wwPDB X-ray Structure Validation Summary Report (i)

Mar 8, 2026 – 05:16 AM UTC

PDB ID	:	3CC2 / pdb_00003cc2
Title	:	The Refined Crystal Structure of the Haloarcula Marismortui Large Ribosomal Subunit at 2.4 Angstrom Resolution with rrnA Sequence for the 23S rRNA and Genome-derived Sequences for r-Proteins
Authors	:	Gurel, G.; Blaha, G.
Deposited on	:	2008-02-23
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

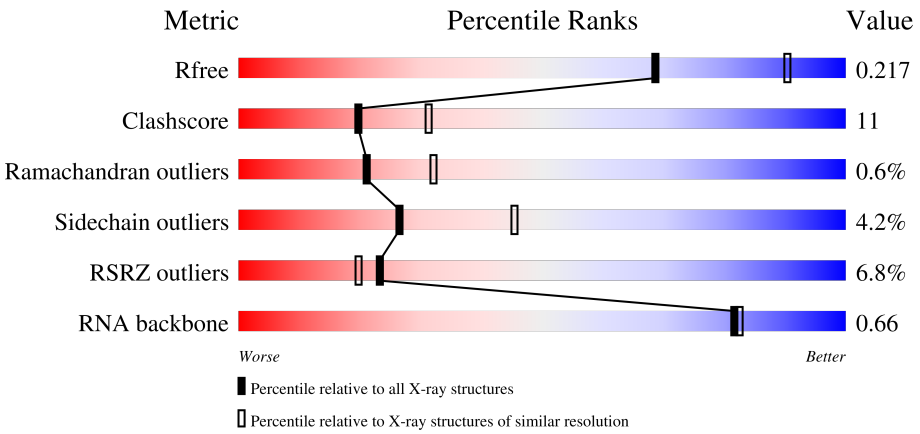
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)
RNA backbone	3983	1155 (2.70-2.10)

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	A	240	5%; 68%; 25%; 5% •
2	B	338	4%; 66%; 28%; 5%
3	C	246	2%; 73%; 22%; 5%
4	D	177	41%; 46%; 31%; • •; 21%

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Mol	Chain	Length	Quality of chain
5	E	178	11% 66% 30%
6	F	120	15% 71% 28%
7	G	348	4% 92%
8	H	177	7% 65% 24% 10%
9	I	162	38% 22% 21% 57%
10	J	145	5% 71% 25%
11	K	132	2% 73% 26%
12	L	165	17% 65% 22% 12%
13	M	196	75% 21%
14	N	187	18% 63% 31% 5%
15	O	116	5% 80% 17%
16	P	149	3% 81% 15%
17	Q	96	2% 80% 15%
18	R	155	% 74% 20%
19	S	85	6% 73% 22% 5%
20	T	120	6% 73% 22%
21	U	67	9% 49% 28% 21%
22	V	71	17% 59% 28% 8%
23	W	154	2% 62% 32% 5%
24	X	92	16% 61% 24% 11%
25	Y	241	2% 45% 12% 41%
26	Z	116	6% 44% 19% 37%
27	1	57	72% 25%
28	2	50	24% 52% 38% 8%
29	3	92	3% 76% 22%

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Mol	Chain	Length	Quality of chain
30	0	2923	2% 61% 27% 5% 6%
31	9	122	4% 48% 40% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	NA	0	8370	-	-	-	X
33	NA	R	8386	-	-	-	X

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 99049 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 protein called 50S ribosomal protein L2P.

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

- Molecule 2 is a protein called 50S ribosomal protein L3P.

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

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	246	1860	1130	345	384	1	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5P.

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

- Molecule 5 is a protein called 50S ribosomal protein L6P.

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

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 7 is a protein called 50S ribosomal protein L10E.

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

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	160	1282	798	240	238	6	0	0	0

- Molecule 9 is a protein called 50S ribosomal protein L11P.

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

- Molecule 10 is a protein called 50S ribosomal protein L13P.

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

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	132	994	609	189	192	4	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L15P.

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

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	194	1558	943	333	281	1	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L18P.

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

- Molecule 15 is a protein called 50S ribosomal protein L18e.

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

- Molecule 16 is a protein called 50S ribosomal protein L19e.

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

- Molecule 17 is a protein called 50S ribosomal protein L21e.

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

- Molecule 18 is a protein called 50S ribosomal protein L22P.

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

- Molecule 19 is a protein called 50S ribosomal protein L23P.

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

- Molecule 20 is a protein called 50S ribosomal protein L24P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24e.

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

- Molecule 22 is a protein called 50S ribosomal protein L29P.

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

- Molecule 23 is a protein called 50S ribosomal protein L30P.

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

- Molecule 24 is a protein called 50S ribosomal protein L31e.

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

- Molecule 25 is a protein called 50S ribosomal protein L32e.

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

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	Z	73	573	343	113	112	5	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	1	56	431	258	86	83	4	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	2	46	396	239	89	67	1	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	3	92	755	458	153	137	7	0	0	0

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
30	0	2754	59021	26349	10873	19054	2745	0	0	0

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
31	9	122	2599	1160	471	847	121	0	0	0

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 33 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
33	A	1	1	1	0	0
33	C	1	1	1	0	0
33	H	1	1	1	0	0
33	J	1	1	1	0	0
33	L	1	1	1	0	0
33	M	1	1	1	0	0
33	Q	1	1	1	0	0
33	R	2	2	2	0	0
33	S	1	1	1	0	0
33	0	73	73	73	0	0
33	9	3	3	3	0	0

- Molecule 34 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
34	3	1	1	1	0	0
			Total	Cl		
34	0	10	10	10	0	0

- Molecule 35 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
35	O	1	1	1	0	0
			Total	Cd		
35	U	1	1	1	0	0
			Total	Cd		
35	Z	1	1	1	0	0
			Total	Cd		
35	1	1	1	1	0	0
			Total	Cd		
35	3	1	1	1	0	0

- Molecule 36 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
36	0	2	2	2	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
37	A	117	117	117	0	0
			Total	O		
37	B	146	146	146	0	0
			Total	O		
37	C	170	170	170	0	0
			Total	O		
37	D	47	47	47	0	0
			Total	O		
37	E	42	42	42	0	0
			Total	O		
37	F	24	24	24	0	0
			Total	O		
37	G	19	19	19	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	H	72	Total O 72 72	0	0
37	I	9	Total O 9 9	0	0
37	J	51	Total O 51 51	0	0
37	K	56	Total O 56 56	0	0
37	L	72	Total O 72 72	0	0
37	M	119	Total O 119 119	0	0
37	N	65	Total O 65 65	0	0
37	O	39	Total O 39 39	0	0
37	P	63	Total O 63 63	0	0
37	Q	52	Total O 52 52	0	0
37	R	80	Total O 80 80	0	0
37	S	33	Total O 33 33	0	0
37	T	38	Total O 38 38	0	0
37	U	27	Total O 27 27	0	0
37	V	14	Total O 14 14	0	0
37	W	66	Total O 66 66	0	0
37	X	29	Total O 29 29	0	0
37	Y	94	Total O 94 94	0	0
37	Z	26	Total O 26 26	0	0
37	1	53	Total O 53 53	0	0
37	2	40	Total O 40 40	0	0

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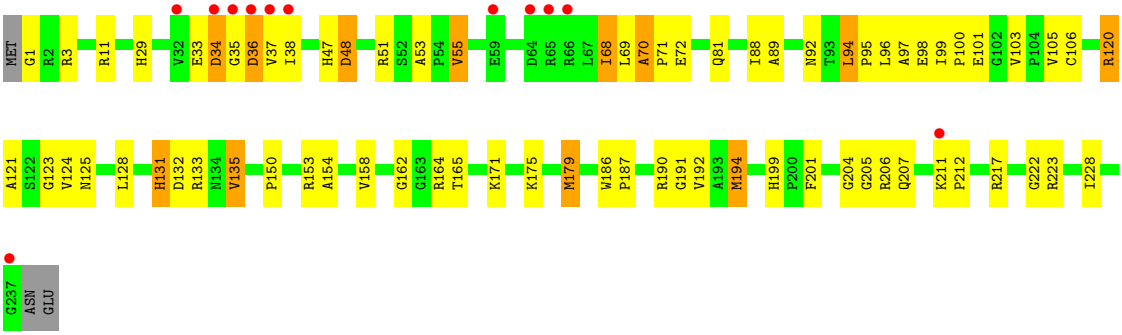
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	3	72	Total O 72 72	0	0
37	0	5949	Total O 5949 5949	0	0
37	9	139	Total O 139 139	0	0

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.

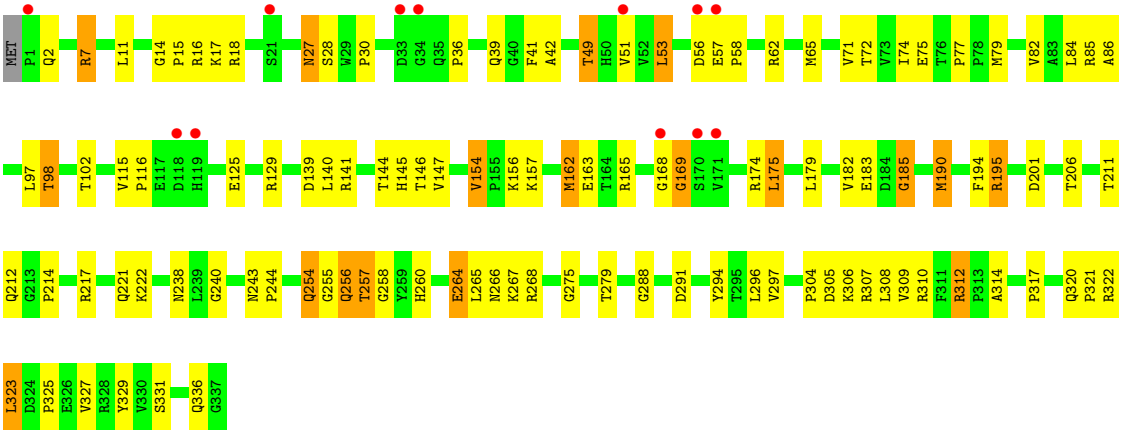
• Molecule 1: 50S ribosomal protein L2P

Chain A: 5% 68% 25% 5%



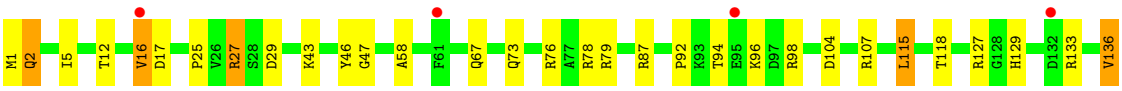
• Molecule 2: 50S ribosomal protein L3P

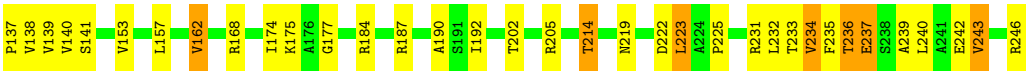
Chain B: 4% 66% 28% 5%



• Molecule 3: 50S ribosomal protein L4P

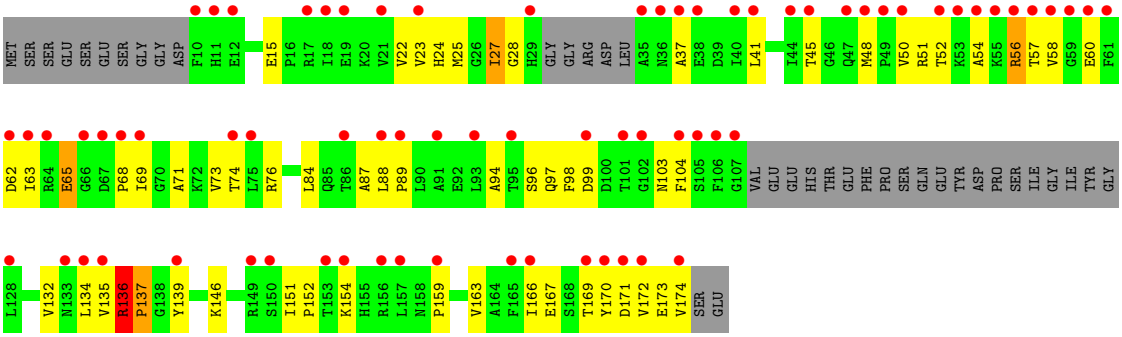
Chain C: 2% 73% 22% 5%





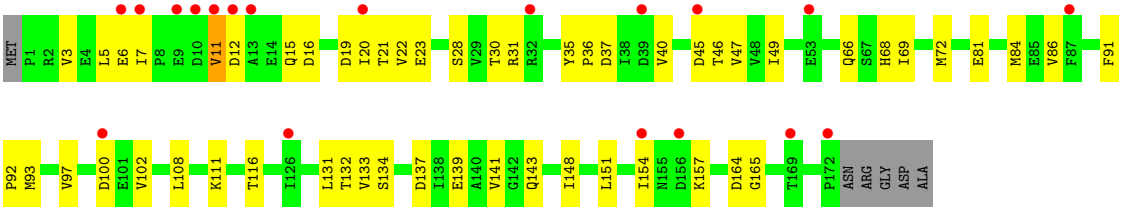
• Molecule 4: 50S ribosomal protein L5P

Chain D:



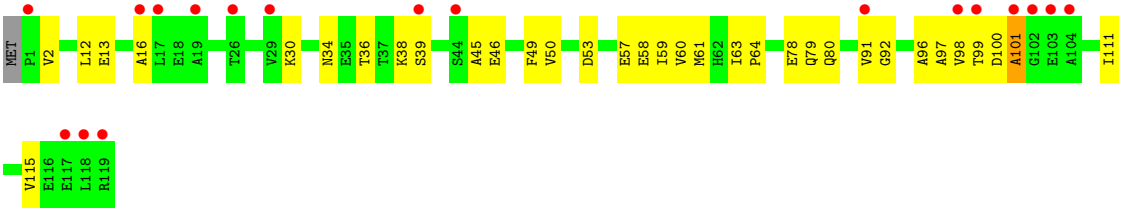
• Molecule 5: 50S ribosomal protein L6P

Chain E:



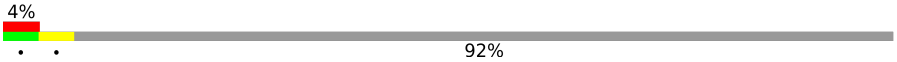
• Molecule 6: 50S ribosomal protein L7Ae

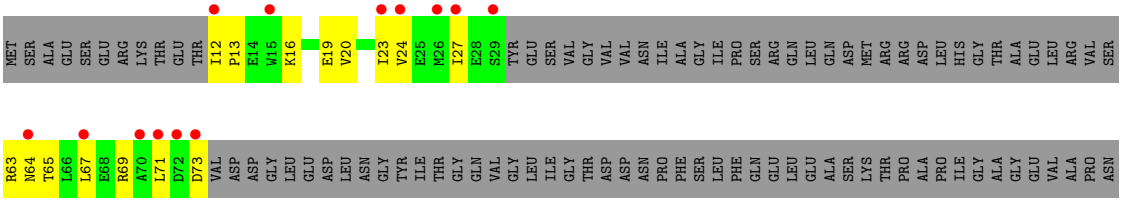
Chain F:

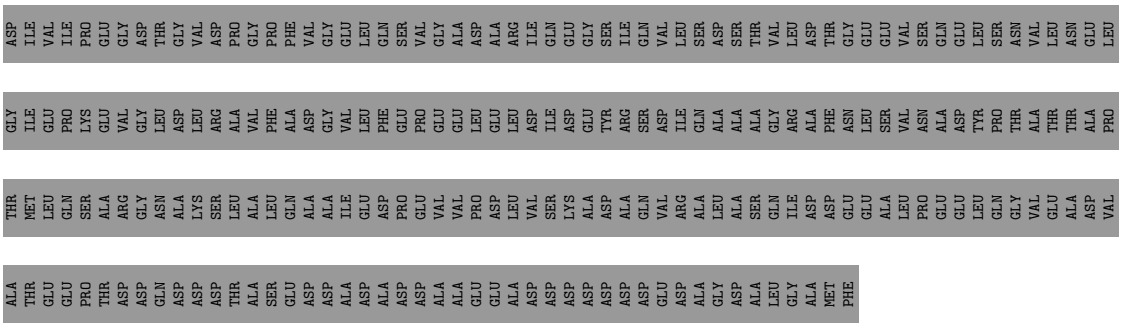


• Molecule 7: 50S ribosomal protein L10E

Chain G:

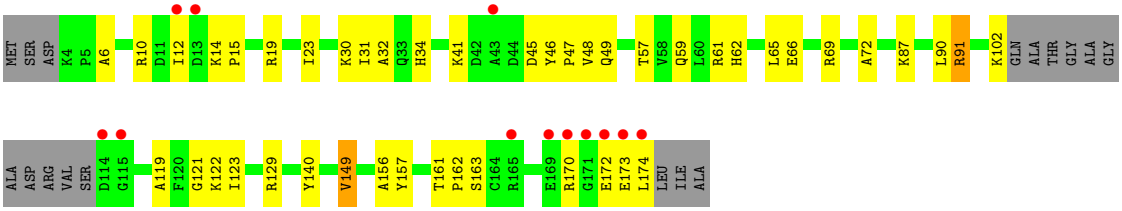






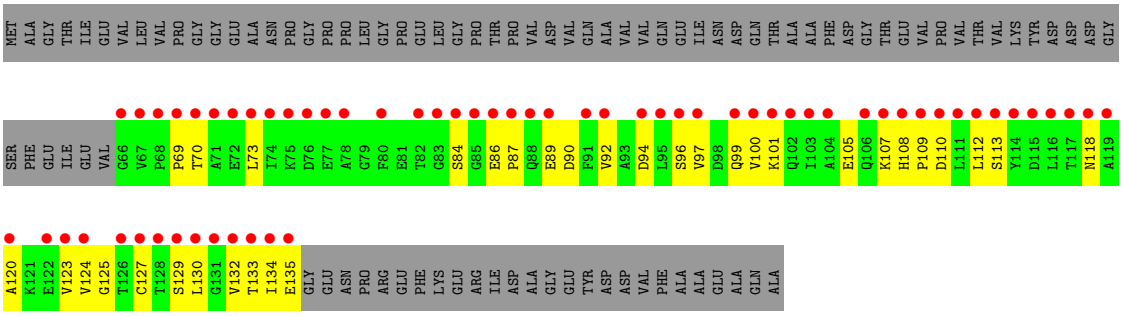
- Molecule 8: 50S ribosomal protein L10e

Chain H:



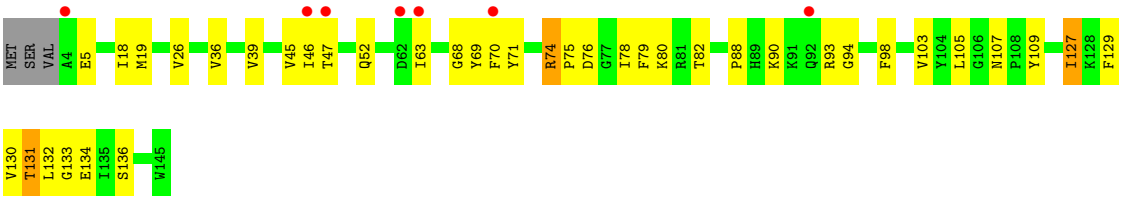
- Molecule 9: 50S ribosomal protein L11P

Chain I:



- Molecule 10: 50S ribosomal protein L13P

Chain J:

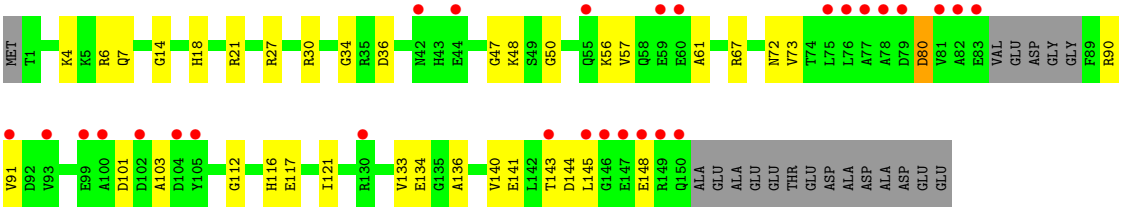


- Molecule 11: 50S ribosomal protein L14P

Chain K:

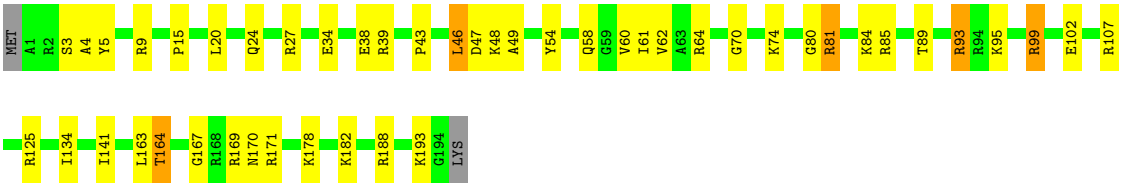
• Molecule 12: 50S ribosomal protein L15P

Chain L:



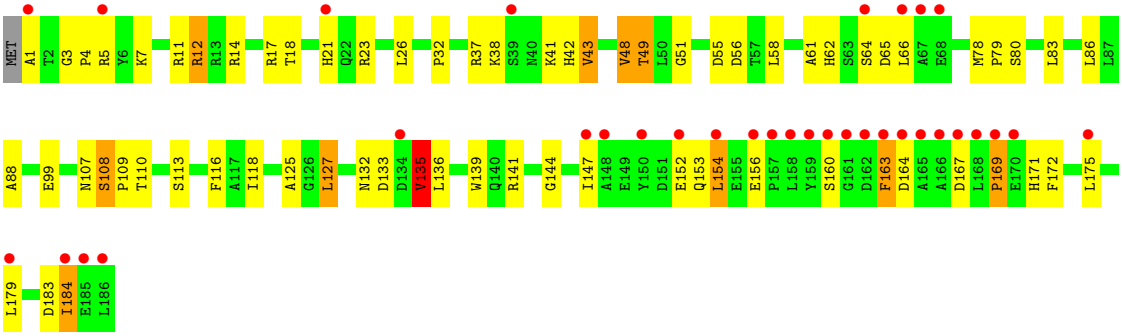
• Molecule 13: 50S ribosomal protein L15e

Chain M:



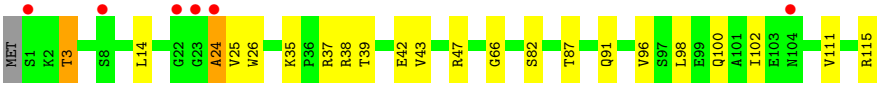
• Molecule 14: 50S ribosomal protein L18P

Chain N:



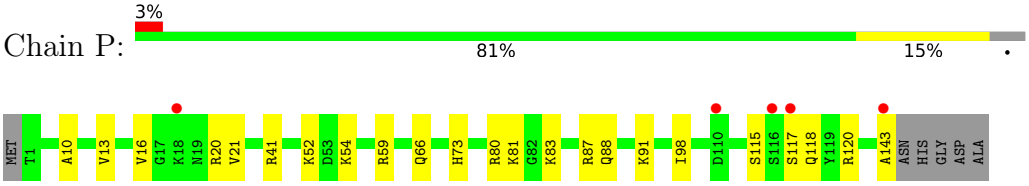
• Molecule 15: 50S ribosomal protein L18e

Chain O:



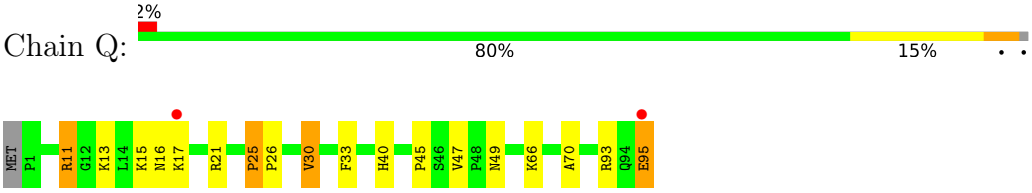
• Molecule 16: 50S ribosomal protein L19e

Chain P:



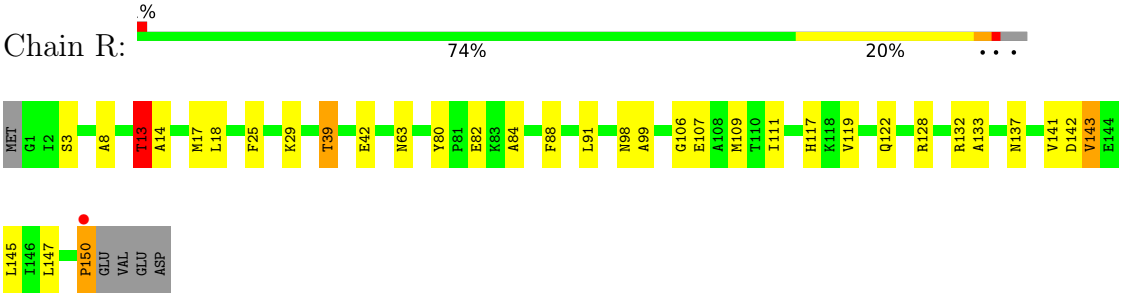
• Molecule 17: 50S ribosomal protein L21e

Chain Q:



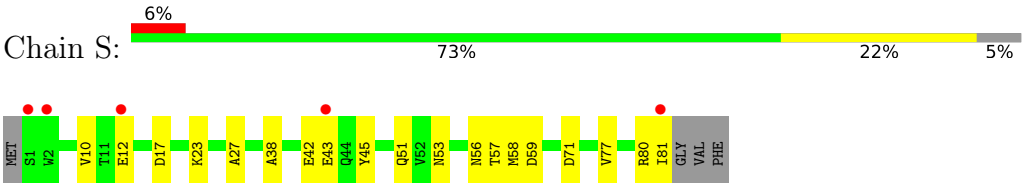
• Molecule 18: 50S ribosomal protein L22P

Chain R:



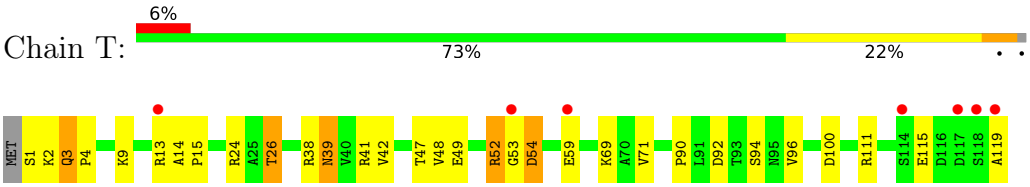
• Molecule 19: 50S ribosomal protein L23P

Chain S:



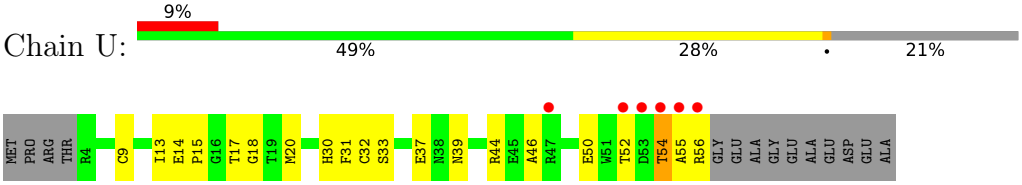
• Molecule 20: 50S ribosomal protein L24P

Chain T:



• Molecule 21: 50S ribosomal protein L24e

Chain U:



• Molecule 22: 50S ribosomal protein L29P

Chain V: 17% 59% 28% • 8%

MET T1 V2 E7 I8 M11 T12 P13 A14 E15 R16 A36 G37 G38 A39 P40 E41 N42 P43 G44 R45 I46 K47 E48 R55 I56 K57 T58 I59 Q60 G64 D65 LEU GLN GLU ASN GLU

• Molecule 23: 50S ribosomal protein L30P

Chain W: 2% 62% 32% 5% •

M1 H2 A3 L4 V5 Q6 G9 E10 V11 N12 M13 I17 Q18 L21 E22 M23 I26 C32 V36 P36 E37 T38 D39 R42 V48 V52 A53 F54 E60 T64 V65 T68 R69 P72 L73 E74 G75 D76 A77 D80 D81 V84 A85 E86 H87

T88 D89 Y90 D91 D92 R108 E109 Q110 P114 T115 H119 P120 P121 R122 H125 D126 G127 H130 G135 G136 Q137 L138 G139 K140 H141 D142 I146 L149 L150 E151 A152 M153 R154

• Molecule 24: 50S ribosomal protein L31e

Chain X: 16% 61% 24% • 11%

MET SER ALA SER ASP PHE GLU E7 I12 R15 R18 P21 N22 H23 K24 R25 M30 L37 V43 D44 E45 D46 R49 A58 W59 A60 R61 A64 N65 T66 I70 R71 V72 R73 A74 A75 R76 F77 E78 E79 E80 G81 E82 A83 I84 V85 E86 A87 E88

THR ALA GLU

• Molecule 25: 50S ribosomal protein L32e

Chain Y: 2% 45% 12% • 41%

MET ALA ASP ASN GLU GLU ASP VAL GLU ALA GLU GLU GLU TYR THR GLU LEU THR ASP ILE SER GLY VAL GLY PRO SER LYS ALA GLU SER LEU ARG GLU ALA GLY PHE GLU SER VAL GLU ASP VAL ARG GLY ALA ASP GLN SER ALA LEU ALA ASP VAL SER GLY ILE GLY ASN ALA LEU

ALA ALA ARG ILE LYS ALA ASP VAL GLY LEU GLU VAL GLU SER GLU THR GLU ALA GLU VAL GLU GLU GLU GLY GLY GLU GLU ALA PRO ASP GLU ASP VAL GLU T95 A99 T103 D108 R115 L116 L117 R122 P126 Q127 F128 D132 H133 H134 T141 S142 W143

R144 R154 R155 R169 T172 A173 V174 E184 V185 R186 V187 H188 N189 D192 T200 E201 A202 V203 R204 I205 K208 R216 I217 E220 Y233 V234 E235 V236 GLU VAL SER GLU

• Molecule 26: 50S ribosomal protein L37Ae

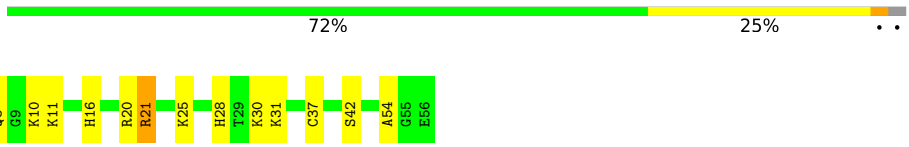
Chain Z: 6% 44% 19% 37%

MET SER PRO ARG ALA ARG ARG GLU PRO ASN LEU GLU GLY LEU MET TRP PRO LEU GLY GLY GLN GLN THR THR MET ALA SER LYS SER GLY LYS THR GLY S34 S35 G36 R37 R41 Y42 G43 R44 R47 R48 D60 H61 N65 C66 G67 E68 D69 R70 V71 G77 Y83

C84 D85 G90 G91 R104 R105 S106 ILE ARG ALA ALA LEU SER GLU ASP GLU GLU

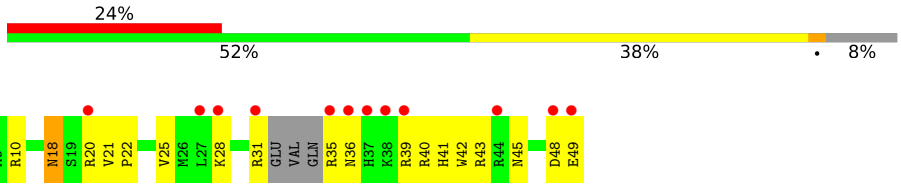
- Molecule 27: 50S ribosomal protein L37e

Chain 1:



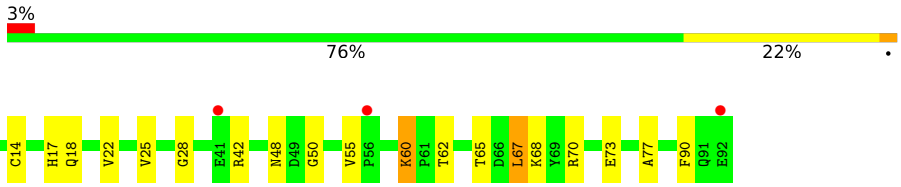
- Molecule 28: 50S ribosomal protein L39e

Chain 2:



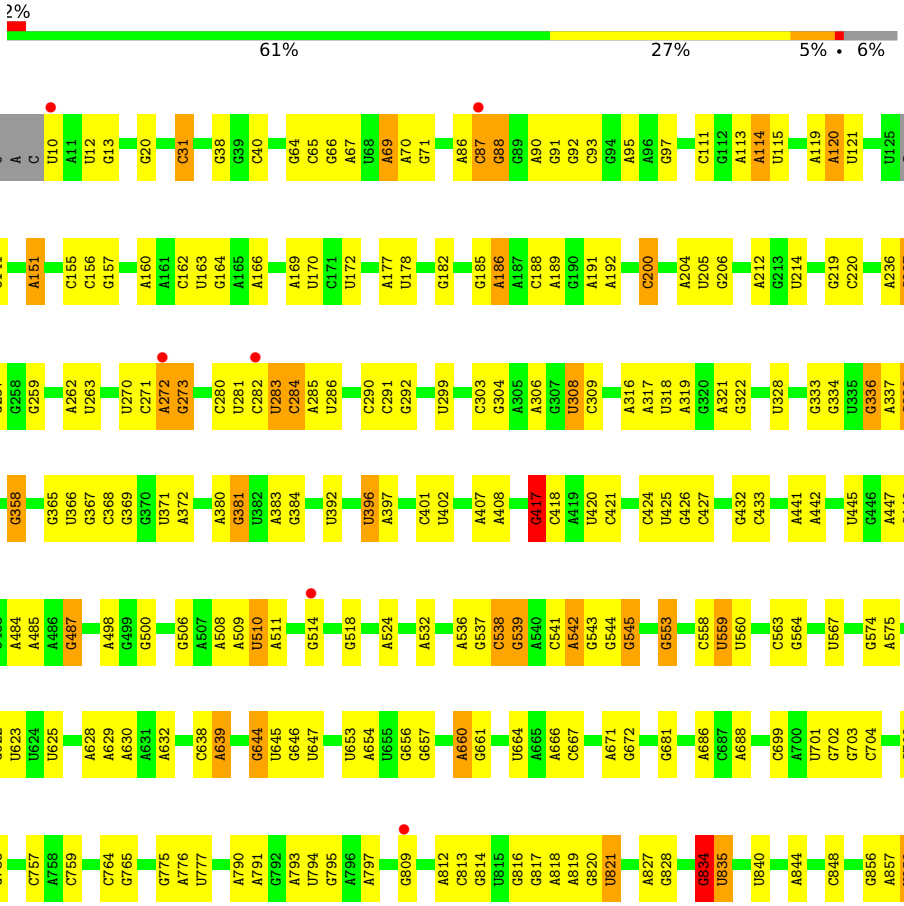
- Molecule 29: 50S ribosomal protein L44E

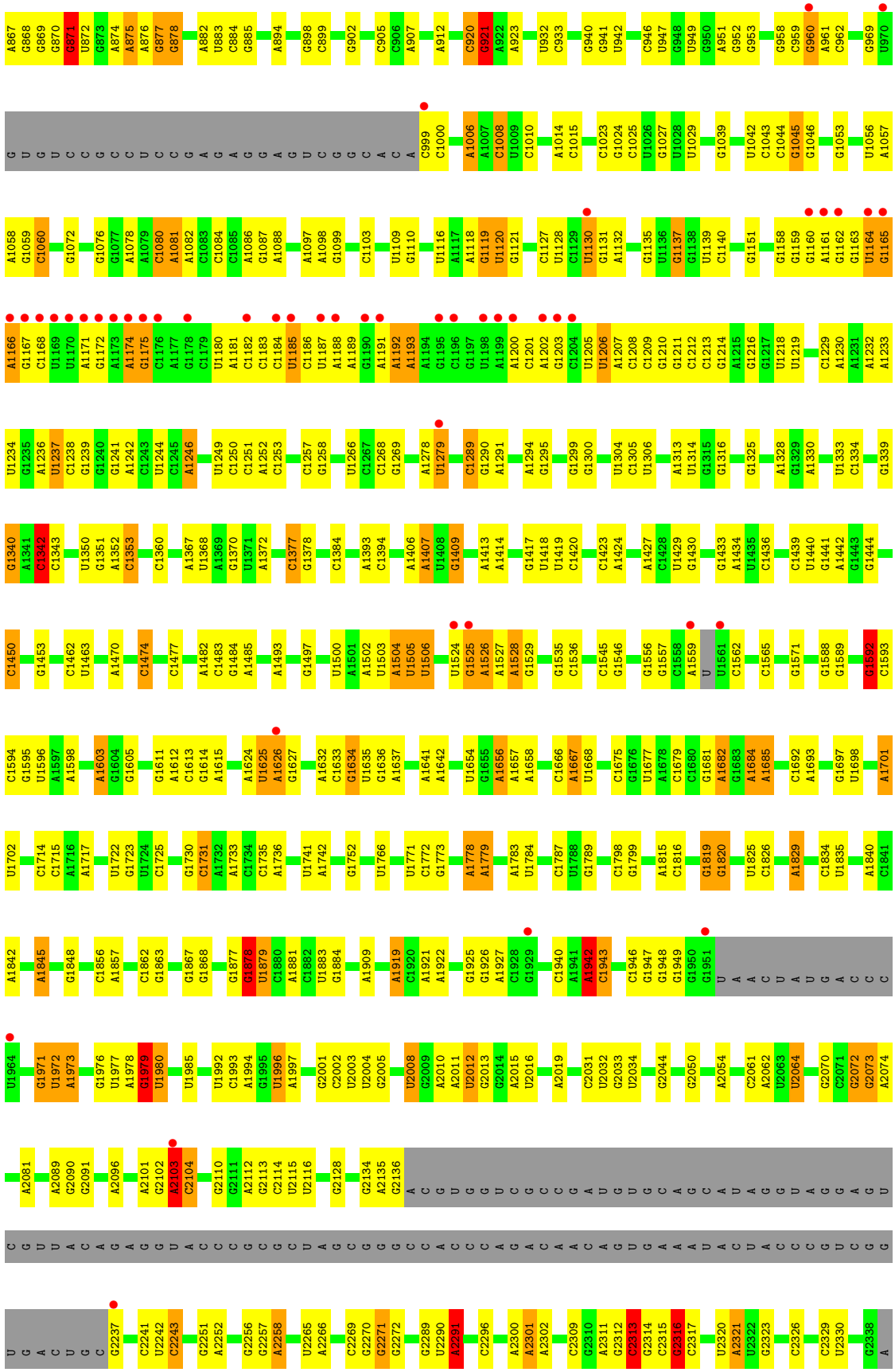
Chain 3:

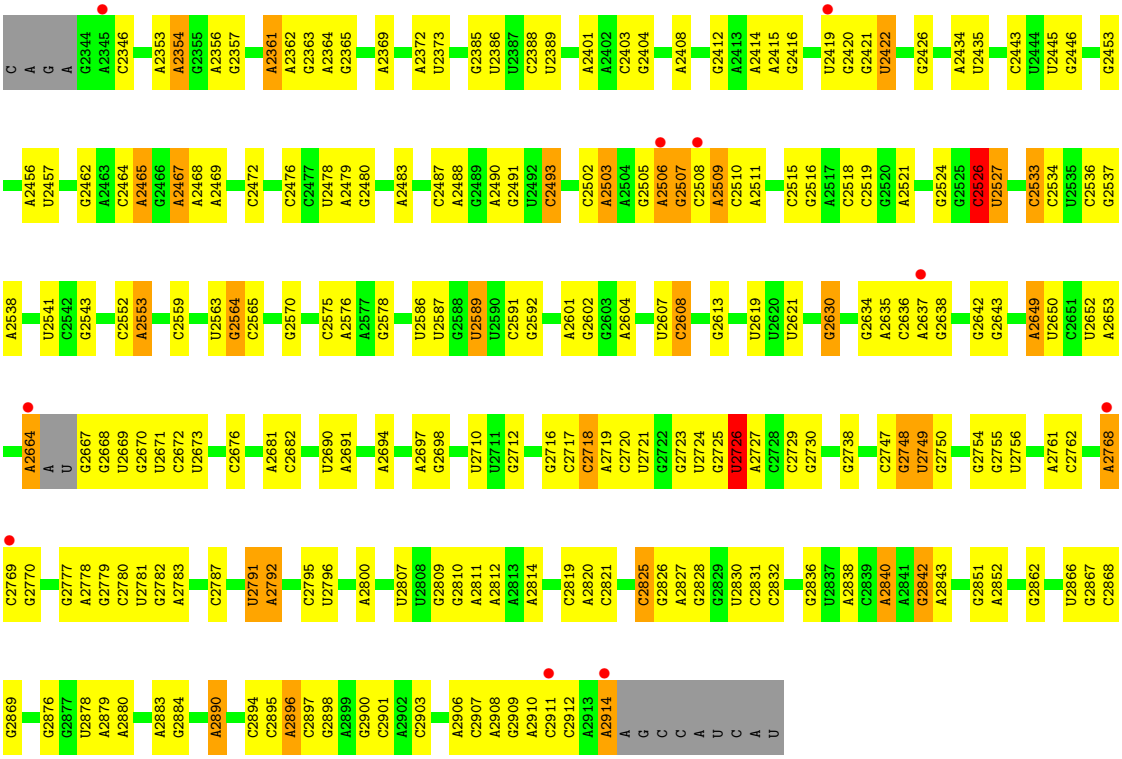


- Molecule 30: 23S RIBOSOMAL RNA

Chain 0:

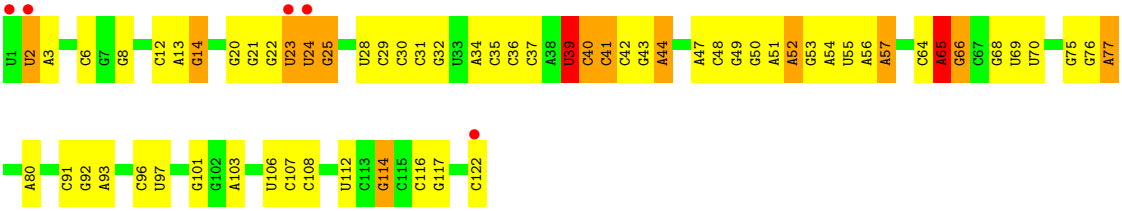



A867 G868 G869 G870 G871 U872 G873 A874 A875 A876 G877 G878 A882 U883 C884 G885 A894 G898 C899 G902 C905 C906 A907 A912 C920 G921 A922 A923 U932 C933 G940 G941 U942 C946 U947 G948 U949 G950 A951 G952 G953 G958 C959 G960 A961 C962 G969 U970
G U G U C C G C C U C C G A G A G G A C U G U C A C C999 C1000 A1006 A1007 C1008 U1009 C1010 A1014 C1015 C1023 G1024 C1025 U1026 G1027 U1028 U1029 G1039 U1042 C1043 C1044 G1045 G1046 G1053 U1056 A1057
A1058 G1059 C1060 G1072 G1076 G1077 A1078 A1079 C1080 A1081 A1082 C1083 C1084 C1085 A1086 G1087 A1088 A1097 A1098 G1099 C1103 U1109 G1110 U1116 A1117 A1118 G1119 U1120 G1121 C1127 U1128 C1129 U1130 G1131 A1132 G1135 U1136 G1137 G1138 U1139 C1140 G1151 G1158 G1159 G1160 A1161 G1162 G1163 U1164 G1165
A1166 G1167 C1168 U1169 U1170 A1171 G1172 A1173 A1174 G1175 C1176 A1177 G1178 C1179 U1180 A1181 C1182 C1183 C1184 U1185 C1186 U1187 A1188 A1189 G1190 A1191 A1192 A1193 A1194 C1195 C1196 G1197 U1198 A1199 A1200 C1201 A1202 G1203 C1204 U1205 U1206 A1207 C1208 C1209 G1210 G1211 C1212 C1213 G1214 A1215 G1216 G1217 U1218 U1219 C1229 A1230 A1231 A1232 A1233
U1234 G1235 A1236 U1237 C1238 G1239 G1240 G1241 A1242 C1243 U1244 C1245 A1246 U1249 C1250 C1251 A1252 C1253 C1257 G1258 U1266 C1267 C1268 G1269 A1278 U1279 C1289 G1290 A1291 A1294 G1295 G1299 G1300 U1304 C1305 U1306 A1313 U1314 G1315 G1316 G1325 A1328 G1329 A1330 U1333 C1334 G1339
G1340 A1341 C1342 C1343 U1350 G1351 A1352 C1353 C1360 A1367 U1368 A1369 G1370 U1371 A1372 C1377 G1378 C1384 A1393 C1394 A1406 A1407 U1408 G1409 A1413 A1414 G1417 U1418 U1419 C1420 C1423 A1424 A1427 C1428 U1429 G1430 G1433 A1434 U1435 C1436 C1439 U1440 G1441 A1442 G1443 G1444
C1450 G1453 C1462 U1463 A1470 C1474 C1477 A1482 C1483 G1484 A1485 A1493 G1497 U1500 A1501 A1502 U1503 A1504 U1505 U1506 U1524 G1525 A1526 A1527 A1528 G1529 G1535 C1536 C1545 G1546 G1556 G1557 C1558 A1559 U U1561 C1562 C1565 G1571 G1588 G1589 G1592 C1593
C1594 G1595 U1596 A1597 A1598 A1603 G1604 G1605 G1611 A1612 C1613 G1614 A1615 A1624 U1625 A1626 G1627 A1632 C1633 G1634 U1635 G1636 A1637 A1641 A1642 U1654 G1655 A1656 A1657 A1658 C1666 A1667 U1668 C1675 G1676 U1677 A1678 C1679 C1680 G1681 A1682 G1683 A1684 A1685 C1692 A1693 G1697 U1698 A1701
U1702 C1714 C1715 A1716 A1717 U1722 G1723 U1724 C1725 G1730 C1731 A1732 A1733 C1734 C1735 A1736 U1741 A1742 G1752 U1766 U1771 C1772 G1773 A1778 A1779 A1783 U1784 C1787 U1788 G1789 C1798 G1799 A1815 C1816 G1819 G1820 U1825 C1826 A1829 C1834 U1835 A1840 G1841
A1842 A1845 G1848 C1856 A1857 C1862 G1863 G1867 G1868 G1877 G1878 U1879 C1880 A1881 C1882 U1883 G1884 A1909 A1919 C1920 A1921 A1922 G1925 G1926 A1927 C1928 G1929 C1940 A1941 A1942 C1943 C1946 G1947 G1948 G1949 G1950 G1951 U A A C U A U G G A C C C
U1964 G1971 U1972 A1973 G1976 U1977 A1978 G1979 U1980 U1985 U1992 C1993 A1994 G1995 U1996 A1997 G2001 C2002 U2003 U2004 G2005 U2008 G2009 A2010 A2011 U2012 G2013 G2014 A2015 U2016 A2019 C2031 U2032 G2033 U2034 G2044 G2050 A2054 C2061 A2062 U2063 U2064 G2070 C2071 G2072 G2073 A2074
A2081 A2089 G2090 G2091 A2096 A2101 G2102 A2103 C2104 C2110 G2111 A2112 C2113 C2114 U2115 U2116 G2128 G2134 A2135 G2136 A C C G U G G U C A C C C G A G C A U U G U G G C A A G G U A U A G G U A C C C C A G G G U C C G A G G U
U G G A C U U G C G2237 C2241 U2242 C2243 G2251 A2252 G2256 G2257 A2258 U2265 A2266 C2269 G2270 G2271 G2272 G2289 U2290 A2291 C2296 A2300 A2301 A2302 C2309 G2310 A2311 G2312 C2313 G2314 C2315 G2316 C2317 U2320 A2321 U2322 G2323 C2326 C2329 U2330 G2338 A



- Molecule 31: 5S RIBOSOMAL RNA

Chain 9:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	211.65Å 299.67Å 573.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 2.40 49.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.5 (49.95-2.40) 90.6 (49.95-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.231 0.185 , 0.217	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å^2)	38.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	99049	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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: K, OMG, CD, UR3, NA, 1MA, OMU, PSU, CL, MG

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	A	0.44	1/1786 (0.1%)	0.98	7/2408 (0.3%)
2	B	0.40	0/2690	0.98	9/3652 (0.2%)
3	C	0.45	0/1885	0.95	5/2552 (0.2%)
4	D	0.40	0/1111	0.93	6/1498 (0.4%)
5	E	0.38	0/1382	0.85	2/1880 (0.1%)
6	F	0.39	0/901	0.91	1/1224 (0.1%)
7	G	0.55	0/241	0.98	0/324
8	H	0.44	0/1302	1.00	8/1743 (0.5%)
9	I	0.43	0/526	1.01	2/716 (0.3%)
10	J	0.38	0/1136	0.91	3/1530 (0.2%)
11	K	0.39	0/1004	0.96	1/1351 (0.1%)
12	L	0.39	0/1130	0.95	5/1509 (0.3%)
13	M	0.41	0/1582	0.89	3/2116 (0.1%)
14	N	0.36	0/1474	1.04	13/1999 (0.7%)
15	O	0.41	0/874	0.93	4/1181 (0.3%)
16	P	0.38	0/1147	0.83	0/1528
17	Q	0.41	0/749	1.06	7/1005 (0.7%)
18	R	1.32	7/1172 (0.6%)	1.37	11/1578 (0.7%)
19	S	0.37	0/648	0.90	1/875 (0.1%)
20	T	0.38	0/958	0.94	4/1289 (0.3%)
21	U	0.38	0/417	0.89	1/562 (0.2%)
22	V	0.43	0/502	1.04	2/675 (0.3%)
23	W	0.47	1/1219 (0.1%)	0.99	5/1655 (0.3%)
24	X	0.45	0/664	0.99	4/895 (0.4%)
25	Y	0.43	0/1146	0.92	1/1536 (0.1%)
26	Z	0.38	0/584	1.00	2/781 (0.3%)
27	1	0.46	0/438	0.90	2/578 (0.3%)
28	2	0.38	0/401	0.78	0/529
29	3	0.39	0/771	0.88	4/1024 (0.4%)
30	0	0.37	0/65958	0.60	27/102869 (0.0%)
31	9	0.36	0/2904	0.58	3/4526 (0.1%)
All	All	0.41	9/98702 (0.0%)	0.72	143/147588 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	1	0
30	0	0	39
31	9	0	1
All	All	1	40

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CA-C	-28.27	0.93	1.52
18	R	150	PRO	N-CA	16.81	1.72	1.47
18	R	150	PRO	CB-CG	16.25	2.31	1.49
18	R	150	PRO	CA-CB	12.17	1.77	1.53
18	R	150	PRO	C-O	11.46	1.46	1.23

The worst 5 of 143 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	R	150	PRO	CB-CA-C	-25.23	62.16	110.10
18	R	150	PRO	N-CA-C	-24.97	49.68	112.10
18	R	150	PRO	CA-C-O	-12.91	80.28	119.00
30	0	1979	G	C2'-C3'-O3'	9.58	123.87	109.50
17	Q	17	LYS	N-CA-C	-8.96	98.46	109.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

5 of 40 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	270	U	Sidechain
30	0	396	U	Sidechain
30	0	417	G	Sidechain
30	0	449	A	Sidechain
30	0	469	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	A	1753	0	1766	79	0
2	B	2625	0	2533	85	0
3	C	1860	0	1813	65	0
4	D	1094	0	1085	46	0
5	E	1357	0	1266	46	0
6	F	890	0	843	27	0
7	G	240	0	231	11	0
8	H	1282	0	1292	34	0
9	I	519	0	500	25	0
10	J	1120	0	1098	39	0
11	K	994	0	1027	40	0
12	L	1118	0	1076	28	0
13	M	1558	0	1572	47	0
14	N	1445	0	1401	57	0
15	O	865	0	873	19	0
16	P	1136	0	1123	20	0
17	Q	735	0	728	11	0
18	R	1149	0	1122	32	0
19	S	641	0	605	14	0
20	T	950	0	923	24	0
21	U	410	0	364	16	0
22	V	499	0	511	20	0
23	W	1196	0	1137	65	0
24	X	654	0	653	20	0
25	Y	1130	0	1133	31	0
26	Z	573	0	532	15	0
27	1	431	0	426	16	0
28	2	396	0	413	24	0
29	3	755	0	728	16	0
30	0	59021	0	29809	873	0
31	9	2599	0	1325	72	0
32	0	109	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	73	0	0	0	0
33	9	3	0	0	0	0
33	A	1	0	0	0	0
33	C	1	0	0	0	0
33	H	1	0	0	0	0
33	J	1	0	0	0	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	Q	1	0	0	0	0
33	R	2	0	0	0	0
33	S	1	0	0	0	0
34	0	10	0	0	0	0
34	3	1	0	0	0	0
34	A	1	0	0	0	0
34	B	1	0	0	0	0
34	J	3	0	0	1	0
34	L	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	O	1	0	0	0	0
34	R	1	0	0	0	0
34	Y	1	0	0	0	0
35	1	1	0	0	0	0
35	3	1	0	0	0	0
35	O	1	0	0	0	0
35	U	1	0	0	0	0
35	Z	1	0	0	1	0
36	0	2	0	0	0	0
37	0	5949	0	0	148	0
37	1	53	0	0	2	0
37	2	40	0	0	4	0
37	3	72	0	0	6	0
37	9	139	0	0	7	0
37	A	117	0	0	15	0
37	B	146	0	0	13	0
37	C	170	0	0	18	0
37	D	47	0	0	5	0
37	E	42	0	0	4	0
37	F	24	0	0	2	0
37	G	19	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	H	72	0	0	5	0
37	I	9	0	0	3	0
37	J	51	0	0	2	0
37	K	56	0	0	4	0
37	L	72	0	0	9	0
37	M	119	0	0	9	0
37	N	65	0	0	10	0
37	O	39	0	0	3	0
37	P	63	0	0	1	0
37	Q	52	0	0	3	0
37	R	80	0	0	2	0
37	S	33	0	0	2	0
37	T	38	0	0	2	0
37	U	27	0	0	1	0
37	V	14	0	0	1	0
37	W	66	0	0	5	0
37	X	29	0	0	5	0
37	Y	94	0	0	10	0
37	Z	26	0	0	2	0
All	All	99049	0	59908	1724	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 11.

The worst 5 of 1724 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)
18:R:150:PRO:CD	18:R:150:PRO:CG	1.89	1.50
14:N:37:ARG:NH1	31:9:6:C:H5”	1.61	1.14
18:R:150:PRO:CG	18:R:150:PRO:C	2.21	1.12
30:0:871:G:H5’	30:0:871:G:C8	1.86	1.10
30:0:960:G:H4’	37:0:6980:HOH:O	1.49	1.09

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	
1	A	235/240 (98%)	220 (94%)	13 (6%)	2 (1%)	14	22
2	B	335/338 (99%)	315 (94%)	17 (5%)	3 (1%)	14	22
3	C	244/246 (99%)	231 (95%)	13 (5%)	0	100	100
4	D	134/177 (76%)	115 (86%)	15 (11%)	4 (3%)	3	3
5	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
6	F	117/120 (98%)	106 (91%)	9 (8%)	2 (2%)	7	10
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
8	H	156/177 (88%)	148 (95%)	8 (5%)	0	100	100
9	I	68/162 (42%)	57 (84%)	11 (16%)	0	100	100
10	J	140/145 (97%)	132 (94%)	7 (5%)	1 (1%)	18	28
11	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	16	25
12	L	141/165 (86%)	126 (89%)	14 (10%)	1 (1%)	18	28
13	M	192/196 (98%)	187 (97%)	5 (3%)	0	100	100
14	N	184/187 (98%)	170 (92%)	11 (6%)	3 (2%)	7	11
15	O	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
16	P	141/149 (95%)	140 (99%)	1 (1%)	0	100	100
17	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
18	R	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
19	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
20	T	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
21	U	51/67 (76%)	48 (94%)	2 (4%)	1 (2%)	6	7
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	7	11
23	W	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
24	X	80/92 (87%)	74 (92%)	5 (6%)	1 (1%)	9	14
25	Y	140/241 (58%)	140 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	71/116 (61%)	63 (89%)	6 (8%)	2 (3%)	4	3
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	42 (100%)	0	0	100	100
29	3	90/92 (98%)	87 (97%)	3 (3%)	0	100	100
All	All	3705/4472 (83%)	3505 (95%)	177 (5%)	23 (1%)	21	32

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
6	F	101	ALA
10	J	5	GLU
12	L	80	ASP
14	N	154	LEU

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	
1	A	179/182 (98%)	170 (95%)	9 (5%)	22	38
2	B	282/283 (100%)	262 (93%)	20 (7%)	13	23
3	C	193/193 (100%)	176 (91%)	17 (9%)	9	15
4	D	117/148 (79%)	114 (97%)	3 (3%)	40	63
5	E	152/156 (97%)	149 (98%)	3 (2%)	48	70
6	F	93/94 (99%)	91 (98%)	2 (2%)	45	67
7	G	27/282 (10%)	26 (96%)	1 (4%)	30	51
8	H	134/145 (92%)	129 (96%)	5 (4%)	30	51
9	I	58/130 (45%)	57 (98%)	1 (2%)	53	74
10	J	118/121 (98%)	113 (96%)	5 (4%)	26	45
11	K	106/106 (100%)	104 (98%)	2 (2%)	50	71
12	L	113/127 (89%)	111 (98%)	2 (2%)	51	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	158/160 (99%)	153 (97%)	5 (3%)	34	56
14	N	149/150 (99%)	142 (95%)	7 (5%)	23	41
15	O	93/94 (99%)	90 (97%)	3 (3%)	34	56
16	P	113/117 (97%)	109 (96%)	4 (4%)	32	53
17	Q	79/80 (99%)	75 (95%)	4 (5%)	21	37
18	R	117/122 (96%)	113 (97%)	4 (3%)	32	54
19	S	71/74 (96%)	68 (96%)	3 (4%)	26	45
20	T	105/106 (99%)	100 (95%)	5 (5%)	23	40
21	U	44/53 (83%)	44 (100%)	0	100	100
22	V	51/57 (90%)	49 (96%)	2 (4%)	28	48
23	W	130/130 (100%)	123 (95%)	7 (5%)	20	35
24	X	66/74 (89%)	61 (92%)	5 (8%)	12	21
25	Y	120/196 (61%)	111 (92%)	9 (8%)	12	21
26	Z	60/94 (64%)	59 (98%)	1 (2%)	53	74
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	43	65
29	3	79/79 (100%)	78 (99%)	1 (1%)	61	80
All	All	3095/3646 (85%)	2964 (96%)	131 (4%)	26	45

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	X	49	ARG
25	Y	103	THR
29	3	42	ARG
4	D	137	PRO
4	D	136	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
19	S	51	GLN
25	Y	133	HIS
19	S	55	GLN
23	W	28	HIS

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Mol	Chain	Res	Type
27	1	8	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	239 (8%)	32 (1%)
31	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3045 (94%)	255 (8%)	33 (1%)

5 of 255 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	2718	C
30	0	2726	U
31	9	65	A
30	0	1237	U
30	0	1232	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
30	PSU	0	2621	30	18,21,22	1.45	2 (11%)	21,30,33	1.28	3 (14%)
30	OMU	0	2587	30	19,22,23	0.25	0	25,31,34	0.35	0
30	1MA	0	628	30,33	21,25,26	0.70	1 (4%)	30,37,40	0.68	1 (3%)
30	OMG	0	2588	30	23,26,27	0.30	0	32,38,41	0.37	0
30	UR3	0	2619	30	19,22,23	0.38	0	26,32,35	0.72	1 (3%)

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
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	OMU	0	2587	30	-	0/9/27/28	0/2/2/2
30	1MA	0	628	30,33	-	1/7/25/26	0/3/3/3
30	OMG	0	2588	30	-	0/9/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	4.98	1.43	1.36
30	0	2621	PSU	C6-C5	2.46	1.38	1.35
30	0	628	1MA	C6-N6	2.37	1.33	1.28

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	0	2621	PSU	C6-C5-C4	3.23	120.35	118.17
30	0	2621	PSU	O2-C2-N1	2.88	125.76	122.79
30	0	2619	UR3	C4-N3-C2	2.86	126.88	124.58
30	0	2621	PSU	C6-N1-C2	-2.77	120.12	122.69
30	0	628	1MA	N1-C2-N3	2.72	129.23	126.00

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	0	628	1MA	C2'-C1'-N9-C8

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides 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)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	237/240 (98%)	0.21	12 (5%)	33	30	19, 38, 77, 98	0
2	B	337/338 (99%)	0.45	12 (3%)	46	42	21, 46, 74, 84	0
3	C	246/246 (100%)	0.11	4 (1%)	70	66	15, 36, 60, 71	0
4	D	140/177 (79%)	2.19	72 (51%)	0	0	47, 90, 115, 123	0
5	E	172/178 (96%)	0.90	19 (11%)	10	8	39, 61, 81, 85	0
6	F	119/120 (99%)	1.12	18 (15%)	5	4	34, 61, 90, 104	0
7	G	29/348 (8%)	2.22	13 (44%)	0	0	69, 86, 95, 98	0
8	H	160/177 (90%)	0.56	12 (7%)	20	17	30, 48, 83, 90	0
9	I	70/162 (43%)	3.74	62 (88%)	0	0	122, 136, 154, 155	0
10	J	142/145 (97%)	0.36	7 (4%)	35	31	29, 43, 66, 89	0
11	K	132/132 (100%)	0.20	3 (2%)	61	57	27, 42, 65, 77	0
12	L	145/165 (87%)	0.86	28 (19%)	3	2	18, 55, 101, 117	0
13	M	194/196 (98%)	-0.23	0	100	100	20, 31, 47, 55	0
14	N	186/187 (99%)	1.10	34 (18%)	3	3	32, 53, 102, 112	0
15	O	115/116 (99%)	0.52	6 (5%)	33	29	29, 44, 62, 70	0
16	P	143/149 (95%)	0.38	5 (3%)	47	43	31, 45, 57, 68	0
17	Q	95/96 (98%)	0.08	2 (2%)	63	59	26, 35, 54, 66	0
18	R	150/155 (96%)	-0.15	1 (0%)	84	81	22, 37, 58, 71	0
19	S	81/85 (95%)	0.53	5 (6%)	26	23	31, 48, 72, 82	0
20	T	119/120 (99%)	0.64	7 (5%)	28	24	29, 46, 78, 98	0
21	U	53/67 (79%)	0.53	6 (11%)	10	7	34, 48, 66, 76	0
22	V	65/71 (91%)	1.26	12 (18%)	3	3	40, 62, 106, 113	0
23	W	154/154 (100%)	0.25	3 (1%)	66	62	28, 42, 59, 71	0
24	X	82/92 (89%)	1.07	15 (18%)	3	3	36, 50, 78, 94	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	Y	142/241 (58%)	0.11	4 (2%) 55 51	22, 36, 60, 80	0
26	Z	73/116 (62%)	0.71	7 (9%) 13 10	34, 48, 68, 87	0
27	1	56/57 (98%)	-0.62	0 100 100	19, 24, 31, 40	0
28	2	46/50 (92%)	1.01	12 (26%) 1 1	26, 50, 75, 89	0
29	3	92/92 (100%)	0.29	3 (3%) 49 45	22, 45, 62, 76	0
30	0	2749/2923 (94%)	-0.61	66 (2%) 59 55	16, 36, 81, 155	0
31	9	122/122 (100%)	0.06	5 (4%) 41 37	31, 54, 77, 138	0
All	All	6646/7517 (88%)	0.07	455 (6%) 23 20	15, 42, 89, 155	0

The worst 5 of 455 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	1	THR	9.9
9	I	128	THR	9.0
4	D	10	PHE	8.9
24	X	88	GLU	8.2
4	D	174	VAL	6.6

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
30	OMU	0	2587	21/22	0.98	0.06	22,25,27,28	0
30	OMG	0	2588	24/25	0.98	0.05	22,25,27,28	0
30	UR3	0	2619	21/22	0.98	0.06	24,27,31,36	0
30	PSU	0	2621	20/21	0.98	0.05	20,23,27,27	0
30	1MA	0	628	23/24	0.99	0.05	20,22,23,25	0

6.3 Carbohydrates (i)

There are no oligosaccharides 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, 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
33	NA	R	8386	1/1	0.59	0.56	80,80,80,80	0
33	NA	0	8370	1/1	0.66	0.53	70,70,70,70	0
32	MG	9	8095	1/1	0.72	0.23	64,64,64,64	0
32	MG	0	8087	1/1	0.78	0.17	57,57,57,57	0
32	MG	0	8090	1/1	0.82	0.14	56,56,56,56	0
33	NA	0	8329	1/1	0.82	0.15	55,55,55,55	0
32	MG	0	8050	1/1	0.82	0.16	66,66,66,66	0
33	NA	0	8376	1/1	0.83	0.16	42,42,42,42	0
33	NA	0	8314	1/1	0.85	0.10	38,38,38,38	0
33	NA	9	8351	1/1	0.85	0.23	45,45,45,45	0
32	MG	0	8094	1/1	0.86	0.18	59,59,59,59	0
32	MG	0	8082	1/1	0.87	0.21	62,62,62,62	0
33	NA	0	8340	1/1	0.87	0.17	49,49,49,49	0
32	MG	0	8047	1/1	0.87	0.11	59,59,59,59	0
33	NA	0	8311	1/1	0.87	0.14	52,52,52,52	0
33	NA	0	8384	1/1	0.87	0.14	53,53,53,53	0
32	MG	0	8104	1/1	0.87	0.13	50,50,50,50	0
32	MG	0	8070	1/1	0.88	0.08	44,44,44,44	0
33	NA	0	8324	1/1	0.88	0.22	48,48,48,48	0
33	NA	0	8307	1/1	0.88	0.11	42,42,42,42	0
33	NA	H	8322	1/1	0.88	0.21	54,54,54,54	0
33	NA	0	8371	1/1	0.89	0.12	48,48,48,48	0
32	MG	0	8105	1/1	0.89	0.06	45,45,45,45	0
33	NA	0	8369	1/1	0.90	0.15	42,42,42,42	0
32	MG	0	8102	1/1	0.90	0.07	48,48,48,48	0
33	NA	0	8366	1/1	0.90	0.13	63,63,63,63	0
33	NA	0	8373	1/1	0.91	0.06	44,44,44,44	0
33	NA	0	8363	1/1	0.91	0.14	50,50,50,50	0
33	NA	0	8381	1/1	0.91	0.08	43,43,43,43	0
33	NA	0	8364	1/1	0.91	0.12	40,40,40,40	0
33	NA	0	8341	1/1	0.91	0.13	41,41,41,41	0
32	MG	0	8066	1/1	0.92	0.16	88,88,88,88	0
33	NA	0	8374	1/1	0.92	0.11	47,47,47,47	0
33	NA	9	8383	1/1	0.92	0.11	46,46,46,46	0
33	NA	0	8372	1/1	0.93	0.25	60,60,60,60	0
33	NA	0	8382	1/1	0.93	0.09	67,67,67,67	0
32	MG	0	8100	1/1	0.93	0.14	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	NA	0	8385	1/1	0.93	0.19	44,44,44,44	0
32	MG	0	8053	1/1	0.93	0.16	33,33,33,33	0
32	MG	0	8103	1/1	0.93	0.13	55,55,55,55	0
33	NA	0	8368	1/1	0.94	0.10	48,48,48,48	0
33	NA	R	8337	1/1	0.94	0.05	33,33,33,33	0
33	NA	0	8326	1/1	0.94	0.08	37,37,37,37	0
33	NA	0	8327	1/1	0.94	0.09	36,36,36,36	0
32	MG	0	8046	1/1	0.94	0.05	39,39,39,39	0
33	NA	0	8335	1/1	0.94	0.06	31,31,31,31	0
32	MG	0	8107	1/1	0.94	0.09	68,68,68,68	0
32	MG	0	8043	1/1	0.94	0.05	32,32,32,32	0
33	NA	0	8377	1/1	0.94	0.12	50,50,50,50	0
33	NA	0	8342	1/1	0.94	0.06	35,35,35,35	0
33	NA	0	8356	1/1	0.94	0.09	35,35,35,35	0
32	MG	0	8049	1/1	0.94	0.09	54,54,54,54	0
33	NA	0	8316	1/1	0.94	0.08	38,38,38,38	0
33	NA	0	8365	1/1	0.94	0.21	31,31,31,31	0
33	NA	0	8318	1/1	0.94	0.10	47,47,47,47	0
33	NA	0	8360	1/1	0.95	0.10	41,41,41,41	0
33	NA	0	8362	1/1	0.95	0.12	46,46,46,46	0
32	MG	0	8076	1/1	0.95	0.04	44,44,44,44	0
33	NA	0	8313	1/1	0.95	0.06	55,55,55,55	0
32	MG	0	8112	1/1	0.95	0.08	39,39,39,39	0
32	MG	0	8113	1/1	0.95	0.07	31,31,31,31	0
33	NA	0	8367	1/1	0.95	0.14	46,46,46,46	0
32	MG	0	8115	1/1	0.95	0.05	41,41,41,41	0
32	MG	0	8116	1/1	0.95	0.07	35,35,35,35	0
32	MG	0	8101	1/1	0.95	0.06	44,44,44,44	0
32	MG	0	8080	1/1	0.95	0.06	40,40,40,40	0
32	MG	0	8092	1/1	0.95	0.10	66,66,66,66	0
33	NA	0	8330	1/1	0.95	0.07	37,37,37,37	0
33	NA	0	8331	1/1	0.95	0.07	35,35,35,35	0
32	MG	0	8062	1/1	0.95	0.05	42,42,42,42	0
33	NA	S	8312	1/1	0.95	0.09	28,28,28,28	0
33	NA	0	8379	1/1	0.95	0.12	46,46,46,46	0
33	NA	0	8302	1/1	0.95	0.09	44,44,44,44	0
32	MG	0	8099	1/1	0.95	0.05	40,40,40,40	0
33	NA	0	8349	1/1	0.95	0.07	32,32,32,32	0
33	NA	0	8350	1/1	0.95	0.12	41,41,41,41	0
33	NA	0	8308	1/1	0.95	0.10	45,45,45,45	0
33	NA	9	8352	1/1	0.95	0.10	41,41,41,41	0
33	NA	0	8358	1/1	0.95	0.18	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	NA	0	8319	1/1	0.96	0.04	31,31,31,31	0
33	NA	0	8301	1/1	0.96	0.07	34,34,34,34	0
33	NA	0	8325	1/1	0.96	0.08	50,50,50,50	0
32	MG	0	8072	1/1	0.96	0.04	47,47,47,47	0
33	NA	0	8359	1/1	0.96	0.09	39,39,39,39	0
33	NA	0	8375	1/1	0.96	0.15	38,38,38,38	0
33	NA	C	8304	1/1	0.96	0.06	29,29,29,29	0
33	NA	0	8361	1/1	0.96	0.08	41,41,41,41	0
33	NA	0	8378	1/1	0.96	0.12	40,40,40,40	0
32	MG	0	8085	1/1	0.96	0.05	37,37,37,37	0
33	NA	M	8347	1/1	0.96	0.04	19,19,19,19	0
33	NA	Q	8348	1/1	0.96	0.06	30,30,30,30	0
33	NA	0	8334	1/1	0.96	0.12	36,36,36,36	0
32	MG	0	8096	1/1	0.96	0.06	34,34,34,34	0
33	NA	0	8315	1/1	0.96	0.07	30,30,30,30	0
32	MG	B	8055	1/1	0.96	0.06	42,42,42,42	0
32	MG	0	8045	1/1	0.96	0.10	55,55,55,55	0
34	CL	J	8502	1/1	0.96	0.07	55,55,55,55	0
34	CL	J	8521	1/1	0.96	0.08	47,47,47,47	0
34	CL	0	8515	1/1	0.96	0.11	53,53,53,53	0
34	CL	0	8517	1/1	0.96	0.06	47,47,47,47	0
36	K	0	8201	1/1	0.96	0.20	60,60,60,60	0
32	MG	0	8089	1/1	0.97	0.05	43,43,43,43	0
33	NA	0	8333	1/1	0.97	0.06	23,23,23,23	0
33	NA	0	8305	1/1	0.97	0.05	33,33,33,33	0
32	MG	0	8063	1/1	0.97	0.06	60,60,60,60	0
32	MG	0	8114	1/1	0.97	0.03	38,38,38,38	0
33	NA	0	8309	1/1	0.97	0.03	25,25,25,25	0
32	MG	0	8064	1/1	0.97	0.05	26,26,26,26	0
33	NA	0	8344	1/1	0.97	0.06	24,24,24,24	0
32	MG	Y	8108	1/1	0.97	0.08	25,25,25,25	0
32	MG	0	8067	1/1	0.97	0.10	28,28,28,28	0
33	NA	0	8354	1/1	0.97	0.04	23,23,23,23	0
33	NA	0	8355	1/1	0.97	0.17	53,53,53,53	0
33	NA	A	8345	1/1	0.97	0.09	43,43,43,43	0
33	NA	0	8357	1/1	0.97	0.07	39,39,39,39	0
32	MG	0	8014	1/1	0.97	0.06	25,25,25,25	0
32	MG	0	8024	1/1	0.97	0.03	22,22,22,22	0
33	NA	J	8346	1/1	0.97	0.04	37,37,37,37	0
33	NA	0	8320	1/1	0.97	0.10	37,37,37,37	0
32	MG	0	8075	1/1	0.97	0.06	27,27,27,27	0
34	CL	A	8509	1/1	0.97	0.07	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	CL	J	8501	1/1	0.97	0.08	46,46,46,46	0
32	MG	0	8041	1/1	0.97	0.12	34,34,34,34	0
32	MG	0	8051	1/1	0.97	0.07	54,54,54,54	0
34	CL	L	8510	1/1	0.97	0.10	40,40,40,40	0
34	CL	0	8514	1/1	0.97	0.07	39,39,39,39	0
32	MG	0	8052	1/1	0.97	0.04	48,48,48,48	0
32	MG	A	8065	1/1	0.97	0.04	23,23,23,23	0
32	MG	K	8069	1/1	0.97	0.04	47,47,47,47	0
33	NA	0	8332	1/1	0.98	0.06	31,31,31,31	0
32	MG	0	8111	1/1	0.98	0.04	23,23,23,23	0
33	NA	0	8306	1/1	0.98	0.16	29,29,29,29	0
32	MG	3	8078	1/1	0.98	0.04	37,37,37,37	0
33	NA	0	8336	1/1	0.98	0.03	37,37,37,37	0
33	NA	0	8338	1/1	0.98	0.03	41,41,41,41	0
33	NA	0	8339	1/1	0.98	0.03	19,19,19,19	0
32	MG	0	8088	1/1	0.98	0.03	24,24,24,24	0
32	MG	0	8026	1/1	0.98	0.03	23,23,23,23	0
33	NA	0	8310	1/1	0.98	0.04	30,30,30,30	0
32	MG	0	8048	1/1	0.98	0.04	41,41,41,41	0
32	MG	0	8037	1/1	0.98	0.03	35,35,35,35	0
32	MG	0	8093	1/1	0.98	0.05	37,37,37,37	0
33	NA	0	8353	1/1	0.98	0.04	17,17,17,17	0
32	MG	0	8006	1/1	0.98	0.04	29,29,29,29	0
32	MG	0	8071	1/1	0.98	0.05	61,61,61,61	0
33	NA	0	8317	1/1	0.98	0.04	28,28,28,28	0
32	MG	0	8098	1/1	0.98	0.11	25,25,25,25	0
32	MG	0	8042	1/1	0.98	0.06	31,31,31,31	0
33	NA	L	8380	1/1	0.98	0.31	44,44,44,44	0
33	NA	0	8321	1/1	0.98	0.11	42,42,42,42	0
32	MG	0	8012	1/1	0.98	0.05	30,30,30,30	0
32	MG	0	8044	1/1	0.98	0.03	33,33,33,33	0
32	MG	0	8079	1/1	0.98	0.03	20,20,20,20	0
34	CL	N	8507	1/1	0.98	0.07	44,44,44,44	0
34	CL	R	8506	1/1	0.98	0.08	40,40,40,40	0
34	CL	Y	8520	1/1	0.98	0.05	35,35,35,35	0
34	CL	0	8505	1/1	0.98	0.06	41,41,41,41	0
34	CL	0	8511	1/1	0.98	0.06	37,37,37,37	0
34	CL	0	8513	1/1	0.98	0.06	44,44,44,44	0
32	MG	0	8057	1/1	0.98	0.07	34,34,34,34	0
32	MG	0	8060	1/1	0.98	0.06	33,33,33,33	0
34	CL	0	8516	1/1	0.98	0.13	41,41,41,41	0
32	MG	T	8073	1/1	0.98	0.04	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	CL	0	8522	1/1	0.98	0.25	44,44,44,44	0
32	MG	0	8086	1/1	0.98	0.04	37,37,37,37	0
32	MG	0	8007	1/1	0.99	0.06	21,21,21,21	0
32	MG	0	8059	1/1	0.99	0.06	22,22,22,22	0
32	MG	0	8027	1/1	0.99	0.02	36,36,36,36	0
32	MG	0	8061	1/1	0.99	0.04	30,30,30,30	0
32	MG	0	8028	1/1	0.99	0.03	27,27,27,27	0
32	MG	0	8029	1/1	0.99	0.03	34,34,34,34	0
32	MG	0	8030	1/1	0.99	0.03	21,21,21,21	0
32	MG	0	8106	1/1	0.99	0.02	31,31,31,31	0
33	NA	0	8323	1/1	0.99	0.09	31,31,31,31	0
32	MG	0	8031	1/1	0.99	0.02	24,24,24,24	0
32	MG	0	8109	1/1	0.99	0.02	25,25,25,25	0
32	MG	0	8034	1/1	0.99	0.04	30,30,30,30	0
32	MG	0	8068	1/1	0.99	0.03	46,46,46,46	0
33	NA	0	8328	1/1	0.99	0.10	31,31,31,31	0
32	MG	0	8035	1/1	0.99	0.02	34,34,34,34	0
32	MG	0	8036	1/1	0.99	0.02	31,31,31,31	0
32	MG	0	8010	1/1	0.99	0.02	24,24,24,24	0
32	MG	0	8074	1/1	0.99	0.04	35,35,35,35	0
32	MG	0	8038	1/1	0.99	0.02	21,21,21,21	0
32	MG	0	8040	1/1	0.99	0.03	38,38,38,38	0
32	MG	0	8011	1/1	0.99	0.02	21,21,21,21	0
32	MG	0	8003	1/1	0.99	0.03	21,21,21,21	0
32	MG	0	8081	1/1	0.99	0.04	39,39,39,39	0
32	MG	0	8013	1/1	0.99	0.03	22,22,22,22	0
32	MG	0	8083	1/1	0.99	0.02	33,33,33,33	0
34	CL	B	8519	1/1	0.99	0.07	34,34,34,34	0
32	MG	0	8084	1/1	0.99	0.02	38,38,38,38	0
32	MG	0	8004	1/1	0.99	0.02	19,19,19,19	0
33	NA	0	8343	1/1	0.99	0.06	28,28,28,28	0
32	MG	0	8016	1/1	0.99	0.06	30,30,30,30	0
34	CL	M	8518	1/1	0.99	0.04	32,32,32,32	0
32	MG	0	8017	1/1	0.99	0.02	11,11,11,11	0
34	CL	O	8508	1/1	0.99	0.06	51,51,51,51	0
32	MG	0	8019	1/1	0.99	0.02	23,23,23,23	0
32	MG	0	8020	1/1	0.99	0.02	22,22,22,22	0
34	CL	3	8504	1/1	0.99	0.03	43,43,43,43	0
34	CL	0	8503	1/1	0.99	0.05	38,38,38,38	0
33	NA	0	8303	1/1	0.99	0.03	32,32,32,32	0
32	MG	0	8021	1/1	0.99	0.02	25,25,25,25	0
34	CL	0	8512	1/1	0.99	0.04	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8091	1/1	0.99	0.06	41,41,41,41	0
32	MG	0	8022	1/1	0.99	0.03	31,31,31,31	0
32	MG	0	8023	1/1	0.99	0.04	28,28,28,28	0
32	MG	0	8002	1/1	0.99	0.06	25,25,25,25	0
32	MG	0	8025	1/1	0.99	0.02	32,32,32,32	0
32	MG	0	8097	1/1	0.99	0.04	30,30,30,30	0
35	CD	O	8405	1/1	0.99	0.06	71,71,71,71	0
35	CD	U	8401	1/1	0.99	0.02	48,48,48,48	0
32	MG	0	8054	1/1	0.99	0.03	16,16,16,16	0
36	K	0	8202	1/1	0.99	0.16	37,37,37,37	0
32	MG	0	8018	1/1	1.00	0.02	30,30,30,30	0
32	MG	0	8039	1/1	1.00	0.01	33,33,33,33	0
32	MG	0	8009	1/1	1.00	0.02	25,25,25,25	0
32	MG	0	8032	1/1	1.00	0.04	26,26,26,26	0
32	MG	0	8077	1/1	1.00	0.01	22,22,22,22	0
32	MG	0	8033	1/1	1.00	0.03	19,19,19,19	0
32	MG	0	8001	1/1	1.00	0.01	24,24,24,24	0
32	MG	0	8015	1/1	1.00	0.02	25,25,25,25	0
32	MG	0	8005	1/1	1.00	0.01	25,25,25,25	0
32	MG	0	8056	1/1	1.00	0.02	34,34,34,34	0
32	MG	0	8110	1/1	1.00	0.03	29,29,29,29	0
35	CD	Z	8403	1/1	1.00	0.02	43,43,43,43	0
35	CD	1	8402	1/1	1.00	0.05	45,45,45,45	0
35	CD	3	8404	1/1	1.00	0.03	45,45,45,45	0
32	MG	0	8008	1/1	1.00	0.02	26,26,26,26	0
32	MG	0	8058	1/1	1.00	0.03	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.