



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2018 – 01:23 am GMT

PDB ID : 1VQ4
Title : The structure of the transition state analogue "DAA" 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

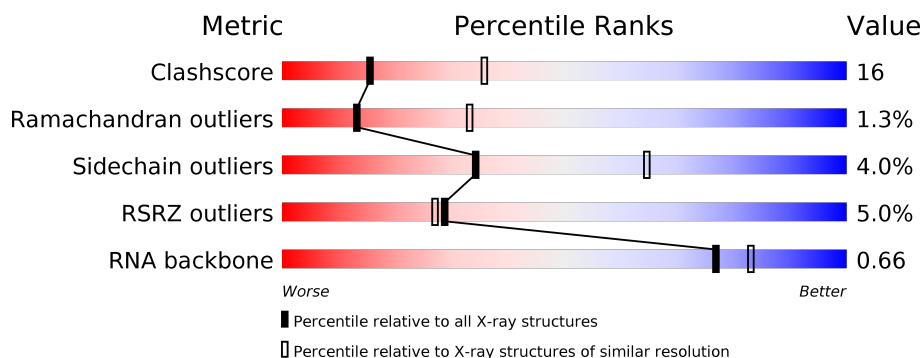
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



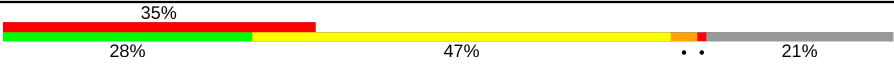
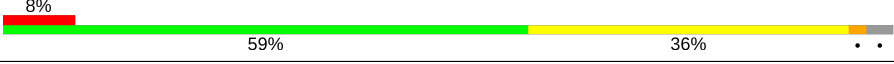

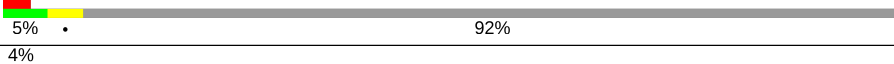

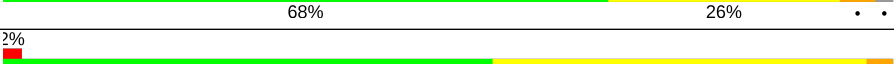

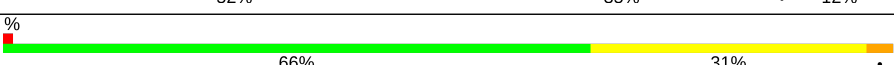



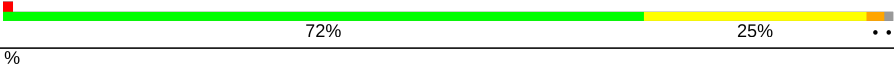


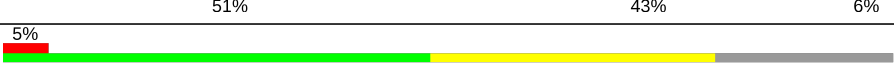
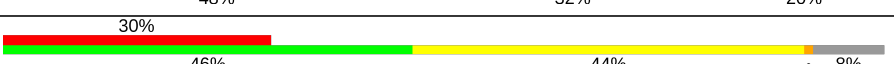
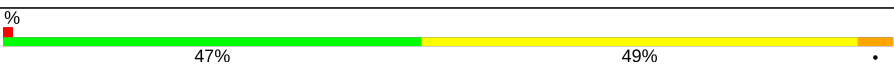

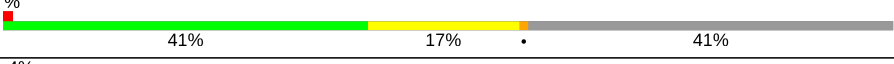






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122126	2756 (2.70-2.70)
Ramachandran outliers	120053	2716 (2.70-2.70)
Sidechain outliers	120020	2716 (2.70-2.70)
RSRZ outliers	108989	2376 (2.70-2.70)
RNA backbone	2636	1009 (3.00-2.40)

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

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>30%</div> <div>5%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>3%</div> <div> <div></div> <div>53%</div> <div>34%</div> <div>11%</div> </div> </div>
3	4	8	<div> <div></div> <div> <div></div> <div>50%</div> <div>38%</div> <div>13%</div> </div> </div>
4	A	240	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>38%</div> </div> </div>
5	B	338	<div> <div>%</div> <div> <div></div> <div>52%</div> <div>42%</div> <div>6%</div> </div> </div>
6	C	246	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>41%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	
15	M	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	83	
29	1	57	
30	2	50	
31	3	92	

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Mol	Chain	Length	Quality of chain
32	I	162	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MG	0	8090	-	-	-	X
33	MG	0	8092	-	-	-	X
35	NA	0	9171	-	-	-	X
35	NA	0	9177	-	-	-	X
35	NA	0	9182	-	-	-	X
35	NA	R	9186	-	-	-	X

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 98999 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal rna.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26350	10878	19048	2745			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	modified residue	GB 3377779
0	2587	OMU	U	modified residue	GB 3377779
0	2588	OMG	G	modified residue	GB 3377779
0	2619	UR3	U	modified residue	GB 3377779
0	2621	PSU	U	modified residue	GB 3377779

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a RNA chain called 5'-R(*CP*CP*(5AA)P*(2OP)P*(PO2)P*(DA)P*C*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	8	Total	C	N	O	P	0	0	0
			127	61	23	38	5			

- Molecule 4 is a protein called 50S ribosomal protein L2P.

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

- Molecule 5 is a protein called 50S ribosomal protein L3P.

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

- Molecule 6 is a protein called 50S ribosomal protein L4E.

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

- Molecule 7 is a protein called 50S ribosomal protein L5P.

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

- Molecule 8 is a protein called 50S ribosomal protein L6P.

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

- Molecule 9 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 10 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L10E.

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

- Molecule 12 is a protein called 50S ribosomal protein L13P.

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

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	CONFLICT	UNP P22450

- Molecule 14 is a protein called 50S ribosomal protein L15P.

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

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	GB 55231501
M	194	ALA	GLY	CONFLICT	GB 55231501

- Molecule 16 is a protein called 50S ribosomal protein L18P.

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

- Molecule 17 is a protein called 50S ribosomal protein L18e.

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

- Molecule 18 is a protein called 50S ribosomal protein L19E.

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

- Molecule 19 is a protein called 50S ribosomal protein L21e.

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

- Molecule 20 is a protein called 50S ribosomal protein L22P.

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

- Molecule 21 is a protein called 50S ribosomal protein L23P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24E.

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

- Molecule 24 is a protein called 50S ribosomal protein L29P.

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

- Molecule 25 is a protein called 50S ribosomal protein L30P.

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

- Molecule 26 is a protein called 50S ribosomal protein L31e.

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

- Molecule 27 is a protein called 50S ribosomal protein L32E.

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

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	CONFLICT	GB 55231162

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	108	Total	Mg	0	0
			108	108		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	2	Total	Mg	0	0
			2	2		
33	T	1	Total	Mg	0	0
			1	1		
33	9	2	Total	Mg	0	0
			2	2		
33	3	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	3	Total	K	0	0
			3	3		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	72	Total Na 72 72	0	0
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	H	2	Total Na 2 2	0	0
35	C	1	Total Na 1 1	0	0
35	A	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	9	2	Total Na 2 2	0	0
35	L	1	Total Na 1 1	0	0
35	S	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0

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

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

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

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	O	1	Total 1	Cd 1	0	0
37	Z	1	Total 1	Cd 1	0	0
37	1	1	Total 1	Cd 1	0	0
37	3	1	Total 1	Cd 1	0	0
37	U	1	Total 1	Cd 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5764	Total 5764	O 5764	0	0
38	9	133	Total 133	O 133	0	0
38	4	3	Total 3	O 3	0	0
38	A	116	Total 116	O 116	0	0
38	B	143	Total 143	O 143	0	0
38	C	173	Total 173	O 173	0	0
38	D	44	Total 44	O 44	0	0
38	E	43	Total 43	O 43	0	0
38	F	24	Total 24	O 24	0	0
38	G	17	Total 17	O 17	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	H	66	Total 66	O 66	0	0
38	J	52	Total 52	O 52	0	0
38	K	57	Total 57	O 57	0	0
38	L	81	Total 81	O 81	0	0
38	M	115	Total 115	O 115	0	0
38	N	61	Total 61	O 61	0	0
38	O	45	Total 45	O 45	0	0
38	P	63	Total 63	O 63	0	0
38	Q	52	Total 52	O 52	0	0
38	R	89	Total 89	O 89	0	0
38	S	31	Total 31	O 31	0	0
38	T	36	Total 36	O 36	0	0
38	U	26	Total 26	O 26	0	0
38	V	13	Total 13	O 13	0	0
38	W	70	Total 70	O 70	0	0
38	X	31	Total 31	O 31	0	0
38	Y	93	Total 93	O 93	0	0
38	Z	31	Total 31	O 31	0	0
38	1	61	Total 61	O 61	0	0
38	2	42	Total 42	O 42	0	0
38	3	71	Total 71	O 71	0	0

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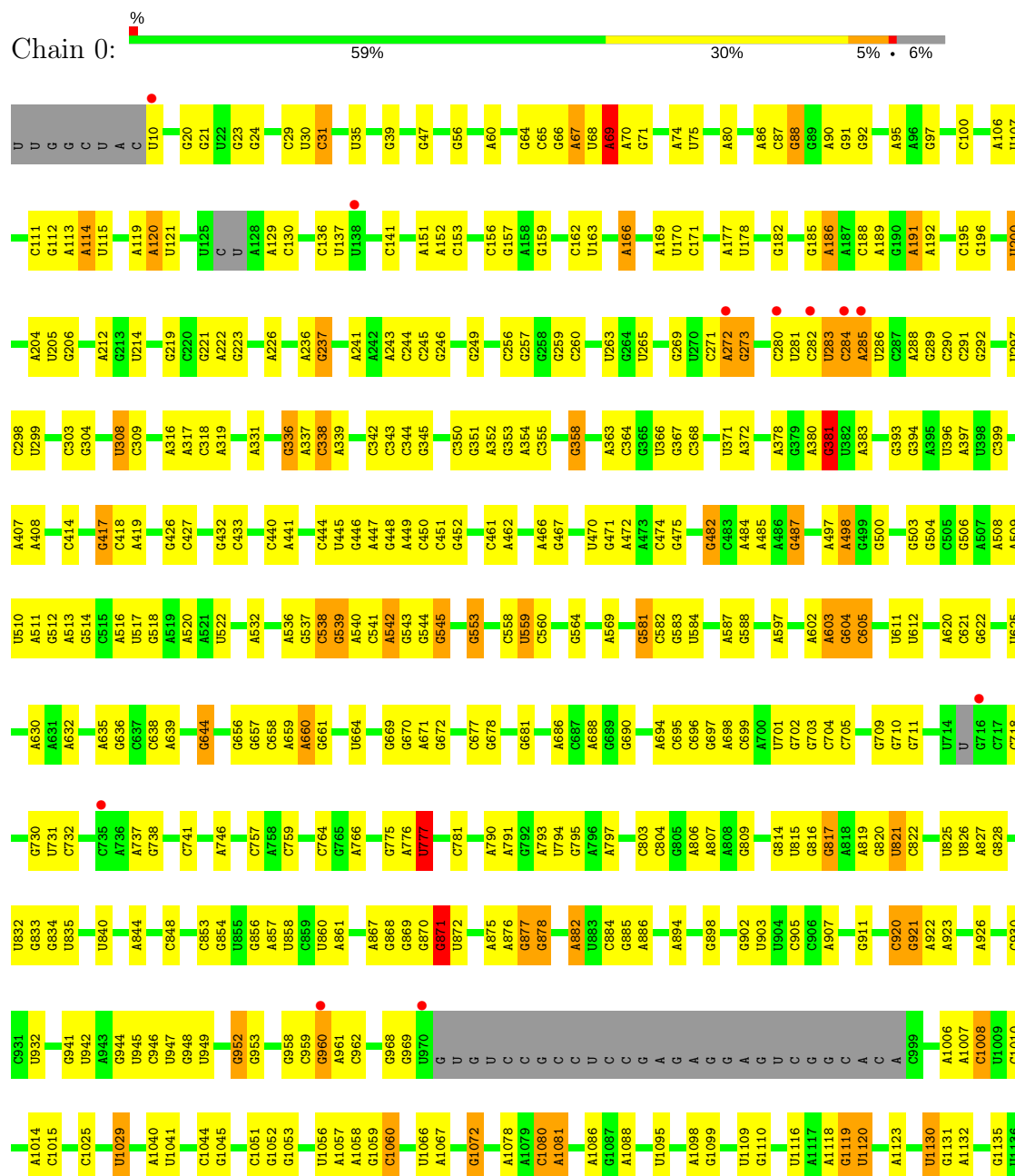
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	I	9	Total	O	0	0
			9	9		

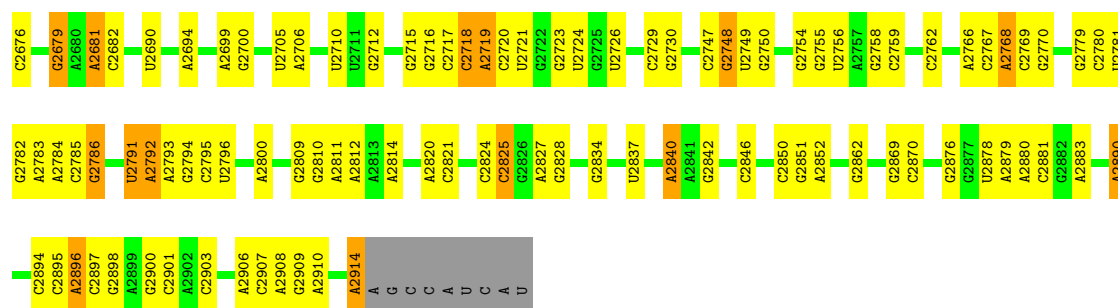
3 Residue-property plots

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.

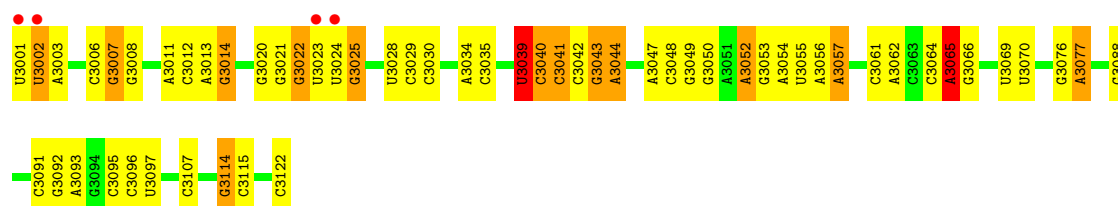
- Molecule 1: 23S ribosomal rna



G1562	C2472	A2353	C2241	U	G2094	U1984	C1882	G1765	G1557	A1329	C1229	G1137
G2563	G2473	A2354	U2242	A	A2095	A1969	G1883	U1766	C1558	U1333	A1230	G1151
G2564	A2474	A2361	C2243	C	A2096	G1970	G1867	A1767	U1559	C1334		
G2565	C2475	A2362	G2250	C	A2101	G1971	G1868	C1769	U	C1335	U1234	G1156
G2570	G2476	A2363	G2251	G	G2102	U1972	U1874		U1561		U1235	G1157
G2576	C2477	A2364	A2252	C	A2105	A1973		C1772	G1562	G1340	A1236	G1158
U2586	U2478	G2365	G2253	G	C2106		G1877	G1773	G1563	A1341	U1237	G1159
U2587	G2480	A2369	G2254	C	G2110	A1978	G1878	G1676	C1564	C1342	U1238	G1160
U2588	U2479	A2370	G2255	U	G2111	G1979	U1879	U1677	U1568	G1343	G1239	A1161
U2589	G2481	A2371	A2256	A	G2112	U1980			U1569	G1344		G1162
G2590	A2482	G2379	A2257	G	G2113	U1986	U1890	G1681	A1471	A1242	A1243	G1163
G2591	G2483	A2380	G2258	C	G2114			A1682	C1472	G1351	G1243	G1164
G2592	U2484	C2381	A2264	G	G2115	U2003	U1903	G1683	U1473	A1352	U1244	U1166
U2597	U2492	A2382	A2265	G	G2116	U2004	A1904	A1684	C1474	C1353	A1245	G1166
U2598	G2493	U2395	A2266	G	G2136	U2005	U1905	A1685		C1360		G1167
A2601	C2502	A2395	C2269	C	A	U2008		C1686	G1589		A1262	
G2602	A2503	G2403	G2270	A	C	G2009	A1909	C1687	G1592	C1366	C1253	U1169
G2603	A2504	G2404	G2271	C	U	A2010	A1910	C1692	C1593			U1170
U2607	G2505	A2408	G2272	C	G	A2011	U1915	A1692	C1594	A1372	U1266	G1171
G2608	A2506	G2412	C2281	G	U	U2012	U1916	U1701	G1595	A1375	C1267	G1172
G2613	U2507	A2413	U2282	G	U	G2013	U1917	U1702	U1596	G1376	C1268	G1173
G2614	G2508	A2414	A2283	C	C	G2014	A1919	C1705	A1597	C1377		A1174
U2619	A2509	A2415	A2284	U	C	U2015	G1920		U1598		G1273	G1175
G2626	G2510	G2416	A2285	C	A	U2016	C1921	A1710	A1603	G1385	A1278	G1176
G2627	A2511	C2417	A2300	A	G	A2030	A1922	A1711	G1604	U1279	U1278	A1177
G2630	G2512	G2418	A2301	C	U	G2033	G1925	A1712	G1605		U1285	U1180
G2634	U2513	U2419	A2302	A	U	U2034	U1926		U1606	G1388	U1285	A1181
U2637	G2514	G2420	C2309	G	U	G2035	A1927	A1717	A1607	A1390	G1289	C1182
G2638	A2515	G2421		U	G	C2036		U1722	C1613	G1391	G1290	C1183
G2639	G2516	A2422	G2312	G	C	A2039	U1937	G1723	G1614	A1392	U1293	C1184
U2641	A2517	G2423	C2313	A	A	G2044	U1939	U1724	C1617	U1506	A1294	U1185
G2642	G2518	A2424	C2314	A	C	G2045	A1941	C1725	U1625	C1507	G1295	U1187
G2643	U2519	G2425	C2315	U	C	G2046	C1942		A1626	U1517		U1188
G2644	C2520	G2426	C2316	A	A	C2047	C1943	G1730		A1406	U1298	A1189
A2649	U2521	G2427	C2317	C	U	G2048	G1944	C1731	A1630	A1407	G1299	G1190
U2652	G2522	U2428		U	G	A2054	G1945	A1732	A1631	U1304	U1304	A1191
A2664	A2523	A2429	U2320	A	A	U2054	C1946	C1735	A1632	A1414	C1305	A1192
U	G2524	G2430	A2321	C	G	G2050	G1947		A1633	U1415	U1306	A1193
G2667	U2525	U2431	G2322	C	U	A2054	U1948	U1838	C1633	G1416	A1307	U1198
G2668	C2526	G2432	G2323	C	A	U2054	G1949	A1839	G1634	G1415	U1308	A1199
U2669	U2527	U2433	G2324	G	G	G2054	G1950	A1840	A1526	G1417	A1308	C1201
G2670	G2528	G2434	C2325	C	A	G2054	G1951	G1743	U1527	U1418	C1201	A1202
U2671	U2529	A2435	U2326	U	G	G2070	U	G1744	G1529	U1419	G1311	G1210
G2672	A2530	G2436	A2332	G	A	C2071	A			G1312	A1321	
U2673	G2531	A2437	A2333	G	C	G2072	A	A1747	G1535	U1422	G1322	C1213
	U2532	G2438	G2334	U	A	G2073	C	A1641	C1536	C1423	U1313	G1214
	G2533	A2439	A2335	A	A	A2074	C	A1642	C1537	U1424	U1314	A1206
	C2534	G2440	C2336	C	U	G2074	U	C1643		G1425	G1315	A1207
	U2535	U2441	G2337	U	A	A2081	U	U1654	G1543	C1426	G1316	C1208
	G2536	G2442	C2338	C	G	A2089	G	G1655	U1544	A1427	A1321	G1210
	U2537	A2443	A2339	C	C	G2090	A	A1656	C1545		G1322	C1213
	U2541	G2444	G2340	G	A	G2091	C	A1657	G1546	A1434	G1325	A1215
A2664	C2542	G2445	G2341	U	C	G2092	C	A1658	G1555	U1435	G1326	G1216
U	U2543	A2446	A2342	C	G	G2093	C	A1659	G1556	C1436	A1328	
	U2544	G2447	U2343	C	G	G2094	C	C1660				
	G2545	G2448	U2344	G	A							
	U2546	A2449	A2345	A	A							
	C2547	G2450	C2346	C	U							
	U2548	U2451		U	U							
	G2549	G2452		C	C							
	C2550	G2453		C	C							
	U2551	A2454		C	C							
	G2552	G2455		C	C							
	A2553	A2456		C	C							
	U2554	G2457		C	C							
	G2555	U2458		C	C							
	U2556	A2459		C	C							



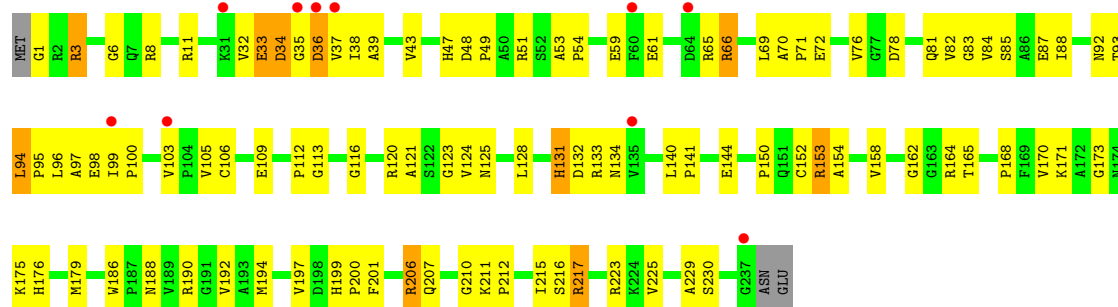
• Molecule 2: 5S ribosomal RNA



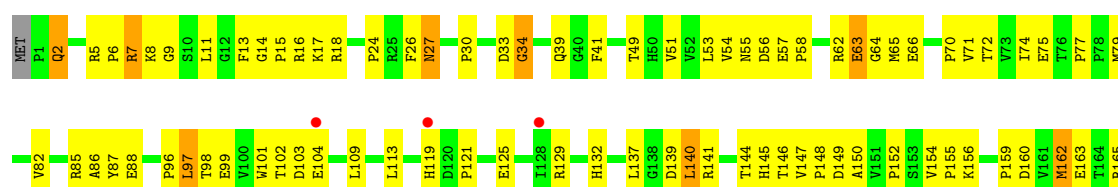
• Molecule 3: 5'-R(*CP*CP*(5AA)P*(2OP)P*(PO2)P*(DA)P*C*C)-3'

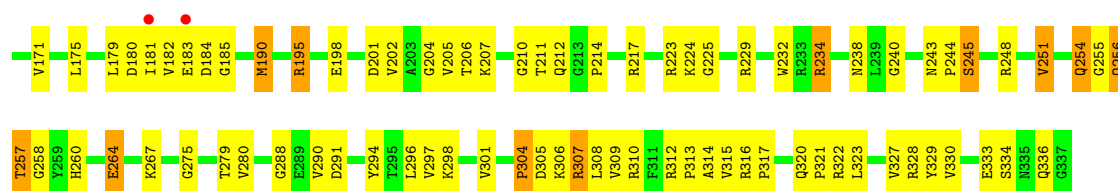


• Molecule 4: 50S ribosomal protein L2P

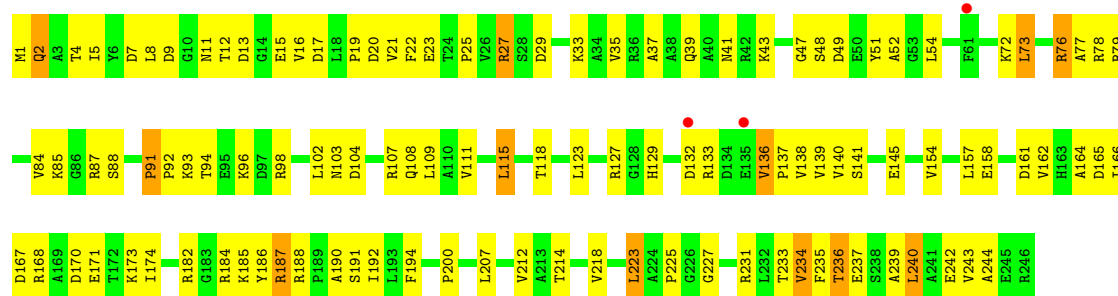


• Molecule 5: 50S ribosomal protein L3P

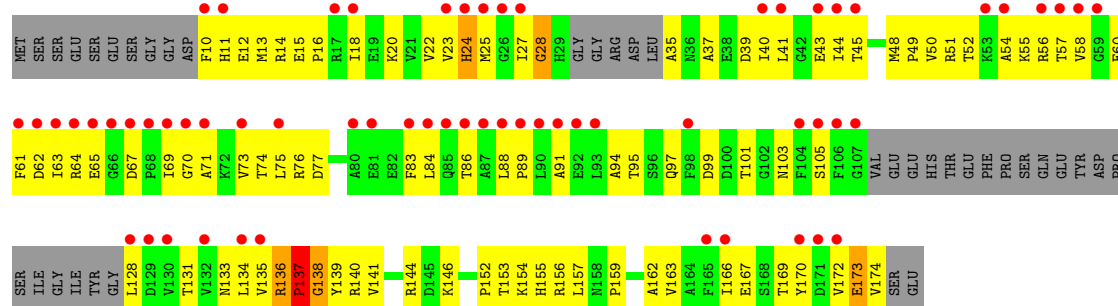




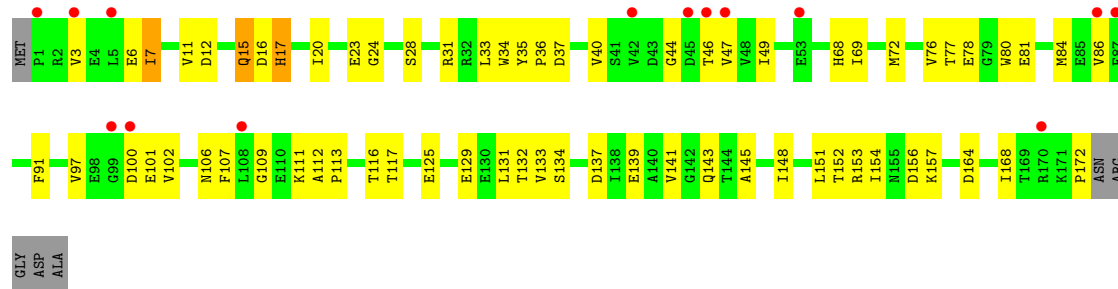
• Molecule 6: 50S ribosomal protein L4E



• Molecule 7: 50S ribosomal protein L5P

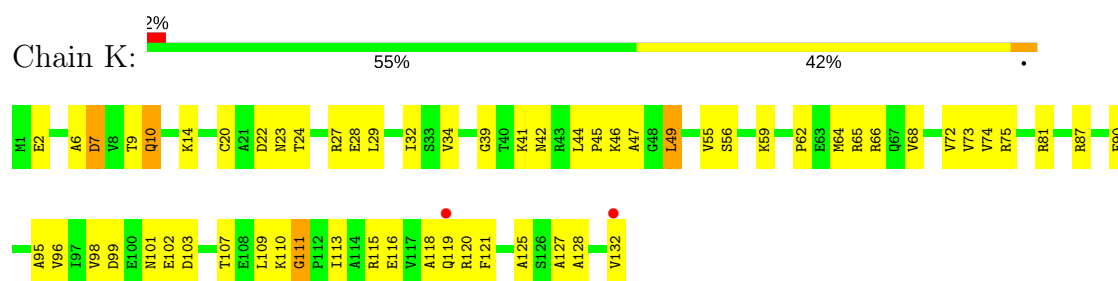


• Molecule 8: 50S ribosomal protein L6P

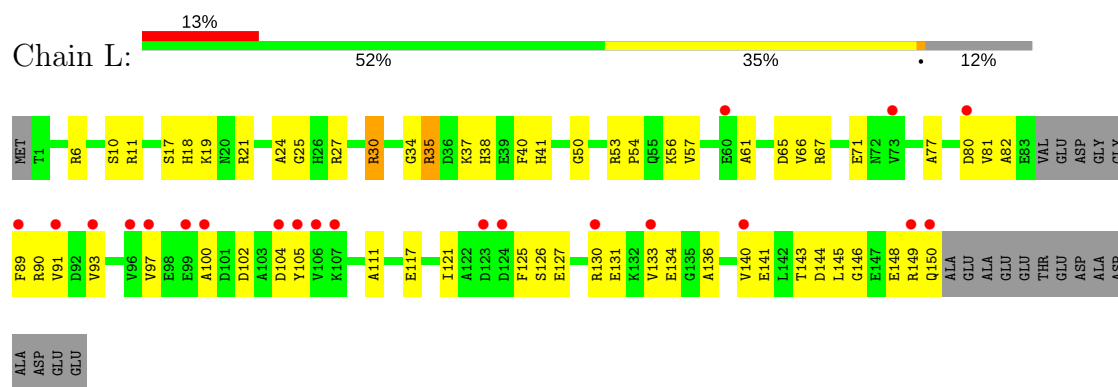


• Molecule 9: 50S ribosomal protein L7AE

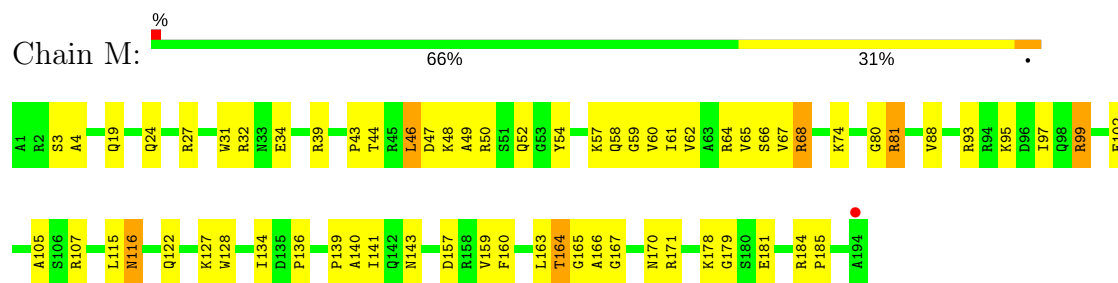




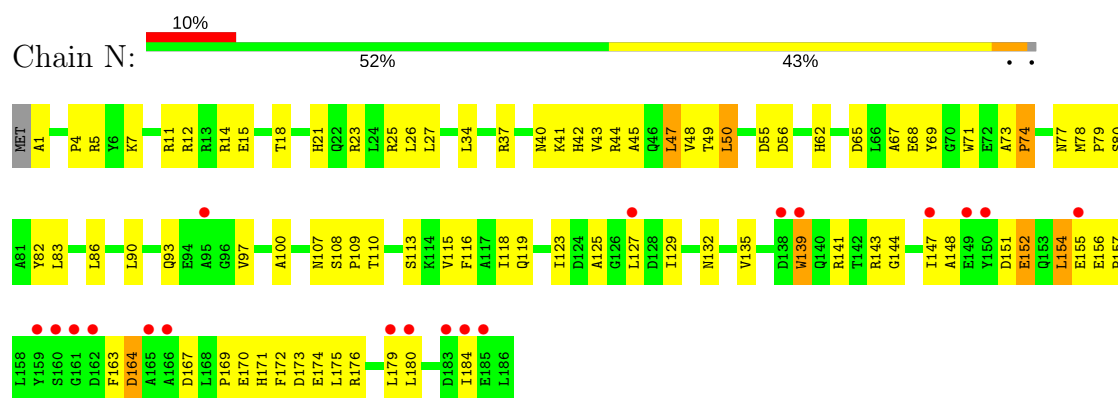
• Molecule 14: 50S ribosomal protein L15P



• Molecule 15: 50S Ribosomal Protein L15E



• Molecule 16: 50S ribosomal protein L18P



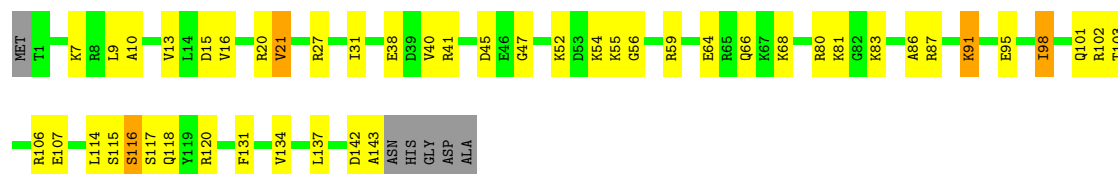
• Molecule 17: 50S ribosomal protein L18e





- Molecule 18: 50S ribosomal protein L19E

Chain P: 64% 29%



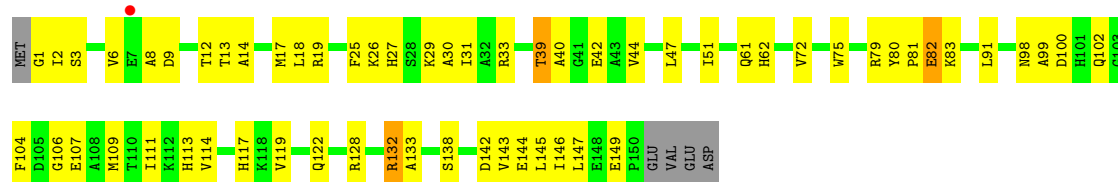
- Molecule 19: 50S ribosomal protein L21e

Chain Q: 72% 25%



- Molecule 20: 50S ribosomal protein L22P

Chain R: 58% 37%



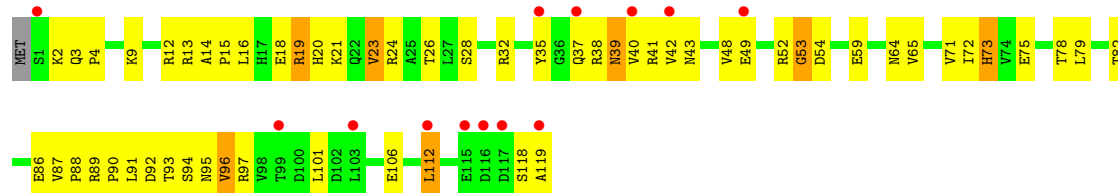
- Molecule 21: 50S ribosomal protein L23P

Chain S: 65% 31% 5%

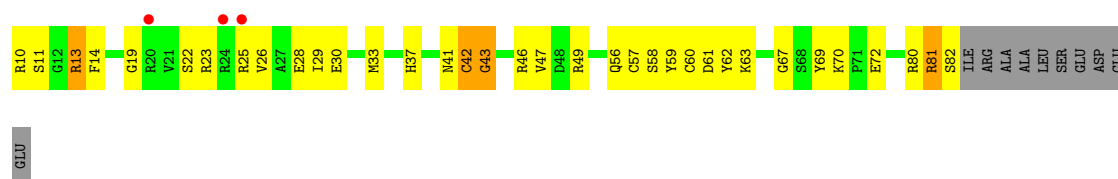


- Molecule 22: 50S ribosomal protein L24P

Chain T: 51% 43% 6%



- Molecule 23: 50S ribosomal protein L24E



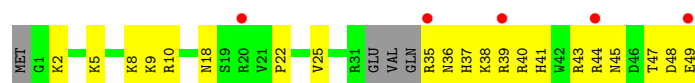
- Molecule 29: 50S ribosomal protein L37e

Chain 1: 65% 33%



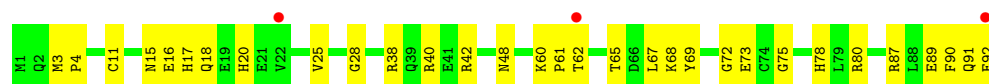
- Molecule 30: 50S ribosomal protein L39e

Chain 2: 10% 50% 42% 8%



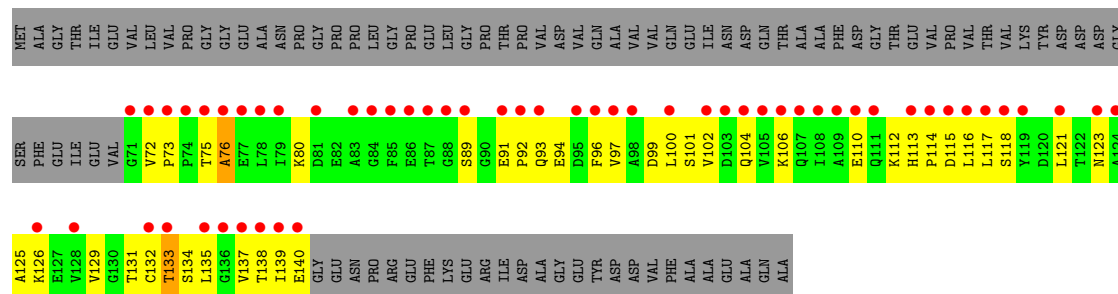
- Molecule 31: 50S ribosomal protein L44E

Chain 3: 3% 66% 34%



- Molecule 32: 50S RIBOSOMAL PROTEIN L11P

Chain I: 34% 19% 23% 57%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	213.00Å 301.03Å 575.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 49.83 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.70) 94.8 (49.83-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.190 , 0.230 0.183 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	53.6	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	98999	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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, PO2, CD, 5AA, OMU, UR3, 2OP, 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	0.38	0/65959	0.69	20/102870 (0.0%)
2	9	0.35	0/2905	0.71	2/4528 (0.0%)
3	4	0.46	0/102	0.73	0/149
4	A	0.31	0/1786	0.65	0/2408
5	B	0.34	0/2690	0.65	0/3652
6	C	0.37	0/1884	0.65	1/2551 (0.0%)
7	D	0.30	0/1111	0.53	0/1498
8	E	0.33	0/1382	0.58	0/1880
9	F	0.30	0/901	0.54	0/1224
10	G	0.30	0/241	0.49	0/324
11	H	0.35	0/1287	0.67	0/1725
12	J	0.37	0/1136	0.63	0/1530
13	K	0.36	0/1001	0.69	0/1347
14	L	0.33	0/1130	0.64	0/1509
15	M	0.33	0/1584	0.61	0/2119
16	N	0.30	0/1474	0.63	0/1999
17	O	0.31	0/874	0.56	0/1181
18	P	0.33	0/1147	0.54	0/1528
19	Q	0.36	0/749	0.72	0/1005
20	R	0.36	0/1172	0.65	0/1578
21	S	0.32	0/648	0.57	0/875
22	T	0.32	0/958	0.61	0/1289
23	U	0.34	0/417	0.58	0/562
24	V	0.27	0/502	0.54	0/675
25	W	0.36	0/1219	0.63	0/1655
26	X	0.36	0/664	0.58	0/895
27	Y	0.37	0/1146	0.64	0/1536
28	Z	0.36	0/589	0.67	0/787
29	1	0.36	0/438	0.62	0/578
30	2	0.33	0/401	0.52	0/529
31	3	0.38	0/771	0.58	0/1024
32	I	0.30	0/526	0.54	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.37	0/98794	0.67	23/147726 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	47
2	9	0	2
3	4	0	1
25	W	0	1
All	All	0	51

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	8.54	128.28	109.50
1	0	1942	A	C5'-C4'-C3'	8.16	129.06	116.00
1	0	1979	G	C2'-C3'-O3'	6.72	124.45	113.70
1	0	871	G	C5'-C4'-O4'	-6.61	101.17	109.10
2	9	3039	U	N1-C1'-C2'	6.29	122.18	114.00

There are no chirality outliers.

5 of 51 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	191	A	Sidechain
1	0	221	G	Sidechain
1	0	24	G	Sidechain
1	0	417	G	Sidechain
1	0	471	G	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29812	849	0
2	9	2600	0	1326	65	0
3	4	127	0	75	4	0
4	A	1753	0	1766	119	0
5	B	2625	0	2533	159	0
6	C	1859	0	1816	127	0
7	D	1094	0	1085	91	0
8	E	1357	0	1266	64	0
9	F	890	0	843	56	0
10	G	240	0	231	13	0
11	H	1266	0	1268	70	0
12	J	1120	0	1098	55	0
13	K	992	0	1031	65	0
14	L	1118	0	1076	55	0
15	M	1560	0	1568	70	0
16	N	1445	0	1401	107	0
17	O	865	0	873	39	0
18	P	1136	0	1123	44	0
19	Q	735	0	729	23	0
20	R	1149	0	1122	62	0
21	S	641	0	605	21	0
22	T	950	0	923	61	0
23	U	410	0	364	24	0
24	V	499	0	511	33	0
25	W	1196	0	1137	95	0
26	X	654	0	653	50	0
27	Y	1130	0	1133	55	0
28	Z	578	0	539	27	0
29	1	431	0	426	30	0
30	2	396	0	413	27	0
31	3	755	0	728	31	0
32	I	519	0	500	54	0
33	0	108	0	0	0	0
33	3	1	0	0	0	0
33	9	2	0	0	0	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	3	0	0	0	0
35	0	72	0	0	0	0
35	9	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	1	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	1	0
36	K	1	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	1	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5764	0	0	97	0
38	1	61	0	0	3	0
38	2	42	0	0	3	0
38	3	71	0	0	5	0
38	4	3	0	0	0	0
38	9	133	0	0	4	0
38	A	116	0	0	18	0
38	B	143	0	0	23	0
38	C	173	0	0	21	0
38	D	44	0	0	8	0
38	E	43	0	0	5	0
38	F	24	0	0	4	0
38	G	17	0	0	0	0
38	H	66	0	0	9	0
38	I	9	0	0	2	0
38	J	52	0	0	3	0
38	K	57	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	L	81	0	0	11	0
38	M	115	0	0	4	0
38	N	61	0	0	10	0
38	O	45	0	0	6	0
38	P	63	0	0	3	0
38	Q	52	0	0	1	0
38	R	89	0	0	5	0
38	S	31	0	0	2	0
38	T	36	0	0	2	0
38	U	26	0	0	0	0
38	V	13	0	0	1	0
38	W	70	0	0	5	0
38	X	31	0	0	5	0
38	Y	93	0	0	7	0
38	Z	31	0	0	1	0
All	All	98999	0	59974	2378	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 16.

The worst 5 of 2378 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)
2:9:3006:C:H5''	16:N:37:ARG:NH1	1.64	1.13
6:C:236:THR:HG22	6:C:239:ALA:H	1.11	1.13
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.32	1.11
2:9:3006:C:H5''	16:N:37:ARG:HH12	1.08	1.07
1:0:1160:G:H5'	1:0:1161:A:H5'	1.34	1.04

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	
4	A	235/240 (98%)	205 (87%)	28 (12%)	2 (1%)	19	44
5	B	335/338 (99%)	303 (90%)	27 (8%)	5 (2%)	11	29
6	C	244/246 (99%)	223 (91%)	20 (8%)	1 (0%)	36	64
7	D	134/177 (76%)	94 (70%)	34 (25%)	6 (4%)	3	5
8	E	170/178 (96%)	161 (95%)	7 (4%)	2 (1%)	14	35
9	F	117/120 (98%)	101 (86%)	13 (11%)	3 (3%)	6	15
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	H	156/171 (91%)	144 (92%)	7 (4%)	5 (3%)	4	10
12	J	140/145 (97%)	128 (91%)	10 (7%)	2 (1%)	12	31
13	K	130/132 (98%)	116 (89%)	12 (9%)	2 (2%)	11	29
14	L	141/165 (86%)	118 (84%)	23 (16%)	0	100	100
15	M	192/194 (99%)	178 (93%)	13 (7%)	1 (0%)	31	58
16	N	184/187 (98%)	167 (91%)	12 (6%)	5 (3%)	5	14
17	O	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
18	P	141/149 (95%)	131 (93%)	9 (6%)	1 (1%)	24	50
19	Q	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	R	148/155 (96%)	133 (90%)	14 (10%)	1 (1%)	24	50
21	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
22	T	117/120 (98%)	108 (92%)	8 (7%)	1 (1%)	19	44
23	U	51/66 (77%)	47 (92%)	3 (6%)	1 (2%)	8	21
24	V	63/71 (89%)	55 (87%)	7 (11%)	1 (2%)	11	27
25	W	152/154 (99%)	144 (95%)	6 (4%)	2 (1%)	13	33
26	X	80/92 (87%)	72 (90%)	7 (9%)	1 (1%)	13	33
27	Y	140/241 (58%)	134 (96%)	6 (4%)	0	100	100
28	Z	71/83 (86%)	57 (80%)	9 (13%)	5 (7%)	1	2
29	1	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
30	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
31	3	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
32	I	68/162 (42%)	55 (81%)	11 (16%)	2 (3%)	5	12
All	All	3705/4430 (84%)	3348 (90%)	308 (8%)	49 (1%)	13	33

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	D	27	ILE
7	D	137	PRO
7	D	173	GLU
9	F	101	ALA
11	H	140	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	179/182 (98%)	167 (93%)	12 (7%)	18	40
5	B	282/283 (100%)	263 (93%)	19 (7%)	18	40
6	C	193/193 (100%)	180 (93%)	13 (7%)	18	40
7	D	117/148 (79%)	112 (96%)	5 (4%)	32	61
8	E	152/156 (97%)	148 (97%)	4 (3%)	49	79
9	F	93/94 (99%)	92 (99%)	1 (1%)	76	91
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	126 (96%)	6 (4%)	30	60
12	J	118/121 (98%)	109 (92%)	9 (8%)	14	33
13	K	106/106 (100%)	103 (97%)	3 (3%)	47	77
14	L	113/127 (89%)	108 (96%)	5 (4%)	31	60
15	M	158/158 (100%)	151 (96%)	7 (4%)	31	60
16	N	149/150 (99%)	145 (97%)	4 (3%)	48	78
17	O	93/94 (99%)	92 (99%)	1 (1%)	76	91
18	P	113/117 (97%)	109 (96%)	4 (4%)	39	69
19	Q	79/80 (99%)	76 (96%)	3 (4%)	36	66
20	R	117/122 (96%)	114 (97%)	3 (3%)	49	79
21	S	71/74 (96%)	69 (97%)	2 (3%)	47	77
22	T	105/106 (99%)	98 (93%)	7 (7%)	18	40
23	U	44/52 (85%)	44 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	V	51/57 (90%)	51 (100%)	0	100	100
25	W	130/130 (100%)	123 (95%)	7 (5%)	24	51
26	X	66/74 (89%)	62 (94%)	4 (6%)	20	45
27	Y	120/196 (61%)	116 (97%)	4 (3%)	41	71
28	Z	60/68 (88%)	59 (98%)	1 (2%)	63	87
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	52	81
31	3	79/79 (100%)	79 (100%)	0	100	100
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3611 (86%)	2968 (96%)	125 (4%)	34	64

5 of 125 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	H	88	ARG
13	K	7	ASP
26	X	15	ARG
11	H	132	GLN
12	J	74	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	58	GLN
19	Q	40	HIS
30	2	16	ASN
15	M	143	ASN
16	N	107	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	237 (8%)	34 (1%)
2	9	121/122 (99%)	17 (14%)	1 (0%)
3	4	1/8 (12%)	0	0
All	All	2867/3052 (93%)	254 (8%)	35 (1%)

5 of 254 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 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1246	A
1	0	1506	U
1	0	2718	C
1	0	1352	A
1	0	1377	C

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	OMU	0	2587	1	14,22,23	0.95	1 (7%)	18,31,34	3.73	2 (11%)
1	OMG	0	2588	1,3	19,26,27	1.08	2 (10%)	22,38,41	2.44	4 (18%)
1	UR3	0	2619	1	13,22,23	0.95	0	15,32,35	0.70	0
1	PSU	0	2621	1	16,21,22	1.60	3 (18%)	20,30,33	5.40	4 (20%)
1	1MA	0	628	1	16,25,26	1.03	1 (6%)	12,37,40	1.24	1 (8%)
3	5AA	4	76	1,3	17,26,27	0.62	0	16,38,41	1.10	2 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3
3	5AA	4	76	1,3	-	0/7/29/30	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.52	1.48	1.52
1	0	2588	OMG	C8-N7	-2.11	1.30	1.34
1	0	2587	OMU	C4-N3	2.44	1.37	1.33
1	0	2621	PSU	C2-N1	2.76	1.43	1.38
1	0	2621	PSU	C4-N3	2.88	1.38	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-16.99	114.75	128.41
1	0	2621	PSU	C5-C4-N3	-8.35	114.60	125.36
1	0	2588	OMG	C5-C6-N1	-8.20	111.81	123.47
1	0	628	1MA	C2-N3-C4	-3.74	110.80	116.51
1	0	2587	OMU	C5-C4-N3	-3.65	114.70	123.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
1	0	2619	UR3	1	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 233 ligands modelled in this entry, 233 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	176:DA	O3'	175:C	P	8.53

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%)	-0.58	31 (1%) 80 81	29, 51, 94, 161	0
2	9	122/122 (100%)	-0.55	4 (3%) 46 46	39, 62, 91, 152	0
3	4	5/8 (62%)	-0.53	0 100 100	41, 43, 47, 47	0
4	A	237/240 (98%)	0.15	10 (4%) 36 34	33, 57, 95, 119	0
5	B	337/338 (99%)	0.01	5 (1%) 73 75	29, 57, 80, 94	0
6	C	246/246 (100%)	-0.10	3 (1%) 79 80	27, 53, 75, 84	0
7	D	140/177 (79%)	2.15	62 (44%) 0 0	58, 101, 127, 137	0
8	E	172/178 (96%)	0.62	14 (8%) 12 9	47, 67, 87, 93	0
9	F	119/120 (99%)	0.92	22 (18%) 1 1	60, 82, 104, 119	0
10	G	29/348 (8%)	1.77	9 (31%) 0 0	65, 90, 102, 105	0
11	H	160/171 (93%)	0.26	7 (4%) 34 32	41, 59, 90, 99	0
12	J	142/145 (97%)	-0.04	1 (0%) 87 88	37, 52, 72, 90	0
13	K	132/132 (100%)	0.01	2 (1%) 73 75	34, 56, 77, 87	0
14	L	145/165 (87%)	0.63	21 (14%) 2 1	30, 72, 118, 132	0
15	M	194/194 (100%)	-0.11	1 (0%) 90 92	34, 50, 67, 74	0
16	N	186/187 (99%)	0.58	19 (10%) 7 5	38, 66, 115, 121	0
17	O	115/116 (99%)	0.10	0 100 100	45, 61, 77, 85	0
18	P	143/149 (95%)	0.26	0 100 100	45, 60, 77, 85	0
19	Q	95/96 (98%)	-0.07	1 (1%) 80 81	40, 48, 60, 75	0
20	R	150/155 (96%)	-0.18	1 (0%) 87 88	37, 48, 68, 75	0
21	S	81/85 (95%)	0.25	2 (2%) 57 58	49, 67, 85, 94	0
22	T	119/120 (99%)	0.70	13 (10%) 5 4	46, 63, 91, 110	0
23	U	53/66 (80%)	0.21	3 (5%) 24 22	43, 57, 74, 85	0
24	V	65/71 (91%)	1.73	21 (32%) 0 0	63, 86, 117, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	-0.07	2 (1%) 77 78	39, 50, 67, 76	0
26	X	82/92 (89%)	0.44	7 (8%) 11 8	45, 59, 77, 95	0
27	Y	142/241 (58%)	-0.00	3 (2%) 63 64	30, 49, 71, 86	0
28	Z	73/83 (87%)	0.17	3 (4%) 37 35	44, 63, 77, 97	0
29	1	56/57 (98%)	-0.43	0 100 100	33, 40, 46, 54	0
30	2	46/50 (92%)	0.52	5 (10%) 5 4	41, 65, 97, 109	0
31	3	92/92 (100%)	0.29	3 (3%) 46 46	37, 59, 73, 84	0
32	I	70/162 (43%)	3.59	55 (78%) 0 0	99, 121, 143, 145	0
All	All	6651/7482 (88%)	-0.05	330 (4%) 29 27	27, 56, 102, 161	0

The worst 5 of 330 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	V	1	THR	11.9
32	I	133	THR	10.3
32	I	71	GLY	9.6
7	D	63	ILE	9.4
32	I	93	GLN	8.5

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	32,36,39,40	0
3	5AA	4	76	24/25	0.98	0.14	38,44,48,48	0
1	1MA	0	628	23/24	0.99	0.15	29,32,34,36	0
1	UR3	0	2619	21/22	0.99	0.16	32,39,41,42	0
1	PSU	0	2621	20/21	0.99	0.13	30,33,37,38	0
1	OMU	0	2587	21/22	0.99	0.13	35,37,39,42	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
37	CD	O	9205	1/1	0.04	0.30	200,200,200,200	0
35	NA	R	9186	1/1	0.30	0.75	84,84,84,84	0
35	NA	9	9151	1/1	0.65	0.35	87,87,87,87	0
35	NA	0	9129	1/1	0.68	0.17	65,65,65,65	0
33	MG	0	8092	1/1	0.72	0.70	115,115,115,115	0
35	NA	0	9171	1/1	0.73	0.40	64,64,64,64	0
35	NA	0	9182	1/1	0.74	0.45	84,84,84,84	0
33	MG	0	8090	1/1	0.76	0.60	69,69,69,69	0
35	NA	0	9177	1/1	0.80	0.41	73,73,73,73	0
33	MG	0	8085	1/1	0.80	0.24	74,74,74,74	0
33	MG	K	8069	1/1	0.84	0.14	49,49,49,49	0
36	CL	0	9322	1/1	0.84	0.53	92,92,92,92	0
33	MG	0	8093	1/1	0.84	0.11	52,52,52,52	0
35	NA	0	9168	1/1	0.84	0.15	56,56,56,56	0
33	MG	0	8024	1/1	0.84	0.64	83,83,83,83	0
35	NA	0	9126	1/1	0.84	0.19	44,44,44,44	0
33	MG	9	8095	1/1	0.85	0.14	75,75,75,75	0
35	NA	R	9137	1/1	0.85	0.12	50,50,50,50	0
36	CL	0	9305	1/1	0.85	0.18	71,71,71,71	0
35	NA	0	9166	1/1	0.85	0.11	68,68,68,68	0
35	NA	0	9170	1/1	0.85	0.47	97,97,97,97	0
35	NA	S	9112	1/1	0.86	0.52	75,75,75,75	0
35	NA	0	9152	1/1	0.86	0.41	65,65,65,65	0
35	NA	0	9124	1/1	0.86	0.17	67,67,67,67	0
35	NA	0	9174	1/1	0.87	0.90	64,64,64,64	0
33	MG	0	8049	1/1	0.87	0.29	80,80,80,80	0
33	MG	0	8082	1/1	0.87	0.20	65,65,65,65	0
35	NA	0	9150	1/1	0.88	0.30	48,48,48,48	0
35	NA	C	9104	1/1	0.89	0.15	41,41,41,41	0
35	NA	9	9183	1/1	0.89	0.14	49,49,49,49	0
36	CL	A	9309	1/1	0.89	0.19	77,77,77,77	0
35	NA	0	9149	1/1	0.90	0.14	42,42,42,42	0
33	MG	0	8054	1/1	0.90	0.15	39,39,39,39	0
35	NA	0	9158	1/1	0.90	0.58	84,84,84,84	0
35	NA	0	9185	1/1	0.90	0.65	54,54,54,54	0
35	NA	0	9161	1/1	0.90	0.30	56,56,56,56	0
35	NA	0	9173	1/1	0.90	0.24	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	T	8073	1/1	0.90	0.09	66,66,66,66	0
34	K	0	9003	1/1	0.90	0.13	66,66,66,66	0
33	MG	0	8041	1/1	0.90	0.22	72,72,72,72	0
33	MG	0	8106	1/1	0.91	0.08	63,63,63,63	0
35	NA	0	9142	1/1	0.91	0.16	53,53,53,53	0
35	NA	R	9138	1/1	0.91	0.06	61,61,61,61	0
33	MG	0	8043	1/1	0.91	0.08	53,53,53,53	0
35	NA	0	9163	1/1	0.91	0.41	63,63,63,63	0
35	NA	0	9107	1/1	0.91	0.20	50,50,50,50	0
33	MG	0	8101	1/1	0.92	0.11	74,74,74,74	0
33	MG	0	8089	1/1	0.92	0.09	60,60,60,60	0
33	MG	0	8047	1/1	0.92	0.17	78,78,78,78	0
35	NA	0	9164	1/1	0.92	0.24	55,55,55,55	0
35	NA	0	9111	1/1	0.92	0.11	59,59,59,59	0
35	NA	0	9133	1/1	0.92	0.11	32,32,32,32	0
35	NA	0	9101	1/1	0.92	0.22	47,47,47,47	0
35	NA	0	9117	1/1	0.92	0.11	46,46,46,46	0
33	MG	0	8050	1/1	0.92	0.08	61,61,61,61	0
35	NA	0	9110	1/1	0.92	0.16	38,38,38,38	0
35	NA	0	9155	1/1	0.92	0.52	78,78,78,78	0
33	MG	A	8066	1/1	0.92	0.05	66,66,66,66	0
35	NA	0	9165	1/1	0.93	0.21	42,42,42,42	0
36	CL	0	9315	1/1	0.93	0.40	84,84,84,84	0
35	NA	0	9167	1/1	0.93	0.08	47,47,47,47	0
35	NA	0	9169	1/1	0.93	0.38	79,79,79,79	0
35	NA	0	9172	1/1	0.93	0.37	61,61,61,61	0
33	MG	0	8039	1/1	0.93	0.06	51,51,51,51	0
35	NA	L	9180	1/1	0.93	0.52	72,72,72,72	0
35	NA	0	9125	1/1	0.93	0.25	69,69,69,69	0
35	NA	0	9135	1/1	0.93	0.28	50,50,50,50	0
33	MG	0	8076	1/1	0.93	0.07	70,70,70,70	0
33	MG	3	8078	1/1	0.93	0.05	55,55,55,55	0
36	CL	3	9304	1/1	0.93	0.15	70,70,70,70	0
33	MG	0	8088	1/1	0.93	0.06	36,36,36,36	0
35	NA	Q	9148	1/1	0.93	0.29	43,43,43,43	0
33	MG	0	8098	1/1	0.93	0.24	40,40,40,40	0
36	CL	N	9307	1/1	0.94	0.19	66,66,66,66	0
33	MG	0	8044	1/1	0.94	0.12	49,49,49,49	0
36	CL	J	9302	1/1	0.94	0.06	61,61,61,61	0
35	NA	0	9184	1/1	0.94	0.54	96,96,96,96	0
33	MG	0	8084	1/1	0.94	0.10	51,51,51,51	0
33	MG	0	8042	1/1	0.94	0.08	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	9132	1/1	0.94	0.09	35,35,35,35	0
36	CL	0	9303	1/1	0.94	0.14	64,64,64,64	0
33	MG	0	8114	1/1	0.94	0.18	56,56,56,56	0
35	NA	0	9159	1/1	0.94	0.23	56,56,56,56	0
33	MG	0	8071	1/1	0.94	0.13	72,72,72,72	0
33	MG	0	8083	1/1	0.94	0.08	42,42,42,42	0
35	NA	0	9113	1/1	0.94	0.16	66,66,66,66	0
35	NA	0	9140	1/1	0.94	0.20	45,45,45,45	0
33	MG	0	8099	1/1	0.95	0.10	63,63,63,63	0
35	NA	0	9127	1/1	0.95	0.10	35,35,35,35	0
35	NA	0	9162	1/1	0.95	0.23	72,72,72,72	0
33	MG	0	8097	1/1	0.95	0.14	40,40,40,40	0
33	MG	0	8094	1/1	0.95	0.12	86,86,86,86	0
33	MG	0	8111	1/1	0.95	0.14	77,77,77,77	0
33	MG	0	8087	1/1	0.95	0.14	54,54,54,54	0
37	CD	3	9204	1/1	0.95	0.09	66,66,66,66	0
33	MG	0	8057	1/1	0.95	0.14	45,45,45,45	0
33	MG	0	8080	1/1	0.95	0.15	46,46,46,46	0
35	NA	0	9116	1/1	0.95	0.11	36,36,36,36	0
33	MG	0	8027	1/1	0.95	0.13	55,55,55,55	0
33	MG	0	8112	1/1	0.95	0.11	47,47,47,47	0
35	NA	H	9109	1/1	0.95	0.13	36,36,36,36	0
35	NA	0	9160	1/1	0.95	0.33	49,49,49,49	0
35	NA	0	9181	1/1	0.95	0.12	48,48,48,48	0
33	MG	0	8063	1/1	0.95	0.15	84,84,84,84	0
35	NA	0	9156	1/1	0.95	0.44	51,51,51,51	0
35	NA	0	9106	1/1	0.95	0.81	51,51,51,51	0
35	NA	0	9157	1/1	0.95	0.10	69,69,69,69	0
35	NA	0	9179	1/1	0.95	0.19	57,57,57,57	0
33	MG	0	8014	1/1	0.95	0.11	41,41,41,41	0
33	MG	0	8059	1/1	0.96	0.07	44,44,44,44	0
35	NA	0	9114	1/1	0.96	0.13	51,51,51,51	0
34	K	0	9001	1/1	0.96	0.24	74,74,74,74	0
36	CL	0	9316	1/1	0.96	0.16	61,61,61,61	0
33	MG	0	8051	1/1	0.96	0.07	61,61,61,61	0
36	CL	R	9306	1/1	0.96	0.12	48,48,48,48	0
35	NA	0	9105	1/1	0.96	0.08	39,39,39,39	0
35	NA	0	9123	1/1	0.96	0.17	43,43,43,43	0
35	NA	0	9121	1/1	0.96	0.33	58,58,58,58	0
35	NA	0	9115	1/1	0.96	0.15	39,39,39,39	0
33	MG	0	8113	1/1	0.96	0.12	45,45,45,45	0
35	NA	A	9145	1/1	0.96	0.16	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8115	1/1	0.96	0.12	49,49,49,49	0
33	MG	0	8081	1/1	0.96	0.18	54,54,54,54	0
36	CL	0	9320	1/1	0.96	0.11	48,48,48,48	0
33	MG	0	8068	1/1	0.96	0.08	59,59,59,59	0
33	MG	0	8075	1/1	0.96	0.06	43,43,43,43	0
35	NA	0	9102	1/1	0.96	0.16	44,44,44,44	0
33	MG	0	8096	1/1	0.96	0.07	51,51,51,51	0
33	MG	0	8104	1/1	0.96	0.22	73,73,73,73	0
33	MG	0	8064	1/1	0.96	0.12	33,33,33,33	0
35	NA	0	9141	1/1	0.96	0.07	47,47,47,47	0
33	MG	0	8046	1/1	0.96	0.10	54,54,54,54	0
33	MG	0	8062	1/1	0.96	0.10	57,57,57,57	0
35	NA	H	9122	1/1	0.96	0.13	59,59,59,59	0
33	MG	0	8048	1/1	0.97	0.16	62,62,62,62	0
33	MG	0	8102	1/1	0.97	0.13	67,67,67,67	0
35	NA	0	9154	1/1	0.97	0.19	38,38,38,38	0
36	CL	J	9321	1/1	0.97	0.13	54,54,54,54	0
35	NA	0	9175	1/1	0.97	0.43	56,56,56,56	0
35	NA	0	9108	1/1	0.97	0.09	61,61,61,61	0
36	CL	0	9317	1/1	0.97	0.08	64,64,64,64	0
35	NA	0	9178	1/1	0.97	0.21	57,57,57,57	0
35	NA	0	9128	1/1	0.97	0.07	35,35,35,35	0
36	CL	K	9312	1/1	0.97	0.10	55,55,55,55	0
33	MG	0	8086	1/1	0.97	0.06	47,47,47,47	0
35	NA	0	9176	1/1	0.97	0.18	42,42,42,42	0
33	MG	0	8108	1/1	0.97	0.10	75,75,75,75	0
33	MG	0	8116	1/1	0.97	0.06	47,47,47,47	0
35	NA	0	9103	1/1	0.97	0.15	39,39,39,39	0
33	MG	0	8040	1/1	0.97	0.18	52,52,52,52	0
33	MG	0	8056	1/1	0.97	0.12	51,51,51,51	0
33	MG	0	8045	1/1	0.97	0.11	62,62,62,62	0
35	NA	0	9144	1/1	0.97	0.10	27,27,27,27	0
36	CL	0	9314	1/1	0.97	0.07	53,53,53,53	0
33	MG	0	8103	1/1	0.97	0.11	81,81,81,81	0
33	MG	0	8012	1/1	0.97	0.16	32,32,32,32	0
36	CL	O	9308	1/1	0.97	0.21	81,81,81,81	0
33	MG	0	8028	1/1	0.97	0.11	44,44,44,44	0
35	NA	0	9131	1/1	0.97	0.08	36,36,36,36	0
33	MG	0	8074	1/1	0.98	0.09	40,40,40,40	0
33	MG	0	8017	1/1	0.98	0.10	33,33,33,33	0
33	MG	0	8022	1/1	0.98	0.07	35,35,35,35	0
33	MG	0	8053	1/1	0.98	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8013	1/1	0.98	0.19	41,41,41,41	0
33	MG	0	8032	1/1	0.98	0.05	35,35,35,35	0
33	MG	0	8011	1/1	0.98	0.15	23,23,23,23	0
36	CL	J	9301	1/1	0.98	0.19	73,73,73,73	0
35	NA	0	9130	1/1	0.98	0.08	44,44,44,44	0
35	NA	0	9136	1/1	0.98	0.07	56,56,56,56	0
35	NA	0	9143	1/1	0.98	0.07	36,36,36,36	0
35	NA	0	9153	1/1	0.98	0.10	25,25,25,25	0
33	MG	0	8035	1/1	0.98	0.07	51,51,51,51	0
36	CL	L	9310	1/1	0.98	0.15	61,61,61,61	0
35	NA	M	9147	1/1	0.98	0.21	33,33,33,33	0
33	MG	0	8034	1/1	0.98	0.10	32,32,32,32	0
36	CL	0	9313	1/1	0.98	0.13	61,61,61,61	0
33	MG	0	8072	1/1	0.98	0.24	55,55,55,55	0
35	NA	J	9146	1/1	0.98	0.10	35,35,35,35	0
33	MG	0	8107	1/1	0.98	0.09	38,38,38,38	0
33	MG	0	8004	1/1	0.98	0.05	27,27,27,27	0
33	MG	B	8055	1/1	0.98	0.14	52,52,52,52	0
33	MG	0	8016	1/1	0.98	0.21	44,44,44,44	0
33	MG	0	8061	1/1	0.98	0.08	45,45,45,45	0
34	K	0	9002	1/1	0.98	0.08	54,54,54,54	0
33	MG	0	8070	1/1	0.98	0.04	45,45,45,45	0
35	NA	0	9119	1/1	0.98	0.08	36,36,36,36	0
33	MG	0	8037	1/1	0.98	0.07	44,44,44,44	0
33	MG	0	8058	1/1	0.98	0.12	57,57,57,57	0
36	CL	M	9318	1/1	0.98	0.15	50,50,50,50	0
35	NA	0	9134	1/1	0.98	0.10	37,37,37,37	0
33	MG	9	8052	1/1	0.98	0.05	47,47,47,47	0
33	MG	0	8023	1/1	0.98	0.18	48,48,48,48	0
33	MG	A	8065	1/1	0.98	0.21	52,52,52,52	0
33	MG	0	8117	1/1	0.98	0.10	40,40,40,40	0
35	NA	0	9118	1/1	0.98	0.21	47,47,47,47	0
33	MG	0	8067	1/1	0.98	0.08	46,46,46,46	0
35	NA	0	9139	1/1	0.99	0.13	22,22,22,22	0
33	MG	0	8018	1/1	0.99	0.15	47,47,47,47	0
33	MG	0	8077	1/1	0.99	0.13	35,35,35,35	0
33	MG	0	8001	1/1	0.99	0.10	38,38,38,38	0
33	MG	0	8118	1/1	0.99	0.09	40,40,40,40	0
33	MG	0	8038	1/1	0.99	0.16	26,26,26,26	0
33	MG	0	8110	1/1	0.99	0.07	40,40,40,40	0
33	MG	Y	8109	1/1	0.99	0.09	39,39,39,39	0
33	MG	0	8003	1/1	0.99	0.14	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	CL	0	9311	1/1	0.99	0.10	52,52,52,52	0
35	NA	0	9120	1/1	0.99	0.10	43,43,43,43	0
37	CD	U	9201	1/1	0.99	0.09	69,69,69,69	0
33	MG	0	8009	1/1	0.99	0.10	35,35,35,35	0
33	MG	0	8020	1/1	0.99	0.11	24,24,24,24	0
33	MG	0	8026	1/1	0.99	0.13	31,31,31,31	0
33	MG	0	8091	1/1	0.99	0.07	57,57,57,57	0
33	MG	0	8060	1/1	0.99	0.31	49,49,49,49	0
33	MG	0	8100	1/1	0.99	0.18	82,82,82,82	0
33	MG	0	8079	1/1	0.99	0.12	38,38,38,38	0
33	MG	0	8007	1/1	0.99	0.07	24,24,24,24	0
33	MG	0	8002	1/1	0.99	0.06	39,39,39,39	0
33	MG	0	8010	1/1	0.99	0.11	29,29,29,29	0
33	MG	0	8021	1/1	0.99	0.17	30,30,30,30	0
33	MG	0	8006	1/1	0.99	0.05	33,33,33,33	0
33	MG	0	8025	1/1	0.99	0.11	35,35,35,35	0
33	MG	0	8019	1/1	0.99	0.09	38,38,38,38	0
33	MG	0	8036	1/1	0.99	0.13	35,35,35,35	0
36	CL	B	9319	1/1	0.99	0.14	60,60,60,60	0
33	MG	0	8015	1/1	0.99	0.12	31,31,31,31	0
33	MG	0	8029	1/1	0.99	0.17	36,36,36,36	0
37	CD	Z	9203	1/1	0.99	0.09	68,68,68,68	0
33	MG	0	8033	1/1	0.99	0.13	32,32,32,32	0
33	MG	0	8008	1/1	0.99	0.08	37,37,37,37	0
33	MG	0	8030	1/1	1.00	0.15	26,26,26,26	0
33	MG	0	8031	1/1	1.00	0.08	37,37,37,37	0
37	CD	1	9202	1/1	1.00	0.05	68,68,68,68	0
33	MG	0	8005	1/1	1.00	0.14	37,37,37,37	0

6.5 Other polymers

There are no such residues in this entry.