



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 12:57 pm BST

PDB ID : 1VQP
Title : The structure of the transition state analogue "RAP" bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.25 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

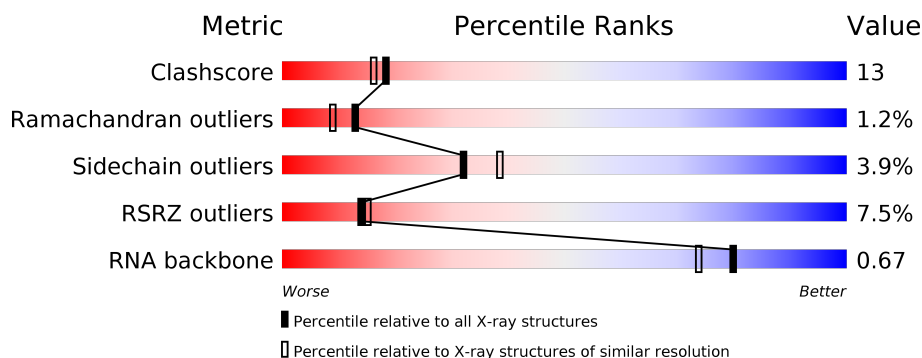
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)
RNA backbone	3102	1016 (2.66-1.86)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>25%</div> <div>5%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>6%</div> <div> <div></div> <div>57%</div> <div>34%</div> <div>7%</div> </div> </div>
3	4	8	<div> <div></div> <div> <div>38%</div> <div>63%</div> </div> </div>
4	A	240	<div> <div>6%</div> <div> <div></div> <div>63%</div> <div>32%</div> <div>5%</div> </div> </div>
5	B	338	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>33%</div> </div> </div>
6	C	246	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>29%</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	8022	-	-	-	X
33	MG	0	8024	-	-	-	X
33	MG	0	8059	-	-	-	X
35	NA	0	9118	-	-	-	X
35	NA	0	9125	-	-	-	X
35	NA	0	9169	-	-	-	X
35	NA	S	9112	-	-	-	X
37	SR	0	9500	-	-	-	X
37	SR	0	9547	-	-	-	X

2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 99070 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*(DC)P*(DC)P*(PPU)*(LOF)P*(PO2)P*AP*C*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	8	Total	C	N	O	P	0	0	0
			132	67	23	37	5			

- 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	A	2	Total	Mg	0	0
			2	2		
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	3	Total	K	0	0
			3	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	64	Total	Na	0	0
			64	64		

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	10	Total 10	Cl 10	0	0
36	J	3	Total 3	Cl 3	0	0
36	B	1	Total 1	Cl 1	0	0
36	A	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	O	1	Total 1	Cl 1	0	0
36	R	1	Total 1	Cl 1	0	0
36	Y	1	Total 1	Cl 1	0	0
36	L	1	Total 1	Cl 1	0	0
36	3	1	Total 1	Cl 1	0	0

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

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

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

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

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

- Molecule 39 is water.

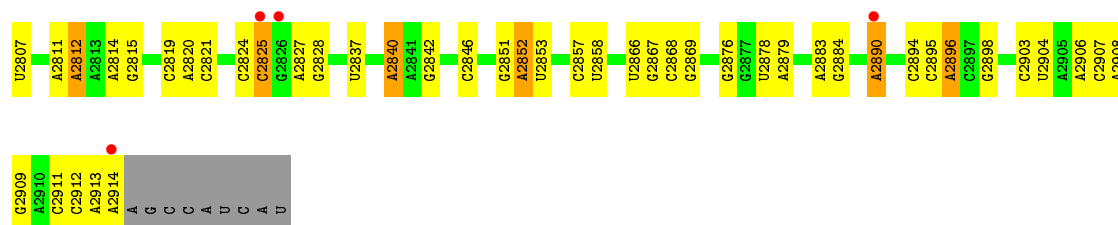
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	0	5757	Total O 5757 5757	0	0
39	9	139	Total O 139 139	0	0
39	4	6	Total O 6 6	0	0
39	A	124	Total O 124 124	0	0
39	B	140	Total O 140 140	0	0
39	C	172	Total O 172 172	0	0
39	D	50	Total O 50 50	0	0
39	E	40	Total O 40 40	0	0
39	F	25	Total O 25 25	0	0
39	G	16	Total O 16 16	0	0
39	H	69	Total O 69 69	0	0
39	J	52	Total O 52 52	0	0
39	K	59	Total O 59 59	0	0
39	L	83	Total O 83 83	0	0
39	M	131	Total O 131 131	0	0
39	N	58	Total O 58 58	0	0
39	O	39	Total O 39 39	0	0
39	P	57	Total O 57 57	0	0
39	Q	51	Total O 51 51	0	0
39	R	87	Total O 87 87	0	0
39	S	32	Total O 32 32	0	0

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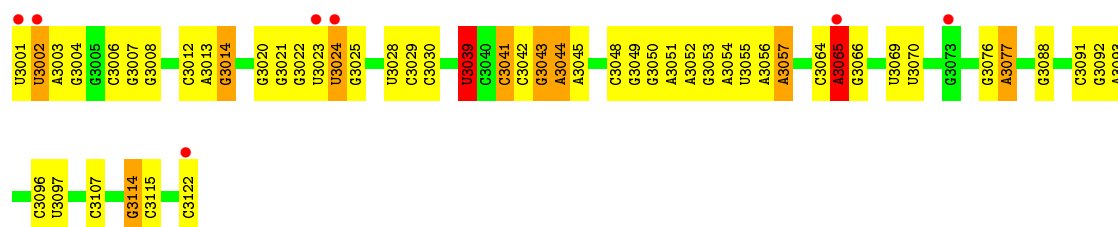
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	T	36	Total 36	O 36	0	0
39	U	30	Total 30	O 30	0	0
39	V	11	Total 11	O 11	0	0
39	W	72	Total 72	O 72	0	0
39	X	24	Total 24	O 24	0	0
39	Y	88	Total 88	O 88	0	0
39	Z	31	Total 31	O 31	0	0
39	1	49	Total 49	O 49	0	0
39	2	38	Total 38	O 38	0	0
39	3	66	Total 66	O 66	0	0
39	I	9	Total 9	O 9	0	0

G2670	A2465	G	C	U	U	G2682	A	U	U1835	U1722	C1593	U1419	A1181
U2671	G2466	A	U	G	A	A2083	U	G	U1838	G1723	C1594	U1422	C1182
C2676	A2467	C	C	A	A	G2090	G	A	A1839	U1724	U1596	C1423	C1183
G2679	A2468	G	G2237	C	C	G2091	C	C	A1840	C1725	A1597	G1426	U1185
A2680	C2346	C	A2238	C	C	A2096	U1964	U1964	A1845	G1730	A1598	U1432	U1186
A2681	C2345	C	C2239	G	G	A2101	U1965	U1965	U1846	C1731	A1603	U1432	U1187
C2682	A2345	C	U2240	G	G	G2102	A1966	A1966	A1847	A1732	G1604	G1441	A1188
U2690	A2346	C	C2243	C	C	A2103	U1967	U1967	A1853	A1733	A1605	A1442	A1189
A2694	C2346	C	A2250	C	C	C2104	G1971	G1971	C1853	A1736	A1607	A458	A1192
U2699	A2347	C	G2251	C	C	G2110	U1972	U1972	C1856	G1739	C1613	A458	A1193
U2699	U2478	C	A2252	G	G	G2111	A1973	A1973	U1846	A1732	G1604	C1462	A1194
A2699	C2347	C	G2253	C	C	A2112	U1974	U1974	A1847	A1733	A1605	A1463	G1195
C2699	A2348	C	A2258	C	C	G2113	U1979	U1979	C1853	A1736	A1607	A458	G1196
U2700	A2349	C	U2265	A	A	G2128	U1980	U1980	U1847	A1733	A1605	A1463	G1197
G2701	A2350	C	A2266	G	G	U2133	A1981	A1981	C1856	G1739	C1613	A458	U1198
A2702	C2349	C	G2270	C	C	G2134	C1982	C1982	U1847	A1733	A1605	A1463	A1199
G2716	A2350	C	G2271	C	C	A2135	U1992	U1992	G1873	U1748	C1630	A1476	A1200
C2717	C2349	C	G2272	C	C	G2136	U1996	U1996	U1874	G1751	A1630	C1477	A1201
A2718	G2379	C	G2283	C	C	A	U1996	U1996	G1877	G1752	C1633	A1482	G1202
A2719	A2502	C	A2291	C	C	U2003	U2003	U2003	U1878	C1753	G1634	C1483	G1203
C2720	A2503	C	A2291	C	C	U2004	U2004	U2004	C1880	A1754	A1641	U1503	C1204
U2721	G2505	C	A2291	C	C	U2005	U2005	U2005	U1879	G1755	A1642	A1504	U1205
G2722	A2506	C	G2299	C	C	U2006	U2006	U2006	C1884	G1756	A1656	U1505	G1211
C2723	A2507	C	A2300	C	C	U2007	U2007	U2007	G1884	G1760	A1656	U1505	C1212
U2724	C2508	C	A2301	C	C	U2008	U2008	U2008	G1902	G1766	A1659	U1506	G1213
G2725	A2509	C	A2302	C	C	U2009	U2009	U2009	U1903	A1767	G1660	U1506	C1214
U2726	C2510	C	A2302	C	C	U2011	U2011	U2011	A1909	C1768	C1666	A1522	A1215
A2727	A2511	C	C2309	C	C	U2012	U2012	U2012	A1919	C1769	A1667	U1524	G1216
G2738	U2512	C	C2309	C	C	U2013	U2013	U2013	C1920	G1773	U1668	U1524	A1217
U2747	A2521	C	C2313	C	C	U2014	U2014	U2014	A1919	A1778	A1683	U1525	U1218
G2748	G2524	C	G2314	C	C	U2015	U2015	U2015	C1920	A1779	A1683	A1526	U1219
U2749	C2525	C	G2315	C	C	U2016	U2016	U2016	A1921	A1779	A1683	A1527	G1226
G2750	A2526	C	G2316	C	C	U2017	U2017	U2017	A1922	A1779	A1683	A1528	A1230
A2761	C2526	C	G2317	C	C	U2018	U2018	U2018	G1926	C1786	A1683	G1529	A1231
C2762	U2531	C	U2320	C	C	U2019	U2019	U2019	A1927	C1787	A1683	G1552	A1232
U2768	A2532	C	A2321	C	C	U2020	U2020	U2020	C1928	C1787	A1683	G1552	A1233
G2769	C2533	C	U2322	C	C	U2021	U2021	U2021	G1929	C1788	A1683	G1555	U1234
U2770	A2534	C	G2323	C	C	U2022	U2022	U2022	A1942	G1789	C1686	U1559	A1235
A2779	C2535	C	U2323	C	C	U2023	U2023	U2023	C1943	U1794	C1687	U1561	A1236
C2780	U2536	C	U2326	C	C	U2024	U2024	U2024	A1943	G1795	C1687	U1561	U1237
U2781	A2537	C	C2329	C	C	U2025	U2025	U2025	C1946	A1796	C1687	U1561	A1238
A2784	C2538	C	U2330	C	C	U2026	U2026	U2026	G1947	A1797	C1687	U1561	G1239
U2795	U2541	C	G2333	C	C	U2027	U2027	U2027	U1948	C1798	C1687	U1561	A1242
U2796	C2542	C	C2334	C	C	U2028	U2028	U2028	G1949	G1799	C1687	U1561	C1243
A2800	U2543	C	C2335	C	C	U2029	U2029	U2029	U1950	G1809	C1687	U1561	C1244
	C2544	C	C2335	C	C	U2030	U2030	U2030	U1951	G1809	C1687	U1561	C1245
	U2545	C	G2338	C	C	U2031	U2031	U2031	U1952	C1818	C1687	U1561	A1246
	C2546	C	A	C	C	U2032	U2032	U2032	U1953	G1819	C1687	U1561	A1247
	U2547	C	C	C	C	U2033	U2033	U2033	U1954	A1820	C1687	U1561	C1250
	C2548	C	A	C	C	U2034	U2034	U2034	U1955	A1821	C1687	U1561	C1251
	U2549	C	A	C	C	U2035	U2035	U2035	U1956	A1822	C1687	U1561	
	C2552	C	A	C	C	U2036	U2036	U2036	U1957	A1823	C1687	U1561	
	A2553	C	A	C	C	U2037	U2037	U2037	U1958	A1824	C1687	U1561	
		C	A	C	C	U2038	U2038	U2038	U1959	A1825	C1687	U1561	
		A	A	C	C	U2039	U2039	U2039	U1960	A1826	C1687	U1561	
		U	A	C	C	U2040	U2040	U2040	U1961	A1827	C1687	U1561	
		C	A	C	C	U2041	U2041	U2041	U1962	A1828	C1687	U1561	
		C	A	C	C	U2042	U2042	U2042	U1963	A1829	C1687	U1561	
		C	A	C	C	U2043	U2043	U2043	U1964	A1830	C1687	U1561	
		C	A	C	C	U2044	U2044	U2044	U1965	A1831	C1687	U1561	
		C	A	C	C	U2045	U2045	U2045	U1966	A1832	C1687	U1561	
		C	A	C	C	U2046	U2046	U2046	U1967	A1833	C1687	U1561	
		C	A	C	C	U2047	U2047	U2047	U1968	A1834	C1687	U1561	
		C	A	C	C	U2048	U2048	U2048	U1969	A1835	C1687	U1561	
		C	A	C	C	U2049	U2049	U2049	U1970	A1836	C1687	U1561	
		C	A	C	C	U2050	U2050	U2050	U1971	A1837	C1687	U1561	
		C	A	C	C	U2051	U2051	U2051	U1972	A1838	C1687	U1561	
		C	A	C	C	U2052	U2052	U2052	U1973	A1839	C1687	U1561	
		C	A	C	C	U2053	U2053	U2053	U1974	A1840	C1687	U1561	
		C	A	C	C	U2054	U2054	U2054	U1975	A1841	C1687	U1561	
		C	A	C	C	U2055	U2055	U2055	U1976	A1842	C1687	U1561	
		C	A	C	C	U2056	U2056	U2056	U1977	A1843	C1687	U1561	
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		C	A	C	C	U2059	U2059	U2059	U1980	A1846	C1687	U1561	
		C	A	C	C	U2060	U2060	U2060	U1981	A1847	C1687	U1561	
		C	A	C	C	U2061	U2061	U2061	U1982	A1848	C1687	U1561	
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		C	A	C	C	U2063	U2063	U2063	U1984	A1850	C1687	U1561	
		C	A	C	C	U2064	U2064	U2064	U1985	A1851	C1687	U1561	
		C	A	C	C	U2065	U2065	U2065	U1986	A1852	C1687	U1561	
		C	A	C	C	U2066	U2066	U2066	U1987	A1853	C1687	U1561	
		C	A	C	C	U2067	U2067	U2067	U1988	A1854	C1687	U1561	
		C	A	C	C	U2068	U2068	U2068	U1989	A1855	C1687	U1561	
		C	A	C	C	U2069	U2069	U2069	U1990	A1856	C1687	U1561	
		C	A	C	C	U2070	U2070	U2070	U1991	A1857	C1687	U1561	
		C	A	C	C	U2071	U2071	U2071	U1992	A1858	C1687	U1561	
		C	A	C	C	U2072	U2072	U2072	U1993	A1859	C1687	U1561	
		C	A	C	C	U2073	U2073	U2073	U1994	A1860	C1687	U1561	
		C	A	C	C	U2074	U2074	U2074	U1995	A1861	C1687	U1561	
		C	A	C	C	U2075	U2075	U2075	U1996	A1862	C1687	U1561	
		C	A	C	C	U2076	U2076	U2076	U1997	A1863	C1687	U1561	
		C	A	C	C	U2077	U2077	U2077	U1998	A1864	C1687	U1561	
		C	A	C	C	U2078	U2078	U2078	U1999	A1865	C1687	U1561	
		C	A	C	C	U2079	U2079	U2079	U2000	A1866	C1687	U1561	
		C	A	C	C	U2080	U2080	U2080	U2001	A1867	C1687	U1561	
		C	A	C	C	U2081	U2081	U2081	U2002	A1868	C1687	U1561	
		C	A	C	C	U2082	U2082	U2082	U2003	A1869	C1687	U1561	
		C	A	C	C	U2083	U2083	U2083	U2004	A1870	C1687	U1561	
		C	A	C	C	U2084	U2084	U2084	U2005	A1871	C1687	U1561	
		C	A	C	C	U2085	U2085	U2085	U2006	A1872	C1687	U1561	
		C	A	C	C	U2086	U2086	U2086	U2007	A1873	C1687	U1561	
		C	A	C	C	U2087	U2087	U2087	U2008	A1874	C1687	U1561	
		C	A	C	C	U2088	U2088	U2088	U2009	A1875	C1687	U1561	
		C	A	C	C	U2089	U2089	U2089	U2010	A1876	C1687	U1561	
		C	A	C	C	U2090	U2090	U2090	U2011	A1877	C1687	U1561	
		C	A	C	C	U2091	U2091	U2091	U2012	A1878	C1687	U1561	
		C	A	C	C	U2092	U2092	U2092	U2013	A18			



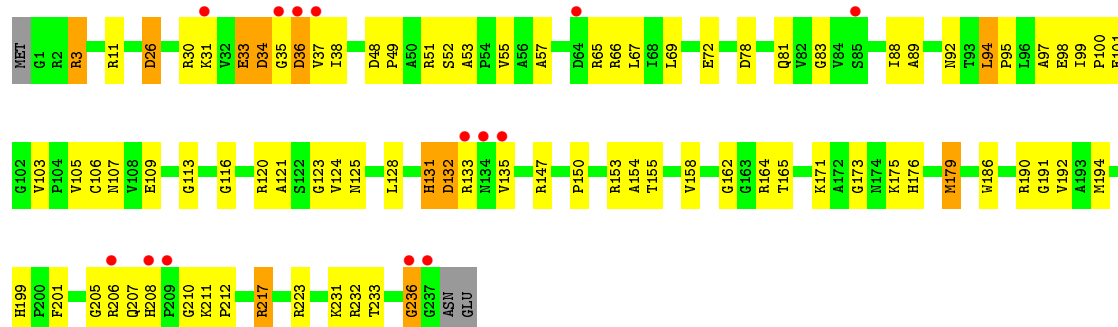
• Molecule 2: 5S ribosomal RNA



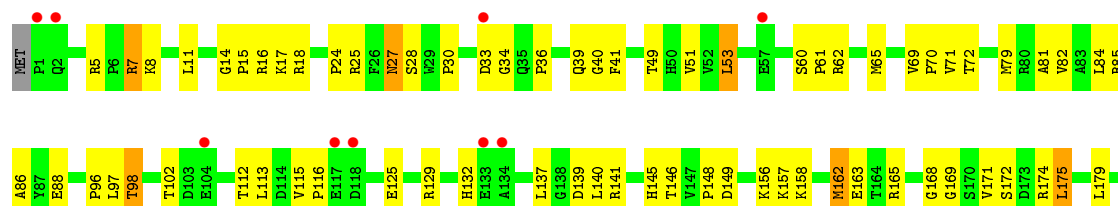
• Molecule 3: 5'-R*(DC)P*(DC)P*(PPU)*(LOF)P*(PO2)P*AP*C*C)-3'

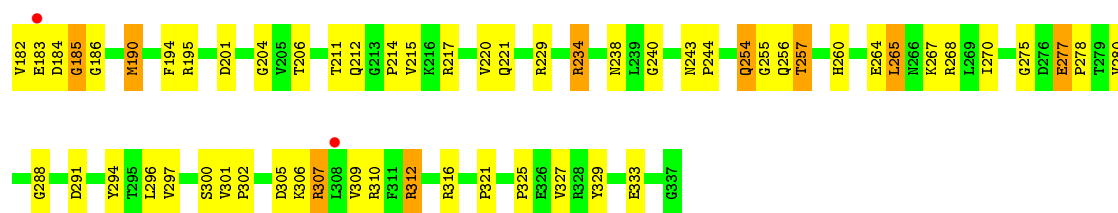


• Molecule 4: 50S ribosomal protein L2P

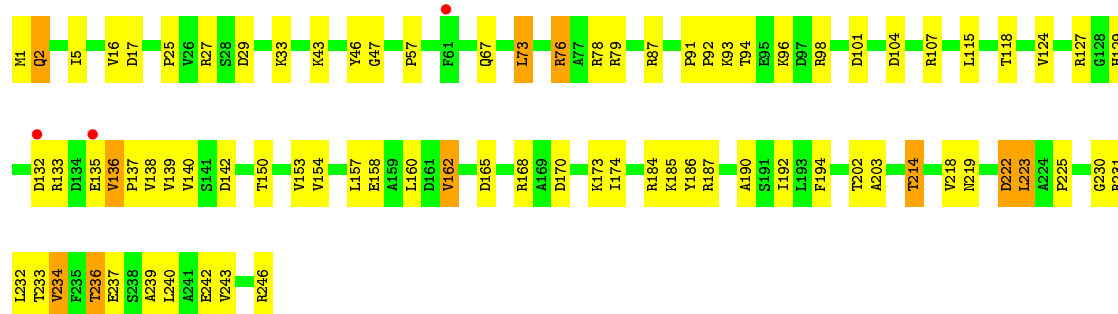


• Molecule 5: 50S ribosomal protein L3P

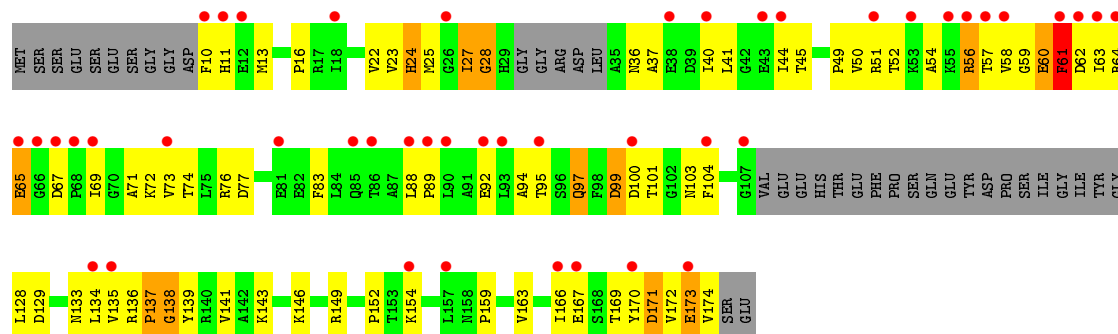




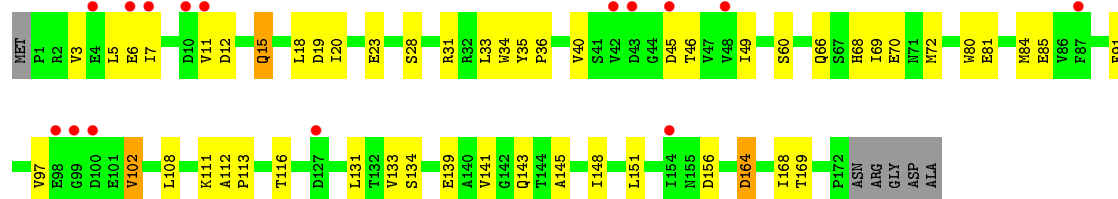
• Molecule 6: 50S ribosomal protein L4E



• Molecule 7: 50S ribosomal protein L5P



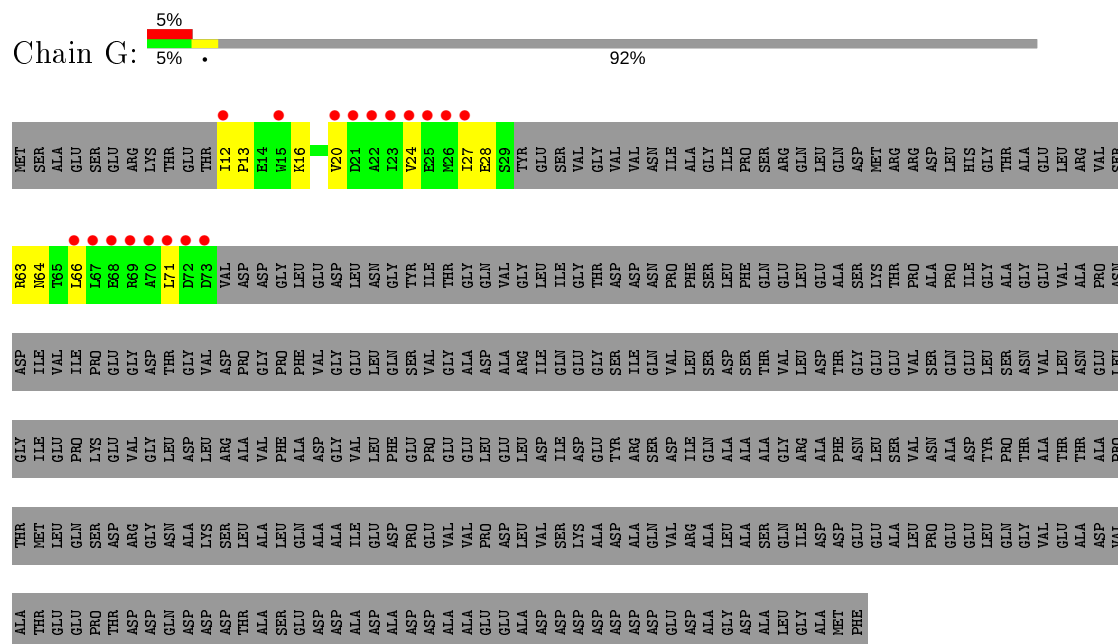
• Molecule 8: 50S ribosomal protein L6P



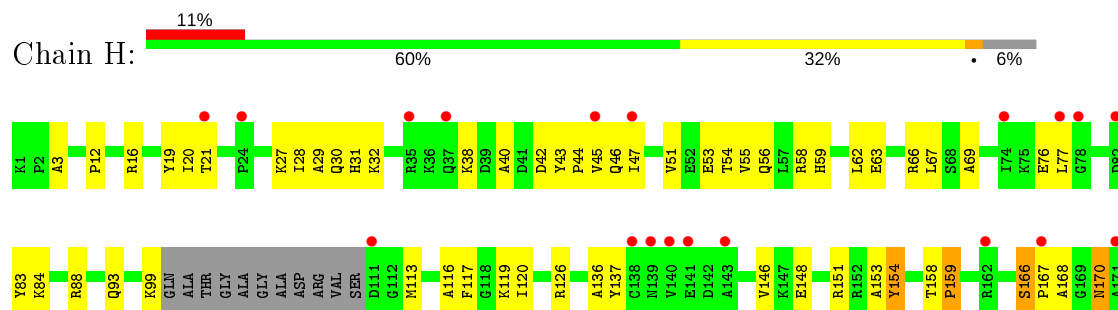
• Molecule 9: 50S ribosomal protein L7AE



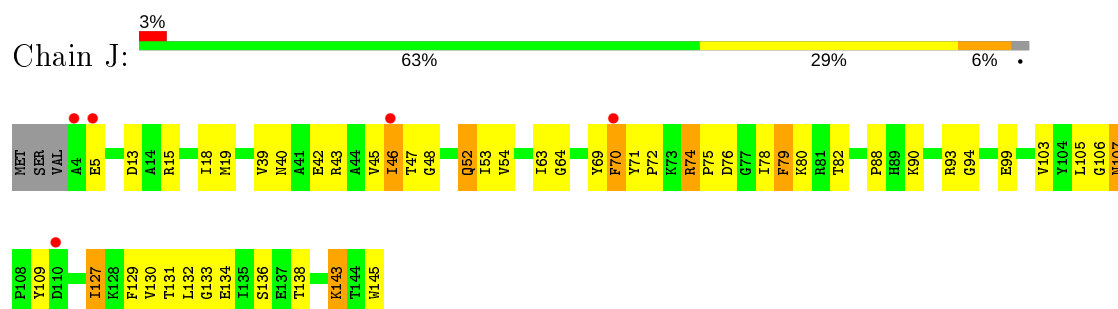
- Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



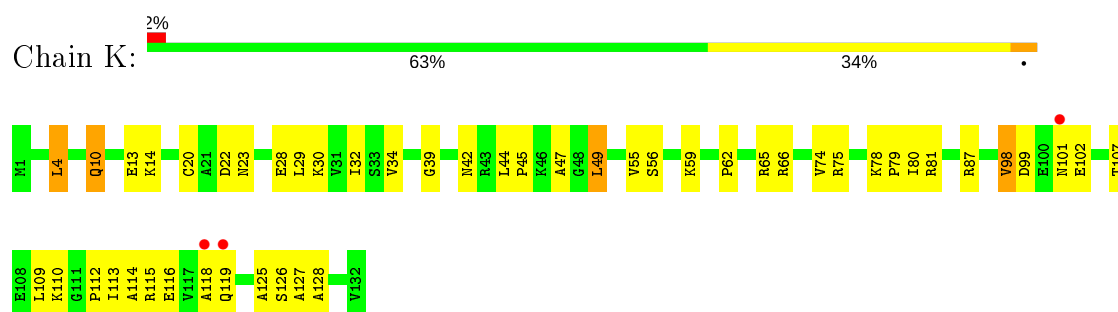
- Molecule 11: 50S RIBOSOMAL PROTEIN L10E



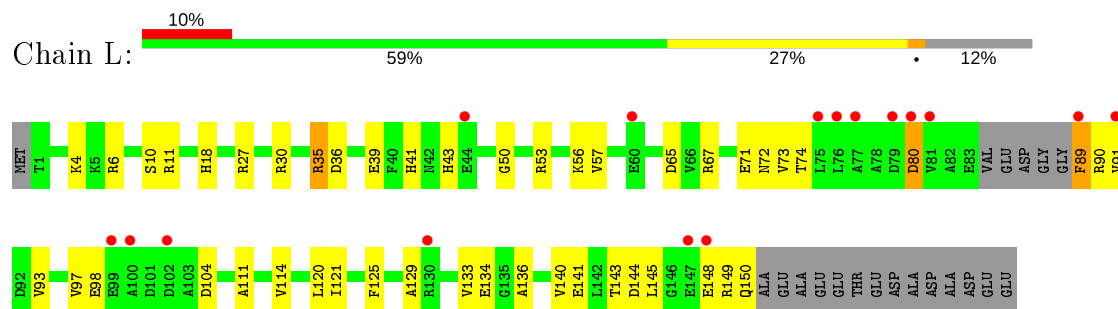
- Molecule 12: 50S ribosomal protein L13P



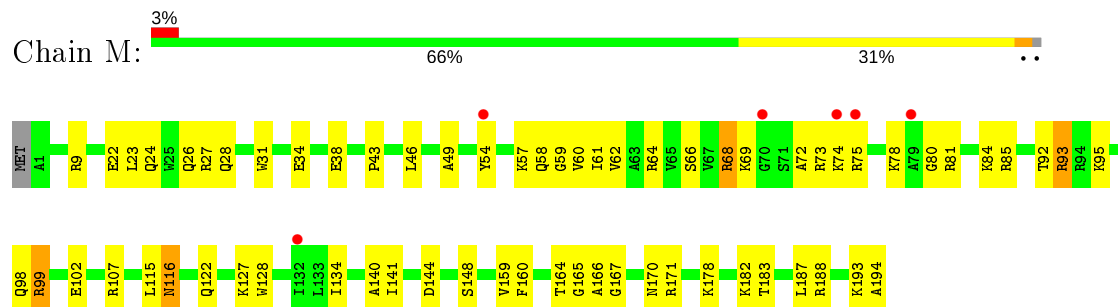
- Molecule 13: 50S ribosomal protein L14P



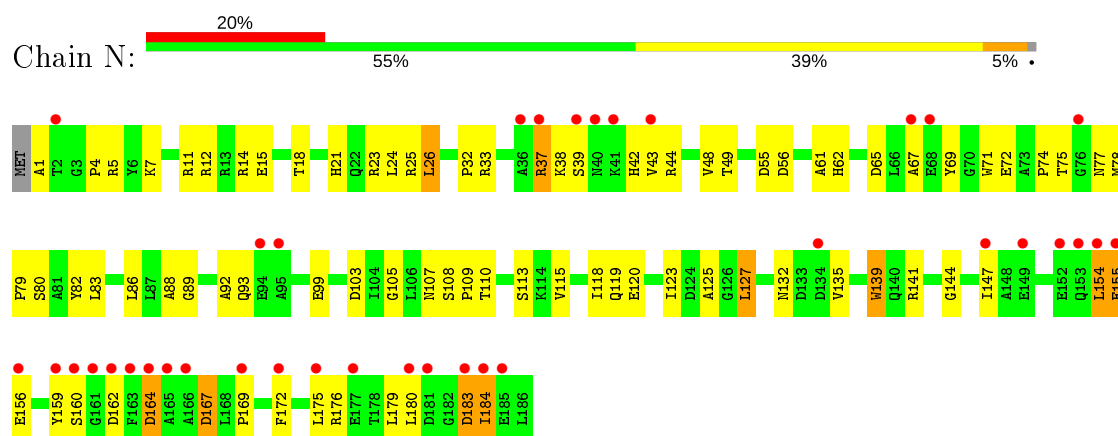
- Molecule 14: 50S ribosomal protein L15P



- Molecule 15: 50S Ribosomal Protein L15E

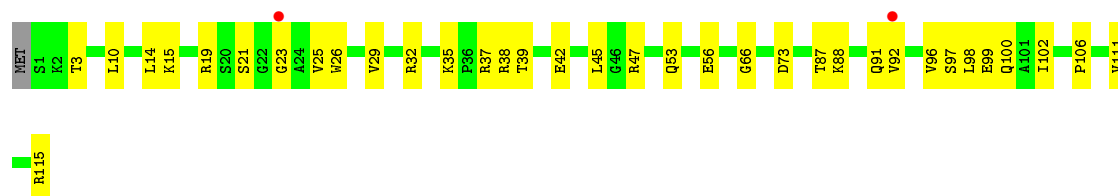


- Molecule 16: 50S ribosomal protein L18P

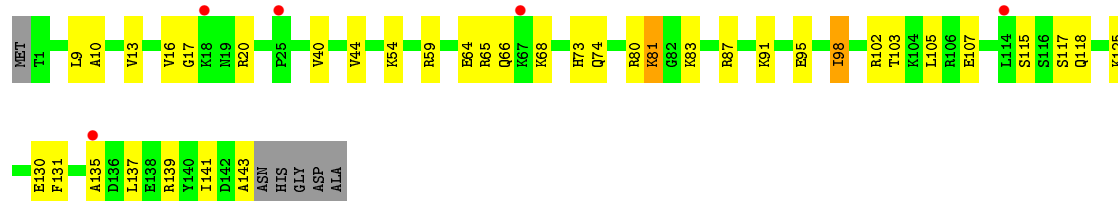


- Molecule 17: 50S ribosomal protein L18e

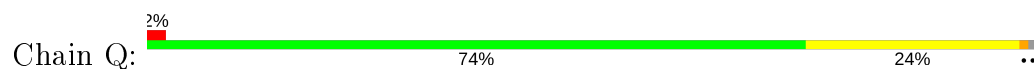




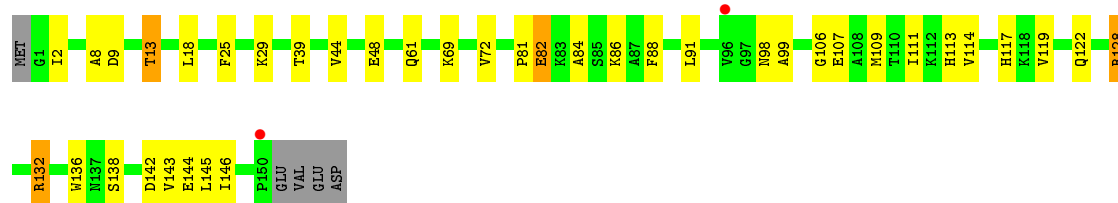
- Molecule 18: 50S ribosomal protein L19E



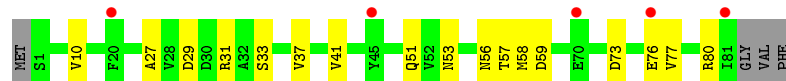
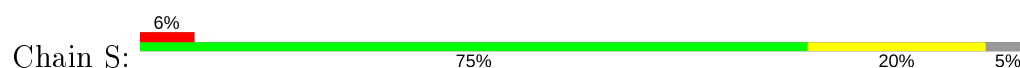
- Molecule 19: 50S ribosomal protein L21e



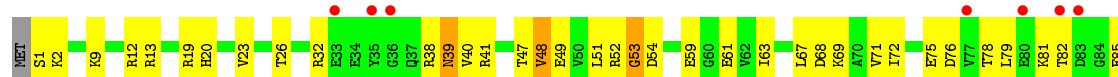
- Molecule 20: 50S ribosomal protein L22P



- Molecule 21: 50S ribosomal protein L23P



- Molecule 22: 50S ribosomal protein L24P

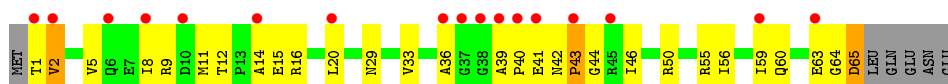




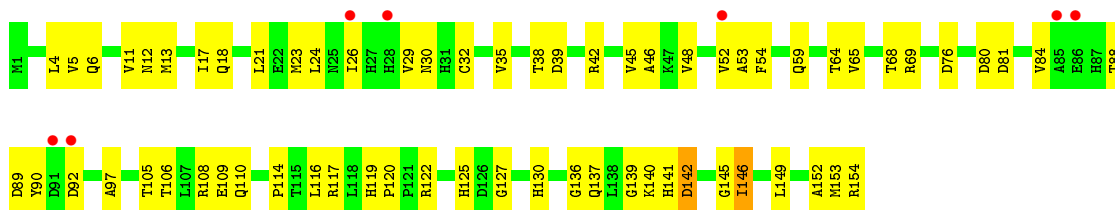
- Molecule 23: 50S ribosomal protein L24E



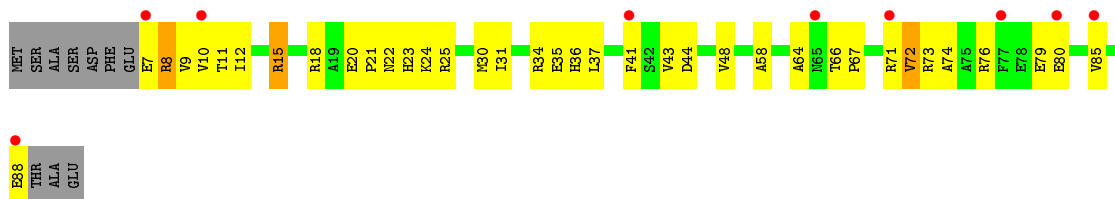
- Molecule 24: 50S ribosomal protein L29P



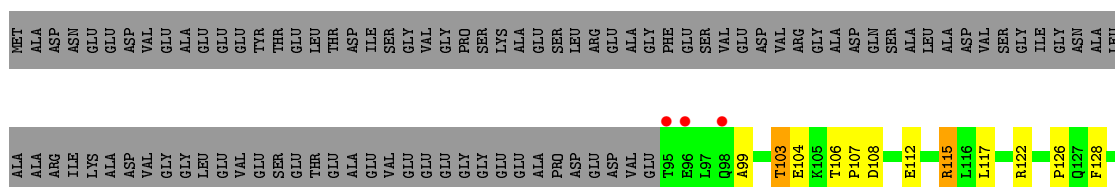
- Molecule 25: 50S ribosomal protein L30P



- Molecule 26: 50S ribosomal protein L31e

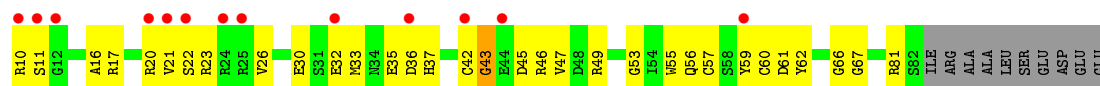


- Molecule 27: 50S ribosomal protein L32E





- Molecule 28: 50S ribosomal protein L37Ae



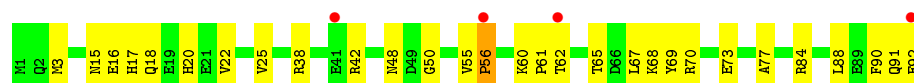
- Molecule 29: 50S ribosomal protein L37e



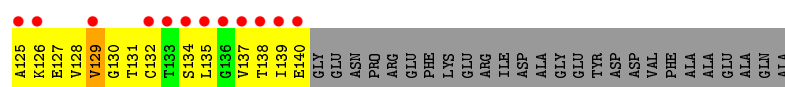
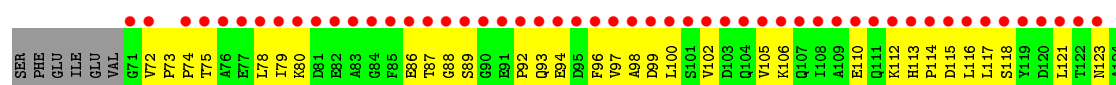
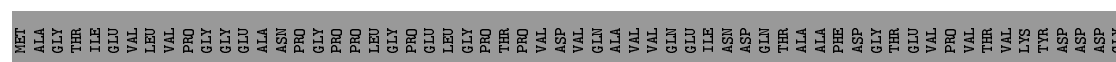
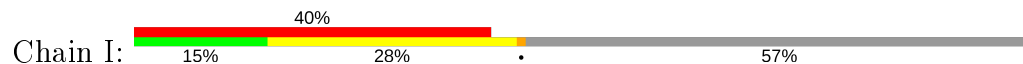
- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E



- Molecule 32: 50S RIBOSOMAL PROTEIN L11P



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.61Å 298.19Å 574.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25 37.18 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.25) 90.5 (37.18-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.74 (at 2.24Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.247 0.209 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99070	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, PPU, CL, SR, NA, K, PO2, CD, HFA, DCZ, 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	0.36	0/65959	0.70	24/102870 (0.0%)
2	9	0.32	0/2905	0.70	1/4528 (0.0%)
3	4	0.51	0/83	0.79	0/119
4	A	0.32	0/1786	0.67	0/2408
5	B	0.32	0/2690	0.65	0/3652
6	C	0.37	0/1884	0.65	1/2551 (0.0%)
7	D	0.28	0/1111	0.53	0/1498
8	E	0.30	0/1382	0.56	0/1880
9	F	0.30	0/901	0.53	0/1224
10	G	0.26	0/241	0.46	0/324
11	H	0.32	0/1287	0.65	0/1725
12	J	0.34	0/1136	0.60	0/1530
13	K	0.34	0/1001	0.67	0/1347
14	L	0.32	0/1130	0.65	0/1509
15	M	0.33	0/1584	0.60	0/2119
16	N	0.28	0/1474	0.61	0/1999
17	O	0.31	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	0/1005
20	R	0.35	0/1172	0.66	1/1578 (0.1%)
21	S	0.32	0/648	0.58	1/875 (0.1%)
22	T	0.29	0/958	0.62	0/1289
23	U	0.32	0/417	0.57	0/562
24	V	0.26	0/502	0.51	0/675
25	W	0.34	0/1219	0.60	0/1655
26	X	0.32	0/664	0.57	0/895
27	Y	0.35	0/1146	0.64	0/1536
28	Z	0.31	0/589	0.60	0/787
29	1	0.43	0/438	0.65	0/578
30	2	0.34	0/401	0.57	0/529
31	3	0.35	0/771	0.58	0/1024
32	I	0.28	0/526	0.50	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.35	0/98775	0.68	29/147696 (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	0	45
2	9	0	2
All	All	0	47

There are no bond length outliers.

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	871	G	C5'-C4'-O4'	-8.48	98.93	109.10
1	0	1942	A	C5'-C4'-C3'	7.65	128.23	116.00
1	0	1819	G	C5'-C4'-C3'	7.08	127.34	116.00
1	0	777	U	O4'-C1'-N1	7.08	113.87	108.20
2	9	3039	U	N1-C1'-C2'	6.91	122.98	114.00

There are no chirality outliers.

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	182	G	Sidechain
1	0	24	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	458	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	29813	686	0
2	9	2600	0	1326	56	0
3	4	132	0	79	4	0
4	A	1753	0	1766	110	0
5	B	2625	0	2531	132	0
6	C	1859	0	1816	92	0
7	D	1094	0	1085	87	0
8	E	1357	0	1266	57	0
9	F	890	0	843	45	0
10	G	240	0	231	10	0
11	H	1266	0	1268	61	0
12	J	1120	0	1098	73	0
13	K	992	0	1031	56	0
14	L	1118	0	1076	48	0
15	M	1560	0	1568	61	0
16	N	1445	0	1401	85	0
17	O	865	0	873	33	0
18	P	1136	0	1123	34	0
19	Q	735	0	729	22	0
20	R	1149	0	1122	39	0
21	S	641	0	605	15	0
22	T	950	0	923	56	0
23	U	410	0	364	17	0
24	V	499	0	511	34	0
25	W	1196	0	1137	85	0
26	X	654	0	653	39	0
27	Y	1130	0	1133	50	0
28	Z	578	0	539	23	0
29	1	431	0	426	22	0
30	2	396	0	413	32	0
31	3	755	0	728	25	0
32	I	519	0	500	56	0
33	0	88	0	0	0	0
33	9	1	0	0	0	0
33	A	2	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	3	0	0	0	0
35	0	64	0	0	0	0
35	9	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	H	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	10	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	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	5757	0	0	88	0
39	1	49	0	0	1	0
39	2	38	0	0	2	0
39	3	66	0	0	2	0
39	4	6	0	0	0	0
39	9	139	0	0	7	0
39	A	124	0	0	16	0
39	B	140	0	0	18	0
39	C	172	0	0	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	D	50	0	0	12	0
39	E	40	0	0	3	0
39	F	25	0	0	2	0
39	G	16	0	0	1	0
39	H	69	0	0	6	0
39	I	9	0	0	0	0
39	J	52	0	0	3	0
39	K	59	0	0	3	0
39	L	83	0	0	9	0
39	M	131	0	0	5	0
39	N	58	0	0	4	0
39	O	39	0	0	5	0
39	P	57	0	0	1	0
39	Q	51	0	0	5	0
39	R	87	0	0	3	0
39	S	32	0	0	0	0
39	T	36	0	0	6	0
39	U	30	0	0	3	0
39	V	11	0	0	1	0
39	W	72	0	0	3	0
39	X	24	0	0	4	0
39	Y	88	0	0	7	0
39	Z	31	0	0	2	0
All	All	99070	0	59977	2013	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 13.

The worst 5 of 2013 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)
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.29	1.14
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.27	1.09
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.28	1.07
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.31	1.06
6:C:236:THR:HG22	6:C:239:ALA:H	1.19	1.06

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%)	212 (90%)	19 (8%)	4 (2%)	9	4
5	B	335/338 (99%)	316 (94%)	16 (5%)	3 (1%)	17	14
6	C	244/246 (99%)	224 (92%)	20 (8%)	0	100	100
7	D	134/177 (76%)	108 (81%)	14 (10%)	12 (9%)	1	0
8	E	170/178 (96%)	166 (98%)	4 (2%)	0	100	100
9	F	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	9	4
10	G	25/348 (7%)	25 (100%)	0	0	100	100
11	H	156/171 (91%)	143 (92%)	11 (7%)	2 (1%)	12	8
12	J	140/145 (97%)	132 (94%)	6 (4%)	2 (1%)	11	7
13	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	19	17
14	L	141/165 (86%)	123 (87%)	17 (12%)	1 (1%)	22	21
15	M	192/195 (98%)	183 (95%)	9 (5%)	0	100	100
16	N	184/187 (98%)	165 (90%)	13 (7%)	6 (3%)	4	1
17	O	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
18	P	141/149 (95%)	138 (98%)	3 (2%)	0	100	100
19	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	R	148/155 (96%)	143 (97%)	4 (3%)	1 (1%)	22	21
21	S	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
22	T	117/120 (98%)	108 (92%)	8 (7%)	1 (1%)	17	14
23	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
24	V	63/71 (89%)	58 (92%)	3 (5%)	2 (3%)	4	1
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%)	140 (100%)	0	0	100	100
28	Z	71/83 (86%)	59 (83%)	8 (11%)	4 (6%)	2	0

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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%)	41 (98%)	1 (2%)	0	100	100
31	3	90/92 (98%)	89 (99%)	0	1 (1%)	14	10
32	I	68/162 (42%)	53 (78%)	14 (21%)	1 (2%)	10	6
All	All	3705/4431 (84%)	3451 (93%)	211 (6%)	43 (1%)	13	9

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	H	166	SER
14	L	80	ASP
16	N	154	LEU
16	N	184	ILE
28	Z	81	ARG

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%)	169 (94%)	10 (6%)	21	21
5	B	282/283 (100%)	261 (93%)	21 (7%)	13	12
6	C	193/193 (100%)	177 (92%)	16 (8%)	11	9
7	D	117/148 (79%)	112 (96%)	5 (4%)	29	33
8	E	152/156 (97%)	148 (97%)	4 (3%)	46	55
9	F	93/94 (99%)	92 (99%)	1 (1%)	73	82
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	127 (96%)	5 (4%)	33	39
12	J	118/121 (98%)	111 (94%)	7 (6%)	19	19
13	K	106/106 (100%)	102 (96%)	4 (4%)	33	39
14	L	113/127 (89%)	109 (96%)	4 (4%)	36	43
15	M	158/159 (99%)	153 (97%)	5 (3%)	39	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	N	149/150 (99%)	145 (97%)	4 (3%)	44	54
17	O	93/94 (99%)	92 (99%)	1 (1%)	73	82
18	P	113/117 (97%)	111 (98%)	2 (2%)	59	68
19	Q	79/80 (99%)	76 (96%)	3 (4%)	33	39
20	R	117/122 (96%)	114 (97%)	3 (3%)	46	55
21	S	71/74 (96%)	71 (100%)	0	100	100
22	T	105/106 (99%)	101 (96%)	4 (4%)	33	39
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	55	64
25	W	130/130 (100%)	126 (97%)	4 (3%)	40	49
26	X	66/74 (89%)	62 (94%)	4 (6%)	18	18
27	Y	120/196 (61%)	108 (90%)	12 (10%)	7	5
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	45 (98%)	1 (2%)	52	61
30	2	42/46 (91%)	41 (98%)	1 (2%)	49	58
31	3	79/79 (100%)	79 (100%)	0	100	100
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3612 (86%)	2971 (96%)	122 (4%)	32	38

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	E	164	ASP
12	J	127	ILE
27	Y	154	ARG
9	F	12	LEU
11	H	170	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	143	ASN
18	P	118	GLN
30	2	16	ASN
15	M	170	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%)	34 (1%)
2	9	121/122 (99%)	14 (11%)	1 (0%)
3	4	0/8	-	-
All	All	2866/3052 (93%)	246 (8%)	35 (1%)

5 of 246 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	21	G
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A

5 of 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1352	A
1	0	1692	C
1	0	2761	A
1	0	1506	U
1	0	1684	A

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

7 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	1MA	0	628	1,35	15,25,26	0.67	0	15,37,40	1.36	1 (6%)
1	OMU	0	2587	1	14,22,23	1.00	2 (14%)	14,31,34	1.16	1 (7%)
1	OMG	0	2588	1,3	18,26,27	1.10	2 (11%)	20,38,41	2.61	4 (20%)
3	PPU	4	76	1,3	18,26,41	0.79	0	15,38,60	0.83	0
3	HFA	4	77	3	10,11,12	1.18	1 (10%)	12,13,15	0.95	1 (8%)
1	UR3	0	2619	1	14,22,23	0.89	1 (7%)	15,32,35	0.58	0
1	PSU	0	2621	1	17,21,22	1.64	3 (17%)	20,30,33	5.42	4 (20%)

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	1MA	0	628	1,35	-	0/3/25/26	0/3/3/3
1	OMU	0	2587	1	-	0/7/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3
3	PPU	4	76	1,3	-	0/7/29/44	0/3/3/4
3	HFA	4	77	3	-	1/5/6/8	0/1/1/1
1	UR3	0	2619	1	-	0/5/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.93	1.48	1.52
1	0	2588	OMG	C6-N1	3.38	1.38	1.33
3	4	77	HFA	OA-CA	3.16	1.49	1.43
1	0	2621	PSU	C4-N3	3.05	1.38	1.33
1	0	2621	PSU	C2-N1	2.74	1.43	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.20	114.75	128.43
1	0	2621	PSU	C4-N3-C2	14.33	127.24	115.14
1	0	2588	OMG	C5-C6-N1	-8.65	111.59	123.43
1	0	2621	PSU	C5-C4-N3	-8.27	114.70	125.36
1	0	2588	OMG	C6-N1-C2	5.84	125.21	115.93

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	4	77	HFA	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
3	4	77	HFA	1	0
1	0	2619	UR3	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 313 ligands modelled in this entry, 313 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	176:A	O3'	175:C	P	8.75

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	-0.08	127 (4%) 32 35	23, 45, 88, 147	0
2	9	122/122 (100%)	0.39	7 (5%) 23 25	40, 63, 89, 149	0
3	4	4/8 (50%)	-0.27	0 100 100	40, 45, 47, 48	0
4	A	237/240 (98%)	0.35	14 (5%) 22 24	27, 48, 83, 102	0
5	B	337/338 (99%)	0.20	11 (3%) 46 48	27, 50, 76, 88	0
6	C	246/246 (100%)	0.05	3 (1%) 79 81	24, 45, 68, 79	0
7	D	140/177 (79%)	1.79	45 (32%) 0 0	55, 93, 121, 129	0
8	E	172/178 (96%)	0.40	15 (8%) 10 11	41, 63, 83, 88	0
9	F	119/120 (99%)	0.72	11 (9%) 9 9	46, 69, 94, 106	0
10	G	29/348 (8%)	2.71	18 (62%) 0 0	67, 89, 97, 100	0
11	H	160/171 (93%)	0.49	19 (11%) 4 3	40, 58, 91, 98	0
12	J	142/145 (97%)	0.05	5 (3%) 44 46	34, 47, 69, 90	0
13	K	132/132 (100%)	0.02	3 (2%) 60 63	33, 44, 68, 78	0
14	L	145/165 (87%)	0.60	16 (11%) 5 5	26, 62, 107, 117	0
15	M	194/195 (99%)	0.27	6 (3%) 49 52	32, 44, 60, 69	0
16	N	186/187 (99%)	0.94	37 (19%) 1 1	44, 61, 107, 115	0
17	O	115/116 (99%)	0.24	2 (1%) 70 73	38, 53, 68, 77	0
18	P	143/149 (95%)	0.32	5 (3%) 44 46	36, 50, 63, 75	0
19	Q	95/96 (98%)	-0.05	2 (2%) 63 66	37, 46, 61, 72	0
20	R	150/155 (96%)	-0.08	2 (1%) 77 79	30, 43, 62, 71	0
21	S	81/85 (95%)	0.39	5 (6%) 20 22	39, 55, 75, 90	0
22	T	119/120 (99%)	0.67	13 (10%) 5 5	39, 53, 79, 104	0
23	U	53/66 (80%)	0.26	2 (3%) 40 43	40, 50, 69, 78	0
24	V	65/71 (91%)	1.93	17 (26%) 0 0	52, 72, 109, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	0.27	7 (4%) 33 36	37, 49, 69, 78	0
26	X	82/92 (89%)	0.56	9 (10%) 5 5	39, 54, 81, 98	0
27	Y	142/241 (58%)	-0.02	5 (3%) 44 46	28, 42, 64, 84	0
28	Z	73/83 (87%)	0.82	13 (17%) 1 1	46, 63, 80, 91	0
29	1	56/57 (98%)	-0.20	0 100 100	28, 33, 40, 48	0
30	2	46/50 (92%)	1.48	12 (26%) 0 0	34, 60, 89, 96	0
31	3	92/92 (100%)	0.23	4 (4%) 35 37	34, 54, 68, 80	0
32	I	70/162 (43%)	6.37	64 (91%) 0 0	105, 117, 137, 138	0
All	All	6650/7483 (88%)	0.28	499 (7%) 14 15	23, 50, 95, 149	0

The worst 5 of 499 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	88	GLY	22.4
24	V	1	THR	18.4
32	I	71	GLY	18.2
32	I	133	THR	17.3
32	I	96	PHE	17.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	HFA	4	77	11/12	0.97	0.16	37,39,42,43	0
1	OMU	0	2587	21/22	0.98	0.11	28,35,37,37	0
1	OMG	0	2588	24/25	0.98	0.13	28,32,36,37	0
3	PPU	4	76	24/38	0.98	0.10	35,39,41,43	0
1	1MA	0	628	23/24	0.98	0.15	30,32,34,39	0
1	UR3	0	2619	21/22	0.98	0.13	34,37,39,41	0
1	PSU	0	2621	20/21	0.98	0.08	28,31,38,39	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
37	SR	0	9500	1/1	0.01	0.64	179,179,179,179	0
33	MG	0	8024	1/1	0.42	1.11	92,92,92,92	0
33	MG	0	8055	1/1	0.48	0.26	102,102,102,102	0
38	CD	O	9205	1/1	0.51	0.23	183,183,183,183	0
35	NA	0	9169	1/1	0.58	0.57	96,96,96,96	0
37	SR	0	9547	1/1	0.63	0.79	194,194,194,194	0
33	MG	0	8052	1/1	0.64	0.23	88,88,88,88	0
35	NA	H	9122	1/1	0.65	0.20	80,80,80,80	0
35	NA	0	9185	1/1	0.66	0.28	50,50,50,50	0
35	NA	S	9112	1/1	0.67	0.43	68,68,68,68	0
35	NA	0	9129	1/1	0.69	0.22	70,70,70,70	0
33	MG	0	8108	1/1	0.70	0.17	111,111,111,111	0
35	NA	0	9174	1/1	0.71	0.33	62,62,62,62	0
33	MG	0	8022	1/1	0.71	1.19	103,103,103,103	0
35	NA	0	9157	1/1	0.71	0.13	44,44,44,44	0
35	NA	0	9182	1/1	0.71	0.26	78,78,78,78	0
33	MG	0	8061	1/1	0.74	0.10	60,60,60,60	0
35	NA	0	9125	1/1	0.74	1.04	93,93,93,93	0
35	NA	0	9173	1/1	0.74	0.26	66,66,66,66	0
35	NA	0	9168	1/1	0.76	0.38	63,63,63,63	0
35	NA	0	9184	1/1	0.76	0.23	75,75,75,75	0
35	NA	0	9118	1/1	0.76	0.44	60,60,60,60	0
35	NA	0	9164	1/1	0.76	0.25	59,59,59,59	0
35	NA	0	9116	1/1	0.76	0.22	44,44,44,44	0
35	NA	D	9151	1/1	0.78	0.13	61,61,61,61	0
33	MG	0	8089	1/1	0.78	0.17	58,58,58,58	0
33	MG	0	8101	1/1	0.79	0.25	78,78,78,78	0
33	MG	0	8082	1/1	0.79	0.32	89,89,89,89	0
33	MG	0	8050	1/1	0.79	0.19	74,74,74,74	0
35	NA	0	9127	1/1	0.80	0.19	45,45,45,45	0
33	MG	0	8059	1/1	0.80	0.49	61,61,61,61	0
35	NA	0	9152	1/1	0.80	0.22	66,66,66,66	0
37	SR	B	9521	1/1	0.80	0.18	165,165,165,165	0
35	NA	0	9126	1/1	0.80	0.31	54,54,54,54	0
35	NA	0	9171	1/1	0.81	0.23	56,56,56,56	0
33	MG	0	8014	1/1	0.81	0.27	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8084	1/1	0.82	0.34	76,76,76,76	0
34	K	0	9001	1/1	0.82	0.35	78,78,78,78	0
35	NA	0	9163	1/1	0.82	0.12	59,59,59,59	0
33	MG	0	8094	1/1	0.83	0.57	92,92,92,92	0
33	MG	0	8042	1/1	0.83	0.08	53,53,53,53	0
35	NA	R	9186	1/1	0.83	0.23	67,67,67,67	0
35	NA	9	9183	1/1	0.83	0.20	73,73,73,73	0
35	NA	0	9140	1/1	0.84	0.13	55,55,55,55	0
33	MG	0	8017	1/1	0.85	0.17	31,31,31,31	0
33	MG	0	8040	1/1	0.85	0.29	69,69,69,69	0
33	MG	0	8093	1/1	0.85	0.13	41,41,41,41	0
33	MG	0	8058	1/1	0.86	0.26	79,79,79,79	0
33	MG	0	8057	1/1	0.86	0.20	69,69,69,69	0
35	NA	0	9158	1/1	0.86	0.31	66,66,66,66	0
37	SR	0	9459	1/1	0.86	0.07	97,97,97,97	0
35	NA	0	9177	1/1	0.86	0.34	62,62,62,62	0
35	NA	0	9179	1/1	0.86	0.33	107,107,107,107	0
33	MG	0	8025	1/1	0.87	0.35	29,29,29,29	0
35	NA	0	9170	1/1	0.87	0.54	82,82,82,82	0
33	MG	0	8045	1/1	0.87	0.31	66,66,66,66	0
35	NA	0	9111	1/1	0.87	0.21	66,66,66,66	0
34	K	0	9003	1/1	0.87	0.23	80,80,80,80	0
33	MG	A	8065	1/1	0.87	0.14	79,79,79,79	0
35	NA	0	9172	1/1	0.87	0.67	71,71,71,71	0
33	MG	0	8047	1/1	0.87	0.29	89,89,89,89	0
37	SR	0	9484	1/1	0.87	0.09	123,123,123,123	0
35	NA	0	9181	1/1	0.87	0.17	52,52,52,52	0
33	MG	0	8085	1/1	0.87	0.30	65,65,65,65	0
33	MG	0	8107	1/1	0.88	0.17	63,63,63,63	0
37	SR	0	9532	1/1	0.88	0.10	123,123,123,123	0
35	NA	C	9104	1/1	0.89	0.17	27,27,27,27	0
35	NA	0	9167	1/1	0.89	0.09	50,50,50,50	0
35	NA	0	9166	1/1	0.89	0.07	59,59,59,59	0
33	MG	0	8113	1/1	0.89	0.11	43,43,43,43	0
37	SR	9	9588	1/1	0.89	0.15	126,126,126,126	0
36	CL	N	9307	1/1	0.89	0.15	55,55,55,55	0
35	NA	0	9150	1/1	0.90	0.18	42,42,42,42	0
35	NA	0	9108	1/1	0.90	0.14	33,33,33,33	0
37	SR	0	9539	1/1	0.90	0.26	134,134,134,134	0
35	NA	0	9141	1/1	0.90	0.09	60,60,60,60	0
33	MG	0	8092	1/1	0.90	0.65	68,68,68,68	0
33	MG	0	8103	1/1	0.90	0.16	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	9130	1/1	0.90	0.09	44,44,44,44	0
36	CL	B	9319	1/1	0.90	0.16	55,55,55,55	0
33	MG	0	8115	1/1	0.91	0.12	51,51,51,51	0
35	NA	0	9124	1/1	0.91	0.27	53,53,53,53	0
37	SR	0	9452	1/1	0.91	0.18	107,107,107,107	0
33	MG	0	8104	1/1	0.91	0.12	50,50,50,50	0
33	MG	0	8013	1/1	0.91	0.16	37,37,37,37	0
33	MG	0	8028	1/1	0.91	0.13	35,35,35,35	0
36	CL	J	9301	1/1	0.91	0.08	51,51,51,51	0
33	MG	0	8063	1/1	0.91	0.18	60,60,60,60	0
37	SR	A	9497	1/1	0.92	0.09	78,78,78,78	0
37	SR	0	9581	1/1	0.92	0.13	106,106,106,106	0
35	NA	0	9113	1/1	0.92	0.10	61,61,61,61	0
33	MG	0	8051	1/1	0.92	0.27	35,35,35,35	0
37	SR	0	9626	1/1	0.92	0.23	114,114,114,114	0
37	SR	0	9475	1/1	0.92	0.07	76,76,76,76	0
35	NA	0	9120	1/1	0.92	0.39	53,53,53,53	0
33	MG	0	8102	1/1	0.92	0.05	61,61,61,61	0
38	CD	Z	9203	1/1	0.92	0.06	57,57,57,57	0
33	MG	0	8083	1/1	0.93	0.05	50,50,50,50	0
35	NA	0	9178	1/1	0.93	0.23	51,51,51,51	0
33	MG	9	8095	1/1	0.93	0.21	49,49,49,49	0
33	MG	0	8114	1/1	0.93	0.40	76,76,76,76	0
36	CL	A	9309	1/1	0.93	0.09	57,57,57,57	0
37	SR	0	9490	1/1	0.93	0.09	89,89,89,89	0
37	SR	0	9590	1/1	0.93	0.05	91,91,91,91	0
37	SR	0	9517	1/1	0.93	0.05	113,113,113,113	0
33	MG	0	8002	1/1	0.93	0.06	45,45,45,45	0
37	SR	0	9468	1/1	0.93	0.07	108,108,108,108	0
33	MG	0	8046	1/1	0.93	0.05	41,41,41,41	0
33	MG	0	8021	1/1	0.93	0.20	53,53,53,53	0
35	NA	0	9165	1/1	0.94	0.17	42,42,42,42	0
35	NA	0	9149	1/1	0.94	0.14	42,42,42,42	0
33	MG	A	8066	1/1	0.94	0.13	56,56,56,56	0
33	MG	0	8054	1/1	0.94	0.18	39,39,39,39	0
35	NA	0	9102	1/1	0.94	0.31	58,58,58,58	0
33	MG	0	8080	1/1	0.94	0.28	48,48,48,48	0
33	MG	0	8039	1/1	0.94	0.15	80,80,80,80	0
37	SR	0	9465	1/1	0.94	0.05	93,93,93,93	0
33	MG	0	8099	1/1	0.94	0.15	62,62,62,62	0
33	MG	0	8072	1/1	0.94	0.25	69,69,69,69	0
37	SR	0	9522	1/1	0.94	0.03	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8019	1/1	0.94	0.12	45,45,45,45	0
35	NA	0	9136	1/1	0.94	0.15	33,33,33,33	0
35	NA	Q	9148	1/1	0.94	0.08	48,48,48,48	0
35	NA	0	9162	1/1	0.94	0.20	49,49,49,49	0
33	MG	0	8079	1/1	0.94	0.16	30,30,30,30	0
35	NA	0	9161	1/1	0.94	0.22	59,59,59,59	0
33	MG	0	8088	1/1	0.94	0.14	36,36,36,36	0
33	MG	0	8090	1/1	0.94	0.62	84,84,84,84	0
35	NA	0	9154	1/1	0.95	0.14	46,46,46,46	0
33	MG	0	8098	1/1	0.95	0.08	43,43,43,43	0
33	MG	0	8027	1/1	0.95	0.16	33,33,33,33	0
37	SR	F	9595	1/1	0.95	0.12	99,99,99,99	0
33	MG	0	8116	1/1	0.95	0.07	49,49,49,49	0
35	NA	0	9107	1/1	0.95	0.28	63,63,63,63	0
35	NA	M	9147	1/1	0.95	0.17	39,39,39,39	0
37	SR	0	9477	1/1	0.95	0.06	83,83,83,83	0
33	MG	0	8003	1/1	0.95	0.11	33,33,33,33	0
33	MG	0	8096	1/1	0.95	0.10	42,42,42,42	0
35	NA	0	9117	1/1	0.95	0.18	43,43,43,43	0
33	MG	0	8020	1/1	0.95	0.20	34,34,34,34	0
33	MG	0	8118	1/1	0.95	0.08	33,33,33,33	0
37	SR	0	9504	1/1	0.95	0.06	90,90,90,90	0
35	NA	R	9137	1/1	0.95	0.06	38,38,38,38	0
37	SR	0	9447	1/1	0.96	0.07	64,64,64,64	0
36	CL	L	9310	1/1	0.96	0.06	49,49,49,49	0
37	SR	0	9566	1/1	0.96	0.05	76,76,76,76	0
37	SR	A	9437	1/1	0.96	0.11	59,59,59,59	0
36	CL	0	9313	1/1	0.96	0.09	51,51,51,51	0
36	CL	0	9305	1/1	0.96	0.09	52,52,52,52	0
33	MG	0	8029	1/1	0.96	0.25	35,35,35,35	0
37	SR	0	9469	1/1	0.96	0.05	81,81,81,81	0
33	MG	0	8068	1/1	0.96	0.20	46,46,46,46	0
36	CL	0	9311	1/1	0.96	0.09	60,60,60,60	0
35	NA	0	9159	1/1	0.96	0.21	55,55,55,55	0
35	NA	0	9114	1/1	0.96	0.26	42,42,42,42	0
33	MG	0	8043	1/1	0.96	0.08	49,49,49,49	0
37	SR	0	9483	1/1	0.96	0.05	68,68,68,68	0
37	SR	0	9585	1/1	0.96	0.05	77,77,77,77	0
35	NA	0	9155	1/1	0.96	0.13	52,52,52,52	0
35	NA	0	9175	1/1	0.96	0.12	51,51,51,51	0
37	SR	0	9435	1/1	0.96	0.08	67,67,67,67	0
35	NA	0	9156	1/1	0.96	0.17	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8044	1/1	0.96	0.07	41,41,41,41	0
36	CL	0	9315	1/1	0.96	0.13	50,50,50,50	0
33	MG	Y	8109	1/1	0.96	0.09	38,38,38,38	0
33	MG	0	8076	1/1	0.96	0.16	56,56,56,56	0
37	SR	0	9455	1/1	0.96	0.07	78,78,78,78	0
33	MG	0	8009	1/1	0.96	0.15	32,32,32,32	0
33	MG	0	8001	1/1	0.96	0.20	23,23,23,23	0
36	CL	O	9308	1/1	0.96	0.10	61,61,61,61	0
35	NA	0	9143	1/1	0.96	0.07	36,36,36,36	0
37	SR	0	9505	1/1	0.96	0.08	79,79,79,79	0
35	NA	0	9139	1/1	0.96	0.12	41,41,41,41	0
36	CL	0	9322	1/1	0.96	0.09	53,53,53,53	0
33	MG	0	8031	1/1	0.96	0.04	44,44,44,44	0
35	NA	0	9110	1/1	0.97	0.12	44,44,44,44	0
33	MG	0	8037	1/1	0.97	0.09	37,37,37,37	0
35	NA	0	9132	1/1	0.97	0.12	45,45,45,45	0
37	SR	0	9601	1/1	0.97	0.06	107,107,107,107	0
37	SR	0	9433	1/1	0.97	0.12	64,64,64,64	0
36	CL	0	9316	1/1	0.97	0.17	71,71,71,71	0
37	SR	S	9470	1/1	0.97	0.12	87,87,87,87	0
36	CL	3	9304	1/1	0.97	0.09	54,54,54,54	0
33	MG	0	8117	1/1	0.97	0.18	39,39,39,39	0
33	MG	0	8112	1/1	0.97	0.07	41,41,41,41	0
35	NA	0	9106	1/1	0.97	0.10	37,37,37,37	0
37	SR	0	9560	1/1	0.97	0.05	91,91,91,91	0
36	CL	0	9314	1/1	0.97	0.14	45,45,45,45	0
35	NA	0	9160	1/1	0.97	0.09	35,35,35,35	0
35	NA	0	9134	1/1	0.97	0.14	48,48,48,48	0
37	SR	0	9570	1/1	0.97	0.06	86,86,86,86	0
33	MG	0	8106	1/1	0.97	0.06	43,43,43,43	0
33	MG	0	8091	1/1	0.97	0.04	47,47,47,47	0
35	NA	0	9115	1/1	0.97	0.11	36,36,36,36	0
37	SR	0	9506	1/1	0.97	0.06	61,61,61,61	0
37	SR	0	9480	1/1	0.97	0.06	85,85,85,85	0
37	SR	0	9467	1/1	0.97	0.04	74,74,74,74	0
36	CL	J	9321	1/1	0.97	0.08	57,57,57,57	0
33	MG	0	8036	1/1	0.97	0.19	56,56,56,56	0
35	NA	0	9131	1/1	0.97	0.17	44,44,44,44	0
37	SR	0	9466	1/1	0.97	0.05	80,80,80,80	0
33	MG	T	8073	1/1	0.97	0.14	40,40,40,40	0
33	MG	0	8060	1/1	0.97	0.11	76,76,76,76	0
37	SR	0	9405	1/1	0.97	0.07	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	CL	0	9317	1/1	0.97	0.06	45,45,45,45	0
37	SR	0	9442	1/1	0.97	0.11	59,59,59,59	0
35	NA	0	9101	1/1	0.97	0.24	46,46,46,46	0
37	SR	B	9458	1/1	0.97	0.09	68,68,68,68	0
33	MG	0	8041	1/1	0.97	0.12	53,53,53,53	0
33	MG	0	8032	1/1	0.97	0.09	41,41,41,41	0
34	K	0	9002	1/1	0.97	0.07	61,61,61,61	0
37	SR	0	9629	1/1	0.97	0.07	71,71,71,71	0
37	SR	0	9515	1/1	0.98	0.17	81,81,81,81	0
37	SR	0	9495	1/1	0.98	0.08	90,90,90,90	0
37	SR	0	9537	1/1	0.98	0.07	119,119,119,119	0
33	MG	0	8110	1/1	0.98	0.08	43,43,43,43	0
36	CL	R	9306	1/1	0.98	0.15	44,44,44,44	0
37	SR	H	9486	1/1	0.98	0.14	97,97,97,97	0
33	MG	0	8056	1/1	0.98	0.13	46,46,46,46	0
37	SR	0	9568	1/1	0.98	0.03	70,70,70,70	0
35	NA	J	9146	1/1	0.98	0.09	43,43,43,43	0
37	SR	0	9429	1/1	0.98	0.07	59,59,59,59	0
37	SR	0	9427	1/1	0.98	0.11	50,50,50,50	0
33	MG	0	8075	1/1	0.98	0.04	37,37,37,37	0
37	SR	0	9482	1/1	0.98	0.25	93,93,93,93	0
36	CL	0	9303	1/1	0.98	0.12	44,44,44,44	0
33	MG	0	8012	1/1	0.98	0.19	40,40,40,40	0
35	NA	R	9138	1/1	0.98	0.17	59,59,59,59	0
37	SR	0	9440	1/1	0.98	0.03	69,69,69,69	0
37	SR	0	9432	1/1	0.98	0.13	61,61,61,61	0
37	SR	0	9426	1/1	0.98	0.04	61,61,61,61	0
37	SR	0	9489	1/1	0.98	0.07	80,80,80,80	0
37	SR	1	9419	1/1	0.98	0.12	41,41,41,41	0
37	SR	0	9453	1/1	0.98	0.05	66,66,66,66	0
37	SR	0	9530	1/1	0.98	0.13	66,66,66,66	0
33	MG	0	8097	1/1	0.98	0.10	56,56,56,56	0
37	SR	0	9509	1/1	0.98	0.08	84,84,84,84	0
36	CL	Y	9320	1/1	0.98	0.08	39,39,39,39	0
35	NA	0	9105	1/1	0.98	0.19	38,38,38,38	0
37	SR	3	9439	1/1	0.98	0.06	57,57,57,57	0
37	SR	0	9434	1/1	0.98	0.09	60,60,60,60	0
33	MG	0	8005	1/1	0.98	0.09	28,28,28,28	0
37	SR	0	9417	1/1	0.98	0.09	55,55,55,55	0
37	SR	0	9508	1/1	0.98	0.04	82,82,82,82	0
33	MG	0	8074	1/1	0.98	0.20	31,31,31,31	0
37	SR	0	9420	1/1	0.98	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8004	1/1	0.98	0.12	33,33,33,33	0
37	SR	0	9457	1/1	0.98	0.06	56,56,56,56	0
35	NA	0	9135	1/1	0.98	0.17	43,43,43,43	0
37	SR	0	9431	1/1	0.98	0.07	61,61,61,61	0
37	SR	9	9503	1/1	0.98	0.07	104,104,104,104	0
37	SR	0	9464	1/1	0.98	0.05	73,73,73,73	0
33	MG	0	8038	1/1	0.99	0.27	27,27,27,27	0
33	MG	K	8069	1/1	0.99	0.28	22,22,22,22	0
37	SR	R	9418	1/1	0.99	0.12	50,50,50,50	0
36	CL	0	9312	1/1	0.99	0.13	48,48,48,48	0
37	SR	0	9425	1/1	0.99	0.12	54,54,54,54	0
37	SR	0	9443	1/1	0.99	0.06	54,54,54,54	0
37	SR	0	9450	1/1	0.99	0.06	65,65,65,65	0
37	SR	0	9423	1/1	0.99	0.04	56,56,56,56	0
37	SR	0	9406	1/1	0.99	0.14	32,32,32,32	0
37	SR	0	9441	1/1	0.99	0.06	62,62,62,62	0
37	SR	0	9451	1/1	0.99	0.07	62,62,62,62	0
37	SR	0	9438	1/1	0.99	0.06	59,59,59,59	0
37	SR	0	9454	1/1	0.99	0.05	65,65,65,65	0
37	SR	0	9422	1/1	0.99	0.09	52,52,52,52	0
37	SR	0	9545	1/1	0.99	0.03	70,70,70,70	0
37	SR	0	9449	1/1	0.99	0.06	60,60,60,60	0
33	MG	0	8026	1/1	0.99	0.20	33,33,33,33	0
36	CL	J	9302	1/1	0.99	0.09	51,51,51,51	0
37	SR	0	9529	1/1	0.99	0.05	89,89,89,89	0
33	MG	0	8015	1/1	0.99	0.07	31,31,31,31	0
33	MG	0	8030	1/1	0.99	0.09	34,34,34,34	0
38	CD	3	9204	1/1	0.99	0.05	57,57,57,57	0
37	SR	0	9414	1/1	0.99	0.10	57,57,57,57	0
37	SR	0	9461	1/1	0.99	0.04	69,69,69,69	0
37	SR	0	9411	1/1	0.99	0.15	42,42,42,42	0
33	MG	0	8067	1/1	0.99	0.08	38,38,38,38	0
37	SR	9	9481	1/1	0.99	0.04	80,80,80,80	0
37	SR	0	9430	1/1	0.99	0.09	47,47,47,47	0
35	NA	0	9123	1/1	0.99	0.08	38,38,38,38	0
37	SR	0	9462	1/1	0.99	0.10	64,64,64,64	0
37	SR	1	9460	1/1	0.99	0.07	47,47,47,47	0
35	NA	0	9128	1/1	0.99	0.09	40,40,40,40	0
33	MG	0	8008	1/1	0.99	0.15	23,23,23,23	0
37	SR	0	9498	1/1	0.99	0.03	58,58,58,58	0
38	CD	U	9201	1/1	0.99	0.07	58,58,58,58	0
37	SR	0	9534	1/1	0.99	0.16	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	SR	0	9413	1/1	0.99	0.10	43,43,43,43	0
36	CL	M	9318	1/1	0.99	0.17	39,39,39,39	0
33	MG	0	8070	1/1	0.99	0.18	27,27,27,27	0
37	SR	0	9416	1/1	0.99	0.08	45,45,45,45	0
37	SR	0	9445	1/1	0.99	0.07	55,55,55,55	0
37	SR	0	9488	1/1	0.99	0.07	69,69,69,69	0
37	SR	0	9446	1/1	0.99	0.09	77,77,77,77	0
37	SR	0	9456	1/1	0.99	0.04	57,57,57,57	0
37	SR	0	9474	1/1	0.99	0.06	57,57,57,57	0
37	SR	0	9421	1/1	0.99	0.05	66,66,66,66	0
38	CD	1	9202	1/1	0.99	0.04	50,50,50,50	0
37	SR	0	9410	1/1	0.99	0.13	36,36,36,36	0
37	SR	0	9444	1/1	0.99	0.04	51,51,51,51	0
37	SR	0	9478	1/1	0.99	0.07	71,71,71,71	0
37	SR	0	9473	1/1	0.99	0.03	69,69,69,69	0
37	SR	L	9409	1/1	1.00	0.10	36,36,36,36	0
37	SR	0	9407	1/1	1.00	0.10	41,41,41,41	0
37	SR	0	9448	1/1	1.00	0.06	52,52,52,52	0
37	SR	0	9408	1/1	1.00	0.11	36,36,36,36	0
37	SR	A	9436	1/1	1.00	0.06	47,47,47,47	0
37	SR	0	9428	1/1	1.00	0.03	49,49,49,49	0
37	SR	0	9501	1/1	1.00	0.07	64,64,64,64	0
37	SR	0	9424	1/1	1.00	0.13	45,45,45,45	0
37	SR	0	9412	1/1	1.00	0.11	38,38,38,38	0
37	SR	0	9415	1/1	1.00	0.10	50,50,50,50	0

6.5 Other polymers

There are no such residues in this entry.