wwPDB X-ray Structure Validation Summary Report (i)

May 26, 2020 – 07:48 pm BST

PDB ID	:	4IOC
Title	:	Crystal structure of compound 4f bound to large ribosomal subunit (50S) from Deinococcus radiodurans
Authors	:	Han, S.; Marr, E.S.
Deposited on	:	2013-01-07
Resolution	:	3.60 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 following versions of software and data (see references (1)) were used in the production of this report:

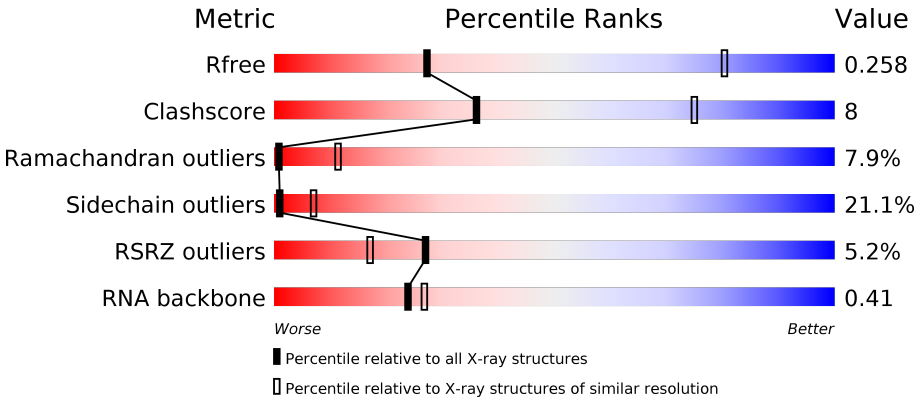
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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 on 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	X	2880	2% 30% 38% 21% 7%
2	Y	123	2% 27% 41% 26% 6%
3	A	274	% 50% 26% 11% 12%
4	B	211	62% 26% 9%

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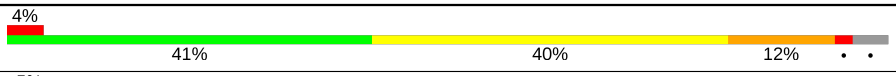
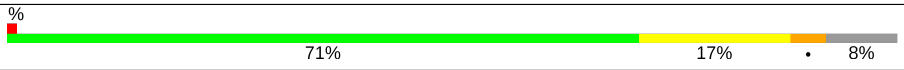
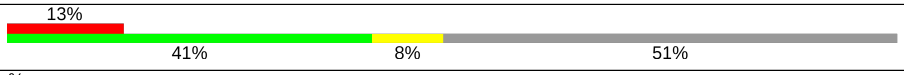
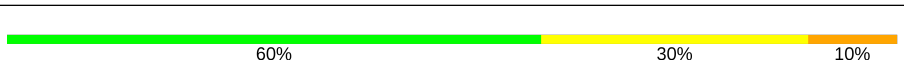
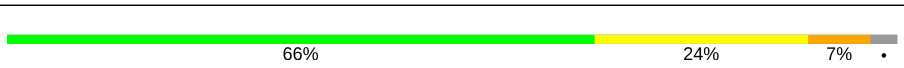
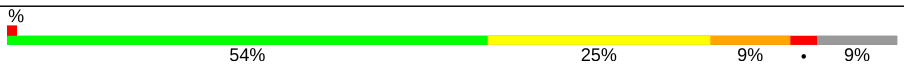
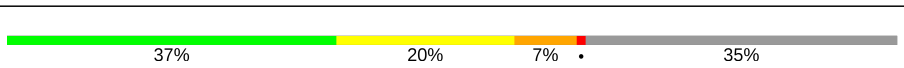
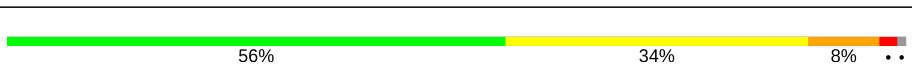
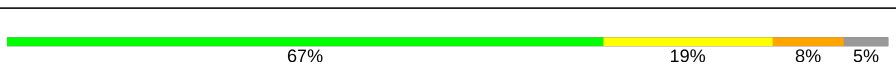
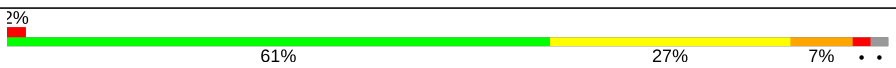
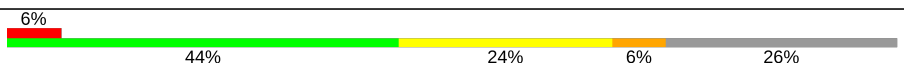
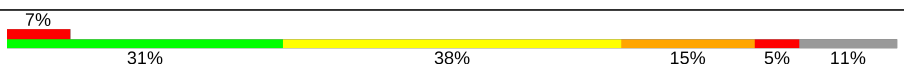
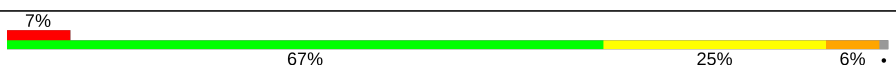
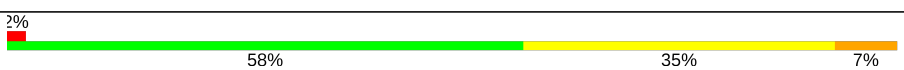
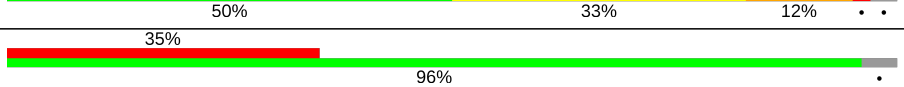
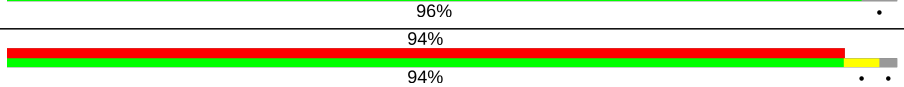
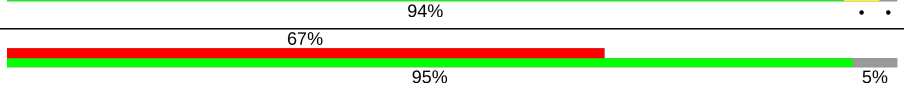
Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	

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Mol	Chain	Length	Quality of chain
30	4	37	

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
31	MG	X	2901	-	-	-	X
31	MG	X	2903	-	-	-	X
31	MG	X	2909	-	-	-	X
31	MG	X	2911	-	-	-	X
31	MG	X	2912	-	-	-	X
31	MG	X	2913	-	-	-	X
31	MG	X	2920	-	-	-	X
31	MG	X	2924	-	-	-	X
31	MG	X	2926	-	-	-	X
31	MG	X	2927	-	-	-	X
31	MG	X	2928	-	-	-	X
31	MG	Y	204	-	-	-	X

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 83877 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	X	2686	57651	25718	10642	18606	2685	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	Y	122	2598	1161	476	840	121	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	240	1826	1137	366	321	2	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	205	1539	965	295	271	8	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	197	1506	935	287	282	2	0	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	D	177	1400	892	247	254	7	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	71	Total	C	N	O	S	0	0	0
			503	310	91	99	3			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	141	Total	C	N	O	0	0	0
			1067	655	216	196			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	104	Total 779	C 476	N 161	O 142	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	M	108	Total 871	C 543	N 172	O 156	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	117	Total 978	C 608	N 210	O 159	S 1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	94	Total 741	C 465	N 139	O 137	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	127	Total 1014	C 639	N 199	O 174	S 2	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	93	Total 726	C 458	N 136	O 130	S 2	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	110	Total 825	C 513	N 160	O 151	S 1	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	175	Total	C	N	O	S	0	0	0
			1345	849	236	254	6			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	84	Total	C	N	O	S	0	0	0
			625	393	122	109	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	U	72	Total	C	N	O	0	0	0
			552	341	116	95			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	66	Total	C	N	O	S	0	0	0
			533	327	107	96	3			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
27	1	53	Total	C	0	0	53
			53	53			

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	2	46	Total C 46 46	0	0	46

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	3	63	Total C 63 63	0	0	63

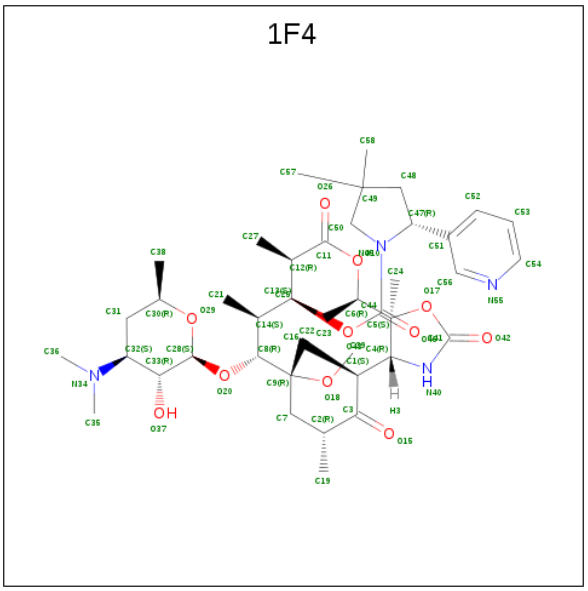
- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	4	37	Total C N O S 297 179 66 47 5	0	0	0

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	28	Total Mg 28 28	0	0
31	Y	6	Total Mg 6 6	0	0
31	M	1	Total Mg 1 1	0	0

- Molecule 32 is (3aS,4R,7R,8S,9S,10R,11R,13R,15S,15aR)-4-ethyl-11-methoxy-3a,7,9,11,13,15-hexamethyl-2,6,14-trioxo-10-{[3,4,6-trideoxy-3-(dimethylamino)-beta-D-xylo-hexopyranosyl]oxy}tetradecahydro-2H-oxacyclotetradecino[4,3-d][1,3]oxazol-8-yl (2R)-4,4-dimethyl-2-(pyridin-3-yl)pyrrolidine-1-carboxylate (three-letter code: 1F4) (formula: $C_{43}H_{68}N_4O_{11}$).



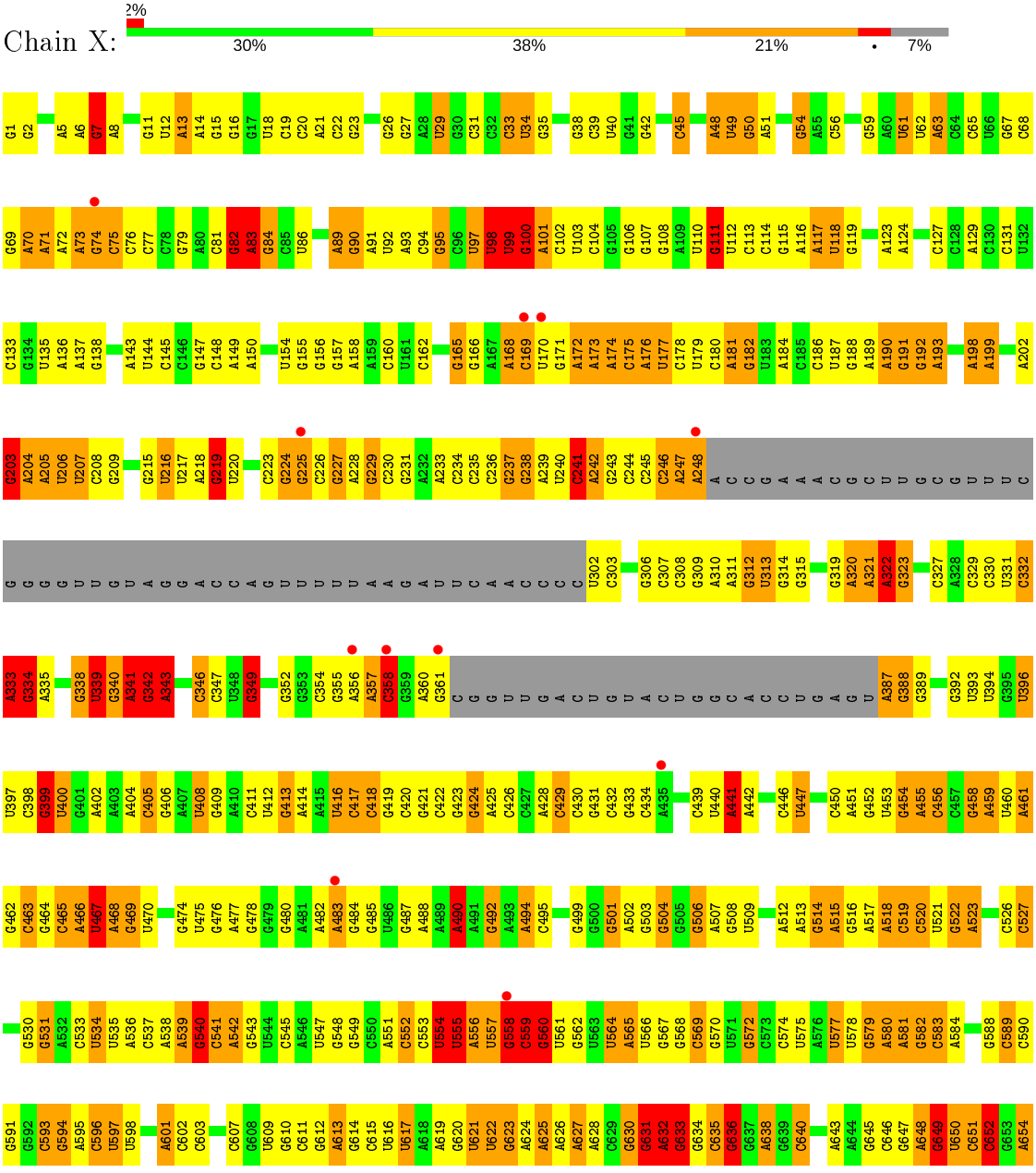
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
32	X	1	58	43	4	11	0	0

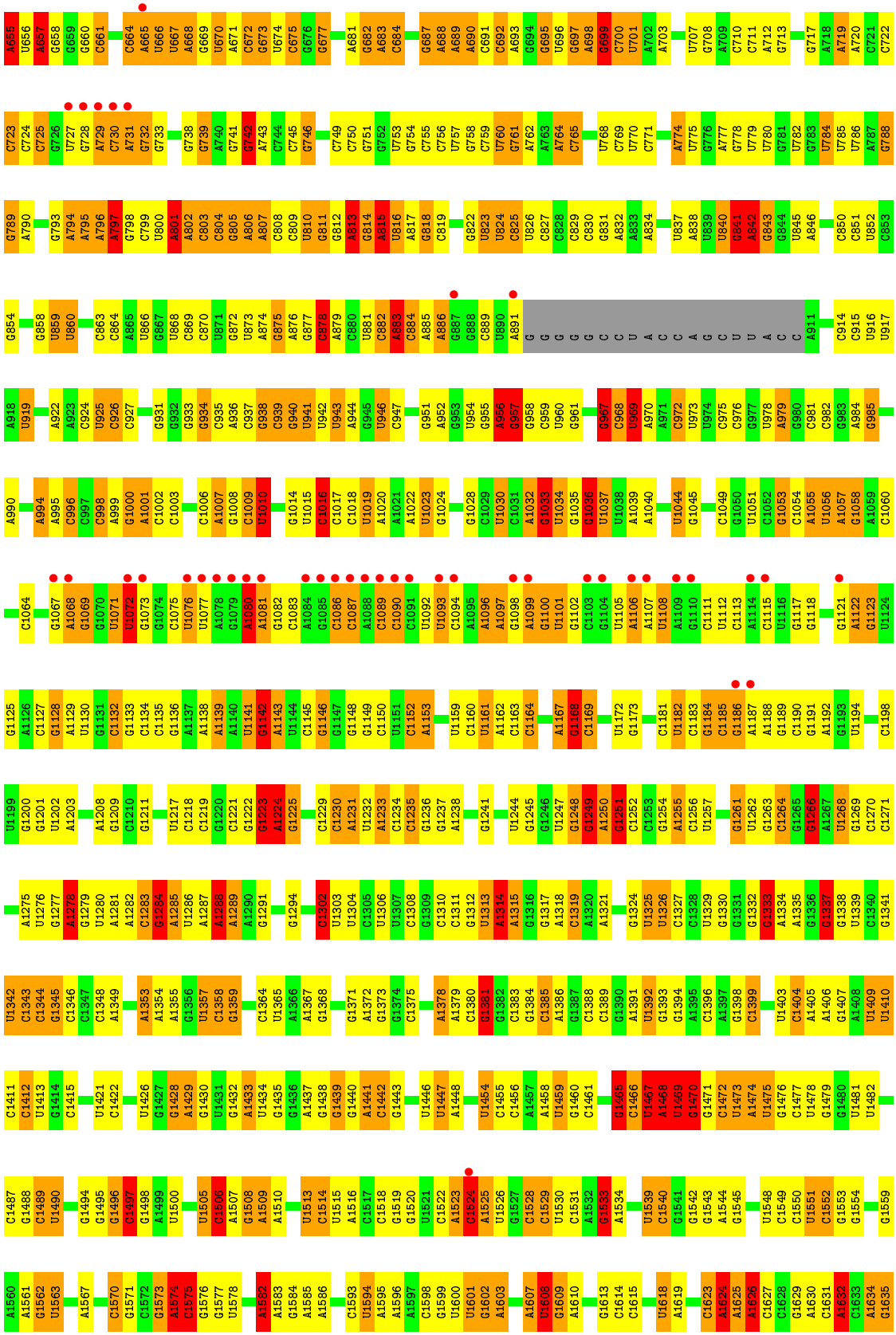
3 Residue-property plots (i)

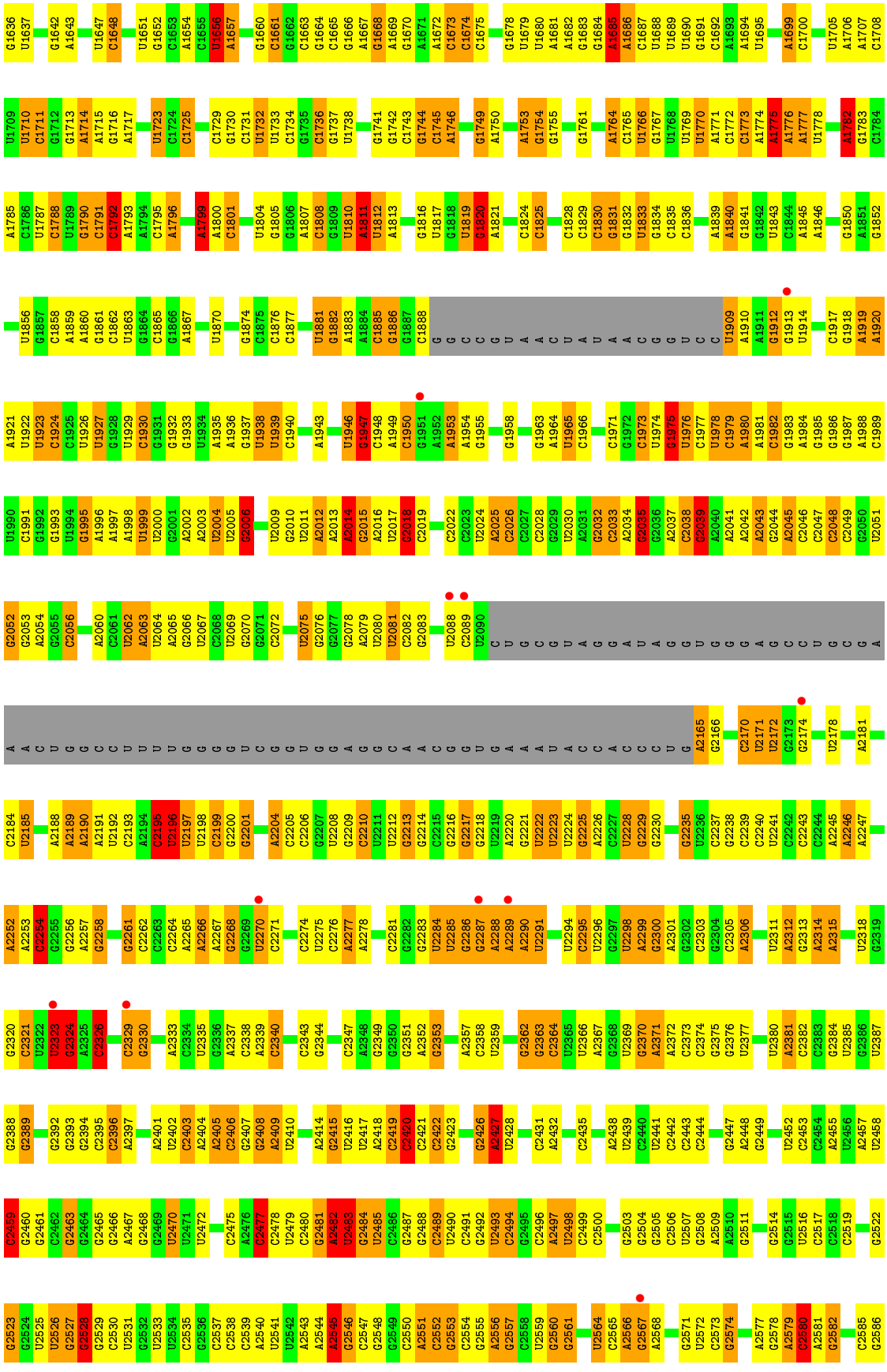
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

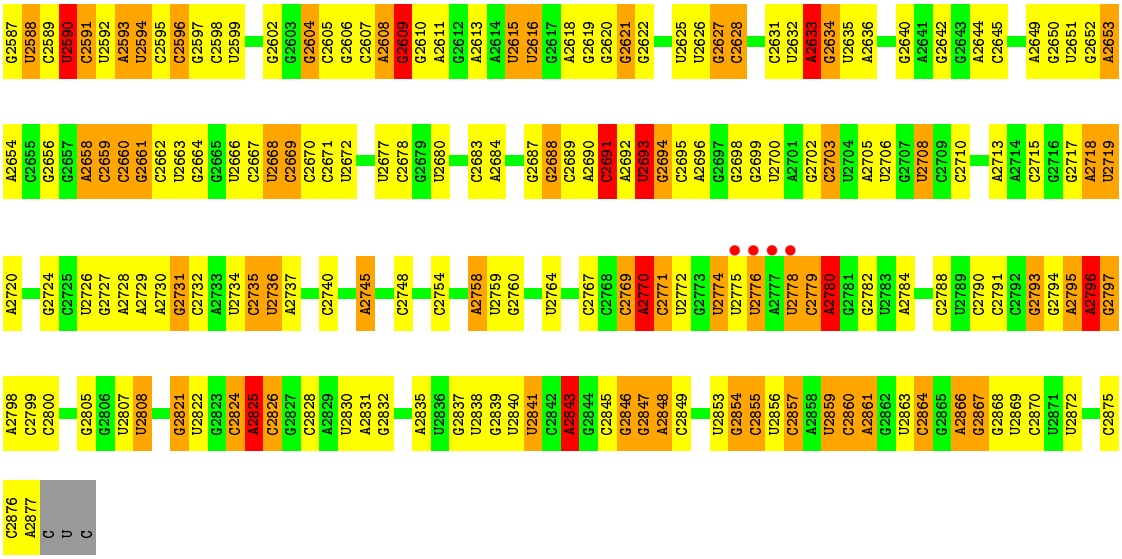
- Molecule 1: 23S ribosomal RNA

Chain X:



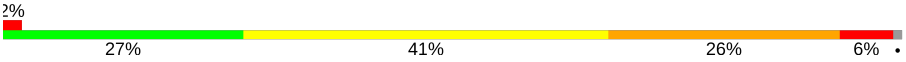

A655 U656 A657 G658 G659 G660 C661 C664 A665 U666 U667 A668 G669 U670 A671 C672 G673 U674 C675 G676 G677 A681 G682 A683 C684 G687 A688 A689 A690 C691 C692 A693 G694 G695 U696 G697 A698 G699 C700 U701 A702 A703 U707 G708 A709 C710 C711 A712 G713 G717 A718 A719 A720 C721 C722
C723 C724 C725 G726 U727 G728 A729 C730 A731 G732 G733 G738 G739 A740 G741 G742 A743 C744 C745 G746 C749 C750 G751 G752 U753 G754 C755 C756 U757 G758 C759 U760 G761 A762 A763 A764 C765 U768 C769 U770 C771 A774 U775 G776 A777 G778 U779 U780 G781 U782 G783 U784 U785 U786 A787 G788
G789 A790 G793 A794 A795 A796 A797 G798 C799 U800 A801 A802 C803 C804 G805 A806 A807 C808 C809 U810 G811 G812 A813 G814 A815 U816 A817 G818 C819 G822 U823 U824 C825 U826 C827 C828 C829 C830 G831 A832 A833 A834 U837 A838 U839 U840 G841 A842 G843 G844 U845 A846 C850 C851 U852 C853
G854 G858 U859 U860 C863 C864 A865 U866 G867 U868 C869 C870 U871 G872 U873 A874 G875 A876 G877 C878 A879 C880 U881 C882 A883 C884 A885 A886 G887 G888 C889 U890 A891 G G G G G C C U A C C A G C U U A C C A911 C914 C915 U916 U917
A918 U919 A922 A923 C924 U925 C926 C927 G931 G932 G933 G934 C935 A936 C937 G938 C939 G940 U941 U942 U943 A944 G945 U946 C947 G951 A952 G953 U954 G955 A956 G957 G958 C959 U960 G961 G967 C968 U969 A970 A971 C972 U973 U974 C975 C976 G977 U978 A979 G980 C981 C982 G983 A984 G985
A990 A994 A995 C996 C997 C998 A999 G1000 A1001 C1002 C1003 C1006 A1007 G1008 C1009 U1010 G1014 U1015 C1016 C1017 C1018 U1019 A1020 A1021 A1022 U1023 G1024 G1028 C1029 U1030 C1031 A1032 G1033 U1034 G1035 G1036 U1037 U1038 A1039 A1040 U1044 G1045 C1049 G1050 U1051 C1052 G1053 C1054 A1055 U1056 A1057 G1058 A1059 C1060
C1064 G1067 A1068 G1069 G1070 U1071 U1072 G1073 G1074 C1075 U1076 U1077 A1078 G1079 A1080 A1081 G1082 C1083 A1084 G1085 C1086 C1087 A1088 C1089 C1090 C1091 U1092 U1093 C1094 A1095 A1096 A1097 G1098 A1099 G1100 U1101 G1102 C1103 G1104 U1105 A1106 A1107 U1108 A1109 G1110 C1111 U1112 C1113 A1114 C1115 U1116 G1117 G1118 G1121 A1122 G1123 U1124
G1125 A1126 C1127 G1128 A1129 U1130 G1131 C1132 G1133 C1134 C1135 G1136 A1137 A1138 A1139 A1140 U1141 A1142 A1143 U1144 C1145 G1146 G1147 G1148 G1149 C1150 U1151 C1152 A1153 U1159 C1160 U1161 A1162 C1163 C1164 A1167 G1168 C1169 U1172 G1173 C1181 U1182 C1183 G1184 C1185 G1186 A1187 A1188 G1189 C1190 G1191 A1192 G1193 U1194 C1198
U1199 G1200 G1201 U1202 A1203 A1208 G1209 C1210 G1211 U1217 C1218 C1219 G1220 C1221 G1222 G1223 A1224 G1225 C1229 C1230 A1231 U1232 A1233 C1234 C1235 G1236 G1237 A1238 G1241 U1244 G1245 G1246 U1247 G1248 G1249 A1250 G1251 C1252 C1253 G1254 A1255 C1256 U1257 G1261 U1262 G1263 C1264 G1265 G1266 A1267 U1268 G1269 C1270 C1271
A1275 U1276 G1277 A1278 G1279 U1280 A1281 A1282 C1283 G1284 A1285 U1286 A1287 A1288 A1289 A1290 G1291 G1294 C1302 U1303 U1304 C1305 U1306 U1307 C1308 G1309 C1310 C1311 G1312 U1313 A1314 A1315 G1316 G1317 A1318 C1319 A1320 A1321 G1324 U1325 U1326 C1327 C1328 U1329 G1330 G1331 G1332 G1333 A1334 A1335 G1336 G1337 G1338 U1339 C1340 G1341
U1342 C1343 C1344 G1345 C1346 C1347 C1348 A1349 A1353 A1354 A1355 G1356 U1357 C1358 G1359 C1364 U1365 A1366 A1367 G1368 G1371 A1372 G1373 G1374 C1375 A1378 A1379 C1380 G1381 G1382 C1383 G1384 C1385 A1386 G1387 C1388 C1389 G1390 A1391 U1392 G1393 G1394 A1395 C1396 A1397 G1398 C1399 U1403 C1404 A1405 A1406 G1407 A1408 U1409 U1410
C1411 C1412 U1413 G1414 C1415 U1421 C1422 U1426 G1427 G1428 A1429 G1430 U1431 G1432 A1433 U1434 G1435 G1436 A1437 G1438 G1439 G1440 A1441 C1442 G1443 U1446 U1447 A1448 U1454 C1455 C1456 A1457 A1458 U1459 C1460 C1461 C1465 C1466 U1467 A1468 U1469 G1470 C1471 C1472 U1473 A1474 U1475 G1476 C1477 U1478 G1479 G1480 U1481 U1482
C1487 G1488 C1489 U1490 G1494 G1495 G1496 C1497 G1498 A1499 U1500 U1505 C1506 A1507 G1508 A1509 A1510 U1513 C1514 U1515 A1516 C1517 C1518 G1519 G1520 U1521 C1522 A1523 C1524 A1525 U1526 G1527 C1528 C1529 U1530 C1531 A1532 G1533 A1534 U1539 C1540 G1541 G1542 G1543 A1544 U1545 U1548 C1549 C1550 U1551 C1552 G1553 G1554 G1559
A1560 A1561 G1562 U1563 A1567 C1570 G1571 C1572 G1573 A1574 C1575 G1576 G1577 U1578 A1582 A1583 G1584 A1585 A1586 C1593 U1594 A1595 A1596 A1597 C1598 G1599 U1600 U1601 G1602 A1603 A1607 U1608 G1609 A1610 G1613 C1614 C1615 U1618 A1619 C1623 A1624 A1625 A1626 C1627 C1628 G1629 A1630 C1631 A1632 C1633 A1634 G1635

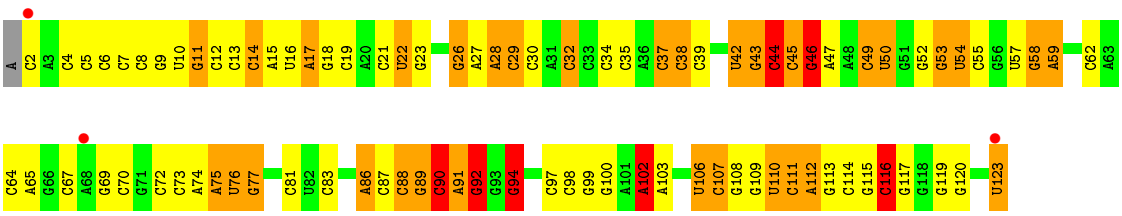




• Molecule 2: 5S ribosomal RNA

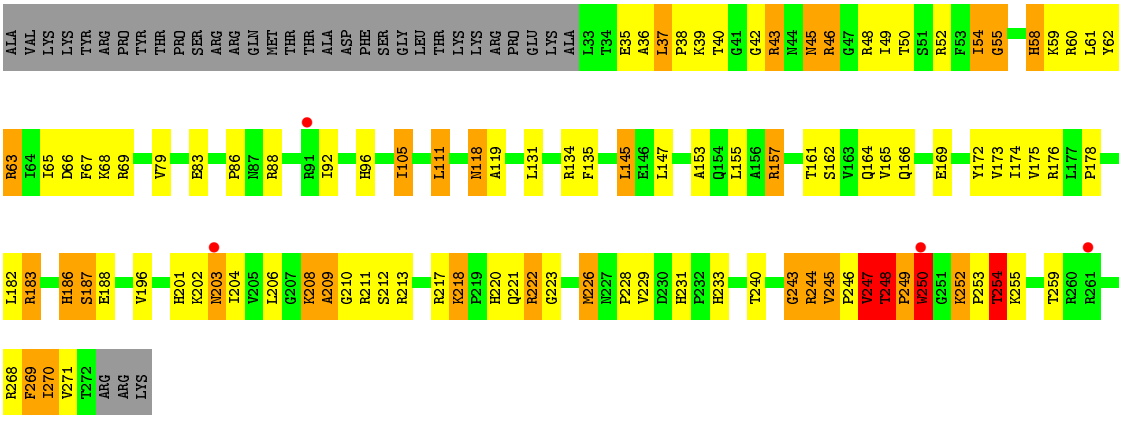
Chain Y:





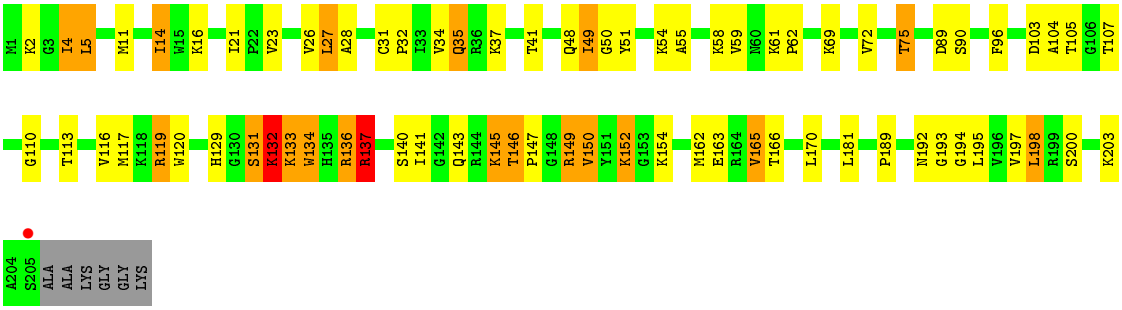
• Molecule 3: 50S ribosomal protein L2

Chain A:



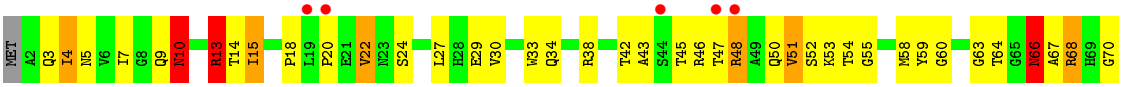
• Molecule 4: 50S ribosomal protein L3

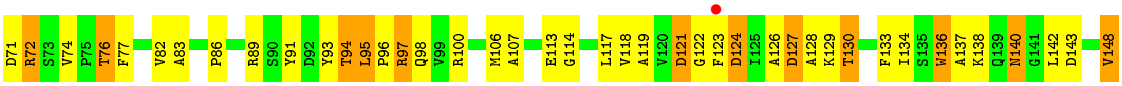
Chain B:

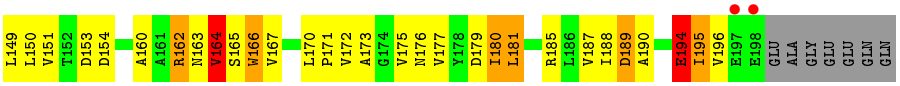


- Molecule 5: 50S ribosomal protein L4

Chain C:

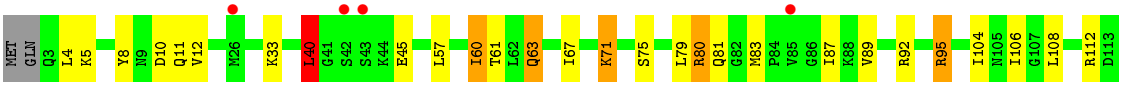


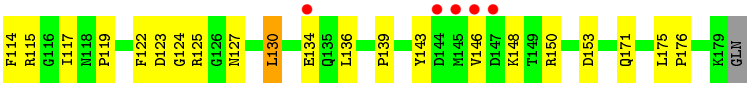




- Molecule 6: 50S ribosomal protein L5

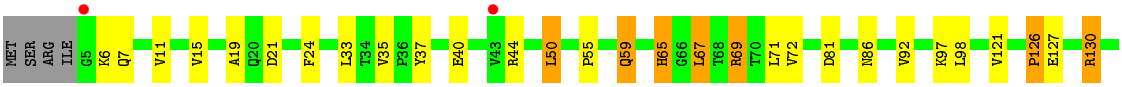
Chain D:

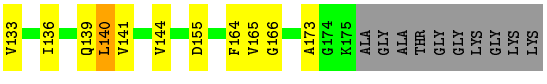




- Molecule 7: 50S ribosomal protein L6

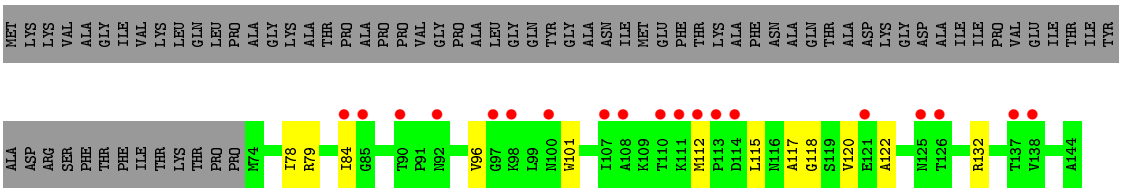
Chain E:





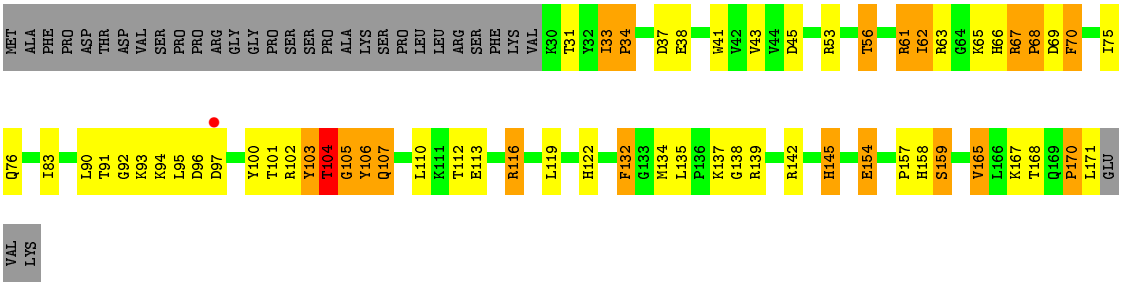
- Molecule 8: 50S ribosomal protein L11

Chain F:



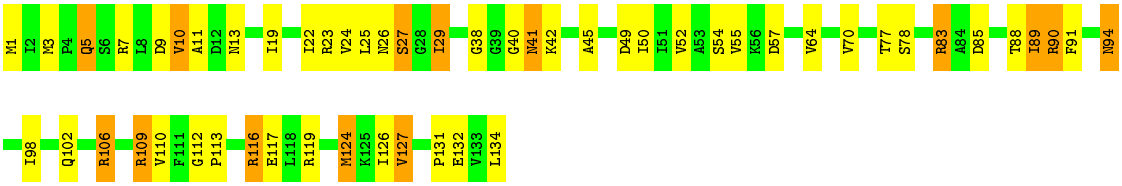
• Molecule 9: 50S ribosomal protein L13

Chain G:



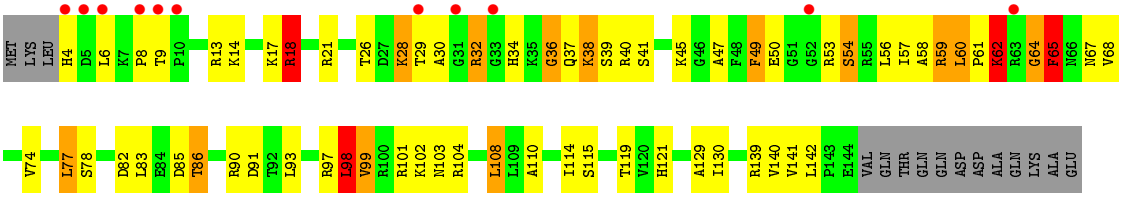
• Molecule 10: 50S ribosomal protein L14

Chain H:



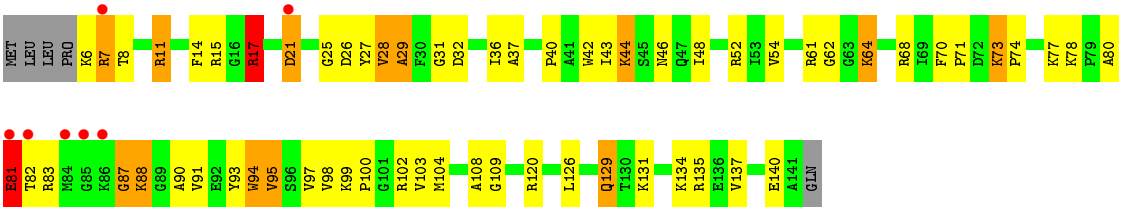
• Molecule 11: 50S ribosomal protein L15

Chain I:



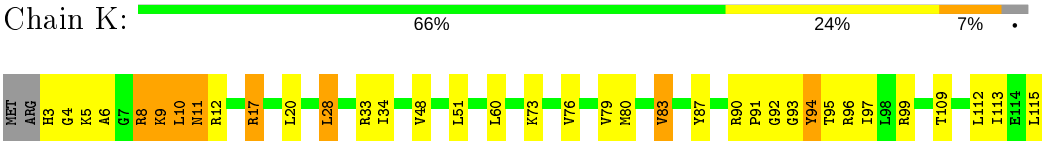
• Molecule 12: 50S ribosomal protein L16

Chain J:



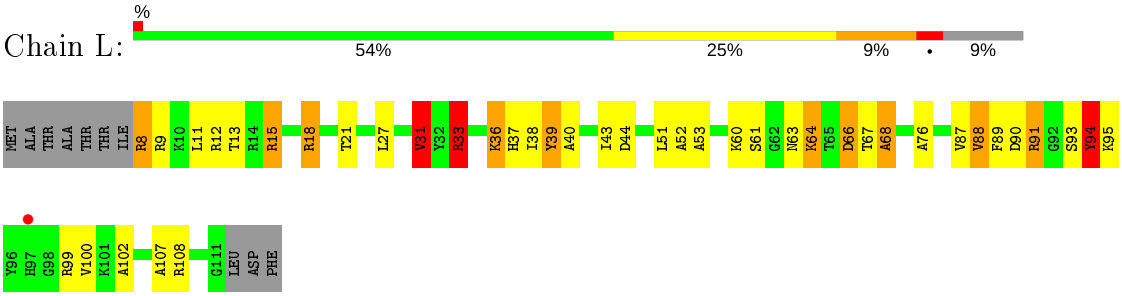
• Molecule 13: 50S ribosomal protein L17

Chain K:



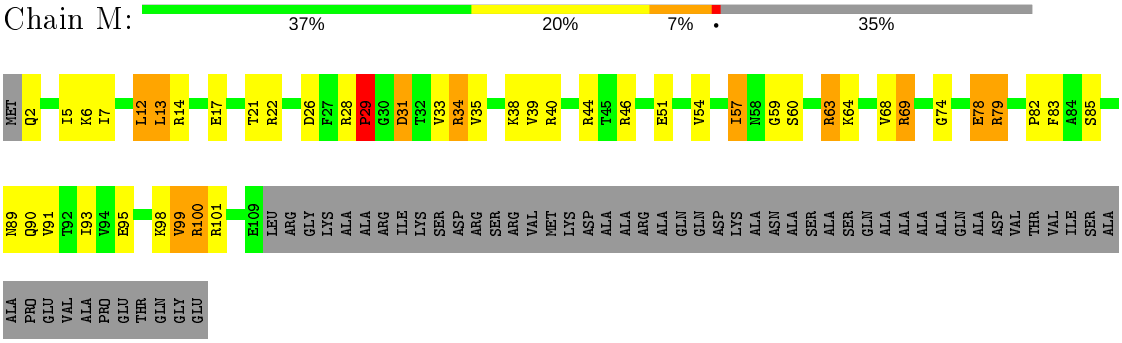
• Molecule 14: 50S ribosomal protein L18

Chain L:



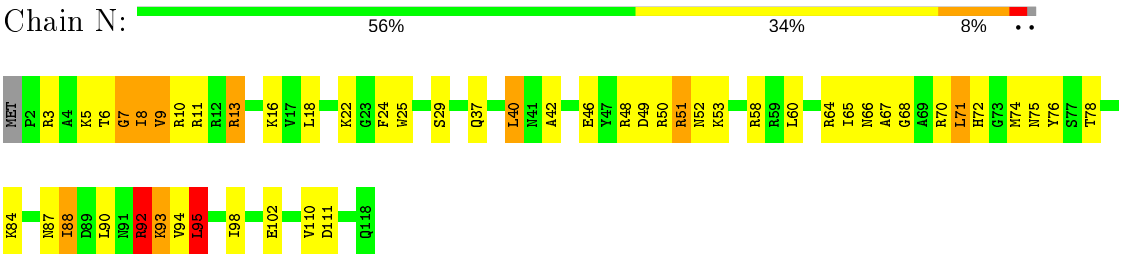
• Molecule 15: 50S ribosomal protein L19

Chain M:



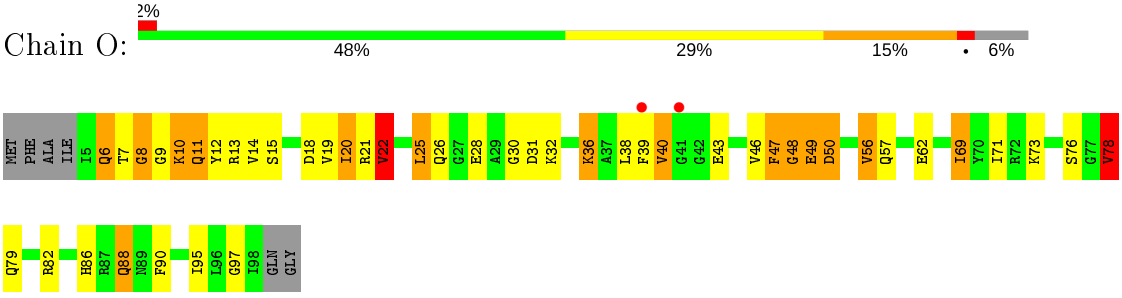
• Molecule 16: 50S ribosomal protein L20

Chain N:



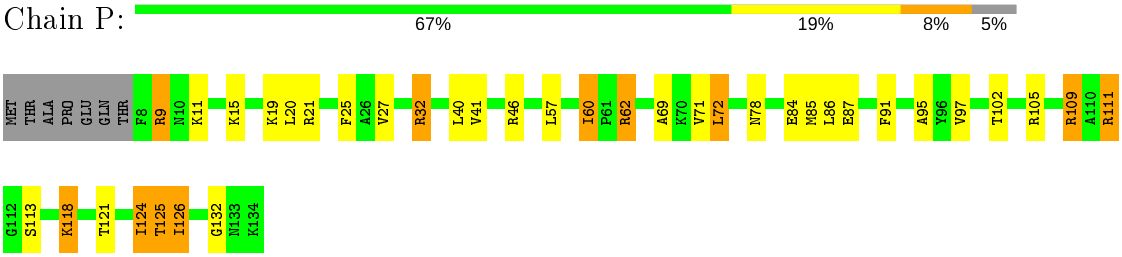
• Molecule 17: 50S ribosomal protein L21

Chain O:



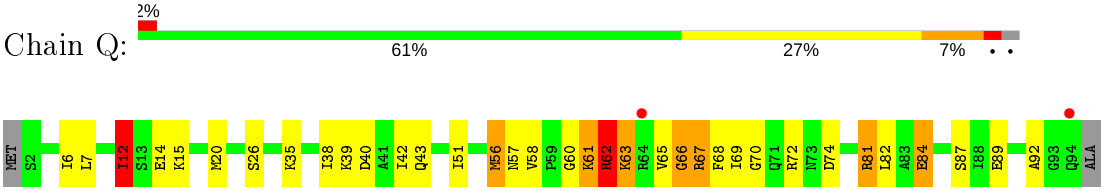
• Molecule 18: 50S ribosomal protein L22

Chain P:



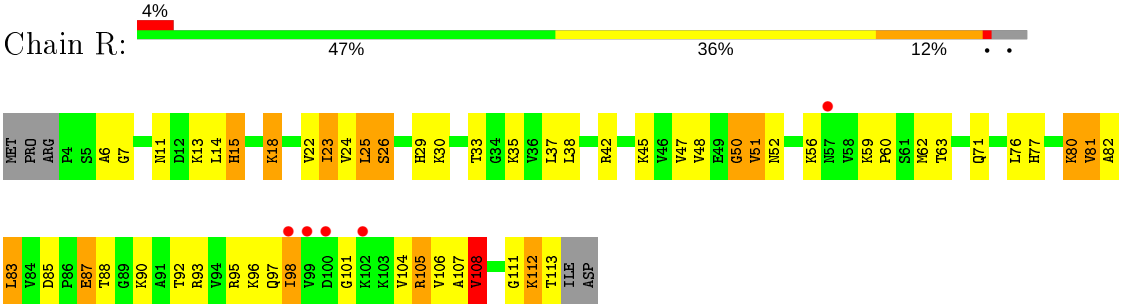
• Molecule 19: 50S ribosomal protein L23

Chain Q:



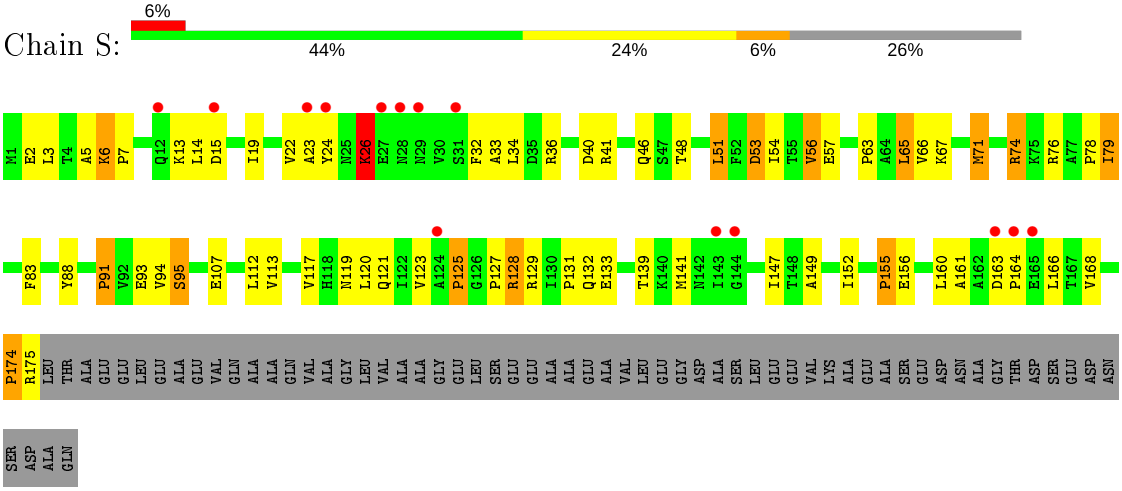
• Molecule 20: 50S ribosomal protein L24

Chain R:



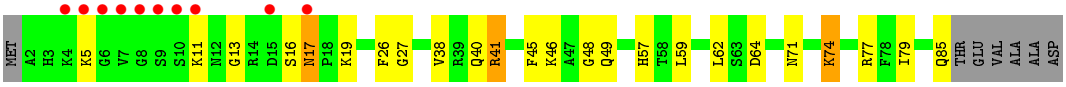
• Molecule 21: 50S ribosomal protein L25

Chain S:



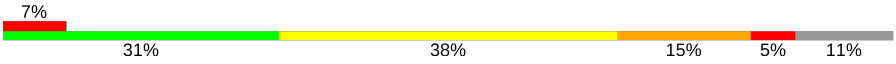
• Molecule 22: 50S ribosomal protein L27

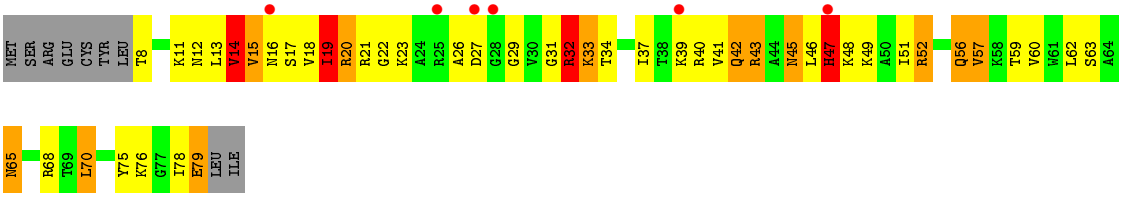
Chain T:



• Molecule 23: 50S ribosomal protein L28

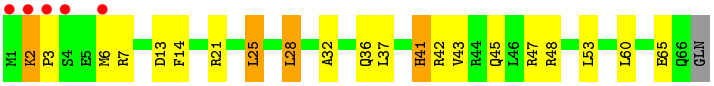
Chain U:





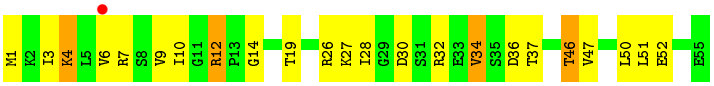
• Molecule 24: 50S ribosomal protein L29

Chain V:



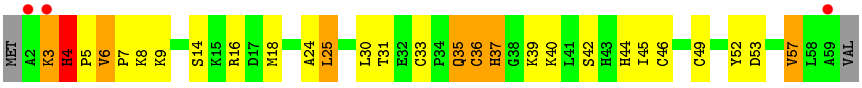
• Molecule 25: 50S ribosomal protein L30

Chain W:



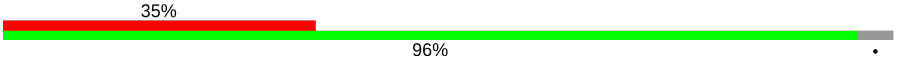
• Molecule 26: 50S ribosomal protein L32

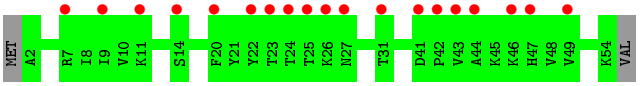
Chain Z:



• Molecule 27: 50S ribosomal protein L33

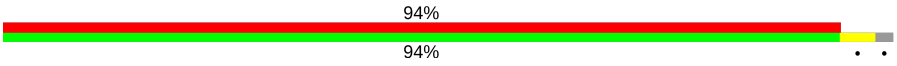
Chain 1:

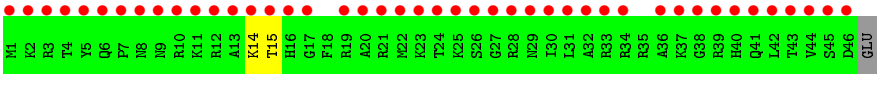




• Molecule 28: 50S ribosomal protein L34

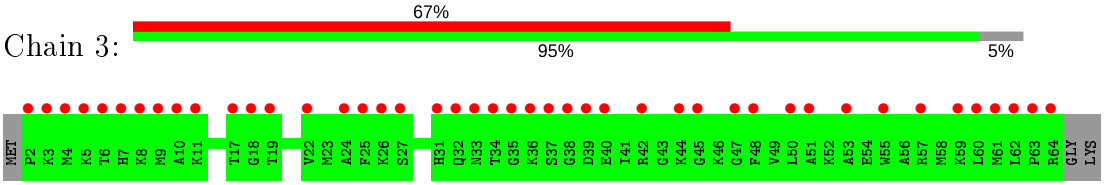
Chain 2:





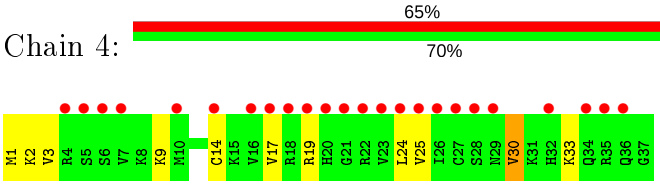
• Molecule 29: 50S ribosomal protein L35

Chain 3:



• Molecule 30: 50S ribosomal protein L36

Chain 4:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	169.64Å 408.49Å 692.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.60 30.11 – 3.61	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.60) 88.4 (30.11-3.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 3.65Å)	Xtriage
Refinement program	autobuster	Depositor
R, R_{free}	0.198 , 0.239 0.215 , 0.258	Depositor DCC
R_{free} test set	12232 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	129.2	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 93.5	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	0.94	EDS
Total number of atoms	83877	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1F4, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	X	1.02	36/64561 (0.1%)	1.86	1991/100708 (2.0%)
2	Y	1.22	2/2904 (0.1%)	1.83	99/4525 (2.2%)
3	A	0.58	0/1862	0.93	4/2510 (0.2%)
4	B	0.55	0/1567	0.88	1/2105 (0.0%)
5	C	0.62	0/1529	0.96	0/2070
6	D	0.46	0/1419	0.68	0/1903
7	E	0.47	0/1308	0.71	0/1771
8	F	0.50	0/508	0.67	0/683
9	G	0.58	0/1138	0.92	2/1539 (0.1%)
10	H	0.53	0/1007	0.84	0/1352
11	I	0.67	0/1081	1.06	2/1448 (0.1%)
12	J	0.86	0/1113	0.96	1/1486 (0.1%)
13	K	0.66	0/886	0.92	0/1188
14	L	0.52	0/785	0.93	0/1048
15	M	0.59	0/884	1.00	2/1186 (0.2%)
16	N	0.53	0/994	0.79	0/1323
17	O	0.52	0/750	0.96	1/1000 (0.1%)
18	P	0.57	0/1027	0.88	0/1373
19	Q	0.56	0/737	0.99	2/988 (0.2%)
20	R	0.59	0/835	1.02	0/1121
21	S	0.61	0/1370	0.76	0/1862
22	T	0.54	0/633	0.88	0/838
23	U	0.71	0/556	1.08	2/741 (0.3%)
24	V	0.52	0/537	0.73	0/714
25	W	0.51	0/426	0.81	0/568
26	Z	0.62	0/469	0.98	0/629
30	4	0.49	0/298	0.73	0/390
All	All	0.94	38/91184 (0.0%)	1.68	2107/137069 (1.5%)

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	X	0	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	559	C	C3'-O3'	8.19	1.53	1.42
1	X	655	A	C3'-O3'	7.84	1.53	1.42
1	X	774	A	C5-C4	7.25	1.43	1.38
1	X	699	G	N9-C4	-6.97	1.32	1.38
1	X	1688	U	C2-N3	6.58	1.42	1.37

The worst 5 of 2107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1288	A	C1'-O4'-C4'	-30.77	85.29	109.90
1	X	1019	U	P-O3'-C3'	19.01	142.51	119.70
1	X	1288	A	C5'-C4'-O4'	18.79	131.64	109.10
1	X	774	A	N1-C6-N6	17.73	129.24	118.60
1	X	559	C	O4'-C1'-N1	17.43	122.14	108.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	1251	G	Sidechain
1	X	699	G	Sidechain
1	X	967	G	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	57651	0	29049	535	0
2	Y	2598	0	1328	22	0
3	A	1826	0	1885	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1539	0	1600	57	0
5	C	1506	0	1525	57	0
6	D	1400	0	1481	17	0
7	E	1286	0	1336	10	0
8	F	503	0	520	5	0
9	G	1114	0	1144	46	0
10	H	997	0	1046	30	0
11	I	1067	0	1103	39	0
12	J	1090	0	1125	31	0
13	K	878	0	930	24	0
14	L	779	0	820	19	0
15	M	871	0	894	25	0
16	N	978	0	1020	33	0
17	O	741	0	756	24	0
18	P	1014	0	1096	23	0
19	Q	726	0	753	11	0
20	R	825	0	881	26	0
21	S	1345	0	1372	30	0
22	T	625	0	655	11	0
23	U	552	0	604	31	0
24	V	533	0	558	7	0
25	W	424	0	470	15	0
26	Z	457	0	462	20	0
27	1	53	0	0	0	0
28	2	46	0	0	1	0
29	3	63	0	0	0	0
30	4	297	0	330	4	0
31	M	1	0	0	0	0
31	X	28	0	0	0	0
31	Y	6	0	0	0	0
32	X	58	0	67	19	0
All	All	83877	0	54810	1080	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 8.

The worst 5 of 1080 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)
4:B:117:MET:SD	4:B:117:MET:CE	2.02	1.47
9:G:100:TYR:HB2	9:G:116:ARG:NH1	1.69	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:33:ILE:HB	9:G:34:PRO:HD3	1.38	1.03
1:X:558:G:H4'	1:X:559:C:H5'	1.40	1.02
1:X:1448:A:H61	1:X:1574:A:H61	1.09	1.00

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	238/274 (87%)	173 (73%)	47 (20%)	18 (8%)	1 12
4	B	203/211 (96%)	173 (85%)	25 (12%)	5 (2%)	5 36
5	C	195/205 (95%)	127 (65%)	40 (20%)	28 (14%)	0 4
6	D	175/180 (97%)	142 (81%)	26 (15%)	7 (4%)	3 26
7	E	169/185 (91%)	134 (79%)	26 (15%)	9 (5%)	2 19
8	F	69/144 (48%)	57 (83%)	9 (13%)	3 (4%)	2 24
9	G	140/174 (80%)	99 (71%)	26 (19%)	15 (11%)	0 7
10	H	132/134 (98%)	117 (89%)	12 (9%)	3 (2%)	6 38
11	I	139/156 (89%)	81 (58%)	39 (28%)	19 (14%)	0 4
12	J	134/141 (95%)	98 (73%)	24 (18%)	12 (9%)	1 9
13	K	111/116 (96%)	92 (83%)	13 (12%)	6 (5%)	2 19
14	L	102/114 (90%)	75 (74%)	15 (15%)	12 (12%)	0 5
15	M	106/166 (64%)	90 (85%)	10 (9%)	6 (6%)	1 18
16	N	115/118 (98%)	91 (79%)	17 (15%)	7 (6%)	1 17
17	O	92/100 (92%)	66 (72%)	13 (14%)	13 (14%)	0 4
18	P	125/134 (93%)	104 (83%)	17 (14%)	4 (3%)	4 31
19	Q	91/95 (96%)	63 (69%)	16 (18%)	12 (13%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
20	R	108/115 (94%)	65 (60%)	26 (24%)	17 (16%)	0 3
21	S	173/237 (73%)	135 (78%)	27 (16%)	11 (6%)	1 17
22	T	82/91 (90%)	65 (79%)	12 (15%)	5 (6%)	1 17
23	U	70/81 (86%)	41 (59%)	15 (21%)	14 (20%)	0 1
24	V	64/67 (96%)	57 (89%)	5 (8%)	2 (3%)	4 32
25	W	53/55 (96%)	47 (89%)	5 (9%)	1 (2%)	8 42
26	Z	56/60 (93%)	45 (80%)	6 (11%)	5 (9%)	1 9
30	4	35/37 (95%)	23 (66%)	11 (31%)	1 (3%)	4 33
All	All	2977/3390 (88%)	2260 (76%)	482 (16%)	235 (8%)	1 11

5 of 235 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	45	ASN
3	A	209	ALA
3	A	217	ARG
3	A	248	THR
3	A	249	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	185/215 (86%)	145 (78%)	40 (22%)	1 6
4	B	155/157 (99%)	119 (77%)	36 (23%)	1 5
5	C	157/163 (96%)	112 (71%)	45 (29%)	0 3
6	D	153/156 (98%)	130 (85%)	23 (15%)	3 19
7	E	136/144 (94%)	115 (85%)	21 (15%)	2 18
8	F	51/107 (48%)	49 (96%)	2 (4%)	32 65
9	G	118/146 (81%)	94 (80%)	24 (20%)	1 8
10	H	103/103 (100%)	80 (78%)	23 (22%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
11	I	108/121 (89%)	79 (73%)	29 (27%)	0 3
12	J	110/115 (96%)	89 (81%)	21 (19%)	1 9
13	K	90/93 (97%)	76 (84%)	14 (16%)	2 18
14	L	74/82 (90%)	51 (69%)	23 (31%)	0 2
15	M	94/134 (70%)	71 (76%)	23 (24%)	0 4
16	N	96/97 (99%)	76 (79%)	20 (21%)	1 7
17	O	75/79 (95%)	56 (75%)	19 (25%)	0 4
18	P	109/115 (95%)	91 (84%)	18 (16%)	2 15
19	Q	75/76 (99%)	60 (80%)	15 (20%)	1 8
20	R	91/96 (95%)	75 (82%)	16 (18%)	2 12
21	S	149/192 (78%)	117 (78%)	32 (22%)	1 6
22	T	62/67 (92%)	53 (86%)	9 (14%)	3 20
23	U	57/66 (86%)	33 (58%)	24 (42%)	0 0
24	V	54/55 (98%)	43 (80%)	11 (20%)	1 8
25	W	48/48 (100%)	37 (77%)	11 (23%)	1 5
26	Z	51/53 (96%)	41 (80%)	10 (20%)	1 8
30	4	35/35 (100%)	29 (83%)	6 (17%)	2 13
All	All	2436/2715 (90%)	1921 (79%)	515 (21%)	1 7

5 of 515 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	I	77	LEU
14	L	43	ILE
23	U	78	ILE
11	I	99	VAL
12	J	131	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	58	ASN
17	O	79	GLN
25	W	54	GLN
15	M	90	GLN

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Mol	Chain	Res	Type
16	N	66	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2683/2880 (93%)	701 (26%)	250 (9%)
2	Y	121/123 (98%)	41 (33%)	12 (9%)
All	All	2804/3003 (93%)	742 (26%)	262 (9%)

5 of 742 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	7	G
1	X	13	A
1	X	14	A
1	X	15	G

5 of 262 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1186	G
1	X	1475	U
1	X	2807	U
1	X	1250	A
1	X	1357	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 36 ligands modelled in this entry, 35 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	$\#\|Z\| > 2$
32	1F4	X	2929	-	60,62,62	1.25	5 (8%)	84,95,95	2.68	38 (45%)

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
32	1F4	X	2929	-	-	34/74/119/119	1/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2929	1F4	C41-N40	4.36	1.39	1.33
32	X	2929	1F4	C52-C51	3.38	1.44	1.39
32	X	2929	1F4	C22-C9	2.72	1.58	1.52
32	X	2929	1F4	O46-C44	2.20	1.24	1.21
32	X	2929	1F4	C4-N40	2.02	1.49	1.45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	X	2929	1F4	C51-C47-N45	-8.14	98.37	112.99
32	X	2929	1F4	C6-O10-C11	6.63	129.97	118.18
32	X	2929	1F4	C58-C49-C50	-5.51	104.57	110.66
32	X	2929	1F4	C22-C9-C7	-5.16	103.00	111.12
32	X	2929	1F4	O43-C13-C14	5.01	119.16	107.50

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	2929	1F4	C4-C5-C6-O10

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Mol	Chain	Res	Type	Atoms
32	X	2929	1F4	C4-C5-C6-C23
32	X	2929	1F4	O17-C5-C6-O10
32	X	2929	1F4	O17-C5-C6-C23
32	X	2929	1F4	C24-C5-C6-O10

All (1) ring outliers are listed below:

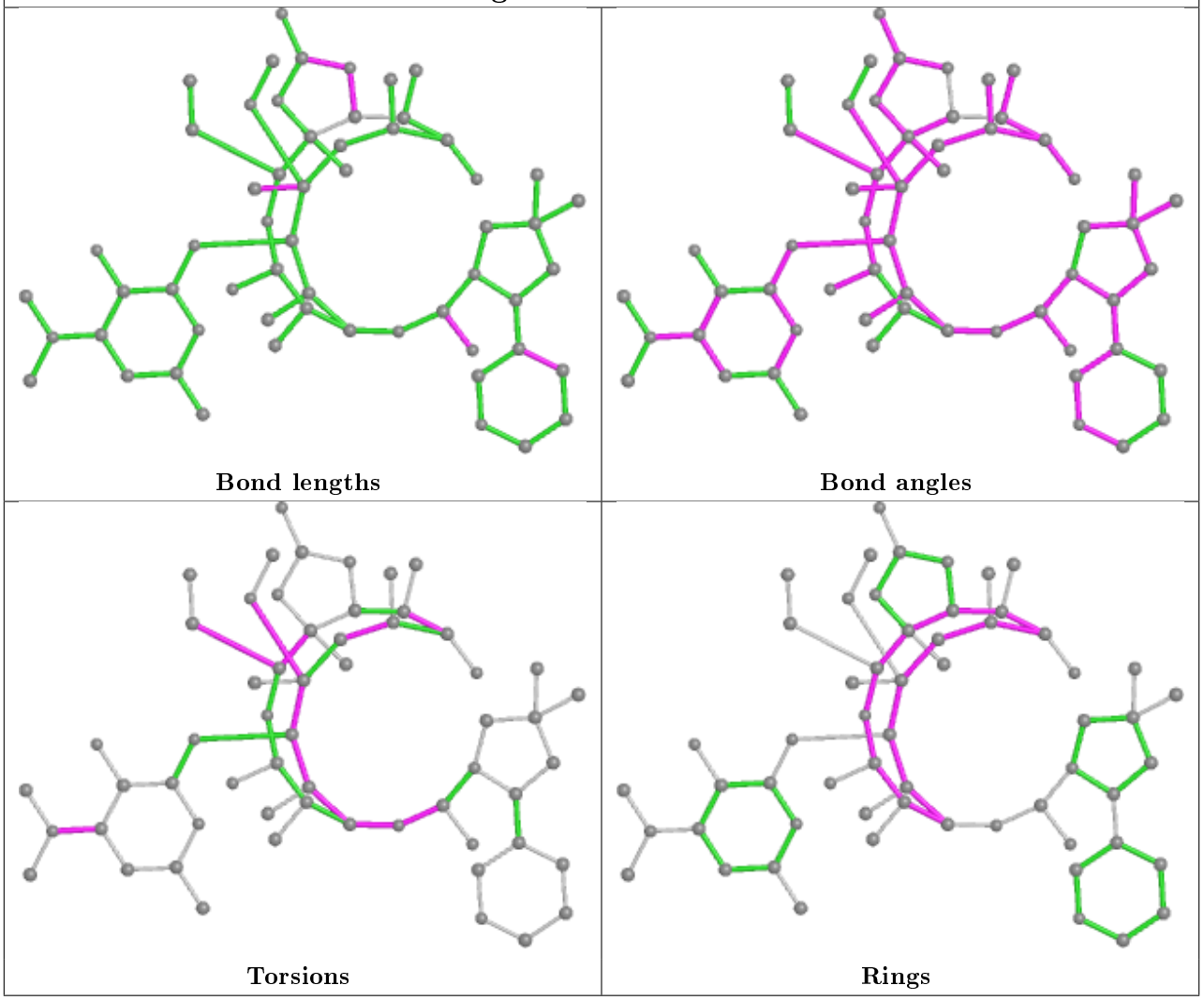
Mol	Chain	Res	Type	Atoms
32	X	2929	1F4	C1-C11-C12-C13-C14-C2-C3-C4-C5-C6-C7-C8-C9-O10

1 monomer is involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	2929	1F4	19	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 1F4 X 2929



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	X	2686/2880 (93%)	-0.14	68 (2%) 57 41	43, 92, 197, 276	0
2	Y	122/123 (99%)	-0.13	3 (2%) 57 41	83, 135, 170, 191	0
3	A	240/274 (87%)	-0.20	4 (1%) 70 55	68, 115, 146, 172	0
4	B	205/211 (97%)	-0.34	1 (0%) 91 83	45, 73, 105, 154	0
5	C	197/205 (96%)	-0.15	8 (4%) 37 24	57, 114, 154, 187	0
6	D	177/180 (98%)	-0.18	9 (5%) 28 17	146, 183, 216, 227	0
7	E	171/185 (92%)	-0.52	2 (1%) 79 66	92, 143, 192, 206	0
8	F	71/144 (49%)	1.53	19 (26%) 0 0	211, 236, 252, 257	0
9	G	142/174 (81%)	-0.32	1 (0%) 87 78	72, 97, 144, 161	0
10	H	134/134 (100%)	-0.40	0 100 100	50, 70, 97, 121	0
11	I	141/156 (90%)	0.30	11 (7%) 13 8	67, 129, 174, 204	0
12	J	136/141 (96%)	0.24	7 (5%) 28 17	74, 103, 149, 184	0
13	K	113/116 (97%)	-0.38	0 100 100	35, 60, 79, 91	0
14	L	104/114 (91%)	-0.15	1 (0%) 82 70	98, 134, 156, 168	0
15	M	108/166 (65%)	-0.62	0 100 100	50, 73, 111, 145	0
16	N	117/118 (99%)	-0.43	0 100 100	59, 90, 128, 159	0
17	O	94/100 (94%)	-0.30	2 (2%) 63 48	66, 115, 157, 173	0
18	P	127/134 (94%)	-0.50	0 100 100	50, 68, 107, 158	0
19	Q	93/95 (97%)	-0.25	2 (2%) 62 45	73, 106, 162, 195	0
20	R	110/115 (95%)	-0.16	5 (4%) 33 21	88, 117, 170, 178	0
21	S	175/237 (73%)	0.35	14 (8%) 12 7	121, 155, 175, 190	0
22	T	84/91 (92%)	0.47	10 (11%) 4 3	79, 107, 186, 200	0
23	U	72/81 (88%)	0.06	6 (8%) 11 7	92, 128, 153, 161	0
24	V	66/67 (98%)	0.02	5 (7%) 13 8	100, 132, 211, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	W	55/55 (100%)	-0.48	1 (1%) 68 53	80, 98, 126, 152	0
26	Z	58/60 (96%)	-0.16	3 (5%) 27 17	49, 70, 105, 114	0
27	1	53/55 (96%)	2.48	19 (35%) 0 0	8, 32, 62, 93	0
28	2	46/47 (97%)	5.92	44 (95%) 0 0	3, 15, 38, 59	0
29	3	63/66 (95%)	3.45	44 (69%) 0 0	3, 25, 40, 61	0
30	4	37/37 (100%)	4.01	24 (64%) 0 0	228, 254, 266, 269	0
All	All	5997/6561 (91%)	-0.01	313 (5%) 27 17	3, 100, 196, 276	0

The worst 5 of 313 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	1	7	ARG	18.8
28	2	27	GLY	13.9
22	T	9	SER	13.0
30	4	25	VAL	12.8
28	2	8	ASN	12.4

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 carbohydrates 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
31	MG	X	2909	1/1	0.34	0.62	97,97,97,97	0
31	MG	Y	204	1/1	0.35	0.93	86,86,86,86	0
31	MG	X	2913	1/1	0.37	1.00	60,60,60,60	0
31	MG	X	2903	1/1	0.45	0.62	89,89,89,89	0

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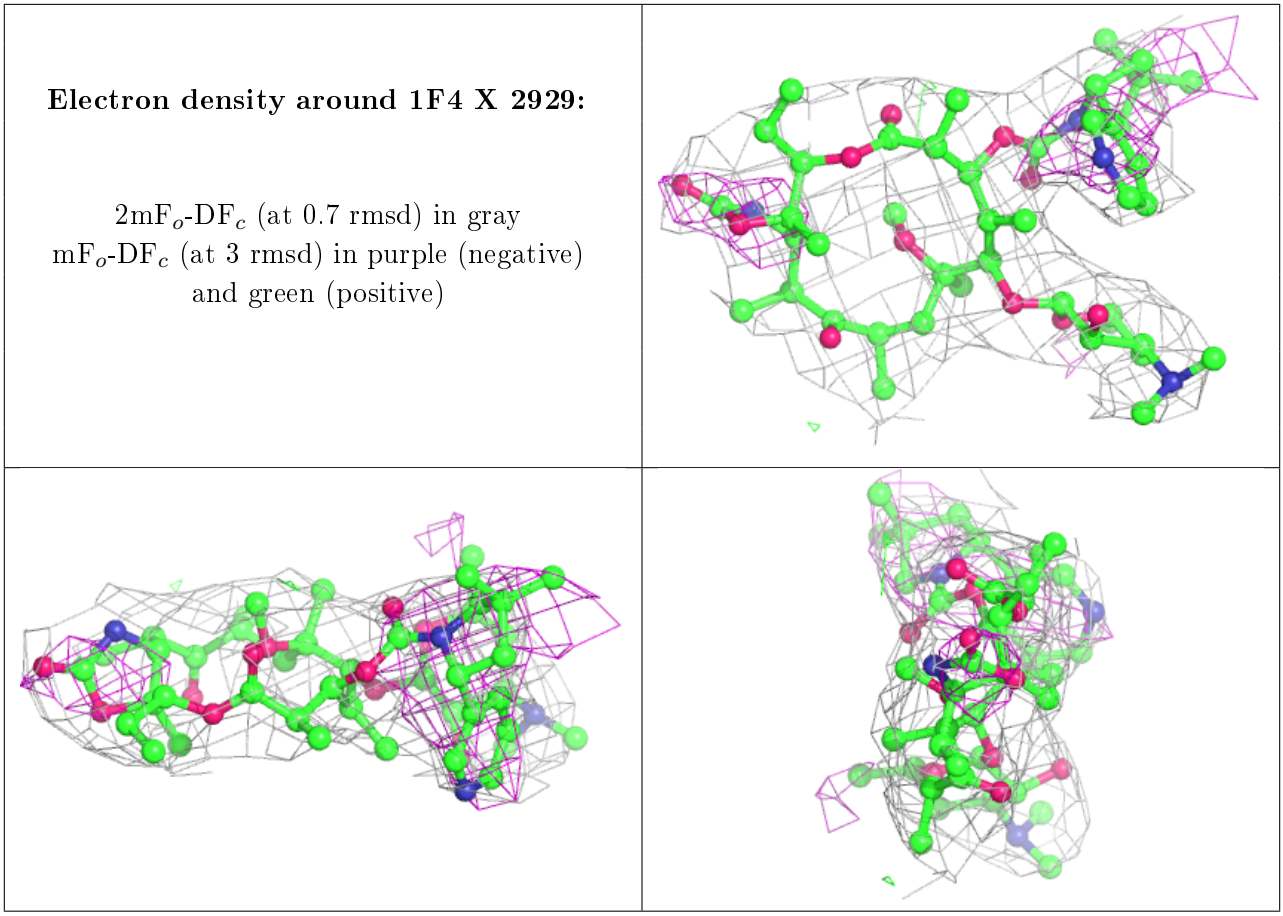
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	X	2901	1/1	0.53	0.69	50,50,50,50	0
31	MG	X	2920	1/1	0.54	0.43	113,113,113,113	0
31	MG	X	2928	1/1	0.58	0.77	61,61,61,61	0
31	MG	X	2927	1/1	0.68	0.53	64,64,64,64	0
31	MG	X	2912	1/1	0.70	0.59	71,71,71,71	0
31	MG	X	2911	1/1	0.77	0.40	68,68,68,68	0
31	MG	X	2926	1/1	0.79	1.78	45,45,45,45	0
31	MG	X	2924	1/1	0.80	1.08	70,70,70,70	0
31	MG	Y	203	1/1	0.81	0.92	59,59,59,59	0
31	MG	X	2908	1/1	0.82	2.35	37,37,37,37	0
31	MG	X	2915	1/1	0.84	0.73	57,57,57,57	0
31	MG	X	2918	1/1	0.84	1.23	42,42,42,42	0
31	MG	Y	206	1/1	0.84	0.29	78,78,78,78	0
31	MG	X	2916	1/1	0.86	1.17	37,37,37,37	0
31	MG	Y	202	1/1	0.88	1.42	88,88,88,88	0
31	MG	X	2905	1/1	0.89	0.49	65,65,65,65	0
31	MG	X	2921	1/1	0.90	0.71	80,80,80,80	0
31	MG	X	2919	1/1	0.92	0.92	30,30,30,30	0
31	MG	X	2904	1/1	0.92	0.29	110,110,110,110	0
31	MG	Y	205	1/1	0.92	0.40	82,82,82,82	0
31	MG	Y	201	1/1	0.93	0.44	98,98,98,98	0
31	MG	X	2902	1/1	0.93	0.31	94,94,94,94	0
31	MG	X	2906	1/1	0.94	0.94	58,58,58,58	0
31	MG	X	2917	1/1	0.94	1.09	55,55,55,55	0
31	MG	X	2922	1/1	0.95	0.84	44,44,44,44	0
31	MG	X	2914	1/1	0.96	0.65	27,27,27,27	0
31	MG	X	2907	1/1	0.96	0.81	51,51,51,51	0
32	1F4	X	2929	58/58	0.96	0.21	20,20,20,20	0
31	MG	X	2923	1/1	0.96	0.34	34,34,34,34	0
31	MG	X	2925	1/1	0.97	0.26	122,122,122,122	0
31	MG	M	201	1/1	0.98	1.39	23,23,23,23	0
31	MG	X	2910	1/1	0.99	0.69	41,41,41,41	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 1F4 X 2929:

$2mF_o$-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

There are no such residues in this entry.