



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:02 PM GMT

PDB ID : 1VQO
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : trunk26765
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

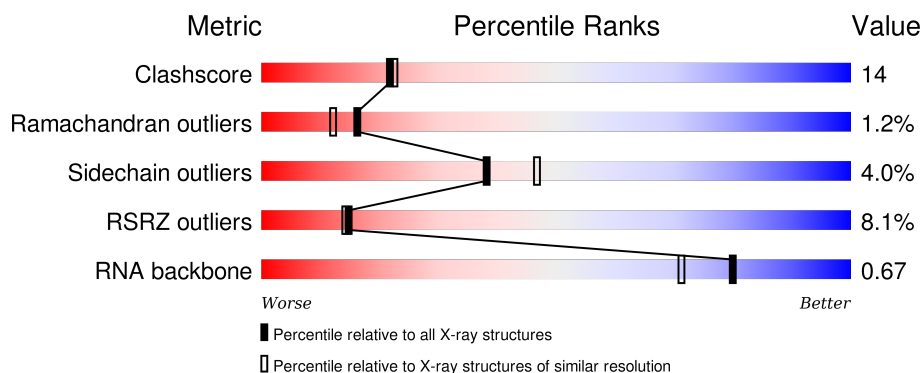
1 Overall quality at a glance

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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)
RNA backbone	2183	1062 (2.80-1.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>3%</div> <div>65%</div> <div>24%</div> <div>6%</div> </div>
2	9	122	<div> <div>4%</div> <div>60%</div> <div>30%</div> <div>9%</div> </div>
3	4	3	<div> <div>33%</div> <div>67%</div> </div>
4	A	240	<div> <div>8%</div> <div>58%</div> <div>38%</div> </div>
5	B	338	<div> <div>2%</div> <div>61%</div> <div>35%</div> </div>

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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	8001	-	-	-	X
33	MG	0	8002	-	-	-	X
33	MG	0	8008	-	-	-	X
33	MG	0	8012	-	-	-	X
33	MG	0	8013	-	-	-	X
33	MG	0	8014	-	-	-	X
33	MG	0	8017	-	-	-	X
33	MG	0	8021	-	-	-	X
33	MG	0	8027	-	-	-	X
33	MG	0	8038	-	-	-	X
33	MG	0	8056	-	-	-	X
33	MG	0	8057	-	-	-	X
33	MG	0	8060	-	-	-	X
33	MG	0	8080	-	-	-	X
33	MG	0	8097	-	-	-	X
33	MG	A	8066	-	-	-	X
34	K	0	9001	-	-	-	X
35	NA	0	9120	-	-	-	X
35	NA	0	9125	-	-	-	X
35	NA	0	9132	-	-	-	X
35	NA	0	9140	-	-	-	X
35	NA	0	9156	-	-	-	X
35	NA	0	9164	-	-	-	X
35	NA	0	9165	-	-	-	X
35	NA	0	9171	-	-	-	X
35	NA	0	9172	-	-	-	X
35	NA	0	9173	-	-	-	X
35	NA	0	9174	-	-	-	X
35	NA	0	9177	-	-	-	X
35	NA	0	9178	-	-	-	X
35	NA	0	9185	-	-	-	X
35	NA	B	9161	-	-	-	X
35	NA	R	9186	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	SR	0	9406	-	-	-	X
37	SR	0	9482	-	-	-	X
37	SR	B	9521	-	-	-	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 (three-letter code: MG) (formula: Mg).

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

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	9	Total Cl 9 9	0	0
36	J	3	Total Cl 3 3	0	0
36	K	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	A	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
36	Y	1	Total Cl 1 1	0	0
36	L	1	Total Cl 1 1	0	0

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

- Molecule 37 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

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

- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	U	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		

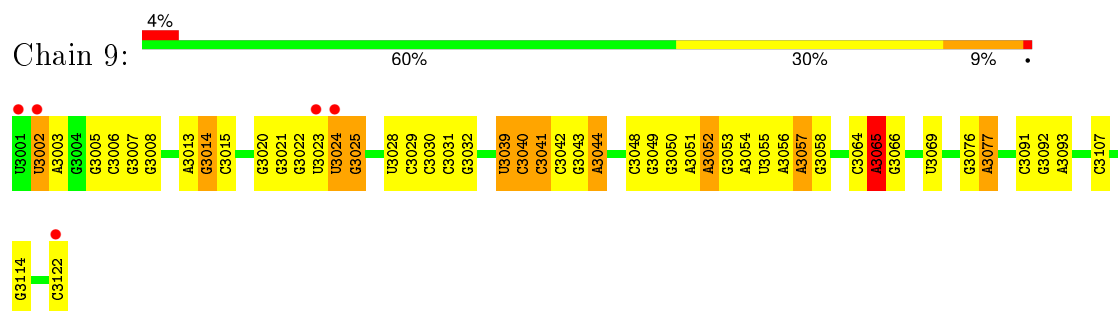
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	Q	49	Total 49	O 49	0	0
39	R	83	Total 83	O 83	0	0
39	S	30	Total 30	O 30	0	0
39	T	36	Total 36	O 36	0	0
39	U	28	Total 28	O 28	0	0
39	V	12	Total 12	O 12	0	0
39	W	68	Total 68	O 68	0	0
39	X	26	Total 26	O 26	0	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

G2867	A2768	U2652	U2535	C2443	C2329	C	G	A2054	C1946	U1788	A1685	G1552	A1372	A1242
G2876	C2769	U2661	C2536	C2443	U2330	C	U	U2064	G1947	G1789	C1686	G1555	U1243	U1244
U2878	G2770	G2662	A2538	C2453	G2337	G	A	U2064	G1948	C1798	C1687		G1376	A1245
A2879		U2663	U2539	A2466	G2338	U	G	A2067	G1950	U1817	C1692	U	G1378	A1246
A2880	C2780	A2664	U2541	U2457	C	G	A	G2068	G1951	C1818	C1700	U1559	A1379	C1250
G2881	U2781	A	U2549	G2462	A	G	A	G2072	U	G1819	A1701	U1561	U1380	C1251
G2882	G2782	G2667	C2549	U2462	C	U	C	A2073	A	G1820	U1702	C1562	A1252	A1252
A2883	A2783		C2552	A2465	A	G	A	G2074	C	U1826	C1705	C1564	C1384	C1253
G2884	A2784		A2553	A2466	A	C	U	A2081	U	G1827	C1714	A1573	C1400	C1268
A2890	G2785		U2563	A2467	U2344	U	A	G2091	G	U1828	C1715	A1574	A1406	
C2894	G2786	C2676	C2564	A2468	C2346	G	C	G2091	A	A1829	A1716	G1592	A1407	A1278
A2896	U2792		C2565	A2469	C2347	C	A	U2091	C	U1835	A1717	C1593	U1408	U1279
C2903	G2795	G2679	A2568	C2472	C2348	A	G	G2094	C	U1838	U1722	C1594	G1409	
A2906	U2796	A2680	A2569	C2476	A2353	G	A	A2095	U1964	U1839	G1723	G1595	U1419	A1287
C2907	U2797	C2681	A2578	C2480	G2355	U	U	A2096	C1965	A1840	U1724	U1596	U1419	U1288
A2908	G2799	A2682	G2578	G2481	A2357	C	G	A2100	U1966	U1845	G1725	G1604	C1426	C1289
C2909	U2800		U2586	G2482	G2357	C	C	A2101	U1967	A1846	G1726	G1605	A1291	A1291
A2910	U2807	A2694	C2586	A2483	A2361	C	C	G2102	G1971	U1847	G1730	A1606	G1430	A1294
C2911	A2811	A2697	U2587	U2484	A2362	C	C	A2103	U1972	A1847	C1731	A1607	U1435	G1295
A2912	G2812	G2698	G2588	U2485	G2363	C	C	C2104	A1973	C1883		A1615	G1441	U1298
A2913	U2813	A2699	U2589	A2486	A2364	G	G		U1974	C1856	C1735	U1625	A1442	G1299
A2914	G2815	G2700	U2590	A2487	A2365	C	C		U1975	G1863	A1736	A1626	C1451	U1304
A	A2816	U2704	C2592	A2490	A2366	C	C		U1980	C1864	U1741	G1627	A1458	C1305
C	G2817	C2493	A2599	G2492	A2369	C	C		U1982					U1306
C	A2820	U2499	A2600	U2493	A2374	C	C		U1996	G1867	G1744	A1630	C1462	U1314
C	C2821	C2500	A2601	A2499	G2375	G	G		U2003	G1868	G1745	G1634	A1463	G1327
U		G2501	G2376	C2502	U2377	G	C		U2004	U1748			A1470	A1328
C	G2824	C2502	U2378	A2503	G2379	C	C		G2005	U1749	U1749	A1641	U1473	A1331
A	C2825	A2504	U2379	A2504	C2388	A	A		C2006	G1878	G1750	A1642	C1474	C1332
U	A2827	G2505	C2507	A2506	A2401	C	C		U2007	U1879	G1751	G1647	G1475	U1333
	G2828	C2507	G2507	G2507	A2402	C	C		U2008	C1880	G1752	U1654	A1476	C1334
		U2607	A2508	A2508	C2403	C	C		A2011	C1882	C1753	G1685	C1477	
	C2831	C2608	A2509	A2509	C2406	C	C		U2012	G1902	A1754	A1657	A1482	G1340
	C2832	G2611	C2510	C2511	U2406	C	C		G2013	U1903	G1756	A1658	A1941	A1941
	U2837	A2612	C2515	A2515	A2414	A	A		G2014	A1904	A1766	G1665	C1942	A1942
	C2838	G2613	G2516	G2516	A2415	C	C		U2015	A1909	U1767	C1666	G1483	C1343
	A2840	U2618	G2516	G2516	G2416	C	C		U2016	U1909	A1768	A1667	G1484	
	G2842	C2627	A2521	G2522	U2419	C	C		A2017	A1919	C1769	U1668	U1503	U1350
	A2841	U2630	G2523	G2523	G2420	U	U		A2018	G1926	U1770	U1505	A1504	G1351
	C2842	G2632	A2524	G2524	G2421	C	C		U2019	U1927	U1771	G1670	A1352	A1352
	G2850	U2633	G2525	G2525	U2422	A	A		U2032	G1928	G1772	C1675	U1506	C1353
	A2851	A2635	G2526	G2526	U2423	C	C		U2034	U1929	G1773	U1524	C1360	
	G2852	C2636	A2527	G2527	G2424	C	C		A2038	C1940	A1778	G1525	G1363	
	U2853	U2637	U2528	G2528	G2425	U	U		A2039	A1941	A1526	A1527	C1366	
		C2644	U2531	U2531	G2426	A	A		U2043	A1942	A1681	G1529	C1366	
	C2857	U2645	C2533	G2534	G2427	C	C		G2044	C1943	A1682			
	U2858	A2534	G2534	G2534	G2428	U	U				A1779	G1683		
	U2866				U2435	A	A				C1787	A1684		

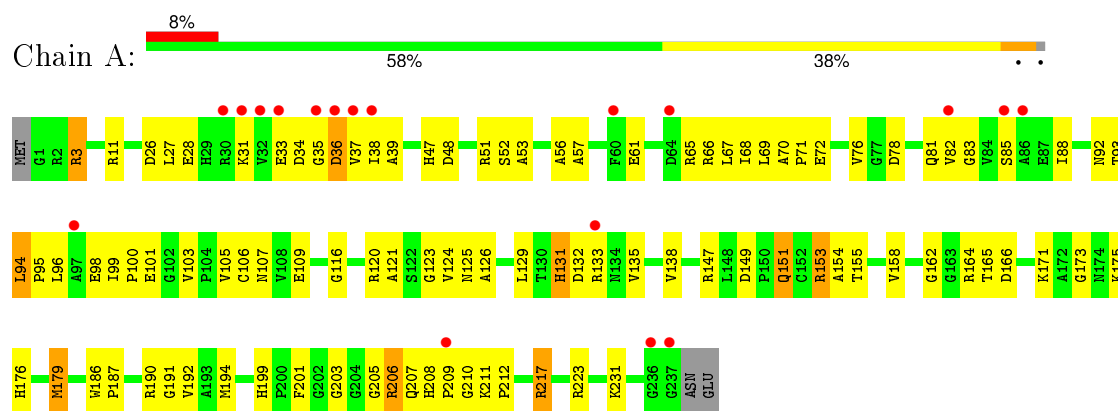
- Molecule 2: 5S ribosomal RNA



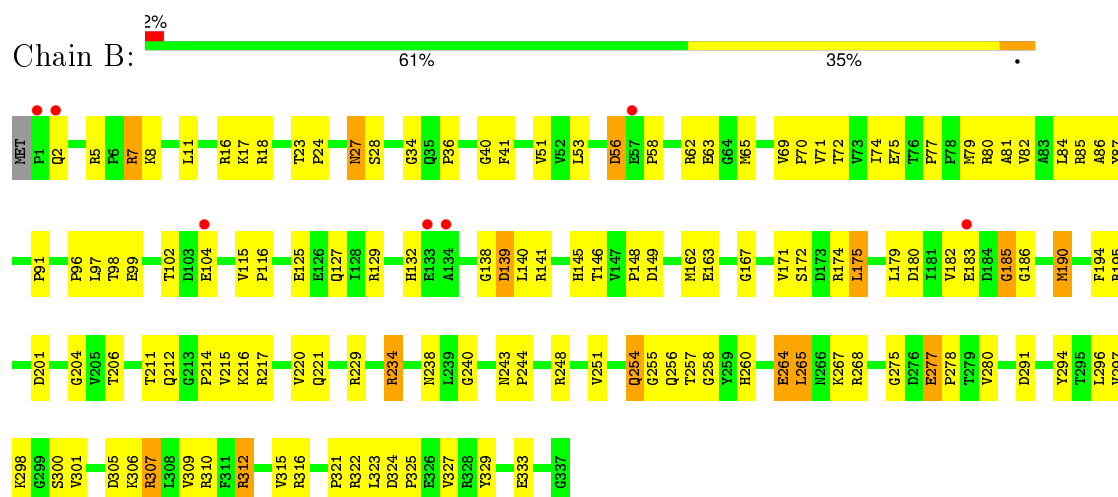
- Molecule 3: 5'-R(*CP*CP*(PPU))-3'



- Molecule 4: 50S ribosomal protein L2P

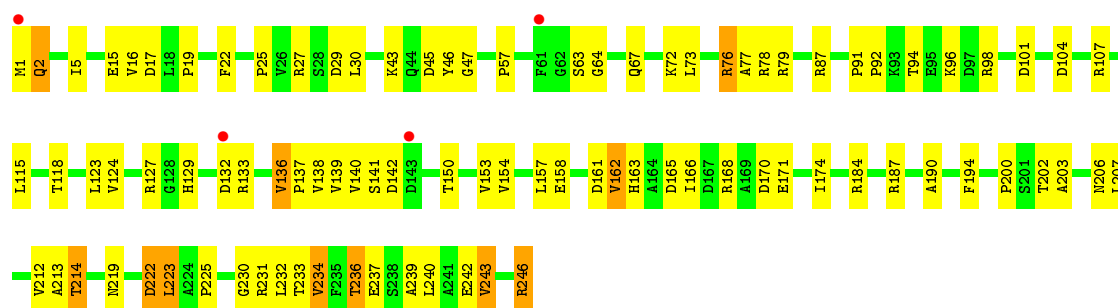


- Molecule 5: 50S ribosomal protein L3P

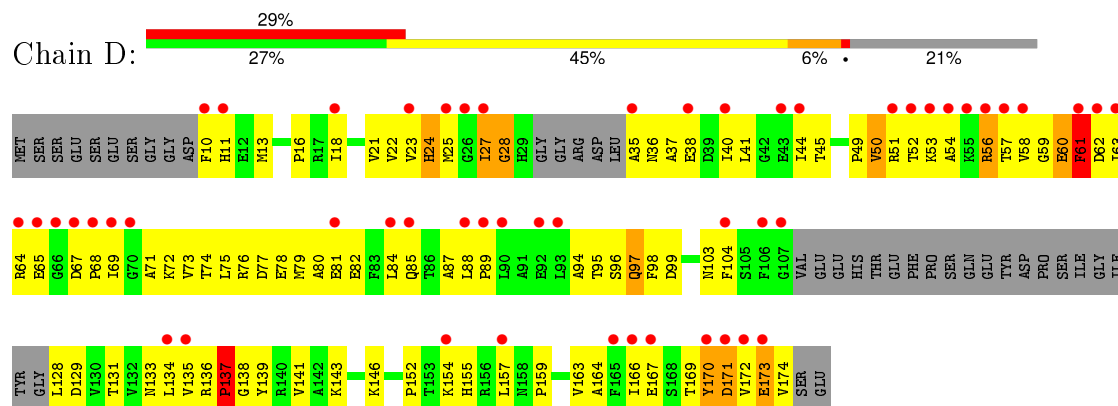


- Molecule 6: 50S ribosomal protein L4E

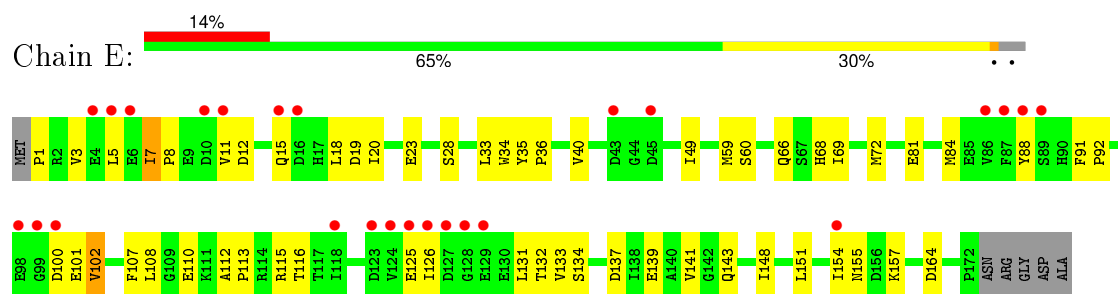




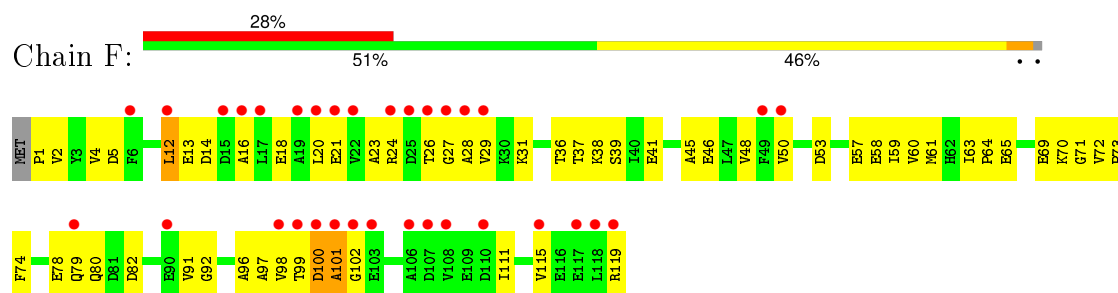
• Molecule 7: 50S ribosomal protein L5P



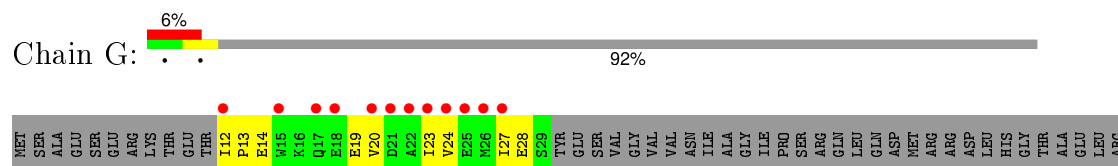
• Molecule 8: 50S ribosomal protein L6P



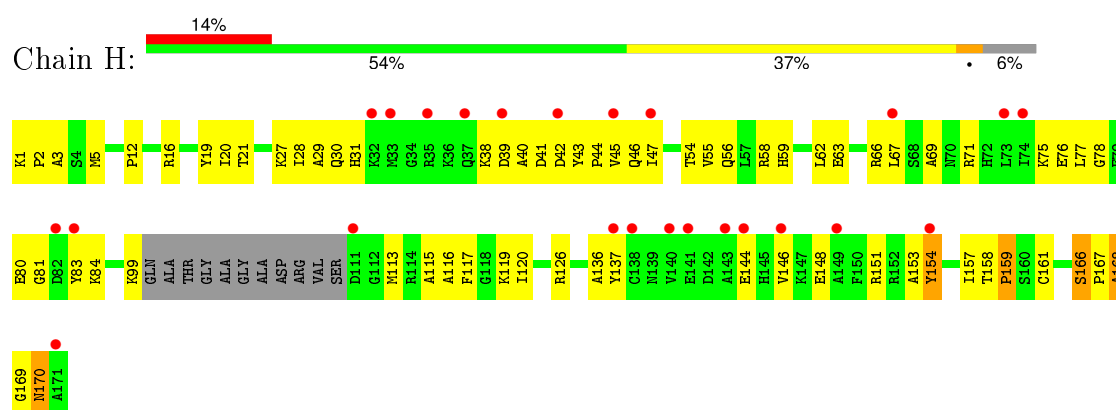
• Molecule 9: 50S ribosomal protein L7AE



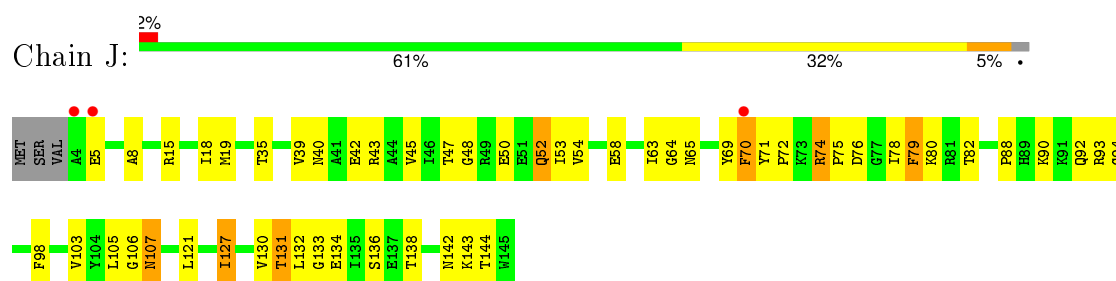
• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



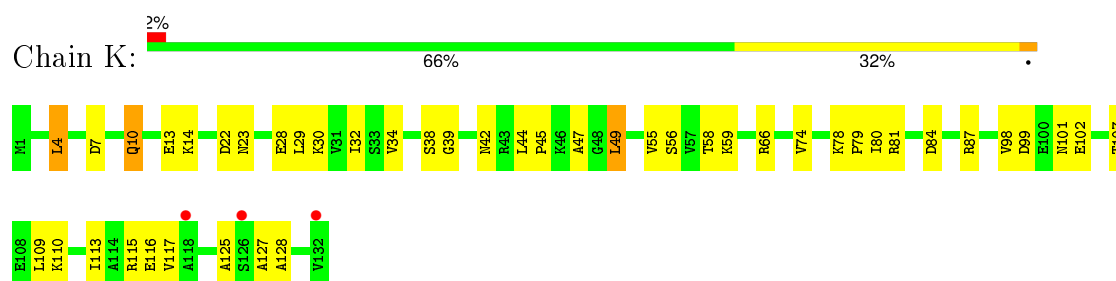
- Molecule 11: 50S RIBOSOMAL PROTEIN L10E



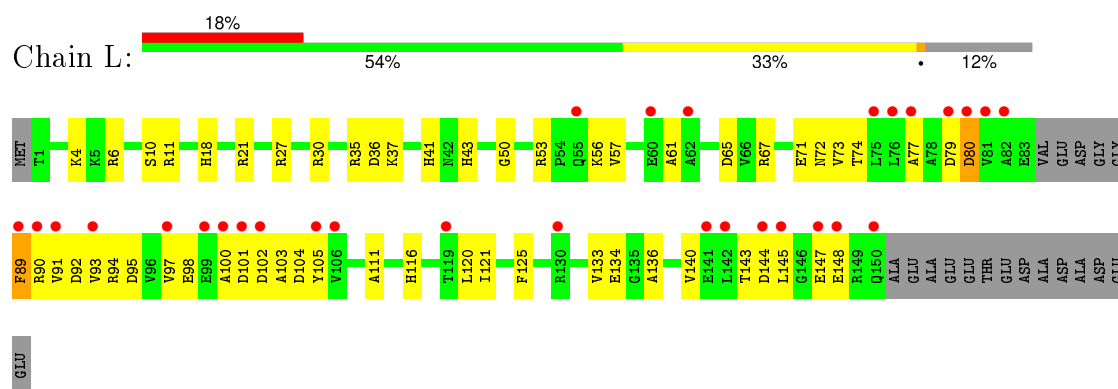
- Molecule 12: 50S ribosomal protein L13P



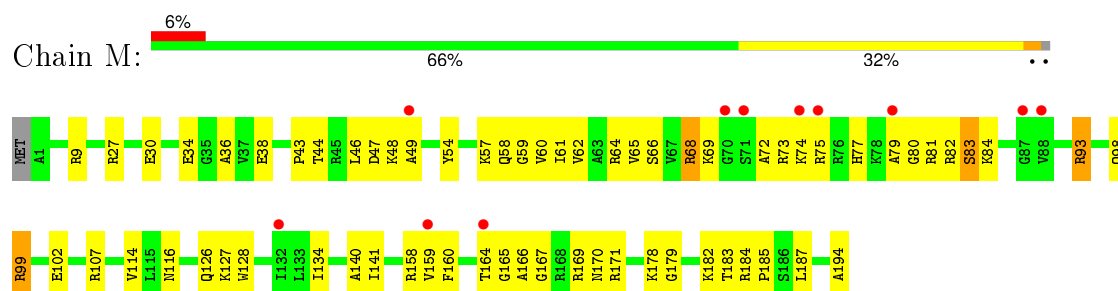
- Molecule 13: 50S ribosomal protein L14P



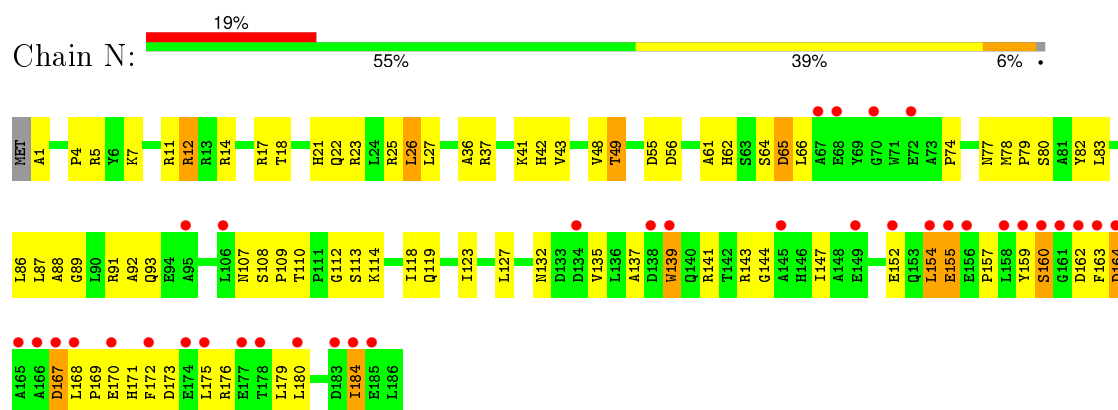
- Molecule 14: 50S ribosomal protein L15P



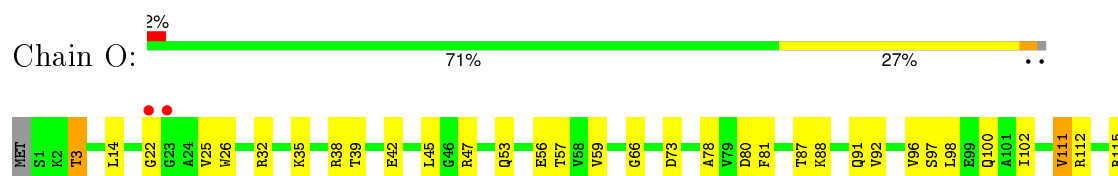
- Molecule 15: 50S Ribosomal Protein L15E



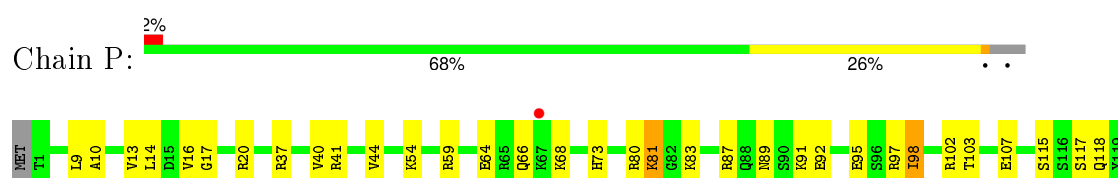
- Molecule 16: 50S ribosomal protein L18P

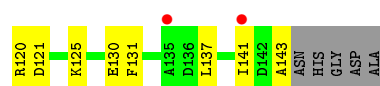


- Molecule 17: 50S ribosomal protein L18e

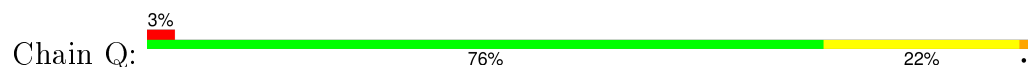


- Molecule 18: 50S ribosomal protein L19E





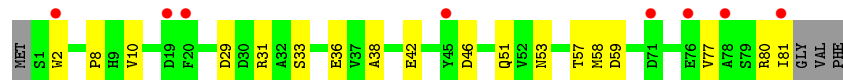
- Molecule 19: 50S ribosomal protein L21e



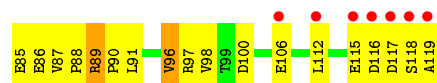
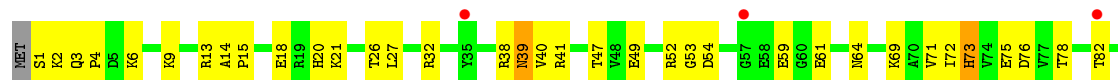
- Molecule 20: 50S ribosomal protein L22P



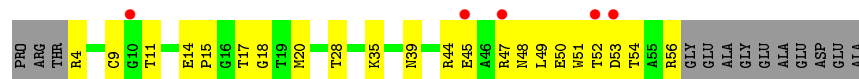
- Molecule 21: 50S ribosomal protein L23P



- Molecule 22: 50S ribosomal protein L24P

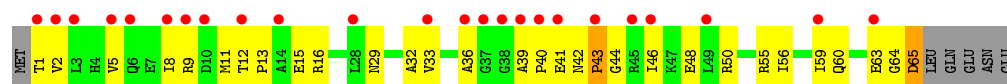


- Molecule 23: 50S ribosomal protein L24E

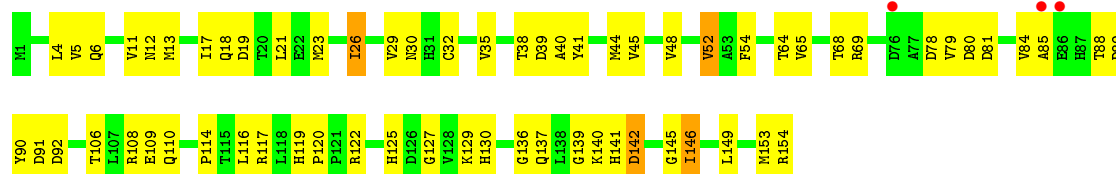


- Molecule 24: 50S ribosomal protein L29P

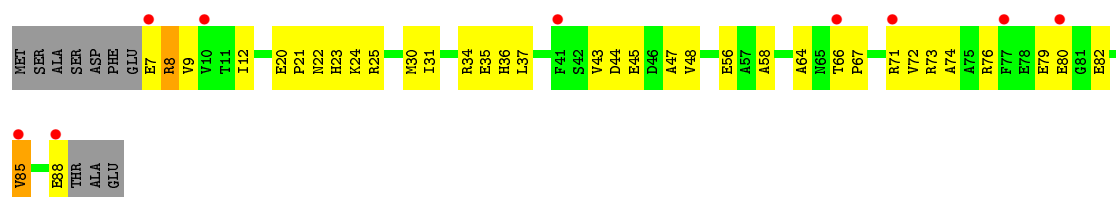




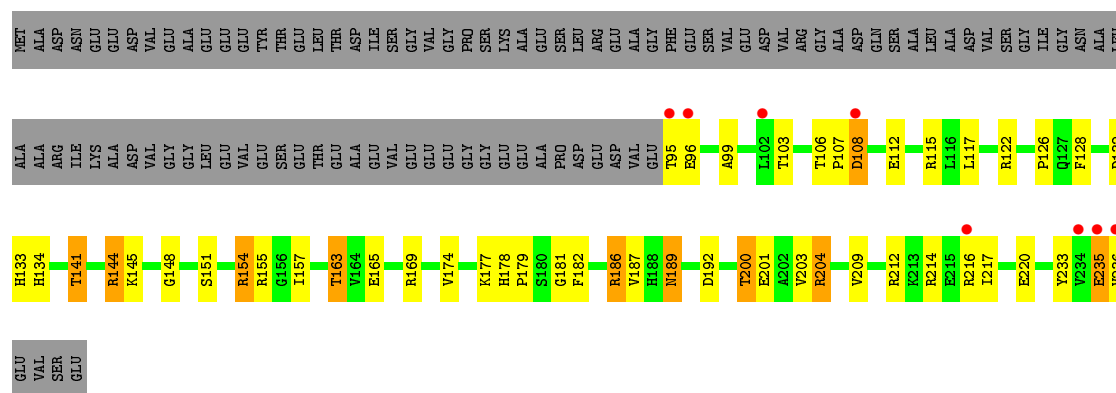
- Molecule 25: 50S ribosomal protein L30P



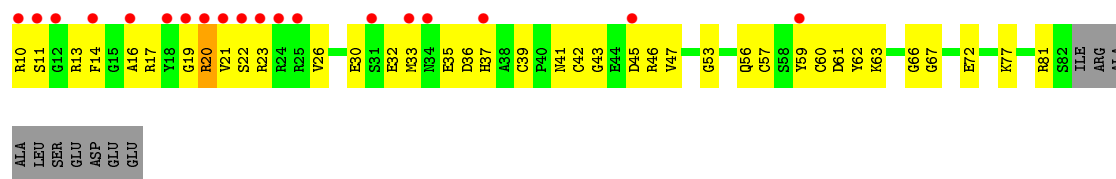
- Molecule 26: 50S ribosomal protein L31e



- Molecule 27: 50S ribosomal protein L32E



- Molecule 28: 50S ribosomal protein L37Ae



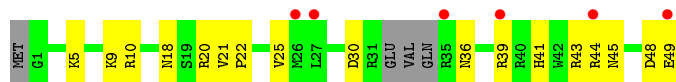
- Molecule 29: 50S ribosomal protein L37e

Chain 1:  75% 23% .



- Molecule 30: 50S ribosomal protein L39e

Chain 2:  12% 58% 34% 8%




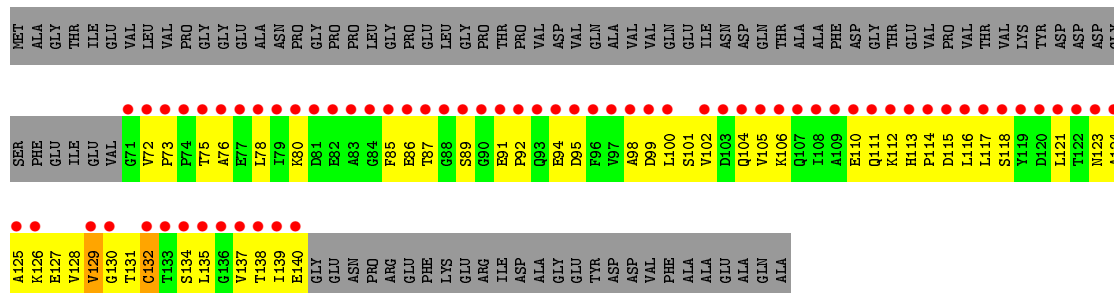
- Molecule 31: 50S ribosomal protein L44E

Chain 3:  4% 71% 28% .



- Molecule 32: 50S RIBOSOMAL PROTEIN L11P

Chain I:  14% 41% 28% 57% .



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 49.39 – 2.21	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-2.20) 88.8 (49.39-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.246 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 892831 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, PPU, CL, SR, NA, K, CD, OMU, UR3, 1MA, PSU

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	0.37	0/65959	0.70	24/102870 (0.0%)
2	9	0.33	0/2905	0.71	1/4528 (0.0%)
3	4	0.43	0/40	0.63	0/60
4	A	0.32	0/1786	0.64	0/2408
5	B	0.35	0/2690	0.67	0/3652
6	C	0.37	0/1884	0.65	0/2551
7	D	0.29	0/1111	0.53	0/1498
8	E	0.32	0/1382	0.57	0/1880
9	F	0.32	0/901	0.53	0/1224
10	G	0.26	0/241	0.46	0/324
11	H	0.33	0/1287	0.64	0/1725
12	J	0.35	0/1136	0.61	0/1530
13	K	0.35	0/1001	0.67	0/1347
14	L	0.32	0/1130	0.66	0/1509
15	M	0.34	0/1584	0.60	0/2119
16	N	0.28	0/1474	0.59	0/1999
17	O	0.32	0/874	0.58	1/1181 (0.1%)
18	P	0.33	0/1147	0.54	0/1528
19	Q	0.34	0/749	0.69	1/1005 (0.1%)
20	R	0.35	0/1172	0.67	1/1578 (0.1%)
21	S	0.31	0/648	0.56	0/875
22	T	0.29	0/958	0.62	0/1289
23	U	0.34	0/417	0.56	0/562
24	V	0.25	0/502	0.51	0/675
25	W	0.34	0/1219	0.61	0/1655
26	X	0.32	0/664	0.59	0/895
27	Y	0.35	0/1146	0.66	0/1536
28	Z	0.32	0/589	0.59	0/787
29	1	0.44	0/438	0.66	0/578
30	2	0.34	0/401	0.58	0/529
31	3	0.35	0/771	0.58	0/1024
32	I	0.28	0/526	0.49	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.36	0/98732	0.68	28/147637 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	40
2	9	0	1
All	All	1	41

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.80	131.06	109.50
1	0	871	G	C5'-C4'-O4'	-8.85	98.48	109.10
1	0	1942	A	C5'-C4'-C3'	8.20	129.12	116.00
1	0	777	U	O4'-C1'-N1	6.82	113.66	108.20
1	0	1819	G	C5'-C4'-C3'	6.76	126.81	116.00

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	718	0
2	9	2600	0	1326	56	0
3	4	74	0	51	2	0
4	A	1753	0	1766	117	0
5	B	2625	0	2532	131	0
6	C	1859	0	1816	111	0
7	D	1094	0	1085	101	0
8	E	1357	0	1266	53	0
9	F	890	0	843	52	0
10	G	240	0	231	15	0
11	H	1266	0	1268	68	0
12	J	1120	0	1098	68	0
13	K	992	0	1031	49	0
14	L	1118	0	1076	59	0
15	M	1560	0	1568	67	0
16	N	1445	0	1401	89	0
17	O	865	0	873	38	0
18	P	1136	0	1123	40	0
19	Q	735	0	728	18	0
20	R	1149	0	1122	46	0
21	S	641	0	605	17	0
22	T	950	0	924	53	0
23	U	410	0	364	26	0
24	V	499	0	511	37	0
25	W	1196	0	1137	76	0
26	X	654	0	653	42	0
27	Y	1130	0	1133	55	0
28	Z	578	0	539	33	0
29	1	431	0	426	24	0
30	2	396	0	413	23	0
31	3	755	0	728	23	0
32	I	519	0	500	54	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	A	124	0	0	12	0
39	B	141	0	0	19	0
39	C	177	0	0	16	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	8	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	4	0
39	P	60	0	0	4	0
39	Q	49	0	0	3	0
39	R	83	0	0	5	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	2117	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 2117 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)
1:0:1160:G:H5'	1:0:1161:A:H5'	1.32	1.10
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
2:9:3006:C:H5''	16:N:37:ARG:NH1	1.68	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	
4	A	235/240 (98%)	208 (88%)	25 (11%)	2 (1%)	21	19
5	B	335/338 (99%)	315 (94%)	16 (5%)	4 (1%)	16	12
6	C	244/246 (99%)	225 (92%)	19 (8%)	0	100	100
7	D	134/177 (76%)	107 (80%)	16 (12%)	11 (8%)	1	0
8	E	170/178 (96%)	164 (96%)	6 (4%)	0	100	100
9	F	117/120 (98%)	105 (90%)	8 (7%)	4 (3%)	5	2
10	G	25/348 (7%)	25 (100%)	0	0	100	100
11	H	156/171 (91%)	137 (88%)	15 (10%)	4 (3%)	7	3
12	J	140/145 (97%)	132 (94%)	5 (4%)	3 (2%)	9	5
13	K	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
14	L	141/165 (86%)	119 (84%)	20 (14%)	2 (1%)	14	10
15	M	192/195 (98%)	183 (95%)	8 (4%)	1 (0%)	34	35
16	N	184/187 (98%)	165 (90%)	12 (6%)	7 (4%)	4	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
21	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
22	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	21	19
23	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
24	V	63/71 (89%)	58 (92%)	4 (6%)	1 (2%)	12	8
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%)	3	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	6	2
All	All	3705/4431 (84%)	3432 (93%)	228 (6%)	45 (1%)	16	12

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%)	168 (94%)	11 (6%)	23	26
5	B	282/283 (100%)	265 (94%)	17 (6%)	24	26
6	C	193/193 (100%)	176 (91%)	17 (9%)	12	12
7	D	117/148 (79%)	111 (95%)	6 (5%)	29	34
8	E	152/156 (97%)	147 (97%)	5 (3%)	45	56
9	F	93/94 (99%)	92 (99%)	1 (1%)	80	89
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	128 (97%)	4 (3%)	48	60
12	J	118/121 (98%)	111 (94%)	7 (6%)	24	27
13	K	106/106 (100%)	102 (96%)	4 (4%)	40	49
14	L	113/127 (89%)	110 (97%)	3 (3%)	52	64
15	M	158/159 (99%)	153 (97%)	5 (3%)	46	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	N	149/150 (99%)	144 (97%)	5 (3%)	44	54
17	O	93/94 (99%)	91 (98%)	2 (2%)	60	72
18	P	113/117 (97%)	111 (98%)	2 (2%)	66	79
19	Q	79/80 (99%)	76 (96%)	3 (4%)	40	49
20	R	117/122 (96%)	115 (98%)	2 (2%)	68	81
21	S	71/74 (96%)	71 (100%)	0	100	100
22	T	105/106 (99%)	101 (96%)	4 (4%)	40	49
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	63	76
25	W	130/130 (100%)	125 (96%)	5 (4%)	40	49
26	X	66/74 (89%)	62 (94%)	4 (6%)	23	26
27	Y	120/196 (61%)	107 (89%)	13 (11%)	8	7
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	57	69
31	3	79/79 (100%)	78 (99%)	1 (1%)	76	87
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3612 (86%)	2970 (96%)	123 (4%)	38	47

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	E	164	ASP
13	K	4	LEU
27	Y	163	THR
11	H	84	LYS
12	J	70	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	170	ASN
19	Q	16	ASN
30	2	18	ASN
16	N	107	ASN

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Mol	Chain	Res	Type
18	P	50	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	232 (8%)	35 (1%)
2	9	121/122 (99%)	16 (13%)	2 (1%)
3	4	1/3 (33%)	0	0
All	All	2867/3047 (94%)	248 (8%)	37 (1%)

5 of 248 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	1506	U
1	0	1692	C
1	0	2852	A
1	0	1563	G
1	0	1684	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	12,22,23	1.10	1 (8%)	19,31,34	3.10	2 (10%)
1	OMG	0	2588	1,3	17,26,27	1.04	1 (5%)	21,38,41	2.55	3 (14%)
1	UR3	0	2619	1	12,22,23	0.88	1 (8%)	16,32,35	0.74	0
1	PSU	0	2621	1	13,21,22	1.58	2 (15%)	18,30,33	6.06	4 (22%)
1	1MA	0	628	1	14,25,26	0.96	1 (7%)	15,37,40	1.14	1 (6%)
3	PPU	4	76	1,3	30,40,41	1.13	1 (3%)	37,57,60	1.02	3 (8%)

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	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3
3	PPU	4	76	1,3	-	0/21/43/44	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	76	PPU	OC-CM	-5.34	1.26	1.42
1	0	2621	PSU	C5-C1'	-4.61	1.48	1.52
1	0	2619	UR3	C6-C5	-2.24	1.33	1.38
1	0	628	1MA	C6-N6	2.55	1.33	1.29
1	0	2621	PSU	C4-N3	2.76	1.38	1.33

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-21.15	114.84	128.33
1	0	2588	OMG	C5-C6-N1	-8.77	111.59	123.59
1	0	628	1MA	C2-N3-C4	-3.55	110.90	116.40
1	0	2587	OMU	C5-C4-N3	-3.27	114.74	123.12
3	4	76	PPU	C4'-C3'-N3'	-2.57	108.25	113.61

There are no chirality outliers.

There are no torsion outliers.

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 carbohydrates 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 [i](#)

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	2749/2922 (94%)	-0.19	94 (3%) 49 47	26, 46, 90, 148	0
2	9	122/122 (100%)	0.04	5 (4%) 41 39	39, 62, 87, 147	0
3	4	2/3 (66%)	-0.51	0 100 100	52, 52, 52, 62	0
4	A	237/240 (98%)	0.49	18 (7%) 17 16	30, 52, 82, 104	0
5	B	337/338 (99%)	0.18	7 (2%) 67 65	31, 50, 72, 85	0
6	C	246/246 (100%)	0.00	4 (1%) 74 73	28, 47, 68, 81	0
7	D	140/177 (79%)	1.89	52 (37%) 0 0	56, 90, 119, 127	0
8	E	172/178 (96%)	0.71	25 (14%) 3 3	42, 60, 78, 83	0
9	F	119/120 (99%)	1.24	33 (27%) 1 1	47, 71, 99, 108	0
10	G	29/348 (8%)	2.72	20 (68%) 0 0	68, 89, 97, 98	0
11	H	160/171 (93%)	0.72	24 (15%) 3 3	44, 60, 92, 99	0
12	J	142/145 (97%)	-0.03	3 (2%) 67 65	36, 47, 66, 86	0
13	K	132/132 (100%)	-0.12	3 (2%) 64 63	34, 45, 66, 69	0
14	L	145/165 (87%)	0.80	30 (20%) 1 1	30, 64, 110, 119	0
15	M	194/195 (99%)	0.47	11 (5%) 27 27	35, 46, 67, 79	0
16	N	186/187 (99%)	0.88	36 (19%) 1 1	44, 62, 104, 112	0
17	O	115/116 (99%)	0.09	2 (1%) 73 72	41, 53, 66, 74	0
18	P	143/149 (95%)	0.19	3 (2%) 67 65	40, 51, 65, 78	0
19	Q	95/96 (98%)	0.07	3 (3%) 51 50	41, 47, 63, 74	0
20	R	150/155 (96%)	-0.05	3 (2%) 68 67	31, 44, 62, 70	0
21	S	81/85 (95%)	0.44	8 (9%) 9 8	43, 62, 82, 95	0
22	T	119/120 (99%)	0.68	10 (8%) 14 13	43, 56, 79, 107	0
23	U	53/66 (80%)	0.37	5 (9%) 11 10	42, 51, 67, 75	0
24	V	65/71 (91%)	2.13	24 (36%) 0 0	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%)	0.03	3 (1%) 70 68	36, 48, 69, 78	0
26	X	82/92 (89%)	0.62	9 (10%) 7 7	41, 53, 79, 97	0
27	Y	142/241 (58%)	0.18	8 (5%) 28 27	31, 43, 62, 82	0
28	Z	73/83 (87%)	1.00	19 (26%) 1 1	49, 73, 86, 92	0
29	1	56/57 (98%)	-0.41	0 100 100	30, 35, 42, 50	0
30	2	46/50 (92%)	0.72	6 (13%) 5 4	38, 58, 73, 83	0
31	3	92/92 (100%)	0.20	4 (4%) 39 38	37, 55, 68, 79	0
32	I	70/162 (43%)	5.65	66 (94%) 0 0	107, 120, 137, 139	0
All	All	6648/7478 (88%)	0.24	538 (8%) 15 14	26, 51, 95, 148	0

The worst 5 of 538 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	17.3
24	V	1	THR	16.0
7	D	63	ILE	14.5
32	I	133	THR	13.7
32	I	96	PHE	12.4

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	PPU	4	76	37/38	0.94	0.14	-	48,54,66,71	0
1	OMU	0	2587	21/22	0.99	0.10	-	33,36,38,39	0
1	PSU	0	2621	20/21	0.97	0.11	-	37,40,50,51	0
1	1MA	0	628	23/24	0.97	0.14	-	29,33,36,37	0
1	UR3	0	2619	21/22	0.97	0.14	-	45,45,49,50	0
1	OMG	0	2588	24/25	0.97	0.12	-	30,35,40,41	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
35	NA	0	9125	1/1	0.93	0.73	52.15	115,115,115,115	0
35	NA	B	9161	1/1	0.84	0.51	46.86	62,62,62,62	0
35	NA	0	9164	1/1	0.79	0.35	30.51	59,59,59,59	0
35	NA	0	9173	1/1	0.74	0.37	26.88	70,70,70,70	0
35	NA	R	9186	1/1	0.92	0.47	20.20	69,69,69,69	0
33	MG	0	8013	1/1	0.96	0.38	18.35	22,22,22,22	0
37	SR	B	9521	1/1	0.70	0.49	18.00	199,199,199,199	0
37	SR	0	9406	1/1	0.99	0.18	16.98	38,38,38,38	0
33	MG	0	8012	1/1	0.96	0.26	16.96	41,41,41,41	0
35	NA	0	9171	1/1	0.61	0.28	15.56	61,61,61,61	0
35	NA	0	9172	1/1	0.90	0.40	15.09	70,70,70,70	0
37	SR	0	9482	1/1	0.99	0.23	12.28	102,102,102,102	0
33	MG	0	8008	1/1	0.99	0.21	12.02	17,17,17,17	0
35	NA	0	9185	1/1	0.83	0.32	11.39	46,46,46,46	0
33	MG	0	8038	1/1	0.99	0.25	10.78	20,20,20,20	0
35	NA	0	9120	1/1	0.94	0.19	10.29	64,64,64,64	0
35	NA	0	9174	1/1	0.93	0.17	9.46	65,65,65,65	0
33	MG	0	8001	1/1	0.95	0.26	8.89	20,20,20,20	0
33	MG	0	8060	1/1	0.93	0.28	7.98	71,71,71,71	0
34	K	0	9001	1/1	0.79	0.45	7.65	116,116,116,116	0
35	NA	0	9177	1/1	0.93	0.23	7.07	63,63,63,63	0
33	MG	0	8021	1/1	0.92	0.20	6.62	55,55,55,55	0
35	NA	0	9178	1/1	0.94	0.22	5.61	51,51,51,51	0
33	MG	0	8017	1/1	0.99	0.15	5.18	28,28,28,28	0
33	MG	0	8027	1/1	0.95	0.19	5.08	39,39,39,39	0
35	NA	0	9156	1/1	0.98	0.14	4.41	53,53,53,53	0
35	NA	0	9132	1/1	0.95	0.21	4.16	51,51,51,51	0
33	MG	0	8014	1/1	0.66	0.34	3.91	73,73,73,73	0
33	MG	0	8080	1/1	0.97	0.18	3.51	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	9140	1/1	0.93	0.25	2.94	60,60,60,60	0
33	MG	0	8097	1/1	0.92	0.16	2.60	62,62,62,62	0
33	MG	0	8057	1/1	0.88	0.23	2.40	85,85,85,85	0
33	MG	0	8002	1/1	0.99	0.16	2.30	28,28,28,28	0
33	MG	A	8066	1/1	0.96	0.19	2.27	53,53,53,53	0
33	MG	0	8056	1/1	0.93	0.20	2.23	46,46,46,46	0
35	NA	0	9165	1/1	0.91	0.21	2.12	47,47,47,47	0
35	NA	0	9117	1/1	0.98	0.19	1.95	39,39,39,39	0
35	NA	0	9135	1/1	0.99	0.16	1.93	50,50,50,50	0
35	NA	0	9154	1/1	0.94	0.16	1.89	59,59,59,59	0
35	NA	0	9162	1/1	0.93	0.16	1.81	58,58,58,58	0
35	NA	0	9168	1/1	0.79	0.12	1.65	57,57,57,57	0
36	CL	0	9316	1/1	0.96	0.17	1.63	69,69,69,69	0
37	SR	0	9515	1/1	0.96	0.15	1.47	87,87,87,87	0
37	SR	0	9407	1/1	0.99	0.12	1.44	43,43,43,43	0
35	NA	9	9183	1/1	0.94	0.15	1.40	66,66,66,66	0
36	CL	0	9315	1/1	0.90	0.11	1.38	58,58,58,58	0
33	MG	0	8070	1/1	0.99	0.16	1.22	26,26,26,26	0
35	NA	C	9104	1/1	0.92	0.20	1.13	34,34,34,34	0
33	MG	0	8074	1/1	0.98	0.19	1.03	23,23,23,23	0
35	NA	0	9105	1/1	0.98	0.14	0.96	43,43,43,43	0
35	NA	M	9147	1/1	0.95	0.18	0.90	43,43,43,43	0
33	MG	0	8003	1/1	0.98	0.17	0.68	32,32,32,32	0
37	SR	H	9486	1/1	0.97	0.15	0.51	109,109,109,109	0
33	MG	0	8004	1/1	0.99	0.11	0.46	30,30,30,30	0
37	SR	A	9437	1/1	0.98	0.14	0.35	67,67,67,67	0
33	MG	0	8015	1/1	0.94	0.12	0.29	34,34,34,34	0
33	MG	0	8020	1/1	0.99	0.15	0.14	37,37,37,37	0
34	K	0	9002	1/1	0.94	0.14	0.11	89,89,89,89	0
33	MG	0	8096	1/1	0.92	0.14	0.01	46,46,46,46	0
37	SR	F	9595	1/1	0.96	0.14	-0.14	105,105,105,105	0
37	SR	1	9419	1/1	0.99	0.11	-0.30	40,40,40,40	0
35	NA	0	9139	1/1	0.92	0.12	-0.38	52,52,52,52	0
35	NA	0	9127	1/1	0.86	0.12	-0.40	57,57,57,57	0
37	SR	0	9509	1/1	0.97	0.12	-0.52	81,81,81,81	0
36	CL	M	9318	1/1	0.97	0.16	-0.53	41,41,41,41	0
37	SR	L	9409	1/1	1.00	0.11	-0.68	40,40,40,40	0
35	NA	0	9124	1/1	0.95	0.09	-0.70	47,47,47,47	0
38	CD	U	9201	1/1	0.99	0.10	-0.74	48,48,48,48	0
35	NA	R	9137	1/1	0.94	0.10	-0.82	36,36,36,36	0
35	NA	0	9114	1/1	0.98	0.10	-0.87	46,46,46,46	0
37	SR	0	9451	1/1	0.99	0.10	-0.90	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	9166	1/1	0.88	0.09	-0.96	67,67,67,67	0
36	CL	B	9319	1/1	0.98	0.11	-0.97	52,52,52,52	0
35	NA	J	9146	1/1	0.84	0.09	-1.01	55,55,55,55	0
33	MG	0	8088	1/1	0.94	0.08	-1.08	45,45,45,45	0
38	CD	Z	9203	1/1	0.98	0.07	-1.10	78,78,78,78	0
37	SR	0	9416	1/1	0.99	0.11	-1.16	43,43,43,43	0
37	SR	0	9450	1/1	0.99	0.09	-1.16	62,62,62,62	0
36	CL	J	9321	1/1	0.97	0.06	-1.26	53,53,53,53	0
37	SR	0	9410	1/1	0.99	0.12	-1.27	37,37,37,37	0
33	MG	T	8073	1/1	0.97	0.12	-1.28	46,46,46,46	0
37	SR	0	9475	1/1	0.91	0.08	-1.44	77,77,77,77	0
37	SR	0	9504	1/1	0.95	0.09	-1.57	105,105,105,105	0
35	NA	0	9143	1/1	0.97	0.10	-1.61	43,43,43,43	0
37	SR	0	9534	1/1	0.92	0.09	-1.71	100,100,100,100	0
37	SR	0	9431	1/1	0.98	0.12	-1.71	55,55,55,55	0
37	SR	0	9490	1/1	0.88	0.08	-1.88	109,109,109,109	0
33	MG	0	8054	1/1	0.83	0.10	-1.88	58,58,58,58	0
35	NA	R	9138	1/1	0.93	0.07	-1.89	56,56,56,56	0
36	CL	O	9308	1/1	0.99	0.06	-1.94	60,60,60,60	0
35	NA	Q	9148	1/1	0.94	0.08	-2.06	44,44,44,44	0
37	SR	0	9424	1/1	1.00	0.13	-2.09	45,45,45,45	0
38	CD	3	9204	1/1	0.98	0.04	-2.09	60,60,60,60	0
37	SR	0	9483	1/1	0.96	0.08	-2.14	68,68,68,68	0
36	CL	3	9304	1/1	0.99	0.08	-2.37	55,55,55,55	0
37	SR	0	9443	1/1	1.00	0.09	-2.55	57,57,57,57	0
33	MG	0	8019	1/1	0.96	0.07	-2.57	58,58,58,58	0
37	SR	A	9436	1/1	0.99	0.04	-2.64	61,61,61,61	0
37	SR	0	9468	1/1	0.92	0.05	-2.71	113,113,113,113	0
36	CL	K	9312	1/1	0.99	0.06	-2.73	46,46,46,46	0
37	SR	0	9455	1/1	0.98	0.07	-2.80	67,67,67,67	0
33	MG	0	8067	1/1	0.95	0.09	-2.82	42,42,42,42	0
33	MG	0	8032	1/1	0.96	0.08	-2.84	43,43,43,43	0
37	SR	0	9532	1/1	0.96	0.07	-2.86	103,103,103,103	0
33	MG	0	8091	1/1	0.94	0.08	-2.90	45,45,45,45	0
37	SR	0	9442	1/1	0.99	0.09	-2.93	59,59,59,59	0
38	CD	1	9202	1/1	0.99	0.04	-3.00	51,51,51,51	0
37	SR	0	9428	1/1	0.99	0.04	-3.14	49,49,49,49	0
37	SR	3	9439	1/1	0.99	0.05	-3.14	63,63,63,63	0
33	MG	0	8044	1/1	0.97	0.08	-3.26	39,39,39,39	0
37	SR	0	9473	1/1	0.99	0.04	-3.37	69,69,69,69	0
33	MG	Y	8109	1/1	0.94	0.07	-3.37	41,41,41,41	0
35	NA	0	9123	1/1	0.96	0.10	-3.57	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	0	9444	1/1	0.99	0.04	-3.58	50,50,50,50	0
36	CL	0	9305	1/1	0.99	0.08	-3.61	54,54,54,54	0
35	NA	0	9150	1/1	0.92	0.11	-3.63	38,38,38,38	0
37	SR	0	9457	1/1	0.99	0.07	-3.72	47,47,47,47	0
37	SR	0	9456	1/1	0.99	0.07	-4.27	69,69,69,69	0
33	MG	0	8112	1/1	0.98	0.04	-4.62	43,43,43,43	0
37	SR	0	9498	1/1	0.98	0.06	-4.88	59,59,59,59	0
35	NA	0	9131	1/1	0.97	0.06	-4.92	48,48,48,48	0
37	SR	0	9506	1/1	0.96	0.03	-5.09	66,66,66,66	0
33	MG	0	8110	1/1	0.97	0.06	-5.21	36,36,36,36	0
37	SR	0	9453	1/1	0.98	0.04	-14.37	69,69,69,69	0
33	MG	0	8005	1/1	0.99	0.07	-	35,35,35,35	0
36	CL	Y	9320	1/1	0.99	0.06	-	43,43,43,43	0
35	NA	0	9134	1/1	0.91	0.07	-	51,51,51,51	0
37	SR	0	9530	1/1	0.92	0.10	-	84,84,84,84	0
35	NA	0	9152	1/1	0.91	0.74	-	78,78,78,78	0
33	MG	0	8050	1/1	0.85	0.17	-	93,93,93,93	0
35	NA	0	9106	1/1	0.99	0.19	-	37,37,37,37	0
37	SR	0	9433	1/1	0.99	0.10	-	76,76,76,76	0
37	SR	0	9440	1/1	0.99	0.03	-	61,61,61,61	0
33	MG	0	8114	1/1	0.94	0.19	-	63,63,63,63	0
35	NA	0	9128	1/1	0.96	0.11	-	45,45,45,45	0
33	MG	0	8031	1/1	0.99	0.07	-	50,50,50,50	0
33	MG	0	8063	1/1	0.91	0.07	-	70,70,70,70	0
33	MG	0	8092	1/1	0.76	0.71	-	81,81,81,81	0
35	NA	0	9118	1/1	0.87	0.23	-	60,60,60,60	0
33	MG	0	8052	1/1	0.82	0.38	-	68,68,68,68	0
37	SR	0	9477	1/1	0.98	0.10	-	84,84,84,84	0
37	SR	0	9501	1/1	0.43	0.38	-	200,200,200,200	0
35	NA	0	9107	1/1	0.97	0.24	-	61,61,61,61	0
35	NA	S	9112	1/1	0.82	0.13	-	59,59,59,59	0
33	MG	0	8039	1/1	0.89	0.07	-	65,65,65,65	0
35	NA	0	9157	1/1	0.87	0.15	-	47,47,47,47	0
33	MG	0	8042	1/1	0.88	0.09	-	60,60,60,60	0
37	SR	0	9517	1/1	0.98	0.06	-	91,91,91,91	0
37	SR	0	9462	1/1	0.99	0.09	-	64,64,64,64	0
33	MG	B	8055	1/1	0.80	0.22	-	108,108,108,108	0
36	CL	0	9311	1/1	0.98	0.08	-	57,57,57,57	0
37	SR	0	9484	1/1	0.87	0.12	-	147,147,147,147	0
37	SR	0	9590	1/1	0.74	0.13	-	178,178,178,178	0
33	MG	0	8079	1/1	0.98	0.12	-	34,34,34,34	0
36	CL	J	9301	1/1	0.99	0.08	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8022	1/1	0.94	0.67	-	74,74,74,74	0
37	SR	0	9447	1/1	0.95	0.09	-	67,67,67,67	0
38	CD	O	9205	1/1	0.99	0.08	-	75,75,75,75	0
35	NA	0	9181	1/1	0.95	0.12	-	50,50,50,50	0
37	SR	0	9466	1/1	0.98	0.03	-	84,84,84,84	0
37	SR	0	9415	1/1	0.99	0.10	-	50,50,50,50	0
37	SR	0	9417	1/1	0.98	0.09	-	59,59,59,59	0
33	MG	0	8098	1/1	0.97	0.07	-	39,39,39,39	0
37	SR	0	9434	1/1	0.98	0.09	-	55,55,55,55	0
37	SR	0	9539	1/1	0.88	0.21	-	162,162,162,162	0
35	NA	0	9179	1/1	0.69	0.98	-	100,100,100,100	0
37	SR	0	9423	1/1	0.99	0.08	-	54,54,54,54	0
36	CL	J	9302	1/1	0.98	0.07	-	48,48,48,48	0
37	SR	0	9454	1/1	0.98	0.05	-	74,74,74,74	0
37	SR	0	9488	1/1	0.96	0.09	-	76,76,76,76	0
35	NA	0	9113	1/1	0.88	0.14	-	65,65,65,65	0
35	NA	0	9160	1/1	0.98	0.09	-	39,39,39,39	0
33	MG	0	8040	1/1	0.84	0.38	-	100,100,100,100	0
35	NA	0	9122	1/1	0.23	0.30	-	96,96,96,96	0
37	SR	0	9429	1/1	0.97	0.09	-	60,60,60,60	0
33	MG	0	8068	1/1	0.99	0.10	-	46,46,46,46	0
33	MG	0	8041	1/1	0.94	0.18	-	50,50,50,50	0
33	MG	0	8043	1/1	0.93	0.05	-	49,49,49,49	0
35	NA	0	9129	1/1	0.57	0.22	-	85,85,85,85	0
37	SR	0	9426	1/1	0.99	0.07	-	67,67,67,67	0
35	NA	0	9110	1/1	0.93	0.14	-	46,46,46,46	0
37	SR	0	9438	1/1	0.98	0.06	-	63,63,63,63	0
33	MG	0	8046	1/1	0.94	0.08	-	40,40,40,40	0
37	SR	0	9601	1/1	-0.14	0.76	-	200,200,200,200	0
35	NA	0	9155	1/1	0.99	0.30	-	55,55,55,55	0
35	NA	0	9102	1/1	0.89	0.28	-	57,57,57,57	0
37	SR	A	9497	1/1	0.99	0.07	-	91,91,91,91	0
37	SR	0	9480	1/1	0.95	0.06	-	87,87,87,87	0
35	NA	0	9182	1/1	0.68	0.20	-	78,78,78,78	0
33	MG	0	8083	1/1	0.98	0.09	-	54,54,54,54	0
33	MG	0	8107	1/1	0.92	0.23	-	67,67,67,67	0
35	NA	0	9184	1/1	0.51	0.50	-	102,102,102,102	0
33	MG	0	8028	1/1	0.94	0.15	-	37,37,37,37	0
37	SR	0	9441	1/1	0.98	0.06	-	60,60,60,60	0
35	NA	0	9159	1/1	0.97	0.11	-	46,46,46,46	0
35	NA	0	9163	1/1	0.84	0.20	-	66,66,66,66	0
37	SR	9	9481	1/1	0.99	0.05	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	9167	1/1	0.92	0.09	-	56,56,56,56	0
37	SR	S	9470	1/1	0.98	0.13	-	100,100,100,100	0
36	CL	N	9307	1/1	0.95	0.14	-	52,52,52,52	0
33	MG	0	8102	1/1	0.96	0.08	-	56,56,56,56	0
37	SR	0	9505	1/1	0.95	0.09	-	85,85,85,85	0
36	CL	0	9303	1/1	0.99	0.12	-	46,46,46,46	0
33	MG	0	8036	1/1	0.95	0.09	-	60,60,60,60	0
33	MG	0	8090	1/1	0.90	0.45	-	80,80,80,80	0
35	NA	0	9136	1/1	0.99	0.11	-	34,34,34,34	0
37	SR	0	9445	1/1	0.98	0.07	-	56,56,56,56	0
33	MG	0	8093	1/1	0.71	0.12	-	42,42,42,42	0
37	SR	B	9458	1/1	0.99	0.06	-	68,68,68,68	0
37	SR	0	9500	1/1	0.80	1.51	-	200,200,200,200	0
37	SR	R	9418	1/1	0.98	0.12	-	54,54,54,54	0
37	SR	0	9425	1/1	0.98	0.10	-	55,55,55,55	0
33	MG	0	8037	1/1	0.94	0.08	-	39,39,39,39	0
35	NA	0	9158	1/1	0.94	0.23	-	63,63,63,63	0
33	MG	0	8076	1/1	0.83	0.12	-	61,61,61,61	0
33	MG	0	8024	1/1	0.81	1.42	-	77,77,77,77	0
36	CL	0	9313	1/1	0.97	0.09	-	51,51,51,51	0
37	SR	0	9435	1/1	0.97	0.08	-	65,65,65,65	0
37	SR	0	9430	1/1	1.00	0.13	-	44,44,44,44	0
35	NA	0	9115	1/1	0.98	0.08	-	39,39,39,39	0
35	NA	0	9108	1/1	0.91	0.10	-	35,35,35,35	0
37	SR	0	9626	1/1	0.89	0.30	-	128,128,128,128	0
37	SR	0	9459	1/1	0.91	0.07	-	101,101,101,101	0
35	NA	0	9101	1/1	0.94	0.15	-	47,47,47,47	0
33	MG	0	8025	1/1	0.99	0.37	-	25,25,25,25	0
35	NA	0	9116	1/1	0.95	0.19	-	58,58,58,58	0
37	SR	0	9412	1/1	0.99	0.12	-	42,42,42,42	0
35	NA	0	9111	1/1	0.95	0.10	-	57,57,57,57	0
37	SR	0	9422	1/1	0.98	0.10	-	54,54,54,54	0
35	NA	0	9141	1/1	0.87	0.10	-	62,62,62,62	0
37	SR	0	9446	1/1	0.98	0.07	-	83,83,83,83	0
33	MG	0	8026	1/1	0.98	0.15	-	27,27,27,27	0
37	SR	9	9503	1/1	0.93	0.04	-	114,114,114,114	0
33	MG	0	8118	1/1	0.85	0.18	-	76,76,76,76	0
33	MG	0	8045	1/1	0.78	0.33	-	84,84,84,84	0
37	SR	0	9452	1/1	0.76	0.20	-	114,114,114,114	0
37	SR	0	9414	1/1	0.98	0.12	-	52,52,52,52	0
37	SR	0	9421	1/1	0.98	0.08	-	64,64,64,64	0
36	CL	0	9322	1/1	0.98	0.15	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	9170	1/1	0.86	0.45	-	94,94,94,94	0
36	CL	A	9309	1/1	0.83	0.14	-	68,68,68,68	0
33	MG	0	8113	1/1	0.88	0.08	-	50,50,50,50	0
33	MG	0	8058	1/1	0.90	0.26	-	45,45,45,45	0
37	SR	0	9448	1/1	1.00	0.05	-	60,60,60,60	0
37	SR	0	9545	1/1	0.98	0.04	-	79,79,79,79	0
37	SR	0	9411	1/1	0.99	0.12	-	40,40,40,40	0
33	MG	0	8106	1/1	0.98	0.04	-	43,43,43,43	0
36	CL	0	9314	1/1	0.99	0.06	-	45,45,45,45	0
37	SR	0	9581	1/1	0.94	0.08	-	121,121,121,121	0
37	SR	0	9465	1/1	0.89	0.07	-	100,100,100,100	0
37	SR	0	9547	1/1	0.54	1.09	-	200,200,200,200	0
33	MG	0	8072	1/1	0.61	0.33	-	96,96,96,96	0
37	SR	0	9560	1/1	0.96	0.07	-	97,97,97,97	0
37	SR	0	9467	1/1	0.96	0.09	-	67,67,67,67	0
37	SR	0	9432	1/1	0.99	0.13	-	62,62,62,62	0
37	SR	0	9537	1/1	0.79	0.14	-	154,154,154,154	0
33	MG	0	8101	1/1	0.92	0.16	-	59,59,59,59	0
37	SR	0	9568	1/1	0.97	0.08	-	75,75,75,75	0
37	SR	0	9461	1/1	0.98	0.04	-	76,76,76,76	0
37	SR	0	9566	1/1	0.96	0.04	-	77,77,77,77	0
37	SR	0	9420	1/1	0.99	0.12	-	56,56,56,56	0
37	SR	0	9508	1/1	0.99	0.05	-	80,80,80,80	0
33	MG	0	8051	1/1	0.96	0.20	-	26,26,26,26	0
37	SR	0	9570	1/1	0.97	0.03	-	98,98,98,98	0
37	SR	0	9522	1/1	0.97	0.04	-	104,104,104,104	0
37	SR	0	9427	1/1	0.98	0.11	-	52,52,52,52	0
35	NA	0	9149	1/1	0.91	0.18	-	42,42,42,42	0
33	MG	0	8115	1/1	0.95	0.12	-	56,56,56,56	0
33	MG	0	8104	1/1	0.89	0.23	-	76,76,76,76	0
33	MG	0	8108	1/1	0.86	0.18	-	74,74,74,74	0
33	MG	0	8061	1/1	0.78	0.11	-	95,95,95,95	0
37	SR	0	9405	1/1	0.95	0.15	-	60,60,60,60	0
33	MG	0	8103	1/1	0.81	0.19	-	62,62,62,62	0
35	NA	D	9151	1/1	0.81	0.11	-	63,63,63,63	0
33	MG	0	8085	1/1	0.87	0.33	-	91,91,91,91	0
37	SR	0	9489	1/1	0.97	0.07	-	85,85,85,85	0
37	SR	0	9495	1/1	0.97	0.08	-	88,88,88,88	0
37	SR	0	9408	1/1	0.99	0.14	-	39,39,39,39	0
36	CL	L	9310	1/1	0.96	0.09	-	54,54,54,54	0
33	MG	0	8117	1/1	0.97	0.09	-	43,43,43,43	0
37	SR	9	9588	1/1	0.94	0.08	-	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8082	1/1	0.45	0.33	-	107,107,107,107	0
35	NA	0	9169	1/1	0.84	0.46	-	104,104,104,104	0
33	MG	0	8047	1/1	0.20	0.48	-	91,91,91,91	0
33	MG	0	8009	1/1	0.98	0.10	-	28,28,28,28	0
37	SR	0	9464	1/1	0.98	0.04	-	74,74,74,74	0
37	SR	0	9469	1/1	0.96	0.05	-	79,79,79,79	0
35	NA	0	9130	1/1	0.97	0.08	-	49,49,49,49	0
37	SR	0	9629	1/1	0.99	0.07	-	65,65,65,65	0
33	MG	9	8095	1/1	0.89	0.20	-	46,46,46,46	0
37	SR	0	9474	1/1	0.94	0.09	-	112,112,112,112	0
33	MG	0	8089	1/1	0.91	0.09	-	54,54,54,54	0
33	MG	0	8084	1/1	0.96	0.73	-	74,74,74,74	0
33	MG	0	8065	1/1	0.69	0.40	-	93,93,93,93	0
33	MG	0	8029	1/1	0.98	0.23	-	33,33,33,33	0
33	MG	0	8099	1/1	0.96	0.10	-	59,59,59,59	0
33	MG	0	8116	1/1	0.95	0.07	-	62,62,62,62	0
35	NA	0	9175	1/1	0.94	0.17	-	52,52,52,52	0
33	MG	0	8059	1/1	0.87	0.37	-	78,78,78,78	0
33	MG	0	8030	1/1	0.92	0.10	-	39,39,39,39	0
37	SR	1	9460	1/1	0.99	0.08	-	52,52,52,52	0
37	SR	0	9413	1/1	1.00	0.10	-	44,44,44,44	0
33	MG	0	8075	1/1	0.97	0.09	-	36,36,36,36	0
33	MG	0	8094	1/1	0.88	0.24	-	67,67,67,67	0
37	SR	0	9529	1/1	0.78	0.15	-	138,138,138,138	0
33	MG	K	8069	1/1	0.98	0.22	-	29,29,29,29	0
37	SR	0	9585	1/1	0.98	0.06	-	83,83,83,83	0
36	CL	0	9317	1/1	0.99	0.05	-	50,50,50,50	0
35	NA	0	9126	1/1	0.86	0.11	-	59,59,59,59	0
37	SR	0	9478	1/1	0.99	0.06	-	70,70,70,70	0
36	CL	R	9306	1/1	0.99	0.14	-	44,44,44,44	0
37	SR	0	9449	1/1	0.99	0.08	-	59,59,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.