



# wwPDB X-ray Structure Validation Summary Report

Nov 23, 2014 – 11:49 AM EST

PDB ID : 4W2D  
Title : Crystal structure of the peptolide 12C bound to bacterial ribosome  
Authors : Fagan, C.E.; Dunham, C.M.  
Deposited on : 2014-03-24  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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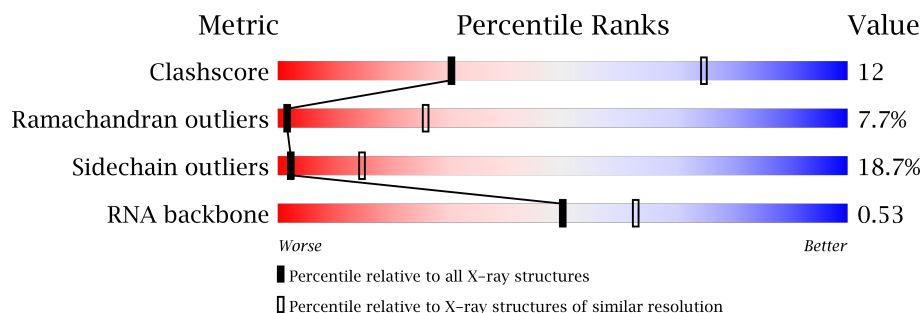
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable24195

# 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))
Clashscore	79885	1155 (3.80-3.40)
Ramachandran outliers	78287	1109 (3.80-3.40)
Sidechain outliers	78261	1108 (3.80-3.40)
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  $\geq 3$ , 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	122	
3	C	276	
4	D	206	
5	E	210	
6	F	182	
7	G	180	
8	H	148	
9	I	140	
10	J	122	
11	K	150	
12	L	141	
13	M	118	
14	N	112	

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Mol	Chain	Length	Quality of chain
15	O	146	
16	P	118	
17	Q	101	
18	R	113	
19	S	96	
20	T	110	
21	U	206	
22	V	85	
23	W	98	
24	X	72	
25	Y	60	
26	Z	71	
27	a	60	
28	b	54	
29	c	49	
30	d	65	
31	e	37	
32	f	12	

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 92327 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	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- 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
			2573	1146	476	832	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	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	K	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	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	M	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	N	111	Total	C	N	O	0	0	0
			882	556	176	150			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	S	92	Total	C	N	O	0	0	0
			725	471	131	123			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	Y	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	a	57	Total	C	N	O	S	0	0	0
			442	278	88	71	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	b	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	c	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	d	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	e	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a protein called T17-GLY-GLY-PRO-LYS-LYS-LYS-LYS-LYS-VAL-GLY-GLY.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
32	f	9	Total	C	N	O	0	0	0
			116	78	18	20			

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	D	2	Total	Mg	0	0
			2	2		
33	K	1	Total	Mg	0	0
			1	1		
33	B	4	Total	Mg	0	0
			4	4		
33	C	1	Total	Mg	0	0
			1	1		
33	c	1	Total	Mg	0	0
			1	1		
33	A	279	Total	Mg	0	0
			279	279		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	L	1	Total	Mg	0	0
			1	1		
33	S	1	Total	Mg	0	0
			1	1		

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	e	1	Total	Zn	0	0
			1	1		

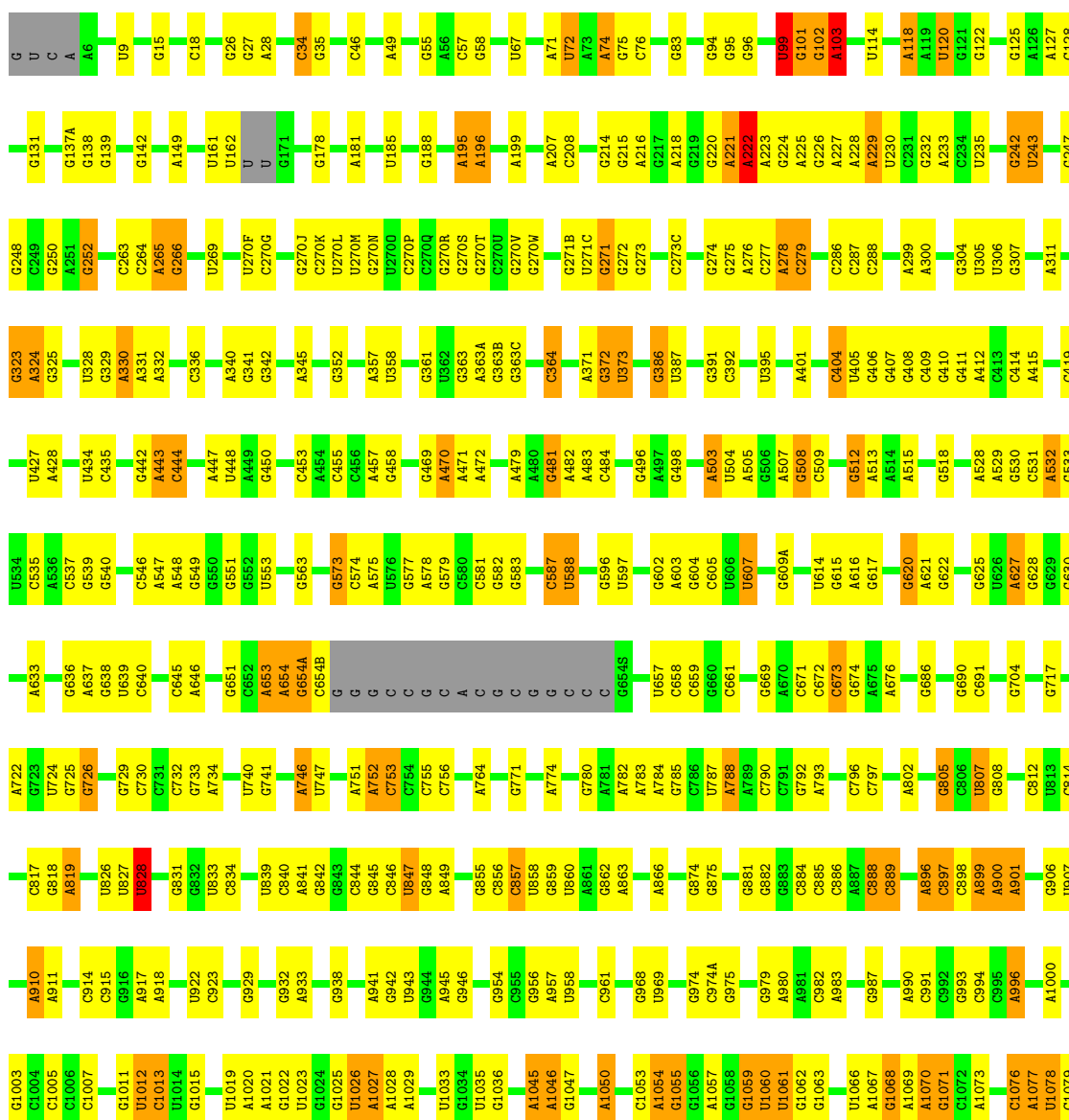
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

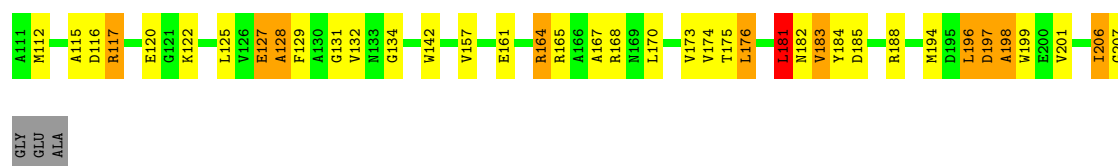
#### • Molecule 1: 23S ribosomal RNA

Chain A:



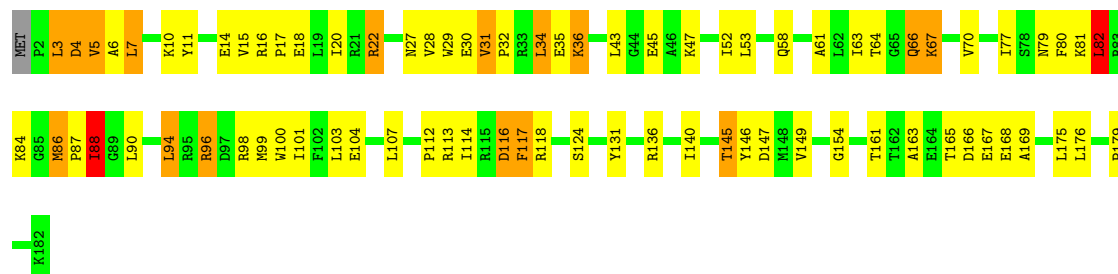
U2609	C2610	G2502	A2393	G2304	G2190	G2110	G1899	A1787	G1674	A1569	C1467	G1368	G1264	G1169	G1080
U2610	C2611	G2503	C2394	A2305	G2191	C2111	C1902	C1790	G1678	A1570	A1471	G1369	A1265	G1170	U1081
C2612	U2504	U2503	C2395	C2306	G2192	G2112	G1903	A1791	G1679	U1578	A1472	G1370	G1266	G1171	U1082
U2613	G2505	G2506	U2401	G2307	G2193	U2113	G1903	A1791	U1680	U1579	G1473	G1371	C1270	G1172	U1083
A2614	U2506	U2511	U2402	A2308	U2197	A2114	G1910	U1794	U1688	A1580	G1479	U1372	U1175	A1085	A1084
U2615	C2616	U2511	C2403	A2310	A2198	G2116	C1914	C1795	U1689	C1585	G1480	A1373	A1272	A1086	A1087
C2617	U2518	U2518	C2404	U2312	G2210	A2117	U1915	U1796	A1689	U1586	G1480	A1374	U1273	A1088	A1088
U2618	C2618	A2518	U2405	A2311	G2211	A2118	U1916	U1797	C1694	A1587	U1482	A1379	A1177	C1178	A1089
C2619	U2619	U2524	U2406	U2312	G2212	A2119	U1917	U1798	G1695	A1588	G1483	C1380	C1180	C1179	U1090
G2620	A2621	G2524	U2406	G2315	A2212	G2120	U1917	G1799	G1696	C1589	A1490	A1384	G1183	U1091	G1092
A2621	U2524	G2524	U2406	G2315	A2212	G2120	U1917	G1799	G1696	C1589	A1490	A1384	G1183	U1091	G1092
U2622	C2623	C2527	G2415	G2318	U2213	G2123	C1920	A1802	A1698	C1592	C1493	C1385	C1291	G1093	G1093
C2627	U2528	U2528	G2415	G2319	G2224	G2124	U1926	A1803	A1699	C1592	C1493	C1386	U1292	U1094	U1094
C2628	U2529	U2529	U2423	A2320	A2225	A2125	U1926	A1803	A1700	G1595	U1497	G1186	G1186	G1187	A1095
A2629	G2530	G2530	U2424	A2321	C2226	G2127	A1928	A1810	G1703	C1598	C1498	A1189	G1296	A1096	A1096
C2630	U2531	G2531	A2425	G2324	A2227	C2128	U1929	A1816	G1703	C1599	G1500	U1394	U1300	U1097	U1097
G2631	C2538	C2538	U2427	G2325	U2232	C2131	U1930	G1816	G1717	C1599	G1500	A1395	A1301	A1098	A1098
A2632	U2542	U2542	G2429	A2328	U2233	G2132	U1930	A1816	G1717	A1603	C1506	U1396	A1301	G1099	G1099
C2633	G2543	G2543	A2430	G2329	U2234	U2133	U1931	A1819	G1718	A1603	C1506	U1396	A1301	G1099	G1099
G2634	U2544	G2544	U2431	G2330	U2235	G2134	U1932	U1820	G1725	C1607	A1507	C1403	G1311	U1101	U1101
C2635	C2545	C2545	A2432	A2331	G2238	G2135	U1933	U1821	G1726	C1607	A1507	C1403	G1311	U1101	U1101
U2636	U2554	U2554	A2433	G2332	G2239	C2136	G1933	U1822	G1727	C1607	A1507	C1403	G1311	U1101	U1101
G2641	U2555	U2555	U2434	A2333	U2240	C2137	U1934	U1823	G1728	C1607	A1507	C1403	G1311	U1101	U1101
C2642	U2556	U2556	U2435	A2334	U2241	G2138	U1935	U1824	A1729	C1607	A1507	C1403	G1311	U1101	U1101
U2643	U2557	U2557	A2436	A2335	U2242	G2139	U1936	U1825	G1730	C1607	A1507	C1403	G1311	U1101	U1101
C2644	U2558	U2558	U2437	A2336	U2243	G2140	U1937	U1826	U1731	C1607	A1507	C1403	G1311	U1101	U1101
U2645	U2559	U2559	U2438	A2337	U2244	G2141	U1938	U1827	G1732	C1607	A1507	C1403	G1311	U1101	U1101
C2646	U2560	U2560	U2439	A2338	U2245	G2142	U1939	U1828	G1733	C1607	A1507	C1403	G1311	U1101	U1101
U2647	U2561	U2561	U2440	A2339	U2246	G2143	U1940	U1829	G1734	C1607	A1507	C1403	G1311	U1101	U1101
C2648	U2562	U2562	U2441	A2340	U2247	G2144	U1941	U1830	G1735	C1607	A1507	C1403	G1311	U1101	U1101
U2649	U2563	U2563	U2442	A2341	U2248	G2145	U1942	U1831	G1736	C1607	A1507	C1403	G1311	U1101	U1101
G2655	U2564	U2564	U2443	A2342	U2249	G2146	U1943	U1832	G1737	C1607	A1507	C1403	G1311	U1101	U1101
U2656	U2565	U2565	U2444	A2343	U2250	G2147	U1944	U1833	G1738	C1607	A1507	C1403	G1311	U1101	U1101
C2657	U2566	U2566	U2445	A2344	U2251	G2148	U1945	U1834	G1739	C1607	A1507	C1403	G1311	U1101	U1101
U2658	U2567	U2567	U2446	A2345	U2252	G2149	U1946	U1835	G1740	C1607	A1507	C1403	G1311	U1101	U1101
C2659	U2568	U2568	U2447	A2346	U2253	G2150	U1947	U1836	G1741	C1607	A1507	C1403	G1311	U1101	U1101
U2660	U2569	U2569	U2448	A2347	U2254	G2151	U1948	U1837	G1742	C1607	A1507	C1403	G1311	U1101	U1101
C2661	U2570	U2570	U2449	A2348	U2255	G2152	U1949	U1838	G1743	C1607	A1507	C1403	G1311	U1101	U1101
U2662	U2571	U2571	U2450	A2349	U2256	G2153	U1950	U1839	G1744	C1607	A1507	C1403	G1311	U1101	U1101
G2663	U2572	U2572	U2451	A2350	U2257	G2154	U1951	U1840	G1745	C1607	A1507	C1403	G1311	U1101	U1101
U2664	U2573	U2573	U2452	A2351	U2258	G2155	U1952	U1841	G1746	C1607	A1507	C1403	G1311	U1101	U1101
C2665	U2574	U2574	U2453	A2352	U2259	G2156	U1953	U1842	G1747	C1607	A1507	C1403	G1311	U1101	U1101
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C2667	U2576	U2576	U2455	A2354	U2261	G2158	U1955	U1844	G1749	C1607	A1507	C1403	G1311	U1101	U1101
U2668	U2577	U2577	U2456	A2355	U2262	G2159	U1956	U1845	G1750	C1607	A1507	C1403	G1311	U1101	U1101
C2669	U2578	U2578	U2457	A2356	U2263	G2160	U1957	U1846	G1751	C1607	A1507	C1403	G1311	U1101	U1101
U2670	U2579	U2579	U2458	A2357	U2264	G2161	U1958	U1847	G1752	C1607	A1507	C1403	G1311	U1101	U1101
C2671	U2580	U2580	U2459	A2358	U2265	G2162	U1959	U1848	G1753	C1607	A1507	C1403	G1311	U1101	U1101
U2672	U2581	U2581	U2460	A2359	U2266	G2163	U1960	U1849	G1754	C1607	A1507	C1403	G1311	U1101	U1101
G2673	U2582	U2582	U2461	A2360	U2267	G2164	U1961	U1850	G1755	C1607	A1507	C1403	G1311	U1101	U1101
C2674	U2583	U2583	U2462	A2361	U2268	G2165	U1962	U1851	G1756	C1607	A1507	C1403	G1311	U1101	U1101
U2675	U2584	U2584	U2463	A2362	U2269	G2166	U1963	U1852	G1757	C1607	A1507	C1403	G1311	U1101	U1101
C2676	U2585	U2585	U2464	A2363	U2270	G2167	U1964	U1853	G1758	C1607	A1507	C1403	G1311	U1101	U1101
U2677	U2586	U2586	U2465	A2364	U2271	G2168	U1965	U1854	G1759	C1607	A1507	C1403	G1311	U1101	U1101
C2678	U2587	U2587	U2466	A2365	U2272	G2169	U1966	U1855	G1760	C1607	A1507	C1403	G1311	U1101	U1101
U2679	U2588	U2588	U2467	A2366	U2273	G2170	U1967	U1856	G1761	C1607	A1507	C1403	G1311	U1101	U1101
C2680	U2589	U2589	U2468	A2367	U2274	G2171	U1968	U1857	G1762	C1607	A1507	C1403	G1311	U1101	U1101
U2681	U2590	U2590	U2469	A2368	U2275	G2172	U1969	U1858	G1763	C1607	A1507	C1403	G1311	U1101	U1101
C2682	U2591	U2591	U2470	A2369	U2276	G2173	U1970	U1859	G1764	C1607	A1507	C1403	G1311	U1101	U1101
G2683	U2592	U2592	U2471	A2370	U2277	G2174	U1971	U1860	G1765	C1607	A1507	C1403	G1311	U1101	U1101
U2684	U2593	U2593	U2472	A2371	U2278	G2175	U1972	U1861	G1766	C1607	A1507	C1403	G1311	U1101	U1101
C2685	U2594	U2594	U2473	A2372	U2279	G2176	U1973	U1862	G1767	C1607	A1507	C1403	G1311	U1101	U1101
U2686	U2595	U2595	U2474	A2373	U2280	G2177	U1974	U1863	G1768	C1607	A1507	C1403	G1311	U1101	U1101
C2687	U2596	U2596	U2475	A2374	U2281	G2178	U1975	U1864	G1769	C1607	A1507	C1403	G1311	U1101	U1101
U2688	U2597	U2597	U2476	A2375	U2282	G2179	U1976	U1865	G1770	C1607	A1507	C1403	G1311	U1101	U1101
C2689	U2598	U2598	U2477	A2376	U2283	G2180	U1977	U1866	G1771	C1607	A1507	C1403	G1311	U1101	U1101
U2689	U2599	U2599	U2478	A2377	U2284	G2181	U1978	U1867	G1772	C1607	A1507	C1403	G1311	U1101	U1101
C2690	U2600	U2600	U2479	A2378	U2285	G2182	U1979	U1868	G1773	C1607	A1507	C1403	G1311	U1101	U1101
U2691	U2601	U2601	U2480	A2379	U2286	G2183	U1980	U1869	G1774	C1607	A1507	C1403	G1311	U1101	U1101
C2692	U2602	U2602	U2481	A2380	U2287	G2184	U1981	U1870	G1775	C1607	A1507	C1403	G1311	U1101	U1101
U2693	U2603	U2603	U2482	A2381	U2288	G2185	U1982	U1871	G1776	C1607	A1507	C1403	G1311	U1101	U1101
C2694	U2604	U2604	U2483	A2382	U2289	G2186	U1983	U1872	G1777	C1607	A1507	C1403	G1311	U1101	U1101
U2695	U2605	U2605	U2484	A2383	U2290	G2187	U1984	U1873	G1778	C1607	A1507	C1403	G1311	U1101	U1101
G2696	U2606	U2606	U2485	A2384	U2291	G2188	U1985	U1874	G1779	C1607	A1507	C1403	G1311	U1101	U1101
U2697	U2607	U2607	U2486	A2385	U2292	G2189	U1986	U1875	G1780	C1607	A1507	C1403	G1311	U1101	U1101
C2698	U2608	U2608	U2487	A2386	U2293	G2190	U1987	U1876	G1781	C1607	A1507	C1403	G1311	U1101	U1101
U2699	U2609	U2609	U2488	A2387	U2294	G2191	U1988	U1877	G1782	C1607	A1507	C1403	G1311	U1101	U1101
C2700	U2610	U2610	U2489	A2388	U2295	G2192	U1989	U1878	G1783	C1607	A1507	C1403	G1311		





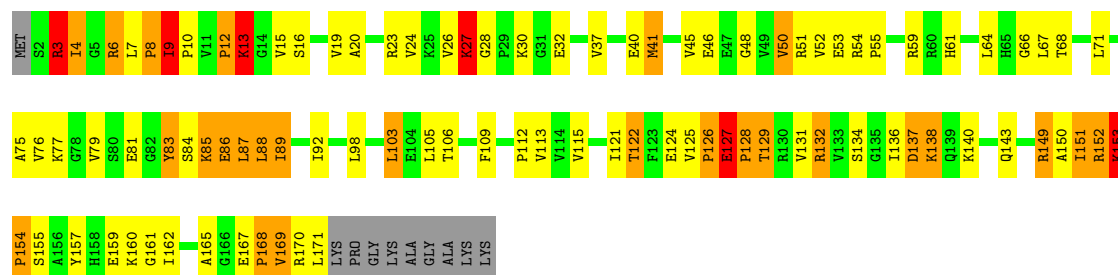
• Molecule 6: 50S ribosomal protein L5

Chain F:



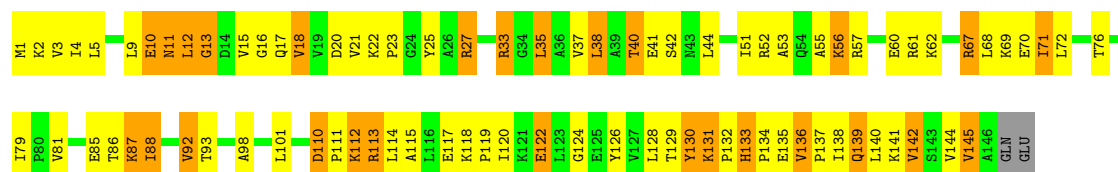
• Molecule 7: 50S ribosomal protein L6

Chain G:



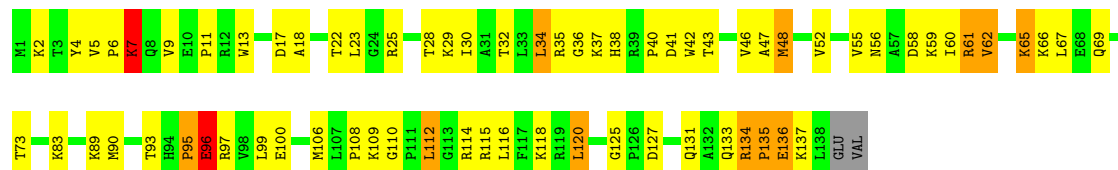
• Molecule 8: 50S ribosomal protein L9

Chain H:



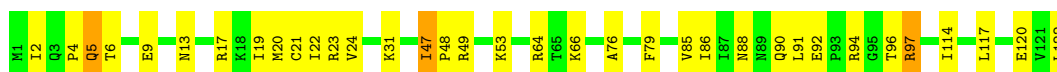
• Molecule 9: 50S ribosomal protein L13

Chain I:



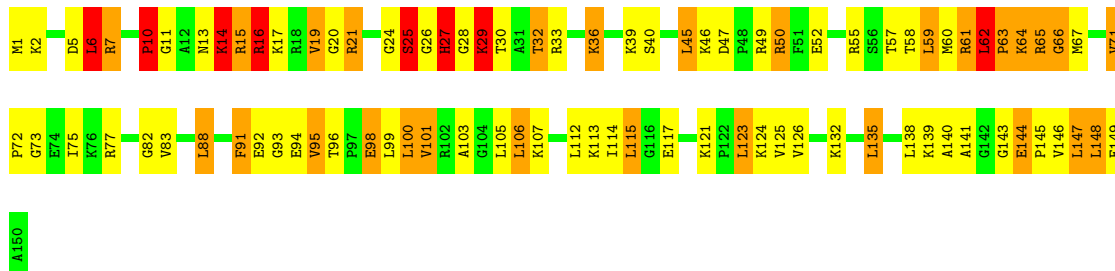
• Molecule 10: 50S ribosomal protein L14

Chain J:



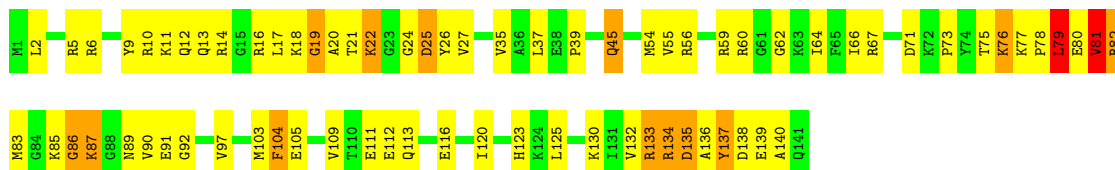
- Molecule 11: 50S ribosomal protein L15

Chain K:



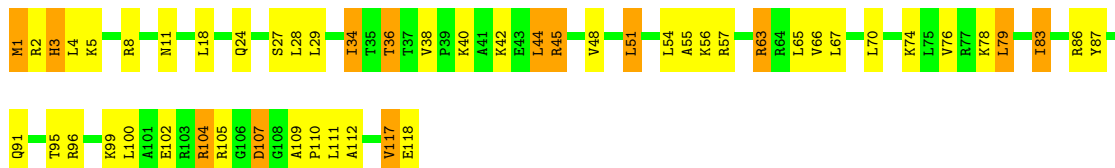
- Molecule 12: 50S ribosomal protein L16

Chain L:



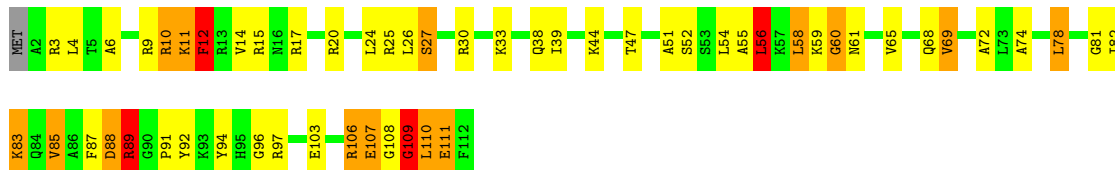
- Molecule 13: 50S ribosomal protein L17

Chain M:



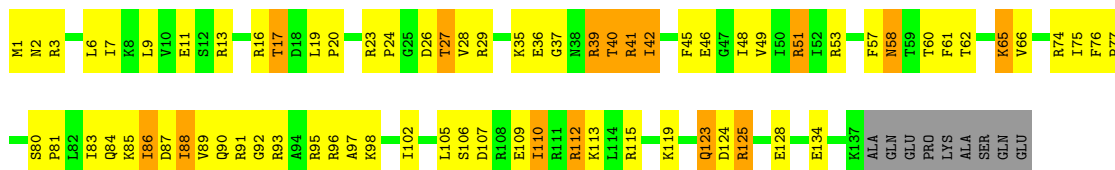
- Molecule 14: 50S ribosomal protein L18

Chain N:



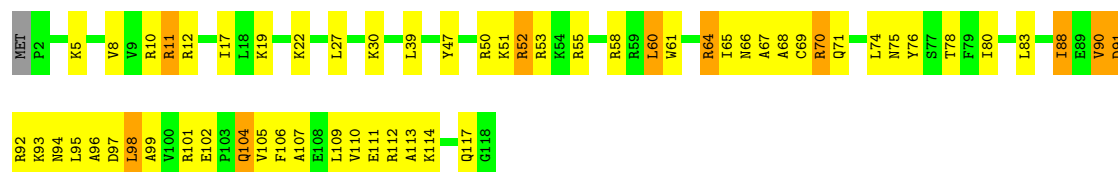
- Molecule 15: 50S ribosomal protein L19

Chain O:



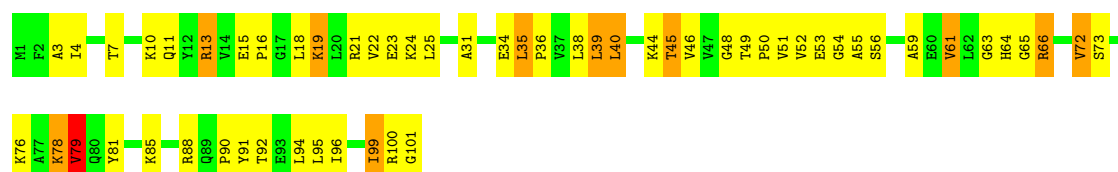
- Molecule 16: 50S ribosomal protein L20

Chain P: 



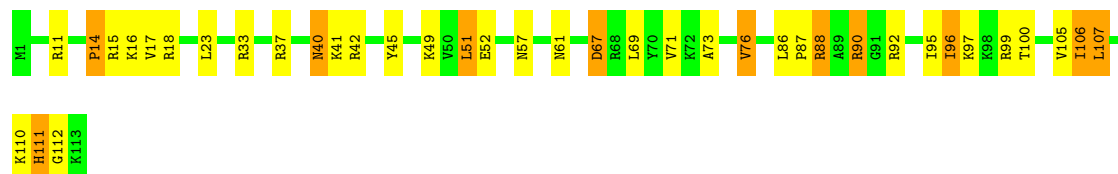
- Molecule 17: 50S ribosomal protein L21

Chain Q: 



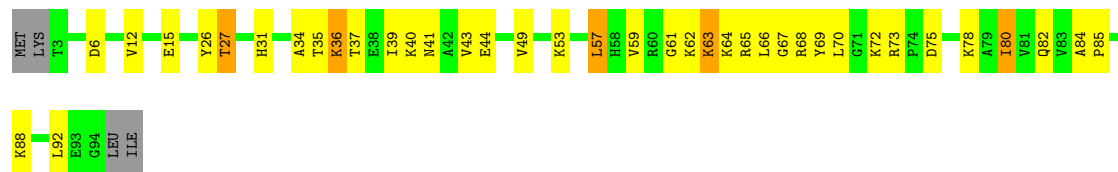
- Molecule 18: 50S ribosomal protein L22

Chain R: 



- Molecule 19: 50S ribosomal protein L23

Chain S: 



- Molecule 20: 50S ribosomal protein L24

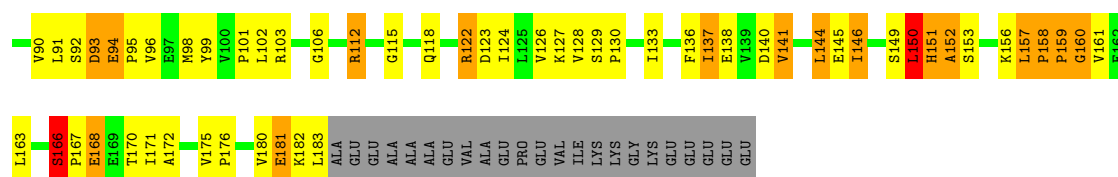
Chain T: 



- Molecule 21: 50S ribosomal protein L25

Chain U: 





- Molecule 22: 50S ribosomal protein L27

Chain V:

- Molecule 23: 50S ribosomal protein L28

Chain W:

- Molecule 24: 50S ribosomal protein L29

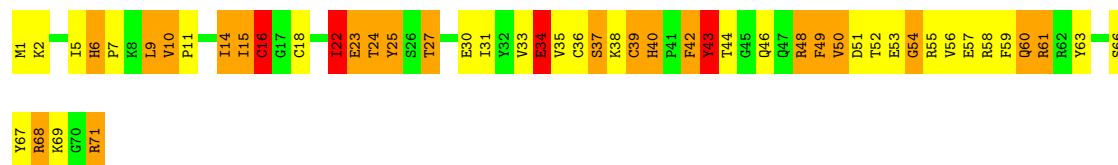
Chain X:

- Molecule 25: 50S ribosomal protein L30

Chain Y:

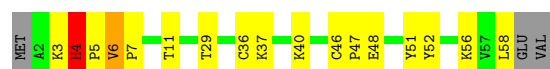
- Molecule 26: 50S ribosomal protein L31

Chain Z:



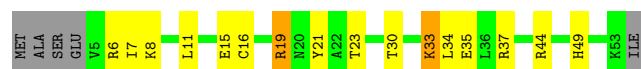
- Molecule 27: 50S ribosomal protein L32

Chain a:



- Molecule 28: 50S ribosomal protein L33

Chain b:





- Molecule 29: 50S ribosomal protein L34

Chain c: 



- Molecule 30: 50S ribosomal protein L35

Chain d: 



- Molecule 31: 50S ribosomal protein L36

Chain e: 



- Molecule 32: T17-GLY-GLY-PRO-LYS-LYS-LYS-LYS-LYS-VAL-GLY-GLY

Chain f: 



## 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, $\alpha$ , $\beta$ , $\gamma$	209.24Å 443.46Å 618.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 3.60	Depositor
% Data completeness (in resolution range)	98.1 (49.79-3.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, $R_{free}$	0.222 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	92327	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	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, T17, 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	0.29	0/69543	0.83	41/108563 (0.0%)
2	B	0.29	0/2878	0.91	11/4490 (0.2%)
3	C	0.57	0/2165	0.77	1/2919 (0.0%)
4	D	0.48	1/1601 (0.1%)	0.74	2/2160 (0.1%)
5	E	0.48	0/1620	0.71	1/2194 (0.0%)
6	F	0.40	0/1499	0.60	0/2016
7	G	0.50	1/1332 (0.1%)	0.76	2/1802 (0.1%)
8	H	0.38	0/1151	0.66	0/1558
9	I	0.43	0/1131	0.64	0/1525
10	J	0.50	0/943	0.65	0/1269
11	K	0.55	2/1162 (0.2%)	0.93	4/1544 (0.3%)
12	L	0.56	0/1143	0.78	0/1527
13	M	0.45	0/982	0.73	0/1312
14	N	0.39	0/892	0.71	0/1187
15	O	0.44	0/1155	0.67	0/1542
16	P	0.50	0/982	0.69	0/1306
17	Q	0.46	0/790	0.73	1/1057 (0.1%)
18	R	0.45	0/911	0.68	0/1220
19	S	0.50	0/739	0.66	0/993
20	T	0.45	0/798	0.69	0/1064
21	U	0.45	2/1493 (0.1%)	0.68	4/2026 (0.2%)
22	V	0.48	0/657	0.69	0/874
23	W	0.46	0/770	0.69	0/1022
24	X	0.52	0/583	0.73	0/771
25	Y	0.41	0/474	0.59	0/635
26	Z	0.37	0/594	0.69	0/795
27	a	0.68	3/456 (0.7%)	0.89	3/617 (0.5%)
28	b	0.37	0/431	0.68	0/575
29	c	0.57	0/438	0.71	0/575
30	d	0.58	0/525	0.82	0/691
31	e	0.32	0/310	0.48	0/407
32	f	0.25	0/56	0.45	0/70

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.35	9/100204 (0.0%)	0.80	70/150306 (0.0%)

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
5	E	0	1
7	G	0	1
14	N	0	1
21	U	0	1
24	X	0	1
30	d	0	2
All	All	0	7

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	63	PRO	N-CD	6.16	1.56	1.47
21	U	159	PRO	N-CD	5.60	1.55	1.47
27	a	5	PRO	N-CD	5.52	1.55	1.47
11	K	10	PRO	N-CD	5.41	1.55	1.47
4	D	22	PRO	N-CD	5.35	1.55	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	771	G	C2-N3-C4	-10.26	106.77	111.90
1	A	771	G	N9-C4-C5	-8.13	102.15	105.40
1	A	673	C	C2-N3-C4	-7.98	115.91	119.90
2	B	81	G	C5-C6-O6	-7.36	124.18	128.60
1	A	1950	G	N3-C4-N9	6.93	130.16	126.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	47	GLY	Peptide
7	G	127	GLU	Peptide
14	N	109	GLY	Peptide

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Mol	Chain	Res	Type	Group
21	U	181	GLU	Peptide
24	X	17	SER	Peptide

## 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	62091	0	31294	688	0
2	B	2573	0	1306	35	0
3	C	2115	0	2195	128	0
4	D	1568	0	1634	78	0
5	E	1585	0	1632	63	0
6	F	1474	0	1535	54	0
7	G	1307	0	1382	89	0
8	H	1136	0	1223	48	0
9	I	1104	0	1180	50	0
10	J	933	0	996	19	0
11	K	1145	0	1228	83	0
12	L	1122	0	1178	50	0
13	M	968	0	1033	33	0
14	N	882	0	943	45	0
15	O	1141	0	1202	50	0
16	P	964	0	1022	52	0
17	Q	779	0	852	43	0
18	R	900	0	964	26	0
19	S	725	0	778	21	0
20	T	785	0	878	40	0
21	U	1461	0	1493	80	0
22	V	648	0	672	29	0
23	W	763	0	848	28	0
24	X	581	0	629	23	0
25	Y	469	0	518	15	0
26	Z	581	0	574	47	0
27	a	442	0	465	0	0
28	b	424	0	450	0	0
29	c	430	0	480	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	d	517	0	582	0	0
31	e	307	0	336	0	0
32	f	116	0	67	0	0
33	A	279	0	0	0	0
33	B	4	0	0	0	0
33	C	1	0	0	0	0
33	D	2	0	0	0	0
33	K	1	0	0	0	0
33	L	1	0	0	0	0
33	S	1	0	0	0	0
33	c	1	0	0	0	0
34	e	1	0	0	0	0
All	All	92327	0	61569	1694	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 12.

The worst 5 of 1694 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:134:ARG:CZ	21:U:122:ARG:HH21	1.34	1.39
4:D:14:ILE:HG22	4:D:21:VAL:CG2	1.56	1.35
3:C:121:PRO:HB3	3:C:135:PHE:CE2	1.64	1.31
4:D:14:ILE:CG2	4:D:21:VAL:HG23	1.62	1.29
21:U:93:ASP:O	21:U:94:GLU:HG2	1.10	1.24

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	C	270/276 (98%)	228 (84%)	33 (12%)	9 (3%)	6	55
4	D	203/206 (98%)	144 (71%)	42 (21%)	17 (8%)	1	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	200/210 (95%)	168 (84%)	24 (12%)	8 (4%)	5	48
6	F	179/182 (98%)	142 (79%)	25 (14%)	12 (7%)	2	31
7	G	168/180 (93%)	124 (74%)	23 (14%)	21 (12%)	1	12
8	H	144/148 (97%)	107 (74%)	20 (14%)	17 (12%)	1	13
9	I	136/140 (97%)	105 (77%)	17 (12%)	14 (10%)	1	16
10	J	120/122 (98%)	108 (90%)	10 (8%)	2 (2%)	14	70
11	K	148/150 (99%)	108 (73%)	22 (15%)	18 (12%)	1	12
12	L	139/141 (99%)	98 (70%)	22 (16%)	19 (14%)	0	9
13	M	116/118 (98%)	99 (85%)	11 (10%)	6 (5%)	3	39
14	N	109/112 (97%)	79 (72%)	17 (16%)	13 (12%)	1	12
15	O	135/146 (92%)	108 (80%)	17 (13%)	10 (7%)	2	28
16	P	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	6	53
17	Q	99/101 (98%)	79 (80%)	12 (12%)	8 (8%)	1	24
18	R	111/113 (98%)	100 (90%)	9 (8%)	2 (2%)	13	68
19	S	90/96 (94%)	82 (91%)	6 (7%)	2 (2%)	10	64
20	T	100/110 (91%)	70 (70%)	18 (18%)	12 (12%)	1	12
21	U	181/206 (88%)	125 (69%)	38 (21%)	18 (10%)	1	18
22	V	80/85 (94%)	73 (91%)	7 (9%)	0	100	100
23	W	95/98 (97%)	72 (76%)	17 (18%)	6 (6%)	2	33
24	X	67/72 (93%)	55 (82%)	6 (9%)	6 (9%)	1	21
25	Y	57/60 (95%)	52 (91%)	4 (7%)	1 (2%)	13	68
26	Z	69/71 (97%)	35 (51%)	15 (22%)	19 (28%)	0	1
27	a	55/60 (92%)	45 (82%)	9 (16%)	1 (2%)	13	68
28	b	47/54 (87%)	22 (47%)	17 (36%)	8 (17%)	0	5
29	c	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	11	65
30	d	62/65 (95%)	48 (77%)	10 (16%)	4 (6%)	2	32
31	e	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
32	f	7/12 (58%)	3 (43%)	3 (43%)	1 (14%)	0	8
All	All	3384/3538 (96%)	2655 (78%)	470 (14%)	259 (8%)	1	26

5 of 259 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	26	LYS
3	C	28	GLU
3	C	122	ASP
3	C	123	ALA
4	D	2	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	C	214/218 (98%)	180 (84%)	34 (16%)	4	24
4	D	165/166 (99%)	135 (82%)	30 (18%)	2	16
5	E	161/166 (97%)	137 (85%)	24 (15%)	4	27
6	F	155/156 (99%)	134 (86%)	21 (14%)	6	32
7	G	142/148 (96%)	116 (82%)	26 (18%)	2	16
8	H	122/124 (98%)	92 (75%)	30 (25%)	1	7
9	I	117/119 (98%)	96 (82%)	21 (18%)	2	17
10	J	100/100 (100%)	89 (89%)	11 (11%)	9	44
11	K	116/116 (100%)	81 (70%)	35 (30%)	0	4
12	L	111/111 (100%)	92 (83%)	19 (17%)	3	20
13	M	101/101 (100%)	80 (79%)	21 (21%)	2	11
14	N	87/88 (99%)	68 (78%)	19 (22%)	1	9
15	O	120/127 (94%)	98 (82%)	22 (18%)	2	16
16	P	93/94 (99%)	77 (83%)	16 (17%)	3	19
17	Q	82/82 (100%)	67 (82%)	15 (18%)	2	16
18	R	92/92 (100%)	75 (82%)	17 (18%)	2	15
19	S	74/78 (95%)	60 (81%)	14 (19%)	2	14
20	T	85/91 (93%)	64 (75%)	21 (25%)	1	7
21	U	162/179 (90%)	133 (82%)	29 (18%)	2	17
22	V	65/67 (97%)	59 (91%)	6 (9%)	13	55
23	W	82/83 (99%)	70 (85%)	12 (15%)	5	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	X	64/67 (96%)	47 (73%)	17 (27%)	1	6
25	Y	51/52 (98%)	43 (84%)	8 (16%)	4	25
26	Z	63/63 (100%)	43 (68%)	20 (32%)	0	3
27	a	49/52 (94%)	36 (74%)	13 (26%)	1	6
28	b	48/52 (92%)	38 (79%)	10 (21%)	2	11
29	c	42/42 (100%)	35 (83%)	7 (17%)	3	21
30	d	54/55 (98%)	41 (76%)	13 (24%)	1	7
31	e	34/34 (100%)	32 (94%)	2 (6%)	28	76
32	f	5/7 (71%)	4 (80%)	1 (20%)	2	12
All	All	2856/2930 (98%)	2322 (81%)	534 (19%)	2	15

5 of 534 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	79	LEU
15	O	51	ARG
27	a	36	CYS
12	L	132	VAL
13	M	105	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2880/2915 (98%)	563 (19%)	57 (1%)
2	B	119/122 (97%)	21 (17%)	1 (0%)
All	All	2999/3037 (98%)	584 (19%)	58 (1%)

5 of 584 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	15	G
1	A	34	C
1	A	35	G
1	A	46	C

5 of 58 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1045	A
1	A	1210	A
1	A	2756	U
1	A	1078	U
1	A	1109	C

## 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 291 ligands modelled in this entry, 291 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.