



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 18, 2024 – 10:42 AM EDT

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

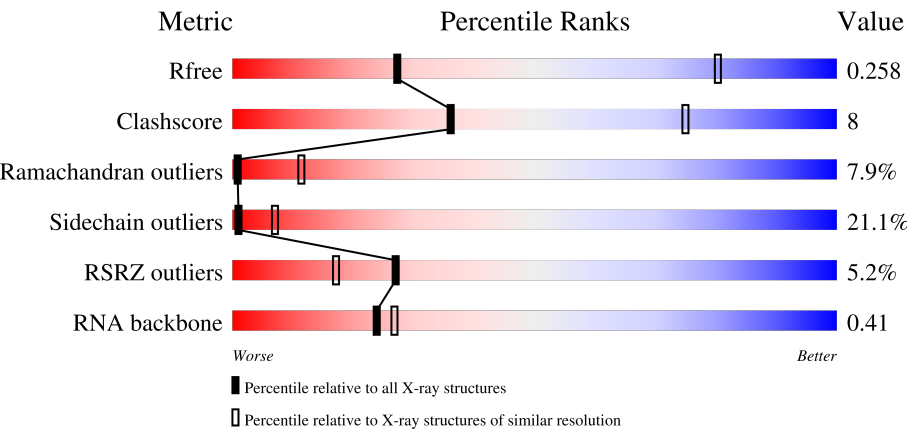
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 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 $\leq 5\%$. 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	<div><div>2%</div><div>30%38%21%7%</div></div>
2	Y	123	<div><div>2%</div><div>27%41%26%6%</div></div>
3	A	274	<div><div>%</div><div>50%26%11%12%</div></div>
4	B	211	<div><div></div><div>62%26%9%</div></div>


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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	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
1	X	2686	Total	C	N	O	P	0	0	0
			57651	25718	10642	18606	2685			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	122	Total	C	N	O	P	0	0	0
			2598	1161	476	840	121			

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

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

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

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

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

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

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

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

- 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	C	N	O	0	0	0
			779	476	161	142			

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

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

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

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

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

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

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

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

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

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

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

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

- 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	S	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

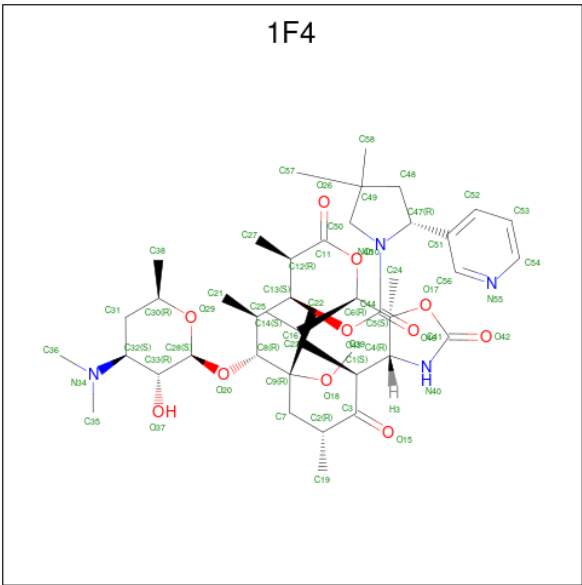
- Molecule 30 is a protein called 50S ribosomal protein L36.

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

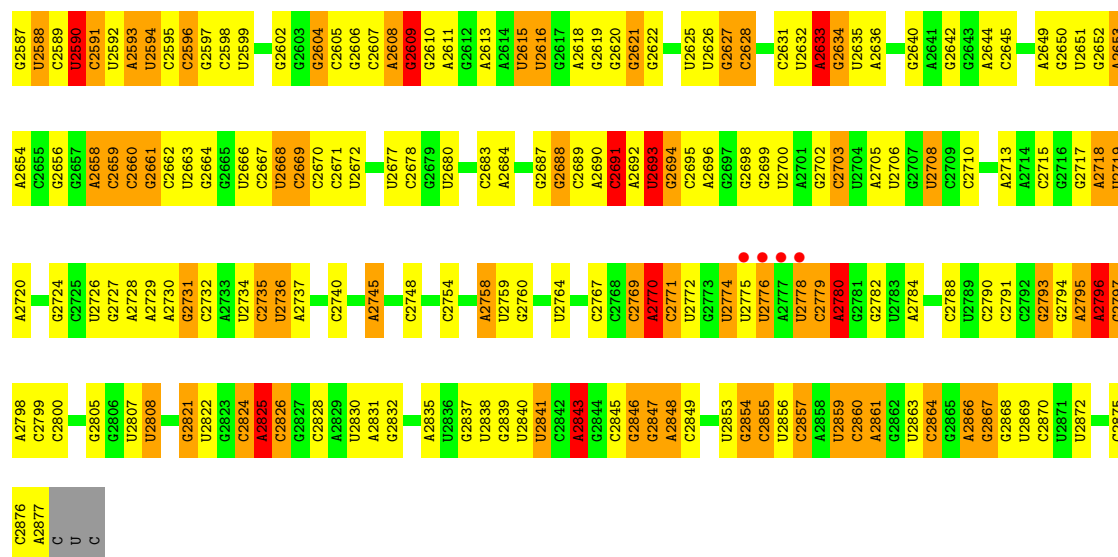
- Molecule 32 is (3aS,4R,7R,8S,9S,10R,11R,13R,15S,15aR)-4-ethyl-11-methoxy-3a,7,9,11,13,15-hexamethyl-2,6,14-trioxo-10-{[3,4,6-trideoxy-3-(dimethylamino)-beta-D-xylo-hexopyranosyl]oxy}tetradecahydro-2H-oxacyclotetradecino[4,3-d][1,3]oxazol-8-yl (2R)-4,4-dimethyl-2-(pyridin-3-yl)pyrrolidine-1-carboxylate (three-letter code: 1F4) (formula: C₄₃H₆₈N₄O₁₁).



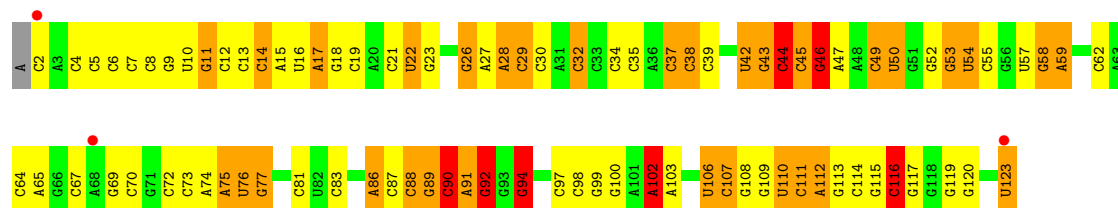
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	N	O	0	0
			58	43	4	11		

A1560	C1487	C1411	U1342	U1199	G1125	C1064	A990	A918	G854	G789	C723	A655
A1561	G1488	C1412	C1343	G1200	A1126	C1064	A994	U919	G858	A790	C724	U656
A1562	C1489	C1413	C1344	U1201	G1127	G1067	A995	A922	U859	G793	C725	A657
U1563	U1490	G1414	C1345	A1202	G1128	G1069	A996	A922	U860	A794	G726	G658
A1567	G1494	C1415	C1346	A1203	U1130	G1070	G997	C924	U863	A795	U727	G659
C1570	U1495	C1421	C1348	A1208	G1131	U1071	A998	U925	C863	A796	G728	G660
G1571	G1496	C1422	A1349	G1209	C1132	U1072	A999	C926	C864	A797	U729	C661
C1572	G1498	U1277	A1281	G1210	G1133	U1073	A1000	C927	A865	G798	C730	C664
A1573	U1500	G1426	C1283	G1211	C1134	G1074	A1001	G931	U866	C799	A731	U666
A1574	G1428	U1280	G1284	U1217	C1135	U1075	A1002	G932	G867	U800	G732	U667
C1575	A1429	U1281	C1285	U1218	C1136	U1076	C1003	G933	U868	A801	G733	U668
G1576	G1430	A1287	A1286	C1219	A1137	U1077	C1006	G934	C870	A802	G738	A668
G1577	U1431	A1288	U1288	G1220	A1138	A1078	A1007	G834	U871	C803	G739	G669
U1578	G1432	A1289	C1289	C1221	A1139	A1079	A1008	C935	U872	C804	A740	U670
A1582	A1433	A1290	U1290	G1222	U1141	A1080	C1009	A936	G872	G805	G741	A671
A1583	U1434	G1291	G1291	G1223	U1142	A1081	U1010	C937	A874	A806	G742	G672
G1584	G1435	G1294	A1224	A1225	A1143	G1082	U1011	G938	U875	A807	A743	G673
A1586	A1367	C1302	G1225	G1229	U1144	C1083	G1014	C939	G876	C808	G744	U674
C1593	G1368	U1303	C1302	C1229	G1145	A1084	U1015	U941	A877	C809	C745	U675
A1594	G1369	C1304	C1303	C1230	G1146	G1085	C1016	U942	G878	U810	G746	G676
A1595	G1371	U1304	C1304	C1231	G1147	C1086	C1017	U943	A879	G811	C749	G677
A1596	G1372	U1305	C1305	A1231	G1148	C1087	C1018	A944	U881	A813	C750	A681
A1597	G1373	U1306	C1306	U1232	G1149	A1088	U1019	G945	C880	A814	G751	G682
C1598	G1374	U1307	C1307	A1233	C1150	C1088	A1020	U946	C882	A815	G752	A683
G1599	G1375	C1308	C1308	C1234	U1151	C1090	A1021	C947	A883	U816	U753	C684
U1600	U1446	G1309	C1309	G1236	A1152	C1091	A1022	G951	A885	A817	C754	G687
A1601	U1447	C1310	C1310	G1237	A1153	U1092	U1023	A952	U886	G818	C755	A688
A1602	A1448	C1311	C1311	A1238	U1159	U1093	G1024	G953	G887	A952	U757	A689
A1603	U1454	G1312	C1312	G1241	U1160	A1095	G1028	U954	G888	C822	C758	A690
A1607	C1455	A1313	G1313	U1241	U1161	A1096	G1029	G955	C889	U823	C759	C691
U1608	C1456	A1314	C1314	U1244	A1162	A1097	U1030	A956	U890	U824	U760	C692
G1609	A1457	G1315	C1315	G1245	C1163	A1098	C1031	G957	A891	C825	G761	A693
A1610	U1458	G1316	C1316	G1246	C1164	A1099	A1032	G958	G	U826	A762	G694
G1613	U1459	A1317	C1317	U1247	A1167	G1100	G1033	C959	G	C827	A763	G695
C1614	G1460	C1318	A1318	U1248	A1168	U1101	U1034	U960	G	C828	A764	U696
C1615	C1461	C1319	C1319	G1249	C1169	G1102	G1035	G961	G	C829	C765	U697
U1618	G1465	A1320	C1320	G1250	U1172	C1103	G1036	C967	C	C830	U768	A698
A1619	U1466	A1321	C1321	A1251	G1173	U1105	U1037	C968	C	C831	C769	C700
C1623	U1467	U1325	C1325	C1252	U1174	A1106	A1039	U969	U	A833	U770	U701
A1624	A1468	U1326	C1326	C1253	G1181	A1107	A1040	A970	A	A834	C771	A702
A1625	U1469	C1327	A1327	G1254	U1182	U1108	U1041	A971	C	U837	A774	A703
A1626	G1470	U1328	C1328	A1255	U1183	A1109	G1045	C972	C	A838	U775	U707
A1627	G1471	C1329	C1329	U1257	C1184	G1110	U1046	U974	A	U839	A776	G708
A1628	U1472	G1330	C1330	U1261	G1185	C1111	C1049	C975	C	U840	A777	A709
C1629	U1473	G1331	C1331	U1262	A1186	C1112	G1050	C976	U	G841	C778	C710
A1630	A1474	G1332	C1332	U1263	A1187	A1113	U1051	G977	U	A842	U779	C711
A1631	U1475	G1333	C1333	G1264	A1188	A1114	C1052	U978	A	G843	U780	A712
A1632	G1476	A1334	C1334	C1265	G1189	U1115	G1053	C979	C	U844	G781	G713
A1633	C1477	A1335	C1335	U1266	C1190	G1117	C1054	G980	U	U845	U782	C714
A1634	U1478	G1336	C1336	G1267	G1191	G1118	A1055	C981	A	A846	G783	G715
A1635	A1479	G1337	C1337	U1268	A1192	G1119	U1056	C982	G	A911	U784	A716
A1636	G1480	G1338	C1338	U1269	G1193	G1121	A1057	G983	C	C914	U785	A717
A1637	U1481	G1339	C1339	C1270	U1194	A1122	G1058	A984	C	C915	U786	A718
A1638	U1482	C1340	C1340	C1271	U1195	G1123	A1059	G985	C	C916	A787	A719
A1639	G1483	G1341	C1341	C1272	C1198	U1124	C1060	G986	C	U917	G788	A720
A1640	A1484	C1342	C1342	C1273	C1199	U1125	C1061	G987	C	C917	C789	C721
A1641	U1485	C1343	C1343	C1274	C1200	U1126	C1062	G988	C	C918	C790	C722
A1642	G1486	C1344	C1344	C1275	U1201	A1127	C1063	G989	C	C919	C791	C723
A1643	U1487	C1345	C1345	U1202	U1202	G1128	C1064	A922	C	C920	C792	C724
A1644	C1488	C1346	C1346	A1203	G1129	G1129	C1065	C924	C	C921	C793	C725
A1645	G1489	C1347	C1347	A1204	U1130	G1130	C1066	U925	C	C922	C794	C726
A1646	U1490	C1348	C1348	A1205	G1131	U1131	C1067	C926	C	C923	C795	C727
A1647	A1491	C1349	C1349	A1206	C1132	U1132	C1068	C927	C	C924	C796	C728
A1648	G1492	C1350	C1350	A1207	G1133	U1133	C1069	C928	C	C925	C797	C729
A1649	U1493	C1351	C1351	A1208	C1134	U1134	C1070	C929	C	C926	C798	C730
A1650	A1494	C1352	C1352	A1209	C1135	U1135	C1071	C930	C	C927	C799	C731
A1651	G1495	C1353	C1353	A1210	C1136	U1136	C1072	C931	C	C928	C800	C732
A1652	U1496	C1354	C1354	U1211	A1137	U1137	C1073	C932	C	C929	C801	C733
A1653	G1497	C1355	C1355	U1212	A1138	U1138	C1074	C933	C	C930	C802	C734
A1654	A1498	C1356	C1356	U1213	A1139	U1139	C1075	C934	C	C931	C803	C735
A1655	U1499	C1357	C1357	U1214	A1140	U1140	C1076	C935	C	C932	C804	C736
A1656	G1499	C1358	C1358	U1215	U1141	U1141	C1077	C936	C	C933	C805	C737
A1657	U1500	C1359	C1359	U1216	U1142	U1142	C1078	C937	C	C934	C806	C738
A1658	A1501	C1360	C1360	U1217	U1143	U1143	C1079	C938	C	C935	C807	C739
A1659	G1501	C1361	C1361	U1218	U1144	U1144	C1080	C939	C	C936	C808	C740
A1660	U1502	C1362	C1362	U1219	U1145	U1145	C1081	C940	C	C937	C809	C741
A1661	A1503	C1363	C1363	U1220	U1146	U1146	C1082	C941	C	C938	C810	C742
A1662	G1503	C1364	C1364	U1221	U1147	U1147	C1083	C942	C	C939	C811	C743
A1663	U1504	C1365	C1365	U1222	U1148	U1148	C1084	C943	C	C940	C812	C744
A1664	G1504	C1366	C1366	U1223	U1149	U1149	C1085	C944	C	C941	C813	C745
A1665	A1505	C1367	C1367	U1224	U1150	U1150	C1086	C945	C	C942	C814	C746
A1666	U1506	C1368	C1368	U1225	U1151	U1151	C1087	C946	C	C943	C815	C747
A1667	G1506	C1369	C1369	U1226	U1152	U1152	C1088	C947	C	C944	C816	C748
A1668	A1507	C1370	C1370	U1227	U1153	U1153	C1089	C948	C	C945	C817	C749
A1669	U1508	C1371	C1371	U1228	U1154	U1154	C1090	C949	C	C946	C818	C750
A1670	G1509	C1372	C1372	U1229	U1155	U1155	C1091	C950	C	C947	C819	C751
A1671	A1510	C1373	C1373	U1230	U1156	U1156	C1092	C951	C	C948	C820	C752
A1672	U1511	C1374	C1374	U1231	U1157	U1157	C1093	C952	C	C949	C821	C753
A1673	G1512	C1375	C1375	U1232	U1158	U1158	C1094	C953	C	C950	C822	C754
A1674	U1513	C1376	C1376	U1233	U1159	U1159	C1095	C954	C	C951	C823	C755
A1675	A1514	C1377	C1377	U1234	U1160	U1160	C1096	C955	C	C952	C824	C756
A1676	G1515	C1378	C1378	U1235	U1161	U1161	C1097	C956	C	C953	C825	C757
A1677	U1516	C1379	C1379	U1236	U1162	U1162	C1098	C957	C	C954	C826	C758
A1678	A1517	C1380	C1380	U1237	U1163	U1163	C1099	C958	C	C955	C827	C759
A1679	G1518	C1381	C1381	U1238	U1164	U1164	C1100	C959	C	C956	C828	C760
A1680	U1519	C1382	C1382	U1239	U1165	U1165	C1101	C960	C	C957	C829	C761
A1681	A1520	C1383	C1383	U1240	U1166	U1166	C1102	C961	C	C958	C830	C762
A1682	G1521	C1384	C1384	U1241	U1167	U1167	C1103	C962	C	C959	C831	C763
A1683	U1522	C1385	C1385	U1242	U1168	U1168	C1104	C963	C	C960	C832	C764
A1684	A1523	C1386	C1386	U1243	U1169	U1169	C1105	C964	C	C961	C833	C765
A1685	G1524	C1387	C1387	U1244	U1170	U1170	C1106	C965	C	C962	C834	C766
A1686	U1525	C1388	C1388	U1245	U1171	U1171	C1107	C966	C	C963	C835	C767
A1687	A1526	C1389	C1389	U1246	U1172	U1172	C1108	C967	C	C964	C836	C768
A1688	G1527	C1390</										

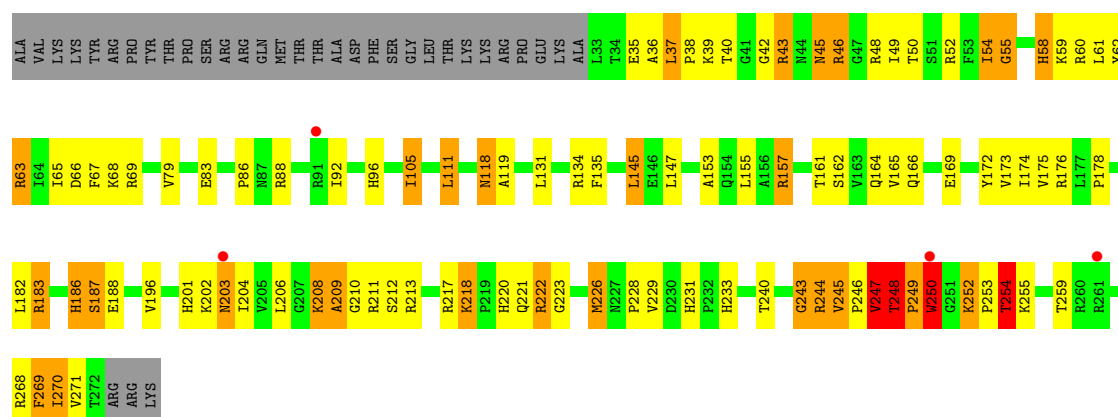
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C2459	G2460	G2461	G2462	G2463	G2464	G2465	G2466	G2467	G2468	G2469	G2470	G2471	U2472	G2475	G2476	G2477	G2478	G2479	G2480	G2481	G2482	G2483	G2484	G2485	G2486	G2487	G2488	G2489	G2490	G2491	G2492	G2493	G2494	G2495	G2496	G2497	G2498	G2499	G2500	G2503	G2504	G2505	G2506	G2507	G2508	A2509	G2510	G2511	G2514	G2515	G2516	G2517	G2518	G2519	G2522			
G2388	G2389	G2392	G2393	G2394	G2395	G2396	A2397	A2401	U2402	G2403	A2404	A2405	G2406	G2407	G2408	A2409	U2410	A2414	G2415	U2416	U2417	A2418	G2419	G2420	G2421	G2422	G2423	G2426	U2427	U2428	C2431	A2432	C2435	A2438	U2439	G2440	U2441	C2442	C2443	C2444	G2447	G2448	G2449	U2452	G2453	C2454	A2455	U2456	U2457	U2458								
G2320	G2321	U2322	G2323	G2324	A2325	G2326	G2329	G2330	A2333	G2334	U2335	G2336	G2337	G2338	G2339	C2340	C2343	G2344	G2347	A2348	G2349	G2350	G2351	G2352	G2353	A2357	G2358	U2359	G2362	G2363	C2364	U2365	A2367	G2368	U2369	G2370	A2371	A2372	C2373	C2374	G2375	G2376	U2377	U2380	A2381	G2382	C2383	G2384	U2385	G2386	U2387							
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U2184	U2185	A2188	A2189	A2190	A2191	U2192	U2193	A2194	G2195	U2196	U2197	U2198	G2199	G2200	G2201	A2204	G2205	G2206	G2207	U2208	G2209	U2210	U2211	U2212	G2213	G2214	G2215	G2216	G2217	G2218	U2219	A2220	G2221	U2222	U2223	U2224	G2225	A2226	G2227	U2228	G2229	G2230	G2236	G2237	G2238	G2239	C2240	U2241	G2242	G2243	G2244	A2245	A2246	U2247				
A2052	G2053	A2054	C2055	G2056	C2056	A2060	G2061	U2062	A2063	U2064	A2065	G2066	U2067	G2068	U2069	G2070	G2071	C2072	U2075	G2076	G2077	G2078	A2079	U2080	U2081	G2082	G2083	U2088	G2089	U2090	C2093	A2095	G2096	G2097	G2098	G2099	U2030	G2032	A2034	G2033	G2034	G2035	G2036	A2037	G2038	G2039	A2040	A2041	A2042	A2043	G2044	A2045	C2046	C2047	G2048	G2049	G2050	U2051
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U1900	C1991	G1992	G1993	U1994	U1995	A1996	A1997	A1998	U1999	U2000	G2001	A2002	A2003	U2004	U2005	G2006	U2009	G2010	U2011	A2012	A2013	A2014	A2015	A2016	U2017	C2018	C2019	C2022	G2023	U2024	A2025	G2026	G2027	C2028	G2029	U2030	G2032	A2034	G2033	G2034	G2035	G2036	A2037	G2038	G2039	A2040	A2041	A2042	A2043	G2044	A2045	C2046	C2047	G2048	G2049	G2050	U2051	
G1785	G1786	G1787	G1788	U1789	A1790	C1791	G1792	A1793	A1794	A1796	A1799	A1800	U1801	U1804	G1805	G1806	U1807	U1808	U1809	U1810	A1811	U1812	A1813	G1816	U1817	G1818	U1819	G1820	A1821	C1824	A1825	C1828	C1829	U1830	G1831	G1832	U1833	G1834	C1835	C1836	A1839	A1840	G1841	G1842	U1843	C1844	A1845	A1846	G1850	A1851	U1852	C1853	C1854					
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U1636	U1637	G1642	A1643	U1647	C1648	U1651	G1652	G1653	G1654	G1655	U1656	U1657	G1660	C1661	G1662	G1663	G1664	G1665	G1666	A1667	G1668	G1669	G1670	A1671	G1672	C1673	C1674	G1675	G1678	U1679	U1680	A1681	G1683	G1684	A1685	C1686	C1687	U1688	U1689	G1691	U1770	C1692	A1693	A1694	U1695	A1699	C1700	U1705	A1706	G1707	C1708							



• Molecule 2: 5S ribosomal RNA

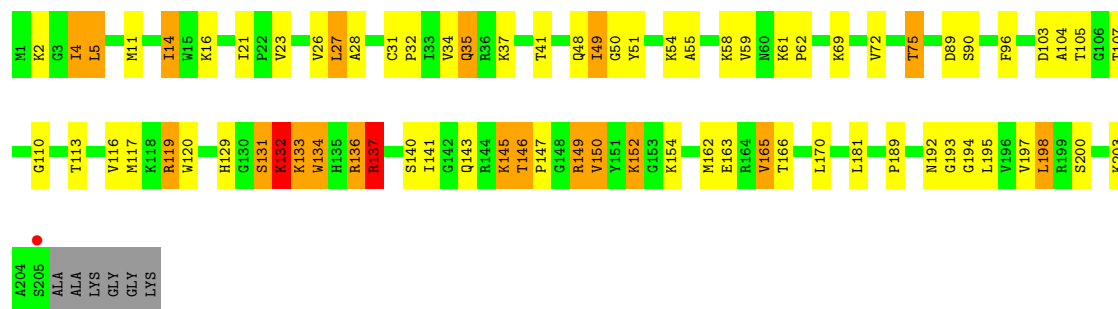


• Molecule 3: 50S ribosomal protein L2

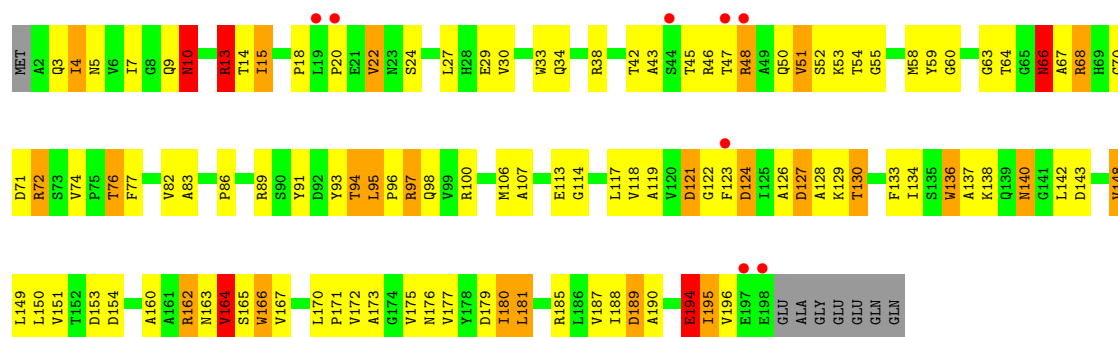


• Molecule 4: 50S ribosomal protein L3

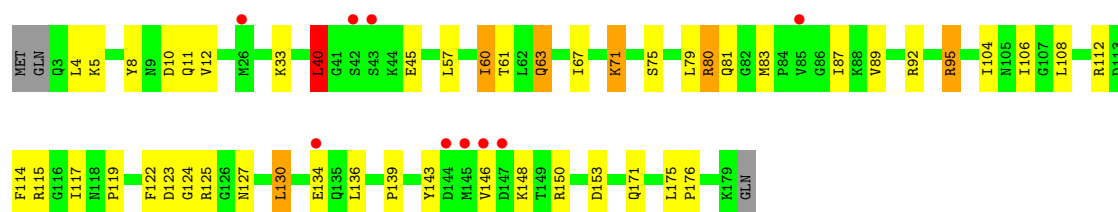




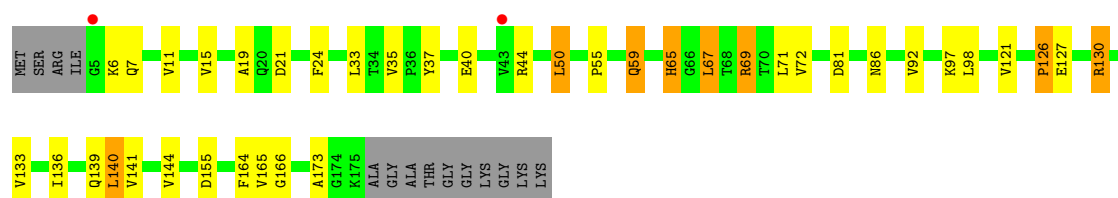
• Molecule 5: 50S ribosomal protein L4



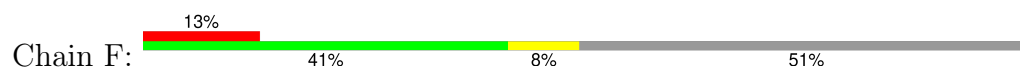
• Molecule 6: 50S ribosomal protein L5

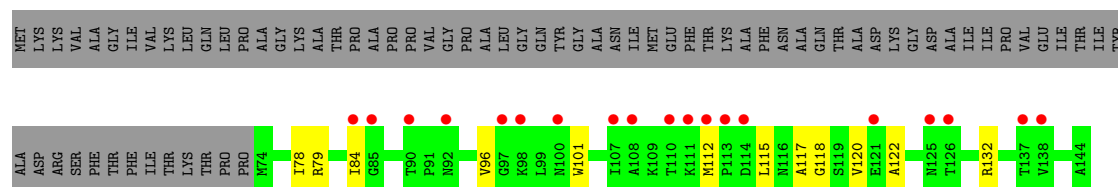


• Molecule 7: 50S ribosomal protein L6

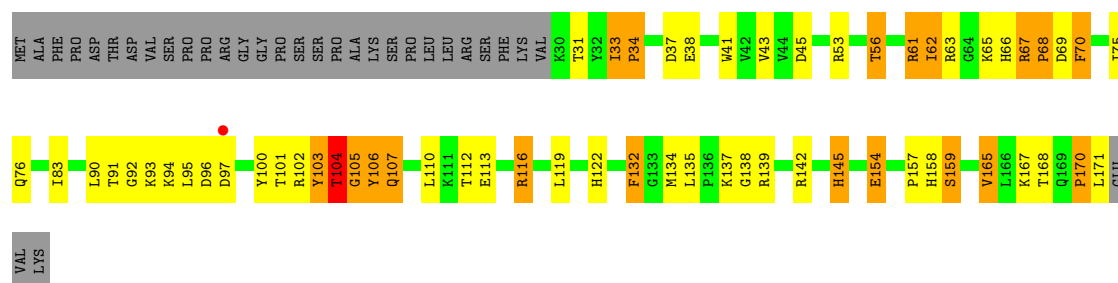


• Molecule 8: 50S ribosomal protein L11

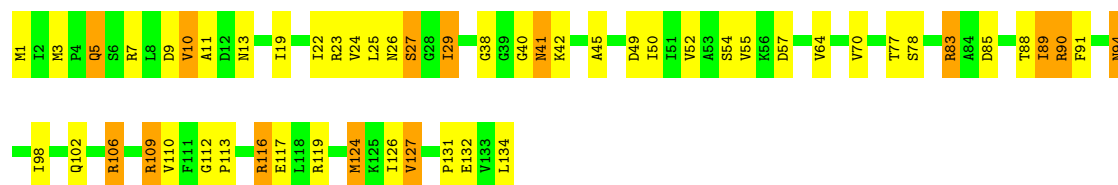




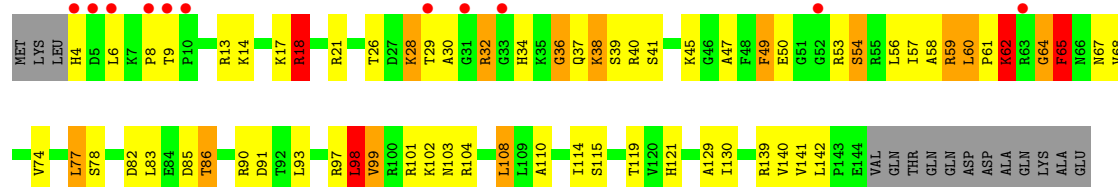
• Molecule 9: 50S ribosomal protein L13



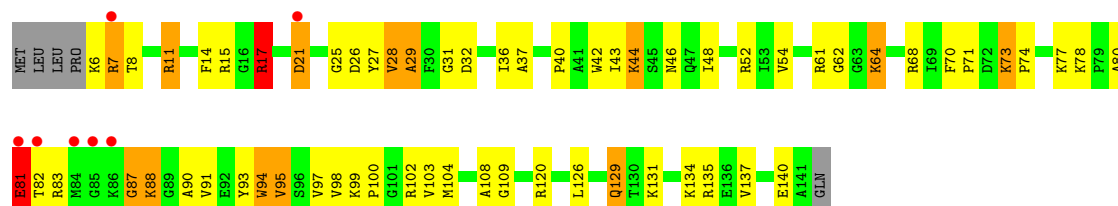
• Molecule 10: 50S ribosomal protein L14



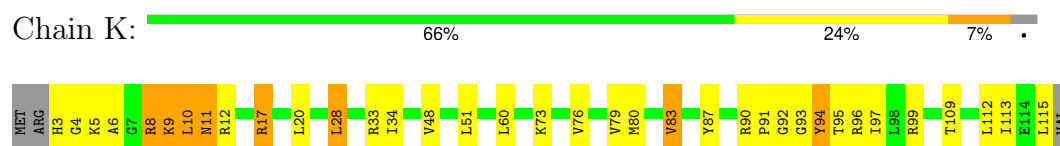
• Molecule 11: 50S ribosomal protein L15



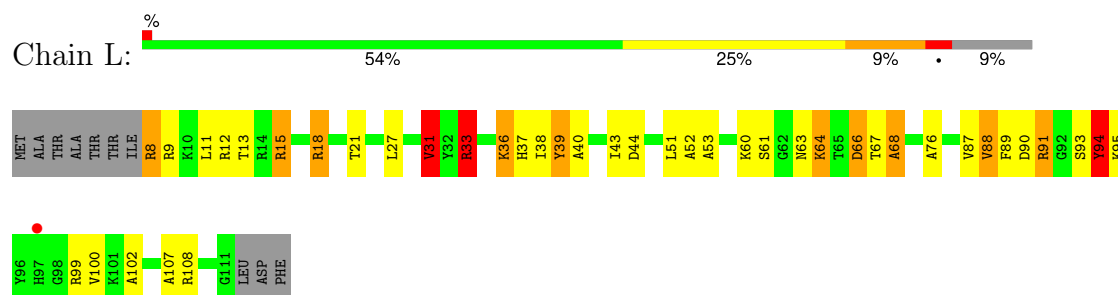
• Molecule 12: 50S ribosomal protein L16



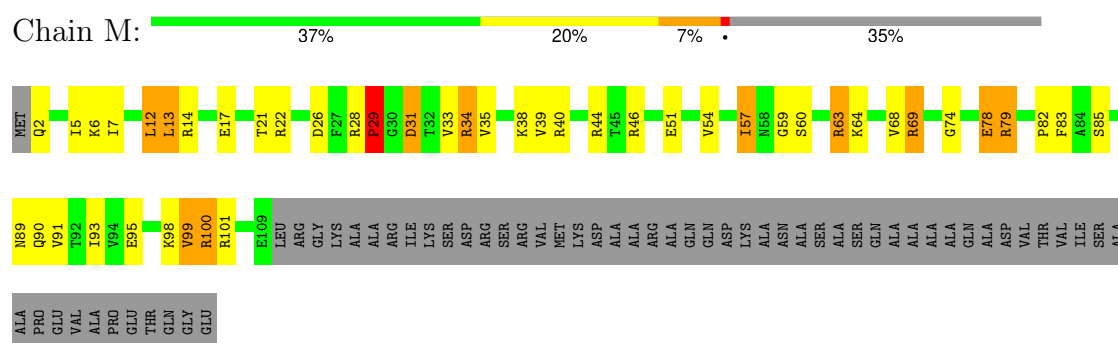
- Molecule 13: 50S ribosomal protein L17



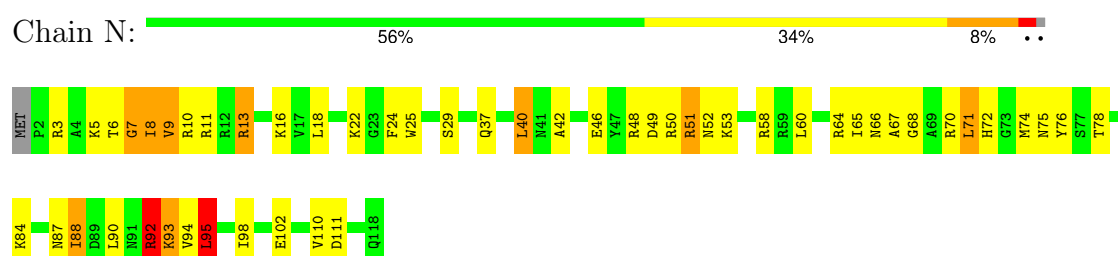
- Molecule 14: 50S ribosomal protein L18



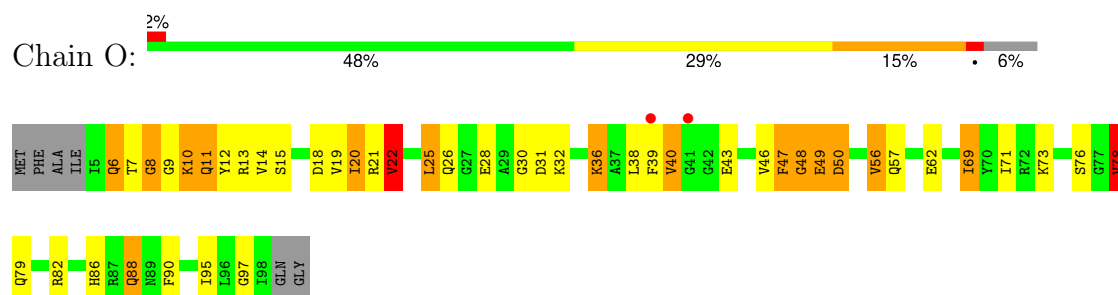
- Molecule 15: 50S ribosomal protein L19



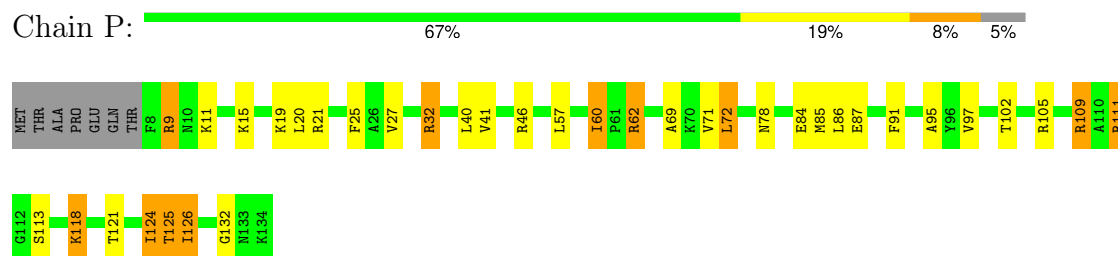
- Molecule 16: 50S ribosomal protein L20



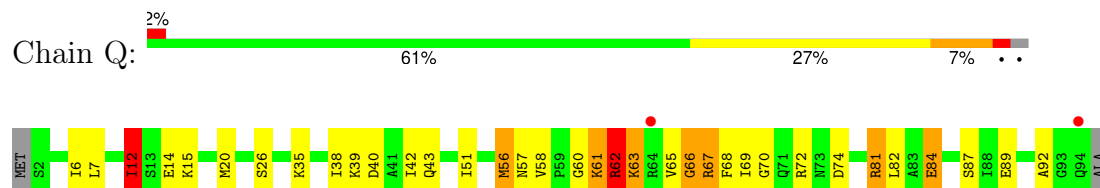
- Molecule 17: 50S ribosomal protein L21



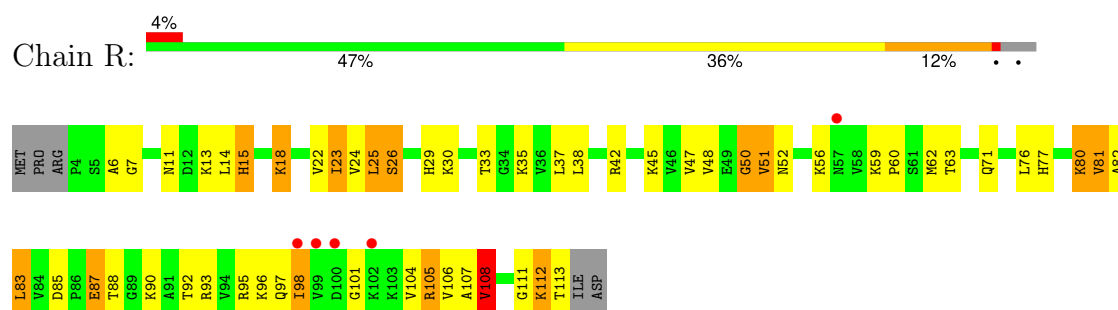
- Molecule 18: 50S ribosomal protein L22



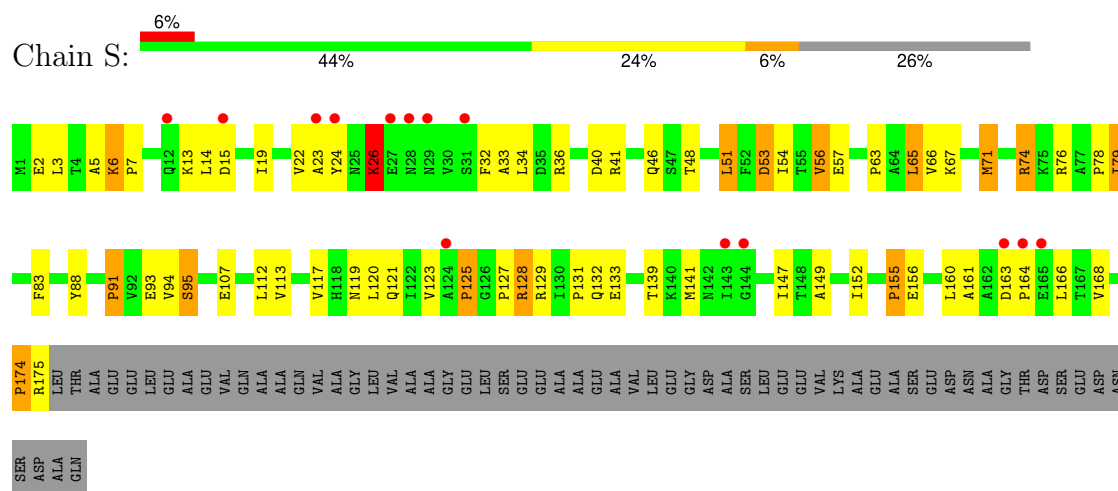
- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24

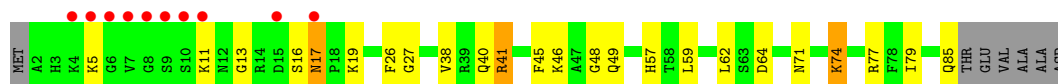


- Molecule 21: 50S ribosomal protein L25

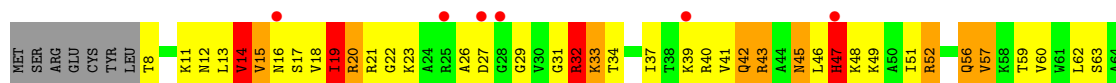


- Molecule 22: 50S ribosomal protein L27





- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



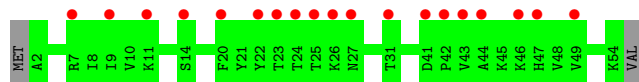
- Molecule 25: 50S ribosomal protein L30



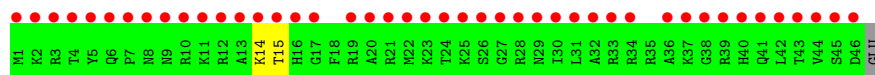
- Molecule 26: 50S ribosomal protein L32



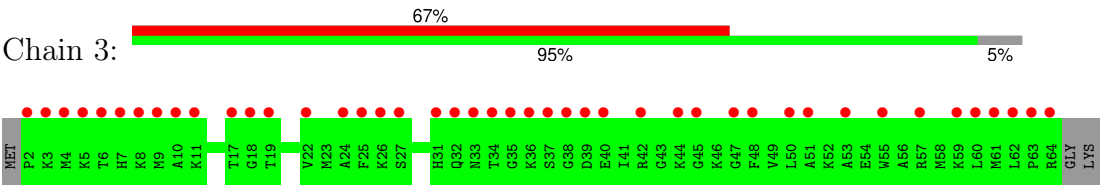
- Molecule 27: 50S ribosomal protein L33



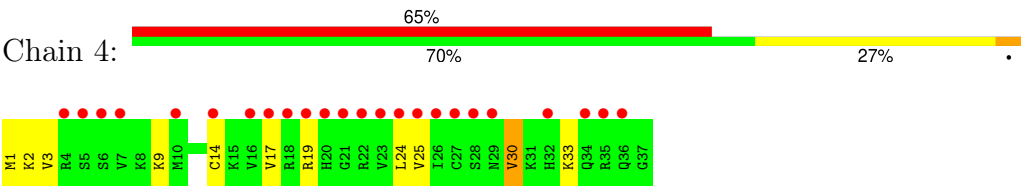
- Molecule 28: 50S ribosomal protein L34



● Molecule 29: 50S ribosomal protein L35



● Molecule 30: 50S ribosomal protein L36



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 , 93.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MG, 1F4

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(°)	Ideal(°)
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

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 ⓘ

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
23	U	40	ARG
23	U	79	GLU
23	U	37	ILE
10	H	10	VAL
9	G	165	VAL

Sometimes 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	90	GLN
23	U	56	GLN
17	O	88	GLN
22	T	71	ASN

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Mol	Chain	Res	Type
26	Z	44	HIS

5.3.3 RNA [i](#)

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	2660	C
1	X	2759	U
2	Y	116	C
1	X	1000	G
1	X	970	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	61,62,62	1.27	6 (9%)	81,95,95	2.75	37 (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	-	-	33/74/119/119	1/5/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2929	1F4	C41-N40	4.52	1.39	1.33
32	X	2929	1F4	C52-C51	3.41	1.44	1.39
32	X	2929	1F4	C22-C9	2.87	1.58	1.52
32	X	2929	1F4	O46-C44	2.19	1.24	1.21
32	X	2929	1F4	C4-N40	2.09	1.49	1.45

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2929	1F4	C51-C47-N45	-8.29	98.37	113.03
32	X	2929	1F4	C6-O10-C11	6.74	129.97	118.20
32	X	2929	1F4	C22-C9-C7	-5.34	103.00	111.17
32	X	2929	1F4	C21-C14-C13	5.10	120.37	111.40
32	X	2929	1F4	O43-C13-C14	5.05	119.16	107.52

There are no chirality outliers.

5 of 33 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

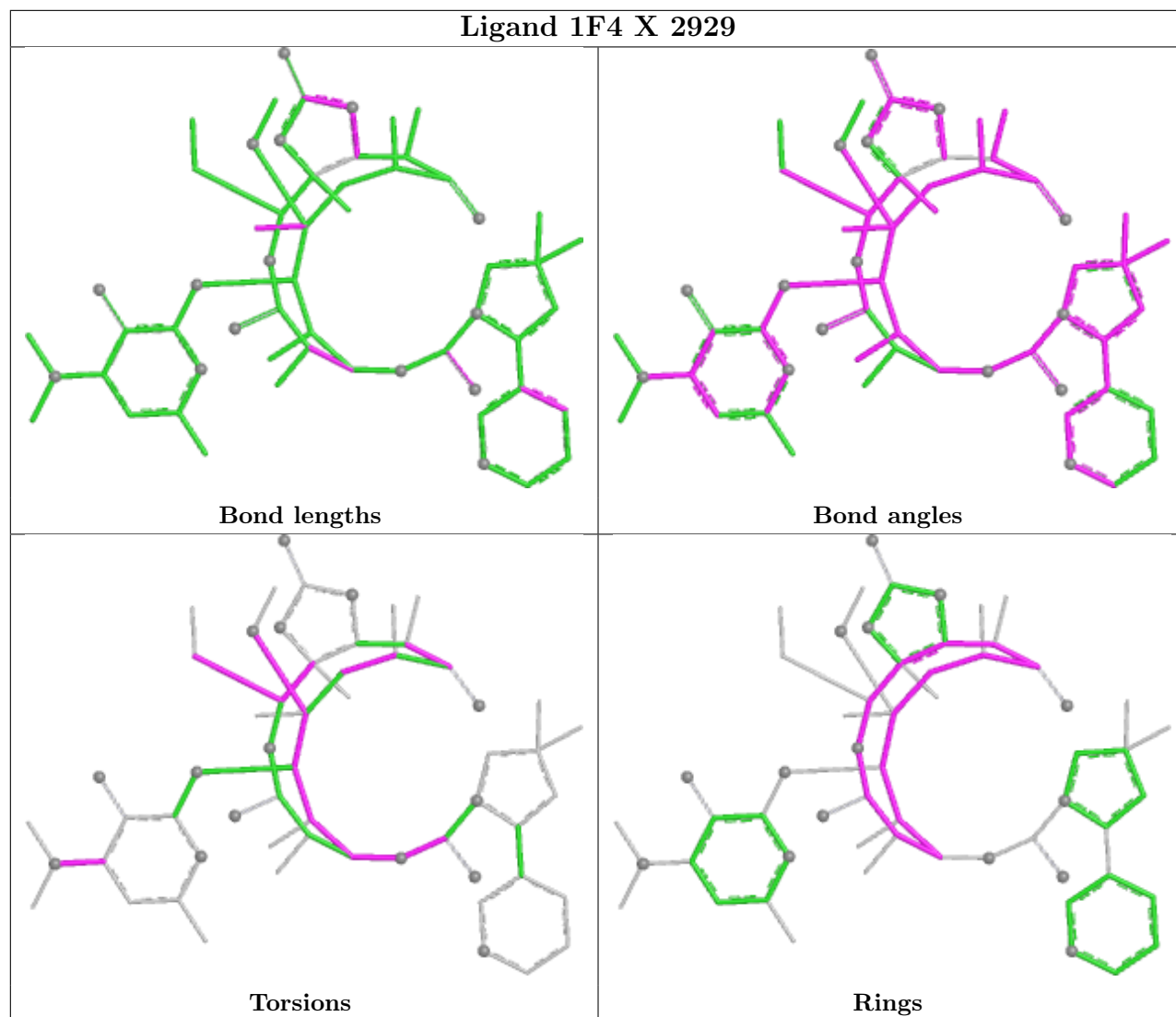
All (1) ring outliers are listed below:

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 than 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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	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%)	-0.17	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%)	5.91	44 (95%) 0 0	3, 15, 38, 59	0
29	3	63/66 (95%)	3.44	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 ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.

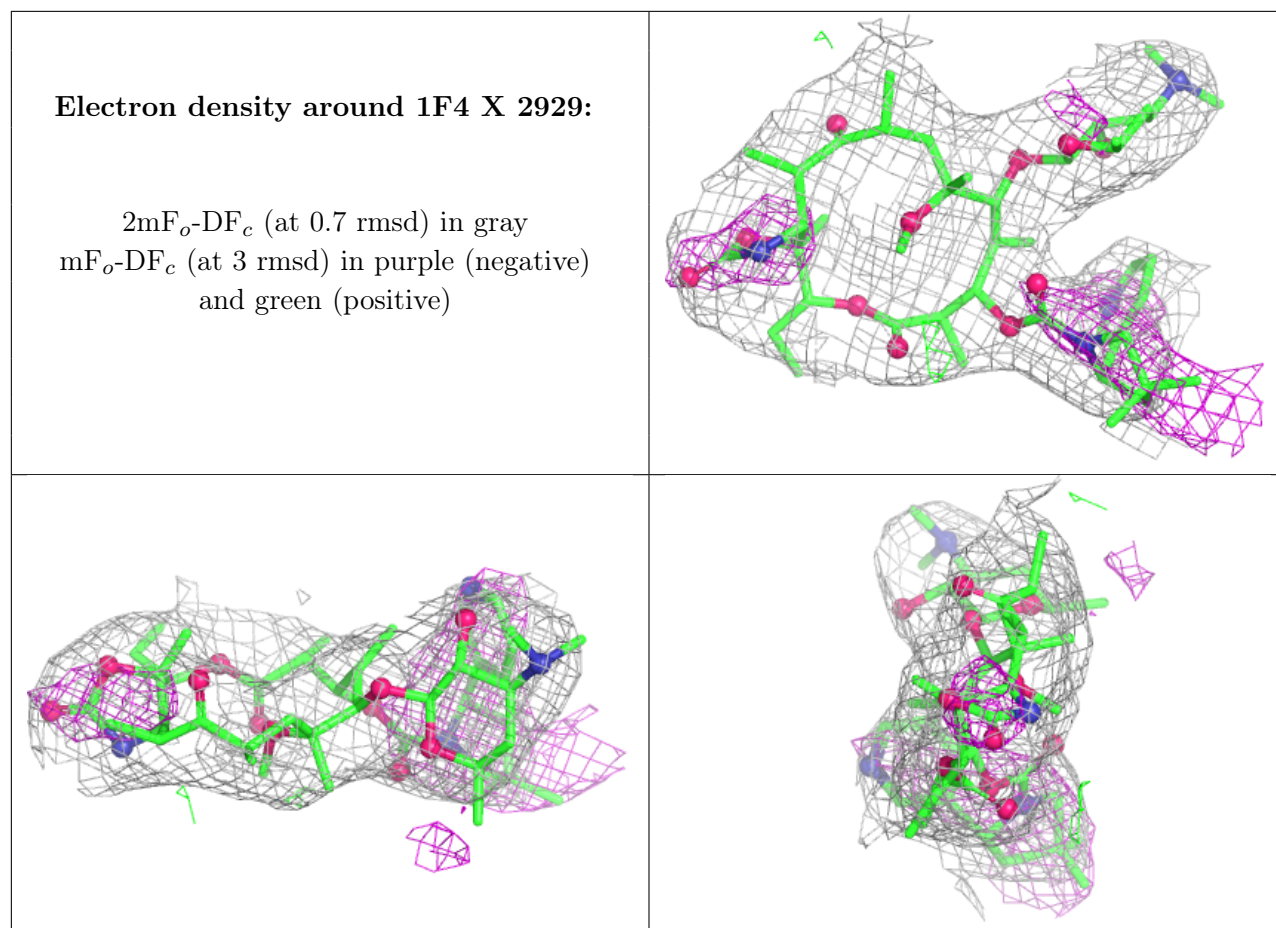
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	MG	X	2909	1/1	0.34	0.62	97,97,97,97	0
31	MG	Y	204	1/1	0.35	0.92	86,86,86,86	0
31	MG	X	2913	1/1	0.37	1.00	60,60,60,60	0
31	MG	X	2903	1/1	0.45	0.62	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^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	0.71	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	0.91	59,59,59,59	0
31	MG	X	2908	1/1	0.82	2.35	37,37,37,37	0
31	MG	X	2918	1/1	0.84	1.23	42,42,42,42	0
31	MG	X	2915	1/1	0.84	0.73	57,57,57,57	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	0.91	0.71	80,80,80,80	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	X	2919	1/1	0.92	0.92	30,30,30,30	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	2923	1/1	0.96	0.34	34,34,34,34	0
32	1F4	X	2929	58/58	0.96	0.21	20,20,20,20	0
31	MG	X	2907	1/1	0.97	0.81	51,51,51,51	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.