wwPDB X-ray Structure Validation Summary Report (i)

Feb 11, 2024 – 07:48 AM EST

PDB ID	:	3CCQ
Title	:	Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation A2488U
Authors	:	Blaha, G.; Gurel, G.
Deposited on	:	2008-02-26
Resolution	:	2.90 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:

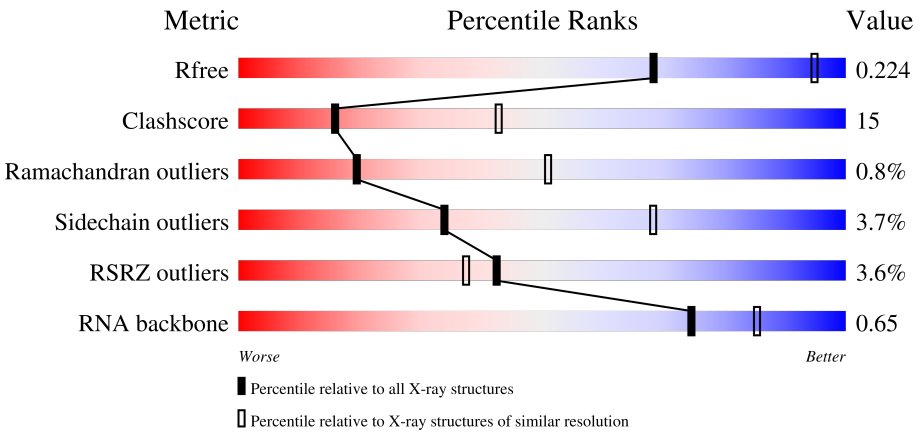
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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	3% 71% 25% • •
2	B	338	% 68% 29% •
3	C	246	2% 72% 26% •
4	D	177	29% 40% 37% • 21%

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Mol	Chain	Length	Quality of chain
5	E	178	5% 67% 29%
6	F	120	5% 66% 30%
7	G	348	% 5% 92%
8	H	177	% 66% 23% 10%
9	I	162	30% 30% 12% 57%
10	J	145	74% 19% 5%
11	K	132	74% 25%
12	L	165	3% 67% 20% 12%
13	M	196	% 65% 32%
14	N	187	9% 67% 30%
15	O	116	84% 16%
16	P	149	% 72% 23%
17	Q	96	72% 25%
18	R	155	70% 24%
19	S	85	2% 75% 20% 5%
20	T	120	2% 80% 18%
21	U	67	% 51% 27% 21%
22	V	71	21% 61% 27% 8%
23	W	154	57% 42%
24	X	92	58% 32% 11%
25	Y	241	43% 15% 41%
26	Z	116	5% 39% 24% 37%
27	1	57	68% 30%
28	2	50	2% 52% 38% 8%
29	3	92	% 79% 20%

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Mol	Chain	Length	Quality of chain
30	0	2923	2% 51% 37% 6% 6%
31	9	122	2% 39% 48% 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
34	SR	0	8947	-	-	-	X
34	SR	0	8982	-	-	-	X
34	SR	0	8986	-	-	-	X
34	SR	0	8994	-	-	-	X
34	SR	0	8996	-	-	-	X
34	SR	0	9006	-	-	-	X
35	NA	0	8509	-	-	-	X
35	NA	0	8528	-	-	-	X
35	NA	0	8560	-	-	-	X
35	NA	0	8562	-	-	-	X
37	K	0	8401	-	-	-	X

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 99120 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	59018	26348	10870	19055	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 (three-letter code: 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	0	87	87	87	0	0
32	9	1	1	1	0	0

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
33	A	1	1	1	0	0
33	B	1	1	1	0	0
33	J	3	3	3	0	0
33	L	1	1	1	0	0
33	M	1	1	1	0	0
33	N	1	1	1	0	0
33	O	1	1	1	0	0
33	Q	1	1	1	0	0
33	R	1	1	1	0	0
33	Y	1	1	1	0	0
33	3	1	1	1	0	0
33	0	9	9	9	0	0

- Molecule 34 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Sr		
34	A	3	3	3	0	0
34	B	2	2	2	0	0
34	F	1	1	1	0	0
34	R	1	1	1	0	0
34	S	1	1	1	0	0
34	1	2	2	2	0	0
34	3	2	2	2	0	0
34	0	93	93	93	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Sr		
34	9	3	3	3	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
35	B	1	1	1	0	0
			Total	Na		
35	C	1	1	1	0	0
			Total	Na		
35	J	1	1	1	0	0
			Total	Na		
35	M	1	1	1	0	0
			Total	Na		
35	Q	1	1	1	0	0
			Total	Na		
35	R	2	2	2	0	0
			Total	Na		
35	S	1	1	1	0	0
			Total	Na		
35	0	65	65	65	0	0
			Total	Na		
35	9	2	2	2	0	0

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

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

- Molecule 37 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	2	Total K 2 2	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	112	Total O 112 112	0	0
38	B	142	Total O 142 142	0	0
38	C	168	Total O 168 168	0	0
38	D	45	Total O 45 45	0	0
38	E	42	Total O 42 42	0	0
38	F	26	Total O 26 26	0	0
38	G	17	Total O 17 17	0	0
38	H	65	Total O 65 65	0	0
38	I	5	Total O 5 5	0	0
38	J	56	Total O 56 56	0	0
38	K	60	Total O 60 60	0	0
38	L	82	Total O 82 82	0	0
38	M	123	Total O 123 123	0	0
38	N	59	Total O 59 59	0	0
38	O	47	Total O 47 47	0	0
38	P	59	Total O 59 59	0	0
38	Q	47	Total O 47 47	0	0
38	R	76	Total O 76 76	0	0
38	S	33	Total O 33 33	0	0

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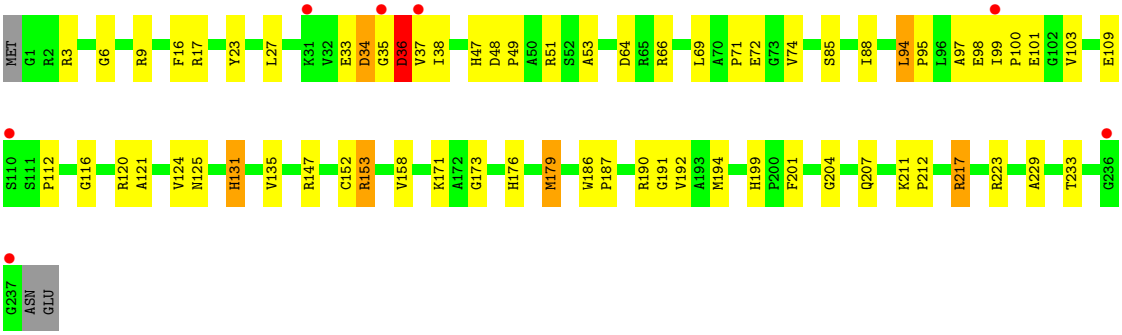
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	T	36	Total O 36 36	0	0
38	U	26	Total O 26 26	0	0
38	V	12	Total O 12 12	0	0
38	W	66	Total O 66 66	0	0
38	X	28	Total O 28 28	0	0
38	Y	97	Total O 97 97	0	0
38	Z	31	Total O 31 31	0	0
38	1	54	Total O 54 54	0	0
38	2	43	Total O 43 43	0	0
38	3	68	Total O 68 68	0	0
38	0	5950	Total O 5950 5950	0	0
38	9	148	Total O 148 148	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.

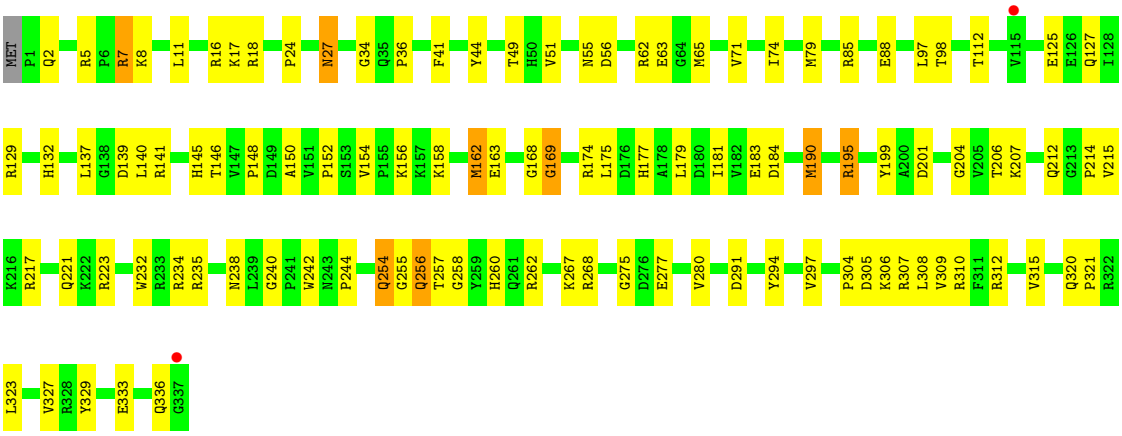
- Molecule 1: 50S ribosomal protein L2P

Chain A:



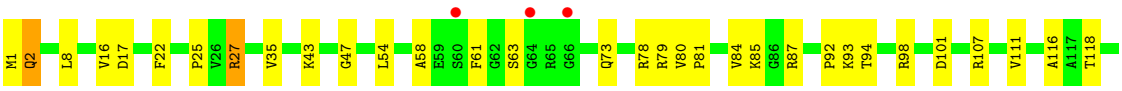
- Molecule 2: 50S ribosomal protein L3P

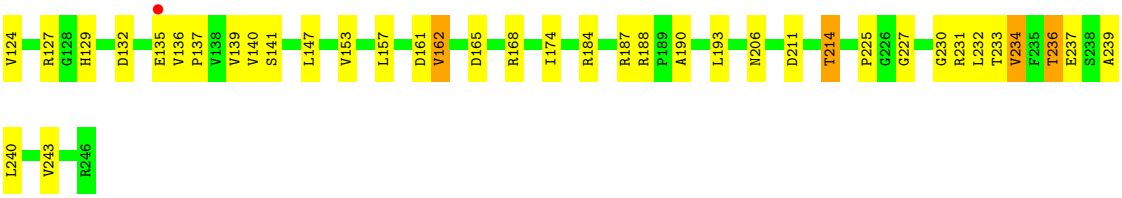
Chain B:



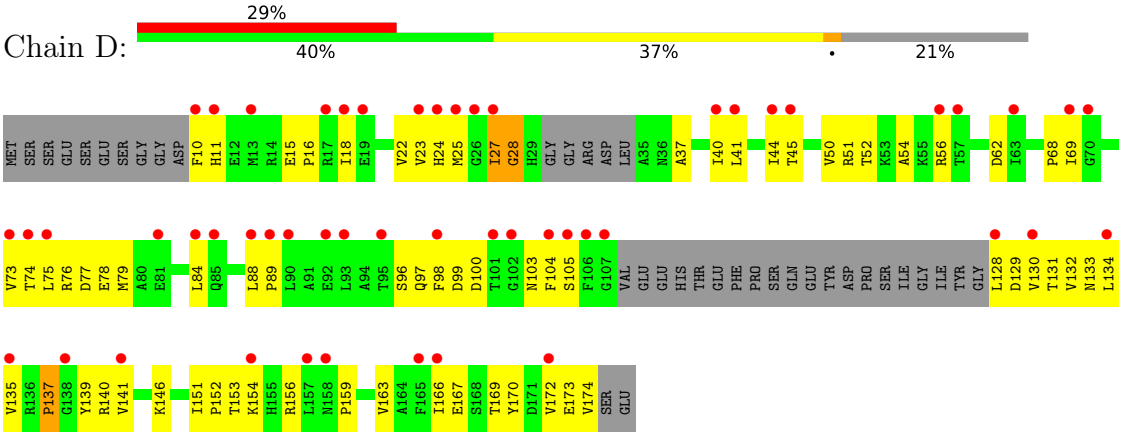
- Molecule 3: 50S ribosomal protein L4P

Chain C:

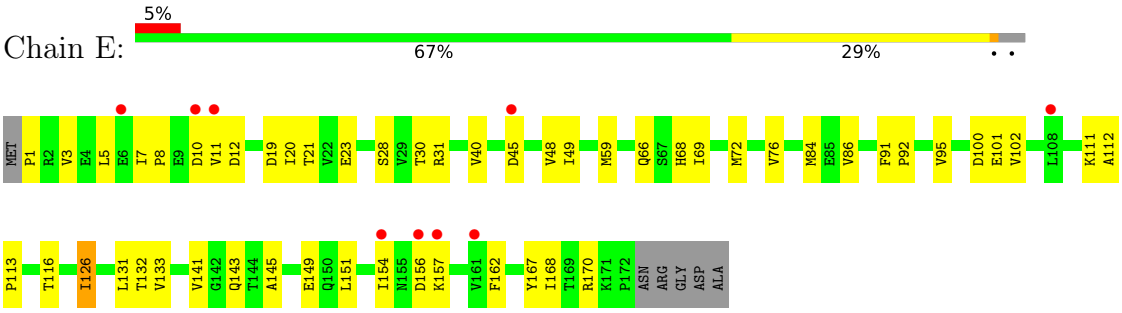




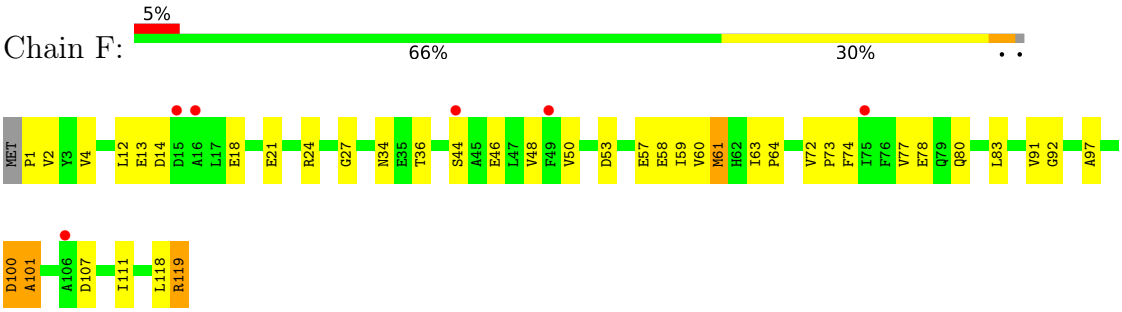
• Molecule 4: 50S ribosomal protein L5P



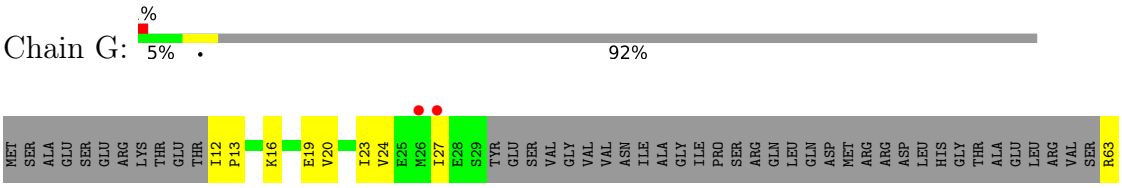
• Molecule 5: 50S ribosomal protein L6P



• Molecule 6: 50S ribosomal protein L7Ae

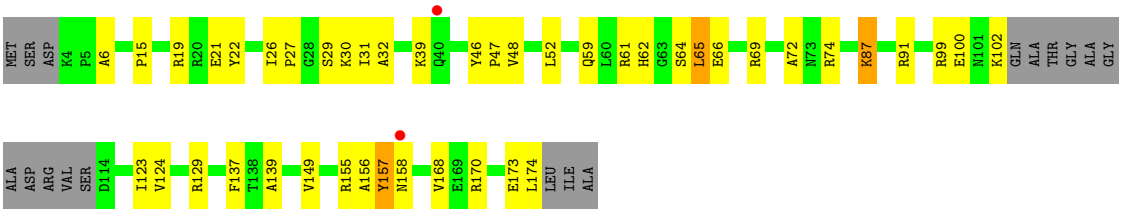


• Molecule 7: 50S ribosomal protein L10E



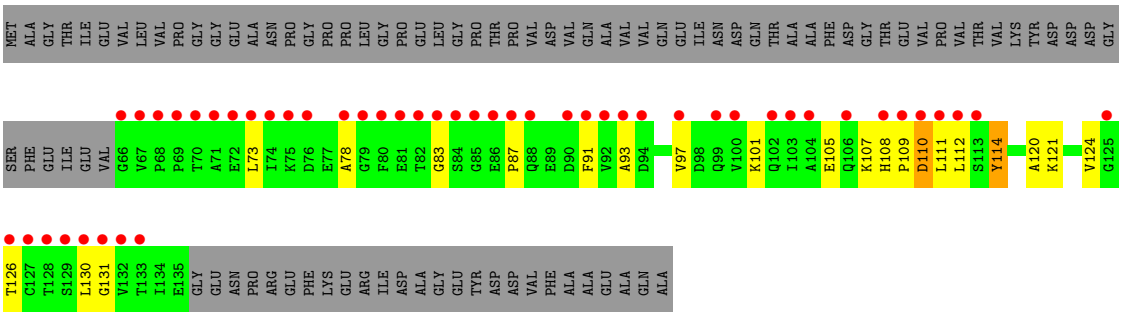
• Molecule 8: 50S ribosomal protein L10e

Chain H:



• Molecule 9: 50S ribosomal protein L11P

Chain I:



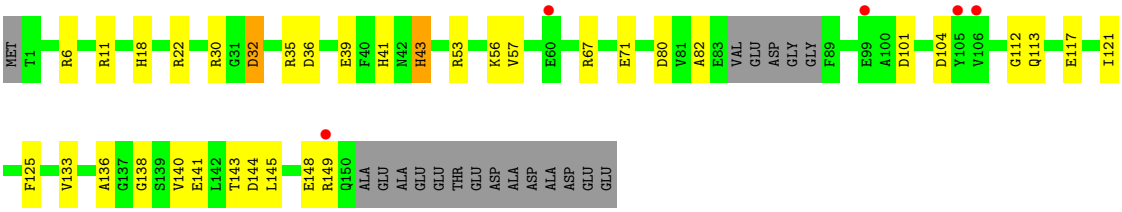
• Molecule 10: 50S ribosomal protein L13P

Chain J:

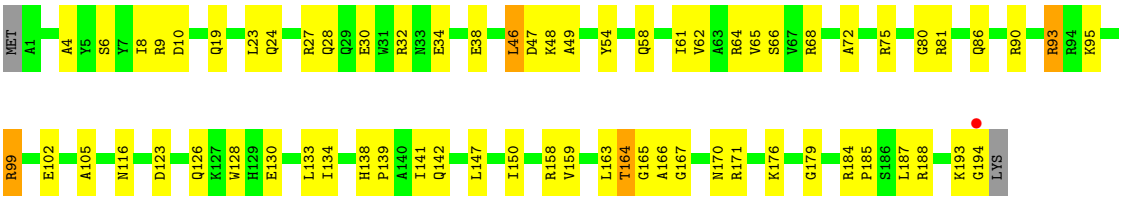
• Molecule 11: 50S ribosomal protein L14P

Chain K:

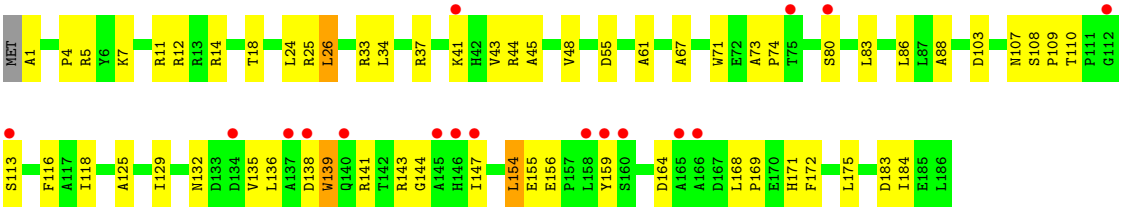
• Molecule 12: 50S ribosomal protein L15P



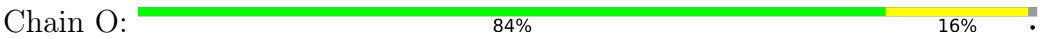
• Molecule 13: 50S ribosomal protein L15e

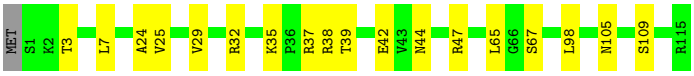


• Molecule 14: 50S ribosomal protein L18P

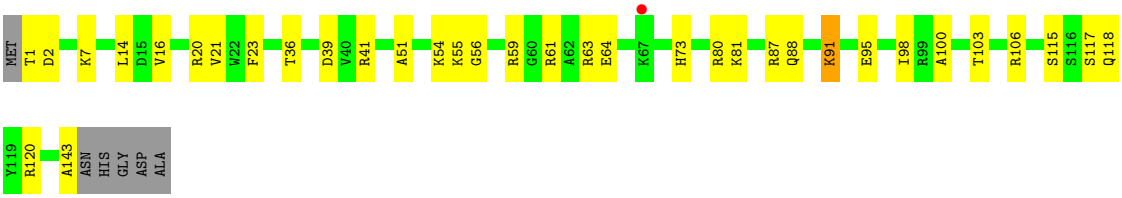


• Molecule 15: 50S ribosomal protein L18e





• Molecule 16: 50S ribosomal protein L19e

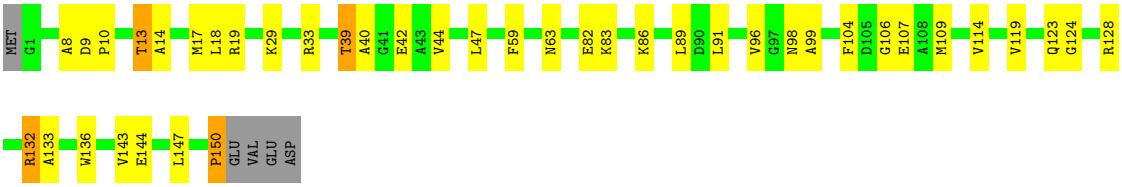


• Molecule 17: 50S ribosomal protein L21e

Chain Q:

• Molecule 18: 50S ribosomal protein L22P

Chain R:



• Molecule 19: 50S ribosomal protein L23P

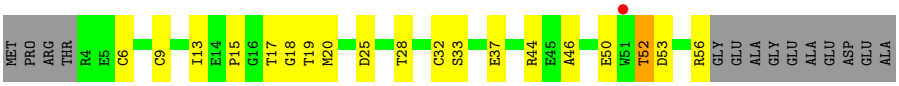
Chain S:

• Molecule 20: 50S ribosomal protein L24P

Chain T:

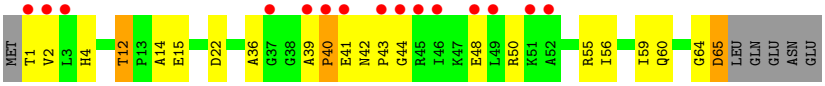
• Molecule 21: 50S ribosomal protein L24e

Chain U:



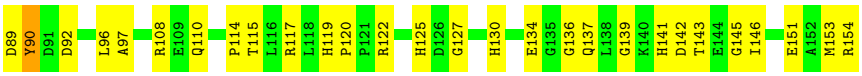
• Molecule 22: 50S ribosomal protein L29P

Chain V:



• Molecule 23: 50S ribosomal protein L30P

Chain W:

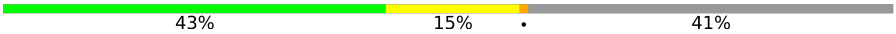


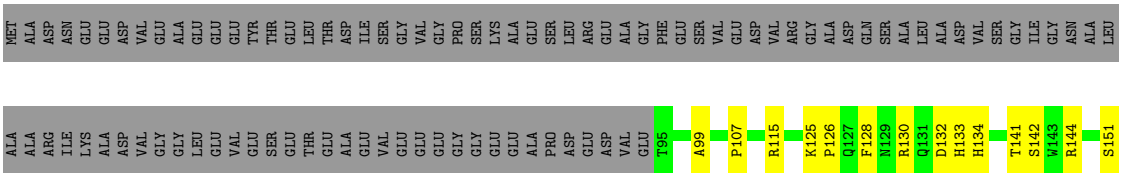
• Molecule 24: 50S ribosomal protein L31e

Chain X:

• Molecule 25: 50S ribosomal protein L32e

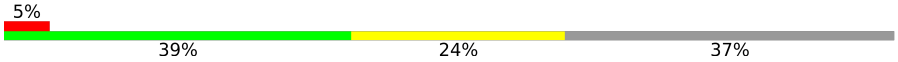
Chain Y:

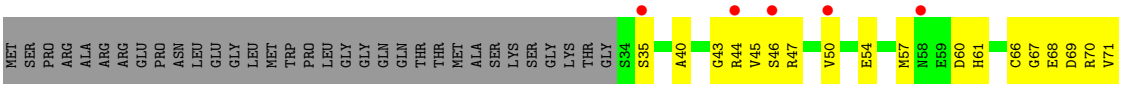


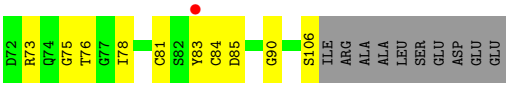


• Molecule 26: 50S ribosomal protein L37Ae

Chain Z:

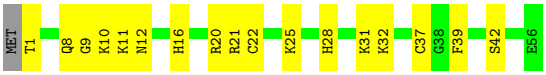




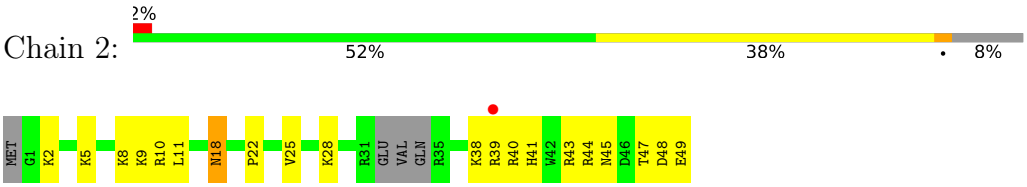


• Molecule 27: 50S ribosomal protein L37e

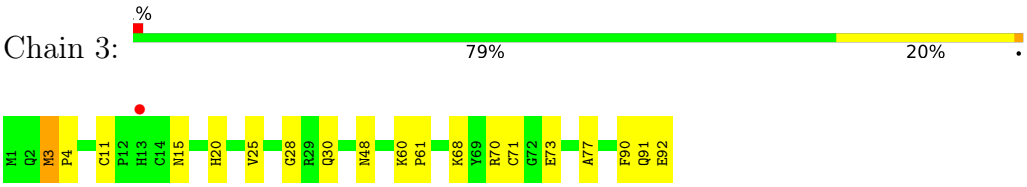
Chain 1:



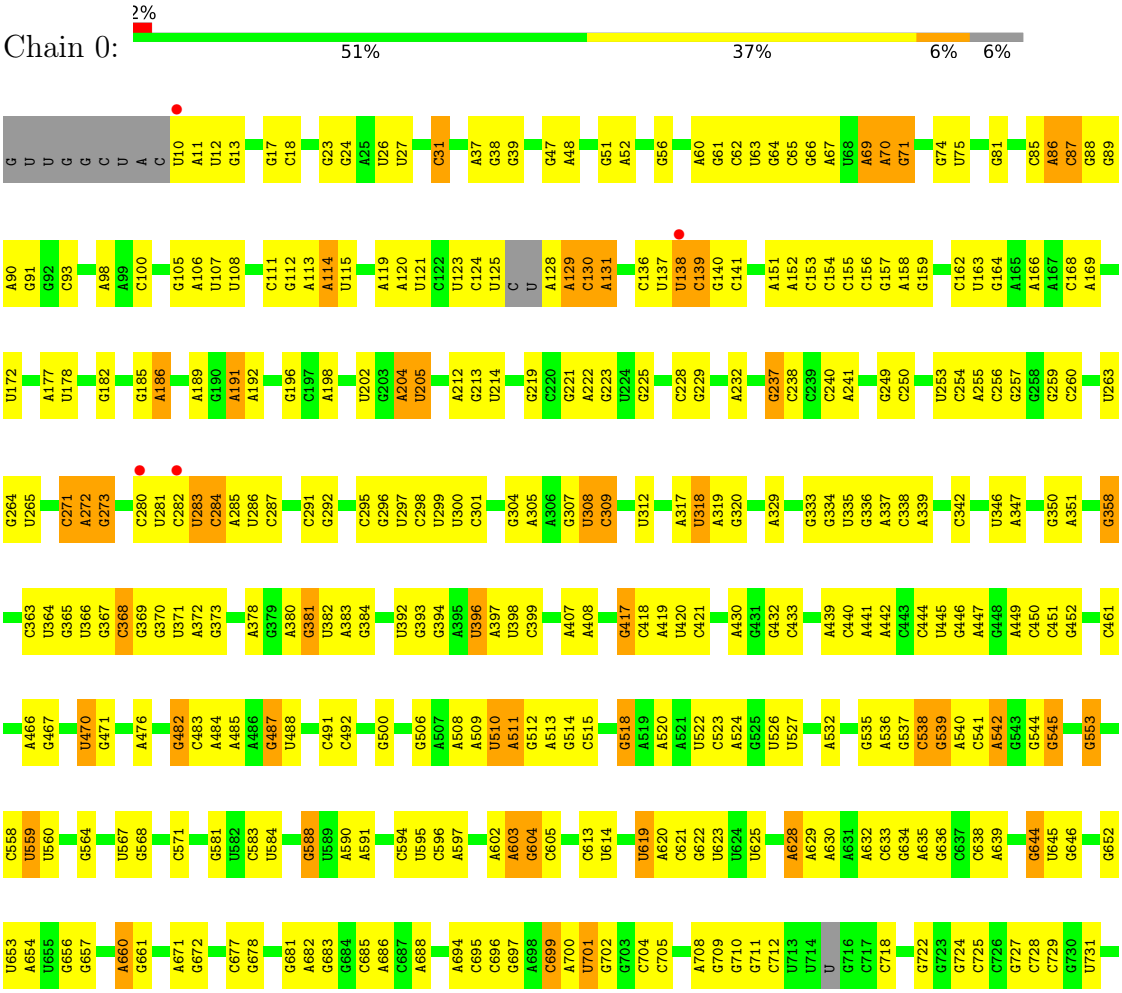
• Molecule 28: 50S ribosomal protein L39e

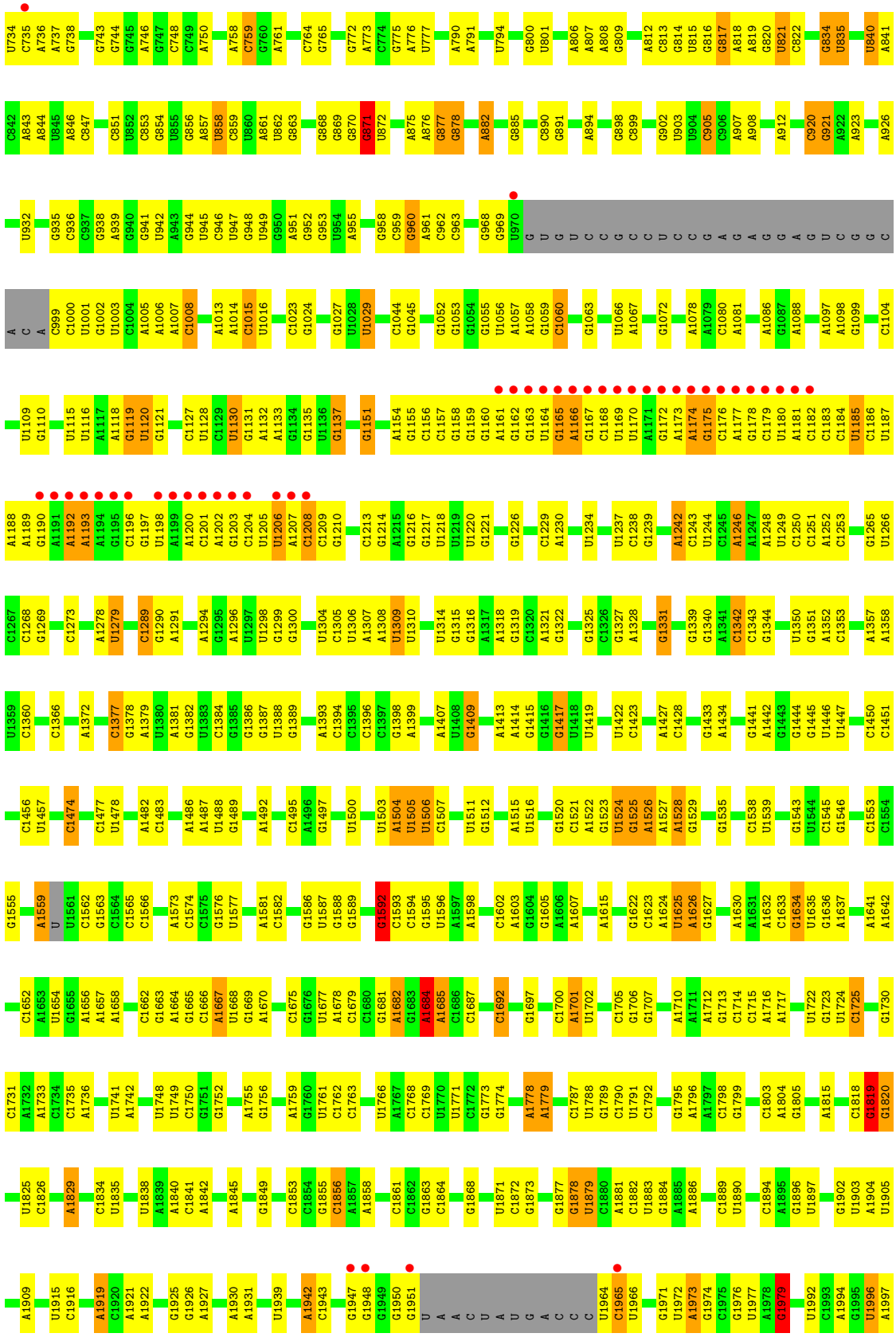


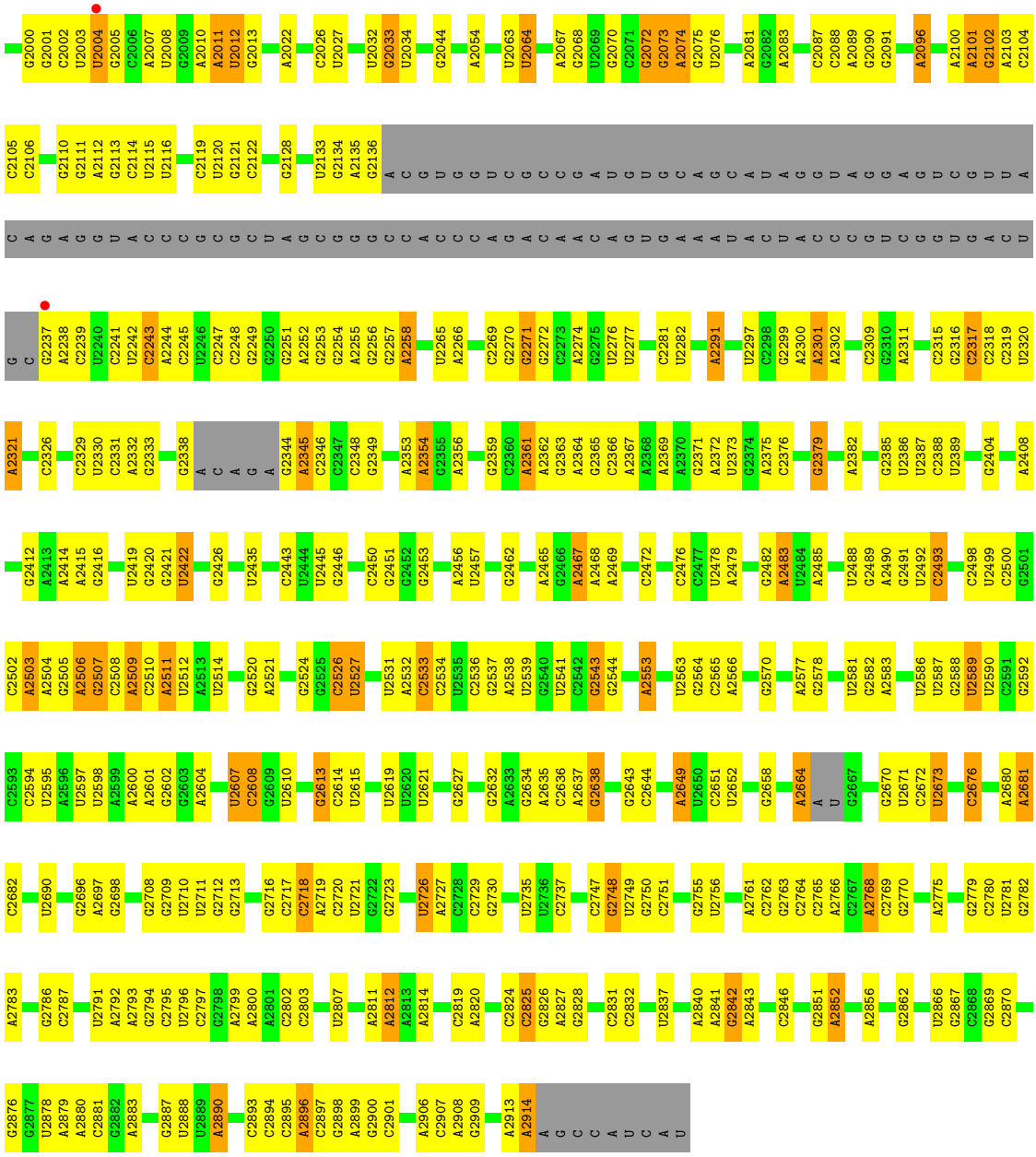
• Molecule 29: 50S ribosomal protein L44E



• Molecule 30: 23S RIBOSOMAL RNA

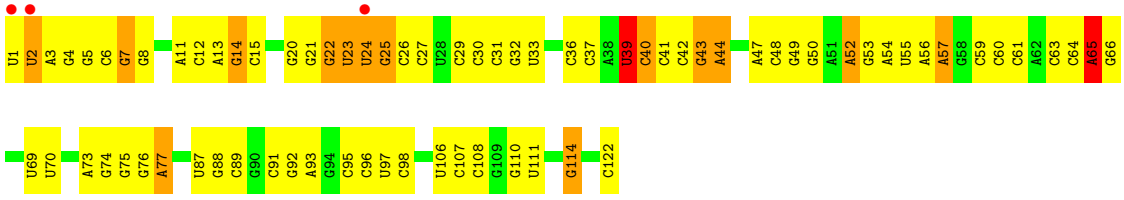



U734 C735 A736 A737 G738 G743 G744 G745 A746 G747 C748 C749 A750 A758 C759 G760 A761 C764 G765 G772 A773 C774 G775 A776 U777 A790 A791 U794 G800 U801 A806 A807 A808 G809 A812 C813 G814 U815 G816 G817 A818 A819 G820 U821 C822 G834 U835 U840 A841
C842 A843 A844 U845 A846 C847 C851 U852 C853 G854 U855 G856 A857 U858 C859 U860 A861 U862 G863 G868 G869 G870 G871 U872 A875 A876 G877 G878 A882 G885 C890 G891 A894 G898 C899 G902 U903 U904 C905 C906 A907 A908 A912 C920 G921 A922 A923 A926
U932 G935 C936 C937 G938 A939 G940 G941 U942 A943 G944 U945 C946 G947 G948 U949 G950 A951 G952 G953 U954 A955 G958 C959 G960 A961 C962 C963 G968 G969 U970 G U G U C C G 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 U1003 C1004 A1005 A1006 A1007 C1008 A1013 A1014 C1015 U1016 C1023 G1024 G1027 U1028 U1029 C1044 G1045 G1052 G1053 G1054 G1055 U1056 A1057 A1058 G1059 C1060 G1063 U1066 A1067 G1072 A1078 A1079 C1080 A1081 A1086 G1087 A1088 A1097 A1098 G1099 C1104
U1109 G1110 U1115 U1116 A1117 A1118 G1119 U1120 G1121 C1127 U1128 C1129 U1130 G1131 A1132 A1133 G1134 G1135 U1136 G1137 G1151 A1154 G1155 C1156 C1157 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 G1195 C1196 G1197 U1198 A1199 A1200 C1201 A1202 G1203 C1204 U1205 U1206 A1207 C1208 C1209 G1210 C1213 G1214 A1215 G1216 G1217 U1218 U1219 U1220 G1221 G1226 C1229 A1230 U1234 U1237 C1238 G1239 A1242 C1243 U1244 C1245 A1246 A1247 A1248 U1249 C1250 C1251 A1252 C1253 G1265 U1266
C1267 C1268 G1269 C1273 A1278 U1279 C1289 G1290 A1291 A1294 G1295 A1296 U1297 U1298 G1299 G1300 U1304 C1305 U1306 A1307 A1308 U1309 U1310 U1314 G1315 G1316 A1317 A1318 G1319 C1320 A1321 G1322 G1325 C1326 G1327 A1328 G1331 G1339 G1340 A1341 C1342 C1343 G1344 U1350 G1351 A1352 C1353 A1357 A1358
U1359 C1360 C1366 A1372 C1377 G1378 A1379 U1380 A1381 G1382 U1383 C1384 G1385 G1386 G1387 U1388 G1389 A1393 C1394 C1395 C1396 C1397 G1398 A1399 A1407 U1408 G1409 A1413 A1414 G1415 G1416 G1417 U1418 U1419 U1422 C1423 A1427 C1428 G1433 A1434 G1441 A1442 G1443 G1444 G1445 U1446 U1447 C1450 C1451
C1456 U1457 C1474 C1477 U1478 A1482 C1483 A1486 A1487 U1488 G1489 A1492 C1495 A1496 G1497 U1500 U1503 A1504 U1505 U1506 C1507 U1511 G1512 A1515 U1516 G1520 C1521 A1522 G1523 U1524 G1525 A1526 A1527 A1528 G1529 G1535 C1538 U1539 G1543 U1544 C1545 G1546 C1553 G1554
G1555 A1559 U U1561 C1562 G1563 C1564 C1565 C1566 A1573 C1574 C1575 G1576 U1577 A1581 C1582 G1586 U1587 G1588 G1589 G1592 C1593 C1594 G1595 U1596 A1597 A1598 C1602 A1603 C1604 G1605 A1606 A1607 A1615 G1622 C1623 A1624 U1625 A1626 G1627 A1630 A1631 A1632 C1633 G1634 U1635 G1636 A1637 A1641 A1642
C1652 A1653 U1654 G1655 A1656 A1657 A1658 C1662 G1663 A1664 G1665 C1666 A1667 U1668 G1669 A1670 C1675 G1676 U1677 A1678 C1679 C1680 G1681 A1682 G1683 A1684 A1685 C1686 C1687 C1692 G1697 C1700 A1701 U1702 C1705 G1706 G1707 A1710 A1711 A1712 G1713 C1714 C1715 A1716 A1717 U1722 G1723 U1724 C1725 G1730
C1731 A1732 A1733 C1734 C1735 A1736 U1741 A1742 U1748 U1749 C1750 G1751 G1752 A1755 G1756 A1759 G1760 U1761 C1762 C1763 U1766 A1767 C1768 C1769 U1770 U1771 C1772 G1773 G1774 A1778 A1779 C1787 U1788 G1789 C1790 U1791 C1792 G1795 A1796 A1797 C1798 G1799 C1803 A1804 G1805 A1815 C1818 G1819 G1820
U1825 C1826 A1829 C1834 U1835 U1838 A1839 A1840 C1841 A1842 A1845 G1849 C1853 C1854 G1855 C1856 A1857 A1858 C1861 C1862 G1863 C1864 G1868 U1871 C1872 G1873 G1877 G1878 U1879 C1880 A1881 C1882 U1883 G1884 A1885 A1886 C1889 U1890 C1894 A1895 G1896 U1897 G1902 U1903 A1904 U1905
A1909 U1915 C1916 A1919 C1920 A1921 A1922 G1925 G1926 A1927 A1930 A1931 U1939 A1942 C1943 G1947 G1948 G1949 G1950 G1951 U A A C U A U G A C C C U1964 C1965 U1966 G1971 U1972 A1973 G1974 C1975 G1976 U1977 A1978 G1979 U1992 C1993 A1994 G1995 U1996 A1997



• 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	212.33Å 299.62Å 575.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 85.65 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.00-2.90) 98.2 (85.65-2.41)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.186 , 0.233 0.177 , 0.224	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å^2)	61.2	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 82.8	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	0.94	EDS
Total number of atoms	99120	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, UR3, OMU, OMG, 1MA, CD, NA, CL, K, SR

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	0.33	0/1786	0.64	0/2408
2	B	0.34	0/2690	0.65	0/3652
3	C	0.36	0/1885	0.62	0/2552
4	D	0.32	0/1111	0.56	1/1498 (0.1%)
5	E	0.33	0/1382	0.57	0/1880
6	F	0.35	0/901	0.57	0/1224
7	G	0.33	0/241	0.51	0/324
8	H	0.33	0/1302	0.63	0/1743
9	I	0.30	0/526	0.50	0/716
10	J	0.36	0/1136	0.61	0/1530
11	K	0.34	0/1004	0.66	0/1351
12	L	0.35	0/1130	0.64	0/1509
13	M	0.36	0/1582	0.61	0/2116
14	N	0.30	0/1474	0.61	0/1999
15	O	0.35	0/874	0.59	0/1181
16	P	0.33	0/1147	0.53	0/1528
17	Q	0.34	0/749	0.65	0/1005
18	R	1.26	7/1172 (0.6%)	1.09	6/1578 (0.4%)
19	S	0.33	0/648	0.54	0/875
20	T	0.32	0/958	0.64	0/1289
21	U	0.32	0/417	0.57	0/562
22	V	0.32	0/502	0.54	0/675
23	W	0.36	0/1219	0.63	0/1655
24	X	0.35	0/664	0.60	0/895
25	Y	0.37	0/1146	0.62	0/1536
26	Z	0.36	0/584	0.63	0/781
27	1	0.39	0/438	0.62	0/578
28	2	0.34	0/401	0.58	0/529
29	3	0.37	0/771	0.57	0/1024
30	0	0.39	0/65954	0.68	9/102862 (0.0%)
31	9	0.33	0/2904	0.68	1/4526 (0.0%)
All	All	0.40	7/98698 (0.0%)	0.67	17/147581 (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
18	R	1	0
23	W	0	1
30	0	0	32
31	9	0	3
All	All	1	36

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.45	2.87	1.50
18	R	150	PRO	CA-C	-18.11	1.16	1.52
18	R	150	PRO	CG-CD	13.90	1.96	1.50
18	R	150	PRO	C-O	11.92	1.47	1.23
18	R	150	PRO	N-CA	11.35	1.66	1.47

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	R	150	PRO	CB-CA-C	-22.47	55.81	112.00
18	R	150	PRO	N-CA-C	-19.38	61.71	112.10
18	R	150	PRO	CA-N-CD	12.28	128.89	111.70
18	R	150	PRO	N-CA-CB	10.98	116.47	103.30
18	R	150	PRO	CA-C-O	-8.52	99.75	120.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	202	U	Sidechain
30	0	205	U	Sidechain
30	0	221	G	Sidechain
30	0	48	A	Sidechain
23	W	90	TYR	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	66	0
2	B	2625	0	2533	94	0
3	C	1860	0	1813	53	0
4	D	1094	0	1085	52	0
5	E	1357	0	1266	36	0
6	F	890	0	843	30	0
7	G	240	0	231	11	0
8	H	1282	0	1292	41	0
9	I	519	0	500	21	0
10	J	1120	0	1098	38	0
11	K	994	0	1027	39	0
12	L	1118	0	1076	33	0
13	M	1558	0	1573	59	0
14	N	1445	0	1401	54	0
15	O	865	0	873	18	0
16	P	1136	0	1123	30	0
17	Q	735	0	729	26	0
18	R	1149	0	1122	32	0
19	S	641	0	605	10	0
20	T	950	0	924	22	0
21	U	410	0	364	17	0
22	V	499	0	511	17	0
23	W	1196	0	1137	66	0
24	X	654	0	653	22	0
25	Y	1130	0	1133	33	0
26	Z	573	0	531	21	0
27	1	431	0	426	21	0
28	2	396	0	413	21	0
29	3	755	0	728	17	0
30	0	59018	0	29809	1329	0
31	9	2599	0	1325	97	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Y	1	0	0	0	0
33	0	9	0	0	3	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	2	0
33	L	1	0	0	0	0
33	M	1	0	0	1	0
33	N	1	0	0	1	0
33	O	1	0	0	0	0
33	Q	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	93	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	3	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	65	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	5950	0	0	203	0
38	1	54	0	0	3	0
38	2	43	0	0	1	0
38	3	68	0	0	6	0
38	9	148	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	A	112	0	0	5	0
38	B	142	0	0	14	0
38	C	168	0	0	13	0
38	D	45	0	0	4	0
38	E	42	0	0	4	0
38	F	26	0	0	1	0
38	G	17	0	0	1	0
38	H	65	0	0	5	0
38	I	5	0	0	0	0
38	J	56	0	0	2	0
38	K	60	0	0	5	0
38	L	82	0	0	8	0
38	M	123	0	0	2	0
38	N	59	0	0	3	0
38	O	47	0	0	4	0
38	P	59	0	0	2	0
38	Q	47	0	0	2	0
38	R	76	0	0	1	0
38	S	33	0	0	0	0
38	T	36	0	0	4	0
38	U	26	0	0	2	0
38	V	12	0	0	1	0
38	W	66	0	0	6	0
38	X	28	0	0	3	0
38	Y	97	0	0	7	0
38	Z	31	0	0	4	0
All	All	99120	0	59910	2191	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 2191 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:CG	18:R:150:PRO:CD	1.96	1.44
30:0:871:G:C8	30:0:871:G:H5'	1.75	1.21
14:N:37:ARG:NH1	31:9:6:C:H5"	1.62	1.12
30:0:1160:G:C5'	30:0:1161:A:H5'	1.79	1.11
31:9:56:A:H2'	31:9:57:A:H5"	1.21	1.11

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%)	213 (91%)	18 (8%)	4 (2%)	9	31
2	B	335/338 (99%)	309 (92%)	22 (7%)	4 (1%)	13	40
3	C	244/246 (99%)	222 (91%)	22 (9%)	0	100	100
4	D	134/177 (76%)	107 (80%)	22 (16%)	5 (4%)	3	13
5	E	170/178 (96%)	156 (92%)	14 (8%)	0	100	100
6	F	117/120 (98%)	104 (89%)	9 (8%)	4 (3%)	3	15
7	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
8	H	156/177 (88%)	145 (93%)	11 (7%)	0	100	100
9	I	68/162 (42%)	54 (79%)	13 (19%)	1 (2%)	10	34
10	J	140/145 (97%)	132 (94%)	8 (6%)	0	100	100
11	K	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
12	L	141/165 (86%)	124 (88%)	14 (10%)	3 (2%)	7	26
13	M	192/196 (98%)	182 (95%)	10 (5%)	0	100	100
14	N	184/187 (98%)	169 (92%)	11 (6%)	4 (2%)	6	24
15	O	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
16	P	141/149 (95%)	138 (98%)	3 (2%)	0	100	100
17	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
18	R	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
19	S	79/85 (93%)	72 (91%)	7 (9%)	0	100	100
20	T	117/120 (98%)	107 (92%)	9 (8%)	1 (1%)	17	48
21	U	51/67 (76%)	48 (94%)	3 (6%)	0	100	100
22	V	63/71 (89%)	58 (92%)	3 (5%)	2 (3%)	4	16
23	W	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	22	54
24	X	80/92 (87%)	71 (89%)	8 (10%)	1 (1%)	12	37
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%)	62 (87%)	8 (11%)	1 (1%)	11	36
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	2	42/50 (84%)	37 (88%)	5 (12%)	0	100	100
29	3	90/92 (98%)	89 (99%)	1 (1%)	0	100	100
All	All	3705/4472 (83%)	3416 (92%)	258 (7%)	31 (1%)	19	51

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	36	ASP
1	A	37	VAL
6	F	101	ALA
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%)	171 (96%)	8 (4%)	27	61
2	B	282/283 (100%)	268 (95%)	14 (5%)	24	57
3	C	193/193 (100%)	180 (93%)	13 (7%)	16	43
4	D	117/148 (79%)	113 (97%)	4 (3%)	37	71
5	E	152/156 (97%)	148 (97%)	4 (3%)	46	77
6	F	93/94 (99%)	91 (98%)	2 (2%)	52	81
7	G	27/282 (10%)	26 (96%)	1 (4%)	34	68
8	H	134/145 (92%)	128 (96%)	6 (4%)	27	61
9	I	58/130 (45%)	56 (97%)	2 (3%)	37	71
10	J	118/121 (98%)	110 (93%)	8 (7%)	16	42
11	K	106/106 (100%)	103 (97%)	3 (3%)	43	76
12	L	113/127 (89%)	108 (96%)	5 (4%)	28	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	158/160 (99%)	151 (96%)	7 (4%)	28	61
14	N	149/150 (99%)	147 (99%)	2 (1%)	69	90
15	O	93/94 (99%)	92 (99%)	1 (1%)	73	92
16	P	113/117 (97%)	111 (98%)	2 (2%)	59	85
17	Q	79/80 (99%)	75 (95%)	4 (5%)	24	56
18	R	117/122 (96%)	112 (96%)	5 (4%)	29	62
19	S	71/74 (96%)	71 (100%)	0	100	100
20	T	105/106 (99%)	101 (96%)	4 (4%)	33	67
21	U	44/53 (83%)	42 (96%)	2 (4%)	27	61
22	V	51/57 (90%)	48 (94%)	3 (6%)	19	49
23	W	130/130 (100%)	127 (98%)	3 (2%)	50	80
24	X	66/74 (89%)	63 (96%)	3 (4%)	27	61
25	Y	120/196 (61%)	116 (97%)	4 (3%)	38	72
26	Z	60/94 (64%)	59 (98%)	1 (2%)	60	86
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	49	79
29	3	79/79 (100%)	78 (99%)	1 (1%)	69	90
All	All	3095/3646 (85%)	2982 (96%)	113 (4%)	34	68

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	74	ARG
26	Z	106	SER
13	M	68	ARG
25	Y	203	VAL
22	V	65	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
22	V	34	GLN
27	1	28	HIS
23	W	2	HIS
24	X	23	HIS

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Mol	Chain	Res	Type
28	2	45	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	242 (8%)	22 (0%)
31	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2866/3045 (94%)	260 (9%)	23 (0%)

5 of 260 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 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1506	U
30	0	2526	C
30	0	2467	A
30	0	2536	C
30	0	857	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	OMU	0	2587	30	19,22,23	0.25	0	26,31,34	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
30	OMG	0	2588	30	18,26,27	1.02	2 (11%)	19,38,41	0.71	1 (5%)
30	1MA	0	628	30,35	16,25,26	1.41	3 (18%)	18,37,40	1.12	2 (11%)
30	UR3	0	2619	30	19,22,23	0.49	0	26,32,35	0.68	1 (3%)
30	PSU	0	2621	30	18,21,22	1.34	2 (11%)	22,30,33	1.27	3 (13%)

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	OMU	0	2587	30	-	0/9/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	1MA	0	628	30,35	-	0/3/25/26	0/3/3/3
30	UR3	0	2619	30	-	0/7/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	4.37	1.42	1.36
30	0	628	1MA	C2-N3	3.84	1.33	1.29
30	0	2588	OMG	C5-C6	-2.63	1.42	1.47
30	0	628	1MA	C6-N6	2.43	1.33	1.27
30	0	2588	OMG	C8-N7	-2.39	1.30	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	0	2621	PSU	C6-C5-C4	3.28	120.49	118.20
30	0	628	1MA	N1-C2-N3	2.85	129.34	126.02
30	0	2621	PSU	C6-N1-C2	-2.76	119.86	122.68
30	0	2621	PSU	O2-C2-N1	2.75	125.82	122.79
30	0	628	1MA	C5-C6-N1	2.62	117.80	113.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	2	0
30	0	628	1MA	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 305 ligands modelled in this entry, 305 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%)	-0.22	7 (2%) 50 45	34, 56, 94, 116	0
2	B	337/338 (99%)	-0.42	2 (0%) 89 89	34, 58, 89, 99	0
3	C	246/246 (100%)	-0.24	4 (1%) 72 71	32, 51, 75, 87	0
4	D	140/177 (79%)	1.64	51 (36%) 0 0	69, 106, 134, 144	0
5	E	172/178 (96%)	-0.10	9 (5%) 27 23	49, 73, 97, 102	0
6	F	119/120 (99%)	-0.01	6 (5%) 28 25	52, 76, 109, 124	0
7	G	29/348 (8%)	0.52	2 (6%) 16 13	79, 103, 110, 113	0
8	H	160/177 (90%)	-0.34	2 (1%) 77 77	53, 73, 107, 111	0
9	I	70/162 (43%)	3.80	49 (70%) 0 0	137, 155, 173, 175	0
10	J	142/145 (97%)	-0.65	0 100 100	43, 57, 77, 99	0
11	K	132/132 (100%)	-0.62	0 100 100	39, 54, 79, 83	0
12	L	145/165 (87%)	0.33	5 (3%) 45 40	32, 71, 123, 134	0
13	M	194/196 (98%)	-0.48	1 (0%) 91 91	35, 49, 64, 71	0
14	N	186/187 (99%)	0.24	17 (9%) 9 6	51, 74, 121, 131	0
15	O	115/116 (99%)	-0.49	0 100 100	44, 61, 78, 85	0
16	P	143/149 (95%)	-0.41	1 (0%) 87 87	47, 61, 74, 83	0
17	Q	95/96 (98%)	-0.49	0 100 100	44, 55, 72, 85	0
18	R	150/155 (96%)	-0.50	0 100 100	37, 51, 73, 84	0
19	S	81/85 (95%)	-0.06	2 (2%) 57 55	49, 64, 87, 97	0
20	T	119/120 (99%)	-0.17	3 (2%) 57 55	42, 62, 92, 121	0
21	U	53/67 (79%)	0.01	1 (1%) 66 65	51, 64, 83, 91	0
22	V	65/71 (91%)	1.07	15 (23%) 0 0	53, 76, 130, 134	0
23	W	154/154 (100%)	-0.69	0 100 100	41, 56, 74, 88	0
24	X	82/92 (89%)	-0.31	0 100 100	49, 66, 91, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	Y	142/241 (58%)	-0.51	1 (0%) 87 87	34, 48, 72, 94	0
26	Z	73/116 (62%)	0.19	6 (8%) 11 9	59, 77, 92, 101	0
27	1	56/57 (98%)	-0.25	0 100 100	33, 39, 48, 56	0
28	2	46/50 (92%)	-0.14	1 (2%) 62 59	41, 69, 102, 114	0
29	3	92/92 (100%)	-0.13	1 (1%) 80 80	43, 65, 78, 91	0
30	0	2749/2923 (94%)	-0.32	51 (1%) 66 65	28, 51, 95, 171	0
31	9	122/122 (100%)	-0.24	3 (2%) 57 55	45, 72, 95, 154	0
All	All	6646/7517 (88%)	-0.20	240 (3%) 42 37	28, 57, 106, 175	0

The worst 5 of 240 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	71	ALA	15.5
9	I	74	ILE	13.2
31	9	1	U	12.1
22	V	1	THR	11.8
9	I	72	GLU	11.1

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	1MA	0	628	23/24	0.98	0.18	33,37,38,39	0
30	OMG	0	2588	24/25	0.98	0.14	36,39,42,43	0
30	UR3	0	2619	21/22	0.98	0.15	42,44,47,47	0
30	PSU	0	2621	20/21	0.98	0.18	34,35,47,48	0
30	OMU	0	2587	21/22	0.99	0.13	38,40,44,45	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, 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
34	SR	0	9006	1/1	-0.21	2.27	200,200,200,200	0
35	NA	0	8560	1/1	0.19	0.88	101,101,101,101	0
35	NA	0	8525	1/1	0.30	0.25	92,92,92,92	0
34	SR	0	8924	1/1	0.32	0.09	154,154,154,154	0
37	K	0	8401	1/1	0.41	0.77	128,128,128,128	0
34	SR	0	8962	1/1	0.53	0.19	169,169,169,169	0
34	SR	0	8947	1/1	0.54	0.51	200,200,200,200	0
34	SR	0	8991	1/1	0.65	0.07	199,199,199,199	0
35	NA	0	8528	1/1	0.65	0.56	66,66,66,66	0
34	SR	0	8955	1/1	0.68	0.20	199,199,199,199	0
35	NA	0	8506	1/1	0.68	0.16	64,64,64,64	0
35	NA	0	8563	1/1	0.69	0.28	88,88,88,88	0
35	NA	0	8562	1/1	0.69	1.31	78,78,78,78	0
35	NA	0	8509	1/1	0.70	0.93	85,85,85,85	0
35	NA	0	8502	1/1	0.72	0.15	66,66,66,66	0
34	SR	0	8982	1/1	0.73	2.26	200,200,200,200	0
35	NA	0	8530	1/1	0.73	0.32	59,59,59,59	0
34	SR	0	8994	1/1	0.74	0.43	200,200,200,200	0
34	SR	0	8993	1/1	0.74	0.10	176,176,176,176	0
35	NA	0	8511	1/1	0.75	0.29	69,69,69,69	0
35	NA	0	8548	1/1	0.75	0.26	58,58,58,58	0
34	SR	0	8979	1/1	0.76	0.14	200,200,200,200	0
35	NA	9	8543	1/1	0.77	0.11	74,74,74,74	0
35	NA	Q	8540	1/1	0.78	0.11	64,64,64,64	0
34	SR	0	8986	1/1	0.78	0.41	200,200,200,200	0
35	NA	0	8568	1/1	0.79	0.20	52,52,52,52	0
34	SR	0	8996	1/1	0.79	1.20	200,200,200,200	0
34	SR	0	8944	1/1	0.79	0.14	169,169,169,169	0
34	SR	B	8987	1/1	0.80	0.56	200,200,200,200	0
32	MG	0	8072	1/1	0.81	0.19	63,63,63,63	0
34	SR	0	9001	1/1	0.81	0.08	173,173,173,173	0
35	NA	0	8527	1/1	0.81	0.27	71,71,71,71	0
35	NA	S	8510	1/1	0.81	0.48	64,64,64,64	0
35	NA	0	8571	1/1	0.82	0.17	76,76,76,76	0
34	SR	0	8998	1/1	0.82	0.19	173,173,173,173	0
35	NA	0	8557	1/1	0.82	0.06	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	SR	A	8977	1/1	0.83	0.06	160,160,160,160	0
35	NA	0	8535	1/1	0.83	0.53	61,61,61,61	0
35	NA	0	8546	1/1	0.83	0.38	65,65,65,65	0
32	MG	0	8067	1/1	0.83	0.16	40,40,40,40	0
35	NA	J	8538	1/1	0.83	0.18	56,56,56,56	0
34	SR	0	8960	1/1	0.83	0.10	141,141,141,141	0
34	SR	0	8997	1/1	0.84	0.84	200,200,200,200	0
32	MG	9	8074	1/1	0.84	0.09	86,86,86,86	0
35	NA	0	8518	1/1	0.85	0.58	88,88,88,88	0
35	NA	0	8544	1/1	0.86	0.17	67,67,67,67	0
35	NA	0	8550	1/1	0.86	0.95	57,57,57,57	0
35	NA	0	8501	1/1	0.87	0.08	40,40,40,40	0
35	NA	0	8565	1/1	0.87	1.24	79,79,79,79	0
34	SR	0	8974	1/1	0.87	0.24	165,165,165,165	0
32	MG	0	8049	1/1	0.88	0.29	69,69,69,69	0
35	NA	0	8567	1/1	0.88	0.36	76,76,76,76	0
34	SR	0	8976	1/1	0.88	0.28	194,194,194,194	0
35	NA	0	8545	1/1	0.88	0.26	47,47,47,47	0
35	NA	0	8573	1/1	0.88	0.34	73,73,73,73	0
34	SR	0	8922	1/1	0.88	0.47	161,161,161,161	0
35	NA	0	8504	1/1	0.88	0.18	44,44,44,44	0
35	NA	0	8574	1/1	0.89	0.26	59,59,59,59	0
32	MG	0	8092	1/1	0.89	0.18	53,53,53,53	0
34	SR	0	8992	1/1	0.89	0.15	136,136,136,136	0
35	NA	0	8522	1/1	0.90	1.12	79,79,79,79	0
34	SR	0	8927	1/1	0.90	0.09	153,153,153,153	0
35	NA	0	8547	1/1	0.90	0.70	80,80,80,80	0
32	MG	0	8038	1/1	0.90	0.15	70,70,70,70	0
35	NA	0	8570	1/1	0.90	0.09	52,52,52,52	0
32	MG	0	8081	1/1	0.90	0.22	73,73,73,73	0
35	NA	0	8554	1/1	0.90	1.00	65,65,65,65	0
34	SR	0	8985	1/1	0.90	0.14	134,134,134,134	0
34	SR	0	8972	1/1	0.90	0.13	146,146,146,146	0
34	SR	0	8951	1/1	0.90	0.04	148,148,148,148	0
33	CL	O	8808	1/1	0.91	0.08	70,70,70,70	0
34	SR	0	8936	1/1	0.91	0.11	94,94,94,94	0
33	CL	0	8815	1/1	0.91	0.12	77,77,77,77	0
34	SR	0	8975	1/1	0.91	0.14	130,130,130,130	0
35	NA	0	8536	1/1	0.91	0.23	61,61,61,61	0
34	SR	0	8946	1/1	0.91	0.22	123,123,123,123	0
32	MG	0	8083	1/1	0.91	0.10	60,60,60,60	0
32	MG	0	8062	1/1	0.91	0.15	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8031	1/1	0.91	0.11	62,62,62,62	0
35	NA	0	8521	1/1	0.91	0.40	61,61,61,61	0
35	NA	0	8549	1/1	0.91	0.52	52,52,52,52	0
34	SR	0	8959	1/1	0.91	0.38	163,163,163,163	0
33	CL	A	8809	1/1	0.91	0.11	80,80,80,80	0
32	MG	0	8011	1/1	0.92	0.23	25,25,25,25	0
32	MG	0	8039	1/1	0.92	0.27	76,76,76,76	0
34	SR	0	9002	1/1	0.92	0.29	177,177,177,177	0
34	SR	0	8989	1/1	0.92	0.16	168,168,168,168	0
34	SR	A	8929	1/1	0.92	0.23	144,144,144,144	0
32	MG	0	8087	1/1	0.92	0.12	51,51,51,51	0
32	MG	0	8066	1/1	0.92	0.18	70,70,70,70	0
34	SR	0	8915	1/1	0.92	0.08	121,121,121,121	0
32	MG	0	8044	1/1	0.92	0.16	50,50,50,50	0
35	NA	0	8529	1/1	0.92	0.15	39,39,39,39	0
32	MG	0	8045	1/1	0.92	0.09	44,44,44,44	0
35	NA	0	8559	1/1	0.92	0.29	91,91,91,91	0
32	MG	0	8091	1/1	0.93	0.07	57,57,57,57	0
32	MG	0	8056	1/1	0.93	0.10	47,47,47,47	0
32	MG	0	8075	1/1	0.93	0.03	42,42,42,42	0
34	SR	0	8965	1/1	0.93	0.09	132,132,132,132	0
32	MG	0	8077	1/1	0.93	0.07	45,45,45,45	0
33	CL	N	8807	1/1	0.93	0.17	69,69,69,69	0
34	SR	0	8928	1/1	0.93	0.06	135,135,135,135	0
35	NA	0	8526	1/1	0.93	0.08	47,47,47,47	0
32	MG	0	8037	1/1	0.93	0.14	88,88,88,88	0
35	NA	0	8564	1/1	0.93	0.39	68,68,68,68	0
34	SR	0	8942	1/1	0.93	0.08	122,122,122,122	0
33	CL	Q	8811	1/1	0.93	0.15	82,82,82,82	0
33	CL	0	8813	1/1	0.93	0.09	66,66,66,66	0
35	NA	0	8569	1/1	0.93	0.15	48,48,48,48	0
35	NA	R	8575	1/1	0.93	0.25	99,99,99,99	0
32	MG	A	8051	1/1	0.93	0.66	70,70,70,70	0
34	SR	0	8988	1/1	0.93	0.05	158,158,158,158	0
32	MG	0	8006	1/1	0.93	0.10	32,32,32,32	0
32	MG	0	8089	1/1	0.93	0.17	72,72,72,72	0
35	NA	0	8505	1/1	0.93	0.87	48,48,48,48	0
34	SR	0	8901	1/1	0.94	0.08	91,91,91,91	0
35	NA	0	8512	1/1	0.94	0.14	52,52,52,52	0
35	NA	0	8551	1/1	0.94	0.37	52,52,52,52	0
35	NA	0	8515	1/1	0.94	0.20	41,41,41,41	0
34	SR	0	9000	1/1	0.94	0.07	176,176,176,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8055	1/1	0.94	0.16	53,53,53,53	0
32	MG	0	8033	1/1	0.94	0.09	55,55,55,55	0
35	NA	0	8561	1/1	0.94	0.22	68,68,68,68	0
32	MG	0	8060	1/1	0.94	0.08	53,53,53,53	0
34	SR	9	8980	1/1	0.94	0.15	175,175,175,175	0
34	SR	9	9003	1/1	0.94	0.09	171,171,171,171	0
33	CL	0	8814	1/1	0.94	0.21	72,72,72,72	0
32	MG	0	8036	1/1	0.94	0.12	56,56,56,56	0
32	MG	0	8014	1/1	0.94	0.20	33,33,33,33	0
34	SR	0	8968	1/1	0.94	0.03	160,160,160,160	0
34	SR	0	8969	1/1	0.94	0.12	159,159,159,159	0
33	CL	L	8810	1/1	0.94	0.09	68,68,68,68	0
34	SR	0	8973	1/1	0.94	0.05	130,130,130,130	0
34	SR	0	8995	1/1	0.94	0.15	136,136,136,136	0
32	MG	T	8057	1/1	0.94	0.12	60,60,60,60	0
34	SR	S	8961	1/1	0.94	0.06	121,121,121,121	0
34	SR	0	8966	1/1	0.95	0.10	107,107,107,107	0
35	NA	0	8537	1/1	0.95	0.18	38,38,38,38	0
35	NA	0	8520	1/1	0.95	0.07	49,49,49,49	0
32	MG	0	8093	1/1	0.95	0.08	42,42,42,42	0
34	SR	0	9008	1/1	0.95	0.17	95,95,95,95	0
35	NA	0	8523	1/1	0.95	0.09	50,50,50,50	0
32	MG	0	8082	1/1	0.95	0.78	89,89,89,89	0
32	MG	0	8053	1/1	0.95	0.19	47,47,47,47	0
33	CL	0	8803	1/1	0.95	0.10	58,58,58,58	0
33	CL	J	8802	1/1	0.95	0.21	75,75,75,75	0
33	CL	J	8821	1/1	0.95	0.14	67,67,67,67	0
32	MG	0	8070	1/1	0.95	0.12	46,46,46,46	0
35	NA	0	8533	1/1	0.95	0.10	55,55,55,55	0
35	NA	0	8516	1/1	0.95	0.11	45,45,45,45	0
32	MG	0	8046	1/1	0.96	0.14	43,43,43,43	0
34	SR	0	8963	1/1	0.96	0.17	112,112,112,112	0
32	MG	0	8047	1/1	0.96	0.32	51,51,51,51	0
35	NA	0	8555	1/1	0.96	0.81	75,75,75,75	0
35	NA	0	8556	1/1	0.96	0.82	64,64,64,64	0
35	NA	R	8532	1/1	0.96	0.12	58,58,58,58	0
32	MG	0	8001	1/1	0.96	0.11	33,33,33,33	0
33	CL	M	8818	1/1	0.96	0.10	40,40,40,40	0
32	MG	0	8035	1/1	0.96	0.10	54,54,54,54	0
34	SR	0	8971	1/1	0.96	0.07	171,171,171,171	0
34	SR	0	8943	1/1	0.96	0.04	124,124,124,124	0
32	MG	0	8040	1/1	0.96	0.21	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8041	1/1	0.96	0.21	29,29,29,29	0
34	SR	0	8908	1/1	0.96	0.08	116,116,116,116	0
32	MG	0	8016	1/1	0.96	0.14	48,48,48,48	0
35	NA	0	8542	1/1	0.96	0.45	49,49,49,49	0
34	SR	0	8953	1/1	0.96	0.13	144,144,144,144	0
34	SR	0	9004	1/1	0.96	0.31	200,200,200,200	0
34	SR	0	8917	1/1	0.96	0.10	107,107,107,107	0
34	SR	0	8921	1/1	0.96	0.15	96,96,96,96	0
35	NA	0	8519	1/1	0.96	0.20	43,43,43,43	0
35	NA	9	8572	1/1	0.96	0.89	81,81,81,81	0
32	MG	0	8003	1/1	0.96	0.19	45,45,45,45	0
34	SR	1	8913	1/1	0.97	0.14	95,95,95,95	0
34	SR	0	8945	1/1	0.97	0.07	106,106,106,106	0
32	MG	0	8071	1/1	0.97	0.09	72,72,72,72	0
34	SR	0	9007	1/1	0.97	0.66	200,200,200,200	0
32	MG	0	8002	1/1	0.97	0.15	36,36,36,36	0
33	CL	Y	8820	1/1	0.97	0.04	48,48,48,48	0
32	MG	0	8013	1/1	0.97	0.06	25,25,25,25	0
35	NA	0	8524	1/1	0.97	0.25	58,58,58,58	0
35	NA	0	8558	1/1	0.97	0.23	49,49,49,49	0
35	NA	C	8503	1/1	0.97	0.21	36,36,36,36	0
34	SR	0	8954	1/1	0.97	0.10	109,109,109,109	0
34	SR	0	8919	1/1	0.97	0.07	170,170,170,170	0
34	SR	0	8957	1/1	0.97	0.13	195,195,195,195	0
34	SR	0	8958	1/1	0.97	0.06	122,122,122,122	0
34	SR	0	8920	1/1	0.97	0.08	135,135,135,135	0
35	NA	0	8531	1/1	0.97	0.06	40,40,40,40	0
32	MG	0	8020	1/1	0.97	0.07	40,40,40,40	0
35	NA	0	8534	1/1	0.97	0.14	44,44,44,44	0
32	MG	0	8079	1/1	0.97	0.11	51,51,51,51	0
32	MG	0	8021	1/1	0.97	0.05	40,40,40,40	0
33	CL	0	8822	1/1	0.97	0.45	81,81,81,81	0
32	MG	0	8022	1/1	0.97	0.22	44,44,44,44	0
32	MG	0	8024	1/1	0.97	0.12	49,49,49,49	0
34	SR	0	8939	1/1	0.97	0.10	149,149,149,149	0
32	MG	0	8026	1/1	0.97	0.08	35,35,35,35	0
32	MG	0	8050	1/1	0.97	0.09	32,32,32,32	0
34	SR	0	8940	1/1	0.98	0.07	97,97,97,97	0
34	SR	0	8941	1/1	0.98	0.14	108,108,108,108	0
32	MG	0	8028	1/1	0.98	0.16	26,26,26,26	0
32	MG	0	8068	1/1	0.98	0.08	51,51,51,51	0
32	MG	0	8069	1/1	0.98	0.30	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8030	1/1	0.98	0.30	68,68,68,68	0
32	MG	0	8052	1/1	0.98	0.07	56,56,56,56	0
34	SR	B	8950	1/1	0.98	0.14	116,116,116,116	0
34	SR	0	8949	1/1	0.98	0.17	122,122,122,122	0
32	MG	0	8017	1/1	0.98	0.19	52,52,52,52	0
33	CL	B	8819	1/1	0.98	0.09	58,58,58,58	0
32	MG	0	8023	1/1	0.98	0.10	37,37,37,37	0
34	SR	1	8952	1/1	0.98	0.15	89,89,89,89	0
35	NA	0	8541	1/1	0.98	0.18	75,75,75,75	0
34	SR	3	8999	1/1	0.98	0.10	110,110,110,110	0
32	MG	0	8034	1/1	0.98	0.16	46,46,46,46	0
32	MG	0	8078	1/1	0.98	0.27	69,69,69,69	0
34	SR	0	8910	1/1	0.98	0.04	100,100,100,100	0
35	NA	B	8552	1/1	0.98	0.10	83,83,83,83	0
34	SR	0	8914	1/1	0.98	0.32	120,120,120,120	0
32	MG	0	8012	1/1	0.98	0.14	18,18,18,18	0
34	SR	0	8964	1/1	0.98	0.09	131,131,131,131	0
32	MG	0	8025	1/1	0.98	0.12	37,37,37,37	0
35	NA	0	8553	1/1	0.98	0.47	65,65,65,65	0
32	MG	0	8063	1/1	0.98	0.14	80,80,80,80	0
32	MG	0	8065	1/1	0.98	0.06	57,57,57,57	0
33	CL	R	8806	1/1	0.98	0.18	57,57,57,57	0
32	MG	0	8085	1/1	0.98	0.53	97,97,97,97	0
34	SR	0	8923	1/1	0.98	0.10	101,101,101,101	0
33	CL	3	8804	1/1	0.98	0.06	63,63,63,63	0
34	SR	0	8926	1/1	0.98	0.17	108,108,108,108	0
35	NA	0	8507	1/1	0.98	0.11	37,37,37,37	0
35	NA	0	8508	1/1	0.98	0.20	35,35,35,35	0
32	MG	K	8054	1/1	0.98	0.16	46,46,46,46	0
33	CL	0	8805	1/1	0.98	0.06	67,67,67,67	0
34	SR	0	8933	1/1	0.98	0.16	139,139,139,139	0
35	NA	0	8566	1/1	0.98	0.12	64,64,64,64	0
35	NA	0	8513	1/1	0.98	0.21	54,54,54,54	0
35	NA	0	8514	1/1	0.98	0.50	56,56,56,56	0
34	SR	0	8981	1/1	0.98	0.33	178,178,178,178	0
34	SR	0	8934	1/1	0.98	0.24	134,134,134,134	0
34	SR	0	8983	1/1	0.98	0.24	170,170,170,170	0
34	SR	0	8984	1/1	0.98	0.03	121,121,121,121	0
33	CL	0	8812	1/1	0.98	0.06	58,58,58,58	0
34	SR	0	8937	1/1	0.98	0.27	112,112,112,112	0
34	SR	0	8938	1/1	0.98	0.02	147,147,147,147	0
32	MG	0	8088	1/1	0.98	0.20	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
37	K	0	8402	1/1	0.98	0.25	76,76,76,76	0
34	SR	0	8904	1/1	0.99	0.18	65,65,65,65	0
34	SR	0	8906	1/1	0.99	0.24	64,64,64,64	0
32	MG	B	8042	1/1	0.99	0.07	44,44,44,44	0
34	SR	0	8909	1/1	0.99	0.15	88,88,88,88	0
34	SR	0	8956	1/1	0.99	0.06	155,155,155,155	0
32	MG	0	8080	1/1	0.99	0.12	75,75,75,75	0
34	SR	0	8911	1/1	0.99	0.08	85,85,85,85	0
32	MG	0	8061	1/1	0.99	0.23	37,37,37,37	0
34	SR	9	8978	1/1	0.99	0.08	135,135,135,135	0
32	MG	0	8043	1/1	0.99	0.06	52,52,52,52	0
32	MG	0	8005	1/1	0.99	0.23	35,35,35,35	0
34	SR	0	8918	1/1	0.99	0.15	80,80,80,80	0
32	MG	0	8084	1/1	0.99	0.15	33,33,33,33	0
32	MG	0	8064	1/1	0.99	0.19	44,44,44,44	0
35	NA	M	8539	1/1	0.99	0.18	34,34,34,34	0
32	MG	0	8032	1/1	0.99	0.05	44,44,44,44	0
34	SR	0	8967	1/1	0.99	0.06	133,133,133,133	0
32	MG	Y	8086	1/1	0.99	0.08	44,44,44,44	0
32	MG	0	8007	1/1	0.99	0.16	32,32,32,32	0
34	SR	0	8970	1/1	0.99	0.02	123,123,123,123	0
32	MG	0	8090	1/1	0.99	0.10	65,65,65,65	0
32	MG	0	8048	1/1	0.99	0.24	33,33,33,33	0
33	CL	0	8816	1/1	0.99	0.08	79,79,79,79	0
33	CL	0	8817	1/1	0.99	0.15	67,67,67,67	0
34	SR	0	8931	1/1	0.99	0.07	113,113,113,113	0
32	MG	0	8015	1/1	0.99	0.13	30,30,30,30	0
32	MG	0	8009	1/1	0.99	0.25	36,36,36,36	0
34	SR	0	8935	1/1	0.99	0.09	79,79,79,79	0
34	SR	A	8930	1/1	0.99	0.06	97,97,97,97	0
32	MG	0	8010	1/1	0.99	0.22	45,45,45,45	0
32	MG	0	8027	1/1	0.99	0.11	51,51,51,51	0
32	MG	0	8073	1/1	0.99	0.35	73,73,73,73	0
34	SR	F	9005	1/1	0.99	0.08	133,133,133,133	0
35	NA	0	8517	1/1	0.99	0.15	31,31,31,31	0
34	SR	R	8912	1/1	0.99	0.16	92,92,92,92	0
33	CL	J	8801	1/1	0.99	0.07	79,79,79,79	0
34	SR	0	8990	1/1	0.99	0.10	139,139,139,139	0
32	MG	0	8019	1/1	0.99	0.20	28,28,28,28	0
32	MG	0	8076	1/1	0.99	0.08	40,40,40,40	0
34	SR	3	8932	1/1	0.99	0.14	76,76,76,76	0
32	MG	0	8029	1/1	0.99	0.15	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8059	1/1	0.99	0.07	57,57,57,57	0
36	CD	O	8705	1/1	0.99	0.06	118,118,118,118	0
36	CD	U	8701	1/1	0.99	0.10	63,63,63,63	0
36	CD	Z	8703	1/1	0.99	0.13	75,75,75,75	0
36	CD	1	8702	1/1	0.99	0.13	67,67,67,67	0
34	SR	0	8948	1/1	0.99	0.10	92,92,92,92	0
34	SR	0	8902	1/1	0.99	0.17	66,66,66,66	0
32	MG	0	8018	1/1	1.00	0.23	40,40,40,40	0
32	MG	0	8008	1/1	1.00	0.09	28,28,28,28	0
34	SR	0	8903	1/1	1.00	0.19	59,59,59,59	0
32	MG	0	8004	1/1	1.00	0.19	32,32,32,32	0
34	SR	0	8905	1/1	1.00	0.27	61,61,61,61	0
32	MG	0	8058	1/1	1.00	0.09	22,22,22,22	0
34	SR	0	8916	1/1	1.00	0.03	120,120,120,120	0
36	CD	3	8704	1/1	1.00	0.10	74,74,74,74	0
34	SR	0	8925	1/1	1.00	0.08	86,86,86,86	0
34	SR	0	8907	1/1	1.00	0.15	56,56,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.