wwPDB X-ray Structure Validation Summary Report (i)

Aug 22, 2023 – 02:47 AM EDT

PDB ID	:	2QA4
Title	:	A more complete structure of the the L7/L12 stalk of the Haloarcula marismortui 50S large ribosomal subunit
Authors	:	Steitz, T.A.; Kavran, J.M.
Deposited on	:	2007-06-14
Resolution	:	3.00 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

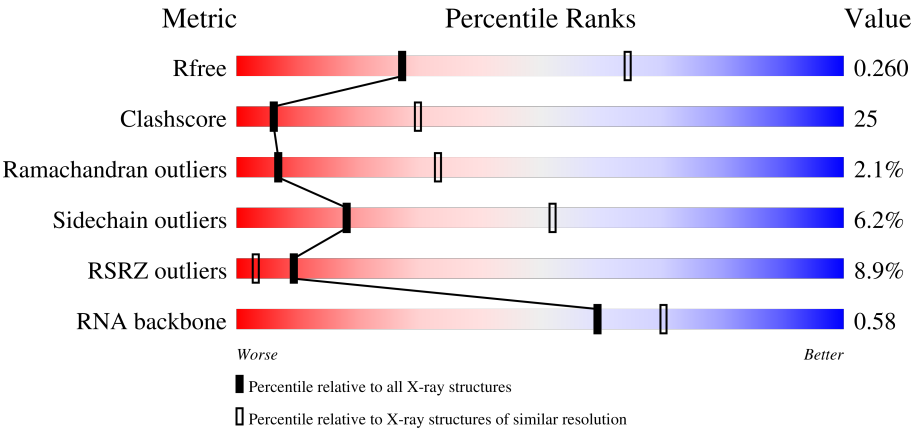
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	28% 57% 9% 6%
2	9	122	17% 69% 13%
3	A	240	10% 61% 34%
4	B	338	4% 59% 36%

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Mol	Chain	Length	Quality of chain
5	C	246	2% 61% 34% 5%
6	D	177	33% 46% 28% 5% 21%
7	E	178	7% 60% 33%
8	F	120	4% 65% 31%
9	G	348	11% 12% 16% 5% 64%
10	H	171	4% 60% 32% 6%
11	I	162	39% 34% 27% 10% 27%
12	J	145	60% 33% 5%
13	K	132	2% 62% 34%
14	L	165	24% 60% 27% 12%
15	M	196	11% 67% 31%
16	N	187	20% 57% 40%
17	O	116	71% 28%
18	P	149	12% 66% 26%
19	Q	96	7% 63% 35%
20	R	155	% 71% 23%
21	S	85	2% 69% 22% 5%
22	T	120	19% 58% 38%
23	U	67	33% 49% 30% 21%
24	V	71	13% 54% 37% 8%
25	W	154	46% 51%
26	X	92	8% 47% 39% 11%
27	Y	241	% 34% 22% 41%
28	Z	92	73% 48% 32% 21%
29	1	57	54% 37% 7%

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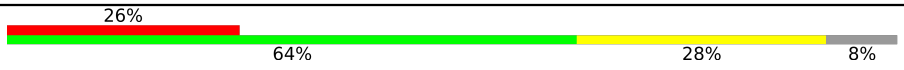
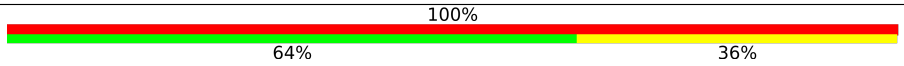
Mol	Chain	Length	Quality of chain
30	2	50	
31	3	92	

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
32	MG	0	2971	-	-	-	X
32	MG	0	2973	-	-	-	X
32	MG	0	2980	-	-	-	X
32	MG	0	2984	-	-	-	X
32	MG	0	2998	-	-	-	X
32	MG	0	3006	-	-	-	X
32	MG	0	3025	-	-	-	X
32	MG	0	3026	-	-	-	X
32	MG	0	3028	-	-	-	X
32	MG	0	3029	-	-	-	X
32	MG	3	93	-	-	-	X
32	MG	A	240	-	-	-	X
32	MG	B	338	-	-	-	X
32	MG	K	133	-	-	-	X
32	MG	Y	241	-	-	-	X
33	K	0	3031	-	-	-	X
33	K	M	196	-	-	-	X
34	NA	0	3033	-	-	-	X
34	NA	0	3034	-	-	-	X
34	NA	0	3039	-	-	-	X
34	NA	0	3044	-	-	-	X
34	NA	0	3050	-	-	-	X
34	NA	0	3052	-	-	-	X
34	NA	0	3057	-	-	-	X
34	NA	0	3059	-	-	-	X
34	NA	0	3075	-	-	-	X
34	NA	0	3077	-	-	-	X
34	NA	0	3082	-	-	-	X
34	NA	0	3084	-	-	-	X
34	NA	0	3094	-	-	-	X
34	NA	0	3098	-	-	-	X
34	NA	0	3099	-	-	-	X
34	NA	0	3100	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	NA	0	3103	-	-	-	X
34	NA	S	85	-	-	-	X
35	CL	0	3106	-	-	-	X
35	CL	0	3109	-	-	-	X
35	CL	0	3112	-	-	-	X
35	CL	3	95	-	-	X	X
35	CL	J	147	-	-	X	-
35	CL	J	149	-	-	X	-
35	CL	O	117	-	-	-	X
35	CL	Q	97	-	-	-	X
36	CD	O	116	-	-	-	X

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 92248 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
			Total	C	N	O	P			
1	0	2753	58979	26332	10869	19036	2742	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	conflict	GB 3377779

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

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

- Molecule 3 is a protein called 50S ribosomal protein L2P.

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

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

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

- Molecule 5 is a protein called 50S ribosomal protein L4P.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	73	LEU	GLN	conflict	UNP P12735

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

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

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

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

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

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

- Molecule 9 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	125	Total	C	N	O	S	0	0	0
			959	592	162	203	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	248	ASP	ALA	conflict	UNP P15825

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

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

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ASP	-	insertion	UNP P60617
H	165	SER	LYS	conflict	UNP P60617
H	166	SER	VAL	conflict	UNP P60617
H	167	PRO	GLU	conflict	UNP P60617
H	168	ALA	ARG	conflict	UNP P60617
H	?	-	GLU	deletion	UNP P60617
H	?	-	GLU	deletion	UNP P60617
H	?	-	LEU	deletion	UNP P60617
H	?	-	LEU	deletion	UNP P60617
H	170	ASN	ILE	conflict	UNP P60617

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	118	Total	C	N	O	S	0	0	0
			876	548	135	192	1			

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 15 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1559	943	332	283	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	UNP P60618
M	194	ALA	GLY	conflict	UNP P60618

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

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

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

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

- Molecule 18 is a protein called 50S ribosomal protein L19e.

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

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

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

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

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

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

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

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

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

- Molecule 23 is a protein called 50S ribosomal protein L24e.

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

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

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

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

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L31E.

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

- Molecule 27 is a protein called 50S ribosomal protein L32e.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	73	Total	C	N	O	S	0	0	0
			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	UNP P60619

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

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

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

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

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

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

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	108	Total	Mg	0	0
			108	108		
32	9	1	Total	Mg	0	0
			1	1		
32	A	2	Total	Mg	0	0
			2	2		
32	B	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	3	1	Total Mg 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	1	Total K 1 1	0	0
33	M	1	Total K 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	73	Total Na 73 73	0	0
34	9	3	Total Na 3 3	0	0
34	A	1	Total Na 1 1	0	0
34	C	1	Total Na 1 1	0	0
34	H	1	Total Na 1 1	0	0
34	J	1	Total Na 1 1	0	0
34	L	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	R	2	Total Na 2 2	0	0
34	S	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	8	Total Cl 8 8	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	1	Total Cl 1 1	0	0
35	B	1	Total Cl 1 1	0	0
35	J	3	Total Cl 3 3	0	0
35	K	1	Total Cl 1 1	0	0
35	L	1	Total Cl 1 1	0	0
35	M	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	Q	1	Total Cl 1 1	0	0
35	R	1	Total Cl 1 1	0	0
35	Y	1	Total Cl 1 1	0	0
35	3	1	Total Cl 1 1	0	0

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

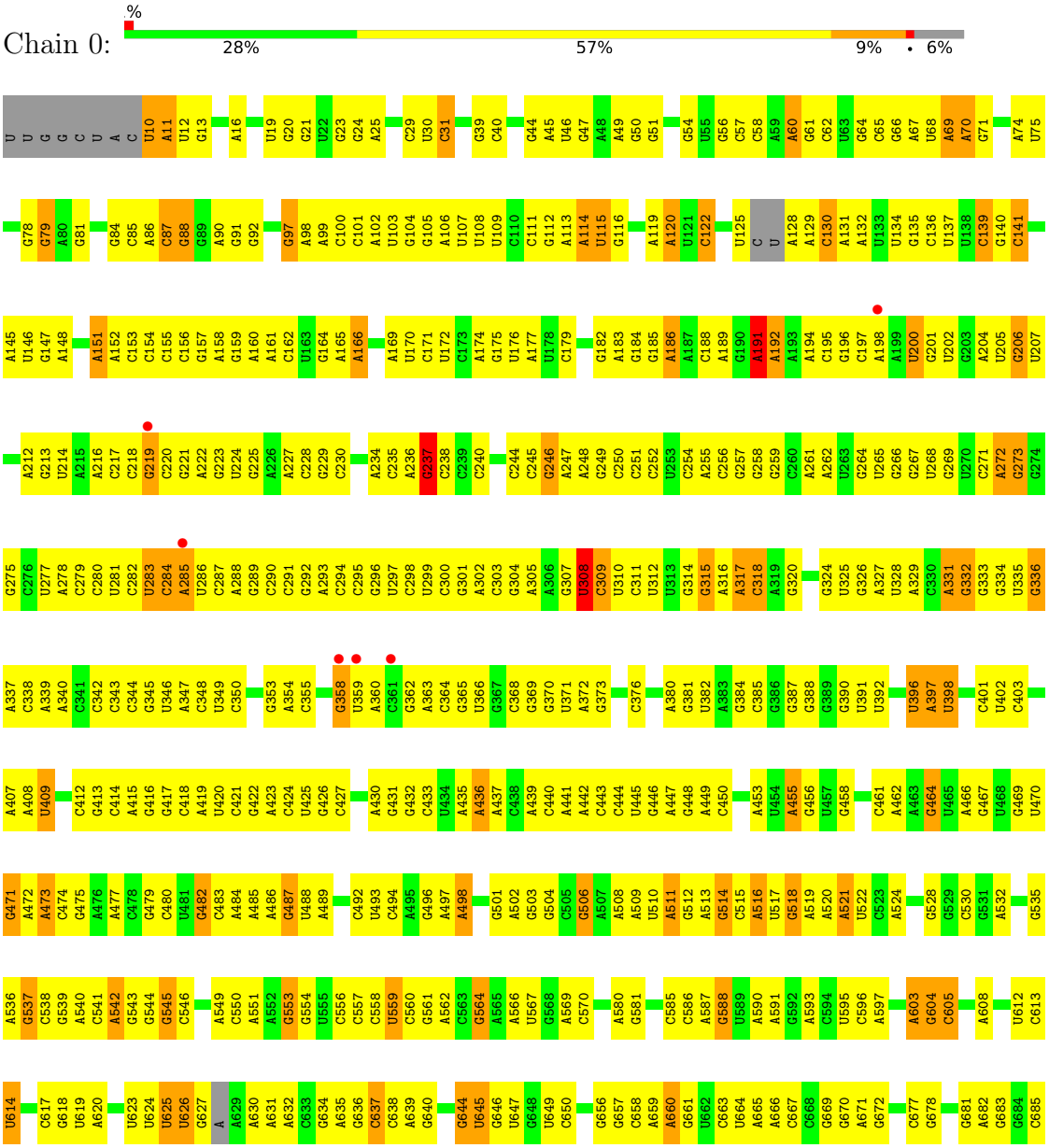
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	O	1	Total Cd 1 1	0	0
36	U	1	Total Cd 1 1	0	0
36	Z	1	Total Cd 1 1	0	0
36	1	1	Total Cd 1 1	0	0
36	3	1	Total Cd 1 1	0	0

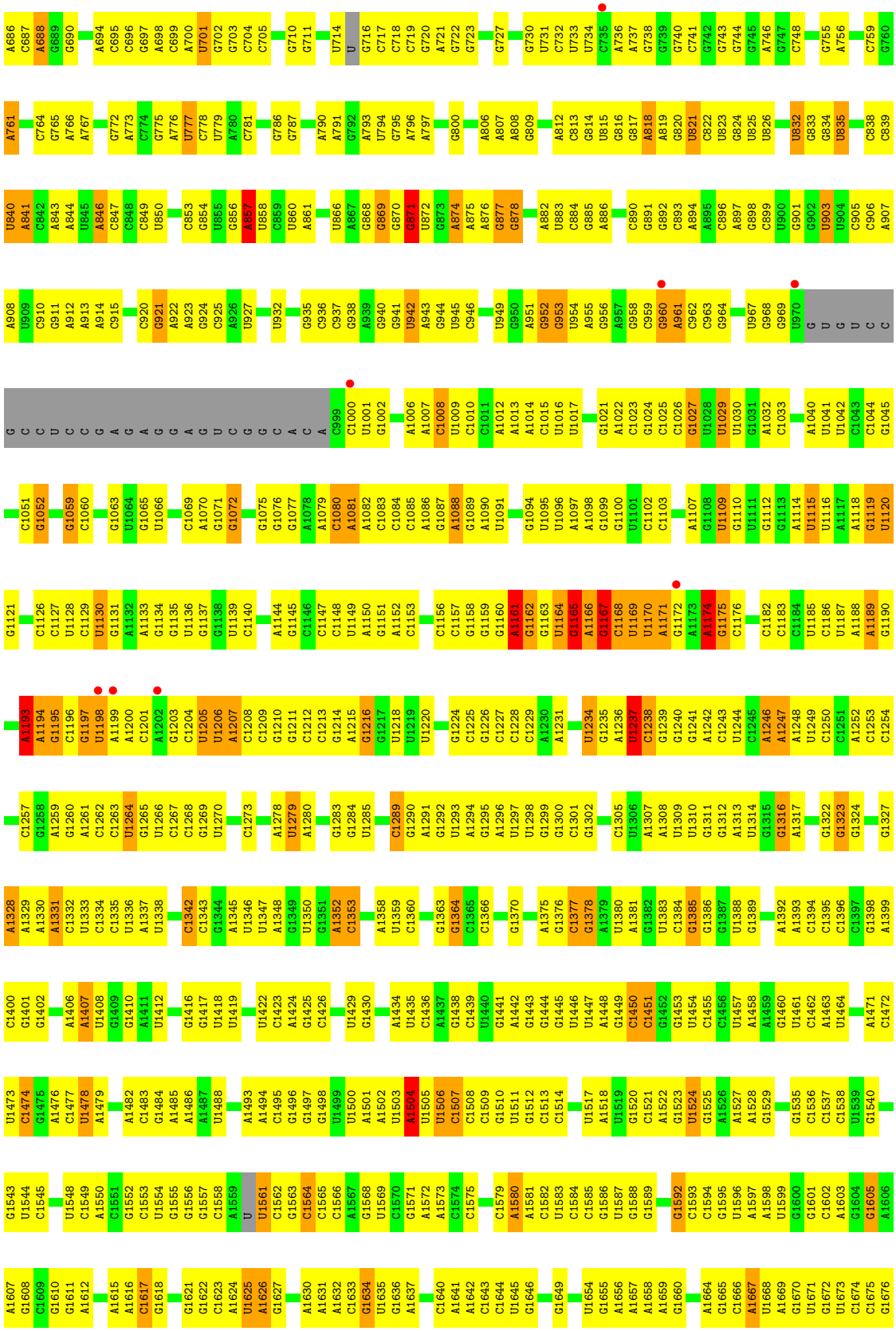
3 Residue-property plots (i)

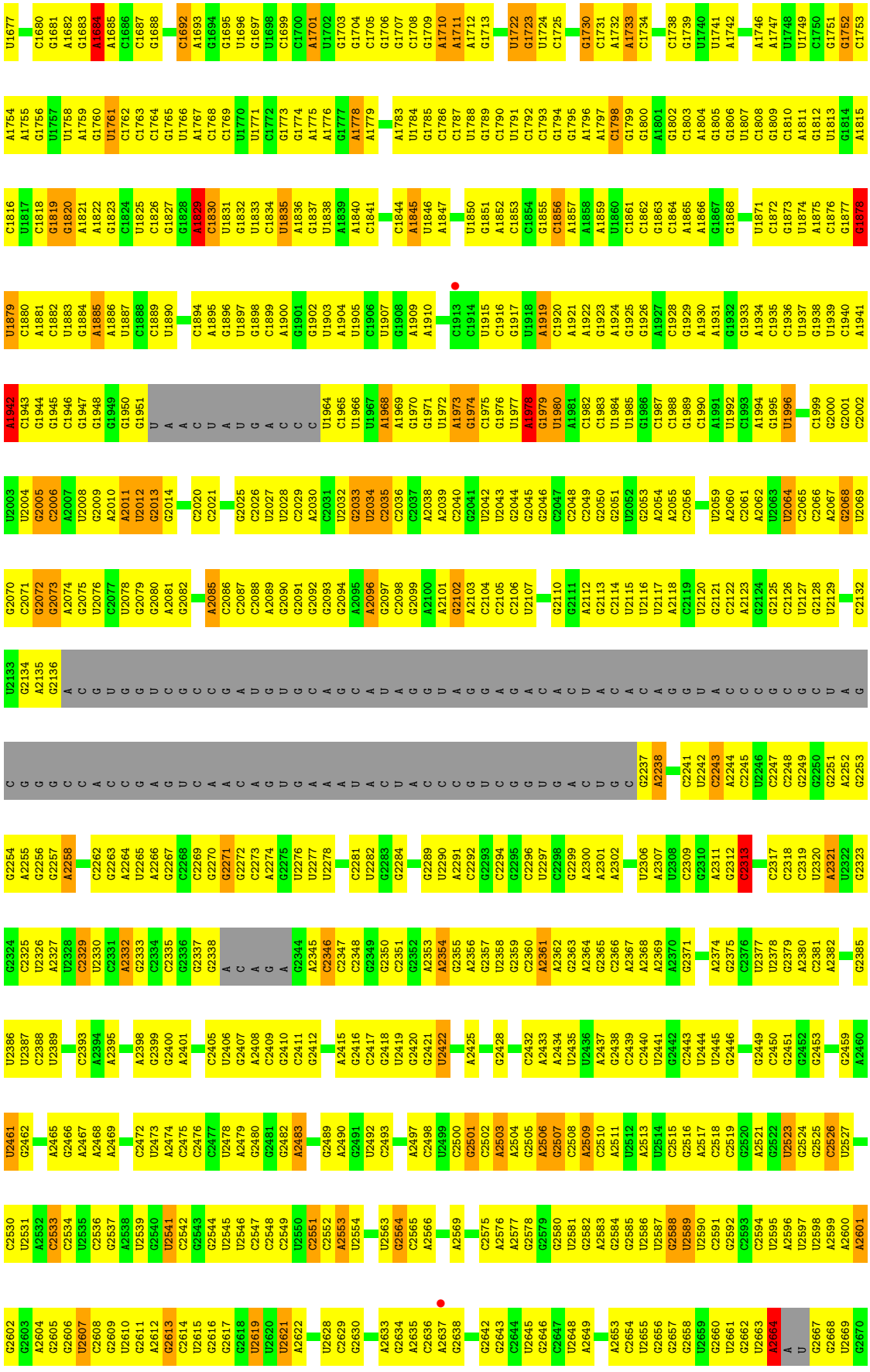
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

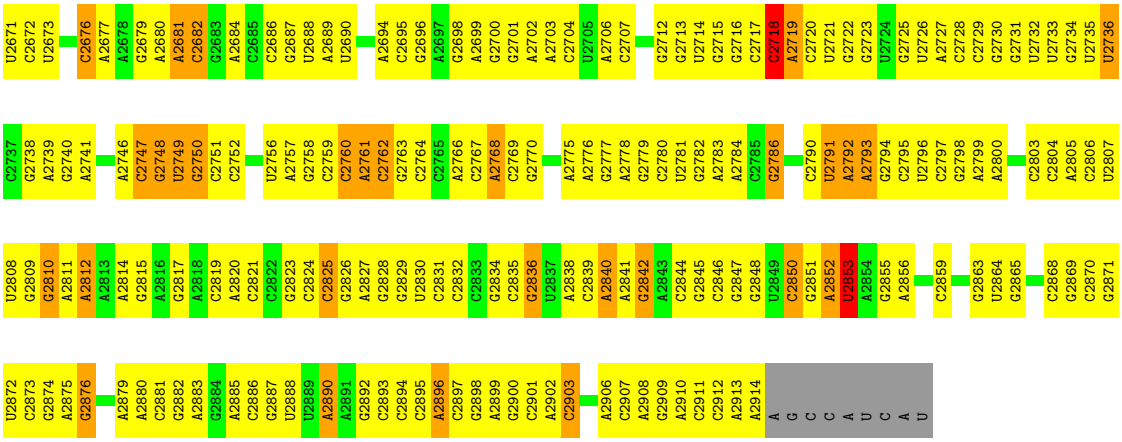
- Molecule 1: 23S RIBOSOMAL RNA

Chain 0:



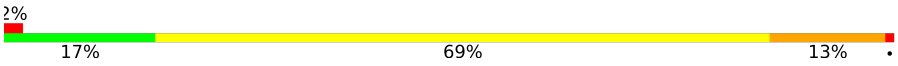

A686 C687 A688 G689 G690
A694 C695 C696 G697 A698 C699 A700 U701 G702 G703 C704 C705
G710 G711
U714 U
G716 C717 C718 C719 G720 A721 G722 G723
G727
G730 U731 C732 U733 U734 C735 A736 A737 G738 G739 G740 C741 G742 G743 G744 G745 A746 G747 C748
G755 A756
C759 G760
A761
C764 G765 A766 A767
G772 A773 C774 G775 A776 U777 C778 U779 A780 C781
G786 G787
A790 A791 G792
A793 U794 G795 A796 A797
G800
A806 A807 A808 G809
A812 C813 G814 U815 G816 G817 A818 A819 G820 U821 C822 U823 G824 U825 U826
U832 G833 G834 U835
C838 C839
U840 A841 C842 A843 A844 U845 A846 C847 C848 C849 U850
C853 G854 U855 G856 A857 U858
C859 U860 A861
U866 A867 G868 G869 G870 G871 U872 G873 A874 A875 A876 G877 G878
A882 U883 C884 G885 A886
C890 G891 G892 C893 A894 A895 C896 A897 G898 C899 U900 G901 G902 U903 U904 C905 C906 A907
A908 U909 C910 G911 A912 A913 A914 C915
C920 G921 A922 A923 G924 C925 A926 U927
U932
G935 C936 C937 G938 A939 G940 G941 U942 A943 G944 U945 C946
U949 G950 A951 G952 G953 U954 A955 G956 A957 G958 C959 G960 A961 C962 C963 G964
U967 G968 G969 U970 G U G U C C
G C C C U C C G A G A G G A G U C G G C A C A
C999 C1000 U1001 G1002 A1006 A1007 C1008 U1009 C1010 C1011 A1012 A1013 A1014 C1015 U1016 U1017 G1021 A1022 C1023 G1024 C1025 C1026 G1027 U1028 U1029 U1030 G1031 A1032 C1033 A1040 U1041 U1042 C1043 C1044 G1045
C1051 G1052 G1059 C1060 G1063 U1064 G1065 U1066 C1069 A1070 G1071 G1072 G1075 G1076 G1077 A1078 A1079 C1080 A1081 A1082 C1083 C1084 C1085 A1086 A1087 A1088 G1089 A1090 U1091 G1094 U1095 U1096 A1097 A1098 G1099 G1100 U1101 C1102 C1103 A1107 G1108 U1109 G1110 U1111 G1112 G1113 A1114 U1115 U1116 A1117 A1118 G1119 U1120
G1121 C1126 C1127 U1128 C1129 U1130 G1131 A1132 A1133 G1134 G1135 U1136 G1137 G1138 U1139 C1140 A1144 G1145 C1146 C1147 C1148 U1149 A1150 G1151 A1152 C1153 C1156 C1157 G1158 G1159 G1160 A1161 G1162 G1163 U1164 G1165 A1166 G1167 C1168 U1169 U1170 A1171 G1172 A1173 A1174 G1175 C1176 C1182 C1183 C1184 U1185 C1186 U1187 A1188 A1189 G1190
A1193 A1194 G1195 C1196 G1197 U1198 A1199 A1200 C1201 A1202 G1203 C1204 U1205 U1206 A1207 C1208 C1209 G1210 G1211 C1212 C1213 G1214 A1215 G1216 G1217 U1218 U1219 U1220 G1224 C1225 G1226 C1227 C1228 C1229 A1230 A1231 U1234 G1235 A1236 U1237 C1238 G1239 G1240 G1241 A1242 C1243 U1244 C1245 A1246 A1247 A1248 U1249 C1250 C1251 A1252 C1253 C1254
C1257 G1258 A1259 G1260 A1261 C1262 C1263 U1264 G1265 U1266 C1267 C1268 G1269 U1270 C1273 A1278 U1279 A1280 G1283 G1284 U1285 C1289 G1290 A1291 G1292 U1293 A1294 G1295 A1296 U1297 U1298 G1299 G1300 C1301 G1302 C1305 U1306 A1307 A1308 U1309 U1310 G1311 G1312 A1313 U1314 G1315 G1316 A1317 G1322 G1323 G1324 G1327
A1328 A1329 A1330 A1331 C1332 U1333 C1334 C1335 U1336 A1337 U1338 C1342 C1343 G1344 A1345 U1346 U1347 A1348 G1349 U1350 G1351 A1352 C1353 A1358 U1359 C1360 G1363 G1364 C1365 C1366 G1370 A1375 G1376 C1377 G1378 A1379 U1380 A1381 G1382 U1383 C1384 G1385 G1386 G1387 U1388 G1389 A1392 A1393 C1394 C1395 C1396 C1397 G1398 A1399
C1400 G1401 C1402 A1406 A1407 U1408 G1409 G1410 A1411 U1412 G1416 G1417 U1418 U1419 U1422 C1423 A1424 G1425 C1426 U1429 G1430 A1434 U1435 C1436 A1437 G1438 C1439 U1440 G1441 A1442 G1443 G1444 G1445 U1446 U1447 A1448 G1449 C1450 C1451 G1452 G1453 U1454 C1455 C1456 U1457 A1458 A1459 G1460 U1461 C1462 A1463 U1464 A1471 C1472
U1473 C1474 G1475 A1476 C1477 U1478 A1479 A1482 C1483 G1484 A1485 A1486 A1487 U1488 A1493 A1494 C1495 G1496 G1497 G1498 U1499 U1500 A1501 A1502 U1503 A1504 U1505 U1506 C1507 C1508 C1509 G1510 U1511 G1512 C1513 C1514 U1517 A1518 U1519 G1520 C1521 A1522 G1523 U1524 G1525 A1526 A1527 A1528 G1529 G1535 C1536 C1537 C1538 U1539 G1540
G1543 U1544 C1545 U1548 C1549 A1550 C1551 G1552 C1553 U1554 G1555 G1556 G1557 C1558 A1559 U A1561 C1562 G1563 C1564 C1565 C1566 A1567 G1568 U1569 C1570 G1571 A1572 A1573 C1574 C1575 C1579 A1580 A1581 C1582 U1583 C1584 C1585 G1586 U1587 G1588 G1589 G1592 C1593 C1594 G1595 U1596 A1597 A1598 U1599 G1600 G1601 C1602 A1603 G1604 G1605 A1606
A1607 G1608 C1609 G1610 G1611 A1612 A1615 A1616 C1617 G1618 G1621 G1622 C1623 A1624 U1625 A1626 G1627 A1630 A1631 A1632 C1633 G1634 U1635 G1636 A1637 C1640 A1641 A1642 C1643 C1644 U1645 G1646 G1649 U1654 G1655 A1656 A1657 A1658 A1659 G1660 A1664 G1665 C1666 A1667 U1668 A1669 G1670 U1671 G1672 U1673 C1674 C1675 G1676

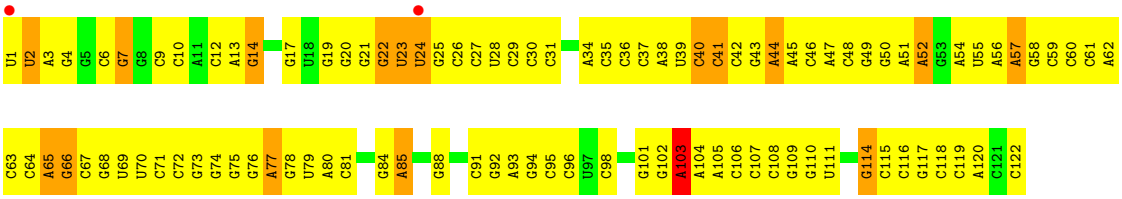




• Molecule 2: 5S RIBOSOMAL RNA

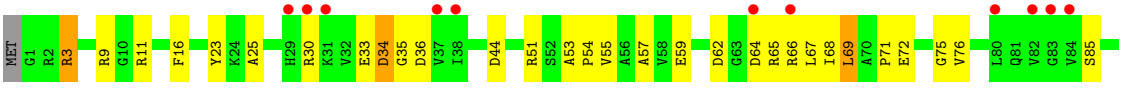
Chain 9:

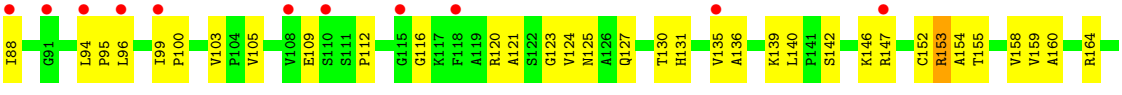


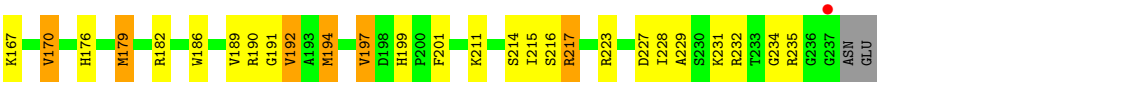


• Molecule 3: 50S ribosomal protein L2P

Chain A:

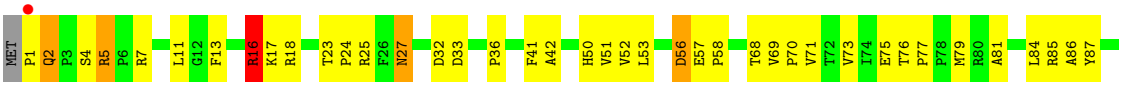


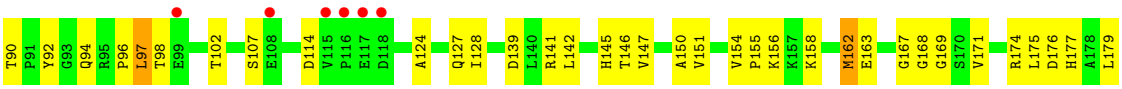


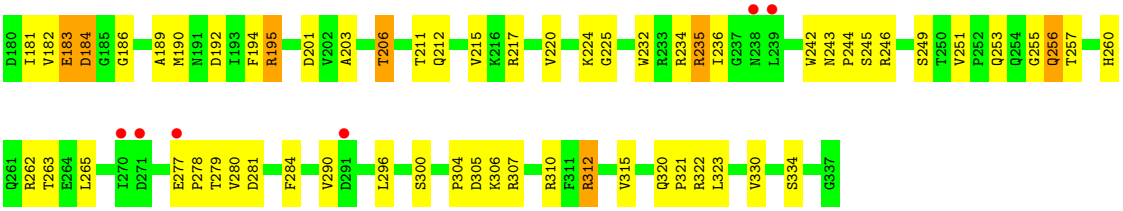


• Molecule 4: 50S ribosomal protein L3P

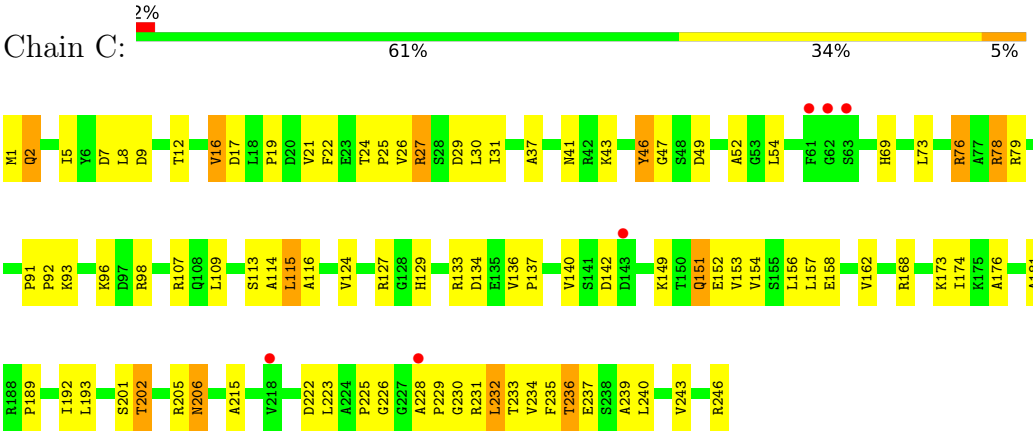
Chain B:



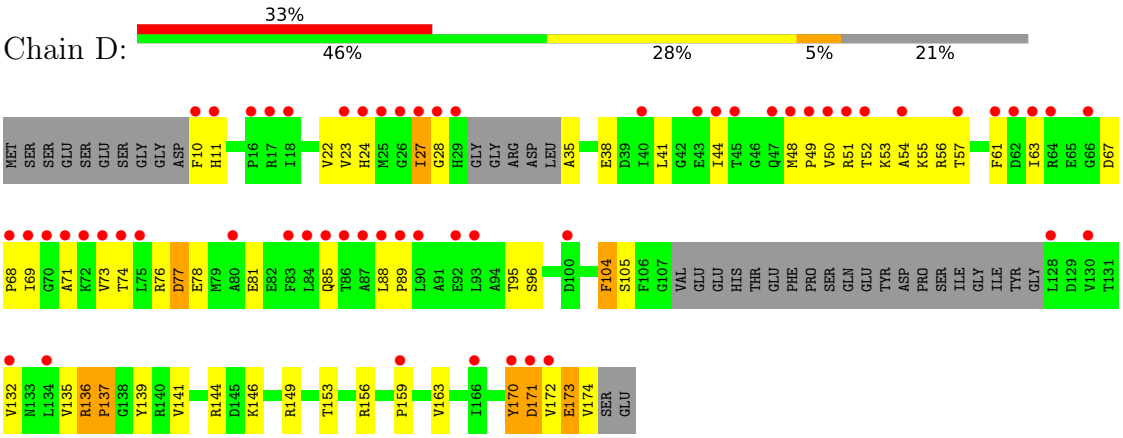




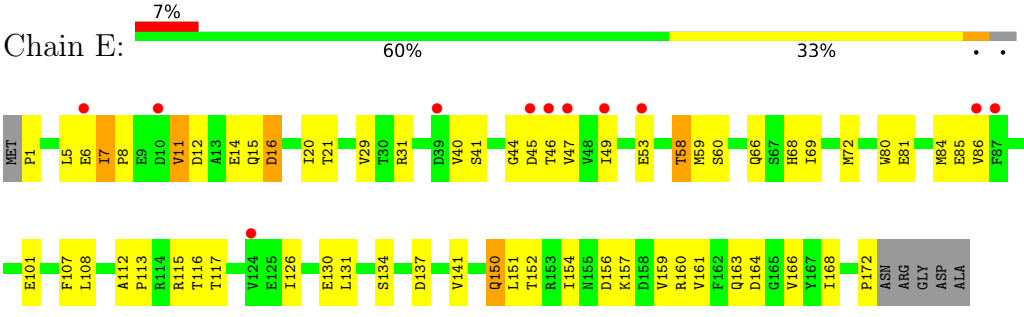
• Molecule 5: 50S ribosomal protein L4P



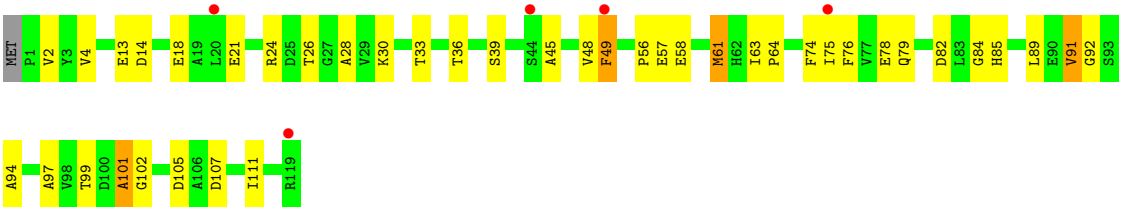
• Molecule 6: 50S ribosomal protein L5P



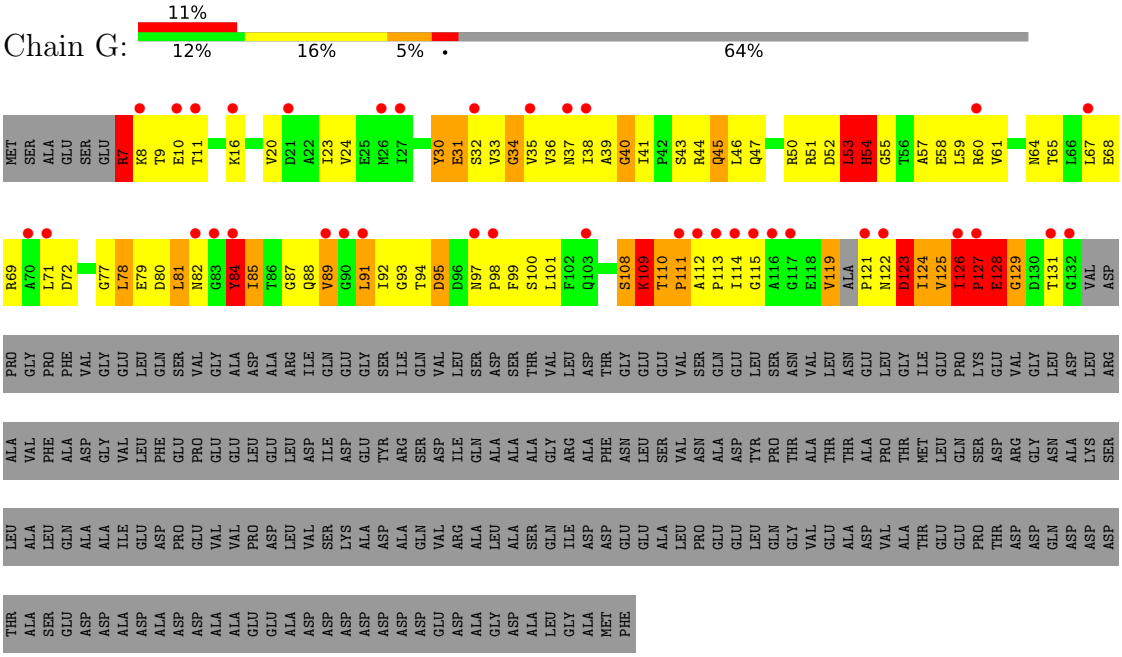
• Molecule 7: 50S ribosomal protein L6P



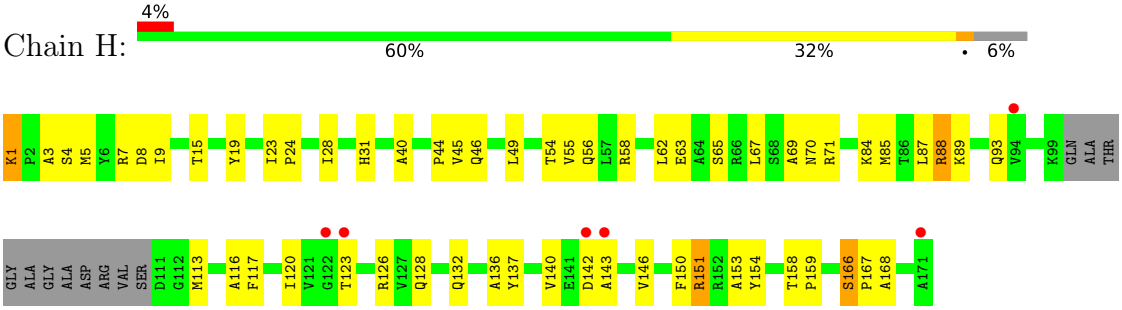
• Molecule 8: 50S ribosomal protein L7Ae



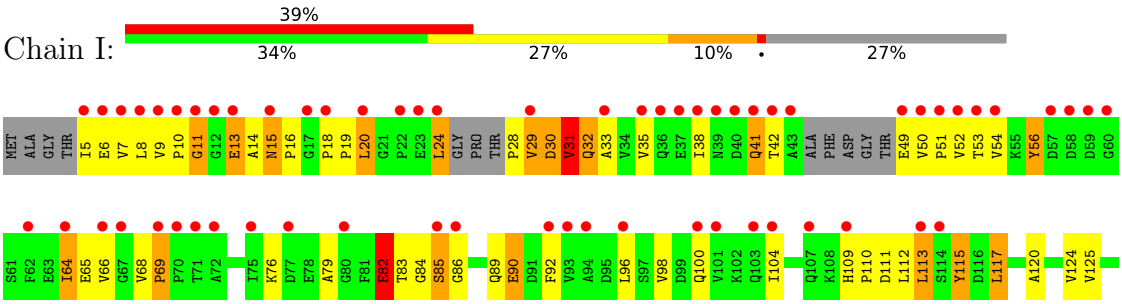
• Molecule 9: ACIDIC RIBOSOMAL PROTEIN P0 HOMO

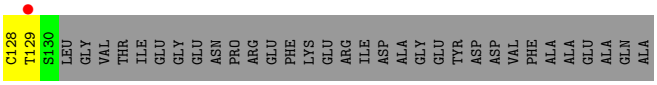


• Molecule 10: 50S ribosomal protein L10e



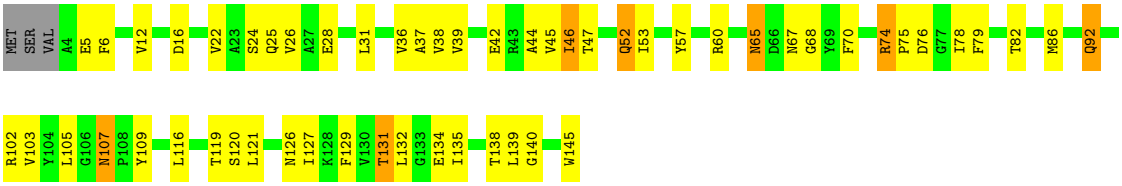
• Molecule 11: 50S ribosomal protein L11P





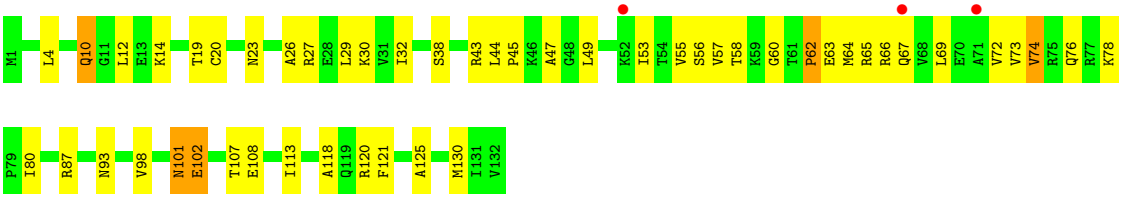
• Molecule 12: 50S ribosomal protein L13P

Chain J:



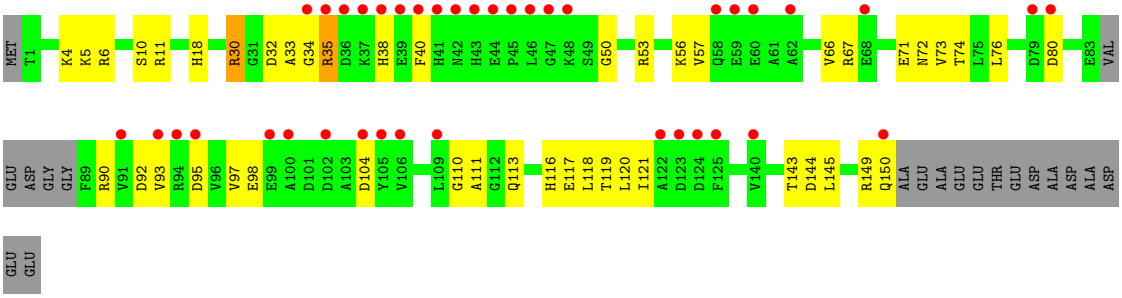
• Molecule 13: 50S ribosomal protein L14P

Chain K:



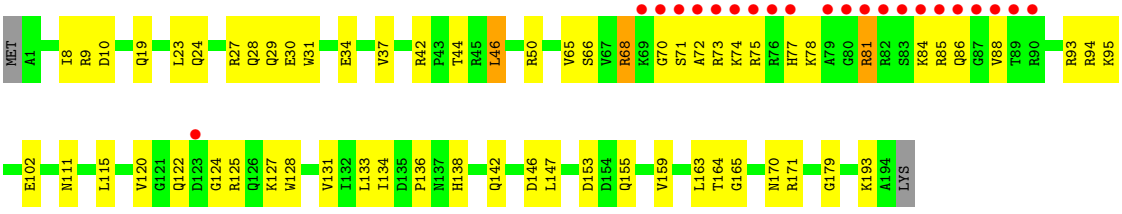
• Molecule 14: 50S ribosomal protein L15P

Chain L:



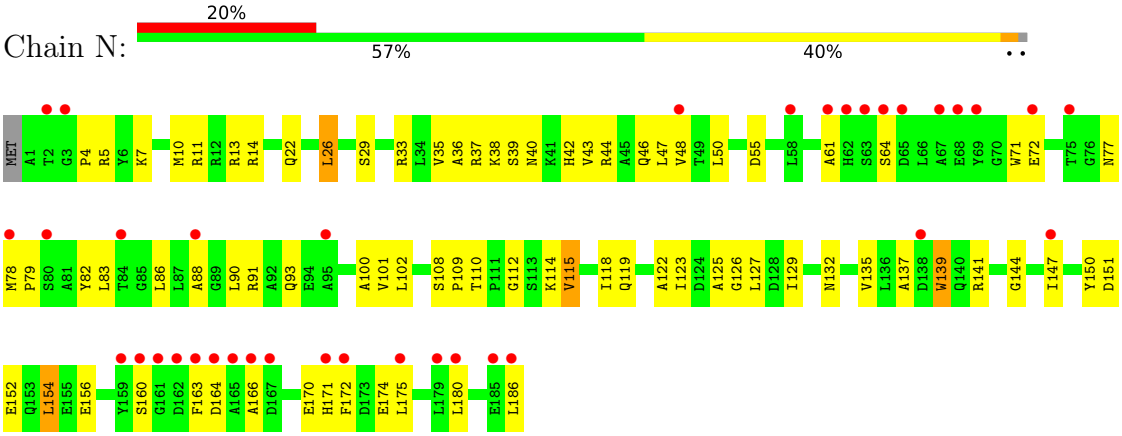
• Molecule 15: 50S ribosomal protein L15e

Chain M:



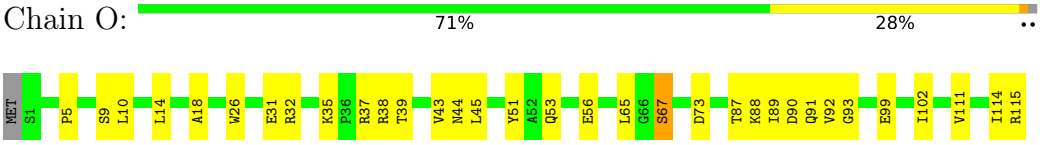
• Molecule 16: 50S ribosomal protein L18P

Chain N:



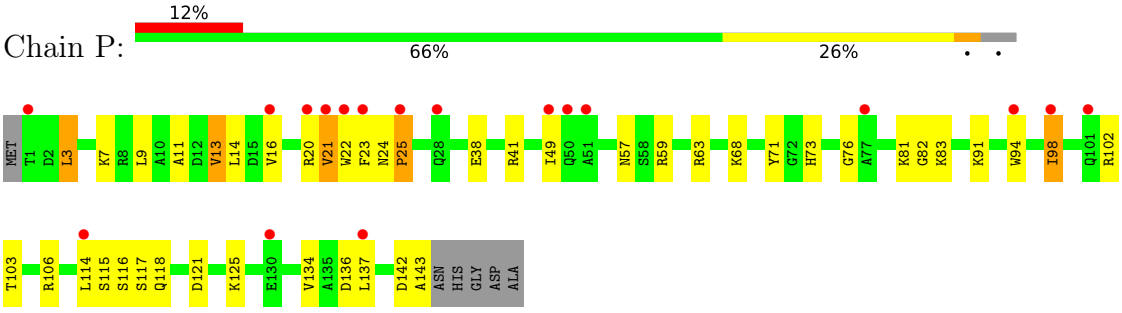
• Molecule 17: 50S ribosomal protein L18e

Chain O:



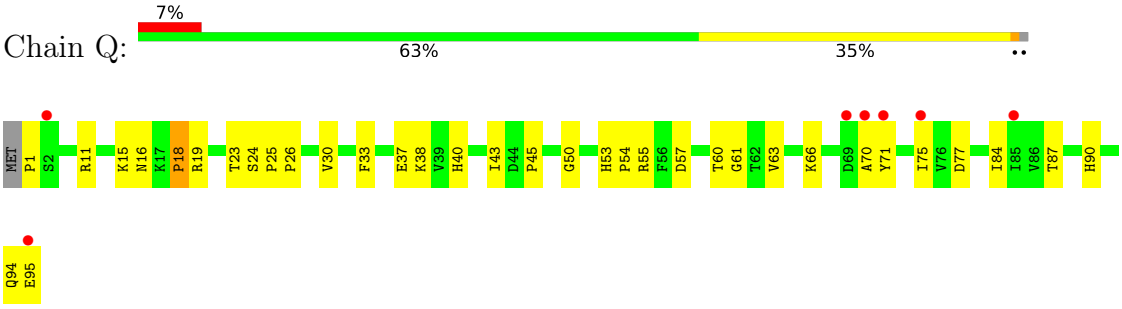
• Molecule 18: 50S ribosomal protein L19e

Chain P:



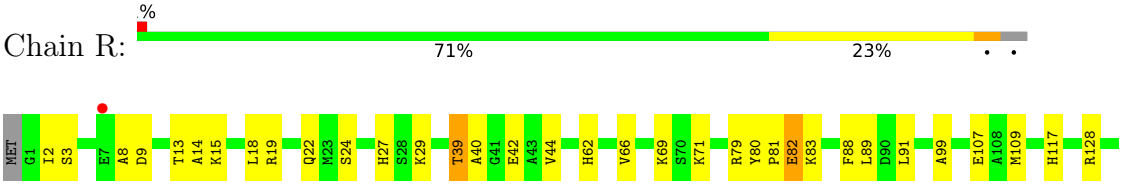
• Molecule 19: 50S ribosomal protein L21e

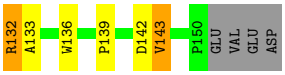
Chain Q:



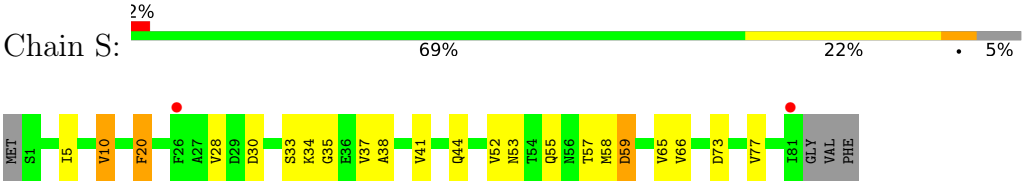
• Molecule 20: 50S ribosomal protein L22P

Chain R:

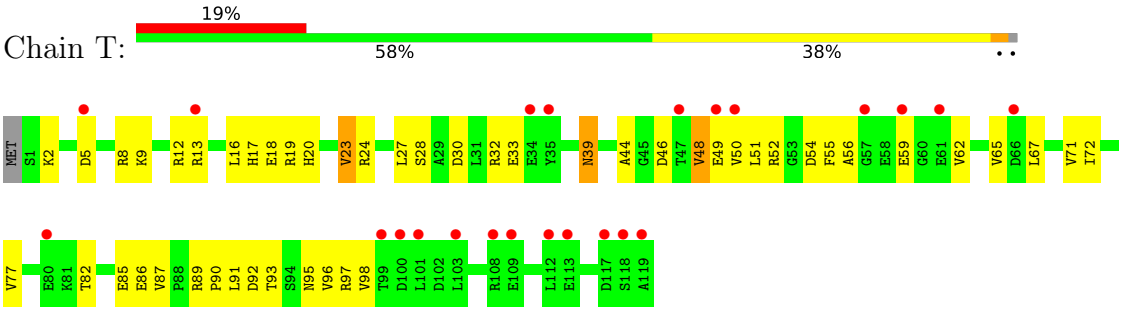




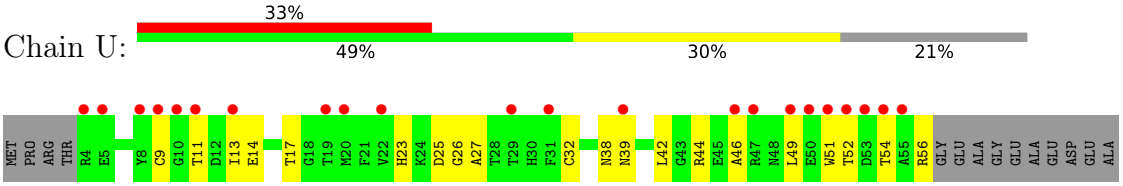
• Molecule 21: 50S ribosomal protein L23P



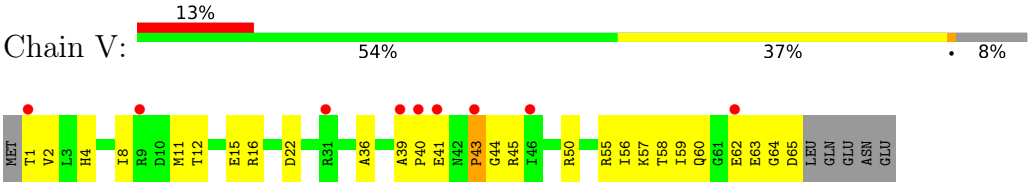
• Molecule 22: 50S ribosomal protein L24P



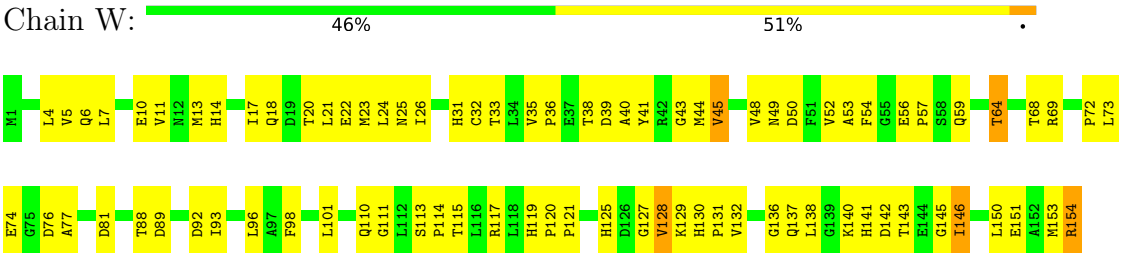
• Molecule 23: 50S ribosomal protein L24e



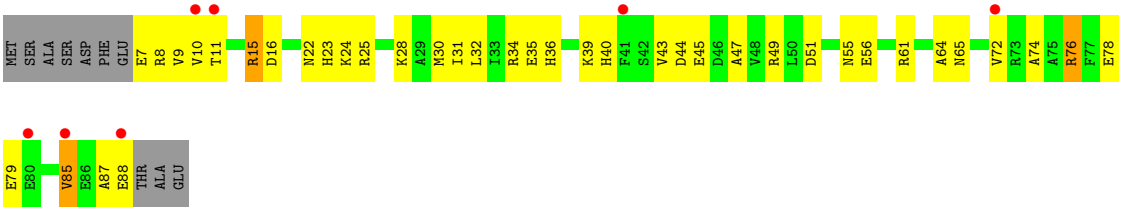
• Molecule 24: 50S ribosomal protein L29P



• Molecule 25: 50S ribosomal protein L30P

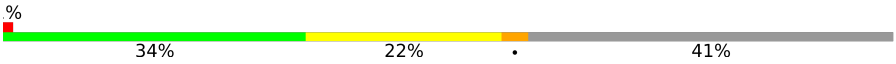


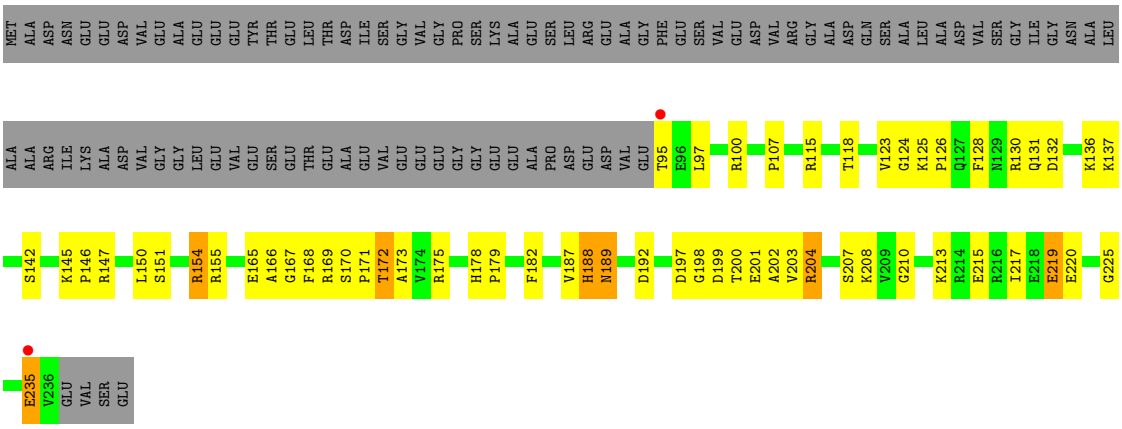
• Molecule 26: 50S RIBOSOMAL PROTEIN L31E



• Molecule 27: 50S ribosomal protein L32e

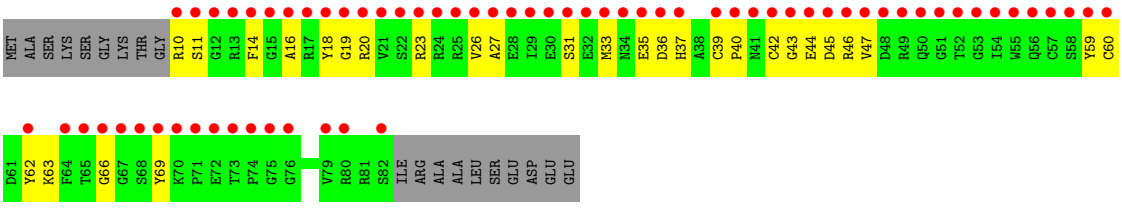
Chain Y:





• Molecule 28: 50S ribosomal protein L37Ae

Chain Z:

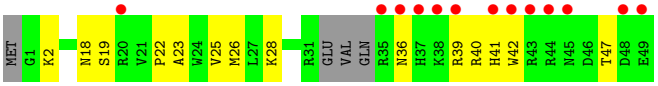


• Molecule 29: 50S ribosomal protein L37e

Chain 1:

• Molecule 30: 50S ribosomal protein L39e

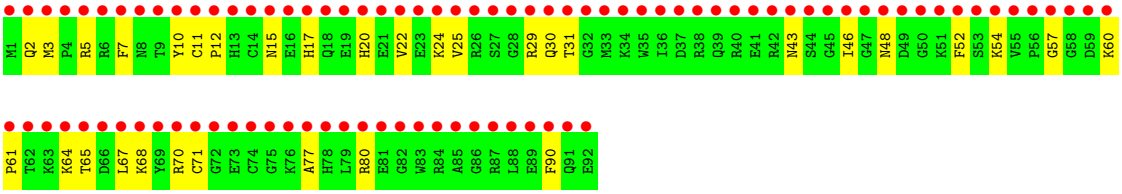
Chain 2:



• Molecule 31: 50S ribosomal protein L44E

Chain 3:


100%
64%
36%


M1 Q2 M3 P4 R5 R6 F7 N8 T9 Y10 C11 P12 H13 C14 N15 E16 H17 Q18 E19 H20 E21 V22 E23 K24 V25 R26 S27 G28 R29 Q30 T31 G32 M33 K34 W35 I36 D37 R38 Q39 R40 E41 R42 N43 S44 G45 I46 G47 N48 D49 G50 K51 F52 S53 K54 V55 P56 G57 G58 D59 K60

P61 T62 K63 K64 T65 D66 L67 K68 Y69 R70 C71 G72 E73 C74 G75 K76 A77 H78 L79 R80 E81 G82 W83 R84 A85 G86 R87 L88 E89 F90 Q91 E92

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	214.49Å 302.43Å 578.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 49.83 – 3.01	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-3.00) 96.9 (49.83-3.01)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.288 0.259 , 0.260	Depositor DCC
R_{free} test set	18014 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	69.6	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 61.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	92248	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PSU, MG, NA, K, CD, OMU, OMG, UR3, CL

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	0.56	0/65932	0.75	36/102817 (0.0%)
2	9	0.42	0/2905	0.72	1/4528 (0.0%)
3	A	0.39	0/1786	0.69	0/2408
4	B	0.46	0/2690	0.76	0/3652
5	C	0.47	0/1884	0.76	1/2551 (0.0%)
6	D	0.36	0/1111	0.60	0/1498
7	E	0.45	0/1382	0.68	0/1880
8	F	0.34	0/901	0.58	0/1224
9	G	1.36	5/971 (0.5%)	1.67	22/1317 (1.7%)
10	H	0.41	0/1287	0.70	0/1725
11	I	4.03	6/890 (0.7%)	2.13	7/1216 (0.6%)
12	J	0.50	0/1136	0.70	0/1530
13	K	0.46	0/1001	0.77	0/1347
14	L	0.39	0/1130	0.68	0/1509
15	M	0.42	0/1583	0.68	0/2119
16	N	0.34	0/1474	0.66	0/1999
17	O	0.45	0/874	0.70	0/1181
18	P	0.42	0/1147	0.60	0/1528
19	Q	0.38	0/749	0.68	0/1005
20	R	0.50	0/1172	0.75	0/1578
21	S	0.42	0/648	0.64	0/875
22	T	0.42	0/958	0.71	0/1289
23	U	0.35	0/417	0.61	0/562
24	V	0.39	0/502	0.61	0/675
25	W	0.47	0/1219	0.77	0/1655
26	X	0.51	0/664	0.72	0/895
27	Y	0.48	0/1146	0.74	0/1536
28	Z	0.36	0/589	0.55	0/787
29	1	0.50	0/438	0.71	0/578
30	2	0.40	0/401	0.60	0/529
31	3	0.35	0/771	0.57	0/1024
All	All	0.66	11/99758 (0.0%)	0.77	67/149017 (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	6	93
2	9	0	1
9	G	0	8
11	I	2	4
All	All	8	106

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	24	LEU	CA-CB	82.97	3.44	1.53
11	I	24	LEU	CG-CD2	57.61	3.65	1.51
11	I	24	LEU	CG-CD1	50.48	3.38	1.51
11	I	24	LEU	CB-CG	34.68	2.53	1.52
9	G	54	HIS	CB-CG	28.65	2.01	1.50

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	I	24	LEU	CB-CA-C	-36.47	40.91	110.20
11	I	24	LEU	CD1-CG-CD2	-30.12	20.15	110.50
11	I	24	LEU	CB-CG-CD1	-29.18	61.40	111.00
11	I	24	LEU	CB-CG-CD2	-25.73	67.26	111.00
11	I	24	LEU	CA-CB-CG	-25.40	56.88	115.30

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1161	A	C1'
1	0	1167	G	C1',C3'
1	0	1193	A	C4',C1',C3'
11	I	24	LEU	CA
11	I	30	ASP	CA

5 of 106 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	116	G	Sidechain
1	0	191	A	Sidechain

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Mol	Chain	Res	Type	Group
1	0	206	G	Sidechain
1	0	49	A	Sidechain
1	0	79	G	Sidechain

5.2 Too-close contacts (i)

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	58979	0	29793	2515	0
2	9	2600	0	1326	157	0
3	A	1753	0	1766	73	0
4	B	2625	0	2533	110	0
5	C	1859	0	1816	84	0
6	D	1094	0	1085	50	0
7	E	1357	0	1266	46	0
8	F	890	0	843	31	0
9	G	959	0	928	154	0
10	H	1266	0	1268	49	0
11	I	876	0	835	60	0
12	J	1120	0	1098	49	0
13	K	992	0	1031	44	0
14	L	1118	0	1076	34	0
15	M	1559	0	1567	63	0
16	N	1445	0	1401	73	0
17	O	865	0	873	28	0
18	P	1136	0	1123	39	0
19	Q	735	0	728	27	0
20	R	1149	0	1122	44	0
21	S	641	0	605	13	0
22	T	950	0	924	50	0
23	U	410	0	367	15	0
24	V	499	0	511	21	0
25	W	1196	0	1137	72	0
26	X	654	0	653	42	0
27	Y	1130	0	1133	51	0
28	Z	578	0	543	36	0
29	1	431	0	427	24	0
30	2	396	0	413	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	3	755	0	732	34	0
32	0	108	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	1	0	0	0	0
33	M	1	0	0	0	0
34	0	73	0	0	0	0
34	9	3	0	0	0	0
34	A	1	0	0	0	0
34	C	1	0	0	0	0
34	H	1	0	0	0	0
34	J	1	0	0	0	0
34	L	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	2	0	0	0	0
34	S	1	0	0	0	0
35	0	8	0	0	1	0
35	3	1	0	0	5	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	4	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	1	0
35	N	1	0	0	0	0
35	O	1	0	0	1	0
35	Q	1	0	0	1	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	1	1	0	0	1	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
All	All	92248	0	60923	3719	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 25.

The worst 5 of 3719 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)
9:G:54:HIS:CG	9:G:54:HIS:CB	2.01	1.43
9:G:108:SER:O	9:G:109:LYS:HE3	1.32	1.30
1:0:1167:G:H5'	1:0:1168:C:OP2	1.34	1.28
9:G:33:VAL:C	9:G:123:ASP:OD2	1.72	1.27
9:G:35:VAL:HG21	9:G:122:ASN:OD1	1.37	1.25

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	235/240 (98%)	206 (88%)	24 (10%)	5 (2%)	7 33
4	B	335/338 (99%)	287 (86%)	38 (11%)	10 (3%)	4 24
5	C	244/246 (99%)	209 (86%)	28 (12%)	7 (3%)	4 24
6	D	134/177 (76%)	95 (71%)	34 (25%)	5 (4%)	3 19
7	E	170/178 (96%)	156 (92%)	12 (7%)	2 (1%)	13 48
8	F	117/120 (98%)	101 (86%)	13 (11%)	3 (3%)	5 27
9	G	121/348 (35%)	79 (65%)	29 (24%)	13 (11%)	0 2
10	H	156/171 (91%)	141 (90%)	11 (7%)	4 (3%)	5 27
11	I	112/162 (69%)	76 (68%)	28 (25%)	8 (7%)	1 5
12	J	140/145 (97%)	129 (92%)	9 (6%)	2 (1%)	11 43
13	K	130/132 (98%)	117 (90%)	11 (8%)	2 (2%)	10 42
14	L	141/165 (86%)	127 (90%)	13 (9%)	1 (1%)	22 60
15	M	192/196 (98%)	161 (84%)	31 (16%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	N	184/187 (98%)	162 (88%)	19 (10%)	3 (2%)	9 40
17	O	113/116 (97%)	103 (91%)	9 (8%)	1 (1%)	17 55
18	P	141/149 (95%)	129 (92%)	11 (8%)	1 (1%)	22 60
19	Q	93/96 (97%)	85 (91%)	5 (5%)	3 (3%)	4 22
20	R	148/155 (96%)	129 (87%)	18 (12%)	1 (1%)	22 60
21	S	79/85 (93%)	65 (82%)	14 (18%)	0	100 100
22	T	117/120 (98%)	105 (90%)	11 (9%)	1 (1%)	17 55
23	U	51/67 (76%)	48 (94%)	3 (6%)	0	100 100
24	V	63/71 (89%)	57 (90%)	5 (8%)	1 (2%)	9 40
25	W	152/154 (99%)	134 (88%)	17 (11%)	1 (1%)	22 60
26	X	80/92 (87%)	66 (82%)	13 (16%)	1 (1%)	12 45
27	Y	140/241 (58%)	130 (93%)	7 (5%)	3 (2%)	7 33
28	Z	71/92 (77%)	64 (90%)	7 (10%)	0	100 100
29	1	54/57 (95%)	45 (83%)	8 (15%)	1 (2%)	8 36
30	2	42/50 (84%)	41 (98%)	1 (2%)	0	100 100
31	3	90/92 (98%)	82 (91%)	7 (8%)	1 (1%)	14 50
All	All	3845/4442 (87%)	3329 (87%)	436 (11%)	80 (2%)	7 33

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	16	ARG
6	D	27	ILE
8	F	91	VAL
9	G	127	PRO
11	I	11	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	179/182 (98%)	164 (92%)	15 (8%)	11	38
4	B	282/283 (100%)	264 (94%)	18 (6%)	17	51
5	C	193/193 (100%)	174 (90%)	19 (10%)	8	30
6	D	117/148 (79%)	109 (93%)	8 (7%)	16	48
7	E	152/156 (97%)	142 (93%)	10 (7%)	16	49
8	F	93/94 (99%)	92 (99%)	1 (1%)	73	90
9	G	106/283 (38%)	95 (90%)	11 (10%)	7	27
10	H	132/138 (96%)	124 (94%)	8 (6%)	18	53
11	I	99/130 (76%)	84 (85%)	15 (15%)	3	14
12	J	118/121 (98%)	107 (91%)	11 (9%)	9	33
13	K	106/106 (100%)	98 (92%)	8 (8%)	13	43
14	L	113/127 (89%)	108 (96%)	5 (4%)	28	65
15	M	158/160 (99%)	150 (95%)	8 (5%)	24	60
16	N	149/150 (99%)	144 (97%)	5 (3%)	37	72
17	O	93/94 (99%)	89 (96%)	4 (4%)	29	66
18	P	113/117 (97%)	107 (95%)	6 (5%)	22	58
19	Q	79/80 (99%)	76 (96%)	3 (4%)	33	69
20	R	117/122 (96%)	113 (97%)	4 (3%)	37	72
21	S	71/74 (96%)	66 (93%)	5 (7%)	15	47
22	T	105/106 (99%)	99 (94%)	6 (6%)	20	56
23	U	44/53 (83%)	44 (100%)	0	100	100
24	V	51/57 (90%)	49 (96%)	2 (4%)	32	69
25	W	130/130 (100%)	121 (93%)	9 (7%)	15	48
26	X	66/74 (89%)	62 (94%)	4 (6%)	18	53
27	Y	120/196 (61%)	111 (92%)	9 (8%)	13	43
28	Z	60/74 (81%)	60 (100%)	0	100	100
29	1	46/47 (98%)	43 (94%)	3 (6%)	17	50
30	2	42/46 (91%)	41 (98%)	1 (2%)	49	79
31	3	79/79 (100%)	78 (99%)	1 (1%)	69	89
All	All	3213/3620 (89%)	3014 (94%)	199 (6%)	18	52

5 of 199 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	131	THR
17	O	43	VAL
13	K	69	LEU
15	M	46	LEU
18	P	98	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
22	T	39	ASN
29	1	16	HIS
24	V	60	GLN
25	W	141	HIS
10	H	70	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2741/2922 (93%)	291 (10%)	35 (1%)
2	9	121/122 (99%)	16 (13%)	4 (3%)
All	All	2862/3044 (94%)	307 (10%)	39 (1%)

5 of 307 RNA backbone outliers are listed below:

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

5 of 39 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	2467	A
2	9	14	G
1	0	2536	C
1	0	2791	U
2	9	65	A

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

4 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	OMG	0	2588	1	18,26,27	1.14	3 (16%)	19,38,41	0.79	1 (5%)
1	OMU	0	2587	1	19,22,23	0.42	0	26,31,34	0.53	0
1	UR3	0	2619	1	19,22,23	0.50	0	26,32,35	0.64	1 (3%)
1	PSU	0	2621	1	18,21,22	1.50	2 (11%)	22,30,33	1.36	4 (18%)

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	OMG	0	2588	1	-	1/5/27/28	0/3/3/3
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	5.20	1.43	1.36
1	0	2588	OMG	C5-C6	-2.82	1.41	1.47
1	0	2588	OMG	C8-N7	-2.53	1.30	1.35
1	0	2621	PSU	C6-C5	2.24	1.37	1.35
1	0	2588	OMG	C5-C4	-2.06	1.37	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	2621	PSU	C6-C5-C4	3.50	120.65	118.20
1	0	2621	PSU	O2-C2-N1	2.69	125.76	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	2621	PSU	C6-N1-C2	-2.69	119.93	122.68
1	0	2621	PSU	O2'-C2'-C1'	-2.47	105.35	111.23
1	0	2619	UR3	C4-N3-C2	2.28	126.71	124.56

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	2588	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2588	OMG	3	0
1	0	2587	OMU	5	0
1	0	2619	UR3	1	0
1	0	2621	PSU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 231 ligands modelled in this entry, 231 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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
9	G	2
1	0	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	0	1207:A	O3'	1208:C	P	2.51
1	G	53:LEU	C	54:HIS	N	1.63
1	G	54:HIS	C	55:GLY	N	0.99

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^{th} 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%)	-0.18	16 (0%) 89 72	17, 56, 120, 184	0
2	9	122/122 (100%)	-0.01	2 (1%) 72 44	41, 89, 136, 181	0
3	A	237/240 (98%)	0.56	23 (9%) 7 2	34, 90, 133, 148	0
4	B	337/338 (99%)	0.15	13 (3%) 39 15	25, 60, 100, 112	0
5	C	246/246 (100%)	0.16	6 (2%) 59 30	29, 58, 91, 106	0
6	D	140/177 (79%)	1.95	58 (41%) 0 0	89, 146, 170, 178	0
7	E	172/178 (96%)	0.48	12 (6%) 16 5	46, 73, 100, 109	0
8	F	119/120 (99%)	0.37	5 (4%) 36 14	74, 110, 150, 166	0
9	G	125/348 (35%)	1.41	37 (29%) 0 0	100, 133, 165, 168	0
10	H	160/171 (93%)	0.34	6 (3%) 40 16	51, 76, 109, 120	0
11	I	118/162 (72%)	2.78	63 (53%) 0 0	20, 181, 199, 200	0
12	J	142/145 (97%)	-0.05	0 100 100	31, 54, 83, 99	0
13	K	132/132 (100%)	0.19	3 (2%) 60 31	33, 61, 98, 103	0
14	L	145/165 (87%)	1.49	39 (26%) 0 0	49, 111, 158, 162	0
15	M	194/196 (98%)	0.77	22 (11%) 5 1	2, 62, 161, 180	0
16	N	186/187 (99%)	1.18	37 (19%) 1 0	62, 106, 176, 189	0
17	O	115/116 (99%)	0.10	0 100 100	48, 70, 88, 91	0
18	P	143/149 (95%)	0.79	18 (12%) 3 1	44, 68, 103, 109	0
19	Q	95/96 (98%)	0.67	7 (7%) 14 4	52, 74, 87, 100	0
20	R	150/155 (96%)	0.04	1 (0%) 87 69	30, 48, 74, 81	0
21	S	81/85 (95%)	0.40	2 (2%) 57 29	56, 87, 108, 123	0
22	T	119/120 (99%)	0.99	23 (19%) 1 0	51, 74, 106, 139	0
23	U	53/67 (79%)	1.90	22 (41%) 0 0	96, 108, 126, 133	0
24	V	65/71 (91%)	0.84	9 (13%) 2 1	66, 105, 145, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	W	154/154 (100%)	-0.02	0 100 100	38, 55, 81, 95	0
26	X	82/92 (89%)	0.57	7 (8%) 10 3	43, 63, 84, 95	0
27	Y	142/241 (58%)	0.26	2 (1%) 75 49	23, 51, 87, 106	0
28	Z	73/92 (79%)	6.73	67 (91%) 0 0	164, 174, 200, 200	0
29	1	56/57 (98%)	0.06	0 100 100	28, 43, 56, 65	0
30	2	46/50 (92%)	1.29	13 (28%) 0 0	48, 87, 150, 152	0
31	3	92/92 (100%)	11.33	92 (100%) 0 0	184, 198, 200, 200	0
All	All	6790/7486 (90%)	0.51	605 (8%) 9 3	2, 67, 162, 200	0

The worst 5 of 605 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	3	9	THR	24.4
31	3	33	MET	23.0
31	3	69	TYR	22.4
31	3	78	HIS	20.9
31	3	25	VAL	20.2

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

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	OMU	0	2587	21/22	0.94	0.18	33,36,42,43	0
1	OMG	0	2588	24/25	0.95	0.18	38,42,48,49	0
1	UR3	0	2619	21/22	0.96	0.18	34,42,44,47	0
1	PSU	0	2621	20/21	0.97	0.15	35,37,44,44	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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^{th} 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
34	NA	0	3103	1/1	-0.15	0.88	198,198,198,198	0
34	NA	0	3050	1/1	-0.11	1.21	137,137,137,137	0
32	MG	0	3027	1/1	-0.00	0.96	110,110,110,110	0
32	MG	0	2946	1/1	0.09	0.34	200,200,200,200	0
32	MG	0	2971	1/1	0.18	0.41	200,200,200,200	0
34	NA	0	3100	1/1	0.30	1.21	56,56,56,56	0
35	CL	O	117	1/1	0.38	1.01	127,127,127,127	0
32	MG	0	3025	1/1	0.41	0.47	57,57,57,57	0
32	MG	0	2998	1/1	0.45	0.50	73,73,73,73	0
34	NA	0	3057	1/1	0.45	0.80	124,124,124,124	0
34	NA	0	3093	1/1	0.45	0.39	116,116,116,116	0
32	MG	0	3029	1/1	0.47	0.99	69,69,69,69	0
32	MG	3	93	1/1	0.49	0.51	69,69,69,69	0
34	NA	0	3054	1/1	0.50	0.34	63,63,63,63	0
35	CL	0	3109	1/1	0.53	0.61	135,135,135,135	0
34	NA	0	3047	1/1	0.55	0.36	53,53,53,53	0
34	NA	0	3082	1/1	0.56	0.48	43,43,43,43	0
35	CL	0	3106	1/1	0.56	1.27	120,120,120,120	0
35	CL	0	3112	1/1	0.59	0.56	96,96,96,96	0
34	NA	S	85	1/1	0.59	0.67	64,64,64,64	0
36	CD	O	116	1/1	0.59	0.47	200,200,200,200	0
34	NA	0	3052	1/1	0.60	0.52	72,72,72,72	0
35	CL	3	95	1/1	0.61	0.65	124,124,124,124	0
32	MG	0	2988	1/1	0.61	0.34	52,52,52,52	0
34	NA	0	3065	1/1	0.64	0.19	27,27,27,27	0
32	MG	0	3028	1/1	0.64	0.97	66,66,66,66	0
34	NA	0	3068	1/1	0.65	0.25	68,68,68,68	0
32	MG	Y	241	1/1	0.66	0.47	68,68,68,68	0
34	NA	0	3075	1/1	0.67	0.46	41,41,41,41	0
34	NA	0	3094	1/1	0.67	0.43	116,116,116,116	0
34	NA	0	3098	1/1	0.67	0.52	62,62,62,62	0
34	NA	0	3046	1/1	0.67	0.28	26,26,26,26	0
32	MG	B	338	1/1	0.68	0.59	43,43,43,43	0
34	NA	0	3038	1/1	0.69	0.32	67,67,67,67	0
34	NA	0	3059	1/1	0.69	0.42	53,53,53,53	0
32	MG	0	2964	1/1	0.69	0.34	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	2980	1/1	0.71	0.47	48,48,48,48	0
32	MG	A	240	1/1	0.72	0.48	56,56,56,56	0
35	CL	0	3111	1/1	0.72	0.25	54,54,54,54	0
34	NA	C	247	1/1	0.73	0.34	41,41,41,41	0
33	K	M	196	1/1	0.73	0.42	127,127,127,127	0
34	NA	0	3044	1/1	0.73	0.85	46,46,46,46	0
34	NA	0	3092	1/1	0.74	0.25	45,45,45,45	0
34	NA	0	3077	1/1	0.74	0.55	119,119,119,119	0
34	NA	A	242	1/1	0.74	0.28	55,55,55,55	0
32	MG	0	2973	1/1	0.75	0.42	51,51,51,51	0
34	NA	9	125	1/1	0.75	0.35	78,78,78,78	0
32	MG	0	2984	1/1	0.75	0.51	59,59,59,59	0
32	MG	0	2987	1/1	0.75	0.16	35,35,35,35	0
34	NA	R	156	1/1	0.76	0.33	53,53,53,53	0
34	NA	0	3099	1/1	0.76	0.90	56,56,56,56	0
34	NA	0	3034	1/1	0.76	0.77	91,91,91,91	0
32	MG	0	2969	1/1	0.77	0.40	38,38,38,38	0
34	NA	0	3064	1/1	0.77	0.30	60,60,60,60	0
32	MG	0	3007	1/1	0.78	0.29	54,54,54,54	0
34	NA	0	3058	1/1	0.78	0.26	61,61,61,61	0
32	MG	0	2985	1/1	0.78	0.29	34,34,34,34	0
32	MG	0	3006	1/1	0.78	0.42	49,49,49,49	0
32	MG	0	3026	1/1	0.79	1.06	79,79,79,79	0
34	NA	9	124	1/1	0.79	0.16	34,34,34,34	0
34	NA	0	3033	1/1	0.79	0.45	60,60,60,60	0
32	MG	0	2974	1/1	0.79	0.19	51,51,51,51	0
33	K	0	3031	1/1	0.79	0.47	153,153,153,153	0
35	CL	Q	97	1/1	0.79	0.57	93,93,93,93	0
34	NA	0	3039	1/1	0.79	0.63	29,29,29,29	0
34	NA	0	3084	1/1	0.79	0.43	62,62,62,62	0
34	NA	0	3060	1/1	0.80	0.15	101,101,101,101	0
32	MG	0	3014	1/1	0.80	0.32	87,87,87,87	0
32	MG	A	241	1/1	0.80	0.38	142,142,142,142	0
34	NA	0	3056	1/1	0.80	0.33	42,42,42,42	0
32	MG	0	3013	1/1	0.80	0.38	41,41,41,41	0
34	NA	J	146	1/1	0.80	0.24	41,41,41,41	0
32	MG	K	133	1/1	0.80	0.45	35,35,35,35	0
34	NA	0	3051	1/1	0.80	0.33	49,49,49,49	0
32	MG	0	3011	1/1	0.81	0.86	71,71,71,71	0
32	MG	0	2989	1/1	0.81	0.67	56,56,56,56	0
35	CL	0	3108	1/1	0.81	0.36	72,72,72,72	0
35	CL	R	157	1/1	0.81	0.24	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	2944	1/1	0.81	0.18	25,25,25,25	0
34	NA	9	126	1/1	0.81	0.85	91,91,91,91	0
34	NA	0	3061	1/1	0.82	0.12	39,39,39,39	0
32	MG	0	3018	1/1	0.82	0.35	78,78,78,78	0
32	MG	0	3030	1/1	0.82	0.18	46,46,46,46	0
34	NA	0	3043	1/1	0.82	0.38	115,115,115,115	0
35	CL	L	166	1/1	0.82	0.27	68,68,68,68	0
32	MG	0	3024	1/1	0.83	0.35	1,1,1,1	0
35	CL	A	243	1/1	0.83	0.40	90,90,90,90	0
34	NA	0	3101	1/1	0.83	0.17	43,43,43,43	0
34	NA	0	3063	1/1	0.83	0.19	162,162,162,162	0
36	CD	Z	93	1/1	0.83	0.35	200,200,200,200	0
34	NA	Q	96	1/1	0.84	0.24	64,64,64,64	0
32	MG	0	2962	1/1	0.84	0.48	60,60,60,60	0
34	NA	0	3067	1/1	0.85	0.30	47,47,47,47	0
32	MG	0	2993	1/1	0.85	0.44	78,78,78,78	0
32	MG	0	2949	1/1	0.85	0.35	45,45,45,45	0
32	MG	0	3004	1/1	0.85	0.53	27,27,27,27	0
32	MG	0	3010	1/1	0.86	0.17	56,56,56,56	0
32	MG	0	2938	1/1	0.86	0.47	42,42,42,42	0
32	MG	0	2947	1/1	0.86	0.27	15,15,15,15	0
35	CL	M	198	1/1	0.86	0.36	77,77,77,77	0
34	NA	0	3041	1/1	0.86	0.36	70,70,70,70	0
32	MG	0	3019	1/1	0.87	0.40	41,41,41,41	0
32	MG	0	3023	1/1	0.87	0.34	29,29,29,29	0
34	NA	0	3032	1/1	0.87	0.45	30,30,30,30	0
32	MG	0	2956	1/1	0.87	0.18	24,24,24,24	0
32	MG	0	3017	1/1	0.87	0.34	166,166,166,166	0
34	NA	0	3035	1/1	0.87	0.17	17,17,17,17	0
32	MG	0	2968	1/1	0.87	0.10	60,60,60,60	0
35	CL	J	149	1/1	0.88	0.15	45,45,45,45	0
34	NA	0	3089	1/1	0.88	0.14	51,51,51,51	0
32	MG	0	2986	1/1	0.88	0.35	53,53,53,53	0
35	CL	N	187	1/1	0.88	0.29	64,64,64,64	0
32	MG	0	3022	1/1	0.88	0.38	44,44,44,44	0
32	MG	0	2950	1/1	0.88	0.23	17,17,17,17	0
32	MG	0	2981	1/1	0.88	0.50	44,44,44,44	0
32	MG	0	2929	1/1	0.88	0.19	14,14,14,14	0
32	MG	0	2943	1/1	0.88	0.37	23,23,23,23	0
34	NA	0	3088	1/1	0.88	0.26	33,33,33,33	0
32	MG	0	2951	1/1	0.89	0.38	11,11,11,11	0
32	MG	0	2963	1/1	0.89	0.15	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	2979	1/1	0.89	0.23	20,20,20,20	0
32	MG	0	2935	1/1	0.89	0.38	28,28,28,28	0
32	MG	0	3015	1/1	0.89	0.49	53,53,53,53	0
32	MG	0	3009	1/1	0.89	0.28	40,40,40,40	0
34	NA	0	3102	1/1	0.90	0.31	47,47,47,47	0
34	NA	0	3073	1/1	0.90	0.27	25,25,25,25	0
32	MG	0	3020	1/1	0.90	0.18	84,84,84,84	0
32	MG	0	2975	1/1	0.90	0.16	45,45,45,45	0
34	NA	0	3078	1/1	0.90	0.16	78,78,78,78	0
34	NA	0	3080	1/1	0.90	0.41	57,57,57,57	0
32	MG	0	2936	1/1	0.90	0.13	17,17,17,17	0
32	MG	0	2999	1/1	0.90	0.19	25,25,25,25	0
34	NA	0	3072	1/1	0.90	0.24	65,65,65,65	0
36	CD	3	94	1/1	0.90	1.15	200,200,200,200	0
32	MG	0	2992	1/1	0.91	0.26	52,52,52,52	0
32	MG	0	3016	1/1	0.91	0.20	43,43,43,43	0
34	NA	H	172	1/1	0.91	0.16	43,43,43,43	0
35	CL	K	134	1/1	0.91	0.34	55,55,55,55	0
34	NA	0	3081	1/1	0.91	0.18	49,49,49,49	0
32	MG	0	1	1/1	0.91	0.20	26,26,26,26	0
34	NA	0	3069	1/1	0.91	0.28	58,58,58,58	0
32	MG	0	2945	1/1	0.91	0.32	27,27,27,27	0
35	CL	0	3105	1/1	0.91	0.17	59,59,59,59	0
32	MG	0	2960	1/1	0.91	0.29	11,11,11,11	0
34	NA	0	3090	1/1	0.91	0.29	81,81,81,81	0
34	NA	0	3055	1/1	0.91	0.14	36,36,36,36	0
35	CL	0	3110	1/1	0.91	0.55	56,56,56,56	0
32	MG	9	123	1/1	0.91	0.17	37,37,37,37	0
34	NA	0	3095	1/1	0.92	0.49	126,126,126,126	0
35	CL	B	339	1/1	0.92	0.46	61,61,61,61	0
35	CL	J	148	1/1	0.92	0.07	49,49,49,49	0
32	MG	0	2959	1/1	0.92	0.18	39,39,39,39	0
34	NA	M	197	1/1	0.92	0.16	28,28,28,28	0
34	NA	0	3040	1/1	0.92	0.18	29,29,29,29	0
32	MG	0	2970	1/1	0.92	0.19	32,32,32,32	0
34	NA	0	3071	1/1	0.92	0.13	27,27,27,27	0
34	NA	0	3085	1/1	0.92	0.41	15,15,15,15	0
32	MG	0	2924	1/1	0.92	0.23	35,35,35,35	0
32	MG	0	3001	1/1	0.92	0.15	38,38,38,38	0
34	NA	0	3074	1/1	0.92	0.47	66,66,66,66	0
32	MG	0	2930	1/1	0.92	0.12	55,55,55,55	0
32	MG	0	3005	1/1	0.92	0.16	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	NA	0	3066	1/1	0.92	0.11	9,9,9,9	0
35	CL	J	147	1/1	0.93	0.16	69,69,69,69	0
34	NA	0	3076	1/1	0.93	0.22	51,51,51,51	0
34	NA	R	155	1/1	0.93	0.21	31,31,31,31	0
34	NA	0	3042	1/1	0.93	0.38	32,32,32,32	0
32	MG	0	3003	1/1	0.93	0.18	26,26,26,26	0
34	NA	0	3104	1/1	0.93	0.59	34,34,34,34	0
34	NA	0	3091	1/1	0.93	0.25	31,31,31,31	0
32	MG	0	2966	1/1	0.93	0.13	46,46,46,46	0
32	MG	0	2937	1/1	0.93	0.24	14,14,14,14	0
32	MG	0	2978	1/1	0.93	0.17	46,46,46,46	0
35	CL	Y	242	1/1	0.93	0.26	27,27,27,27	0
34	NA	0	3083	1/1	0.93	0.17	27,27,27,27	0
32	MG	0	2990	1/1	0.93	0.15	31,31,31,31	0
32	MG	0	2991	1/1	0.93	0.16	20,20,20,20	0
34	NA	0	3086	1/1	0.93	0.40	26,26,26,26	0
32	MG	0	2928	1/1	0.94	0.14	32,32,32,32	0
34	NA	0	3045	1/1	0.94	0.22	33,33,33,33	0
32	MG	0	3000	1/1	0.94	0.20	7,7,7,7	0
32	MG	0	2957	1/1	0.94	0.14	37,37,37,37	0
34	NA	0	3048	1/1	0.94	0.21	46,46,46,46	0
32	MG	0	3012	1/1	0.94	0.27	39,39,39,39	0
32	MG	0	2977	1/1	0.94	0.52	43,43,43,43	0
32	MG	0	2942	1/1	0.94	0.41	16,16,16,16	0
32	MG	0	2954	1/1	0.94	0.18	29,29,29,29	0
32	MG	0	2997	1/1	0.94	0.27	59,59,59,59	0
32	MG	0	2967	1/1	0.94	0.30	50,50,50,50	0
34	NA	0	3070	1/1	0.94	0.10	27,27,27,27	0
32	MG	0	3008	1/1	0.94	0.30	52,52,52,52	0
32	MG	0	2939	1/1	0.95	0.31	20,20,20,20	0
32	MG	0	2982	1/1	0.95	0.25	14,14,14,14	0
32	MG	0	2983	1/1	0.95	0.29	43,43,43,43	0
34	NA	0	3079	1/1	0.95	0.12	53,53,53,53	0
34	NA	0	3087	1/1	0.95	0.08	22,22,22,22	0
34	NA	0	3096	1/1	0.95	0.21	47,47,47,47	0
34	NA	0	3097	1/1	0.95	0.17	50,50,50,50	0
32	MG	0	2995	1/1	0.95	0.16	13,13,13,13	0
32	MG	0	2931	1/1	0.95	0.11	27,27,27,27	0
32	MG	0	2952	1/1	0.95	0.23	4,4,4,4	0
32	MG	0	2932	1/1	0.96	0.14	10,10,10,10	0
32	MG	0	2976	1/1	0.96	0.18	19,19,19,19	0
34	NA	L	165	1/1	0.96	0.07	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	2941	1/1	0.96	0.16	15,15,15,15	0
32	MG	0	2933	1/1	0.96	0.32	1,1,1,1	0
32	MG	0	2994	1/1	0.96	0.20	14,14,14,14	0
32	MG	0	3021	1/1	0.96	0.23	20,20,20,20	0
34	NA	0	3062	1/1	0.96	0.07	38,38,38,38	0
32	MG	0	2925	1/1	0.96	0.19	5,5,5,5	0
36	CD	U	67	1/1	0.96	0.10	134,134,134,134	0
34	NA	0	3037	1/1	0.96	0.34	61,61,61,61	0
35	CL	0	3107	1/1	0.96	0.15	55,55,55,55	0
32	MG	0	2972	1/1	0.97	0.20	109,109,109,109	0
32	MG	0	2958	1/1	0.97	0.43	33,33,33,33	0
32	MG	T	120	1/1	0.97	0.25	38,38,38,38	0
32	MG	0	2955	1/1	0.97	0.30	11,11,11,11	0
34	NA	0	3049	1/1	0.97	0.27	28,28,28,28	0
32	MG	0	2953	1/1	0.97	0.11	8,8,8,8	0
34	NA	0	3036	1/1	0.97	0.36	49,49,49,49	0
32	MG	0	2940	1/1	0.97	0.33	24,24,24,24	0
34	NA	0	3053	1/1	0.97	0.07	19,19,19,19	0
32	MG	0	2961	1/1	0.98	0.19	41,41,41,41	0
32	MG	0	2965	1/1	0.98	0.22	47,47,47,47	0
32	MG	0	2934	1/1	0.98	0.34	22,22,22,22	0
32	MG	0	2926	1/1	0.98	0.15	17,17,17,17	0
32	MG	0	2996	1/1	0.98	0.24	21,21,21,21	0
32	MG	0	3002	1/1	0.98	0.06	20,20,20,20	0
32	MG	0	2927	1/1	0.99	0.19	18,18,18,18	0
36	CD	1	57	1/1	0.99	0.06	76,76,76,76	0
32	MG	0	2948	1/1	0.99	0.27	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.