



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 03:57 PM GMT

PDB ID : 4IOC
Title : Crystal structure of compound 4f bound to large ribosomal subunit (50S) from *Deinococcus radiodurans*
Authors : Han, S.; Marr, E.S.
Deposited on : 2013-01-07
Resolution : 3.60 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

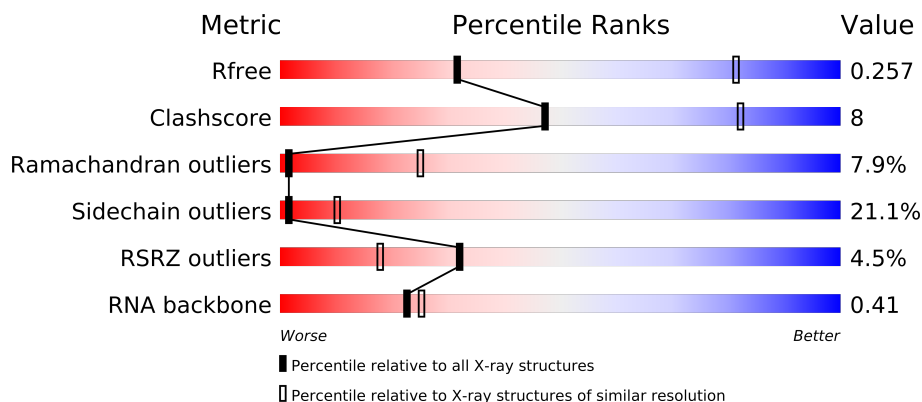
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1020 (3.86-3.34)
Clashscore	79885	1155 (3.80-3.40)
Ramachandran outliers	78287	1109 (3.80-3.40)
Sidechain outliers	78261	1108 (3.80-3.40)
RSRZ outliers	66119	1000 (3.84-3.36)
RNA backbone	1838	1012 (4.40-2.76)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	X	2880	
2	Y	123	
3	A	274	
4	B	211	
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	

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Mol	Chain	Length	Quality of chain
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	
30	4	37	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
31	MG	M	201	-	X
31	MG	X	2901	-	X
31	MG	X	2902	-	X
31	MG	X	2903	-	X
31	MG	X	2904	-	X
31	MG	X	2905	-	X
31	MG	X	2906	-	X
31	MG	X	2907	-	X
31	MG	X	2908	-	X
31	MG	X	2909	-	X
31	MG	X	2910	-	X
31	MG	X	2911	-	X
31	MG	X	2912	-	X
31	MG	X	2913	-	X
31	MG	X	2914	-	X
31	MG	X	2915	-	X
31	MG	X	2916	-	X
31	MG	X	2917	-	X
31	MG	X	2918	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
31	MG	X	2919	-	X
31	MG	X	2920	-	X
31	MG	X	2921	-	X
31	MG	X	2922	-	X
31	MG	X	2923	-	X
31	MG	X	2924	-	X
31	MG	X	2926	-	X
31	MG	X	2927	-	X
31	MG	X	2928	-	X
31	MG	Y	201	-	X
31	MG	Y	202	-	X
31	MG	Y	203	-	X
31	MG	Y	204	-	X
31	MG	Y	205	-	X
31	MG	Y	206	-	X

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 83877 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2686	Total	C	N	O	P	0	0	0
			57651	25718	10642	18606	2685			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

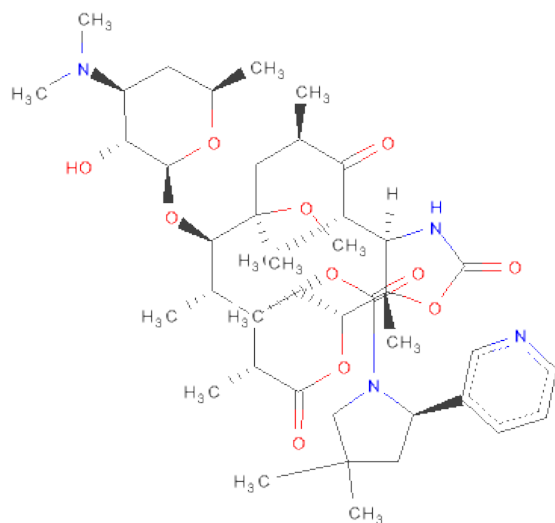
- Molecule 30 is a protein called 50S ribosomal protein L36.

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

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

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

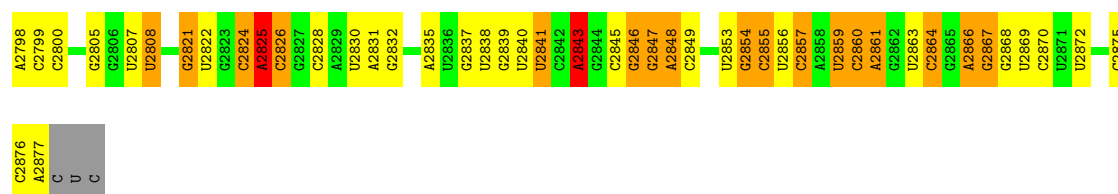
- Molecule 32 is (3AS,4R,7R,8S,9S,10R,11R,13R,15S,15AR)-4-ETHYL-11-METHOXY-3A,7,9,11,13,15-HEXAMETHYL-2,6,14-TRIOXO-10-{[3,4,6-TRIDEOXY-3-(DIMETHYLAMINO)-BETA-D-XYLO-HEXOPYRANOSYL]OXY}TETRADECAHYDRO-2H-OXACYCLO TETRADECINO[4,3-D][1,3]OXAZOL-8-YL(2R)-4,4-DIMETHYL-2-(PYRIDIN-3-YL)PYRROLIDINE-1-CARBOXYLATE (three-letter code: 1F4) (formula: C₄₃H₆₈N₄O₁₁).



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

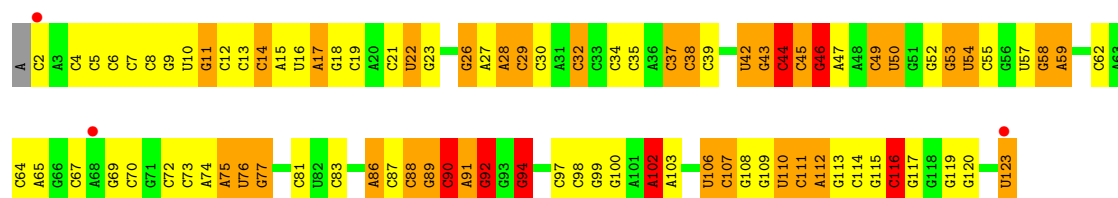
U1710	C1711	G1712	G1713	A1714	A1715	G1716	A1717	A1561	G1488	C1412	C1343	A1275	G1200	A1196	C1064	A994	U919	G854	G789	C723
G1642	G1643	A1643	U1647	C1648	U1651	G1652	C1653	A1563	C1489	U1413	C1344	A1277	G1201	C1127	G1067	A995	A922	G858	A790	C724
A1643	U1647	C1648	U1651	G1652	C1653	A1563	A1567	U1563	G1494	C1415	G1346	A1278	A1202	A1129	G1068	A996	A923	U859	G793	C725
U1647	C1648	U1651	G1652	C1653	A1563	A1567	U1563	U1563	G1495	U1421	C1347	A1279	A1203	U1130	G1069	C997	C924	U860	A794	C726
C1648	U1651	G1652	C1653	A1563	A1567	U1563	U1563	U1563	G1496	C1422	A1348	U1280	A1208	G1131	G1070	C998	U925	C963	A795	C727
U1651	G1652	C1653	A1563	A1567	U1563	U1563	U1563	U1563	G1497	U1426	A1349	U1281	A1209	C1132	U1071	A999	C926	C964	A796	C728
C1653	A1563	A1567	U1563	U1563	U1563	U1563	U1563	U1563	G1498	U1427	A1353	U1282	C1210	G1133	U1072	G1000	C927	A965	A797	C729
A1654	C1655	G1656	U1657	U1658	U1659	U1660	U1661	U1662	G1499	G1428	A1354	U1284	C1211	C1134	G1073	A1001	C931	U866	G798	C730
C1655	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	G1500	C1432	A1355	U1285	G1212	C1135	G1074	C1002	C932	U867	G799	C731
U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	G1501	U1431	A1356	U1286	C1213	C1136	G1075	C1003	C933	U868	U800	C732
U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1505	U1436	A1357	U1287	C1214	A1137	U1076	C1006	C934	U869	A801	C733
U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	C1506	U1437	C1358	U1288	G1220	A1138	U1077	C1007	C935	A802	G738	
U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1507	U1438	G1359	U1289	C1221	A1139	U1078	A1007	C936	A803	G739	
U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1508	U1439	A1360	U1290	G1222	A1140	U1079	G1008	C937	A804	A740	
C1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	A1509	U1441	A1361	U1291	G1223	A1141	U1080	C1009	C938	A805	G741	
U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	A1510	U1442	A1362	U1292	G1224	A1142	U1081	C1010	C939	A806	G742	
G1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1511	U1443	A1363	U1293	G1225	A1143	U1082	C1011	C940	A807	G743	
U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1512	U1444	A1364	U1294	G1226	A1144	U1083	C1012	C941	A808	G744	
U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1513	U1445	A1365	U1295	G1227	A1145	U1084	C1013	C942	A809	G745	
U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1514	U1446	A1366	U1296	G1228	A1146	U1085	C1014	C943	A810	G746	
U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1515	U1447	A1367	U1297	G1229	A1147	U1086	C1015	C944	A811		
U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1516	U1448	A1368	U1298	G1230	A1148	U1087	C1016	C945	A812		
U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1517	U1449	A1369	U1299	G1231	A1149	U1088	C1017	C946	A813		
U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1518	U1450	A1370	U1300	G1232	A1150	U1089	C1018	C947	A814		
U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1519	U1451	A1371	U1301	G1233	A1151	U1090	C1019	C948	A815		
U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1520	U1452	A1372	U1302	G1234	A1152	U1091	C1020	C949	A816		
U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1521	U1453	A1373	U1303	G1235	A1153	U1092	C1021	C950	A817		
U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1522	U1454	A1374	U1304	G1236	A1154	U1093	C1022	C951	A818		
U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1684	U1523	U1455	A1375	U1305	G1237	A1155	U1094	C1023	C952	A819		
U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1684	U1685	U1524	U1456	A1376	U1306	G1238	A1156	U1095	C1024	C953	A820		
U1678	U1679	U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1525	U1457	A1377	U1307	G1239	A1157	U1096	C1025	C954	A821		
U1679	U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1526	U1458	A1378	U1308	G1240	A1158	U1097	C1026	C955	A822		
U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1688	U1527	U1459	A1379	U1309	G1241	A1159	U1098	C1027	C956	A823		
U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1688	U1689	U1528	U1460	A1380	U1310	G1242	A1160	U1099	C1028	C957	A824		
U1682	U1683	U1684	U1685	U1686	U1687	U1688	U1689	U1690	U1529	U1461	A1381	U1311	G1243	A1161	U1100	C1029	C958	A825		
U1683	U1684	U1685	U1686	U1687	U1688	U1689	U1690	U1691	U1530	U1462	A1382	U1312	G1244	A1162	U1101	C1030	C959	A826		
U1684	U1685	U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1531	U1463	A1383	U1313	G1245	A1163	U1102	C1031	C960	A827		
U1685	U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1532	U1464	A1384	U1314	G1246	A1164	U1103	C1032	C961	A828		
U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1533	U1465	A1385	U1315	G1247	A1165	U1104	C1033	C962	A829		
U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1534	U1466	A1386	U1316	G1248	A1166	U1105	C1034	C963	A830		
U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1535	U1467	A1387	U1317	G1249	A1167	U1106	C1035	C964	A831		
U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1536	U1468	A1388	U1318	G1250	A1168	U1107	C1036	C965	A832		
U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1537	U1469	A1389	U1319	G1251	A1169	U1108	C1037	C966	A833		
U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1538	U1470	A1390	U1320	G1252	A1170	U1109	C1038	C967	A834		
U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1539	U1471	A1391	U1321	G1253	A1171	U1110	C1039	C968	A835		
U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1540	U1472	A1392	U1322	G1254	A1172	U1111	C1040	C969	A836		
U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1702	U1541	U1473	A1393	U1323	G1255	A1173	U1112	C1041	C970	A837		
U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1702	U1703	U1542	U1474	A1394	U1324	G1256	A1174	U1113	C1042	C971	A838		
U1696	U1697	U1698	U1699	U1700	U1701	U1702	U1703	U1704	U1543	U1475	A1395	U1325	G1257	A1175	U1114	C1043	C972	A839		
U1697	U1698	U1699	U1700	U1701	U1702	U1703	U1704	U1705	U1544	U1476	A1396	U1326	G1258	A1176	U1115	C1044	C973	A840		
U1698	U1699	U1700	U1701	U1702	U1703	U1704	U1705	U1706	U1545	U1477	A1397	U1327	G1259	A1177	U1116	C1045	C974	A841		
U1699	U1700	U1701	U1702	U1703	U1704	U1705	U1706	U1707	U1546	U1478	A1398	U1328	G1260	A1178	U1117	C1046	C975	A842		
U1700	U1701	U1702	U1703	U1704	U1705	U1706	U1707	U1708	U1547	U1479	A1399	U1329	G1261	A1179	U1118	C1047	C976	A843		
U1701	U1702	U1703	U1704	U1705	U1706	U1707	U1708	U1709	U1548	U1480	A1400	U1330	G1262	A1180	U1119	C1048	C977	A844		
U1702	U1703	U1704	U1705	U1706	U1707	U1708	U1709	U1710	U1549	U1481	A1401	U1331	G1263	A1181	U1120	C1049	C978	A845		
U1703	U1704	U1705	U1706	U1707	U1708	U1709	U1710	U1711	U1550	U1482	A1402	U1332	G1264	A1182	U1121	C1050	C979	A846		
U1704	U1705	U1706	U1707	U1708	U1709	U1710	U1711	U1712	U1551	U1483	A1403	U1333	G1265	A1183	U1122	C1051	C980	A847		
U1705	U1706	U1707	U1708	U1709	U1710	U1711	U1712	U1713	U1552	U1484	A1404	U1334	G1266	A1184	U1123	C1052	C981	A848		
U1706	U1707	U1708	U1709	U1710	U1711	U1712	U1713	U1714	U1553	U1485	A1405	U1335	G1267	A1185	U1124	C1053	C982	A849		
U1707	U1708	U1709	U1710	U1711	U1712	U1713	U1714	U1715	U1554	U1486	A1406	U1336	G1268	A1186	U1125	C1054	C983	A850		
U1708	U1709	U1710	U1711	U1712	U1713	U1714	U1715	U1716	U1555	U1487	A1407	U1337	G1269	A1187	U1126	C1055	C984	A851		
U1709	U1710	U1711	U1712	U1713	U1714	U1715	U1716	U1717	U1556	U1488	A1408	U1338	G1270	A1188	U1127	C1056	C985	A852		
U1710	U1711	U1712	U1713	U1714	U1715	U1716	U1717	U1718	U1557	U1489	A1409	U1339	G1271	A1189	U1128	C1057	C986			

A2720	A2654	G2587	G2593	C2459	G2388	G2320	A2252	C2184	A	G2053	C1991	U1922	U1856	C1786
G2695	G2655	U2588	G2524	G2460	G2389	C2321	A2253	U2185	C	A2054	G1992	U1923	G1857	U1787
G2657	G2656	C2589	U2525	C2461	G2392	U2322	C2254		G	G2055	G1993	C1924	C1858	C1788
U2726	U2590	U2526	G2526	C2462	G2392	U2323	G2255	A2188	U	G2056	U1994	C1925	C1859	U1789
G2658	G2591	G2527	G2463	G2463	G2393	G2324	G2256	A2189	C	A2060	G1995	U1926	G1861	G1790
G2660	U2592	G2464	G2464	G2464	G2394	A2325	A2257	A2190	G	G2061	A1996	U1927	G1862	C1791
G2661	G2593	G2465	G2465	G2465	G2395	C2326	G2258	A2191	C	U2062	A1997	G1928	G1863	G1792
A2729	U2594	G2466	G2466	G2466	C2396	C2329	G2261	U2192	U	U2063	A1998	U1929	U1863	A1793
G2662	C2595	A2467	G2467	G2467	G2397	G2330	C2262	C2193	U	U2064	U1999	C1930	G1865	A1794
G2663	G2596	G2468	G2468	G2468	A2401	A2333	C2263	G2194	U	U2065	G2001	G1932	G1866	A1796
G2664	G2597	U2470	G2469	U2470	A2402	A2334	C2264	C2195	G	G2066	G2002	G1933	A1867	
G2665	U2598	U2471	G2471	U2471	G2403	U2335	A2265	U2197	G	G2067	A2003	U1934		A1798
G2667	G2599	U2472	U2472	U2472	A2404	U2336	A2266	U2198	G	G2068	G2004	A1935		A1800
U2736	G2602	C2475	C2475	C2475	A2405	G2337	A2267	C2199	G	U2069	U2005	A1936	U1870	A1801
G2668	G2603	C2476	C2476	C2476	C2406	A2337	G2268	C2200	U	G2070	G2006	G1937	G1874	
G2670	G2604	A2477	A2477	A2477	G2407	C2338	G2269	G2201	C	G2071		U1938	C1875	U1804
C2740	C2605	C2478	C2478	C2478	G2408	A2339	U2270		G	G2072	U2009	U1939	C1876	G1805
	G2606	U2479	U2479	U2479	A2409	C2340	C2271		C		G2010	C1940	C1877	G1806
A2745	C2607	U2480	U2480	U2480	U2410			A2204	G	U2075	U2011			A1807
	A2608	A2543	A2543	A2543	G2411	C2343	C2274	C2205	U	G2076	A2012	A1943	U1881	A1808
C2748	G2609	A2544	A2544	A2544	A2414	G2344	U2275	C2206	G	G2077	A2013		G1882	G1809
G2679	G2610	A2545	A2545	A2545	G2415	G2345	G2276	U2208	A	G2078	A2014	U1946	G1883	U1810
U2680	A2611	G2546	G2546	G2546	U2416	C2347	A2277	G2209	G	A2079	G2015	G1947	A1884	A1811
	G2612	C2547	G2547	G2547	U2417	G2348	A2278	G2210	G	U2080	A2016	C1948	C1885	U1812
C2683	A2613	G2548	G2548	G2548	A2418	U2349		U2211	C	U2081	U2017	A1949	G1886	A1813
A2694	A2614	G2549	G2549	G2549	C2419	G2350	C2281	U2212	A	G2082	G2018	C1950	G1887	
	U2615	C2550	C2550	C2550	C2420	G2351	G2282	G2213	C	U2083	C2019	G1951	G1888	G1816
G2687	G2616	A2551	A2551	A2551	G2421	A2352	G2283	G2214	G			A1952	G	U1817
G2688	U2617	G2552	G2552	G2552	G2422	G2353	U2284	C2215	G	U2088	C2022	A1953	C	U1818
C2689	A2618	G2553	G2553	G2553	G2423	A2357	U2285	G2216	U	C2089	G2023	A1954	C	U1819
A2690	G2619	C2554	C2554	C2554		C2358	G2286	G2217	G	U2090	U2024	G1955	C	G1820
G2691	G2620	U2555	U2555	U2555	G2426	C2359	G2287	G2218	G	C	A2025		C	A1821
G2692	A2621	G2556	G2556	G2556	A2427	U2359	A2288	U2219	A	U	C2026	G1958	U	
U2693	G2622	G2557	G2557	G2557	U2428		A2290	G2221	A	G	C2027		A	C1824
G2694		C2558	C2558	C2558	C2429	G2362	A2291	U2222	U	C	C2028	G1963	C	C1825
C2767	U2625	U2559	U2559	U2559	C2431	G2363		U2223	A	U	G2029	A1964	U	
G2768	U2626	G2560	G2560	G2560	A2432	C2364	U2294	U2224	C	A	U2030	U1965	A	G1828
U2774	G2627	G2561		U2498		U2365	U2296	U2225	C	G	A2031	C1966	U	C1829
U2775	C2628		C2435	C2499	C2435	G2366	G2295	A2226	C	A	C2032	U1967	U	G1830
A2776		U2564	U2564	C2500		A2367	U2296	A2227	A	G	A2033	G1972	A	G1831
G2769	C2631	C2565	A2566	G2503	A2438	G2368	G2297	C2227	C	U	G2035	C1973	C	G1832
U2770	U2632	A2567	A2567	G2504	U2439	G2369	U2298	U2228	C	A	G2036	G1974	C	U1833
C2779	A2633	G2567	G2567	G2505	G2440	G2370	A2299	G2229	C	A		G1975	G	G1834
G2780	G2634	U2568	U2568	G2506	U2441	A2371	G2300	G2230	U	G	A2037	U1976	U	C1835
U2704	U2635			C2507	C2442	C2372	A2301		G	G	C2038	C1977	C	C1836
G2782	A2636	U2572	U2572	U2508	C2443	C2373	G2302	A2165		U	G2039	U1978	C	A1839
U2706	U2637	G2573	G2573	A2509	C2444	G2374	G2303	G2166		G	A2041	C1979	U1909	A1840
U2708	G2640	U2574	U2574	G2510	G2447	G2375	G2304	C2169		U	A2042	A1980	A1910	G1841
C2709	A2641			G2511	U2448	G2376	C2305	U2170		A	G2043	A1981	A1911	G1842
G2710	G2642			G2514	G2449	U2377	A2306	U2171		G	G2044	C1982	G1912	U1843
	U2643	A2577	G2578	G2515	U2452	U2380	U2311	U2172		C	A2045	A1983	G1913	C1844
A2713	C2645	G2579	A2580	U2516	C2453	A2381	G2312	G2173		C	C2046	A1984	U1914	A1845
C2792		C2581	C2581	U2517	G2454	C2382	G2313	G2174		U	C2047	G1985		A1846
G2793	A2649	G2582	G2582	G2518	A2455	G2384	A2314			C	C2048	G1986	C1917	
G2794	G2650			C2519	U2456	G2385	A2315	U2178		C	C2049	G1987	G1918	G1850
A2795	U2651			G2519	A2457	U2386	U2318	A2247		A	U2051	A1988	A1919	A1851
G2796	G2652			G2522	U2458	U2387	G2319	A2248			G2052	C1989	A1920	G1852
G2797	A2653											U1990	A1921	



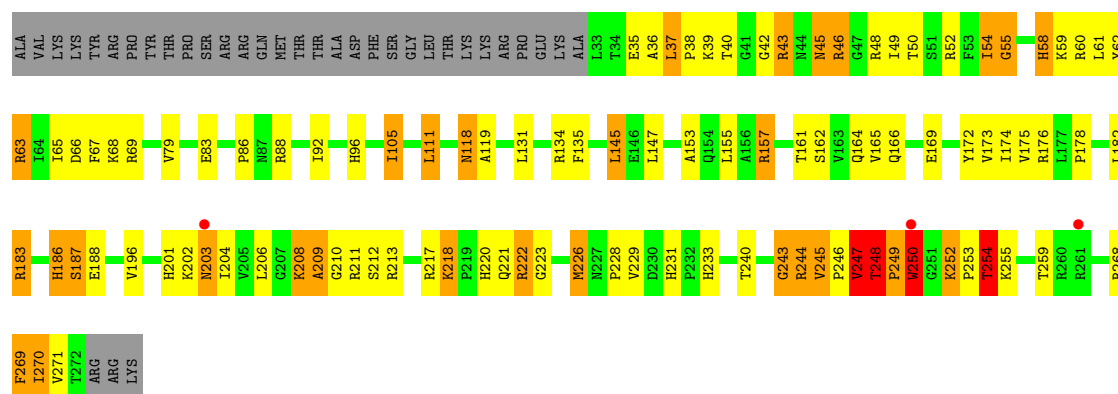
- Molecule 2: 5S ribosomal RNA

Chain Y:



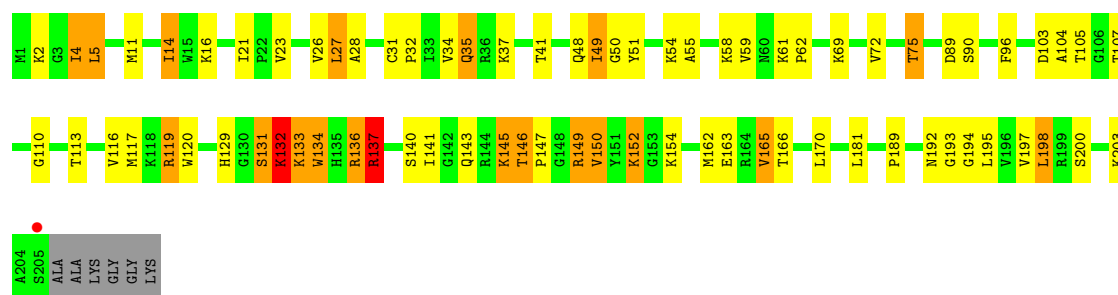
- Molecule 3: 50S ribosomal protein L2

Chain A:



- Molecule 4: 50S ribosomal protein L3

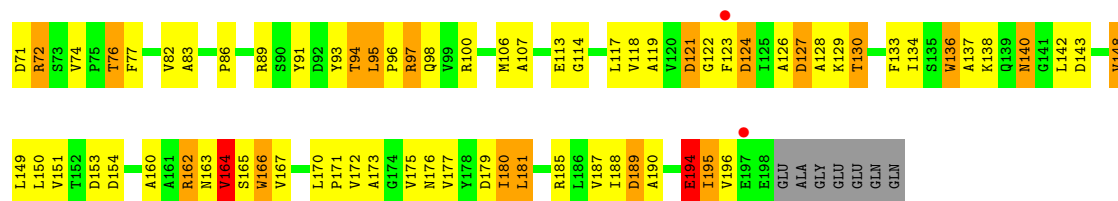
Chain B:



- Molecule 5: 50S ribosomal protein L4

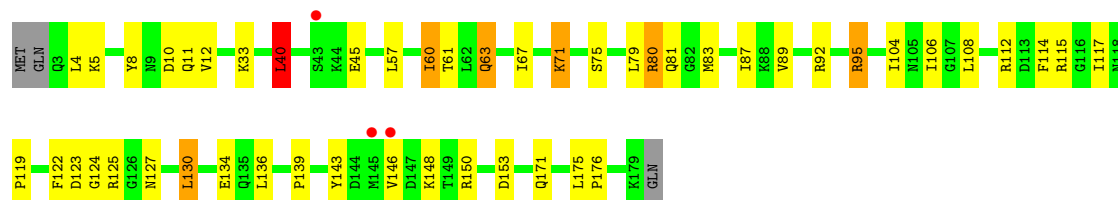
Chain C:





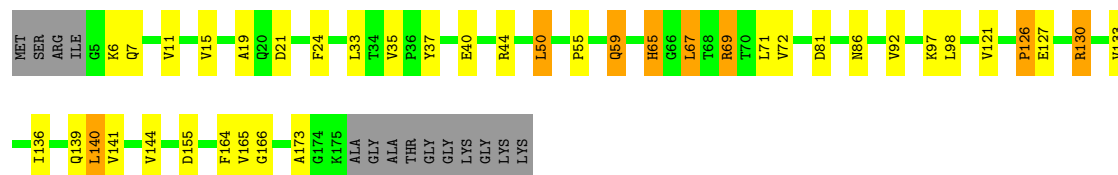
• Molecule 6: 50S ribosomal protein L5

Chain D:



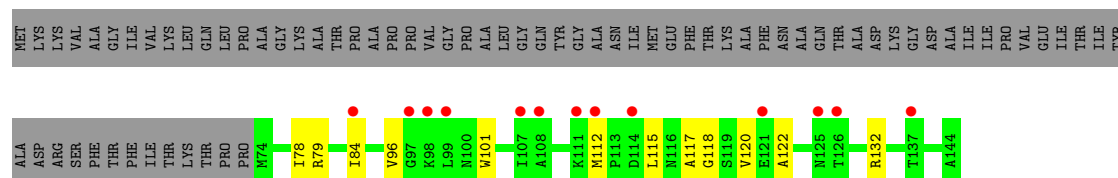
• Molecule 7: 50S ribosomal protein L6

Chain E:



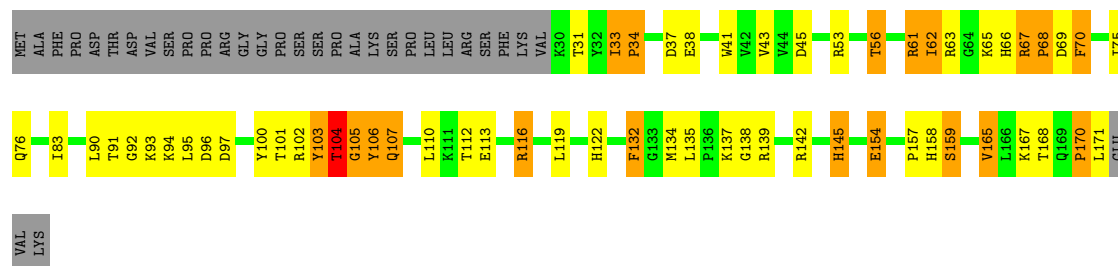
• Molecule 8: 50S ribosomal protein L11

Chain F:



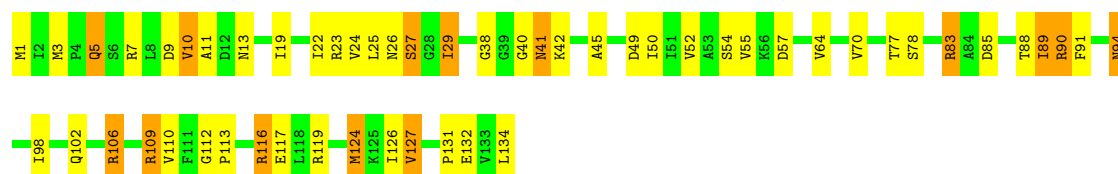
• Molecule 9: 50S ribosomal protein L13

Chain G:



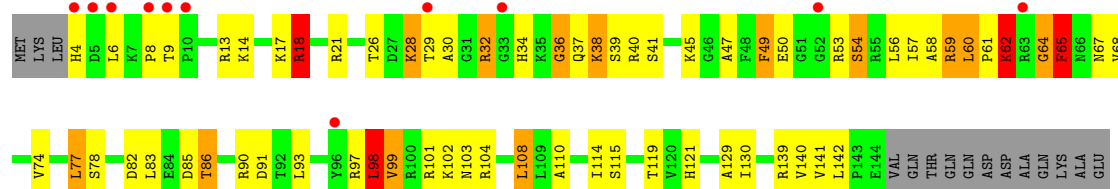
• Molecule 10: 50S ribosomal protein L14

Chain H:



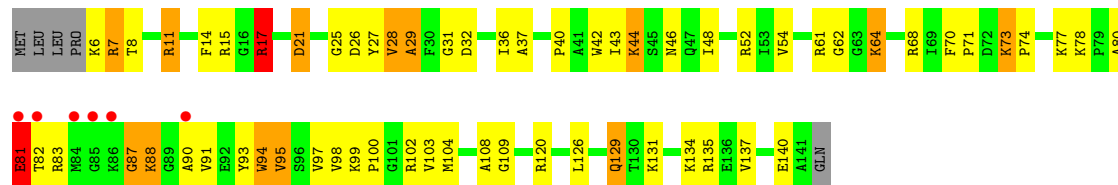
• Molecule 11: 50S ribosomal protein L15

Chain I:



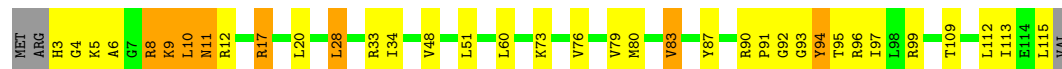
• Molecule 12: 50S ribosomal protein L16

Chain J:



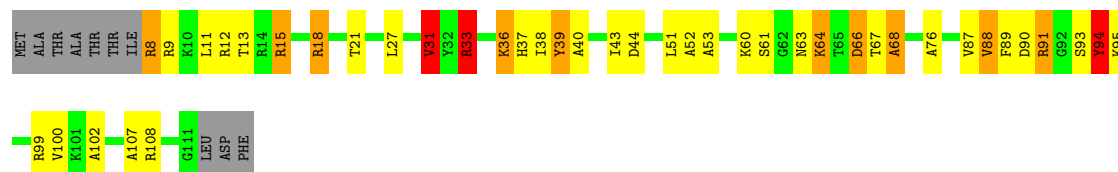
• Molecule 13: 50S ribosomal protein L17

Chain K:



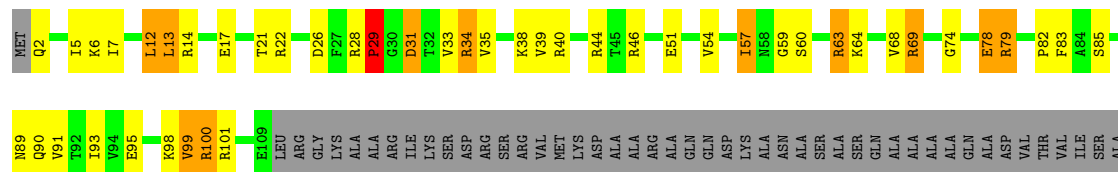
• Molecule 14: 50S ribosomal protein L18

Chain L:



• Molecule 15: 50S ribosomal protein L19

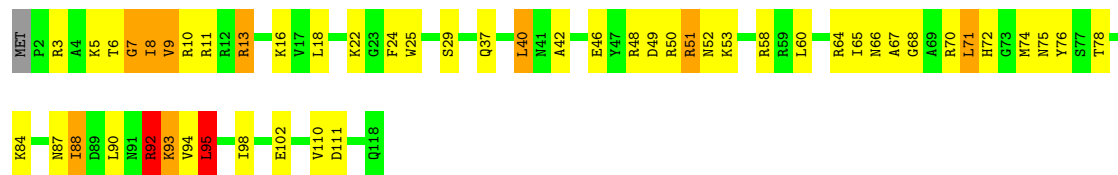
Chain M:



ALA
PRO
GLU
VAL
ALA
GLU
PRO
THR
GLN
GLY
GLU

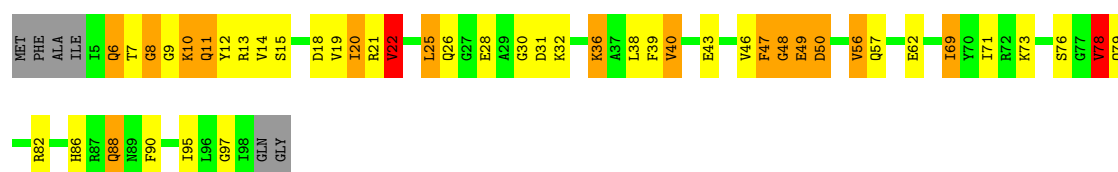
- Molecule 16: 50S ribosomal protein L20

Chain N:



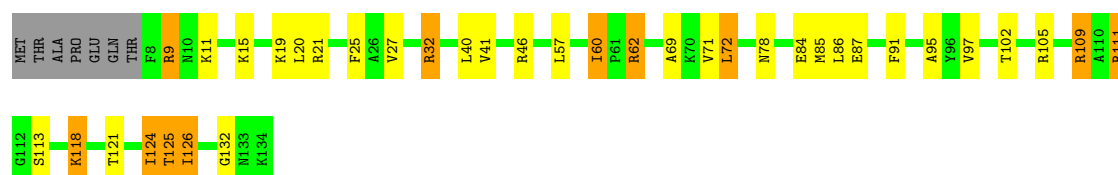
- Molecule 17: 50S ribosomal protein L21

Chain O:



- Molecule 18: 50S ribosomal protein L22

Chain P:



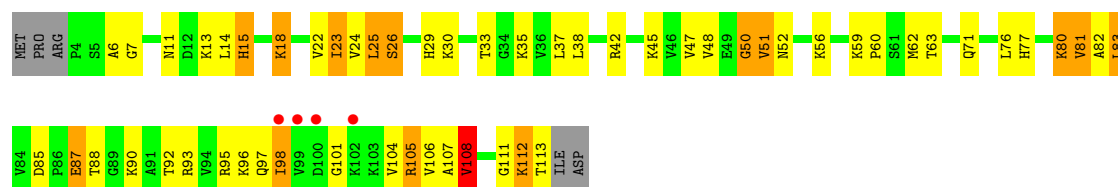
- Molecule 19: 50S ribosomal protein L23

Chain Q:



- Molecule 20: 50S ribosomal protein L24

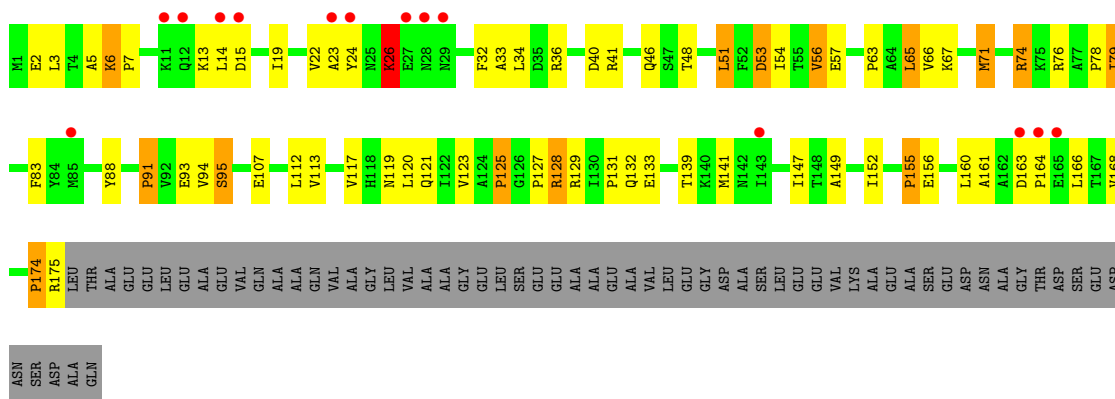
Chain R:



- Molecule 21: 50S ribosomal protein L25

Chain S:





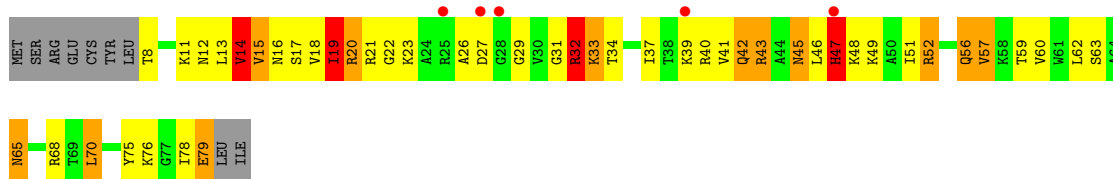
- Molecule 22: 50S ribosomal protein L27

Chain T:



- Molecule 23: 50S ribosomal protein L28

Chain U:



- Molecule 24: 50S ribosomal protein L29

Chain V:



- Molecule 25: 50S ribosomal protein L30

Chain W:



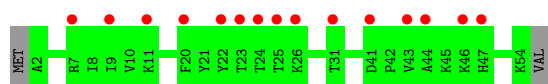
- Molecule 26: 50S ribosomal protein L32

Chain Z:



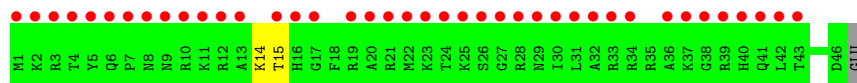
- Molecule 27: 50S ribosomal protein L33

Chain 1:



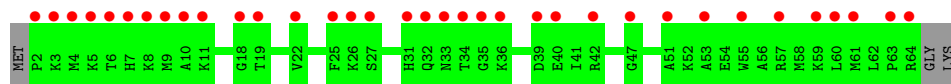
- Molecule 28: 50S ribosomal protein L34

Chain 2:



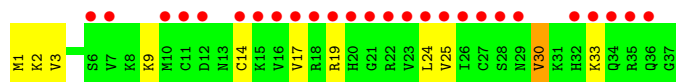
- Molecule 29: 50S ribosomal protein L35

Chain 3:



- Molecule 30: 50S ribosomal protein L36

Chain 4:



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.64Å 408.49Å 692.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.60 30.11 – 3.61	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.60) 88.5 (30.11-3.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 3.65Å)	Xtriage
Refinement program	autobuster	Depositor
R, R_{free}	0.198 , 0.239 0.215 , 0.257	Depositor DCC
R_{free} test set	12232 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	129.2	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 49.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 242941 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	83877	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is

detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	3

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

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

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

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

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	57651	0	29049	535	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Y	2598	0	1328	22	0
3	A	1826	0	1885	83	0
4	B	1539	0	1600	57	0
5	C	1506	0	1525	57	0
6	D	1400	0	1481	17	0
7	E	1286	0	1336	10	0
8	F	503	0	520	5	0
9	G	1114	0	1144	46	0
10	H	997	0	1046	30	0
11	I	1067	0	1103	39	0
12	J	1090	0	1125	31	0
13	K	878	0	930	24	0
14	L	779	0	820	19	0
15	M	871	0	894	25	0
16	N	978	0	1020	33	0
17	O	741	0	756	24	0
18	P	1014	0	1096	23	0
19	Q	726	0	753	11	0
20	R	825	0	881	26	0
21	S	1345	0	1372	30	0
22	T	625	0	655	11	0
23	U	552	0	604	31	0
24	V	533	0	558	7	0
25	W	424	0	470	15	0
26	Z	457	0	462	20	0
27	1	53	0	0	0	0
28	2	46	0	0	1	0
29	3	63	0	0	0	0
30	4	297	0	330	4	0
31	M	1	0	0	0	0
31	X	28	0	0	0	0
31	Y	6	0	0	0	0
32	X	58	0	67	19	0
All	All	83877	0	54810	1080	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

The worst 5 of 1080 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:117:MET:SD	4:B:117:MET:CE	2.02	1.47
9:G:100:TYR:HB2	9:G:116:ARG:NH1	1.69	1.08

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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	238/274 (87%)	173 (73%)	47 (20%)	18 (8%)	2	26
4	B	203/211 (96%)	173 (85%)	25 (12%)	5 (2%)	9	61
5	C	195/205 (95%)	127 (65%)	40 (20%)	28 (14%)	0	8
6	D	175/180 (97%)	142 (81%)	26 (15%)	7 (4%)	5	48
7	E	169/185 (91%)	134 (79%)	26 (15%)	9 (5%)	3	38
8	F	69/144 (48%)	57 (83%)	9 (13%)	3 (4%)	4	46
9	G	140/174 (80%)	99 (71%)	26 (19%)	15 (11%)	1	15
10	H	132/134 (98%)	117 (89%)	12 (9%)	3 (2%)	10	63
11	I	139/156 (89%)	81 (58%)	39 (28%)	19 (14%)	0	9
12	J	134/141 (95%)	98 (73%)	24 (18%)	12 (9%)	1	21
13	K	111/116 (96%)	92 (83%)	13 (12%)	6 (5%)	3	38
14	L	102/114 (90%)	75 (74%)	15 (15%)	12 (12%)	1	13
15	M	106/166 (64%)	90 (85%)	10 (9%)	6 (6%)	3	36
16	N	115/118 (98%)	91 (79%)	17 (15%)	7 (6%)	2	34
17	O	92/100 (92%)	66 (72%)	13 (14%)	13 (14%)	0	9
18	P	125/134 (93%)	104 (83%)	17 (14%)	4 (3%)	6	55
19	Q	91/95 (96%)	63 (69%)	16 (18%)	12 (13%)	0	10
20	R	108/115 (94%)	65 (60%)	26 (24%)	17 (16%)	0	6
21	S	173/237 (73%)	135 (78%)	27 (16%)	11 (6%)	2	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	T	82/91 (90%)	65 (79%)	12 (15%)	5 (6%)	2	34
23	U	70/81 (86%)	41 (59%)	15 (21%)	14 (20%)	0	3
24	V	64/67 (96%)	57 (89%)	5 (8%)	2 (3%)	7	57
25	W	53/55 (96%)	47 (89%)	5 (9%)	1 (2%)	12	67
26	Z	56/60 (93%)	45 (80%)	6 (11%)	5 (9%)	1	21
30	4	35/37 (95%)	23 (66%)	11 (31%)	1 (3%)	7	58
All	All	2977/3390 (88%)	2260 (76%)	482 (16%)	235 (8%)	1	25

5 of 235 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	185/215 (86%)	145 (78%)	40 (22%)	1	10
4	B	155/157 (99%)	119 (77%)	36 (23%)	1	8
5	C	157/163 (96%)	112 (71%)	45 (29%)	0	4
6	D	153/156 (98%)	130 (85%)	23 (15%)	4	27
7	E	136/144 (94%)	115 (85%)	21 (15%)	4	25
8	F	51/107 (48%)	49 (96%)	2 (4%)	43	85
9	G	118/146 (81%)	94 (80%)	24 (20%)	2	11
10	H	103/103 (100%)	80 (78%)	23 (22%)	1	9
11	I	108/121 (89%)	79 (73%)	29 (27%)	1	5
12	J	110/115 (96%)	89 (81%)	21 (19%)	2	14
13	K	90/93 (97%)	76 (84%)	14 (16%)	4	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	L	74/82 (90%)	51 (69%)	23 (31%)	0	4
15	M	94/134 (70%)	71 (76%)	23 (24%)	1	7
16	N	96/97 (99%)	76 (79%)	20 (21%)	2	11
17	O	75/79 (95%)	56 (75%)	19 (25%)	1	7
18	P	109/115 (95%)	91 (84%)	18 (16%)	3	22
19	Q	75/76 (99%)	60 (80%)	15 (20%)	2	12
20	R	91/96 (95%)	75 (82%)	16 (18%)	3	18
21	S	149/192 (78%)	117 (78%)	32 (22%)	1	10
22	T	62/67 (92%)	53 (86%)	9 (14%)	5	28
23	U	57/66 (86%)	33 (58%)	24 (42%)	0	1
24	V	54/55 (98%)	43 (80%)	11 (20%)	2	11
25	W	48/48 (100%)	37 (77%)	11 (23%)	1	8
26	Z	51/53 (96%)	41 (80%)	10 (20%)	2	13
30	4	35/35 (100%)	29 (83%)	6 (17%)	3	20
All	All	2436/2715 (90%)	1921 (79%)	515 (21%)	1	10

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

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

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

Mol	Chain	Res	Type
15	M	58	ASN
17	O	79	GLN
25	W	54	GLN
15	M	90	GLN
16	N	66	ASN

5.3.3 RNA ⓘ

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

5 of 742 RNA backbone outliers are listed below:

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

5 of 262 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1186	G
1	X	1475	U
1	X	2807	U
1	X	1250	A
1	X	1357	U

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 35 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	1F4	X	2929	-	62,62,62	1.22	4 (6%)	95,95,95	3.39	47 (49%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	1F4	X	2929	-	-	0/74/119/119	0/3/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2929	1F4	C41-N40	4.34	1.39	1.33
32	X	2929	1F4	C52-C51	3.20	1.44	1.39
32	X	2929	1F4	C22-C9	2.46	1.58	1.52
32	X	2929	1F4	O46-C44	2.06	1.24	1.21

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2929	1F4	C5-O17-C41	-13.94	99.90	108.91
32	X	2929	1F4	C51-C47-N45	-11.68	98.37	112.97
32	X	2929	1F4	C6-C5-C4	-6.73	102.72	110.30
32	X	2929	1F4	C4-N40-C41	-6.52	106.10	112.50
32	X	2929	1F4	C6-O10-C11	6.42	129.97	118.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.24	53 (1%) 62 36	43, 92, 197, 276	0
2	Y	122/123 (99%)	-0.22	3 (2%) 54 31	83, 135, 170, 191	0
3	A	240/274 (87%)	0.04	3 (1%) 74 47	68, 115, 146, 172	0
4	B	205/211 (97%)	-0.09	1 (0%) 88 71	45, 73, 105, 154	0
5	C	197/205 (96%)	0.08	5 (2%) 54 31	57, 114, 154, 187	0
6	D	177/180 (98%)	0.07	3 (1%) 67 40	146, 183, 216, 227	0
7	E	171/185 (92%)	-0.19	0 100 100	92, 143, 192, 206	0
8	F	71/144 (49%)	1.26	13 (18%) 2 2	211, 236, 252, 257	0
9	G	142/174 (81%)	-0.07	0 100 100	72, 97, 144, 161	0
10	H	134/134 (100%)	-0.13	0 100 100	50, 70, 97, 121	0
11	I	141/156 (90%)	0.42	11 (7%) 13 8	67, 129, 174, 204	0
12	J	136/141 (96%)	0.45	6 (4%) 33 18	74, 103, 149, 184	0
13	K	113/116 (97%)	-0.11	0 100 100	35, 60, 79, 91	0
14	L	104/114 (91%)	0.06	0 100 100	98, 134, 156, 168	0
15	M	108/166 (65%)	-0.23	0 100 100	50, 73, 111, 145	0
16	N	117/118 (99%)	-0.14	0 100 100	59, 90, 128, 159	0
17	O	94/100 (94%)	-0.09	0 100 100	66, 115, 157, 173	0
18	P	127/134 (94%)	-0.20	0 100 100	50, 68, 107, 158	0
19	Q	93/95 (97%)	0.02	2 (2%) 59 34	73, 106, 162, 195	0
20	R	110/115 (95%)	0.08	4 (3%) 41 23	88, 117, 170, 178	0
21	S	175/237 (73%)	0.48	14 (8%) 12 8	121, 155, 175, 190	0
22	T	84/91 (92%)	0.46	10 (11%) 5 5	79, 107, 186, 200	0
23	U	72/81 (88%)	0.26	5 (6%) 17 9	92, 128, 153, 161	0
24	V	66/67 (98%)	0.25	5 (7%) 14 8	100, 132, 211, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	55/55 (100%)	-0.14	1 (1%) 65 39	80, 98, 126, 152	0
26	Z	58/60 (96%)	0.03	2 (3%) 43 24	49, 70, 105, 114	0
27	1	53/55 (96%)	2.01	15 (28%) 1 1	8, 32, 62, 93	0
28	2	46/47 (97%)	4.61	40 (86%) 0 1	3, 15, 38, 59	0
29	3	63/66 (95%)	2.74	35 (55%) 0 1	3, 25, 40, 61	0
30	4	37/37 (100%)	3.53	26 (70%) 0 1	228, 254, 266, 269	0
All	All	5997/6561 (91%)	0.04	257 (4%) 32 19	3, 100, 196, 276	0

The worst 5 of 257 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	1	7	ARG	19.9
30	4	25	VAL	10.6
28	2	37	LYS	10.0
28	2	27	GLY	9.8
24	V	1	MET	9.8

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
31	MG	Y	203	1/1	1.04	134.09	59,59,59,59	0
31	MG	X	2912	1/1	0.65	109.67	71,71,71,71	0
31	MG	X	2921	1/1	0.68	76.20	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	X	2908	1/1	2.36	61.45	37,37,37,37	0
31	MG	X	2926	1/1	1.75	56.01	45,45,45,45	0
31	MG	X	2928	1/1	0.76	53.57	61,61,61,61	0
31	MG	X	2909	1/1	0.66	51.87	97,97,97,97	0
31	MG	X	2919	1/1	0.86	41.55	30,30,30,30	0
31	MG	X	2913	1/1	0.98	40.79	60,60,60,60	0
31	MG	X	2917	1/1	1.09	36.99	55,55,55,55	0
31	MG	M	201	1/1	1.34	32.55	23,23,23,23	0
31	MG	X	2920	1/1	0.65	30.81	113,113,113,113	0
31	MG	X	2924	1/1	1.21	27.74	70,70,70,70	0
31	MG	X	2918	1/1	1.28	26.91	42,42,42,42	0
31	MG	X	2916	1/1	1.15	25.06	37,37,37,37	0
31	MG	X	2905	1/1	0.50	24.26	65,65,65,65	0
31	MG	Y	204	1/1	1.00	22.71	86,86,86,86	0
31	MG	X	2903	1/1	0.62	22.17	89,89,89,89	0
31	MG	X	2907	1/1	0.83	21.72	51,51,51,51	0
31	MG	X	2927	1/1	0.59	21.40	64,64,64,64	0
31	MG	X	2915	1/1	0.72	17.75	57,57,57,57	0
31	MG	Y	202	1/1	1.50	17.40	88,88,88,88	0
31	MG	Y	206	1/1	0.32	15.69	78,78,78,78	0
31	MG	X	2901	1/1	0.61	14.84	50,50,50,50	0
31	MG	X	2910	1/1	0.68	14.76	41,41,41,41	0
31	MG	X	2906	1/1	0.98	14.02	58,58,58,58	0
31	MG	X	2922	1/1	0.81	10.50	44,44,44,44	0
31	MG	X	2911	1/1	0.29	6.53	68,68,68,68	0
31	MG	X	2923	1/1	0.36	5.84	34,34,34,34	0
31	MG	Y	205	1/1	0.42	5.30	82,82,82,82	0
31	MG	Y	201	1/1	0.40	3.88	98,98,98,98	0
31	MG	X	2904	1/1	0.29	3.65	110,110,110,110	0
31	MG	X	2914	1/1	0.59	3.59	27,27,27,27	0
31	MG	X	2902	1/1	0.37	2.93	94,94,94,94	0
32	1F4	X	2929	58/58	0.22	-0.18	20,20,20,20	0
31	MG	X	2925	1/1	0.13	-0.24	122,122,122,122	0

6.5 Other polymers ⓘ

There are no such residues in this entry.