



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:16 am GMT

PDB ID : 5JVH
Title : The crystal structure large ribosomal subunit (50S) of *Deinococcus radiodurans* in complex with evernimicin
Authors : Yonath, A.
Deposited on : 2016-05-11
Resolution : 3.58 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

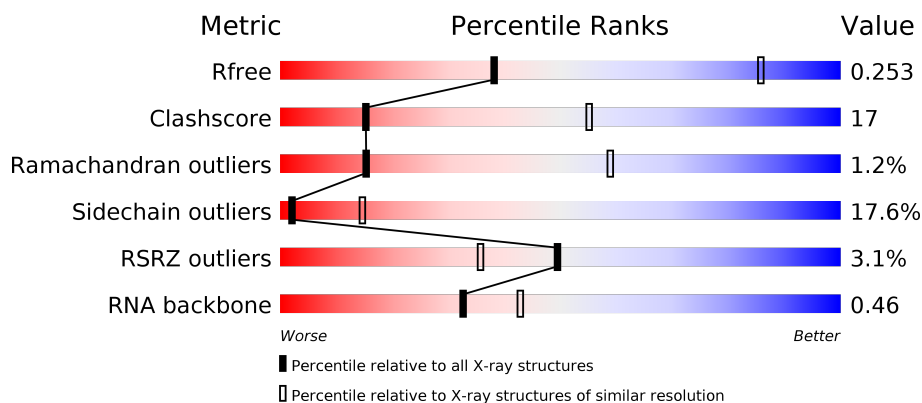
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.58 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.






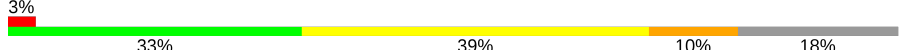

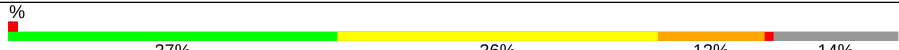
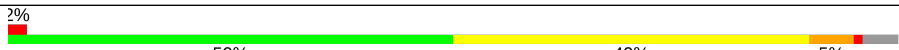
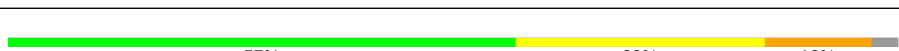
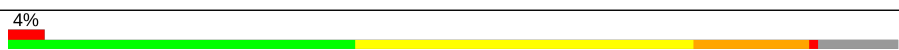
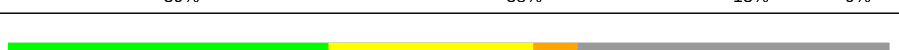
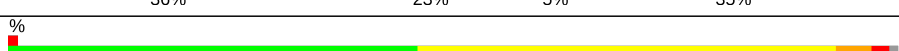

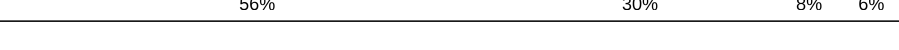
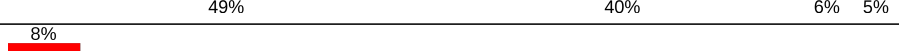
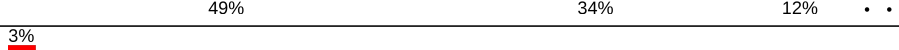
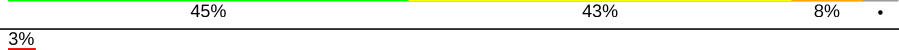


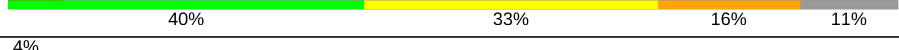

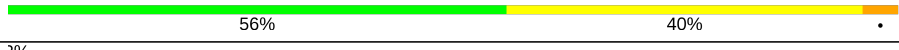
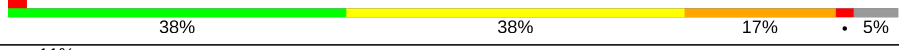
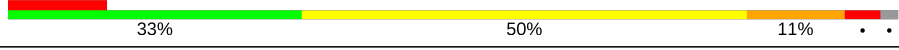
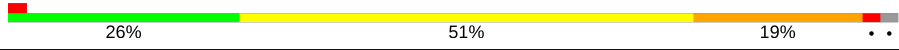
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1009 (3.70-3.46)
Clashscore	112137	1128 (3.70-3.46)
Ramachandran outliers	110173	1088 (3.70-3.46)
Sidechain outliers	110143	1088 (3.70-3.46)
RSRZ outliers	101464	1034 (3.70-3.46)
RNA backbone	2435	1005 (4.26-2.88)

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	<div> <div>3%</div> <div> <div>36%</div> <div>40%</div> <div>14%</div> <div>8%</div> </div> </div>
2	Y	123	<div> <div>2%</div> <div> <div>46%</div> <div>41%</div> <div>11%</div> </div> </div>
3	A	275	<div> <div>0%</div> <div> <div>40%</div> <div>45%</div> <div>9%</div> <div>6%</div> </div> </div>
4	B	211	<div> <div>0%</div> <div> <div>53%</div> <div>38%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	G	174	
9	H	134	
10	I	156	
11	J	141	
12	K	116	
13	L	114	
14	M	166	
15	N	118	
16	O	100	
17	P	134	
18	Q	95	
19	R	115	
20	S	237	
21	T	91	
22	U	81	
23	V	67	
24	W	55	
25	Z	60	
26	1	54	
27	2	47	
28	3	66	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	6O1	X	2901	-	-	-	X
30	MG	K	201	-	-	-	X
30	MG	X	2903	-	-	-	X
30	MG	X	2906	-	-	-	X
30	MG	X	2907	-	-	-	X
30	MG	X	2910	-	-	-	X
30	MG	X	2911	-	-	-	X
30	MG	X	2912	-	-	-	X
30	MG	X	2915	-	-	-	X
30	MG	X	2916	-	-	-	X
30	MG	X	2918	-	-	-	X
30	MG	X	2921	-	-	-	X
30	MG	X	2924	-	-	-	X
30	MG	X	2925	-	-	-	X
30	MG	X	2926	-	-	-	X
30	MG	X	2931	-	-	-	X
30	MG	X	2935	-	-	-	X
30	MG	X	2936	-	-	-	X
30	MG	X	2939	-	-	-	X
30	MG	X	2941	-	-	-	X
30	MG	X	2946	-	-	-	X
30	MG	X	2947	-	-	-	X
30	MG	X	2952	-	-	-	X
30	MG	X	2953	-	-	-	X
30	MG	X	2954	-	-	-	X
30	MG	X	2957	-	-	-	X
30	MG	X	2959	-	-	-	X
30	MG	X	2963	-	-	-	X
30	MG	X	2964	-	-	-	X
30	MG	X	2969	-	-	-	X
30	MG	X	2970	-	-	-	X
30	MG	X	2975	-	-	-	X
30	MG	X	2977	-	-	-	X
30	MG	X	2978	-	-	-	X
30	MG	X	2980	-	-	-	X
30	MG	X	2981	-	-	-	X
30	MG	X	2983	-	-	-	X
30	MG	X	2990	-	-	-	X
30	MG	X	2992	-	-	-	X
30	MG	X	2993	-	-	-	X
30	MG	X	3008	-	-	-	X
30	MG	X	3011	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MG	X	3014	-	-	-	X
30	MG	X	3017	-	-	-	X
30	MG	X	3020	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 83681 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	2658	Total	C	N	O	P	0	0	0
			57052	25450	10532	18413	2657			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	C	conflict	GB 1026245073

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	120	Total	C	N	O	P	0	0	0
			2561	1143	471	827	120			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	259	Total	C	N	O	S	0	0	0
			1973	1226	395	349	3			

- 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	194	Total	C	N	O	S	0	0	0
			1481	920	284	275	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 L13.

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

- Molecule 9 is a protein called 50S ribosomal protein L14.

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

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	134	Total	C	N	O	S	0	0	0
			1011	619	206	186				

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	136	Total	C	N	O	S	0	0	0
			1078	690	196	185	7			

- Molecule 12 is a protein called 50S ribosomal protein L17.

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

- Molecule 13 is a protein called 50S ribosomal protein L18.

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

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	108	Total	C	N	O	0	0	0
			859	537	166	156			

- Molecule 15 is a protein called 50S ribosomal protein L20.

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

- Molecule 16 is a protein called 50S ribosomal protein L21.

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

- Molecule 17 is a protein called 50S ribosomal protein L22.

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

- Molecule 18 is a protein called 50S ribosomal protein L23.

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

- Molecule 19 is a protein called 50S ribosomal protein L24.

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

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	179	Total	C	N	O	S	0	0	0
			1374	867	240	261	6			

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	74	Total	C	N	O	S	0	0	0
			556	351	107	97	1			

- Molecule 22 is a protein called 50S ribosomal protein L28.

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

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	S	0	0	0
			525	322	106	95	2			

- Molecule 24 is a protein called 50S ribosomal protein L30.

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

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	57	Total	C	N	O	S	0	0	0
			452	278	93	76	5			

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1	53	Total	C	N	O	S	0	0	0
			427	271	79	76	1			

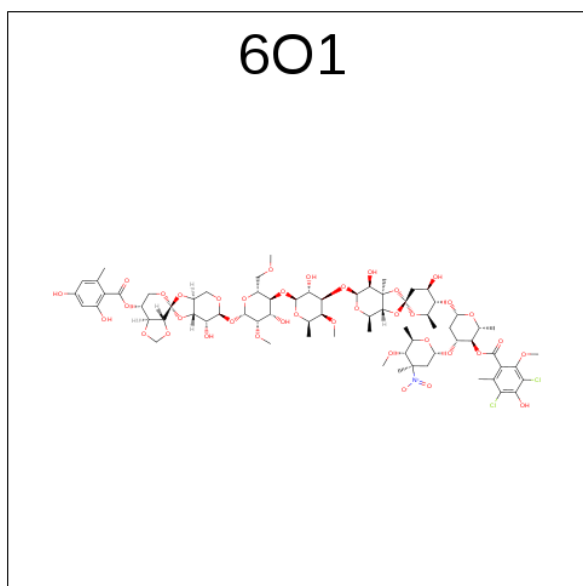
- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	59	Total	C	N	O	S	0	0	0
			462	290	95	73	4			

- Molecule 29 is Evernimicin (three-letter code: 6O1) (formula: $C_{70}H_{97}Cl_2NO_{38}$).

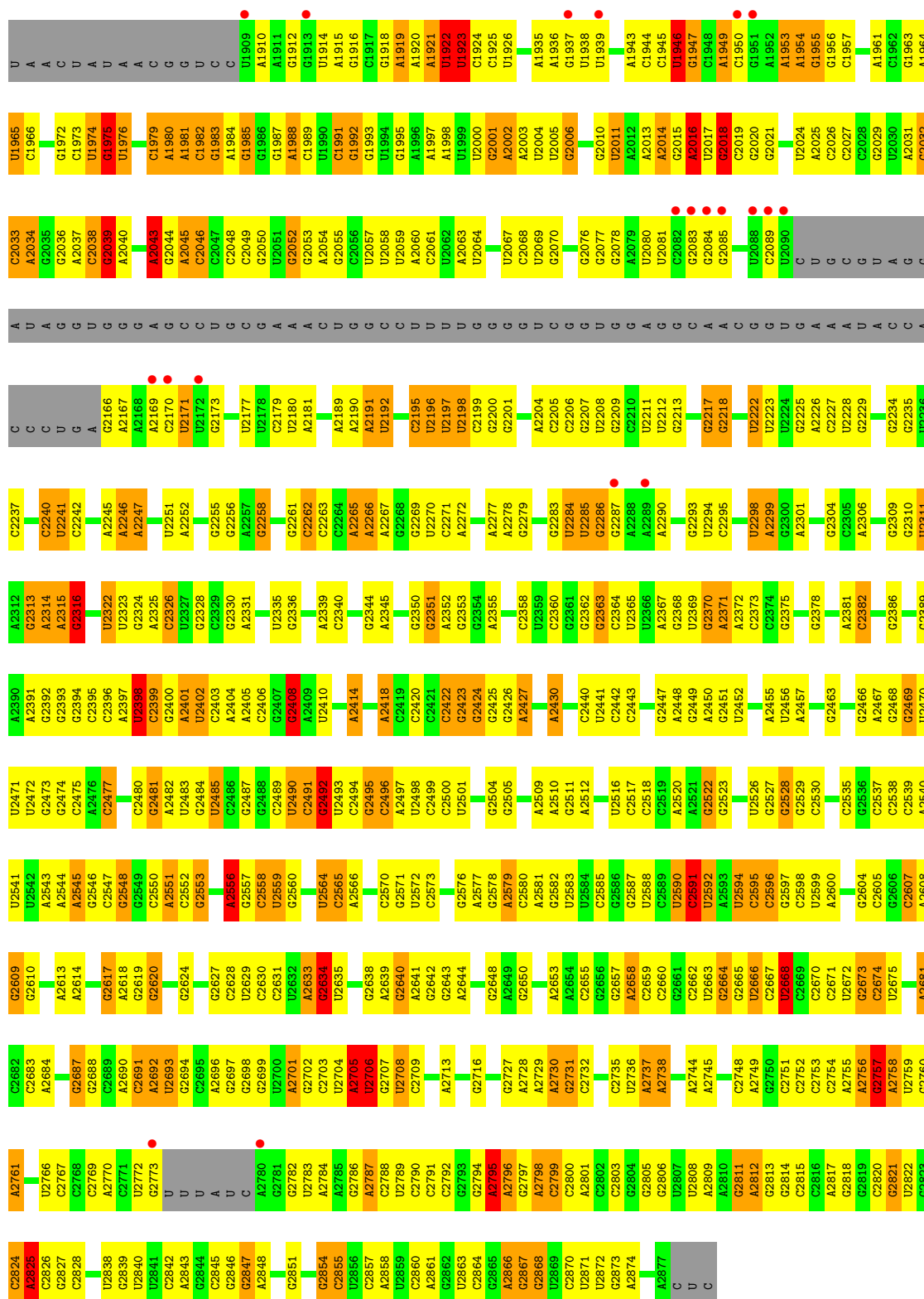


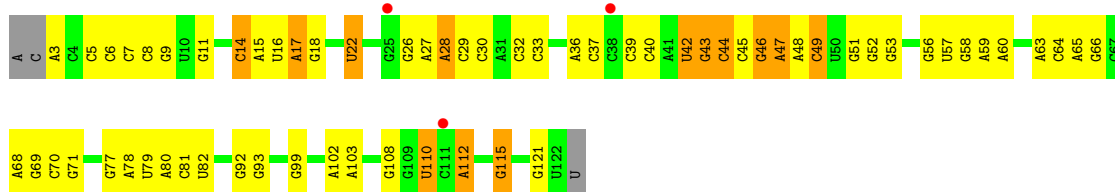
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	X	1	Total	C	Cl	N	O	0	0
			111	70	2	1	38		

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

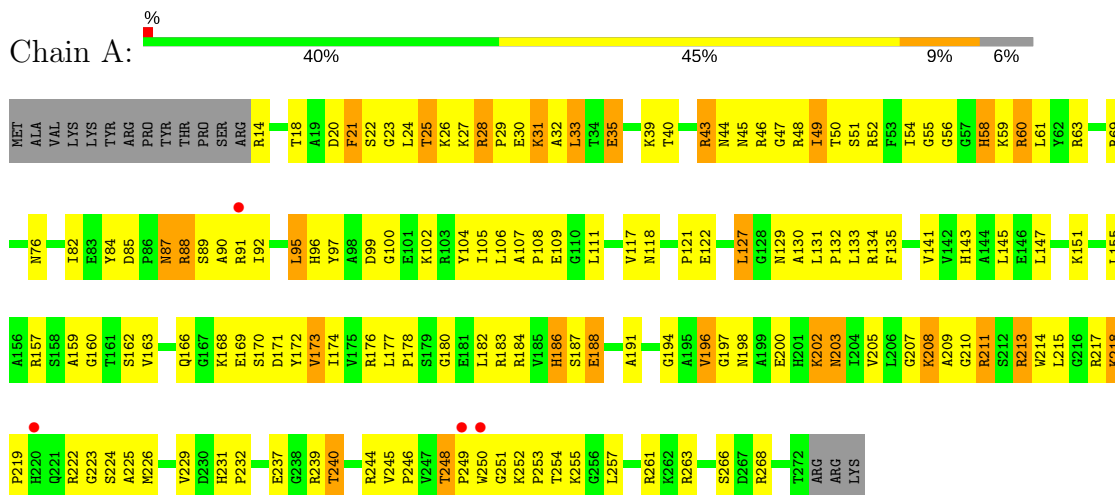
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	119	Total	Mg	0	0
			119	119		
30	Y	1	Total	Mg	0	0
			1	1		
30	K	2	Total	Mg	0	0
			2	2		
30	M	1	Total	Mg	0	0
			1	1		

G1822	G1754	C1517	G1438	G1360	G1223	A1153	A1022	U946	A876	C808
G1823	G1755	G1520	G1439	G1361	A1224	A1154	U1023	C947	G877	C809
C1824	C1756	U1521	G1440	C1362	G1225	G1155	G1024	C948	C878	U810
G1825	G1757	U1522	C1441	C1363	G1226	U1161	C1029	G951	C879	G811
G1826	U1601	C1523	C1442	G1296	A1227	A1162	U1030	G952	C880	G812
G1827	G1502	C1524	C1443	A1299	C1229	C1163	G1031	G953	C881	G813
C1830	A1603	G1525	C1444	G1371	C1230	C1164	A1032	U954	C882	G814
G1760	A1604	A1526	A1448	A1372	C1231	G1165	G1033	U955	U890	A817
G1761	A1605	G1527	U1454	G1374	A1231	A1166	U1034	A956	A	C818
G1762	C1606	C1528	U1455	A1378	C1235	A1167	G1035	G957	G	C819
G1763	U1608	G1531	U1456	A1378	G1236	G1173	G1036	G958	G	U820
A1764	U1609	A1532	U1459	G1381	G1237	G1174	U1037	C959	G	A821
G1765	A1610	G1533	U1460	G1382	G1240	G1175	U1038	A964	G	G822
U1688	C1614	C1534	C1461	G1383	A1242	U1176	A1039	G967	G	G823
G1688	C1615	C1535	C1462	A1386	A1245	U1177	A1040	U969	C	U824
G1688	G1542	G1543	A1463	A1386	G1246	C1178	G1041	U970	U	C825
G1688	A1544	A1544	G1464	G1390	G1247	A1179	U1044	U971	A	C829
G1688	U1547	U1548	G1465	A1391	U1247	C1180	U1045	A971	C	C830
G1688	U1549	C1550	G1466	G1392	G1248	U1182	U1046	C972	C	A832
G1688	U1551	U1551	U1467	G1393	G1249	C1183	U1047	A972	A	A833
G1688	C1552	C1553	U1468	G1393	A1250	G1184	U1048	U977	G	A834
G1688	G1553	G1554	U1469	G1393	G1251	C1185	G1050	U978	U	U835
G1688	U1555	U1556	G1470	A1397	C1252	G1186	U1051	A979	U	G836
G1688	C1557	C1558	G1480	G1398	G1253	U1187	U1052	A984	A	U837
G1688	U1564	U1565	U1481	C1399	A1255	A1188	C1053	G985	C	U840
G1688	G1566	G1567	U1482	G1403	C1256	U1189	G1054	G986	C	G841
G1688	C1570	C1571	G1483	C1404	G1260	C1190	U1055	G987	C	A842
G1688	G1573	G1574	A1486	C1412	G1261	G1191	U1056	G988	C	U845
G1688	A1574	A1575	C1487	G1416	U1262	A1192	U1057	G989	C	A846
G1688	C1575	C1576	U1490	C1417	G1263	U1193	G1058	C991	C	C847
G1688	G1576	G1577	C1491	C1418	G1264	U1194	U1059	G992	U	A848
G1688	U1578	U1579	A1493	G1419	G1265	U1195	C1120	G993	C	G849
G1688	G1582	G1583	U1494	A1420	G1266	G1196	C1121	G994	C	C850
G1688	A1584	A1585	G1495	U1421	A1267	U1197	G1122	G995	C	C851
G1688	U1586	U1587	G1496	C1422	G1268	U1198	U1060	G996	C	U852
G1688	A1588	A1589	U1497	C1423	U1269	C1199	G1061	C997	C	U853
G1688	G1590	G1591	U1498	U1424	G1270	U1200	U1062	G998	C	C854
G1688	U1592	U1593	U1499	U1425	C1271	A1203	G1063	A999	C	U857
G1688	G1594	G1595	U1500	G1426	G1272	G1204	C1064	C1003	C	G858
G1688	A1596	A1597	U1501	G1427	C1273	G1205	U1065	A1004	C	U859
G1688	U1598	U1599	C1501	G1428	C1274	G1206	G1006	G928	C	U860
G1688	G1600	G1601	U1505	A1429	A1275	U1207	A1007	A929	C	G861
G1688	C1602	C1603	U1506	G1430	U1276	A1208	G1008	G931	C	A862
G1688	U1604	U1605	U1507	C1431	G1277	G1209	C1009	G932	C	C863
G1688	G1606	G1607	U1508	A1432	G1278	U1210	A1010	G933	C	U864
G1688	U1608	U1609	U1509	G1433	G1279	U1211	G1011	G934	C	A865
G1688	A1610	A1611	U1510	U1434	C1283	U1212	U1012	G938	C	U866
G1688	C1612	C1613	U1511	U1435	G1284	U1213	G1013	U939	C	G870
G1688	G1614	G1615	U1512	G1436	A1285	G1214	U1014	G940	C	U871
G1688	U1616	U1617	U1513	U1437	A1286	U1215	U1015	G941	C	G872
G1688	A1618	A1619	U1514	U1438	A1287	G1216	G1016	U942	C	U873
G1688	U1620	U1621	U1515	U1439	A1288	U1217	C1017	U943	C	A874
G1688	C1622	C1623	U1516	U1440	U1289	G1218	U1018	U944	C	G875
G1688	U1624	U1625	U1517	U1441	A1290	U1219	G1019	A1021	C	
G1688	A1626	A1627	U1518	U1442	G1291	G1220	U1020			
G1688	U1628	U1629	U1519	U1443	G1292	G1221	U1021			
G1688	C1630	C1631	U1520	U1444	G1293	G1222	U1022			
G1688	U1632	U1633	U1521	U1445	G1294	G1223	U1023			
G1688	A1634	A1635	U1522	U1446	G1295	G1224	U1024			
G1688	U1636	U1637	U1523	U1447	G1296	G1225	U1025			
G1688	C1638	C1639	U1524	U1448	G1297	G1226	U1026			
G1688	U1640	U1641	U1525	U1449	G1298	G1227	U1027			
G1688	A1642	A1643	U1526	U1450	G1299	G1228	U1028			
G1688	U1644	U1645	U1527	U1451	G1300	G1229	U1029			
G1688	C1646	C1647	U1528	U1452	G1301	G1230	U1030			
G1688	U1648	U1649	U1529	U1453	G1302	G1231	U1031			
G1688	A1650	A1651	U1530	U1454	C1303	G1232	U1032			
G1688	U1652	U1653	U1531	U1455	U1304	G1233	U1033			
G1688	C1654	C1655	U1532	U1456	U1305	G1234	U1034			
G1688	U1656	U1657	U1533	U1457	G1306	G1235	U1035			
G1688	A1658	A1659	U1534	U1458	G1307	G1236	U1036			
G1688	U1660	U1661	U1535	U1459	U1308	G1237	U1037			
G1688	G1662	G1663	U1536	U1460	G1309	G1238	U1038			
G1688	U1664	U1665	U1537	U1461	U1310	G1239	U1039			
G1688	C1666	C1667	U1538	U1462	G1311	G1240	U1040			
G1688	A1668	A1669	U1539	U1463	C1312	G1241	U1041			
G1688	U1670	U1671	U1540	U1464	U1313	G1242	U1042			
G1688	G1672	G1673	U1541	U1465	U1314	G1243	U1043			
G1688	A1674	A1675	U1542	U1466	A1315	G1244	U1044			
G1688	U1676	U1677	U1543	U1467	G1316	G1245	U1045			
G1688	C1678	C1679	U1544	U1468	G1317	G1246	U1046			
G1688	A1680	A1681	U1545	U1469	A1318	U1247	U1047			
G1688	U1682	U1683	U1546	U1470	G1319	G1248	U1048			
G1688	C1684	C1685	U1547	U1471	U1320	G1249	U1049			
G1688	U1686	U1687	U1548	U1472	G1321	G1250	G1050			
G1688	A1688	A1689	U1549	U1473	G1322	G1251	U1051			
G1688	U1690	U1691	U1550	U1474	G1323	C1252	U1052			
G1688	C1692	C1693	U1551	U1475	G1324	G1253	U1053			
G1688	U1694	U1695	U1552	U1476	U1325	A1255	G1054			
G1688	A1696	A1697	U1553	U1477	U1326	C1256	U1055			
G1688	U1698	U1699	U1554	U1478	G1327	G1257	U1056			
G1688	C1700	C1701	U1555	U1479	G1328	G1258	U1057			
G1688	U1702	U1703	U1556	U1480	U1329	G1259	U1058			
G1688	A1704	A1705	U1557	U1481	G1330	G1260	U1059			
G1688	U1706	U1707	U1558	U1482	U1331	U1261	G1060			
G1688	C1708	C1709	U1559	U1483	G1332	U1262	U1061			
G1688	U1710	U1711	U1560	U1484	U1333	G1263	U1062			
G1688	A1712	A1713	U1561	U1485	A1334	G1264	U1063			
G1688	U1714	U1715	U1562	U1486	G1335	G1265	U1064			
G1688	C1716	C1717	U1563	U1487	U1336	A1267	U1065			
G1688	U1718	U1719	U1564	U1488	G1337	U1268	U1066			
G1688	A1720	A1721	U1565	U1489	U1338	U1269	U1067			
G1688	U1722	U1723	U1566	U1490	U1339	G1270	U1068			
G1688	C1724	C1725	U1567	C1491	C1340	G1271	U1069			
G1688	U1726	U1727	U1568	U1492	G1341	G1272	U1070			
G1688	A1728	A1729	U1569	U1493	U1342	G1273	U1071			
G1688	C1730	C1731	U1570	U1494	C1343	C1274	U1072			
G1688	U1732	U1733	U1571	U1495	G1344	A1275	G1073			
G1688	A1734	A1735	U1572	U1496	C1345	U1276	G1074			
G1688	U1736	U1737	U1573	U1497	G1346	G1277	C1075			
G1688	C1738	C1739	U1574	U1498	U1347	G1278	U1076			
G1688	U1740	U1741	U1575	U1499	G1348	A1279	U1077			
G1688	A1742	A1743	U1576	U1500	U1349	G1279	U1078			
G1688	U1744	U1745	U1577	U1501	G1350	G1280	U1079			
G1688	C1746	C1747	U1578	U1502	C1351	C1283	A1012			
G1688	A1748	A1749	U1579	U1503	G1352	G1284	G1013			
G1688	U1750	U1751	U1580	U1504	C1353	A1285	U1014			
G1688	C1752	C1753	U1581	U1505	A1353	U1286	G1015			
G1688	A1754	A1755	U1582	U1506	G1354	A1287	U1016			
G1688	U1756	U1757	U1583	U1507	C1355	U1288	G1017			
G1688	C1758	C1759	U1584	U1508	G1356	U1289	C1018			
G1688	A1760	A1761	U1585	U1509	U1357	A1290	U1019			
G1688	U1762	U1763	U1586	U1510	G1358	G1291	A1020			
G1688	C1764	C1765	U1587	U1511	U1359	G1292	U1021			
G1688	A1766	A1767	U1588	U1512	G1360	G1293	U1022			
G1688	U1768	U1769	U1589	U1513	U1361	G1294	U1023			
G1688	C1770	C1771	U1590	U1514	C1362	G1295	U1024			
G1688	A1772	A1773	U1591	U1515	U1363	G1296	U1025			
G1688	U1774	U1								





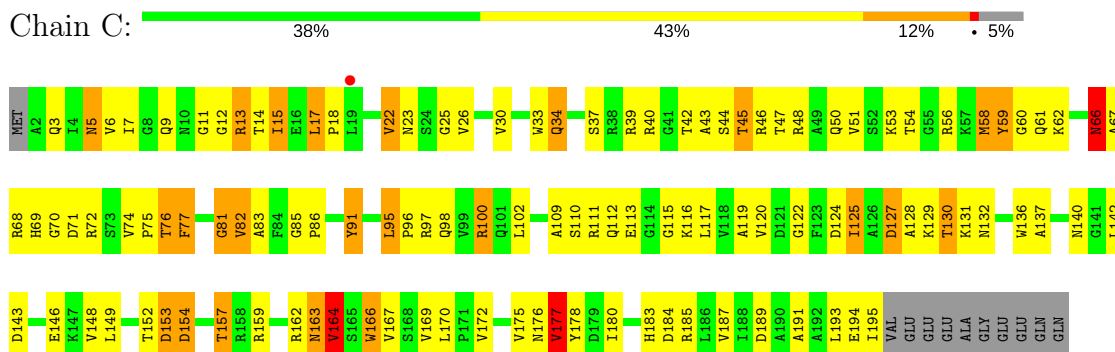
• Molecule 3: 50S ribosomal protein L2



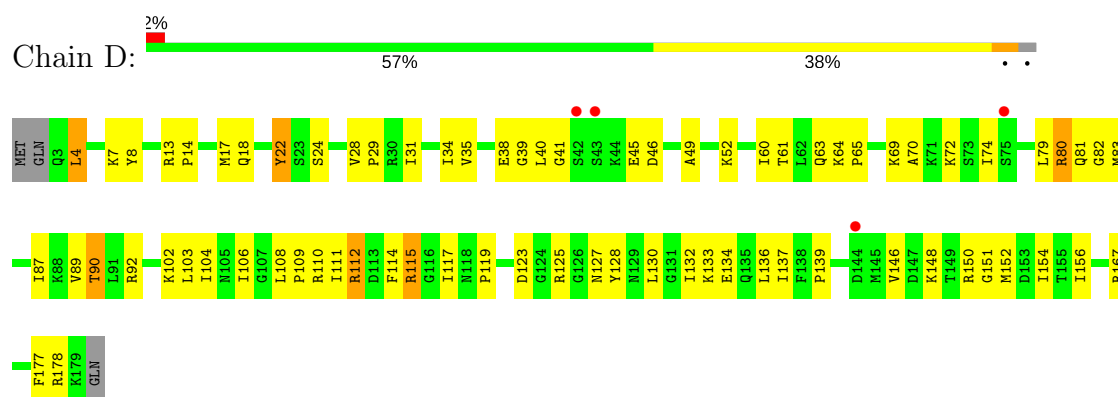
• Molecule 4: 50S ribosomal protein L3



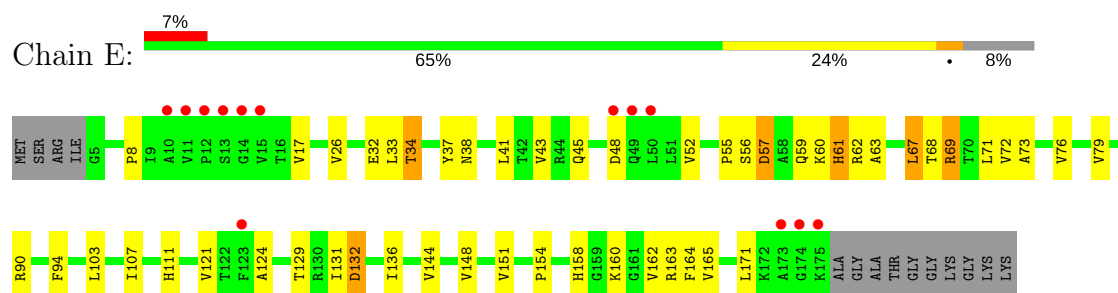
• Molecule 5: 50S ribosomal protein L4



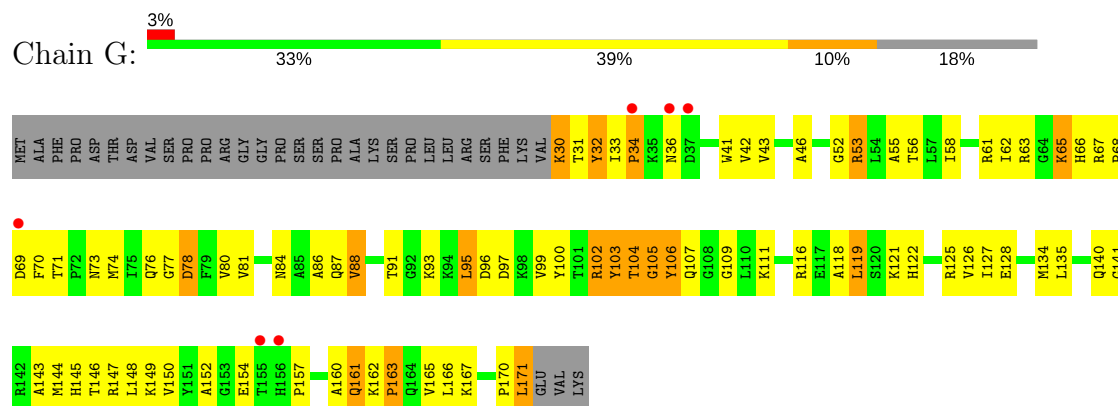
• Molecule 6: 50S ribosomal protein L5



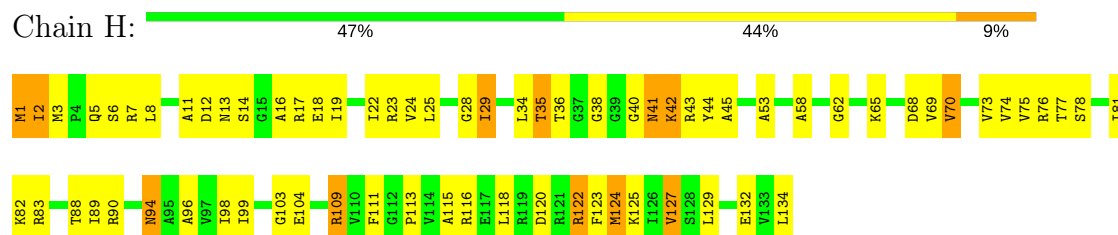
• Molecule 7: 50S ribosomal protein L6



• Molecule 8: 50S ribosomal protein L13

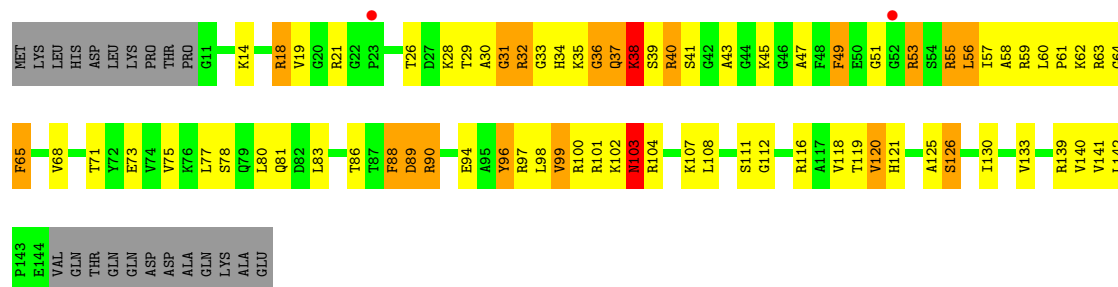


• Molecule 9: 50S ribosomal protein L14

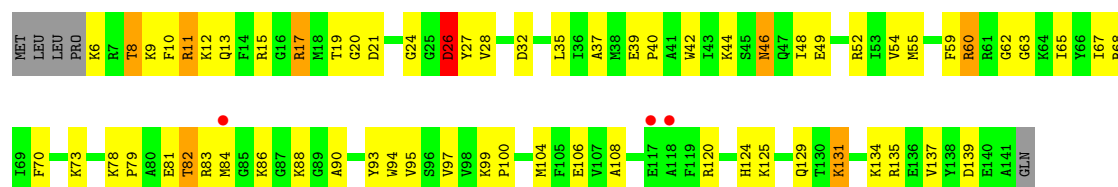


• Molecule 10: 50S ribosomal protein L15

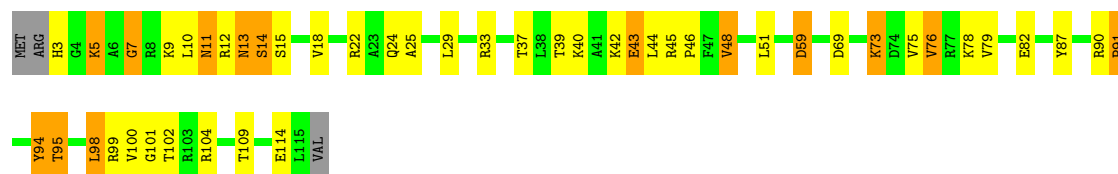




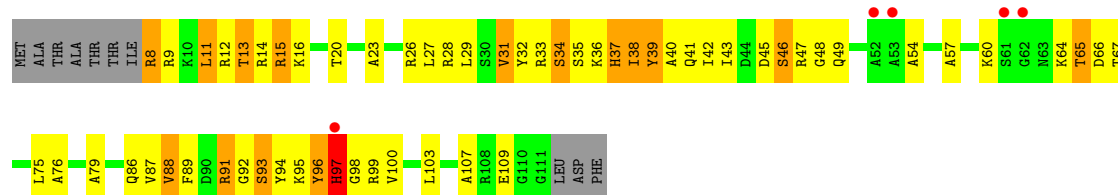
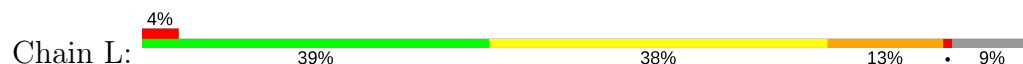
- Molecule 11: 50S ribosomal protein L16



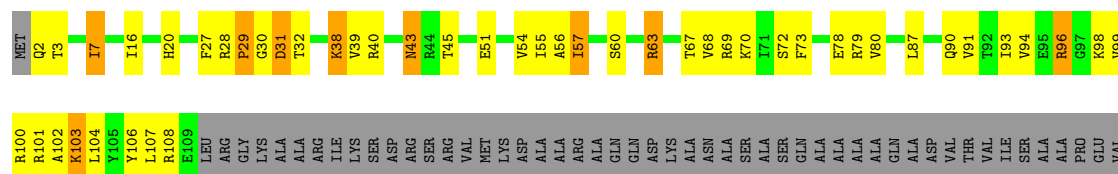
- Molecule 12: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L18

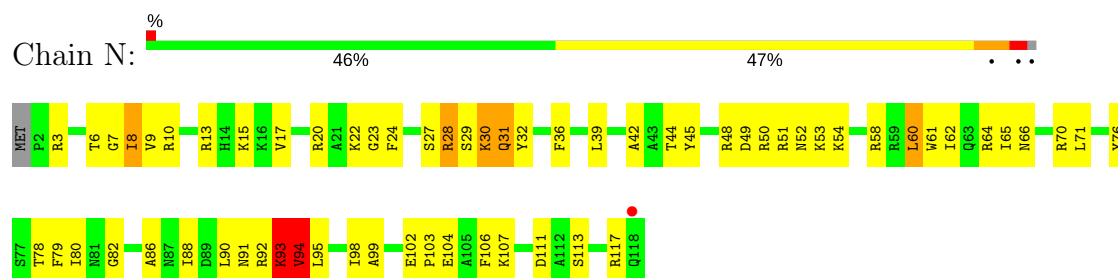


- Molecule 14: 50S ribosomal protein L19

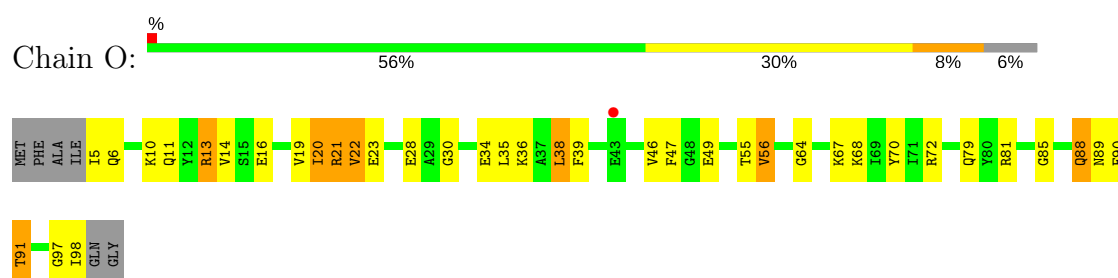


ALA
PRO
GLU
THR
GLN
GLY
GLU

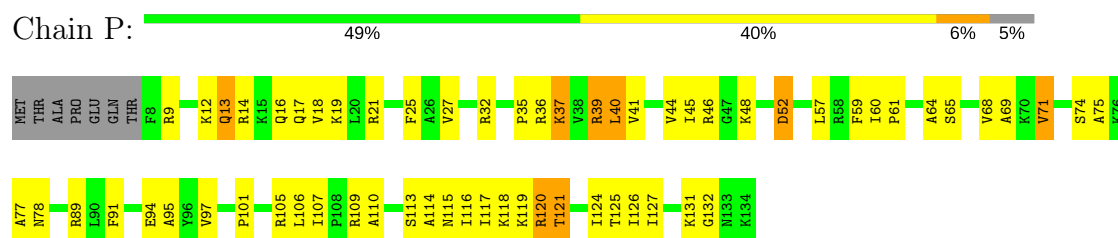
• Molecule 15: 50S ribosomal protein L20



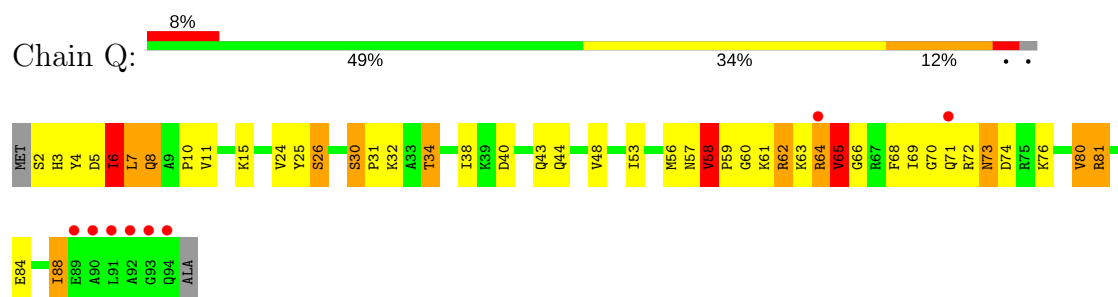
• Molecule 16: 50S ribosomal protein L21



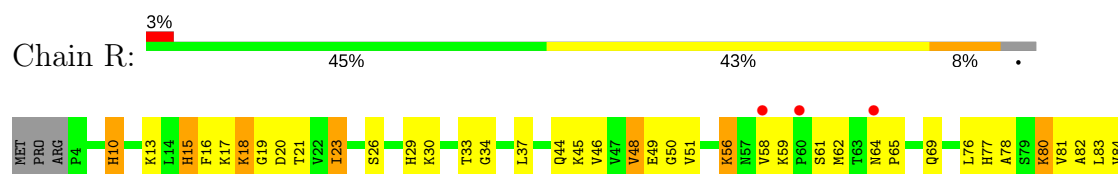
• Molecule 17: 50S ribosomal protein L22



• Molecule 18: 50S ribosomal protein L23

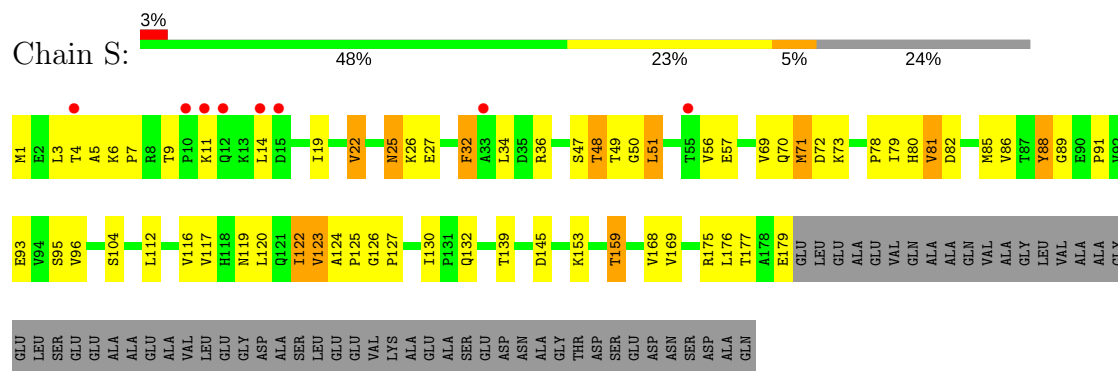


• Molecule 19: 50S ribosomal protein L24

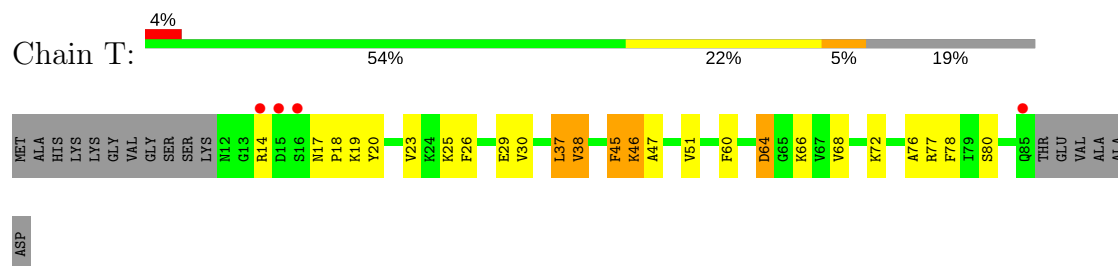




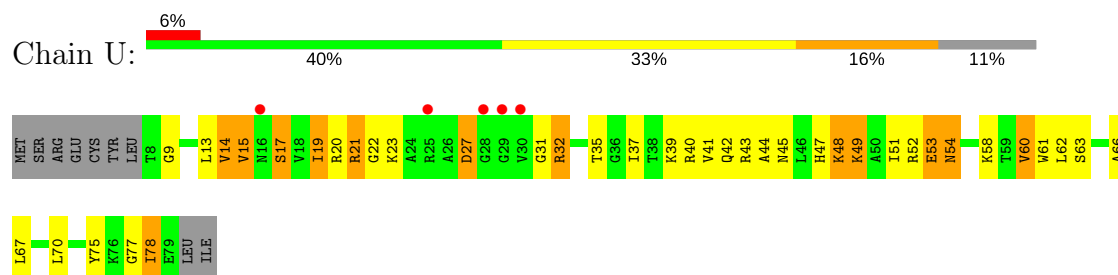
• Molecule 20: 50S ribosomal protein L25



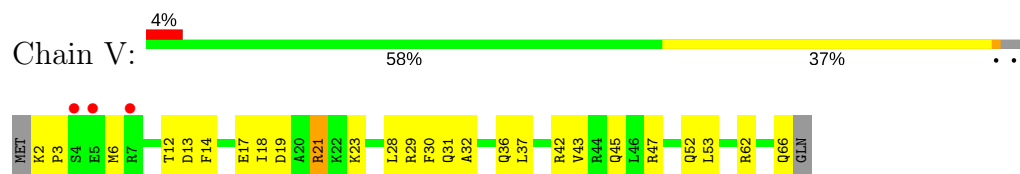
• Molecule 21: 50S ribosomal protein L27



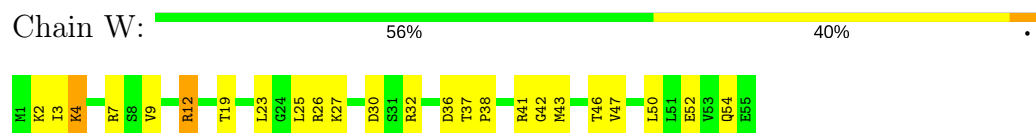
• Molecule 22: 50S ribosomal protein L28



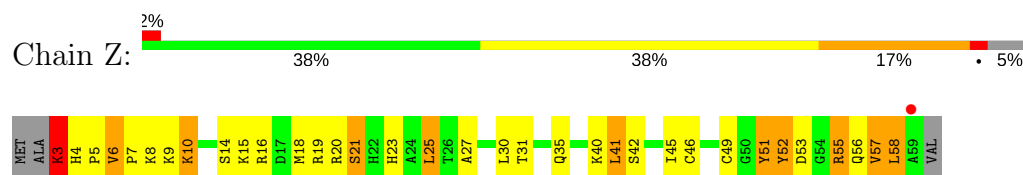
• Molecule 23: 50S ribosomal protein L29



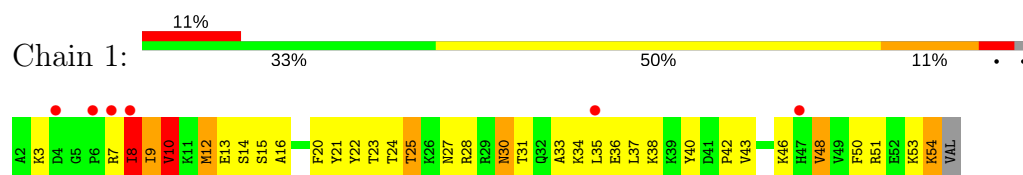
• Molecule 24: 50S ribosomal protein L30



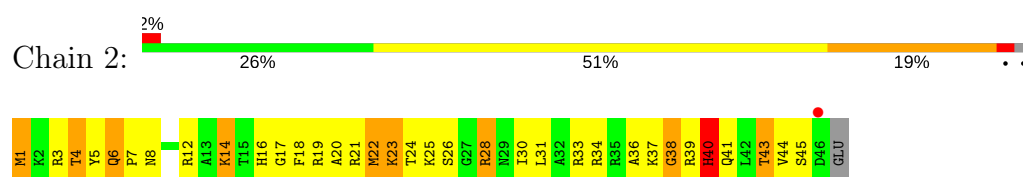
- Molecule 25: 50S ribosomal protein L32



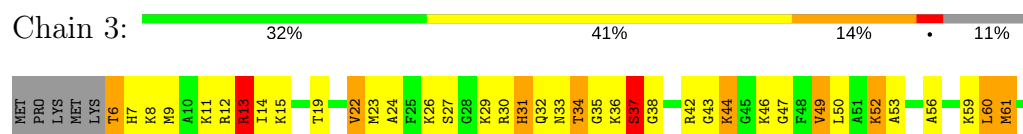
- Molecule 26: 50S ribosomal protein L33



- Molecule 27: 50S ribosomal protein L34



- Molecule 28: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.47Å 407.38Å 692.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.58 29.84 – 3.57	Depositor EDS
% Data completeness (in resolution range)	94.3 (29.84-3.58) 94.2 (29.84-3.57)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.56Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.204 , 0.247 0.208 , 0.253	Depositor DCC
R_{free} test set	13342 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	112.0	Xtriage
Anisotropy	0.654	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	83681	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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, 6O1

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	0.69	20/63887 (0.0%)	1.25	500/99650 (0.5%)
2	Y	0.41	0/2863	0.93	0/4461
3	A	0.49	0/2011	0.79	4/2708 (0.1%)
4	B	0.58	0/1567	0.85	0/2105
5	C	0.49	0/1504	0.77	1/2036 (0.0%)
6	D	0.30	0/1419	0.51	0/1903
7	E	0.30	0/1308	0.54	0/1771
8	G	0.51	0/1138	0.81	1/1539 (0.1%)
9	H	0.56	0/1007	0.74	0/1352
10	I	0.61	0/1022	0.93	3/1366 (0.2%)
11	J	0.48	0/1101	0.71	0/1472
12	K	0.67	0/886	0.89	2/1188 (0.2%)
13	L	0.39	0/785	0.69	0/1048
14	M	0.67	1/872 (0.1%)	0.91	2/1172 (0.2%)
15	N	0.52	0/994	0.77	0/1323
16	O	0.46	0/750	0.81	2/1000 (0.2%)
17	P	0.58	0/1027	0.71	0/1373
18	Q	0.49	0/737	0.82	2/988 (0.2%)
19	R	0.45	0/835	0.75	0/1121
20	S	0.31	0/1399	0.57	0/1902
21	T	0.45	0/563	0.75	0/747
22	U	0.46	0/556	0.73	0/741
23	V	0.34	0/529	0.52	0/704
24	W	0.43	0/426	0.67	0/568
25	Z	0.56	0/464	0.77	0/622
26	1	0.55	0/434	0.83	0/579
27	2	0.58	0/387	1.04	2/509 (0.4%)
28	3	0.59	0/468	0.98	2/614 (0.3%)
All	All	0.63	21/90939 (0.0%)	1.14	521/136562 (0.4%)

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
3	A	0	1
4	B	0	1
5	C	0	2
8	G	0	4
10	I	0	5
11	J	0	1
13	L	0	1
15	N	0	2
19	R	0	1
25	Z	0	1
27	2	0	3
28	3	0	2
All	All	0	24

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	774	A	C5-C4	7.18	1.43	1.38
1	X	542	A	N9-C4	-7.12	1.33	1.37
14	M	29	PRO	CA-C	6.60	1.66	1.52
1	X	540	G	C2-N3	6.49	1.38	1.32
1	X	2548	G	C6-O6	6.47	1.29	1.24

The worst 5 of 521 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	774	A	N7-C8-N9	14.67	121.13	113.80
1	X	774	A	C8-N9-C4	-14.58	99.97	105.80
1	X	542	A	C2-N3-C4	-13.70	103.75	110.60
1	X	1333	G	N3-C4-N9	-12.51	118.49	126.00
1	X	2018	G	C4-C5-N7	11.72	115.49	110.80

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	58	HIS	Peptide
4	B	122	PHE	Peptide
5	C	176	ASN	Peptide

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Continued from previous page...

Mol	Chain	Res	Type	Group
5	C	66	ASN	Peptide
8	G	34	PRO	Peptide

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	57052	0	28750	1265	0
2	Y	2561	0	1306	59	0
3	A	1973	0	2034	131	0
4	B	1539	0	1600	81	0
5	C	1481	0	1504	97	0
6	D	1400	0	1481	60	0
7	E	1286	0	1336	31	0
8	G	1114	0	1144	83	0
9	H	997	0	1046	55	0
10	I	1011	0	1047	76	0
11	J	1078	0	1103	47	0
12	K	878	0	930	34	0
13	L	779	0	820	49	0
14	M	859	0	872	35	0
15	N	978	0	1020	66	0
16	O	741	0	756	34	0
17	P	1014	0	1096	49	0
18	Q	726	0	753	29	0
19	R	825	0	881	57	0
20	S	1374	0	1401	44	0
21	T	556	0	579	24	0
22	U	552	0	604	42	0
23	V	525	0	546	14	0
24	W	424	0	470	16	0
25	Z	452	0	457	34	0
26	1	427	0	445	35	0
27	2	383	0	414	37	0
28	3	462	0	506	36	0
29	X	111	0	0	2	0
30	K	2	0	0	0	0
30	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	X	119	0	0	0	0
30	Y	1	0	0	0	0
All	All	83681	0	54901	2278	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 17.

The worst 5 of 2278 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:356:A:HO2'	1:X:357:A:H8	1.10	0.99
8:G:100:TYR:HB2	8:G:116:ARG:HE	1.25	0.96
10:I:56:LEU:H	10:I:59:ARG:HD3	1.30	0.94
1:X:1277:G:OP1	25:Z:19:ARG:NH2	2.01	0.93
1:X:1264:C:H5''	15:N:13:ARG:HH12	1.34	0.93

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	257/275 (94%)	219 (85%)	37 (14%)	1 (0%)	38	76
4	B	203/211 (96%)	183 (90%)	15 (7%)	5 (2%)	6	44
5	C	192/205 (94%)	161 (84%)	25 (13%)	6 (3%)	5	39
6	D	175/180 (97%)	151 (86%)	24 (14%)	0	100	100
7	E	169/185 (91%)	155 (92%)	13 (8%)	1 (1%)	28	70
8	G	140/174 (80%)	124 (89%)	15 (11%)	1 (1%)	25	68
9	H	132/134 (98%)	123 (93%)	8 (6%)	1 (1%)	22	65
10	I	132/156 (85%)	98 (74%)	30 (23%)	4 (3%)	5	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	J	134/141 (95%)	117 (87%)	16 (12%)	1 (1%)	25	68
12	K	111/116 (96%)	101 (91%)	9 (8%)	1 (1%)	20	64
13	L	102/114 (90%)	80 (78%)	22 (22%)	0	100	100
14	M	106/166 (64%)	100 (94%)	6 (6%)	0	100	100
15	N	115/118 (98%)	100 (87%)	13 (11%)	2 (2%)	11	52
16	O	92/100 (92%)	83 (90%)	9 (10%)	0	100	100
17	P	125/134 (93%)	121 (97%)	4 (3%)	0	100	100
18	Q	91/95 (96%)	69 (76%)	19 (21%)	3 (3%)	4	38
19	R	108/115 (94%)	80 (74%)	28 (26%)	0	100	100
20	S	177/237 (75%)	150 (85%)	25 (14%)	2 (1%)	17	61
21	T	72/91 (79%)	63 (88%)	9 (12%)	0	100	100
22	U	70/81 (86%)	51 (73%)	17 (24%)	2 (3%)	5	41
23	V	63/67 (94%)	58 (92%)	5 (8%)	0	100	100
24	W	53/55 (96%)	49 (92%)	4 (8%)	0	100	100
25	Z	55/60 (92%)	45 (82%)	10 (18%)	0	100	100
26	1	51/54 (94%)	36 (71%)	12 (24%)	3 (6%)	2	23
27	2	44/47 (94%)	37 (84%)	5 (11%)	2 (4%)	3	29
28	3	57/66 (86%)	44 (77%)	11 (19%)	2 (4%)	4	37
All	All	3026/3377 (90%)	2598 (86%)	391 (13%)	37 (1%)	15	59

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	N	94	VAL
18	Q	6	ILE
5	C	177	VAL
20	S	122	ILE
26	1	9	ILE

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	200/216 (93%)	160 (80%)	40 (20%)	1	10
4	B	155/157 (99%)	132 (85%)	23 (15%)	3	23
5	C	154/163 (94%)	117 (76%)	37 (24%)	1	6
6	D	153/156 (98%)	144 (94%)	9 (6%)	23	62
7	E	136/144 (94%)	124 (91%)	12 (9%)	12	47
8	G	118/146 (81%)	100 (85%)	18 (15%)	3	22
9	H	103/103 (100%)	83 (81%)	20 (19%)	1	11
10	I	101/121 (84%)	77 (76%)	24 (24%)	1	6
11	J	108/115 (94%)	89 (82%)	19 (18%)	2	15
12	K	90/93 (97%)	74 (82%)	16 (18%)	2	14
13	L	74/82 (90%)	50 (68%)	24 (32%)	0	2
14	M	92/134 (69%)	76 (83%)	16 (17%)	2	15
15	N	96/97 (99%)	87 (91%)	9 (9%)	10	44
16	O	75/79 (95%)	64 (85%)	11 (15%)	3	24
17	P	109/115 (95%)	90 (83%)	19 (17%)	2	15
18	Q	75/76 (99%)	53 (71%)	22 (29%)	0	3
19	R	91/96 (95%)	77 (85%)	14 (15%)	3	21
20	S	152/192 (79%)	130 (86%)	22 (14%)	4	24
21	T	55/67 (82%)	47 (86%)	8 (14%)	4	24
22	U	57/66 (86%)	43 (75%)	14 (25%)	1	5
23	V	53/55 (96%)	49 (92%)	4 (8%)	16	53
24	W	48/48 (100%)	42 (88%)	6 (12%)	5	30
25	Z	51/53 (96%)	36 (71%)	15 (29%)	0	3
26	1	45/47 (96%)	33 (73%)	12 (27%)	0	4
27	2	39/40 (98%)	29 (74%)	10 (26%)	0	5
28	3	46/52 (88%)	34 (74%)	12 (26%)	0	5
All	All	2476/2713 (91%)	2040 (82%)	436 (18%)	2	15

5 of 436 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	106	GLU

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Mol	Chain	Res	Type
14	M	31	ASP
26	1	8	ILE
12	K	11	ASN
13	L	15	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
10	I	103	ASN
12	K	35	GLN
25	Z	44	HIS
11	J	58	HIS
13	L	41	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2649/2880 (91%)	580 (21%)	0
2	Y	119/123 (96%)	23 (19%)	0
All	All	2768/3003 (92%)	603 (21%)	0

5 of 603 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	4	C
1	X	7	G
1	X	10	A
1	X	14	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 124 ligands modelled in this entry, 123 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	$\# Z > 2$
29	6O1	X	2901	-	116,123,123	1.61	13 (11%)	154,191,191	1.86	28 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	6O1	X	2901	-	-	0/50/234/234	0/13/13/13

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	2901	6O1	C08-C05	-5.99	1.39	1.51
29	X	2901	6O1	C62-C61	-5.36	1.40	1.51
29	X	2901	6O1	C04-C09	-4.19	1.40	1.50
29	X	2901	6O1	C56-C55	-3.69	1.41	1.50
29	X	2901	6O1	C51-C50	-2.79	1.48	1.53

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2901	6O1	O50-C50-C51	-10.81	97.90	106.55
29	X	2901	6O1	O51-C51-C50	-6.18	98.11	106.36
29	X	2901	6O1	C44-O44-C36	-5.04	105.27	114.37
29	X	2901	6O1	C36-C37-C38	-4.76	102.16	110.37
29	X	2901	6O1	C29-O33-C33	-3.59	107.33	113.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	2901	6O1	2	0

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	2658/2880 (92%)	-0.12	96 (3%) 43 31	30, 77, 204, 337	0
2	Y	120/123 (97%)	-0.07	3 (2%) 58 43	80, 150, 187, 207	0
3	A	259/275 (94%)	-0.19	4 (1%) 74 60	50, 105, 160, 212	0
4	B	205/211 (97%)	-0.49	0 100 100	30, 51, 113, 199	0
5	C	194/205 (94%)	-0.38	1 (0%) 90 83	35, 103, 180, 254	0
6	D	177/180 (98%)	-0.14	4 (2%) 61 46	128, 183, 249, 280	0
7	E	171/185 (92%)	-0.08	13 (7%) 15 11	70, 142, 203, 254	0
8	G	142/174 (81%)	-0.12	6 (4%) 37 26	38, 78, 188, 245	0
9	H	134/134 (100%)	-0.43	0 100 100	40, 55, 108, 175	0
10	I	134/156 (85%)	-0.10	2 (1%) 74 60	50, 120, 191, 236	0
11	J	136/141 (96%)	-0.04	3 (2%) 62 47	65, 106, 170, 225	0
12	K	113/116 (97%)	-0.53	0 100 100	30, 37, 91, 200	0
13	L	104/114 (91%)	0.01	5 (4%) 31 22	120, 154, 189, 241	0
14	M	108/166 (65%)	-0.66	0 100 100	37, 50, 117, 169	0
15	N	117/118 (99%)	-0.47	1 (0%) 84 72	42, 82, 136, 279	0
16	O	94/100 (94%)	-0.37	1 (1%) 80 67	48, 101, 170, 216	0
17	P	127/134 (94%)	-0.53	0 100 100	34, 53, 105, 192	0
18	Q	93/95 (97%)	-0.28	8 (8%) 11 9	49, 88, 174, 215	0
19	R	110/115 (95%)	-0.28	4 (3%) 43 31	62, 117, 213, 259	0
20	S	179/237 (75%)	-0.10	8 (4%) 34 24	97, 158, 213, 289	0
21	T	74/91 (81%)	-0.09	4 (5%) 26 19	67, 104, 157, 206	0
22	U	72/81 (88%)	0.10	5 (6%) 18 12	70, 125, 187, 215	0
23	V	65/67 (97%)	-0.23	3 (4%) 33 23	83, 125, 197, 216	0
24	W	55/55 (100%)	-0.61	0 100 100	68, 90, 135, 182	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	57/60 (95%)	-0.28	1 (1%) 69 54	32, 43, 104, 182	0
26	1	53/54 (98%)	0.36	6 (11%) 6 5	101, 129, 224, 259	0
27	2	46/47 (97%)	-0.29	1 (2%) 62 47	44, 59, 103, 162	0
28	3	59/66 (89%)	0.04	0 100 100	72, 100, 161, 239	0
All	All	5856/6380 (91%)	-0.19	179 (3%) 49 36	30, 91, 201, 337	0

The worst 5 of 179 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	1523	A	15.4
6	D	43	SER	8.2
22	U	29	GLY	6.4
1	X	1522	C	6.3
1	X	1073	G	6.0

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
30	MG	X	2977	1/1	0.96	1.03	85.12	78,78,78,78	0
30	MG	X	2935	1/1	0.88	2.21	66.25	41,41,41,41	0
30	MG	X	2952	1/1	0.97	1.28	43.51	54,54,54,54	0
30	MG	X	2992	1/1	0.90	1.05	42.15	34,34,34,34	0
30	MG	X	2970	1/1	0.94	1.03	33.37	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	MG	X	2947	1/1	0.94	1.18	32.51	52,52,52,52	0
30	MG	X	2921	1/1	0.96	0.98	30.70	37,37,37,37	0
30	MG	X	2975	1/1	0.89	1.38	30.37	49,49,49,49	0
30	MG	X	3020	1/1	0.54	1.57	29.07	64,64,64,64	0
30	MG	X	2910	1/1	0.94	0.62	27.03	34,34,34,34	0
30	MG	X	3008	1/1	0.94	0.62	23.65	39,39,39,39	0
30	MG	X	2911	1/1	0.97	0.66	19.97	46,46,46,46	0
30	MG	X	2906	1/1	0.91	0.87	19.73	42,42,42,42	0
30	MG	X	2916	1/1	0.82	1.05	18.56	51,51,51,51	0
30	MG	X	2912	1/1	0.95	0.46	16.76	34,34,34,34	0
30	MG	X	2939	1/1	0.96	0.61	15.65	30,30,30,30	0
30	MG	X	2907	1/1	0.90	1.25	14.61	49,49,49,49	0
30	MG	K	201	1/1	0.83	0.69	14.53	31,31,31,31	0
30	MG	X	2963	1/1	0.98	0.67	14.51	71,71,71,71	0
30	MG	X	2925	1/1	0.92	0.53	11.43	43,43,43,43	0
30	MG	X	2918	1/1	0.98	0.47	10.87	45,45,45,45	0
30	MG	X	2969	1/1	0.99	0.64	10.71	43,43,43,43	0
30	MG	X	2964	1/1	0.92	0.53	10.70	60,60,60,60	0
30	MG	X	2946	1/1	0.98	0.43	10.65	34,34,34,34	0
30	MG	X	2993	1/1	0.98	0.42	10.22	44,44,44,44	0
30	MG	X	2959	1/1	0.96	0.69	9.95	54,54,54,54	0
30	MG	X	2990	1/1	0.96	0.63	9.85	39,39,39,39	0
30	MG	X	2924	1/1	0.99	0.39	9.74	30,30,30,30	0
30	MG	X	2931	1/1	0.96	0.58	9.73	32,32,32,32	0
30	MG	X	2941	1/1	0.97	0.43	9.41	55,55,55,55	0
30	MG	X	2915	1/1	0.98	0.36	9.06	36,36,36,36	0
30	MG	X	2978	1/1	0.92	0.42	9.04	49,49,49,49	0
30	MG	X	2903	1/1	0.95	0.61	8.38	37,37,37,37	0
30	MG	X	2936	1/1	0.98	0.48	7.90	53,53,53,53	0
30	MG	X	2954	1/1	0.99	0.56	7.77	41,41,41,41	0
30	MG	X	2980	1/1	0.97	0.44	5.83	49,49,49,49	0
30	MG	X	3017	1/1	0.88	0.76	5.60	52,52,52,52	0
30	MG	X	2981	1/1	0.92	0.61	5.30	99,99,99,99	0
30	MG	X	2983	1/1	0.98	0.30	4.80	63,63,63,63	0
30	MG	X	2926	1/1	0.97	0.32	4.77	32,32,32,32	0
30	MG	X	2957	1/1	0.96	0.33	4.75	42,42,42,42	0
30	MG	X	3014	1/1	0.97	0.29	3.61	43,43,43,43	0
29	6O1	X	2901	111/111	0.91	0.39	3.50	106,116,136,139	0
30	MG	X	3011	1/1	0.94	0.34	3.27	58,58,58,58	0
30	MG	X	2953	1/1	0.97	0.29	2.01	38,38,38,38	0
30	MG	X	2943	1/1	0.95	0.29	1.75	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	MG	X	2942	1/1	0.91	0.25	1.23	31,31,31,31	0
30	MG	X	3018	1/1	0.96	0.28	0.90	32,32,32,32	0
30	MG	X	2917	1/1	0.94	0.21	0.73	33,33,33,33	0
30	MG	X	2951	1/1	0.97	0.22	0.71	35,35,35,35	0
30	MG	X	2998	1/1	0.94	0.22	0.47	35,35,35,35	0
30	MG	X	2996	1/1	0.98	0.19	0.03	43,43,43,43	0
30	MG	K	202	1/1	0.95	0.19	-0.39	31,31,31,31	0
30	MG	X	2932	1/1	0.95	0.32	-	53,53,53,53	0
30	MG	X	2902	1/1	0.94	1.16	-	32,32,32,32	0
30	MG	X	2967	1/1	0.90	0.37	-	55,55,55,55	0
30	MG	X	3013	1/1	0.98	0.49	-	47,47,47,47	0
30	MG	X	2973	1/1	0.94	0.35	-	52,52,52,52	0
30	MG	X	3005	1/1	0.96	0.92	-	66,66,66,66	0
30	MG	X	3002	1/1	0.95	0.31	-	44,44,44,44	0
30	MG	X	2965	1/1	0.97	0.48	-	40,40,40,40	0
30	MG	X	2997	1/1	0.99	0.36	-	38,38,38,38	0
30	MG	X	2999	1/1	0.80	0.77	-	74,74,74,74	0
30	MG	X	2955	1/1	0.96	0.39	-	31,31,31,31	0
30	MG	Y	201	1/1	0.96	0.90	-	77,77,77,77	0
30	MG	X	2909	1/1	0.94	0.72	-	36,36,36,36	0
30	MG	X	3001	1/1	0.79	1.63	-	86,86,86,86	0
30	MG	X	2950	1/1	0.97	0.51	-	36,36,36,36	0
30	MG	X	2961	1/1	0.96	0.68	-	68,68,68,68	0
30	MG	X	3006	1/1	0.74	0.50	-	34,34,34,34	0
30	MG	X	2940	1/1	0.92	0.41	-	34,34,34,34	0
30	MG	X	2982	1/1	0.89	0.86	-	31,31,31,31	0
30	MG	X	2937	1/1	0.93	0.73	-	32,32,32,32	0
30	MG	X	2986	1/1	0.96	0.48	-	46,46,46,46	0
30	MG	X	2987	1/1	0.93	0.46	-	43,43,43,43	0
30	MG	X	2908	1/1	0.95	0.67	-	34,34,34,34	0
30	MG	X	2974	1/1	0.87	0.85	-	30,30,30,30	0
30	MG	X	2920	1/1	0.95	0.74	-	34,34,34,34	0
30	MG	X	3016	1/1	0.71	1.26	-	74,74,74,74	0
30	MG	X	2938	1/1	0.94	0.33	-	36,36,36,36	0
30	MG	X	2968	1/1	0.94	0.26	-	35,35,35,35	0
30	MG	X	3009	1/1	0.99	0.33	-	41,41,41,41	0
30	MG	X	2923	1/1	0.98	0.38	-	30,30,30,30	0
30	MG	X	3019	1/1	0.83	1.06	-	46,46,46,46	0
30	MG	X	2928	1/1	0.91	0.17	-	41,41,41,41	0
30	MG	X	2995	1/1	0.93	0.82	-	83,83,83,83	0
30	MG	X	2966	1/1	0.98	0.34	-	37,37,37,37	0
30	MG	X	2930	1/1	0.97	0.64	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	MG	X	2913	1/1	0.91	0.63	-	36,36,36,36	0
30	MG	X	2976	1/1	0.94	0.49	-	53,53,53,53	0
30	MG	X	3015	1/1	0.89	0.55	-	98,98,98,98	0
30	MG	X	2945	1/1	0.93	1.19	-	55,55,55,55	0
30	MG	X	3012	1/1	0.74	0.39	-	52,52,52,52	0
30	MG	X	2985	1/1	0.98	0.27	-	55,55,55,55	0
30	MG	X	2905	1/1	0.97	0.82	-	30,30,30,30	0
30	MG	X	2933	1/1	0.88	1.35	-	38,38,38,38	0
30	MG	X	3004	1/1	0.96	0.30	-	54,54,54,54	0
30	MG	X	3007	1/1	0.88	0.50	-	40,40,40,40	0
30	MG	X	2948	1/1	0.97	0.26	-	30,30,30,30	0
30	MG	X	2927	1/1	0.79	0.54	-	57,57,57,57	0
30	MG	X	2971	1/1	0.92	0.62	-	33,33,33,33	0
30	MG	X	3010	1/1	0.97	0.27	-	41,41,41,41	0
30	MG	X	2972	1/1	0.92	0.63	-	36,36,36,36	0
30	MG	X	3000	1/1	0.98	0.28	-	39,39,39,39	0
30	MG	X	2962	1/1	0.98	0.20	-	41,41,41,41	0
30	MG	X	2922	1/1	0.95	0.45	-	35,35,35,35	0
30	MG	X	3003	1/1	0.95	0.87	-	63,63,63,63	0
30	MG	X	2984	1/1	0.97	0.56	-	49,49,49,49	0
30	MG	X	2956	1/1	0.95	0.58	-	32,32,32,32	0
30	MG	X	2904	1/1	0.91	1.01	-	32,32,32,32	0
30	MG	X	2989	1/1	0.96	0.67	-	56,56,56,56	0
30	MG	X	2979	1/1	0.90	0.29	-	46,46,46,46	0
30	MG	X	2994	1/1	0.94	0.37	-	77,77,77,77	0
30	MG	X	2949	1/1	0.96	0.35	-	32,32,32,32	0
30	MG	X	2914	1/1	0.96	0.46	-	43,43,43,43	0
30	MG	X	2944	1/1	0.93	0.88	-	37,37,37,37	0
30	MG	X	2991	1/1	0.96	0.69	-	72,72,72,72	0
30	MG	M	201	1/1	0.92	1.59	-	35,35,35,35	0
30	MG	X	2934	1/1	0.98	0.81	-	39,39,39,39	0
30	MG	X	2958	1/1	0.96	0.86	-	38,38,38,38	0
30	MG	X	2988	1/1	0.94	0.64	-	55,55,55,55	0
30	MG	X	2929	1/1	0.98	0.73	-	39,39,39,39	0
30	MG	X	2960	1/1	0.80	0.88	-	34,34,34,34	0
30	MG	X	2919	1/1	0.98	0.31	-	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.