



wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 06:24 am BST

PDB ID : 1S72
Title : REFINED CRYSTAL STRUCTURE OF THE HALOARCUA MARISMORTUI LARGE RIBOSOMAL SUBUNIT AT 2.4 ANGSTROM RESOLUTION
Authors : Klein, D.J.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on : 2004-01-28
Resolution : 2.40 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

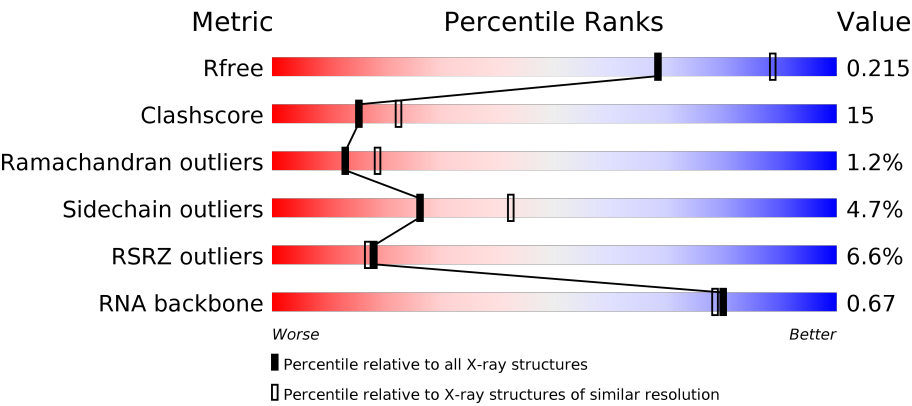
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
R _{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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>2%</div><div><div></div><div>65%</div><div>24%</div><div>5%</div><div>6%</div></div></div>
2	9	122	<div><div>4%</div><div><div></div><div>56%</div><div>35%</div><div>7%</div><div></div></div></div>
3	A	240	<div><div>8%</div><div><div></div><div>63%</div><div>30%</div><div>6%</div><div></div></div></div>
4	B	338	<div><div>4%</div><div><div></div><div>57%</div><div>37%</div><div>6%</div><div></div></div></div>

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	171	
11	I	162	
12	J	145	
13	K	132	
14	L	165	
15	M	194	
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	73	
29	1	57	

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Mol	Chain	Length	Quality of chain
30	2	50	<div><div></div><div>12%</div><div>54%</div><div>36%</div><div>• 8%</div></div>
31	3	92	<div><div></div><div>3%</div><div>64%</div><div>33%</div><div>• •</div></div>

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 99039 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 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	CONFLICT	GB 3377779
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 protein called 50S ribosomal protein L2P.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	SER	ASP	CONFLICT	UNP P20276
A	160	ALA	GLY	CONFLICT	UNP P20276

- Molecule 4 is a protein called 50S ribosomal protein L3P.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	310	ARG	PRO	CONFLICT	UNP P20279

- Molecule 5 is a protein called 50S ribosomal protein L4E.

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

- Molecule 6 is a protein called 50S ribosomal protein L5P.

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

- Molecule 7 is a protein called 50S ribosomal protein L6P.

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

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	103	GLU	ALA	CONFLICT	UNP P12743
F	105	ASP	ALA	CONFLICT	UNP P12743
F	106	ALA	THR	CONFLICT	UNP P12743
F	107	ASP	VAL	CONFLICT	UNP P12743
F	108	VAL	LEU	CONFLICT	UNP P12743
F	110	ASP	GLU	CONFLICT	UNP P12743

- Molecule 9 is a protein called Acidic ribosomal protein P0 homolog.

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

- Molecule 10 is a protein called 50S ribosomal protein L10e.

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

- Molecule 11 is a protein called 50S ribosomal protein L11P.

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

- 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	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			

- 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	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
			579	346	116	112	5			

- 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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	109	Total	Mg	0	0
			109	109		
32	Y	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	9	1	Total	Mg	0	0
			1	1		
32	3	1	Total	Mg	0	0
			1	1		

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	2	Total	K	0	0
			2	2		

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	72	Total Na 72 72	0	0
34	J	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	H	2	Total Na 2 2	0	0
34	C	1	Total Na 1 1	0	0
34	A	1	Total Na 1 1	0	0
34	T	1	Total Na 1 1	0	0
34	R	2	Total Na 2 2	0	0
34	9	2	Total Na 2 2	0	0
34	L	1	Total Na 1 1	0	0
34	S	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	10	Total Cl 10 10	0	0
35	J	3	Total Cl 3 3	0	0
35	B	1	Total Cl 1 1	0	0
35	A	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	R	1	Total Cl 1 1	0	0
35	Y	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	L	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total 1	Cd 1	0	0
36	Z	1	Total 1	Cd 1	0	0
36	1	1	Total 1	Cd 1	0	0
36	3	1	Total 1	Cd 1	0	0
36	U	1	Total 1	Cd 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	5893	Total 5893	O 5893	0	0
37	9	136	Total 136	O 136	0	0
37	A	127	Total 127	O 127	0	0
37	B	153	Total 153	O 153	0	0
37	C	172	Total 172	O 172	0	0
37	D	49	Total 49	O 49	0	0
37	E	44	Total 44	O 44	0	0
37	F	25	Total 25	O 25	0	0
37	G	20	Total 20	O 20	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	H	71	Total 71	O 71	0	0
37	I	9	Total 9	O 9	0	0
37	J	55	Total 55	O 55	0	0
37	K	61	Total 61	O 61	0	0
37	L	85	Total 85	O 85	0	0
37	M	121	Total 121	O 121	0	0
37	N	64	Total 64	O 64	0	0
37	O	44	Total 44	O 44	0	0
37	P	65	Total 65	O 65	0	0
37	Q	52	Total 52	O 52	0	0
37	R	83	Total 83	O 83	0	0
37	S	33	Total 33	O 33	0	0
37	T	40	Total 40	O 40	0	0
37	U	25	Total 25	O 25	0	0
37	V	14	Total 14	O 14	0	0
37	W	67	Total 67	O 67	0	0
37	X	28	Total 28	O 28	0	0
37	Y	96	Total 96	O 96	0	0
37	Z	29	Total 29	O 29	0	0
37	1	51	Total 51	O 51	0	0
37	2	40	Total 40	O 40	0	0

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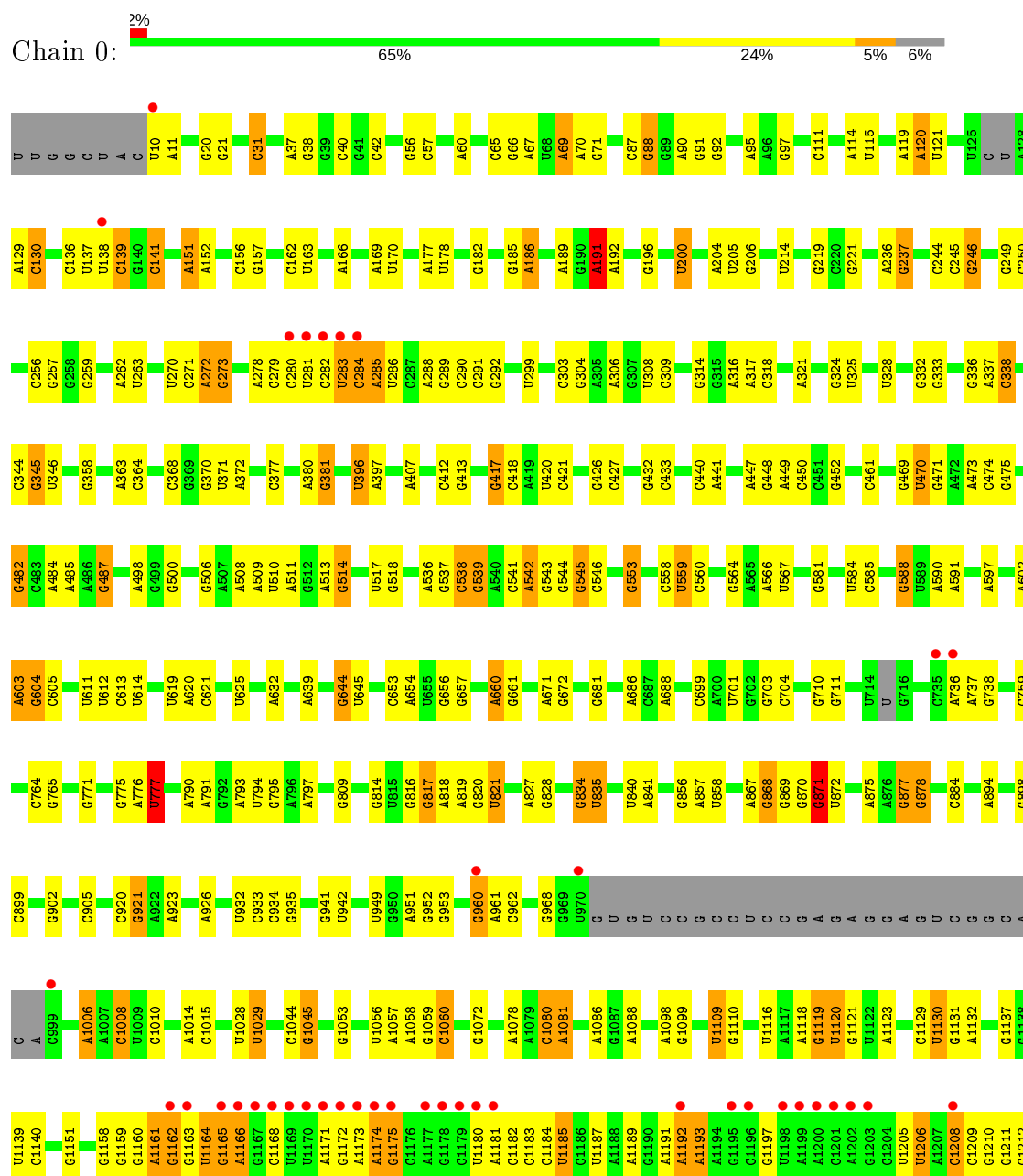
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	3	71	Total	O	0	0
			71	71		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

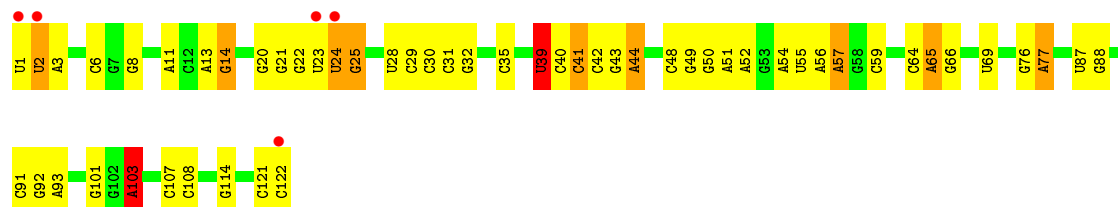
• Molecule 1: 23S ribosomal RNA



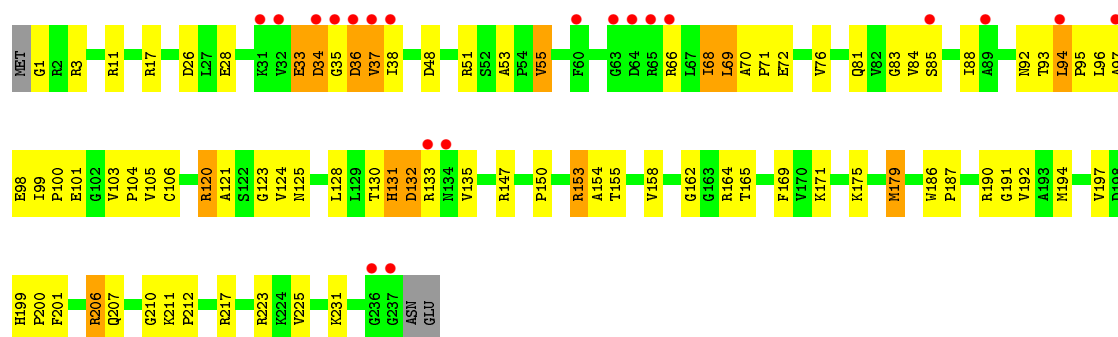
G1216	G1217	G1218	G1219	G1229	A1232	U1234	G1235	A1236	U1237	G1238	G1239	A1242	C1243	U1244	A1246	U1249	C1250	G1251	U1266	C1267	G1268	G1269	C1273	U1279	C1289	G1290	A1291	G1292	U1298	G1299	U1306	U1314	G1327	A1328	A1329	U1333	C1334	G1340	A1341	C1342	C1343					
G1351	A1352	C1353	C1360	A1367	U1368	A1372	C1377	U1384	G1385	A1406	A1407	U1408	G1409	A1414	U1417	U1418	U1419	C1423	A1424	G1430	G1438	C1439	U1440	G1441	A1442	U14596	A14597	C1450	C1451	A1458	C1462	A1463	A1470	C1474	C1477	U1478	G1484	A1485	A1341	C1342	C1343					
U1500	U1503	A1504	U1505	U1506	A1515	C1516	G1523	U1524	G1525	A1526	A1527	A1528	G1529	C1545	G1546	G1555	A1559	U	U1561	G1562	G1563	C1564	C1565	A1580	G1592	C1593	C1594	G1595	A1596	A1597	A1598	A1603	G1604	G1605	C1609	G1610	G1613	G1614	A1615	U1625	G1627	A1630	C1633			
G1634	U1635	G1636	A1637	A1641	A1642	A1656	A1657	A1658	C1666	A1667	U1668	A1669	G1670	C1679	G1680	G1681	A1682	G1683	A1684	A1685	C1692	C1699	G1700	A1701	U1702	A1710	A1717	U1722	G1723	U1724	C1725	G1730	C1731	A1732	A1733	C1734	C1735	A1736	U1741	A1742	G1751	G1752	C1753	U1766	A1767	C1768
C1769	A1778	A1779	A1787	C1787	U1788	G1789	G1794	A1798	G1809	G1819	G1820	A1829	C1834	U1835	G1836	A1840	A1845	G1848	C1853	C1856	A1857	C1862	G1863	G1867	G1868	U1874	G1877	G1878	U1879	U1883	G1884	G1902	U1903	A1904	A1909	A1919	G1923	G1926	A1930	C1931	C1932	C1933				
A1927	C1940	A1941	A1942	C1943	G1947	G1948	G1949	G1950	G1951	U	A	A	C	C	U	A	U1964	C1965	U1966	U1967	G1970	G1971	U1972	A1973	G1974	A1978	G1979	U1980	U1996	A1997	G2001	C2002	U2003	U2004	G2005	U2008	G2009	A2010	A2011	U2012	G2013	A2019	G2033	U2034	G	
G2044	G2050	A2054	C2061	A2062	U2063	U2064	G2072	G2073	A2074	U2078	A2081	G2082	A2083	A2089	G2090	G2091	G2094	A2095	A2096	A2101	G2102	G2110	G2111	G2112	G2113	C2114	U2115	U2116	G2128	G2136	A	C	C	A	G	U	U	G	C	C	A	C	C	G		
C	A	G	A	U	A	G	G	G	A	A	G	C	U	A	C	C	G	G	U	A	C	C	U	U	A	A	C	C	G	G	G	A	U	C	U	G	C	C	A	A	C	A	U	U	G	
A	A	U	A	C	C	C	G	U	C	C	G	A	C	C	C	C	G2237	A2238	C2241	U2242	C2247	G2251	A2252	G2253	G2254	A2255	G2256	G2257	A2258	U2265	A2266	G2267	G2270	G2271	G2272	C2281	U2282	G2289	U2290	A2291	A2300	A2301	A2302	C2309		
G2310	A2311	C2312	C2313	G2314	C2315	G2316	C2317	U2320	A2321	U2326	C2329	U2330	G2338	A	C	A	G2344	A2345	C2346	A2353	A2354	G2355	A2356	C2357	U2358	G2359	C2360	A2361	A2362	G2363	A2364	G2365	A2369	G2383	U2386	G2387	C2388	A2395	A2401	A2402	C2403	G2412	A2413	A2414	A2415	G2416
U2419	G2420	G2421	U2422	G2426	A2434	G2438	C2443	G2453	U2456	U2457	G2462	A2465	G2466	A2467	A2468	A2469	C2472	C2476	C2477	U2478	A2479	G2480	A2483	A2488	G2489	A2490	C2493	C2502	A2503	A2504	G2505	A2506	G2507	C2508	A2509	A2511	C2515	G2516	A2521	G2524						
G2525	C2526	U2527	C2533	C2534	U2535	G2536	U2537	U2541	C2542	G2543	C2547	C2548	C2552	A2553	C2559	G2560	C2561	G2562	U2563	G2564	C2565	G2570	G2578	U2586	U2587	G2588	U2589	U2590	C2591	G2592	A2601	G2602	G2603	A2604	U2607	G2608	G2613	G2616	G2630	G2634	A2635	C2636	A2637	G2638		
G2642	G2643	A2649	U2652	A2653	G2654	A2664	U	G2667	G2668	U2669	G2670	U2671	G2672	U2673	C2676	G2679	U2791	A2680	A2681	C2682	U2690	A2691	A2694	U2710	U2711	G2712	G2716	C2717	C2718	C2719	C2720	G2721	G2722	G2723	U2724	G2725	U2726	G2730	G2731	G2738	A2741	G2742	G2743	C2747	G2748	G2750
U2756	A2761	C2762	A2768	C2769	G2770	G2777	A2778	G2779	C2780	U2781	G2782	A2783	G2786	C2787	C2790	U2791	A2792	C2795	U2796	A2800	U2807	A2811	A2812	A2813	A2814	G2815	A2820	C2821	C2825	G2826	G2827	G2828	G2829	U2830	C2831	C2832	U2837	A2840	A2841	G2842	A2843	C2850	G2851	A2852		



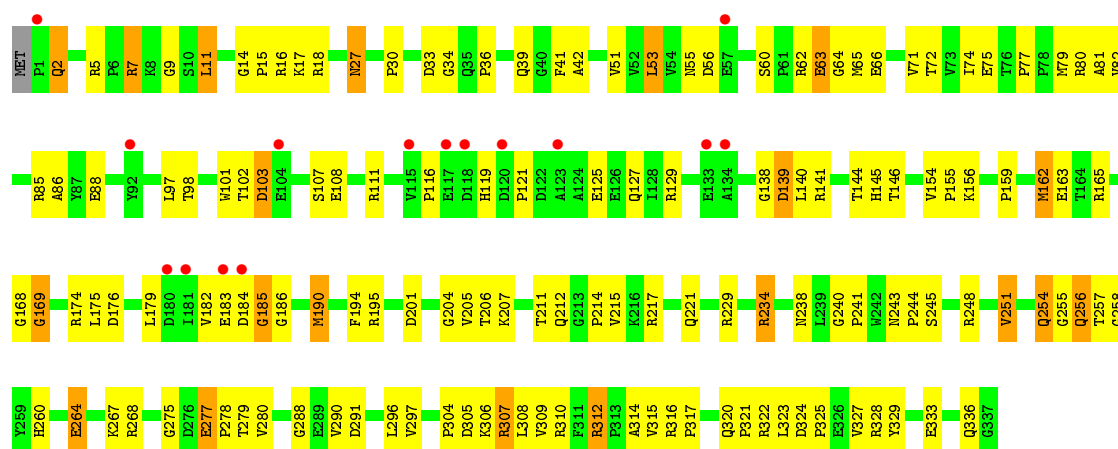
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 50S ribosomal protein L2P

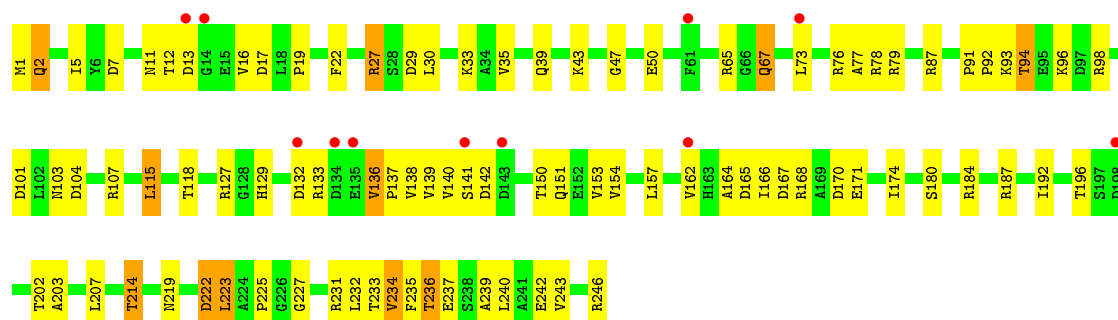


• Molecule 4: 50S ribosomal protein L3P

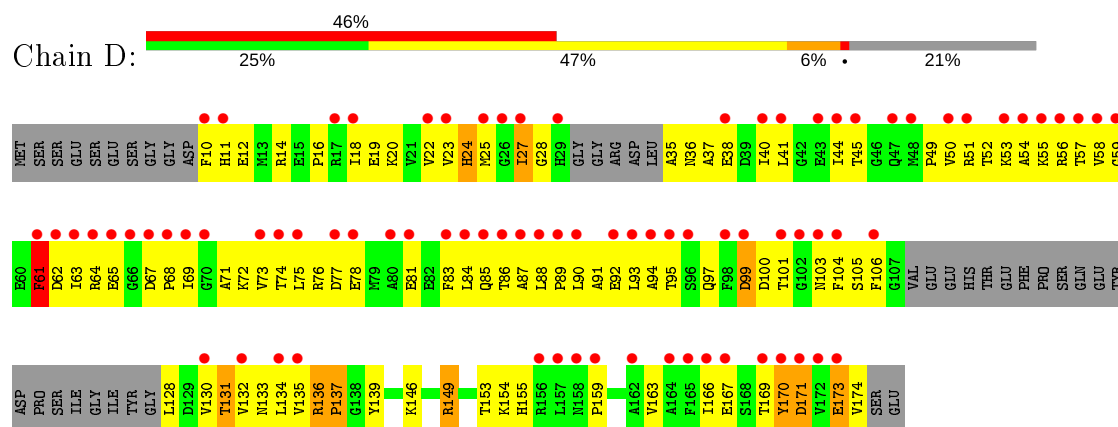


• Molecule 5: 50S ribosomal protein L4E

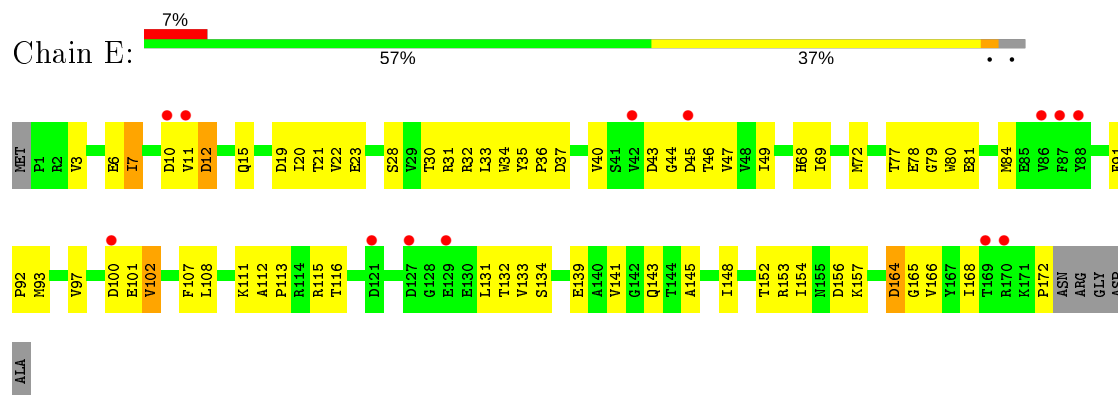




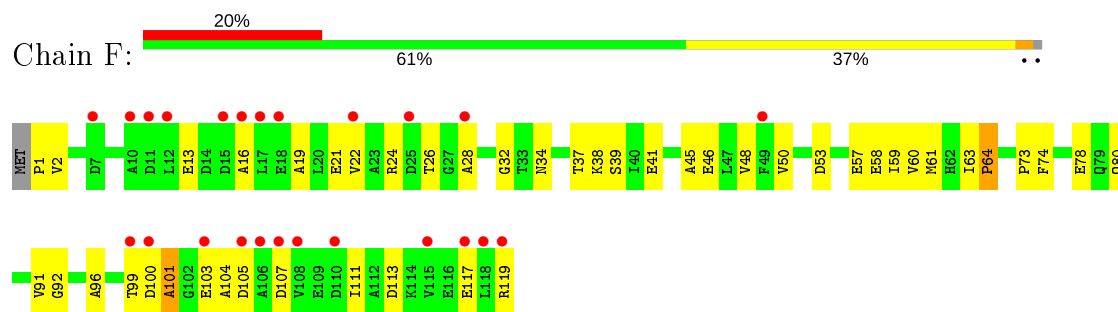
• Molecule 6: 50S ribosomal protein L5P



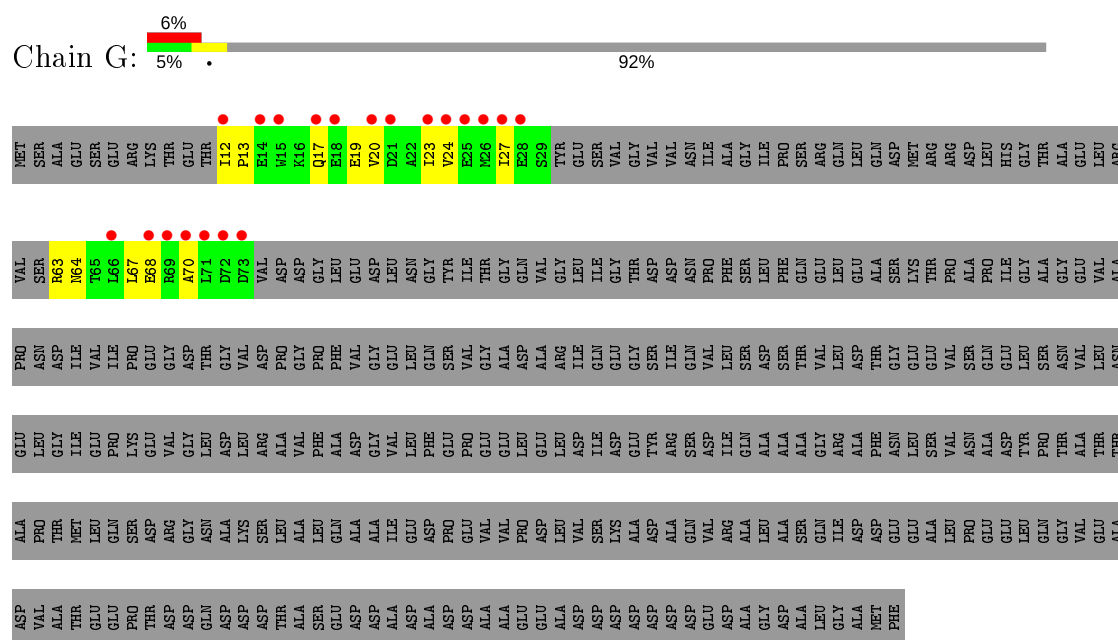
• Molecule 7: 50S ribosomal protein L6P



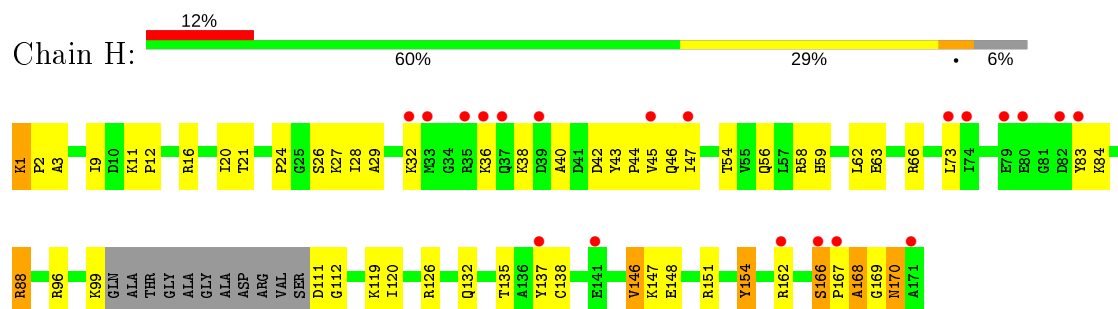
• Molecule 8: 50S ribosomal protein L7Ae



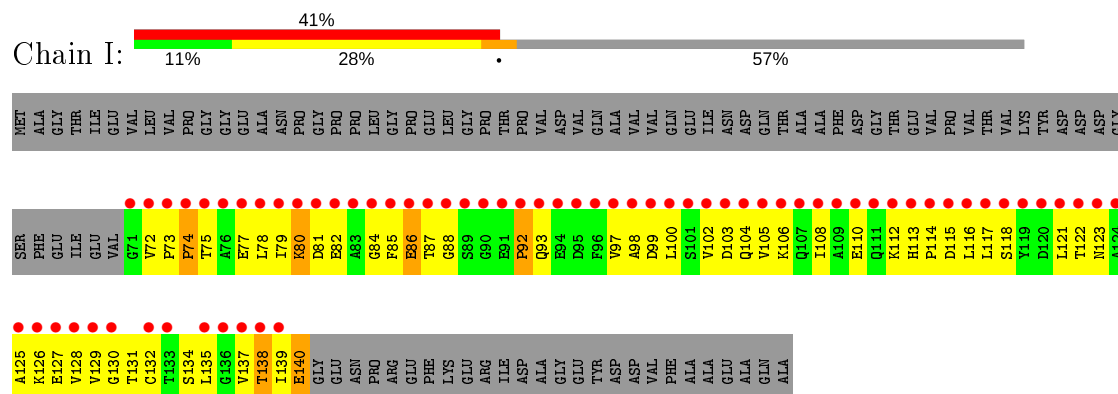
• Molecule 9: Acidic ribosomal protein P0 homolog



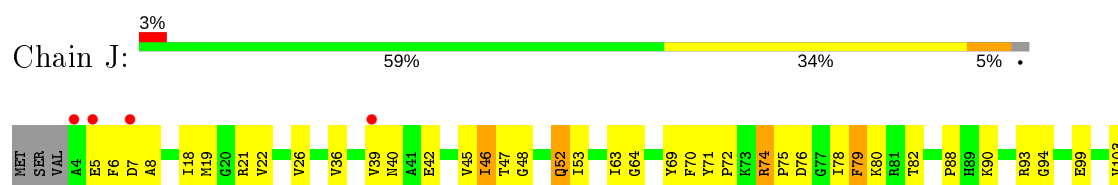
- Molecule 10: 50S ribosomal protein L10e



- Molecule 11: 50S ribosomal protein L11P

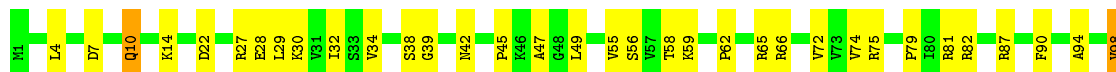


- Molecule 12: 50S ribosomal protein L13P

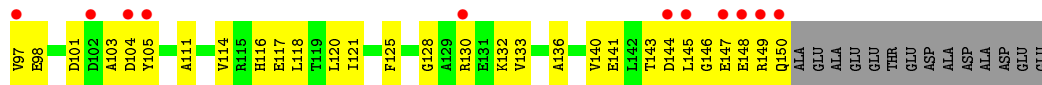




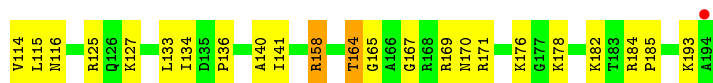
• Molecule 13: 50S ribosomal protein L14P



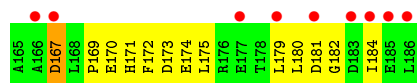
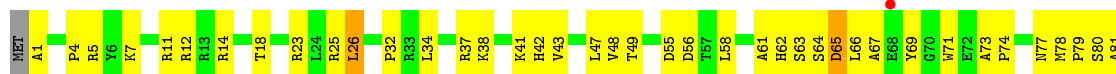
• Molecule 14: 50S ribosomal protein L15P



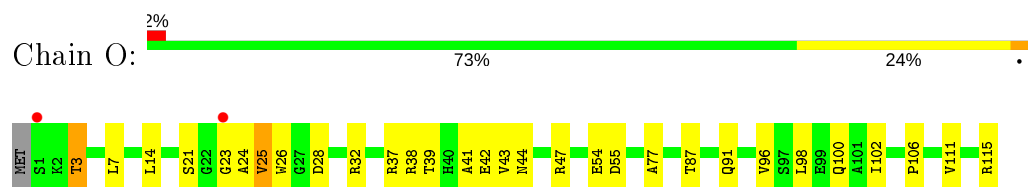
• Molecule 15: 50S ribosomal protein L15e



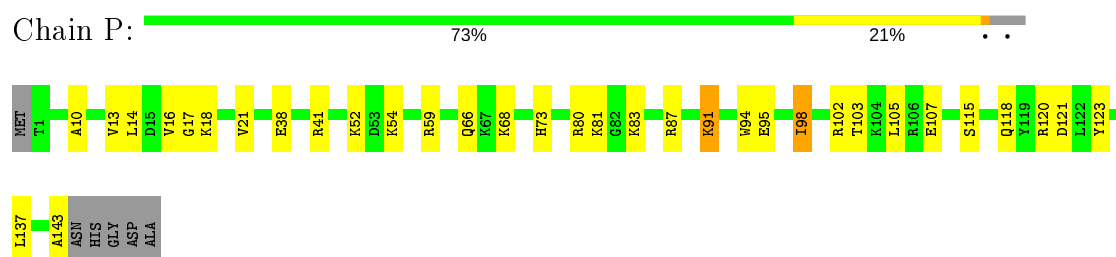
• Molecule 16: 50S ribosomal protein L18P



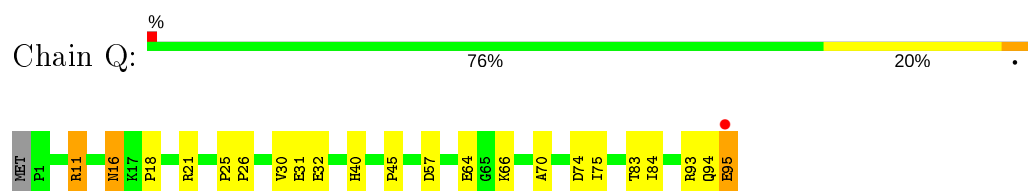
- Molecule 17: 50S ribosomal protein L18e



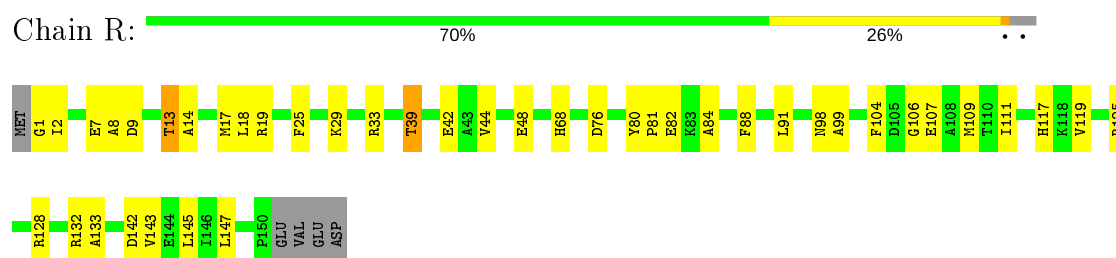
- Molecule 18: 50S ribosomal protein L19E



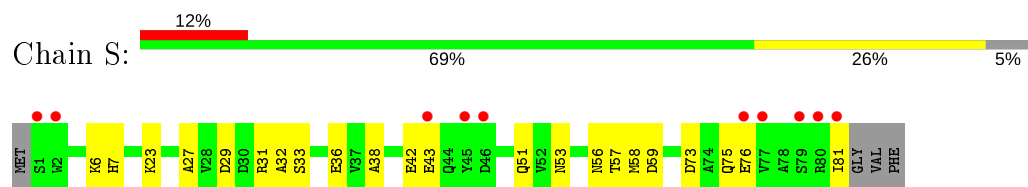
- Molecule 19: 50S ribosomal protein L21e



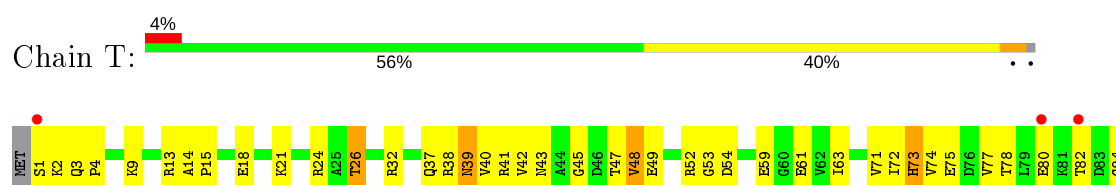
- Molecule 20: 50S ribosomal protein L22P

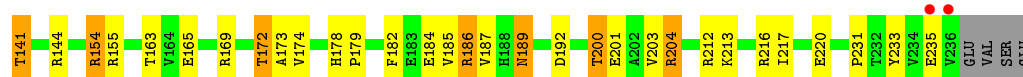


- Molecule 21: 50S ribosomal protein L23P



- Molecule 22: 50S ribosomal protein L24P





- Molecule 28: 50S ribosomal protein L37Ae



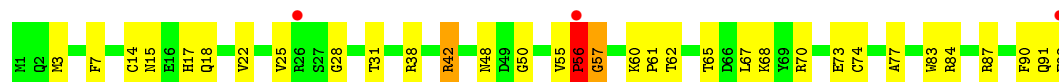
- Molecule 29: 50S ribosomal protein L37e



- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.66Å 299.67Å 573.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 85.48 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.2 (15.00-2.40) 90.6 (85.48-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.188 , 0.222 0.182 , 0.215	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.3	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	99039	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.37	0/65959	0.70	27/102870 (0.0%)
2	9	0.35	0/2905	0.73	4/4528 (0.1%)
3	A	0.34	0/1786	0.67	0/2408
4	B	0.34	0/2690	0.65	0/3652
5	C	0.39	0/1884	0.67	0/2551
6	D	0.32	0/1111	0.57	0/1498
7	E	0.32	0/1382	0.57	0/1880
8	F	0.38	0/901	0.57	0/1224
9	G	0.28	0/241	0.48	0/324
10	H	0.33	0/1287	0.66	0/1725
11	I	0.36	0/526	0.56	0/716
12	J	0.34	0/1136	0.61	0/1530
13	K	0.34	0/1001	0.65	0/1347
14	L	0.34	0/1130	0.68	0/1509
15	M	0.36	0/1584	0.64	0/2119
16	N	0.37	0/1474	0.70	0/1999
17	O	0.33	0/874	0.61	0/1181
18	P	0.35	0/1147	0.54	0/1528
19	Q	0.35	0/749	0.69	0/1005
20	R	0.36	0/1172	0.66	0/1578
21	S	0.34	0/648	0.59	0/875
22	T	0.32	0/958	0.64	0/1289
23	U	0.35	0/417	0.58	0/562
24	V	0.31	0/502	0.55	0/675
25	W	0.34	0/1219	0.63	0/1655
26	X	0.33	0/664	0.60	0/895
27	Y	0.35	0/1146	0.63	0/1536
28	Z	0.35	0/590	0.66	0/787
29	1	0.44	0/438	0.68	0/578
30	2	0.37	0/401	0.55	0/529
31	3	0.38	0/771	0.62	0/1024
All	All	0.36	0/98693	0.68	31/147577 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	60
2	9	0	2
All	All	1	62

There are no bond length outliers.

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	0	1563	G	C2'-C3'-O3'	9.56	130.53	109.50
1	0	1942	A	C5'-C4'-C3'	9.41	131.06	116.00
1	0	871	G	C5'-C4'-O4'	-8.49	98.91	109.10
1	0	1942	A	C5'-C4'-O4'	7.87	118.55	109.10
1	0	1979	G	C2'-C3'-O3'	7.87	126.82	109.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 62 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	191	A	Sidechain
1	0	196	G	Sidechain
1	0	221	G	Sidechain
1	0	246	G	Sidechain
1	0	270	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	29813	712	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	9	2600	0	1326	54	0
3	A	1753	0	1766	103	0
4	B	2625	0	2533	163	0
5	C	1859	0	1816	109	0
6	D	1094	0	1085	116	0
7	E	1357	0	1266	76	0
8	F	890	0	843	56	0
9	G	240	0	231	17	0
10	H	1266	0	1268	78	0
11	I	519	0	500	72	0
12	J	1120	0	1098	68	0
13	K	992	0	1031	55	0
14	L	1118	0	1076	56	0
15	M	1560	0	1568	59	0
16	N	1445	0	1401	114	0
17	O	865	0	873	29	0
18	P	1136	0	1123	35	0
19	Q	735	0	728	18	0
20	R	1149	0	1122	45	0
21	S	641	0	605	20	0
22	T	950	0	923	48	0
23	U	410	0	364	31	0
24	V	499	0	511	29	0
25	W	1196	0	1137	96	0
26	X	654	0	653	42	0
27	Y	1130	0	1133	53	0
28	Z	579	0	539	27	0
29	1	431	0	426	21	0
30	2	396	0	413	28	0
31	3	755	0	728	29	0
32	0	109	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	72	0	0	0	0
34	9	2	0	0	0	0
34	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	C	1	0	0	0	0
34	H	2	0	0	0	0
34	J	1	0	0	0	0
34	L	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	2	0	0	0	0
34	S	1	0	0	0	0
34	T	1	0	0	0	0
35	0	10	0	0	0	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	1	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	5893	0	0	145	0
37	1	51	0	0	1	0
37	2	40	0	0	5	0
37	3	71	0	0	9	0
37	9	136	0	0	8	0
37	A	127	0	0	18	0
37	B	153	0	0	28	0
37	C	172	0	0	28	0
37	D	49	0	0	20	0
37	E	44	0	0	11	0
37	F	25	0	0	7	0
37	G	20	0	0	3	0
37	H	71	0	0	16	0
37	I	9	0	0	9	0
37	J	55	0	0	5	0
37	K	61	0	0	13	0
37	L	85	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	M	121	0	0	10	0
37	N	64	0	0	13	0
37	O	44	0	0	6	0
37	P	65	0	0	3	0
37	Q	52	0	0	2	0
37	R	83	0	0	8	0
37	S	33	0	0	5	0
37	T	40	0	0	5	0
37	U	25	0	0	4	0
37	V	14	0	0	4	0
37	W	67	0	0	10	0
37	X	28	0	0	3	0
37	Y	96	0	0	15	0
37	Z	29	0	0	5	0
All	All	99039	0	59899	2245	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 15.

The worst 5 of 2245 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)
5:C:236:THR:HG22	5:C:239:ALA:H	1.04	1.11
1:0:1160:G:H5'	1:0:1161:A:H5'	1.26	1.09
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.31	1.09
1:0:960:G:H4'	37:0:6920:HOH:O	1.51	1.08
5:C:5:ILE:HD11	5:C:16:VAL:HG23	1.36	1.07

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	235/240 (98%)	217 (92%)	15 (6%)	3 (1%)	12	17
4	B	335/338 (99%)	314 (94%)	14 (4%)	7 (2%)	7	8
5	C	244/246 (99%)	224 (92%)	20 (8%)	0	100	100
6	D	134/177 (76%)	104 (78%)	23 (17%)	7 (5%)	2	1
7	E	170/178 (96%)	159 (94%)	10 (6%)	1 (1%)	25	36
8	F	117/120 (98%)	105 (90%)	10 (8%)	2 (2%)	9	11
9	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	H	156/171 (91%)	145 (93%)	9 (6%)	2 (1%)	12	17
11	I	68/162 (42%)	53 (78%)	12 (18%)	3 (4%)	2	2
12	J	140/145 (97%)	132 (94%)	5 (4%)	3 (2%)	7	8
13	K	130/132 (98%)	120 (92%)	8 (6%)	2 (2%)	10	14
14	L	141/165 (86%)	120 (85%)	20 (14%)	1 (1%)	22	32
15	M	192/194 (99%)	186 (97%)	6 (3%)	0	100	100
16	N	184/187 (98%)	171 (93%)	8 (4%)	5 (3%)	5	5
17	O	113/116 (97%)	108 (96%)	5 (4%)	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	32
21	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
22	T	117/120 (98%)	111 (95%)	6 (5%)	0	100	100
23	U	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
24	V	63/71 (89%)	58 (92%)	3 (5%)	2 (3%)	4	3
25	W	152/154 (99%)	147 (97%)	4 (3%)	1 (1%)	22	32
26	X	80/92 (87%)	71 (89%)	7 (9%)	2 (2%)	5	6
27	Y	140/241 (58%)	140 (100%)	0	0	100	100
28	Z	71/73 (97%)	61 (86%)	9 (13%)	1 (1%)	11	15
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	42 (100%)	0	0	100	100
31	3	90/92 (98%)	86 (96%)	2 (2%)	2 (2%)	6	7
All	All	3705/4420 (84%)	3442 (93%)	218 (6%)	45 (1%)	13	19

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	139	ASP
6	D	137	PRO
6	D	173	GLU
10	H	166	SER
10	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	
3	A	179/182 (98%)	166 (93%)	13 (7%)	14	22
4	B	282/283 (100%)	263 (93%)	19 (7%)	16	26
5	C	193/193 (100%)	179 (93%)	14 (7%)	14	22
6	D	117/148 (79%)	108 (92%)	9 (8%)	13	20
7	E	152/156 (97%)	148 (97%)	4 (3%)	46	66
8	F	93/94 (99%)	93 (100%)	0	100	100
9	G	27/283 (10%)	27 (100%)	0	100	100
10	H	132/138 (96%)	125 (95%)	7 (5%)	22	37
11	I	58/130 (45%)	54 (93%)	4 (7%)	15	25
12	J	118/121 (98%)	110 (93%)	8 (7%)	16	25
13	K	106/106 (100%)	103 (97%)	3 (3%)	43	63
14	L	113/127 (89%)	109 (96%)	4 (4%)	36	55
15	M	158/158 (100%)	151 (96%)	7 (4%)	28	45
16	N	149/150 (99%)	142 (95%)	7 (5%)	26	42
17	O	93/94 (99%)	88 (95%)	5 (5%)	22	36
18	P	113/117 (97%)	110 (97%)	3 (3%)	44	65
19	Q	79/80 (99%)	75 (95%)	4 (5%)	24	39
20	R	117/122 (96%)	114 (97%)	3 (3%)	46	66
21	S	71/74 (96%)	71 (100%)	0	100	100
22	T	105/106 (99%)	100 (95%)	5 (5%)	25	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	55	74
25	W	130/130 (100%)	122 (94%)	8 (6%)	18	29
26	X	66/74 (89%)	63 (96%)	3 (4%)	27	44
27	Y	120/196 (61%)	110 (92%)	10 (8%)	11	17
28	Z	60/60 (100%)	60 (100%)	0	100	100
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	49	68
31	3	79/79 (100%)	76 (96%)	3 (4%)	33	51
All	All	3093/3603 (86%)	2948 (95%)	145 (5%)	26	42

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	H	170	ASN
14	L	30	ARG
27	Y	172	THR
11	I	93	GLN
12	J	79	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	24	GLN
17	O	53	GLN
29	1	28	HIS
15	M	26	GLN
15	M	170	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2746/2922 (93%)	236 (8%)	34 (1%)
2	9	121/122 (99%)	17 (14%)	2 (1%)
All	All	2867/3044 (94%)	253 (8%)	36 (1%)

5 of 253 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A

5 of 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1352	A
1	0	1692	C
1	0	2791	U
1	0	1450	C
1	0	1856	C

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

5 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	PSU	0	2621	1	17,21,22	1.50	3 (17%)	20,30,33	5.44	4 (20%)
1	OMG	0	2588	1	18,26,27	1.12	2 (11%)	20,38,41	2.62	5 (25%)
1	UR3	0	2619	1	14,22,23	0.86	0	15,32,35	0.66	0
1	OMU	0	2587	1	14,22,23	1.03	1 (7%)	14,31,34	1.16	1 (7%)
1	1MA	0	628	1	15,25,26	0.71	0	15,37,40	1.38	1 (6%)

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	PSU	0	2621	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/5/25/26	0/2/2/2
1	OMU	0	2587	1	-	0/7/27/28	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.56	1.48	1.52
1	0	2588	OMG	C6-N1	3.52	1.39	1.33
1	0	2621	PSU	C4-N3	2.84	1.38	1.33
1	0	2587	OMU	C4-N3	2.74	1.37	1.33
1	0	2621	PSU	C2-N1	2.54	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	-17.10	114.84	128.43
1	0	2621	PSU	C4-N3-C2	14.53	127.41	115.14
1	0	2588	OMG	C5-C6-N1	-8.73	111.50	123.43
1	0	2621	PSU	C5-C4-N3	-8.35	114.60	125.36
1	0	2588	OMG	C6-N1-C2	5.88	125.27	115.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 231 ligands modelled in this entry, 231 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	-0.38	56 (2%) 65 63	18, 37, 80, 136	0
2	9	122/122 (100%)	-0.39	5 (4%) 37 36	32, 54, 75, 144	0
3	A	237/240 (98%)	0.38	20 (8%) 11 10	20, 39, 73, 93	0
4	B	337/338 (99%)	0.38	15 (4%) 33 31	21, 46, 72, 83	0
5	C	246/246 (100%)	0.32	11 (4%) 33 31	15, 36, 58, 70	0
6	D	140/177 (79%)	2.55	82 (58%) 0 0	44, 89, 112, 117	0
7	E	172/178 (96%)	0.60	13 (7%) 13 12	38, 59, 78, 83	0
8	F	119/120 (99%)	0.92	24 (20%) 1 0	38, 58, 83, 90	0
9	G	29/348 (8%)	2.54	20 (68%) 0 0	65, 81, 89, 93	0
10	H	160/171 (93%)	0.57	20 (12%) 3 3	32, 47, 77, 88	0
11	I	70/162 (43%)	5.30	67 (95%) 0 0	88, 102, 119, 122	0
12	J	142/145 (97%)	0.25	4 (2%) 53 51	30, 43, 63, 85	0
13	K	132/132 (100%)	0.15	6 (4%) 33 31	28, 43, 62, 71	0
14	L	145/165 (87%)	0.73	17 (11%) 4 4	20, 55, 93, 106	0
15	M	194/194 (100%)	-0.11	1 (0%) 91 89	19, 32, 46, 54	0
16	N	186/187 (99%)	0.62	17 (9%) 9 8	32, 51, 94, 109	0
17	O	115/116 (99%)	0.00	2 (1%) 70 68	28, 44, 61, 69	0
18	P	143/149 (95%)	0.12	0 100 100	31, 45, 57, 64	0
19	Q	95/96 (98%)	0.09	1 (1%) 80 79	27, 35, 52, 59	0
20	R	150/155 (96%)	-0.03	0 100 100	23, 36, 54, 63	0
21	S	81/85 (95%)	0.50	10 (12%) 4 3	32, 47, 68, 72	0
22	T	119/120 (99%)	0.42	5 (4%) 36 35	29, 46, 67, 82	0
23	U	53/66 (80%)	0.36	2 (3%) 40 39	34, 47, 64, 73	0
24	V	65/71 (91%)	1.63	12 (18%) 1 1	40, 59, 99, 103	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	0.35	6 (3%) 39 38	28, 42, 58, 67	0
26	X	82/92 (89%)	0.43	4 (4%) 29 28	36, 49, 74, 91	0
27	Y	142/241 (58%)	0.01	5 (3%) 44 43	22, 36, 60, 75	0
28	Z	73/73 (100%)	0.39	4 (5%) 25 24	37, 49, 68, 85	0
29	1	56/57 (98%)	0.20	0 100 100	18, 25, 33, 37	0
30	2	46/50 (92%)	0.52	6 (13%) 3 3	29, 50, 75, 86	0
31	3	92/92 (100%)	0.19	3 (3%) 46 45	24, 45, 59, 73	0
All	All	6646/7464 (89%)	0.15	438 (6%) 18 17	15, 42, 85, 144	0

The worst 5 of 438 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	I	96	PHE	14.9
24	V	1	THR	11.9
11	I	71	GLY	11.5
11	I	133	THR	10.5
11	I	109	ALA	10.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
1	OMG	0	2588	24/25	0.98	0.13	22,25,27,30	0
1	UR3	0	2619	21/22	0.98	0.14	23,27,31,37	0
1	OMU	0	2587	21/22	0.98	0.13	24,26,28,30	0
1	1MA	0	628	23/24	0.98	0.17	21,24,25,27	0
1	PSU	0	2621	20/21	0.99	0.15	20,25,28,28	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
32	MG	0	8087	1/1	0.52	0.31	71,71,71,71	0
32	MG	0	8050	1/1	0.64	0.15	62,62,62,62	0
32	MG	0	8072	1/1	0.71	0.10	51,51,51,51	0
32	MG	0	8103	1/1	0.73	0.27	57,57,57,57	0
32	MG	9	8095	1/1	0.77	0.14	67,67,67,67	0
34	NA	0	8371	1/1	0.78	0.37	52,52,52,52	0
34	NA	0	8384	1/1	0.79	0.16	54,54,54,54	0
32	MG	0	8102	1/1	0.80	0.10	54,54,54,54	0
34	NA	0	8370	1/1	0.82	0.43	60,60,60,60	0
32	MG	0	8070	1/1	0.83	0.14	41,41,41,41	0
32	MG	0	8047	1/1	0.83	0.10	55,55,55,55	0
34	NA	0	8329	1/1	0.83	0.13	50,50,50,50	0
34	NA	C	8304	1/1	0.84	0.20	32,32,32,32	0
32	MG	0	8094	1/1	0.84	0.07	62,62,62,62	0
32	MG	0	8049	1/1	0.85	0.12	55,55,55,55	0
34	NA	9	8351	1/1	0.86	0.15	43,43,43,43	0
34	NA	R	8386	1/1	0.87	0.41	75,75,75,75	0
32	MG	0	8112	1/1	0.87	0.13	38,38,38,38	0
34	NA	0	8311	1/1	0.87	0.14	48,48,48,48	0
34	NA	H	8322	1/1	0.87	0.26	53,53,53,53	0
32	MG	0	8034	1/1	0.87	0.09	32,32,32,32	0
34	NA	0	8308	1/1	0.88	0.20	43,43,43,43	0
32	MG	0	8101	1/1	0.88	0.29	48,48,48,48	0
34	NA	0	8307	1/1	0.88	0.14	42,42,42,42	0
34	NA	9	8383	1/1	0.88	0.22	44,44,44,44	0
34	NA	0	8363	1/1	0.89	0.31	52,52,52,52	0
32	MG	0	8052	1/1	0.89	0.07	47,47,47,47	0
32	MG	0	8066	1/1	0.90	0.49	76,76,76,76	0
32	MG	0	8090	1/1	0.90	0.34	55,55,55,55	0
32	MG	0	8089	1/1	0.90	0.08	52,52,52,52	0
34	NA	0	8376	1/1	0.90	0.40	40,40,40,40	0
34	NA	0	8341	1/1	0.91	0.13	38,38,38,38	0
34	NA	0	8372	1/1	0.91	0.45	55,55,55,55	0
34	NA	0	8327	1/1	0.91	0.26	38,38,38,38	0
32	MG	0	8077	1/1	0.91	0.13	24,24,24,24	0
32	MG	0	8076	1/1	0.91	0.05	43,43,43,43	0
32	MG	0	8067	1/1	0.91	0.14	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	NA	0	8373	1/1	0.91	0.13	44,44,44,44	0
32	MG	0	8014	1/1	0.92	0.09	25,25,25,25	0
32	MG	0	8116	1/1	0.92	0.16	38,38,38,38	0
34	NA	0	8358	1/1	0.92	0.38	67,67,67,67	0
32	MG	0	8043	1/1	0.92	0.06	34,34,34,34	0
32	MG	0	8045	1/1	0.92	0.07	51,51,51,51	0
34	NA	0	8324	1/1	0.92	0.15	51,51,51,51	0
32	MG	0	8062	1/1	0.92	0.07	42,42,42,42	0
34	NA	0	8314	1/1	0.92	0.30	39,39,39,39	0
32	MG	0	8085	1/1	0.92	0.08	35,35,35,35	0
34	NA	0	8385	1/1	0.92	0.38	48,48,48,48	0
34	NA	0	8340	1/1	0.92	0.25	46,46,46,46	0
34	NA	0	8350	1/1	0.92	0.36	36,36,36,36	0
34	NA	0	8382	1/1	0.93	0.10	66,66,66,66	0
35	CL	J	8521	1/1	0.93	0.17	48,48,48,48	0
34	NA	0	8325	1/1	0.93	0.24	49,49,49,49	0
32	MG	0	8022	1/1	0.93	0.12	31,31,31,31	0
34	NA	0	8310	1/1	0.93	0.12	28,28,28,28	0
32	MG	0	8082	1/1	0.93	0.19	59,59,59,59	0
32	MG	0	8080	1/1	0.93	0.07	42,42,42,42	0
34	NA	0	8357	1/1	0.93	0.09	40,40,40,40	0
32	MG	0	8068	1/1	0.93	0.04	45,45,45,45	0
34	NA	0	8369	1/1	0.93	0.21	41,41,41,41	0
32	MG	0	8071	1/1	0.93	0.04	61,61,61,61	0
32	MG	B	8055	1/1	0.93	0.07	43,43,43,43	0
32	MG	0	8012	1/1	0.94	0.14	34,34,34,34	0
34	NA	S	8312	1/1	0.94	0.08	28,28,28,28	0
32	MG	0	8016	1/1	0.94	0.09	32,32,32,32	0
32	MG	K	8069	1/1	0.94	0.12	47,47,47,47	0
34	NA	0	8377	1/1	0.94	0.23	51,51,51,51	0
34	NA	0	8361	1/1	0.94	0.22	38,38,38,38	0
32	MG	0	8051	1/1	0.94	0.11	56,56,56,56	0
34	NA	0	8321	1/1	0.94	0.24	40,40,40,40	0
32	MG	0	8046	1/1	0.94	0.06	38,38,38,38	0
34	NA	0	8362	1/1	0.94	0.35	51,51,51,51	0
34	NA	0	8356	1/1	0.94	0.20	37,37,37,37	0
32	MG	0	8093	1/1	0.94	0.12	37,37,37,37	0
34	NA	0	8365	1/1	0.94	0.19	30,30,30,30	0
34	NA	A	8345	1/1	0.94	0.09	47,47,47,47	0
34	NA	0	8313	1/1	0.94	0.11	48,48,48,48	0
34	NA	0	8302	1/1	0.94	0.20	45,45,45,45	0
32	MG	0	8099	1/1	0.94	0.23	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8013	1/1	0.95	0.15	22,22,22,22	0
32	MG	0	8079	1/1	0.95	0.16	20,20,20,20	0
34	NA	0	8349	1/1	0.95	0.17	36,36,36,36	0
34	NA	0	8318	1/1	0.95	0.29	51,51,51,51	0
34	NA	0	8334	1/1	0.95	0.09	35,35,35,35	0
34	NA	0	8364	1/1	0.95	0.26	38,38,38,38	0
34	NA	0	8333	1/1	0.95	0.09	25,25,25,25	0
34	NA	0	8315	1/1	0.95	0.18	32,32,32,32	0
34	NA	0	8366	1/1	0.95	0.24	57,57,57,57	0
32	MG	0	8104	1/1	0.95	0.14	47,47,47,47	0
34	NA	0	8368	1/1	0.95	0.15	50,50,50,50	0
32	MG	0	8006	1/1	0.95	0.07	27,27,27,27	0
33	K	0	8201	1/1	0.95	0.15	64,64,64,64	0
32	MG	0	8039	1/1	0.95	0.07	34,34,34,34	0
32	MG	0	8028	1/1	0.95	0.06	26,26,26,26	0
34	NA	0	8326	1/1	0.95	0.19	38,38,38,38	0
32	MG	0	8064	1/1	0.95	0.14	26,26,26,26	0
35	CL	0	8515	1/1	0.95	0.10	50,50,50,50	0
34	NA	0	8355	1/1	0.96	0.35	48,48,48,48	0
34	NA	L	8380	1/1	0.96	0.34	42,42,42,42	0
32	MG	0	8097	1/1	0.96	0.08	32,32,32,32	0
34	NA	0	8330	1/1	0.96	0.08	38,38,38,38	0
34	NA	0	8317	1/1	0.96	0.11	27,27,27,27	0
34	NA	R	8337	1/1	0.96	0.08	34,34,34,34	0
34	NA	0	8379	1/1	0.96	0.45	49,49,49,49	0
32	MG	0	8091	1/1	0.96	0.09	42,42,42,42	0
34	NA	0	8336	1/1	0.96	0.07	37,37,37,37	0
35	CL	J	8502	1/1	0.96	0.12	53,53,53,53	0
34	NA	0	8316	1/1	0.96	0.21	37,37,37,37	0
32	MG	0	8037	1/1	0.96	0.06	34,34,34,34	0
32	MG	0	8105	1/1	0.96	0.13	43,43,43,43	0
34	NA	Q	8348	1/1	0.96	0.07	32,32,32,32	0
32	MG	0	8098	1/1	0.96	0.06	27,27,27,27	0
32	MG	3	8078	1/1	0.96	0.09	40,40,40,40	0
32	MG	0	8023	1/1	0.96	0.13	31,31,31,31	0
34	NA	0	8303	1/1	0.97	0.18	34,34,34,34	0
34	NA	0	8319	1/1	0.97	0.11	29,29,29,29	0
35	CL	R	8506	1/1	0.97	0.12	40,40,40,40	0
34	NA	0	8378	1/1	0.97	0.18	42,42,42,42	0
32	MG	0	8061	1/1	0.97	0.15	34,34,34,34	0
32	MG	0	8044	1/1	0.97	0.09	33,33,33,33	0
32	MG	0	8020	1/1	0.97	0.09	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	NA	0	8359	1/1	0.97	0.26	40,40,40,40	0
34	NA	0	8381	1/1	0.97	0.14	42,42,42,42	0
34	NA	0	8342	1/1	0.97	0.26	33,33,33,33	0
34	NA	0	8352	1/1	0.97	0.13	40,40,40,40	0
34	NA	M	8347	1/1	0.97	0.17	20,20,20,20	0
35	CL	0	8522	1/1	0.97	0.17	46,46,46,46	0
32	MG	0	8113	1/1	0.97	0.10	36,36,36,36	0
32	MG	0	8106	1/1	0.97	0.03	31,31,31,31	0
35	CL	3	8504	1/1	0.97	0.07	45,45,45,45	0
32	MG	0	8033	1/1	0.97	0.10	20,20,20,20	0
32	MG	0	8040	1/1	0.97	0.12	38,38,38,38	0
32	MG	0	8096	1/1	0.97	0.12	38,38,38,38	0
34	NA	T	8343	1/1	0.97	0.06	31,31,31,31	0
32	MG	0	8018	1/1	0.97	0.06	29,29,29,29	0
34	NA	0	8331	1/1	0.97	0.28	40,40,40,40	0
34	NA	0	8360	1/1	0.97	0.17	43,43,43,43	0
32	MG	0	8107	1/1	0.97	0.07	65,65,65,65	0
32	MG	0	8031	1/1	0.97	0.12	24,24,24,24	0
34	NA	0	8335	1/1	0.97	0.19	32,32,32,32	0
32	MG	0	8081	1/1	0.97	0.10	39,39,39,39	0
34	NA	0	8301	1/1	0.97	0.12	35,35,35,35	0
32	MG	0	8002	1/1	0.97	0.08	28,28,28,28	0
32	MG	0	8063	1/1	0.97	0.14	62,62,62,62	0
32	MG	0	8042	1/1	0.97	0.09	29,29,29,29	0
32	MG	0	8059	1/1	0.97	0.08	26,26,26,26	0
35	CL	L	8510	1/1	0.97	0.10	38,38,38,38	0
34	NA	0	8367	1/1	0.97	0.28	45,45,45,45	0
32	MG	0	8027	1/1	0.97	0.07	36,36,36,36	0
32	MG	0	8011	1/1	0.97	0.10	24,24,24,24	0
34	NA	0	8332	1/1	0.97	0.12	33,33,33,33	0
32	MG	Y	8108	1/1	0.97	0.09	27,27,27,27	0
34	NA	0	8374	1/1	0.97	0.20	44,44,44,44	0
32	MG	0	8001	1/1	0.97	0.11	25,25,25,25	0
32	MG	0	8032	1/1	0.97	0.06	24,24,24,24	0
32	MG	0	8074	1/1	0.97	0.06	35,35,35,35	0
35	CL	Y	8520	1/1	0.97	0.14	39,39,39,39	0
32	MG	0	8084	1/1	0.98	0.07	39,39,39,39	0
32	MG	0	8092	1/1	0.98	0.11	68,68,68,68	0
35	CL	0	8505	1/1	0.98	0.11	42,42,42,42	0
32	MG	0	8053	1/1	0.98	0.10	29,29,29,29	0
36	CD	O	8405	1/1	0.98	0.08	73,73,73,73	0
32	MG	0	8038	1/1	0.98	0.13	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8041	1/1	0.98	0.10	34,34,34,34	0
35	CL	0	8503	1/1	0.98	0.17	42,42,42,42	0
32	MG	0	8088	1/1	0.98	0.08	21,21,21,21	0
32	MG	0	8036	1/1	0.98	0.09	36,36,36,36	0
35	CL	J	8501	1/1	0.98	0.09	46,46,46,46	0
32	MG	0	8003	1/1	0.98	0.10	22,22,22,22	0
34	NA	0	8344	1/1	0.98	0.11	25,25,25,25	0
35	CL	O	8508	1/1	0.98	0.08	53,53,53,53	0
34	NA	0	8306	1/1	0.98	0.13	31,31,31,31	0
32	MG	0	8029	1/1	0.98	0.09	36,36,36,36	0
34	NA	0	8339	1/1	0.98	0.20	21,21,21,21	0
35	CL	0	8511	1/1	0.98	0.11	38,38,38,38	0
32	MG	0	8083	1/1	0.98	0.08	30,30,30,30	0
32	MG	T	8073	1/1	0.98	0.05	39,39,39,39	0
32	MG	0	8010	1/1	0.98	0.16	25,25,25,25	0
35	CL	M	8518	1/1	0.98	0.20	35,35,35,35	0
32	MG	0	8048	1/1	0.98	0.07	40,40,40,40	0
35	CL	0	8517	1/1	0.98	0.10	50,50,50,50	0
32	MG	0	8058	1/1	0.98	0.06	28,28,28,28	0
32	MG	0	8114	1/1	0.98	0.07	37,37,37,37	0
34	NA	0	8354	1/1	0.98	0.17	26,26,26,26	0
32	MG	0	8115	1/1	0.98	0.09	44,44,44,44	0
32	MG	0	8054	1/1	0.98	0.15	18,18,18,18	0
32	MG	0	8019	1/1	0.98	0.05	25,25,25,25	0
34	NA	0	8305	1/1	0.98	0.23	33,33,33,33	0
35	CL	N	8507	1/1	0.98	0.09	46,46,46,46	0
34	NA	H	8309	1/1	0.98	0.09	28,28,28,28	0
32	MG	0	8035	1/1	0.98	0.07	37,37,37,37	0
32	MG	0	8100	1/1	0.98	0.06	62,62,62,62	0
32	MG	0	8015	1/1	0.98	0.18	27,27,27,27	0
32	MG	0	8007	1/1	0.98	0.15	22,22,22,22	0
32	MG	0	8008	1/1	0.98	0.10	24,24,24,24	0
32	MG	0	8009	1/1	0.98	0.14	25,25,25,25	0
32	MG	0	8021	1/1	0.98	0.09	24,24,24,24	0
34	NA	J	8346	1/1	0.98	0.08	36,36,36,36	0
32	MG	0	8075	1/1	0.98	0.06	30,30,30,30	0
32	MG	0	8026	1/1	0.98	0.16	27,27,27,27	0
32	MG	0	8057	1/1	0.98	0.12	36,36,36,36	0
35	CL	0	8514	1/1	0.98	0.20	38,38,38,38	0
35	CL	0	8513	1/1	0.99	0.11	45,45,45,45	0
35	CL	B	8519	1/1	0.99	0.14	34,34,34,34	0
34	NA	0	8323	1/1	0.99	0.15	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	CD	Z	8403	1/1	0.99	0.14	48,48,48,48	0
32	MG	0	8109	1/1	0.99	0.13	26,26,26,26	0
32	MG	0	8024	1/1	0.99	0.15	23,23,23,23	0
35	CL	A	8509	1/1	0.99	0.11	49,49,49,49	0
32	MG	0	8025	1/1	0.99	0.09	37,37,37,37	0
36	CD	1	8402	1/1	0.99	0.07	44,44,44,44	0
32	MG	0	8086	1/1	0.99	0.09	33,33,33,33	0
33	K	0	8202	1/1	0.99	0.07	38,38,38,38	0
34	NA	0	8320	1/1	0.99	0.30	38,38,38,38	0
32	MG	0	8005	1/1	0.99	0.12	24,24,24,24	0
32	MG	A	8065	1/1	0.99	0.07	24,24,24,24	0
32	MG	0	8111	1/1	0.99	0.09	25,25,25,25	0
35	CL	0	8512	1/1	0.99	0.12	35,35,35,35	0
34	NA	0	8353	1/1	0.99	0.14	20,20,20,20	0
32	MG	0	8110	1/1	0.99	0.11	32,32,32,32	0
36	CD	U	8401	1/1	0.99	0.11	52,52,52,52	0
34	NA	0	8328	1/1	0.99	0.12	30,30,30,30	0
32	MG	0	8060	1/1	0.99	0.22	32,32,32,32	0
36	CD	3	8404	1/1	0.99	0.09	49,49,49,49	0
32	MG	0	8056	1/1	0.99	0.04	31,31,31,31	0
35	CL	0	8516	1/1	0.99	0.14	42,42,42,42	0
32	MG	0	8004	1/1	0.99	0.14	22,22,22,22	0
34	NA	0	8338	1/1	0.99	0.06	38,38,38,38	0
34	NA	0	8375	1/1	0.99	0.22	43,43,43,43	0
32	MG	0	8017	1/1	1.00	0.14	13,13,13,13	0
32	MG	0	8030	1/1	1.00	0.07	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.