



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 03:56 AM EDT

PDB ID : 1VQO / pdb_00001vqo
Title : The structure of CCPMN bound to the large ribosomal subunit haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.20 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

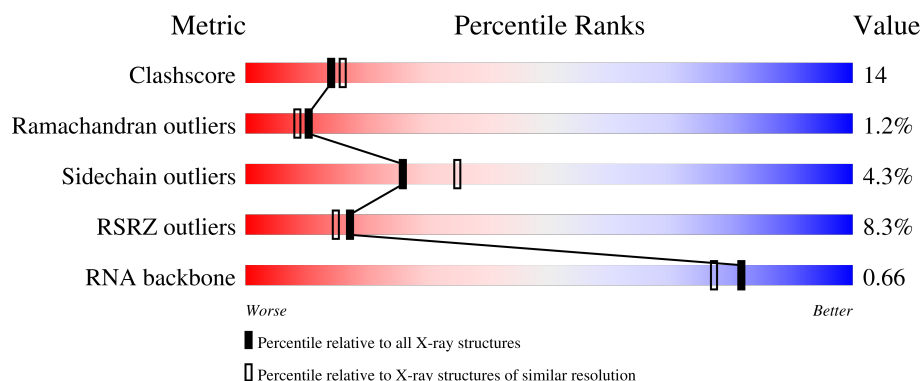
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)
RNA backbone	3983	1052 (2.50-1.90)

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	 3% 65% 25% 6%
2	9	122	 7% 60% 30% 9%
3	4	3	 33% 33% 33%
4	A	240	 9% 56% 37% 6%
5	B	338	 3% 57% 37% 6%

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Mol	Chain	Length	Quality of chain
6	C	246	
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	
15	M	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	

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Mol	Chain	Length	Quality of chain
31	3	92	
32	I	162	

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
33	MG	0	8040	-	-	-	X
33	MG	0	8082	-	-	-	X
34	K	0	9001	-	-	-	X
35	NA	0	9122	-	-	-	X
35	NA	0	9152	-	-	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99040 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 ribosomal rna.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26350	10878	19048	2745			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	modified residue	GB 3377779
0	2587	OMU	U	modified residue	GB 3377779
0	2588	OMG	G	modified residue	GB 3377779
0	2619	UR3	U	modified residue	GB 3377779
0	2621	PSU	U	modified residue	GB 3377779

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

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 RNA chain called 5'-R(*CP*CP*(PPU))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 4 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 5 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 6 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 7 is a protein called 50S ribosomal protein L5P.

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

- Molecule 8 is a protein called 50S ribosomal protein L6P.

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

- Molecule 9 is a protein called 50S ribosomal protein L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 10 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

- Molecule 12 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	conflict	UNP P22450

- Molecule 14 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	145	Total	C	N	O	S	0	0	0
			1118	670	222	226				

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	GB 55231501
M	194	ALA	GLY	conflict	GB 55231501

- Molecule 16 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 17 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	115	Total	C	N	O	0	0	0
			865	529	161	175			

- Molecule 18 is a protein called 50S ribosomal protein L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	P	143	Total	C	N	O	0	0	0
			1136	683	229	224			

- Molecule 19 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	Q	95	Total	C	N	O	0	0	0
			735	450	141	144			

- Molecule 20 is a protein called 50S ribosomal protein L22P.

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

- Molecule 21 is a protein called 50S ribosomal protein L23P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	T	119	Total	C	N	O	0	0	0
			950	568	180	202			

- Molecule 23 is a protein called 50S ribosomal protein L24E.

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

- Molecule 24 is a protein called 50S ribosomal protein L29P.

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

- Molecule 25 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 26 is a protein called 50S ribosomal protein L31e.

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

- Molecule 27 is a protein called 50S ribosomal protein L32E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Y	142	Total	C	N	O	S	0	0	0
			1130	686	228	216				

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	conflict	GB 55231162

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	88	Total	Mg	0	0
			88	88		
33	9	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	2	Total	K	0	0
			2	2		

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	64	Total Na 64 64	0	0
35	9	1	Total Na 1 1	0	0
35	B	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	D	1	Total Na 1 1	0	0
35	J	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	S	1	Total Na 1 1	0	0

- Molecule 36 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	9	Total Cl 9 9	0	0
36	A	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	J	3	Total Cl 3 3	0	0
36	K	1	Total Cl 1 1	0	0
36	L	1	Total Cl 1 1	0	0
36	M	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	O	1	Total Cl 1 1	0	0
36	R	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	Y	1	Total 1	Cl 1	0	0
36	3	1	Total 1	Cl 1	0	0

- Molecule 37 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	98	Total 98	Sr 98	0	0
37	9	3	Total 3	Sr 3	0	0
37	A	3	Total 3	Sr 3	0	0
37	B	2	Total 2	Sr 2	0	0
37	F	1	Total 1	Sr 1	0	0
37	H	1	Total 1	Sr 1	0	0
37	L	1	Total 1	Sr 1	0	0
37	R	1	Total 1	Sr 1	0	0
37	S	1	Total 1	Sr 1	0	0
37	1	2	Total 2	Sr 2	0	0
37	3	1	Total 1	Sr 1	0	0

- Molecule 38 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	1	Total 1	Cd 1	0	0
38	U	1	Total 1	Cd 1	0	0
38	Z	1	Total 1	Cd 1	0	0
38	1	1	Total 1	Cd 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	3	1	Total	Cd	0	0
			1	1		

- Molecule 39 is water.

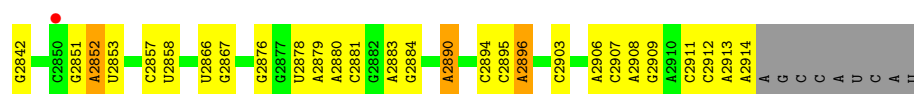
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5780	Total	O	0	0
			5780	5780		
39	9	136	Total	O	0	0
			136	136		
39	4	4	Total	O	0	0
			4	4		
39	A	124	Total	O	0	0
			124	124		
39	B	141	Total	O	0	0
			141	141		
39	C	177	Total	O	0	0
			177	177		
39	D	46	Total	O	0	0
			46	46		
39	E	43	Total	O	0	0
			43	43		
39	F	25	Total	O	0	0
			25	25		
39	G	16	Total	O	0	0
			16	16		
39	H	71	Total	O	0	0
			71	71		
39	J	58	Total	O	0	0
			58	58		
39	K	60	Total	O	0	0
			60	60		
39	L	82	Total	O	0	0
			82	82		
39	M	125	Total	O	0	0
			125	125		
39	N	62	Total	O	0	0
			62	62		
39	O	40	Total	O	0	0
			40	40		
39	P	60	Total	O	0	0
			60	60		

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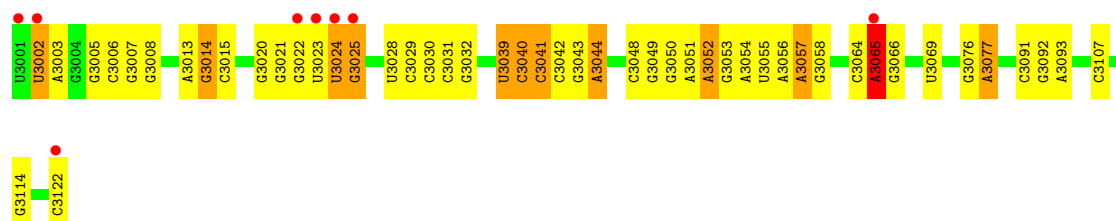
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	Q	49	Total 49	O 49	0	0
39	R	83	Total 83	O 83	0	0
39	S	30	Total 30	O 30	0	0
39	T	36	Total 36	O 36	0	0
39	U	28	Total 28	O 28	0	0
39	V	12	Total 12	O 12	0	0
39	W	68	Total 68	O 68	0	0
39	X	26	Total 26	O 26	0	0
39	Y	93	Total 93	O 93	0	0
39	Z	29	Total 29	O 29	0	0
39	1	52	Total 52	O 52	0	0
39	2	40	Total 40	O 40	0	0
39	3	66	Total 66	O 66	0	0
39	I	8	Total 8	O 8	0	0

G2748	G2633	G2595	G2420	G2313	U	U1919	U1766	C1666	U1503	C1353	U1234
U2749	G2634	C2526	G2421	G2313	G	G1926	A1767	A1667	A1504	A1358	G1235
G2750	A2635	U2531	U2422	C2317	C	U1927	C1768	U1668	U1505	U1359	U1236
G2754	A2636	U2532	G2426	U2320	A	G1928	U1770	U1669	U1506	C1360	C1238
G2755	A2637	C2533	U2435	A2321	U	G1929	C1772	G1670	G1523	G1363	G1239
A2761	C2644	U2534	U2435	A2321	A	C1940	G1773	C1675	U1524	G1363	A1242
C2762	U2645	U2535	C2443	G2324	C	A1941	A1778	G1681	U1525	C1366	C1243
A2766	A2649	C2536	G2443	G2324	U	A1942	A1778	A1682	A1526	C1366	A1244
C2765	U2650	C2537	G2453	C2329	A	C1943	A1779	G1683	A1527	A1369	C1245
A2768	C2651	U2539	A2456	U2330	C	G1946	C1787	A1684	G1528	A1372	A1246
C2769	U2652	C2540	U2457	G2337	C	C1946	U1786	A1685	G1529	A1372	A1247
G2770	U2661	U2541	U2457	G2338	G	G1951	G1789	C1686	G1532	A1372	A1247
G2779	G2662	C2549	G2462	G2338	U	U1951	G1789	C1687	G1532	G1376	C1250
C2780	U2663	C2552	A2465	C	A	U	C1798	C1692	G1555	C1377	C1251
U2781	A2664	A2553	A2465	A	A	A	C1798	A1693	A1559	G1378	A1252
G2782	U	G	A2467	G	C	C	U1817	C1700	U	U1380	A1261
A2783	G2667	U2563	G2468	G2344	C	U1964	C1818	A1701	U1561	C1384	A1268
A2784	A2668	C2564	A2469	A2345	A	C1965	G1820	U1702	G1562	C1400	A1278
C2785	G2670	C2565	C2472	C2346	U	U1966	G1820	U1702	G1563	C1400	A1278
G2786	U2671	C2566	C2472	C2347	G	U1967	C1826	C1705	C1564	A1406	U1279
U2791	C2676	A2568	C2476	C2348	C	C	A1827	C1714	A1573	A1407	U1287
A2792	G2679	C2578	G2480	A2353	C	C	G1827	C1715	C1574	A1407	U1287
C2795	A2680	G2578	G2481	A2354	A	U1967	G1827	C1715	G1592	U1408	C1289
U2796	A2681	U2586	G2482	A2355	G	U1967	U1835	A1717	C1593	G1409	C1290
C2797	C2682	C2587	U2483	A2356	C	U1967	U1838	U1722	C1594	U1419	A1291
A2800	A2694	U2588	U2484	C2357	A	U1967	U1838	G1723	U1595	C1426	A1299
U2807	A2697	U2590	A2485	A2361	C	G1971	A1839	G1723	U1596	C1426	A1299
A2811	C2698	C2591	A2490	A2362	C	U1972	A1840	U1724	A1603	G1430	A1299
C2812	A2699	G2592	G2491	A2363	G	A1973	A1845	G1726	G1604	G1430	A1299
A2813	G2700	A2599	U2492	A2364	C	U1973	A1846	G1726	G1605	U1435	U1298
A2814	C2704	A2600	C2493	A2365	C	G1973	U1847	G1730	A1606	U1435	U1298
G2815	U2705	C2601	U2499	A2369	U	U1980	C1853	C1731	A1607	G1441	U1304
A2816	G2706	G2602	C2500	A2374	A	A1981	C1856	C1734	A1615	A1442	C1305
G2817	U2711	U2607	G2501	C2375	G	U1992	C1856	A1735	U1625	G1451	U1306
A2820	G2712	C2608	C2502	U2376	G	U1996	G1863	A1736	A1626	G1452	U1314
C2821	G2715	G2611	A2503	U2377	G	U2003	C1864	U1741	G1627	A1458	U1314
G2824	G2716	A2612	G2504	U2378	G	U2004	G1867	G1744	A1630	G1327	G1327
C2825	C2717	G2613	C2505	G2379	C	U2005	G1868	G1745	A1630	A1328	A1328
A2826	C2718	C2613	C2506	G2379	C	C2006	U1877	U1748	G1634	A1331	A1331
A2827	A2719	G2618	A2507	C2388	C	U2007	U1878	U1749	A1641	G1332	C1332
G2828	U2720	U2619	C2508	A2401	C	U2008	U1879	G1750	A1642	U1473	C1333
C2831	U2721	U2620	A2511	A2402	G	A2011	C1880	G1751	G1647	C1474	C1334
C2832	U2724	U2621	C2515	C2403	A	U2012	C1882	C1753	A1654	A1476	G1340
G2833	G2725	C2626	G2516	U2406	C	G2013	U1881	G1753	G1475	C1342	C1342
U2837	U2726	C2627	A2521	A2414	C	G2014	C1882	A1754	C1477	C1477	C1343
A2838	U2735	G2630	A2522	A2415	A	A2015	G1902	A1755	A1656	A1482	U1350
C2839	U2735	U2631	U2523	G2416	C	U2016	U1903	G1756	A1657	C1483	G1351
A2840	C2747	U2632	G2524	U2419	A	U2017	A1909	A1759	A1658	G1484	A1352
A2841	C2747	G2632	G2524	U2419	G	A2019	A1909	A1759	A1658	G1484	A1352



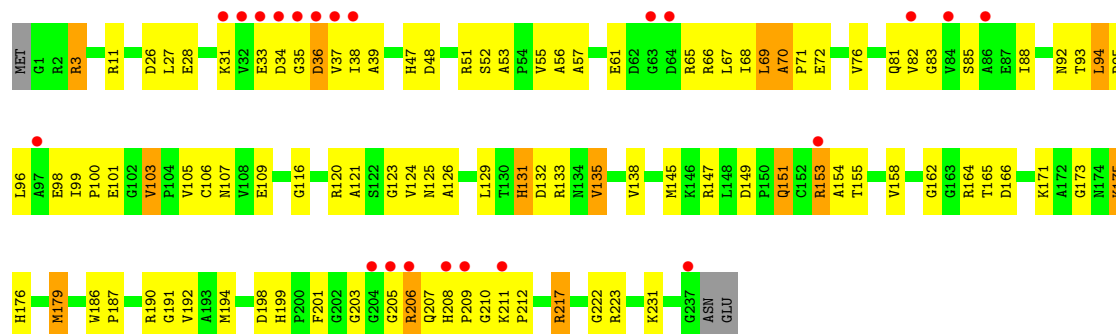
• Molecule 2: 5S ribosomal RNA



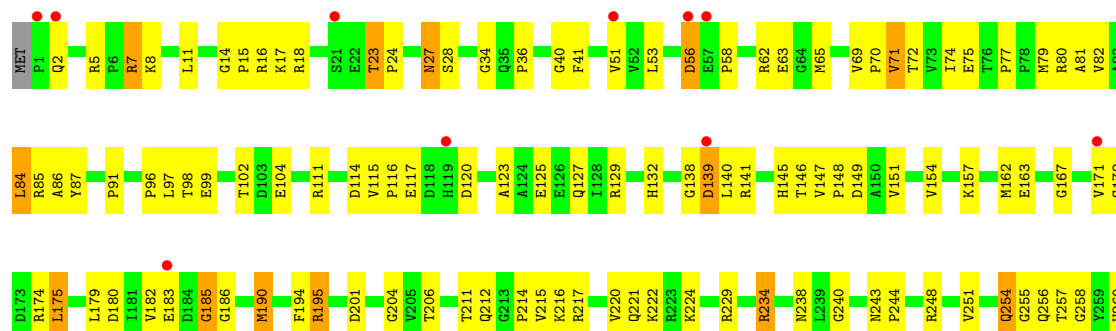
• Molecule 3: 5'-R(*CP*CP*(PPU))-3'



• Molecule 4: 50S ribosomal protein L2P

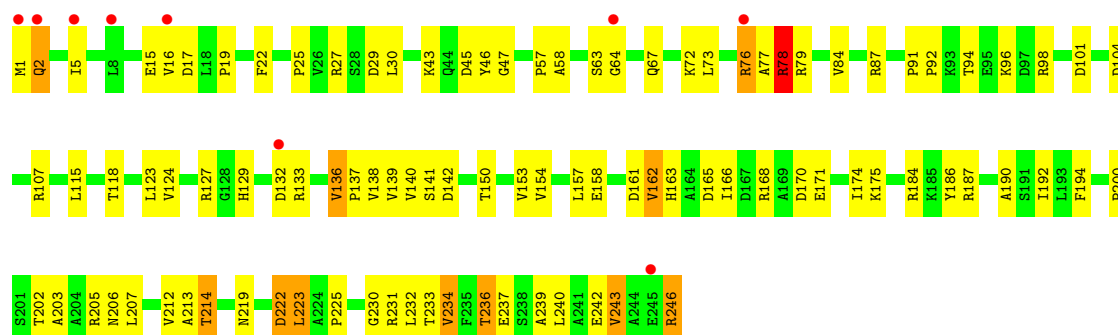


• Molecule 5: 50S ribosomal protein L3P

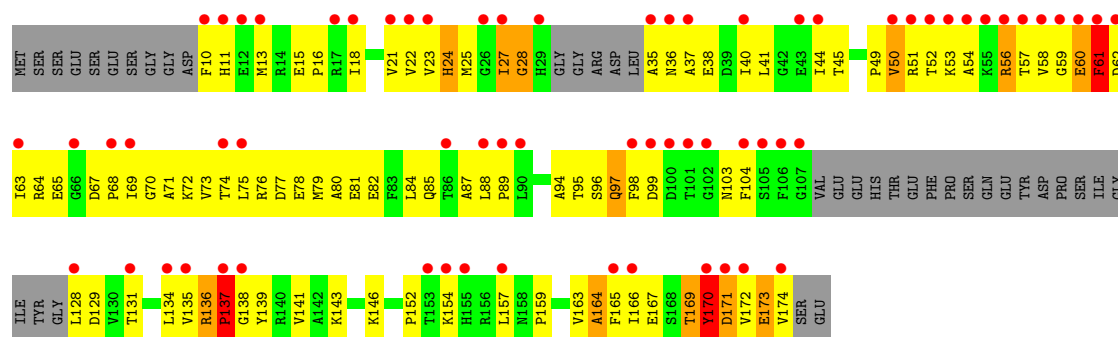




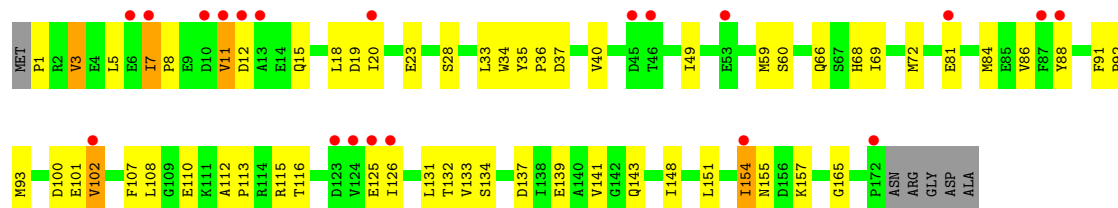
• Molecule 6: 50S ribosomal protein L4E



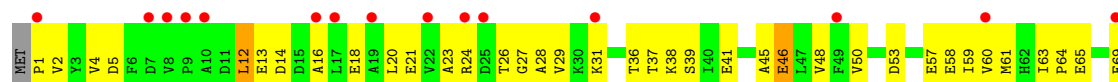
• Molecule 7: 50S ribosomal protein L5P

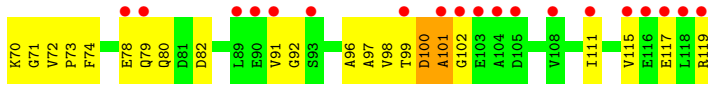


• Molecule 8: 50S ribosomal protein L6P

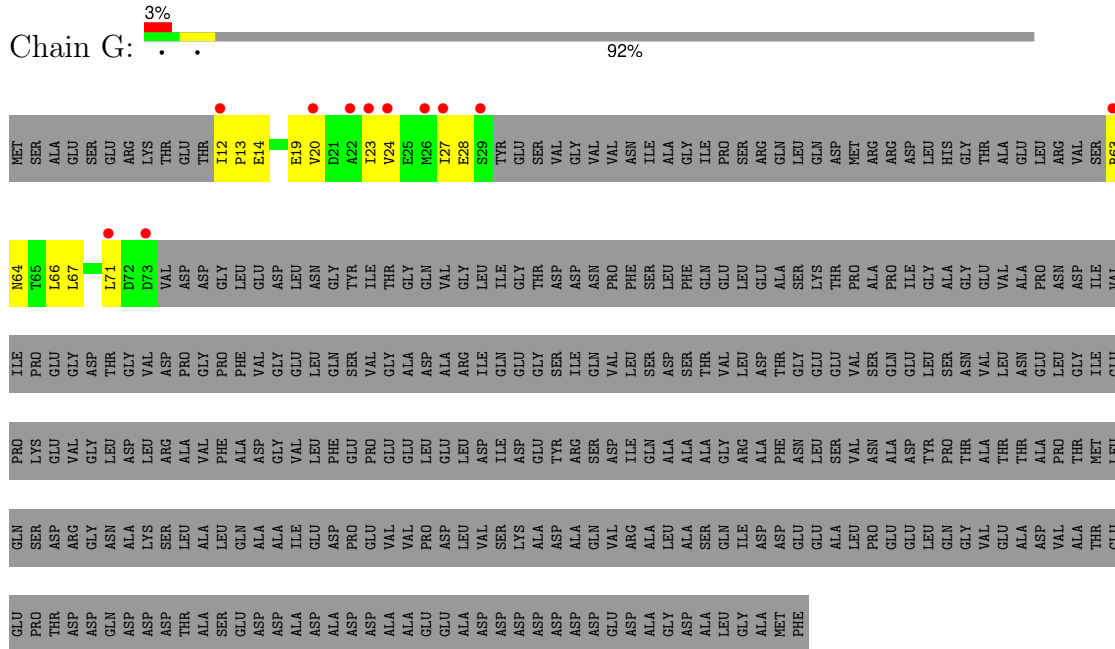


• Molecule 9: 50S ribosomal protein L7AE

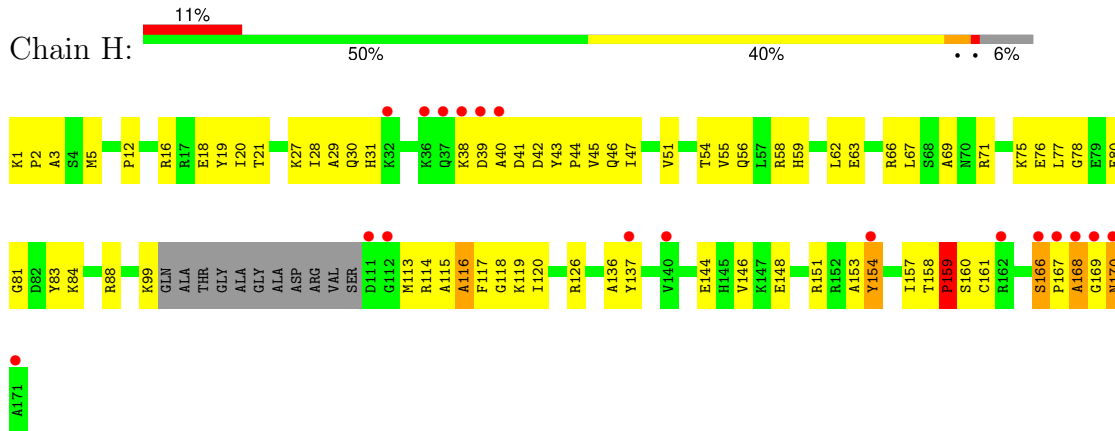




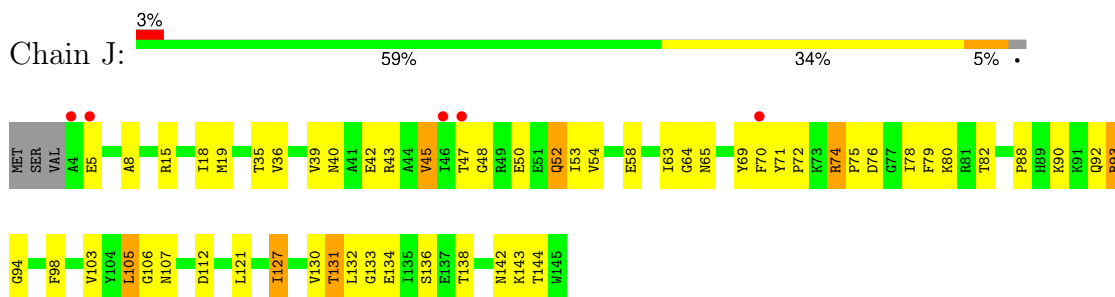
● Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



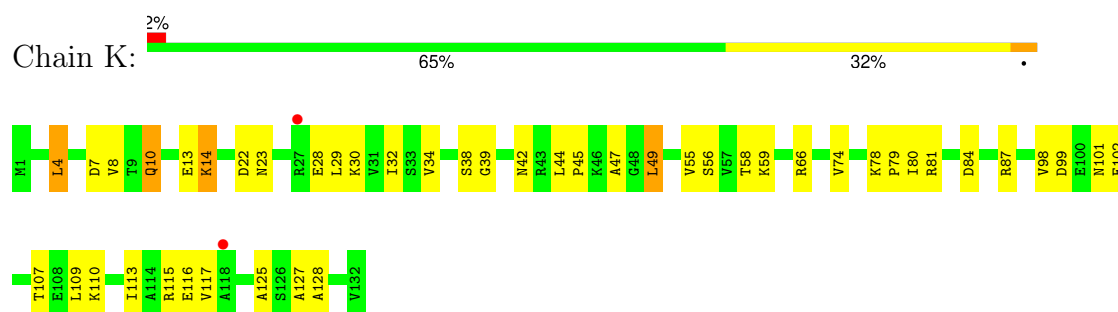
- Molecule 11: 50S RIBOSOMAL PROTEIN L10E



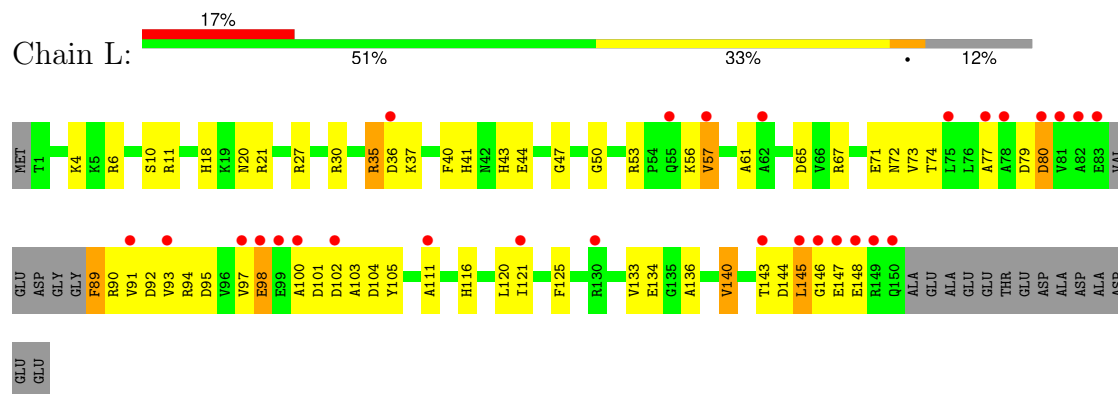
- Molecule 12: 50S ribosomal protein L13P



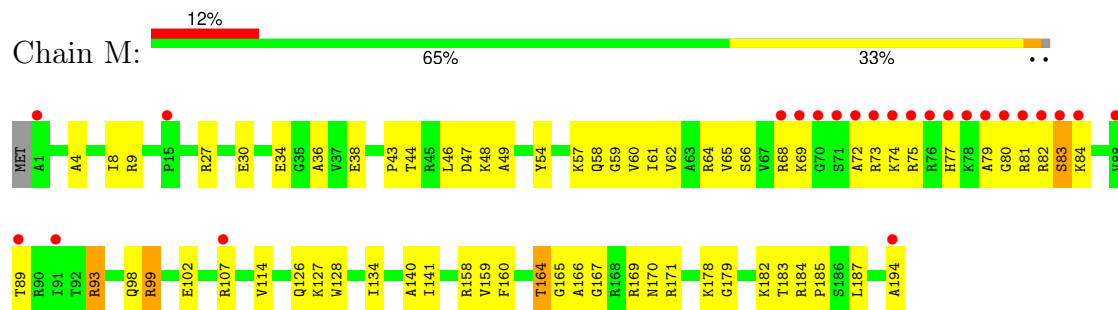
- Molecule 13: 50S ribosomal protein L14P



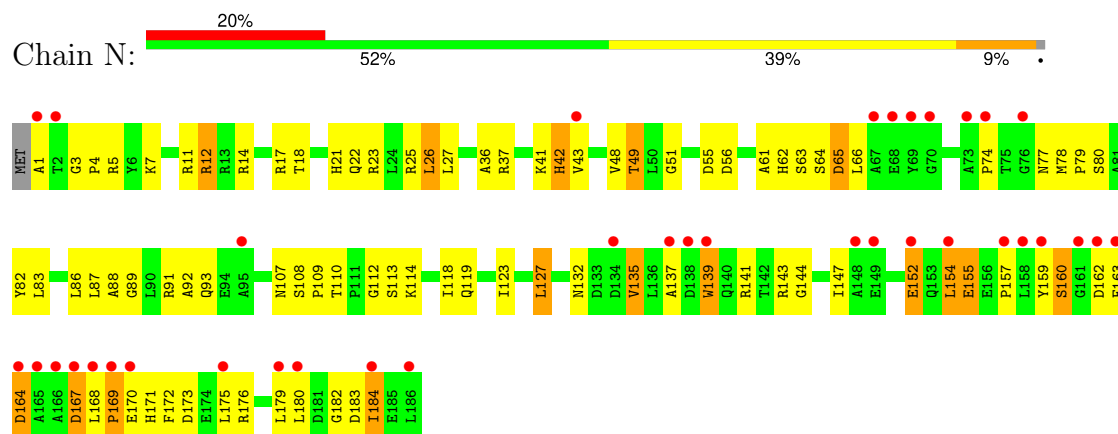
- Molecule 14: 50S ribosomal protein L15P



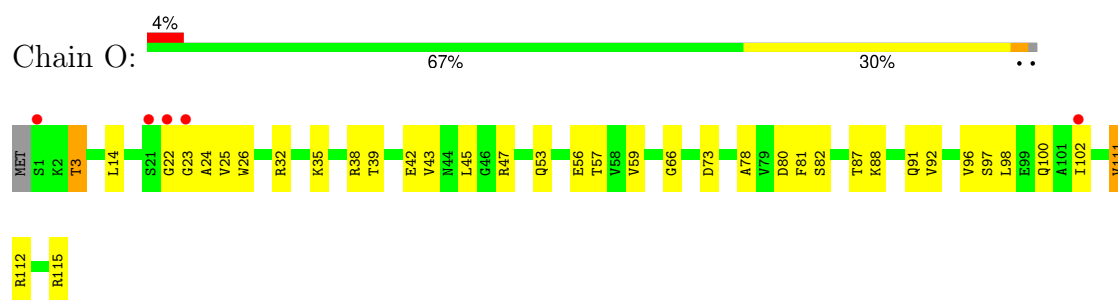
- Molecule 15: 50S Ribosomal Protein L15E



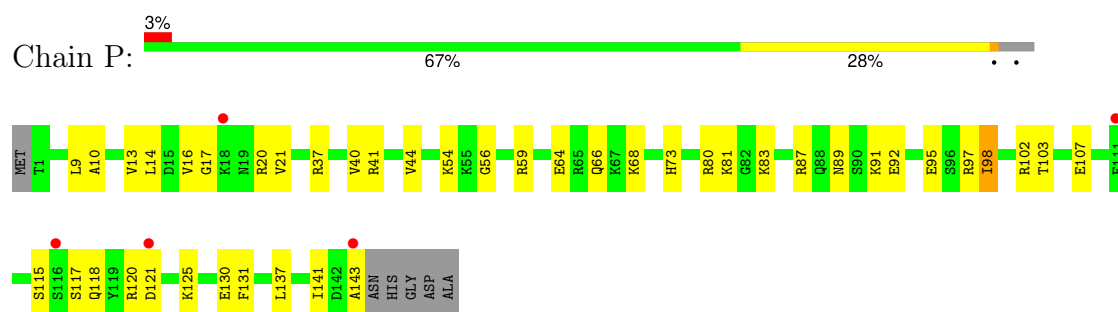
- Molecule 16: 50S ribosomal protein L18P



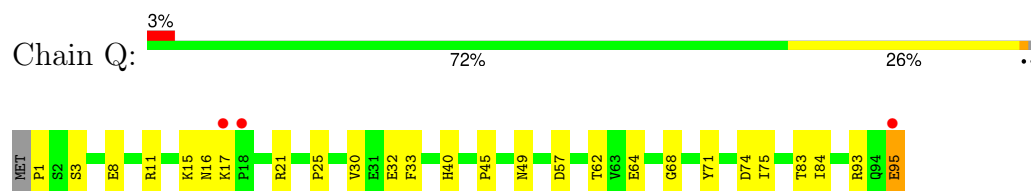
- Molecule 17: 50S ribosomal protein L18e



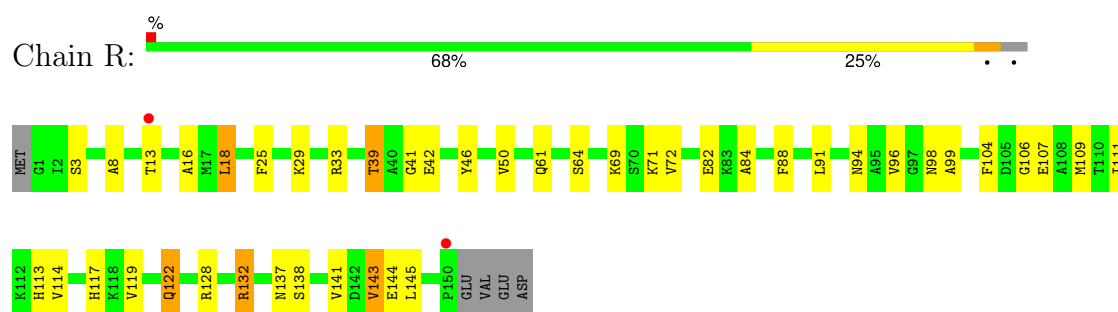
• Molecule 18: 50S ribosomal protein L19E



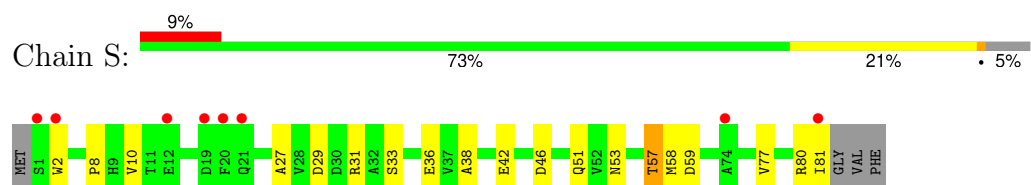
• Molecule 19: 50S ribosomal protein L21e



• Molecule 20: 50S ribosomal protein L22P

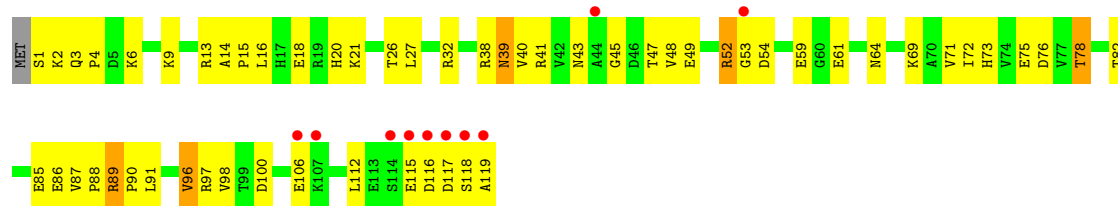


• Molecule 21: 50S ribosomal protein L23P



• Molecule 22: 50S ribosomal protein L24P

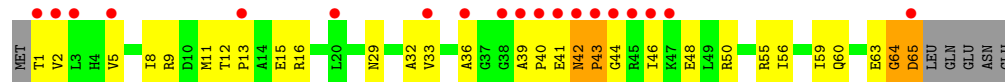




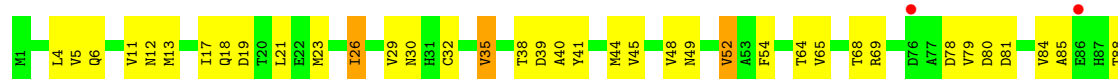
• Molecule 23: 50S ribosomal protein L24E



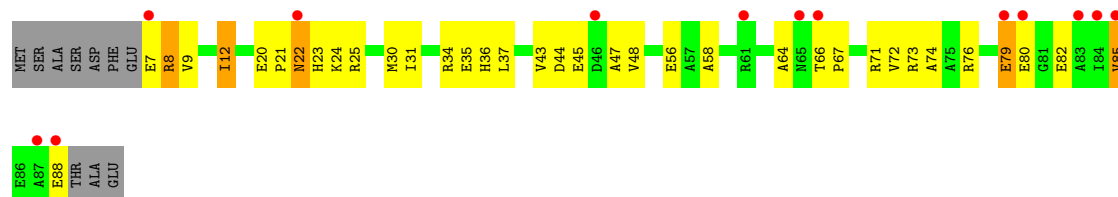
• Molecule 24: 50S ribosomal protein L29P



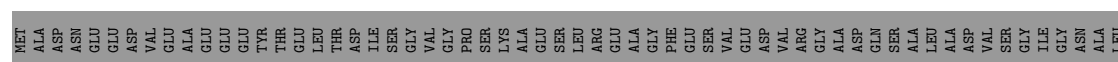
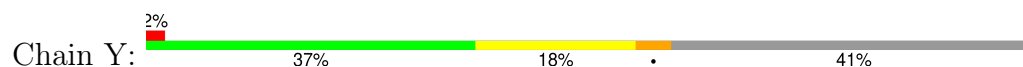
• Molecule 25: 50S ribosomal protein L30P

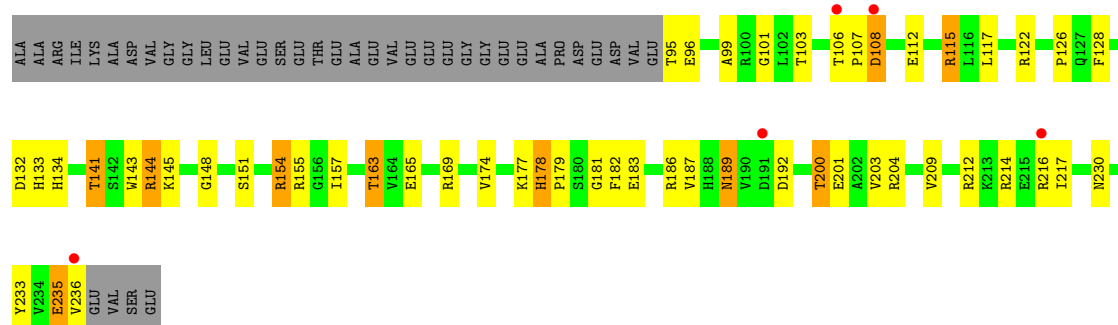


• Molecule 26: 50S ribosomal protein L31e

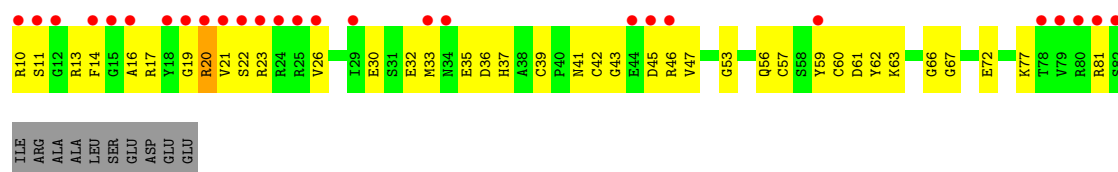


• Molecule 27: 50S ribosomal protein L32E





• Molecule 28: 50S ribosomal protein L37Ae



• Molecule 29: 50S ribosomal protein L37e



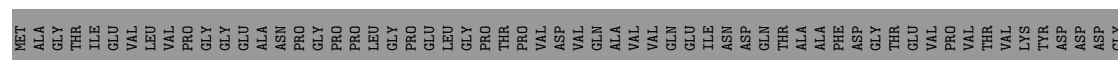
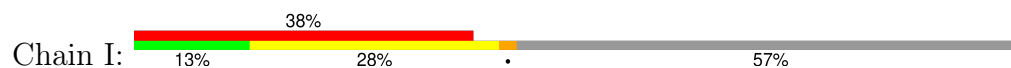
• Molecule 30: 50S ribosomal protein L39e

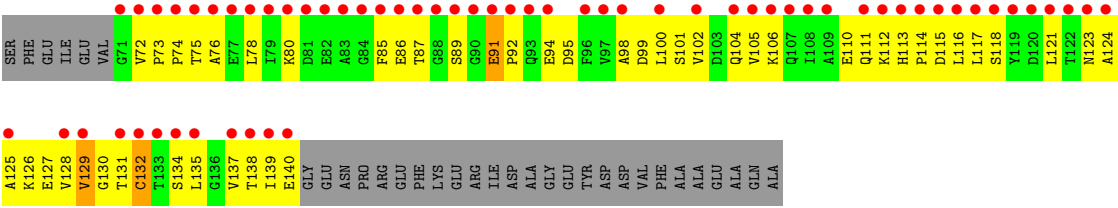


• Molecule 31: 50S ribosomal protein L44E



• Molecule 32: 50S RIBOSOMAL PROTEIN L11P





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.04Å 299.41Å 575.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.21	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-2.20) 88.8 (50.00-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.69 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.246 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99040	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% 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: CD, MG, 1MA, NA, PPU, OMG, UR3, SR, K, OMU, PSU, CL

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	0.38	0/65959	0.62	33/102870 (0.0%)
2	9	0.37	0/2905	0.60	1/4528 (0.0%)
3	4	0.35	0/40	0.68	0/60
4	A	0.40	0/1786	0.95	5/2408 (0.2%)
5	B	0.44	0/2690	1.01	19/3652 (0.5%)
6	C	0.44	0/1884	0.98	6/2551 (0.2%)
7	D	0.34	0/1111	0.85	6/1498 (0.4%)
8	E	0.38	0/1382	0.86	2/1880 (0.1%)
9	F	0.38	0/901	0.83	0/1224
10	G	0.31	0/241	0.76	0/324
11	H	0.37	0/1287	0.95	5/1725 (0.3%)
12	J	0.41	0/1136	0.94	3/1530 (0.2%)
13	K	0.42	0/1001	1.00	2/1347 (0.1%)
14	L	0.38	0/1130	0.99	6/1509 (0.4%)
15	M	0.41	0/1584	0.88	3/2119 (0.1%)
16	N	0.34	0/1474	1.02	9/1999 (0.5%)
17	O	0.41	0/874	0.91	4/1181 (0.3%)
18	P	0.39	0/1147	0.87	1/1528 (0.1%)
19	Q	0.41	0/749	1.03	3/1005 (0.3%)
20	R	0.44	0/1172	0.95	5/1578 (0.3%)
21	S	0.35	0/648	0.86	2/875 (0.2%)
22	T	0.36	0/958	0.95	3/1289 (0.2%)
23	U	0.40	0/417	0.87	1/562 (0.2%)
24	V	0.32	0/502	0.89	3/675 (0.4%)
25	W	0.49	1/1219 (0.1%)	0.95	3/1655 (0.2%)
26	X	0.43	0/664	0.94	3/895 (0.3%)
27	Y	0.44	0/1146	0.98	6/1536 (0.4%)
28	Z	0.34	0/589	0.88	0/787
29	1	0.48	0/438	0.94	1/578 (0.2%)
30	2	0.41	0/401	0.83	0/529
31	3	0.39	0/771	0.86	0/1024
32	I	0.34	0/526	0.89	2/716 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.39	1/98732 (0.0%)	0.72	137/147637 (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	40
2	9	0	1
All	All	1	41

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	W	35	VAL	CA-CB	5.70	1.58	1.54

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	14.37	131.06	109.50
19	Q	17	LYS	N-CA-C	-10.11	96.99	109.83
16	N	163	PHE	N-CA-C	-9.00	102.43	113.41
1	0	1942	A	C5'-C4'-C3'	8.75	129.12	116.00
1	0	1563	G	C4'-C3'-O3'	8.47	122.11	109.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 41 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	191	A	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	458	G	Sidechain
1	0	469	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	59021	0	29812	719	0
2	9	2600	0	1326	55	0
3	4	74	0	51	2	0
4	A	1753	0	1766	120	0
5	B	2625	0	2532	132	0
6	C	1859	0	1816	114	0
7	D	1094	0	1085	105	0
8	E	1357	0	1266	59	0
9	F	890	0	843	53	0
10	G	240	0	231	15	0
11	H	1266	0	1268	72	0
12	J	1120	0	1098	70	0
13	K	992	0	1031	50	0
14	L	1118	0	1076	63	0
15	M	1560	0	1568	68	0
16	N	1445	0	1401	93	0
17	O	865	0	873	39	0
18	P	1136	0	1123	40	0
19	Q	735	0	728	20	0
20	R	1149	0	1122	45	0
21	S	641	0	605	17	0
22	T	950	0	924	54	0
23	U	410	0	364	26	0
24	V	499	0	511	35	0
25	W	1196	0	1137	77	0
26	X	654	0	653	42	0
27	Y	1130	0	1133	56	0
28	Z	578	0	539	33	0
29	1	431	0	426	23	0
30	2	396	0	413	23	0
31	3	755	0	728	22	0
32	I	519	0	500	57	0
33	0	88	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	64	0	0	0	0
35	9	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	9	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	2	0
36	K	1	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	98	0	0	0	0
37	1	2	0	0	0	0
37	3	1	0	0	0	0
37	9	3	0	0	0	0
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5780	0	0	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	1	52	0	0	3	0
39	2	40	0	0	2	0
39	3	66	0	0	4	0
39	4	4	0	0	0	0
39	9	136	0	0	10	0
39	A	124	0	0	12	0
39	B	141	0	0	19	0
39	C	177	0	0	17	0
39	D	46	0	0	10	0
39	E	43	0	0	1	0
39	F	25	0	0	4	0
39	G	16	0	0	3	0
39	H	71	0	0	8	0
39	I	8	0	0	0	0
39	J	58	0	0	3	0
39	K	60	0	0	7	0
39	L	82	0	0	12	0
39	M	125	0	0	6	0
39	N	62	0	0	7	0
39	O	40	0	0	5	0
39	P	60	0	0	4	0
39	Q	49	0	0	3	0
39	R	83	0	0	4	0
39	S	30	0	0	0	0
39	T	36	0	0	4	0
39	U	28	0	0	4	0
39	V	12	0	0	1	0
39	W	68	0	0	4	0
39	X	26	0	0	6	0
39	Y	93	0	0	11	0
39	Z	29	0	0	2	0
All	All	99040	0	59949	2156	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 14.

The worst 5 of 2156 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)
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.29	1.14
1:0:1160:G:H5'	1:0:1161:A:H5'	1.32	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:236:THR:HG22	6:C:239:ALA:H	1.10	1.10
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.34	1.10
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.32	1.08

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
4	A	235/240 (98%)	208 (88%)	25 (11%)	2 (1%)	14	14
5	B	335/338 (99%)	315 (94%)	16 (5%)	4 (1%)	10	8
6	C	244/246 (99%)	225 (92%)	19 (8%)	0	100	100
7	D	134/177 (76%)	107 (80%)	16 (12%)	11 (8%)	0	0
8	E	170/178 (96%)	164 (96%)	6 (4%)	0	100	100
9	F	117/120 (98%)	105 (90%)	8 (7%)	4 (3%)	3	1
10	G	25/348 (7%)	25 (100%)	0	0	100	100
11	H	156/171 (91%)	137 (88%)	15 (10%)	4 (3%)	4	2
12	J	140/145 (97%)	132 (94%)	5 (4%)	3 (2%)	5	3
13	K	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
14	L	141/165 (86%)	119 (84%)	20 (14%)	2 (1%)	9	7
15	M	192/195 (98%)	183 (95%)	8 (4%)	1 (0%)	24	27
16	N	184/187 (98%)	165 (90%)	12 (6%)	7 (4%)	2	1
17	O	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
18	P	141/149 (95%)	136 (96%)	5 (4%)	0	100	100
19	Q	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
22	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	14	14
23	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
24	V	63/71 (89%)	58 (92%)	4 (6%)	1 (2%)	7	6
25	W	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
26	X	80/92 (87%)	72 (90%)	8 (10%)	0	100	100
27	Y	140/241 (58%)	137 (98%)	3 (2%)	0	100	100
28	Z	71/83 (86%)	62 (87%)	6 (8%)	3 (4%)	2	1
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
31	3	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
32	I	68/162 (42%)	56 (82%)	10 (15%)	2 (3%)	3	2
All	All	3705/4431 (84%)	3432 (93%)	228 (6%)	45 (1%)	10	8

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	27	LEU
5	B	139	ASP
11	H	166	SER
11	H	168	ALA
12	J	143	LYS

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	
4	A	179/182 (98%)	166 (93%)	13 (7%)	13	15
5	B	282/283 (100%)	262 (93%)	20 (7%)	13	16
6	C	193/193 (100%)	175 (91%)	18 (9%)	8	9
7	D	117/148 (79%)	112 (96%)	5 (4%)	26	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	E	152/156 (97%)	145 (95%)	7 (5%)	24	32
9	F	93/94 (99%)	91 (98%)	2 (2%)	45	61
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	126 (96%)	6 (4%)	24	33
12	J	118/121 (98%)	112 (95%)	6 (5%)	21	27
13	K	106/106 (100%)	102 (96%)	4 (4%)	29	40
14	L	113/127 (89%)	109 (96%)	4 (4%)	32	43
15	M	158/159 (99%)	154 (98%)	4 (2%)	42	56
16	N	149/150 (99%)	143 (96%)	6 (4%)	28	38
17	O	93/94 (99%)	91 (98%)	2 (2%)	45	61
18	P	113/117 (97%)	111 (98%)	2 (2%)	51	68
19	Q	79/80 (99%)	76 (96%)	3 (4%)	29	40
20	R	117/122 (96%)	113 (97%)	4 (3%)	32	44
21	S	71/74 (96%)	71 (100%)	0	100	100
22	T	105/106 (99%)	101 (96%)	4 (4%)	29	40
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	48	64
25	W	130/130 (100%)	125 (96%)	5 (4%)	29	40
26	X	66/74 (89%)	62 (94%)	4 (6%)	17	20
27	Y	120/196 (61%)	109 (91%)	11 (9%)	8	9
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	45 (98%)	1 (2%)	45	61
30	2	42/46 (91%)	42 (100%)	0	100	100
31	3	79/79 (100%)	78 (99%)	1 (1%)	61	76
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3612 (86%)	2960 (96%)	133 (4%)	26	35

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	W	146	ILE
26	X	85	VAL
27	Y	235	GLU

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Mol	Chain	Res	Type
6	C	240	LEU
6	C	236	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
20	R	113	HIS
23	U	48	ASN
20	R	122	GLN
21	S	75	GLN
25	W	110	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	242 (8%)	35 (1%)
2	9	121/122 (99%)	16 (13%)	2 (1%)
3	4	1/3 (33%)	0	0
All	All	2867/3047 (94%)	258 (8%)	37 (1%)

5 of 258 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G

5 of 37 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	2467	A
2	9	3043	G
1	0	2536	C
1	0	2761	A
1	0	1232	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	OMU	0	2587	1	19,22,23	0.24	0	25,31,34	0.46	0
1	PSU	0	2621	1	18,21,22	1.67	2 (11%)	21,30,33	1.38	3 (14%)
1	1MA	0	628	1	21,25,26	0.69	1 (4%)	30,37,40	0.78	1 (3%)
1	OMG	0	2588	3,1	23,26,27	0.28	0	32,38,41	0.41	0
3	PPU	4	76	3,1	37,40,41	1.03	1 (2%)	47,57,60	0.79	2 (4%)
1	UR3	0	2619	1	19,22,23	0.50	0	26,32,35	0.73	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	2/7/25/26	0/3/3/3
1	OMG	0	2588	3,1	-	0/9/27/28	0/3/3/3
3	PPU	4	76	3,1	-	0/25/43/44	0/4/4/4
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	76	PPU	OC-CM	-5.82	1.26	1.42
1	0	2621	PSU	C2-N1	5.56	1.43	1.36
1	0	2621	PSU	C6-C5	3.48	1.39	1.35
1	0	628	1MA	C6-N6	2.39	1.33	1.28

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.55	120.57	118.17
1	0	2621	PSU	C6-N1-C2	-3.35	119.58	122.69
1	0	2619	UR3	C4-N3-C2	2.94	126.94	124.58
3	4	76	PPU	C2-N1-C6	2.94	119.00	111.83
1	0	628	1MA	N1-C2-N3	2.78	129.30	126.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	628	1MA	C2'-C1'-N9-C8
1	0	628	1MA	C2'-C1'-N9-C4

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
3	4	76	PPU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 312 ligands modelled in this entry, 312 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	2749/2922 (94%)	-0.19	81 (2%) 53 50	26, 46, 90, 148	0
2	9	122/122 (100%)	0.41	8 (6%) 24 21	39, 62, 87, 147	0
3	4	2/3 (66%)	0.14	0 100 100	52, 52, 52, 62	0
4	A	237/240 (98%)	0.69	22 (9%) 14 12	30, 52, 82, 104	0
5	B	337/338 (99%)	0.54	10 (2%) 52 49	31, 50, 72, 85	0
6	C	246/246 (100%)	0.50	9 (3%) 45 42	28, 47, 68, 81	0
7	D	140/177 (79%)	2.19	66 (47%) 0 0	56, 90, 119, 127	0
8	E	172/178 (96%)	1.01	20 (11%) 9 7	42, 60, 78, 83	0
9	F	119/120 (99%)	1.45	34 (28%) 1 1	47, 71, 99, 108	0
10	G	29/348 (8%)	1.91	11 (37%) 1 0	68, 89, 97, 98	0
11	H	160/171 (93%)	1.02	18 (11%) 10 8	44, 60, 92, 99	0
12	J	142/145 (97%)	0.49	5 (3%) 47 44	36, 47, 66, 86	0
13	K	132/132 (100%)	0.26	2 (1%) 72 69	34, 45, 66, 69	0
14	L	145/165 (87%)	1.12	28 (19%) 3 2	30, 64, 110, 119	0
15	M	194/195 (99%)	0.64	24 (12%) 8 6	35, 46, 67, 79	0
16	N	186/187 (99%)	1.29	37 (19%) 3 2	44, 62, 104, 112	0
17	O	115/116 (99%)	0.74	5 (4%) 40 36	41, 53, 66, 74	0
18	P	143/149 (95%)	0.66	5 (3%) 47 44	40, 51, 65, 78	0
19	Q	95/96 (98%)	0.48	3 (3%) 50 47	41, 47, 63, 74	0
20	R	150/155 (96%)	0.16	2 (1%) 75 73	31, 44, 62, 70	0
21	S	81/85 (95%)	0.89	8 (9%) 13 10	43, 62, 82, 95	0
22	T	119/120 (99%)	0.94	10 (8%) 17 14	43, 56, 79, 107	0
23	U	53/66 (80%)	0.69	2 (3%) 44 41	42, 51, 67, 75	0
24	V	65/71 (91%)	1.74	19 (29%) 1 1	54, 78, 111, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	0.49	3 (1%) 66 63	36, 48, 69, 78	0
26	X	82/92 (89%)	0.94	13 (15%) 5 3	41, 53, 79, 97	0
27	Y	142/241 (58%)	0.33	5 (3%) 47 44	31, 43, 62, 82	0
28	Z	73/83 (87%)	1.70	27 (36%) 1 0	49, 73, 86, 92	0
29	1	56/57 (98%)	-0.11	0 100 100	30, 35, 42, 50	0
30	2	46/50 (92%)	1.02	8 (17%) 4 3	38, 58, 73, 83	0
31	3	92/92 (100%)	0.72	3 (3%) 49 46	37, 55, 68, 79	0
32	I	70/162 (43%)	3.46	61 (87%) 0 0	107, 120, 137, 139	0
All	All	6648/7478 (88%)	0.41	549 (8%) 17 15	26, 51, 94, 148	0

The worst 5 of 549 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	V	1	THR	9.7
7	D	10	PHE	9.1
32	I	133	THR	8.3
15	M	70	GLY	8.0
16	N	166	ALA	7.6

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

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
3	PPU	4	76	37/38	0.93	0.12	48,54,66,71	0
1	PSU	0	2621	20/21	0.96	0.07	37,40,50,51	0
1	UR3	0	2619	21/22	0.96	0.08	45,45,49,50	0
1	OMG	0	2588	24/25	0.97	0.07	30,35,40,41	0
1	1MA	0	628	23/24	0.98	0.06	29,33,36,37	0
1	OMU	0	2587	21/22	0.98	0.06	33,36,38,39	0

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
37	SR	0	9601	1/1	0.57	0.28	200,200,200,200	0
37	SR	0	9547	1/1	0.60	0.34	200,200,200,200	0
33	MG	0	8050	1/1	0.64	0.22	93,93,93,93	0
35	NA	0	9122	1/1	0.66	0.46	96,96,96,96	0
35	NA	0	9171	1/1	0.66	0.27	61,61,61,61	0
35	NA	0	9184	1/1	0.68	0.37	102,102,102,102	0
33	MG	0	8014	1/1	0.69	0.30	73,73,73,73	0
33	MG	0	8045	1/1	0.71	0.32	84,84,84,84	0
33	MG	0	8082	1/1	0.72	0.50	107,107,107,107	0
33	MG	0	8065	1/1	0.73	0.29	93,93,93,93	0
33	MG	B	8055	1/1	0.74	0.15	108,108,108,108	0
34	K	0	9001	1/1	0.75	0.43	116,116,116,116	0
35	NA	0	9129	1/1	0.76	0.38	85,85,85,85	0
33	MG	0	8092	1/1	0.77	0.35	81,81,81,81	0
35	NA	0	9164	1/1	0.77	0.29	59,59,59,59	0
35	NA	0	9173	1/1	0.78	0.20	70,70,70,70	0
33	MG	0	8040	1/1	0.78	0.43	100,100,100,100	0
37	SR	0	9501	1/1	0.79	0.20	200,200,200,200	0
33	MG	0	8047	1/1	0.79	0.38	91,91,91,91	0
35	NA	0	9152	1/1	0.79	0.50	78,78,78,78	0
33	MG	0	8090	1/1	0.80	0.26	80,80,80,80	0
35	NA	0	9170	1/1	0.82	0.42	94,94,94,94	0
33	MG	0	8024	1/1	0.83	0.49	77,77,77,77	0
33	MG	0	8052	1/1	0.83	0.30	68,68,68,68	0
35	NA	0	9168	1/1	0.83	0.24	57,57,57,57	0
35	NA	0	9179	1/1	0.83	0.34	100,100,100,100	0
37	SR	0	9590	1/1	0.84	0.18	178,178,178,178	0
33	MG	0	8059	1/1	0.85	0.14	78,78,78,78	0
33	MG	0	8061	1/1	0.85	0.16	95,95,95,95	0
37	SR	0	9484	1/1	0.86	0.16	147,147,147,147	0
37	SR	0	9500	1/1	0.86	0.46	200,200,200,200	0
35	NA	0	9172	1/1	0.86	0.26	70,70,70,70	0
33	MG	0	8085	1/1	0.86	0.23	91,91,91,91	0
35	NA	0	9185	1/1	0.86	0.24	46,46,46,46	0
35	NA	D	9151	1/1	0.86	0.18	63,63,63,63	0
37	SR	0	9537	1/1	0.87	0.18	154,154,154,154	0
33	MG	0	8072	1/1	0.88	0.20	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	0	9529	1/1	0.88	0.16	138,138,138,138	0
35	NA	0	9120	1/1	0.88	0.18	64,64,64,64	0
37	SR	0	9452	1/1	0.88	0.14	114,114,114,114	0
35	NA	0	9182	1/1	0.88	0.11	78,78,78,78	0
35	NA	0	9140	1/1	0.88	0.16	60,60,60,60	0
34	K	0	9002	1/1	0.89	0.21	89,89,89,89	0
33	MG	0	8101	1/1	0.89	0.13	59,59,59,59	0
33	MG	0	8084	1/1	0.89	0.49	74,74,74,74	0
35	NA	0	9166	1/1	0.89	0.19	67,67,67,67	0
35	NA	0	9126	1/1	0.89	0.16	59,59,59,59	0
35	NA	0	9127	1/1	0.89	0.14	57,57,57,57	0
33	MG	0	8094	1/1	0.89	0.17	67,67,67,67	0
35	NA	S	9112	1/1	0.89	0.11	59,59,59,59	0
36	CL	0	9316	1/1	0.89	0.23	69,69,69,69	0
37	SR	B	9521	1/1	0.89	0.44	199,199,199,199	0
33	MG	0	8076	1/1	0.90	0.09	61,61,61,61	0
33	MG	0	8022	1/1	0.90	0.35	74,74,74,74	0
33	MG	0	8107	1/1	0.90	0.24	67,67,67,67	0
33	MG	9	8095	1/1	0.90	0.19	46,46,46,46	0
35	NA	0	9157	1/1	0.90	0.18	47,47,47,47	0
35	NA	0	9163	1/1	0.90	0.14	66,66,66,66	0
35	NA	0	9174	1/1	0.90	0.20	65,65,65,65	0
33	MG	0	8057	1/1	0.90	0.18	85,85,85,85	0
33	MG	0	8060	1/1	0.91	0.20	71,71,71,71	0
35	NA	0	9165	1/1	0.91	0.25	47,47,47,47	0
35	NA	0	9113	1/1	0.91	0.10	65,65,65,65	0
35	NA	0	9181	1/1	0.91	0.10	50,50,50,50	0
35	NA	0	9167	1/1	0.91	0.15	56,56,56,56	0
33	MG	0	8097	1/1	0.91	0.12	62,62,62,62	0
35	NA	0	9169	1/1	0.91	0.31	104,104,104,104	0
33	MG	0	8063	1/1	0.91	0.10	70,70,70,70	0
35	NA	0	9124	1/1	0.91	0.14	47,47,47,47	0
37	SR	0	9626	1/1	0.91	0.43	128,128,128,128	0
33	MG	0	8104	1/1	0.91	0.16	76,76,76,76	0
33	MG	0	8103	1/1	0.92	0.18	62,62,62,62	0
35	NA	9	9183	1/1	0.92	0.18	66,66,66,66	0
35	NA	0	9175	1/1	0.92	0.19	52,52,52,52	0
35	NA	0	9154	1/1	0.92	0.19	59,59,59,59	0
37	SR	0	9539	1/1	0.92	0.46	162,162,162,162	0
33	MG	T	8073	1/1	0.92	0.15	46,46,46,46	0
35	NA	0	9162	1/1	0.92	0.14	58,58,58,58	0
37	SR	0	9459	1/1	0.92	0.11	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	0	9468	1/1	0.92	0.12	113,113,113,113	0
33	MG	0	8093	1/1	0.92	0.15	42,42,42,42	0
33	MG	0	8116	1/1	0.93	0.09	62,62,62,62	0
35	NA	0	9125	1/1	0.93	0.27	115,115,115,115	0
33	MG	0	8118	1/1	0.93	0.21	76,76,76,76	0
37	SR	0	9474	1/1	0.93	0.07	112,112,112,112	0
33	MG	0	8039	1/1	0.93	0.09	65,65,65,65	0
37	SR	0	9490	1/1	0.93	0.21	109,109,109,109	0
35	NA	0	9116	1/1	0.93	0.17	58,58,58,58	0
33	MG	0	8001	1/1	0.93	0.16	20,20,20,20	0
37	SR	0	9504	1/1	0.93	0.10	105,105,105,105	0
35	NA	B	9161	1/1	0.93	0.35	62,62,62,62	0
35	NA	C	9104	1/1	0.93	0.10	34,34,34,34	0
35	NA	0	9141	1/1	0.93	0.11	62,62,62,62	0
35	NA	J	9146	1/1	0.93	0.07	55,55,55,55	0
35	NA	R	9186	1/1	0.93	0.15	69,69,69,69	0
33	MG	0	8108	1/1	0.93	0.15	74,74,74,74	0
35	NA	0	9177	1/1	0.93	0.17	63,63,63,63	0
36	CL	A	9309	1/1	0.93	0.30	68,68,68,68	0
33	MG	0	8046	1/1	0.94	0.07	40,40,40,40	0
37	SR	0	9475	1/1	0.94	0.09	77,77,77,77	0
35	NA	0	9132	1/1	0.94	0.16	51,51,51,51	0
35	NA	0	9118	1/1	0.94	0.24	60,60,60,60	0
33	MG	0	8042	1/1	0.94	0.08	60,60,60,60	0
35	NA	0	9149	1/1	0.94	0.15	42,42,42,42	0
36	CL	0	9315	1/1	0.94	0.11	58,58,58,58	0
33	MG	0	8099	1/1	0.94	0.13	59,59,59,59	0
35	NA	0	9102	1/1	0.94	0.36	57,57,57,57	0
36	CL	B	9319	1/1	0.94	0.24	52,52,52,52	0
36	CL	L	9310	1/1	0.94	0.12	54,54,54,54	0
37	SR	0	9405	1/1	0.94	0.11	60,60,60,60	0
35	NA	0	9107	1/1	0.94	0.12	61,61,61,61	0
35	NA	0	9111	1/1	0.94	0.11	57,57,57,57	0
33	MG	0	8041	1/1	0.94	0.12	50,50,50,50	0
37	SR	0	9482	1/1	0.95	0.40	102,102,102,102	0
35	NA	0	9158	1/1	0.95	0.12	63,63,63,63	0
33	MG	A	8066	1/1	0.95	0.17	53,53,53,53	0
33	MG	0	8089	1/1	0.95	0.09	54,54,54,54	0
33	MG	0	8080	1/1	0.95	0.12	47,47,47,47	0
35	NA	0	9134	1/1	0.95	0.16	51,51,51,51	0
37	SR	0	9505	1/1	0.95	0.30	85,85,85,85	0
35	NA	0	9139	1/1	0.95	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8114	1/1	0.95	0.13	63,63,63,63	0
33	MG	0	8067	1/1	0.95	0.10	42,42,42,42	0
35	NA	0	9143	1/1	0.95	0.06	43,43,43,43	0
37	SR	0	9581	1/1	0.95	0.11	121,121,121,121	0
33	MG	0	8021	1/1	0.95	0.09	55,55,55,55	0
33	MG	0	8013	1/1	0.95	0.22	22,22,22,22	0
35	NA	0	9108	1/1	0.95	0.07	35,35,35,35	0
37	SR	9	9588	1/1	0.95	0.07	114,114,114,114	0
35	NA	0	9110	1/1	0.95	0.12	46,46,46,46	0
37	SR	H	9486	1/1	0.95	0.35	109,109,109,109	0
33	MG	0	8058	1/1	0.96	0.11	45,45,45,45	0
35	NA	0	9123	1/1	0.96	0.10	41,41,41,41	0
33	MG	0	8088	1/1	0.96	0.05	45,45,45,45	0
35	NA	0	9150	1/1	0.96	0.11	38,38,38,38	0
33	MG	0	8043	1/1	0.96	0.07	49,49,49,49	0
35	NA	M	9147	1/1	0.96	0.07	43,43,43,43	0
33	MG	0	8098	1/1	0.96	0.09	39,39,39,39	0
33	MG	0	8113	1/1	0.96	0.10	50,50,50,50	0
35	NA	0	9114	1/1	0.96	0.10	46,46,46,46	0
37	SR	0	9509	1/1	0.96	0.06	81,81,81,81	0
37	SR	0	9515	1/1	0.96	0.31	87,87,87,87	0
35	NA	0	9159	1/1	0.96	0.10	46,46,46,46	0
37	SR	0	9534	1/1	0.96	0.29	100,100,100,100	0
35	NA	0	9160	1/1	0.96	0.07	39,39,39,39	0
35	NA	0	9178	1/1	0.96	0.20	51,51,51,51	0
35	NA	0	9130	1/1	0.96	0.10	49,49,49,49	0
36	CL	N	9307	1/1	0.96	0.12	52,52,52,52	0
35	NA	0	9115	1/1	0.96	0.10	39,39,39,39	0
37	SR	0	9447	1/1	0.96	0.06	67,67,67,67	0
33	MG	0	8054	1/1	0.96	0.06	58,58,58,58	0
33	MG	0	8115	1/1	0.96	0.05	56,56,56,56	0
37	SR	0	9465	1/1	0.96	0.06	100,100,100,100	0
37	SR	F	9595	1/1	0.96	0.10	105,105,105,105	0
33	MG	0	8044	1/1	0.96	0.06	39,39,39,39	0
37	SR	0	9469	1/1	0.97	0.07	79,79,79,79	0
33	MG	0	8051	1/1	0.97	0.08	26,26,26,26	0
35	NA	Q	9148	1/1	0.97	0.04	44,44,44,44	0
37	SR	0	9477	1/1	0.97	0.06	84,84,84,84	0
35	NA	R	9138	1/1	0.97	0.06	56,56,56,56	0
37	SR	0	9483	1/1	0.97	0.05	68,68,68,68	0
33	MG	0	8102	1/1	0.97	0.06	56,56,56,56	0
33	MG	0	8096	1/1	0.97	0.06	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	0	9495	1/1	0.97	0.06	88,88,88,88	0
36	CL	0	9303	1/1	0.97	0.07	46,46,46,46	0
36	CL	0	9313	1/1	0.97	0.06	51,51,51,51	0
33	MG	0	8091	1/1	0.97	0.13	45,45,45,45	0
35	NA	0	9135	1/1	0.97	0.08	50,50,50,50	0
36	CL	0	9322	1/1	0.97	0.34	53,53,53,53	0
35	NA	0	9105	1/1	0.97	0.06	43,43,43,43	0
37	SR	0	9517	1/1	0.97	0.07	91,91,91,91	0
37	SR	0	9522	1/1	0.97	0.06	104,104,104,104	0
35	NA	0	9106	1/1	0.97	0.15	37,37,37,37	0
37	SR	0	9530	1/1	0.97	0.06	84,84,84,84	0
36	CL	J	9301	1/1	0.97	0.18	53,53,53,53	0
36	CL	J	9321	1/1	0.97	0.09	53,53,53,53	0
33	MG	0	8117	1/1	0.97	0.05	43,43,43,43	0
33	MG	0	8106	1/1	0.97	0.05	43,43,43,43	0
37	SR	0	9560	1/1	0.97	0.08	97,97,97,97	0
37	SR	0	9570	1/1	0.97	0.15	98,98,98,98	0
33	MG	0	8083	1/1	0.97	0.05	54,54,54,54	0
37	SR	0	9433	1/1	0.97	0.07	76,76,76,76	0
33	MG	0	8025	1/1	0.97	0.20	25,25,25,25	0
33	MG	0	8112	1/1	0.97	0.06	43,43,43,43	0
37	SR	9	9503	1/1	0.97	0.06	114,114,114,114	0
35	NA	0	9128	1/1	0.97	0.10	45,45,45,45	0
37	SR	A	9437	1/1	0.97	0.05	67,67,67,67	0
35	NA	0	9155	1/1	0.97	0.19	55,55,55,55	0
37	SR	0	9467	1/1	0.97	0.06	67,67,67,67	0
35	NA	0	9156	1/1	0.97	0.11	53,53,53,53	0
35	NA	0	9131	1/1	0.98	0.06	48,48,48,48	0
37	SR	0	9480	1/1	0.98	0.05	87,87,87,87	0
33	MG	0	8027	1/1	0.98	0.10	39,39,39,39	0
36	CL	0	9317	1/1	0.98	0.08	50,50,50,50	0
33	MG	0	8028	1/1	0.98	0.04	37,37,37,37	0
37	SR	0	9488	1/1	0.98	0.05	76,76,76,76	0
37	SR	0	9489	1/1	0.98	0.09	85,85,85,85	0
33	MG	0	8070	1/1	0.98	0.06	26,26,26,26	0
33	MG	0	8056	1/1	0.98	0.05	46,46,46,46	0
33	MG	K	8069	1/1	0.98	0.09	29,29,29,29	0
36	CL	J	9302	1/1	0.98	0.05	48,48,48,48	0
33	MG	0	8075	1/1	0.98	0.04	36,36,36,36	0
33	MG	Y	8109	1/1	0.98	0.09	41,41,41,41	0
37	SR	0	9506	1/1	0.98	0.15	66,66,66,66	0
37	SR	0	9508	1/1	0.98	0.09	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	CL	M	9318	1/1	0.98	0.05	41,41,41,41	0
33	MG	0	8031	1/1	0.98	0.05	50,50,50,50	0
36	CL	R	9306	1/1	0.98	0.05	44,44,44,44	0
36	CL	Y	9320	1/1	0.98	0.10	43,43,43,43	0
36	CL	3	9304	1/1	0.98	0.05	55,55,55,55	0
33	MG	0	8110	1/1	0.98	0.14	36,36,36,36	0
37	SR	0	9532	1/1	0.98	0.10	103,103,103,103	0
37	SR	0	9427	1/1	0.98	0.04	52,52,52,52	0
37	SR	0	9429	1/1	0.98	0.04	60,60,60,60	0
37	SR	0	9431	1/1	0.98	0.04	55,55,55,55	0
37	SR	0	9545	1/1	0.98	0.09	79,79,79,79	0
35	NA	0	9101	1/1	0.98	0.07	47,47,47,47	0
37	SR	0	9446	1/1	0.98	0.04	83,83,83,83	0
37	SR	0	9566	1/1	0.98	0.11	77,77,77,77	0
37	SR	0	9568	1/1	0.98	0.04	75,75,75,75	0
33	MG	0	8079	1/1	0.98	0.03	34,34,34,34	0
35	NA	R	9137	1/1	0.98	0.04	36,36,36,36	0
37	SR	0	9454	1/1	0.98	0.08	74,74,74,74	0
37	SR	0	9455	1/1	0.98	0.05	67,67,67,67	0
33	MG	0	8036	1/1	0.98	0.04	60,60,60,60	0
37	SR	9	9481	1/1	0.98	0.08	80,80,80,80	0
33	MG	0	8037	1/1	0.98	0.09	39,39,39,39	0
33	MG	0	8015	1/1	0.98	0.03	34,34,34,34	0
33	MG	0	8019	1/1	0.98	0.05	58,58,58,58	0
37	SR	A	9497	1/1	0.98	0.04	91,91,91,91	0
36	CL	0	9305	1/1	0.98	0.07	54,54,54,54	0
36	CL	0	9311	1/1	0.98	0.07	57,57,57,57	0
33	MG	0	8012	1/1	0.98	0.13	41,41,41,41	0
37	SR	S	9470	1/1	0.98	0.04	100,100,100,100	0
38	CD	O	9205	1/1	0.98	0.06	75,75,75,75	0
37	SR	0	9466	1/1	0.99	0.10	84,84,84,84	0
33	MG	0	8020	1/1	0.99	0.03	37,37,37,37	0
36	CL	O	9308	1/1	0.99	0.10	60,60,60,60	0
33	MG	0	8029	1/1	0.99	0.08	33,33,33,33	0
37	SR	0	9473	1/1	0.99	0.07	69,69,69,69	0
33	MG	0	8030	1/1	0.99	0.03	39,39,39,39	0
36	CL	0	9314	1/1	0.99	0.14	45,45,45,45	0
33	MG	0	8002	1/1	0.99	0.03	28,28,28,28	0
37	SR	0	9478	1/1	0.99	0.03	70,70,70,70	0
37	SR	0	9406	1/1	0.99	0.06	38,38,38,38	0
37	SR	0	9407	1/1	0.99	0.02	43,43,43,43	0
37	SR	0	9410	1/1	0.99	0.02	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	0	9411	1/1	0.99	0.02	40,40,40,40	0
37	SR	0	9412	1/1	0.99	0.02	42,42,42,42	0
37	SR	0	9413	1/1	0.99	0.03	44,44,44,44	0
37	SR	0	9414	1/1	0.99	0.03	52,52,52,52	0
37	SR	0	9416	1/1	0.99	0.03	43,43,43,43	0
37	SR	0	9498	1/1	0.99	0.07	59,59,59,59	0
37	SR	0	9417	1/1	0.99	0.03	59,59,59,59	0
37	SR	0	9420	1/1	0.99	0.03	56,56,56,56	0
37	SR	0	9421	1/1	0.99	0.03	64,64,64,64	0
37	SR	0	9422	1/1	0.99	0.04	54,54,54,54	0
37	SR	0	9423	1/1	0.99	0.04	54,54,54,54	0
37	SR	0	9425	1/1	0.99	0.04	55,55,55,55	0
37	SR	0	9426	1/1	0.99	0.04	67,67,67,67	0
33	MG	0	8032	1/1	0.99	0.07	43,43,43,43	0
35	NA	0	9117	1/1	0.99	0.12	39,39,39,39	0
33	MG	0	8003	1/1	0.99	0.03	32,32,32,32	0
37	SR	0	9432	1/1	0.99	0.06	62,62,62,62	0
33	MG	0	8004	1/1	0.99	0.03	30,30,30,30	0
37	SR	0	9434	1/1	0.99	0.03	55,55,55,55	0
37	SR	0	9435	1/1	0.99	0.04	65,65,65,65	0
37	SR	0	9438	1/1	0.99	0.05	63,63,63,63	0
37	SR	0	9440	1/1	0.99	0.06	61,61,61,61	0
37	SR	0	9441	1/1	0.99	0.06	60,60,60,60	0
37	SR	0	9442	1/1	0.99	0.05	59,59,59,59	0
37	SR	0	9443	1/1	0.99	0.04	57,57,57,57	0
37	SR	0	9444	1/1	0.99	0.07	50,50,50,50	0
37	SR	0	9445	1/1	0.99	0.05	56,56,56,56	0
35	NA	0	9136	1/1	0.99	0.05	34,34,34,34	0
33	MG	0	8038	1/1	0.99	0.10	20,20,20,20	0
37	SR	0	9585	1/1	0.99	0.06	83,83,83,83	0
37	SR	0	9449	1/1	0.99	0.04	59,59,59,59	0
37	SR	0	9451	1/1	0.99	0.04	62,62,62,62	0
33	MG	0	8068	1/1	0.99	0.10	46,46,46,46	0
37	SR	0	9629	1/1	0.99	0.05	65,65,65,65	0
37	SR	0	9453	1/1	0.99	0.06	69,69,69,69	0
33	MG	0	8008	1/1	0.99	0.10	17,17,17,17	0
36	CL	K	9312	1/1	0.99	0.09	46,46,46,46	0
37	SR	A	9436	1/1	0.99	0.10	61,61,61,61	0
37	SR	0	9456	1/1	0.99	0.07	69,69,69,69	0
37	SR	0	9457	1/1	0.99	0.04	47,47,47,47	0
37	SR	B	9458	1/1	0.99	0.06	68,68,68,68	0
33	MG	0	8026	1/1	0.99	0.05	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	0	9461	1/1	0.99	0.09	76,76,76,76	0
37	SR	0	9462	1/1	0.99	0.04	64,64,64,64	0
37	SR	R	9418	1/1	0.99	0.03	54,54,54,54	0
37	SR	0	9464	1/1	0.99	0.08	74,74,74,74	0
37	SR	1	9460	1/1	0.99	0.05	52,52,52,52	0
37	SR	3	9439	1/1	0.99	0.06	63,63,63,63	0
33	MG	0	8009	1/1	0.99	0.02	28,28,28,28	0
38	CD	Z	9203	1/1	0.99	0.04	78,78,78,78	0
38	CD	1	9202	1/1	0.99	0.09	51,51,51,51	0
38	CD	3	9204	1/1	0.99	0.06	60,60,60,60	0
37	SR	0	9428	1/1	1.00	0.06	49,49,49,49	0
37	SR	0	9448	1/1	1.00	0.06	60,60,60,60	0
37	SR	L	9409	1/1	1.00	0.01	40,40,40,40	0
37	SR	0	9415	1/1	1.00	0.02	50,50,50,50	0
37	SR	0	9450	1/1	1.00	0.04	62,62,62,62	0
37	SR	1	9419	1/1	1.00	0.02	40,40,40,40	0
37	SR	0	9430	1/1	1.00	0.01	44,44,44,44	0
33	MG	0	8074	1/1	1.00	0.10	23,23,23,23	0
37	SR	0	9424	1/1	1.00	0.02	45,45,45,45	0
38	CD	U	9201	1/1	1.00	0.02	48,48,48,48	0
33	MG	0	8017	1/1	1.00	0.06	28,28,28,28	0
37	SR	0	9408	1/1	1.00	0.03	39,39,39,39	0
33	MG	0	8005	1/1	1.00	0.03	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.