• Molecule 28: 50S ribosomal protein L2

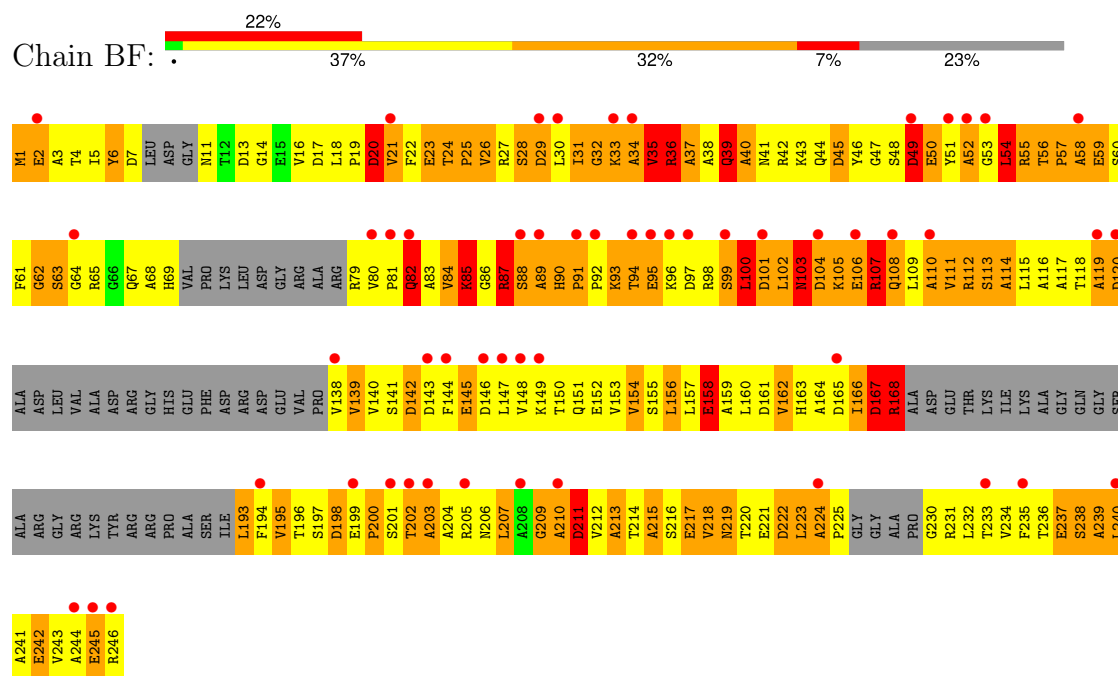


• Molecule 29: 50S ribosomal protein L3

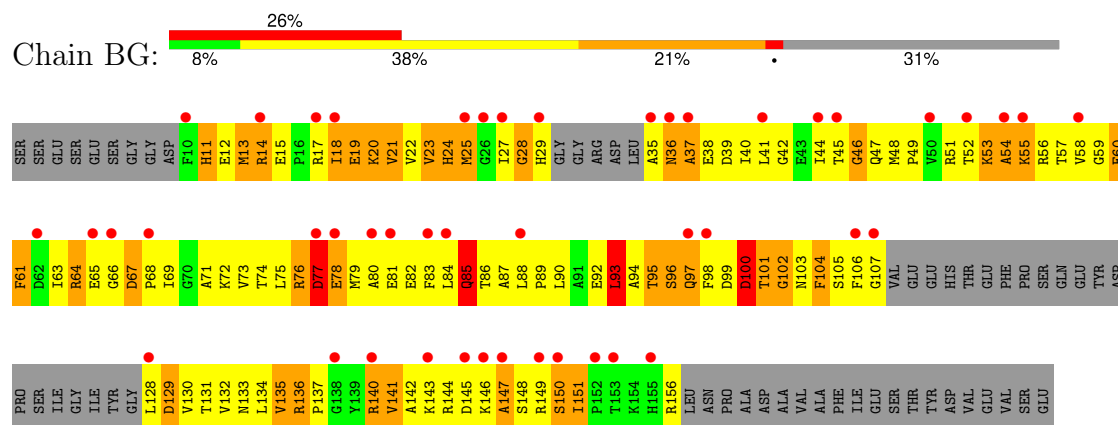




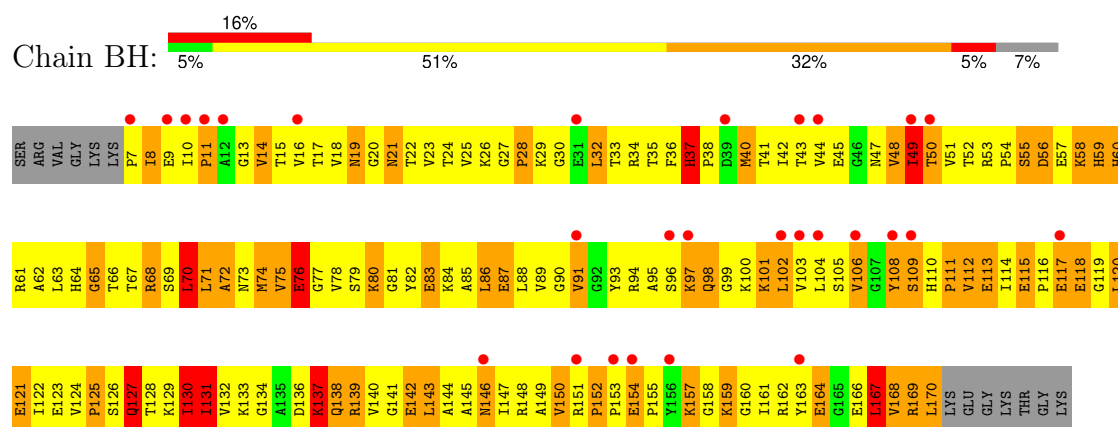
• Molecule 30: 50S ribosomal protein L4



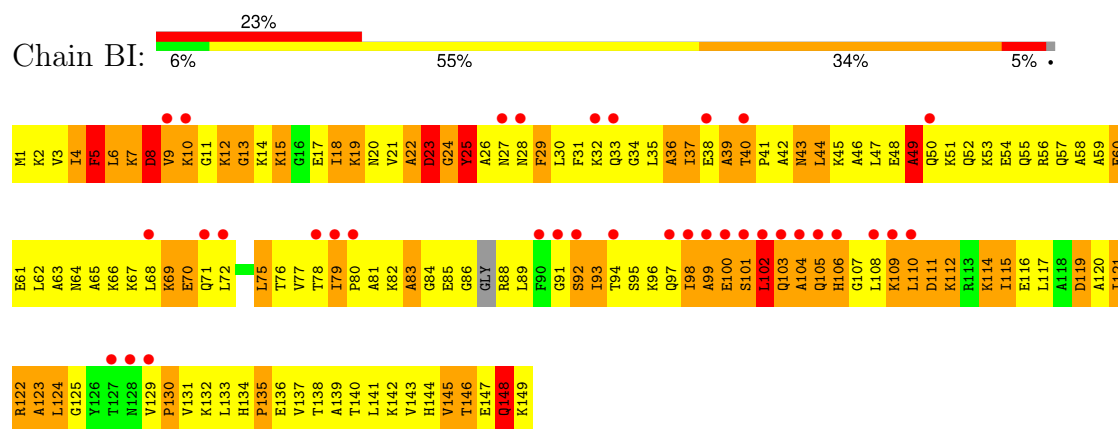
• Molecule 31: 50S ribosomal protein L5



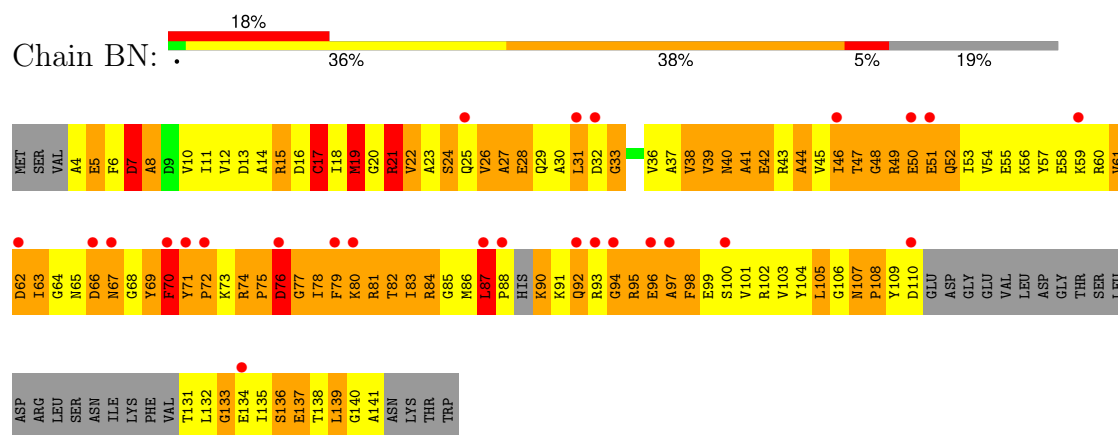
• Molecule 32: 50S ribosomal protein L6



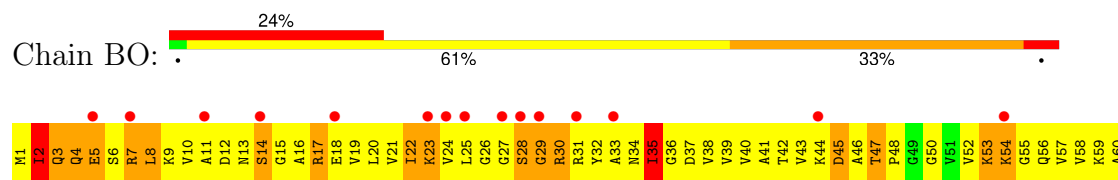
• Molecule 33: 50S ribosomal protein L9

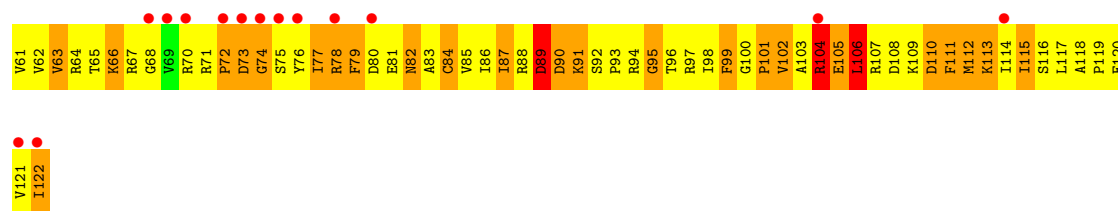


• Molecule 34: 50S ribosomal protein L13

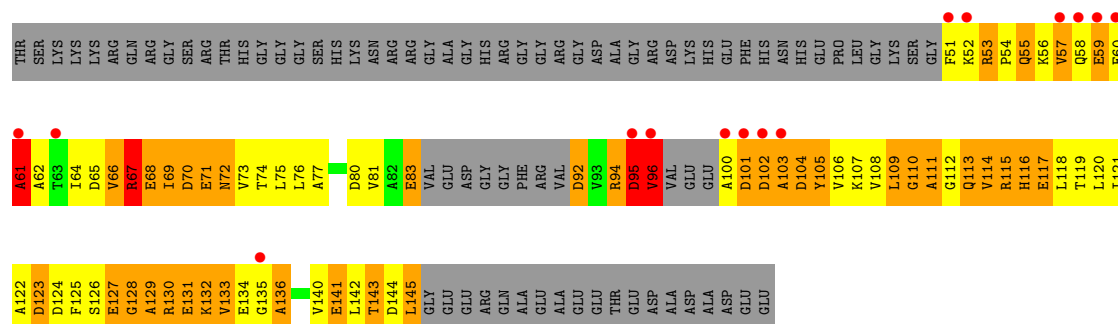
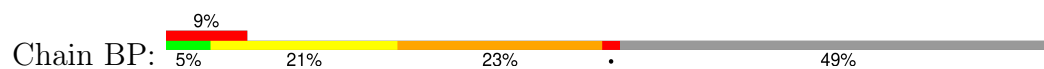


• Molecule 35: 50S ribosomal protein L14

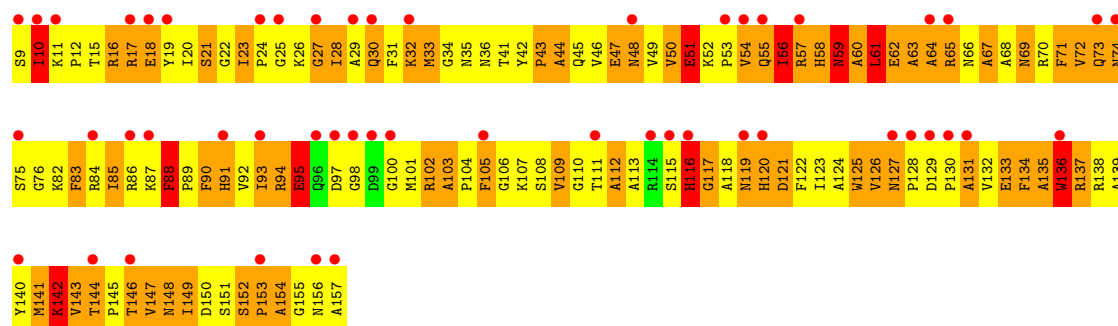




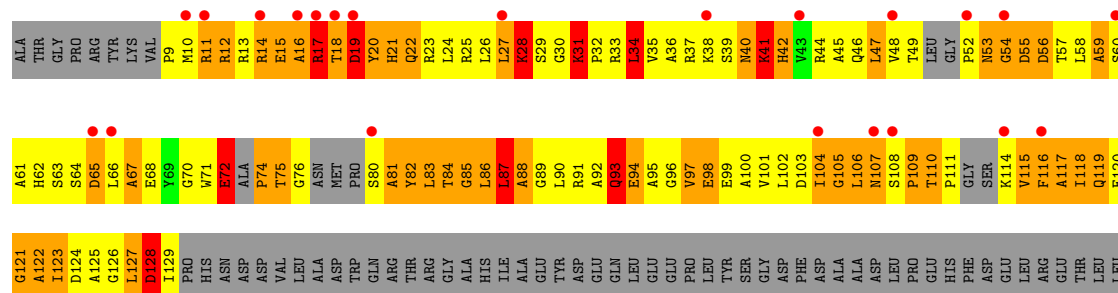
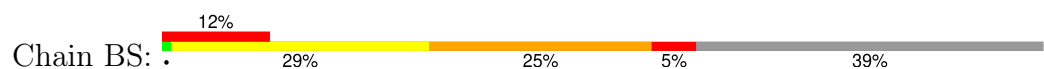
• Molecule 36: 50S ribosomal protein L15



• Molecule 37: 50S ribosomal protein L16



• Molecule 38: 50S ribosomal protein L18



ASP  
GLY  
ASP  
ILE  
GLU  
LEU

• Molecule 39: 50S ribosomal protein L19

Chain BT: 30%  
6% 35% 29% 9% 21%

PRO ARG THR R4 E5 C6 D7 Y8 C9 G10 T11 D12 S13 E14 P15 G16 T17 T18 T19 M20 F21 V22 H23 K24 D25 G26 A27 T28 T29 H30 F31 G32 S33 S34 K35 C36 E37 N38 N39 L42 L43 R44 E45 A46 R47 N48 L49 E50 E51 T52 D53 T54 A55 R56 GLY GLU ALA GLY

ALA  
GLU  
ASP  
GLU  
ALA

• Molecule 40: 50S ribosomal protein L22

Chain BW: 26%  
41% 49%

MET E2 A3 K4 I5 A6 R7 Y8 Y9 V10 R11 I12 S13 P14 R15 K16 V17 R18 L19 V20 V21 D22 L23 I24 R25 G26 P27 K28 L29 E30 E31 A32 R33 R34 I35 L36 R37 Y38 T39 N40 K41 R42 G43 A44 Y45 F46 V47 K48 K49 V50 L51 E52 S53 A54 A55 A56 N57 V58 V59 N60

N61 H62 D63 MET L65 E66 D67 R68 L69 V70 V71 W72 K73 A74 Y75 V76 D77 E78 G79 P80 A81 L82 K83 R84 V85 L86 P87 R88 A89 R90 R91 G92 R93 A94 I95 I96 K97 K98 R99 T100 S101 H102 T103 T104 V105 I106 L107 G108 E109 K110 H11 S11 LYS

• Molecule 41: 50S ribosomal protein L23

Chain BX: 24%  
40% 31% 15% 10%

S1 W2 D3 V4 I5 K6 H7 P8 H9 V10 T11 E12 K13 A14 M15 N16 D17 M18 D19 F20 G21 N22 K23 L24 Q25 F26 A27 V28 D29 D30 R31 A32 A33 K34 G35 Y36 E37 V37 A38 D39 V40 V41 E42 E43 E44 Y45 D46 Y47 T48 V49 E50 Q51 V52 N53 T54 Q55 T56 M57 D58 G59 G60

E61 K62 A63 A64 V65 V66 R67 L68 S69 D70 E71 D72 D73 A74 Q75 E76 V77 A78 S79 ARG ILE GLY VAL PHE

• Molecule 42: 50S ribosomal protein 24

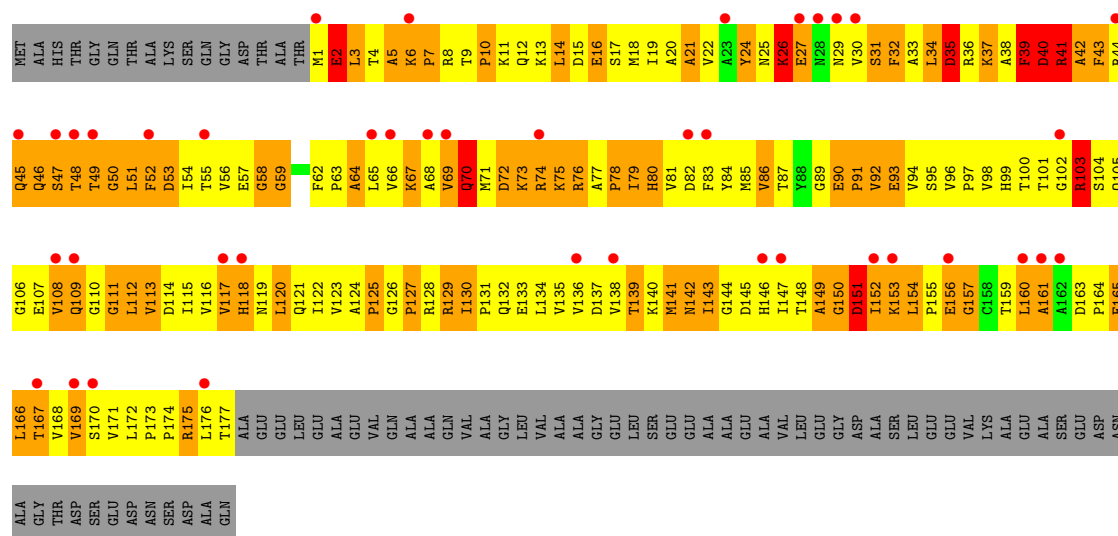
Chain BY: 34%  
49% 31% 8% 8%

S1 K2 Q3 N4 P4 D5 K6 Q7 Q8 K9 S10 Q11 R12 R13 A14 P15 L16 H17 E18 T19 H20 K21 V22 V23 R24 A25 T26 L27 R28 A29 L30 L31 R32 E33 E34 Y35 E36 G37 GLN ARG ASN V40 R41 V42 V43 N44 A45 G46 D47 T48 V49 E50 L51 R52 G53 D54 F55 A56 G57 E58 E59 G60

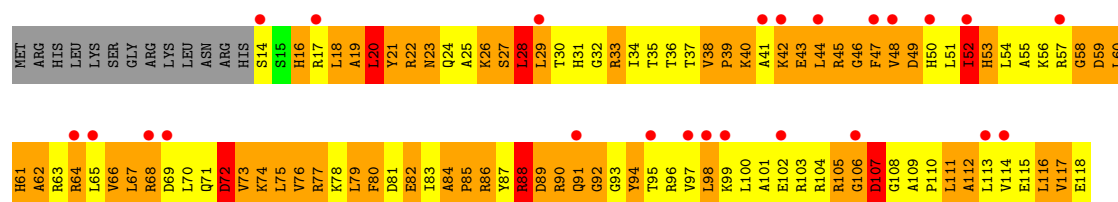
E61 V62 I63 N64 V65 D66 L67 D68 K69 A70 A71 H72 H73 R74 E75 D76 T77 T78 L79 E80 K81 D82 D83 G84 E85 E86 H87 P88 R89 P90 L91 D92 T93 S94 N95 Y96 V97 V98 V99 D100 L101 D102 D103 L104 E105 D106 K107 R108 E109 A110 R111 L112 E113 SER GLU ASP ASP SER ALA

• Molecule 43: 50S ribosomal protein CTC

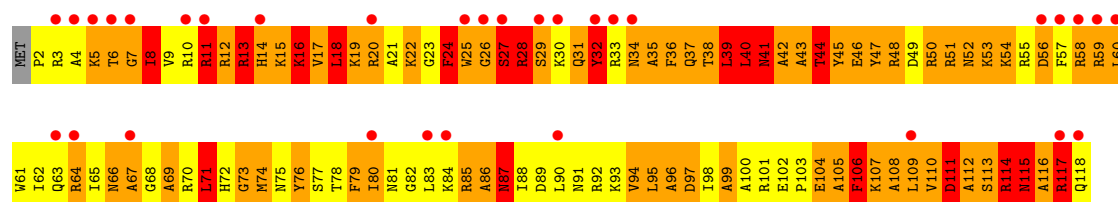
Chain BZ: 16%  
35% 29% 30%



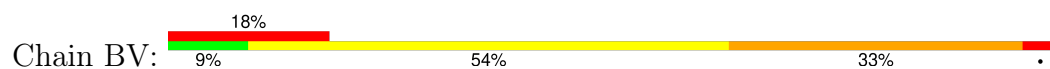
• Molecule 44: 50S ribosomal protein L17



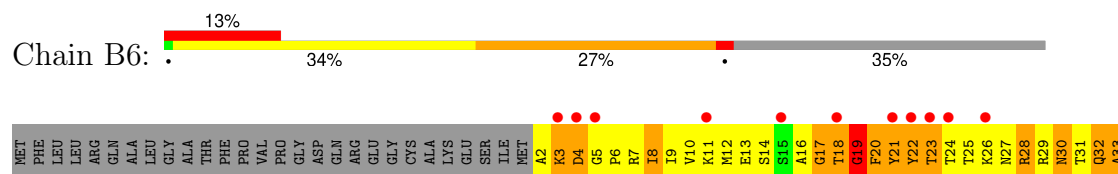
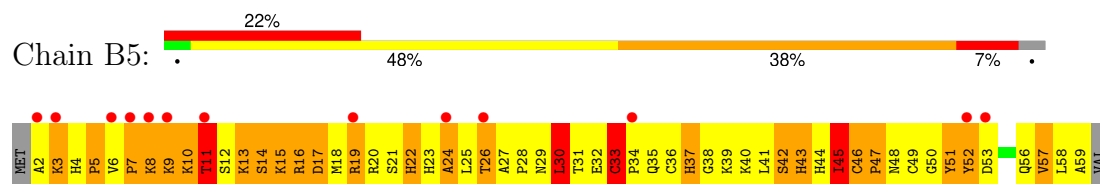
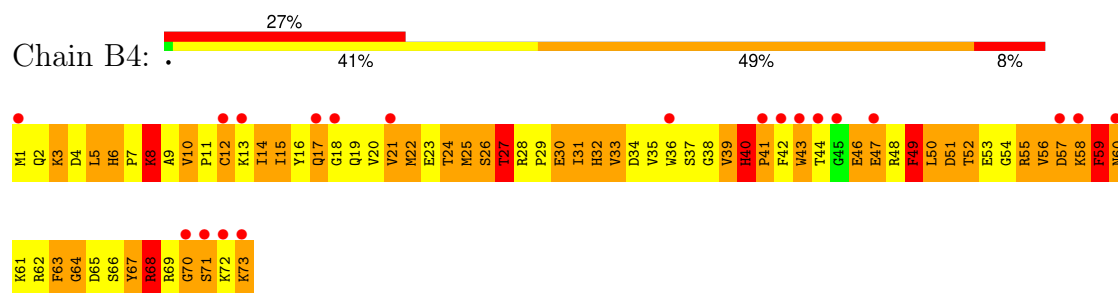
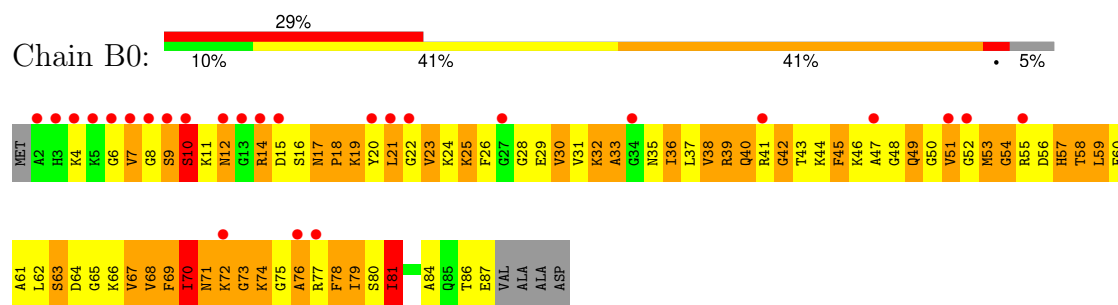
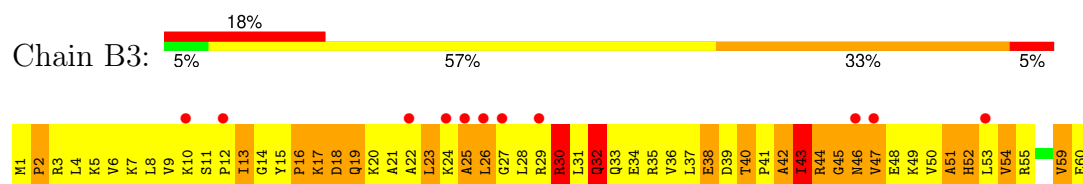
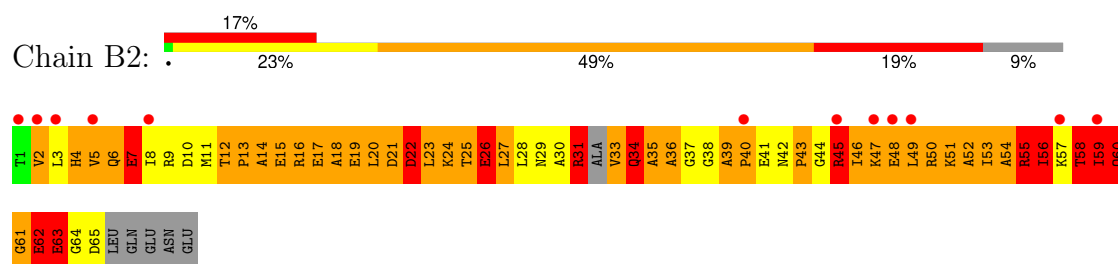
• Molecule 45: 50S ribosomal protein L20



• Molecule 46: 50S ribosomal protein L21



• Molecule 47: 50S ribosomal protein L29



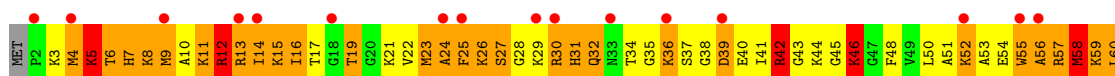




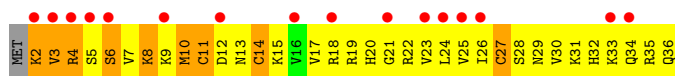
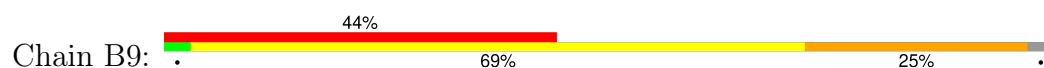
- Molecule 53: 50S ribosomal protein L34



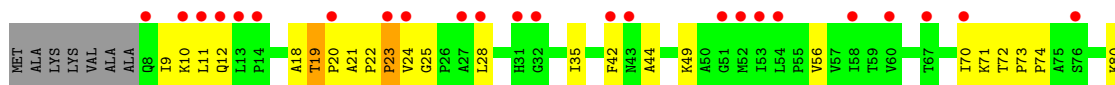
- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



- Molecule 56: 50S ribosomal protein L11



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	518.99Å 518.99Å 365.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 5.90 40.00 – 5.90	Depositor EDS
% Data completeness (in resolution range)	97.4 (40.00-5.90) 97.0 (40.00-5.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.41 (at 5.39Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.351 , 0.371 0.338 , 0.359	Depositor DCC
$R_{free}$ test set	6319 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	223.1	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.14 , 141.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	142780	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	236.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	AA	1.25	68/36411 (0.2%)	1.47	415/56769 (0.7%)
2	AV	2.34	3/1813 (0.2%)	1.16	11/2823 (0.4%)
3	AW	1.82	17/1739 (1.0%)	1.97	36/2698 (1.3%)
4	AX	0.18	0/139	0.66	0/213
5	AB	0.63	1/1935 (0.1%)	0.66	4/2609 (0.2%)
6	AC	0.60	2/1636 (0.1%)	1.10	6/2205 (0.3%)
7	AD	0.65	4/1733 (0.2%)	0.97	9/2318 (0.4%)
8	AE	0.46	0/1161	0.61	1/1561 (0.1%)
9	AF	0.35	0/856	0.54	0/1154
10	AG	0.60	1/1276 (0.1%)	0.59	2/1709 (0.1%)
11	AH	0.41	0/1136	0.66	0/1527
12	AI	0.34	0/1029	0.54	0/1378
13	AJ	0.35	0/807	0.56	0/1085
14	AK	0.87	1/900 (0.1%)	0.56	0/1213
15	AL	0.49	1/986 (0.1%)	0.70	1/1320 (0.1%)
16	AM	1.15	2/1008 (0.2%)	1.16	3/1347 (0.2%)
17	AN	0.49	1/501 (0.2%)	0.64	1/664 (0.2%)
18	AO	0.32	0/745	0.54	0/992
19	AP	0.40	0/716	0.59	1/963 (0.1%)
20	AQ	1.15	2/870 (0.2%)	1.38	5/1159 (0.4%)
21	AR	0.40	0/603	0.70	0/799
22	AS	0.34	0/661	0.53	0/890
23	AT	0.32	0/764	0.57	1/1006 (0.1%)
24	AU	0.33	0/212	0.48	0/277
26	BB	1.11	5/2950 (0.2%)	1.43	23/4602 (0.5%)
27	BA	1.21	152/67844 (0.2%)	1.45	897/105838 (0.8%)
28	BD	0.37	0/1328	0.61	0/1783
29	BE	0.64	3/1540 (0.2%)	1.07	7/2078 (0.3%)
30	BF	0.69	3/1444 (0.2%)	0.82	1/1954 (0.1%)
31	BG	0.25	0/971	0.46	0/1304
32	BH	0.58	1/1272 (0.1%)	0.48	0/1721
33	BI	0.39	1/1156 (0.1%)	0.64	3/1544 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
34	BN	0.35	0/927	0.55	0/1245
35	BO	0.32	0/946	0.57	0/1269
36	BP	1.55	3/643 (0.5%)	1.32	5/870 (0.6%)
37	BQ	0.32	0/1106	0.53	0/1490
38	BS	0.79	2/877 (0.2%)	0.87	5/1179 (0.4%)
39	BT	0.39	0/412	0.70	0/554
40	BW	0.37	0/869	0.59	0/1166
41	BX	0.49	1/608 (0.2%)	1.04	3/820 (0.4%)
42	BY	0.25	0/887	0.83	3/1195 (0.3%)
43	BZ	0.32	1/1385 (0.1%)	0.55	3/1883 (0.2%)
44	BR	0.31	0/867	0.49	0/1162
45	BU	0.70	1/994 (0.1%)	0.65	3/1323 (0.2%)
46	BV	0.75	1/796 (0.1%)	0.89	3/1058 (0.3%)
47	B2	0.37	0/497	1.00	2/668 (0.3%)
48	B3	0.31	0/482	0.50	0/646
49	B0	0.29	0/649	1.15	3/860 (0.3%)
50	B4	0.77	2/620 (0.3%)	0.57	0/831
51	B5	0.36	0/469	0.79	3/629 (0.5%)
52	B6	0.32	0/438	0.55	1/583 (0.2%)
53	B7	0.38	0/387	0.64	0/509
54	B8	0.73	2/503 (0.4%)	1.23	5/657 (0.8%)
55	B9	0.33	0/286	0.59	0/375
56	BK	0.30	0/1010	0.60	3/1349 (0.2%)
All	All	1.11	281/154800 (0.2%)	1.32	1469/231824 (0.6%)

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
3	AW	1	5
5	AB	0	1
6	AC	0	2
7	AD	0	1
15	AL	0	1
16	AM	0	1
20	AQ	0	2
28	BD	0	1
29	BE	0	3
30	BF	0	3
32	BH	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
33	BI	0	1
36	BP	0	1
38	BS	0	1
41	BX	0	1
42	BY	0	1
47	B2	0	1
54	B8	0	1
56	BK	0	1
All	All	1	29

The worst 5 of 281 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BA	2199	A	O3'-P	-71.12	0.75	1.61
2	AV	45	G	O3'-P	-70.03	0.77	1.61
2	AV	65	G	O3'-P	-62.91	0.85	1.61
27	BA	2196	C	O3'-P	-59.20	0.90	1.61
1	AA	1211	U	O3'-P	-53.33	0.97	1.61

The worst 5 of 1469 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BA	712(A)	A	P-O3'-C3'	-48.47	61.54	119.70
1	AA	196	A	P-O3'-C3'	44.40	172.99	119.70
3	AW	25	C	O3'-P-O5'	-43.47	21.42	104.00
27	BA	2199	A	O3'-P-O5'	-43.09	22.13	104.00
26	BB	24	G	P-O3'-C3'	29.89	155.56	119.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	AW	37	YYG	C15

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AW	16	U	Sidechain
3	AW	17	U	Sidechain
3	AW	18	G	Sidechain
3	AW	19	G	Sidechain
3	AW	62	A	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	32551	0	16464	1921	4
2	AV	1622	0	823	187	0
3	AW	1638	0	835	235	0
4	AX	136	0	63	35	0
5	AB	1900	0	1950	97	0
6	AC	1612	0	1675	104	0
7	AD	1703	0	1762	190	0
8	AE	1146	0	1206	57	0
9	AF	843	0	857	27	0
10	AG	1257	0	1294	141	0
11	AH	1116	0	1177	79	0
12	AI	1011	0	1041	80	0
13	AJ	794	0	840	118	0
14	AK	885	0	904	50	0
15	AL	970	0	1056	79	0
16	AM	997	0	1071	129	0
17	AN	492	0	529	111	0
18	AO	734	0	771	31	0
19	AP	700	0	720	68	0
20	AQ	857	0	929	96	0
21	AR	597	0	668	31	0
22	AS	647	0	672	146	0
23	AT	762	0	859	43	0
24	AU	208	0	221	22	0
25	AY	333	0	0	47	0
26	BB	2637	0	1338	198	0
27	BA	60600	0	30513	10828	139
28	BD	1308	0	1345	1087	0
29	BE	1507	0	1474	1127	3
30	BF	1430	0	1359	1069	0
31	BG	957	0	950	685	0
32	BH	1251	0	1289	743	0
33	BI	1145	0	1225	635	4
34	BN	917	0	896	775	1
35	BO	937	0	993	614	0
36	BP	639	0	605	490	0
37	BQ	1081	0	1048	916	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BS	866	0	867	686	0
39	BT	406	0	360	166	0
40	BW	860	0	911	559	0
41	BX	602	0	558	457	0
42	BY	879	0	860	748	0
43	BZ	1360	0	1377	887	0
44	BR	855	0	904	580	0
45	BU	978	0	995	924	0
46	BV	787	0	783	652	0
47	B2	494	0	504	385	0
48	B3	477	0	528	446	0
49	B0	641	0	657	501	0
50	B4	604	0	587	493	0
51	B5	457	0	457	293	0
52	B6	431	0	454	288	0
53	B7	383	0	409	396	0
54	B8	496	0	541	358	0
55	B9	285	0	312	203	0
56	BK	999	0	1068	144	0
All	All	142780	0	94554	28116	146

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 119.

The worst 5 of 28116 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)
51:B5:33:CYS:SG	51:B5:36:CYS:HB2	1.24	1.69
27:BA:2470:G:C2	27:BA:2471:C:C5	1.81	1.68
27:BA:994:C:C2	45:BU:53:LYS:HD3	1.16	1.68
53:B7:30:ILE:HA	53:B7:33:ARG:CD	1.21	1.67
27:BA:2580:U:C6	27:BA:2581:G:C8	1.82	1.66

The worst 5 of 146 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:6:A:C4'	27:BA:2902:C:O2'[8_554]	0.49	1.71
1:AA:359:U:OP1	33:BI:82:LYS:NZ[3_454]	0.68	1.52
27:BA:6:A:N9	27:BA:2902:C:C6[8_554]	0.88	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:BA:1:G:O6	27:BA:2898:U:C2[8_554]	0.92	1.28
27:BA:6:A:O4'	27:BA:2902:C:C2'[8_554]	0.97	1.23

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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	
5	AB	232/256 (91%)	183 (79%)	34 (15%)	15 (6%)	1	12
6	AC	204/239 (85%)	165 (81%)	23 (11%)	16 (8%)	1	10
7	AD	206/209 (99%)	156 (76%)	34 (16%)	16 (8%)	1	10
8	AE	146/162 (90%)	114 (78%)	29 (20%)	3 (2%)	5	30
9	AF	99/101 (98%)	85 (86%)	10 (10%)	4 (4%)	2	18
10	AG	153/156 (98%)	131 (86%)	18 (12%)	4 (3%)	4	25
11	AH	136/138 (99%)	101 (74%)	25 (18%)	10 (7%)	1	10
12	AI	125/128 (98%)	87 (70%)	30 (24%)	8 (6%)	1	12
13	AJ	96/105 (91%)	73 (76%)	14 (15%)	9 (9%)	0	8
14	AK	117/129 (91%)	89 (76%)	23 (20%)	5 (4%)	2	17
15	AL	122/135 (90%)	91 (75%)	14 (12%)	17 (14%)	0	3
16	AM	123/126 (98%)	96 (78%)	21 (17%)	6 (5%)	2	16
17	AN	58/61 (95%)	42 (72%)	12 (21%)	4 (7%)	1	11
18	AO	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	11	44
19	AP	81/88 (92%)	64 (79%)	10 (12%)	7 (9%)	0	9
20	AQ	102/105 (97%)	78 (76%)	17 (17%)	7 (7%)	1	11
21	AR	71/88 (81%)	54 (76%)	11 (16%)	6 (8%)	0	9
22	AS	78/93 (84%)	60 (77%)	15 (19%)	3 (4%)	2	19
23	AT	97/106 (92%)	79 (81%)	12 (12%)	6 (6%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	AU	22/27 (82%)	17 (77%)	3 (14%)	2 (9%)	0	8
28	BD	169/173 (98%)	60 (36%)	34 (20%)	75 (44%)	0	0
29	BE	183/338 (54%)	89 (49%)	35 (19%)	59 (32%)	0	0
30	BF	179/246 (73%)	51 (28%)	47 (26%)	81 (45%)	0	0
31	BG	116/176 (66%)	46 (40%)	31 (27%)	39 (34%)	0	0
32	BH	162/177 (92%)	74 (46%)	39 (24%)	49 (30%)	0	0
33	BI	144/149 (97%)	71 (49%)	29 (20%)	44 (31%)	0	0
34	BN	111/145 (77%)	34 (31%)	21 (19%)	56 (50%)	0	0
35	BO	120/122 (98%)	61 (51%)	27 (22%)	32 (27%)	0	0
36	BP	82/164 (50%)	28 (34%)	21 (26%)	33 (40%)	0	0
37	BQ	130/138 (94%)	38 (29%)	35 (27%)	57 (44%)	0	0
38	BS	105/186 (56%)	36 (34%)	20 (19%)	49 (47%)	0	0
39	BT	48/66 (73%)	17 (35%)	13 (27%)	18 (38%)	0	0
40	BW	104/113 (92%)	42 (40%)	15 (14%)	47 (45%)	0	0
41	BX	72/84 (86%)	26 (36%)	18 (25%)	28 (39%)	0	0
42	BY	108/119 (91%)	49 (45%)	20 (18%)	39 (36%)	0	0
43	BZ	175/253 (69%)	52 (30%)	53 (30%)	70 (40%)	0	0
44	BR	103/118 (87%)	35 (34%)	20 (19%)	48 (47%)	0	0
45	BU	115/118 (98%)	22 (19%)	23 (20%)	70 (61%)	0	0
46	BV	96/100 (96%)	39 (41%)	25 (26%)	32 (33%)	0	0
47	B2	62/70 (89%)	8 (13%)	9 (14%)	45 (73%)	0	0
48	B3	58/60 (97%)	24 (41%)	13 (22%)	21 (36%)	0	0
49	B0	84/91 (92%)	33 (39%)	16 (19%)	35 (42%)	0	0
50	B4	71/73 (97%)	21 (30%)	16 (22%)	34 (48%)	0	0
51	B5	56/60 (93%)	16 (29%)	17 (30%)	23 (41%)	0	0
52	B6	51/82 (62%)	21 (41%)	9 (18%)	21 (41%)	0	0
53	B7	44/47 (94%)	4 (9%)	7 (16%)	33 (75%)	0	0
54	B8	61/64 (95%)	23 (38%)	9 (15%)	29 (48%)	0	0
55	B9	33/36 (92%)	14 (42%)	9 (27%)	10 (30%)	0	0
56	BK	124/141 (88%)	93 (75%)	26 (21%)	5 (4%)	2	18
All	All	5320/6250 (85%)	2968 (56%)	1021 (19%)	1331 (25%)	0	1

5 of 1331 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AB	24	TRP
5	AB	104	ASN
5	AB	153	ARG
5	AB	154	LEU
5	AB	161	ALA

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	
5	AB	202/220 (92%)	173 (86%)	29 (14%)	2	12
6	AC	160/188 (85%)	146 (91%)	14 (9%)	8	25
7	AD	180/181 (99%)	162 (90%)	18 (10%)	6	20
8	AE	115/123 (94%)	94 (82%)	21 (18%)	1	8
9	AF	90/90 (100%)	83 (92%)	7 (8%)	10	29
10	AG	126/127 (99%)	116 (92%)	10 (8%)	10	29
11	AH	119/119 (100%)	91 (76%)	28 (24%)	0	4
12	AI	98/99 (99%)	90 (92%)	8 (8%)	9	28
13	AJ	88/92 (96%)	77 (88%)	11 (12%)	3	15
14	AK	90/99 (91%)	85 (94%)	5 (6%)	17	38
15	AL	104/111 (94%)	93 (89%)	11 (11%)	5	19
16	AM	100/101 (99%)	87 (87%)	13 (13%)	3	14
17	AN	49/50 (98%)	43 (88%)	6 (12%)	4	15
18	AO	79/80 (99%)	70 (89%)	9 (11%)	4	16
19	AP	72/74 (97%)	62 (86%)	10 (14%)	3	12
20	AQ	96/97 (99%)	87 (91%)	9 (9%)	7	23
21	AR	64/77 (83%)	57 (89%)	7 (11%)	5	18
22	AS	71/80 (89%)	64 (90%)	7 (10%)	6	21
23	AT	76/82 (93%)	68 (90%)	8 (10%)	5	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	AU	19/22 (86%)	19 (100%)	0	100	100
28	BD	135/135 (100%)	99 (73%)	36 (27%)	0	3
29	BE	156/284 (55%)	128 (82%)	28 (18%)	1	8
30	BF	152/193 (79%)	124 (82%)	28 (18%)	1	8
31	BG	102/147 (69%)	93 (91%)	9 (9%)	8	25
32	BH	137/147 (93%)	111 (81%)	26 (19%)	1	7
33	BI	119/119 (100%)	98 (82%)	21 (18%)	1	8
34	BN	95/121 (78%)	80 (84%)	15 (16%)	2	10
35	BO	101/101 (100%)	81 (80%)	20 (20%)	1	7
36	BP	67/126 (53%)	56 (84%)	11 (16%)	2	9
37	BQ	110/110 (100%)	83 (76%)	27 (24%)	0	3
38	BS	89/149 (60%)	73 (82%)	16 (18%)	1	8
39	BT	44/52 (85%)	30 (68%)	14 (32%)	0	2
40	BW	88/92 (96%)	74 (84%)	14 (16%)	2	10
41	BX	67/73 (92%)	44 (66%)	23 (34%)	0	1
42	BY	97/105 (92%)	80 (82%)	17 (18%)	1	8
43	BZ	151/203 (74%)	129 (85%)	22 (15%)	2	12
44	BR	89/101 (88%)	71 (80%)	18 (20%)	1	6
45	BU	96/97 (99%)	68 (71%)	28 (29%)	0	2
46	BV	79/79 (100%)	69 (87%)	10 (13%)	3	14
47	B2	51/56 (91%)	37 (72%)	14 (28%)	0	2
48	B3	52/52 (100%)	47 (90%)	5 (10%)	7	22
49	B0	64/67 (96%)	57 (89%)	7 (11%)	5	18
50	B4	66/66 (100%)	54 (82%)	12 (18%)	1	8
51	B5	51/53 (96%)	43 (84%)	8 (16%)	2	10
52	B6	46/69 (67%)	39 (85%)	7 (15%)	2	11
53	B7	39/40 (98%)	31 (80%)	8 (20%)	1	6
54	B8	50/51 (98%)	39 (78%)	11 (22%)	1	5
55	B9	34/35 (97%)	30 (88%)	4 (12%)	4	16
56	BK	108/113 (96%)	105 (97%)	3 (3%)	38	57
All	All	4533/5148 (88%)	3840 (85%)	693 (15%)	2	11

5 of 693 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	BS	87	LEU
44	BR	105	ARG
39	BT	25	ASP
38	BS	83	LEU
42	BY	31	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 124 such sidechains are listed below:

Mol	Chain	Res	Type
29	BE	318	ASN
47	B2	42	ASN
34	BN	92	GLN
47	B2	29	ASN
52	B6	27	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1498/1522 (98%)	518 (34%)	166 (11%)
2	AV	74/76 (97%)	16 (21%)	4 (5%)
26	BB	122/123 (99%)	44 (36%)	3 (2%)
27	BA	2785/2916 (95%)	1488 (53%)	360 (12%)
3	AW	70/76 (92%)	14 (20%)	4 (5%)
4	AX	5/18 (27%)	0	0
All	All	4554/4731 (96%)	2080 (45%)	537 (11%)

5 of 2080 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	8	A
1	AA	9	G
1	AA	12	U

5 of 537 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	BA	2426	A

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Mol	Chain	Res	Type
27	BA	2493	U
27	BA	2425	A
27	BA	2777	G
27	BA	197	A

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

3 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$
3	PSU	AW	39	3	18,21,22	0.74	1 (5%)	21,30,33	0.73	0
3	PSU	AW	55	3	18,21,22	0.72	0	21,30,33	0.91	1 (4%)
3	YYG	AW	37	3	30,42,43	0.95	1 (3%)	32,62,65	2.77	10 (31%)

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
3	PSU	AW	39	3	-	0/7/25/26	0/2/2/2
3	PSU	AW	55	3	-	0/7/25/26	0/2/2/2
3	YYG	AW	37	3	1/1/8/9	7/20/42/43	0/3/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AW	37	YYG	C8-N7	-2.26	1.31	1.34
3	AW	39	PSU	C6-N1	-2.04	1.33	1.36

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AW	37	YYG	C11-C12-N1	8.60	111.38	106.53
3	AW	37	YYG	C24-O23-C21	6.47	123.12	115.63
3	AW	37	YYG	C3-N3-C4	5.81	125.54	116.76
3	AW	37	YYG	O23-C21-N20	4.58	118.47	110.77
3	AW	37	YYG	C4-N3-C2	-3.88	111.82	122.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	AW	37	YYG	C15

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AW	37	YYG	C12-C13-C14-C15
3	AW	37	YYG	C15-C16-O18-C19
3	AW	37	YYG	O17-C16-O18-C19
3	AW	37	YYG	C13-C14-C15-C16
3	AW	37	YYG	C13-C14-C15-N20

There are no ring outliers.

2 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AW	39	PSU	5	0
3	AW	37	YYG	40	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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
27	BA	104
1	AA	67
3	AW	8
56	BK	5
2	AV	4
37	BQ	3
26	BB	3
46	BV	2
6	AC	2
28	BD	1
8	AE	1
16	AM	1
5	AB	1
36	BP	1
10	AG	1
38	BS	1
30	BF	1
15	AL	1
43	BZ	1
33	BI	1
7	AD	1
32	BH	1
45	BU	1
14	AK	1
20	AQ	1

The worst 5 of 214 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BK	70:ILE	C	71:LYS	N	5.81
1	BK	73:PRO	C	74:PRO	N	5.30
1	BK	72:THR	C	73:PRO	N	5.11
1	AA	30(D):A	O3'	1031:G	P	4.82
1	BA	142(A):A	O3'	1143:A	P	4.82

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	AA	1515/1522 (99%)	0.55	75 (4%)	35	30	236, 236, 236, 236	0
2	AV	76/76 (100%)	0.72	5 (6%)	26	24	236, 236, 236, 236	0
3	AW	73/76 (96%)	0.89	5 (6%)	25	23	236, 236, 236, 236	0
4	AX	17/18 (94%)	4.23	12 (70%)	0	1	236, 236, 236, 236	0
5	AB	234/256 (91%)	0.97	36 (15%)	6	10	236, 236, 236, 236	0
6	AC	206/239 (86%)	1.18	47 (22%)	2	6	236, 236, 236, 236	0
7	AD	208/209 (99%)	1.91	75 (36%)	1	4	236, 236, 236, 236	0
8	AE	150/162 (92%)	0.93	27 (18%)	4	8	236, 236, 236, 236	0
9	AF	101/101 (100%)	1.14	18 (17%)	4	8	236, 236, 236, 236	0
10	AG	155/156 (99%)	1.33	37 (23%)	2	6	236, 236, 236, 236	0
11	AH	138/138 (100%)	0.67	24 (17%)	5	9	236, 236, 236, 236	0
12	AI	127/128 (99%)	1.27	33 (25%)	2	5	236, 236, 236, 236	0
13	AJ	98/105 (93%)	1.51	34 (34%)	1	4	236, 236, 236, 236	0
14	AK	119/129 (92%)	0.81	13 (10%)	12	15	236, 236, 236, 236	0
15	AL	124/135 (91%)	1.57	38 (30%)	1	4	236, 236, 236, 236	0
16	AM	125/126 (99%)	1.91	44 (35%)	1	4	236, 236, 236, 236	0
17	AN	60/61 (98%)	1.38	19 (31%)	1	4	236, 236, 236, 236	0
18	AO	88/89 (98%)	1.23	22 (25%)	2	6	236, 236, 236, 236	0
19	AP	83/88 (94%)	1.54	24 (28%)	1	5	236, 236, 236, 236	0
20	AQ	104/105 (99%)	1.01	15 (14%)	7	11	236, 236, 236, 236	0
21	AR	73/88 (82%)	0.91	13 (17%)	4	8	236, 236, 236, 236	0
22	AS	80/93 (86%)	1.81	30 (37%)	1	3	236, 236, 236, 236	0
23	AT	99/106 (93%)	1.50	29 (29%)	1	5	236, 236, 236, 236	0
24	AU	24/27 (88%)	2.50	12 (50%)	0	3	236, 236, 236, 236	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	AY	333/354 (94%)	6.43	264 (79%) 0 1	236, 236, 236, 236	0
26	BB	123/123 (100%)	0.29	1 (0%) 82 70	236, 236, 236, 236	0
27	BA	2814/2916 (96%)	0.80	309 (10%) 12 14	236, 236, 236, 236	0
28	BD	173/173 (100%)	1.45	59 (34%) 1 4	236, 236, 236, 236	0
29	BE	191/338 (56%)	1.55	58 (30%) 1 4	236, 236, 236, 236	0
30	BF	189/246 (76%)	1.59	54 (28%) 1 5	236, 236, 236, 236	0
31	BG	122/176 (69%)	1.64	46 (37%) 1 3	236, 236, 236, 236	0
32	BH	164/177 (92%)	1.00	28 (17%) 5 9	236, 236, 236, 236	0
33	BI	148/149 (99%)	1.27	35 (23%) 2 6	236, 236, 236, 236	0
34	BN	117/145 (80%)	1.45	26 (22%) 3 6	236, 236, 236, 236	0
35	BO	122/122 (100%)	1.46	29 (23%) 2 6	236, 236, 236, 236	0
36	BP	84/164 (51%)	1.07	15 (17%) 4 8	236, 236, 236, 236	0
37	BQ	138/138 (100%)	1.91	51 (36%) 1 3	236, 236, 236, 236	0
38	BS	113/186 (60%)	1.01	22 (19%) 4 8	236, 236, 236, 236	0
39	BT	52/66 (78%)	1.87	20 (38%) 1 3	236, 236, 236, 236	0
40	BW	108/113 (95%)	1.41	29 (26%) 2 5	236, 236, 236, 236	0
41	BX	76/84 (90%)	1.15	20 (26%) 2 5	236, 236, 236, 236	0
42	BY	110/119 (92%)	1.87	40 (36%) 1 3	236, 236, 236, 236	0
43	BZ	177/253 (69%)	1.26	40 (22%) 3 6	236, 236, 236, 236	0
44	BR	105/118 (88%)	1.16	24 (22%) 2 6	236, 236, 236, 236	0
45	BU	117/118 (99%)	1.43	32 (27%) 2 5	236, 236, 236, 236	0
46	BV	100/100 (100%)	1.07	18 (18%) 4 8	236, 236, 236, 236	0
47	B2	64/70 (91%)	0.89	12 (18%) 4 8	236, 236, 236, 236	0
48	B3	60/60 (100%)	0.85	11 (18%) 4 8	236, 236, 236, 236	0
49	B0	86/91 (94%)	1.36	26 (30%) 1 4	236, 236, 236, 236	0
50	B4	73/73 (100%)	1.31	20 (27%) 2 5	236, 236, 236, 236	0
51	B5	58/60 (96%)	1.61	13 (22%) 3 6	236, 236, 236, 236	0
52	B6	53/82 (64%)	0.92	11 (20%) 3 7	236, 236, 236, 236	0
53	B7	46/47 (97%)	1.51	11 (23%) 2 6	236, 236, 236, 236	0
54	B8	63/64 (98%)	1.58	17 (26%) 2 5	236, 236, 236, 236	0
55	B9	35/36 (97%)	1.69	16 (45%) 1 3	236, 236, 236, 236	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
56	BK	133/141 (94%)	1.79	48 (36%) 1 4	236, 236, 236, 236	0
All	All	10424/11335 (91%)	1.23	2092 (20%) 3 7	236, 236, 236, 236	0

The worst 5 of 2092 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	AY	284	ARG	66.1
25	AY	165	PRO	43.3
25	AY	287	LYS	35.9
25	AY	166	GLY	35.8
25	AY	283	GLU	35.8

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	PSU	AW	55	20/21	0.27	0.14	236,236,236,236	0
3	YYG	AW	37	39/40	0.48	0.35	236,236,236,236	0
3	PSU	AW	39	20/21	0.81	0.23	236,236,236,236	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.