wwPDB X-ray Structure Validation Summary Report (i)

Feb 3, 2025 – 10:27 PM EST

PDB ID	:	4JI5
Title	:	Crystal Structure of 30S ribosomal subunit from Thermus thermophilus
Authors	:	Demirci, H.; Wang, L.; Murphy IV, F.; Murphy, E.; Carr, J.; Blanchard, S.; Jogl, G.; Dahlberg, A.E.; Gregory, S.T.
Deposited on	:	2013-03-05
Resolution	:	3.85 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:

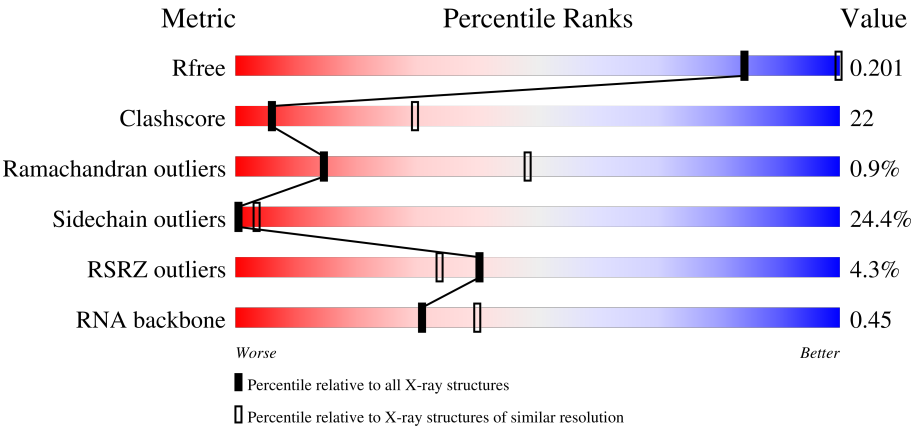
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.85 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}	164625	1056 (4.02-3.70)
Clashscore	180529	1117 (4.02-3.70)
Ramachandran outliers	177936	1077 (4.02-3.70)
Sidechain outliers	177891	1070 (4.02-3.70)
RSRZ outliers	164620	1056 (4.02-3.70)
RNA backbone	3690	1134 (4.70-3.00)

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	1522	3% 19% 39% 33% 9%
2	B	256	2% 42% 33% 14% 9%
3	C	239	2% 33% 40% 12% 14%
4	D	209	10% 41% 44% 15%

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Mol	Chain	Length	Quality of chain
5	E	162	6% 36% 43% 12% 7%
6	F	101	3% 38% 46% 17%
7	G	156	8% 53% 38% 9%
8	H	138	7% 41% 39% 20%
9	I	128	5% 40% 50% 9%
10	J	105	4% 30% 44% 16% 7%
11	K	129	2% 47% 36% 7% 10%
12	L	135	5% 39% 42% 11% 8%
13	M	126	7% 39% 43% 11% 6%
14	N	61	30% 44% 23%
15	O	89	34% 51% 13%
16	P	88	% 44% 43% 7% 6%
17	Q	105	10% 28% 48% 18% 6%
18	R	88	23% 41% 15% 20%
19	S	93	5% 34% 34% 16% 14%
20	T	106	5% 39% 38% 16% 7%
21	U	27	11% 59% 26% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1630	-	-	-	X
22	MG	A	1632	-	-	-	X
22	MG	A	1745	-	-	-	X
22	MG	A	1749	-	-	-	X
22	MG	A	1757	-	-	-	X
22	MG	K	201	-	-	-	X

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 52228 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 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1514	32687	14559	6046	10562	1520	0	6	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1534	C	A	conflict	GB M26923.1
A	1535	A	C	conflict	GB M26923.1

- Molecule 2 is a protein called RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	234	1900	1213	341	341	5	0	0	0

- Molecule 3 is a protein called RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	206	1612	1016	314	281	1	0	0	0

- Molecule 4 is a protein called RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	208	1703	1066	339	291	7	0	0	0

- Molecule 5 is a protein called RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	150	1146	724	217	201	4	0	0	0

- Molecule 6 is a protein called RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- Molecule 10 is a protein called RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 11 is a protein called RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			972	612	195	163	2			

- Molecule 13 is a protein called RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

- Molecule 14 is a protein called RIBOSOMAL PROTEIN S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 17 is a protein called RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

- Molecule 20 is a protein called RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	164	Total	Mg	0	0
			164	164		
22	D	1	Total	Mg	0	0
			1	1		
22	E	1	Total	Mg	0	0
			1	1		
22	F	1	Total	Mg	0	0
			1	1		
22	G	1	Total	Mg	0	0
			1	1		
22	H	1	Total	Mg	0	0
			1	1		
22	K	2	Total	Mg	0	0
			2	2		
22	S	1	Total	Mg	0	0
			1	1		

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	D	1	Total	Zn	0	0
			1	1		
23	N	1	Total	Zn	0	0
			1	1		

- Molecule 24 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	271	Total	O	0	0
			271	271		

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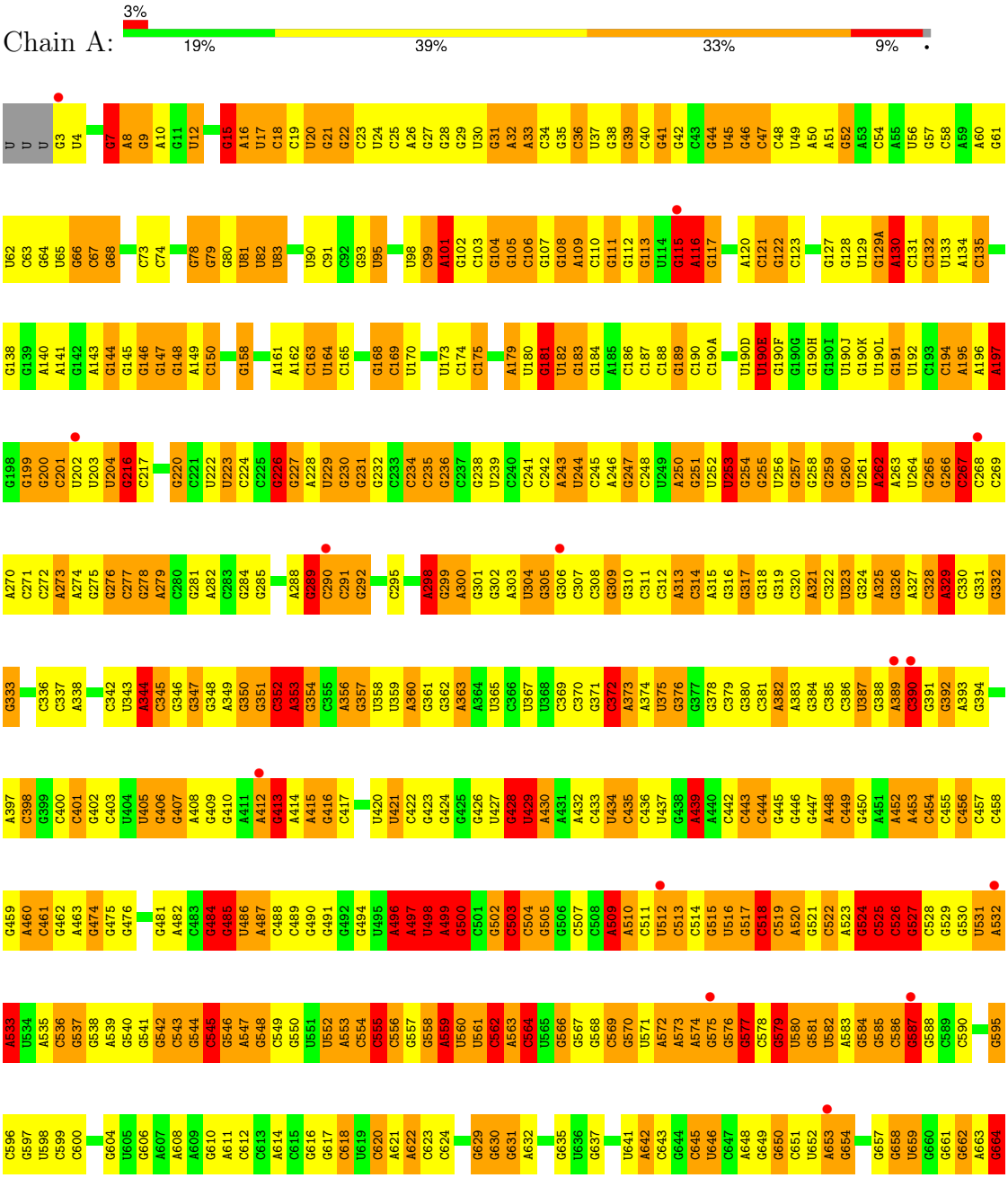
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total O 1 1	0	0
24	E	3	Total O 3 3	0	0
24	L	1	Total O 1 1	0	0
24	N	1	Total O 1 1	0	0
24	P	1	Total O 1 1	0	0
24	T	1	Total O 1 1	0	0

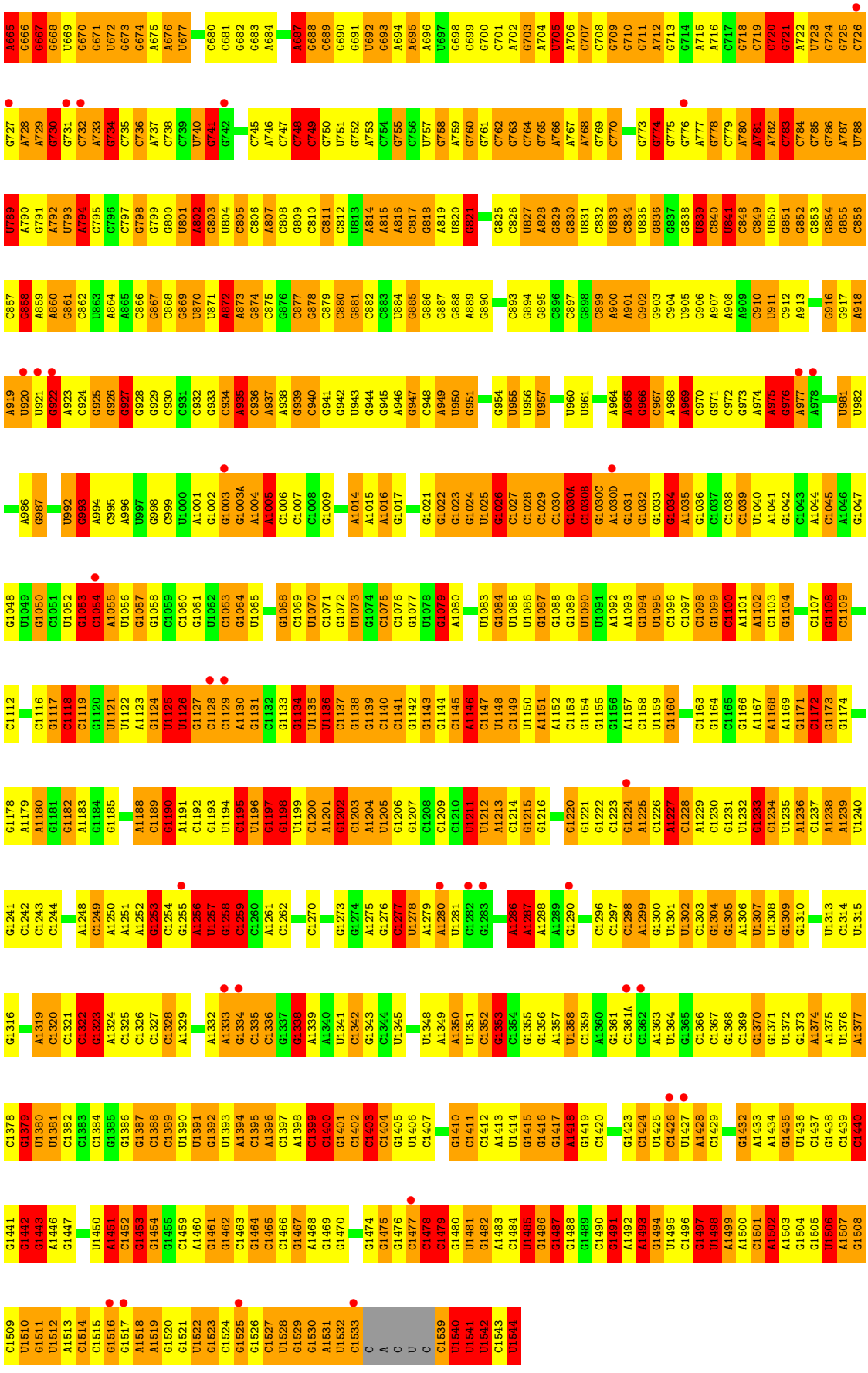
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

Chain A:

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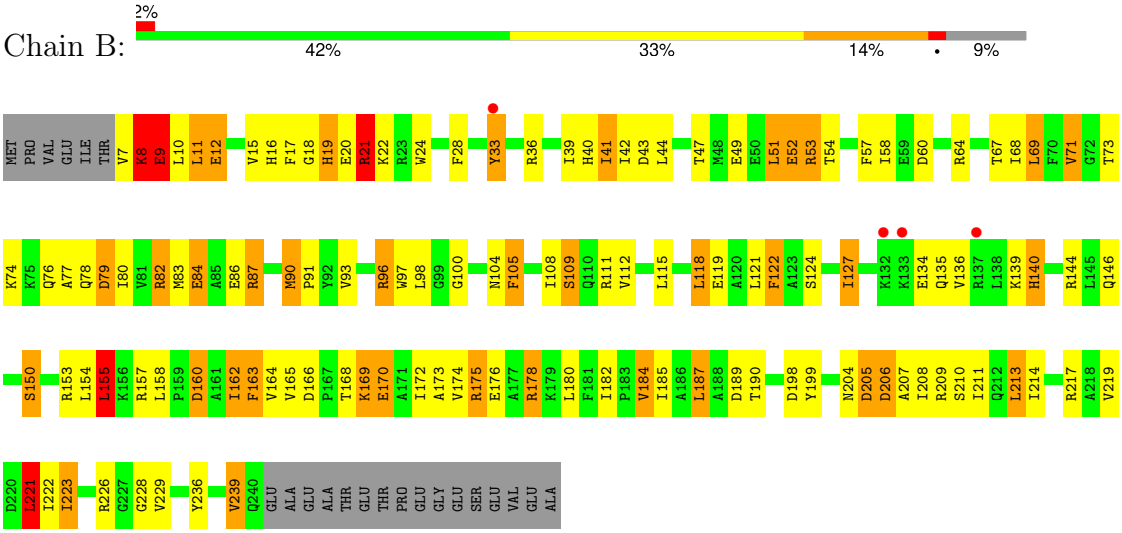
G727 A728 A729 G730 G731 C732 A733 G734 C735 C736 A737 C738 C739 U740 G741 G742 C745 A746 C747 C748 C749 G750 U751 G752 A753 C754 G755 C756 U757 G758 A759 G760 G761 C762 G763 C764 G765 A766 A767 A768 G769 C770 G773 G774 G775 G776 A777 G778 C779 A780 A781 A782 C783 C784 G785 G786 A787 U788
U789 A790 G791 A792 U793 A794 C795 C796 C797 G798 G799 G800 U801 A802 G803 U804 C805 C806 A807 C808 G809 C810 C811 C812 U813 A814 A815 A816 C817 G818 A819 U820 G821 G825 C826 U827 A828 G829 G830 U831 C832 U833 C834 U835 G836 G837 G838 U839 C840 U841 C848 G849 U850 G851 G852 G853 G854 G855 C856
C857 G858 A859 A860 G861 C862 U863 A864 A865 C866 G867 C868 G869 U870 U871 A872 A873 G874 C875 G876 C877 G878 C879 C880 G881 C882 C883 U884 G885 G886 G887 G888 A889 G890 C893 G894 G895 G896 C897 G898 C899 A900 A901 G902 G903 C904 U905 G906 A907 A908 A909 C910 U911 C912 A913 G916 G917 A918
A919 U920 U921 G922 A923 C924 G925 G926 G927 G928 G929 C930 C931 C932 G933 C934 A935 C936 A937 A938 G939 C940 G941 G942 U943 G944 G945 A946 G947 C948 A949 U950 G951 G954 U955 U956 U957 U960 U961 A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 U981 U982
A986 G987 U992 G993 A994 C995 A996 U997 G998 C999 U1000 A1001 G1002 G1003 G1003A A1004 A1005 C1006 C1007 C1008 G1009 A1014 A1015 A1016 G1017 G1021 G1022 G1023 G1024 U1025 G1026 C1027 C1028 C1029 C1030 G1030A C1030B G1030C A1030D G1031 G1032 G1033 G1034 A1035 G1036 C1037 C1038 C1039 U1040 A1041 G1042 C1043 A1044 C1045 A1046 G1047
G1048 U1049 G1050 C1051 U1052 G1053 C1054 A1055 U1056 G1057 G1058 C1059 C1060 G1061 U1062 C1063 G1064 U1065 G1068 C1069 U1070 C1071 C1072 U1073 G1074 C1075 C1076 G1077 U1078 G1079 A1080 U1083 G1084 U1085 U1086 G1087 G1088 G1089 U1090 U1091 A1092 A1093 G1094 U1095 C1096 C1097 C1098 G1099 C1100 A1101 A1102 C1103 G1104 C1107 G1108 C1109
C1112 C1116 G1117 C1118 C1119 G1120 U1121 U1122 A1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 C1132 G1133 G1134 U1135 U1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 G1154 G1155 G1156 A1157 C1158 U1159 G1160 C1163 G1164 C1165 G1166 A1167 A1168 A1169 C1171 C1172 G1173 G1174
G1178 A1179 A1180 G1181 G1182 A1183 G1184 G1185 A1188 C1189 G1190 A1191 C1192 G1193 U1194 C1195 U1196 G1197 G1198 U1199 C1200 A1201 G1202 C1203 A1204 U1205 G1206 G1207 C1208 C1209 C1210 U1211 U1212 A1213 C1214 G1215 G1216 G1220 G1221 G1222 C1223 G1224 A1225 C1226 A1227 C1228 A1229 C1230 G1231 U1232 G1233 C1234 U1235 A1236 C1237 A1238 A1239 U1240
G1241 C1242 C1243 C1244 A1248 C1249 A1250 A1251 A1252 G1253 C1254 G1255 A1256 U1257 G1258 C1259 C1260 A1261 C1262 C1270 G1273 G1274 A1275 G1276 C1277 U1278 A1279 A1280 U1281 C1282 G1283 A1286 A1287 A1288 A1289 G1290 C1296 C1297 C1298 A1299 G1300 U1301 U1302 C1303 G1304 G1305 A1306 U1307 U1308 G1309 G1310 U1313 C1314 U1315
G1316 A1319 C1320 C1321 C1322 G1323 A1324 C1325 C1326 C1327 C1328 A1329 A1332 A1333 G1334 C1335 C1336 G1337 G1338 A1339 A1340 U1341 C1342 G1343 C1344 U1345 U1348 A1349 A1350 U1351 C1352 G1353 C1354 G1355 G1356 A1357 U1358 C1359 A1360 G1361 C1361A C1362 A1363 U1364 G1365 C1366 C1367 G1368 C1369 G1370 G1371 U1372 G1373 A1374 A1375 U1376 A1377
C1378 G1379 U1380 U1381 C1382 C1383 C1384 G1385 C1386 G1387 C1388 C1389 U1390 U1391 C1392 U1393 A1394 C1395 A1396 C1397 A1398 C1399 C1400 G1401 C1402 C1403 C1404 G1405 U1406 C1407 G1410 C1411 C1412 A1413 U1414 G1415 G1416 G1417 A1418 G1419 C1420 G1423 C1424 U1425 C1426 U1427 A1428 C1429 G1432 A1433 A1434 G1435 U1436 C1437 C1438 C1439 C1440
G1441 G1442 G1443 A1446 G1447 U1450 A1451 C1452 G1453 G1454 G1455 C1459 A1460 G1461 G1462 C1463 G1464 C1465 C1466 G1467 A1468 G1469 G1470 G1474 G1475 G1476 C1477 C1478 C1479 G1480 U1481 G1482 A1483 C1484 U1485 G1486 G1487 G1488 G1489 C1490 G1491 A1492 A1493 G1494 U1495 C1496 G1497 U1498 A1499 A1500 C1501 A1502 A1503 G1504 G1505 U1506 A1507 G1508
C1509 U1510 G1511 U1512 A1513 C1514 C1515 G1516 G1517 A1518 A1519 G1520 G1521 U1522 G1523 C1524 G1525 G1526 C1527 U1528 G1529 G1530 A1531 U1532 C1533 C A C U C C1539 U1540 U1541 U1542 C1543 U1544

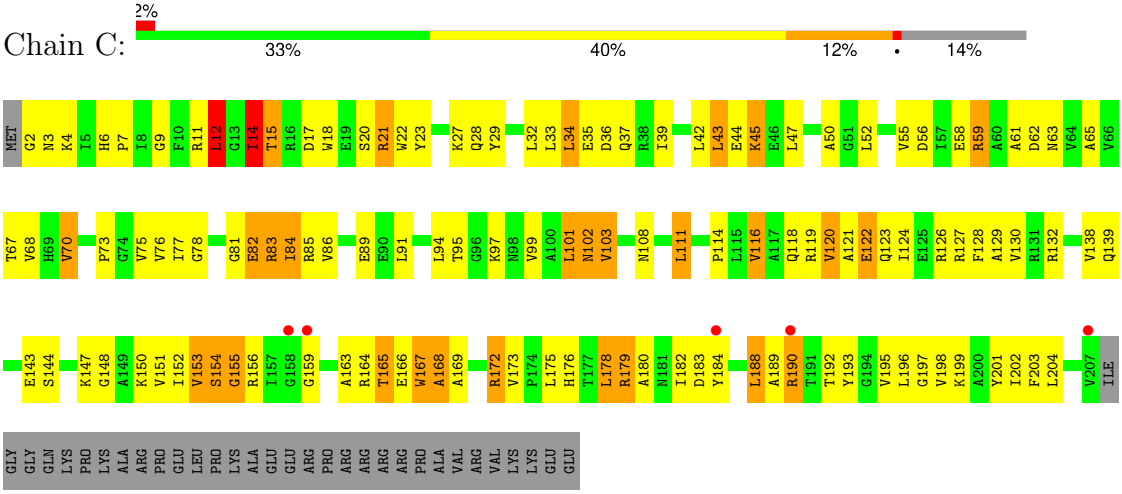
• Molecule 2: RIBOSOMAL PROTEIN S2

Chain B:



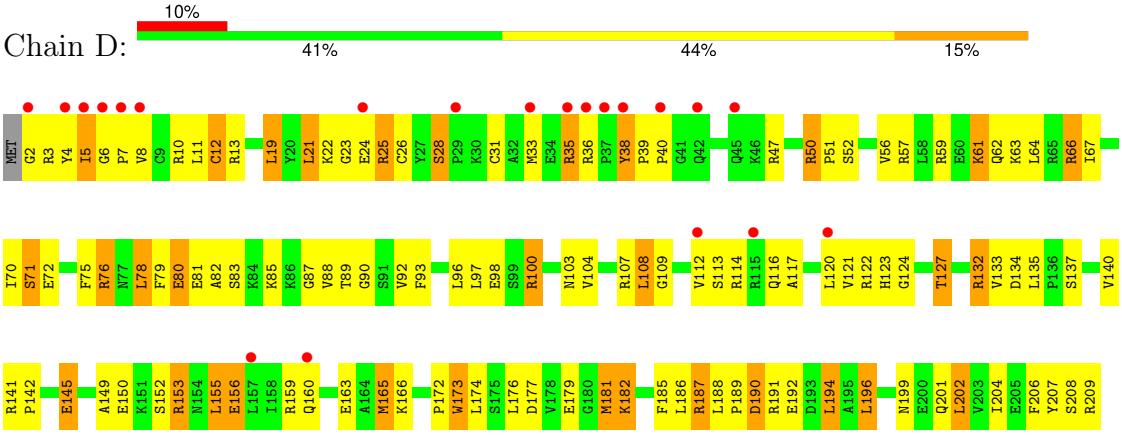
• Molecule 3: RIBOSOMAL PROTEIN S3

Chain C:



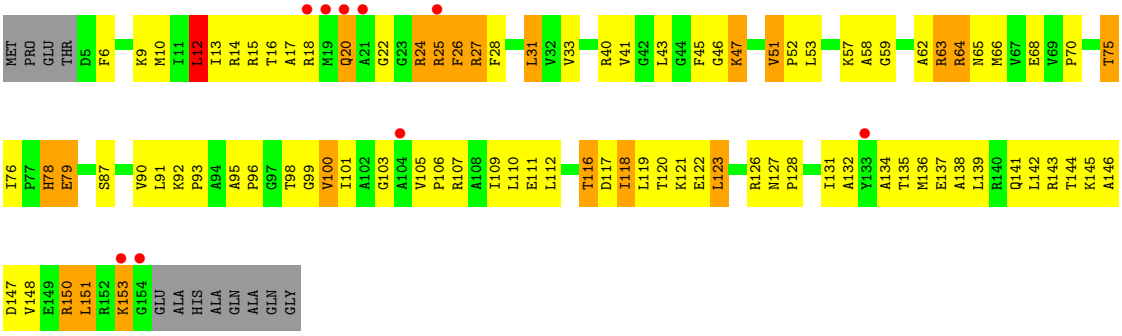
• Molecule 4: RIBOSOMAL PROTEIN S4

Chain D:



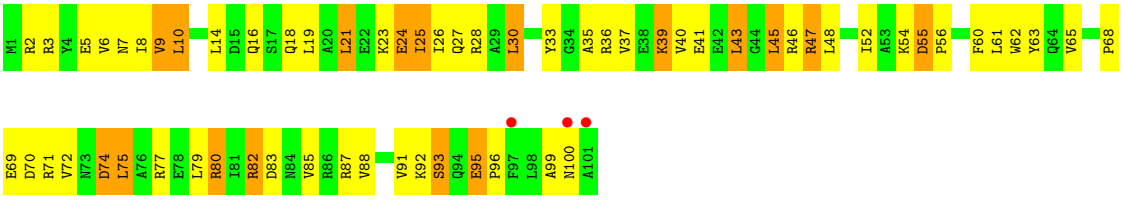
• Molecule 5: RIBOSOMAL PROTEIN S5

Chain E:



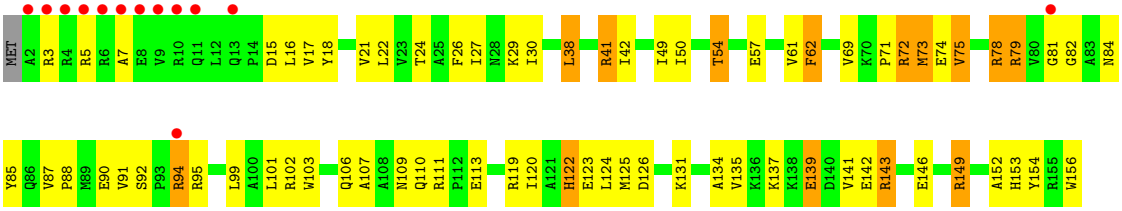
• Molecule 6: RIBOSOMAL PROTEIN S6

Chain F:



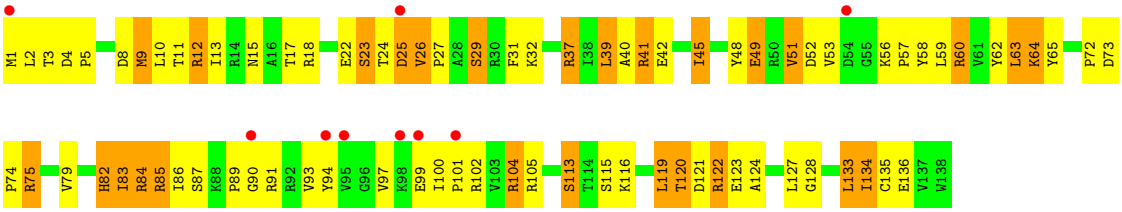
• Molecule 7: RIBOSOMAL PROTEIN S7

Chain G:



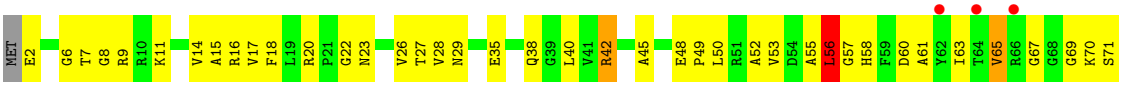
• Molecule 8: RIBOSOMAL PROTEIN S8

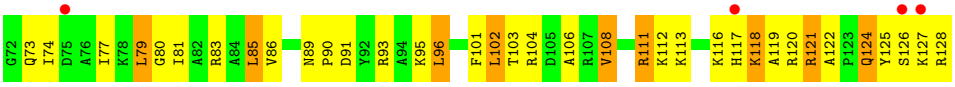
Chain H:



• Molecule 9: RIBOSOMAL PROTEIN S9

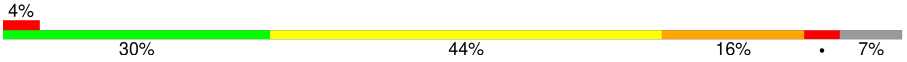
Chain I:

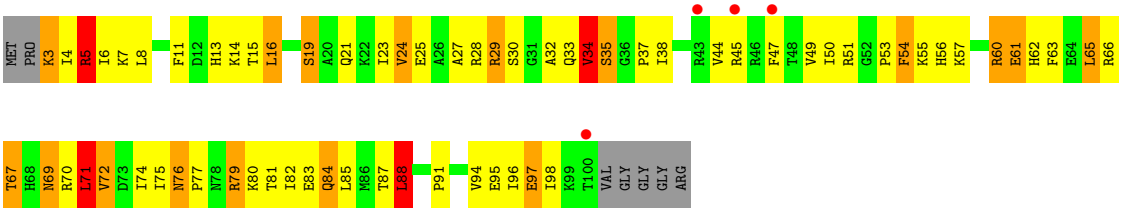




• Molecule 10: RIBOSOMAL PROTEIN S10

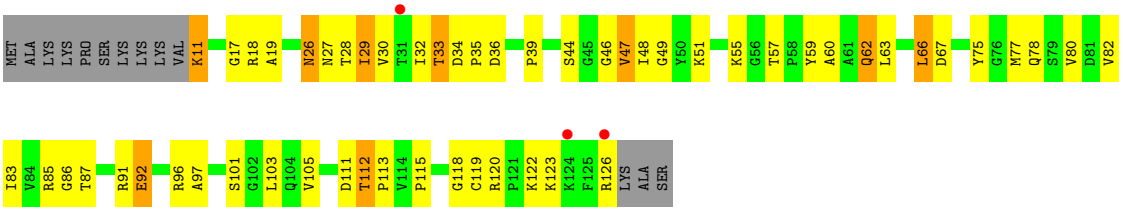
Chain J:





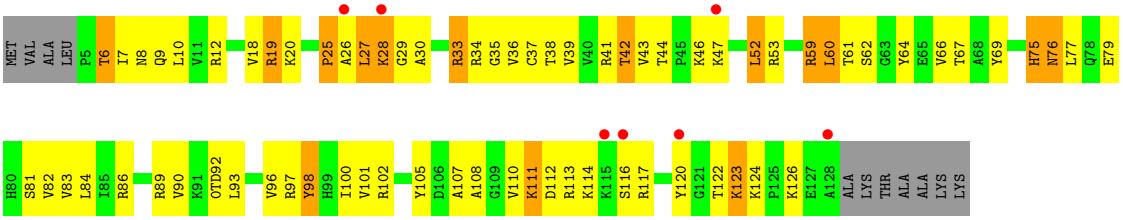
• Molecule 11: RIBOSOMAL PROTEIN S11

Chain K:



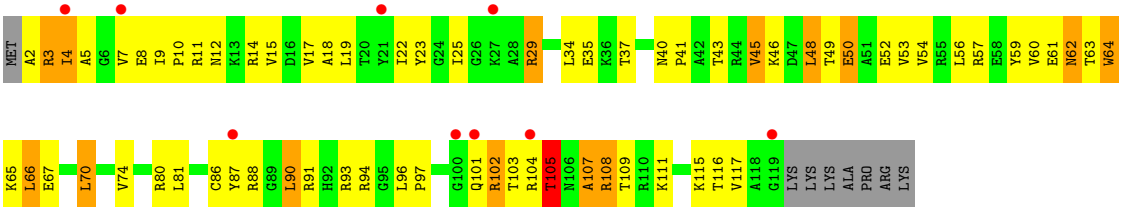
• Molecule 12: RIBOSOMAL PROTEIN S12

Chain L:



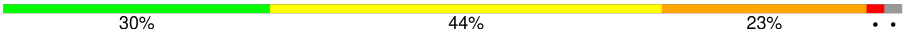
• Molecule 13: RIBOSOMAL PROTEIN S13

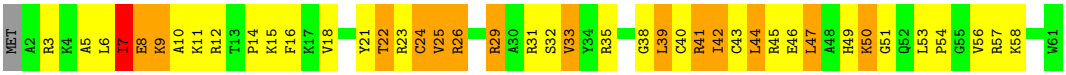
Chain M:



• Molecule 14: RIBOSOMAL PROTEIN S14

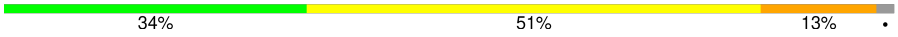
Chain N:

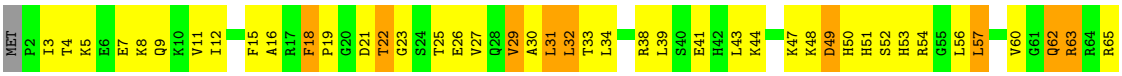


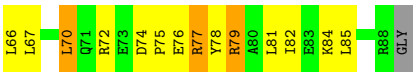


• Molecule 15: RIBOSOMAL PROTEIN S15

Chain O:

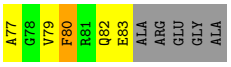






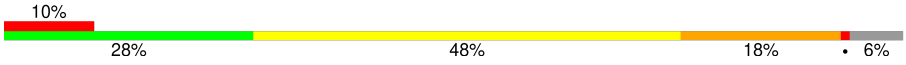
• Molecule 16: RIBOSOMAL PROTEIN S16

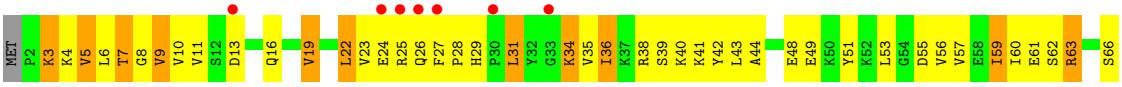
Chain P:

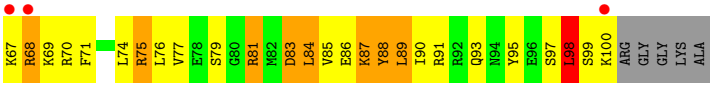


• Molecule 17: RIBOSOMAL PROTEIN S17

Chain Q:

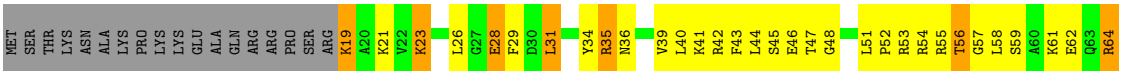


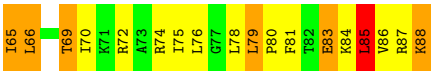




• Molecule 18: RIBOSOMAL PROTEIN S18

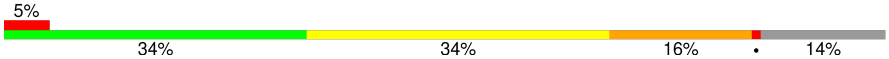
Chain R:

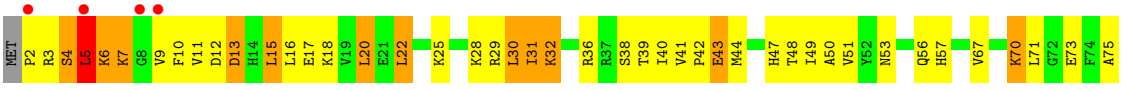




• Molecule 19: RIBOSOMAL PROTEIN S19

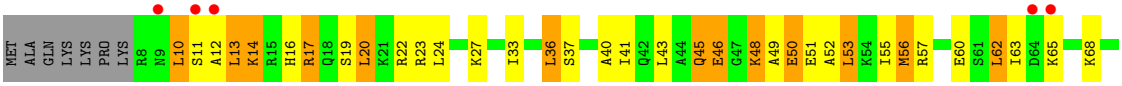
Chain S:

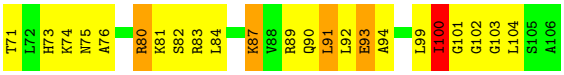




• Molecule 20: RIBOSOMAL PROTEIN S20

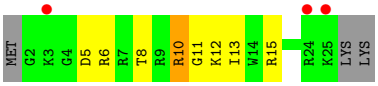
Chain T:





• Molecule 21: RIBOSOMAL PROTEIN THX

Chain U:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	399.62Å 399.62Å 216.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.29 – 3.85 47.29 – 3.85	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.29-3.85) 99.2 (47.29-3.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 3.88Å)	Xtriage
Refinement program	PHENIX dev_1119	Depositor
R, R_{free}	0.153 , 0.202 0.154 , 0.201	Depositor DCC
R_{free} test set	8213 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	157.0	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 161.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	52228	wwPDB-VP
Average B, all atoms (Å^2)	162.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% 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: MA6, MG, 4OC, UR3, 2MG, 7MG, 0TD, ZN, PSU, M2G, 5MC

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	1.18	129/36187 (0.4%)	2.02	1881/56471 (3.3%)
2	B	0.76	0/1935	1.00	6/2609 (0.2%)
3	C	0.79	0/1636	0.98	6/2205 (0.3%)
4	D	0.77	1/1733 (0.1%)	0.97	1/2318 (0.0%)
5	E	0.82	0/1162	1.05	4/1564 (0.3%)
6	F	0.83	0/856	1.02	3/1154 (0.3%)
7	G	0.73	0/1276	0.87	1/1709 (0.1%)
8	H	0.83	0/1136	0.98	0/1527
9	I	0.63	0/1029	0.88	1/1379 (0.1%)
10	J	0.77	0/805	1.03	4/1082 (0.4%)
11	K	0.71	0/879	0.91	0/1187
12	L	0.97	2/977 (0.2%)	1.15	2/1306 (0.2%)
13	M	0.59	0/947	0.84	0/1270
14	N	0.77	0/501	1.04	3/664 (0.5%)
15	O	0.69	0/740	0.94	0/987
16	P	0.74	0/716	0.92	0/963
17	Q	0.87	0/836	1.05	3/1117 (0.3%)
18	R	0.71	0/579	0.99	2/768 (0.3%)
19	S	0.60	0/661	1.01	4/890 (0.4%)
20	T	0.74	0/765	1.03	2/1007 (0.2%)
21	U	0.71	0/212	0.83	0/277
All	All	1.06	132/55568 (0.2%)	1.76	1923/82454 (2.3%)

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
2	B	0	2
3	C	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1
9	I	0	2
10	J	0	2
13	M	0	3
14	N	0	1
16	P	0	1
20	T	0	3
All	All	0	18

The worst 5 of 132 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	672	U	C4-O4	8.76	1.30	1.23
1	A	563	A	N9-C4	-7.63	1.33	1.37
1	A	729	A	N3-C4	-7.49	1.30	1.34
1	A	1512	U	C4-O4	7.36	1.29	1.23
1	A	372	C	C2-O2	7.33	1.31	1.24

The worst 5 of 1923 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1528	U	O5'-P-OP2	-17.17	90.09	110.70
1	A	309	G	N1-C6-O6	16.92	130.05	119.90
1	A	922	G	N1-C6-O6	15.33	129.10	119.90
1	A	558	G	C5-C6-N1	-15.09	103.95	111.50
1	A	1335	C	N1-C2-O2	14.44	127.56	118.90

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	8	LYS	Peptide
2	B	9	GLU	Peptide
3	C	154	SER	Peptide
3	C	166	GLU	Peptide
3	C	168	ALA	Peptide

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	32687	0	16528	920	0
2	B	1900	0	1951	96	0
3	C	1612	0	1677	97	0
4	D	1703	0	1763	104	0
5	E	1146	0	1207	78	0
6	F	843	0	857	62	0
7	G	1257	0	1296	69	0
8	H	1116	0	1177	74	0
9	I	1010	0	1037	65	0
10	J	792	0	835	73	0
11	K	864	0	881	44	0
12	L	972	0	1058	59	0
13	M	937	0	995	59	0
14	N	492	0	529	47	0
15	O	729	0	768	49	0
16	P	700	0	720	34	0
17	Q	823	0	891	55	0
18	R	574	0	644	49	0
19	S	647	0	673	48	0
20	T	763	0	861	51	0
21	U	208	0	221	9	0
22	A	164	0	0	0	0
22	D	1	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	G	1	0	0	0	0
22	H	1	0	0	0	0
22	K	2	0	0	0	0
22	S	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	271	0	0	14	0
24	C	1	0	0	0	0
24	E	3	0	0	0	0
24	L	1	0	0	0	0
24	N	1	0	0	0	0
24	P	1	0	0	0	0
24	T	1	0	0	0	0
All	All	52228	0	36569	1946	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 22.

The worst 5 of 1946 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.48	0.95
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.49	0.94
1:A:664:G:H22	1:A:741:G:H1	1.17	0.92
1:A:1002:G:N1	1:A:1003(A):G:O6	2.04	0.91
4:D:187:ARG:HH22	4:D:188:LEU:HD12	1.36	0.91

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
2	B	232/256 (91%)	198 (85%)	29 (12%)	5 (2%)	5 32
3	C	204/239 (85%)	175 (86%)	27 (13%)	2 (1%)	13 46
4	D	206/209 (99%)	190 (92%)	16 (8%)	0	100 100
5	E	148/162 (91%)	139 (94%)	6 (4%)	3 (2%)	6 34
6	F	99/101 (98%)	97 (98%)	2 (2%)	0	100 100
7	G	153/156 (98%)	137 (90%)	16 (10%)	0	100 100
8	H	136/138 (99%)	127 (93%)	9 (7%)	0	100 100
9	I	125/128 (98%)	111 (89%)	12 (10%)	2 (2%)	8 37
10	J	96/105 (91%)	81 (84%)	13 (14%)	2 (2%)	5 33
11	K	114/129 (88%)	99 (87%)	15 (13%)	0	100 100
12	L	121/135 (90%)	106 (88%)	12 (10%)	3 (2%)	4 30
13	M	116/126 (92%)	94 (81%)	21 (18%)	1 (1%)	14 48
14	N	58/61 (95%)	48 (83%)	10 (17%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	O	85/89 (96%)	78 (92%)	7 (8%)	0	100 100
16	P	81/88 (92%)	70 (86%)	11 (14%)	0	100 100
17	Q	97/105 (92%)	89 (92%)	8 (8%)	0	100 100
18	R	68/88 (77%)	59 (87%)	9 (13%)	0	100 100
19	S	78/93 (84%)	67 (86%)	9 (12%)	2 (3%)	4 29
20	T	97/106 (92%)	79 (81%)	16 (16%)	2 (2%)	5 33
21	U	22/27 (82%)	21 (96%)	1 (4%)	0	100 100
All	All	2336/2541 (92%)	2065 (88%)	249 (11%)	22 (1%)	14 48

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
12	L	28	LYS
19	S	31	ILE
2	B	9	GLU
3	C	62	ASP

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
2	B	202/220 (92%)	150 (74%)	52 (26%)	0 3
3	C	160/188 (85%)	121 (76%)	39 (24%)	0 3
4	D	180/181 (99%)	135 (75%)	45 (25%)	0 3
5	E	115/123 (94%)	88 (76%)	27 (24%)	0 4
6	F	90/90 (100%)	72 (80%)	18 (20%)	1 6
7	G	126/127 (99%)	103 (82%)	23 (18%)	1 9
8	H	119/119 (100%)	83 (70%)	36 (30%)	0 2
9	I	98/99 (99%)	77 (79%)	21 (21%)	1 5
10	J	87/92 (95%)	63 (72%)	24 (28%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	K	88/99 (89%)	69 (78%)	19 (22%)	1 5
12	L	103/110 (94%)	78 (76%)	25 (24%)	0 3
13	M	94/101 (93%)	71 (76%)	23 (24%)	0 3
14	N	49/50 (98%)	34 (69%)	15 (31%)	0 2
15	O	79/80 (99%)	61 (77%)	18 (23%)	0 4
16	P	72/74 (97%)	61 (85%)	11 (15%)	2 13
17	Q	94/97 (97%)	64 (68%)	30 (32%)	0 1
18	R	61/77 (79%)	45 (74%)	16 (26%)	0 3
19	S	71/80 (89%)	52 (73%)	19 (27%)	0 3
20	T	76/82 (93%)	54 (71%)	22 (29%)	0 2
21	U	19/22 (86%)	18 (95%)	1 (5%)	19 45
All	All	1983/2111 (94%)	1499 (76%)	484 (24%)	0 3

5 of 484 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	102	ARG
19	S	5	LEU
11	K	26	ASN
18	R	83	GLU
20	T	48	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	13	HIS
10	J	33	GLN
20	T	16	HIS
15	O	62	GLN
9	I	29	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1505/1522 (98%)	357 (23%)	27 (1%)

5 of 357 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	7	G
1	A	9	G
1	A	12	U
1	A	15	G

5 of 27 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	559	A
1	A	992	U
1	A	1319	A
1	A	793	U
1	A	1125	U

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

17 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	MA6	A	1519[A]	1	19,26,27	1.23	3 (15%)	18,38,41	0.89	0
1	PSU	A	516	1,22	18,21,22	1.28	3 (16%)	21,30,33	1.14	3 (14%)
1	M2G	A	966	1	20,27,28	1.57	2 (10%)	19,40,43	1.51	2 (10%)
1	MA6	A	1518[B]	1	19,26,27	1.43	4 (21%)	18,38,41	0.82	0
12	0TD	L	92	12	8,9,10	1.58	1 (12%)	6,11,13	2.34	2 (33%)
1	MA6	A	1519[B]	1	19,26,27	1.86	5 (26%)	18,38,41	0.76	0
1	7MG	A	527	1	23,26,27	3.88	6 (26%)	27,39,42	2.37	8 (29%)
1	UR3	A	1498	1	19,22,23	1.33	3 (15%)	26,32,35	1.42	4 (15%)
1	4OC	A	1402	1	20,23,24	1.14	2 (10%)	25,32,35	0.98	2 (8%)
1	5MC	A	1400	1	19,22,23	1.56	5 (26%)	26,32,35	1.15	4 (15%)
1	PSU	A	1540	1	18,21,22	1.01	1 (5%)	21,30,33	1.64	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	5MC	A	1407	1	19,22,23	1.08	2 (10%)	26,32,35	1.29	2 (7%)
1	2MG	A	1207	1,22	18,26,27	1.39	2 (11%)	16,38,41	1.23	2 (12%)
1	PSU	A	1541	1	18,21,22	1.08	3 (16%)	21,30,33	1.94	6 (28%)
1	5MC	A	1404	1	19,22,23	1.40	3 (15%)	26,32,35	1.15	3 (11%)
1	5MC	A	967	1	19,22,23	1.14	2 (10%)	26,32,35	1.15	3 (11%)
1	MA6	A	1518[A]	1	19,26,27	1.24	1 (5%)	18,38,41	0.83	1 (5%)

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	MA6	A	1519[A]	1	-	4/7/29/30	0/3/3/3
1	PSU	A	516	1,22	-	0/7/25/26	0/2/2/2
1	M2G	A	966	1	-	2/7/29/30	0/3/3/3
1	MA6	A	1518[B]	1	-	6/7/29/30	0/3/3/3
12	0TD	L	92	12	-	3/7/12/14	-
1	MA6	A	1519[B]	1	-	4/7/29/30	0/3/3/3
1	7MG	A	527	1	-	1/7/37/38	0/3/3/3
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1,22	-	0/5/27/28	0/3/3/3
1	PSU	A	1541	1	-	3/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	3/7/29/30	0/3/3/3

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-16.46	1.35	1.45
1	A	1519[B]	MA6	C6-N1	5.09	1.39	1.32
1	A	527	7MG	C5-N7	4.67	1.41	1.35
1	A	1518[A]	MA6	C6-C5	-4.57	1.37	1.44
1	A	1207	2MG	C5-C6	-4.27	1.39	1.47

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	527	7MG	C5-C6-N1	5.06	119.84	110.94
12	L	92	0TD	CSB-SB-CB	-4.67	93.96	102.36
1	A	527	7MG	N9-C8-N7	4.66	109.97	103.37
1	A	527	7MG	C2-N3-C4	4.54	120.12	112.30
1	A	527	7MG	C5-C4-N3	-4.43	119.81	128.13

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1518[A]	MA6	O4'-C4'-C5'-O5'
1	A	1518[A]	MA6	C3'-C4'-C5'-O5'

There are no ring outliers.

14 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1519[A]	MA6	2	0
1	A	516	PSU	1	0
1	A	966	M2G	2	0
1	A	1518[B]	MA6	4	0
1	A	1519[B]	MA6	4	0
1	A	527	7MG	3	0
1	A	1498	UR3	1	0
1	A	1402	4OC	1	0
1	A	1400	5MC	2	0
1	A	1540	PSU	1	0
1	A	1541	PSU	1	0
1	A	1404	5MC	2	0
1	A	967	5MC	5	0
1	A	1518[A]	MA6	3	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 174 ligands modelled in this entry, 174 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	1500/1522 (98%)	-0.27	47 (3%) 51 40	59, 152, 229, 333	4 (0%)
2	B	234/256 (91%)	-0.48	4 (1%) 69 52	122, 170, 240, 274	0
3	C	206/239 (86%)	-0.12	5 (2%) 59 46	121, 156, 199, 229	0
4	D	208/209 (99%)	0.16	21 (10%) 14 15	104, 151, 206, 237	0
5	E	150/162 (92%)	-0.12	9 (6%) 29 26	93, 132, 172, 216	0
6	F	101/101 (100%)	-0.15	3 (2%) 52 41	135, 171, 201, 254	0
7	G	155/156 (99%)	0.05	13 (8%) 18 18	145, 183, 228, 254	0
8	H	138/138 (100%)	-0.11	9 (6%) 26 24	114, 143, 181, 226	0
9	I	127/128 (99%)	0.12	7 (5%) 32 27	149, 182, 222, 246	0
10	J	98/105 (93%)	0.23	4 (4%) 42 34	136, 186, 225, 252	0
11	K	116/129 (89%)	-0.01	3 (2%) 57 44	134, 168, 207, 226	0
12	L	123/135 (91%)	-0.10	7 (5%) 30 27	106, 137, 168, 224	0
13	M	118/126 (93%)	0.10	9 (7%) 21 20	149, 192, 225, 299	0
14	N	60/61 (98%)	0.01	0 100 100	133, 161, 214, 240	0
15	O	87/89 (97%)	-0.56	0 100 100	128, 160, 194, 201	0
16	P	83/88 (94%)	-0.20	1 (1%) 76 60	126, 148, 181, 205	0
17	Q	99/105 (94%)	0.41	10 (10%) 14 15	120, 144, 178, 199	0
18	R	70/88 (79%)	-0.56	0 100 100	131, 165, 237, 266	0
19	S	80/93 (86%)	-0.01	5 (6%) 27 25	157, 197, 240, 268	0
20	T	99/106 (93%)	0.33	5 (5%) 34 30	123, 154, 196, 214	0
21	U	24/27 (88%)	1.05	3 (12%) 9 13	172, 194, 241, 254	0
All	All	3876/4063 (95%)	-0.13	165 (4%) 40 34	59, 159, 221, 333	4 (0%)

The worst 5 of 165 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	8	GLU	15.5
7	G	6	ARG	10.8
7	G	9	VAL	8.7
1	A	1516[A]	G	8.5
7	G	11	GLN	8.0

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PSU	A	1540	20/21	0.89	0.18	234,259,275,280	0
1	2MG	A	1207	24/25	0.93	0.08	148,156,161,163	0
1	MA6	A	1518[A]	24/25	0.93	0.19	109,121,135,142	24
1	MA6	A	1518[B]	24/25	0.93	0.19	126,134,140,141	24
1	PSU	A	516	20/21	0.93	0.07	143,152,163,165	0
1	PSU	A	1541	20/21	0.93	0.15	232,243,250,252	0
1	7MG	A	527	24/25	0.94	0.09	127,137,152,160	0
1	M2G	A	966	25/26	0.96	0.12	120,145,181,186	0
1	4OC	A	1402	22/23	0.96	0.09	117,134,153,154	0
1	5MC	A	1407	21/22	0.96	0.06	140,145,154,161	0
1	UR3	A	1498	21/22	0.96	0.12	115,130,138,144	0
1	5MC	A	1400	21/22	0.97	0.07	106,127,151,157	0
1	MA6	A	1519[A]	24/25	0.98	0.11	104,118,124,129	24
1	MA6	A	1519[B]	24/25	0.98	0.11	105,117,131,134	24
1	5MC	A	967	21/22	0.98	0.07	134,149,157,162	0
1	5MC	A	1404	21/22	0.98	0.17	132,137,141,146	0
12	0TD	L	92	10/11	0.99	0.07	130,141,148,274	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1632	1/1	-0.09	0.54	161,161,161,161	0
22	MG	A	1732	1/1	0.08	0.34	161,161,161,161	0
22	MG	A	1731	1/1	0.34	0.29	185,185,185,185	0
22	MG	A	1730	1/1	0.34	0.23	181,181,181,181	0
22	MG	A	1733	1/1	0.35	0.30	143,143,143,143	0
22	MG	A	1653	1/1	0.51	0.35	100,100,100,100	0
22	MG	A	1746	1/1	0.51	0.20	185,185,185,185	0
22	MG	G	201	1/1	0.51	0.38	157,157,157,157	0
22	MG	A	1630	1/1	0.52	0.47	127,127,127,127	0
22	MG	A	1749	1/1	0.58	0.41	134,134,134,134	0
22	MG	A	1650	1/1	0.60	0.34	120,120,120,120	0
22	MG	A	1728	1/1	0.62	0.32	120,120,120,120	0
22	MG	A	1684	1/1	0.62	0.23	128,128,128,128	0
22	MG	A	1755	1/1	0.69	0.10	148,148,148,148	0
22	MG	A	1706	1/1	0.70	0.13	400,400,400,400	0
22	MG	A	1671	1/1	0.70	0.22	108,108,108,108	0
22	MG	A	1737	1/1	0.72	0.28	143,143,143,143	0
22	MG	A	1639	1/1	0.73	0.16	133,133,133,133	0
22	MG	A	1757	1/1	0.73	0.43	121,121,121,121	0
22	MG	A	1673	1/1	0.73	0.24	121,121,121,121	0
22	MG	A	1675	1/1	0.74	0.35	95,95,95,95	0
22	MG	A	1735	1/1	0.74	0.17	143,143,143,143	0
22	MG	A	1734	1/1	0.75	0.22	136,136,136,136	0
22	MG	A	1619	1/1	0.76	0.19	132,132,132,132	0
22	MG	A	1628	1/1	0.76	0.18	127,127,127,127	0
22	MG	F	201	1/1	0.76	0.28	127,127,127,127	0
22	MG	A	1750	1/1	0.76	0.35	137,137,137,137	0
22	MG	A	1752	1/1	0.77	0.19	156,156,156,156	0
22	MG	A	1679	1/1	0.79	0.23	140,140,140,140	0
22	MG	A	1647	1/1	0.79	0.13	141,141,141,141	0
22	MG	A	1736	1/1	0.79	0.26	112,112,112,112	0
22	MG	A	1745	1/1	0.80	0.44	107,107,107,107	0
22	MG	A	1762	1/1	0.80	0.18	136,136,136,136	0
22	MG	K	201	1/1	0.80	0.62	93,93,93,93	0
22	MG	A	1751	1/1	0.81	0.40	170,170,170,170	0
22	MG	A	1674	1/1	0.81	0.26	114,114,114,114	0
22	MG	A	1741	1/1	0.82	0.18	111,111,111,111	0
22	MG	A	1754	1/1	0.83	0.17	121,121,121,121	0
22	MG	A	1631	1/1	0.83	0.10	277,277,277,277	0
22	MG	A	1756	1/1	0.83	0.10	132,132,132,132	0
22	MG	A	1726	1/1	0.83	0.08	127,127,127,127	0
22	MG	A	1711	1/1	0.84	0.11	398,398,398,398	0
22	MG	A	1760	1/1	0.84	0.07	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1758	1/1	0.85	0.41	139,139,139,139	0
22	MG	A	1693	1/1	0.85	0.30	94,94,94,94	0
22	MG	A	1748	1/1	0.85	0.40	97,97,97,97	0
22	MG	A	1698	1/1	0.85	0.10	424,424,424,424	0
22	MG	A	1617	1/1	0.85	0.36	109,109,109,109	0
22	MG	A	1622	1/1	0.85	0.18	88,88,88,88	0
22	MG	S	101	1/1	0.85	0.15	137,137,137,137	0
22	MG	A	1761	1/1	0.86	0.10	148,148,148,148	0
22	MG	A	1607	1/1	0.86	0.10	134,134,134,134	0
22	MG	A	1738	1/1	0.87	0.30	126,126,126,126	0
22	MG	A	1764	1/1	0.87	0.18	132,132,132,132	0
22	MG	D	302	1/1	0.87	0.20	130,130,130,130	0
22	MG	A	1614	1/1	0.87	0.17	113,113,113,113	0
22	MG	A	1753	1/1	0.87	0.25	118,118,118,118	0
22	MG	A	1743	1/1	0.87	0.22	104,104,104,104	0
22	MG	A	1720	1/1	0.87	0.07	324,324,324,324	0
22	MG	A	1640	1/1	0.88	0.25	141,141,141,141	0
22	MG	A	1729	1/1	0.88	0.21	94,94,94,94	0
22	MG	A	1667	1/1	0.88	0.17	93,93,93,93	0
22	MG	A	1747	1/1	0.88	0.24	102,102,102,102	0
22	MG	A	1740	1/1	0.88	0.13	130,130,130,130	0
22	MG	A	1689	1/1	0.88	0.36	107,107,107,107	0
22	MG	A	1744	1/1	0.89	0.10	115,115,115,115	0
22	MG	A	1646	1/1	0.89	0.11	153,153,153,153	0
22	MG	A	1701	1/1	0.89	0.10	383,383,383,383	0
22	MG	A	1643	1/1	0.89	0.07	245,245,245,245	0
22	MG	A	1692	1/1	0.89	0.20	126,126,126,126	0
22	MG	A	1660	1/1	0.89	0.20	107,107,107,107	0
22	MG	A	1697	1/1	0.90	0.09	411,411,411,411	0
22	MG	A	1719	1/1	0.90	0.22	320,320,320,320	0
22	MG	A	1634	1/1	0.90	0.17	113,113,113,113	0
22	MG	A	1601	1/1	0.90	0.33	96,96,96,96	0
22	MG	A	1686	1/1	0.90	0.17	118,118,118,118	0
22	MG	A	1710	1/1	0.90	0.09	470,470,470,470	0
22	MG	A	1685	1/1	0.91	0.12	136,136,136,136	0
22	MG	A	1681	1/1	0.91	0.19	107,107,107,107	0
22	MG	A	1683	1/1	0.92	0.09	264,264,264,264	0
22	MG	A	1623	1/1	0.92	0.24	90,90,90,90	0
22	MG	A	1705	1/1	0.92	0.07	310,310,310,310	0
22	MG	A	1636	1/1	0.92	0.12	186,186,186,186	0
22	MG	A	1742	1/1	0.92	0.15	97,97,97,97	0
22	MG	A	1642	1/1	0.92	0.09	191,191,191,191	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1661	1/1	0.92	0.10	105,105,105,105	0
22	MG	A	1676	1/1	0.92	0.07	153,153,153,153	0
22	MG	A	1649	1/1	0.92	0.29	102,102,102,102	0
22	MG	A	1668	1/1	0.92	0.34	115,115,115,115	0
22	MG	A	1677	1/1	0.93	0.22	89,89,89,89	0
22	MG	A	1702	1/1	0.93	0.10	259,259,259,259	0
22	MG	A	1721	1/1	0.93	0.19	259,259,259,259	0
22	MG	A	1615	1/1	0.93	0.21	92,92,92,92	0
22	MG	A	1616	1/1	0.93	0.13	127,127,127,127	0
22	MG	A	1611	1/1	0.93	0.14	153,153,153,153	0
22	MG	H	201	1/1	0.93	0.06	83,83,83,83	0
22	MG	A	1759	1/1	0.93	0.14	132,132,132,132	0
22	MG	A	1699	1/1	0.93	0.13	426,426,426,426	0
22	MG	A	1682	1/1	0.94	0.18	126,126,126,126	0
22	MG	A	1625	1/1	0.94	0.18	123,123,123,123	0
22	MG	A	1669	1/1	0.94	0.27	89,89,89,89	0
22	MG	A	1652	1/1	0.94	0.18	127,127,127,127	0
22	MG	A	1662	1/1	0.94	0.26	110,110,110,110	0
22	MG	A	1605	1/1	0.94	0.17	293,293,293,293	0
22	MG	A	1690	1/1	0.94	0.22	96,96,96,96	0
22	MG	A	1727	1/1	0.95	0.18	92,92,92,92	0
22	MG	A	1635	1/1	0.95	0.09	129,129,129,129	0
22	MG	A	1704	1/1	0.95	0.20	436,436,436,436	0
22	MG	A	1620	1/1	0.95	0.07	114,114,114,114	0
22	MG	A	1678	1/1	0.95	0.18	79,79,79,79	0
22	MG	A	1707	1/1	0.95	0.10	411,411,411,411	0
22	MG	A	1708	1/1	0.95	0.10	262,262,262,262	0
22	MG	A	1763	1/1	0.95	0.07	148,148,148,148	0
22	MG	A	1645	1/1	0.95	0.14	141,141,141,141	0
22	MG	A	1659	1/1	0.95	0.14	100,100,100,100	0
22	MG	A	1713	1/1	0.95	0.22	192,192,192,192	0
22	MG	A	1672	1/1	0.95	0.07	129,129,129,129	0
22	MG	A	1638	1/1	0.95	0.29	95,95,95,95	0
22	MG	A	1629	1/1	0.95	0.06	192,192,192,192	0
22	MG	A	1606	1/1	0.95	0.11	154,154,154,154	0
22	MG	A	1633	1/1	0.96	0.11	171,171,171,171	0
22	MG	A	1644	1/1	0.96	0.08	279,279,279,279	0
22	MG	A	1651	1/1	0.96	0.12	95,95,95,95	0
22	MG	A	1663	1/1	0.96	0.33	122,122,122,122	0
22	MG	A	1687	1/1	0.96	0.12	157,157,157,157	0
22	MG	A	1666	1/1	0.96	0.20	97,97,97,97	0
22	MG	A	1613	1/1	0.96	0.34	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1691	1/1	0.96	0.04	109,109,109,109	0
22	MG	A	1618	1/1	0.96	0.11	147,147,147,147	0
22	MG	A	1657	1/1	0.96	0.19	95,95,95,95	0
22	MG	E	201	1/1	0.96	0.25	95,95,95,95	0
22	MG	A	1696	1/1	0.96	0.17	390,390,390,390	0
22	MG	A	1716	1/1	0.96	0.20	497,497,497,497	0
22	MG	A	1717	1/1	0.96	0.10	254,254,254,254	0
22	MG	A	1670	1/1	0.96	0.31	111,111,111,111	0
22	MG	A	1612	1/1	0.96	0.08	104,104,104,104	0
22	MG	A	1665	1/1	0.97	0.07	102,102,102,102	0
22	MG	A	1658	1/1	0.97	0.18	130,130,130,130	0
22	MG	A	1700	1/1	0.97	0.05	129,129,129,129	0
22	MG	A	1723	1/1	0.97	0.11	181,181,181,181	0
22	MG	A	1724	1/1	0.97	0.11	290,290,290,290	0
22	MG	A	1709	1/1	0.97	0.27	354,354,354,354	0
22	MG	A	1739	1/1	0.97	0.17	96,96,96,96	0
22	MG	A	1688	1/1	0.97	0.17	84,84,84,84	0
22	MG	A	1694	1/1	0.97	0.10	244,244,244,244	0
22	MG	A	1703	1/1	0.97	0.14	475,475,475,475	0
22	MG	A	1714	1/1	0.97	0.11	200,200,200,200	0
22	MG	A	1603	1/1	0.97	0.05	184,184,184,184	0
22	MG	A	1648	1/1	0.97	0.11	227,227,227,227	0
22	MG	A	1680	1/1	0.98	0.05	134,134,134,134	0
22	MG	A	1664	1/1	0.98	0.13	101,101,101,101	0
22	MG	A	1627	1/1	0.98	0.04	121,121,121,121	0
22	MG	A	1604	1/1	0.98	0.08	90,90,90,90	0
22	MG	A	1602	1/1	0.98	0.12	114,114,114,114	0
22	MG	A	1715	1/1	0.98	0.04	167,167,167,167	0
22	MG	A	1624	1/1	0.98	0.05	114,114,114,114	0
22	MG	A	1695	1/1	0.98	0.06	184,184,184,184	0
22	MG	A	1621	1/1	0.98	0.11	107,107,107,107	0
22	MG	A	1654	1/1	0.98	0.06	105,105,105,105	0
22	MG	A	1655	1/1	0.98	0.11	96,96,96,96	0
22	MG	A	1722	1/1	0.98	0.05	73,73,73,73	0
22	MG	A	1656	1/1	0.99	0.04	68,68,68,68	0
22	MG	A	1610	1/1	0.99	0.09	87,87,87,87	0
22	MG	A	1626	1/1	0.99	0.08	108,108,108,108	0
22	MG	A	1725	1/1	0.99	0.06	114,114,114,114	0
22	MG	A	1608	1/1	0.99	0.05	143,143,143,143	0
22	MG	A	1641	1/1	0.99	0.15	96,96,96,96	0
22	MG	A	1718	1/1	0.99	0.11	111,111,111,111	0
22	MG	A	1609	1/1	0.99	0.06	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1637	1/1	0.99	0.10	235,235,235,235	0
22	MG	K	202	1/1	0.99	0.04	110,110,110,110	0
22	MG	A	1712	1/1	0.99	0.08	376,376,376,376	0
23	ZN	D	301	1/1	0.99	0.14	136,136,136,136	0
23	ZN	N	101	1/1	1.00	0.01	148,148,148,148	0

6.5 Other polymers (i)

There are no such residues in this entry.