wwPDB X-ray Structure Validation Summary Report (i)

Feb 6, 2024 – 03:09 AM EST

PDB ID	:	1YJ9
Title	:	Crystal Structure Of The Mutant 50S Ribosomal Subunit Of Haloarcula Marismortui Containing a three residue deletion in L22
Authors	:	Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on	:	2005-01-13
Resolution	:	2.80 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:

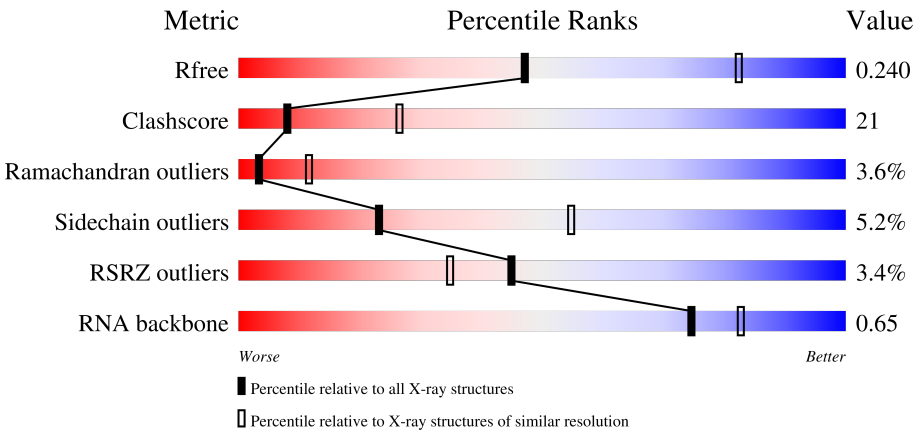
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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

Mol	Chain	Length	Quality of chain
1	0	2922	51% 38% 5% 6%
2	9	122	2% 38% 53% 8% •
3	A	240	3% 50% 41% 7% •
4	B	338	% 43% 49% 8%

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Mol	Chain	Length	Quality of chain
5	C	246	43% 50% 6%
6	D	177	22% 22% 48% 7% • 21%
7	E	178	7% 46% 48% • •
8	F	120	11% 36% 58% 5% •
9	G	348	3% • 5% 92%
10	H	177	% 46% 39% 6% 10%
11	I	162	27% 9% 30% • 57%
12	J	145	% 50% 43% 5% •
13	K	132	51% 47% •
14	L	165	7% 41% 43% • 12%
15	M	195	51% 46% • •
16	N	187	5% 36% 58% • ••
17	O	116	47% 50% • •
18	P	149	% 54% 37% 5% •
19	Q	96	59% 36% • •
20	R	152	7% 53% 39% 5% •
21	S	85	4% 42% 51% • 5%
22	T	120	5% 39% 53% 7% •
23	U	66	5% 39% 39% • 20%
24	V	71	18% 32% 52% 6% • 8%
25	W	154	42% 54% 5%
26	X	92	9% 36% 46% 7% • 11%
27	Y	241	2% 34% 22% • 41%
28	Z	83	36% 46% 6% 12%
29	1	57	58% 40% •

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Mol	Chain	Length	Quality of chain
30	2	50	6% 48% 46%
31	3	92	% 63% 34%

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	NA	0	8526	-	-	-	X
34	NA	0	8552	-	-	-	X
34	NA	0	8556	-	-	-	X
34	NA	0	8563	-	-	-	X
34	NA	0	8568	-	-	-	X
34	NA	R	8586	-	-	-	X
35	CL	0	8815	-	-	-	X
35	CL	J	8801	-	-	X	-
35	CL	J	8802	-	-	X	-

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 99031 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	0	2754	59041	26358	10875	19062	2746	0	1	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	modified residue	GB 55229667
0	2587	OMU	U	modified residue	GB 55229667
0	2588	OMG	G	modified residue	GB 55229667
0	2619	UR3	U	modified residue	GB 55229667
0	2621	PSU	U	modified residue	GB 55229667

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	9	122	2599	1160	471	847	121	0	0	0

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

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

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

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

- Molecule 5 is a protein called 50S ribosomal protein L4E.

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

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

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

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

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

- Molecule 8 is a protein called 50S ribosomal protein L7AE.

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

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

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

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L10E.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	M	194	1558	942	332	283	1	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	GB 55231501

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	R	147	1123	699	204	216	4	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	?	-	GLN	deletion	UNP P10970
R	?	-	GLN	deletion	UNP P10970
R	?	-	GLY	deletion	UNP P10970

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	2	49	421	254	93	73	1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
32	0	107	107	107	0	0
32	9	1	1	1	0	0
32	A	2	2	2	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	2	1	1	1	0	0
32	3	1	1	1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
33	0	2	2	2	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
34	0	74	74	74	0	0

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	9	Total Cl 9 9	0	0
35	A	1	Total Cl 1 1	0	0
35	B	1	Total Cl 1 1	0	0
35	J	3	Total Cl 3 3	0	0
35	L	1	Total Cl 1 1	0	0
35	M	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	Q	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	R	1	Total Cl 1 1	0	0
35	Y	1	Total Cl 1 1	0	0
35	3	1	Total Cl 1 1	0	0

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

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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	5866	Total O 5866 5866	0	0
37	9	143	Total O 143 143	0	0
37	A	119	Total O 119 119	0	0
37	B	148	Total O 148 148	0	0
37	C	180	Total O 180 180	0	0
37	D	46	Total O 46 46	0	0
37	E	45	Total O 45 45	0	0
37	F	27	Total O 27 27	0	0
37	G	19	Total O 19 19	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	H	69	Total O 69 69	0	0
37	I	9	Total O 9 9	0	0
37	J	57	Total O 57 57	0	0
37	K	54	Total O 54 54	0	0
37	L	84	Total O 84 84	0	0
37	M	130	Total O 130 130	0	0
37	N	64	Total O 64 64	0	0
37	O	45	Total O 45 45	0	0
37	P	64	Total O 64 64	0	0
37	Q	53	Total O 53 53	0	0
37	R	58	Total O 58 58	0	0
37	S	34	Total O 34 34	0	0
37	T	32	Total O 32 32	0	0
37	U	26	Total O 26 26	0	0
37	V	14	Total O 14 14	0	0
37	W	72	Total O 72 72	0	0
37	X	24	Total O 24 24	0	0
37	Y	104	Total O 104 104	0	0
37	Z	34	Total O 34 34	0	0
37	1	63	Total O 63 63	0	0
37	2	32	Total O 32 32	0	0

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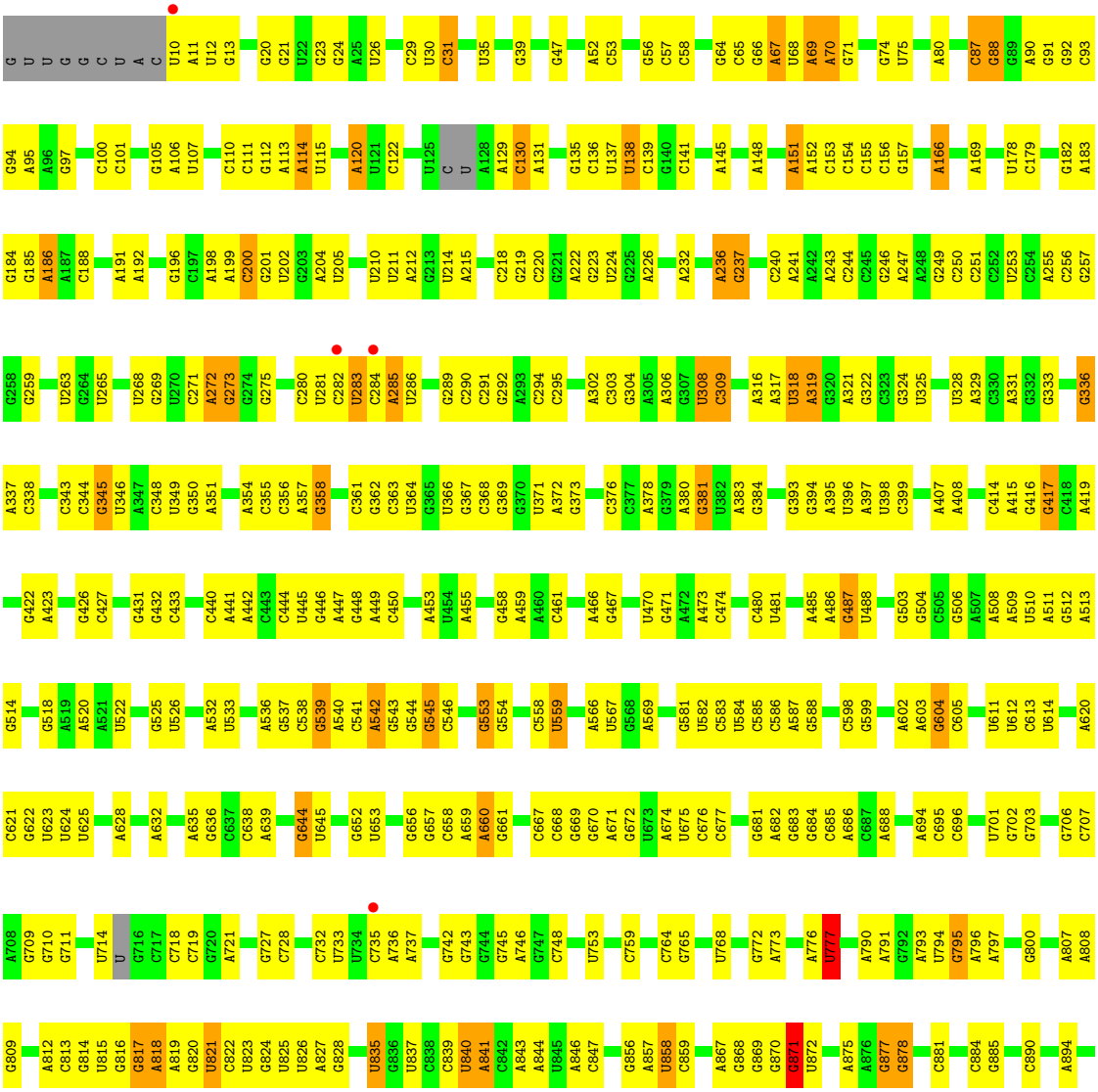
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
37	3	69	69	69	0	0

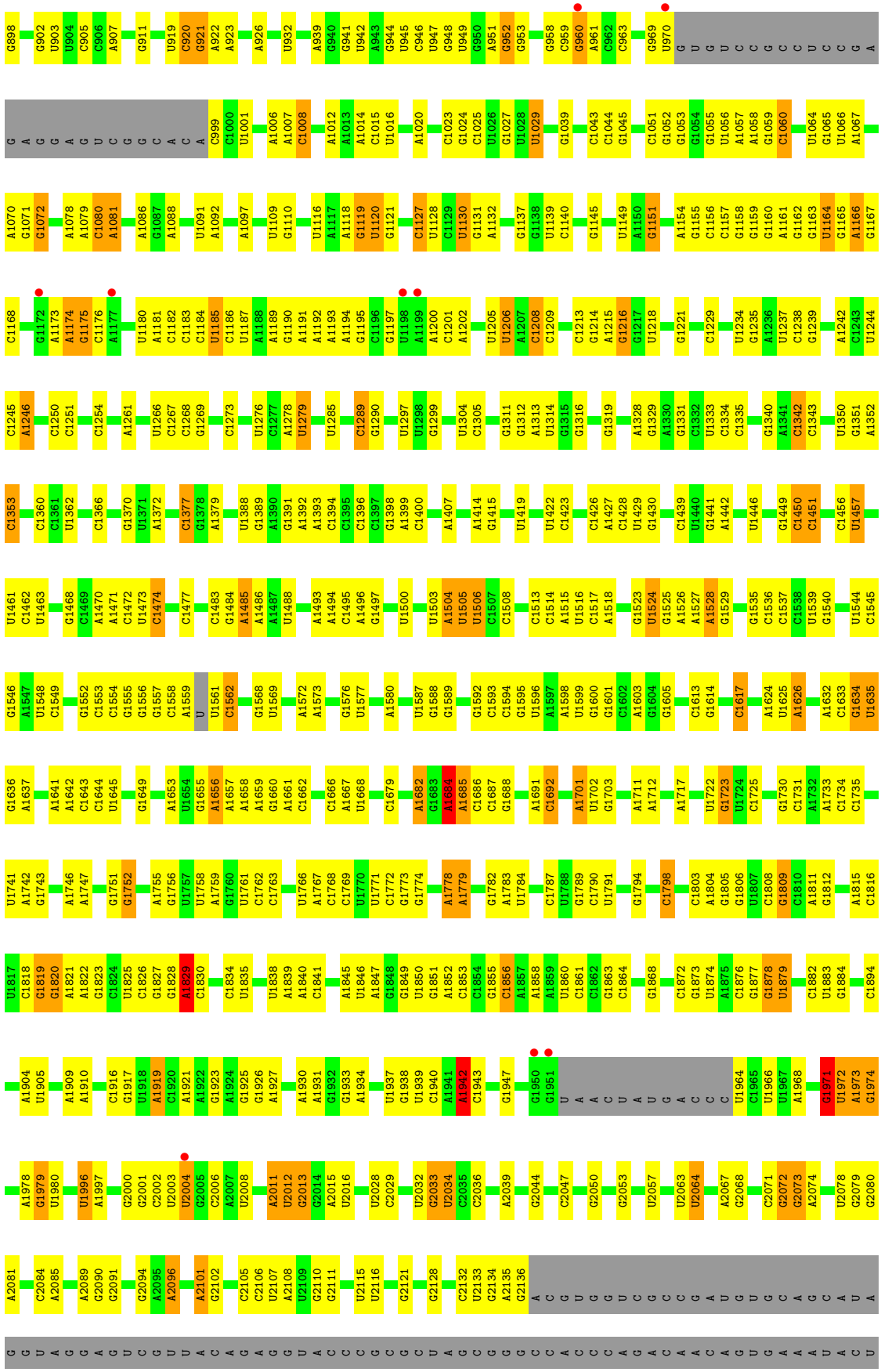
3 Residue-property plots (i)

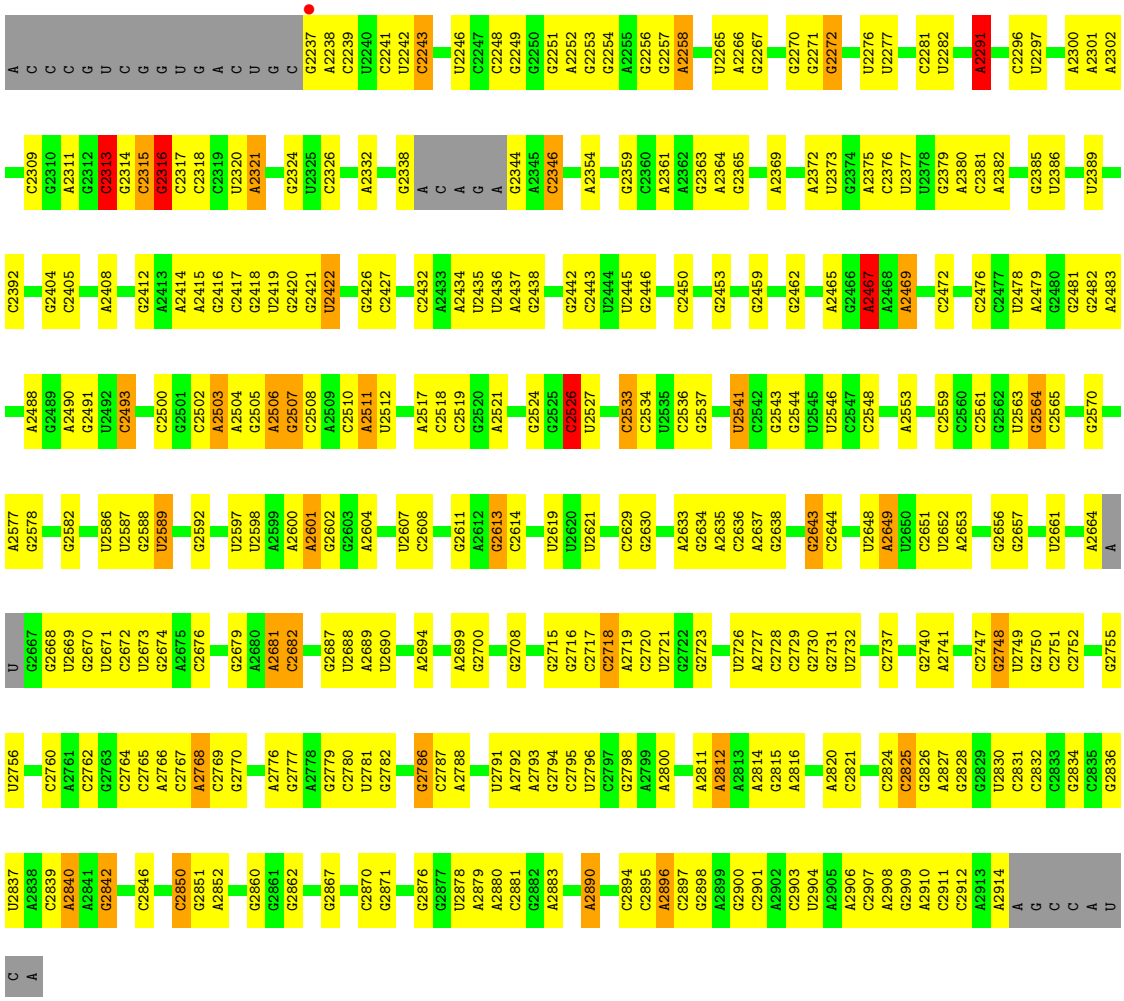
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S Ribosomal RNA

Chain 0:

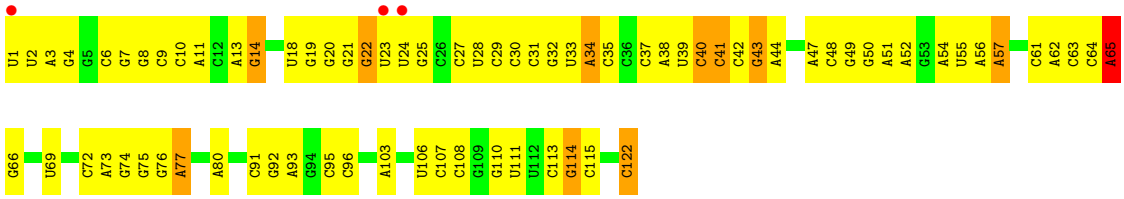



G898 G902 U903 U904 C905 C906 A907 G911 U919 C920 G921 A922 A923 A926 U932 A939 G940 G941 U942 A943 G944 U945 C946 U947 G948 U949 G950 A951 G952 G953 G958 C959 G960 A961 C962 C963 G969 U970
G A G G A G U C G G C A C A C999 C1000 U1001 A1006 A1007 C1008 A1012 A1013 A1014 C1015 U1016 A1020 C1023 G1024 C1025 U1026 G1027 U1028 U1029 G1039 C1043 C1044 G1045 C1051 G1052 G1053 G1054 G1055 U1056 A1057 A1058 G1059 G1060 U1064 G1065 U1066 A1067
A1070 G1071 G1072 A1078 A1079 C1080 A1081 A1086 G1087 A1088 U1091 A1092 A1097 U1109 G1110 U1116 A1117 A1118 G1119 U1120 G1121 C1127 U1128 C1129 U1130 G1131 A1132 G1137 G1138 U1139 C1140 G1145 U1149 A1150 G1151 A1154 G1155 C1156 C1157 G1158 G1159 G1160 A1161 G1162 G1163 U1164 G1165 A1166 G1167
C1168 G1172 A1173 A1174 G1175 C1176 A1177 U1180 A1181 C1182 C1183 C1184 U1185 C1186 U1187 A1188 A1189 G1190 A1191 A1192 A1193 A1194 G1195 C1196 G1197 U1198 A1199 A1200 C1201 A1202 U1205 U1206 A1207 C1208 C1209 C1213 G1214 A1215 G1216 G1217 U1218 G1221 C1229 U1234 G1235 A1236 U1237 C1238 G1239 A1242 C1243 U1244
C1245 A1246 C1250 C1251 C1254 A1261 U1266 C1267 C1268 G1269 C1273 U1276 C1277 A1278 U1279 U1285 C1289 G1290 U1297 U1298 G1299 U1304 C1305 G1311 G1312 A1313 U1314 G1315 G1316 G1319 A1328 G1329 A1330 G1331 C1332 U1333 C1334 C1335 G1340 A1341 C1342 C1343 U1350 G1351 A1352
C1353 C1360 C1361 U1362 C1366 G1370 U1371 A1372 C1377 G1378 A1379 U1388 G1389 A1390 G1391 A1392 A1393 C1394 C1395 C1396 C1397 G1398 A1399 C1400 A1407 A1414 G1415 U1419 U1422 C1423 C1426 A1427 C1428 U1429 G1430 C1439 U1440 G1441 A1442 U1446 G1449 C1450 C1451 C1456 U1457
U1461 C1462 U1463 G1468 C1469 A1470 A1471 C1472 U1473 C1474 C1477 C1483 G1484 A1485 A1486 A1487 U1488 A1493 A1494 C1495 A1496 G1497 U1500 U1503 A1504 U1505 U1506 C1507 C1508 C1513 C1514 A1515 U1516 C1517 A1518 G1523 U1524 G1525 A1526 A1527 A1528 G1529 G1535 C1536 C1537 C1538 U1539 G1540 U1544 C1545
G1546 A1547 U1548 C1549 G1552 C1553 C1554 G1555 G1556 G1557 C1558 A1559 U U1561 C1562 G1568 U1569 A1572 A1573 G1576 U1577 A1580 U1587 G1588 G1589 G1592 C1593 C1594 G1595 U1596 A1597 A1598 U1599 G1600 G1601 C1602 A1603 G1604 G1605 C1613 G1614 C1617 A1624 U1625 A1626 A1632 C1633 G1634 U1635
G1636 A1637 A1641 A1642 C1643 C1644 U1645 G1649 A1653 U1654 G1655 A1656 A1657 A1658 A1659 G1660 A1661 C1662 C1666 A1667 U1668 C1679 A1682 G1683 A1684 A1685 C1686 C1687 G1688 A1691 C1692 A1701 U1702 G1703 A1711 A1712 A1717 U1722 G1723 U1724 C1725 G1730 C1731 A1732 A1733 C1734 C1735
U1741 A1742 G1743 A1746 A1747 G1751 G1752 A1755 G1756 U1757 U1758 A1759 G1760 U1761 C1762 C1763 U1766 A1767 C1768 C1769 U1770 U1771 C1772 G1773 G1774 A1778 A1779 G1782 A1783 U1784 C1787 U1788 G1789 C1790 U1791 G1794 C1798 C1803 A1804 G1805 G1806 U1807 C1808 G1809 C1810 A1811 G1812 A1815 C1816
U1817 C1818 G1819 G1820 A1821 A1822 G1823 C1824 U1825 C1826 G1827 G1828 A1829 C1830 C1834 U1835 U1838 A1839 A1840 C1841 A1845 U1846 A1847 G1848 G1849 U1850 G1851 A1852 C1853 C1854 G1855 C1856 A1857 A1858 A1859 U1860 C1861 C1862 G1863 C1864 G1868 C1872 G1873 U1874 A1875 C1876 G1877 G1878 U1879 C1882 U1883 G1884 C1894
A1904 U1905 A1909 A1910 C1916 G1917 U1918 A1919 C1920 A1921 A1922 G1923 A1924 G1925 G1926 A1927 A1930 A1931 G1932 G1933 A1934 U1937 G1938 U1939 C1940 A1941 A1942 C1943 G1947 G1950 G1951 U A A C U A U G A C C C U1964 C1965 U1966 U1967 A1968 G1971 U1972 A1973 G1974
A1978 G1979 U1980 U1996 A1997 G2000 G2001 C2002 U2003 U2004 G2005 C2006 A2007 U2008 A2011 U2012 G2013 G2014 A2015 U2016 U2028 C2029 U2032 G2033 U2034 C2035 C2036 A2039 G2044 C2047 G2050 G2053 U2057 U2063 U2064 A2067 G2068 C2071 G2072 G2073 A2074 U2078 G2079 G2080
A2081 C2084 A2085 A2089 G2090 G2091 G2094 A2095 A2096 A2101 G2102 C2105 C2106 U2107 A2108 U2109 G2110 G2111 U2115 U2116 G2121 G2128 C2132 U2133 G2134 A2135 G2136 A C G U G G U C G G U U A C A G A C C C G G C U A G C C G G C C A G G A C C A A U A C U A
G G U A G G A G U C G U A C A G A C C C G G C U A G C C G G C C A G G A C C A A U A C U A



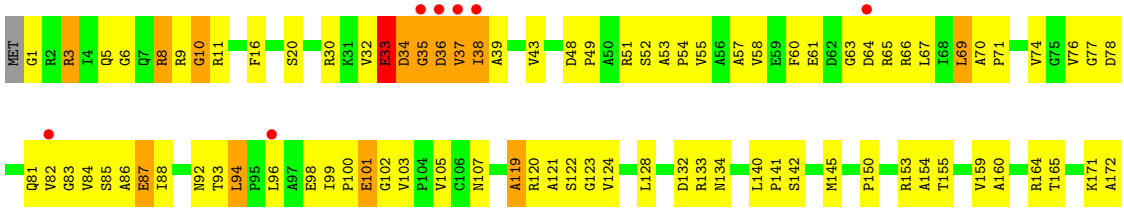
- Molecule 2: 5S Ribosomal RNA

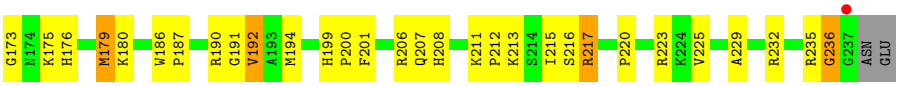
Chain 9:



- Molecule 3: 50S ribosomal protein L2P

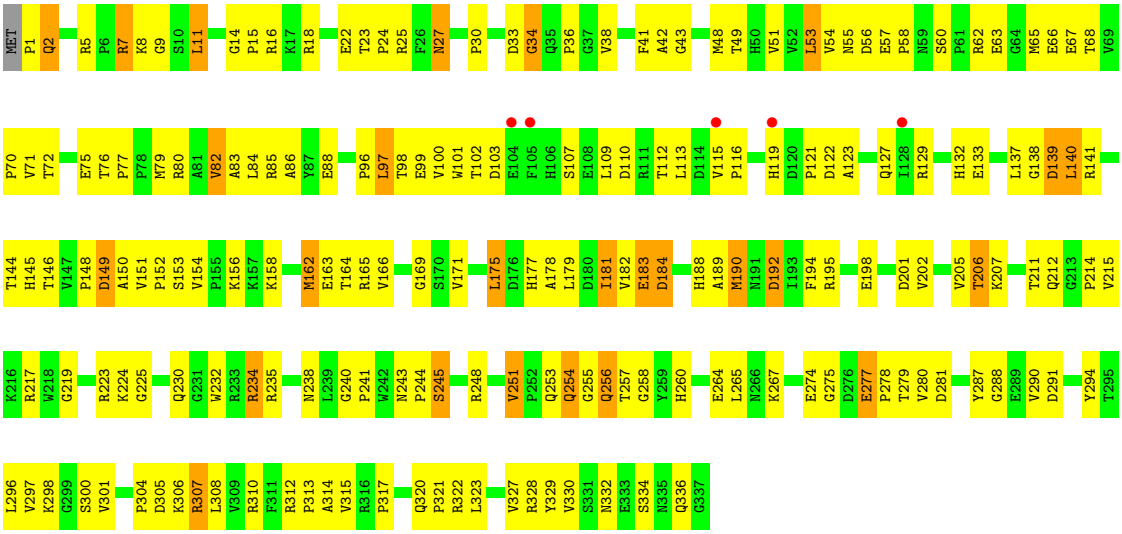
Chain A:





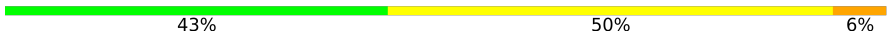
• Molecule 4: 50S ribosomal protein L3P

Chain B:



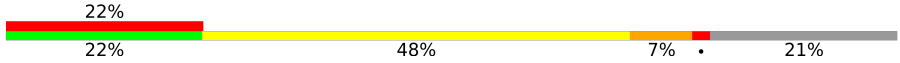
• Molecule 5: 50S ribosomal protein L4E

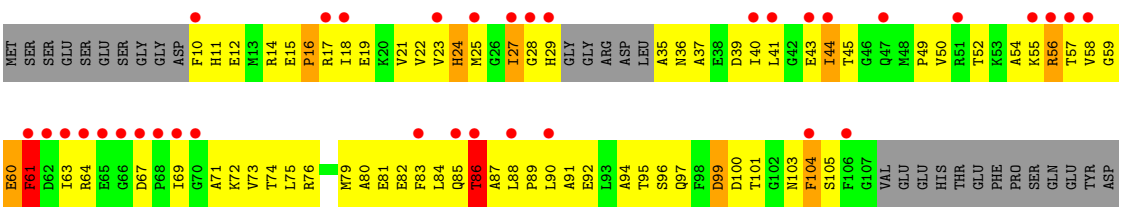
Chain C:



• Molecule 6: 50S ribosomal protein L5P

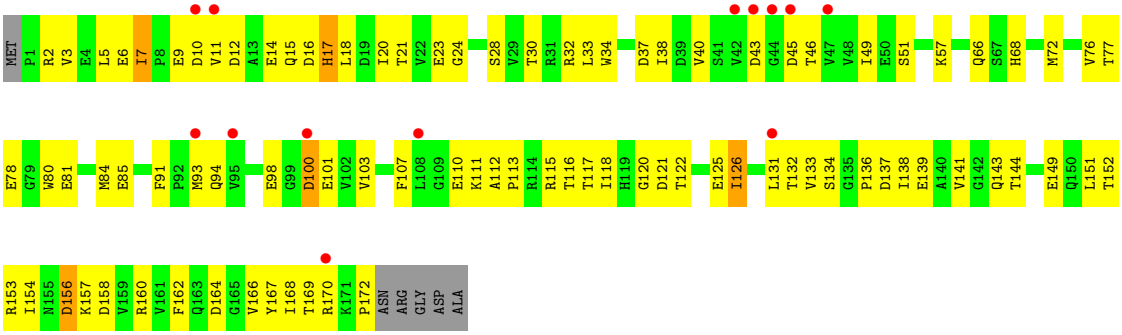
Chain D:





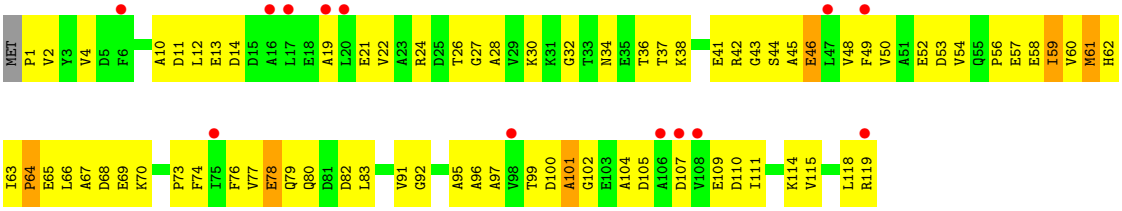
• Molecule 7: 50S ribosomal protein L6P

Chain E:



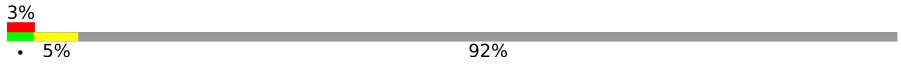
• Molecule 8: 50S ribosomal protein L7AE

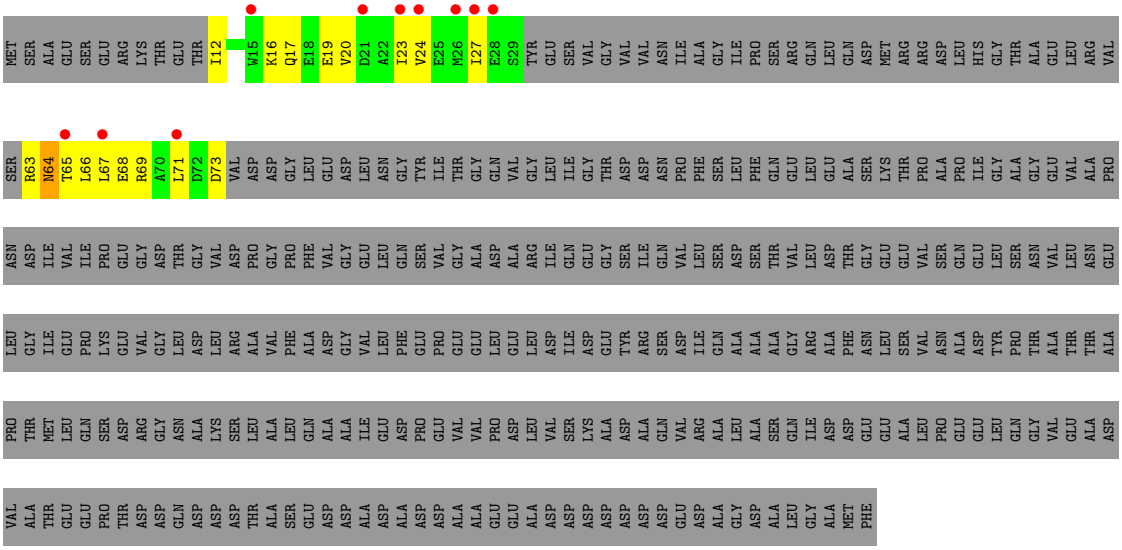
Chain F:



• Molecule 9: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

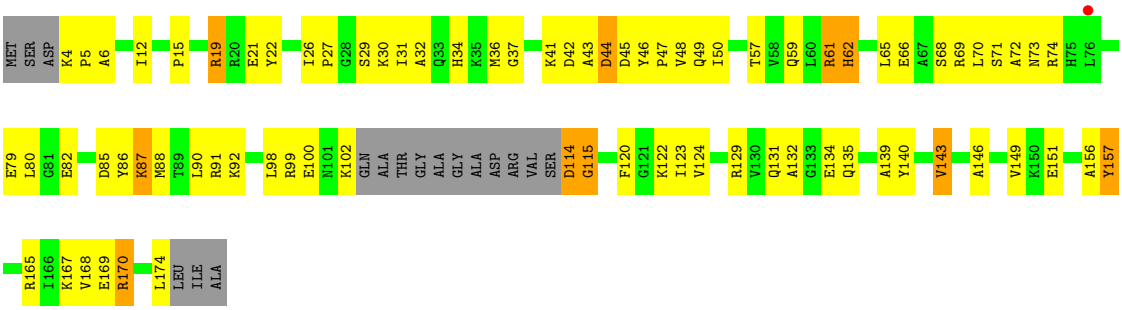
Chain G:





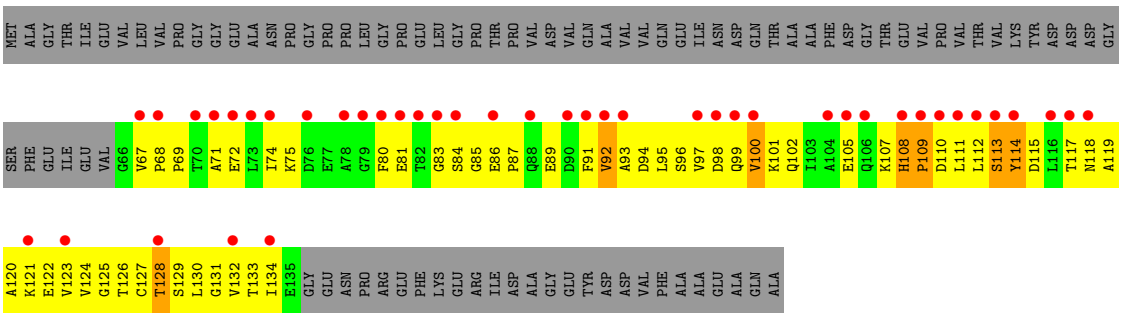
• Molecule 10: 50S RIBOSOMAL PROTEIN L10E

Chain H:



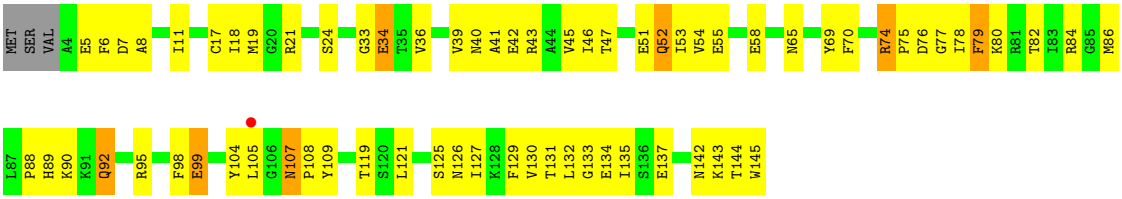
• Molecule 11: 50S RIBOSOMAL PROTEIN L11P

Chain I:



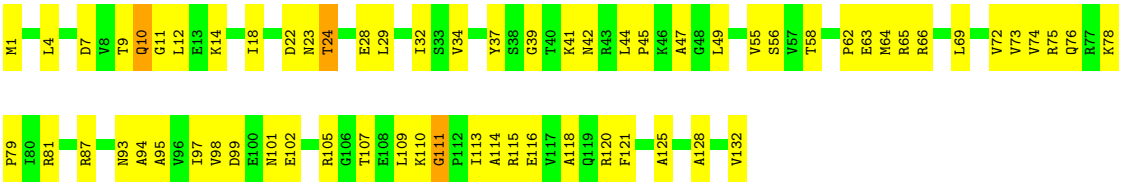
• Molecule 12: 50S ribosomal protein L13P

Chain J:



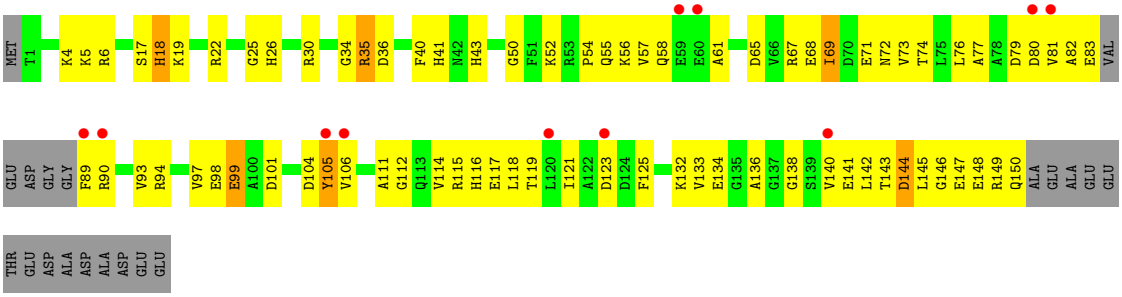
• Molecule 13: 50S ribosomal protein L14P

Chain K:



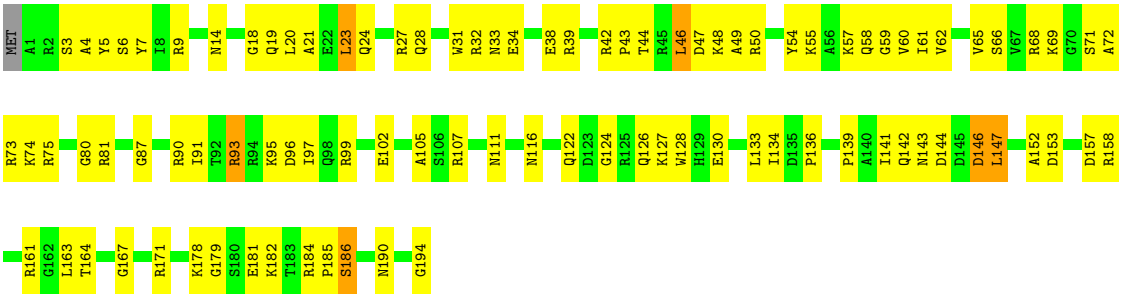
• Molecule 14: 50S ribosomal protein L15P

Chain L:



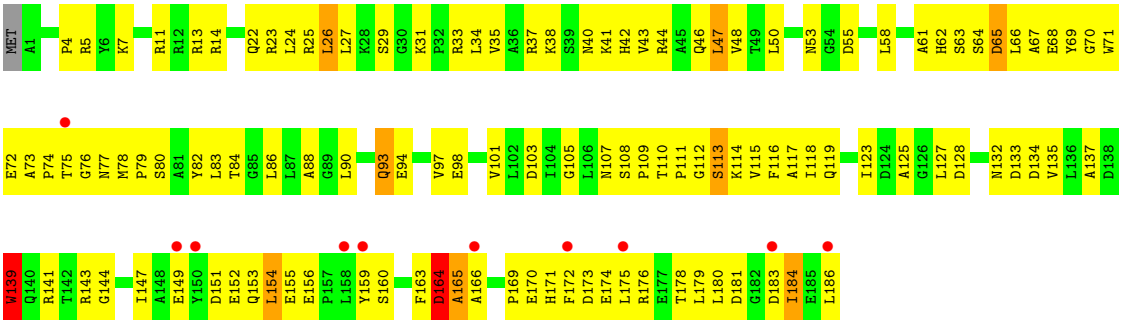
- Molecule 15: 50S Ribosomal Protein L15E

Chain M:



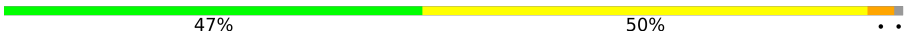
- Molecule 16: 50S ribosomal protein L18P

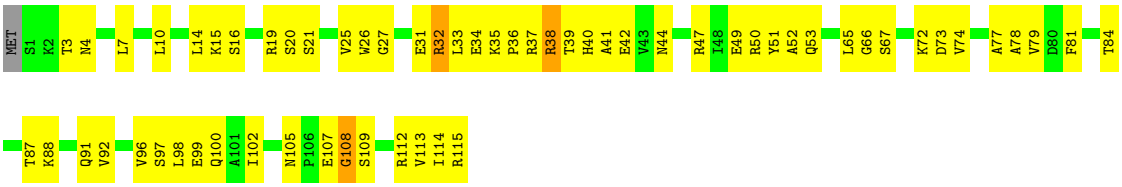
Chain N:



- Molecule 17: 50S ribosomal protein L18e

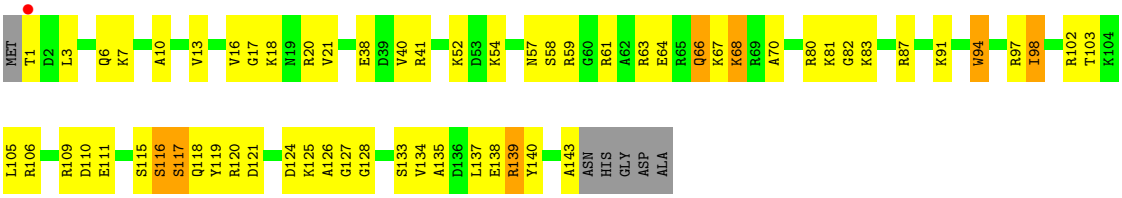
Chain O:





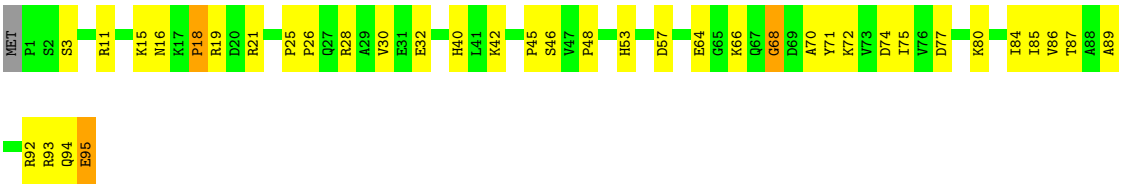
- Molecule 18: 50S ribosomal protein L19E

Chain P:



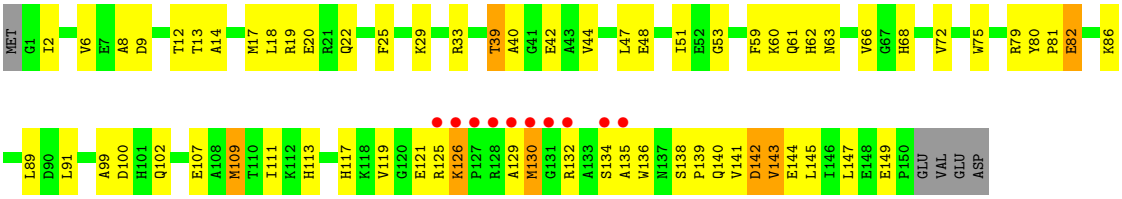
• Molecule 19: 50S ribosomal protein L21e

Chain Q:



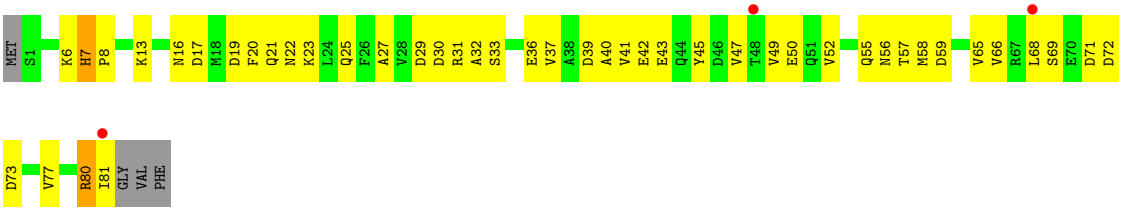
• Molecule 20: 50S ribosomal protein L22P

Chain R:



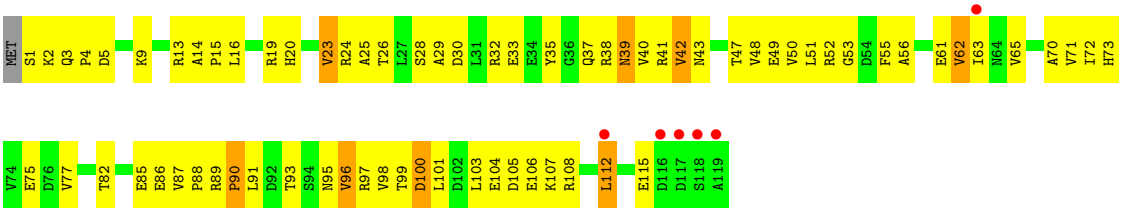
• Molecule 21: 50S ribosomal protein L23P

Chain S:



• Molecule 22: 50S ribosomal protein L24P

Chain T:



• Molecule 23: 50S ribosomal protein L24E

Chain U: 5% 39% 39% • 20%

PRO ARG THR R4 E5 C6 D7 Y8 C9 G10 T11 D12 I13 E14 P15 G16 T17 G18 V22 H23 K24 D25 G26 A27 H30 F31 C32 S33 S34 K35 C36 E37 N38 N39 R44 N48 W51 T52 D53 T54 A55 R56 GLY GLU ALA GLY GLU ALA GLU ASP GLU ALA

• Molecule 24: 50S ribosomal protein L29P

Chain V: 18% 32% 52% 6% • 8%

MET T1 V2 L3 H4 V5 I8 R9 D10 M11 T12 P13 A14 E15 R16 E17 A18 E19 L20 D21 D22 L27 A30 R31 A32 V33 G37 G38 A39 P40 E41 N42 P43 G44 E48 L49 R50 K51 A52 I53 A54 R55 I56 K57 T58 I59 Q60 G61 E62 E63 G64 D65 LEU GLN GLU

ASN GLU

• Molecule 25: 50S ribosomal protein L30P

Chain W: 42% 54% 5%

M1 H2 A3 L4 V5 Q6 L7 R8 V11 N12 M13 I17 Q18 L21 E22 M23 L24 N25 I26 V29 N30 H31 C32 P36 E37 T38 D39 A40 Y41 R42 C43 M44 V45 A46 K47 V48 N49 V52 A53 F54 G55 E56 Q59 E60 T61 L62 E63 T64 V65 T68 R69

P72 L73 E74 G75 D76 A77 D80 D81 E82 T88 D89 Y90 D91 D92 I93 L96 A97 F98 A99 E103 T106 L107 R108 E109 Q110 G111 L112 S113 P114 T115 L116 R117 L118 H119 H125 D126 G127 V128 K129 H130 P131 V132 K133 E134 G135 G136 Q137 L138 G139 K140 H141 D142 T143 E144

G145 I146 L150 E151 A152 M153 R154

• Molecule 26: 50S ribosomal protein L31e

Chain X: 9% 36% 46% 7% • 11%

MET SER ALA SER ASP PHE GLU E7 R8 V9 V10 T11 I12 R15 R18 A19 E20 P21 N22 H23 K24 R25 A26 D27 M30 I31 E35 H36 L37 A38 K39 H40 F41 S42 V43 D44 E45 D46 A47 V48 R49 N55 E56 A57 A58 R63 A64 N65 T66 K69 I70 R71 V72

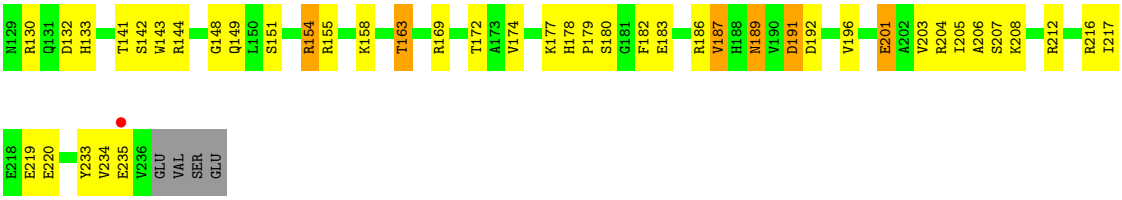
R73 A74 A75 R76 F77 E78 E79 E80 G81 E82 A83 I84 V85 E86 A87 E88 THR ALA GLU

• Molecule 27: 50S ribosomal protein L32E

Chain Y: 2% 34% 22% • 41%

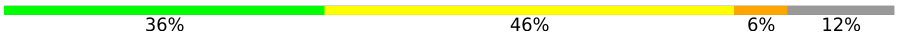
MET ALA ASP ASN GLU GLU ASP VAL GLU ALA GLU GLU GLU TYR THR GLU LEU THR ASP ILE SER GLY VAL GLY PRO SER LYS ALA GLU SER LEU ARG GLU ALA GLY PHE GLU SER VAL GLU ASP VAL ARG GLY ALA ASP GLN SER ALA LEU ALA ASP VAL SER GLY ILE GLY ASN ALA LEU

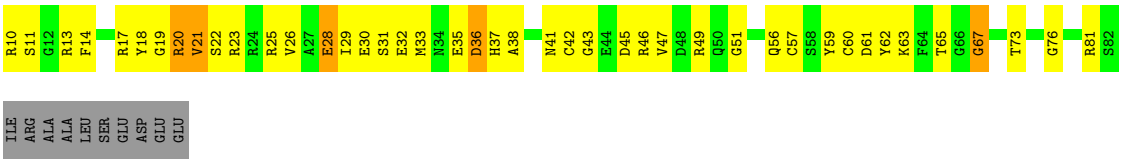
ALA ALA ARG ILE LYS ALA ASP VAL GLY GLY LEU GLU VAL GLU SER GLU THR GLU ALA GLU VAL GLU GLU GLU GLY GLY GLU GLU ALA PRO ASP GLU ASP VAL GLU T95 E96 L97 Q98 A99 L102 T103 T106 P107 D108 L109 S110 D111 E112 R115 R122 K125 P126 Q127 F128



- Molecule 28: 50S ribosomal protein L37Ae

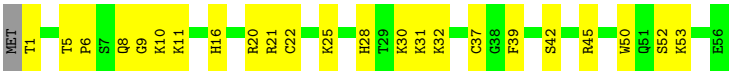
Chain Z:





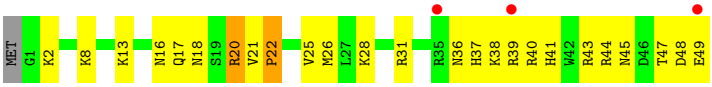
- Molecule 29: 50S ribosomal protein L37e

Chain 1:



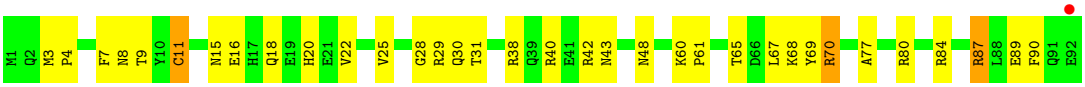
- Molecule 30: 50S ribosomal protein L39e

Chain 2:



- Molecule 31: 50S ribosomal protein L44E

Chain 3:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	213.08Å 300.75Å 575.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 2.80 49.56 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.3 (29.94-2.80) 89.2 (49.56-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.184 , 0.242 0.185 , 0.240	Depositor DCC
R_{free} test set	3987 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å^2)	55.8	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 63.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	99031	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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, UR3, OMG, MG, CD, PSU, NA, 1MA, CL, OMU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	0	0.42	0/65980	0.69	13/102903 (0.0%)
2	9	0.38	0/2904	0.70	1/4526 (0.0%)
3	A	0.35	0/1786	0.66	0/2408
4	B	0.35	0/2690	0.66	0/3652
5	C	0.39	0/1884	0.66	0/2551
6	D	0.33	0/1111	0.57	0/1498
7	E	0.35	0/1382	0.59	0/1880
8	F	0.34	0/901	0.59	0/1224
9	G	0.31	0/241	0.53	0/324
10	H	0.38	0/1302	0.70	1/1743 (0.1%)
11	I	0.31	0/526	0.59	0/716
12	J	0.40	0/1136	0.61	0/1530
13	K	0.37	0/1001	0.69	0/1347
14	L	0.36	0/1130	0.65	0/1509
15	M	0.36	0/1582	0.62	1/2117 (0.0%)
16	N	0.32	0/1474	0.64	0/1999
17	O	0.35	0/874	0.58	0/1181
18	P	0.37	0/1147	0.55	0/1528
19	Q	0.40	0/749	0.74	1/1005 (0.1%)
20	R	0.42	0/1146	0.63	0/1544
21	S	0.36	0/648	0.59	0/875
22	T	0.34	0/958	0.64	0/1289
23	U	0.34	0/417	0.58	0/562
24	V	0.31	0/502	0.56	0/675
25	W	0.37	0/1219	0.65	0/1655
26	X	0.36	0/664	0.62	0/895
27	Y	0.38	0/1146	0.65	0/1536
28	Z	0.38	0/589	0.63	0/787
29	1	0.40	0/438	0.64	0/578
30	2	0.41	0/427	0.61	0/566
31	3	0.40	0/771	0.58	0/1024
All	All	0.40	0/98725	0.68	17/147627 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	46
2	9	0	1
All	All	0	47

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	1942	A	C5'-C4'-C3'	7.17	127.47	116.00
1	0	1504	A	C1'-O4'-C4'	-6.38	104.80	109.90
1	0	2291	A	N9-C1'-C2'	6.19	122.05	114.00
19	Q	68	GLY	N-CA-C	-5.89	98.36	113.10
1	0	1504	A	N9-C1'-C2'	5.75	121.48	114.00

There are no chirality outliers.

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	148	A	Sidechain
1	0	26	U	Sidechain
1	0	333	G	Sidechain
1	0	398	U	Sidechain
1	0	458	G	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59041	0	29817	1161	0
2	9	2599	0	1325	86	0
3	A	1753	0	1766	148	0
4	B	2625	0	2533	200	0
5	C	1859	0	1816	160	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1094	0	1085	138	0
7	E	1357	0	1266	77	0
8	F	890	0	843	79	0
9	G	240	0	231	22	0
10	H	1282	0	1292	95	0
11	I	519	0	500	63	0
12	J	1120	0	1098	80	0
13	K	992	0	1031	77	0
14	L	1118	0	1076	81	0
15	M	1558	0	1566	98	0
16	N	1445	0	1401	147	0
17	O	865	0	873	62	0
18	P	1136	0	1123	71	0
19	Q	735	0	729	37	0
20	R	1123	0	1099	69	0
21	S	641	0	605	39	0
22	T	950	0	923	99	0
23	U	410	0	364	31	0
24	V	499	0	511	44	0
25	W	1196	0	1137	120	0
26	X	654	0	653	57	0
27	Y	1130	0	1133	66	0
28	Z	578	0	539	39	0
29	1	431	0	426	36	0
30	2	421	0	437	35	0
31	3	755	0	728	31	0
32	0	107	0	0	0	0
32	2	1	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	74	0	0	0	0
34	9	2	0	0	0	0
34	A	1	0	0	0	0
34	C	1	0	0	0	0
34	J	1	0	0	0	0
34	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	2	0	0	0	0
34	S	1	0	0	0	0
34	T	1	0	0	0	0
35	0	9	0	0	1	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	4	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	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	5866	0	0	246	0
37	1	63	0	0	8	0
37	2	32	0	0	2	0
37	3	69	0	0	8	0
37	9	143	0	0	12	0
37	A	119	0	0	21	0
37	B	148	0	0	31	0
37	C	180	0	0	34	0
37	D	46	0	0	17	0
37	E	45	0	0	10	0
37	F	27	0	0	8	0
37	G	19	0	0	2	0
37	H	69	0	0	12	0
37	I	9	0	0	5	0
37	J	57	0	0	8	0
37	K	54	0	0	10	0
37	L	84	0	0	17	0
37	M	130	0	0	10	0
37	N	64	0	0	22	0
37	O	45	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	P	64	0	0	10	0
37	Q	53	0	0	7	0
37	R	58	0	0	5	0
37	S	34	0	0	3	0
37	T	32	0	0	9	0
37	U	26	0	0	3	0
37	V	14	0	0	5	0
37	W	72	0	0	12	0
37	X	24	0	0	5	0
37	Y	104	0	0	15	0
37	Z	34	0	0	3	0
All	All	99031	0	59926	3232	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 21.

The worst 5 of 3232 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)
5:C:127:ARG:NH2	5:C:225:PRO:HG2	1.66	1.09
5:C:236:THR:HG22	5:C:239:ALA:H	0.95	1.08
1:0:1160:G:H5'	1:0:1161:A:H5'	1.13	1.07
4:B:264:GLU:HG2	4:B:267:LYS:HE2	1.36	1.04
29:1:25:LYS:HD2	30:2:49:GLU:H	1.20	1.03

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	235/240 (98%)	191 (81%)	31 (13%)	13 (6%)	2 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B	335/338 (99%)	291 (87%)	35 (10%)	9 (3%)	5	17
5	C	244/246 (99%)	201 (82%)	32 (13%)	11 (4%)	2	8
6	D	134/177 (76%)	85 (63%)	31 (23%)	18 (13%)	0	0
7	E	170/178 (96%)	150 (88%)	15 (9%)	5 (3%)	4	15
8	F	117/120 (98%)	93 (80%)	17 (14%)	7 (6%)	1	4
9	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
10	H	156/177 (88%)	134 (86%)	17 (11%)	5 (3%)	4	13
11	I	68/162 (42%)	49 (72%)	14 (21%)	5 (7%)	1	2
12	J	140/145 (97%)	121 (86%)	14 (10%)	5 (4%)	3	11
13	K	130/132 (98%)	111 (85%)	17 (13%)	2 (2%)	10	33
14	L	141/165 (86%)	114 (81%)	25 (18%)	2 (1%)	11	34
15	M	192/195 (98%)	169 (88%)	20 (10%)	3 (2%)	9	31
16	N	184/187 (98%)	149 (81%)	23 (12%)	12 (6%)	1	3
17	O	113/116 (97%)	102 (90%)	8 (7%)	3 (3%)	5	17
18	P	141/149 (95%)	125 (89%)	12 (8%)	4 (3%)	5	17
19	Q	93/96 (97%)	86 (92%)	5 (5%)	2 (2%)	6	22
20	R	145/152 (95%)	122 (84%)	18 (12%)	5 (3%)	3	13
21	S	79/85 (93%)	69 (87%)	9 (11%)	1 (1%)	12	36
22	T	117/120 (98%)	92 (79%)	19 (16%)	6 (5%)	2	6
23	U	51/66 (77%)	43 (84%)	7 (14%)	1 (2%)	7	24
24	V	63/71 (89%)	50 (79%)	9 (14%)	4 (6%)	1	3
25	W	152/154 (99%)	136 (90%)	14 (9%)	2 (1%)	12	36
26	X	80/92 (87%)	69 (86%)	8 (10%)	3 (4%)	3	10
27	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
28	Z	71/83 (86%)	56 (79%)	10 (14%)	5 (7%)	1	3
29	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
30	2	47/50 (94%)	44 (94%)	1 (2%)	2 (4%)	2	8
31	3	90/92 (98%)	84 (93%)	6 (7%)	0	100	100
All	All	3707/4434 (84%)	3148 (85%)	424 (11%)	135 (4%)	3	11

5 of 135 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	34	ASP
4	B	34	GLY
4	B	139	ASP
4	B	206	THR
5	C	8	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	
3	A	179/182 (98%)	171 (96%)	8 (4%)	27	60
4	B	282/283 (100%)	258 (92%)	24 (8%)	10	31
5	C	193/193 (100%)	182 (94%)	11 (6%)	20	50
6	D	117/148 (79%)	109 (93%)	8 (7%)	16	42
7	E	152/156 (97%)	147 (97%)	5 (3%)	38	72
8	F	93/94 (99%)	90 (97%)	3 (3%)	39	73
9	G	27/283 (10%)	26 (96%)	1 (4%)	34	68
10	H	134/145 (92%)	125 (93%)	9 (7%)	16	43
11	I	58/130 (45%)	55 (95%)	3 (5%)	23	55
12	J	118/121 (98%)	111 (94%)	7 (6%)	19	49
13	K	106/106 (100%)	104 (98%)	2 (2%)	57	85
14	L	113/127 (89%)	108 (96%)	5 (4%)	28	61
15	M	158/159 (99%)	151 (96%)	7 (4%)	28	61
16	N	149/150 (99%)	143 (96%)	6 (4%)	31	65
17	O	93/94 (99%)	88 (95%)	5 (5%)	22	53
18	P	113/117 (97%)	107 (95%)	6 (5%)	22	54
19	Q	79/80 (99%)	77 (98%)	2 (2%)	47	80
20	R	114/120 (95%)	109 (96%)	5 (4%)	28	61
21	S	71/74 (96%)	66 (93%)	5 (7%)	15	40
22	T	105/106 (99%)	99 (94%)	6 (6%)	20	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	U	44/52 (85%)	41 (93%)	3 (7%)	16	42
24	V	51/57 (90%)	48 (94%)	3 (6%)	19	49
25	W	130/130 (100%)	125 (96%)	5 (4%)	33	67
26	X	66/74 (89%)	60 (91%)	6 (9%)	9	27
27	Y	120/196 (61%)	114 (95%)	6 (5%)	24	56
28	Z	60/68 (88%)	58 (97%)	2 (3%)	38	72
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	45/46 (98%)	42 (93%)	3 (7%)	16	43
31	3	79/79 (100%)	75 (95%)	4 (5%)	24	55
All	All	3095/3617 (86%)	2935 (95%)	160 (5%)	23	55

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	R	142	ASP
26	X	82	GLU
21	S	71	ASP
23	U	53	ASP
27	Y	201	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
20	R	98	ASN
25	W	87	HIS
20	R	117	HIS
22	T	64	ASN
25	W	141	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2744/2922 (93%)	247 (9%)	26 (0%)
2	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2865/3044 (94%)	264 (9%)	27 (0%)

5 of 264 RNA backbone outliers are listed below:

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

5 of 27 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1450	C
1	0	1979	G
1	0	2718	C
1	0	1942	A
1	0	2011	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	$\#\|Z\| > 2$
1	UR3	0	2619	1	19,22,23	0.35	0	26,32,35	0.64	1 (3%)
1	OMG	0	2588	1	18,26,27	1.07	2 (11%)	19,38,41	0.75	1 (5%)
1	OMU	0	2587	1	19,22,23	0.34	0	26,31,34	0.42	0
1	1MA	0	628	1	16,25,26	1.38	3 (18%)	18,37,40	1.13	2 (11%)
1	PSU	0	2621	1	18,21,22	1.52	2 (11%)	22,30,33	1.16	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
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	0	2588	1	-	1/5/27/28	0/3/3/3
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3
1	PSU	0	2621	1	-	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)
1	0	2621	PSU	C2-N1	5.13	1.43	1.36
1	0	628	1MA	C2-N3	3.66	1.33	1.29
1	0	2621	PSU	C6-C5	3.06	1.38	1.35
1	0	2588	OMG	C5-C6	-2.88	1.41	1.47
1	0	628	1MA	C6-N6	2.61	1.34	1.27

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	628	1MA	N1-C2-N3	2.86	129.36	126.02
1	0	2621	PSU	C6-C5-C4	2.79	120.15	118.20
1	0	2621	PSU	O2-C2-N1	2.71	125.78	122.79
1	0	2621	PSU	C6-N1-C2	-2.59	120.04	122.68
1	0	628	1MA	C5-C6-N1	2.50	117.62	113.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	2588	OMG	C3'-C2'-O2'-CM2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	0	2749/2922 (94%)	-0.26	14 (0%)	91	88	29, 55, 100, 157	0
2	9	122/122 (100%)	-0.22	3 (2%)	57	47	44, 68, 95, 159	0
3	A	237/240 (98%)	0.12	8 (3%)	45	35	34, 62, 95, 116	0
4	B	337/338 (99%)	-0.06	5 (1%)	73	68	32, 64, 90, 97	0
5	C	246/246 (100%)	-0.21	1 (0%)	92	91	29, 58, 81, 90	0
6	D	140/177 (79%)	1.27	39 (27%)	0	0	62, 107, 129, 138	0
7	E	172/178 (96%)	0.58	13 (7%)	13	7	52, 75, 97, 101	0
8	F	119/120 (99%)	0.64	13 (10%)	5	3	65, 84, 105, 117	0
9	G	29/348 (8%)	1.78	10 (34%)	0	0	76, 98, 106, 107	0
10	H	160/177 (90%)	-0.02	1 (0%)	89	86	40, 61, 96, 107	0
11	I	70/162 (43%)	2.71	43 (61%)	0	0	112, 126, 144, 147	0
12	J	142/145 (97%)	-0.21	1 (0%)	87	84	43, 58, 82, 95	0
13	K	132/132 (100%)	-0.05	0	100	100	40, 61, 84, 89	0
14	L	145/165 (87%)	0.28	11 (7%)	13	7	29, 75, 115, 126	0
15	M	194/195 (99%)	-0.24	0	100	100	40, 55, 69, 79	0
16	N	186/187 (99%)	0.25	10 (5%)	25	17	46, 71, 115, 125	0
17	O	115/116 (99%)	-0.05	0	100	100	47, 65, 81, 83	0
18	P	143/149 (95%)	0.20	1 (0%)	87	84	44, 66, 80, 86	0
19	Q	95/96 (98%)	-0.12	0	100	100	39, 51, 64, 79	0
20	R	147/152 (96%)	0.24	10 (6%)	17	10	41, 56, 114, 128	0
21	S	81/85 (95%)	0.21	3 (3%)	41	31	52, 72, 88, 95	0
22	T	119/120 (99%)	0.51	6 (5%)	28	19	51, 69, 94, 111	0
23	U	53/66 (80%)	0.13	3 (5%)	23	15	51, 64, 79, 85	0
24	V	65/71 (91%)	0.99	13 (20%)	1	0	63, 85, 118, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	W	154/154 (100%)	-0.20	0 100 100	41, 56, 76, 85	0
26	X	82/92 (89%)	0.38	8 (9%) 7 4	49, 66, 87, 101	0
27	Y	142/241 (58%)	0.04	5 (3%) 44 34	31, 53, 79, 95	0
28	Z	73/83 (87%)	-0.11	0 100 100	53, 69, 86, 102	0
29	1	56/57 (98%)	-0.42	0 100 100	35, 43, 49, 58	0
30	2	49/50 (98%)	0.20	3 (6%) 21 13	40, 66, 94, 104	0
31	3	92/92 (100%)	0.07	1 (1%) 80 75	42, 63, 76, 91	0
All	All	6646/7478 (88%)	-0.00	225 (3%) 45 35	29, 61, 106, 159	0

The worst 5 of 225 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	V	1	THR	9.6
20	R	131	GLY	7.2
22	T	119	ALA	6.8
6	D	69	ILE	6.4
20	R	134	SER	6.1

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
1	OMU	0	2587	21/22	0.98	0.14	39,42,43,46	0
1	OMG	0	2588	24/25	0.98	0.14	40,42,44,44	0
1	UR3	0	2619	21/22	0.98	0.14	40,42,43,46	0
1	PSU	0	2621	20/21	0.98	0.14	40,41,43,44	0
1	1MA	0	628	23/24	0.99	0.16	32,37,39,39	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	NA	0	8568	1/1	0.49	0.46	84,84,84,84	0
34	NA	0	8513	1/1	0.60	0.18	72,72,72,72	0
34	NA	R	8586	1/1	0.61	0.50	81,81,81,81	0
34	NA	0	8526	1/1	0.64	0.83	78,78,78,78	0
32	MG	0	8031	1/1	0.70	0.19	34,34,34,34	0
35	CL	0	8815	1/1	0.70	0.76	112,112,112,112	0
34	NA	0	8556	1/1	0.71	0.69	58,58,58,58	0
34	NA	0	8552	1/1	0.73	0.65	62,62,62,62	0
34	NA	0	8571	1/1	0.75	0.28	61,61,61,61	0
32	MG	0	8104	1/1	0.78	0.29	61,61,61,61	0
34	NA	0	8563	1/1	0.79	0.46	51,51,51,51	0
32	MG	0	8050	1/1	0.80	0.11	97,97,97,97	0
34	NA	0	8507	1/1	0.82	0.46	61,61,61,61	0
32	MG	9	8095	1/1	0.82	0.09	54,54,54,54	0
34	NA	0	8564	1/1	0.83	0.17	40,40,40,40	0
32	MG	0	8038	1/1	0.84	0.21	38,38,38,38	0
34	NA	L	8580	1/1	0.85	0.72	72,72,72,72	0
34	NA	0	8572	1/1	0.85	0.31	69,69,69,69	0
34	NA	9	8551	1/1	0.85	0.19	46,46,46,46	0
34	NA	0	8567	1/1	0.86	0.17	70,70,70,70	0
34	NA	0	8530	1/1	0.86	0.30	72,72,72,72	0
34	NA	0	8582	1/1	0.86	0.25	78,78,78,78	0
34	NA	0	8585	1/1	0.86	0.53	60,60,60,60	0
34	NA	0	8541	1/1	0.87	0.24	53,53,53,53	0
34	NA	0	8524	1/1	0.87	0.26	68,68,68,68	0
32	MG	0	8041	1/1	0.87	0.22	59,59,59,59	0
34	NA	R	8537	1/1	0.87	0.14	51,51,51,51	0
32	MG	0	8097	1/1	0.87	0.19	51,51,51,51	0
34	NA	0	8538	1/1	0.87	0.09	61,61,61,61	0
35	CL	0	8816	1/1	0.87	0.47	79,79,79,79	0
34	NA	0	8522	1/1	0.88	0.19	68,68,68,68	0
34	NA	0	8532	1/1	0.88	0.36	47,47,47,47	0
32	MG	0	8043	1/1	0.88	0.12	62,62,62,62	0
32	MG	0	8099	1/1	0.88	0.14	62,62,62,62	0
34	NA	0	8528	1/1	0.88	0.74	61,61,61,61	0
35	CL	N	8807	1/1	0.88	0.33	74,74,74,74	0
34	NA	0	8506	1/1	0.89	0.71	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8107	1/1	0.89	0.19	65,65,65,65	0
35	CL	0	8805	1/1	0.89	0.23	77,77,77,77	0
34	NA	9	8583	1/1	0.89	0.64	71,71,71,71	0
34	NA	C	8504	1/1	0.89	0.34	48,48,48,48	0
35	CL	0	8817	1/1	0.89	0.17	74,74,74,74	0
34	NA	0	8508	1/1	0.89	0.23	73,73,73,73	0
35	CL	R	8806	1/1	0.89	0.18	63,63,63,63	0
32	MG	0	8114	1/1	0.90	0.16	47,47,47,47	0
32	MG	0	8049	1/1	0.90	0.31	70,70,70,70	0
32	MG	0	8040	1/1	0.90	0.12	57,57,57,57	0
34	NA	0	8566	1/1	0.91	0.33	68,68,68,68	0
32	MG	0	8082	1/1	0.91	0.10	76,76,76,76	0
32	MG	0	8115	1/1	0.91	0.14	70,70,70,70	0
34	NA	0	8569	1/1	0.91	0.59	66,66,66,66	0
32	MG	0	8085	1/1	0.91	0.13	62,62,62,62	0
35	CL	B	8819	1/1	0.91	0.40	74,74,74,74	0
32	MG	T	8073	1/1	0.91	0.21	68,68,68,68	0
34	NA	0	8581	1/1	0.91	0.14	52,52,52,52	0
34	NA	0	8579	1/1	0.92	0.27	62,62,62,62	0
32	MG	0	8103	1/1	0.92	0.16	67,67,67,67	0
35	CL	0	8822	1/1	0.92	0.20	79,79,79,79	0
34	NA	S	8512	1/1	0.92	0.14	48,48,48,48	0
32	MG	2	8076	1/1	0.92	0.17	69,69,69,69	0
32	MG	0	8092	1/1	0.92	0.24	80,80,80,80	0
35	CL	Y	8820	1/1	0.92	0.14	55,55,55,55	0
35	CL	3	8804	1/1	0.92	0.29	74,74,74,74	0
34	NA	0	8540	1/1	0.93	0.24	40,40,40,40	0
34	NA	0	8529	1/1	0.93	0.15	79,79,79,79	0
34	NA	0	8550	1/1	0.93	0.26	56,56,56,56	0
34	NA	0	8511	1/1	0.93	0.13	43,43,43,43	0
32	MG	0	8062	1/1	0.93	0.13	65,65,65,65	0
34	NA	0	8570	1/1	0.93	0.16	66,66,66,66	0
35	CL	J	8802	1/1	0.93	0.12	75,75,75,75	0
34	NA	0	8559	1/1	0.93	0.41	66,66,66,66	0
34	NA	0	8560	1/1	0.93	0.65	61,61,61,61	0
34	NA	0	8574	1/1	0.93	0.79	63,63,63,63	0
34	NA	0	8510	1/1	0.93	0.24	40,40,40,40	0
36	CD	3	8704	1/1	0.93	0.08	72,72,72,72	0
32	MG	0	8112	1/1	0.94	0.18	64,64,64,64	0
35	CL	0	8814	1/1	0.94	0.17	71,71,71,71	0
34	NA	0	8584	1/1	0.94	0.17	70,70,70,70	0
34	NA	0	8561	1/1	0.94	0.34	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	NA	0	8533	1/1	0.94	0.14	49,49,49,49	0
34	NA	0	8535	1/1	0.94	0.20	73,73,73,73	0
35	CL	A	8809	1/1	0.94	0.23	82,82,82,82	0
34	NA	0	8573	1/1	0.94	0.64	73,73,73,73	0
32	MG	0	8070	1/1	0.94	0.12	54,54,54,54	0
35	CL	L	8810	1/1	0.94	0.13	73,73,73,73	0
34	NA	M	8547	1/1	0.94	0.22	45,45,45,45	0
34	NA	0	8578	1/1	0.94	0.58	77,77,77,77	0
34	NA	0	8557	1/1	0.94	0.11	65,65,65,65	0
32	MG	0	8111	1/1	0.94	0.07	48,48,48,48	0
35	CL	0	8803	1/1	0.94	0.20	80,80,80,80	0
32	MG	0	8024	1/1	0.95	0.14	45,45,45,45	0
32	MG	0	8042	1/1	0.95	0.11	55,55,55,55	0
32	MG	0	8089	1/1	0.95	0.08	69,69,69,69	0
34	NA	0	8514	1/1	0.95	0.09	39,39,39,39	0
34	NA	0	8515	1/1	0.95	0.26	65,65,65,65	0
34	NA	0	8521	1/1	0.95	0.38	73,73,73,73	0
34	NA	0	8549	1/1	0.95	0.16	54,54,54,54	0
32	MG	K	8069	1/1	0.95	0.09	62,62,62,62	0
35	CL	J	8801	1/1	0.95	0.10	67,67,67,67	0
32	MG	0	8015	1/1	0.95	0.06	41,41,41,41	0
32	MG	0	8109	1/1	0.95	0.05	33,33,33,33	0
34	NA	Q	8548	1/1	0.95	0.17	49,49,49,49	0
35	CL	O	8808	1/1	0.95	0.40	99,99,99,99	0
32	MG	0	8093	1/1	0.95	0.20	50,50,50,50	0
32	MG	0	8044	1/1	0.95	0.16	51,51,51,51	0
34	NA	0	8576	1/1	0.95	0.18	51,51,51,51	0
32	MG	0	8113	1/1	0.95	0.12	49,49,49,49	0
32	MG	0	8088	1/1	0.96	0.10	34,34,34,34	0
34	NA	A	8545	1/1	0.96	0.10	46,46,46,46	0
34	NA	0	8516	1/1	0.96	0.23	61,61,61,61	0
34	NA	0	8517	1/1	0.96	0.10	52,52,52,52	0
32	MG	0	8014	1/1	0.96	0.10	20,20,20,20	0
34	NA	0	8562	1/1	0.96	0.31	81,81,81,81	0
32	MG	0	8091	1/1	0.96	0.13	53,53,53,53	0
34	NA	0	8523	1/1	0.96	0.10	37,37,37,37	0
32	MG	0	8051	1/1	0.96	0.15	67,67,67,67	0
34	NA	T	8543	1/1	0.96	0.14	43,43,43,43	0
32	MG	0	8052	1/1	0.96	0.06	44,44,44,44	0
32	MG	0	8059	1/1	0.96	0.10	44,44,44,44	0
32	MG	Y	8108	1/1	0.96	0.15	48,48,48,48	0
32	MG	0	8003	1/1	0.96	0.10	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	K	0	8401	1/1	0.96	0.41	91,91,91,91	0
33	K	0	8402	1/1	0.96	0.13	69,69,69,69	0
34	NA	0	8505	1/1	0.96	0.17	49,49,49,49	0
34	NA	0	8536	1/1	0.96	0.09	52,52,52,52	0
34	NA	0	8575	1/1	0.96	0.25	58,58,58,58	0
32	MG	0	8100	1/1	0.96	0.13	66,66,66,66	0
34	NA	0	8577	1/1	0.96	0.20	72,72,72,72	0
32	MG	0	8063	1/1	0.96	0.23	73,73,73,73	0
32	MG	0	8068	1/1	0.96	0.05	70,70,70,70	0
32	MG	0	8004	1/1	0.96	0.07	43,43,43,43	0
35	CL	Q	8811	1/1	0.96	0.16	72,72,72,72	0
32	MG	0	8048	1/1	0.96	0.09	62,62,62,62	0
32	MG	0	8027	1/1	0.96	0.09	63,63,63,63	0
34	NA	0	8554	1/1	0.96	0.15	38,38,38,38	0
32	MG	0	8087	1/1	0.96	0.10	81,81,81,81	0
32	MG	0	8094	1/1	0.97	0.04	67,67,67,67	0
32	MG	0	8096	1/1	0.97	0.11	53,53,53,53	0
32	MG	0	8116	1/1	0.97	0.08	39,39,39,39	0
32	MG	0	8074	1/1	0.97	0.06	40,40,40,40	0
32	MG	0	8081	1/1	0.97	0.14	74,74,74,74	0
34	NA	0	8558	1/1	0.97	0.70	107,107,107,107	0
34	NA	0	8518	1/1	0.97	0.18	32,32,32,32	0
34	NA	0	8519	1/1	0.97	0.07	34,34,34,34	0
32	MG	0	8007	1/1	0.97	0.09	29,29,29,29	0
32	MG	0	8101	1/1	0.97	0.09	70,70,70,70	0
32	MG	0	8102	1/1	0.97	0.19	71,71,71,71	0
32	MG	3	8078	1/1	0.97	0.07	43,43,43,43	0
34	NA	0	8525	1/1	0.97	0.10	50,50,50,50	0
35	CL	0	8812	1/1	0.97	0.14	65,65,65,65	0
35	CL	0	8813	1/1	0.97	0.10	67,67,67,67	0
32	MG	0	8053	1/1	0.97	0.15	47,47,47,47	0
34	NA	0	8527	1/1	0.97	0.12	69,69,69,69	0
32	MG	0	8046	1/1	0.97	0.06	55,55,55,55	0
34	NA	0	8501	1/1	0.97	0.11	29,29,29,29	0
34	NA	0	8502	1/1	0.97	0.23	49,49,49,49	0
34	NA	0	8503	1/1	0.97	0.20	70,70,70,70	0
32	MG	0	8105	1/1	0.97	0.08	63,63,63,63	0
34	NA	0	8534	1/1	0.97	0.11	55,55,55,55	0
32	MG	0	8025	1/1	0.97	0.12	58,58,58,58	0
35	CL	J	8821	1/1	0.97	0.10	54,54,54,54	0
32	MG	0	8008	1/1	0.97	0.08	35,35,35,35	0
32	MG	0	8064	1/1	0.97	0.19	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	NA	0	8539	1/1	0.97	0.10	26,26,26,26	0
34	NA	0	8509	1/1	0.97	0.12	37,37,37,37	0
32	MG	0	8016	1/1	0.97	0.13	48,48,48,48	0
34	NA	0	8542	1/1	0.97	0.20	51,51,51,51	0
34	NA	0	8544	1/1	0.97	0.07	33,33,33,33	0
32	MG	0	8033	1/1	0.97	0.13	37,37,37,37	0
32	MG	0	8011	1/1	0.98	0.11	32,32,32,32	0
32	MG	0	8057	1/1	0.98	0.20	67,67,67,67	0
32	MG	0	8013	1/1	0.98	0.16	54,54,54,54	0
32	MG	0	8028	1/1	0.98	0.06	48,48,48,48	0
32	MG	A	8066	1/1	0.98	0.06	88,88,88,88	0
32	MG	0	8029	1/1	0.98	0.12	55,55,55,55	0
32	MG	0	8018	1/1	0.98	0.11	50,50,50,50	0
32	MG	0	8045	1/1	0.98	0.10	59,59,59,59	0
34	NA	0	8520	1/1	0.98	0.06	33,33,33,33	0
32	MG	0	8032	1/1	0.98	0.07	32,32,32,32	0
32	MG	0	8047	1/1	0.98	0.09	59,59,59,59	0
32	MG	0	8075	1/1	0.98	0.09	54,54,54,54	0
32	MG	0	8077	1/1	0.98	0.07	32,32,32,32	0
32	MG	0	8022	1/1	0.98	0.06	42,42,42,42	0
32	MG	0	8035	1/1	0.98	0.03	58,58,58,58	0
32	MG	0	8083	1/1	0.98	0.04	52,52,52,52	0
32	MG	0	8084	1/1	0.98	0.07	54,54,54,54	0
32	MG	0	8036	1/1	0.98	0.08	44,44,44,44	0
35	CL	M	8818	1/1	0.98	0.19	60,60,60,60	0
32	MG	0	8110	1/1	0.98	0.04	59,59,59,59	0
34	NA	0	8531	1/1	0.98	0.17	55,55,55,55	0
34	NA	J	8546	1/1	0.98	0.11	48,48,48,48	0
32	MG	0	8086	1/1	0.98	0.07	46,46,46,46	0
34	NA	0	8565	1/1	0.98	0.29	49,49,49,49	0
32	MG	0	8037	1/1	0.98	0.08	51,51,51,51	0
36	CD	O	8705	1/1	0.98	0.08	98,98,98,98	0
32	MG	0	8010	1/1	0.98	0.10	45,45,45,45	0
32	MG	0	8012	1/1	0.99	0.10	33,33,33,33	0
32	MG	0	8023	1/1	0.99	0.07	42,42,42,42	0
32	MG	0	8079	1/1	0.99	0.11	43,43,43,43	0
32	MG	0	8080	1/1	0.99	0.09	47,47,47,47	0
32	MG	0	8001	1/1	0.99	0.09	33,33,33,33	0
32	MG	0	8106	1/1	0.99	0.09	38,38,38,38	0
32	MG	0	8002	1/1	0.99	0.06	35,35,35,35	0
32	MG	0	8026	1/1	0.99	0.09	28,28,28,28	0
32	MG	0	8054	1/1	0.99	0.10	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8056	1/1	0.99	0.11	49,49,49,49	0
32	MG	0	8009	1/1	0.99	0.04	36,36,36,36	0
32	MG	0	8005	1/1	0.99	0.09	45,45,45,45	0
32	MG	0	8060	1/1	0.99	0.13	50,50,50,50	0
32	MG	0	8061	1/1	0.99	0.10	36,36,36,36	0
32	MG	0	8090	1/1	0.99	0.10	59,59,59,59	0
32	MG	0	8017	1/1	0.99	0.04	33,33,33,33	0
32	MG	A	8065	1/1	0.99	0.08	43,43,43,43	0
34	NA	0	8553	1/1	0.99	0.10	36,36,36,36	0
32	MG	0	8030	1/1	0.99	0.13	34,34,34,34	0
34	NA	0	8555	1/1	0.99	0.23	67,67,67,67	0
32	MG	B	8055	1/1	0.99	0.07	46,46,46,46	0
32	MG	0	8006	1/1	0.99	0.06	37,37,37,37	0
32	MG	0	8019	1/1	0.99	0.03	39,39,39,39	0
32	MG	0	8021	1/1	0.99	0.10	31,31,31,31	0
32	MG	0	8071	1/1	0.99	0.08	80,80,80,80	0
32	MG	0	8098	1/1	0.99	0.11	30,30,30,30	0
32	MG	0	8072	1/1	0.99	0.11	61,61,61,61	0
36	CD	U	8701	1/1	0.99	0.10	76,76,76,76	0
36	CD	Z	8703	1/1	0.99	0.11	71,71,71,71	0
32	MG	0	8034	1/1	0.99	0.10	36,36,36,36	0
32	MG	0	8058	1/1	1.00	0.09	46,46,46,46	0
32	MG	0	8067	1/1	1.00	0.07	54,54,54,54	0
32	MG	0	8039	1/1	1.00	0.07	44,44,44,44	0
36	CD	1	8702	1/1	1.00	0.07	68,68,68,68	0
32	MG	0	8020	1/1	1.00	0.06	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.