



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:30 am GMT

PDB ID : 3DLL
Title : The oxazolidinone antibiotics perturb the ribosomal peptidyl-transferase center and effect tRNA positioning
Authors : Wilson, D.N.; Schlutzen, F.; Harms, J.M.; Starosta, A.L.; Connell, S.R.; Fucini, P.
Deposited on : 2008-06-27
Resolution : 3.50 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

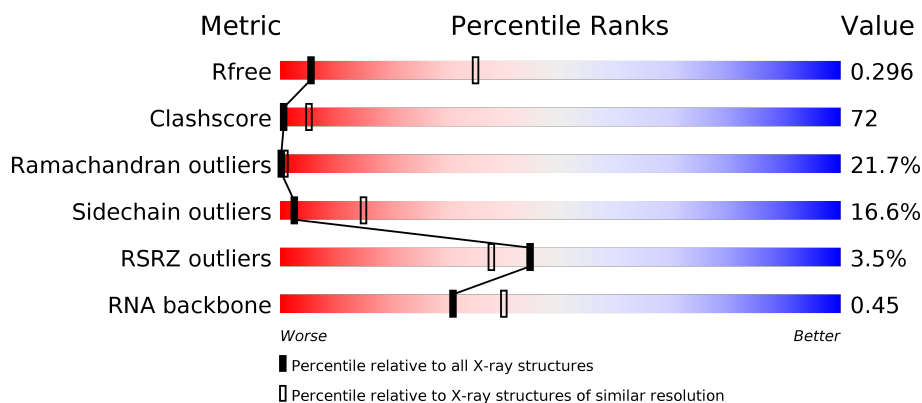
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)
RNA backbone	2435	1024 (4.10-2.86)

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. 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	
2	Z	123	
3	A	274	
4	B	211	

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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	142	
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	Y	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
32	MG	M	167	-	-	-	X
32	MG	X	2885	-	-	-	X
32	MG	X	2889	-	-	-	X
32	MG	X	2896	-	-	-	X
32	MG	X	2899	-	-	-	X
32	MG	X	2903	-	-	-	X
32	MG	X	2907	-	-	-	X
32	MG	X	2909	-	-	-	X
33	ZLD	X	2911	-	-	X	X

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 83657 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 rRNA-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 rRNA-5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Z	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	218	Total	C	N	O	S	0	0	0
			1637	1017	326	292	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	70	Total	C	N	O	S	0	0	0
			504	314	90	97	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			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	MET	-	INITIATING METHIONINE	UNP Q9RXJ5

- 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	Y	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 53 53	0	0	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

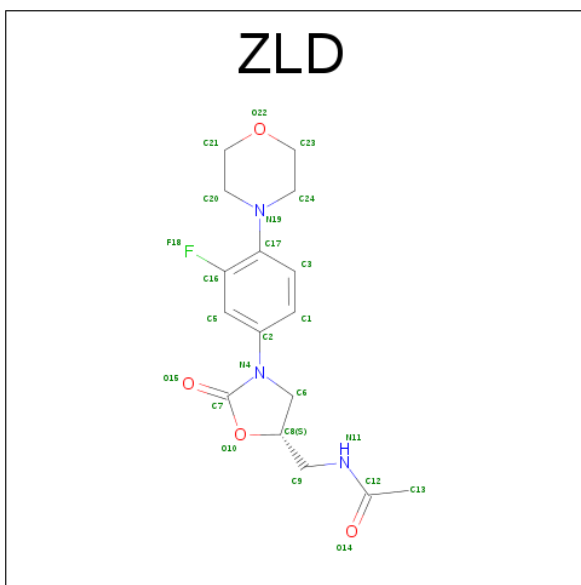
- Molecule 31 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	Y	1	Total Zn 1 1	0	0
31	4	1	Total Zn 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	X	30	Total Mg 30 30	0	0
32	Z	4	Total Mg 4 4	0	0
32	M	1	Total Mg 1 1	0	0

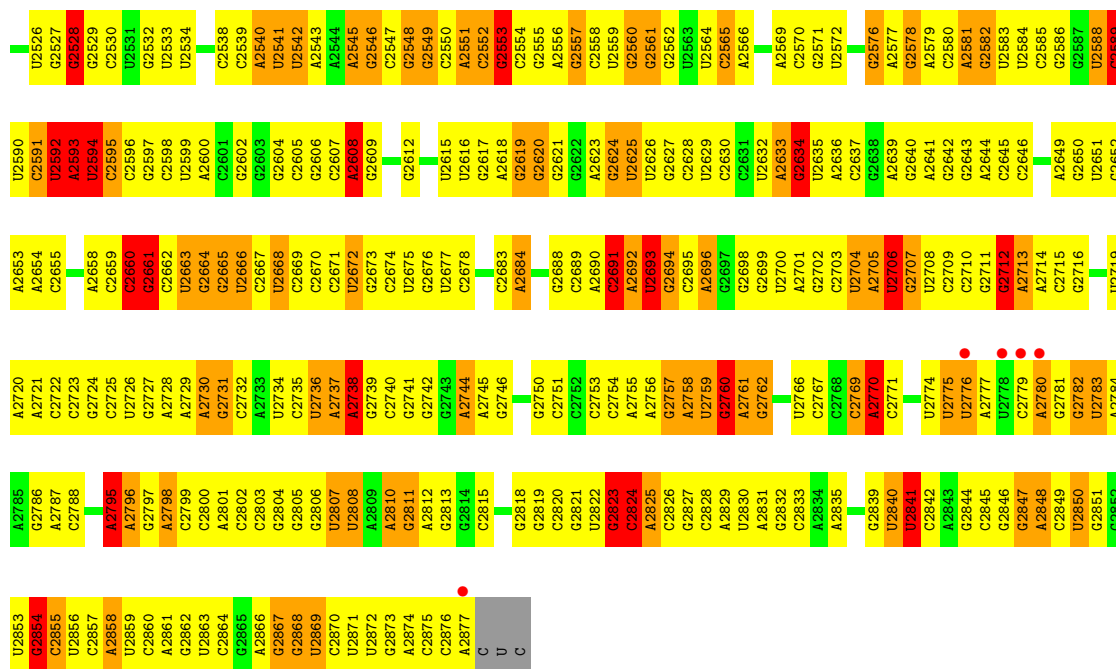
- Molecule 33 is N- $\{[(5S)-3-(3-FLUORO-4-MORPHOLIN-4-YLPHENYL)-2-OXO-1,3-OXAZOLIDIN-5-YL]METHYL\}$ ACETAMIDE (three-letter code: ZLD) (formula: C₁₆H₂₀FN₃O₄).



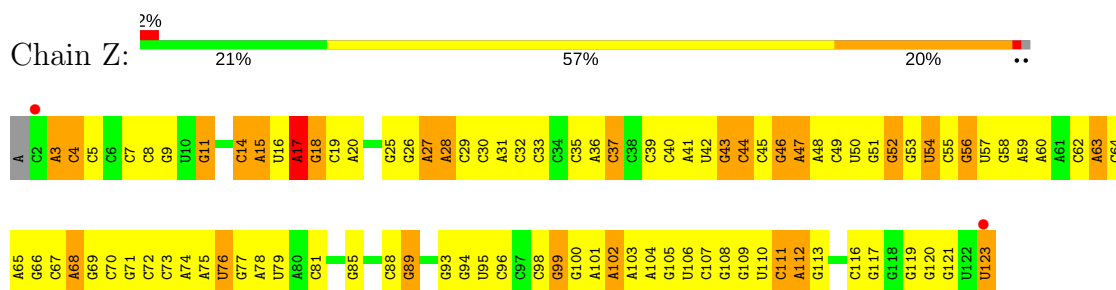
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	X	1	Total	C	F	N	O	0	0
			24	16	1	3	4		

A1534	A1474	U1409	C1348	U1286	A1224	G1104	A1043	C982	A921	U860	A797	G735	G673
A1538	U1475	U1410	A1349	A1287	G1225	U1105	U1044	G983	A922	C861	G796	G736	U674
U1539	G1476	C1411	G1350	A1288	A1226	A1106	G1045	G984	A923	A862	G799	G737	G676
G1540	G1477	C1412	G1351	A1289	A1227	A1107	U1046	G985	C924	C863	C799	G738	G677
G1479	G1478	U1413	G1352	A1290	G1228	U1108	U1047	A986	U925	C864	A801	G739	G678
G1480	G1479	G1414	A1353	G1291	C1229	U1109	C1049	G987	C926	A865	A802	A740	G679
U1481	U1481	C1415	A1354	A1292	G1330	G1110	G1050	G988	C927	U866	C903	G741	C679
U1482	U1482	A1416	A1355	U1295	A1231	C1111	U1051	G989	G928	C867	C804	G742	U680
G1483	G1483	C1417	G1356	A1296	U1232	C1112	C1052	A990	A929	U868	G905	A743	A681
G1484	G1484	U1418	U1357	A1297	A1233	C1113	C1053	A991	G930	C869	A906		G682
U1485	U1485	C1419	C1358	A1298	G1234	C1114	C1054	A992	A931	C870	A907	G746	A683
U1547	U1485	A1420	G1359	G1298	A1235	C1115	C1055	A993	G932	U871	C908	A747	C684
U1548	U1486	U1421	G1360	A1299	A1236	U1116	U1056	A994	G933	C872	C909	A748	U685
C1487	C1487	C1422	G1361	G1237	U1177	G1117	A1057	A995	G934	U873	C910	C749	C686
C1550	G1488	A1423	A1362	U1301	C1178	G1118	U1058	C996	C935	A874	G911	C750	C688
C1552	U1490	U1424	C1363	C1302	A1179	U1119	A1059		A936	G875	G912	G751	A688
G1553	G1491	G1428	G1364	U1303	G1240	C1120	A1060	A999	G937	A876	G813	G752	U753
G1554	A1492	A1429	U1365	U1304	C1241	C1121	A1061	G1000	C938	C877	G814	U754	A690
A1555	A1493	G1430	A1366	U1307	A1242	A1122	G1062	A1001	C939	C878	A815	G754	C691
A1556	G1494	U1431	A1367	C1308	U1243	G1123	C1063	C1002	G940	A879	U816	C755	C692
G1557	G1495	G1432	G1368	U1309	G1184	U1124	C1064	C1003	U941	C882	G818	C756	A693
C1558	G1496	A1433	G1369	C1310	C1185	G1125	A1065	A1004	U942	A883	C919	U757	G694
G1497	G1497	U1434	U1370	C1311	G1186	A1126	G1066	U1005	U943	A884	C920	U758	G695
G1498	G1498	G1435	A1371	G1312	A1187	A1127	G1067	C1006	A944	C885	U821	C759	U696
A1560	G1499	A1436	A1372	U1313	U1188	G1128	U1068	A1007	G945	A886	A820	U760	G697
A1561	U1500	A1437	G1373	U1314	G1189	A1129	G1069	G1008	U946	A887	G822	G761	A698
G1562	G1501	C1438	G1374	A1315	C1190	U1130	G1070	C1009	C947	C887	G823	A762	G699
U1564	C1502	G1439	C1375	A1316	G1191	U1131	U1071	U1010	C948	A888	U824	A763	C700
G1565	G1503	U1440	G1376	G1317	A1192	C1132	U1072	A1011	C889	C925	U825	A764	U701
G1566	U1504	A1441	G1377	G1318	G1193	G1133	G1073	A1012	A956	U890	U826	C765	A702
U1505	U1505	C1442	A1378	A1319	U1194	C1134	G1074	G1013	A952	C891	C927	A766	G703
G1506	G1506	G1443	A1379	C1319	U1195	C1135	C1075	G1014	G953	C828	C928	G767	G704
A1569	A1507	C1444	C1380	A1320	G1196	G1136	U1076	U1015	U954	C829	C929	U768	C705
C1570	G1508	U1445	G1381	A1321	U1197	A1137	U1077	C1016	G955	G830	C930	C769	A706
G1571	A1509	U1446	C1382	G1322	C1198	A1138	A1078	C1017	A957	G831	U770	C771	U707
C1572	U1510	U1447	C1383	G1323	U1199	A1139	G1079	C1018	G957	A832	U771	G772	G708
G1573	A1511	A1448	A1384	G1324	G1200	A1140	A1080	U1019	G958	C833	A834	G773	A709
A1574	A1512	C1449	C1385	U1325	G1201	U1141	A1081	A1020	C959	C834	U835	A774	C710
G1575	U1513	G1450	A1386	U1326	U1202	G1142	G1082	A1021	U960	C835	U836	A775	C711
G1576	C1514	C1451	C1389	C1327	G1263	A1143	C1083	A1022	G961	A836	G836	U776	A712
G1577	U1515	U1452	G1390	C1328	G1264	U1144	A1084	U1023	C962	C837	U837	G777	G713
U1578	U1516	A1453	U1391	U1329	G1205	C1145	G1085	G1024	G963	C838	U838	A778	G714
C1579	C1517	U1454	U1392	G1330	G1206	G1146	C1086	A1025	A964	A839	U839	G779	U715
C1580	C1518		G1393	G1331	G1207	G1147	C1087	U1026	G965	C840	U840	U779	U716
C1581	G1519	U1459	G1394	G1332	C1270	G1148	A1088	C1027	A966	C841	G841	U780	G717
A1582	G1520	A1460	A1395	G1333	G1271	G1149	C1089	G1028	C967	U842	G842	G783	A718
G1583	U1521	C1461	C1396	A1335	G1272	C1150	C1090	C1029	C968	A843	G843	U784	A719
A1584	C1522	C1462	G1397	G1336	C1273	U1151	C1091	U1030	U969	A844	G844	U785	A720
A1585	A1523	A1463	G1398	G1337	A1275	G1152	U1092	C1031	A970	C847	U786	U786	C721
A1586	C1524	A1464	C1399	G1338	U1276	A1153	U1093	A1032	A971	C848	A848	A787	C725
A1587	U1525	G1465	A1400	U1339	G1277	G1154	C1094	G1033	C972	A849	G849	G788	G726
A1588	U1526	C1466	G1401	C1340	A1278	U1155	A1095	U1034	U973	G850	G850	G789	U727
G1589	G1527	U1467	G1402	G1341	G1279	G1157	A1097	G1035	U974	G851	G851	A790	G728
C1590	C1528	U1468	U1403	U1342	U1280	A1158	G1098	G1036	C975	C914	U852	G791	G729
U1591	U1529	A1469	C1404	C1343	C1281	U1159	A1099	U1037	C976	C915	C853	G792	C730
U1592	U1530	G1470	A1405	C1344	A1282	C1160	G1100	U1038	U978	U917	A856	G793	A731
C1593	C1531	G1471	A1406	G1345	C1283	U1161	U1101	A1039	A979	U918	U857	A794	G732
U1594	U1532	G1472	G1407	C1346	G1284	A1162	G1102	A1040	G980	U919	G858	A795	G733
A1595	G1533	U1473	A1408	C1347	A1285	C1163	C1103	G1042	C981	G920	U859	A796	G734

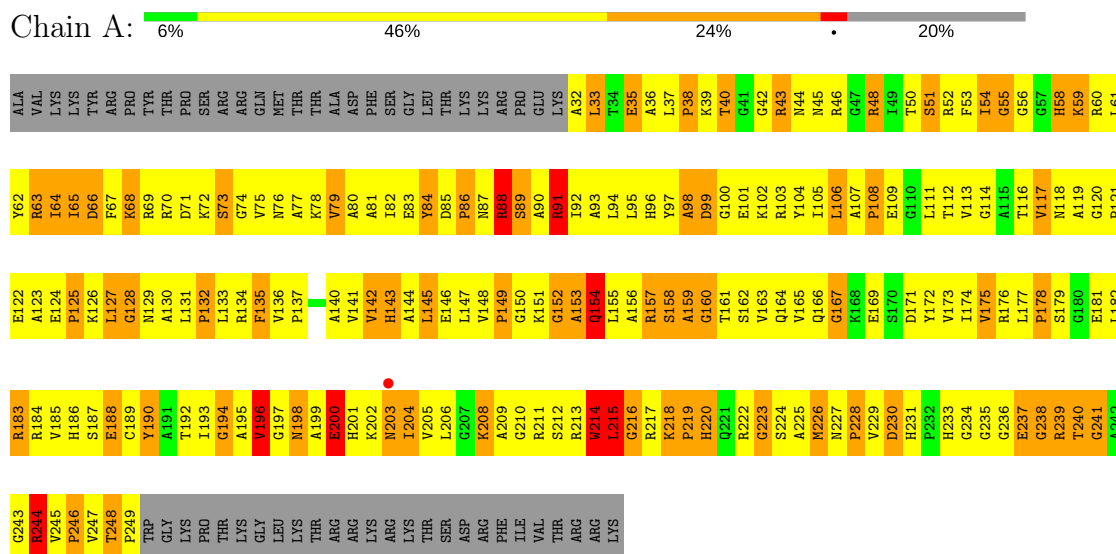
G2464	G2465	A2404	U2342	C2281	G2215	A	C	G2032	G1972	A1911	G1850	U1787	C1727	A1596
G2466	G2467	A2405	G2343	G2282	G2216	U	G	C2033	C1973	G1912	G1851	C1788	A1728	A1597
A2407	A2408	G2217	G2344	G2283	G2217	A	U	A2034	U1974	U1913	G1854	U1789	C1729	C1598
G2468	G2469	G2218	A2345	U2284	C	A	A	G2035	G1975	U1914	G1855	G1790	C1730	C1599
G2470	U2471	G2219	G2346	U2285	C	G	G	A2036	U1976	A1915	U1856	C1791	C1731	U1600
A2411	A2412	G2220	G2347	U2286	A	A	A	G2037	U1977	G1916	U1857	G1792	U1732	U1601
A2413	A2414	G2221	A2348	G2287	C	U	U	C2038	U1978	C1917	G1858	A1793	U1733	G1602
G2415	G2416	G2222	G2349	A2288	U2223	C	U	A2039	C1979	G1918	C1859	G1794	C1734	A1603
A2417	A2418	G2223	G2350	A2289	G2224	C	A	G2040	A1980	A1919	A1859	G1795	C1735	A1604
A2419	A2420	G2224	G2351	U2290	U2225	U	G	A2041	A1981	A1920	A1860	G1796	C1736	A1605
C2421	C2422	G2225	A2352	U2291	G2226	G	G	A2042	C1982	A1921	G1861	G1797	C1737	C1606
G2423	G2424	C2226	G2353	C2292	A2227	U	U	A2043	G1983	U1922	G1862	U1798	U1738	A1607
G2425	G2426	C2227	G2354	C2293	C2228	G	G	G2044	G1984	U1923	U1863	G1799	C1739	U1608
A2427	A2428	G2228	U2294	U2294	U2228	G	G	A2045	A1985	C1924	G1864	G1740	U1676	G1609
G2476	G2477	G2229	A2356	C2295	G2229	G	G	A2046	G1986	U1925	G1865	G1741	U1679	C1615
A2478	U2479	G2230	A2357	A2299	G2231	A	A	C2047	G1987	U1926	G1866	G1742	U1680	C1616
C2480	C2481	G2231	U2358	U2217	G2231	C	C	C2048	A1988	U1927	A1867	G1743	A1681	G1617
A2482	U2483	G2232	G2359	U2172	G2231	C	C	C2049	A1989	G1928	A1868	G1744	U1682	U1618
G2484	G2485	C2233	G2360	G2173	G2235	U	U	G2050	U1990	U1929	A1869	C1745	U1683	A1619
U2486	G2487	G2234	G2361	G2174	U2236	G	G	U2051	C1991	C1930	U1870	A1746	C1620	C1623
A2488	C2489	G2235	G2362	A2175	U2237	U	U	G2052	G1992	G1931	U1871	G1747	G1684	A1625
A2490	C2491	G2236	G2363	G2176	G2238	G	G	C2053	U1993	U1932	A1872	U1748	A1685	A1626
G2492	G2493	G2237	G2364	U2177	C2239	C	C	A2054	U1994	G1933	A1873	G1749	C1622	C1627
C2494	C2495	G2238	G2365	U2178	A2240	G	G	G2055	G1995	U1934	A1874	U1750	C1628	C1629
G2496	C2497	G2239	U2366	U2179	U2241	A	A	C2056	A1996	G1935	C1875	A1751	A1694	A1630
U2498	U2499	G2240	G2367	G2180	C2242	C	C	U2057	A1997	U1936	C1876	G1752	C1631	C1632
C2500	U2501	G2241	G2368	U2181	C2243	U	U	G2058	U2003	C1944	A1883	C1758	A1697	A1632
G2502	G2503	G2242	G2369	A2182	U2244	C	C	U2059	U2004	G1945	A1884	C1759	A1698	C1633
G2504	G2505	G2243	G2370	C2183	A2245	U	U	G2060	G2005	U1946	C1885	G1760	A1699	A1634
C2506	C2507	G2244	A2371	G2184	A2246	G	G	U2061	G2006	G1947	G1886	G1761	G1635	G1636
U2507	G2508	G2245	G2372	U2185	A2247	C	C	G2070	G2007	C1948	G1887	G1762	G1703	U1639
A2509	A2510	G2246	G2373	G2186	A2248	U	U	G2071	U2008	A1949	C1888	A1764	G1704	C1640
G2511	G2512	G2247	U2374	A2187	U2249	C	C	C2072	G2010	C1950	G	C1765	U1705	C1641
A2513	G2514	G2248	G2375	G2188	G2250	U	U	U2073	U2011	G1951	C	U1766	G1706	G1642
C2515	C2516	G2249	G2376	A2189	U2251	U	U	A2074	A2012	A1952	C	G1767	A1707	U1643
G2517	G2518	G2250	G2377	U2190	C2252	G	G	U2075	A2013	A1953	C	U1768	C1708	A1643
A2519	A2520	G2251	G2378	U2191	G2253	U	U	G2076	A2014	A1954	U	U1769	U1709	G1644
G2521	G2522	G2252	G2379	U2192	C2254	C	C	G2077	G2015	G1955	A	U1770	U1710	U1645
C2523	C2524	G2253	U2380	U2193	G2255	G	G	G2078	A2016	G1956	A	A1771	C1711	G1646
G2525	G2526	G2254	G2381	A2194	G2256	U	U	U2079	U2017	C1957	A	C1772	G1712	U1647
C2527	C2528	G2255	G2382	U2195	A2257	G	G	U2080	G2018	G1958	C	C1773	G1713	C1648
A2529	A2530	G2256	G2383	U2196	G2258	C	C	C2081	C2019	U1959	U	A1774	A1714	A1649
G2531	G2532	G2257	G2384	U2197	G2259	G	G	G2082	G2020	A1960	A	A1775	A1715	A1650
C2533	C2534	G2258	U2385	U2198	G2260	U	U	G2083	G2021	A1961	U	A1776	G1716	U1651
A2535	A2536	G2259	G2386	G2199	C2261	C	C	G2084	C2022	C1962	A	A1777	G1717	G1652
G2537	G2538	G2260	U2387	G2200	C2262	A	A	U2085	G2023	G1963	A	U1778	C1718	C1653
C2539	C2540	G2261	G2388	G2201	C2263	C	C	U2086	U2024	G1964	C	G1779	G1719	A1654
A2541	A2542	G2262	G2389	G2202	C2264	U	U	U2087	A2025	A1965	G	A1774	G1720	C1655
C2543	C2544	G2263	G2390	G2203	A2265	G	G	G2088	C2026	G1966	U	A1775	C1721	U1656
A2545	A2546	G2264	G2391	G2204	A2266	C	C	U2089	G2027	U1967	C	A1776	G1722	A1657
G2547	G2548	G2265	G2392	A2205	A2267	G	G	G2090	C2028	G1968	C	A1777	U1723	A1658
C2549	C2550	G2266	G2393	C2206	G2268	A	A	U2091	C2029	G1969	C	A1778	C1724	G1659
A2551	A2552	G2267	G2394	G2207	G2269	C	C	U2092	U2030	G1970	U	C1779	C1725	G1660
G2553	G2554	G2268	G2395	U2208	U2270	G	G	U2093	A2031	C1971	A	C1780	C1726	C1661
C2555	C2556	G2269	G2396	U2209	G2271	U	U	C						
A2557	A2558	G2270	G2397	G2210	A2272	G	G	U						
G2559	G2560	G2271	G2398	U2211	C2273	A	A							
C2561	C2562	G2272	U2399	U2212	U2274	G	G							
A2563	A2564	G2273	A2401	G2213	C2275	A	A							
G2565	G2566	G2274	C2403	G2214	U2276	A	A							
C2567	C2568	G2275		G2215	G2277									
A2569	A2570	G2276		G2216	G2278									
G2571	G2572	G2277		G2217	G2279									
C2573	C2574	G2278		G2218	G2280									
A2575	A2576	G2279		G2219	G2281									
G2577	G2578	G2280		G2220	G2282									
C2579	C2580	G2281		G2221	G2283									
A2581	A2582	G2282		G2222	G2284									
G2583	G2584	G2283		G2223	G2285									
C2585	C2586	G2284		G2224	G2286									
A2587	A2588	G2285		G2225	G2287									
G2589	G2590	G2286		G2226	G2288									
C2591	C2592	G2287		G2227	G2289									
A2593	A2594	G2288		G2228	G2290									
G2595	G2596	G2289		G2229	G2291									
C2597	C2598	G2290		G2230	G2292									
A2599	A2600	G2291		G2231	G2293									
G2601	G2602	G2292		G2232	G2294									
C2603	C2604	G2293		G2233	G2295									
A2605	A2606	G2294		G2234	G2296									
G2607	G2608	G2295		G2235	G2297									
C2609	C2610	G2296		G2236	G2298									
A2611	A2612	G2297		G2237	G2299									
G2613	G2614	G2298		G2238	G2300									
C2615	C2616	G2299		G2239	G2301									
A2617	A2618	G2300		G2240	G2302									
G2619	G2620	G2301		G2241	G2303									
C2621	C2622	G2302		G2242	G2304									
A2623	A2624	G2303		G2243	G2305									
G2625	G2626	G2304		G2244	G2306									
C2627	C2628	G2305		G2245	G2307									
A2629	A2630	G2306		G2246	G2308									
G2631	G2632	G2307		G2247	G2309									
C2633	C2634	G2308		G2248	G2310									
A2635	A2636	G2309		G2249	G2311									
G2637	G2638	G2310		G2250	G2312									
C2639	C2640	G2311		G2251	G2313									
A2641	A2642	G2312		G2252	G2314									
G2643	G2644	G2313		G2253	G2315									
C2645	C2646	G2314		G2254	G2316									
A2647	A2648	G2315		G2255	G2317									
G2649	G2650	G2316		G2256	G2318									
C2651	C2652	G2317		G2257	G2319									
A2653	A2654	G2318		G2258	G2320									
G2655	G2656	G2319		G2259	G2321									
C2657	C2658	G2320		G2260	G2322									
A2659	A2660	G2321		G2261	G2323									
G2661	G2662	G2322		G2262	G2324									
C2663	C2664	G2323		G2263	G2325									
A2665	A2666	G2324		G2264	G2326									
G2667	G2668	G2325		G2265	G2327									



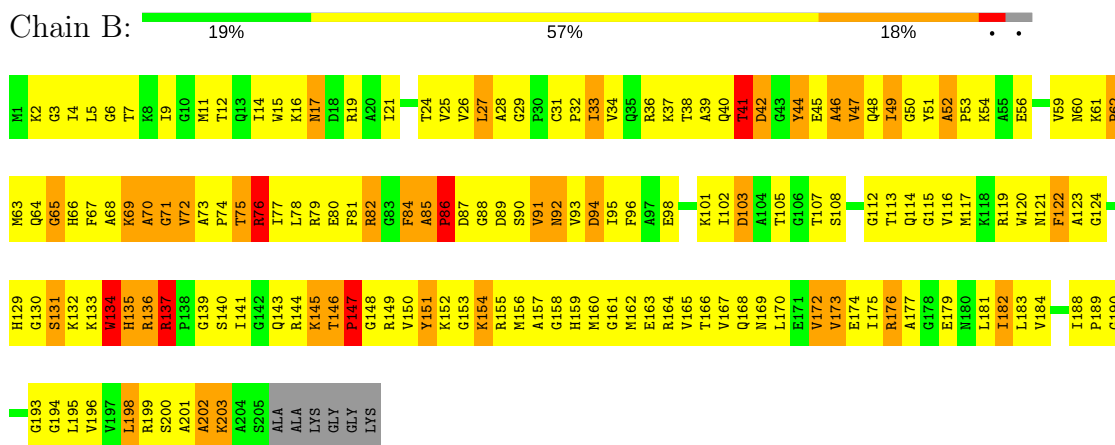
• Molecule 2: rRNA-5S ribosomal RNA



• Molecule 3: 50S ribosomal protein L2

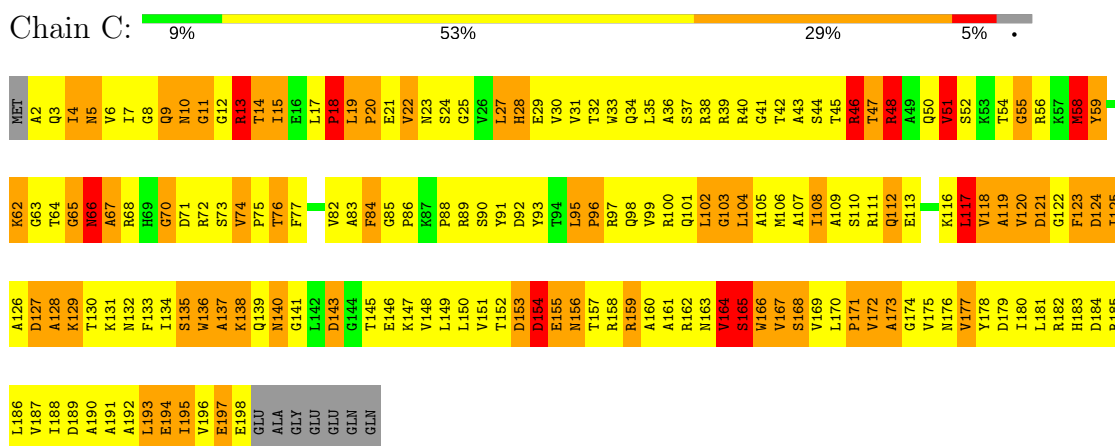


Chain B:



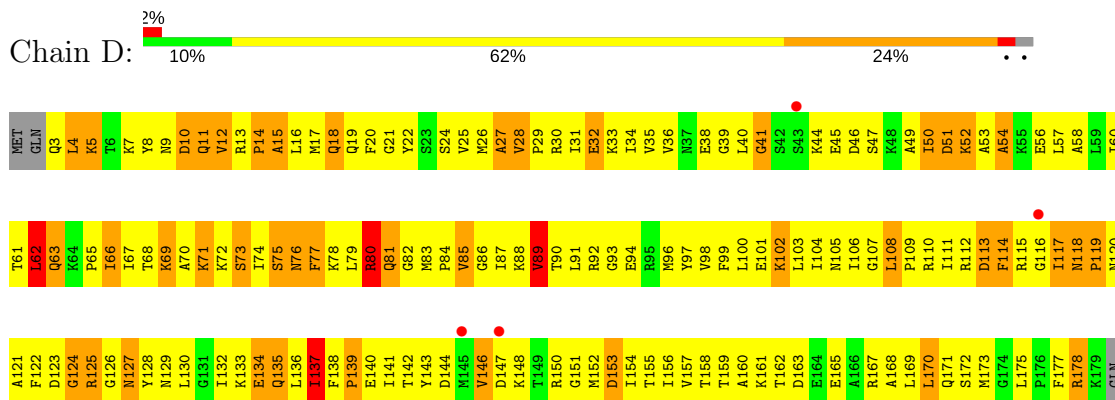
• Molecule 5: 50S ribosomal protein L4

Chain C:



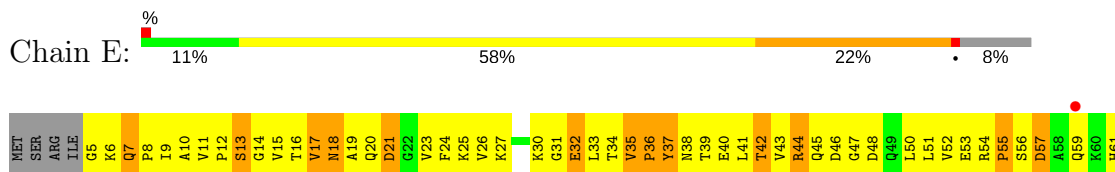
• Molecule 6: 50S ribosomal protein L5

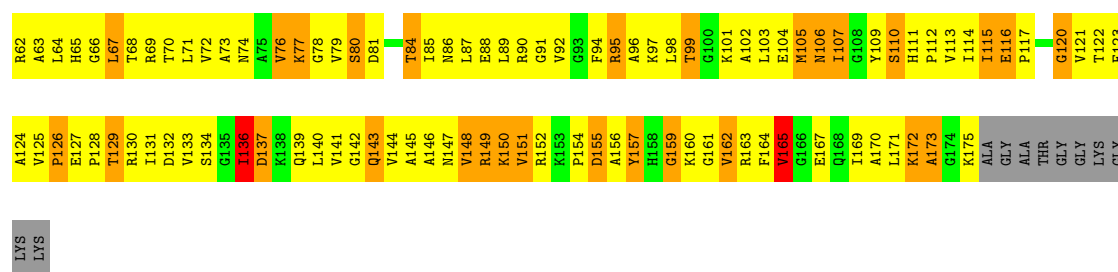
Chain D:



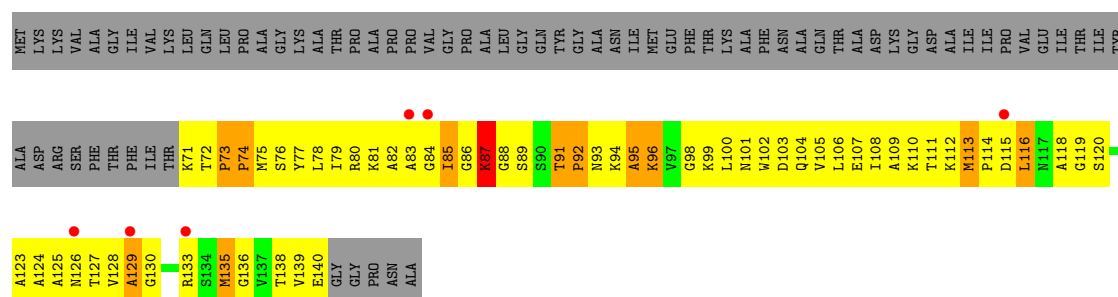
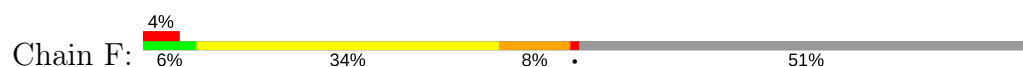
• Molecule 7: 50S ribosomal protein L6

Chain E:

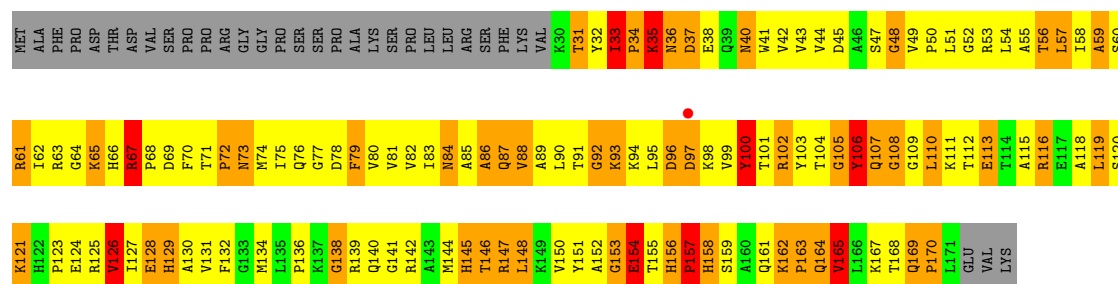




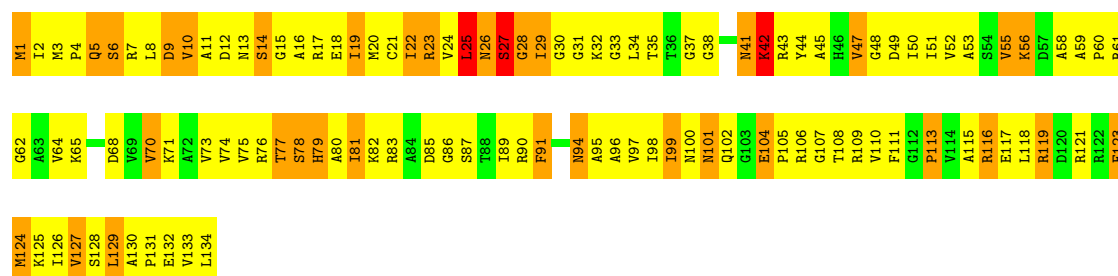
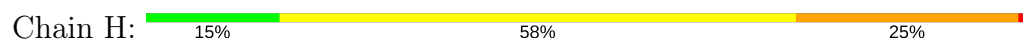
• Molecule 8: 50S ribosomal protein L11



• Molecule 9: 50S ribosomal protein L13

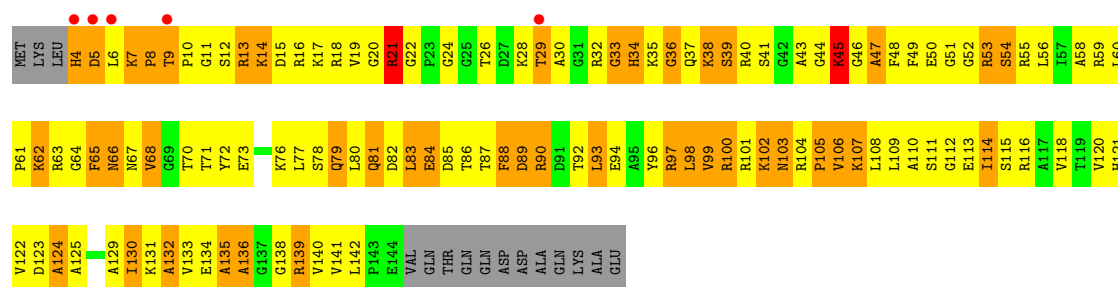


• Molecule 10: 50S ribosomal protein L14

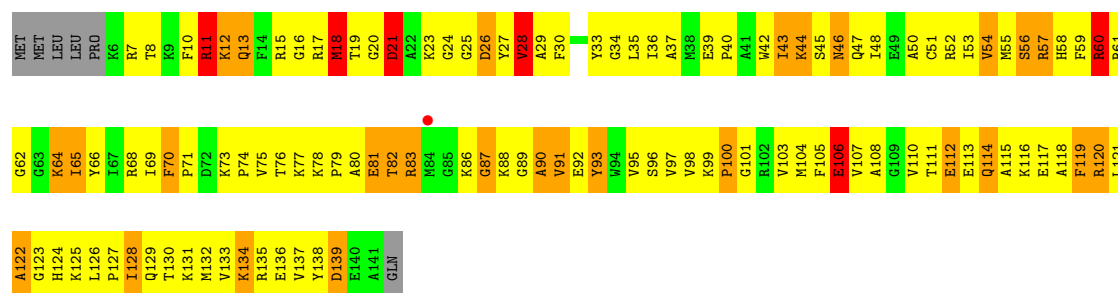
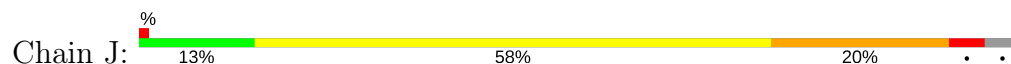


• Molecule 11: 50S ribosomal protein L15

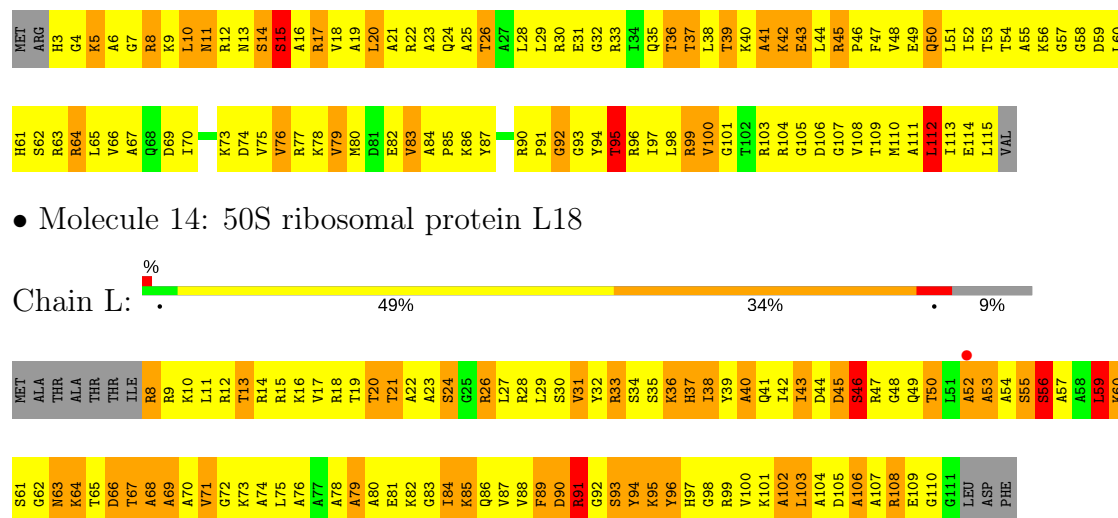
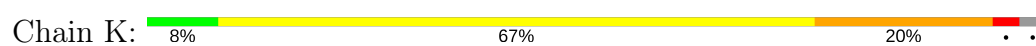




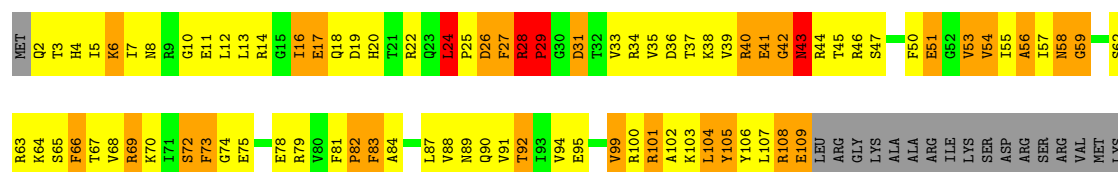
• Molecule 12: 50S ribosomal protein L16



• Molecule 13: 50S ribosomal protein L17



• Molecule 14: 50S ribosomal protein L18



ASP
ALA
ALA
ARG
ALA
GLN
GLN
ASP
LYS
ASN
ALA
SER
ALA
SER
GLN
ALA
ALA
ALA
GLN
ALA
ALA
GLN
ASP
VAL
THR
VAL
ILE
SER
ALA
ALA
PRO
GLU
VAL
ALA
PRO
THR
GLN
GLY
GLU

• Molecule 16: 50S ribosomal protein L20

Chain N: 9% 56% 31% • •

MET F2 R3 A4 K5 T6 G7 I8 V9 R10 R11 R12 R13 R14 R15 R16 R17 R18 R19 R20 R21 R22 R23 R24 R25 R26 R27 R28 R29 R30 R31 R32 R33 R34 R35 R36 R37 R38 R39 R40 R41 R42 R43 R44 R45 R46 R47 R48 R49 R50 R51 R52 R53 R54 R55 R56 R57 R58 R59 R60

• Molecule 17: 50S ribosomal protein L21

Chain O: 11% 56% 25% • 6%

MET PHE ILE A6 K6 Q6 T7 G8 G9 K10 K11 K12 K13 K14 K15 K16 K17 K18 K19 K20 K21 K22 K23 K24 K25 K26 K27 K28 K29 K30 K31 K32 K33 K34 K35 K36 K37 K38 K39 K40 K41 K42 K43 K44 K45 K46 K47 K48 K49 K50 K51 K52 K53 K54 K55 K56 K57 K58 K59 K60

• Molecule 18: 50S ribosomal protein L22

Chain P: 16% 63% 13% • 5%

MET THR ALA PRO GLU THR F8 R9 R10 R11 R12 R13 R14 R15 R16 R17 R18 R19 R20 R21 R22 R23 R24 R25 R26 R27 R28 R29 R30 R31 R32 R33 R34 R35 R36 R37 R38 R39 R40 R41 R42 R43 R44 R45 R46 R47 R48 R49 R50 R51 R52 R53 R54 R55 R56 R57 R58 R59 R60

• Molecule 19: 50S ribosomal protein L23

Chain Q: 9% 52% 33% • •

MET S2 R3 Y4 D5 I6 L7 Q8 Q9 R10 R11 R12 R13 R14 R15 R16 R17 R18 R19 R20 R21 R22 R23 R24 R25 R26 R27 R28 R29 R30 R31 R32 R33 R34 R35 R36 R37 R38 R39 R40 R41 R42 R43 R44 R45 R46 R47 R48 R49 R50 R51 R52 R53 R54 R55 R56 R57 R58 R59 R60

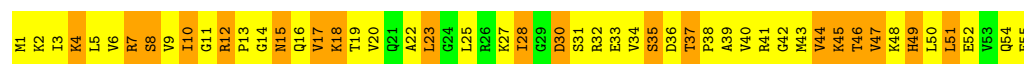
• Molecule 20: 50S ribosomal protein L24

Chain R: 5% 53% 32% 5% •

MET PRO ARG P4 S5 A6 G7 S8 H9 H10 H11 H12 H13 H14 H15 H16 H17 H18 H19 H20 H21 H22 H23 H24 H25 H26 H27 H28 H29 H30 H31 H32 H33 H34 H35 H36 H37 H38 H39 H40 H41 H42 H43 H44 H45 H46 H47 H48 H49 H50 H51 H52 H53 H54 H55 H56 H57 H58 H59 H60



Chain W: 



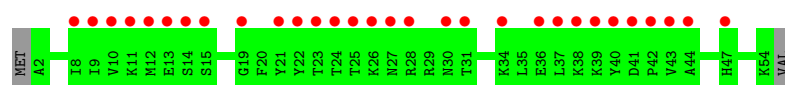
- Molecule 26: 50S ribosomal protein L32

Chain Y: 




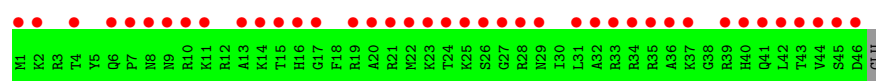
- Molecule 27: 50S ribosomal protein L33

Chain 1: 



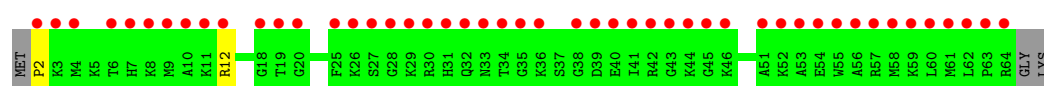
- Molecule 28: 50S ribosomal protein L34

Chain 2: 




- Molecule 29: 50S ribosomal protein L35

Chain 3: 



- Molecule 30: 50S ribosomal protein L36

Chain 4: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.70Å 410.00Å 695.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.50 30.06 – 3.30	Depositor EDS
% Data completeness (in resolution range)	90.5 (29.98-3.50) 85.7 (30.06-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.259 , 0.280 0.250 , 0.296	Depositor DCC
R_{free} test set	13552 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	68.5	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.14 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	83657	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: ZLD, ZN, 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	0.83	19/64561 (0.0%)	0.93	192/100708 (0.2%)
2	Z	0.56	0/2904	0.78	0/4525
3	A	0.62	0/1669	0.95	1/2254 (0.0%)
4	B	0.76	0/1567	0.99	1/2105 (0.0%)
5	C	0.62	0/1529	0.92	1/2070 (0.0%)
6	D	0.50	0/1419	0.79	0/1903
7	E	0.49	0/1308	0.80	0/1771
8	F	0.51	0/510	0.82	0/688
9	G	0.62	0/1138	0.95	2/1539 (0.1%)
10	H	0.75	0/1007	0.99	2/1352 (0.1%)
11	I	0.66	1/1081 (0.1%)	0.98	0/1448
12	J	0.68	1/1113 (0.1%)	0.87	0/1486
13	K	0.90	0/886	1.07	1/1188 (0.1%)
14	L	0.53	0/785	0.84	0/1048
15	M	0.76	0/884	1.24	5/1186 (0.4%)
16	N	0.64	0/994	0.84	0/1323
17	O	0.60	0/750	0.92	1/1000 (0.1%)
18	P	0.76	0/1027	0.99	1/1373 (0.1%)
19	Q	0.62	0/737	0.93	2/988 (0.2%)
20	R	0.53	0/835	0.91	3/1121 (0.3%)
21	S	0.51	0/1370	0.82	0/1862
22	T	0.59	0/633	0.89	0/838
23	U	0.57	0/556	0.92	0/741
24	V	0.51	0/537	0.82	0/714
25	W	0.54	0/426	0.86	0/568
26	Y	0.71	0/469	1.01	0/629
30	4	0.48	0/298	0.77	0/390
All	All	0.78	21/90993 (0.0%)	0.92	212/136818 (0.2%)

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	228
2	Z	0	4
9	G	0	1
17	O	0	1
All	All	0	234

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	2594	U	P-OP2	17.32	1.78	1.49
1	X	2594	U	P-OP1	-13.28	1.26	1.49
1	X	2592	U	P-OP2	-12.20	1.28	1.49
1	X	28	A	C5-C6	-6.98	1.34	1.41
1	X	1333	G	N9-C4	-6.33	1.32	1.38

The worst 5 of 212 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	M	28	ARG	C-N-CD	-19.65	77.37	120.60
1	X	2594	U	O5'-P-OP2	-18.88	88.04	110.70
1	X	2592	U	O5'-P-OP2	-15.03	92.18	105.70
1	X	2592	U	N1-C1'-C2'	14.74	133.17	114.00
1	X	2592	U	C1'-O4'-C4'	-12.24	100.11	109.90

There are no chirality outliers.

5 of 234 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	10	A	Sidechain
1	X	24	G	Sidechain
1	X	25	U	Sidechain
1	X	34	U	Sidechain
1	X	98	U	Sidechain

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	57651	0	29049	4430	0
2	Z	2598	0	1328	213	0
3	A	1637	0	1673	471	0
4	B	1539	0	1600	358	0
5	C	1506	0	1525	400	0
6	D	1400	0	1481	437	0
7	E	1286	0	1336	330	0
8	F	504	0	530	125	0
9	G	1114	0	1144	371	0
10	H	997	0	1046	213	1
11	I	1067	0	1103	324	0
12	J	1090	0	1125	259	0
13	K	878	0	930	165	1
14	L	779	0	820	275	0
15	M	871	0	894	204	0
16	N	978	0	1020	288	0
17	O	741	0	756	242	0
18	P	1014	0	1096	191	0
19	Q	726	0	753	197	0
20	R	825	0	881	271	0
21	S	1345	0	1372	323	0
22	T	625	0	655	144	0
23	U	552	0	604	192	0
24	V	533	0	558	133	0
25	W	424	0	470	103	0
26	Y	457	0	462	86	0
27	1	53	0	0	0	0
28	2	46	0	0	0	0
29	3	63	0	0	2	0
30	4	297	0	329	83	0
31	4	1	0	0	0	0
31	Y	1	0	0	0	0
32	M	1	0	0	0	0
32	X	30	0	0	0	0
32	Z	4	0	0	0	0
33	X	24	0	19	22	0
All	All	83657	0	54559	9938	1

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 72.

The worst 5 of 9938 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)
1:X:1281:A:H1'	1:X:2592:U:C5	1.68	1.26
1:X:2198:U:H3'	1:X:2199:C:C4'	1.66	1.24
1:X:2198:U:C3'	1:X:2199:C:H4'	1.68	1.23
1:X:1781:C:OP1	3:A:219:PRO:HB2	1.41	1.20
1:X:1281:A:C1'	1:X:2592:U:H5	1.55	1.20

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:107:GLY:O	13:K:86:LYS:NZ[8_555]	2.03	0.17

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	216/274 (79%)	109 (50%)	52 (24%)	55 (26%)	0	0
4	B	203/211 (96%)	124 (61%)	47 (23%)	32 (16%)	0	3
5	C	195/205 (95%)	92 (47%)	46 (24%)	57 (29%)	0	0
6	D	175/180 (97%)	78 (45%)	54 (31%)	43 (25%)	0	1
7	E	169/185 (91%)	91 (54%)	42 (25%)	36 (21%)	0	1
8	F	68/144 (47%)	37 (54%)	21 (31%)	10 (15%)	0	3
9	G	140/174 (80%)	66 (47%)	32 (23%)	42 (30%)	0	0
10	H	132/134 (98%)	91 (69%)	26 (20%)	15 (11%)	0	6
11	I	139/156 (89%)	51 (37%)	50 (36%)	38 (27%)	0	0
12	J	134/142 (94%)	63 (47%)	46 (34%)	25 (19%)	0	2
13	K	111/116 (96%)	61 (55%)	31 (28%)	19 (17%)	0	2
14	L	102/114 (90%)	48 (47%)	25 (24%)	29 (28%)	0	0
15	M	106/166 (64%)	68 (64%)	17 (16%)	21 (20%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	N	115/118 (98%)	56 (49%)	30 (26%)	29 (25%)	0	0
17	O	92/100 (92%)	52 (56%)	19 (21%)	21 (23%)	0	1
18	P	125/134 (93%)	75 (60%)	35 (28%)	15 (12%)	0	6
19	Q	91/95 (96%)	44 (48%)	23 (25%)	24 (26%)	0	0
20	R	108/115 (94%)	63 (58%)	17 (16%)	28 (26%)	0	0
21	S	173/237 (73%)	97 (56%)	40 (23%)	36 (21%)	0	1
22	T	82/91 (90%)	51 (62%)	16 (20%)	15 (18%)	0	2
23	U	70/81 (86%)	39 (56%)	15 (21%)	16 (23%)	0	1
24	V	64/67 (96%)	32 (50%)	19 (30%)	13 (20%)	0	1
25	W	53/55 (96%)	22 (42%)	18 (34%)	13 (24%)	0	1
26	Y	56/60 (93%)	31 (55%)	17 (30%)	8 (14%)	0	3
30	4	35/37 (95%)	22 (63%)	11 (31%)	2 (6%)	2	21
All	All	2954/3391 (87%)	1563 (53%)	749 (25%)	642 (22%)	0	1

5 of 642 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	33	LEU
3	A	58	HIS
3	A	66	ASP
3	A	91	ARG
3	A	98	ALA

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	164/215 (76%)	130 (79%)	34 (21%)	1	7
4	B	155/157 (99%)	132 (85%)	23 (15%)	3	20
5	C	157/163 (96%)	126 (80%)	31 (20%)	1	8
6	D	153/156 (98%)	139 (91%)	14 (9%)	11	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	E	136/144 (94%)	119 (88%)	17 (12%)	5	26
8	F	53/107 (50%)	48 (91%)	5 (9%)	10	40
9	G	118/146 (81%)	96 (81%)	22 (19%)	2	10
10	H	103/103 (100%)	80 (78%)	23 (22%)	1	5
11	I	108/121 (89%)	91 (84%)	17 (16%)	3	18
12	J	110/116 (95%)	92 (84%)	18 (16%)	2	15
13	K	90/93 (97%)	71 (79%)	19 (21%)	1	7
14	L	74/82 (90%)	54 (73%)	20 (27%)	0	3
15	M	94/134 (70%)	81 (86%)	13 (14%)	4	23
16	N	96/97 (99%)	80 (83%)	16 (17%)	2	14
17	O	75/79 (95%)	69 (92%)	6 (8%)	14	48
18	P	109/115 (95%)	92 (84%)	17 (16%)	3	18
19	Q	75/76 (99%)	62 (83%)	13 (17%)	2	13
20	R	91/96 (95%)	70 (77%)	21 (23%)	1	5
21	S	149/192 (78%)	123 (83%)	26 (17%)	2	13
22	T	62/67 (92%)	53 (86%)	9 (14%)	4	21
23	U	57/66 (86%)	46 (81%)	11 (19%)	1	9
24	V	54/55 (98%)	45 (83%)	9 (17%)	2	14
25	W	48/48 (100%)	41 (85%)	7 (15%)	3	20
26	Y	51/53 (96%)	45 (88%)	6 (12%)	6	29
30	4	35/35 (100%)	30 (86%)	5 (14%)	4	22
All	All	2417/2716 (89%)	2015 (83%)	402 (17%)	2	15

5 of 402 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	I	88	PHE
14	L	24	SER
23	U	61	TRP
12	J	10	PHE
13	K	5	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
11	I	121	HIS
15	M	48	GLN
24	V	36	GLN
12	J	13	GLN
14	L	86	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2680/2880 (93%)	678 (25%)	0
2	Z	121/123 (98%)	24 (19%)	0
All	All	2801/3003 (93%)	702 (25%)	0

5 of 702 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	13	A
1	X	14	A
1	X	27	G
1	X	34	U
1	X	35	G

There are no RNA pucker outliers to report.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 37 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	$\# Z > 2$
33	ZLD	X	2911	-	26,26,26	1.24	2 (7%)	35,36,36	2.15	8 (22%)

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
33	ZLD	X	2911	-	-	0/13/33/33	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	X	2911	ZLD	C5-C16	2.10	1.41	1.37
33	X	2911	ZLD	O10-C7	3.39	1.40	1.35

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	X	2911	ZLD	C2-N4-C7	-5.66	119.25	125.86
33	X	2911	ZLD	O10-C7-N4	-5.37	106.55	109.97
33	X	2911	ZLD	C5-C16-C17	-4.15	119.97	123.37
33	X	2911	ZLD	C5-C2-N4	2.16	122.59	119.93
33	X	2911	ZLD	F18-C16-C17	2.43	120.61	118.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	X	2911	ZLD	22	0

5.7 Other polymers [i](#)

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, 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%)	-0.46	54 (2%) 65 57	1, 35, 97, 115	0
2	Z	122/123 (99%)	0.01	2 (1%) 72 64	28, 74, 94, 101	0
3	A	218/274 (79%)	-0.53	1 (0%) 90 86	8, 44, 57, 63	0
4	B	205/211 (97%)	-0.88	0 100 100	1, 12, 35, 53	0
5	C	197/205 (96%)	-0.55	0 100 100	2, 45, 62, 78	0
6	D	177/180 (98%)	-0.12	4 (2%) 61 51	54, 65, 73, 76	0
7	E	171/185 (92%)	-0.48	1 (0%) 89 84	38, 59, 72, 76	0
8	F	70/144 (48%)	0.70	6 (8%) 11 11	62, 71, 75, 76	0
9	G	142/174 (81%)	-0.62	1 (0%) 87 82	19, 37, 53, 57	0
10	H	134/134 (100%)	-0.91	0 100 100	1, 8, 30, 42	0
11	I	141/156 (90%)	-0.08	5 (3%) 44 38	10, 54, 69, 84	0
12	J	136/142 (95%)	-0.52	1 (0%) 87 82	25, 44, 59, 66	0
13	K	113/116 (97%)	-0.91	0 100 100	1, 2, 13, 23	0
14	L	104/114 (91%)	-0.27	1 (0%) 82 75	38, 54, 61, 67	0
15	M	108/166 (65%)	-0.95	0 100 100	1, 11, 40, 46	0
16	N	117/118 (99%)	-0.76	0 100 100	2, 33, 55, 64	0
17	O	94/100 (94%)	-0.69	0 100 100	13, 46, 63, 66	0
18	P	127/134 (94%)	-0.88	0 100 100	1, 10, 40, 57	0
19	Q	93/95 (97%)	-0.62	0 100 100	23, 36, 60, 63	0
20	R	110/115 (95%)	-0.55	0 100 100	32, 44, 66, 70	0
21	S	175/237 (73%)	-0.13	5 (2%) 52 43	53, 62, 72, 79	0
22	T	84/91 (92%)	-0.04	5 (5%) 23 19	23, 47, 66, 69	0
23	U	72/81 (88%)	-0.37	0 100 100	39, 52, 63, 64	0
24	V	66/67 (98%)	-0.76	0 100 100	34, 52, 72, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
25	W	55/55 (100%)	-0.67	0	100	32, 41, 57, 66	0
26	Y	58/60 (96%)	-0.81	0	100	1, 7, 32, 34	0
27	1	53/55 (96%)	2.49	30 (56%)	0	33, 47, 62, 65	0
28	2	46/47 (97%)	3.36	40 (86%)	0	1, 12, 25, 35	0
29	3	63/66 (95%)	3.45	48 (76%)	0	23, 34, 43, 50	0
30	4	37/37 (100%)	0.50	3 (8%)	13	52, 65, 72, 73	0
All	All	5974/6562 (91%)	-0.38	207 (3%)	44	1, 41, 84, 115	0

The worst 5 of 207 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	3	34	THR	8.7
29	3	33	ASN	8.6
27	1	40	TYR	8.4
29	3	39	ASP	7.8
29	3	32	GLN	7.3

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
32	MG	X	2907	1/1	0.97	0.62	47.48	1,1,1,1	0
32	MG	X	2899	1/1	0.99	0.53	45.13	1,1,1,1	0
32	MG	M	167	1/1	0.98	0.55	19.63	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	X	2889	1/1	0.95	0.43	12.66	1,1,1,1	0
32	MG	X	2909	1/1	0.98	0.36	12.09	1,1,1,1	0
32	MG	X	2903	1/1	0.93	0.31	11.39	1,1,1,1	0
33	ZLD	X	2911	24/24	0.90	0.48	8.50	28,31,37,37	0
32	MG	X	2896	1/1	0.99	0.28	5.66	1,1,1,1	0
32	MG	X	2885	1/1	0.88	0.21	2.47	45,45,45,45	0
32	MG	X	2883	1/1	0.97	0.19	1.61	1,1,1,1	0
31	ZN	Y	61	1/1	0.98	0.13	-0.27	89,89,89,89	0
31	ZN	4	38	1/1	0.98	0.03	-1.94	78,78,78,78	0
32	MG	X	2887	1/1	0.96	0.17	-	37,37,37,37	0
32	MG	X	2888	1/1	0.99	0.38	-	1,1,1,1	0
32	MG	Z	125	1/1	0.98	0.17	-	1,1,1,1	0
32	MG	X	2884	1/1	0.97	0.23	-	19,19,19,19	0
32	MG	X	2900	1/1	0.92	0.52	-	1,1,1,1	0
32	MG	X	2901	1/1	0.98	0.35	-	1,1,1,1	0
32	MG	X	2895	1/1	0.98	0.31	-	1,1,1,1	0
32	MG	Z	127	1/1	0.97	0.20	-	3,3,3,3	0
32	MG	X	2893	1/1	0.95	0.20	-	3,3,3,3	0
32	MG	X	2902	1/1	0.97	0.80	-	61,61,61,61	0
32	MG	X	2881	1/1	0.95	0.50	-	10,10,10,10	0
32	MG	X	2886	1/1	0.96	0.25	-	15,15,15,15	0
32	MG	X	2905	1/1	0.96	0.36	-	18,18,18,18	0
32	MG	X	2882	1/1	0.96	0.38	-	49,49,49,49	0
32	MG	Z	126	1/1	0.95	0.13	-	12,12,12,12	0
32	MG	X	2892	1/1	0.98	0.19	-	1,1,1,1	0
32	MG	X	2897	1/1	0.90	0.27	-	1,1,1,1	0
32	MG	X	2908	1/1	0.96	0.46	-	48,48,48,48	0
32	MG	Z	124	1/1	0.90	0.19	-	11,11,11,11	0
32	MG	X	2891	1/1	0.94	0.11	-	23,23,23,23	0
32	MG	X	2904	1/1	0.94	0.40	-	1,1,1,1	0
32	MG	X	2906	1/1	0.99	0.09	-	40,40,40,40	0
32	MG	X	2890	1/1	0.95	0.65	-	1,1,1,1	0
32	MG	X	2910	1/1	0.94	0.26	-	14,14,14,14	0
32	MG	X	2898	1/1	0.97	0.40	-	1,1,1,1	0
32	MG	X	2894	1/1	0.94	0.36	-	2,2,2,2	0

6.5 Other polymers ⓘ

There are no such residues in this entry.