



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:39 PM UTC

PDB ID : 1JJ2 / pdb_00001jj2
Title : Fully Refined Crystal Structure of the Haloarcula marismortui Large Ribosomal Subunit at 2.4 Angstrom Resolution
Authors : Klein, D.J.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on : 2001-07-03
Resolution : 2.40 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

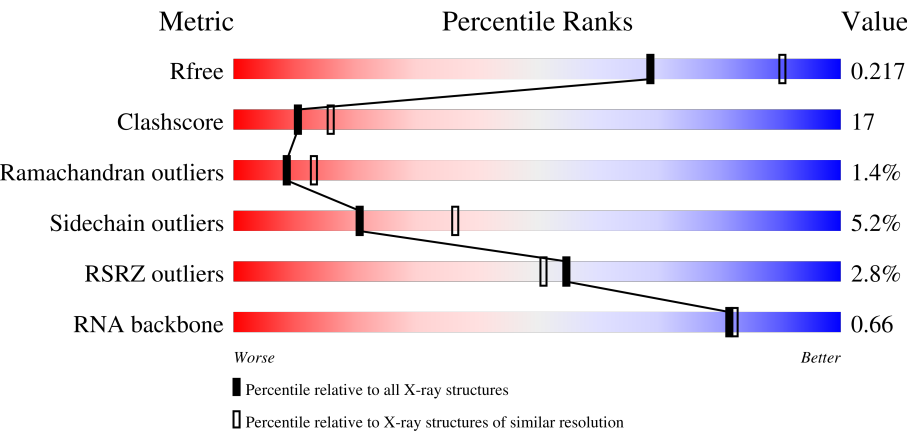
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)
RNA backbone	3983	1155 (2.70-2.10)

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 ≥ 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	0	2922	2% 64% 24% 6% 6%
2	9	122	5% 55% 33% 8%
3	A	239	2% 60% 32% 7%
4	B	337	51% 42% 7%

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	176	
7	E	177	
8	F	119	
9	G	348	
10	H	167	
11	I	145	
12	J	132	
13	K	164	
14	L	194	
15	M	186	
16	N	115	
17	O	148	
18	P	95	
19	Q	154	
20	R	84	
21	S	119	
22	T	66	
23	U	70	
24	V	154	
25	W	91	
26	X	240	
27	Y	73	
28	Z	56	
29	1	48	

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Mol	Chain	Length	Quality of chain
30	2	92	2% 59% 34% 7%

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 98543 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 23S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	conflict	GB 3377779

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	237	Total	C	N	O	S	0	0	0
			1754	1072	352	325	5			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	337	Total	C	N	O	S	0	0	0
			2624	1616	493	510	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP P20279
B	310	ARG	PHE	conflict	UNP P20279

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	145	Total	C	N	O		0	0	0
			1114	668	222	224				

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	115	Total	C	N	O		0	0	0
			864	529	161	174				

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	O	143	Total	C	N	O		0	0	0
			1133	680	230	223				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	71	LYS	TYR	conflict	UNP P14119

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	P	95	Total	C	N	O	0	0	0
			734	450	141	143			

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	S	119	Total	C	N	O	0	0	0
			949	568	180	201			

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	154	Total	C	N	O	S	0	0	0
			1195	737	209	243	6			

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L31E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L32E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	X	142	Total	C	N	O		0	0	0
			1130	686	228	216				

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Y	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	?	-	ARG	deletion	UNP P22452

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	0	109	Total Mg 109 109	0	0
31	9	1	Total Mg 1 1	0	0
31	A	2	Total Mg 2 2	0	0
31	B	1	Total Mg 1 1	0	0
31	J	1	Total Mg 1 1	0	0
31	S	1	Total Mg 1 1	0	0
31	X	1	Total Mg 1 1	0	0
31	2	1	Total Mg 1 1	0	0

- Molecule 32 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	0	2	Total K 2 2	0	0

- Molecule 33 is SODIUM ION (CCD ID: Na) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	72	Total Na 72 72	0	0
33	9	2	Total Na 2 2	0	0
33	A	1	Total Na 1 1	0	0
33	C	1	Total Na 1 1	0	0
33	H	2	Total Na 2 2	0	0
33	I	1	Total Na 1 1	0	0
33	K	1	Total Na 1 1	0	0
33	L	1	Total Na 1 1	0	0
33	P	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	Q	2	Total 2	Na 2	0	0
33	R	1	Total 1	Na 1	0	0
33	S	1	Total 1	Na 1	0	0

- Molecule 34 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	10	Total 10	Cl 10	0	0
34	A	1	Total 1	Cl 1	0	0
34	B	1	Total 1	Cl 1	0	0
34	I	3	Total 3	Cl 3	0	0
34	K	1	Total 1	Cl 1	0	0
34	L	1	Total 1	Cl 1	0	0
34	M	1	Total 1	Cl 1	0	0
34	N	1	Total 1	Cl 1	0	0
34	Q	1	Total 1	Cl 1	0	0
34	X	1	Total 1	Cl 1	0	0
34	2	1	Total 1	Cl 1	0	0

- Molecule 35 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	N	1	Total 1	Cd 1	0	0
35	T	1	Total 1	Cd 1	0	0
35	Y	1	Total 1	Cd 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	Z	1	Total	Cd	0	0
			1	1		
35	2	1	Total	Cd	0	0
			1	1		

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	5938	Total	O	0	0
			5938	5938		
36	9	135	Total	O	0	0
			135	135		
36	A	126	Total	O	0	0
			126	126		
36	B	150	Total	O	0	0
			150	150		
36	C	172	Total	O	0	0
			172	172		
36	D	53	Total	O	0	0
			53	53		
36	E	46	Total	O	0	0
			46	46		
36	F	28	Total	O	0	0
			28	28		
36	G	21	Total	O	0	0
			21	21		
36	H	74	Total	O	0	0
			74	74		
36	I	56	Total	O	0	0
			56	56		
36	J	62	Total	O	0	0
			62	62		
36	K	80	Total	O	0	0
			80	80		
36	L	127	Total	O	0	0
			127	127		
36	M	70	Total	O	0	0
			70	70		
36	N	43	Total	O	0	0
			43	43		
36	O	68	Total	O	0	0
			68	68		

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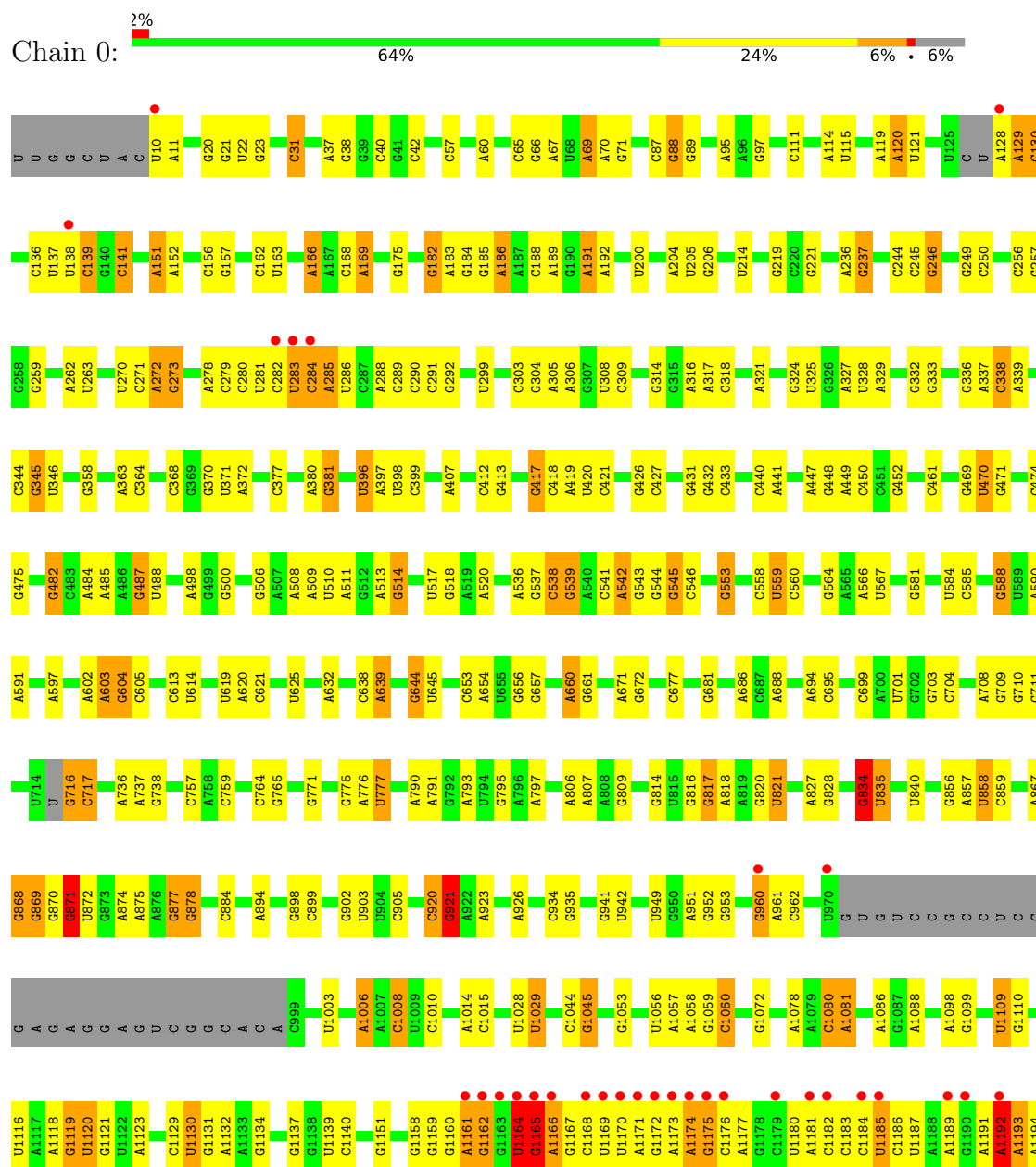
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	P	53	Total 53	O 53	0	0
36	Q	81	Total 81	O 81	0	0
36	R	32	Total 32	O 32	0	0
36	S	39	Total 39	O 39	0	0
36	T	25	Total 25	O 25	0	0
36	U	15	Total 15	O 15	0	0
36	V	67	Total 67	O 67	0	0
36	W	29	Total 29	O 29	0	0
36	X	99	Total 99	O 99	0	0
36	Y	39	Total 39	O 39	0	0
36	Z	53	Total 53	O 53	0	0
36	1	40	Total 40	O 40	0	0
36	2	72	Total 72	O 72	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

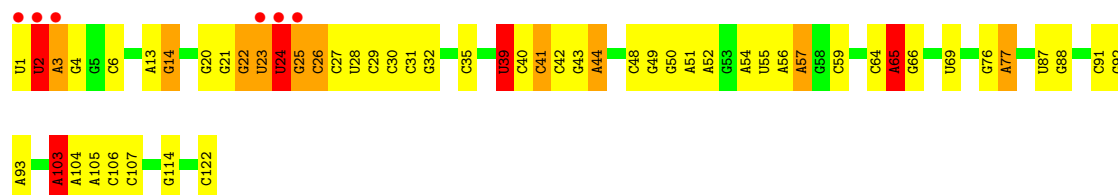
• Molecule 1: 23S rRNA



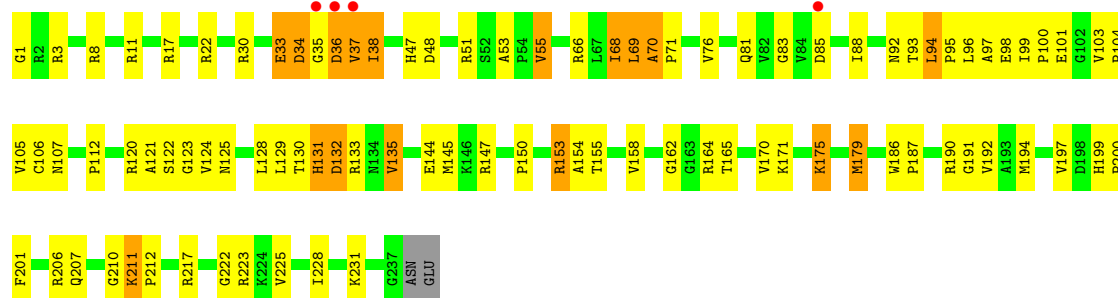
A2697	U2590	G2480	C2346	C2247	A	A2101	G1970	C1853	A1710	C1593	U1440	G1292	G1195
G2698	C2591	A2483	A2354	G2251	C	G2102	G1971	C1854	A1717	C1594	G1441	G1299	C1196
U2710	G2592	A2488	A2354	A2252	C	G2110	U1972	G1855	U1722	U1596	A1442	G1299	U1198
G2711	U2598	G2489	A2361	A2255	C	G2111	A1973	A1857	U1723	A1597	C1450	U1306	G1201
G2712	U2598	A2490	A2362	A2256	C	A2112	G1974	C1862	U1724	A1598	A1451	U1314	A1202
G2716	A2601	G2493	A2363	G2257	C	G2113	A1978	G1863	C1725	A1603	A1458	U1328	G1203
G2717	G2602	G2493	A2364	A2258	U	G2114	G1979	G1867	G1730	G1604	C1462	A1328	U1205
G2718	A2604	G2501	G2365	A2259	G	U2115	U1980	G1868	G1731	G1605	A1463	A1329	U1206
A2719	G2502	G2501	A2369	U2265	C	U2116	A1981	G1868	A1732	C1613	C1467	U1333	A1207
G2720	A2503	A2503	G2383	A2266	G	G2128	C1982	G1877	A1733	C1614	C1470	U1334	C1208
G2722	G2505	G2505	G	A2266	G	G2136	U1986	G1878	C1734	A1615	A1470	U1339	C1209
G2723	G2506	G2506	G	G2270	C	A	A1997	U1879	A1735	U1625	A1470	G1340	G1211
G2724	G2507	G2507	C	G2271	C	C	G2001	C1880	A1736	U1626	C1474	G1340	C1212
G2725	G2508	G2508	A	G2272	C	G	C2002	G1881	U1741	G1627	C1342	C1342	C1213
U2726	A2509	C2723	C	C2723	C	U	U2003	U1883	A1742	A1630	C1477	C1343	G1214
A2727	G2510	A2274	C	A2274	C	G	U2004	G1884	G	A1630	G	U1219	A1215
G2728	A2511	G2281	G	U2297	C	G	G2005	U1887	G1751	C1633	G1484	G1351	G1216
G2729	G2515	C2282	G	C2282	A	U	U2008	U1887	G1752	C1633	A1485	U1368	G1217
G2730	G2516	G2281	G	U2297	C	U	G2009	U1887	C1753	U1634	A1488	U1368	U1218
G2731	G2516	G2281	G	U2297	C	U	A2010	U1887	G1756	U1635	U1488	G1360	G1229
C2747	A2637	G2289	C	U2297	C	U	A2011	U1887	U1766	U1637	A1484	G1367	A1232
U2748	G2638	U2296	C	U2297	C	U	U2012	U1887	U1766	U1637	A1484	U1367	A1232
G2749	G2638	A2291	C	U2297	C	U	G2013	U1887	U1766	U1637	A1484	U1367	A1232
G2750	G2642	U2297	C	U2297	C	U	G2013	U1887	U1766	U1637	A1484	U1367	A1232
U2756	G2643	U2297	C	U2297	C	U	G2013	U1887	U1766	U1637	A1484	U1367	A1232
A2761	A2649	A2300	U	A2300	U	U	A2019	A1919	A1778	U1654	U1500	A1372	U1234
C2762	U2650	A2301	G	A2301	G	U	G2033	C1920	A1779	G1655	A1501	A1372	U1234
U2768	G2653	A2302	C	A2302	C	C	U2034	A1921	A1779	G1655	A1501	A1372	U1234
C2769	U2652	C2309	A	C2309	A	A	G2044	G1926	C1787	U1656	A1502	C1377	A1236
G2770	C2654	G2310	U	G2310	U	C	U2054	G1928	U1788	A1557	U1503	G1378	U1237
G2777	A2664	G2312	C	G2312	C	U	A2054	G1929	G1789	U1506	U1506	U1380	C1238
A2778	U	C2313	U	C2313	U	A	C2061	C1940	G1794	A1667	G1523	G1384	G1240
G2779	G2667	G2314	A	G2314	A	G	A2062	A1941	C1798	U1668	U1524	G1385	A1242
G2780	U2668	C2315	C	C2315	C	G	U2064	A1942	A1804	A1669	G1525	A1393	C1243
U2781	G2669	G2316	C	G2316	C	U	U2064	C1943	A1805	G1670	A1526	C1394	C1245
G2782	G2670	C2317	C	C2317	C	A	G2072	G1947	G1809	U1677	A1527	A1406	A1246
A2783	U2671	U2320	G	U2320	G	G	G2073	G1948	G1809	C1678	A1528	A1406	A1247
G2786	C2672	A2321	U	A2321	U	A	A2074	G1951	G1819	C1679	U1529	U1407	A1248
C2787	U2563	U2326	G	U2326	G	A	U2078	U	G1820	C1680	C1545	U1408	U1249
C2790	G2564	U2329	G	U2329	G	A	A2081	A	A1829	G1681	G1546	G1409	C1251
U2791	A2565	U2330	C	U2330	C	A	G2082	A	A1829	G1682	G1546	A1413	U1266
A2792	G2570	G2338	C	G2338	C	U	A2083	C	A1829	G1683	G1546	A1413	U1266
G2795	G2578	A	C	A	C	A	A2089	U	C1834	A1684	A1559	G1417	C1267
U2796	U2586	A	C	A	C	A	G2090	A	U1835	A1685	U	U1418	G1268
A2800	U2587	G2344	G	G2344	G	A	G2091	C	A1840	C1692	C1561	U1419	C1269
A2811	U2588	A2345	G	A2345	G	U	C2094	C	A1845	U1700	C1563	A1423	C1273
	U2589		U2242		U		A2095	C	G1848	U1702	C1564	A1424	U1279
							A2096	C			A1580	G1430	C1289
											G1592	C1439	A1291



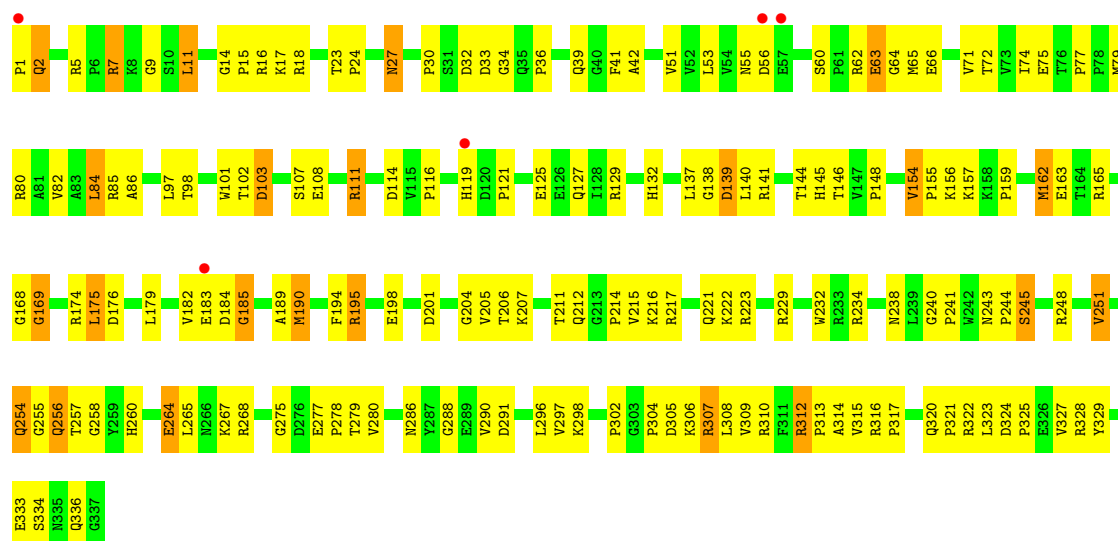
• Molecule 2: 5S RRNA



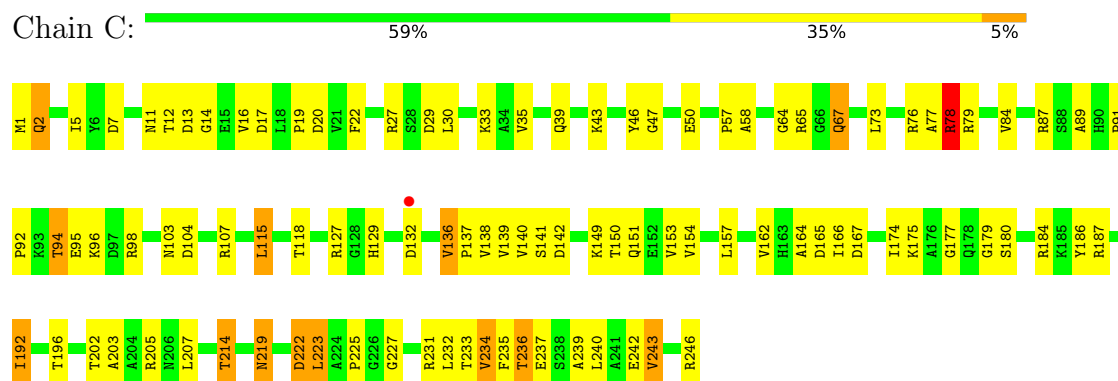
• Molecule 3: RIBOSOMAL PROTEIN L2



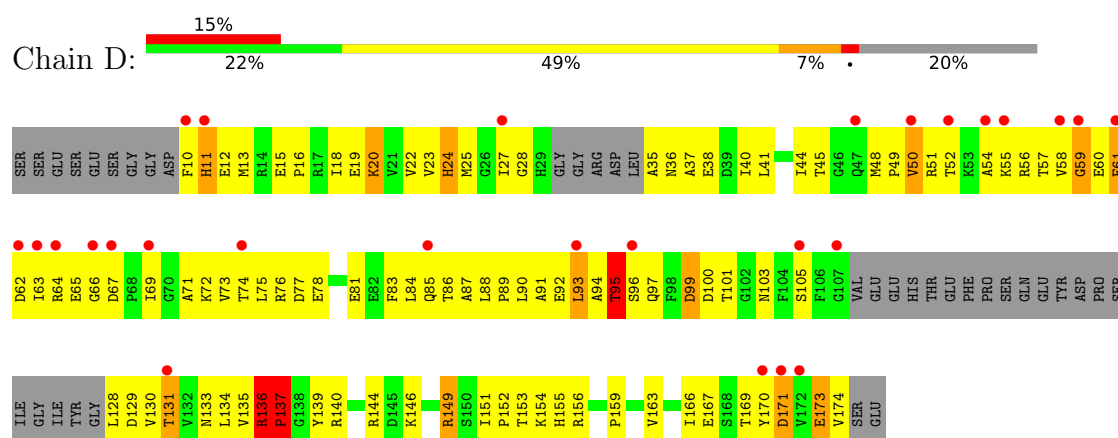
• Molecule 4: RIBOSOMAL PROTEIN L3



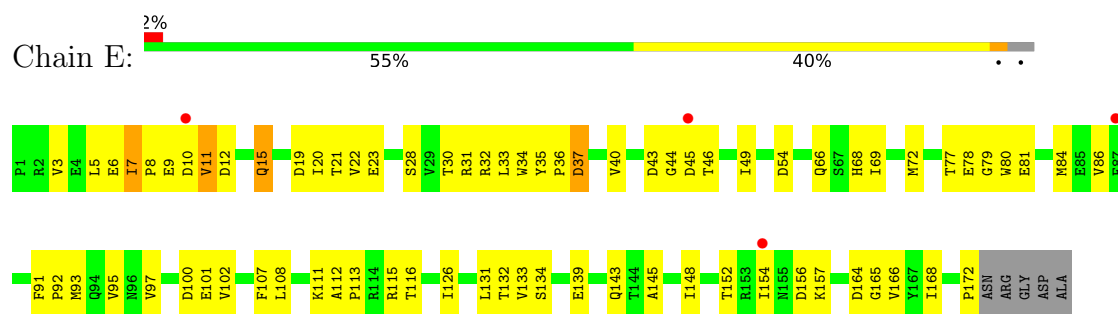
• Molecule 5: RIBOSOMAL PROTEIN L4



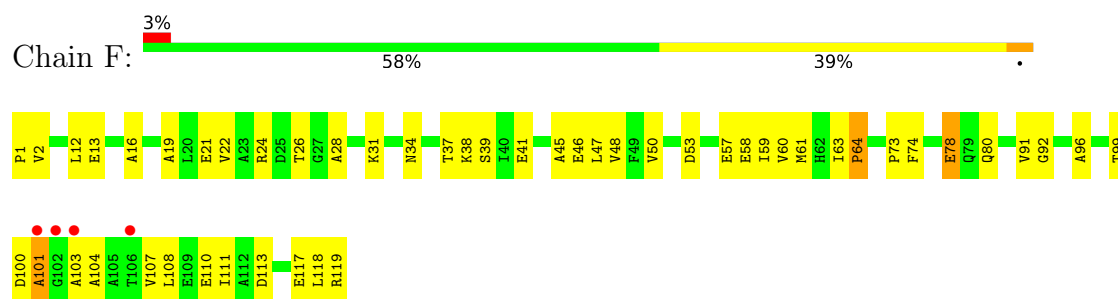
• Molecule 6: RIBOSOMAL PROTEIN L5



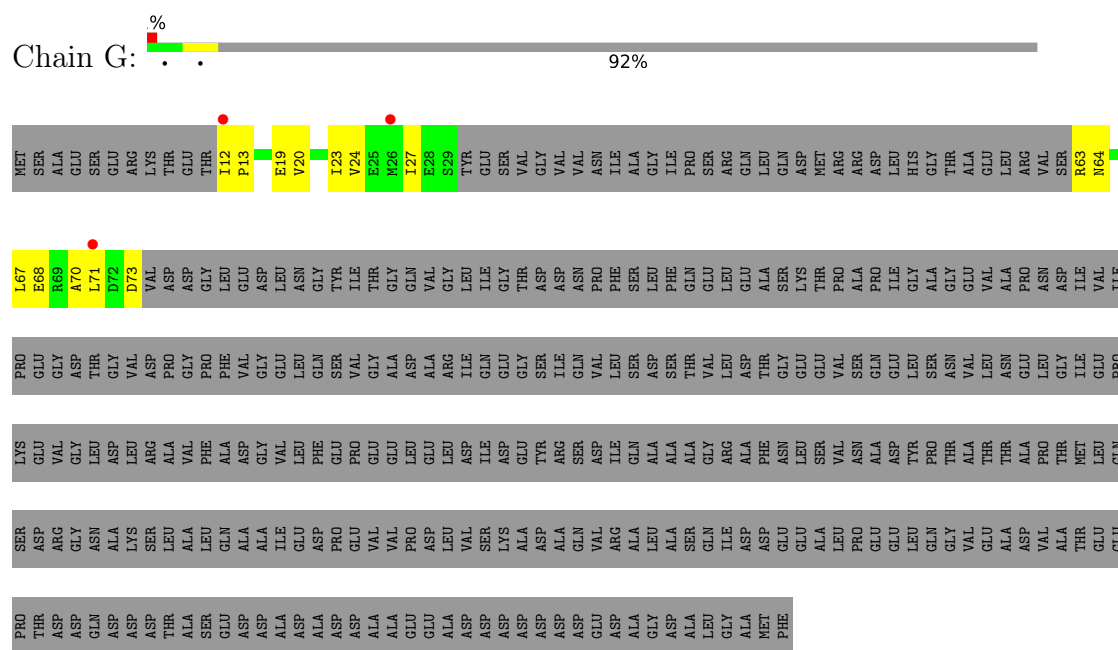
• Molecule 7: RIBOSOMAL PROTEIN L6



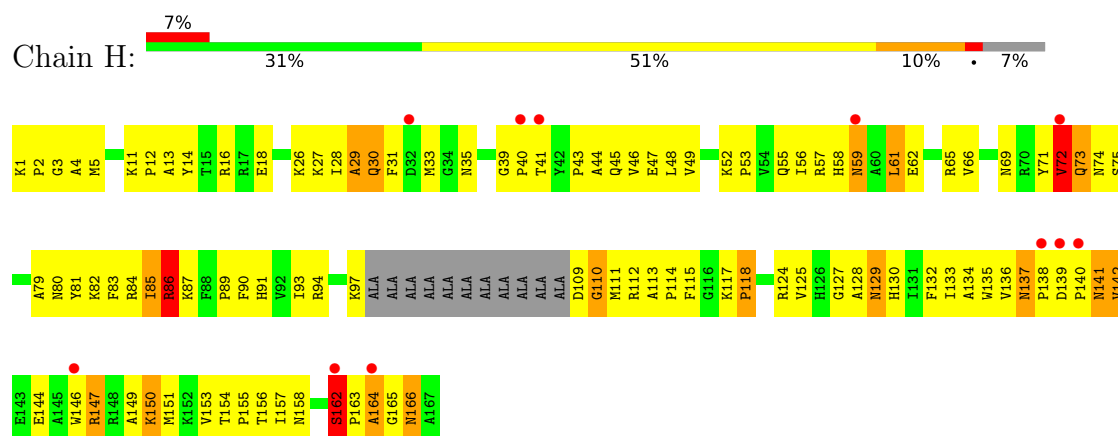
• Molecule 8: RIBOSOMAL PROTEIN L7AE



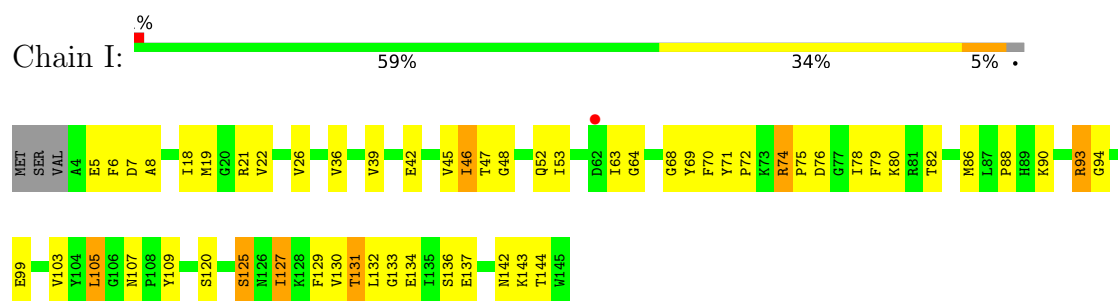
• Molecule 9: RIBOSOMAL PROTEIN L10



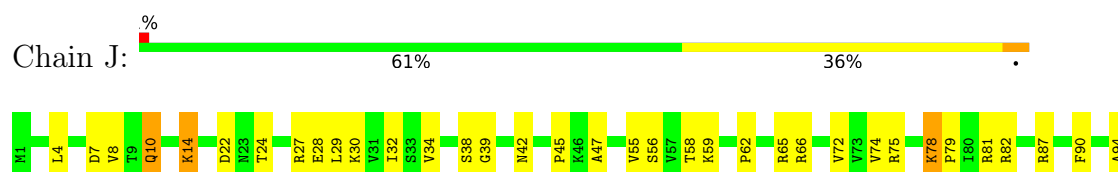
• Molecule 10: RIBOSOMAL PROTEIN L10E



• Molecule 11: RIBOSOMAL PROTEIN L13

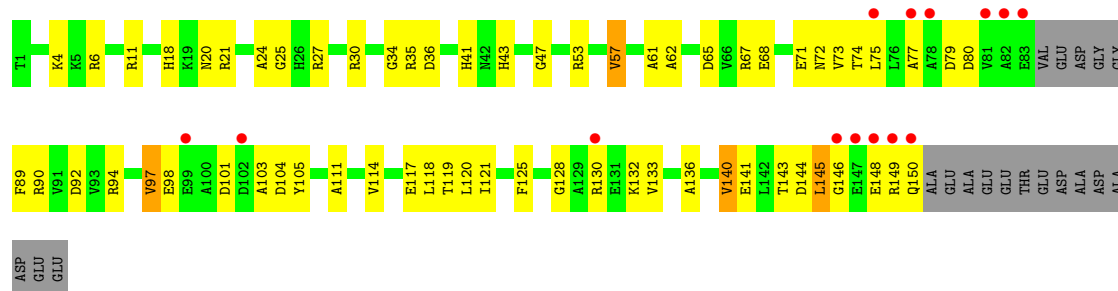


• Molecule 12: RIBOSOMAL PROTEIN L14

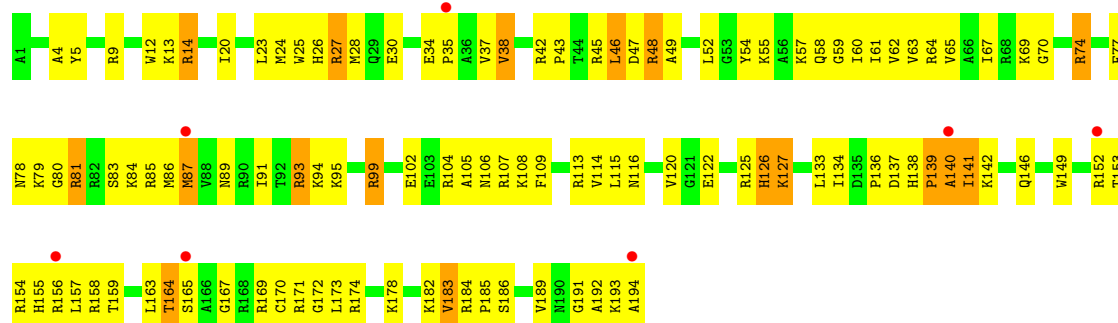




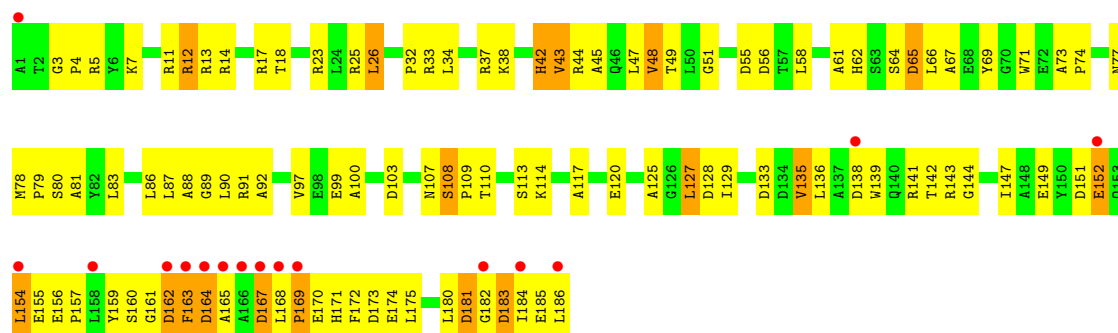
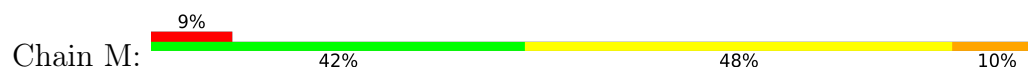
• Molecule 13: RIBOSOMAL PROTEIN L15



• Molecule 14: RIBOSOMAL PROTEIN L15E



• Molecule 15: RIBOSOMAL PROTEIN L18



• Molecule 16: RIBOSOMAL PROTEIN L18E





• Molecule 17: RIBOSOMAL PROTEIN L19E



• Molecule 18: RIBOSOMAL PROTEIN L21E



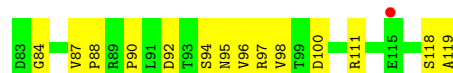
• Molecule 19: RIBOSOMAL PROTEIN L22



• Molecule 20: RIBOSOMAL PROTEIN L23



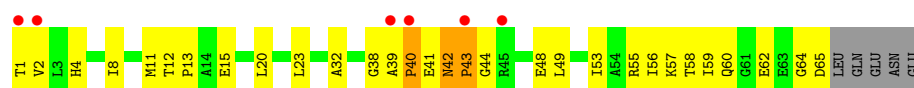
• Molecule 21: RIBOSOMAL PROTEIN L24



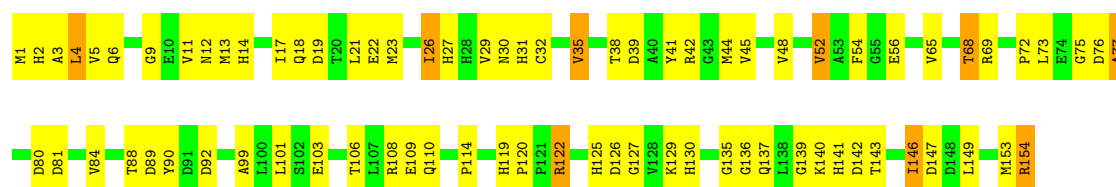
• Molecule 22: RIBOSOMAL PROTEIN L24E



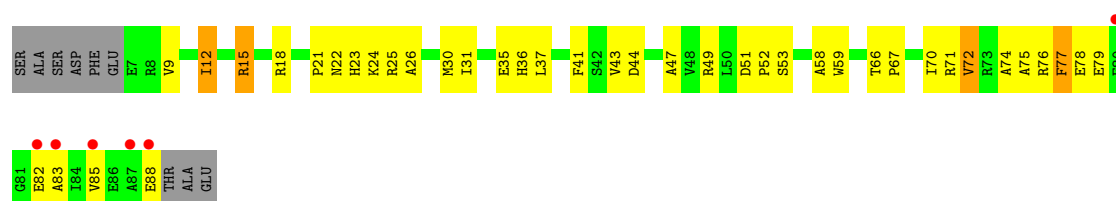
Chain U:



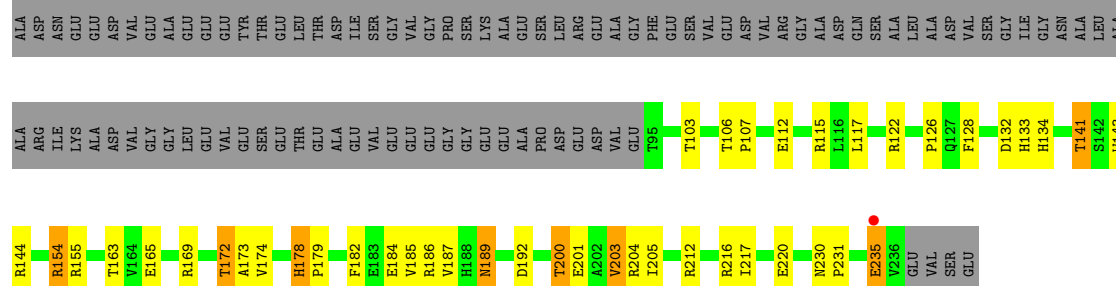
Chain V: 49% 45% 6%



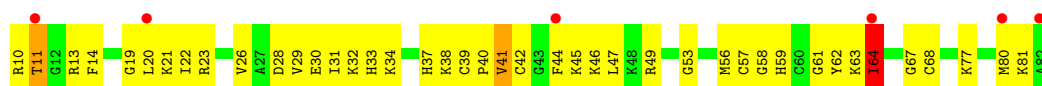
Chain W:



Chain X: 41% 15% 41%



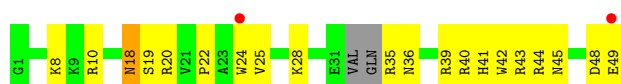
Chain Y:



• Molecule 28: RIBOSOMAL PROTEIN L37E



• Molecule 29: RIBOSOMAL PROTEIN L39E



• Molecule 30: RIBOSOMAL PROTEIN L44E



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.66Å 299.67Å 573.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 15.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.2 (15.00-2.40) 90.2 (15.00-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.189 , 0.222 0.184 , 0.217	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	98543	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: K, CL, CD, NA, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.39	1/66076 (0.0%)	0.63	42/103052 (0.0%)
2	9	0.45	2/2905 (0.1%)	0.79	15/4528 (0.3%)
3	A	0.43	0/1787	1.00	6/2409 (0.2%)
4	B	0.42	0/2689	0.98	8/3652 (0.2%)
5	C	0.48	0/1883	0.99	13/2551 (0.5%)
6	D	0.36	0/1111	0.94	5/1498 (0.3%)
7	E	0.37	0/1382	0.87	3/1880 (0.2%)
8	F	0.40	0/896	0.89	1/1219 (0.1%)
9	G	0.34	0/241	0.76	0/324
10	H	0.46	0/1246	1.20	14/1686 (0.8%)
11	I	0.40	0/1135	0.92	2/1530 (0.1%)
12	J	0.40	0/1003	0.97	4/1351 (0.3%)
13	K	0.39	0/1126	1.01	6/1504 (0.4%)
14	L	0.49	0/1633	1.04	10/2180 (0.5%)
15	M	0.36	0/1473	1.04	14/1999 (0.7%)
16	N	0.41	0/873	0.93	3/1181 (0.3%)
17	O	0.40	0/1143	0.84	1/1521 (0.1%)
18	P	0.43	0/748	1.04	5/1005 (0.5%)
19	Q	0.44	0/1172	0.99	6/1578 (0.4%)
20	R	0.37	0/648	0.90	3/875 (0.3%)
21	S	0.38	0/957	0.95	5/1289 (0.4%)
22	T	0.35	0/417	0.86	0/562
23	U	0.37	0/502	0.96	2/675 (0.3%)
24	V	0.46	0/1218	1.00	6/1655 (0.4%)
25	W	0.42	0/664	0.99	2/895 (0.2%)
26	X	0.42	0/1146	0.95	4/1536 (0.3%)
27	Y	0.45	0/575	1.02	1/763 (0.1%)
28	Z	0.48	0/437	0.98	3/578 (0.5%)
29	1	0.44	0/398	0.75	0/527
30	2	0.41	0/771	0.97	5/1024 (0.5%)
All	All	0.40	3/98255 (0.0%)	0.74	189/147027 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	62
2	9	0	2
All	All	1	64

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	9	3	A	O5'-C5'	7.70	1.54	1.42
2	9	3	A	C2'-O2'	-6.86	1.31	1.41
1	0	1206	U	P-OP2	5.29	1.59	1.49

The worst 5 of 189 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1164	U	OP1-P-O3'	-16.18	59.47	108.00
1	0	1563	G	C2'-C3'-O3'	14.05	130.57	109.50
2	9	24	U	C2'-C3'-O3'	13.09	129.14	109.50
10	H	74	ASN	N-CA-C	-12.22	95.28	113.61
1	0	1979	G	C2'-C3'-O3'	11.99	127.49	109.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 64 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	182	G	Sidechain
1	0	191	A	Sidechain
1	0	22	U	Sidechain
1	0	221	G	Sidechain
1	0	246	G	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	0	59017	0	29807	766	0
2	9	2600	0	1326	78	0
3	A	1754	0	1763	114	0
4	B	2624	0	2533	183	0
5	C	1858	0	1816	107	0
6	D	1094	0	1085	137	0
7	E	1357	0	1266	82	0
8	F	885	0	854	61	0
9	G	240	0	231	20	0
10	H	1215	0	1215	157	0
11	I	1119	0	1098	65	0
12	J	993	0	1027	60	0
13	K	1114	0	1072	55	0
14	L	1605	0	1676	151	0
15	M	1444	0	1401	124	0
16	N	864	0	873	32	0
17	O	1133	0	1127	38	0
18	P	734	0	728	19	0
19	Q	1149	0	1122	49	0
20	R	641	0	605	21	0
21	S	949	0	923	52	0
22	T	410	0	364	33	0
23	U	499	0	511	30	0
24	V	1195	0	1137	96	0
25	W	654	0	653	43	0
26	X	1130	0	1133	53	0
27	Y	563	0	597	56	0
28	Z	430	0	426	21	0
29	1	393	0	406	32	0
30	2	755	0	728	37	0
31	0	109	0	0	0	0
31	2	1	0	0	0	0
31	9	1	0	0	0	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	J	1	0	0	0	0
31	S	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	X	1	0	0	0	0
32	0	2	0	0	0	0
33	0	72	0	0	0	0
33	9	2	0	0	0	0
33	A	1	0	0	0	0
33	C	1	0	0	0	0
33	H	2	0	0	0	0
33	I	1	0	0	0	0
33	K	1	0	0	0	0
33	L	1	0	0	0	0
33	P	1	0	0	0	0
33	Q	2	0	0	0	0
33	R	1	0	0	0	0
33	S	1	0	0	0	0
34	0	10	0	0	0	0
34	2	1	0	0	0	0
34	A	1	0	0	0	0
34	B	1	0	0	0	0
34	I	3	0	0	1	0
34	K	1	0	0	0	0
34	L	1	0	0	1	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	Q	1	0	0	0	0
34	X	1	0	0	0	0
35	2	1	0	0	0	0
35	N	1	0	0	0	0
35	T	1	0	0	0	0
35	Y	1	0	0	0	0
35	Z	1	0	0	0	0
36	0	5938	0	0	174	0
36	1	40	0	0	6	0
36	2	72	0	0	10	0
36	9	135	0	0	14	0
36	A	126	0	0	21	0
36	B	150	0	0	31	0
36	C	172	0	0	30	0
36	D	53	0	0	18	0
36	E	46	0	0	12	0
36	F	28	0	0	7	0
36	G	21	0	0	4	0
36	H	74	0	0	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	I	56	0	0	5	0
36	J	62	0	0	14	0
36	K	80	0	0	16	0
36	L	127	0	0	20	0
36	M	70	0	0	16	0
36	N	43	0	0	6	0
36	O	68	0	0	1	0
36	P	53	0	0	1	0
36	Q	81	0	0	8	0
36	R	32	0	0	5	0
36	S	39	0	0	4	0
36	T	25	0	0	6	0
36	U	15	0	0	4	0
36	V	67	0	0	10	0
36	W	29	0	0	3	0
36	X	99	0	0	15	0
36	Y	39	0	0	12	0
36	Z	53	0	0	1	0
All	All	98543	0	59503	2525	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 17.

The worst 5 of 2525 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)
1:O:1134:G:H4'	10:H:151:MET:HE1	1.27	1.16
1:O:1160:G:H5'	1:O:1161:A:H5'	1.26	1.14
10:H:86:ARG:NH1	10:H:133:ILE:HG13	1.62	1.12
19:Q:99:ALA:HB1	19:Q:109:MET:HE1	1.27	1.12
5:C:5:ILE:HD11	5:C:16:VAL:HG23	1.35	1.07

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
3	A	235/239 (98%)	216 (92%)	14 (6%)	5 (2%)	5	7
4	B	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	5	7
5	C	244/246 (99%)	226 (93%)	18 (7%)	0	100	100
6	D	134/176 (76%)	97 (72%)	28 (21%)	9 (7%)	1	0
7	E	170/177 (96%)	161 (95%)	8 (5%)	1 (1%)	21	32
8	F	117/119 (98%)	106 (91%)	9 (8%)	2 (2%)	7	10
9	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	H	152/167 (91%)	135 (89%)	12 (8%)	5 (3%)	3	2
11	I	140/145 (97%)	130 (93%)	7 (5%)	3 (2%)	5	7
12	J	130/132 (98%)	121 (93%)	8 (6%)	1 (1%)	16	25
13	K	141/164 (86%)	121 (86%)	19 (14%)	1 (1%)	18	28
14	L	192/194 (99%)	181 (94%)	10 (5%)	1 (0%)	24	37
15	M	184/186 (99%)	167 (91%)	10 (5%)	7 (4%)	2	2
16	N	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
17	O	141/148 (95%)	138 (98%)	3 (2%)	0	100	100
18	P	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
19	Q	148/154 (96%)	143 (97%)	4 (3%)	1 (1%)	18	28
20	R	79/84 (94%)	75 (95%)	4 (5%)	0	100	100
21	S	117/119 (98%)	112 (96%)	5 (4%)	0	100	100
22	T	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
23	U	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	3	3
24	V	152/154 (99%)	147 (97%)	4 (3%)	1 (1%)	18	28
25	W	80/91 (88%)	70 (88%)	8 (10%)	2 (2%)	4	5
26	X	140/240 (58%)	140 (100%)	0	0	100	100
27	Y	71/73 (97%)	64 (90%)	5 (7%)	2 (3%)	4	3
28	Z	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
29	1	42/48 (88%)	42 (100%)	0	0	100	100
30	2	90/92 (98%)	86 (96%)	2 (2%)	2 (2%)	5	6
All	All	3633/4235 (86%)	3372 (93%)	209 (6%)	52 (1%)	9	13

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	139	ASP
6	D	93	LEU
6	D	95	THR
6	D	137	PRO
6	D	173	GLU

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	
3	A	179/181 (99%)	167 (93%)	12 (7%)	15	26
4	B	282/282 (100%)	262 (93%)	20 (7%)	13	23
5	C	193/193 (100%)	179 (93%)	14 (7%)	13	22
6	D	117/147 (80%)	108 (92%)	9 (8%)	12	20
7	E	152/155 (98%)	148 (97%)	4 (3%)	40	63
8	F	92/92 (100%)	89 (97%)	3 (3%)	33	55
9	G	27/283 (10%)	27 (100%)	0	100	100
10	H	122/122 (100%)	107 (88%)	15 (12%)	4	6
11	I	118/121 (98%)	111 (94%)	7 (6%)	18	31
12	J	106/106 (100%)	103 (97%)	3 (3%)	38	60
13	K	112/126 (89%)	109 (97%)	3 (3%)	39	62
14	L	166/166 (100%)	157 (95%)	9 (5%)	20	35
15	M	149/149 (100%)	140 (94%)	9 (6%)	17	31
16	N	93/93 (100%)	89 (96%)	4 (4%)	26	44
17	O	113/116 (97%)	110 (97%)	3 (3%)	39	62
18	P	79/79 (100%)	75 (95%)	4 (5%)	21	37
19	Q	117/121 (97%)	114 (97%)	3 (3%)	40	63
20	R	71/73 (97%)	70 (99%)	1 (1%)	59	79
21	S	105/105 (100%)	100 (95%)	5 (5%)	23	40
22	T	44/52 (85%)	44 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	U	51/56 (91%)	50 (98%)	1 (2%)	48	70
24	V	130/130 (100%)	121 (93%)	9 (7%)	14	24
25	W	66/73 (90%)	64 (97%)	2 (3%)	36	58
26	X	120/195 (62%)	110 (92%)	10 (8%)	10	17
27	Y	56/56 (100%)	54 (96%)	2 (4%)	31	52
28	Z	46/46 (100%)	46 (100%)	0	100	100
29	1	42/44 (96%)	41 (98%)	1 (2%)	43	65
30	2	79/79 (100%)	75 (95%)	4 (5%)	21	37
All	All	3027/3441 (88%)	2870 (95%)	157 (5%)	21	36

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	P	11	ARG
26	X	163	THR
19	Q	13	THR
24	V	26	ILE
27	Y	11	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	153	GLN
20	R	51	GLN
28	Z	28	HIS
17	O	66	GLN
19	Q	22	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2747/2922 (94%)	253 (9%)	35 (1%)
2	9	121/122 (99%)	18 (14%)	5 (4%)
All	All	2868/3044 (94%)	271 (9%)	40 (1%)

5 of 271 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A

5 of 40 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	2526	C
2	9	2	U
1	0	2536	C
1	0	2726	U
2	9	24	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 232 ligands modelled in this entry, 232 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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, 95th 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 ²)	Q<0.9
1	0	2754/2922 (94%)	-0.77	50 (1%) 67 63	17, 36, 79, 126	0
2	9	122/122 (100%)	-0.10	6 (4%) 35 31	31, 54, 78, 136	0
3	A	237/239 (99%)	-0.28	4 (1%) 69 65	19, 38, 71, 92	0
4	B	337/337 (100%)	-0.13	5 (1%) 72 68	21, 45, 71, 82	0
5	C	246/246 (100%)	-0.32	1 (0%) 88 86	15, 35, 58, 70	0
6	D	140/176 (79%)	1.29	27 (19%) 3 2	43, 86, 105, 108	0
7	E	172/177 (97%)	0.27	4 (2%) 61 57	37, 59, 77, 81	0
8	F	119/119 (100%)	0.45	4 (3%) 48 44	37, 58, 83, 88	0
9	G	29/348 (8%)	1.12	3 (10%) 12 9	64, 79, 86, 91	0
10	H	156/167 (93%)	0.29	11 (7%) 22 18	30, 47, 75, 79	0
11	I	142/145 (97%)	-0.18	1 (0%) 84 81	29, 42, 63, 84	0
12	J	132/132 (100%)	-0.18	1 (0%) 82 80	27, 42, 61, 71	0
13	K	145/164 (88%)	0.19	14 (9%) 13 10	18, 54, 90, 102	0
14	L	194/194 (100%)	-0.29	7 (3%) 46 42	19, 32, 50, 62	0
15	M	186/186 (100%)	0.36	16 (8%) 16 13	31, 50, 91, 103	0
16	N	115/115 (100%)	-0.00	3 (2%) 57 53	27, 44, 60, 69	0
17	O	143/148 (96%)	-0.15	0 100 100	30, 44, 56, 64	0
18	P	95/95 (100%)	-0.40	1 (1%) 78 74	25, 34, 50, 60	0
19	Q	150/154 (97%)	-0.57	0 100 100	23, 36, 54, 63	0
20	R	81/84 (96%)	-0.10	1 (1%) 76 73	31, 46, 68, 72	0
21	S	119/119 (100%)	0.02	2 (1%) 69 65	28, 45, 69, 81	0
22	T	53/66 (80%)	0.06	0 100 100	33, 47, 63, 71	0
23	U	65/70 (92%)	0.56	6 (9%) 14 12	39, 59, 97, 101	0
24	V	154/154 (100%)	-0.26	0 100 100	27, 40, 57, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	82/91 (90%)	0.25	6 (7%) 21 17	35, 48, 73, 91	0
26	X	142/240 (59%)	-0.35	1 (0%) 84 81	22, 35, 59, 74	0
27	Y	73/73 (100%)	0.59	6 (8%) 17 14	36, 49, 63, 77	0
28	Z	56/56 (100%)	-0.86	0 100 100	17, 24, 32, 35	0
29	1	46/48 (95%)	0.22	2 (4%) 40 36	27, 49, 77, 86	0
30	2	92/92 (100%)	-0.06	2 (2%) 62 58	23, 44, 59, 72	0
All	All	6577/7279 (90%)	-0.33	184 (2%) 55 51	15, 41, 80, 136	0

The worst 5 of 184 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	U	1	THR	8.2
3	A	37	VAL	6.2
25	W	88	GLU	6.0
2	9	25	G	5.8
1	0	1169	U	5.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th 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 ²)	Q<0.9
31	MG	0	8087	1/1	0.56	0.22	72,72,72,72	0
31	MG	9	8095	1/1	0.69	0.26	69,69,69,69	0
33	NA	Q	8386	1/1	0.69	0.26	74,74,74,74	0
31	MG	0	8066	1/1	0.75	0.19	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	NA	0	8370	1/1	0.78	0.26	61,61,61,61	0
31	MG	0	8102	1/1	0.78	0.10	51,51,51,51	0
31	MG	0	8070	1/1	0.80	0.07	40,40,40,40	0
31	MG	0	8090	1/1	0.83	0.09	53,53,53,53	0
33	NA	0	8307	1/1	0.84	0.08	42,42,42,42	0
33	NA	0	8376	1/1	0.84	0.10	39,39,39,39	0
33	NA	0	8329	1/1	0.84	0.08	48,48,48,48	0
31	MG	0	8101	1/1	0.86	0.11	48,48,48,48	0
33	NA	9	8383	1/1	0.86	0.16	43,43,43,43	0
33	NA	0	8314	1/1	0.86	0.10	40,40,40,40	0
31	MG	0	8106	1/1	0.87	0.06	42,42,42,42	0
33	NA	0	8340	1/1	0.87	0.13	47,47,47,47	0
31	MG	0	8050	1/1	0.87	0.05	56,56,56,56	0
33	NA	9	8351	1/1	0.88	0.16	42,42,42,42	0
31	MG	0	8043	1/1	0.88	0.07	33,33,33,33	0
31	MG	0	8103	1/1	0.88	0.08	54,54,54,54	0
33	NA	0	8311	1/1	0.89	0.09	48,48,48,48	0
33	NA	0	8371	1/1	0.89	0.12	49,49,49,49	0
33	NA	0	8324	1/1	0.89	0.16	48,48,48,48	0
31	MG	0	8082	1/1	0.90	0.14	56,56,56,56	0
33	NA	0	8358	1/1	0.90	0.35	74,74,74,74	0
33	NA	H	8322	1/1	0.90	0.13	52,52,52,52	0
33	NA	0	8364	1/1	0.90	0.12	38,38,38,38	0
33	NA	0	8384	1/1	0.91	0.09	52,52,52,52	0
33	NA	0	8369	1/1	0.91	0.10	40,40,40,40	0
31	MG	0	8094	1/1	0.91	0.12	59,59,59,59	0
33	NA	0	8350	1/1	0.91	0.08	36,36,36,36	0
33	NA	Q	8337	1/1	0.91	0.04	33,33,33,33	0
33	NA	0	8366	1/1	0.91	0.09	54,54,54,54	0
33	NA	0	8385	1/1	0.92	0.18	48,48,48,48	0
31	MG	0	8047	1/1	0.92	0.10	54,54,54,54	0
33	NA	0	8372	1/1	0.92	0.12	54,54,54,54	0
33	NA	0	8373	1/1	0.92	0.07	43,43,43,43	0
33	NA	0	8363	1/1	0.92	0.12	52,52,52,52	0
33	NA	0	8357	1/1	0.92	0.05	39,39,39,39	0
33	NA	0	8342	1/1	0.93	0.07	33,33,33,33	0
31	MG	0	8076	1/1	0.93	0.04	46,46,46,46	0
31	MG	0	8046	1/1	0.93	0.05	38,38,38,38	0
31	MG	0	8092	1/1	0.93	0.09	66,66,66,66	0
31	MG	0	8093	1/1	0.93	0.05	35,35,35,35	0
33	NA	R	8312	1/1	0.93	0.05	26,26,26,26	0
33	NA	0	8360	1/1	0.94	0.07	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	NA	0	8379	1/1	0.94	0.14	48,48,48,48	0
31	MG	0	8104	1/1	0.94	0.04	45,45,45,45	0
33	NA	0	8330	1/1	0.94	0.09	39,39,39,39	0
31	MG	0	8049	1/1	0.94	0.08	56,56,56,56	0
33	NA	0	8341	1/1	0.94	0.06	37,37,37,37	0
33	NA	0	8313	1/1	0.94	0.06	48,48,48,48	0
31	MG	0	8113	1/1	0.94	0.06	36,36,36,36	0
31	MG	0	8051	1/1	0.94	0.07	56,56,56,56	0
33	NA	0	8327	1/1	0.94	0.11	38,38,38,38	0
31	MG	0	8114	1/1	0.95	0.03	35,35,35,35	0
33	NA	0	8374	1/1	0.95	0.10	44,44,44,44	0
33	NA	0	8336	1/1	0.95	0.03	37,37,37,37	0
33	NA	0	8362	1/1	0.95	0.10	51,51,51,51	0
33	NA	0	8382	1/1	0.95	0.07	64,64,64,64	0
31	MG	0	8053	1/1	0.95	0.13	28,28,28,28	0
31	MG	0	8099	1/1	0.95	0.05	44,44,44,44	0
33	NA	0	8326	1/1	0.95	0.07	37,37,37,37	0
33	NA	0	8367	1/1	0.95	0.06	45,45,45,45	0
33	NA	0	8310	1/1	0.95	0.09	27,27,27,27	0
33	NA	P	8348	1/1	0.95	0.04	32,32,32,32	0
33	NA	0	8352	1/1	0.95	0.05	40,40,40,40	0
33	NA	0	8356	1/1	0.95	0.10	37,37,37,37	0
31	MG	0	8100	1/1	0.95	0.06	64,64,64,64	0
34	CL	I	8521	1/1	0.95	0.07	47,47,47,47	0
33	NA	0	8301	1/1	0.96	0.05	33,33,33,33	0
33	NA	0	8302	1/1	0.96	0.09	44,44,44,44	0
31	MG	0	8091	1/1	0.96	0.03	41,41,41,41	0
31	MG	0	8045	1/1	0.96	0.06	51,51,51,51	0
33	NA	0	8349	1/1	0.96	0.06	37,37,37,37	0
31	MG	0	8071	1/1	0.96	0.04	62,62,62,62	0
33	NA	0	8375	1/1	0.96	0.17	39,39,39,39	0
31	MG	0	8062	1/1	0.96	0.06	41,41,41,41	0
33	NA	0	8377	1/1	0.96	0.11	50,50,50,50	0
33	NA	0	8378	1/1	0.96	0.11	39,39,39,39	0
31	MG	0	8064	1/1	0.96	0.04	26,26,26,26	0
33	NA	0	8381	1/1	0.96	0.05	41,41,41,41	0
33	NA	0	8318	1/1	0.96	0.11	49,49,49,49	0
31	MG	0	8012	1/1	0.96	0.07	32,32,32,32	0
33	NA	0	8359	1/1	0.96	0.08	39,39,39,39	0
31	MG	0	8117	1/1	0.96	0.09	36,36,36,36	0
33	NA	0	8361	1/1	0.96	0.05	38,38,38,38	0
33	NA	C	8304	1/1	0.96	0.04	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	0	8067	1/1	0.96	0.07	34,34,34,34	0
33	NA	L	8347	1/1	0.96	0.04	18,18,18,18	0
31	MG	J	8069	1/1	0.96	0.05	46,46,46,46	0
32	K	0	8201	1/1	0.96	0.13	62,62,62,62	0
33	NA	0	8333	1/1	0.96	0.04	23,23,23,23	0
33	NA	0	8335	1/1	0.96	0.06	31,31,31,31	0
34	CL	0	8517	1/1	0.96	0.06	50,50,50,50	0
34	CL	I	8502	1/1	0.96	0.05	53,53,53,53	0
33	NA	0	8368	1/1	0.96	0.12	48,48,48,48	0
31	MG	0	8108	1/1	0.97	0.08	62,62,62,62	0
31	MG	0	8037	1/1	0.97	0.03	35,35,35,35	0
31	MG	0	8096	1/1	0.97	0.04	37,37,37,37	0
33	NA	0	8344	1/1	0.97	0.06	24,24,24,24	0
31	MG	0	8115	1/1	0.97	0.03	36,36,36,36	0
33	NA	0	8316	1/1	0.97	0.06	35,35,35,35	0
31	MG	0	8085	1/1	0.97	0.06	35,35,35,35	0
33	NA	0	8355	1/1	0.97	0.14	47,47,47,47	0
33	NA	0	8319	1/1	0.97	0.03	29,29,29,29	0
33	NA	0	8321	1/1	0.97	0.12	40,40,40,40	0
31	MG	0	8052	1/1	0.97	0.04	45,45,45,45	0
33	NA	0	8325	1/1	0.97	0.07	47,47,47,47	0
31	MG	0	8089	1/1	0.97	0.05	51,51,51,51	0
31	MG	X	8109	1/1	0.97	0.05	25,25,25,25	0
31	MG	0	8048	1/1	0.97	0.04	39,39,39,39	0
31	MG	0	8040	1/1	0.97	0.05	38,38,38,38	0
33	NA	I	8346	1/1	0.97	0.04	34,34,34,34	0
33	NA	K	8380	1/1	0.97	0.22	42,42,42,42	0
33	NA	0	8331	1/1	0.97	0.05	39,39,39,39	0
33	NA	0	8365	1/1	0.97	0.20	28,28,28,28	0
31	MG	0	8072	1/1	0.97	0.04	47,47,47,47	0
33	NA	0	8334	1/1	0.97	0.08	33,33,33,33	0
31	MG	0	8041	1/1	0.97	0.10	33,33,33,33	0
33	NA	S	8343	1/1	0.97	0.05	29,29,29,29	0
33	NA	0	8308	1/1	0.97	0.04	42,42,42,42	0
34	CL	A	8509	1/1	0.97	0.05	50,50,50,50	0
33	NA	0	8338	1/1	0.97	0.02	36,36,36,36	0
33	NA	0	8339	1/1	0.97	0.04	20,20,20,20	0
34	CL	K	8510	1/1	0.97	0.08	36,36,36,36	0
31	MG	0	8074	1/1	0.98	0.03	36,36,36,36	0
31	MG	2	8078	1/1	0.98	0.04	39,39,39,39	0
31	MG	0	8097	1/1	0.98	0.05	30,30,30,30	0
31	MG	0	8098	1/1	0.98	0.06	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	0	8075	1/1	0.98	0.05	28,28,28,28	0
33	NA	0	8305	1/1	0.98	0.04	32,32,32,32	0
33	NA	0	8306	1/1	0.98	0.13	28,28,28,28	0
31	MG	0	8003	1/1	0.98	0.02	21,21,21,21	0
31	MG	0	8080	1/1	0.98	0.05	41,41,41,41	0
31	MG	0	8081	1/1	0.98	0.03	39,39,39,39	0
31	MG	0	8042	1/1	0.98	0.06	29,29,29,29	0
31	MG	0	8014	1/1	0.98	0.09	25,25,25,25	0
31	MG	0	8086	1/1	0.98	0.04	33,33,33,33	0
33	NA	0	8354	1/1	0.98	0.06	25,25,25,25	0
33	NA	0	8315	1/1	0.98	0.06	30,30,30,30	0
31	MG	0	8044	1/1	0.98	0.04	32,32,32,32	0
33	NA	H	8309	1/1	0.98	0.04	28,28,28,28	0
33	NA	0	8317	1/1	0.98	0.03	27,27,27,27	0
31	MG	0	8112	1/1	0.98	0.08	23,23,23,23	0
31	MG	0	8022	1/1	0.98	0.03	32,32,32,32	0
33	NA	0	8320	1/1	0.98	0.08	38,38,38,38	0
31	MG	0	8024	1/1	0.98	0.03	22,22,22,22	0
33	NA	0	8323	1/1	0.98	0.11	31,31,31,31	0
31	MG	0	8025	1/1	0.98	0.04	36,36,36,36	0
31	MG	0	8116	1/1	0.98	0.03	42,42,42,42	0
31	MG	0	8035	1/1	0.98	0.02	36,36,36,36	0
34	CL	0	8503	1/1	0.98	0.04	40,40,40,40	0
34	CL	0	8505	1/1	0.98	0.04	41,41,41,41	0
34	CL	0	8513	1/1	0.98	0.04	44,44,44,44	0
34	CL	0	8515	1/1	0.98	0.10	48,48,48,48	0
34	CL	0	8516	1/1	0.98	0.07	42,42,42,42	0
31	MG	0	8006	1/1	0.98	0.04	27,27,27,27	0
34	CL	0	8522	1/1	0.98	0.19	44,44,44,44	0
31	MG	A	8105	1/1	0.98	0.03	27,27,27,27	0
34	CL	B	8519	1/1	0.98	0.04	33,33,33,33	0
34	CL	I	8501	1/1	0.98	0.03	44,44,44,44	0
31	MG	0	8007	1/1	0.98	0.04	21,21,21,21	0
31	MG	S	8073	1/1	0.98	0.03	39,39,39,39	0
33	NA	0	8332	1/1	0.98	0.06	33,33,33,33	0
34	CL	N	8508	1/1	0.98	0.03	52,52,52,52	0
34	CL	Q	8506	1/1	0.98	0.04	40,40,40,40	0
34	CL	X	8520	1/1	0.98	0.05	38,38,38,38	0
35	CD	N	8405	1/1	0.98	0.04	71,71,71,71	0
31	MG	0	8002	1/1	0.99	0.05	26,26,26,26	0
31	MG	0	8110	1/1	0.99	0.02	24,24,24,24	0
31	MG	0	8111	1/1	0.99	0.04	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	NA	0	8328	1/1	0.99	0.07	28,28,28,28	0
31	MG	0	8068	1/1	0.99	0.03	44,44,44,44	0
31	MG	0	8036	1/1	0.99	0.03	35,35,35,35	0
31	MG	0	8013	1/1	0.99	0.03	22,22,22,22	0
31	MG	0	8038	1/1	0.99	0.02	22,22,22,22	0
31	MG	0	8039	1/1	0.99	0.02	32,32,32,32	0
31	MG	0	8008	1/1	0.99	0.03	22,22,22,22	0
31	MG	0	8015	1/1	0.99	0.02	26,26,26,26	0
31	MG	A	8065	1/1	0.99	0.05	24,24,24,24	0
31	MG	0	8077	1/1	0.99	0.02	23,23,23,23	0
33	NA	A	8345	1/1	0.99	0.03	46,46,46,46	0
31	MG	B	8055	1/1	0.99	0.03	40,40,40,40	0
31	MG	0	8079	1/1	0.99	0.02	19,19,19,19	0
31	MG	0	8016	1/1	0.99	0.04	32,32,32,32	0
31	MG	0	8017	1/1	0.99	0.03	12,12,12,12	0
31	MG	0	8018	1/1	0.99	0.03	27,27,27,27	0
31	MG	0	8009	1/1	0.99	0.03	24,24,24,24	0
32	K	0	8202	1/1	0.99	0.15	37,37,37,37	0
31	MG	0	8023	1/1	0.99	0.02	30,30,30,30	0
33	NA	0	8353	1/1	0.99	0.04	18,18,18,18	0
31	MG	0	8010	1/1	0.99	0.02	24,24,24,24	0
33	NA	0	8303	1/1	0.99	0.06	32,32,32,32	0
31	MG	0	8088	1/1	0.99	0.06	20,20,20,20	0
31	MG	0	8011	1/1	0.99	0.02	23,23,23,23	0
34	CL	0	8511	1/1	0.99	0.03	37,37,37,37	0
34	CL	0	8512	1/1	0.99	0.03	34,34,34,34	0
31	MG	0	8026	1/1	0.99	0.01	26,26,26,26	0
34	CL	0	8514	1/1	0.99	0.05	36,36,36,36	0
31	MG	0	8027	1/1	0.99	0.03	37,37,37,37	0
31	MG	0	8028	1/1	0.99	0.02	25,25,25,25	0
31	MG	0	8029	1/1	0.99	0.03	35,35,35,35	0
31	MG	0	8031	1/1	0.99	0.02	24,24,24,24	0
31	MG	0	8056	1/1	0.99	0.04	31,31,31,31	0
31	MG	0	8057	1/1	0.99	0.04	35,35,35,35	0
31	MG	0	8058	1/1	0.99	0.02	27,27,27,27	0
31	MG	0	8059	1/1	0.99	0.06	25,25,25,25	0
31	MG	0	8060	1/1	0.99	0.04	31,31,31,31	0
31	MG	0	8061	1/1	0.99	0.01	32,32,32,32	0
34	CL	L	8518	1/1	0.99	0.03	32,32,32,32	0
34	CL	M	8507	1/1	0.99	0.05	45,45,45,45	0
31	MG	0	8032	1/1	0.99	0.04	23,23,23,23	0
31	MG	0	8063	1/1	0.99	0.05	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	0	8033	1/1	0.99	0.02	20,20,20,20	0
34	CL	2	8504	1/1	0.99	0.03	45,45,45,45	0
31	MG	0	8034	1/1	0.99	0.03	31,31,31,31	0
35	CD	T	8401	1/1	0.99	0.01	49,49,49,49	0
35	CD	Y	8403	1/1	0.99	0.05	49,49,49,49	0
35	CD	Z	8402	1/1	0.99	0.09	37,37,37,37	0
35	CD	2	8404	1/1	0.99	0.02	47,47,47,47	0
31	MG	0	8054	1/1	1.00	0.02	18,18,18,18	0
31	MG	0	8020	1/1	1.00	0.01	24,24,24,24	0
31	MG	0	8021	1/1	1.00	0.01	24,24,24,24	0
31	MG	0	8004	1/1	1.00	0.02	21,21,21,21	0
31	MG	0	8005	1/1	1.00	0.02	24,24,24,24	0
31	MG	0	8030	1/1	1.00	0.03	22,22,22,22	0
31	MG	0	8001	1/1	1.00	0.01	25,25,25,25	0
31	MG	0	8019	1/1	1.00	0.01	23,23,23,23	0
31	MG	0	8083	1/1	1.00	0.03	30,30,30,30	0
31	MG	0	8084	1/1	1.00	0.04	39,39,39,39	0
31	MG	0	8107	1/1	1.00	0.02	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.