



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:02 am GMT

PDB ID : 2D3O
Title : Structure of Ribosome Binding Domain of the Trigger Factor on the 50S ribosomal subunit from *D. radiodurans*
Authors : Schlutzen, F.; Wilson, D.N.; Hansen, H.A.; Tian, P.; Harms, J.M.; McInnes, S.J.; Albrecht, R.; Buerger, J.; Wilbanks, S.M.; Fucini, P.
Deposited on : 2005-09-30
Resolution : 3.35 Å(reported)

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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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

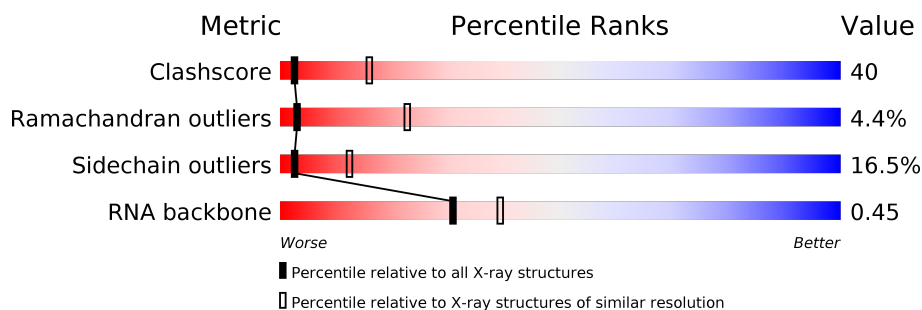
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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))
Clashscore	112137	1231 (3.42-3.30)
Ramachandran outliers	110173	1212 (3.42-3.30)
Sidechain outliers	110143	1211 (3.42-3.30)
RNA backbone	2435	1005 (3.90-2.82)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	2880	
2	R	95	
3	S	115	
4	W	67	
5	1	112	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 63004 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	0	2802	Total	C	N	O	P	0	0	0
			60132	26824	11089	19418	2801			

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 5 is a protein called Trigger Factor.

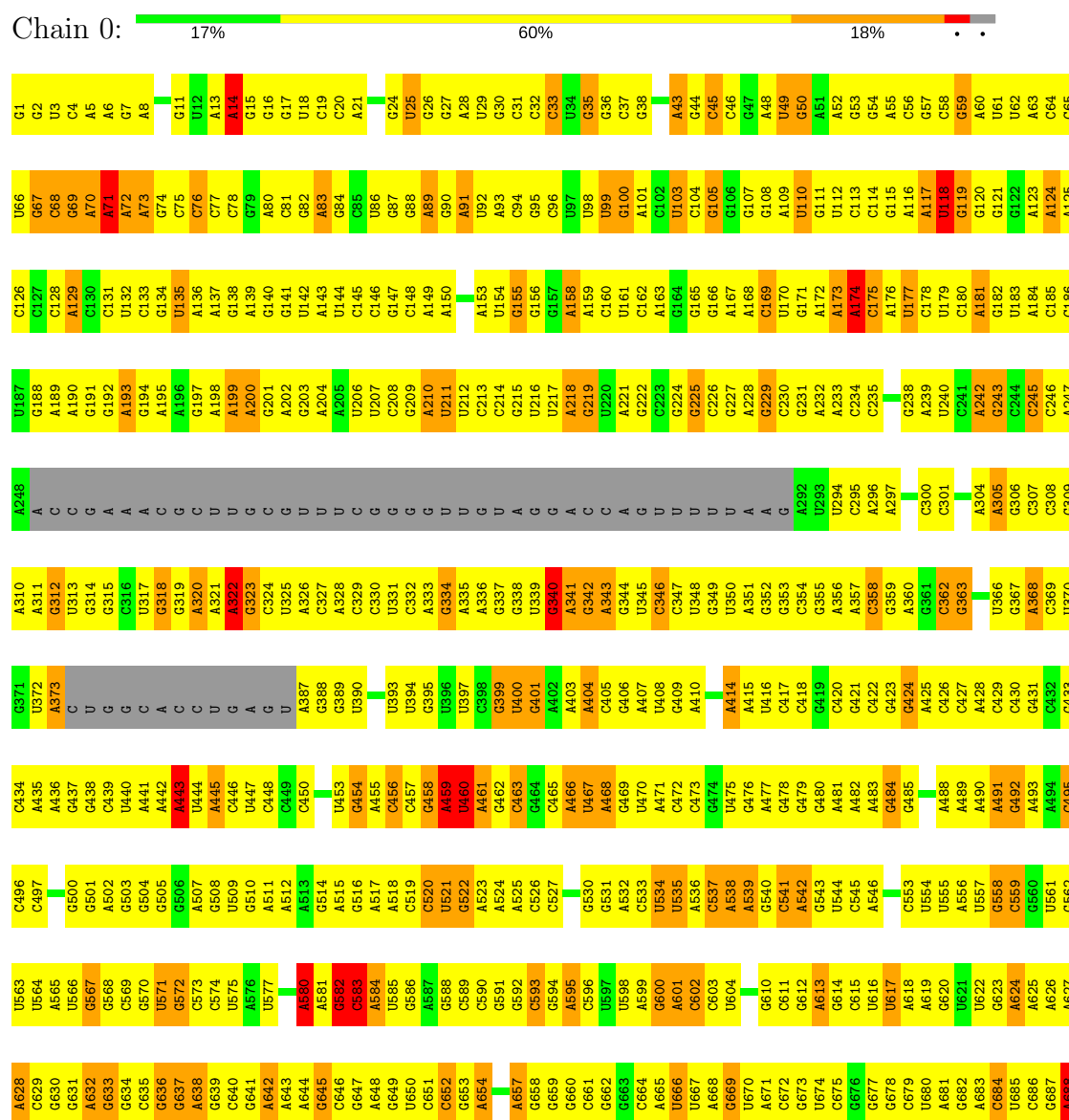
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	1	100	Total	C	N	O	0	0	0
			788	494	146	148			

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

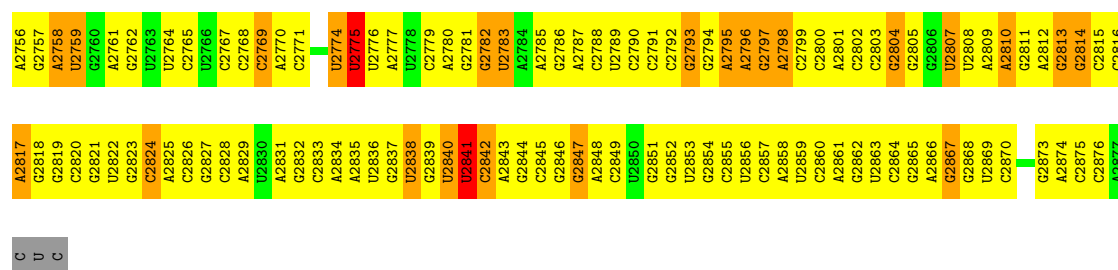
Note EDS was not executed.

• Molecule 1: 23S RIBOSOMAL RNA



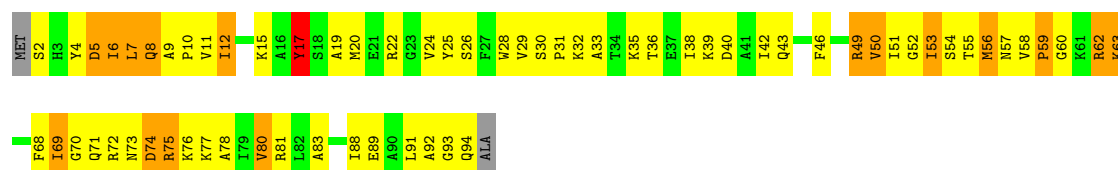
C1648	C1580	C1514	A1453	U1392	C1328	C1256	U1195	G1133	G1000	C935	U873	A813	G752	A689
A1651	C1581	U1515	U1454	G1393	U1329	U1257	G1196	C1134	A1001	A936	A874	G814	U752	A690
G1652	A1582	A1516	C1455	G1394	G1330	G1258	G1197	C1135	C1002	C937	G875	A815	U754	C691
C1653	A1583	C1517	C1456	A1395	A1259	A1259	C1198	C1003	C1003	G938	A876	U816	C755	C692
A1654	C1585	G1519	A1457	C1396	G1332	A1260	U1199	A1137	U1005	C939	G877	A817	C756	A693
C1655	A1586	U1520	U1459	G1398	G1333	G1261	G1200	A1138	U1005	G940	C878	G818	U757	G694
U1656	A1587	C1522	C1460	A1399	A1334	U1262	G1201	A1139	C1006	U941	A879	C819	G758	G695
A1658	C1588	U1522	G1461	G1336	A1335	G1263	U1202	U1076	A1007	U942	A880	U820	U759	U696
G1659	A1589	A1523	C1462	A1400	G1337	G1264	A1203	U1077	G1008	U943	U881	A821	U760	G697
C1660	C1590	C1524	A1463	G1401	G1338	G1265	G1204	A1078	G1009	A944	A882	U822	A761	A698
G1661	U1591	U1403	G1464	G1402	U1339	G1269	G1206	A1080	U1010	G945	A883	U823	A762	G699
C1662	A1592	C1404	G1465	G1403	C1340	C1270	A1208	A1081	A1011	U946	C884	U824	A763	C700
G1663	C1593	A1405	C1466	U1406	G1341	C1271	G1209	G1082	A1012	C947	A885	C825	A764	U701
C1664	U1594	U1407	U1467	U1342	U1342	C1271	G1209	G1083	G1013	C948	A886	U826	C765	A702
A1665	C1595	G1408	A1468	C1343	C1344	C1274	G1211	C1086	U1015	U951	G887	C927	A766	A703
G1666	A1596	A1532	U1469	A1408	G1345	C1274	C1210	C1087	C1016	A952	A888	C928	G767	G704
U1667	G1597	U1537	G1470	U1409	G1346	A1278	G1211	C1088	C1017	A953	C889	C929	U770	C705
C1668	A1598	A1534	G1471	U1410	C1346	G1279	U1212	A1089	C1018	U954	U890	G831	C771	U707
G1670	C1599	U1535	C1411	C1411	C1347	G1279	A1215	C1089	U1019	G955	A891	A832	C772	G708
A1681	U1600	G1536	U1473	C1412	C1348	G1284	G1216	C1090	A1020	A956	G	A833	C773	A709
C1672	G1601	A1537	A1474	U1413	A1349	A1285	U1217	C1091	A1021	G957	G	A834	A774	C710
C1673	G1602	U1475	G1476	G1414	G1350	A1286	C1218	U1092	A1022	G958	G	U835	U775	G711
A1603	A1603	C1415	G1477	G1415	G1351	U1287	C1219	U1093	U1023	C959	C	G836	G776	A712
A1605	C1540	C1416	C1477	C1416	G1352	A1287	G1220	C1094	G1024	U960	C	U837	A777	G713
G1606	G1541	C1417	U1478	C1417	A1353	A1288	C1221	A1095	A1025	G961	C	A838	G778	G714
C1607	G1542	G1418	G1479	C1418	A1354	A1289	G1222	A1096	U1026	C962	U	U839	U779	U715
G1608	A1543	G1419	A1480	G1419	A1355	A1290	G1223	A1097	C1027	U	A	U840	U780	U716
A1685	U1544	A1420	U1481	G1420	G1356	G1291	A1162	U1098	G1028	C968	C	G841	G781	G717
A1686	C1546	U1482	U1482	U1421	U1357	A1292	C1163	A1099	C1029	U969	C	A842	U782	A718
C1687	U1611	G1422	G1483	C1422	C1358	A1293	A1226	G1100	U1030	A970	A	G843	G783	A719
U1690	U1612	A1423	U1484	A1423	G1359	G1294	A1227	U1101	C1031	A971	C	G844	U784	A720
C1691	G1613	U1485	U1485	U1424	C1363	U1295	G1228	G1102	A1032	C972	C	U845	U785	C721
C1692	U1551	G1425	A1486	U1426	G1364	G1296	C1229	C1103	G1033	U973	U	A846	U786	C722
G1693	G1552	G1427	U1488	U1427	U1365	G1298	A1231	G1104	A1040	C980	U	C847	U787	C723
A1694	U1553	G1428	C1489	G1428	A1366	A1299	U1232	A1106	G1036	C975	C	A848	G788	C724
C1696	G1557	A1429	U1490	A1429	A1367	A1300	A1233	A1107	U1037	G977	C	G849	A790	G726
U1697	C1558	G1430	C1491	G1430	G1368	U1301	C1234	U1108	U1038	U978	A911	C850	U727	G727
A1699	G1559	A1433	A1492	A1433	G1369	C1302	C1235	A1109	G1039	U979	A912	U852	U792	G728
C1699	A1560	G1434	U1493	U1434	U1370	U1303	G1236	C1113	A1041	C981	C914	G854	A794	G732
A1699	G1561	G1435	G1494	G1435	G1371	U1304	G1237	A1114	G1042	C982	C915	G855	A795	G733
C1700	U1625	G1436	G1496	G1436	A1372	C1305	A1238	C1115	U1043	G983	U	A856	A796	U
C1701	A1626	C1437	C1497	A1437	G1373	U1306	A1239	U1116	U1044	A984	A918	U857	A797	G736
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A1706	A1630	C1501	C1500	A1441	A1379	C1311	A1242	C1120	U1046	A986	A921	U860	U800	G739
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C1708	A1632	G1503	G1503	G1443	G1381	U1313	G1245	A1122	U1054	G988	A923	A862	A802	G741
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G1711	G1635	C1572	A1446	U1446	G1384	G1317	A1249	G1125	U1057	A992	C927	A865	A806	C745
G1712	C1636	G1573	U1447	C1447	C1385	A1318	G1251	A1126	G1058	A994	A929	U866	A807	C745
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C1715	U1577	A1511	C1511	C1389	C1389	U1325	C1253	U1130	C1064	C997	G932	C869	U810	C749
G1716	U1578	A1512	G1450	U1325	U1325	U1325	G1131	G1131	C1064	C998	G933	U871	G811	C750
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G2698	C2630	C2443	G2567	G2505	C2441	A2381	G2320	C2254	A2190	G2110	A2042	C1979	A2199	A1845	A1782	G1721
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G2710	G2643	A2455	A2581	C2518	A2455	G2394	G2332	A2267	G2203	U2128	G2055	G1995	G1932	A1860	A1794	G1735
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G2723	C2659	C2472	C2595	G2532	U2472	G2408	G2346	A2280	G2217	C2148	U2069	U2009	U1945	A1874	U1811	U1748
G2724	C2660	G2473	G2596	U2533	G2473	A2409	A2348	C2281	U2219	G2149	G2070	U2010	U1946	U1875	G1749	G1749
U2725	G2661	G2474	G2597	G2534	G2474	U2410	A2349	U2284	A2220	U2150	G2071	U2011	G1947	U1881	A1750	A1750
G2726	A2662	C2475	C2598	G2535	C2475	A2411	G2349	U2285	A2221	G2151	C2072	U2012	C1948	G1814	A1751	A1751
G2727	G2663	U2476	U2599	G2536	A2476	A2412	A2352	G2286	U2222	A2152	A2073	A2013	C1950	A1883	U1752	A1752
A2728	U2664	C2477	C2600	C2537	C2477	A2413	G2353	G2287	U2223	A2153	U2074	A2014	G1951	A1884	G1816	A1753
A2729	U2665	U2478	G2601	G2538	C2478	G2414	G2354	A2288	U2224	A2154	U2075	G2015	A1952	G1885	G1818	G1754
G2730	C2666	U2479	G2602	C2539	C2479	G2415	A2355	A2289	G2225	U2155	G2076	A2016	A1953	G1886	G1755	G1755
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C2732	C2668	G2481	G2604	U2541	G2481	U2417	A2357	U2291	C2227	G2166	G2078	G2018	G1955	G1888	C1757	C1757
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U2734	C2670	U2483	C2419	A2543	C2483	C2419	U2359	G2293	G2229	G2167	U2080	G2020	C1957	C1890	G1759	A1759
G2735	C2671	G2484	C2420	G2544	C2484	C2420	C2360	U2294	G2230	G2168	U2081	G2021	U1959	C1891	G1761	G1761
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A2738	C2674	G2487	G2493	G2547	G2487	G2423	G2363	G2297	C2233	U2172	G2084	U2024	A1961	U1827	U1826	G1764
G2739	U2675	G2488	C2494	G2548	G2488	G2424	G2364	U2298	G2234	U2173	G2085	A2025	C1962	C1828	C1828	A1764
C2740	C2676	C2489	G2495	U2549	C2489	G2425	U2365	A2299	G2235	G2174	U2086	C2026	G1963	C1829	C1765	C1765
G2741	U2677	U2490	C2496	G2550	G2490	G2426	U2366	G2300	U2236	A2175	U2087	C2027	A1964	C1830	U1766	U1766
A2742	C2678	C2491	C2497	A2551	C2491	A2427	G2367	A2301	C2237	U2176	G2087	C2028	U1965	G1904	G1767	G1767
G2743	A2681	U2615	U2616	G2552	U2492	U2428	G2368	A2302	G2238	U2177	G2088	C2029	C1966	G1905	U1768	U1768
A2744	C2682	G2610	G2611	C2553	C2493	A2429	U2369	G2303	C2239	U2178	G2089	G2030	U1967	U1906	U1769	U1769
A2745	G2687	A2618	G2619	G2554	C2494	A2430	U2370	A2306	C2240	U2179	U2096	A2031	G1968	C1907	U1770	U1770
U2749	G2688	C2620	G2620	G2555	C2495	C2431	A2371	A2307	C2241	U2180	A2097	U2032	G1969	U1909	C1834	A1771
G2750	C2689	A2497	A2556	U2556	C2496	A2432	A2372	A2308	C2242	U2181	G2098	C2033	G1970	A1910	C1772	C1772
C2751	A2690	G2621	C2557	C2558	U2497	A2433	C2373	G2309	A2245	A2182	G2099	A2034	C1971	A1911	G1836	C1773
C2752	C2691	G2622	U2559	C2559	U2498	G2434	C2374	G2310	A2246	C2183	A2100	G2035	C1972	G1912	G1837	A1774
G2753	C2692	U2623	G2560	C2560	U2499	C2435	C2375	U2311	A2247	C2184	G2036	A2037	C1973	G1913	G1838	A1775
C2754	A2692	U2624	C2561	C2561	C2500	U2436	G2376	A2312	A2248	U2185	U2105	G2037	U1974	U1914	A1839	A1776
A2755	U2693	G2625	U2625	G2561	U2501	G2437	U2377	G2313	G2249	G2186	G2106	C2038	G1975	A1915	A1840	U1778



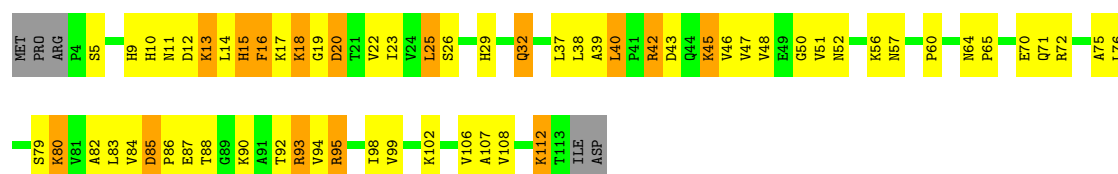
• Molecule 2: 50S RIBOSOMAL PROTEIN L23

Chain R: 28% 52% 17% ..



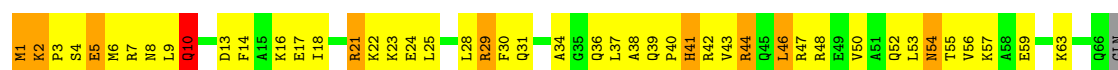
• Molecule 3: 50S RIBOSOMAL PROTEIN L24

Chain S: 41% 42% 13% .



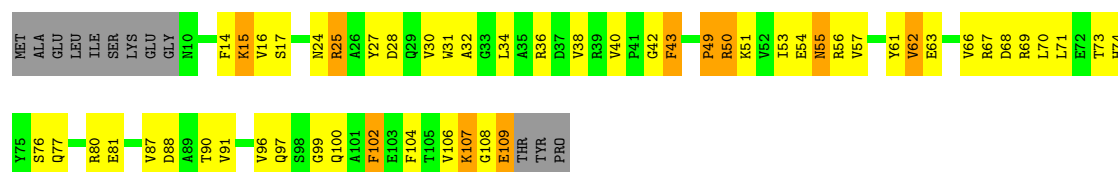
• Molecule 4: 50S RIBOSOMAL PROTEIN L29

Chain W: 30% 54% 13% ..



• Molecule 5: Trigger Factor

Chain 1: 41% 39% 9% 11%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.50Å 410.50Å 695.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.35	Depositor
% Data completeness (in resolution range)	(Not available) (29.84-3.35)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.299 , 0.322	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	63004	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0	0.67	3/67338 (0.0%)	0.82	72/105044 (0.1%)
2	R	0.48	0/737	0.80	0/988
3	S	0.42	0/835	0.73	1/1121 (0.1%)
4	W	0.44	0/537	0.58	0/714
5	1	0.48	0/802	0.68	0/1084
All	All	0.66	3/70249 (0.0%)	0.82	73/108951 (0.1%)

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	0	0	169
2	R	0	1
All	All	0	170

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2776	U	C1'-N1	6.38	1.58	1.48
1	0	2775	U	C1'-N1	6.21	1.58	1.48
1	0	567	G	C5-C6	-5.13	1.37	1.42

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2034	A	N9-C1'-C2'	10.22	127.28	114.00
1	0	1342	U	N1-C1'-C2'	9.78	126.71	114.00
1	0	1467	U	N1-C1'-C2'	8.63	125.23	114.00
1	0	2775	U	C2-N1-C1'	-8.26	107.78	117.70
1	0	1631	C	N1-C1'-C2'	8.21	124.68	114.00

There are no chirality outliers.

5 of 170 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	118	U	Sidechain
1	0	14	A	Sidechain
1	0	25	U	Sidechain
1	0	43	A	Sidechain
1	0	71	A	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	60132	0	30298	3519	0
2	R	726	0	753	126	0
3	S	825	0	881	117	0
4	W	533	0	558	81	0
5	1	788	0	784	74	0
All	All	63004	0	33274	3848	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 40.

The worst 5 of 3848 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)
2:R:69:ILE:CG2	2:R:70:GLY:H	1.26	1.38
1:0:1325:U:H1'	1:0:1619:A:N1	1.50	1.25
2:R:69:ILE:HG22	2:R:70:GLY:N	1.30	1.19
3:S:92:THR:HB	3:S:95:ARG:HH22	1.05	1.18
1:0:67:G:H21	1:0:72:A:H2'	1.09	1.16

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	
2	R	91/95 (96%)	70 (77%)	16 (18%)	5 (6%)	2	16
3	S	108/115 (94%)	79 (73%)	24 (22%)	5 (5%)	3	21
4	W	64/67 (96%)	54 (84%)	8 (12%)	2 (3%)	5	32
5	1	98/112 (88%)	81 (83%)	13 (13%)	4 (4%)	3	25
All	All	361/389 (93%)	284 (79%)	61 (17%)	16 (4%)	3	23

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	S	42	ARG
3	S	65	PRO
4	W	2	LYS
5	1	49	PRO
2	R	69	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	75/76 (99%)	61 (81%)	14 (19%)	2	8
3	S	91/96 (95%)	77 (85%)	14 (15%)	3	15
4	W	54/55 (98%)	43 (80%)	11 (20%)	1	5
5	1	83/93 (89%)	72 (87%)	11 (13%)	4	20
All	All	303/320 (95%)	253 (84%)	50 (16%)	2	12

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	S	40	LEU
3	S	112	LYS
5	1	88	ASP
3	S	43	ASP
3	S	80	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	S	64	ASN
3	S	71	GLN
5	1	55	ASN
3	S	57	ASN
5	1	24	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2798/2880 (97%)	580 (20%)	0

5 of 580 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	14	A
1	0	25	U
1	0	33	C
1	0	35	G
1	0	45	C

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 [i](#)

There are no ligands in this entry.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.