wwPDB X-ray Structure Validation Summary Report (i)

Aug 7, 2023 – 01:37 PM EDT

PDB ID	:	1Q82
Title	:	Crystal Structure of CC-Puromycin bound to the A-site of the 50S ribosomal subunit
Authors	:	Hansen, J.L.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on	:	2003-08-20
Resolution	:	2.98 Å(reported)

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

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

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

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

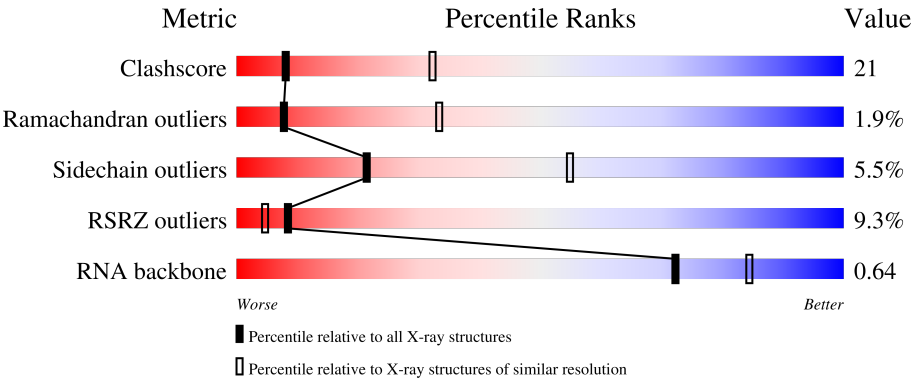
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.98 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)
RNA backbone	3102	1088 (3.26-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	2922	3% 50% 36% 7% • 6%
2	B	122	5% 51% 35% 10% •
3	5	2	50% 50% 50%
4	C	239	11% 54% 40% 5% •
5	D	337	2% 48% 46% 6%

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Mol	Chain	Length	Quality of chain
6	E	246	2% 54% 40% 5%
7	F	176	38% 25% 45% 8% 20%
8	G	177	10% 50% 46%
9	H	119	20% 53% 45%
10	I	348	5% 5% 92%
11	J	167	10% 34% 51% 7% 7%
12	K	145	% 59% 32% 6%
13	L	132	2% 57% 42%
14	M	164	24% 48% 38% 12%
15	N	194	11% 41% 53% 6%
16	O	186	19% 40% 54% 6%
17	P	115	% 70% 29%
18	Q	148	5% 62% 34%
19	R	95	3% 63% 34%
20	S	154	66% 28%
21	T	84	5% 69% 26%
22	U	119	9% 61% 36%
23	V	66	44% 39% 38% 20%
24	W	70	30% 51% 37% 7%
25	X	154	49% 45% 6%
26	Y	91	11% 43% 42% 5% 10%
27	Z	240	2% 38% 18% 41%
28	1	73	73% 27% 67% 5%
29	2	56	52% 48%
30	3	48	15% 60% 33%

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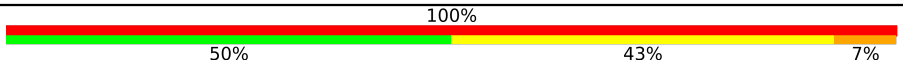
Mol	Chain	Length	Quality of chain
31	4	92	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	1	8105	-	-	-	X
32	MG	A	8011	-	-	X	-
32	MG	A	8024	-	-	-	X
32	MG	A	8049	-	-	-	X
32	MG	A	8092	-	-	-	X
32	MG	A	8102	-	-	-	X
32	MG	A	8114	-	-	-	X
34	NA	A	8307	-	-	-	X
34	NA	A	8310	-	-	-	X
34	NA	A	8326	-	-	-	X
34	NA	A	8328	-	-	-	X
34	NA	A	8332	-	-	-	X
34	NA	A	8340	-	-	-	X
34	NA	A	8363	-	-	-	X
34	NA	A	8365	-	-	-	X
34	NA	A	8371	-	-	-	X
34	NA	A	8372	-	-	-	X
34	NA	A	8382	-	-	-	X
34	NA	A	8384	-	-	-	X
34	NA	B	8383	-	-	-	X
34	NA	S	8386	-	-	-	X
34	NA	T	8312	-	-	-	X
35	CL	A	8522	-	-	-	X
35	CL	M	8510	-	-	-	X
35	CL	N	8518	-	-	X	-
37	CD	4	8404	-	-	-	X

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 98593 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	A	2754	59017	26346	10878	19048	2745	0	0	0

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

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

- Molecule 3 is a RNA chain called CC-puromycin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	5	2	40	18	6	14	2	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	C	237	1754	1072	352	325	5	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	D	337	2624	1616	493	510	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	deletion	UNP P20279
D	310	ARG	PHE	conflict	UNP P20279

- Molecule 6 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 7 is a protein called 50S ribosomal protein L5P.

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

- Molecule 8 is a protein called 50S ribosomal protein L6P.

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

- Molecule 9 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 10 is a protein called Acidic ribosomal protein P0 homolog.

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

- Molecule 11 is a protein called L10 Ribosomal Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	145	Total	C	N	O	0	0	0
			1114	668	222	224			

- Molecule 15 is a protein called L15 Ribosomal Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	P	115	Total	C	N	O	0	0	0
			864	529	161	174			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	Q	143	Total	C	N	O	0	0	0
			1133	680	230	223			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	71	LYS	TYR	conflict	UNP P14119

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	R	95	Total	C	N	O	0	0	0
			734	450	141	143			

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	119	Total	C	N	O	0	0	0
			949	568	180	201			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	X	154	Total	C	N	O	S	0	0	0
			1195	737	209	243	6			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	ARG	deletion	UNP P22452

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	109	Total Mg 109 109	0	0
32	B	1	Total Mg 1 1	0	0
32	C	1	Total Mg 1 1	0	0
32	D	1	Total Mg 1 1	0	0
32	L	1	Total Mg 1 1	0	0
32	U	1	Total Mg 1 1	0	0
32	Z	1	Total Mg 1 1	0	0
32	1	1	Total Mg 1 1	0	0
32	4	1	Total Mg 1 1	0	0

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	71	Total Na 71 71	0	0
34	B	2	Total Na 2 2	0	0
34	C	1	Total Na 1 1	0	0
34	E	1	Total Na 1 1	0	0
34	J	2	Total Na 2 2	0	0
34	K	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0
34	N	1	Total Na 1 1	0	0

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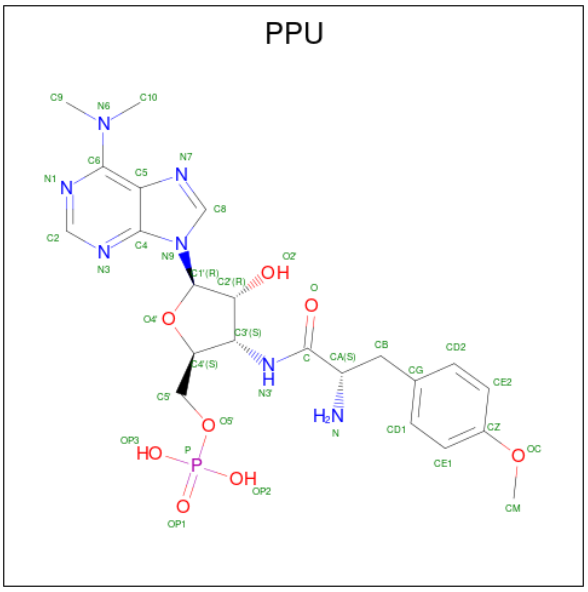
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	R	1	Total Na 1 1	0	0
34	S	2	Total Na 2 2	0	0
34	T	1	Total Na 1 1	0	0
34	U	1	Total Na 1 1	0	0
34	4	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	7	Total Cl 7 7	0	0
35	C	1	Total Cl 1 1	0	0
35	D	1	Total Cl 1 1	0	0
35	K	4	Total Cl 4 4	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	P	1	Total Cl 1 1	0	0
35	R	1	Total Cl 1 1	0	0
35	S	1	Total Cl 1 1	0	0
35	Z	2	Total Cl 2 2	0	0
35	4	1	Total Cl 1 1	0	0

- Molecule 36 is PUROMYCIN-5'-MONOPHOSPHATE (three-letter code: PPU) (formula: $C_{22}H_{30}N_7O_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	5	1	Total C N O P 37 22 7 7 1	0	0

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	P	1	Total Cd 1 1	0	0
37	V	1	Total Cd 1 1	0	0
37	1	1	Total Cd 1 1	0	0
37	2	1	Total Cd 1 1	0	0
37	4	1	Total Cd 1 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	5860	Total O 5860 5860	0	0
38	B	146	Total O 146 146	0	0
38	5	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	C	140	Total O 140 140	0	0
38	D	146	Total O 146 146	0	0
38	E	176	Total O 176 176	0	0
38	F	52	Total O 52 52	0	0
38	G	45	Total O 45 45	0	0
38	H	32	Total O 32 32	0	0
38	I	22	Total O 22 22	0	0
38	J	78	Total O 78 78	0	0
38	K	54	Total O 54 54	0	0
38	L	64	Total O 64 64	0	0
38	M	86	Total O 86 86	0	0
38	N	138	Total O 138 138	0	0
38	O	64	Total O 64 64	0	0
38	P	44	Total O 44 44	0	0
38	Q	70	Total O 70 70	0	0
38	R	57	Total O 57 57	0	0
38	S	83	Total O 83 83	0	0
38	T	36	Total O 36 36	0	0
38	U	38	Total O 38 38	0	0
38	V	22	Total O 22 22	0	0
38	W	16	Total O 16 16	0	0

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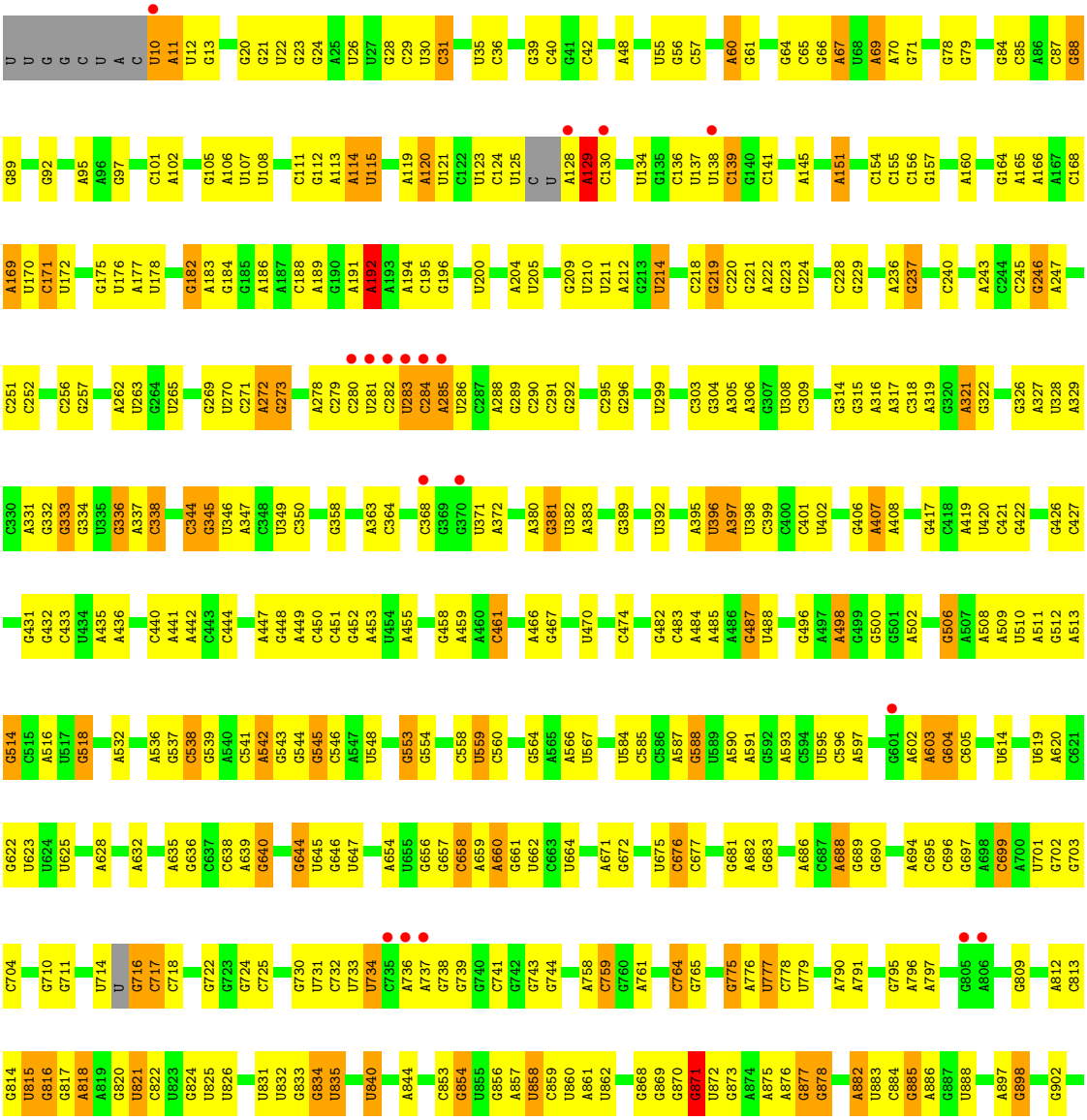
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	X	67	Total O 67 67	0	0
38	Y	28	Total O 28 28	0	0
38	Z	100	Total O 100 100	0	0
38	1	36	Total O 36 36	0	0
38	2	58	Total O 58 58	0	0
38	3	37	Total O 37 37	0	0
38	4	70	Total O 70 70	0	0

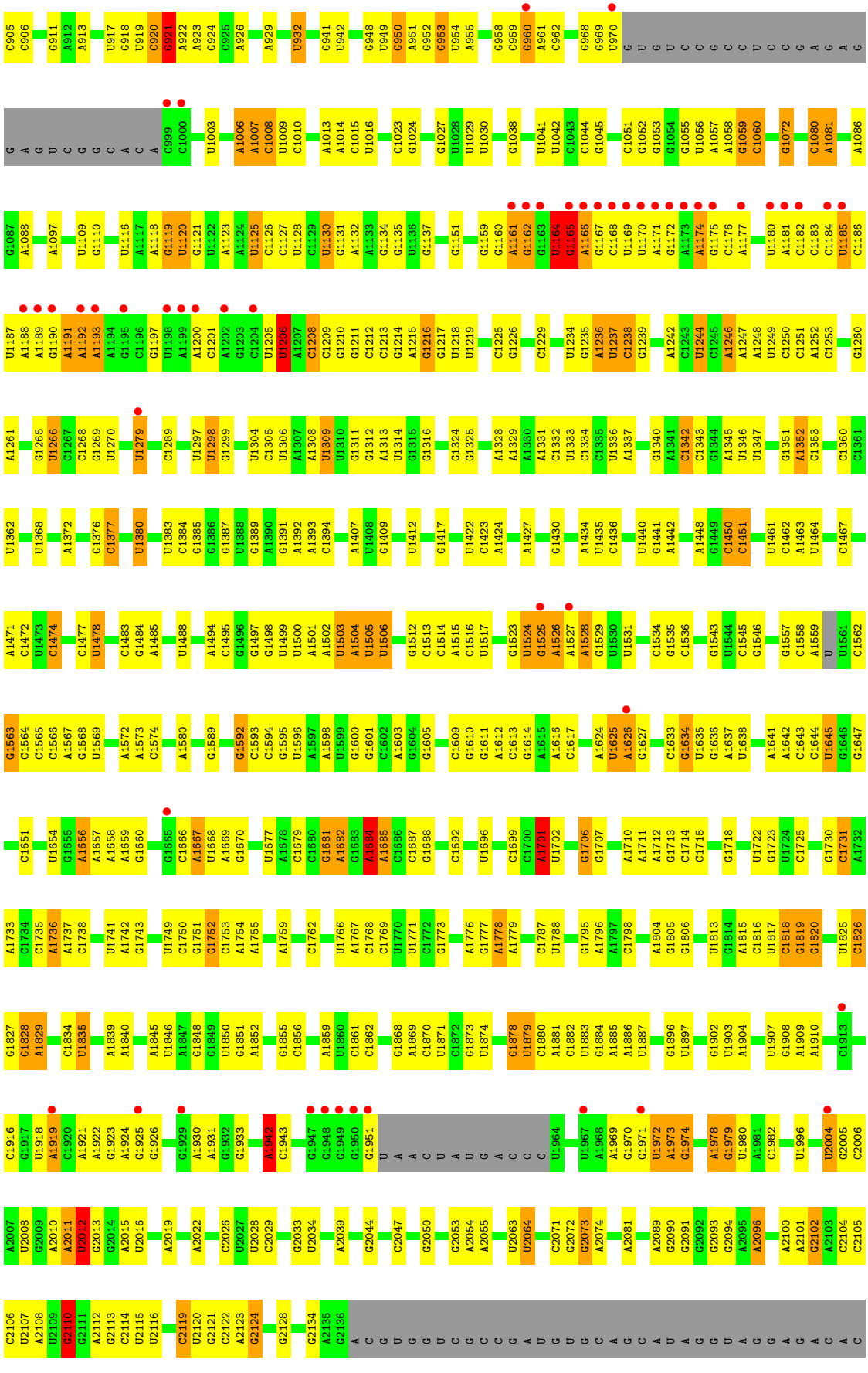
3 Residue-property plots (i)

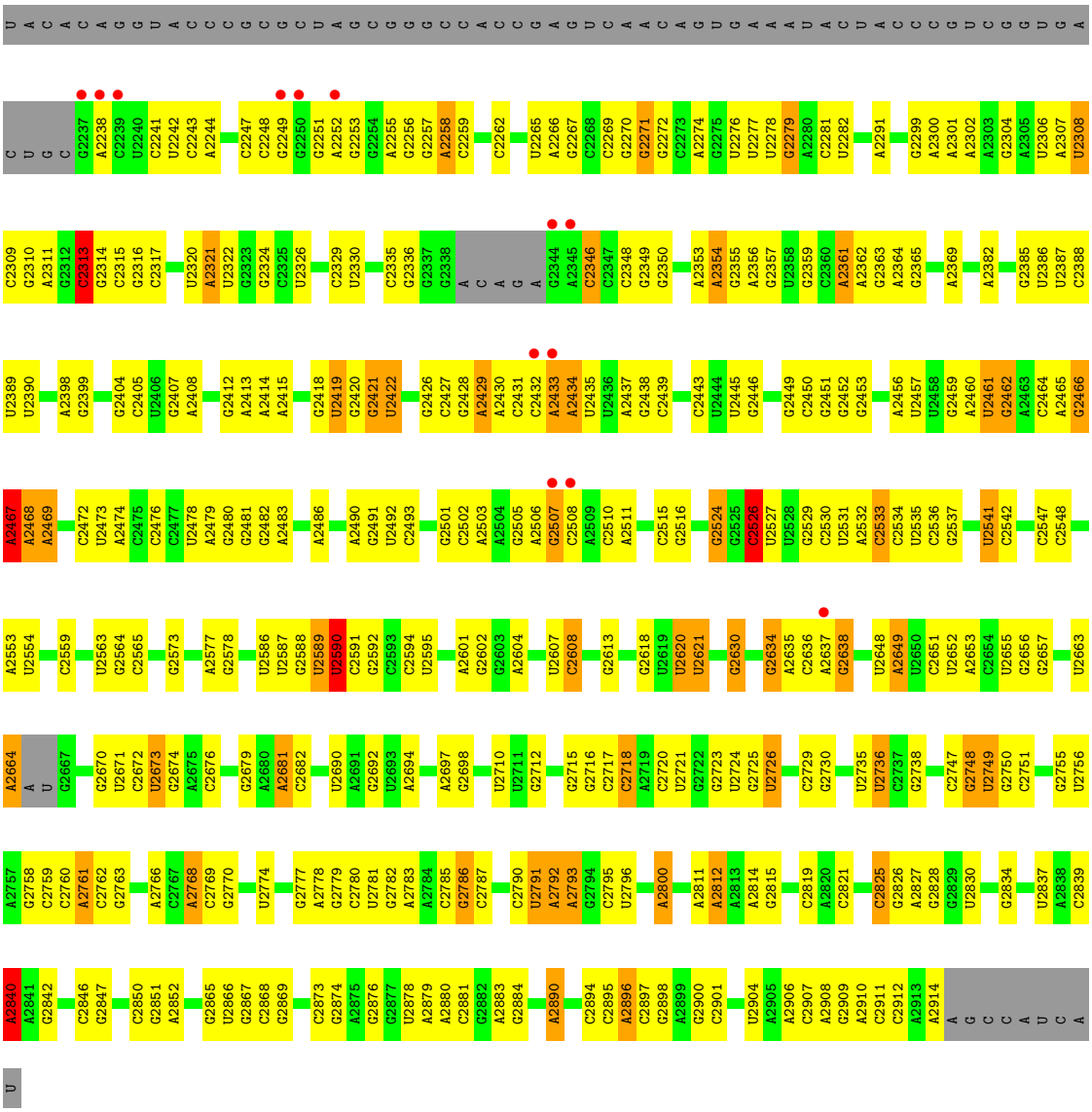
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

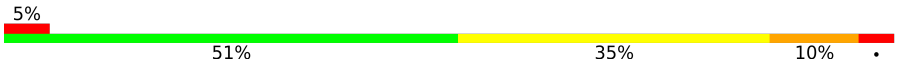


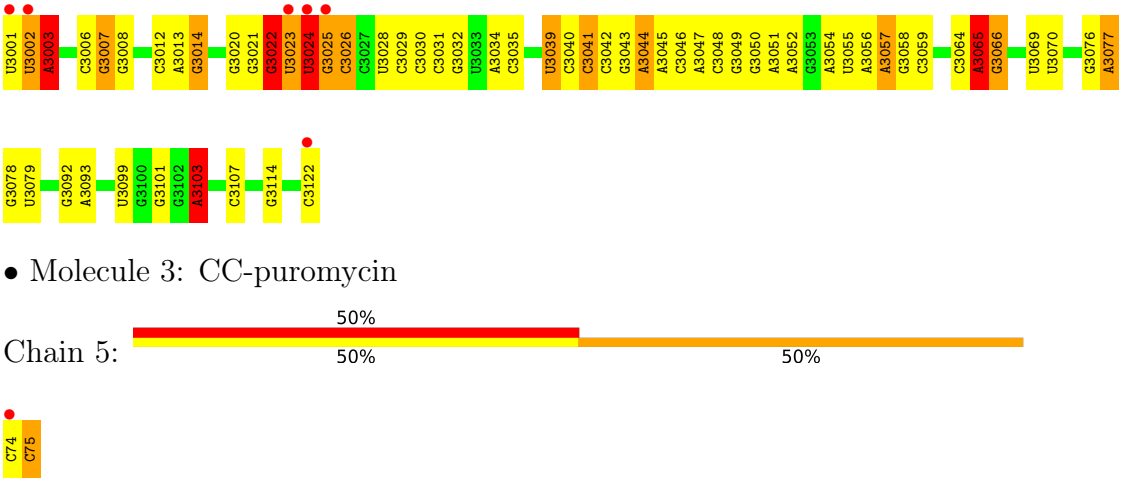

C905 C906 G911 A912 A913 U917 G918 U919 C920 G921 A922 A923 G924 C925 A926 A929 U932 G941 U942 G948 U949 G950 A951 G952 G953 U954 A955 G958 C959 G960 A961 C962 G968 G969 U970
G C A G U C G G C A C A C999 C1000 U1003 A1006 A1007 C1008 U1009 C1010 A1013 A1014 C1015 U1016 C1023 G1024 G1027 U1028 U1029 U1030 G1038 U1041 U1042 C1043 C1044 G1045 C1051 G1052 G1053 G1054 G1055 U1056 A1057 A1058 G1059 C1060 G1072 C1080 A1081 A1086
G1087 A1088 A1097 U1109 G1110 U1116 A1117 A1118 G1119 U1120 G1121 U1122 A1123 A1124 U1125 C1126 C1127 U1128 C1129 U1130 G1131 A1132 A1133 G1134 G1135 U1136 G1137 G1151 G1159 G1160 A1161 G1162 G1163 U1164 G1165 A1166 G1167 C1168 U1169 U1170 A1171 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 G1203 C1204 U1205 U1206 A1207 C1208 C1209 G1210 G1211 C1212 C1213 G1214 A1215 G1216 G1217 U1218 U1219 C1225 G1226 C1229 U1234 G1235 A1236 U1237 C1238 G1239 A1242 C1243 U1244 C1245 A1246 A1247 A1248 U1249 C1250 C1251 A1252 C1253 G1260
A1261 G1265 U1266 C1267 C1268 G1269 U1270 U1279 C1289 U1297 U1298 G1299 U1304 C1305 U1306 A1307 A1308 U1309 U1310 G1311 G1312 A1313 U1314 G1315 G1316 G1324 G1325 A1328 A1329 A1330 A1331 C1332 U1333 C1334 C1335 U1336 A1337 G1340 A1341 C1342 C1343 G1344 A1345 U1346 U1347 G1351 A1362 C1353 C1360 C1361
U1362 U1368 A1372 G1376 C1377 U1380 U1383 C1384 G1385 C1386 G1387 U1388 G1389 A1390 G1391 A1392 A1393 C1394 A1407 U1408 G1409 U1412 G1417 U1422 C1423 A1424 A1427 G1430 A1434 U1435 C1436 U1440 G1441 A1442 A1448 G1449 C1450 C1451 U1461 C1462 A1463 U1464 C1467
A1471 C1472 U1473 C1474 C1477 U1478 C1483 G1484 A1485 U1488 A1494 C1495 G1496 G1497 G1498 U1499 U1500 A1501 A1502 U1503 A1504 U1505 U1506 G1512 C1513 C1514 A1515 C1516 U1517 G1523 U1524 G1525 A1526 A1527 A1528 G1529 U1530 U1531 C1534 G1535 C1536 G1543 U1544 C1545 G1546 G1557 C1558 A1559 U U1561 C1562
G1563 C1564 C1565 C1566 A1567 G1568 U1569 A1572 A1573 C1574 A1580 G1589 G1592 C1593 C1594 G1595 U1596 A1597 A1598 U1599 G1600 G1601 C1602 A1603 G1604 G1605 C1609 G1610 G1611 A1612 C1613 G1614 A1615 A1616 C1617 A1624 U1625 A1626 G1627 C1633 G1634 U1635 G1636 A1637 U1638 A1641 A1642 C1643 C1644 U1645 G1646 G1647
C1651 U1654 G1655 A1656 A1657 A1658 A1659 G1660 G1665 C1666 A1667 U1668 A1669 G1670 U1677 A1678 C1679 C1680 G1681 A1682 G1683 A1684 A1685 C1686 C1687 G1688 C1692 U1696 C1699 C1700 A1701 U1702 G1706 G1707 A1710 A1711 A1712 G1713 C1714 C1715 G1718 U1722 G1723 U1724 C1725 G1730 C1731 A1732
A1733 C1734 C1735 A1736 A1737 C1738 U1741 A1742 G1743 U1749 C1750 G1751 G1752 C1753 A1754 A1755 A1759 C1762 U1766 A1767 C1768 C1769 U1770 U1771 C1772 G1773 A1776 G1777 A1778 A1779 C1787 U1788 G1795 A1796 A1797 C1798 A1804 G1805 G1806 U1813 G1814 A1815 C1816 U1817 C1818 G1819 G1820 U1825 C1826
G1827 G1828 A1829 C1834 U1835 A1839 A1840 A1845 U1846 A1847 G1848 G1849 U1850 G1851 A1852 G1855 C1856 A1859 U1860 C1861 C1862 G1868 A1869 C1870 U1871 C1872 G1873 U1874 G1878 U1879 C1880 A1881 C1882 U1883 G1884 A1885 A1886 U1887 G1896 U1897 G1902 U1903 A1904 U1907 G1908 A1909 A1910 C1913
C1916 G1917 U1918 A1919 C1920 A1921 A1922 G1923 A1924 G1925 G1926 G1929 A1930 A1931 G1932 G1933 A1942 C1943 G1947 G1948 G1949 G1950 G1951 U A A A C U A U G A C C C U1964 U1967 A1968 A1969 G1970 G1971 U1972 A1973 G1974 A1978 G1979 U1980 A1981 C1982 U1996 U2004 G2005 C2006
A2007 U2008 G2009 A2010 A2011 U2012 G2013 G2014 A2015 U2016 A2019 A2022 C2026 U2027 U2028 C2029 G2033 U2034 A2039 G2044 C2047 G2050 G2053 A2054 A2055 U2063 U2064 C2071 G2072 G2073 A2074 A2081 A2089 G2090 G2091 G2092 G2093 G2094 A2095 A2096 A2100 A2101 G2102 A2103 C2104 C2105
C2106 U2107 A2108 U2109 C2110 G2111 A2112 G2113 C2114 U2115 U2116 C2119 U2120 C2121 C2122 A2123 G2124 G2128 G2134 A2135 G2136 A C G U G U C G C A G C C C G A U G U G C A G C A A C



• Molecule 2: 5S ribosomal RNA

Chain B:



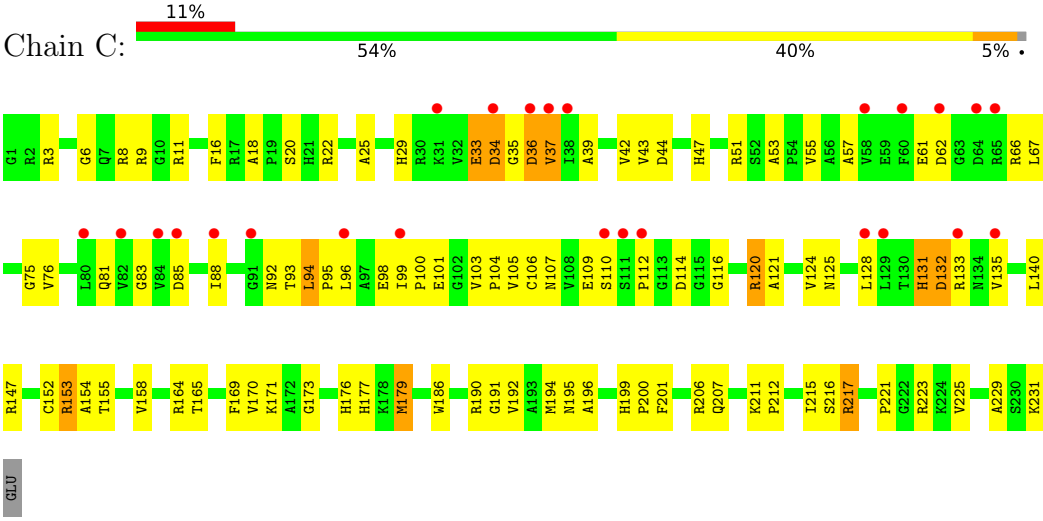


• Molecule 3: CC-puromycin

Chain 5:

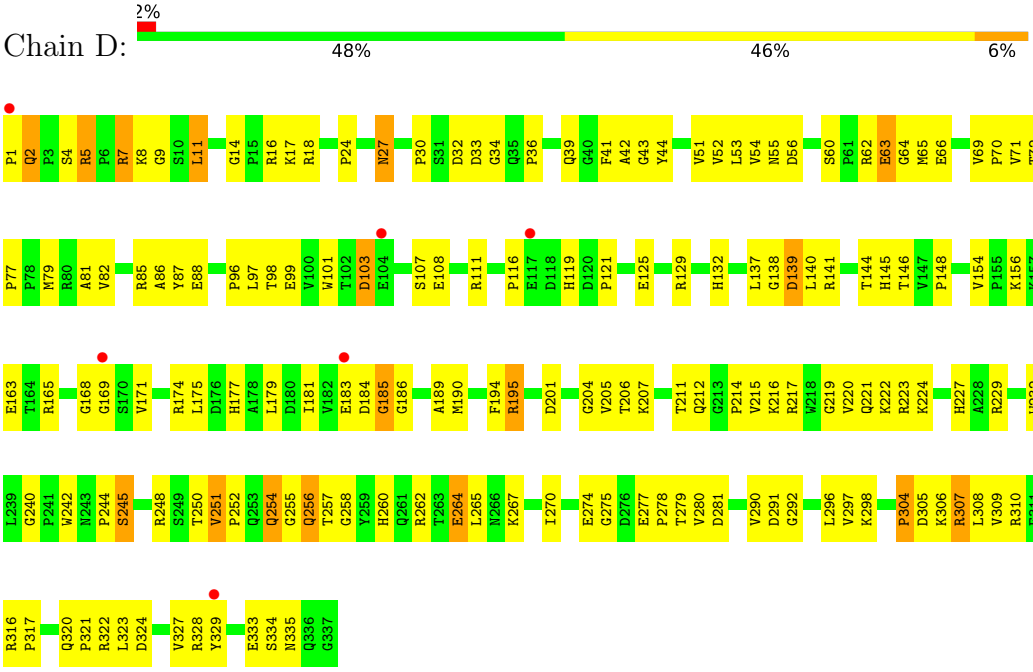
• Molecule 4: 50S ribosomal protein L2P

Chain C:



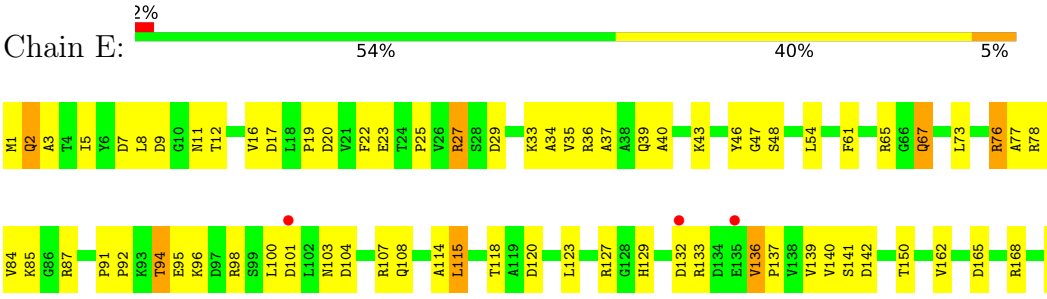
• Molecule 5: 50S ribosomal protein L3P

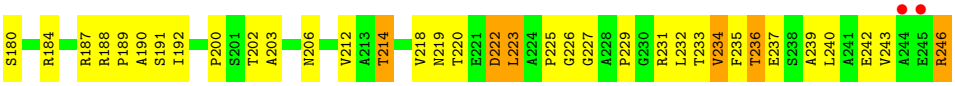
Chain D:



• Molecule 6: 50S ribosomal protein L4E

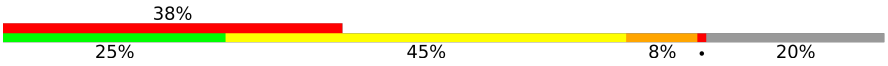
Chain E:

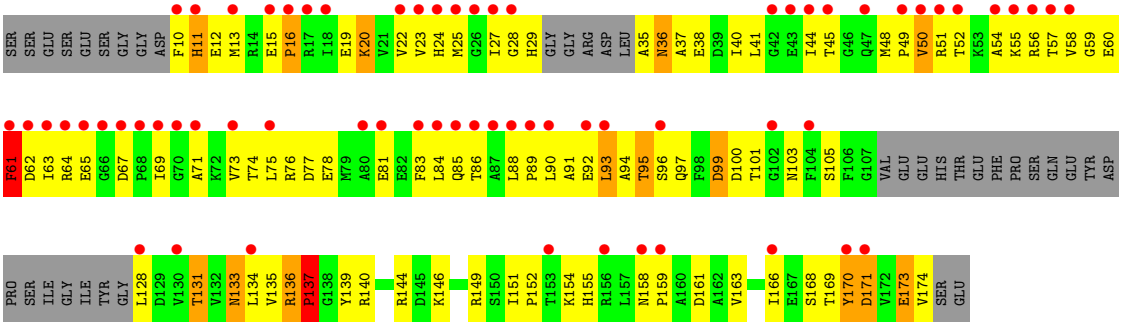




• Molecule 7: 50S ribosomal protein L5P

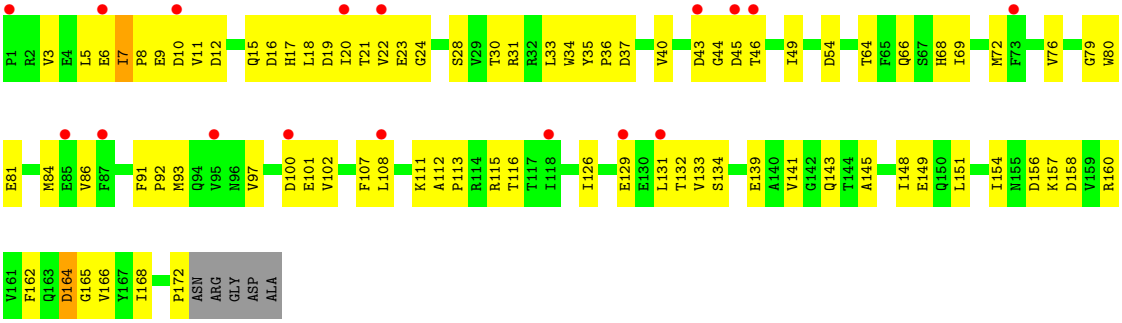
Chain F:





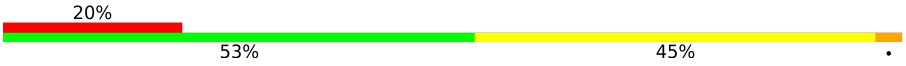
• Molecule 8: 50S ribosomal protein L6P

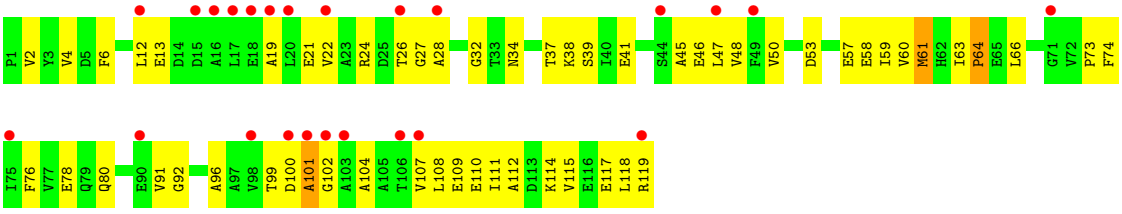
Chain G:



• Molecule 9: 50S ribosomal protein L7Ae

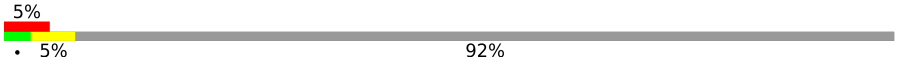
Chain H:

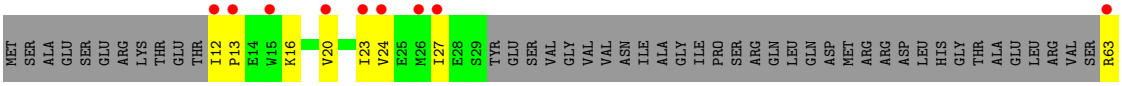




• Molecule 10: Acidic ribosomal protein P0 homolog

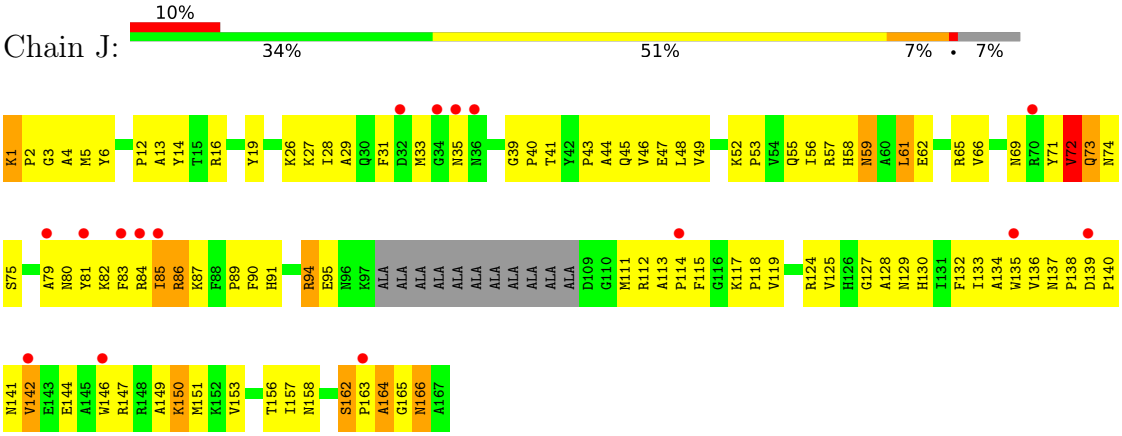
Chain I:





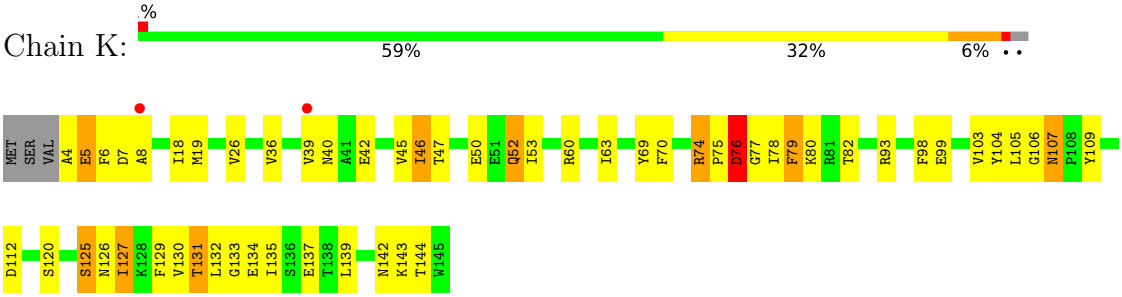
• Molecule 11: L10 Ribosomal Protein

Chain J:



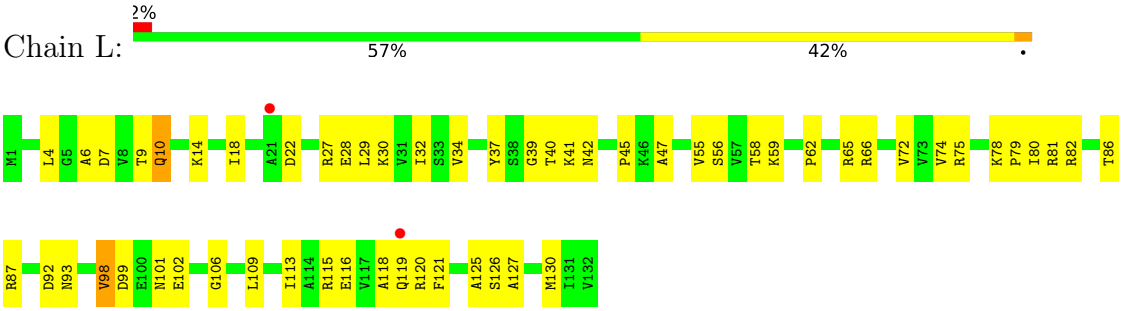
• Molecule 12: 50S ribosomal protein L13P

Chain K:

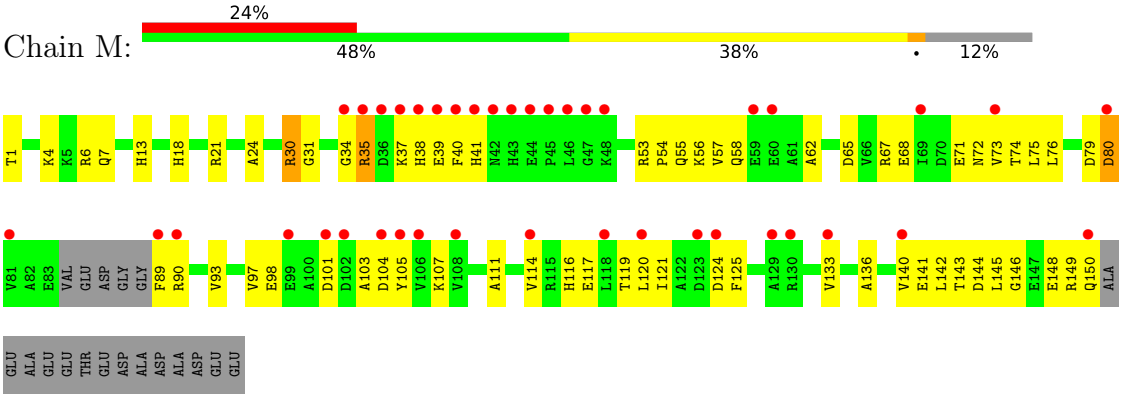


• Molecule 13: 50S ribosomal protein L14P

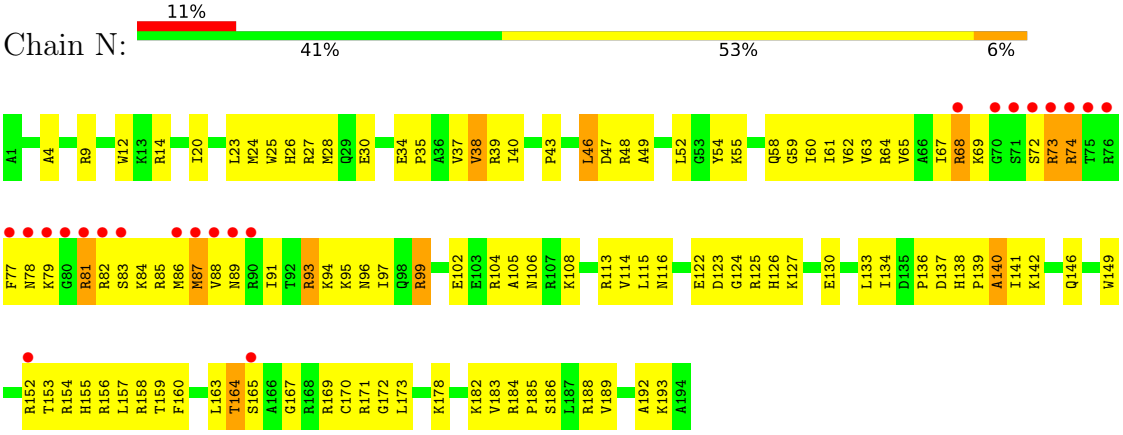
Chain L:



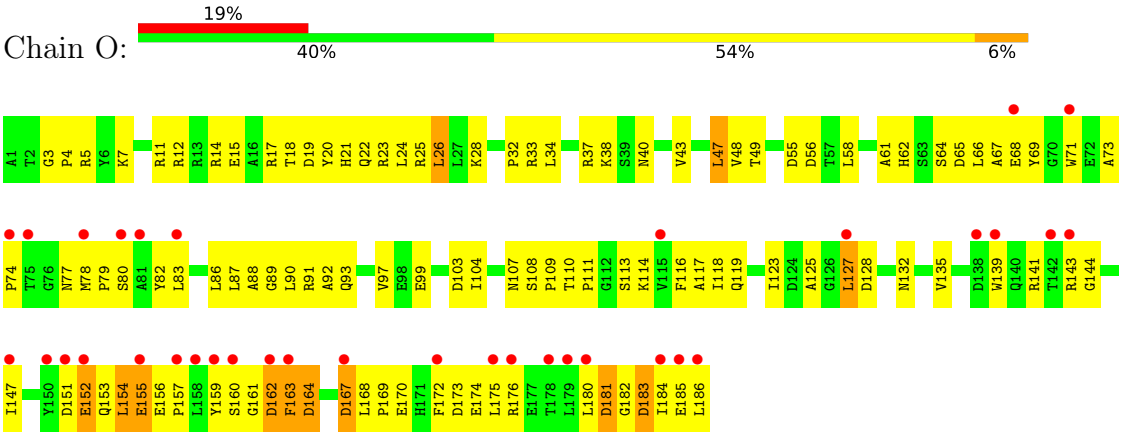
• Molecule 14: 50S ribosomal protein L15P



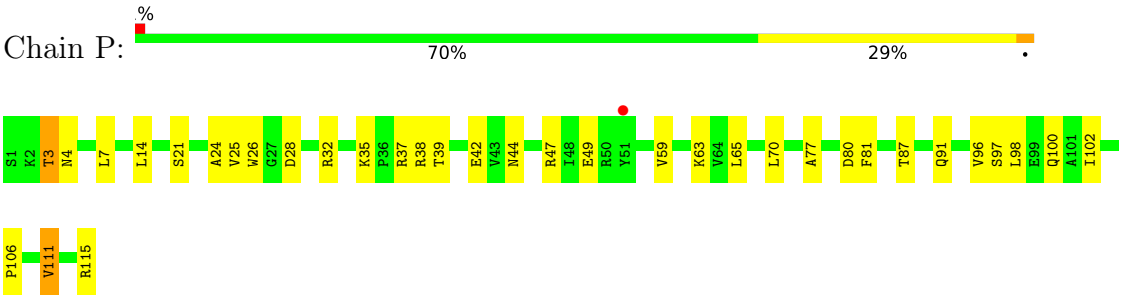
• Molecule 15: L15 Ribosomal Protein



• Molecule 16: 50S ribosomal protein L18P

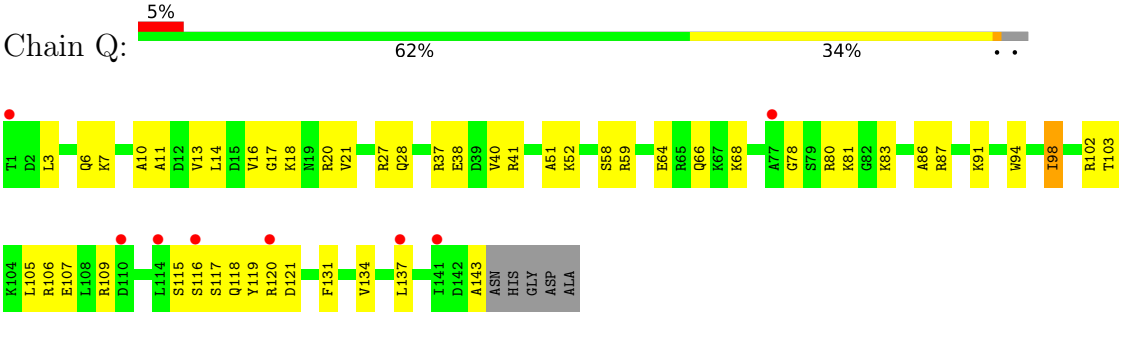


• Molecule 17: 50S ribosomal protein L18e



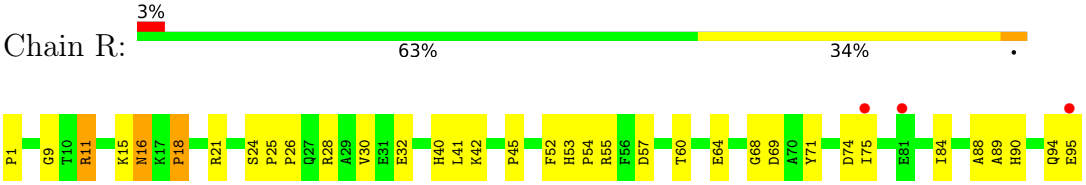
• Molecule 18: 50S ribosomal protein L19E

Chain Q:



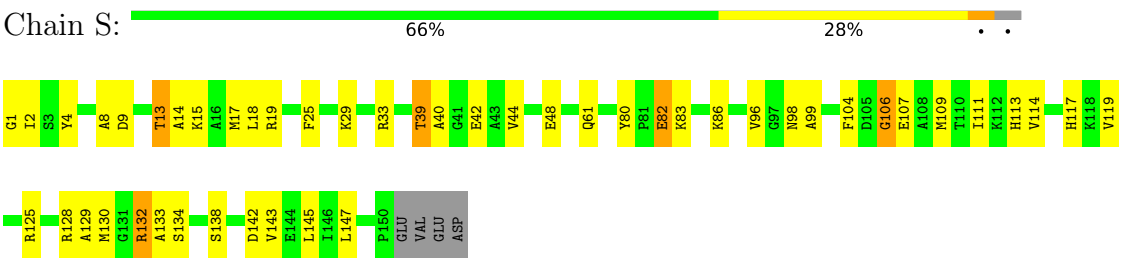
• Molecule 19: 50S ribosomal protein L21e

Chain R:



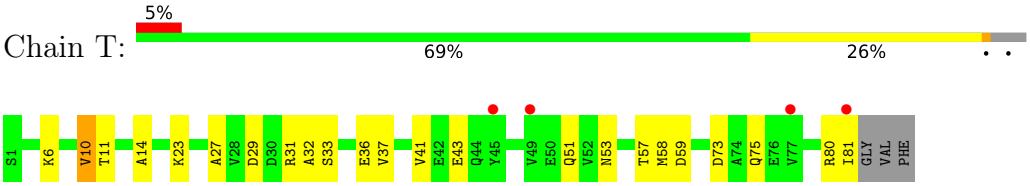
• Molecule 20: 50S ribosomal protein L22P

Chain S:



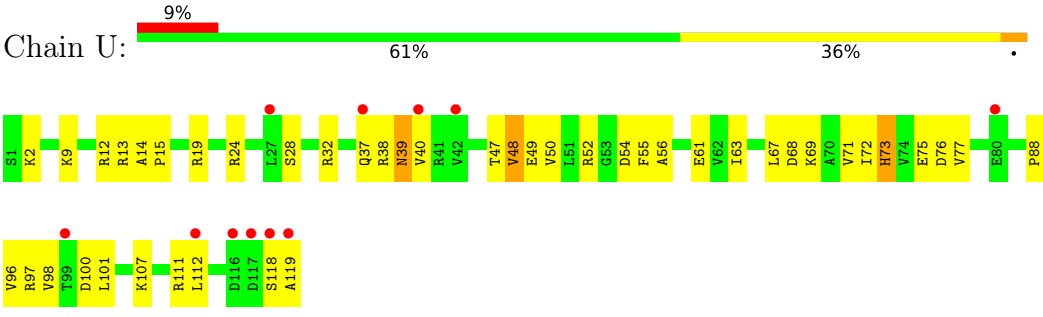
• Molecule 21: 50S ribosomal protein L23P

Chain T:



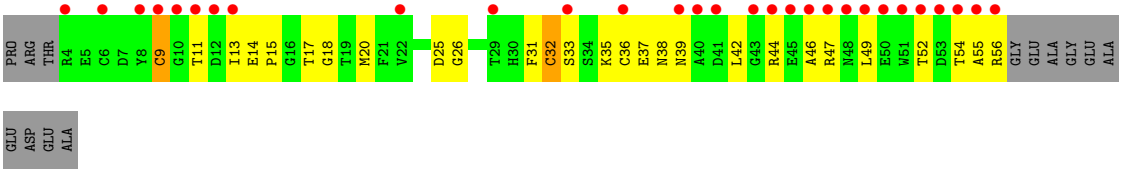
• Molecule 22: 50S ribosomal protein L24P

Chain U:



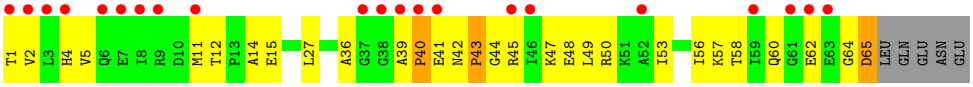
• Molecule 23: 50S ribosomal protein L24E

Chain V:



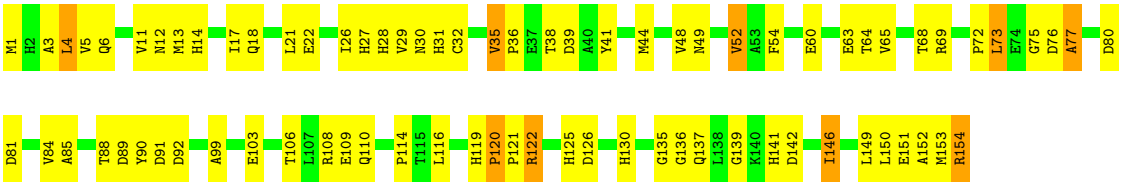
• Molecule 24: 50S ribosomal protein L29P

Chain W:



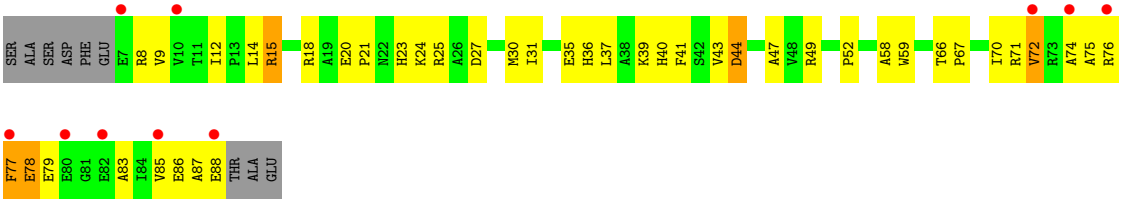
• Molecule 25: 50S ribosomal protein L30P

Chain X:



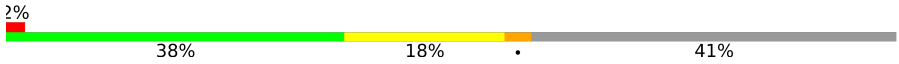
• Molecule 26: 50S ribosomal protein L31e

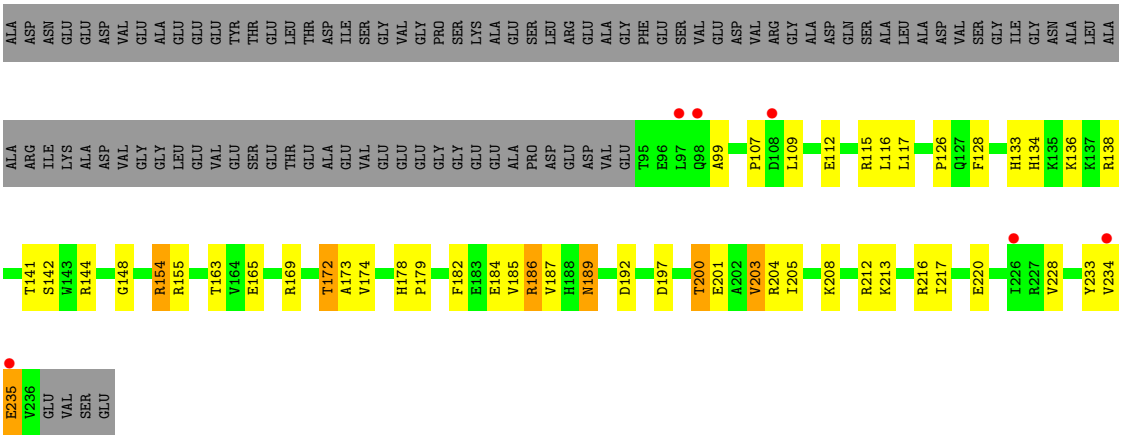
Chain Y:



• Molecule 27: 50S ribosomal protein L32E

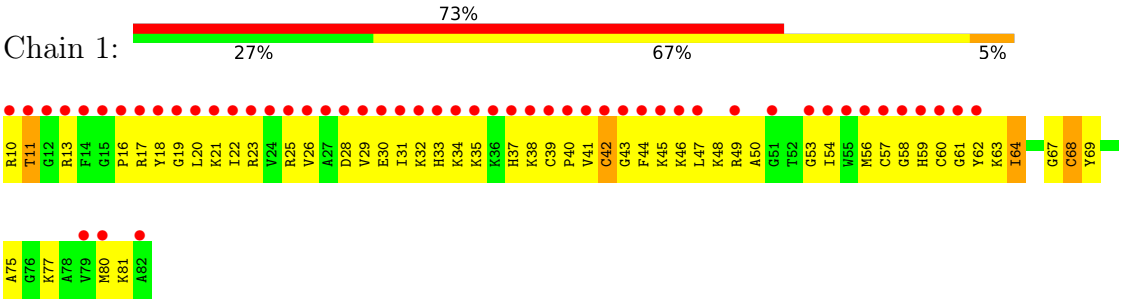
Chain Z:





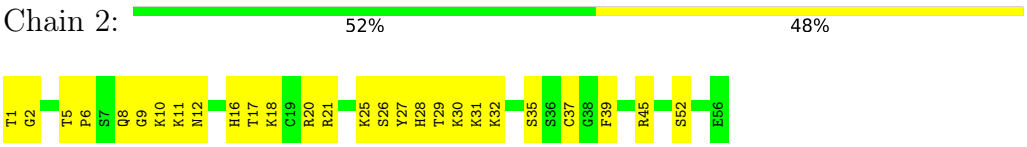
• Molecule 28: L37Ae 50S ribosomal protein

Chain 1:



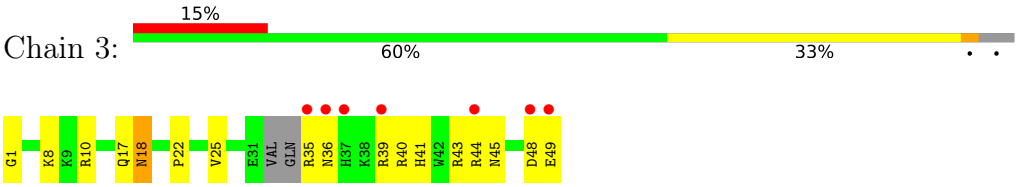
• Molecule 29: 50S ribosomal protein L37e

Chain 2:



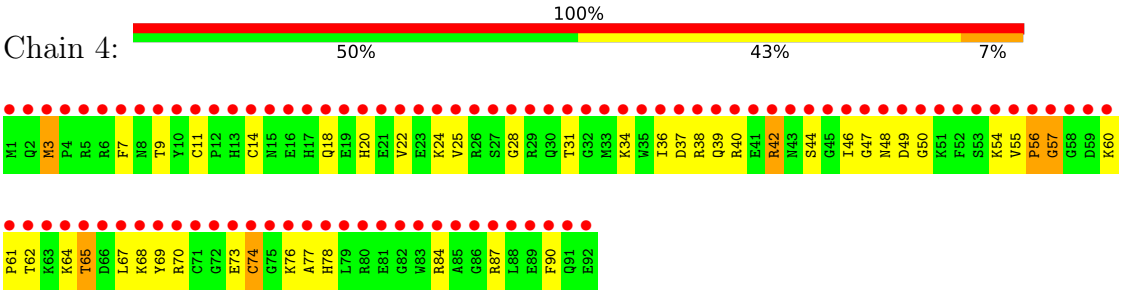
• Molecule 30: 50S ribosomal protein L39e

Chain 3:



• Molecule 31: 50S ribosomal protein L44E

Chain 4:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	213.16Å 301.29Å 575.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.98 49.62 – 2.98	Depositor EDS
% Data completeness (in resolution range)	91.7 (20.00-2.98) 91.8 (49.62-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.50 (at 2.96Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.251 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	46.6	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 63.9	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	0.91	EDS
Total number of atoms	98593	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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: NA, MG, CL, K, CD, PPU

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	0.58	2/66076 (0.0%)	0.76	28/103052 (0.0%)
2	B	0.54	0/2905	0.82	4/4528 (0.1%)
3	5	2.09	1/43 (2.3%)	1.94	0/64
4	C	0.45	0/1787	0.75	0/2409
5	D	0.44	0/2689	0.70	0/3652
6	E	0.48	0/1883	0.72	0/2551
7	F	0.40	0/1111	0.63	0/1498
8	G	0.45	0/1382	0.65	0/1880
9	H	0.39	0/896	0.62	0/1219
10	I	0.38	0/241	0.56	0/324
11	J	0.48	0/1246	0.81	2/1686 (0.1%)
12	K	0.49	0/1135	0.70	0/1530
13	L	0.46	0/1003	0.76	0/1351
14	M	0.49	0/1126	0.76	0/1504
15	N	0.61	0/1633	0.83	2/2180 (0.1%)
16	O	0.40	0/1473	0.71	0/1999
17	P	0.47	0/873	0.70	0/1181
18	Q	0.44	0/1143	0.62	0/1521
19	R	0.44	0/748	0.75	1/1005 (0.1%)
20	S	0.49	0/1172	0.73	0/1578
21	T	0.41	0/648	0.65	0/875
22	U	0.39	0/957	0.70	0/1289
23	V	0.58	0/417	0.74	1/562 (0.2%)
24	W	0.38	0/502	0.60	0/675
25	X	0.50	0/1218	0.72	0/1655
26	Y	0.46	0/664	0.71	0/895
27	Z	0.48	0/1146	0.71	0/1536
28	1	0.77	0/575	0.84	0/763
29	2	0.55	0/437	0.77	0/578
30	3	0.44	0/398	0.61	0/527
31	4	0.93	0/771	0.80	0/1024
All	All	0.56	3/98298 (0.0%)	0.75	38/147091 (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	A	1	143
2	B	1	4
All	All	2	147

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1206	U	N1-C2	5.33	1.43	1.38
1	A	1206	U	C3'-O3'	-5.24	1.34	1.42
3	5	75	C	C4'-C3'	-5.04	1.47	1.52

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1164	U	OP1-P-O3'	-18.53	64.43	105.20
1	A	1164	U	OP2-P-O3'	-18.53	64.44	105.20
1	A	1165	G	O5'-P-OP1	-11.90	94.99	105.70
2	B	3024	U	C2'-C3'-O3'	9.55	130.52	109.50
1	A	1563	G	C2'-C3'-O3'	9.10	129.51	109.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'
2	B	3024	U	C3'

5 of 147 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	U	Sidechain
1	A	26	U	Sidechain
1	A	28	G	Sidechain
1	A	48	A	Sidechain
1	A	55	U	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	59017	0	29798	1217	0
2	B	2600	0	1326	82	0
3	5	40	0	22	5	0
4	C	1754	0	1763	125	0
5	D	2624	0	2533	189	0
6	E	1858	0	1816	137	0
7	F	1094	0	1085	137	0
8	G	1357	0	1266	83	0
9	H	885	0	854	57	0
10	I	240	0	231	25	0
11	J	1215	0	1215	155	0
12	K	1119	0	1098	70	0
13	L	993	0	1027	67	0
14	M	1114	0	1072	67	0
15	N	1605	0	1676	179	0
16	O	1444	0	1401	142	0
17	P	864	0	873	40	0
18	Q	1133	0	1127	60	0
19	R	734	0	728	28	0
20	S	1149	0	1122	56	0
21	T	641	0	605	28	0
22	U	949	0	923	49	0
23	V	410	0	368	36	0
24	W	499	0	511	27	0
25	X	1195	0	1137	99	0
26	Y	654	0	653	51	0
27	Z	1130	0	1133	63	0
28	1	563	0	601	80	0
29	2	430	0	426	39	0
30	3	393	0	406	30	0
31	4	755	0	732	62	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	A	109	0	0	2	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	2	0	0	0	0
34	4	1	0	0	0	0
34	A	71	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	0	0
34	E	1	0	0	0	0
34	J	2	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	2	0	0	0	0
34	T	1	0	0	0	0
34	U	1	0	0	0	0
35	4	1	0	0	1	0
35	A	7	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	4	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	2	0
35	O	1	0	0	1	0
35	P	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
35	Z	2	0	0	1	0
36	5	37	0	28	4	0
37	1	1	0	0	0	0
37	2	1	0	0	0	0
37	4	1	0	0	0	0
37	P	1	0	0	0	0
37	V	1	0	0	0	0
38	1	36	0	0	13	0
38	2	58	0	0	4	0
38	3	37	0	0	4	0
38	4	70	0	0	11	0
38	5	1	0	0	0	0
38	A	5860	0	0	268	0
38	B	146	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	C	140	0	0	15	0
38	D	146	0	0	32	0
38	E	176	0	0	34	0
38	F	52	0	0	20	0
38	G	45	0	0	11	0
38	H	32	0	0	9	0
38	I	22	0	0	8	0
38	J	78	0	0	20	0
38	K	54	0	0	4	0
38	L	64	0	0	16	0
38	M	86	0	0	15	0
38	N	138	0	0	27	0
38	O	64	0	0	19	0
38	P	44	0	0	12	0
38	Q	70	0	0	11	0
38	R	57	0	0	4	0
38	S	83	0	0	10	0
38	T	36	0	0	5	0
38	U	38	0	0	2	0
38	V	22	0	0	6	0
38	W	16	0	0	3	0
38	X	67	0	0	10	0
38	Y	28	0	0	6	0
38	Z	100	0	0	16	0
All	All	98593	0	59556	3185	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 3185 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)
11:J:165:GLY:HA3	38:J:8398:HOH:O	1.43	1.15
11:J:86:ARG:NH1	11:J:133:ILE:HG13	1.63	1.13
15:N:164:THR:HG22	15:N:167:GLY:H	1.10	1.12
1:A:1751:G:H2'	1:A:1752:G:H5"	1.30	1.10
28:1:46:LYS:HD3	28:1:59:HIS:HB2	1.30	1.10

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
4	C	235/239 (98%)	202 (86%)	29 (12%)	4 (2%)	9 36
5	D	335/337 (99%)	299 (89%)	28 (8%)	8 (2%)	6 27
6	E	244/246 (99%)	222 (91%)	21 (9%)	1 (0%)	34 70
7	F	134/176 (76%)	93 (69%)	29 (22%)	12 (9%)	1 3
8	G	170/177 (96%)	158 (93%)	11 (6%)	1 (1%)	25 61
9	H	117/119 (98%)	100 (86%)	14 (12%)	3 (3%)	5 25
10	I	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	3 15
11	J	152/167 (91%)	130 (86%)	17 (11%)	5 (3%)	4 19
12	K	140/145 (97%)	129 (92%)	6 (4%)	5 (4%)	3 17
13	L	130/132 (98%)	118 (91%)	10 (8%)	2 (2%)	10 39
14	M	141/164 (86%)	122 (86%)	18 (13%)	1 (1%)	22 58
15	N	192/194 (99%)	173 (90%)	18 (9%)	1 (0%)	29 66
16	O	184/186 (99%)	163 (89%)	13 (7%)	8 (4%)	2 14
17	P	113/115 (98%)	107 (95%)	6 (5%)	0	100 100
18	Q	141/148 (95%)	135 (96%)	5 (4%)	1 (1%)	22 58
19	R	93/95 (98%)	85 (91%)	5 (5%)	3 (3%)	4 20
20	S	148/154 (96%)	135 (91%)	12 (8%)	1 (1%)	22 58
21	T	79/84 (94%)	74 (94%)	5 (6%)	0	100 100
22	U	117/119 (98%)	110 (94%)	7 (6%)	0	100 100
23	V	51/66 (77%)	47 (92%)	4 (8%)	0	100 100
24	W	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	4 20
25	X	152/154 (99%)	143 (94%)	7 (5%)	2 (1%)	12 43
26	Y	80/91 (88%)	71 (89%)	6 (8%)	3 (4%)	3 16
27	Z	140/240 (58%)	138 (99%)	2 (1%)	0	100 100
28	1	71/73 (97%)	63 (89%)	6 (8%)	2 (3%)	5 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
29	2	54/56 (96%)	52 (96%)	2 (4%)	0	100 100
30	3	42/48 (88%)	42 (100%)	0	0	100 100
31	4	90/92 (98%)	84 (93%)	4 (4%)	2 (2%)	6 29
All	All	3633/4235 (86%)	3276 (90%)	289 (8%)	68 (2%)	8 33

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	139	ASP
7	F	93	LEU
7	F	95	THR
7	F	137	PRO
7	F	173	GLU

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
4	C	179/181 (99%)	167 (93%)	12 (7%)	16 47
5	D	282/282 (100%)	264 (94%)	18 (6%)	17 49
6	E	193/193 (100%)	176 (91%)	17 (9%)	10 34
7	F	117/147 (80%)	107 (92%)	10 (8%)	10 36
8	G	152/155 (98%)	148 (97%)	4 (3%)	46 76
9	H	92/92 (100%)	91 (99%)	1 (1%)	73 90
10	I	27/283 (10%)	27 (100%)	0	100 100
11	J	122/122 (100%)	110 (90%)	12 (10%)	8 29
12	K	118/121 (98%)	107 (91%)	11 (9%)	9 31
13	L	106/106 (100%)	103 (97%)	3 (3%)	43 75
14	M	112/126 (89%)	108 (96%)	4 (4%)	35 68
15	N	166/166 (100%)	157 (95%)	9 (5%)	22 55
16	O	149/149 (100%)	143 (96%)	6 (4%)	31 66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	P	93/93 (100%)	89 (96%)	4 (4%)	29 64
18	Q	113/116 (97%)	110 (97%)	3 (3%)	44 75
19	R	79/79 (100%)	75 (95%)	4 (5%)	24 57
20	S	117/121 (97%)	113 (97%)	4 (3%)	37 70
21	T	71/73 (97%)	70 (99%)	1 (1%)	67 86
22	U	105/105 (100%)	102 (97%)	3 (3%)	42 74
23	V	44/52 (85%)	42 (96%)	2 (4%)	27 62
24	W	51/56 (91%)	49 (96%)	2 (4%)	32 66
25	X	130/130 (100%)	121 (93%)	9 (7%)	15 46
26	Y	66/73 (90%)	61 (92%)	5 (8%)	13 41
27	Z	120/195 (62%)	112 (93%)	8 (7%)	16 47
28	1	56/56 (100%)	50 (89%)	6 (11%)	6 24
29	2	46/46 (100%)	46 (100%)	0	100 100
30	3	42/44 (96%)	41 (98%)	1 (2%)	49 78
31	4	79/79 (100%)	73 (92%)	6 (8%)	13 41
All	All	3027/3441 (88%)	2862 (94%)	165 (6%)	21 55

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	R	16	ASN
26	Y	72	VAL
20	S	39	THR
25	X	4	LEU
27	Z	203	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
20	S	117	HIS
25	X	141	HIS
21	T	53	ASN
25	X	27	HIS
27	Z	189	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	248 (9%)	36 (1%)
2	B	121/122 (99%)	18 (14%)	5 (4%)
3	5	1/2 (50%)	0	0
All	All	2869/3046 (94%)	266 (9%)	41 (1%)

5 of 266 RNA backbone outliers are listed below:

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

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2466	G
1	A	2791	U
1	A	2467	A
1	A	2649	A
2	B	3024	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 233 ligands modelled in this entry, 232 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
36	PPU	5	76	3	32,40,41	2.22	12 (37%)	33,57,60	1.72	6 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	PPU	5	76	3	-	2/21/43/44	0/4/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	76	PPU	CB-CG	4.78	1.62	1.51
36	5	76	PPU	C-N3'	4.39	1.43	1.34
36	5	76	PPU	C10-N6	-4.04	1.36	1.45
36	5	76	PPU	CE2-CD2	-3.75	1.31	1.38
36	5	76	PPU	O-C	3.58	1.30	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	5	76	PPU	CA-C-N3'	-4.23	110.28	116.15
36	5	76	PPU	C3'-N3'-C	-4.06	117.09	123.21
36	5	76	PPU	CG-CB-CA	-3.92	105.98	114.13
36	5	76	PPU	CM-OC-CZ	3.20	124.45	117.51
36	5	76	PPU	O4'-C1'-C2'	2.99	111.29	106.93

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	5	76	PPU	O-C-CA-CB
36	5	76	PPU	N3'-C-CA-CB

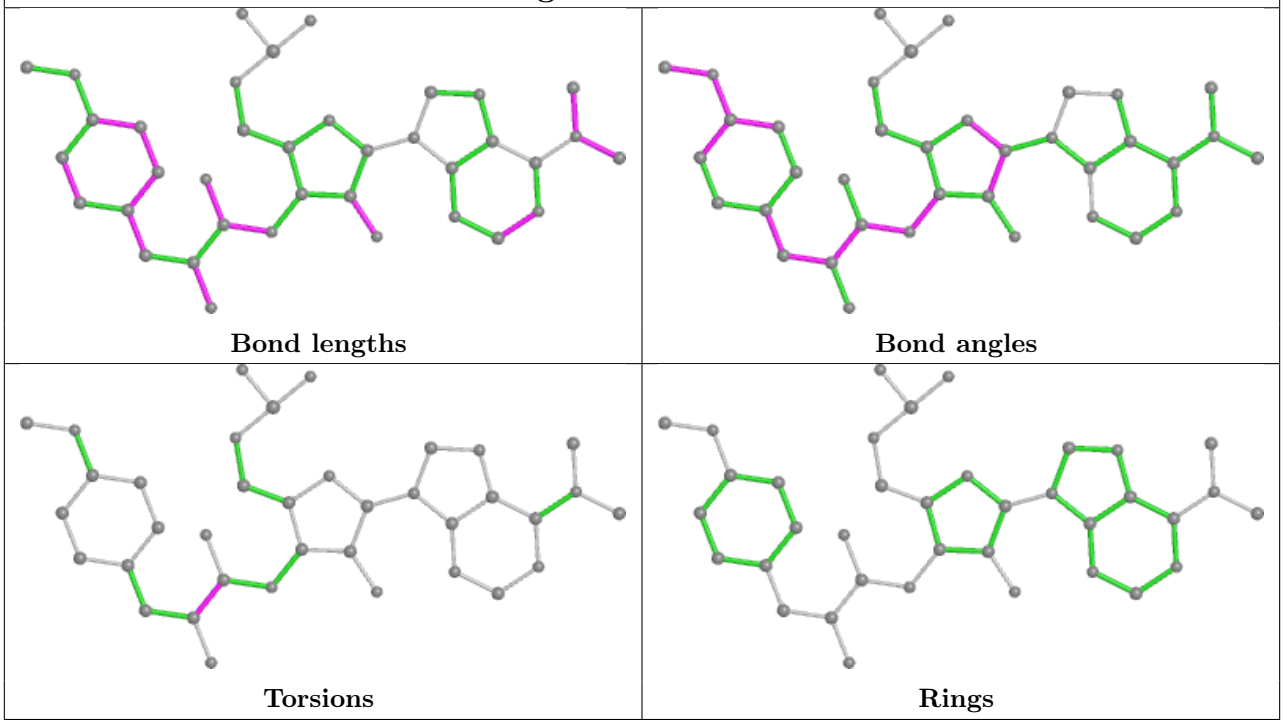
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	5	76	PPU	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PPU 5 76



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	2754/2922 (94%)	0.09	83 (3%) 50 31	19, 45, 94, 144	0
2	B	122/122 (100%)	0.48	6 (4%) 29 17	33, 67, 97, 147	0
3	5	2/2 (100%)	2.10	1 (50%) 0 0	65, 65, 65, 87	0
4	C	237/239 (99%)	0.59	26 (10%) 5 3	30, 62, 97, 109	0
5	D	337/337 (100%)	0.18	6 (1%) 68 48	22, 50, 77, 89	0
6	E	246/246 (100%)	0.06	5 (2%) 65 45	20, 44, 69, 78	0
7	F	140/176 (79%)	2.16	66 (47%) 0 0	65, 101, 122, 128	0
8	G	172/177 (97%)	0.94	17 (9%) 7 4	38, 62, 84, 89	0
9	H	119/119 (100%)	0.96	24 (20%) 1 0	51, 76, 99, 107	0
10	I	29/348 (8%)	2.38	17 (58%) 0 0	66, 87, 95, 99	0
11	J	156/167 (93%)	0.76	16 (10%) 6 3	35, 59, 82, 89	0
12	K	142/145 (97%)	0.08	2 (1%) 75 57	32, 44, 67, 78	0
13	L	132/132 (100%)	0.26	2 (1%) 73 54	33, 49, 75, 82	0
14	M	145/164 (88%)	1.29	40 (27%) 0 0	26, 79, 106, 111	0
15	N	194/194 (100%)	0.63	22 (11%) 5 3	28, 47, 106, 118	0
16	O	186/186 (100%)	1.10	35 (18%) 1 0	46, 73, 112, 125	0
17	P	115/115 (100%)	0.26	1 (0%) 84 69	36, 53, 68, 72	0
18	Q	143/148 (96%)	0.56	8 (5%) 24 13	34, 53, 76, 85	0
19	R	95/95 (100%)	0.21	3 (3%) 47 29	36, 47, 63, 82	0
20	S	150/154 (97%)	-0.00	0 100 100	26, 40, 61, 72	0
21	T	81/84 (96%)	0.52	4 (4%) 29 17	44, 62, 82, 88	0
22	U	119/119 (100%)	0.82	11 (9%) 9 5	40, 55, 84, 104	0
23	V	53/66 (80%)	2.37	29 (54%) 0 0	77, 92, 100, 108	0
24	W	65/70 (92%)	1.43	21 (32%) 0 0	46, 76, 111, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	X	154/154 (100%)	0.08	0 100 100	28, 42, 59, 70	0
26	Y	82/91 (90%)	0.71	10 (12%) 4 2	37, 53, 77, 91	0
27	Z	142/240 (59%)	0.17	6 (4%) 36 21	25, 40, 64, 82	0
28	1	73/73 (100%)	5.61	53 (72%) 0 0	93, 115, 125, 127	0
29	2	56/56 (100%)	-0.25	0 100 100	22, 32, 40, 45	0
30	3	46/48 (95%)	0.88	7 (15%) 2 1	34, 63, 96, 105	0
31	4	92/92 (100%)	8.87	92 (100%) 0 0	110, 125, 133, 136	0
All	All	6579/7281 (90%)	0.56	613 (9%) 8 5	19, 52, 105, 147	0

The worst 5 of 613 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	4	82	GLY	29.1
28	1	11	THR	19.9
31	4	37	ASP	18.9
31	4	83	TRP	18.6
31	4	62	THR	17.9

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

There are no non-standard protein/DNA/RNA residues in this entry.

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	A	8384	1/1	0.14	0.75	82,82,82,82	0
32	MG	A	8049	1/1	0.33	0.69	95,95,95,95	0
32	MG	A	8076	1/1	0.34	0.17	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	A	8024	1/1	0.37	0.60	110,110,110,110	0
34	NA	T	8312	1/1	0.39	0.57	80,80,80,80	0
35	CL	4	8504	1/1	0.40	0.36	101,101,101,101	0
35	CL	M	8510	1/1	0.41	0.43	97,97,97,97	0
34	NA	A	8382	1/1	0.47	0.52	79,79,79,79	0
34	NA	A	8371	1/1	0.53	0.60	54,54,54,54	0
34	NA	A	8329	1/1	0.53	0.35	61,61,61,61	0
34	NA	A	8340	1/1	0.53	0.59	58,58,58,58	0
34	NA	B	8351	1/1	0.56	0.39	75,75,75,75	0
34	NA	A	8365	1/1	0.56	0.55	46,46,46,46	0
34	NA	A	8363	1/1	0.58	0.78	48,48,48,48	0
32	MG	1	8105	1/1	0.59	0.72	58,58,58,58	0
34	NA	S	8386	1/1	0.62	0.53	70,70,70,70	0
32	MG	A	8102	1/1	0.62	1.13	135,135,135,135	0
34	NA	S	8337	1/1	0.64	0.25	52,52,52,52	0
34	NA	A	8372	1/1	0.65	0.54	80,80,80,80	0
34	NA	R	8348	1/1	0.69	0.21	57,57,57,57	0
34	NA	B	8383	1/1	0.69	0.94	77,77,77,77	0
32	MG	A	8114	1/1	0.70	1.03	124,124,124,124	0
34	NA	A	8373	1/1	0.70	0.27	54,54,54,54	0
34	NA	A	8328	1/1	0.71	0.57	47,47,47,47	0
34	NA	A	8385	1/1	0.72	0.34	46,46,46,46	0
34	NA	A	8381	1/1	0.73	0.16	46,46,46,46	0
37	CD	1	8403	1/1	0.73	0.31	203,203,203,203	0
32	MG	A	8092	1/1	0.74	0.47	91,91,91,91	0
37	CD	4	8404	1/1	0.74	0.42	203,203,203,203	0
34	NA	A	8357	1/1	0.76	0.10	49,49,49,49	0
32	MG	A	8113	1/1	0.76	0.32	54,54,54,54	0
34	NA	A	8310	1/1	0.76	0.53	40,40,40,40	0
34	NA	A	8326	1/1	0.76	0.64	60,60,60,60	0
34	NA	A	8327	1/1	0.77	0.20	40,40,40,40	0
34	NA	A	8307	1/1	0.77	0.64	58,58,58,58	0
34	NA	A	8352	1/1	0.78	0.33	39,39,39,39	0
34	NA	4	8369	1/1	0.79	0.33	66,66,66,66	0
35	CL	A	8522	1/1	0.79	0.62	83,83,83,83	0
34	NA	A	8368	1/1	0.79	0.24	56,56,56,56	0
32	MG	A	8093	1/1	0.80	0.23	44,44,44,44	0
34	NA	A	8319	1/1	0.80	0.15	44,44,44,44	0
34	NA	A	8332	1/1	0.80	0.46	68,68,68,68	0
35	CL	K	8502	1/1	0.80	0.19	71,71,71,71	0
35	CL	D	8519	1/1	0.81	0.40	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	D	8055	1/1	0.82	0.15	81,81,81,81	0
34	NA	A	8374	1/1	0.82	0.65	60,60,60,60	0
34	NA	A	8355	1/1	0.82	0.62	64,64,64,64	0
32	MG	A	8045	1/1	0.82	0.13	50,50,50,50	0
34	NA	A	8301	1/1	0.82	0.14	31,31,31,31	0
35	CL	R	8511	1/1	0.83	0.38	67,67,67,67	0
32	MG	A	8046	1/1	0.83	0.10	53,53,53,53	0
32	MG	B	8095	1/1	0.83	0.08	72,72,72,72	0
35	CL	C	8509	1/1	0.83	0.32	86,86,86,86	0
34	NA	J	8322	1/1	0.84	0.37	72,72,72,72	0
32	MG	A	8089	1/1	0.84	0.22	82,82,82,82	0
34	NA	A	8378	1/1	0.84	0.55	52,52,52,52	0
32	MG	U	8073	1/1	0.84	0.21	48,48,48,48	0
34	NA	A	8303	1/1	0.84	0.36	51,51,51,51	0
32	MG	A	8085	1/1	0.85	0.16	95,95,95,95	0
32	MG	A	8088	1/1	0.85	0.15	65,65,65,65	0
35	CL	A	8505	1/1	0.85	0.25	74,74,74,74	0
34	NA	A	8356	1/1	0.85	0.81	57,57,57,57	0
34	NA	A	8377	1/1	0.85	0.33	86,86,86,86	0
32	MG	A	8115	1/1	0.85	0.09	59,59,59,59	0
35	CL	K	8516	1/1	0.86	0.27	61,61,61,61	0
34	NA	A	8354	1/1	0.86	0.38	51,51,51,51	0
34	NA	K	8346	1/1	0.86	0.19	37,37,37,37	0
34	NA	A	8341	1/1	0.87	0.17	55,55,55,55	0
35	CL	O	8507	1/1	0.87	0.23	65,65,65,65	0
32	MG	A	8101	1/1	0.87	0.10	50,50,50,50	0
34	NA	A	8316	1/1	0.88	0.21	45,45,45,45	0
34	NA	A	8353	1/1	0.88	0.22	53,53,53,53	0
32	MG	A	8099	1/1	0.88	0.24	68,68,68,68	0
32	MG	A	8064	1/1	0.88	0.24	24,24,24,24	0
32	MG	Z	8109	1/1	0.89	0.15	38,38,38,38	0
34	NA	A	8364	1/1	0.89	0.34	54,54,54,54	0
32	MG	A	8051	1/1	0.89	0.11	86,86,86,86	0
32	MG	A	8103	1/1	0.89	0.23	45,45,45,45	0
34	NA	A	8358	1/1	0.89	0.45	105,105,105,105	0
34	NA	A	8335	1/1	0.90	0.26	57,57,57,57	0
34	NA	A	8302	1/1	0.90	0.20	31,31,31,31	0
32	MG	A	8112	1/1	0.90	0.21	57,57,57,57	0
34	NA	A	8375	1/1	0.90	0.26	55,55,55,55	0
35	CL	N	8518	1/1	0.90	0.19	46,46,46,46	0
34	NA	A	8366	1/1	0.90	0.43	47,47,47,47	0
35	CL	A	8503	1/1	0.90	0.24	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	A	8071	1/1	0.90	0.07	93,93,93,93	0
34	NA	A	8308	1/1	0.90	0.15	63,63,63,63	0
34	NA	N	8347	1/1	0.90	0.11	24,24,24,24	0
32	MG	A	8053	1/1	0.91	0.19	41,41,41,41	0
34	NA	A	8311	1/1	0.91	0.13	31,31,31,31	0
35	CL	A	8515	1/1	0.91	0.31	68,68,68,68	0
32	MG	A	8116	1/1	0.91	0.16	55,55,55,55	0
34	NA	E	8304	1/1	0.91	0.14	25,25,25,25	0
35	CL	S	8506	1/1	0.91	0.20	60,60,60,60	0
32	MG	A	8047	1/1	0.91	0.16	31,31,31,31	0
36	PPU	5	76	37/38	0.91	0.27	60,64,69,71	0
35	CL	K	8501	1/1	0.91	0.17	58,58,58,58	0
34	NA	A	8370	1/1	0.91	0.32	52,52,52,52	0
34	NA	A	8362	1/1	0.92	0.20	74,74,74,74	0
32	MG	A	8041	1/1	0.92	0.17	55,55,55,55	0
33	K	A	8202	1/1	0.92	0.15	89,89,89,89	0
34	NA	J	8309	1/1	0.92	0.18	42,42,42,42	0
32	MG	A	8104	1/1	0.92	0.20	52,52,52,52	0
32	MG	A	8108	1/1	0.92	0.06	53,53,53,53	0
35	CL	Z	8520	1/1	0.92	0.15	35,35,35,35	0
34	NA	A	8331	1/1	0.92	0.15	76,76,76,76	0
32	MG	A	8016	1/1	0.92	0.13	36,36,36,36	0
34	NA	A	8306	1/1	0.92	0.62	44,44,44,44	0
34	NA	A	8324	1/1	0.92	0.25	51,51,51,51	0
32	MG	A	8082	1/1	0.93	0.16	56,56,56,56	0
32	MG	A	8027	1/1	0.93	0.05	54,54,54,54	0
35	CL	K	8521	1/1	0.93	0.24	60,60,60,60	0
32	MG	A	8106	1/1	0.93	0.20	76,76,76,76	0
32	MG	A	8094	1/1	0.93	0.17	65,65,65,65	0
32	MG	A	8096	1/1	0.93	0.07	51,51,51,51	0
32	MG	A	8059	1/1	0.93	0.10	47,47,47,47	0
32	MG	4	8078	1/1	0.93	0.19	74,74,74,74	0
34	NA	A	8333	1/1	0.93	0.08	33,33,33,33	0
32	MG	A	8063	1/1	0.93	0.11	85,85,85,85	0
34	NA	A	8336	1/1	0.93	0.10	49,49,49,49	0
34	NA	M	8380	1/1	0.93	0.17	65,65,65,65	0
32	MG	A	8090	1/1	0.93	0.19	70,70,70,70	0
34	NA	A	8325	1/1	0.94	0.25	40,40,40,40	0
34	NA	A	8359	1/1	0.94	0.45	60,60,60,60	0
34	NA	A	8361	1/1	0.94	0.45	62,62,62,62	0
32	MG	A	8077	1/1	0.94	0.06	32,32,32,32	0
32	MG	A	8079	1/1	0.94	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	A	8043	1/1	0.94	0.10	32,32,32,32	0
32	MG	A	8056	1/1	0.94	0.15	56,56,56,56	0
34	NA	A	8330	1/1	0.94	0.20	35,35,35,35	0
32	MG	A	8057	1/1	0.94	0.17	46,46,46,46	0
35	CL	A	8514	1/1	0.94	0.27	50,50,50,50	0
32	MG	A	8010	1/1	0.94	0.05	30,30,30,30	0
32	MG	A	8062	1/1	0.94	0.14	49,49,49,49	0
34	NA	A	8334	1/1	0.94	0.09	46,46,46,46	0
32	MG	A	8013	1/1	0.94	0.11	42,42,42,42	0
32	MG	A	8035	1/1	0.94	0.06	48,48,48,48	0
34	NA	A	8339	1/1	0.94	0.09	30,30,30,30	0
32	MG	A	8066	1/1	0.94	0.16	65,65,65,65	0
32	MG	A	8008	1/1	0.94	0.08	42,42,42,42	0
34	NA	A	8342	1/1	0.94	0.14	28,28,28,28	0
34	NA	A	8344	1/1	0.94	0.07	27,27,27,27	0
34	NA	A	8349	1/1	0.94	0.23	67,67,67,67	0
34	NA	A	8350	1/1	0.94	0.16	37,37,37,37	0
34	NA	A	8313	1/1	0.94	0.10	74,74,74,74	0
32	MG	A	8075	1/1	0.94	0.12	45,45,45,45	0
32	MG	A	8100	1/1	0.94	0.14	79,79,79,79	0
34	NA	A	8321	1/1	0.94	0.42	48,48,48,48	0
37	CD	P	8405	1/1	0.94	0.07	89,89,89,89	0
34	NA	A	8323	1/1	0.94	0.22	45,45,45,45	0
32	MG	A	8042	1/1	0.94	0.17	34,34,34,34	0
32	MG	A	8070	1/1	0.95	0.78	69,69,69,69	0
32	MG	A	8052	1/1	0.95	0.08	51,51,51,51	0
32	MG	A	8030	1/1	0.95	0.12	34,34,34,34	0
34	NA	A	8314	1/1	0.95	0.10	43,43,43,43	0
32	MG	A	8097	1/1	0.95	0.20	32,32,32,32	0
34	NA	C	8345	1/1	0.95	0.12	35,35,35,35	0
34	NA	A	8317	1/1	0.95	0.06	32,32,32,32	0
32	MG	A	8044	1/1	0.95	0.15	54,54,54,54	0
34	NA	A	8320	1/1	0.95	0.23	42,42,42,42	0
32	MG	A	8034	1/1	0.95	0.05	36,36,36,36	0
32	MG	A	8004	1/1	0.95	0.07	53,53,53,53	0
32	MG	A	8081	1/1	0.95	0.08	39,39,39,39	0
32	MG	A	8060	1/1	0.95	0.19	44,44,44,44	0
32	MG	A	8039	1/1	0.95	0.05	51,51,51,51	0
32	MG	A	8087	1/1	0.95	0.09	49,49,49,49	0
32	MG	A	8018	1/1	0.95	0.08	42,42,42,42	0
34	NA	U	8343	1/1	0.95	0.09	27,27,27,27	0
32	MG	A	8050	1/1	0.95	0.10	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	A	8029	1/1	0.95	0.10	38,38,38,38	0
32	MG	A	8068	1/1	0.95	0.11	46,46,46,46	0
32	MG	C	8065	1/1	0.96	0.13	68,68,68,68	0
34	NA	A	8367	1/1	0.96	0.14	43,43,43,43	0
32	MG	A	8040	1/1	0.96	0.13	100,100,100,100	0
32	MG	A	8028	1/1	0.96	0.07	37,37,37,37	0
32	MG	A	8067	1/1	0.96	0.14	41,41,41,41	0
32	MG	A	8061	1/1	0.96	0.06	45,45,45,45	0
34	NA	A	8360	1/1	0.96	0.73	61,61,61,61	0
35	CL	A	8513	1/1	0.96	0.12	56,56,56,56	0
35	CL	Z	8517	1/1	0.96	0.31	61,61,61,61	0
32	MG	A	8091	1/1	0.96	0.10	67,67,67,67	0
32	MG	A	8023	1/1	0.96	0.12	45,45,45,45	0
32	MG	A	8058	1/1	0.96	0.08	39,39,39,39	0
32	MG	A	8072	1/1	0.96	0.07	53,53,53,53	0
37	CD	V	8401	1/1	0.96	0.15	129,129,129,129	0
34	NA	A	8379	1/1	0.96	0.24	48,48,48,48	0
34	NA	A	8338	1/1	0.96	0.09	44,44,44,44	0
32	MG	A	8111	1/1	0.97	0.07	61,61,61,61	0
32	MG	A	8083	1/1	0.97	0.08	37,37,37,37	0
35	CL	A	8512	1/1	0.97	0.10	31,31,31,31	0
32	MG	A	8021	1/1	0.97	0.11	32,32,32,32	0
32	MG	A	8022	1/1	0.97	0.05	32,32,32,32	0
34	NA	A	8318	1/1	0.97	0.28	43,43,43,43	0
32	MG	A	8002	1/1	0.97	0.05	36,36,36,36	0
32	MG	A	8009	1/1	0.97	0.06	32,32,32,32	0
32	MG	A	8117	1/1	0.97	0.08	33,33,33,33	0
32	MG	A	8003	1/1	0.97	0.07	23,23,23,23	0
32	MG	A	8012	1/1	0.97	0.10	44,44,44,44	0
32	MG	A	8001	1/1	0.97	0.09	33,33,33,33	0
32	MG	A	8014	1/1	0.97	0.07	20,20,20,20	0
32	MG	A	8048	1/1	0.97	0.07	33,33,33,33	0
32	MG	A	8031	1/1	0.97	0.04	32,32,32,32	0
32	MG	A	8032	1/1	0.97	0.06	34,34,34,34	0
33	K	A	8201	1/1	0.97	0.24	71,71,71,71	0
32	MG	A	8033	1/1	0.97	0.12	25,25,25,25	0
32	MG	A	8074	1/1	0.97	0.05	42,42,42,42	0
32	MG	A	8006	1/1	0.97	0.09	57,57,57,57	0
32	MG	A	8017	1/1	0.97	0.05	35,35,35,35	0
32	MG	A	8054	1/1	0.97	0.06	33,33,33,33	0
32	MG	A	8037	1/1	0.97	0.09	43,43,43,43	0
32	MG	A	8038	1/1	0.97	0.05	33,33,33,33	0

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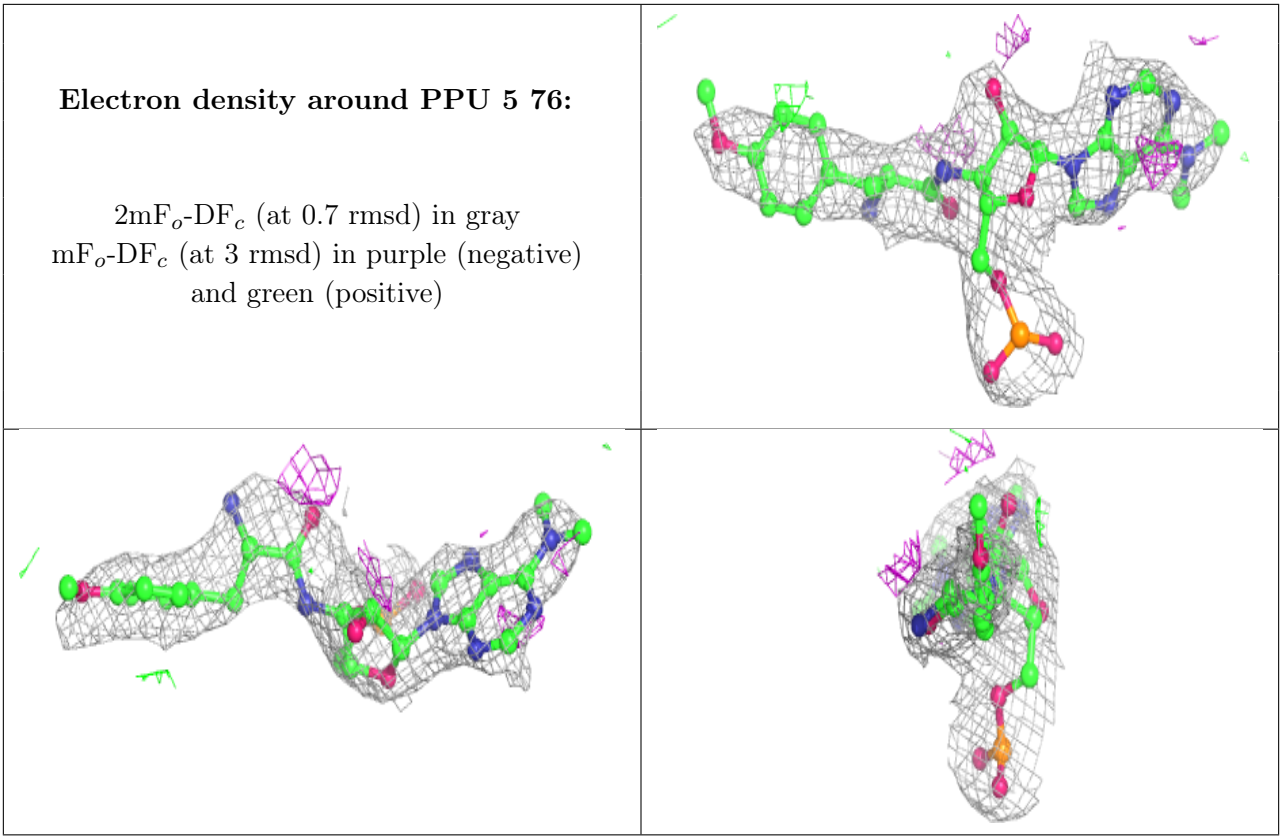
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	A	8007	1/1	0.97	0.03	28,28,28,28	0
32	MG	A	8110	1/1	0.97	0.07	30,30,30,30	0
35	CL	P	8508	1/1	0.98	0.32	82,82,82,82	0
32	MG	L	8069	1/1	0.98	0.09	81,81,81,81	0
34	NA	A	8376	1/1	0.98	0.17	79,79,79,79	0
32	MG	A	8020	1/1	0.98	0.05	46,46,46,46	0
32	MG	A	8015	1/1	0.98	0.05	50,50,50,50	0
34	NA	A	8315	1/1	0.98	0.16	43,43,43,43	0
34	NA	A	8305	1/1	0.98	0.09	27,27,27,27	0
32	MG	A	8098	1/1	0.98	0.18	33,33,33,33	0
32	MG	A	8084	1/1	0.98	0.05	50,50,50,50	0
32	MG	A	8036	1/1	0.98	0.06	38,38,38,38	0
32	MG	A	8107	1/1	0.98	0.06	36,36,36,36	0
32	MG	A	8011	1/1	0.99	0.13	24,24,24,24	0
32	MG	A	8005	1/1	0.99	0.07	38,38,38,38	0
32	MG	A	8086	1/1	0.99	0.09	49,49,49,49	0
32	MG	A	8080	1/1	0.99	0.06	35,35,35,35	0
32	MG	A	8025	1/1	0.99	0.06	40,40,40,40	0
32	MG	A	8026	1/1	0.99	0.05	33,33,33,33	0
37	CD	2	8402	1/1	0.99	0.07	57,57,57,57	0
32	MG	A	8019	1/1	0.99	0.07	30,30,30,30	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PPU 5 76:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.