



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 01:45 AM UTC

PDB ID : 1VQ6 / pdb_00001vq6
Title : The structure of c-hpmn and CCA-PHE-CAP-BIO bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

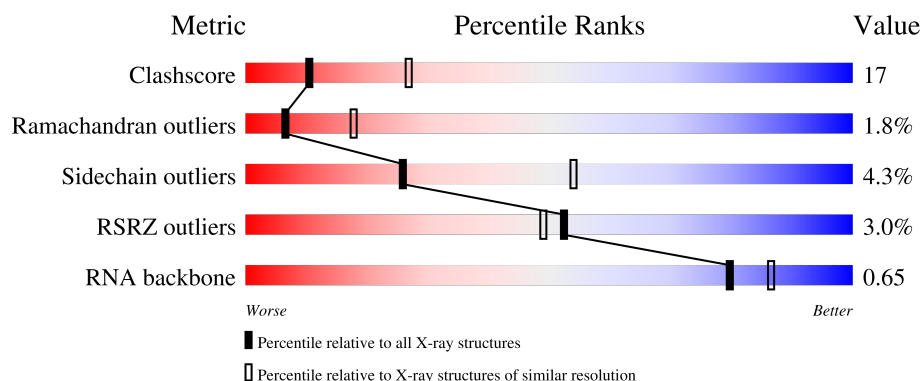
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



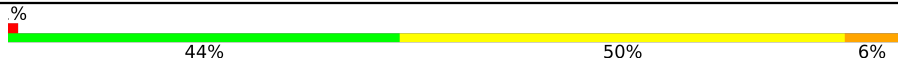
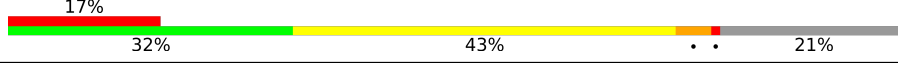
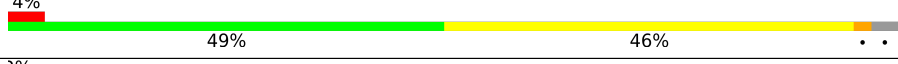
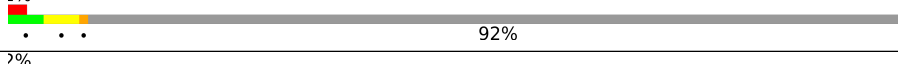
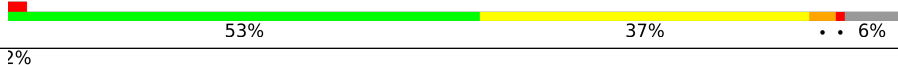
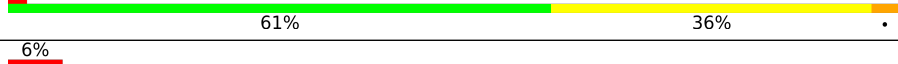
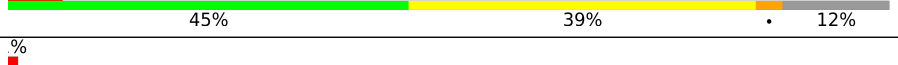
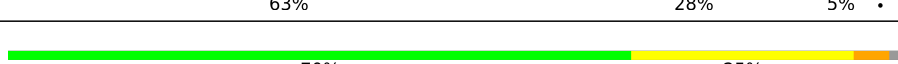
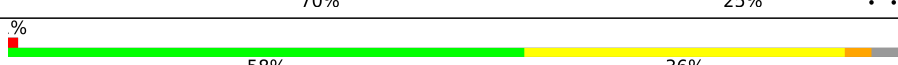
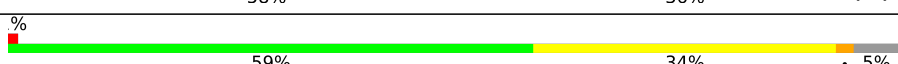
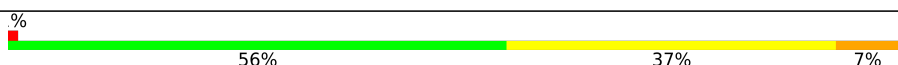
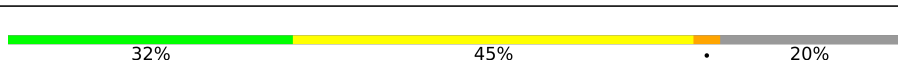
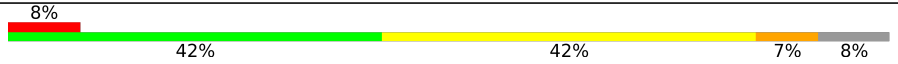
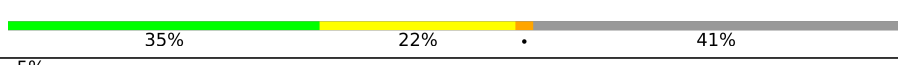
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	2922	57% 31% 5% 6%
2	9	122	50% 42% 7%
3	4	3	33% 67%
4	5	6	17% 50% 33% 17%
5	A	240	52% 40% 6%

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Mol	Chain	Length	Quality of chain
6	B	338	
7	C	246	
8	D	177	
9	E	178	
10	F	120	
11	G	348	
12	H	171	
13	J	145	
14	K	132	
15	L	165	
16	M	194	
17	N	187	
18	O	116	
19	P	149	
20	Q	96	
21	R	155	
22	S	85	
23	T	120	
24	U	66	
25	V	71	
26	W	154	
27	X	92	
28	Y	241	
29	Z	83	
30	1	57	

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Mol	Chain	Length	Quality of chain
31	2	50	
32	3	92	
33	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
36	NA	0	9152	-	-	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99029 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			

- 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*(5AA)*(HFA))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	3	Total	C	N	O	P	0	0	0
			52	30	9	12	1			

- Molecule 4 is a RNA chain called 5'-R(*CP*CP*AP*(PHE)*(ACA)*(BTN))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	5	6	Total	C	N	O	P	0	0	0
			82	46	13	21	2			

- Molecule 5 is a protein called 50S ribosomal protein L2P.

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

- Molecule 6 is a protein called 50S ribosomal protein L3P.

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

- Molecule 7 is a protein called 50S ribosomal protein L4E.

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

- Molecule 8 is a protein called 50S ribosomal protein L5P.

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

- Molecule 9 is a protein called 50S ribosomal protein L6P.

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

- Molecule 10 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 11 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L10E.

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

- Molecule 13 is a protein called 50S ribosomal protein L13P.

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

- Molecule 14 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	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 15 is a protein called 50S ribosomal protein L15P.

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

- Molecule 16 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	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 17 is a protein called 50S ribosomal protein L18P.

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

- Molecule 18 is a protein called 50S ribosomal protein L18e.

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

- Molecule 19 is a protein called 50S ribosomal protein L19E.

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

- Molecule 20 is a protein called 50S ribosomal protein L21e.

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

- Molecule 21 is a protein called 50S ribosomal protein L22P.

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

- Molecule 22 is a protein called 50S ribosomal protein L23P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24P.

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

- Molecule 24 is a protein called 50S ribosomal protein L24E.

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

- Molecule 25 is a protein called 50S ribosomal protein L29P.

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

- Molecule 26 is a protein called 50S ribosomal protein L30P.

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

- Molecule 27 is a protein called 50S ribosomal protein L31e.

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

- Molecule 28 is a protein called 50S ribosomal protein L32E.

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

- Molecule 29 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	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 30 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 31 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 32 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	107	Total	Mg	0	0
			107	107		
34	9	1	Total	Mg	0	0
			1	1		
34	5	1	Total	Mg	0	0
			1	1		
34	A	2	Total	Mg	0	0
			2	2		
34	B	2	Total	Mg	0	0
			2	2		
34	K	1	Total	Mg	0	0
			1	1		
34	T	1	Total	Mg	0	0
			1	1		
34	Y	1	Total	Mg	0	0
			1	1		
34	3	1	Total	Mg	0	0
			1	1		

- Molecule 35 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	2	Total	K	0	0
			2	2		

- Molecule 36 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	73	Total	Na	0	0
			73	73		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	9	2	Total 2	Na 2	0	0
36	A	1	Total 1	Na 1	0	0
36	C	1	Total 1	Na 1	0	0
36	H	1	Total 1	Na 1	0	0
36	J	1	Total 1	Na 1	0	0
36	L	1	Total 1	Na 1	0	0
36	M	1	Total 1	Na 1	0	0
36	Q	1	Total 1	Na 1	0	0
36	R	3	Total 3	Na 3	0	0
36	S	1	Total 1	Na 1	0	0

- Molecule 37 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	8	Total 8	Cl 8	0	0
37	A	1	Total 1	Cl 1	0	0
37	B	1	Total 1	Cl 1	0	0
37	J	3	Total 3	Cl 3	0	0
37	K	1	Total 1	Cl 1	0	0
37	L	1	Total 1	Cl 1	0	0
37	M	1	Total 1	Cl 1	0	0
37	N	1	Total 1	Cl 1	0	0
37	O	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	R	1	Total 1	Cl 1	0	0
37	Y	2	Total 2	Cl 2	0	0
37	3	1	Total 1	Cl 1	0	0

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

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

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5764	Total 5764	O 5764	0	0
39	9	135	Total 135	O 135	0	0
39	4	1	Total 1	O 1	0	0
39	5	1	Total 1	O 1	0	0
39	A	120	Total 120	O 120	0	0
39	B	156	Total 156	O 156	0	0
39	C	168	Total 168	O 168	0	0
39	D	45	Total 45	O 45	0	0
39	E	49	Total 49	O 49	0	0

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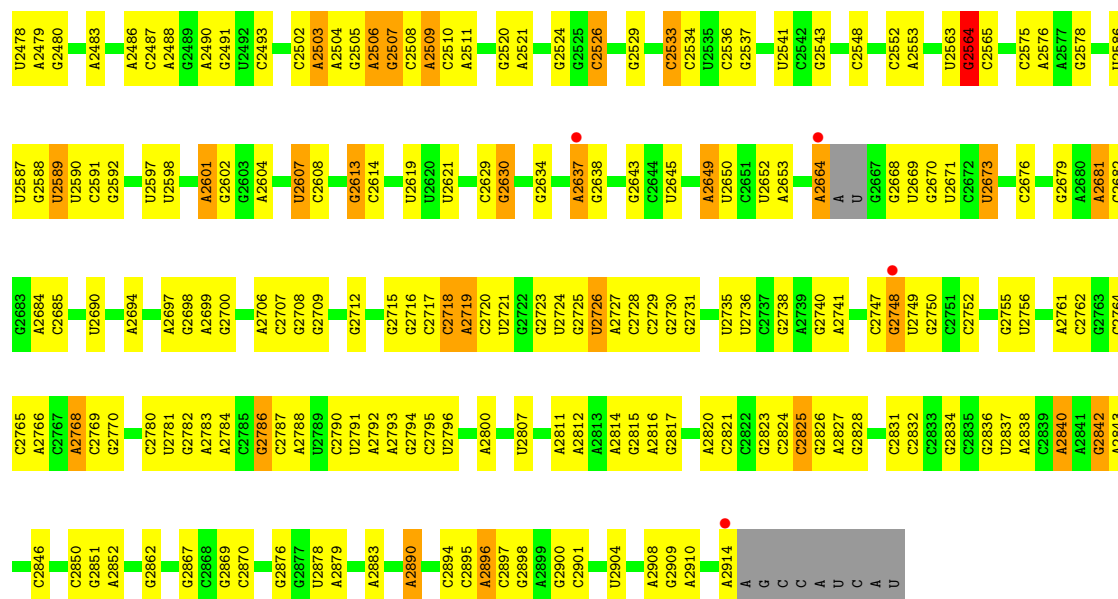
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39	F	23	Total 23	O 23	0	0
39	G	16	Total 16	O 16	0	0
39	H	68	Total 68	O 68	0	0
39	J	50	Total 50	O 50	0	0
39	K	55	Total 55	O 55	0	0
39	L	89	Total 89	O 89	0	0
39	M	125	Total 125	O 125	0	0
39	N	64	Total 64	O 64	0	0
39	O	42	Total 42	O 42	0	0
39	P	63	Total 63	O 63	0	0
39	Q	50	Total 50	O 50	0	0
39	R	81	Total 81	O 81	0	0
39	S	35	Total 35	O 35	0	0
39	T	35	Total 35	O 35	0	0
39	U	29	Total 29	O 29	0	0
39	V	13	Total 13	O 13	0	0
39	W	70	Total 70	O 70	0	0
39	X	25	Total 25	O 25	0	0
39	Y	95	Total 95	O 95	0	0
39	Z	30	Total 30	O 30	0	0
39	1	59	Total 59	O 59	0	0

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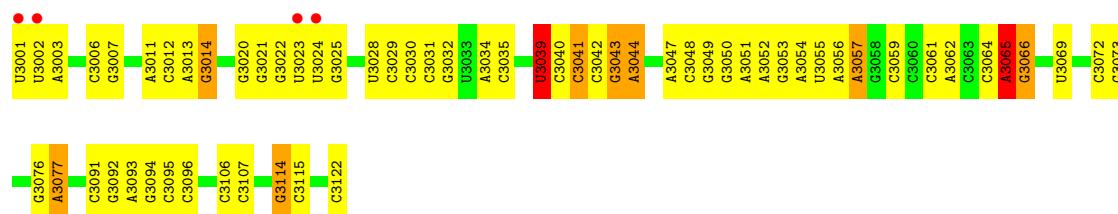
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	2	42	Total 42	O 42	0	0
39	3	71	Total 71	O 71	0	0
39	I	10	Total 10	O 10	0	0

G2385	A1181	C1253	A1372	A1482	C1593	A1710	G1805	A1922	C2036	A	G	A2300	G2385
U2386	C1182	A1261	A1373	C1483	C1594	A1717	G1806	G1923	A2039	G	U	A2301	U2386
C2388	C1183	A1261	C1374	G1484	G1595	A1717	A1811	G1926	G2043	U	G	A2302	C2388
C2392	C1184	U1266	C1375	A1494	U1596	U1722	A1815	A1927	G2044	A	C	A2303	C2392
A2401	U1185	U1266	A1376	C1495	A1597	U1723	C1816	A1930	G2045	A	C	C2309	A2401
A2402	U1087	U1266	G1376	C1496	A1598	U1724	U1817	A1931	G2046	A	C	G2310	A2402
C2403	U1088	C1268	C1377	G1497	A1599	C1725	C1818	C1940	A2054	U	C	A2311	C2403
G2404	U1187	G1269	G1378	G1498	U1500	G1730	G1819	A1941	A2054	C	U	C2312	G2404
A2408	U1095	A1188	A1379	U1380	A1603	G1731	G1820	A1942	A2054	A	G	C2314	A2408
C2411	U1096	A1189	U1379	U1380	G1604	A1732	U1825	C1943	U2064	C	U	C2315	C2411
G2412	U1097	A1190	U1380	U1380	G1605	A1733	C1826	G1951	A2067	C	U	G2316	G2412
A2413	A1097	A1191	U1380	U1380	G1605	A1733	G1827	U	A2067	G	G	C2317	A2413
A2414	A1098	A1192	U1380	U1380	G1605	A1733	A1829	A	G2068	A	G	U2320	A2414
A2415	G1099	A1193	U1380	U1380	G1605	A1733	A1834	C	G2072	C	G	A2321	A2415
G2418	A1106	A1196	U1380	U1380	G1605	A1733	U1835	U	G2073	A	C	G2324	G2418
U2419	U1109	G1196	U1380	U1380	G1605	A1733	U1835	C	G2074	C	C	C2325	U2419
G2420	G1110	G1197	U1380	U1380	G1605	A1733	A1839	U	G2075	A	C	U2326	G2420
U2421	A1114	C1201	U1407	U1408	A1630	A1746	C1840	A	G2076	C	U	C2329	U2421
U2422	U1115	G1202	U1408	U1408	A1631	A1747	U1835	C	G2077	C	C	U2330	U2422
G2426	U1116	G1203	U1408	U1408	A1632	A1755	U1846	C	G2078	C	C	C2335	G2426
G2433	U1117	C1204	U1408	U1408	A1633	G1751	U1847	U	G2079	C	C	G2336	G2433
A2434	U1205	U1206	U1408	U1408	G1634	G1752	A1849	A	G2080	C	C	G2337	A2434
G2438	U1119	U1207	U1408	U1408	U1635	A1755	A1845	C	G2081	C	C	A	G2438
C2439	U1120	A1207	U1408	U1408	G1636	G1756	U1846	C	A2081	C	C	C	C2439
C2443	G1121	C1209	U1408	U1408	A1637	G1756	U1847	C	A2082	C	C	G	C2443
G2451	U1122	G1210	U1408	U1408	A1637	G1756	G1847	C	G2083	C	C	G	G2451
G2452	U1130	G1211	U1408	U1408	A1637	G1756	G1848	C	G2084	C	C	G	G2452
C2453	G1131	C1212	U1408	U1408	A1637	G1756	G1849	C	G2085	C	C	G	C2453
G2454	A1132	C1213	U1408	U1408	A1637	G1756	G1850	C	G2086	C	C	G	G2454
A2455	U1136	G1216	U1408	U1408	A1637	G1756	G1851	C	G2087	C	C	G	A2455
A2456	G1137	G1217	U1408	U1408	A1637	G1756	G1852	C	G2088	C	C	G	A2456
U2457	U1138	U1218	U1408	U1408	A1637	G1756	G1853	C	G2089	C	C	G	U2457
A2460	G1138	G1226	U1408	U1408	A1637	G1756	G1854	C	G2090	C	C	G	A2460
U2461	C1157	C1229	U1408	U1408	A1637	G1756	G1855	C	G2091	C	C	G	U2461
A2462	G1158	A1230	U1408	U1408	A1637	G1756	G1856	C	G2092	C	C	G	A2462
A2465	G1159	A1231	U1408	U1408	A1637	G1756	G1857	C	G2093	C	C	G	A2465
G2466	G1160	A1232	U1408	U1408	A1637	G1756	G1858	C	G2094	C	C	G	G2466
A2467	A1161	A1233	U1408	U1408	A1637	G1756	G1859	C	G2095	C	C	G	A2467
A2468	G1162	G1234	U1408	U1408	A1637	G1756	G1860	C	G2096	C	C	G	A2468
A2469	G1163	G1235	U1408	U1408	A1637	G1756	G1861	C	G2097	C	C	G	G2469
G2472	U1164	A1236	U1408	U1408	A1637	G1756	G1862	C	G2098	C	C	G	A2472
U2473	U1165	U1237	U1408	U1408	A1637	G1756	G1863	C	G2099	C	C	G	U2473
A2474	A1166	G1238	U1408	U1408	A1637	G1756	G1864	C	G2100	C	C	G	A2474
C2475	G1167	G1239	U1408	U1408	A1637	G1756	G1865	C	G2101	C	C	G	C2475
C2476	C1168	C1240	U1408	U1408	A1637	G1756	G1866	C	G2102	C	C	G	C2476
C2477	U1169	A1242	U1408	U1408	A1637	G1756	G1867	C	G2103	C	C	G	C2477
	U1170	C1243	U1408	U1408	A1637	G1756	G1868	C	G2104	C	C	G	
	A1171	U1244	U1408	U1408	A1637	G1756	G1869	C	G2105	C	C	G	
	G1172	C1245	U1408	U1408	A1637	G1756	G1870	C	G2106	C	C	G	
	A1173	A1246	U1408	U1408	A1637	G1756	G1871	C	G2107	C	C	G	
	U1174	U1249	U1408	U1408	A1637	G1756	G1872	C	G2108	C	C	G	
	G1175	C1250	U1408	U1408	A1637	G1756	G1873	C	G2109	C	C	G	
	C1176	C1251	U1408	U1408	A1637	G1756	G1874	C	G2110	C	C	G	
	U1180	A1252	U1408	U1408	A1637	G1756	G1875	C	G2111	C	C	G	



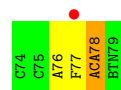
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 5'-R(*CP*(5AA)*(HFA))-3'

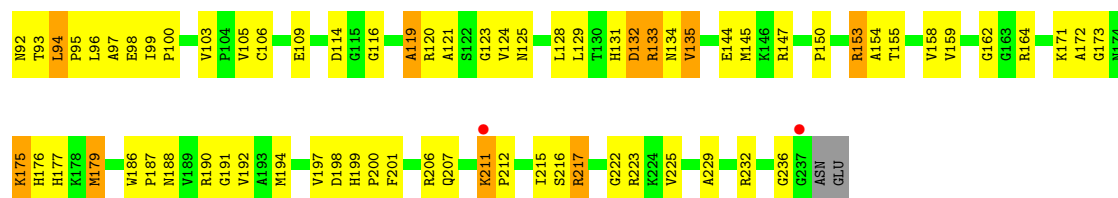


• Molecule 4: 5'-R(*CP*CP*AP*(PHE)*(ACA)*(BTN))-3'

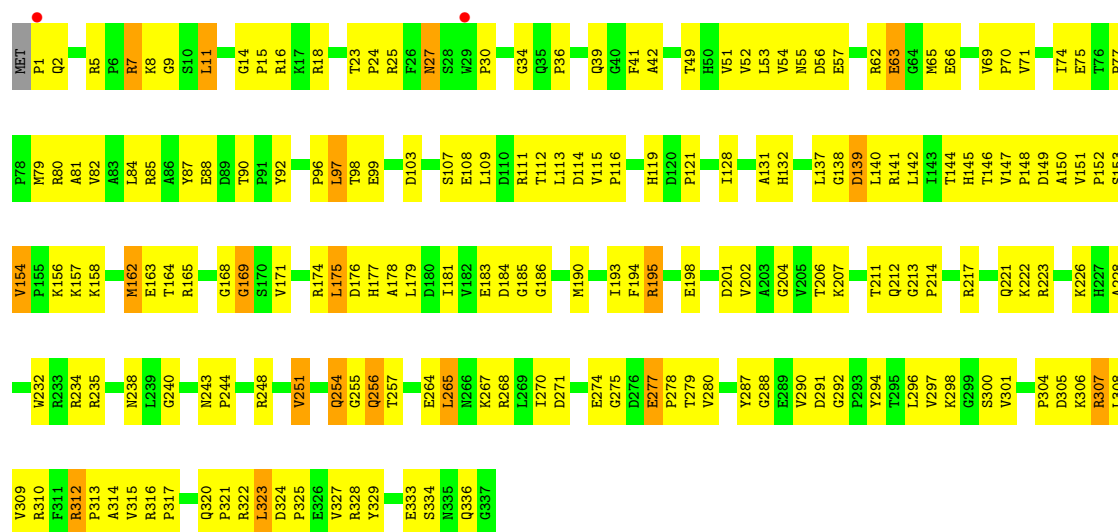
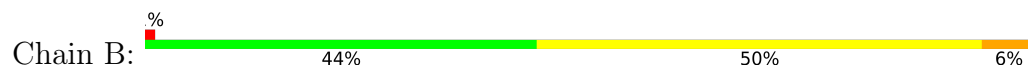


• Molecule 5: 50S ribosomal protein L2P

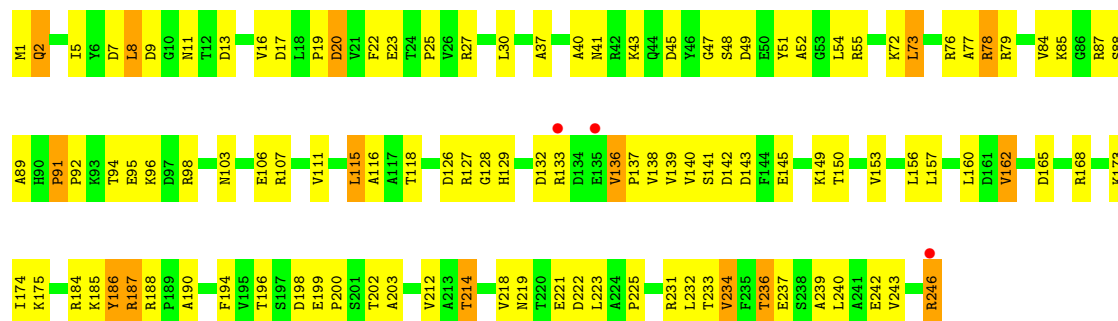




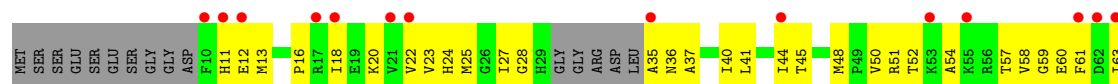
• Molecule 6: 50S ribosomal protein L3P

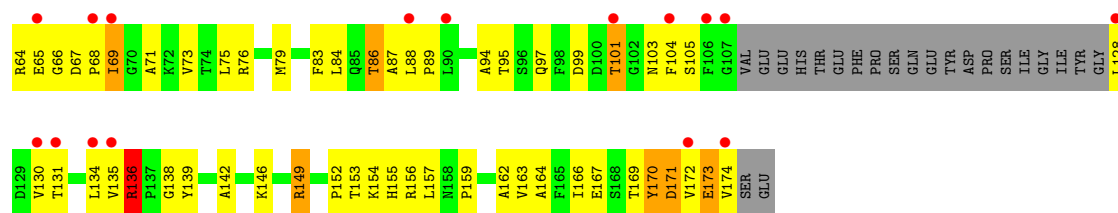


• Molecule 7: 50S ribosomal protein L4E

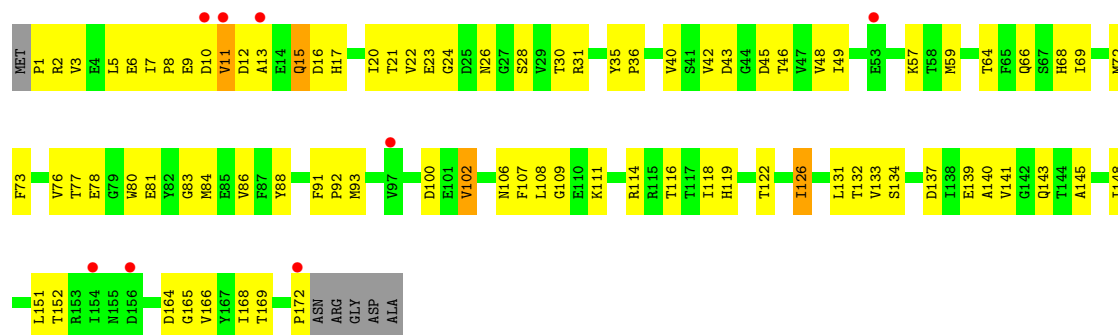


• Molecule 8: 50S ribosomal protein L5P

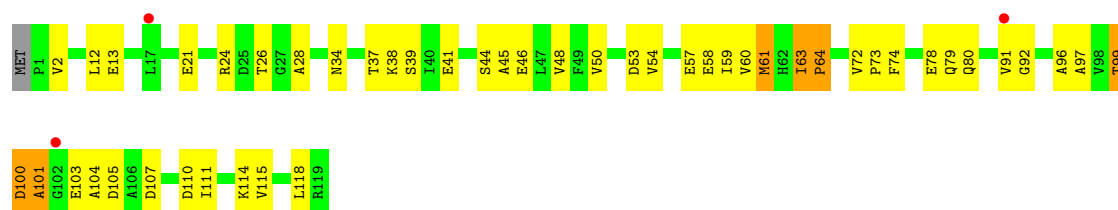




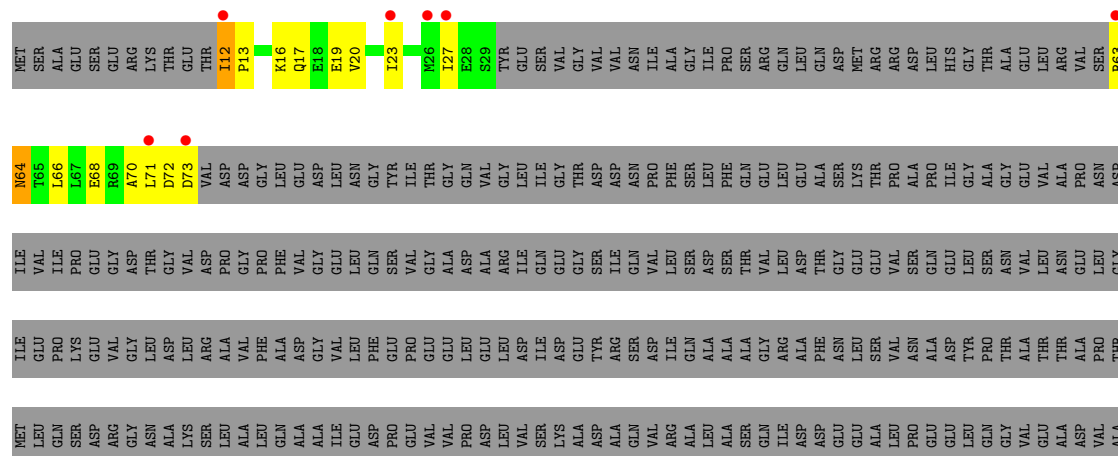
● Molecule 9: 50S ribosomal protein L6P



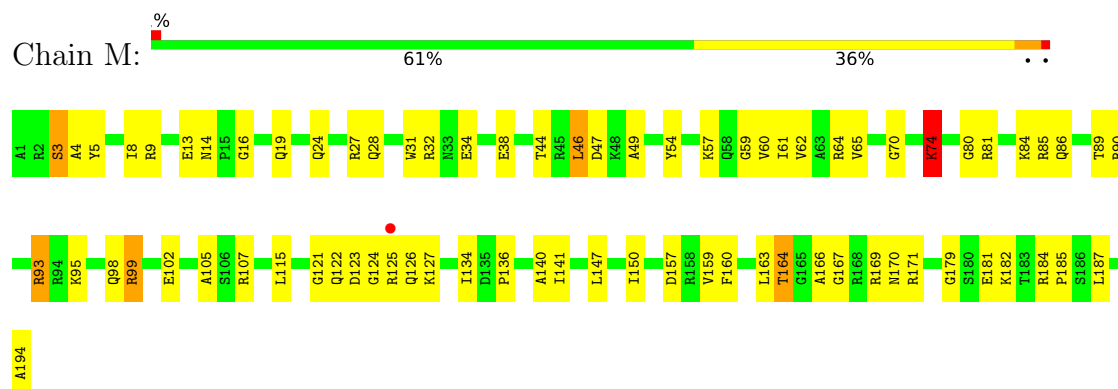
● Molecule 10: 50S ribosomal protein L7AE



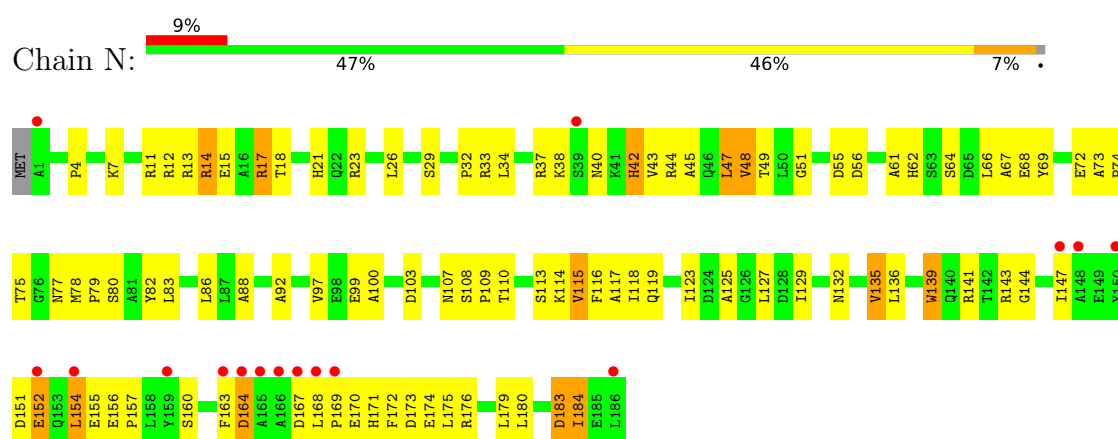
● Molecule 11: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



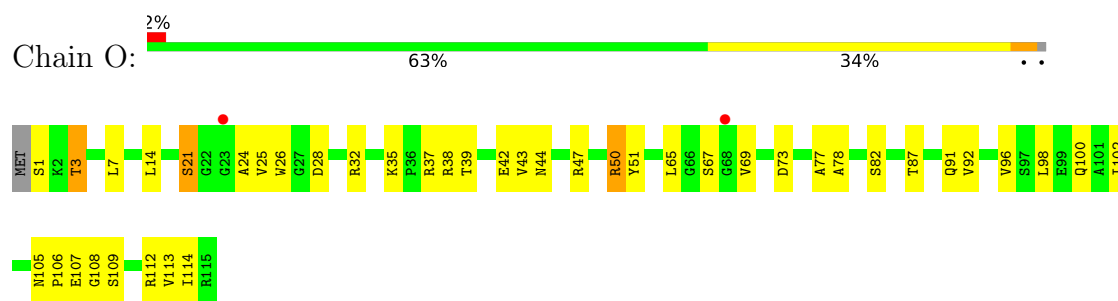
- Molecule 16: 50S Ribosomal Protein L15E



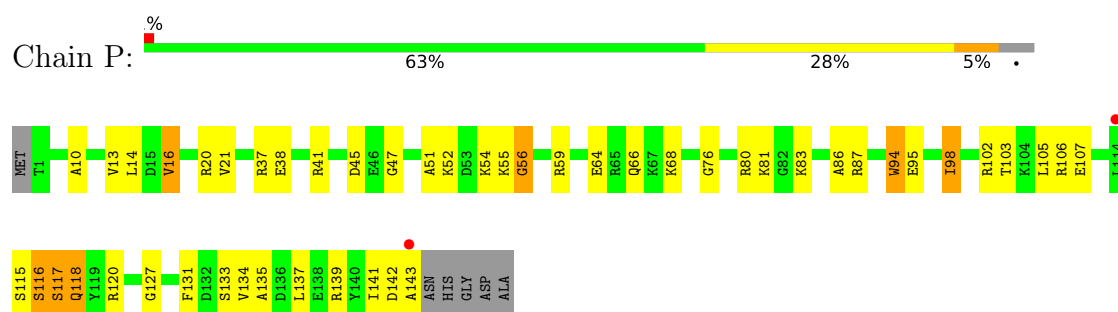
- Molecule 17: 50S ribosomal protein L18P



- Molecule 18: 50S ribosomal protein L18e



- Molecule 19: 50S ribosomal protein L19E



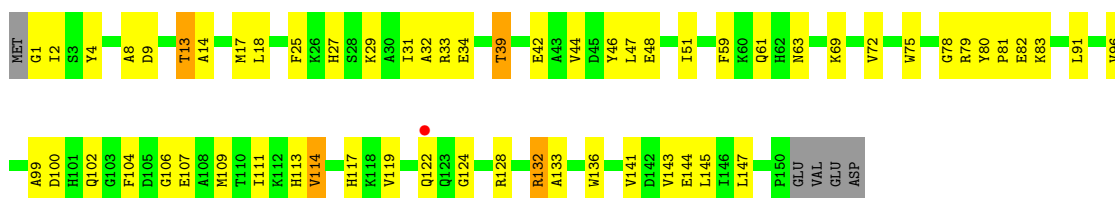
- Molecule 20: 50S ribosomal protein L21e

Chain Q:  70% 25% . .



- Molecule 21: 50S ribosomal protein L22P

Chain R:  58% 36% . .



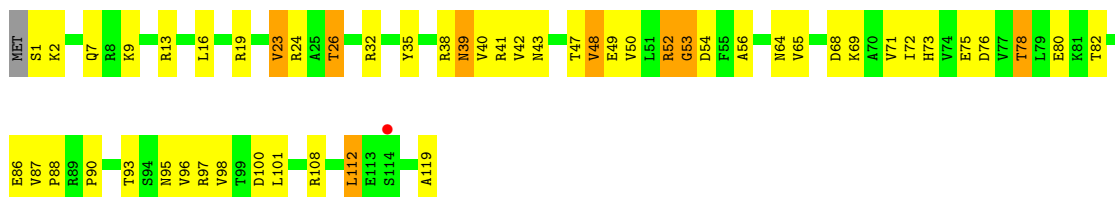
- Molecule 22: 50S ribosomal protein L23P

Chain S:  59% 34% . 5%



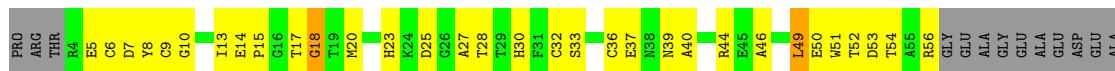
- Molecule 23: 50S ribosomal protein L24P

Chain T:  56% 37% 7% .



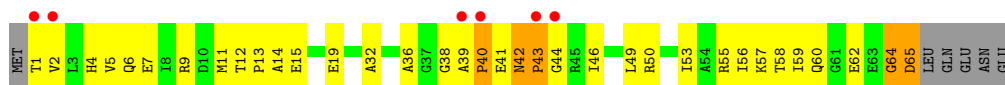
- Molecule 24: 50S ribosomal protein L24E

Chain U:  32% 45% . 20%



- Molecule 25: 50S ribosomal protein L29P

Chain V:  8% 42% 42% 7% 8%

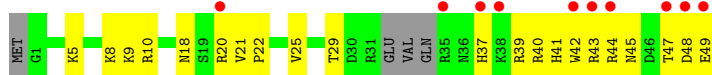


- Molecule 26: 50S ribosomal protein L30P





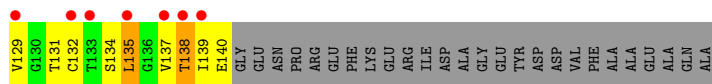
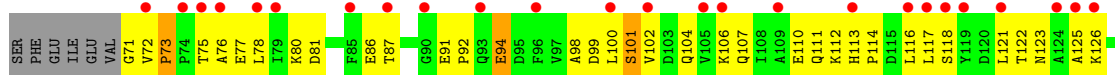
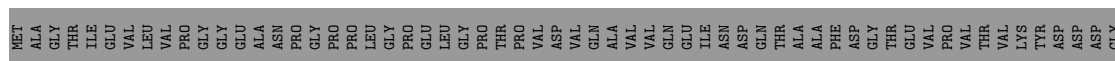
- Molecule 31: 50S ribosomal protein L39e



- Molecule 32: 50S ribosomal protein L44E



- Molecule 33: 50S RIBOSOMAL PROTEIN L11P



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.05Å 300.19Å 573.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.70) 93.2 (50.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.194 , 0.233 0.185 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	56.1	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.1	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	99029	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% 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: UR3, CD, BTN, CL, OMG, 1MA, PSU, ACA, K, 5AA, OMU, NA, MG, HFA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.38	0/65959	0.61	30/102870 (0.0%)
2	9	0.37	0/2905	0.60	3/4528 (0.1%)
3	4	0.28	0/18	0.76	0/26
4	5	0.45	0/76	1.08	1/112 (0.9%)
5	A	0.42	0/1786	1.00	9/2408 (0.4%)
6	B	0.42	0/2690	1.02	14/3652 (0.4%)
7	C	0.48	0/1884	0.99	6/2551 (0.2%)
8	D	0.34	0/1111	0.82	3/1498 (0.2%)
9	E	0.38	0/1382	0.87	1/1880 (0.1%)
10	F	0.39	0/901	0.90	2/1224 (0.2%)
11	G	0.37	0/241	0.71	0/324
12	H	0.39	0/1287	0.97	6/1725 (0.3%)
13	J	0.43	0/1136	0.94	2/1530 (0.1%)
14	K	0.45	0/1001	1.03	3/1347 (0.2%)
15	L	0.39	0/1130	0.97	4/1509 (0.3%)
16	M	0.44	0/1584	0.92	8/2119 (0.4%)
17	N	0.37	0/1474	1.01	7/1999 (0.4%)
18	O	0.42	0/874	0.93	3/1181 (0.3%)
19	P	0.41	0/1147	0.89	3/1528 (0.2%)
20	Q	0.45	0/749	1.05	3/1005 (0.3%)
21	R	0.44	0/1172	0.94	2/1578 (0.1%)
22	S	0.37	0/648	0.91	4/875 (0.5%)
23	T	0.39	0/958	0.99	2/1289 (0.2%)
24	U	0.39	0/417	0.97	2/562 (0.4%)
25	V	0.38	0/502	0.98	3/675 (0.4%)
26	W	0.48	0/1219	1.01	4/1655 (0.2%)
27	X	0.43	0/664	0.95	2/895 (0.2%)
28	Y	0.45	0/1146	0.98	5/1536 (0.3%)
29	Z	0.39	0/589	0.90	1/787 (0.1%)
30	1	0.45	0/438	0.97	1/578 (0.2%)
31	2	0.40	0/401	0.77	0/529
32	3	0.43	0/771	0.91	6/1024 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	I	0.37	0/526	1.01	4/716 (0.6%)
All	All	0.39	0/98786	0.72	144/147715 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	49
2	9	0	2
26	W	0	1
All	All	1	52

There are no bond length outliers.

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	14.17	130.76	109.50
20	Q	17	LYS	N-CA-C	-9.29	98.03	109.83
5	A	222	GLY	N-CA-C	-9.21	103.52	114.48
17	N	135	VAL	N-CA-C	-9.11	104.15	112.90
1	0	1563	G	C4'-C3'-O3'	8.68	122.42	109.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	174	A	Sidechain
1	0	26	U	Sidechain
1	0	270	U	Sidechain
1	0	333	G	Sidechain
1	0	396	U	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	29810	912	0
2	9	2600	0	1326	61	0
3	4	52	0	36	2	0
4	5	82	0	50	3	0
5	A	1753	0	1766	133	0
6	B	2625	0	2533	204	0
7	C	1859	0	1816	115	0
8	D	1094	0	1085	91	0
9	E	1357	0	1266	90	0
10	F	890	0	843	46	0
11	G	240	0	231	15	0
12	H	1266	0	1268	71	0
13	J	1120	0	1098	75	0
14	K	992	0	1031	65	0
15	L	1118	0	1076	65	0
16	M	1560	0	1568	67	0
17	N	1445	0	1401	109	0
18	O	865	0	873	40	0
19	P	1136	0	1123	51	0
20	Q	735	0	729	21	0
21	R	1149	0	1122	58	0
22	S	641	0	605	23	0
23	T	950	0	923	55	0
24	U	410	0	364	33	0
25	V	499	0	511	36	0
26	W	1196	0	1137	105	0
27	X	654	0	653	53	0
28	Y	1130	0	1133	64	0
29	Z	578	0	539	27	0
30	1	431	0	426	24	0
31	2	396	0	413	31	0
32	3	755	0	728	27	0
33	I	519	0	500	49	0
34	0	107	0	0	0	0
34	3	1	0	0	0	0
34	5	1	0	0	0	0
34	9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	A	2	0	0	0	0
34	B	2	0	0	0	0
34	K	1	0	0	0	0
34	T	1	0	0	0	0
34	Y	1	0	0	0	0
35	0	2	0	0	0	0
36	0	73	0	0	0	0
36	9	2	0	0	0	0
36	A	1	0	0	0	0
36	C	1	0	0	0	0
36	H	1	0	0	0	0
36	J	1	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	3	0	0	0	0
36	S	1	0	0	0	0
37	0	8	0	0	0	0
37	3	1	0	0	0	0
37	A	1	0	0	0	0
37	B	1	0	0	0	0
37	J	3	0	0	0	0
37	K	1	0	0	0	0
37	L	1	0	0	0	0
37	M	1	0	0	0	0
37	N	1	0	0	0	0
37	O	1	0	0	0	0
37	R	1	0	0	0	0
37	Y	2	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	5764	0	0	115	0
39	1	59	0	0	2	0
39	2	42	0	0	1	0
39	3	71	0	0	5	0
39	4	1	0	0	0	0
39	5	1	0	0	0	0
39	9	135	0	0	2	0
39	A	120	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	B	156	0	0	21	0
39	C	168	0	0	18	0
39	D	45	0	0	8	0
39	E	49	0	0	8	0
39	F	23	0	0	3	0
39	G	16	0	0	1	0
39	H	68	0	0	6	0
39	I	10	0	0	2	0
39	J	50	0	0	2	0
39	K	55	0	0	7	0
39	L	89	0	0	15	0
39	M	125	0	0	3	0
39	N	64	0	0	8	0
39	O	42	0	0	7	0
39	P	63	0	0	3	0
39	Q	50	0	0	6	0
39	R	81	0	0	3	0
39	S	35	0	0	2	0
39	T	35	0	0	3	0
39	U	29	0	0	1	0
39	V	13	0	0	1	0
39	W	70	0	0	4	0
39	X	25	0	0	6	0
39	Y	95	0	0	8	0
39	Z	30	0	0	1	0
All	All	99029	0	59983	2550	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

The worst 5 of 2550 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)
25:V:12:THR:HG22	25:V:15:GLU:HG3	1.27	1.14
1:O:1160:G:H5'	1:O:1161:A:H5'	1.18	1.10
12:H:46:GLN:HB3	12:H:167:PRO:HD2	1.30	1.08
1:O:1242:A:H5'	13:J:82:THR:HG23	1.37	1.07
8:D:25:MET:HE2	8:D:41:LEU:HG	1.38	1.04

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	
5	A	235/240 (98%)	205 (87%)	24 (10%)	6 (3%)	4	11
6	B	335/338 (99%)	295 (88%)	33 (10%)	7 (2%)	5	15
7	C	244/246 (99%)	215 (88%)	28 (12%)	1 (0%)	30	54
8	D	134/177 (76%)	94 (70%)	33 (25%)	7 (5%)	1	3
9	E	170/178 (96%)	156 (92%)	14 (8%)	0	100	100
10	F	117/120 (98%)	104 (89%)	7 (6%)	6 (5%)	1	3
11	G	25/348 (7%)	24 (96%)	0	1 (4%)	2	5
12	H	156/171 (91%)	142 (91%)	11 (7%)	3 (2%)	6	17
13	J	140/145 (97%)	126 (90%)	11 (8%)	3 (2%)	5	15
14	K	130/132 (98%)	116 (89%)	12 (9%)	2 (2%)	8	22
15	L	141/165 (86%)	122 (86%)	17 (12%)	2 (1%)	9	23
16	M	192/194 (99%)	176 (92%)	16 (8%)	0	100	100
17	N	184/187 (98%)	166 (90%)	13 (7%)	5 (3%)	4	10
18	O	113/116 (97%)	109 (96%)	2 (2%)	2 (2%)	6	18
19	P	141/149 (95%)	131 (93%)	7 (5%)	3 (2%)	5	15
20	Q	93/96 (97%)	84 (90%)	9 (10%)	0	100	100
21	R	148/155 (96%)	135 (91%)	11 (7%)	2 (1%)	9	23
22	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
23	T	117/120 (98%)	107 (92%)	9 (8%)	1 (1%)	14	35
24	U	51/66 (77%)	46 (90%)	4 (8%)	1 (2%)	6	16
25	V	63/71 (89%)	54 (86%)	7 (11%)	2 (3%)	3	7
26	W	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	18	41
27	X	80/92 (87%)	70 (88%)	8 (10%)	2 (2%)	4	11
28	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
29	Z	71/83 (86%)	55 (78%)	9 (13%)	7 (10%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
31	2	42/50 (84%)	39 (93%)	3 (7%)	0	100	100
32	3	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	11	29
33	I	68/162 (42%)	49 (72%)	16 (24%)	3 (4%)	2	4
All	All	3705/4430 (84%)	3316 (90%)	321 (9%)	68 (2%)	6	18

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	139	ASP
6	B	184	ASP
10	F	101	ALA
12	H	166	SER
12	H	168	ALA

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	
5	A	179/182 (98%)	171 (96%)	8 (4%)	24	52
6	B	282/283 (100%)	268 (95%)	14 (5%)	22	48
7	C	193/193 (100%)	178 (92%)	15 (8%)	11	29
8	D	117/148 (79%)	112 (96%)	5 (4%)	26	54
9	E	152/156 (97%)	148 (97%)	4 (3%)	40	70
10	F	93/94 (99%)	90 (97%)	3 (3%)	34	64
11	G	27/283 (10%)	25 (93%)	2 (7%)	13	32
12	H	132/138 (96%)	124 (94%)	8 (6%)	17	40
13	J	118/121 (98%)	112 (95%)	6 (5%)	21	48
14	K	106/106 (100%)	104 (98%)	2 (2%)	50	77
15	L	113/127 (89%)	111 (98%)	2 (2%)	51	78
16	M	158/158 (100%)	152 (96%)	6 (4%)	29	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	N	149/150 (99%)	143 (96%)	6 (4%)	28	56
18	O	93/94 (99%)	91 (98%)	2 (2%)	45	74
19	P	113/117 (97%)	108 (96%)	5 (4%)	25	53
20	Q	79/80 (99%)	74 (94%)	5 (6%)	16	39
21	R	117/122 (96%)	113 (97%)	4 (3%)	32	62
22	S	71/74 (96%)	71 (100%)	0	100	100
23	T	105/106 (99%)	98 (93%)	7 (7%)	15	36
24	U	44/52 (85%)	42 (96%)	2 (4%)	24	52
25	V	51/57 (90%)	49 (96%)	2 (4%)	28	57
26	W	130/130 (100%)	123 (95%)	7 (5%)	20	45
27	X	66/74 (89%)	59 (89%)	7 (11%)	6	17
28	Y	120/196 (61%)	114 (95%)	6 (5%)	22	48
29	Z	60/68 (88%)	60 (100%)	0	100	100
30	1	46/47 (98%)	44 (96%)	2 (4%)	26	54
31	2	42/46 (91%)	41 (98%)	1 (2%)	43	72
32	3	79/79 (100%)	78 (99%)	1 (1%)	61	83
33	I	58/130 (45%)	57 (98%)	1 (2%)	53	79
All	All	3093/3611 (86%)	2960 (96%)	133 (4%)	26	54

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

Mol	Chain	Res	Type
27	X	15	ARG
27	X	79	GLU
31	2	18	ASN
10	F	105	ASP
10	F	99	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
21	R	94	ASN
26	W	6	GLN
21	R	113	HIS
23	T	39	ASN

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Mol	Chain	Res	Type
26	W	119	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	244 (8%)	30 (1%)
2	9	121/122 (99%)	16 (13%)	1 (0%)
3	4	0/3	-	-
4	5	2/6 (33%)	0	0
All	All	2868/3053 (93%)	260 (9%)	31 (1%)

5 of 260 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A
1	0	70	A

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1377	C
1	0	2718	C
1	0	1563	G
1	0	2791	U
1	0	2467	A

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

8 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	36,1	19,22,23	0.34	0	25,31,34	0.38	0
1	1MA	0	628	36,1	21,25,26	0.71	1 (4%)	30,37,40	0.79	1 (3%)
3	5AA	4	76	3,1	23,26,27	0.38	0	29,38,41	0.96	1 (3%)
1	UR3	0	2619	1	19,22,23	0.53	0	26,32,35	0.70	1 (3%)
1	OMG	0	2588	3,1	23,26,27	0.28	0	32,38,41	0.33	0
4	ACA	5	78	4	6,7,8	1.89	1 (16%)	5,6,8	0.77	0
1	PSU	0	2621	1	18,21,22	1.59	2 (11%)	21,30,33	1.41	3 (14%)
3	HFA	4	77	3	10,11,12	1.23	1 (10%)	11,13,15	0.53	0

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	36,1	-	0/9/27/28	0/2/2/2
1	1MA	0	628	36,1	-	2/7/25/26	0/3/3/3
3	5AA	4	76	3,1	-	0/11/29/30	0/3/3/3
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
1	OMG	0	2588	3,1	-	0/9/27/28	0/3/3/3
4	ACA	5	78	4	-	3/5/5/6	-
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
3	HFA	4	77	3	-	0/5/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	5.18	1.43	1.36
4	5	78	ACA	C3-C2	-4.28	1.34	1.52
3	4	77	HFA	OA-CA	3.29	1.49	1.43
1	0	2621	PSU	C6-C5	3.22	1.38	1.35
1	0	628	1MA	C6-N6	2.56	1.34	1.28

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.56	120.58	118.17
1	0	2621	PSU	C6-N1-C2	-3.40	119.53	122.69
3	4	76	5AA	C2-N1-C6	2.89	118.89	111.83
1	0	2621	PSU	O2-C2-N1	2.81	125.68	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	628	1MA	N1-C2-N3	2.79	129.31	126.00

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	5	78	ACA	O-C-C2-C3
4	5	78	ACA	C2-C3-C4-C5
1	0	628	1MA	C2'-C1'-N9-C8
4	5	78	ACA	C4-C5-C6-N
1	0	628	1MA	C2'-C1'-N9-C4

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
3	4	76	5AA	1	0
1	0	2588	OMG	1	0
4	5	78	ACA	1	0
3	4	77	HFA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	76:A	O3'	77:PHE	C	1.60

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	-0.42	32 (1%) 76 75	30, 56, 102, 163	0
2	9	122/122 (100%)	-0.05	4 (3%) 49 45	51, 72, 98, 158	0
3	4	1/3 (33%)	0.45	0 100 100	75, 75, 75, 75	0
4	5	4/6 (66%)	1.07	1 (25%) 2 1	63, 63, 71, 81	0
5	A	237/240 (98%)	0.12	6 (2%) 58 55	37, 61, 97, 120	0
6	B	337/338 (99%)	0.31	2 (0%) 85 85	38, 68, 95, 104	0
7	C	246/246 (100%)	0.08	3 (1%) 76 75	32, 55, 81, 89	0
8	D	140/177 (79%)	1.30	30 (21%) 2 2	67, 111, 136, 143	0
9	E	172/178 (96%)	0.72	8 (4%) 36 33	58, 83, 108, 116	0
10	F	119/120 (99%)	0.54	3 (2%) 58 55	58, 84, 112, 127	0
11	G	29/348 (8%)	1.06	7 (24%) 2 1	78, 96, 110, 112	0
12	H	160/171 (93%)	0.21	4 (2%) 58 55	46, 66, 98, 104	0
13	J	142/145 (97%)	0.21	3 (2%) 63 61	49, 63, 82, 103	0
14	K	132/132 (100%)	0.42	2 (1%) 72 70	41, 67, 88, 94	0
15	L	145/165 (87%)	0.55	10 (6%) 23 20	34, 77, 120, 133	0
16	M	194/194 (100%)	-0.13	1 (0%) 87 86	38, 51, 68, 77	0
17	N	186/187 (99%)	0.54	16 (8%) 16 13	47, 72, 120, 126	0
18	O	115/116 (99%)	0.39	2 (1%) 69 67	47, 66, 83, 96	0
19	P	143/149 (95%)	0.47	2 (1%) 73 72	47, 68, 83, 91	0
20	Q	95/96 (98%)	0.00	0 100 100	45, 54, 68, 87	0
21	R	150/155 (96%)	-0.16	1 (0%) 84 83	42, 55, 73, 84	0
22	S	81/85 (95%)	0.15	1 (1%) 76 75	52, 68, 87, 94	0
23	T	119/120 (99%)	0.29	1 (0%) 82 81	48, 67, 99, 115	0
24	U	53/66 (80%)	0.32	0 100 100	52, 67, 84, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	V	65/71 (91%)	0.76	6 (9%) 14 12	62, 85, 123, 128	0
26	W	154/154 (100%)	0.15	0 100 100	46, 61, 81, 92	0
27	X	82/92 (89%)	0.50	5 (6%) 27 24	53, 69, 89, 106	0
28	Y	142/241 (58%)	0.00	1 (0%) 84 83	35, 56, 79, 97	0
29	Z	73/83 (87%)	0.53	4 (5%) 30 27	54, 72, 84, 105	0
30	1	56/57 (98%)	-0.43	0 100 100	37, 42, 48, 60	0
31	2	46/50 (92%)	0.88	10 (21%) 2 2	42, 71, 124, 132	0
32	3	92/92 (100%)	0.08	1 (1%) 78 76	42, 62, 77, 89	0
33	I	70/162 (43%)	2.08	32 (45%) 0 0	118, 134, 156, 158	0
All	All	6651/7483 (88%)	0.02	198 (2%) 52 49	30, 62, 110, 163	0

The worst 5 of 198 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	V	1	THR	9.2
33	I	133	THR	6.8
8	D	10	PHE	5.9
25	V	2	VAL	5.2
2	9	3001	U	4.9

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
4	ACA	5	78	8/9	0.85	0.29	77,82,89,90	0
3	HFA	4	77	11/12	0.92	0.18	86,86,87,88	0
3	5AA	4	76	24/25	0.93	0.12	77,82,86,87	0
1	UR3	0	2619	21/22	0.97	0.07	40,46,49,54	0
1	PSU	0	2621	20/21	0.98	0.05	34,37,42,43	0
1	OMU	0	2587	21/22	0.98	0.07	41,43,46,49	0
1	OMG	0	2588	24/25	0.98	0.07	38,40,45,46	0
1	1MA	0	628	23/24	0.98	0.07	39,41,42,44	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	NA	R	9186	1/1	0.66	0.31	80,80,80,80	0
36	NA	0	9129	1/1	0.72	0.19	68,68,68,68	0
36	NA	0	9124	1/1	0.75	0.36	69,69,69,69	0
36	NA	0	9184	1/1	0.76	0.17	103,103,103,103	0
36	NA	0	9152	1/1	0.76	0.43	76,76,76,76	0
36	NA	0	9185	1/1	0.80	0.29	61,61,61,61	0
36	NA	0	9171	1/1	0.80	0.26	74,74,74,74	0
34	MG	0	8114	1/1	0.81	0.11	62,62,62,62	0
36	NA	9	9151	1/1	0.81	0.25	80,80,80,80	0
34	MG	0	8046	1/1	0.81	0.11	68,68,68,68	0
36	NA	0	9170	1/1	0.83	0.56	85,85,85,85	0
36	NA	0	9163	1/1	0.83	0.22	75,75,75,75	0
34	MG	0	8045	1/1	0.84	0.24	87,87,87,87	0
36	NA	0	9166	1/1	0.85	0.17	71,71,71,71	0
36	NA	0	9110	1/1	0.86	0.11	44,44,44,44	0
34	MG	0	8082	1/1	0.86	0.20	72,72,72,72	0
34	MG	0	8050	1/1	0.86	0.10	86,86,86,86	0
37	CL	J	9302	1/1	0.86	0.18	86,86,86,86	0
36	NA	0	9175	1/1	0.87	0.37	61,61,61,61	0
34	MG	0	8106	1/1	0.87	0.07	57,57,57,57	0
36	NA	0	9164	1/1	0.88	0.20	55,55,55,55	0
36	NA	0	9182	1/1	0.89	0.17	78,78,78,78	0
34	MG	0	8092	1/1	0.89	0.24	102,102,102,102	0
34	MG	0	8100	1/1	0.89	0.20	79,79,79,79	0
36	NA	0	9111	1/1	0.89	0.21	71,71,71,71	0
36	NA	H	9122	1/1	0.89	0.19	75,75,75,75	0
34	MG	0	8024	1/1	0.89	0.10	61,61,61,61	0
36	NA	S	9112	1/1	0.89	0.14	74,74,74,74	0
36	NA	0	9177	1/1	0.89	0.21	78,78,78,78	0
36	NA	0	9126	1/1	0.90	0.09	51,51,51,51	0
36	NA	0	9160	1/1	0.90	0.28	48,48,48,48	0
34	MG	0	8087	1/1	0.90	0.10	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	CL	0	9315	1/1	0.90	0.24	89,89,89,89	0
36	NA	0	9181	1/1	0.90	0.09	69,69,69,69	0
34	MG	0	8053	1/1	0.91	0.09	57,57,57,57	0
36	NA	0	9168	1/1	0.91	0.22	69,69,69,69	0
34	MG	0	8072	1/1	0.91	0.12	56,56,56,56	0
36	NA	0	9133	1/1	0.91	0.11	38,38,38,38	0
34	MG	0	8097	1/1	0.91	0.07	46,46,46,46	0
34	MG	0	8047	1/1	0.91	0.15	85,85,85,85	0
36	NA	0	9121	1/1	0.91	0.19	69,69,69,69	0
37	CL	0	9322	1/1	0.91	0.46	90,90,90,90	0
34	MG	0	8102	1/1	0.91	0.07	64,64,64,64	0
36	NA	0	9141	1/1	0.92	0.10	52,52,52,52	0
36	NA	0	9113	1/1	0.92	0.16	71,71,71,71	0
36	NA	0	9155	1/1	0.92	0.16	80,80,80,80	0
36	NA	0	9159	1/1	0.92	0.16	62,62,62,62	0
36	NA	0	9114	1/1	0.92	0.11	44,44,44,44	0
34	MG	0	8094	1/1	0.92	0.13	80,80,80,80	0
34	MG	0	8043	1/1	0.92	0.06	55,55,55,55	0
36	NA	0	9165	1/1	0.92	0.15	45,45,45,45	0
36	NA	0	9107	1/1	0.92	0.07	55,55,55,55	0
34	MG	0	8041	1/1	0.92	0.10	87,87,87,87	0
36	NA	0	9169	1/1	0.92	0.24	65,65,65,65	0
34	MG	0	8049	1/1	0.92	0.15	93,93,93,93	0
36	NA	0	9140	1/1	0.92	0.10	53,53,53,53	0
38	CD	O	9205	1/1	0.92	0.14	146,146,146,146	0
35	K	0	9001	1/1	0.93	0.28	70,70,70,70	0
36	NA	0	9102	1/1	0.93	0.07	54,54,54,54	0
36	NA	0	9174	1/1	0.93	0.18	74,74,74,74	0
34	MG	0	8044	1/1	0.93	0.08	52,52,52,52	0
36	NA	0	9176	1/1	0.93	0.11	49,49,49,49	0
36	NA	0	9108	1/1	0.93	0.08	57,57,57,57	0
34	MG	0	8057	1/1	0.93	0.07	49,49,49,49	0
36	NA	0	9157	1/1	0.93	0.10	75,75,75,75	0
34	MG	T	8073	1/1	0.93	0.11	68,68,68,68	0
36	NA	0	9172	1/1	0.94	0.18	64,64,64,64	0
36	NA	0	9127	1/1	0.94	0.07	46,46,46,46	0
36	NA	9	9183	1/1	0.94	0.07	63,63,63,63	0
34	MG	0	8113	1/1	0.94	0.06	56,56,56,56	0
34	MG	0	8085	1/1	0.94	0.07	68,68,68,68	0
34	MG	5	8118	1/1	0.94	0.07	47,47,47,47	0
36	NA	0	9179	1/1	0.94	0.14	72,72,72,72	0
34	MG	A	8065	1/1	0.94	0.10	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	NA	0	9162	1/1	0.94	0.19	61,61,61,61	0
36	NA	0	9149	1/1	0.94	0.07	43,43,43,43	0
34	MG	0	8051	1/1	0.95	0.09	87,87,87,87	0
34	MG	0	8101	1/1	0.95	0.12	74,74,74,74	0
36	NA	C	9104	1/1	0.95	0.06	43,43,43,43	0
34	MG	0	8064	1/1	0.95	0.06	38,38,38,38	0
34	MG	0	8090	1/1	0.95	0.12	77,77,77,77	0
36	NA	0	9116	1/1	0.95	0.07	48,48,48,48	0
36	NA	0	9136	1/1	0.95	0.11	68,68,68,68	0
36	NA	0	9117	1/1	0.95	0.04	62,62,62,62	0
37	CL	B	9319	1/1	0.95	0.17	57,57,57,57	0
34	MG	K	8069	1/1	0.95	0.05	48,48,48,48	0
37	CL	N	9307	1/1	0.95	0.14	74,74,74,74	0
37	CL	Y	9320	1/1	0.95	0.07	55,55,55,55	0
37	CL	3	9304	1/1	0.95	0.09	67,67,67,67	0
36	NA	0	9173	1/1	0.95	0.08	62,62,62,62	0
36	NA	0	9178	1/1	0.96	0.16	75,75,75,75	0
34	MG	0	8093	1/1	0.96	0.06	65,65,65,65	0
36	NA	0	9123	1/1	0.96	0.08	47,47,47,47	0
36	NA	0	9101	1/1	0.96	0.09	47,47,47,47	0
36	NA	0	9161	1/1	0.96	0.07	62,62,62,62	0
34	MG	0	8088	1/1	0.96	0.05	41,41,41,41	0
34	MG	0	8096	1/1	0.96	0.04	63,63,63,63	0
34	MG	0	8042	1/1	0.96	0.07	47,47,47,47	0
36	NA	0	9132	1/1	0.96	0.05	34,34,34,34	0
34	MG	0	8116	1/1	0.96	0.11	67,67,67,67	0
36	NA	R	9137	1/1	0.96	0.06	47,47,47,47	0
36	NA	0	9134	1/1	0.96	0.13	46,46,46,46	0
34	MG	9	8095	1/1	0.96	0.10	73,73,73,73	0
37	CL	0	9311	1/1	0.96	0.15	58,58,58,58	0
37	CL	0	9313	1/1	0.96	0.06	64,64,64,64	0
36	NA	0	9139	1/1	0.96	0.07	30,30,30,30	0
37	CL	0	9316	1/1	0.96	0.19	75,75,75,75	0
34	MG	0	8098	1/1	0.96	0.08	46,46,46,46	0
34	MG	0	8099	1/1	0.96	0.06	55,55,55,55	0
37	CL	J	9301	1/1	0.96	0.13	69,69,69,69	0
34	MG	0	8091	1/1	0.96	0.06	74,74,74,74	0
37	CL	L	9310	1/1	0.96	0.09	72,72,72,72	0
36	NA	0	9150	1/1	0.96	0.05	46,46,46,46	0
34	MG	0	8070	1/1	0.96	0.07	66,66,66,66	0
36	NA	0	9120	1/1	0.96	0.07	35,35,35,35	0
36	NA	0	9156	1/1	0.96	0.14	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	NA	J	9146	1/1	0.97	0.05	41,41,41,41	0
36	NA	L	9180	1/1	0.97	0.10	61,61,61,61	0
34	MG	0	8062	1/1	0.97	0.07	64,64,64,64	0
36	NA	R	9138	1/1	0.97	0.06	67,67,67,67	0
36	NA	0	9158	1/1	0.97	0.17	122,122,122,122	0
36	NA	0	9135	1/1	0.97	0.08	55,55,55,55	0
34	MG	0	8104	1/1	0.97	0.05	59,59,59,59	0
36	NA	0	9106	1/1	0.97	0.45	49,49,49,49	0
36	NA	0	9115	1/1	0.97	0.07	41,41,41,41	0
34	MG	0	8040	1/1	0.97	0.04	55,55,55,55	0
36	NA	0	9142	1/1	0.97	0.06	45,45,45,45	0
37	CL	A	9309	1/1	0.97	0.08	72,72,72,72	0
36	NA	0	9128	1/1	0.97	0.06	43,43,43,43	0
34	MG	Y	8109	1/1	0.97	0.05	62,62,62,62	0
36	NA	0	9131	1/1	0.97	0.09	35,35,35,35	0
36	NA	0	9153	1/1	0.97	0.04	35,35,35,35	0
36	NA	0	9154	1/1	0.97	0.12	38,38,38,38	0
37	CL	R	9306	1/1	0.97	0.07	67,67,67,67	0
37	CL	Y	9317	1/1	0.97	0.07	72,72,72,72	0
36	NA	A	9145	1/1	0.97	0.04	41,41,41,41	0
36	NA	0	9119	1/1	0.97	0.08	45,45,45,45	0
34	MG	0	8076	1/1	0.97	0.04	68,68,68,68	0
36	NA	0	9103	1/1	0.98	0.09	48,48,48,48	0
36	NA	0	9105	1/1	0.98	0.08	45,45,45,45	0
34	MG	0	8108	1/1	0.98	0.11	58,58,58,58	0
34	MG	0	8111	1/1	0.98	0.06	59,59,59,59	0
34	MG	0	8112	1/1	0.98	0.12	43,43,43,43	0
36	NA	Q	9148	1/1	0.98	0.09	46,46,46,46	0
34	MG	0	8039	1/1	0.98	0.14	50,50,50,50	0
36	NA	0	9167	1/1	0.98	0.07	56,56,56,56	0
34	MG	0	8081	1/1	0.98	0.06	59,59,59,59	0
34	MG	0	8115	1/1	0.98	0.07	54,54,54,54	0
37	CL	0	9303	1/1	0.98	0.12	63,63,63,63	0
34	MG	0	8019	1/1	0.98	0.03	35,35,35,35	0
34	MG	0	8117	1/1	0.98	0.04	34,34,34,34	0
37	CL	0	9314	1/1	0.98	0.07	57,57,57,57	0
34	MG	0	8084	1/1	0.98	0.04	47,47,47,47	0
36	NA	0	9143	1/1	0.98	0.05	38,38,38,38	0
36	NA	0	9144	1/1	0.98	0.04	37,37,37,37	0
34	MG	0	8067	1/1	0.98	0.06	52,52,52,52	0
36	NA	0	9118	1/1	0.98	0.11	54,54,54,54	0
34	MG	0	8068	1/1	0.98	0.05	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	MG	0	8059	1/1	0.98	0.04	52,52,52,52	0
37	CL	J	9321	1/1	0.98	0.06	60,60,60,60	0
37	CL	K	9312	1/1	0.98	0.05	60,60,60,60	0
34	MG	0	8089	1/1	0.98	0.04	65,65,65,65	0
37	CL	M	9318	1/1	0.98	0.09	45,45,45,45	0
34	MG	0	8071	1/1	0.98	0.06	62,62,62,62	0
37	CL	O	9308	1/1	0.98	0.08	81,81,81,81	0
34	MG	0	8103	1/1	0.98	0.05	66,66,66,66	0
36	NA	0	9125	1/1	0.98	0.10	62,62,62,62	0
35	K	0	9002	1/1	0.98	0.18	47,47,47,47	0
34	MG	0	8060	1/1	0.98	0.08	45,45,45,45	0
34	MG	0	8075	1/1	0.98	0.04	48,48,48,48	0
34	MG	0	8063	1/1	0.99	0.03	68,68,68,68	0
34	MG	0	8033	1/1	0.99	0.02	44,44,44,44	0
36	NA	0	9109	1/1	0.99	0.05	35,35,35,35	0
34	MG	0	8037	1/1	0.99	0.04	47,47,47,47	0
34	MG	0	8006	1/1	0.99	0.02	43,43,43,43	0
34	MG	0	8007	1/1	0.99	0.02	25,25,25,25	0
34	MG	0	8008	1/1	0.99	0.02	31,31,31,31	0
36	NA	M	9147	1/1	0.99	0.02	32,32,32,32	0
34	MG	0	8012	1/1	0.99	0.03	43,43,43,43	0
34	MG	0	8074	1/1	0.99	0.04	38,38,38,38	0
34	MG	0	8110	1/1	0.99	0.05	36,36,36,36	0
34	MG	0	8013	1/1	0.99	0.04	43,43,43,43	0
34	MG	0	8014	1/1	0.99	0.03	50,50,50,50	0
34	MG	0	8080	1/1	0.99	0.04	43,43,43,43	0
37	CL	0	9305	1/1	0.99	0.05	62,62,62,62	0
34	MG	0	8015	1/1	0.99	0.02	37,37,37,37	0
34	MG	0	8016	1/1	0.99	0.07	40,40,40,40	0
34	MG	0	8083	1/1	0.99	0.08	45,45,45,45	0
34	MG	0	8018	1/1	0.99	0.08	49,49,49,49	0
34	MG	0	8048	1/1	0.99	0.06	63,63,63,63	0
34	MG	0	8086	1/1	0.99	0.04	58,58,58,58	0
34	MG	0	8002	1/1	0.99	0.02	48,48,48,48	0
34	MG	A	8066	1/1	0.99	0.03	67,67,67,67	0
36	NA	0	9130	1/1	0.99	0.03	49,49,49,49	0
34	MG	B	8055	1/1	0.99	0.04	60,60,60,60	0
34	MG	0	8020	1/1	0.99	0.02	33,33,33,33	0
34	MG	0	8023	1/1	0.99	0.05	53,53,53,53	0
34	MG	0	8052	1/1	0.99	0.02	51,51,51,51	0
34	MG	3	8078	1/1	0.99	0.03	41,41,41,41	0
34	MG	0	8003	1/1	0.99	0.03	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	MG	0	8054	1/1	0.99	0.03	35,35,35,35	0
34	MG	0	8025	1/1	0.99	0.04	45,45,45,45	0
34	MG	0	8027	1/1	0.99	0.04	48,48,48,48	0
34	MG	0	8028	1/1	0.99	0.03	43,43,43,43	0
34	MG	0	8061	1/1	0.99	0.03	36,36,36,36	0
34	MG	0	8029	1/1	0.99	0.04	39,39,39,39	0
38	CD	Z	9203	1/1	0.99	0.02	76,76,76,76	0
38	CD	3	9204	1/1	0.99	0.04	64,64,64,64	0
34	MG	0	8005	1/1	1.00	0.01	38,38,38,38	0
34	MG	0	8009	1/1	1.00	0.02	35,35,35,35	0
34	MG	0	8010	1/1	1.00	0.02	42,42,42,42	0
34	MG	0	8026	1/1	1.00	0.05	31,31,31,31	0
34	MG	0	8017	1/1	1.00	0.01	31,31,31,31	0
34	MG	0	8011	1/1	1.00	0.07	29,29,29,29	0
34	MG	0	8001	1/1	1.00	0.02	37,37,37,37	0
34	MG	0	8030	1/1	1.00	0.03	36,36,36,36	0
34	MG	0	8031	1/1	1.00	0.02	29,29,29,29	0
34	MG	0	8032	1/1	1.00	0.02	47,47,47,47	0
34	MG	0	8004	1/1	1.00	0.02	38,38,38,38	0
34	MG	0	8034	1/1	1.00	0.02	38,38,38,38	0
34	MG	0	8035	1/1	1.00	0.04	49,49,49,49	0
34	MG	0	8077	1/1	1.00	0.02	28,28,28,28	0
34	MG	B	8056	1/1	1.00	0.02	57,57,57,57	0
34	MG	0	8079	1/1	1.00	0.03	34,34,34,34	0
34	MG	0	8036	1/1	1.00	0.02	32,32,32,32	0
34	MG	0	8021	1/1	1.00	0.02	33,33,33,33	0
34	MG	0	8038	1/1	1.00	0.03	33,33,33,33	0
34	MG	0	8058	1/1	1.00	0.03	48,48,48,48	0
38	CD	U	9201	1/1	1.00	0.02	78,78,78,78	0
34	MG	0	8022	1/1	1.00	0.02	39,39,39,39	0
38	CD	1	9202	1/1	1.00	0.07	65,65,65,65	0
34	MG	0	8107	1/1	1.00	0.03	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.