



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 02:56 am BST

PDB ID : 1VQN  
Title : The structure of CC-HPMN AND CCA-PHE-CAP-BIO bound to the large ribosomal subunit of haloarcula marismortui  
Authors : Schmeing, T.M.; Steitz, T.A.  
Deposited on : 2004-12-16  
Resolution : 2.40 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

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

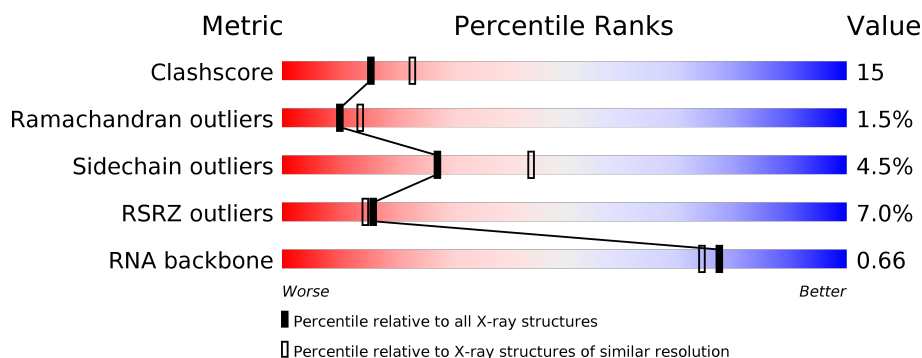
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
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  $\geq 3$ , 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>62%</div> <div>27%</div> <div>5%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>5%</div> <div> <div></div> <div>57%</div> <div>32%</div> <div>11%</div> </div> </div>
3	4	4	<div> <div></div> <div> <div></div> <div>50%</div> <div>50%</div> </div> </div>
4	5	6	<div> <div>17%</div> <div> <div></div> <div>17%</div> <div>67%</div> <div>17%</div> </div> </div>
5	A	240	<div> <div>5%</div> <div> <div></div> <div>61%</div> <div>33%</div> <div>5%</div> </div> </div>
6	B	338	<div> <div>3%</div> <div> <div></div> <div>57%</div> <div>39%</div> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	C	246	
8	D	177	
9	E	178	
10	F	120	
11	G	348	
12	H	171	
13	J	145	
14	K	132	
15	L	165	
16	M	194	
17	N	187	
18	O	116	
19	P	149	
20	Q	96	
21	R	155	
22	S	85	
23	T	120	
24	U	66	
25	V	71	
26	W	154	
27	X	92	
28	Y	241	
29	Z	83	
30	1	57	
31	2	50	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
32	3	92	
33	I	162	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	MG	0	8047	-	-	-	X
36	NA	0	9152	-	-	-	X
36	NA	0	9184	-	-	-	X
38	SR	B	9521	-	-	-	X

## 2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 99077 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

- Molecule 3 is a RNA chain called 5'-R(\*CP\*CP\*(PPU)\*(LOF))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	4	Total	C	N	O	P	0	0	0
			72	39	12	19	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	5	6	Total	C	N	O	P	S	0	0	0
			93	53	15	22	2	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 15 is a protein called 50S ribosomal protein L15P.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 17 is a protein called 50S ribosomal protein L18P.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 30 is a protein called 50S ribosomal protein L37e.

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

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

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

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

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

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

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

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	87	Total	Mg	0	0
			87	87		
34	Y	1	Total	Mg	0	0
			1	1		
34	K	1	Total	Mg	0	0
			1	1		
34	A	1	Total	Mg	0	0
			1	1		
34	T	1	Total	Mg	0	0
			1	1		
34	5	1	Total	Mg	0	0
			1	1		
34	2	1	Total	Mg	0	0
			1	1		
34	9	1	Total	Mg	0	0
			1	1		

- Molecule 35 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 36 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	66	Total	Na	0	0
			66	66		
36	J	1	Total	Na	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	Q	1	Total 1	Na 1	0	0
36	D	1	Total 1	Na 1	0	0
36	C	1	Total 1	Na 1	0	0
36	R	2	Total 2	Na 2	0	0
36	9	1	Total 1	Na 1	0	0
36	S	1	Total 1	Na 1	0	0
36	M	1	Total 1	Na 1	0	0

- Molecule 37 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	10	Total 10	Cl 10	0	0
37	J	3	Total 3	Cl 3	0	0
37	B	1	Total 1	Cl 1	0	0
37	A	1	Total 1	Cl 1	0	0
37	N	1	Total 1	Cl 1	0	0
37	O	1	Total 1	Cl 1	0	0
37	R	1	Total 1	Cl 1	0	0
37	Y	1	Total 1	Cl 1	0	0
37	L	1	Total 1	Cl 1	0	0
37	3	1	Total 1	Cl 1	0	0
37	M	1	Total 1	Cl 1	0	0

- Molecule 38 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	98	Total 98	Sr 98	0	0
38	1	2	Total 2	Sr 2	0	0
38	H	1	Total 1	Sr 1	0	0
38	B	2	Total 2	Sr 2	0	0
38	3	1	Total 1	Sr 1	0	0
38	A	3	Total 3	Sr 3	0	0
38	R	1	Total 1	Sr 1	0	0
38	9	3	Total 3	Sr 3	0	0
38	L	1	Total 1	Sr 1	0	0
38	S	1	Total 1	Sr 1	0	0
38	F	1	Total 1	Sr 1	0	0

- Molecule 39 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	O	1	Total 1	Cd 1	0	0
39	Z	1	Total 1	Cd 1	0	0
39	1	1	Total 1	Cd 1	0	0
39	3	1	Total 1	Cd 1	0	0
39	U	1	Total 1	Cd 1	0	0

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	0	5727	Total 5727	O 5727	0	0
40	9	137	Total 137	O 137	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	4	1	Total 1	O 1	0	0
40	5	2	Total 2	O 2	0	0
40	A	120	Total 120	O 120	0	0
40	B	138	Total 138	O 138	0	0
40	C	180	Total 180	O 180	0	0
40	D	48	Total 48	O 48	0	0
40	E	44	Total 44	O 44	0	0
40	F	24	Total 24	O 24	0	0
40	G	14	Total 14	O 14	0	0
40	H	72	Total 72	O 72	0	0
40	J	54	Total 54	O 54	0	0
40	K	61	Total 61	O 61	0	0
40	L	83	Total 83	O 83	0	0
40	M	128	Total 128	O 128	0	0
40	N	58	Total 58	O 58	0	0
40	O	39	Total 39	O 39	0	0
40	P	61	Total 61	O 61	0	0
40	Q	51	Total 51	O 51	0	0
40	R	78	Total 78	O 78	0	0
40	S	31	Total 31	O 31	0	0
40	T	35	Total 35	O 35	0	0

*Continued on next page...*

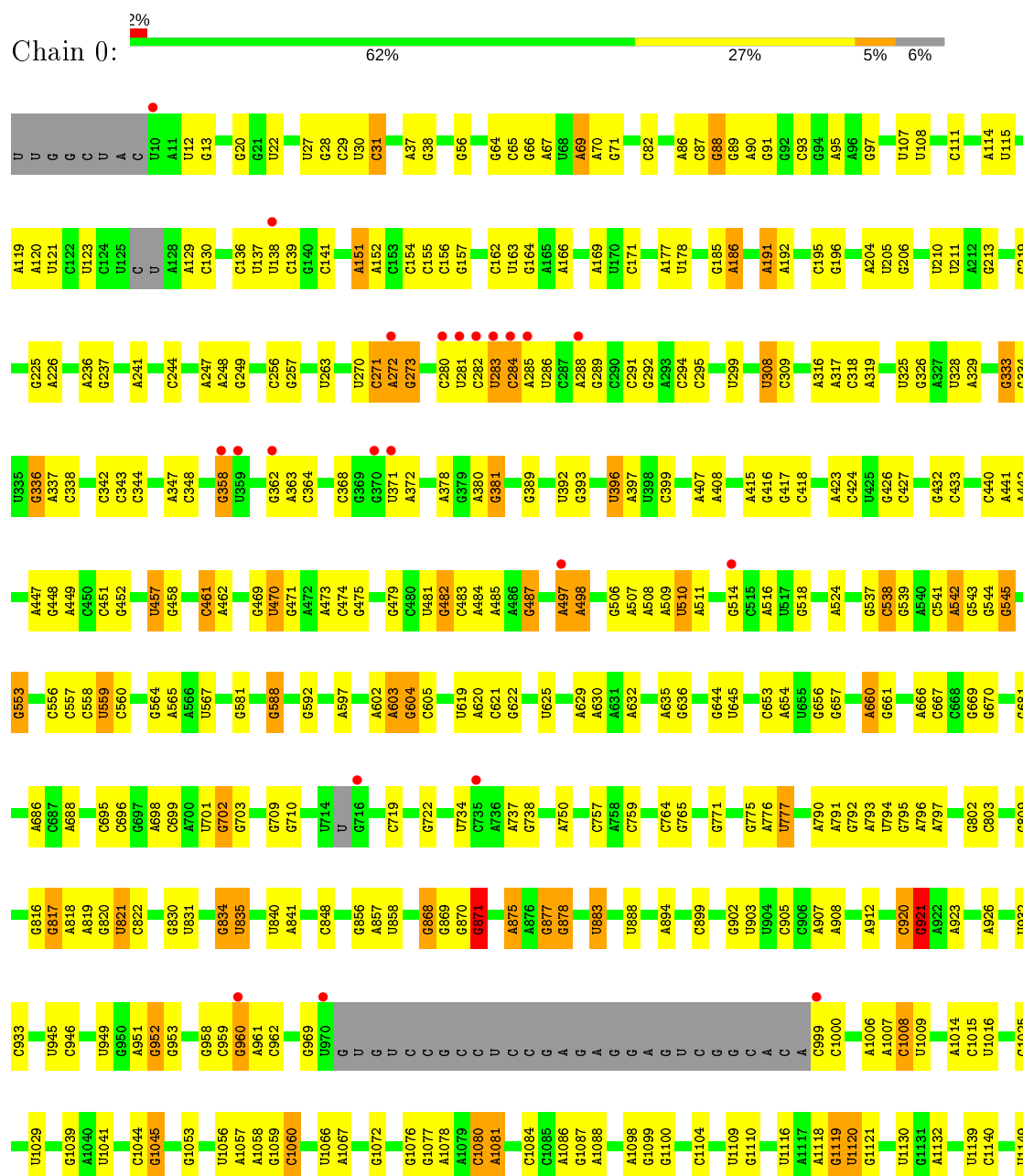
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	U	28	Total 28	O 28	0	0
40	V	12	Total 12	O 12	0	0
40	W	62	Total 62	O 62	0	0
40	X	21	Total 21	O 21	0	0
40	Y	93	Total 93	O 93	0	0
40	Z	34	Total 34	O 34	0	0
40	1	59	Total 59	O 59	0	0
40	2	40	Total 40	O 40	0	0
40	3	71	Total 71	O 71	0	0
40	I	10	Total 10	O 10	0	0

### 3 Residue-property plots

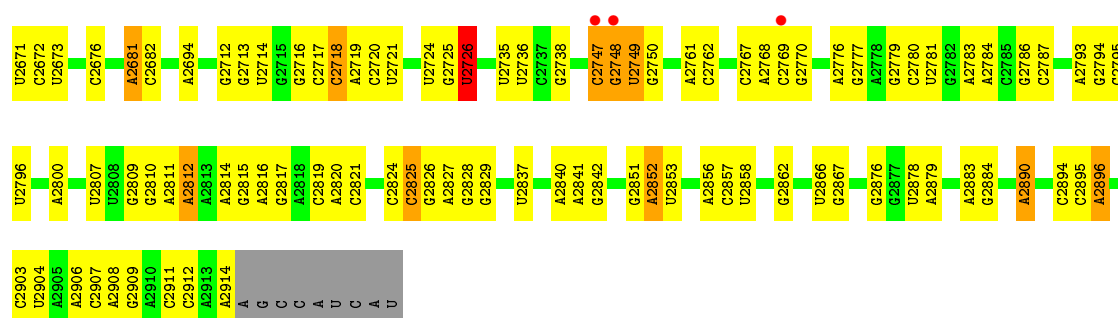
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

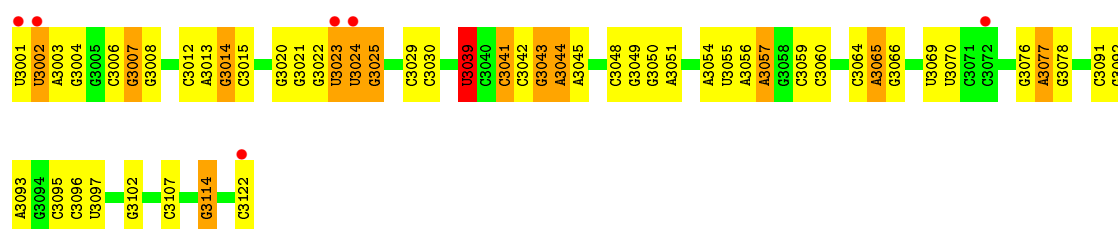


G2564	A2467	C2476	C2351	C2243	G2091	C	U1845	U1741	C1633	A1482	C1343	A1232	A1150
C2565	A2468	C2477	G2352	C2248	A2096	U1964	A1847	G1744	C1634	A1483	U1350	A1233	G1151
A2568	A2469	C2478	C2353	C2249	C	U1965	G1948	G1745	U1635	G1484	G1351	U1234	G1158
A2569	C2472	C2479	A2354	G2250	A2100	U1967	G1949	U1748	G1636	A1352	A1352	G1235	G1159
G2578	C2476	C2477	G2355	G2251	G2102	C	C1853	U1748	A1637	G1491	C1353	U1237	G1160
U2586	C2477	C2478	A2356	G2252	A2103	G	C1856	U1748	A1637	G1491	C1353	C1238	A1161
U2587	C2478	C2479	G2357	A2253	G2110	C	U1856	G1751	A1641	U1503	C1360	G1239	G1162
G2588	C2479	C2480	A2361	G2254	G2115	U	G1863	G1752	A1642	A1504	G1363	U1242	G1163
U2589	G2481	G2482	G2362	A2255	U2133	U1979	G1867	G1755	U1654	U1505	G1363	C1243	U1164
U2590	G2482	G2483	G2363	A2256	U2134	U1980	G1868	G1756	A1656	U1506	U1367	C1244	A1166
C2591	A2483	C2484	G2364	G2257	U2135	A1981	G1869	U1766	A1657	U1511	U1368	C1245	G1167
G2592	C2487	C2488	G2365	A2258	G2136	U1982	G1877	U1766	A1658	G1512	A1372	A1246	C1168
C2599	C2487	C2488	A2369	U2265	A2136	U1982	G1878	U1771	A1666	U1524	A1372	C1250	U1169
A2600	A2490	C2489	A2372	A2266	G2136	U1982	G1878	U1771	A1666	G1525	A1372	C1250	U1170
A2601	U2491	C2490	U2373	A2267	C	U1982	U1879	G1772	A1667	G1525	A1372	C1251	G1171
G2602	U2492	C2491	A2374	G2270	C	U1982	U1880	G1773	U1668	A1528	A1379	C1253	G1172
U2607	C2493	C2494	G2375	G2271	A	G2001	C1881	G1773	U1668	A1528	A1379	C1253	A1173
C2608	C2502	C2503	C2376	G2272	C	C2002	U1882	G1777	A1669	G1529	U1380	C1257	A1174
U2613	C2504	C2505	U2377	A2291	C	U2003	G1884	A1778	U1670	C1535	C1384	G1258	G1175
U2619	A2506	C2507	U2378	A2292	U	U2004	A1885	A1779	C1679	C1536	C1384	C1257	A1177
U2620	C2508	C2509	G2379	C2296	C	C2006	A1886	A1783	G1680	A1406	A1406	A1261	U1180
C2626	C2510	C2511	A2413	U2297	C	A2007	G1902	U1784	G1681	A1407	U1407	U1266	A1181
C2627	C2512	C2513	A2414	A2301	C	U2008	U1903	G1785	A1682	U1408	U1408	C1267	G1182
G2630	C2515	C2516	A2415	A2302	C	C	G1903	C1786	G1683	G1409	G1409	C1268	C1183
U2631	C2517	C2518	G2417	A2303	C	U2010	U1904	C1787	U1684	U1554	U1554	C1268	C1184
U2632	C2519	C2520	U2418	A2304	C	U2011	A1919	U1788	A1685	U1559	G1415	A1278	U1185
A2634	C2521	C2522	U2419	A2305	C	U2012	A1920	G1789	G1686	U	G1415	U1279	C1186
U2637	C2524	C2525	G2421	A2306	C	U2013	A1921	G1794	C1687	U1561	U1418	C1289	U1187
G2642	C2526	C2527	U2422	A2307	C	U2014	A1922	G1795	C1692	U1562	U1418	C1289	A1188
C2644	C2528	C2529	G2423	A2308	C	U2015	G1926	G1796	C1700	C1574	U1422	G1290	A1189
U2645	C2531	C2532	U2424	A2309	C	U2016	A1927	A1797	C1700	C1575	C1423	A1294	G1190
U2648	C2533	C2534	U2444	A2310	C	U2017	G1928	C1798	A1701	C1575	C1423	A1294	A1191
U2649	C2535	C2536	U2445	A2311	C	U2018	G1929	G1799	U1702	G1589	U1427	U1298	A1193
U2652	C2537	C2538	G2446	A2312	C	U2019	G1930	G1799	U1702	G1589	U1427	U1298	A1193
A2653	C2541	C2542	G2447	A2313	C	U2020	C1940	C1816	A1710	G1592	U1435	G1299	U1198
U2661	C2543	C2544	U2448	A2314	C	U2021	A1941	U1817	C1714	G1593	U1435	U1306	A1199
U2662	C2545	C2546	U2449	A2315	C	U2022	A1942	C1818	C1715	C1594	U1440	A1307	A1200
U2663	C2547	C2548	U2450	A2316	C	U2023	C1943	G1820	A1716	G1595	G1441	A1308	C1201
A	C2549	C2550	U2451	A2317	C	U2024	C1944	G1821	A1717	U1596	A1442	G1311	G1203
U	C2551	C2552	U2452	A2318	C	U2025	G1945	A1822	G1718	A1597	C1451	G1312	C1204
G2667	C2553	C2554	U2453	A2319	C	U2026	G1946	C1826	U1722	A1598	C1451	A1313	U1205
U2670	C2555	C2556	U2454	A2320	C	U2027	G1947	G1827	G1723	A1603	G1453	U1314	U1206
	C2557	C2558	U2455	A2321	C	U2028	G1948	G1828	U1724	G1604	U1454	G1315	A1207
	C2559	C2560	U2456	A2322	C	U2029	G1949	A1829	C1725	G1605	U1458	G1325	C1208
	C2561	C2562	U2457	A2323	C	U2030	G1950	C1834	G1730	A1606	U1458	C1209	C1209
	C2563	C2564	U2458	A2324	C	U2031	G1951	U1835	C1731	A1607	U1458	G1210	G1210
	C2565	C2566	U2459	A2325	C	U2032	U	A1836	A1732	A1615	C1462	A1328	G1211
	C2567	C2568	U2460	A2326	C	U2033	A	G1837	A1733	U1625	U1473	C1333	C1212
	C2569	C2570	U2461	A2327	C	U2034	A	U1838	A1734	A1826	C1474	C1334	G1216
	C2571	C2572	U2462	A2328	C	U2035	A	U1839	A1735	A1827	C1475	C1335	G1217
	C2573	C2574	U2463	A2329	C	U2036	A	A1840	A1736	G1627	U1218	U1219	U1218
	C2575	C2576	U2464	A2330	C	U2037	A	A1841	A1737	A1630	C1477	C1340	U1219
	C2577	C2578	U2465	A2331	C	U2038	A	A1842	A1738	A1631	C1478	C1341	C1342





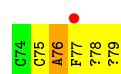
- Molecule 2: 5S ribosomal RNA



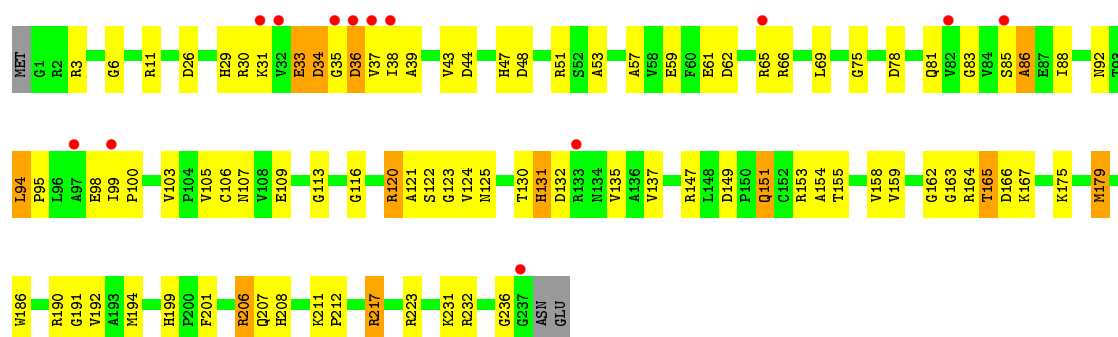
- Molecule 3: 5'-R(\*CP\*CP\*(PPU)\*(LOF))-3'



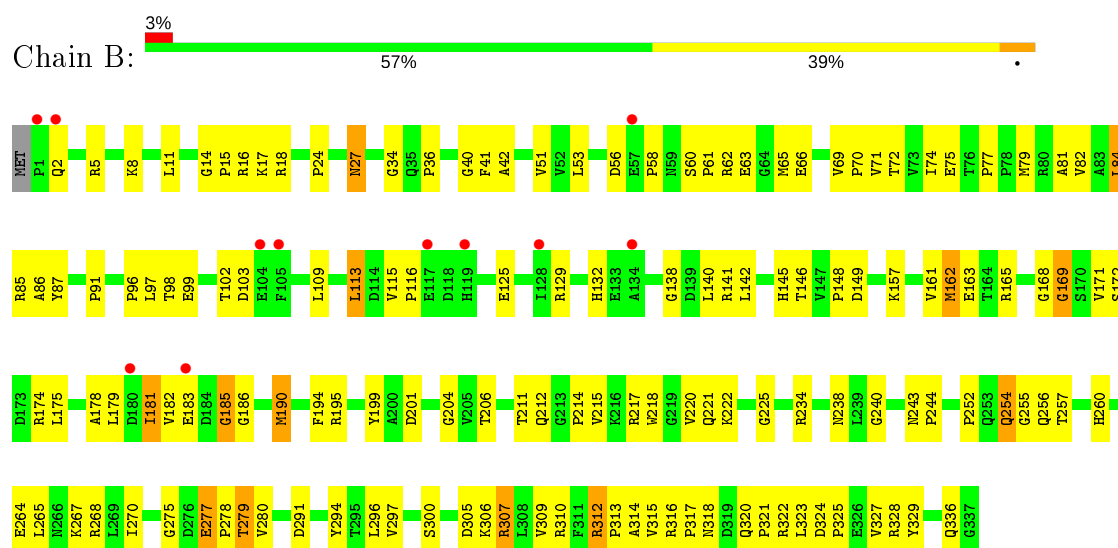
- Molecule 4: 5'-R(\*CP\*CP\*AP\*(PHE)\*(ACA)\*(BTN))-3'



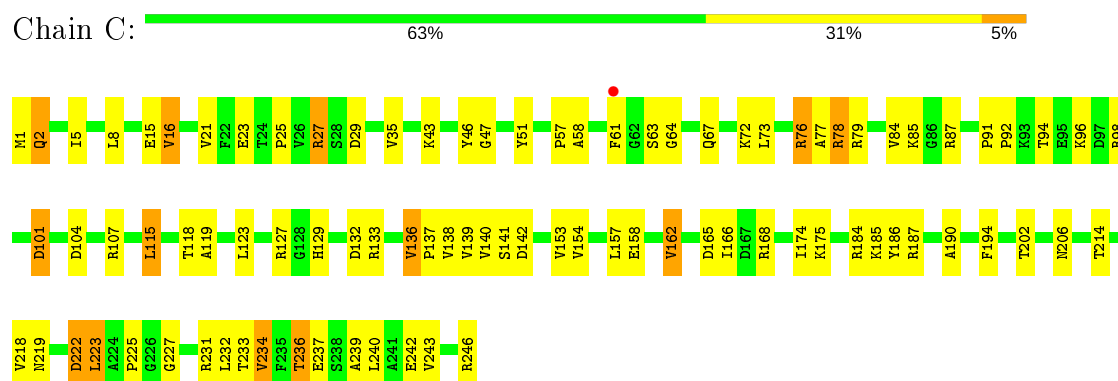
- Molecule 5: 50S ribosomal protein L2P



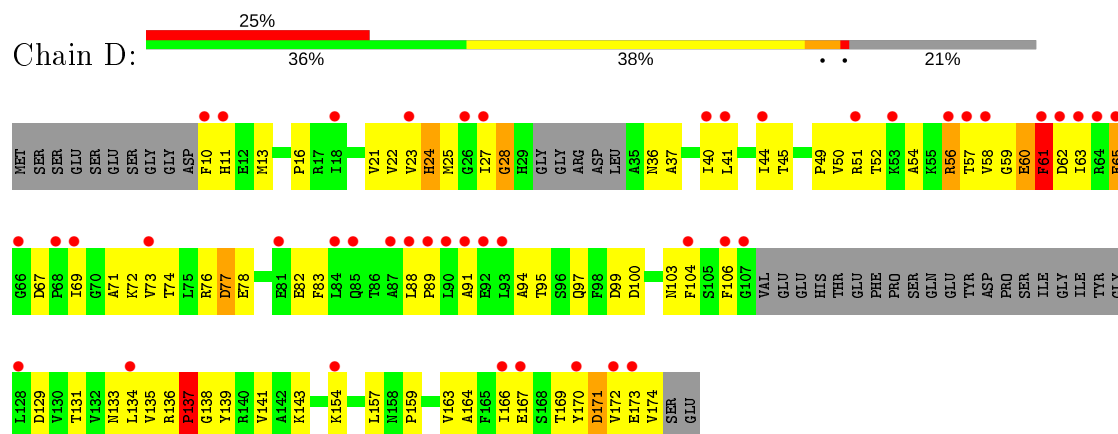
- Molecule 6: 50S ribosomal protein L3P



• Molecule 7: 50S ribosomal protein L4E



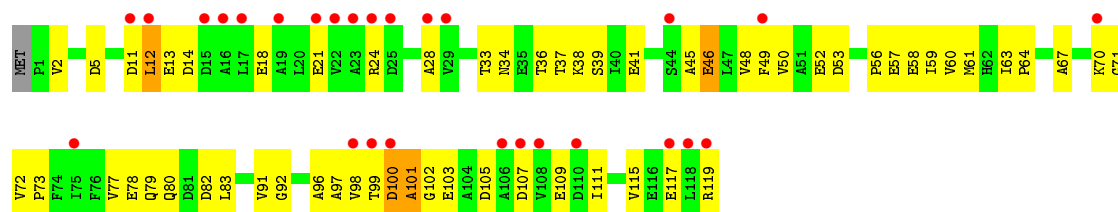
• Molecule 8: 50S ribosomal protein L5P



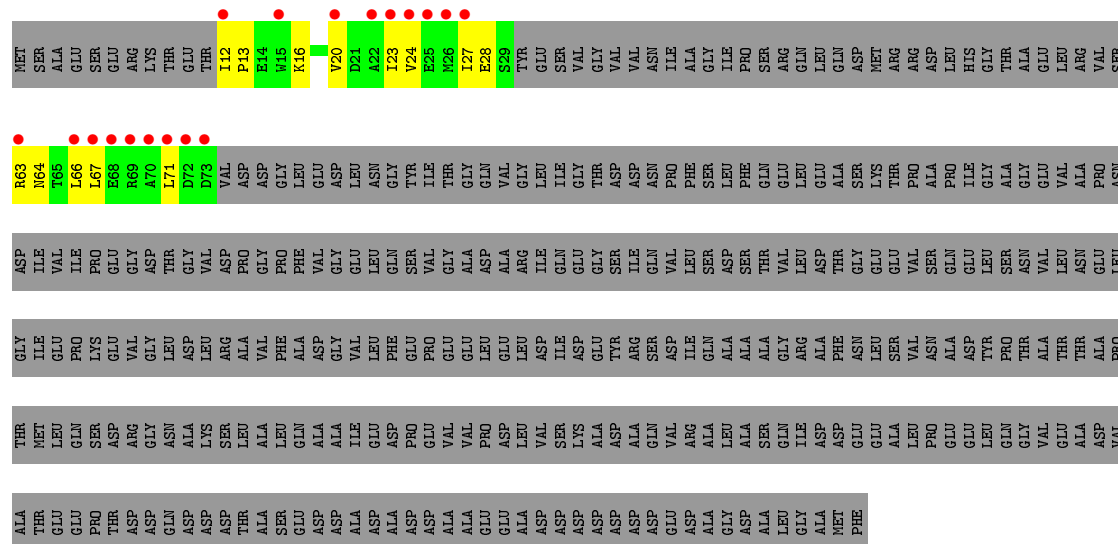
• Molecule 9: 50S ribosomal protein L6P



- Molecule 10: 50S ribosomal protein L7AE

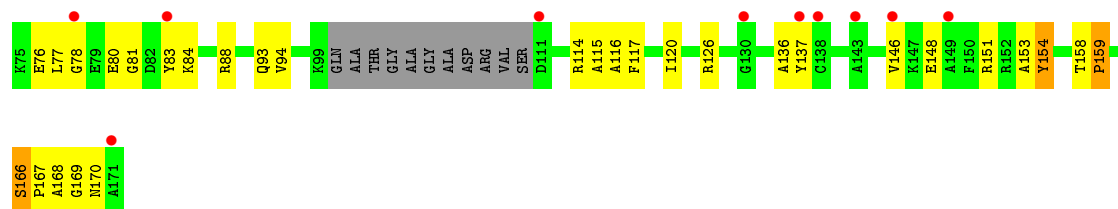


- Molecule 11: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

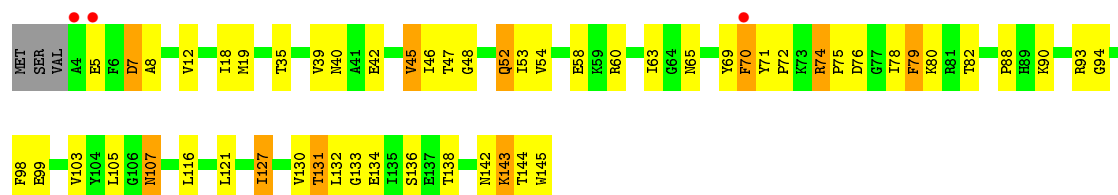


- Molecule 12: 50S RIBOSOMAL PROTEIN L10E

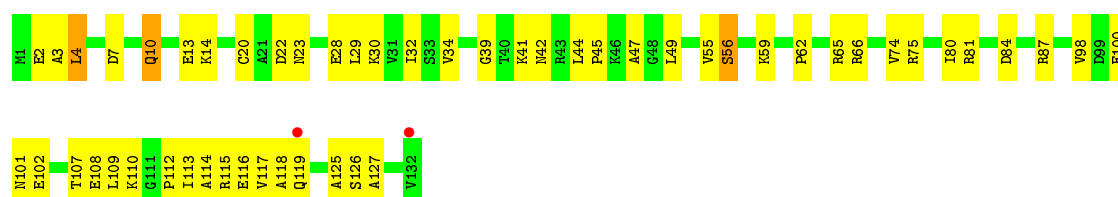




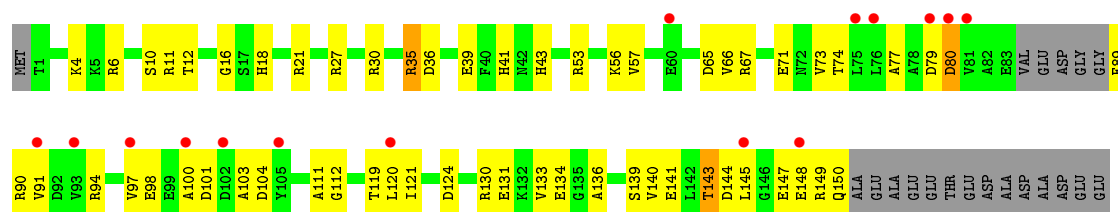
• Molecule 13: 50S ribosomal protein L13P



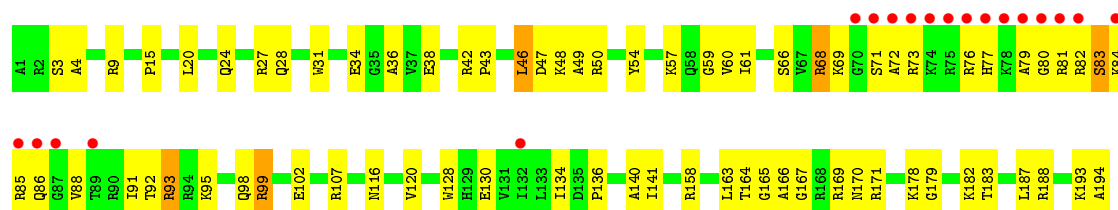
• Molecule 14: 50S ribosomal protein L14P



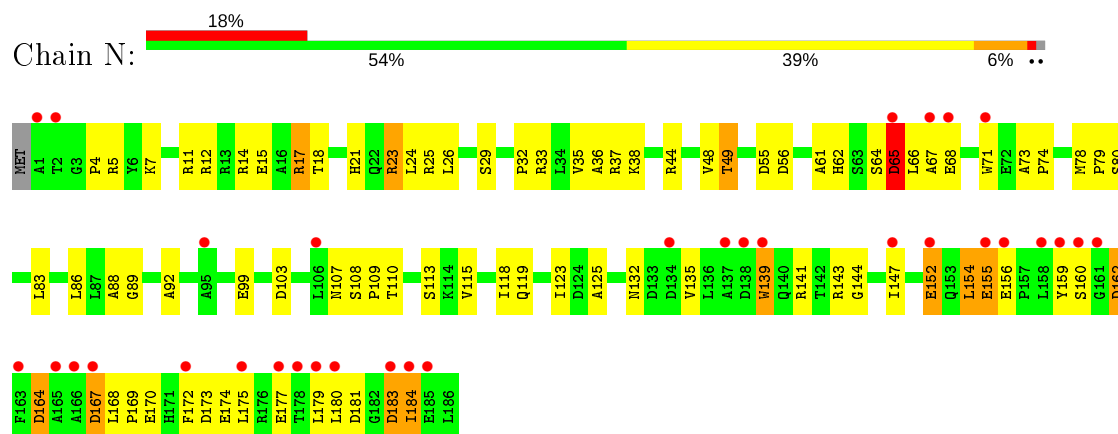
• Molecule 15: 50S ribosomal protein L15P



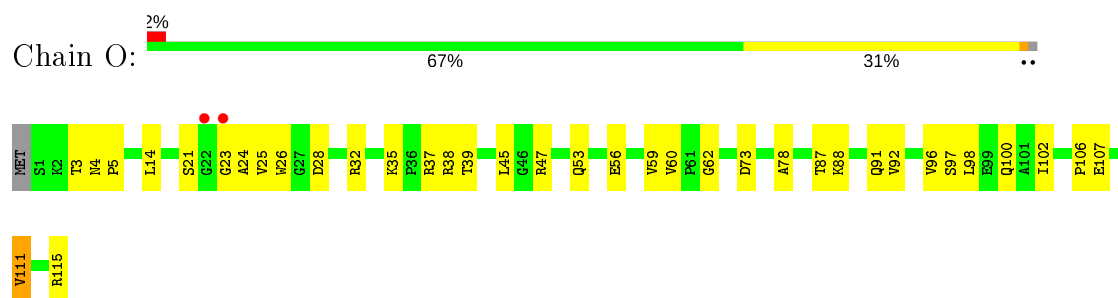
• Molecule 16: 50S Ribosomal Protein L15E



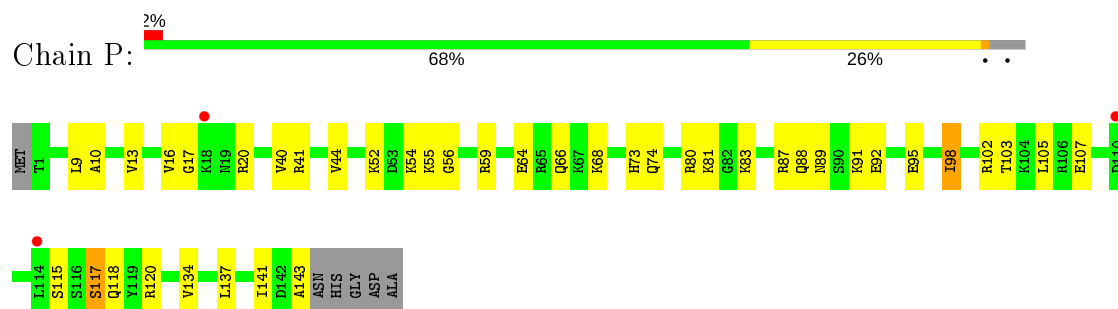
- Molecule 17: 50S ribosomal protein L18P



- Molecule 18: 50S ribosomal protein L18e

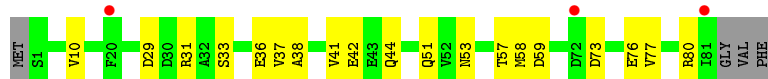
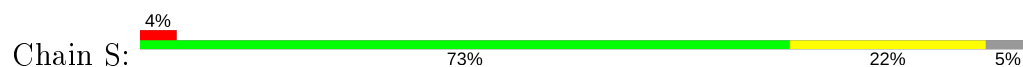


- Molecule 19: 50S ribosomal protein L19E

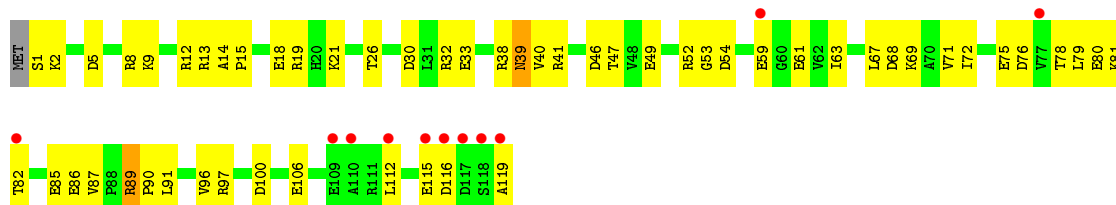




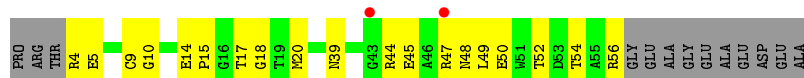
- Molecule 22: 50S ribosomal protein L23P



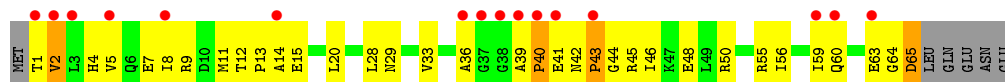
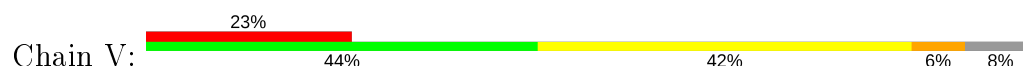
- Molecule 23: 50S ribosomal protein L24P



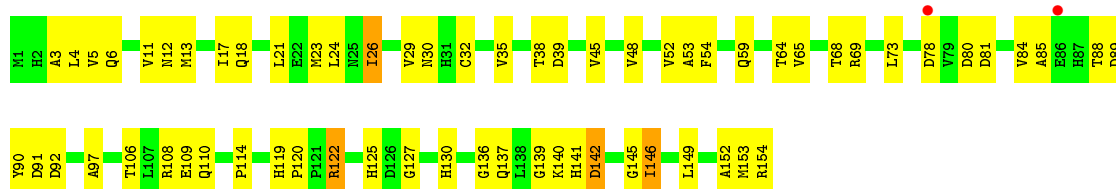
- Molecule 24: 50S ribosomal protein L24E



- Molecule 25: 50S ribosomal protein L29P

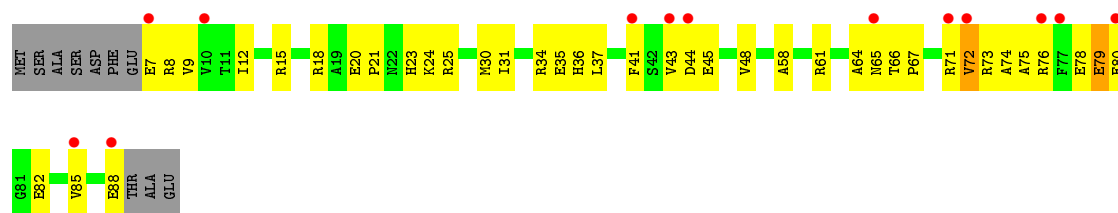


- Molecule 26: 50S ribosomal protein L30P

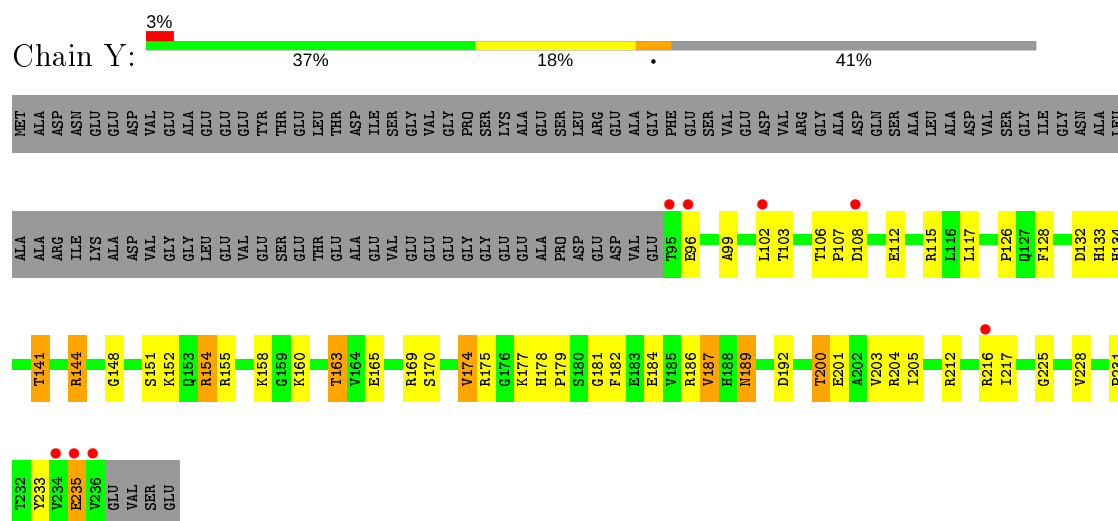


- Molecule 27: 50S ribosomal protein L31e

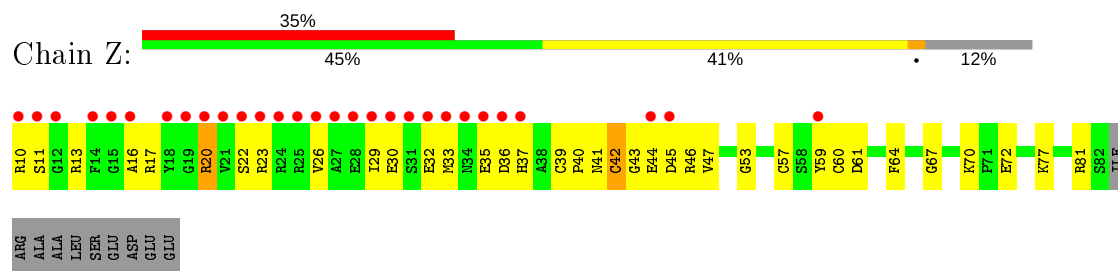




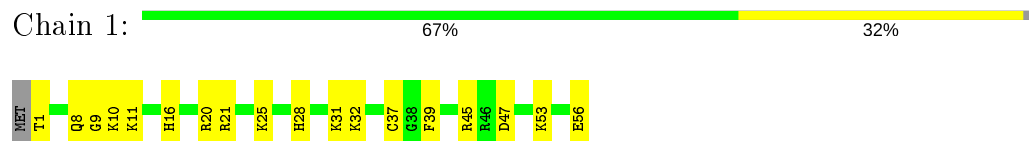
- Molecule 28: 50S ribosomal protein L32E



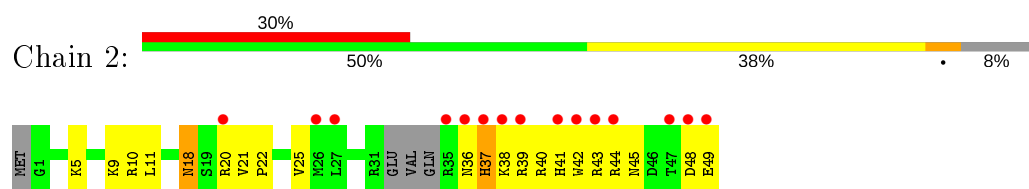
- Molecule 29: 50S ribosomal protein L37Ae



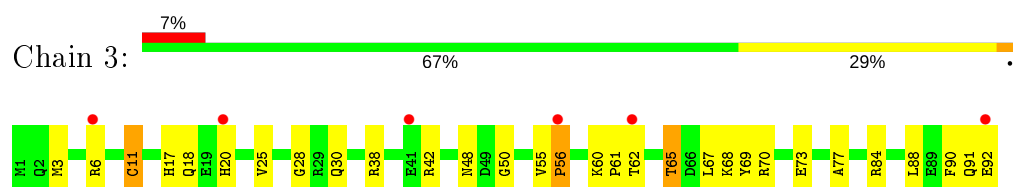
- Molecule 30: 50S ribosomal protein L37e



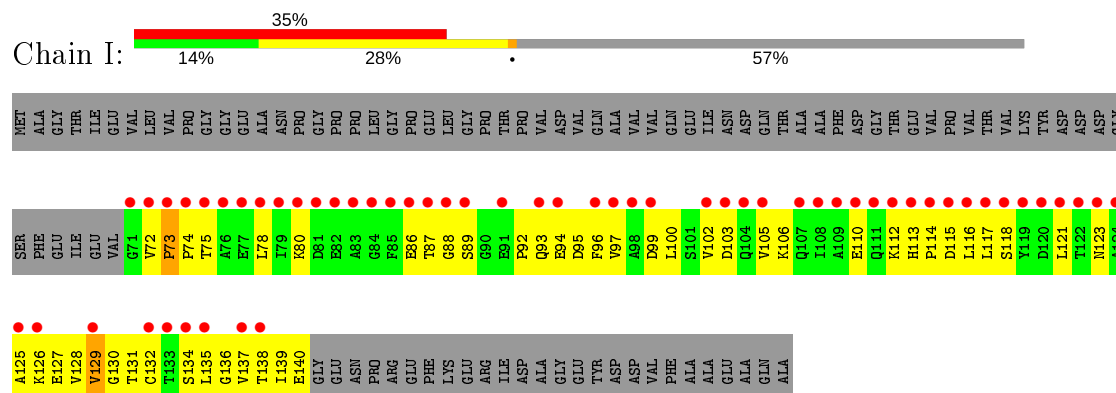
- Molecule 31: 50S ribosomal protein L39e



- Molecule 32: 50S ribosomal protein L44E



● Molecule 33: 50S RIBOSOMAL PROTEIN L11P





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.72Å 298.78Å 575.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 49.32 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.40) 89.2 (49.32-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.74 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.212 , 0.248 0.208 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.3	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 64.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	99077	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACA, OMG, PPU, CL, SR, NA, K, MG, CD, HFA, OMU, UR3, 1MA, BTN, 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	0.70	25/102870 (0.0%)
2	9	0.33	0/2905	0.70	1/4528 (0.0%)
3	4	0.47	0/40	0.68	0/60
4	5	0.51	0/76	0.79	0/112
5	A	0.33	0/1786	0.65	0/2408
6	B	0.34	0/2690	0.65	0/3652
7	C	0.38	0/1884	0.65	0/2551
8	D	0.29	0/1111	0.54	0/1498
9	E	0.32	0/1382	0.58	0/1880
10	F	0.33	0/901	0.54	0/1224
11	G	0.28	0/241	0.48	0/324
12	H	0.34	0/1287	0.64	0/1725
13	J	0.35	0/1136	0.62	0/1530
14	K	0.36	0/1001	0.68	0/1347
15	L	0.32	0/1130	0.64	0/1509
16	M	0.34	0/1584	0.59	0/2119
17	N	0.29	0/1474	0.61	0/1999
18	O	0.32	0/874	0.58	0/1181
19	P	0.35	0/1147	0.55	0/1528
20	Q	0.34	0/749	0.69	0/1005
21	R	0.37	0/1172	0.67	0/1578
22	S	0.32	0/648	0.56	0/875
23	T	0.31	0/958	0.63	0/1289
24	U	0.35	0/417	0.58	0/562
25	V	0.27	0/502	0.52	0/675
26	W	0.35	0/1219	0.60	0/1655
27	X	0.34	0/664	0.61	0/895
28	Y	0.37	0/1146	0.66	0/1536
29	Z	0.32	0/589	0.57	0/787
30	1	0.43	0/438	0.63	0/578
31	2	0.32	0/401	0.57	0/529
32	3	0.35	0/771	0.57	0/1024

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	I	0.29	0/526	0.51	0/716
All	All	0.37	0/98808	0.67	26/147749 (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	55
2	9	0	1
All	All	0	56

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	871	G	C5'-C4'-O4'	-7.44	100.17	109.10
1	0	1942	A	C5'-C4'-C3'	7.11	127.37	116.00
1	0	1592	G	N9-C1'-C2'	6.67	122.67	114.00
1	0	1819	G	C5'-C4'-C3'	6.40	126.24	116.00
1	0	883	U	N1-C1'-C2'	6.20	122.06	114.00

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	191	A	Sidechain
1	0	22	U	Sidechain
1	0	270	U	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29812	769	0
2	9	2600	0	1326	58	0
3	4	72	0	47	1	0
4	5	93	0	68	4	0
5	A	1753	0	1765	111	0
6	B	2625	0	2532	151	0
7	C	1859	0	1816	97	0
8	D	1094	0	1085	92	0
9	E	1357	0	1266	50	0
10	F	890	0	843	55	0
11	G	240	0	231	12	0
12	H	1266	0	1268	63	0
13	J	1120	0	1098	69	0
14	K	992	0	1031	58	0
15	L	1118	0	1076	61	0
16	M	1560	0	1568	75	0
17	N	1445	0	1401	87	0
18	O	865	0	873	42	0
19	P	1136	0	1123	42	0
20	Q	735	0	728	22	0
21	R	1149	0	1122	39	0
22	S	641	0	605	17	0
23	T	950	0	923	52	0
24	U	410	0	364	22	0
25	V	499	0	511	43	0
26	W	1196	0	1137	83	0
27	X	654	0	653	41	0
28	Y	1130	0	1133	60	0
29	Z	578	0	539	39	0
30	1	431	0	426	29	0
31	2	396	0	413	30	0
32	3	755	0	728	30	0
33	I	519	0	500	60	0
34	0	87	0	0	0	0
34	2	1	0	0	0	0
34	5	1	0	0	0	0
34	9	1	0	0	0	0
34	A	1	0	0	0	0
34	K	1	0	0	0	0
34	T	1	0	0	0	0
34	Y	1	0	0	0	0
35	0	2	0	0	0	0
36	0	66	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	9	1	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
36	J	1	0	0	0	0
36	M	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	2	0	0	0	0
36	S	1	0	0	0	0
37	0	10	0	0	0	0
37	3	1	0	0	0	0
37	A	1	0	0	0	0
37	B	1	0	0	0	0
37	J	3	0	0	1	0
37	L	1	0	0	0	0
37	M	1	0	0	0	0
37	N	1	0	0	0	0
37	O	1	0	0	0	0
37	R	1	0	0	0	0
37	Y	1	0	0	0	0
38	0	98	0	0	0	0
38	1	2	0	0	0	0
38	3	1	0	0	0	0
38	9	3	0	0	0	0
38	A	3	0	0	0	0
38	B	2	0	0	0	0
38	F	1	0	0	0	0
38	H	1	0	0	0	0
38	L	1	0	0	0	0
38	R	1	0	0	0	0
38	S	1	0	0	0	0
39	1	1	0	0	0	0
39	3	1	0	0	0	0
39	O	1	0	0	0	0
39	U	1	0	0	0	0
39	Z	1	0	0	0	0
40	0	5727	0	0	102	0
40	1	59	0	0	3	0
40	2	40	0	0	1	0
40	3	71	0	0	5	0
40	4	1	0	0	0	0
40	5	2	0	0	0	0
40	9	137	0	0	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	A	120	0	0	8	0
40	B	138	0	0	18	0
40	C	180	0	0	19	0
40	D	48	0	0	11	0
40	E	44	0	0	4	0
40	F	24	0	0	2	0
40	G	14	0	0	0	0
40	H	72	0	0	6	0
40	I	10	0	0	2	0
40	J	54	0	0	3	0
40	K	61	0	0	4	0
40	L	83	0	0	12	0
40	M	128	0	0	3	0
40	N	58	0	0	4	0
40	O	39	0	0	3	0
40	P	61	0	0	2	0
40	Q	51	0	0	5	0
40	R	78	0	0	4	0
40	S	31	0	0	1	0
40	T	35	0	0	4	0
40	U	28	0	0	3	0
40	V	12	0	0	2	0
40	W	62	0	0	6	0
40	X	21	0	0	5	0
40	Y	93	0	0	10	0
40	Z	34	0	0	2	0
All	All	99077	0	60011	2220	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 2220 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)
26:W:21:LEU:HD21	26:W:48:VAL:HG11	1.35	1.08
14:K:29:LEU:HB3	14:K:55:VAL:HG11	1.33	1.07
1:0:1160:G:H5'	1:0:1161:A:H5'	1.36	1.07
27:X:37:LEU:HD13	27:X:85:VAL:HG21	1.39	1.04
2:9:3076:G:H3'	2:9:3077:A:H5''	1.36	1.04

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A	235/240 (98%)	207 (88%)	25 (11%)	3 (1%)	12	17
6	B	335/338 (99%)	309 (92%)	21 (6%)	5 (2%)	10	14
7	C	244/246 (99%)	223 (91%)	19 (8%)	2 (1%)	19	29
8	D	134/177 (76%)	104 (78%)	19 (14%)	11 (8%)	1	0
9	E	170/178 (96%)	162 (95%)	8 (5%)	0	100	100
10	F	117/120 (98%)	103 (88%)	11 (9%)	3 (3%)	5	5
11	G	25/348 (7%)	25 (100%)	0	0	100	100
12	H	156/171 (91%)	136 (87%)	16 (10%)	4 (3%)	5	5
13	J	140/145 (97%)	130 (93%)	6 (4%)	4 (3%)	4	4
14	K	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	19	29
15	L	141/165 (86%)	118 (84%)	21 (15%)	2 (1%)	11	15
16	M	192/194 (99%)	178 (93%)	13 (7%)	1 (0%)	29	41
17	N	184/187 (98%)	161 (88%)	14 (8%)	9 (5%)	2	1
18	O	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
19	P	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
20	Q	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
21	R	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
22	S	79/85 (93%)	73 (92%)	6 (8%)	0	100	100
23	T	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	9	11
24	U	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
25	V	63/71 (89%)	59 (94%)	1 (2%)	3 (5%)	2	1
26	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
27	X	80/92 (87%)	72 (90%)	8 (10%)	0	100	100
28	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
29	Z	71/83 (86%)	58 (82%)	10 (14%)	3 (4%)	3	2

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
31	2	42/50 (84%)	41 (98%)	0	1 (2%)	6	6
32	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	14	20
33	I	68/162 (42%)	54 (79%)	12 (18%)	2 (3%)	4	4
All	All	3705/4430 (84%)	3385 (91%)	263 (7%)	57 (2%)	10	14

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	169	GLY
8	D	60	GLU
8	D	137	PRO
10	F	101	ALA
12	H	166	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	A	179/182 (98%)	165 (92%)	14 (8%)	12	19
6	B	282/283 (100%)	267 (95%)	15 (5%)	22	37
7	C	193/193 (100%)	173 (90%)	20 (10%)	7	10
8	D	117/148 (79%)	112 (96%)	5 (4%)	29	46
9	E	152/156 (97%)	146 (96%)	6 (4%)	32	50
10	F	93/94 (99%)	91 (98%)	2 (2%)	52	71
11	G	27/283 (10%)	27 (100%)	0	100	100
12	H	132/138 (96%)	127 (96%)	5 (4%)	33	51
13	J	118/121 (98%)	108 (92%)	10 (8%)	10	16
14	K	106/106 (100%)	101 (95%)	5 (5%)	26	42
15	L	113/127 (89%)	110 (97%)	3 (3%)	44	65
16	M	158/158 (100%)	153 (97%)	5 (3%)	39	59

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	N	149/150 (99%)	142 (95%)	7 (5%)	26	42
18	O	93/94 (99%)	92 (99%)	1 (1%)	73	87
19	P	113/117 (97%)	110 (97%)	3 (3%)	44	65
20	Q	79/80 (99%)	75 (95%)	4 (5%)	24	39
21	R	117/122 (96%)	114 (97%)	3 (3%)	46	66
22	S	71/74 (96%)	71 (100%)	0	100	100
23	T	105/106 (99%)	101 (96%)	4 (4%)	33	51
24	U	44/52 (85%)	44 (100%)	0	100	100
25	V	51/57 (90%)	50 (98%)	1 (2%)	55	74
26	W	130/130 (100%)	124 (95%)	6 (5%)	27	43
27	X	66/74 (89%)	63 (96%)	3 (4%)	27	44
28	Y	120/196 (61%)	109 (91%)	11 (9%)	9	13
29	Z	60/68 (88%)	59 (98%)	1 (2%)	60	78
30	1	46/47 (98%)	45 (98%)	1 (2%)	52	71
31	2	42/46 (91%)	41 (98%)	1 (2%)	49	68
32	3	79/79 (100%)	77 (98%)	2 (2%)	47	67
33	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3611 (86%)	2955 (96%)	138 (4%)	27	44

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	H	18	GLU
14	K	4	LEU
28	Y	174	VAL
12	H	88	ARG
13	J	52	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
19	P	50	GLN
21	R	61	GLN
31	2	16	ASN
19	P	66	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
19	P	89	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	233 (8%)	32 (1%)
2	9	121/122 (99%)	15 (12%)	1 (0%)
3	4	1/4 (25%)	0	0
4	5	2/6 (33%)	1 (50%)	0
All	All	2869/3054 (93%)	249 (8%)	33 (1%)

5 of 249 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1506	U
1	0	1730	G
1	0	2761	A
1	0	1684	A
1	0	1685	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	0	2621	1	17,21,22	1.65	3 (17%)	20,30,33	5.47	4 (20%)
1	1MA	0	628	1,36	15,25,26	0.70	0	15,37,40	1.37	1 (6%)
4	ACA	5	78	4	7,7,8	1.98	1 (14%)	6,6,8	0.91	0
1	OMG	0	2588	1,3	18,26,27	1.12	2 (11%)	20,38,41	2.60	4 (20%)
1	OMU	0	2587	1	14,22,23	1.02	2 (14%)	14,31,34	1.14	1 (7%)
3	PPU	4	76	1,3	18,26,41	0.81	0	15,38,60	0.77	0
3	HFA	4	77	3	10,11,12	0.91	1 (10%)	12,13,15	0.61	0
1	UR3	0	2619	1,38	14,22,23	0.95	1 (7%)	15,32,35	0.58	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1,36	-	0/3/25/26	0/3/3/3
4	ACA	5	78	4	-	0/4/5/6	-
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3
1	OMU	0	2587	1	-	0/7/27/28	0/2/2/2
3	PPU	4	76	1,3	-	0/7/29/44	0/3/3/4
3	HFA	4	77	3	-	0/5/6/8	0/1/1/1
1	UR3	0	2619	1,38	-	0/5/25/26	0/2/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	78	ACA	C3-C2	-4.87	1.32	1.52
1	0	2621	PSU	C5-C1'	-4.79	1.48	1.52
1	0	2588	OMG	C6-N1	3.42	1.39	1.33
1	0	2621	PSU	C4-N3	3.27	1.38	1.33
1	0	2587	OMU	C4-N3	2.74	1.37	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.45	114.56	128.43
1	0	2621	PSU	C4-N3-C2	14.33	127.24	115.14
1	0	2588	OMG	C5-C6-N1	-8.59	111.69	123.43
1	0	2621	PSU	C5-C4-N3	-8.31	114.65	125.36
1	0	2588	OMG	C6-N1-C2	5.80	125.14	115.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	5	78	ACA	1	0
1	0	2587	OMU	3	0
3	4	76	PPU	1	0
1	0	2619	UR3	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 312 ligands modelled in this entry, 312 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	0	2749/2922 (94%)	-0.63	62 (2%) 60 58	24, 49, 93, 153	0
2	9	122/122 (100%)	-0.24	6 (4%) 29 28	41, 69, 93, 152	0
3	4	2/4 (50%)	-1.10	0 100 100	43, 43, 43, 52	0
4	5	4/6 (66%)	-0.08	1 (25%) 0 0	55, 57, 58, 66	0
5	A	237/240 (98%)	0.33	13 (5%) 25 24	31, 54, 86, 106	0
6	B	337/338 (99%)	0.14	11 (3%) 46 45	31, 55, 79, 93	0
7	C	246/246 (100%)	-0.06	1 (0%) 92 91	27, 49, 70, 87	0
8	D	140/177 (79%)	1.71	44 (31%) 0 0	64, 96, 125, 132	0
9	E	172/178 (96%)	0.74	24 (13%) 2 2	44, 66, 86, 92	0
10	F	119/120 (99%)	1.00	27 (22%) 0 0	49, 74, 100, 112	0
11	G	29/348 (8%)	2.39	18 (62%) 0 0	74, 92, 103, 105	0
12	H	160/171 (93%)	0.60	16 (10%) 7 6	47, 65, 96, 103	0
13	J	142/145 (97%)	-0.01	3 (2%) 63 61	37, 52, 72, 93	0
14	K	132/132 (100%)	-0.15	2 (1%) 73 72	37, 48, 71, 84	0
15	L	145/165 (87%)	0.60	15 (10%) 6 6	29, 69, 112, 121	0
16	M	194/194 (100%)	0.52	19 (9%) 7 7	37, 48, 85, 93	0
17	N	186/187 (99%)	0.90	33 (17%) 1 1	49, 68, 112, 119	0
18	O	115/116 (99%)	0.16	2 (1%) 70 68	40, 59, 73, 81	0
19	P	143/149 (95%)	0.24	3 (2%) 63 61	39, 55, 66, 79	0
20	Q	95/96 (98%)	0.05	4 (4%) 36 35	42, 52, 67, 76	0
21	R	150/155 (96%)	-0.14	0 100 100	33, 47, 66, 75	0
22	S	81/85 (95%)	0.30	3 (3%) 41 41	43, 61, 84, 97	0
23	T	119/120 (99%)	0.67	11 (9%) 9 8	41, 59, 85, 110	0
24	U	53/66 (80%)	0.26	2 (3%) 40 39	42, 56, 73, 82	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	V	65/71 (91%)	1.61	16 (24%) 0 0	56, 78, 115, 120	0
26	W	154/154 (100%)	0.02	2 (1%) 77 75	40, 53, 74, 82	0
27	X	82/92 (89%)	0.67	13 (15%) 1 1	44, 58, 84, 103	0
28	Y	142/241 (58%)	0.10	8 (5%) 24 23	29, 45, 68, 90	0
29	Z	73/83 (87%)	1.74	29 (39%) 0 0	52, 83, 97, 105	0
30	1	56/57 (98%)	-0.43	0 100 100	31, 36, 46, 55	0
31	2	46/50 (92%)	1.44	15 (32%) 0 0	41, 68, 96, 102	0
32	3	92/92 (100%)	0.33	6 (6%) 18 17	41, 61, 73, 86	0
33	I	70/162 (43%)	5.01	57 (81%) 0 0	111, 125, 142, 144	0
All	All	6652/7484 (88%)	0.03	466 (7%) 16 15	24, 54, 100, 153	0

The worst 5 of 466 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	I	71	GLY	15.4
25	V	1	THR	14.2
33	I	79	ILE	12.3
33	I	76	ALA	12.1
33	I	133	THR	11.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	ACA	5	78	8/9	0.88	0.30	66,72,83,86	0
3	HFA	4	77	11/12	0.95	0.20	42,44,47,48	0
1	UR3	0	2619	21/22	0.97	0.15	39,42,45,48	0
1	OMG	0	2588	24/25	0.98	0.13	31,34,39,41	0
1	OMU	0	2587	21/22	0.98	0.13	32,37,40,40	0
3	PPU	4	76	24/38	0.98	0.13	41,44,45,49	0
1	1MA	0	628	23/24	0.98	0.12	32,35,37,38	0
1	PSU	0	2621	20/21	0.98	0.14	36,38,43,43	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
38	SR	0	9529	1/1	-0.08	0.27	131,131,131,131	0
38	SR	0	9484	1/1	0.32	0.14	149,149,149,149	0
36	NA	0	9184	1/1	0.40	0.41	87,87,87,87	0
38	SR	0	9537	1/1	0.50	0.23	157,157,157,157	0
38	SR	0	9547	1/1	0.52	0.39	194,194,194,194	0
34	MG	0	8047	1/1	0.56	0.54	107,107,107,107	0
36	NA	0	9122	1/1	0.57	0.40	90,90,90,90	0
38	SR	9	9588	1/1	0.59	0.14	143,143,143,143	0
38	SR	B	9521	1/1	0.59	0.63	200,200,200,200	0
34	MG	0	8101	1/1	0.61	0.29	80,80,80,80	0
36	NA	0	9182	1/1	0.63	0.39	90,90,90,90	0
38	SR	0	9501	1/1	0.65	0.20	159,159,159,159	0
34	MG	0	8108	1/1	0.68	0.14	103,103,103,103	0
36	NA	D	9151	1/1	0.70	0.23	68,68,68,68	0
36	NA	0	9181	1/1	0.72	0.16	54,54,54,54	0
36	NA	0	9135	1/1	0.72	0.30	55,55,55,55	0
36	NA	0	9141	1/1	0.74	0.13	73,73,73,73	0
36	NA	9	9183	1/1	0.75	0.38	75,75,75,75	0
35	K	0	9002	1/1	0.75	0.18	88,88,88,88	0
39	CD	Z	9203	1/1	0.75	0.13	84,84,84,84	0
36	NA	0	9114	1/1	0.76	0.20	65,65,65,65	0
36	NA	0	9116	1/1	0.77	0.35	52,52,52,52	0
36	NA	0	9152	1/1	0.77	1.03	83,83,83,83	0
36	NA	0	9126	1/1	0.78	0.11	63,63,63,63	0
34	MG	0	8093	1/1	0.79	0.13	49,49,49,49	0
36	NA	J	9146	1/1	0.79	0.11	55,55,55,55	0
36	NA	0	9129	1/1	0.80	0.13	72,72,72,72	0
34	MG	0	8090	1/1	0.80	0.35	68,68,68,68	0
34	MG	0	8092	1/1	0.82	0.34	77,77,77,77	0
34	MG	0	8065	1/1	0.82	0.34	107,107,107,107	0
34	MG	0	8059	1/1	0.83	0.42	84,84,84,84	0
34	MG	0	8052	1/1	0.83	0.25	99,99,99,99	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	NA	0	9172	1/1	0.83	0.35	76,76,76,76	0
34	MG	0	8037	1/1	0.84	0.10	46,46,46,46	0
34	MG	0	8104	1/1	0.84	0.13	57,57,57,57	0
36	NA	R	9186	1/1	0.84	0.38	80,80,80,80	0
34	MG	0	8107	1/1	0.84	0.17	65,65,65,65	0
34	MG	0	8013	1/1	0.84	0.34	25,25,25,25	0
34	MG	0	8102	1/1	0.85	0.12	68,68,68,68	0
36	NA	0	9158	1/1	0.85	0.44	66,66,66,66	0
36	NA	0	9185	1/1	0.85	0.61	54,54,54,54	0
34	MG	0	8022	1/1	0.85	0.94	112,112,112,112	0
36	NA	0	9132	1/1	0.86	0.22	68,68,68,68	0
36	NA	0	9161	1/1	0.86	0.72	68,68,68,68	0
34	MG	0	8061	1/1	0.86	0.19	87,87,87,87	0
36	NA	0	9169	1/1	0.86	0.39	116,116,116,116	0
36	NA	0	9164	1/1	0.87	0.57	61,61,61,61	0
34	MG	0	8113	1/1	0.87	0.12	52,52,52,52	0
36	NA	0	9102	1/1	0.87	0.22	63,63,63,63	0
36	NA	S	9112	1/1	0.87	0.23	80,80,80,80	0
35	K	0	9001	1/1	0.87	0.31	74,74,74,74	0
34	MG	0	8030	1/1	0.87	0.08	37,37,37,37	0
38	SR	0	9581	1/1	0.87	0.08	130,130,130,130	0
38	SR	0	9500	1/1	0.88	1.54	200,200,200,200	0
34	MG	0	8089	1/1	0.88	0.17	61,61,61,61	0
34	MG	0	8024	1/1	0.88	0.41	86,86,86,86	0
34	MG	5	8118	1/1	0.88	0.34	45,45,45,45	0
34	MG	0	8050	1/1	0.88	0.22	89,89,89,89	0
34	MG	0	8106	1/1	0.88	0.09	51,51,51,51	0
38	SR	0	9539	1/1	0.88	0.38	157,157,157,157	0
34	MG	0	8091	1/1	0.89	0.15	64,64,64,64	0
38	SR	0	9532	1/1	0.89	0.05	120,120,120,120	0
34	MG	0	8072	1/1	0.89	0.65	89,89,89,89	0
36	NA	0	9143	1/1	0.89	0.14	40,40,40,40	0
36	NA	0	9165	1/1	0.89	0.30	45,45,45,45	0
36	NA	0	9140	1/1	0.89	0.15	57,57,57,57	0
34	MG	0	8103	1/1	0.89	0.17	67,67,67,67	0
36	NA	0	9170	1/1	0.89	0.28	77,77,77,77	0
36	NA	0	9166	1/1	0.89	0.09	74,74,74,74	0
38	SR	0	9590	1/1	0.89	0.12	131,131,131,131	0
34	MG	0	8040	1/1	0.90	0.21	92,92,92,92	0
34	MG	0	8058	1/1	0.90	0.21	41,41,41,41	0
34	MG	0	8025	1/1	0.90	0.42	27,27,27,27	0
36	NA	0	9131	1/1	0.90	0.14	47,47,47,47	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
38	SR	0	9482	1/1	0.90	0.35	135,135,135,135	0
36	NA	0	9128	1/1	0.90	0.15	49,49,49,49	0
34	MG	0	8014	1/1	0.90	0.38	73,73,73,73	0
34	MG	0	8051	1/1	0.90	0.21	36,36,36,36	0
38	SR	9	9503	1/1	0.90	0.05	122,122,122,122	0
36	NA	0	9168	1/1	0.90	0.17	69,69,69,69	0
38	SR	0	9626	1/1	0.91	0.25	154,154,154,154	0
34	MG	0	8055	1/1	0.91	0.31	97,97,97,97	0
36	NA	0	9111	1/1	0.91	0.31	63,63,63,63	0
36	NA	0	9167	1/1	0.91	0.10	65,65,65,65	0
38	SR	0	9504	1/1	0.91	0.11	108,108,108,108	0
36	NA	0	9177	1/1	0.91	0.35	77,77,77,77	0
34	MG	0	8099	1/1	0.91	0.14	75,75,75,75	0
38	SR	0	9459	1/1	0.91	0.10	103,103,103,103	0
38	SR	0	9468	1/1	0.91	0.05	128,128,128,128	0
34	MG	0	8043	1/1	0.91	0.06	52,52,52,52	0
36	NA	0	9174	1/1	0.91	0.38	65,65,65,65	0
36	NA	0	9179	1/1	0.91	0.60	121,121,121,121	0
37	CL	L	9310	1/1	0.92	0.12	58,58,58,58	0
34	MG	0	8094	1/1	0.92	0.50	72,72,72,72	0
36	NA	0	9101	1/1	0.92	0.13	46,46,46,46	0
34	MG	0	8019	1/1	0.92	0.06	51,51,51,51	0
34	MG	0	8063	1/1	0.92	0.10	65,65,65,65	0
38	SR	0	9465	1/1	0.92	0.10	107,107,107,107	0
38	SR	0	9509	1/1	0.92	0.15	95,95,95,95	0
37	CL	A	9309	1/1	0.92	0.19	66,66,66,66	0
34	MG	0	8032	1/1	0.92	0.10	48,48,48,48	0
34	MG	9	8095	1/1	0.92	0.35	55,55,55,55	0
37	CL	J	9301	1/1	0.93	0.18	60,60,60,60	0
36	NA	0	9113	1/1	0.93	0.11	60,60,60,60	0
36	NA	M	9147	1/1	0.93	0.18	42,42,42,42	0
36	NA	0	9159	1/1	0.93	0.35	58,58,58,58	0
36	NA	0	9173	1/1	0.93	0.34	69,69,69,69	0
36	NA	0	9117	1/1	0.93	0.07	51,51,51,51	0
34	MG	0	8085	1/1	0.93	0.21	63,63,63,63	0
36	NA	0	9106	1/1	0.93	0.44	44,44,44,44	0
34	MG	0	8115	1/1	0.93	0.09	59,59,59,59	0
36	NA	0	9171	1/1	0.93	0.31	61,61,61,61	0
36	NA	0	9124	1/1	0.93	0.19	50,50,50,50	0
34	MG	0	8054	1/1	0.93	0.16	63,63,63,63	0
36	NA	0	9175	1/1	0.93	0.33	55,55,55,55	0
36	NA	0	9120	1/1	0.93	0.21	61,61,61,61	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	MG	0	8036	1/1	0.94	0.11	65,65,65,65	0
34	MG	0	8097	1/1	0.94	0.13	57,57,57,57	0
38	SR	0	9452	1/1	0.94	0.16	106,106,106,106	0
38	SR	0	9508	1/1	0.94	0.08	97,97,97,97	0
34	MG	T	8073	1/1	0.94	0.11	43,43,43,43	0
36	NA	0	9157	1/1	0.94	0.18	47,47,47,47	0
36	NA	0	9150	1/1	0.94	0.21	47,47,47,47	0
36	NA	0	9163	1/1	0.94	0.17	73,73,73,73	0
34	MG	2	8076	1/1	0.94	0.17	64,64,64,64	0
36	NA	0	9110	1/1	0.94	0.33	46,46,46,46	0
39	CD	O	9205	1/1	0.94	0.05	132,132,132,132	0
38	SR	0	9570	1/1	0.94	0.07	111,111,111,111	0
36	NA	0	9149	1/1	0.94	0.29	49,49,49,49	0
34	MG	0	8057	1/1	0.94	0.20	77,77,77,77	0
38	SR	0	9522	1/1	0.95	0.04	114,114,114,114	0
36	NA	0	9155	1/1	0.95	0.18	60,60,60,60	0
34	MG	0	8003	1/1	0.95	0.13	35,35,35,35	0
37	CL	0	9317	1/1	0.95	0.06	52,52,52,52	0
34	MG	0	8068	1/1	0.95	0.14	48,48,48,48	0
34	MG	0	8004	1/1	0.95	0.10	35,35,35,35	0
37	CL	0	9322	1/1	0.95	0.38	61,61,61,61	0
36	NA	0	9125	1/1	0.95	0.81	92,92,92,92	0
38	SR	H	9486	1/1	0.95	0.15	125,125,125,125	0
38	SR	0	9517	1/1	0.95	0.06	110,110,110,110	0
34	MG	0	8082	1/1	0.95	0.20	82,82,82,82	0
38	SR	0	9505	1/1	0.95	0.07	106,106,106,106	0
38	SR	0	9483	1/1	0.95	0.06	77,77,77,77	0
37	CL	J	9321	1/1	0.95	0.11	66,66,66,66	0
34	MG	0	8045	1/1	0.95	0.26	72,72,72,72	0
38	SR	0	9560	1/1	0.95	0.08	101,101,101,101	0
34	MG	0	8116	1/1	0.95	0.10	64,64,64,64	0
34	MG	0	8083	1/1	0.95	0.11	53,53,53,53	0
36	NA	C	9104	1/1	0.95	0.16	33,33,33,33	0
38	SR	0	9495	1/1	0.95	0.14	111,111,111,111	0
37	CL	M	9318	1/1	0.95	0.17	41,41,41,41	0
34	MG	0	8098	1/1	0.95	0.07	45,45,45,45	0
34	MG	0	8079	1/1	0.95	0.13	33,33,33,33	0
36	NA	0	9139	1/1	0.95	0.10	43,43,43,43	0
34	MG	0	8029	1/1	0.95	0.22	35,35,35,35	0
34	MG	0	8067	1/1	0.95	0.11	40,40,40,40	0
34	MG	0	8021	1/1	0.95	0.16	56,56,56,56	0
34	MG	0	8070	1/1	0.96	0.14	24,24,24,24	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	NA	0	9162	1/1	0.96	0.15	52,52,52,52	0
37	CL	J	9302	1/1	0.96	0.07	53,53,53,53	0
36	NA	R	9137	1/1	0.96	0.08	36,36,36,36	0
38	SR	F	9595	1/1	0.96	0.16	109,109,109,109	0
36	NA	0	9156	1/1	0.96	0.16	57,57,57,57	0
38	SR	0	9490	1/1	0.96	0.13	116,116,116,116	0
38	SR	0	9530	1/1	0.96	0.11	72,72,72,72	0
34	MG	0	8060	1/1	0.96	0.07	82,82,82,82	0
38	SR	0	9440	1/1	0.96	0.05	72,72,72,72	0
37	CL	Y	9320	1/1	0.96	0.08	47,47,47,47	0
36	NA	0	9178	1/1	0.96	0.45	54,54,54,54	0
38	SR	0	9585	1/1	0.96	0.08	94,94,94,94	0
37	CL	3	9304	1/1	0.96	0.07	61,61,61,61	0
36	NA	0	9107	1/1	0.96	0.40	71,71,71,71	0
38	SR	0	9433	1/1	0.96	0.12	75,75,75,75	0
36	NA	0	9115	1/1	0.96	0.18	41,41,41,41	0
34	MG	0	8042	1/1	0.96	0.11	48,48,48,48	0
34	MG	Y	8109	1/1	0.96	0.12	45,45,45,45	0
34	MG	0	8112	1/1	0.96	0.06	46,46,46,46	0
36	NA	0	9105	1/1	0.96	0.09	44,44,44,44	0
37	CL	N	9307	1/1	0.96	0.16	65,65,65,65	0
38	SR	0	9447	1/1	0.97	0.07	73,73,73,73	0
34	MG	0	8027	1/1	0.97	0.24	36,36,36,36	0
37	CL	0	9316	1/1	0.97	0.26	78,78,78,78	0
34	MG	0	8002	1/1	0.97	0.09	34,34,34,34	0
34	MG	A	8066	1/1	0.97	0.10	57,57,57,57	0
37	CL	0	9311	1/1	0.97	0.15	71,71,71,71	0
38	SR	0	9426	1/1	0.97	0.08	71,71,71,71	0
34	MG	0	8009	1/1	0.97	0.10	21,21,21,21	0
34	MG	0	8114	1/1	0.97	0.47	83,83,83,83	0
38	SR	0	9466	1/1	0.97	0.06	96,96,96,96	0
38	SR	0	9545	1/1	0.97	0.06	85,85,85,85	0
38	SR	A	9437	1/1	0.97	0.10	70,70,70,70	0
37	CL	0	9315	1/1	0.97	0.09	52,52,52,52	0
34	MG	0	8012	1/1	0.97	0.22	39,39,39,39	0
38	SR	0	9601	1/1	0.97	0.06	119,119,119,119	0
38	SR	0	9438	1/1	0.97	0.09	70,70,70,70	0
34	MG	0	8117	1/1	0.97	0.12	46,46,46,46	0
38	SR	0	9446	1/1	0.97	0.07	88,88,88,88	0
34	MG	0	8044	1/1	0.97	0.06	35,35,35,35	0
38	SR	0	9534	1/1	0.97	0.14	111,111,111,111	0
36	NA	0	9127	1/1	0.97	0.10	60,60,60,60	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
38	SR	0	9442	1/1	0.97	0.10	66,66,66,66	0
38	SR	A	9436	1/1	0.97	0.06	60,60,60,60	0
34	MG	0	8088	1/1	0.97	0.11	28,28,28,28	0
34	MG	0	8046	1/1	0.97	0.05	39,39,39,39	0
36	NA	0	9108	1/1	0.97	0.10	34,34,34,34	0
36	NA	0	9160	1/1	0.97	0.17	46,46,46,46	0
36	NA	0	9138	1/1	0.97	0.07	62,62,62,62	0
38	SR	0	9568	1/1	0.97	0.07	80,80,80,80	0
34	MG	K	8069	1/1	0.97	0.17	25,25,25,25	0
38	SR	0	9405	1/1	0.97	0.16	59,59,59,59	0
38	SR	0	9432	1/1	0.97	0.14	68,68,68,68	0
34	MG	0	8041	1/1	0.97	0.09	55,55,55,55	0
36	NA	0	9134	1/1	0.97	0.10	47,47,47,47	0
34	MG	0	8084	1/1	0.97	0.40	89,89,89,89	0
37	CL	R	9306	1/1	0.97	0.10	45,45,45,45	0
34	MG	0	8110	1/1	0.97	0.11	45,45,45,45	0
38	SR	0	9489	1/1	0.98	0.11	94,94,94,94	0
34	MG	0	8075	1/1	0.98	0.07	47,47,47,47	0
38	SR	0	9464	1/1	0.98	0.05	81,81,81,81	0
38	SR	0	9477	1/1	0.98	0.10	86,86,86,86	0
38	SR	0	9421	1/1	0.98	0.10	78,78,78,78	0
34	MG	0	8001	1/1	0.98	0.19	22,22,22,22	0
38	SR	0	9629	1/1	0.98	0.08	75,75,75,75	0
38	SR	0	9566	1/1	0.98	0.04	80,80,80,80	0
38	SR	9	9481	1/1	0.98	0.08	89,89,89,89	0
34	MG	0	8020	1/1	0.98	0.16	36,36,36,36	0
34	MG	0	8056	1/1	0.98	0.23	44,44,44,44	0
38	SR	0	9454	1/1	0.98	0.10	82,82,82,82	0
38	SR	0	9435	1/1	0.98	0.08	76,76,76,76	0
37	CL	0	9305	1/1	0.98	0.07	61,61,61,61	0
38	SR	0	9427	1/1	0.98	0.12	56,56,56,56	0
38	SR	0	9443	1/1	0.98	0.10	63,63,63,63	0
34	MG	0	8031	1/1	0.98	0.12	49,49,49,49	0
38	SR	0	9475	1/1	0.98	0.13	83,83,83,83	0
38	SR	0	9445	1/1	0.98	0.09	57,57,57,57	0
36	NA	0	9118	1/1	0.98	0.21	66,66,66,66	0
38	SR	0	9506	1/1	0.98	0.04	68,68,68,68	0
36	NA	0	9154	1/1	0.98	0.15	54,54,54,54	0
36	NA	0	9130	1/1	0.98	0.15	50,50,50,50	0
38	SR	0	9461	1/1	0.98	0.06	82,82,82,82	0
34	MG	0	8039	1/1	0.98	0.17	49,49,49,49	0
34	MG	0	8096	1/1	0.98	0.05	41,41,41,41	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
38	SR	0	9456	1/1	0.98	0.10	67,67,67,67	0
38	SR	0	9469	1/1	0.98	0.05	85,85,85,85	0
38	SR	0	9455	1/1	0.98	0.10	88,88,88,88	0
36	NA	0	9136	1/1	0.98	0.12	34,34,34,34	0
34	MG	0	8005	1/1	0.98	0.06	29,29,29,29	0
38	SR	0	9457	1/1	0.98	0.08	51,51,51,51	0
38	SR	0	9414	1/1	0.98	0.12	57,57,57,57	0
38	SR	0	9441	1/1	0.98	0.07	68,68,68,68	0
34	MG	0	8017	1/1	0.98	0.14	31,31,31,31	0
36	NA	Q	9148	1/1	0.98	0.09	49,49,49,49	0
38	SR	0	9462	1/1	0.98	0.10	74,74,74,74	0
34	MG	0	8080	1/1	0.98	0.17	57,57,57,57	0
38	SR	A	9497	1/1	0.98	0.09	96,96,96,96	0
37	CL	0	9312	1/1	0.99	0.10	57,57,57,57	0
38	SR	0	9478	1/1	0.99	0.06	77,77,77,77	0
34	MG	0	8026	1/1	0.99	0.15	30,30,30,30	0
34	MG	0	8028	1/1	0.99	0.13	37,37,37,37	0
38	SR	0	9428	1/1	0.99	0.07	55,55,55,55	0
37	CL	0	9314	1/1	0.99	0.06	51,51,51,51	0
38	SR	0	9449	1/1	0.99	0.09	67,67,67,67	0
38	SR	0	9473	1/1	0.99	0.03	82,82,82,82	0
38	SR	0	9467	1/1	0.99	0.10	86,86,86,86	0
34	MG	0	8008	1/1	0.99	0.19	16,16,16,16	0
38	SR	0	9410	1/1	0.99	0.14	41,41,41,41	0
38	SR	0	9431	1/1	0.99	0.13	65,65,65,65	0
38	SR	0	9430	1/1	0.99	0.10	49,49,49,49	0
38	SR	0	9515	1/1	0.99	0.14	100,100,100,100	0
37	CL	B	9319	1/1	0.99	0.17	54,54,54,54	0
38	SR	0	9488	1/1	0.99	0.11	86,86,86,86	0
39	CD	1	9202	1/1	0.99	0.05	54,54,54,54	0
38	SR	0	9451	1/1	0.99	0.12	60,60,60,60	0
38	SR	0	9413	1/1	0.99	0.12	49,49,49,49	0
38	SR	0	9408	1/1	0.99	0.12	36,36,36,36	0
36	NA	0	9123	1/1	0.99	0.09	52,52,52,52	0
38	SR	L	9409	1/1	0.99	0.07	37,37,37,37	0
38	SR	0	9425	1/1	0.99	0.15	56,56,56,56	0
38	SR	0	9434	1/1	0.99	0.14	64,64,64,64	0
39	CD	3	9204	1/1	0.99	0.03	64,64,64,64	0
38	SR	1	9419	1/1	0.99	0.09	40,40,40,40	0
38	SR	0	9480	1/1	0.99	0.05	93,93,93,93	0
38	SR	3	9439	1/1	0.99	0.05	72,72,72,72	0
34	MG	0	8015	1/1	0.99	0.09	35,35,35,35	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
38	SR	0	9417	1/1	0.99	0.08	63,63,63,63	0
38	SR	0	9474	1/1	0.99	0.08	73,73,73,73	0
37	CL	0	9313	1/1	0.99	0.10	59,59,59,59	0
38	SR	1	9460	1/1	0.99	0.10	52,52,52,52	0
37	CL	O	9308	1/1	0.99	0.09	67,67,67,67	0
34	MG	0	8074	1/1	0.99	0.18	27,27,27,27	0
34	MG	0	8038	1/1	0.99	0.25	25,25,25,25	0
37	CL	0	9303	1/1	0.99	0.13	53,53,53,53	0
38	SR	S	9470	1/1	0.99	0.16	101,101,101,101	0
38	SR	0	9411	1/1	0.99	0.14	43,43,43,43	0
38	SR	0	9450	1/1	0.99	0.07	72,72,72,72	0
38	SR	0	9429	1/1	0.99	0.10	72,72,72,72	0
38	SR	0	9453	1/1	0.99	0.06	72,72,72,72	0
38	SR	R	9418	1/1	0.99	0.15	57,57,57,57	0
38	SR	0	9444	1/1	0.99	0.05	55,55,55,55	0
38	SR	0	9422	1/1	0.99	0.10	58,58,58,58	0
38	SR	0	9412	1/1	0.99	0.13	45,45,45,45	0
38	SR	0	9498	1/1	0.99	0.05	63,63,63,63	0
38	SR	B	9458	1/1	0.99	0.05	82,82,82,82	0
38	SR	0	9407	1/1	1.00	0.13	47,47,47,47	0
38	SR	0	9424	1/1	1.00	0.16	49,49,49,49	0
38	SR	0	9448	1/1	1.00	0.07	63,63,63,63	0
38	SR	0	9423	1/1	1.00	0.05	64,64,64,64	0
38	SR	0	9406	1/1	1.00	0.13	35,35,35,35	0
38	SR	0	9415	1/1	1.00	0.10	56,56,56,56	0
38	SR	0	9416	1/1	1.00	0.08	43,43,43,43	0
39	CD	U	9201	1/1	1.00	0.09	53,53,53,53	0
38	SR	0	9420	1/1	1.00	0.17	70,70,70,70	0

## 6.5 Other polymers

There are no such residues in this entry.