



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:41 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : trunk28620

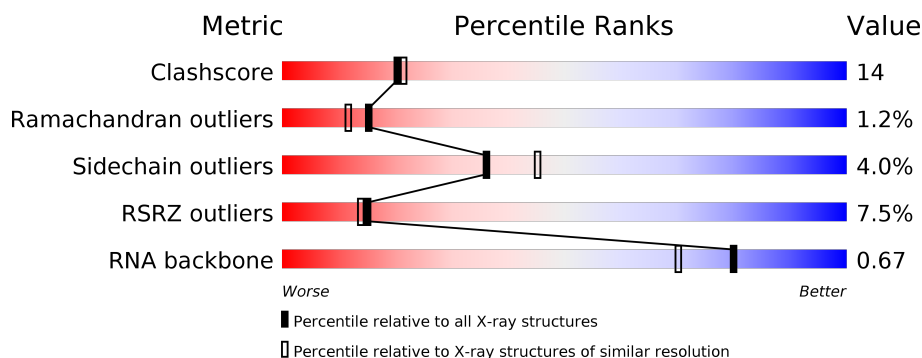
# 1 Overall quality at a glance

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	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)
RNA backbone	2435	1007 (2.74-1.66)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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> <div></div> <div>65%</div> <div>25%</div> <div>• 6%</div> </div> </div>
2	9	122	<div> <div>4%</div> <div> <div></div> <div>60%</div> <div>30%</div> <div>10%</div> </div> </div>
3	4	3	<div> <div></div> <div> <div>33%</div> <div>67%</div> </div> </div>
4	A	240	<div> <div>7%</div> <div> <div></div> <div>58%</div> <div>38%</div> <div>• •</div> </div> </div>
5	B	338	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>35%</div> <div>•</div> </div> </div>
6	C	246	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>33%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
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	
31	3	92	

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Mol	Chain	Length	Quality of chain
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
37	SR	0	9406	-	-	-	X
37	SR	0	9482	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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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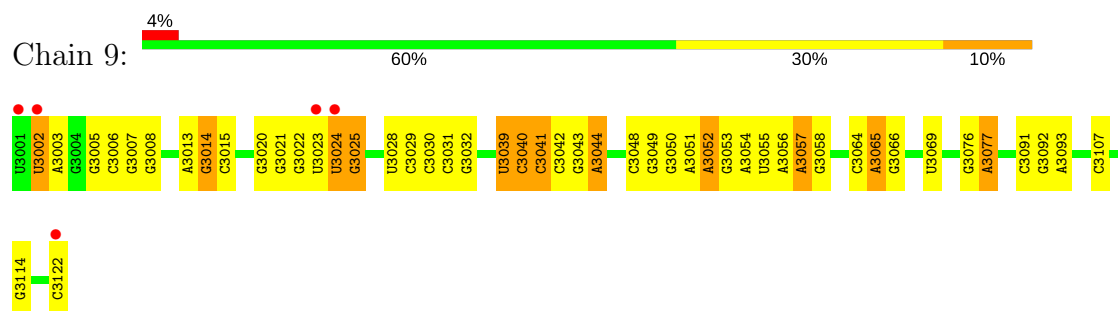
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	Q	49	Total 49	O 49	0	0
39	R	83	Total 83	O 83	0	0
39	S	30	Total 30	O 30	0	0
39	T	36	Total 36	O 36	0	0
39	U	28	Total 28	O 28	0	0
39	V	12	Total 12	O 12	0	0
39	W	68	Total 68	O 68	0	0
39	X	26	Total 26	O 26	0	0
39	Y	93	Total 93	O 93	0	0
39	Z	29	Total 29	O 29	0	0
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





C2881	U2781	A2664	U2541	G2338	C	A	A2067	G1951	U1817	C1700	U	U1561	G1378	A1246
G2882	G2782	A	U2457	A	G	G	G2068	U	C1818	C1701	A	C1562	A1379	C1250
A2883	A2783	U	G2462	C	A	G	G2072	A	G1820	A1701	C	G1563	U1380	C1251
G2884	G2785	G2667	G2465	G	A	G	G2073	C	C1826	U1702	C	C1564	C1384	A1252
A2890	G2786	A2670	G2466	A	C	A	A2074	U	G1827	C1705	A	A1573	C1400	C1253
C2894	U2791	G2670	G2467	C2344	C	U	A2081	A	A1828	C1714	U	C1574	C1268	
C2895	A2792	G2676	A2467	A2345	U	A	G	U	G1828	C1715	G	A1406	A1406	
A2896	G2795	G2679	A2469	C2346	C	C	G2090	A	A1829	A1716	C	G1593	A1407	A1278
C2903	U2796	G2680	C2472	C2347	C	A	G2091	C	U1835	A1717	C	G1594	U1408	U1279
A2906	A2800	A2681	A2476	C2348	A	A	G2094	C	U1838	U1722	U	G1595	G1409	
C2907	U2807	C2682	C2477	A2353	G	G	A2095	U1964	A1839	G1723	U	U1596	U1419	A1287
A2908	U2807	A2694	A2480	A2354	U	A	A2096	C1965	A1840	U1724	C	G1597	A1406	U1288
G2910	U2811	G2697	G2481	A2355	C	U	A2100	U1966	U1845	C1725	C	G1598	C1426	C1289
C2911	A2812	G2698	G2482	G2357	C	C	A2101	U1967	A1846	G1726	C	G1605	G1430	A1291
C2912	A2813	A2699	A2483	A2361	C	C	G2102	G1971	U1847	G1730	C	A1606	G1430	A1294
A2913	G2814	G2700	U2484	A2362	G	G	A2103	U1972	C1883	G1731	C	A1607	U1435	G1295
A2914	G2815	G2704	A2485	A2363	C	C	C2104	G1979	C1856	C1734	C	A1615	G1441	U1298
A	A2816	U2705	A2490	A2365	C	C	G2110	U1980	U1856	C1735	C	U1625	A1442	G1299
G	G2817	G2705	G2491	A2366	U	U	G2118	U1982	G1863	A1736	C	A1626	C1451	U1304
C	A2599	U2711	U2492	A2369	A	A	U2128	U1986	C1864	U1741	C	G1627	A1458	U1306
C	A2600	G2712	C2493	U2265	C	C	U2133	U1996	G1867	G1744	C	A1630	A1462	U1314
A	A2601	U2712	G2374	A2266	G	G	G2134	U2003	G1868	G1745	C	G1634	A1463	
U	G2602	G2715	G2375	U2267	C	C	A2135	U2004	U1877	U1748	C	A1641	A1470	G1327
C	U2607	G2716	U2376	G2270	C	C	G2136	G2005	G1878	U1749	C	A1642	A1470	A1328
A	G2608	G2717	U2377	G2271	C	C	A	C2006	U1879	C1750	C	A1647	U1473	C1331
C	C2608	C2718	U2378	G2272	C	C	G	U2007	C1880	G1751	C	G1647	C1332	C1332
G2831	G2611	A2719	G2503	G2281	C	C	U	U2008	C1881	G1752	C	U1654	U1474	U1333
C2832	A2612	C2720	A2504	G2282	C	C	G	A2011	C1882	C1753	C	G1655	G1476	C1334
U2837	G2613	U2721	G2505	G2283	A	A	U	U2012	G1902	A1754	C	U1656	G1477	
A2838	G2618	G2724	A2506	A2291	G	G	C	U2013	U1903	A1755	C	A1657	A1482	G1340
C2839	C2626	G2725	G2507	G2282	U	U	A	G2014	U1904	G1756	C	A1658	C1483	A1341
A2840	G2627	U2726	A2510	G2283	C	C	G	U2016	A1909	C	C	G1665	C1484	C1343
G2841	U2630	U2735	G2515	A2292	A	A	U	U2017	A1919	U1766	C	U1666	U1503	U1350
G2842	G2631	G2747	G2516	A2293	C	C	A	A2018	A1919	A1767	C	A1667	A1504	G1351
C2850	G2632	U2749	A2414	G2299	G	G	G	A2019	G1926	C1768	C	U1668	U1505	A1352
G2851	A2634	G2750	A2415	A2300	U	U	U	U2032	A1927	C1769	C	A1669	U1506	C1353
A2852	G2635	G2754	G2420	A2301	C	C	A	G2033	G1928	U1770	C	G1670		
U2853	G2636	G2755	G2421	A2302	A	A	C	U2034	C1929	U1771	C	C1675	U1524	C1360
C2857	A2637	G2755	U2422	A2302	A	A	G	A2038	C1940	G1772	C		G1525	
U2858	C2644	C2762	G2426	A2309	U	U	C	A2039	C1941	G1773	C	G1681	A1526	G1363
C2866	U2645	G2765	C2427	G2310	A	A	A	U2043	A1942	A1778	C	A1682	A1527	C1366
G2867	A2649	C2765	G2428	G2313	C	C	U	G2044	C1943	A1779	C	G1683	G1529	
U2876	U2652	A2768	U2435	G2317	C	C	G	A2054	C1946	C1787	C	A1685	A1369	
G2877	G2661	C2769	C2443	G2329	C	C	U	U2064	G1947	U1788	C	G1686	G1552	A1372
U2878	U2662	G2770	G2443	G2330	C	C	G		G1948	G1789	C	C1687	G1555	G1376
A2879	G2663	G2779	G2453	G2337	C	C	U		G1950	C1798	C		A1559	C1377
A2880		C2780	G2453	G2337	U	U	G							

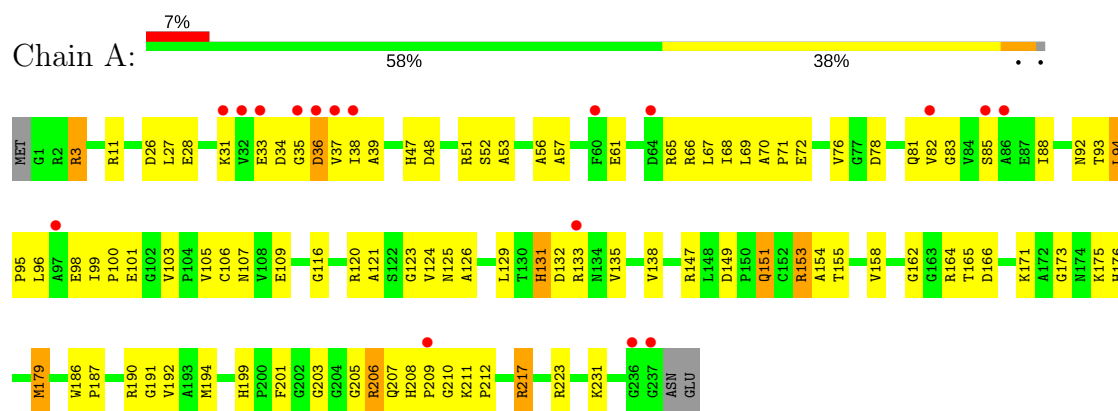
- Molecule 2: 5S ribosomal RNA



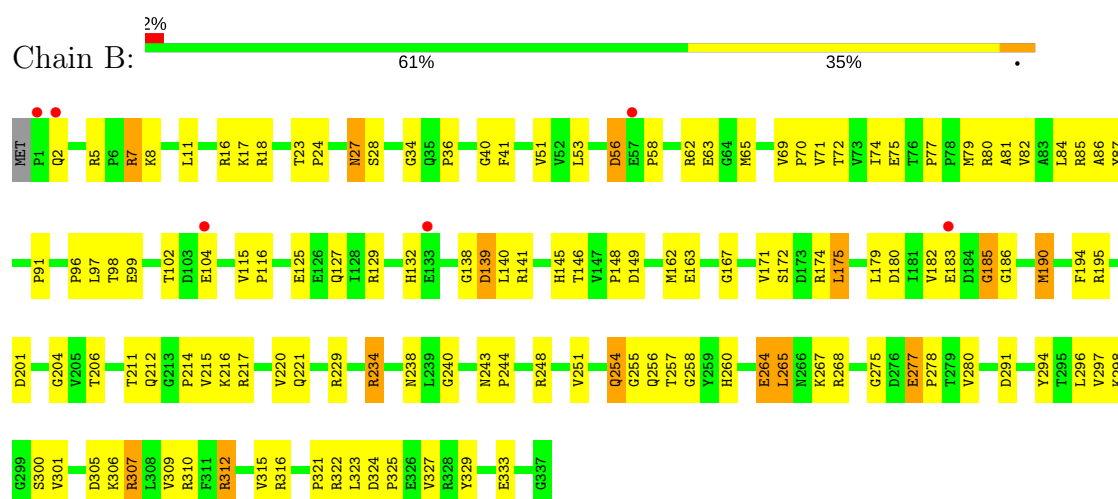
- Molecule 3: 5'-R(\*CP\*CP\*(PPU))-3'



- Molecule 4: 50S ribosomal protein L2P

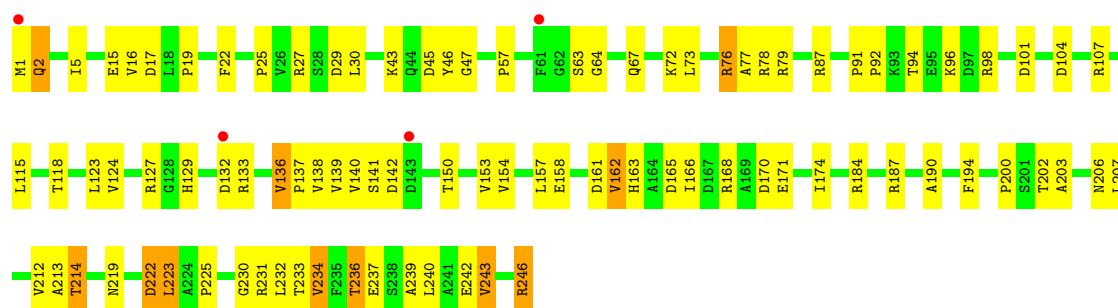


- Molecule 5: 50S ribosomal protein L3P

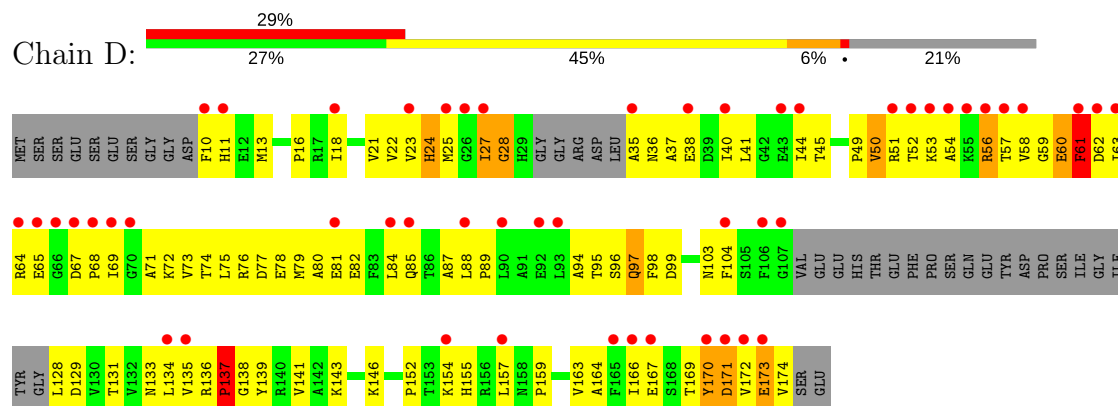


- Molecule 6: 50S ribosomal protein L4E

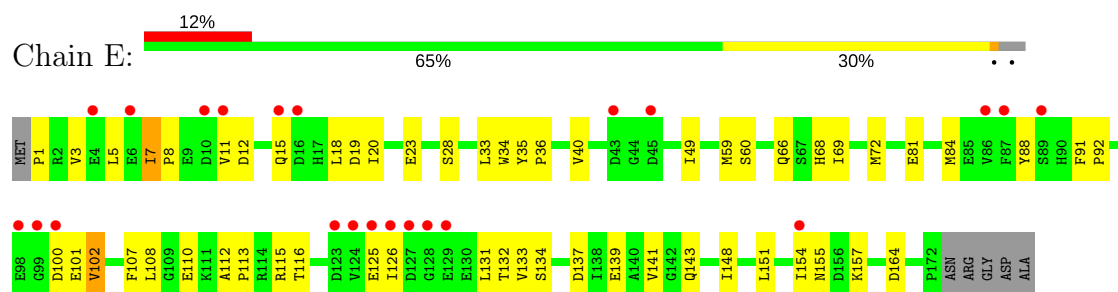




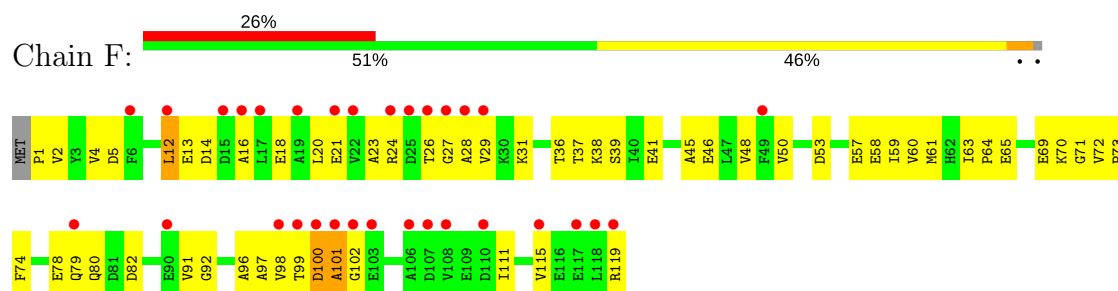
• Molecule 7: 50S ribosomal protein L5P



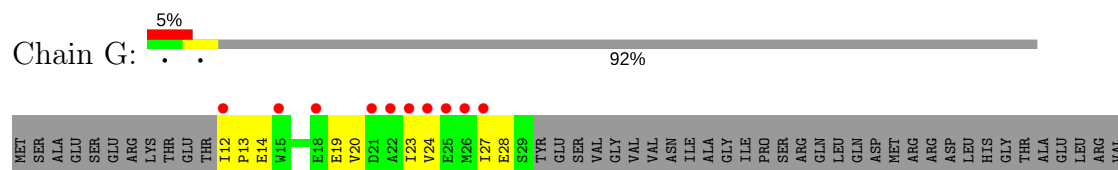
• Molecule 8: 50S ribosomal protein L6P



• Molecule 9: 50S ribosomal protein L7AE

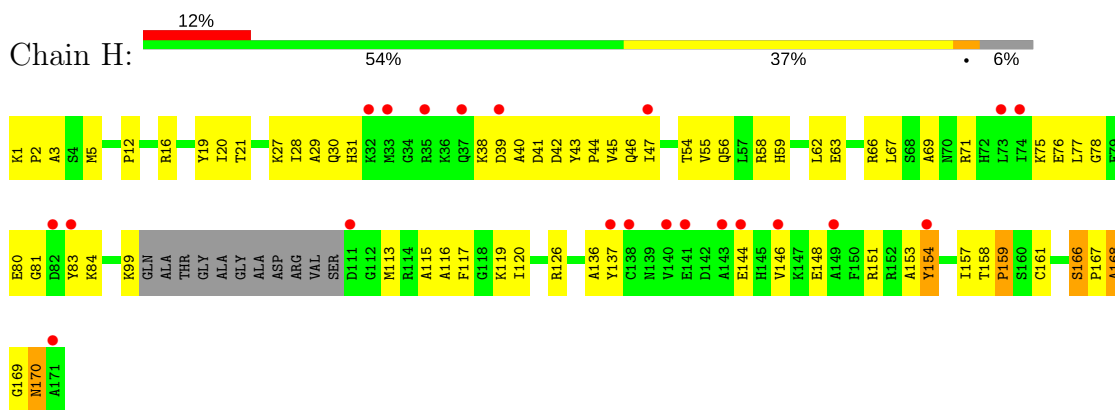


• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

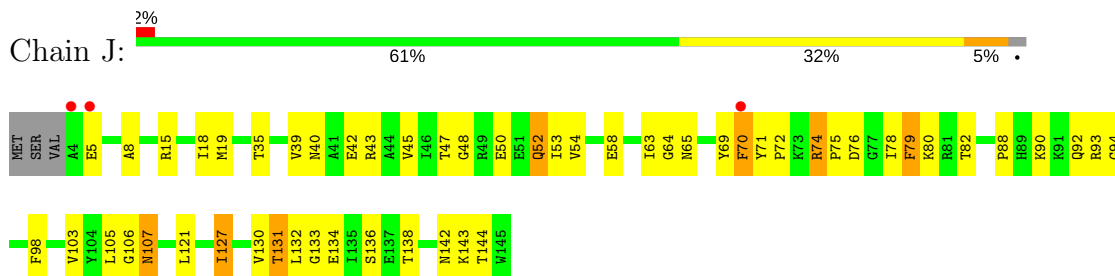




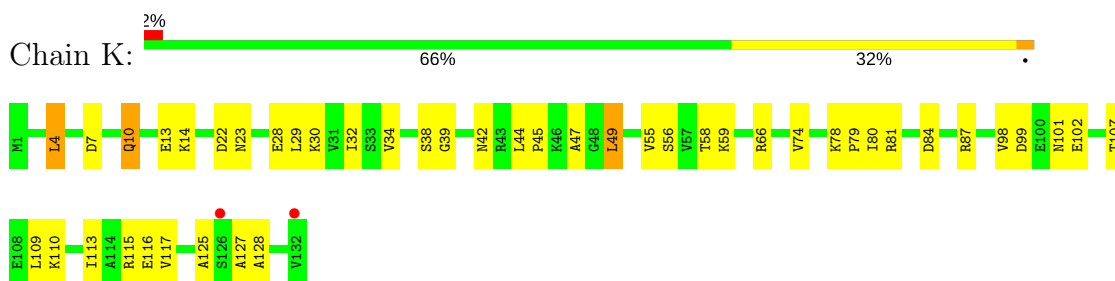
- Molecule 11: 50S RIBOSOMAL PROTEIN L10E



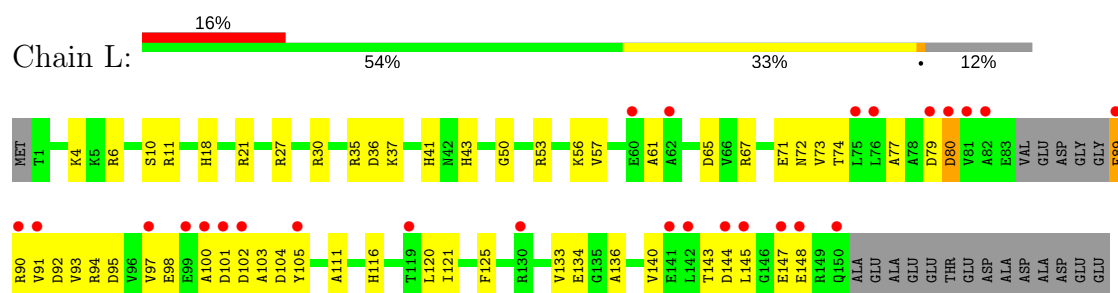
- Molecule 12: 50S ribosomal protein L13P



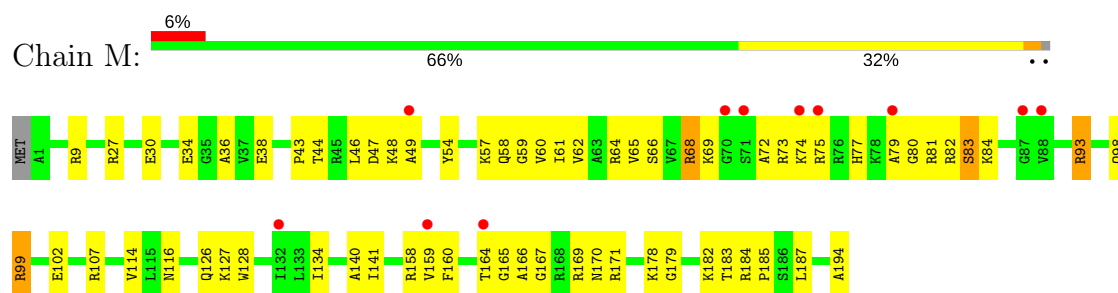
- Molecule 13: 50S ribosomal protein L14P



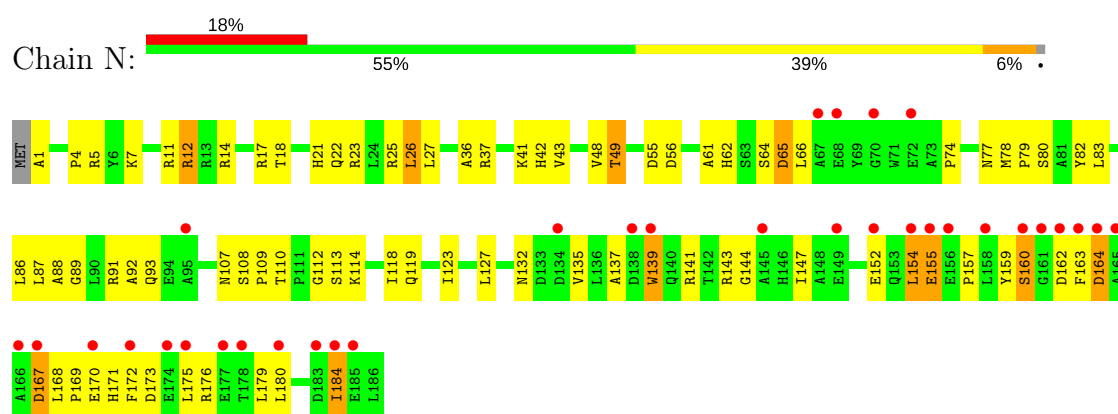
- Molecule 14: 50S ribosomal protein L15P



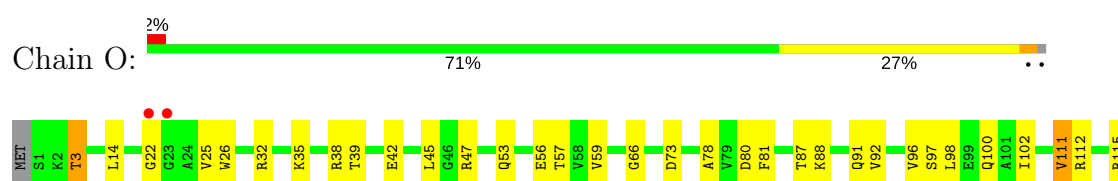
• Molecule 15: 50S Ribosomal Protein L15E



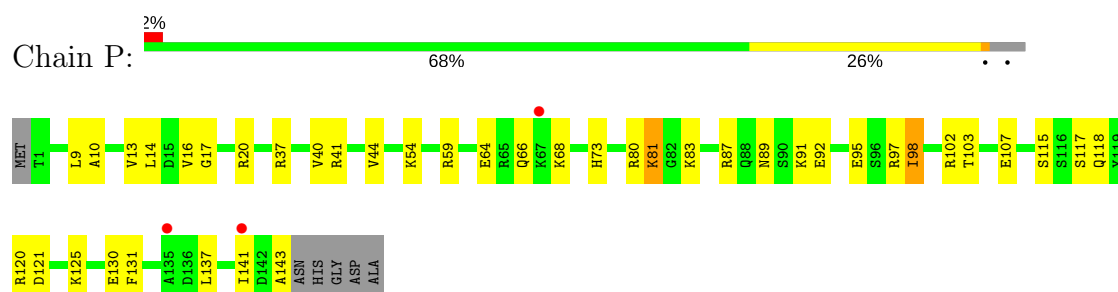
• Molecule 16: 50S ribosomal protein L18P



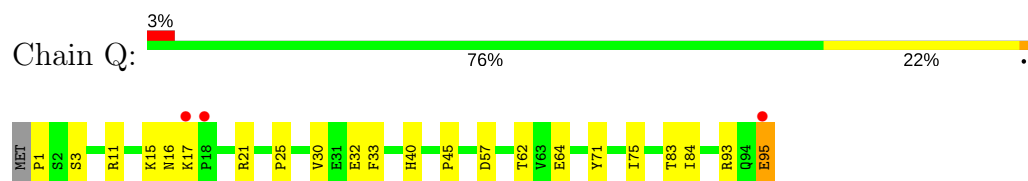
• Molecule 17: 50S ribosomal protein L18e



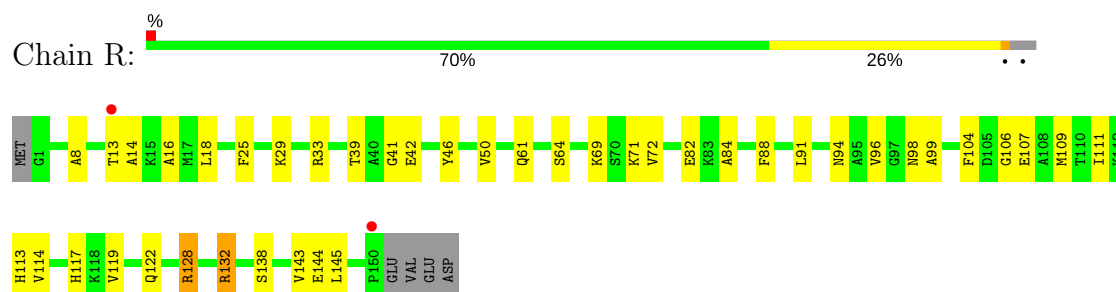
• Molecule 18: 50S ribosomal protein L19E



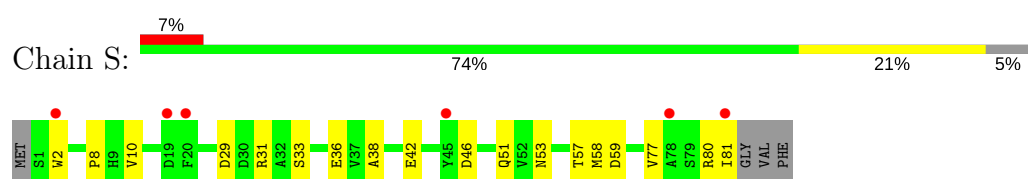
- Molecule 19: 50S ribosomal protein L21e



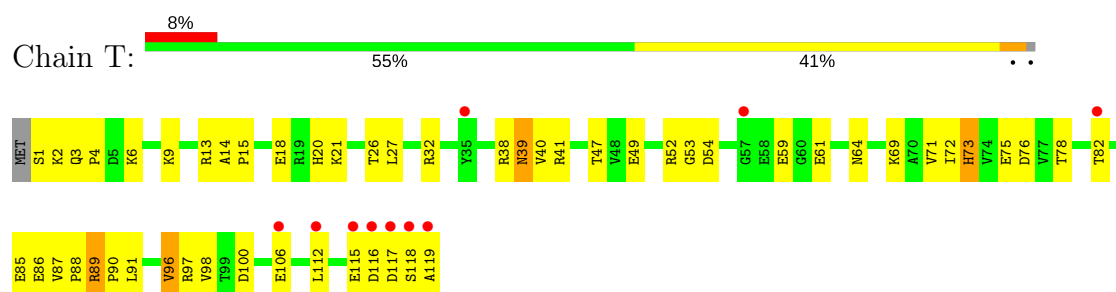
- Molecule 20: 50S ribosomal protein L22P



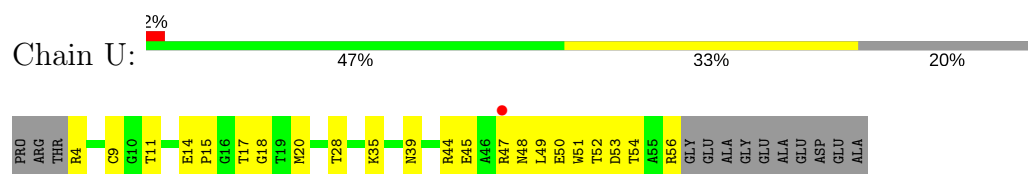
- Molecule 21: 50S ribosomal protein L23P



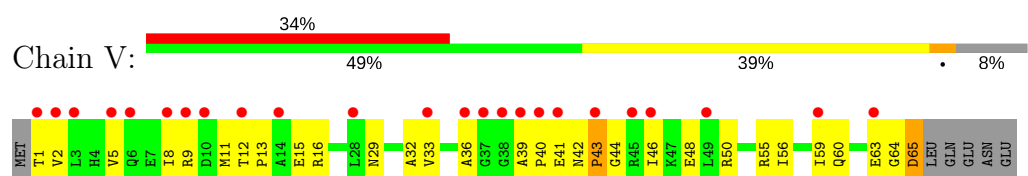
- Molecule 22: 50S ribosomal protein L24P



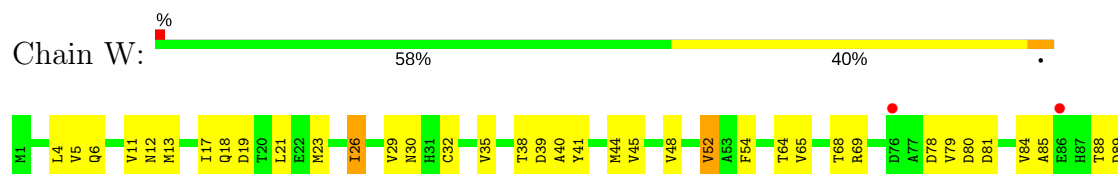
- Molecule 23: 50S ribosomal protein L24E



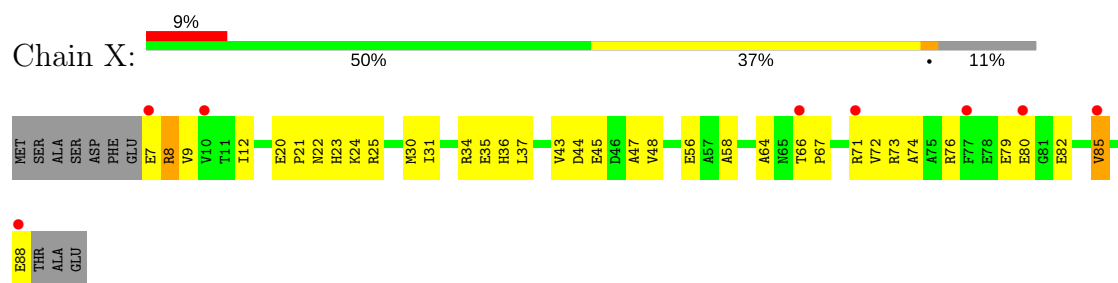
- Molecule 24: 50S ribosomal protein L29P



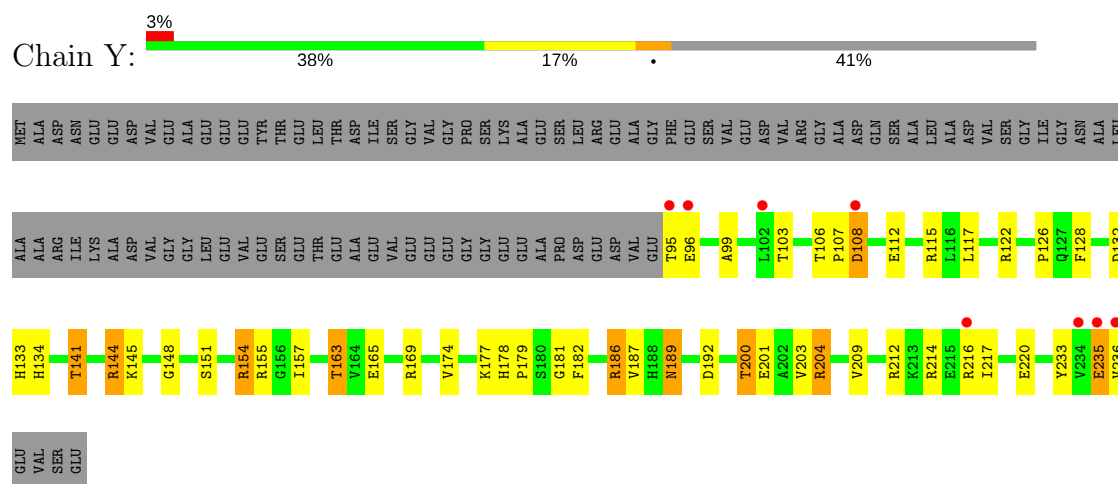
- Molecule 25: 50S ribosomal protein L30P



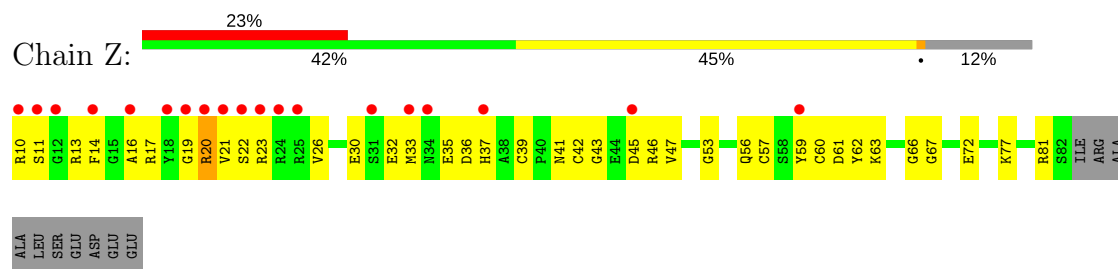
• Molecule 26: 50S ribosomal protein L31e



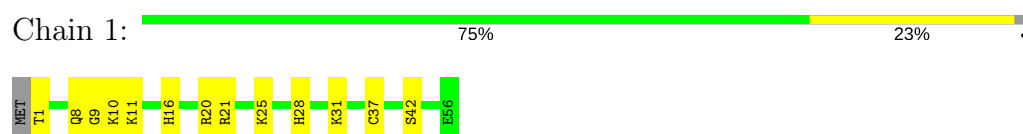
• Molecule 27: 50S ribosomal protein L32E



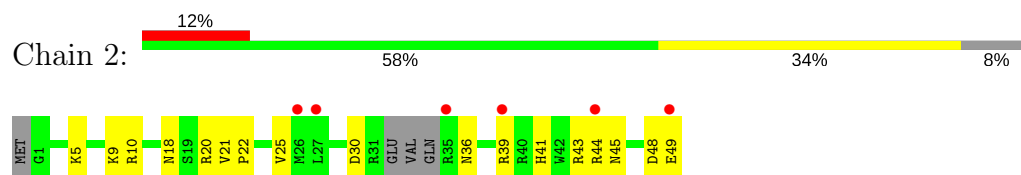
• Molecule 28: 50S ribosomal protein L37Ae



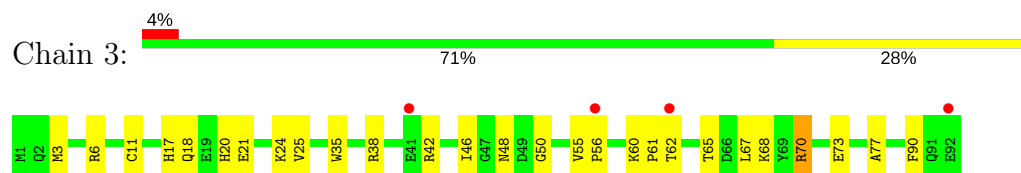
• Molecule 29: 50S ribosomal protein L37e



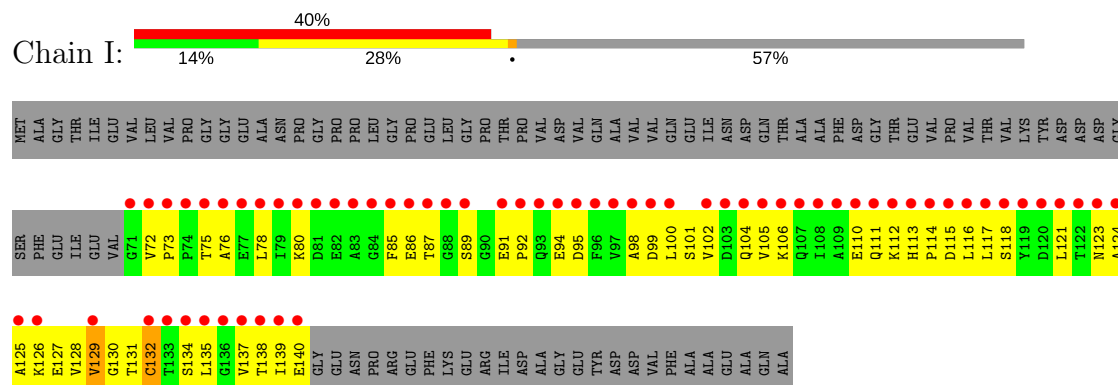
## ● Molecule 30: 50S ribosomal protein L39e



## ● 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	42.0	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	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 <sup>2</sup> )	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.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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:O:1160:G:H5'	1:O: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%)	20	18
5	B	335/338 (99%)	315 (94%)	16 (5%)	4 (1%)	15	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%)	4	2
10	G	25/348 (7%)	25 (100%)	0	0	100	100
11	H	156/171 (91%)	137 (88%)	15 (10%)	4 (3%)	6	3
12	J	140/145 (97%)	132 (94%)	5 (4%)	3 (2%)	8	5
13	K	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
14	L	141/165 (86%)	119 (84%)	20 (14%)	2 (1%)	13	10
15	M	192/195 (98%)	183 (95%)	8 (4%)	1 (0%)	32	34
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%)	20	18
23	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
24	V	63/71 (89%)	58 (92%)	4 (6%)	1 (2%)	11	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%)	5	2
All	All	3705/4431 (84%)	3432 (93%)	228 (6%)	45 (1%)	15	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%)	22	25
5	B	282/283 (100%)	265 (94%)	17 (6%)	22	25
6	C	193/193 (100%)	176 (91%)	17 (9%)	12	11
7	D	117/148 (79%)	111 (95%)	6 (5%)	28	33
8	E	152/156 (97%)	147 (97%)	5 (3%)	43	54
9	F	93/94 (99%)	92 (99%)	1 (1%)	78	88
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	128 (97%)	4 (3%)	46	58
12	J	118/121 (98%)	111 (94%)	7 (6%)	23	26
13	K	106/106 (100%)	102 (96%)	4 (4%)	38	47
14	L	113/127 (89%)	110 (97%)	3 (3%)	50	62
15	M	158/159 (99%)	153 (97%)	5 (3%)	44	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	N	149/150 (99%)	144 (97%)	5 (3%)	42	53
17	O	93/94 (99%)	91 (98%)	2 (2%)	57	70
18	P	113/117 (97%)	111 (98%)	2 (2%)	64	77
19	Q	79/80 (99%)	76 (96%)	3 (4%)	38	47
20	R	117/122 (96%)	115 (98%)	2 (2%)	66	79
21	S	71/74 (96%)	71 (100%)	0	100	100
22	T	105/106 (99%)	101 (96%)	4 (4%)	38	47
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	60	74
25	W	130/130 (100%)	125 (96%)	5 (4%)	38	47
26	X	66/74 (89%)	62 (94%)	4 (6%)	22	25
27	Y	120/196 (61%)	107 (89%)	13 (11%)	7	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%)	54	67
31	3	79/79 (100%)	78 (99%)	1 (1%)	73	85
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3612 (86%)	2970 (96%)	123 (4%)	36	45

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%)	0
2	9	121/122 (99%)	16 (13%)	0
3	4	1/3 (33%)	0	0
All	All	2867/3047 (94%)	248 (8%)	0

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

There are no RNA pucker outliers to report.

## 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	14,22,23	1.05	1 (7%)	18,31,34	3.63	2 (11%)
1	OMG	0	2588	1,3	18,26,27	1.03	1 (5%)	22,38,41	2.49	5 (22%)
1	UR3	0	2619	1	14,22,23	0.82	1 (7%)	16,32,35	0.72	0
1	PSU	0	2621	1	16,21,22	1.63	3 (18%)	20,30,33	6.10	5 (25%)
1	1MA	0	628	1	16,25,26	0.99	1 (6%)	13,37,40	1.13	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PPU	4	76	1,3	31,40,41	1.12	1 (3%)	34,57,60	0.93	2 (5%)

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 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	76	PPU	OC-CM	-5.46	1.26	1.42
1	0	2621	PSU	C5-C1'	-4.64	1.48	1.52
1	0	2619	UR3	C6-C5	-2.24	1.33	1.38
1	0	628	1MA	C6-N6	2.75	1.33	1.27
1	0	2621	PSU	C4-N3	2.86	1.38	1.33

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-18.86	114.84	128.40
1	0	2621	PSU	C5-C4-N3	-13.21	114.59	125.43
1	0	2588	OMG	C5-C6-N1	-8.35	111.59	123.48
1	0	628	1MA	C2-N3-C4	-3.59	110.90	116.41
1	0	2587	OMU	C5-C4-N3	-3.51	114.74	123.12

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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 [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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	0	2749/2922 (94%)	-0.24	90 (3%) 47 44	26, 46, 90, 148	0
2	9	122/122 (100%)	-0.01	5 (4%) 38 36	39, 62, 87, 147	0
3	4	2/3 (66%)	-0.54	0 100 100	52, 52, 52, 62	0
4	A	237/240 (98%)	0.43	17 (7%) 16 15	30, 52, 82, 104	0
5	B	337/338 (99%)	0.12	6 (1%) 69 66	31, 50, 72, 85	0
6	C	246/246 (100%)	-0.05	4 (1%) 72 70	28, 47, 68, 81	0
7	D	140/177 (79%)	1.79	51 (36%) 0 0	56, 90, 119, 127	0
8	E	172/178 (96%)	0.64	22 (12%) 4 4	42, 60, 78, 83	0
9	F	119/120 (99%)	1.16	31 (26%) 1 1	47, 71, 99, 108	0
10	G	29/348 (8%)	2.60	17 (58%) 0 0	68, 89, 97, 98	0
11	H	160/171 (93%)	0.65	21 (13%) 4 3	44, 60, 92, 99	0
12	J	142/145 (97%)	-0.08	3 (2%) 64 61	36, 47, 66, 86	0
13	K	132/132 (100%)	-0.17	2 (1%) 74 72	34, 45, 66, 69	0
14	L	145/165 (87%)	0.73	26 (17%) 2 1	30, 64, 110, 119	0
15	M	194/195 (99%)	0.41	11 (5%) 24 24	35, 46, 67, 79	0
16	N	186/187 (99%)	0.80	33 (17%) 2 1	44, 62, 104, 112	0
17	O	115/116 (99%)	0.03	2 (1%) 70 68	41, 53, 66, 74	0
18	P	143/149 (95%)	0.13	3 (2%) 64 61	40, 51, 65, 78	0
19	Q	95/96 (98%)	0.01	3 (3%) 48 46	41, 47, 63, 74	0
20	R	150/155 (96%)	-0.11	2 (1%) 77 75	31, 44, 62, 70	0
21	S	81/85 (95%)	0.38	6 (7%) 15 14	43, 62, 82, 95	0
22	T	119/120 (99%)	0.61	10 (8%) 12 10	43, 56, 79, 107	0
23	U	53/66 (80%)	0.31	1 (1%) 67 65	42, 51, 67, 75	0
24	V	65/71 (91%)	2.03	24 (36%) 0 0	54, 78, 111, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	154/154 (100%)	-0.03	2 (1%) 77 75	36, 48, 69, 78	0
26	X	82/92 (89%)	0.56	8 (9%) 8 7	41, 53, 79, 97	0
27	Y	142/241 (58%)	0.12	8 (5%) 25 24	31, 43, 62, 82	0
28	Z	73/83 (87%)	0.93	19 (26%) 1 1	49, 73, 86, 92	0
29	1	56/57 (98%)	-0.45	0 100 100	30, 35, 42, 50	0
30	2	46/50 (92%)	0.66	6 (13%) 4 3	38, 58, 73, 83	0
31	3	92/92 (100%)	0.15	4 (4%) 36 34	37, 55, 68, 79	0
32	I	70/162 (43%)	5.46	64 (91%) 0 0	107, 120, 137, 139	0
All	All	6648/7478 (88%)	0.19	501 (7%) 15 14	26, 51, 95, 148	0

The worst 5 of 501 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	16.8
24	V	1	THR	15.5
7	D	63	ILE	14.0
32	I	133	THR	13.3
32	I	96	PHE	12.1

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	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 [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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( $\text{\AA}^2$ )	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

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	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.