



wwPDB X-ray Structure Validation Summary Report

Oct 10, 2014 – 01:25 PM EDT

PDB ID : 4RB8
Title : Crystal structure of the Thermus thermophilus 70S ribosome in complex with amicoumacin, mRNA and three deacylated tRNAs in the A, P and E sites
Authors : Polikanov, Y.S.; Osterman, I.A.; Szal, T.; Tashlitsky, V.N.; Serebryakova, M.V.; Kusochev, P.; Bulkley, D.; Malanicheva, I.A.; Efimenko, T.A.; Efremenkova, O.V.; Konevega, A.L.; Shaw, K.J.; Bogdanov, A.A.; Rodnina, M.V.; Dontsova, O.A.; Mankin, A.S.; Steitz, T.A.; Sergiev, P.V.
Deposited on : 2014-09-12
Resolution : 2.40 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>

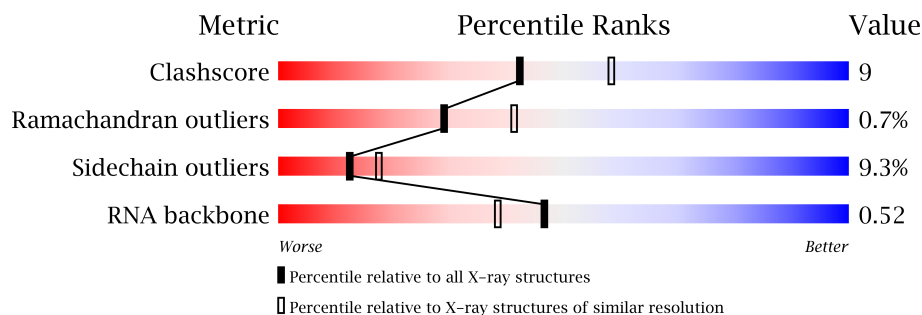
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 23426
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk24003

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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	88313	3035 (2.40-2.40)
Ramachandran outliers	86584	2982 (2.40-2.40)
C α geometry	86677	2981 (2.40-2.40)
Sidechain outliers	86556	2983 (2.40-2.40)
RNA backbone	2044	1127 (3.00-1.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2915	
2	B	121	
3	D	276	
4	E	206	
5	F	210	
6	G	182	
7	H	180	
8	I	148	
9	N	140	
10	O	122	
11	P	150	
12	Q	141	
13	R	118	

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Mol	Chain	Length	Quality of chain
14	S	112	
15	T	146	
16	U	118	
17	V	101	
18	W	113	
19	X	96	
20	Y	110	
21	Z	206	
22	0	85	
23	1	98	
24	2	72	
25	3	60	
26	4	71	
27	5	60	
28	6	54	
29	7	49	
30	8	65	
31	9	37	

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 91678 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	A	2800	Total	C	N	O	P	0	0	0
			60314	26840	11284	19390	2800			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

- Molecule 3 is a protein called 50S Ribosomal Protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 5 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

- Molecule 6 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	4			

- Molecule 7 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 8 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	146	Total	C	N	O	S	0	0	0
			1064	681	186	196	1			

- Molecule 9 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 10 is a protein called 50S Ribosomal Protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 12 is a protein called 50S Ribosomal Protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S Ribosomal Protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	S	110	Total	C	N	O			
			870	549	173	148	0	0	0

- Molecule 15 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	T	131	Total	C	N	O	S		
			1083	675	224	183	1	0	0

- Molecule 16 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	U	116	Total	C	N	O	S		
			959	608	201	149	1	0	0

- Molecule 17 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	V	101	Total	C	N	O	S		
			771	495	140	135	1	0	0

- Molecule 18 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	W	112	Total	C	N	O	S		
			886	557	174	153	2	0	0

- Molecule 19 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	X	95	Total	C	N	O	S		
			750	488	135	126	1	0	0

- Molecule 20 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	Y	107	Total	C	N	O	S		
			806	517	152	131	6	0	0

- Molecule 21 is a protein called 50S Ribosomal Protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Z	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	2			

- Molecule 22 is a protein called 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	0	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 23 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	1	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 24 is a protein called 50S Ribosomal Protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 25 is a protein called 50S Ribosomal Protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	3	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 26 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	4	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 27 is a protein called 50S Ribosomal Protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 28 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 29 is a protein called 50S Ribosomal Protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S Ribosomal Protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	P	1	Total	Mg	0	0
			1	1		
32	B	21	Total	Mg	0	0
			21	21		
32	W	3	Total	Mg	0	0
			3	3		
32	X	1	Total	Mg	0	0
			1	1		
32	E	7	Total	Mg	0	0
			7	7		
32	V	2	Total	Mg	0	0
			2	2		
32	A	673	Total	Mg	0	0
			673	673		
32	5	2	Total	Mg	0	0
			2	2		
32	R	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	1	1	Total 1	Mg 1	0	0
32	D	6	Total 6	Mg 6	0	0
32	Z	1	Total 1	Mg 1	0	0
32	U	4	Total 4	Mg 4	0	0
32	0	1	Total 1	Mg 1	0	0
32	G	1	Total 1	Mg 1	0	0
32	Q	3	Total 3	Mg 3	0	0
32	T	1	Total 1	Mg 1	0	0
32	8	2	Total 2	Mg 2	0	0
32	O	1	Total 1	Mg 1	0	0
32	Y	1	Total 1	Mg 1	0	0
32	3	1	Total 1	Mg 1	0	0
32	F	7	Total 7	Mg 7	0	0

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	9	1	Total 1	Zn 1	0	0
33	Y	1	Total 1	Zn 1	0	0
33	4	1	Total 1	Zn 1	0	0
33	6	1	Total 1	Zn 1	0	0
33	5	1	Total 1	Zn 1	0	0

- Molecule 34 is water.

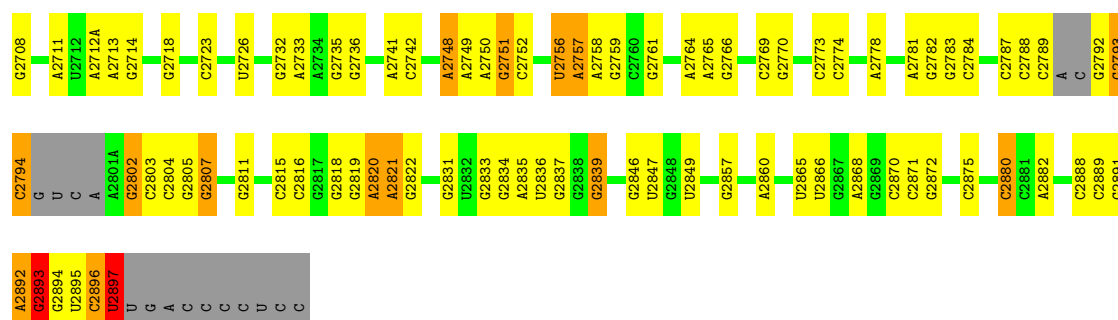
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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34	B	10	Total 10	O 10	0	0
34	D	17	Total 17	O 17	0	0
34	E	8	Total 8	O 8	0	0
34	F	6	Total 6	O 6	0	0
34	I	2	Total 2	O 2	0	0
34	N	1	Total 1	O 1	0	0
34	O	3	Total 3	O 3	0	0
34	P	12	Total 12	O 12	0	0
34	Q	1	Total 1	O 1	0	0
34	R	3	Total 3	O 3	0	0
34	T	3	Total 3	O 3	0	0
34	U	1	Total 1	O 1	0	0
34	V	1	Total 1	O 1	0	0
34	W	2	Total 2	O 2	0	0
34	X	2	Total 2	O 2	0	0
34	Y	1	Total 1	O 1	0	0
34	Z	2	Total 2	O 2	0	0
34	0	4	Total 4	O 4	0	0
34	1	4	Total 4	O 4	0	0
34	2	1	Total 1	O 1	0	0
34	3	1	Total 1	O 1	0	0

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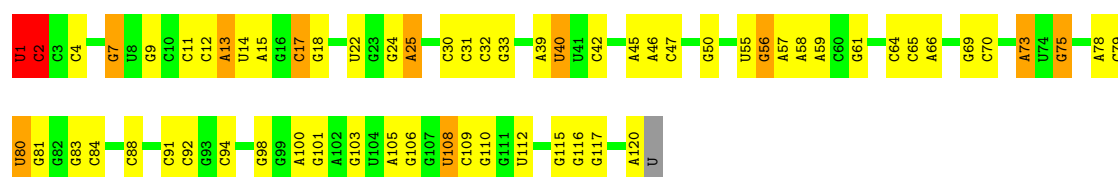
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	5	2	Total	O	0	0
			2	2		
34	7	5	Total	O	0	0
			5	5		
34	8	5	Total	O	0	0
			5	5		
34	9	1	Total	O	0	0
			1	1		

C2573	A2469	G2353	G2270	G2159	G2099	G1996	C1836	G1753	G1622	G1529	C1417	G1309	U1211	C
G2578	C2470	G2354	G2271	G2160	G2100	C1997	C1843	G1756	G1623	C1530	U1420	G1310	G1212	C
G2582	C2472	U2357	A2273	C2162	G2102	G1998	G1843	G1766	A1631A	C1532	G1421	U1313	C1218	A
G2589	U2473	C2364	A2274	C2163	C2103	G1999	A1847	A1759	G1636	G1533	A1427	C1314	A1220	C
G2592	C2474	C2365	G2275	C2164	G2104	G2000	A1848	A1762	A1637	U	C1428	G1315	G1113	C
U2593	C2475	G2366	G2277	G2165	C2105	G2010	G1856	G1763	G1638	A	G1434	U1335	G1114	A
A2602	A2476	G2367	A2278	G2166	G2106	A2013	G1857	G1764	C1639	G1536	A1435	A1336	G1115	G
U2611	A2477	A2376	G2279	U2167	C2107	A2014	G1858	G1769	C1640	U1539	G1436	G1337	G1116	G
C2612	C2478	G2377	C2283	A2170	G2110	G2018	A1877	G1770	A1641	U1540	G1437	G1338	G1117	A
U2615	G2483	G2380	C2284	A2171	C2111	A2019	C1877	G1771	G1642	G1541	U1340	U1339	C1118	G
C2617	C2484	A2287	A2286	A2173	G2112	A2019	C1879	G1772	G1647	A1542	C1445	U1341	U1130	U
A2629	U2487	C2383	C2384	C2174	U2113	U2022	A1885	A1773	C1648	U1543	G1446	A1342	G1232	U
G2630	G2495	G2384	G2385	C2175	G2115	G2023	C1886	U1777	G1651	C1548	C1447	U1352	C1135	G
A2632	G2496	C2386	C2387	C2176	G2116	G2024	C1886	U1778	A1652	C1549	G1448	G1353	G1137	C
C2646	U2503	U2291	U2290	C2177	G2117	G2025	G1891	U1779	G1653	U1554	A1449	G1354	G1138	U
U2647	G2504	G2393	G2394	C2178	U2118	U2028	G1899	C1781	A1654	A1554	G1450	G1355	G1139	U
C2648	U2505	G2395	A2305	G2182	G2120	A2030	A1900	A1783	A1665	C1557	A1452	U1357	C1140	G
U2649	C2507	G2396	G2397	C2183	G2121	G2031	G1906	A1784	G1667	G1558	G1455	G1358	U1141	A
G2650	G2508	G2398	G2399	C2184	G2122	G2032	A1912	A1785	A1668	G1560	U1453	U1142	G1142A	A
C2651	C2404	G2405	G2406	C2185	G2123	G2033	A1913	A1786	A1669	G1561	A1359	A1143	A1143	C
U2652	U2514	U2311	U2312	C2186	G2124	A2034	A1914	U1794	C1670	A1562	A1460	A1360	G1149	A
A2653	C2515	G2315	G2316	G2187	G2125	U2042	A1915	C1795	A1677	A1566	G1461	C1363	C1150	G
G2655	U2516	G2315	G2316	C2188	G2126	C2043	A1916	U1796	C1671	G1567	G1465	G1364	C1251	C
A2657	G2518	G2316	G2317	C2189	G2127	C2044	A1917	C1797	C1684	A1568	G1466	A1365	G1153	C
C2658	U2519	U2317	U2318	G2191	G2128	G2037	U1917	A1798	C1684	G1569	C1467	G1370	G1154	C
U2659	C2520	G2319	G2320	C2192	G2129	G2038	U1917	G1799	A1689	U1578	A1471	G1371	A1155	U
G2663	U2526	U2321	U2322	C2193	U2130	A2042	G1929	U1794	A1677	C1584	G1477	U1372	U1159	C
C2664	G2529	G2321	G2322	G2194	G2131	C2043	U1930	C1795	A1677	A1579	A1477	A1374	G1180	U
U2671	U2535	G2323	G2324	C2198	G2132	C2044	U1931	U1796	C1683	A1580	G1478	G1375	G1170	U
G2672	G2543	G2325	G2326	U2203	G2133	A2051	A1932	U1798	C1684	C1582	U1263	U1263	G1171	A
C2673	U2544	G2326	G2327	C2205	G2134	C2055	A1933	G1799	A1689	A1583	G1264	A1378	G	A
A2675	G2552	G2327	G2328	C2206	G2135	C2056	A1936	G1800	U1693	C1584	U1265	A1379	A	A
C2683	U2553	G2329	G2330	G2207	G2136	G2056	A1937	G1801	A1696	A1586	G1266	G1380	U	G
U2689	G2554	U2344	U2345	G2208	G2140	A2060	A1938	A1802	G1696	C1589	C1493	A1384	A	G
C2690	U2557	G2346	G2347	U2218	G2141	G2061	A1955	U1803	G1697	U1590	A1494	A1268	C1178	U
A2693	C2558	G2347	G2348	C2224	G2142	A2062	U1956	U1805	A1698	G1591	A1495	G1385	G	G
G2694	U2562	U2349	U2350	G2224	G2143	C2063	C1957	A1810	G1699	C1592	A1496	U1394	G1183	C
U2702	G2565	G2351	G2352	A2225	C2144	C2064	C1958	A1811	A1700	G1593	U1497	A1395	G1184	G
C2703	U2566	G2352	G2353	G2226	C2145	C2065	U1963	A1812	U1713	G1594	C1506	G1399	C1185	U
G2705	A2567	G2353	G2354	G2227	G2146	G2066	U1967	A1815	G1714	G1595	A1507	C1400	G1187	A
C2707	U2568	G2354	G2355	G2228	G2147	G2067	C1967	G1816	G1717	C1599	A1508	G1401	U1187	A
U2709	A2569	G2355	G2356	G2229	G2148	A2071	G1968	G1817	G1718	C1607	C1509	U1291	U1198	U
G2710	C2569	G2356	G2357	U2243	G2149	G2072	A1969	G1823	U1721	A1608	U1405	U1292	U1199	G
C2712	U2570	G2357	G2358	U2244	G2150	G2073	A1970	G1823	A1722	A1509B	U1406	U1292	U1199	G
U2713	A2571	G2359	G2360	U2245	G2151	G2074	A1971	A1829	A1722	G1510	U1407	C1298	C1201	C
C2714	U2572	G2360	G2361	U2246	G2152	G2075	A1972	C1830	G1740	A1610	C1408	G1299	U1300	C
U2715	G2573	G2361	G2362	U2247	G2153	G2076	G1973	C1830	G1740	A1614	A1412	U1301	A1204	A
C2716	U2574	G2362	G2363	U2248	G2154	G2077	U1991	U1833	G1746	G1615	G1413	U1301	U1205	C
U2717	A2575	G2363	G2364	U2249	G2155	G2078	U1992	U1834	C1752	A1616	G1416	C1306	U1206	U
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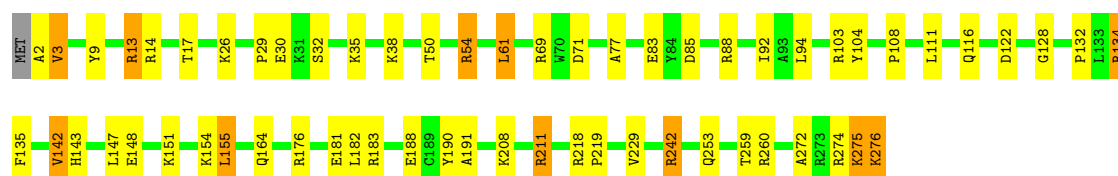
• Molecule 2: 5S Ribosomal RNA

Chain B:



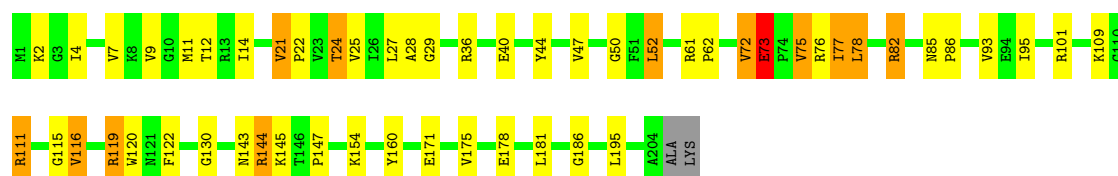
• Molecule 3: 50S Ribosomal Protein L2

Chain D:



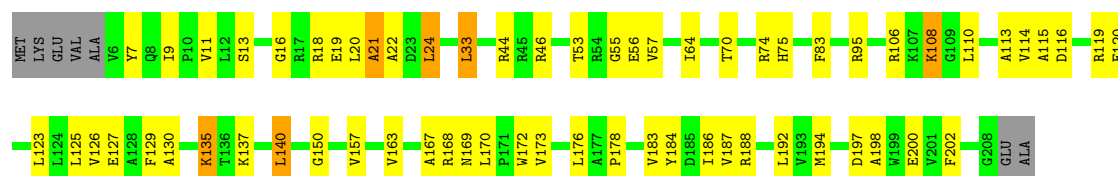
• Molecule 4: 50S Ribosomal Protein L3

Chain E:



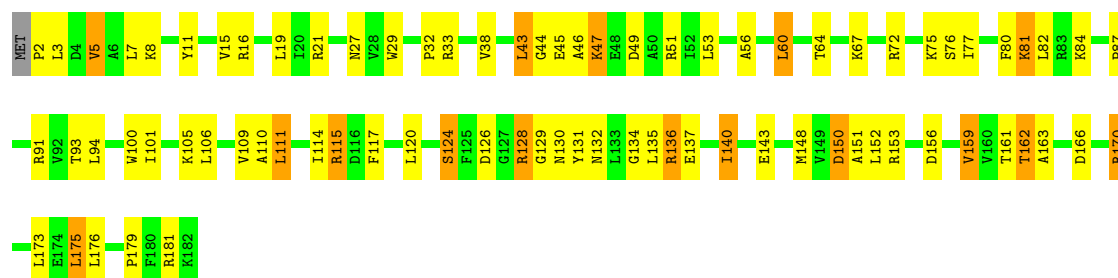
• Molecule 5: 50S Ribosomal Protein L4

Chain F:



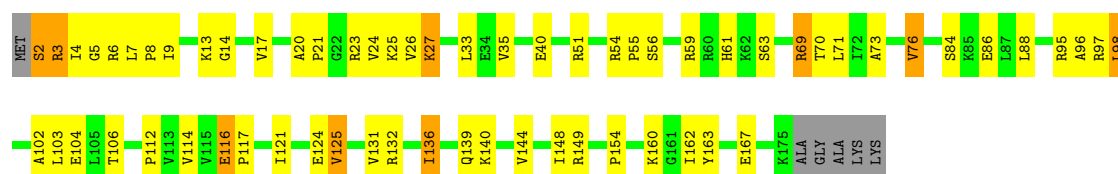
• Molecule 6: 50S Ribosomal Protein L5

Chain G:



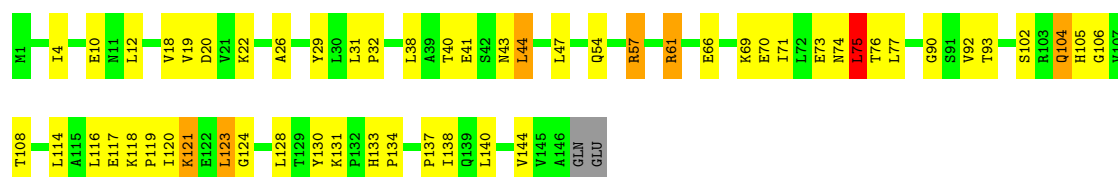
• Molecule 7: 50S Ribosomal Protein L6

Chain H:



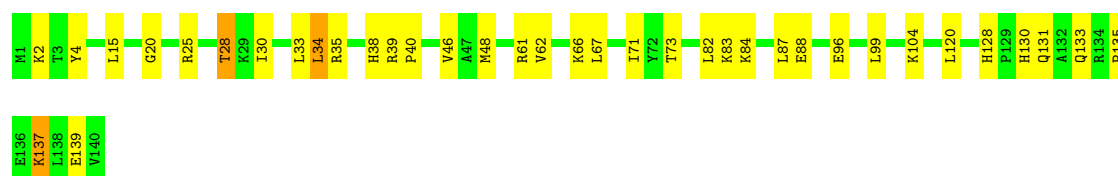
• Molecule 8: 50S Ribosomal Protein L9

Chain I:



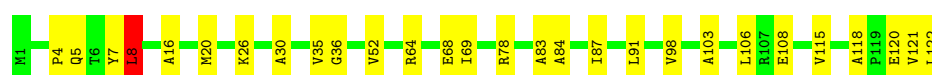
• Molecule 9: 50S Ribosomal Protein L13

Chain N:



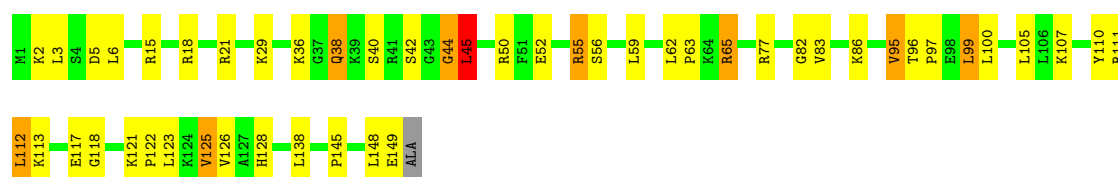
• Molecule 10: 50S Ribosomal Protein L14

Chain O:



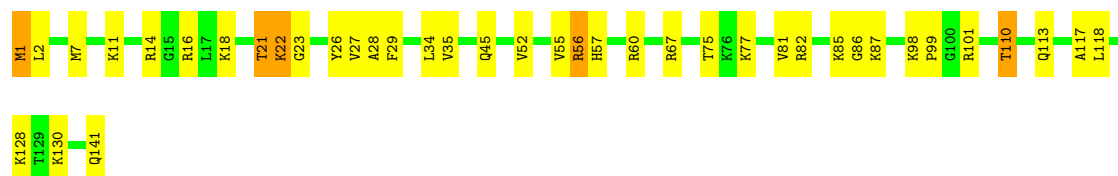
• Molecule 11: 50S Ribosomal Protein L15

Chain P:



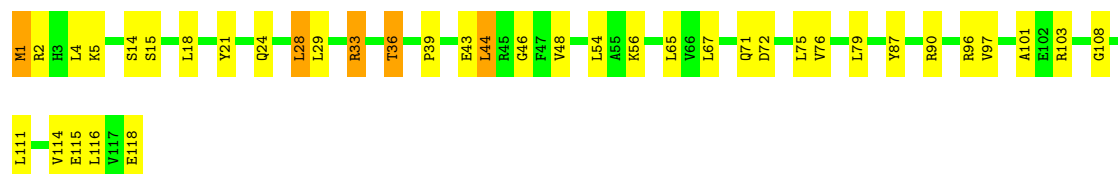
- Molecule 12: 50S Ribosomal Protein L16

Chain Q: 



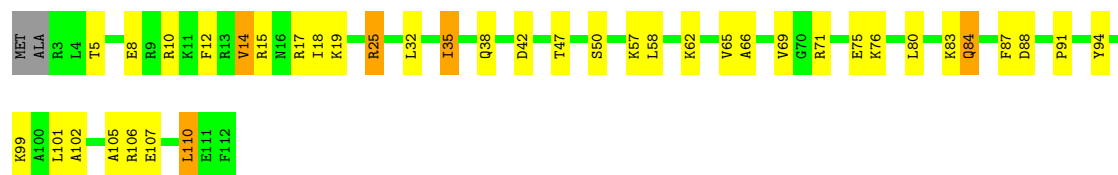
- Molecule 13: 50S Ribosomal Protein L17

Chain R: 



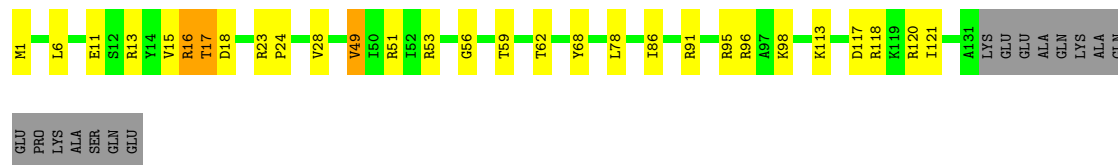
- Molecule 14: 50S Ribosomal Protein L18

Chain S: 



- Molecule 15: 50S Ribosomal Protein L19

Chain T: 



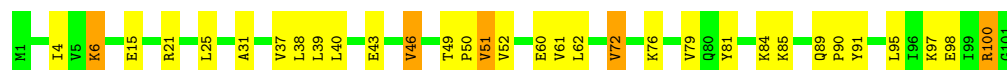
- Molecule 16: 50S Ribosomal Protein L20

Chain U: 



- Molecule 17: 50S Ribosomal Protein L21

Chain V: 



- Molecule 18: 50S Ribosomal Protein L22

R1	E2			V9	L10	R11	L12	S13	P14	R15	K16	V17	R18	L19		L23		K27		R42		Y45		K49	V50	L51		A54		N60		V71	K72		E78		K83		L86	F87	R88		D94	I95	I96		T100		L107		G12	H12S
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P1	K2	T3	A4		I8		P11	V12		K16	E23	G24	K25		V29	V30	H31	P32	K33	A34	T35		E38		A42	V43		K50		K53	L57	R65		K78		V81	Q82	V83		A84		Q87		E90	A91	L92		L95		T97
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M1	R2	H6	K9	G10	D11	T12	V13	Y20	K21	G22	R23	I38	M42	M43	I44	K63	P66	L67	H68	V72	R73	P74	R84	H85	R86	K87	K88	F89	L90	E91	K94	K95	C99	A100	D107	THR	GLU	CTD
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K6	A7	Y8	E11	L18	R19	V27	M28	Y29	N30	H31	R32	H33	L33	N34	Y38	D45	K46	Q50	A51	S52	I53	H54	H55	T69	R72	Q73	V74	D77	R78	R79	R82	P83	E84	H85	T86	D87	F88	F89	V90	L91	S92	E97	V100	P101
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V105	THR	PRO	ALA	GLY	VAL	ARG	ALA	GLY	GLY	VAL	LEU	GLN	GLU	ILE	H121	H122	D123	D126	D127	V128	S129	F130	R131	N132	I133	P134	E135	F136	I137	E138	V139	D140	V141	L144	E145	I146	G147	D148	S153	D154	L155	K156	L157	F158	P159	G160	V161	F162	L163	A164	V165	S166	P167	T170
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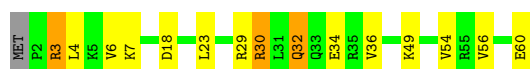
I171	V174	VAL	PRO	PRO	GLU	ASP	VAL	LYS	LEU	ALA	GLU	GLU	ALA	ALA	ALA	GLU	VAL	ALA	GLU	PRO	GLU	VAL	IIE	LYS	LYS	GLY	LYS	GLU	GLU	GLU	GLU	GLU
------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

MET
 A2
 K5
 G6
 L7
 T10
 R11
 N12
 G13
 R14
 R20
 E27
 R32
 N35
 I36
 L37
 T43
 R55
 F60
 Q70
 R77
 H80
 L94
 ALA

MET	S2	K3	V4	C5	R21	K32	T35	R40	L46	R50	V51	R52	T59	V62	A63	A64	I67	P68	K69	V74	E75	R76	E83	G84	L85	E89	E93	L94	L95	L98
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Category	Count
M1	100
P18	100
E22	100
K28	100
L32	100
L35	100
R36	100
L44	100
L53	100
N65	100
R69	100
Q70	100
ASN	100
ALA	100

Chain 3:



• Molecule 26: 50S Ribosomal Protein L31

Chain 4:



• Molecule 27: 50S Ribosomal Protein L32

Chain 5:



• Molecule 28: 50S Ribosomal Protein L33

Chain 6:



• Molecule 29: 50S Ribosomal Protein L34

Chain 7:



• Molecule 30: 50S Ribosomal Protein L35

Chain 8:



• Molecule 31: 50S Ribosomal Protein L36

Chain 9:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.06Å 448.57Å 623.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	256.12 – 2.40	Depositor
% Data completeness (in resolution range)	99.7 (256.12-2.40)	Depositor
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.237 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	91678	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	0/67545	0.92	63/105432 (0.1%)
2	B	0.47	1/2879 (0.0%)	0.91	2/4487 (0.0%)
3	D	0.34	0/2186	0.56	0/2944
4	E	0.34	0/1592	0.61	1/2149 (0.0%)
5	F	0.33	0/1615	0.55	0/2188
6	G	0.29	0/1453	0.52	0/1963
7	H	0.30	0/1356	0.54	0/1834
8	I	0.27	0/1079	0.55	1/1475 (0.1%)
9	N	0.32	0/1144	0.53	0/1543
10	O	0.32	0/943	0.56	1/1269 (0.1%)
11	P	0.32	0/1152	0.59	1/1533 (0.1%)
12	Q	0.32	0/1143	0.53	0/1527
13	R	0.34	0/982	0.55	0/1312
14	S	0.31	0/880	0.53	0/1172
15	T	0.30	0/1097	0.53	0/1468
16	U	0.34	0/977	0.53	0/1301
17	V	0.29	0/782	0.54	0/1049
18	W	0.33	0/897	0.55	0/1205
19	X	0.34	0/764	0.53	1/1025 (0.1%)
20	Y	0.33	0/819	0.54	0/1095
21	Z	0.30	0/1299	0.55	0/1763
22	0	0.30	0/662	0.49	0/881
23	1	0.33	0/762	0.52	0/1014
24	2	0.28	0/590	0.47	0/781
25	3	0.27	0/469	0.50	0/630
26	4	0.33	0/545	0.65	0/737
27	5	0.33	0/469	0.59	0/635
28	6	0.29	0/456	0.49	0/608
29	7	0.34	0/426	0.54	0/561
30	8	0.30	0/525	0.51	0/691
31	9	0.31	0/310	0.53	0/407
All	All	0.40	1/97798 (0.0%)	0.84	70/146679 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	U	OP3-P	-10.22	1.48	1.61

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1614	A	O5'-P-OP1	-8.54	98.02	105.70
1	A	2897	U	C2-N1-C1'	7.67	126.90	117.70
1	A	2139	C	N1-C2-O2	7.39	123.33	118.90
1	A	1298	C	O5'-P-OP2	-7.32	99.11	105.70
1	A	645	C	C2-N1-C1'	7.22	126.74	118.80

There are no chirality outliers.

There are no planarity outliers.

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	A	60314	0	30412	730	0
2	B	2575	0	1303	51	0
3	D	2136	0	2218	53	0
4	E	1559	0	1617	38	0
5	F	1580	0	1619	42	0
6	G	1428	0	1438	55	0
7	H	1330	0	1407	41	0
8	I	1064	0	1082	29	0
9	N	1117	0	1184	21	0
10	O	933	0	996	14	0
11	P	1135	0	1212	47	0
12	Q	1122	0	1179	31	0
13	R	968	0	1033	32	0
14	S	870	0	923	23	0
15	T	1083	0	1136	18	0
16	U	959	0	1019	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	V	771	0	830	18	0
18	W	886	0	940	15	0
19	X	750	0	814	18	0
20	Y	806	0	881	18	0
21	Z	1271	0	1273	52	0
22	0	653	0	674	17	0
23	1	755	0	826	14	0
24	2	588	0	643	5	0
25	3	464	0	514	9	0
26	4	532	0	503	27	0
27	5	455	0	465	8	0
28	6	449	0	469	11	0
29	7	418	0	467	11	0
30	8	517	0	582	23	0
31	9	307	0	335	9	0
32	0	1	0	0	0	0
32	1	1	0	0	0	0
32	3	1	0	0	0	0
32	5	2	0	0	0	0
32	8	2	0	0	0	0
32	A	673	0	0	0	0
32	B	21	0	0	0	0
32	D	6	0	0	0	0
32	E	7	0	0	0	0
32	F	7	0	0	0	0
32	G	1	0	0	0	0
32	O	1	0	0	0	0
32	P	1	0	0	0	0
32	Q	3	0	0	0	0
32	R	1	0	0	0	0
32	T	1	0	0	0	0
32	U	4	0	0	0	0
32	V	2	0	0	0	0
32	W	3	0	0	0	0
32	X	1	0	0	0	0
32	Y	1	0	0	0	0
32	Z	1	0	0	0	0
33	4	1	0	0	0	0
33	5	1	0	0	0	0
33	6	1	0	0	0	0
33	9	1	0	0	0	0
33	Y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	0	4	0	0	0	0
34	1	4	0	0	1	0
34	2	1	0	0	0	0
34	3	1	0	0	0	0
34	5	2	0	0	0	0
34	7	5	0	0	0	0
34	8	5	0	0	0	0
34	9	1	0	0	0	0
34	A	1039	0	0	58	0
34	B	10	0	0	1	0
34	D	17	0	0	0	0
34	E	8	0	0	1	0
34	F	6	0	0	0	0
34	I	2	0	0	0	0
34	N	1	0	0	0	0
34	O	3	0	0	0	0
34	P	12	0	0	3	0
34	Q	1	0	0	0	0
34	R	3	0	0	0	0
34	T	3	0	0	0	0
34	U	1	0	0	0	0
34	V	1	0	0	0	0
34	W	2	0	0	0	0
34	X	2	0	0	0	0
34	Y	1	0	0	1	0
34	Z	2	0	0	0	0
All	All	91678	0	59994	1308	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 9.

The worst 5 of 1308 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2124:G:H1	1:A:2174:C:H42	1.12	0.97
1:A:2121:G:H1	1:A:2177:C:H42	1.13	0.91
1:A:2807:G:N1	1:A:2893:G:O6	2.04	0.90
31:9:25:VAL:HB	31:9:34:GLN:HB2	1.55	0.89
2:B:7:G:H21	14:S:38:GLN:HE22	1.20	0.89

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	D	273/276 (99%)	265 (97%)	7 (3%)	1 (0%)	42	59
4	E	202/206 (98%)	196 (97%)	4 (2%)	2 (1%)	21	30
5	F	201/210 (96%)	198 (98%)	1 (0%)	2 (1%)	21	30
6	G	179/182 (98%)	167 (93%)	10 (6%)	2 (1%)	20	27
7	H	172/180 (96%)	165 (96%)	7 (4%)	0	100	100
8	I	144/148 (97%)	133 (92%)	10 (7%)	1 (1%)	29	41
9	N	138/140 (99%)	136 (99%)	1 (1%)	1 (1%)	29	41
10	O	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
11	P	147/150 (98%)	138 (94%)	6 (4%)	3 (2%)	11	12
12	Q	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	29	41
13	R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	S	108/112 (96%)	106 (98%)	1 (1%)	1 (1%)	23	33
15	T	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
16	U	114/118 (97%)	114 (100%)	0	0	100	100
17	V	99/101 (98%)	97 (98%)	1 (1%)	1 (1%)	21	30
18	W	110/113 (97%)	110 (100%)	0	0	100	100
19	X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	20	27
20	Y	105/110 (96%)	100 (95%)	5 (5%)	0	100	100
21	Z	156/206 (76%)	149 (96%)	6 (4%)	1 (1%)	32	46
22	0	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
23	1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	20	27
24	2	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	4	67/71 (94%)	55 (82%)	6 (9%)	6 (9%)	1	0
27	5	57/60 (95%)	57 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	7	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	10	10
30	8	62/65 (95%)	62 (100%)	0	0	100	100
31	9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	3364/3526 (95%)	3248 (97%)	91 (3%)	25 (1%)	29	41

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	52	LEU
4	E	73	GLU
5	F	21	ALA
5	F	130	ALA
6	G	81	LYS

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	D	215/218 (99%)	201 (94%)	14 (6%)	23	35
4	E	164/166 (99%)	147 (90%)	17 (10%)	10	14
5	F	159/166 (96%)	144 (91%)	15 (9%)	12	17
6	G	143/156 (92%)	119 (83%)	24 (17%)	3	3
7	H	144/148 (97%)	129 (90%)	15 (10%)	10	14
8	I	105/124 (85%)	88 (84%)	17 (16%)	3	4
9	N	118/119 (99%)	106 (90%)	12 (10%)	10	14
10	O	100/100 (100%)	97 (97%)	3 (3%)	52	74
11	P	115/116 (99%)	106 (92%)	9 (8%)	17	26
12	Q	111/111 (100%)	101 (91%)	10 (9%)	13	19
13	R	101/101 (100%)	88 (87%)	13 (13%)	6	7
14	S	85/88 (97%)	76 (89%)	9 (11%)	9	13
15	T	113/127 (89%)	105 (93%)	8 (7%)	20	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	U	93/94 (99%)	88 (95%)	5 (5%)	30	46
17	V	80/82 (98%)	71 (89%)	9 (11%)	8	11
18	W	90/92 (98%)	84 (93%)	6 (7%)	22	33
19	X	77/78 (99%)	74 (96%)	3 (4%)	42	62
20	Y	85/91 (93%)	76 (89%)	9 (11%)	9	13
21	Z	137/179 (76%)	123 (90%)	14 (10%)	10	14
22	0	65/67 (97%)	62 (95%)	3 (5%)	36	54
23	1	80/83 (96%)	72 (90%)	8 (10%)	11	15
24	2	65/67 (97%)	60 (92%)	5 (8%)	18	26
25	3	50/52 (96%)	45 (90%)	5 (10%)	11	15
26	4	53/63 (84%)	39 (74%)	14 (26%)	1	0
27	5	50/52 (96%)	45 (90%)	5 (10%)	11	15
28	6	50/52 (96%)	49 (98%)	1 (2%)	66	85
29	7	41/42 (98%)	38 (93%)	3 (7%)	19	29
30	8	54/55 (98%)	52 (96%)	2 (4%)	44	65
31	9	34/34 (100%)	33 (97%)	1 (3%)	53	74
All	All	2777/2923 (95%)	2518 (91%)	259 (9%)	12	17

5 of 259 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	P	15	ARG
13	R	54	LEU
26	4	48	ARG
11	P	65	ARG
12	Q	22	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
11	P	38	GLN
12	Q	57	HIS
21	Z	50	GLN
12	Q	13	GLN
12	Q	123	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2791/2915 (95%)	485 (17%)	29 (1%)
2	B	119/121 (98%)	20 (16%)	1 (0%)
All	All	2910/3036 (95%)	505 (17%)	30 (1%)

5 of 505 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	10	G
1	A	11	G
1	A	12	U
1	A	15	G

5 of 30 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	856	C
1	A	1300	U
1	A	2689	U
1	A	1210	A
1	A	1420	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 746 ligands modelled in this entry, 746 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.