



wwPDB X-ray Structure Validation Summary Report

Sep 15, 2014 – 10:58 AM EDT

PDB ID : 1VVO
Title : Crystal Structure of Frameshift Suppressor tRNA SufA6 Bound to Codon CCC-U on the Ribosome
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-06-07
Resolution : 3.22 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>

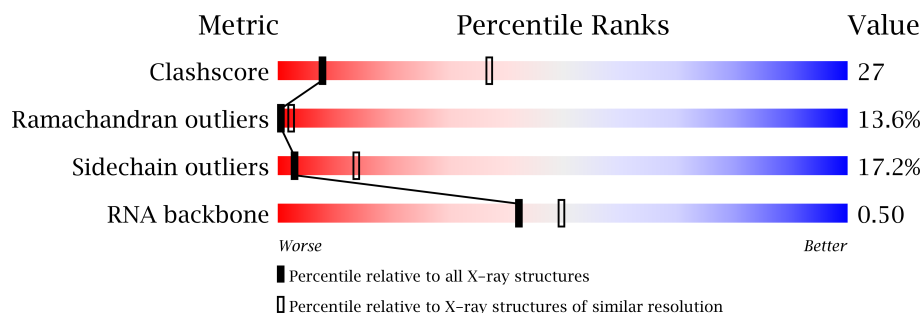
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 3.22 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	1072 (3.28-3.16)
Ramachandran outliers	78287	1052 (3.28-3.16)
Sidechain outliers	78261	1051 (3.28-3.16)
RNA backbone	1838	1004 (3.74-2.70)

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	2916	
2	B	122	
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	
14	S	112	

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Mol	Chain	Length	Quality of chain
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	
32	a	3	

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 92290 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 rRNA.

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 rRNA.

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	D	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	E	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	F	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	G	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	H	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	I	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	N	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	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	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	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	111	Total	C	N	O			
			882	556	176	150	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	U	117	Total	C	N	O	S			
			964	610	202	151	1	0	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			
			779	501	142	135	1	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Z	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	0	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	1	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	2	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	3	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	4	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	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	6	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	7	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	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 a RNA chain called tRNA acceptor end mimic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	a	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	D	1	Total	Mg	0	0
			1	1		
33	E	2	Total	Mg	0	0
			2	2		
33	B	3	Total	Mg	0	0
			3	3		
33	7	1	Total	Mg	0	0
			1	1		
33	A	269	Total	Mg	0	0
			269	269		
33	5	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	X	1	Total	Mg	0	0
			1	1		

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

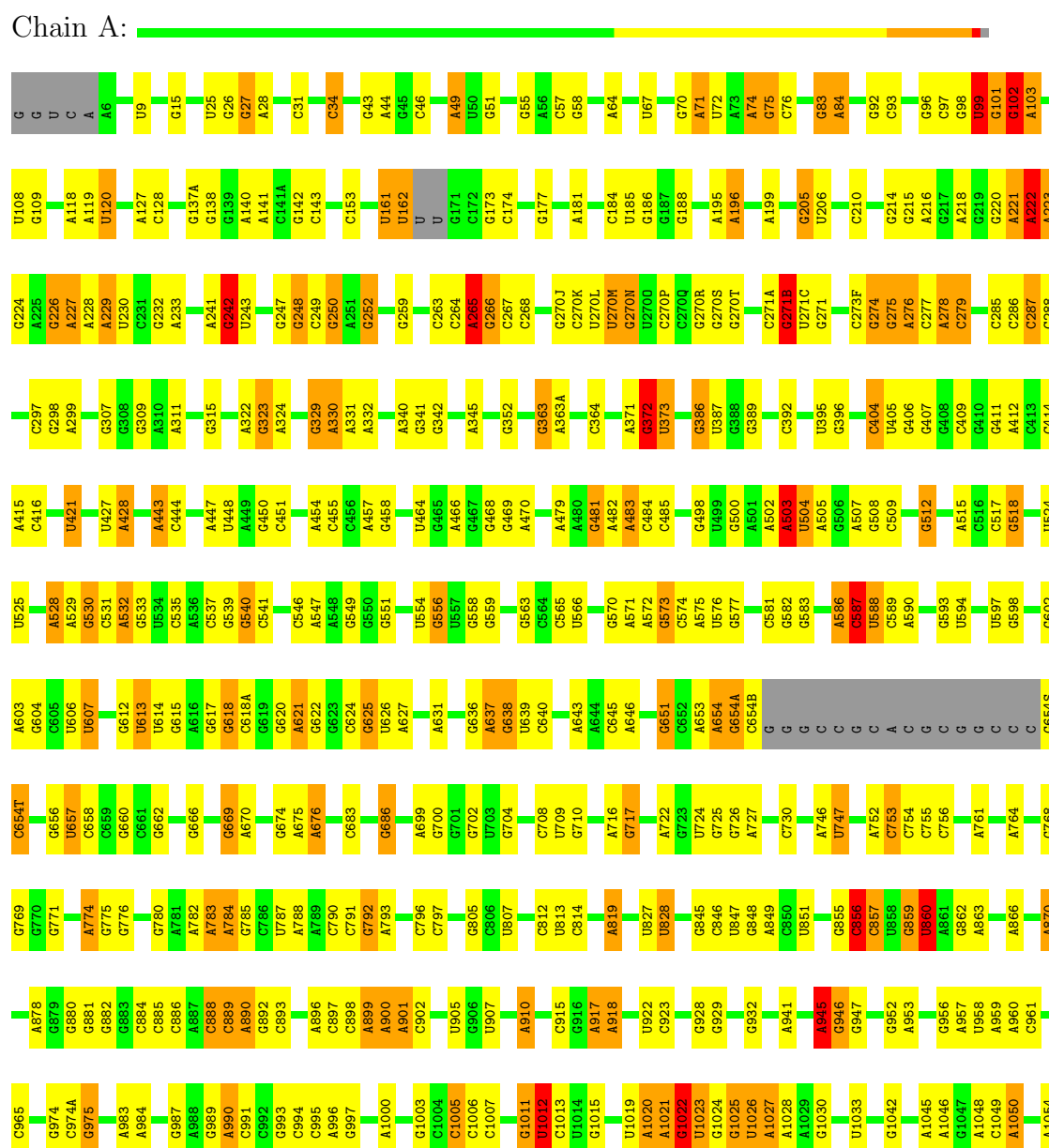
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	9	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

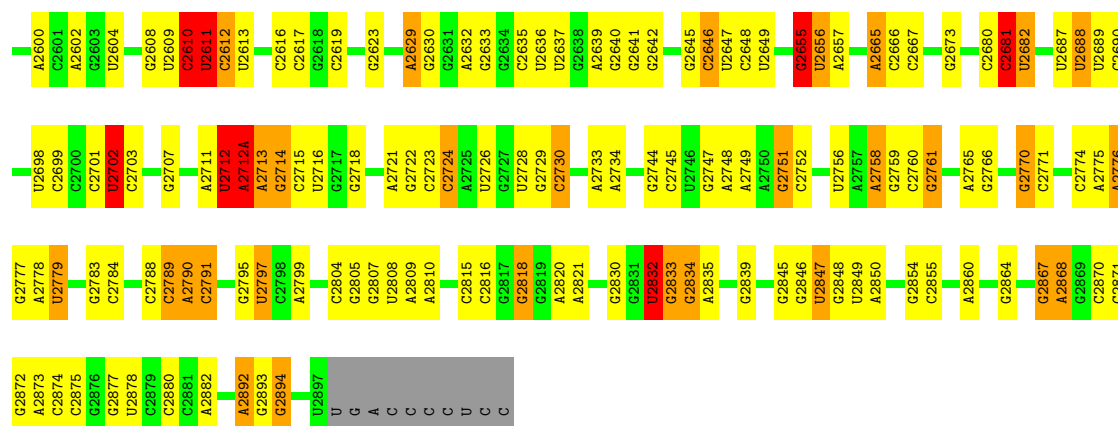
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 rRNA

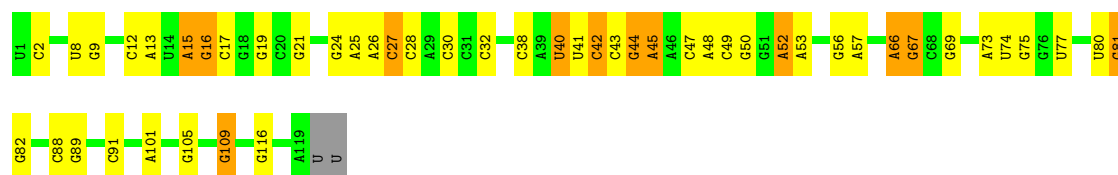


G2494	G2410	G2318	G2226	C2128	A2030	U1931	G1816	G1717	A1587	C1493	C1408	A1317	G1209	A1128	G1055
G2502	A2411	A2320	A2227	G2131	A2031	A1932	G1817	G1718	C1588	A1494	C1411	A1321	A1129	A1129	G1056
U2504	G2414	G2321	U2232	U2132	A2032	G1933	U1818	G1725	C1589	A1495	C1411	A1321	U1211	A1130	G1057
G2505	G2415	G2323	G2234	G2133	A2033	A1936	U1820	G1728	C1592	U1497	G1416	G1328	C1217	G1131	G1058
U2506	C2416	C2324	G2238	A2135	C2040	U1939	G1824	A1729	G1595	C1505	C1417	U1329	C1135	C1135	U1060
C2507	U2419	G2326	G2239	C2136	U2041	U1940	A1825	U1730	G1598	C1506	A1418	C1330	A1220	G1136	U1061
G2508	U2420	A2327	G2239	A2135	C2043	C1941	G1826	A1732	C1599	A1507	A1419	G1332	C1221	G1137	G1062
C2512	U2423	A2328	U2243	C2146	A2051	G1950	A1829	C1734	C1600	C1509	G1422	A1336	G1228	G1139	G1063
G2513	U2424	G2329	U2244	G2147	G2052	U1951	A1835	A1734	G1595	A1510	G1423	G1337	C1230	C1140	U1066
A2518	C2424	G2330	U2245	G2148	G2053	A1952	G1836	G1743	C1607	A1511	G1424	U1340	G1231	U1141	A1067
U2519	A2426	G2331	G2246	U2149	A2054	A1953	C1836	G1743	A1608	C1512	G1425	U1340	A1142A	U1142	A1068
G2524	A2429	G2334	G2250	G2151	G2056	U1955	G1846	G1750	A1610	U1514	A1427	U1341	G1238	G1149	A1070
G2525	A2335	A2336	G2251	G2152	A2059	U1956	A1847	C1754	A1614	U1520	G1428	G1348	A1241	G1150	G1071
G2529	C2343	A2337	G2252	G2157	A2060	C1957	A1848	A1755	A1614	U1520	G1429	A1349	G1151	C1151	C1076
U2537	U2344	G2345	A2267	A2160	G2061	G1958	A1853	G1756	C1617	A1528	C1430	U1352	G1244	C1152	U1077
C2538	A2346	A2346	A2268	G2160	C2063	A1960	G1858	U1757	A1618	A1529	U1431	U1352	G1250	G1153	U1078
U2438	U2347	C2347	G2275	C2164	U2068	U1963	A1859	A1759	G1622	G1530	A1434	A1353	G1251	G1154	C1079
A2439	U2348	U2348	G2276	G2165	G2069	C1967	U1864	A1762	U1639	C1533	G1441	G1356	G1252	A1155	C1080
G2543	C2440	G2349	G2277	C2166	A2069	G1968	C1870	G1764	C1640	G1534	G1442	A1359	C1256	G1162	U1082
C2441	C2441	C2350	U2167	U2167	U2074	A1969	C1870	G1764	G1648	U1535	A1444A	G1364	C1257	U1165	U1083
G2545	G2447	C2355	G2280	A2169	U2075	A1970	A1871	A1772	C1648	C1537	C1445	G1364	C1166	C1166	A1086
U2547	A2448	C2356	C2283	A2170	U2086	A1972	G1878	G1770	G1653	G1539	A1449	A1365	U1263	G1169	G1087
G2548	U2449	U2357	C2284	A2173	G2087	U1978	C1882	C1771	A1654	U1540	G1449A	G1368	G1266	G1170	A1088
U2554	G2455	A2361	C2285	A2176	G2093	C1979	G1883	A1773	G1666	U1541	G1454	G1371	A1269	A1174	G1093
C2558	U2456	A2361	A2287	C2179	G2094	A1981	A1885	A1780	G1667	G1542	G1455	A1373	C1270	U1175	U1094
U2562	G2459	C2364	G2289	C2179	C2095	C1982	G1888	A1783	G1674	A1545	C1458	A1379	G1271	G1176	A1095
U2563	C2466	G2365	U2291	U2180	U2096	U1989	A1889	A1783	A1677	C1547	G1458	A1379	G1271	G1176	A1096
A2565	C2467	A2369	C2292	G2181	C2097	C1990	A1889	A1786	C1677	G1547	G1459	A1384	U1273	C1177	U1097
A2566	G2468	C2373	C2293	C2183	U2099	U1991	G1899	A1787	G1678	C1550	G1460	G1385	C1180	A1098	G1099
C2567	A2469	G2376	C2294	G2187	U2102	G1993	G1902	C1790	G1681	C1551	C1464	C1386	G1279	C1180	C1100
G2568	G2470	A2377	C2295	G2187	U2102	U1993	G1903	A1791	G1681	C1551	C1464	C1386	G1279	C1180	C1101
G2569	C2475	A2377	A2298	G2190	C2105	G1998	G1906	A1794	U1688	A1554	G1465	G1389	A1287	G1184	C1102
A2572	A2476	G2382	G2299	G2191	G2106	G1998	G1906	C1795	A1689	A1554	G1466	U1390	A1287	G1187	A1103
C2573	A2477	G2383	G2302	G2192	G2106	G1998	A1913	U1796	C1694	C1557	G1467	U1391	C1291	U1188	C1104
G2473	A2478	G2384	G2303	G2193	C2111	G2009	A1913	C1797	G1695	G1559	A1471	U1391	C1291	A1189	U1105
G2481	G2481	C2385	G2304	A2198	G2112	G2012	A1918	U1798	G1696	A1569	G1478	U1394	U1300	G1195	C1109
G2482	C2482	G2385	A2305	A2199	U2113	A2013	A1919	G1799	U1693	A1569	G1478	U1394	U1300	G1195	C1109
G2483	A2392	G2386	A2306	A2199	A2014	A2014	A1919	C1799	C1697	A1569	G1478	U1394	A1301	G1195	A1111
G2484	A2393	G2387	G2307	G2210	A2015	A2015	C1920	C1800	A1698	C1575	U1482	U1397	A1302	U1199	G1112
U2580	C2394	G2308	G2308	G2211	G2115	A2015	G1920	G1801	G1699	U1576	U1482	C1399	G1303	C1200	G1113
G2485	G2485	C2394	A2309	G2212	G2116	A2020	U1923	A1802	A1700	C1577	G1484	G1400	C1304	C1201	G1114
G2581	G2485	C2394	A2309	G2212	A2117	C2021	C1924	A1803	A1700	U1578	G1485	G1401	C1304	C1201	G1114
G2582	U2401	U2401	A2310	G2213	U2118	U2022	C1924	A1803	A1700	U1578	G1485	G1401	C1304	C1201	G1114
G2583	G2489	C2402	A2311	G2213	A2119	G2023	U1926	G1811	G1705	A1579	G1486	C1402	G1203	G1203	G1120
U2584	C2490	C2403	U2312	G2216	A2119	G2023	U1926	A1812	U1706	A1579	G1486	C1402	G1203	G1203	G1120
U2491	U2491	C2404	U2312	G2216	G2120	G1581	A1927	A1813	A1813	A1580	G1487	C1404	A1204	G1121	G1122
U2585	U2492	G2405	G2315	G2224	A2126	C2025	A1928	G1814	U1709	G1581	G1488	C1404	G1206	G1206	G1125
U2591	U2493	U2493	G2315	G2224	A2126	C2026	G1929	G1814	C1710	C1585	A1490	C1407	U1313	G1207	G1125
U2591	U2493	U2493	G2315	G2224	A2126	C2026	G1929	G1814	C1710	C1585	A1490	C1407	U1313	G1207	G1125



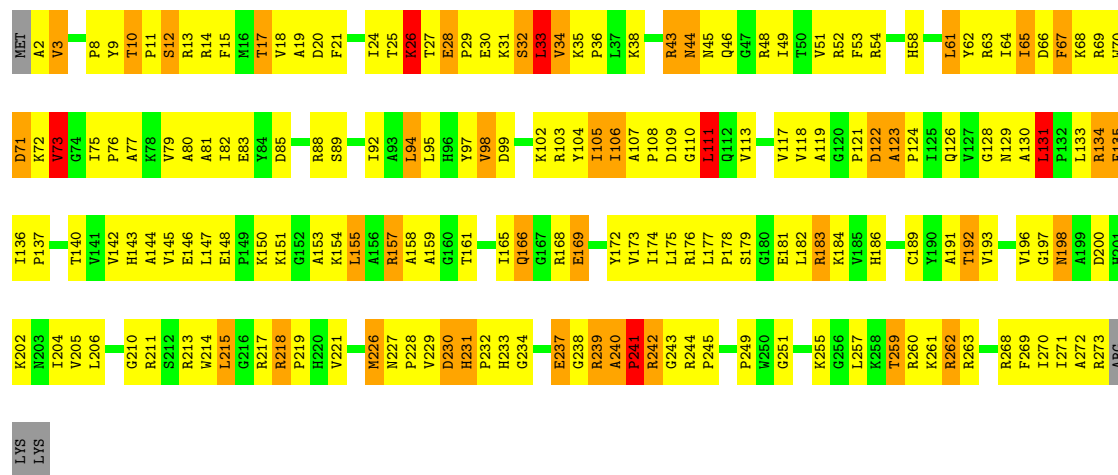
• Molecule 2: 5S rRNA

Chain B:



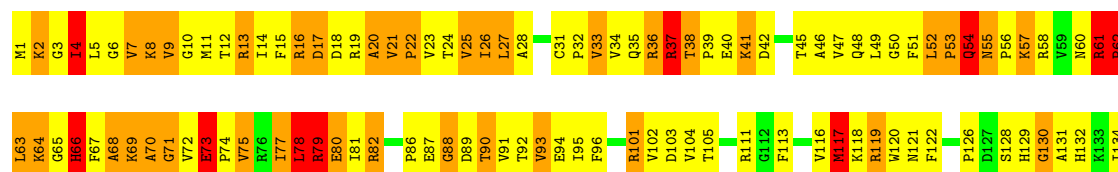
• Molecule 3: 50S ribosomal protein L2

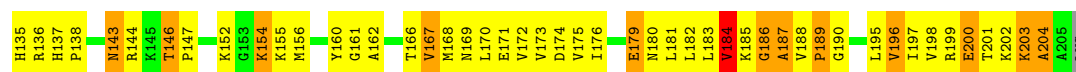
Chain D:



• Molecule 4: 50S ribosomal protein L3

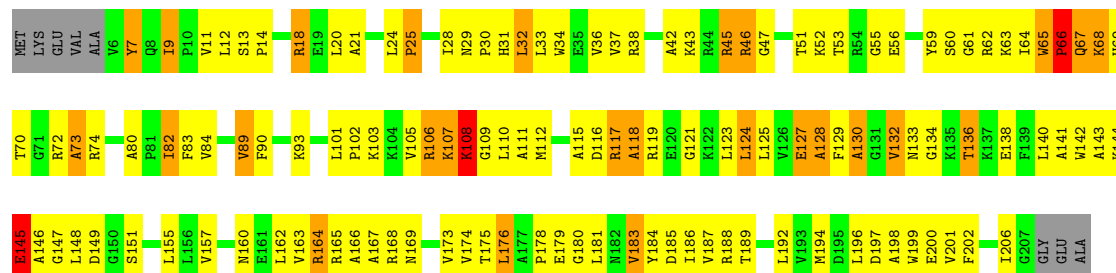
Chain E:





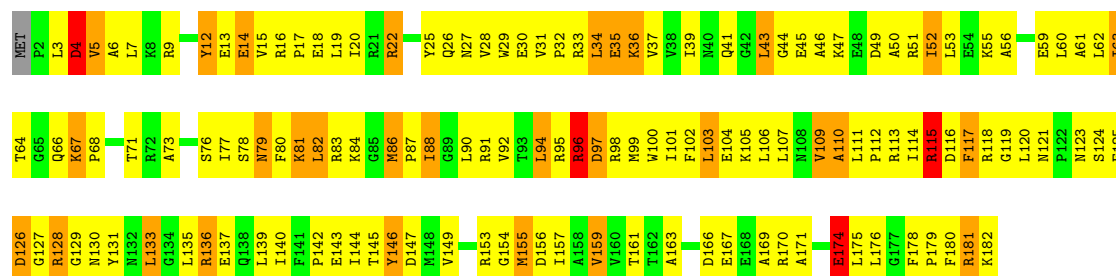
• Molecule 5: 50S ribosomal protein L4

Chain F:



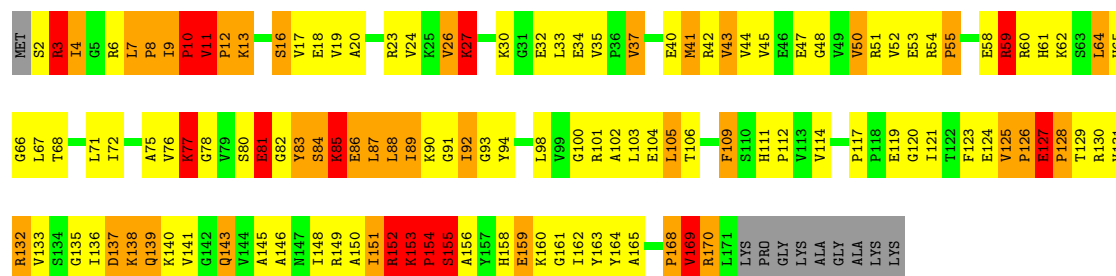
• Molecule 6: 50S ribosomal protein L5

Chain G:



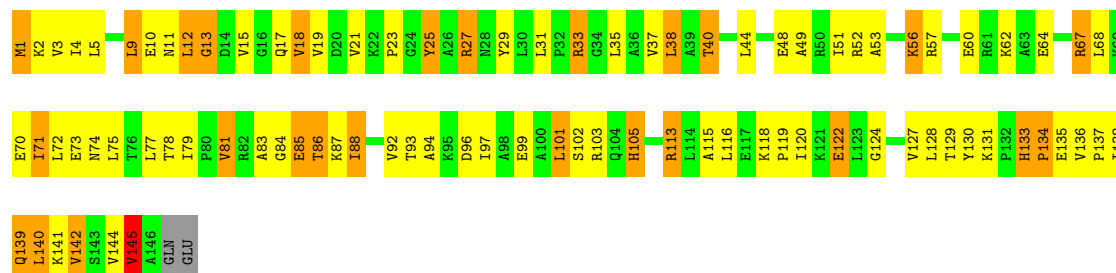
• Molecule 7: 50S ribosomal protein L6

Chain H:



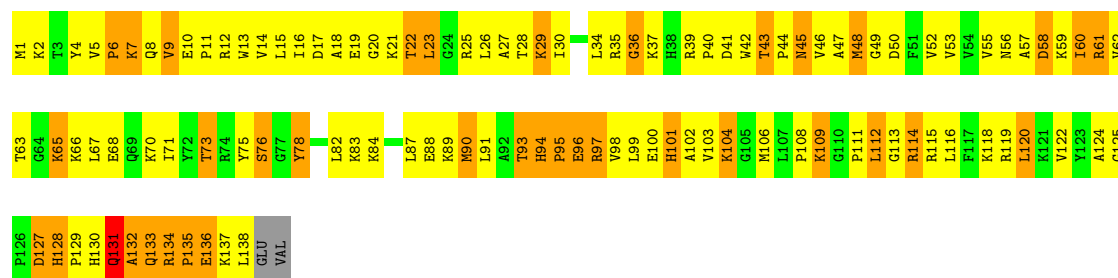
• Molecule 8: 50S ribosomal protein L9

Chain I:



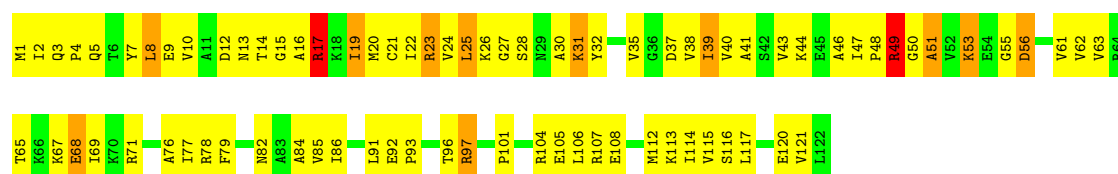
- Molecule 9: 50S ribosomal protein L13

Chain N:



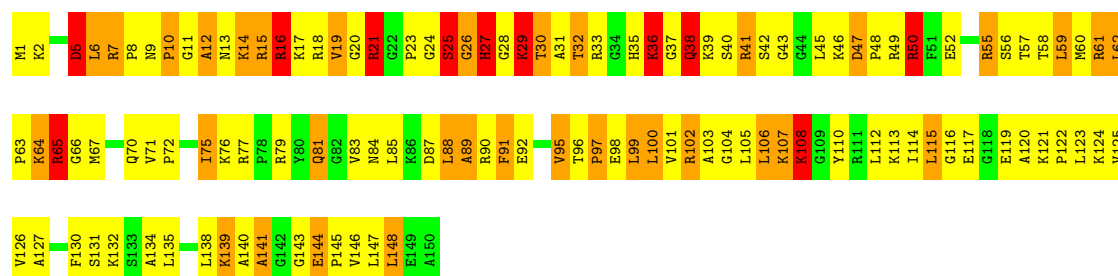
- Molecule 10: 50S ribosomal protein L14

Chain O:



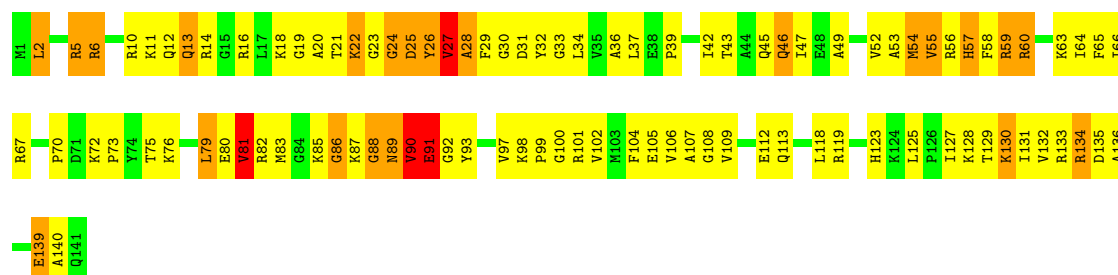
- Molecule 11: 50S ribosomal protein L15

Chain P:



- Molecule 12: 50S ribosomal protein L16

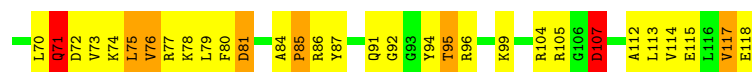
Chain Q:



- Molecule 13: 50S ribosomal protein L17

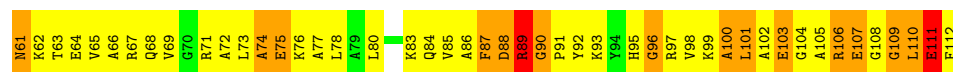
Chain R:





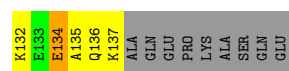
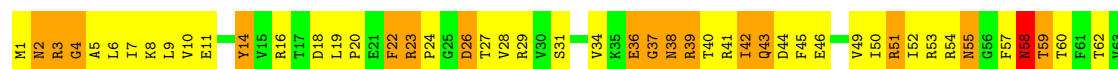
• Molecule 14: 50S ribosomal protein L18

Chain S:



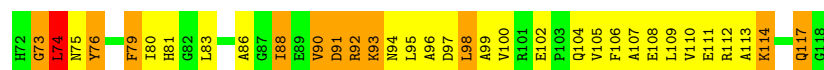
• Molecule 15: 50S ribosomal protein L19

Chain T:



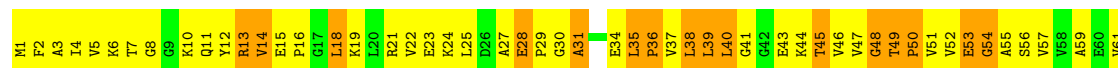
• Molecule 16: 50S ribosomal protein L20

Chain U:



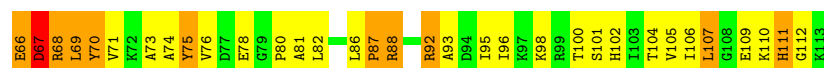
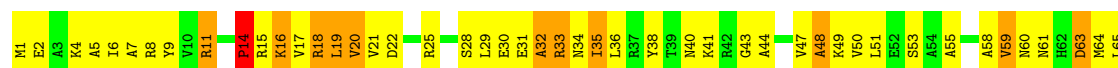
• Molecule 17: 50S ribosomal protein L21

Chain V:



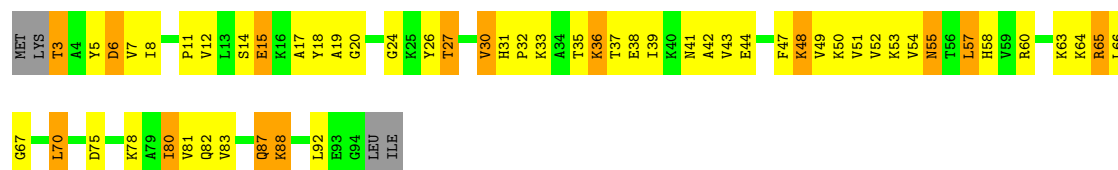
• Molecule 18: 50S ribosomal protein L22

Chain W:



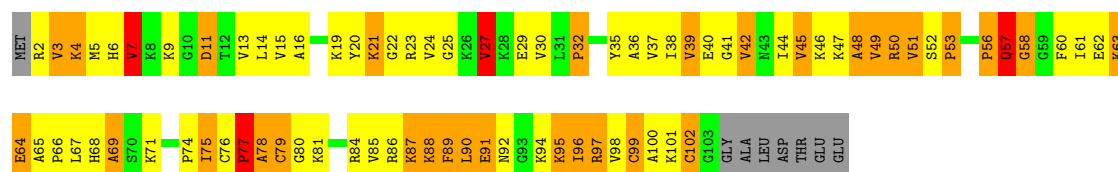
- Molecule 19: 50S ribosomal protein L23

Chain X:



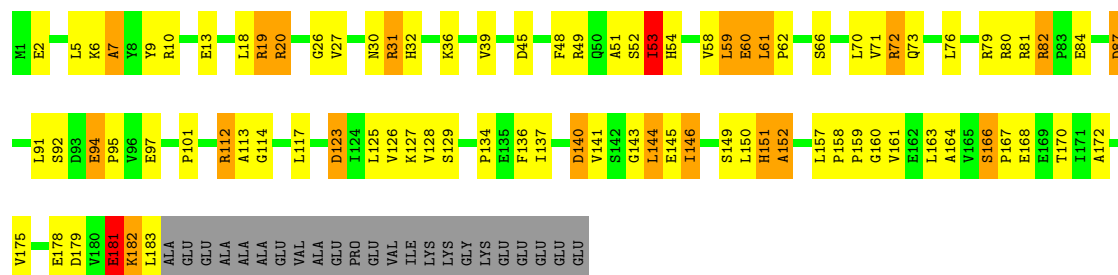
- Molecule 20: 50S ribosomal protein L24

Chain Y:



- Molecule 21: 50S ribosomal protein L25

Chain Z:



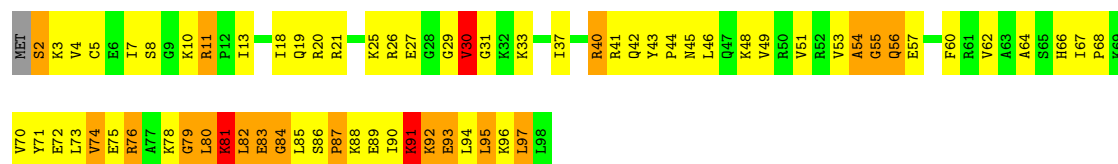
- Molecule 22: 50S ribosomal protein L27

Chain 0:



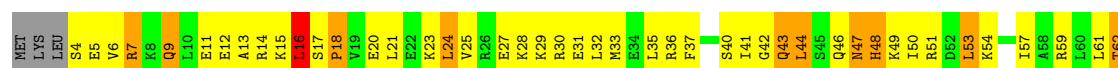
- Molecule 23: 50S ribosomal protein L28

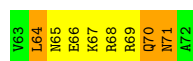
Chain 1:



- Molecule 24: 50S ribosomal protein L29

Chain 2:





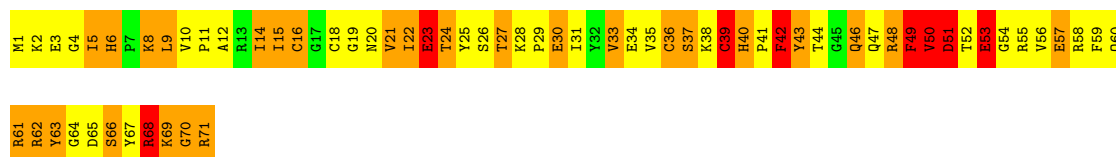
- Molecule 25: 50S ribosomal protein L30

Chain 3:



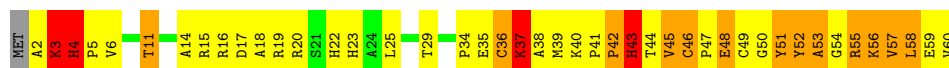
- Molecule 26: 50S ribosomal protein L31

Chain 4:



- Molecule 27: 50S ribosomal protein L32

Chain 5:



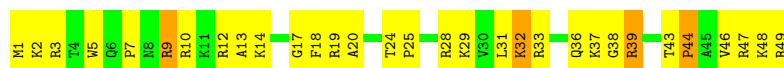
- Molecule 28: 50S ribosomal protein L33

Chain 6:



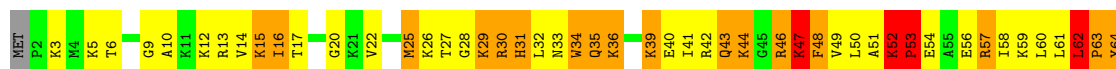
- Molecule 29: 50S ribosomal protein L34

Chain 7:



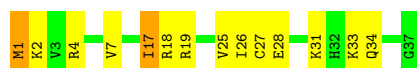
- Molecule 30: 50S ribosomal protein L35

Chain 8:



- Molecule 31: 50S ribosomal protein L36

Chain 9:



- Molecule 32: tRNA acceptor end mimic

Chain a: 



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	210.20Å 450.23Å 621.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.97 – 3.22	Depositor
% Data completeness (in resolution range)	98.5 (34.97-3.22)	Depositor
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX	Depositor
R, R_{free}	0.229 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	92290	wwPDB-VP
Average B, all atoms (Å ²)	78.0	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, PPU

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	0.44	3/69543 (0.0%)	0.94	121/108563 (0.1%)
2	B	0.35	0/2878	0.89	0/4490
3	D	0.56	1/2165 (0.0%)	0.90	4/2919 (0.1%)
4	E	0.52	0/1601	0.91	2/2160 (0.1%)
5	F	0.50	0/1620	0.76	0/2194
6	G	0.40	0/1499	0.66	0/2016
7	H	0.45	0/1332	0.85	4/1802 (0.2%)
8	I	0.30	0/1151	0.63	0/1558
9	N	0.46	0/1131	0.78	1/1525 (0.1%)
10	O	0.53	0/943	0.71	0/1269
11	P	0.49	0/1162	0.95	3/1544 (0.2%)
12	Q	0.54	0/1143	0.89	3/1527 (0.2%)
13	R	0.45	0/982	0.80	1/1312 (0.1%)
14	S	0.45	0/892	0.82	1/1187 (0.1%)
15	T	0.46	0/1155	0.73	2/1542 (0.1%)
16	U	0.48	0/982	0.77	0/1306
17	V	0.47	0/790	0.82	0/1057
18	W	0.45	0/911	0.75	0/1220
19	X	0.56	0/739	0.77	0/993
20	Y	0.52	0/798	0.80	0/1064
21	Z	0.33	0/1493	0.63	0/2026
22	0	0.31	0/657	0.53	0/874
23	1	0.49	0/770	0.85	1/1022 (0.1%)
24	2	0.50	0/583	0.83	1/771 (0.1%)
25	3	0.43	0/474	0.71	0/635
26	4	0.38	0/594	0.78	1/795 (0.1%)
27	5	0.51	0/473	0.74	0/639
28	6	0.42	0/431	0.76	0/575
29	7	0.56	0/438	0.76	0/575
30	8	0.62	0/525	0.93	1/691 (0.1%)
31	9	0.37	0/310	0.61	0/407
32	a	0.78	0/40	1.81	1/60 (1.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.45	4/100205 (0.0%)	0.90	147/150318 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1762	A	N9-C4	6.24	1.41	1.37
1	A	676	A	N9-C4	-5.26	1.34	1.37
1	A	654(T)	C	C1'-N1	5.14	1.56	1.48
3	D	241	PRO	N-CD	5.01	1.54	1.47

The worst 5 of 147 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1929	G	C6-C5-N7	-11.06	123.77	130.40
1	A	1929	G	C5-C6-O6	-10.55	122.27	128.60
1	A	1929	G	C4-C5-N7	10.40	114.96	110.80
4	E	21	VAL	C-N-CD	-10.12	98.35	120.60
1	A	945	A	O4'-C1'-N9	10.00	116.20	108.20

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	62091	0	31296	832	0
2	B	2573	0	1306	35	0
3	D	2115	0	2195	311	0
4	E	1568	0	1634	264	0
5	F	1585	0	1632	174	0
6	G	1474	0	1535	183	0
7	H	1307	0	1382	226	0
8	I	1136	0	1223	48	0
9	N	1104	0	1180	189	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	O	933	0	996	122	0
11	P	1145	0	1228	242	0
12	Q	1122	0	1179	154	0
13	R	968	0	1033	111	0
14	S	882	0	943	154	0
15	T	1141	0	1202	152	0
16	U	964	0	1022	135	0
17	V	779	0	852	135	1
18	W	900	0	964	98	0
19	X	725	0	778	68	0
20	Y	785	0	878	152	0
21	Z	1461	0	1493	59	0
22	0	648	0	672	20	0
23	1	763	0	848	140	0
24	2	581	0	629	76	0
25	3	469	0	518	42	0
26	4	581	0	574	132	0
27	5	459	0	480	75	1
28	6	424	0	450	88	0
29	7	430	0	480	41	0
30	8	517	0	582	103	0
31	9	307	0	336	16	0
32	a	74	0	51	0	0
33	5	1	0	0	0	0
33	7	1	0	0	0	0
33	A	269	0	0	0	0
33	B	3	0	0	0	0
33	D	1	0	0	0	0
33	E	2	0	0	0	0
33	X	1	0	0	0	0
34	9	1	0	0	0	0
All	All	92290	0	61571	4158	1

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 27.

The worst 5 of 4158 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:127:GLU:CG	7:H:128:PRO:HD3	1.36	1.52
23:1:81:LYS:NZ	23:1:81:LYS:HA	1.42	1.34
23:1:81:LYS:HE2	23:1:81:LYS:N	1.50	1.26
7:H:127:GLU:HG2	7:H:128:PRO:CD	1.70	1.21

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:127:GLU:CB	7:H:128:PRO:HD3	1.69	1.20

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:V:51:VAL:N	27:5:60:VAL:O[4.445]	2.16	0.04

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	270/276 (98%)	204 (76%)	47 (17%)	19 (7%)	2	14
4	E	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	0
5	F	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	7
6	G	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	1	4
7	H	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	0
8	I	144/148 (97%)	103 (72%)	24 (17%)	17 (12%)	1	4
9	N	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	1
10	O	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	2	12
11	P	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	0
12	Q	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	1	7
13	R	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	1	4
14	S	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	1
15	T	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	1
16	U	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	11
17	V	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	7
18	W	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	X	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	3	23
20	Y	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0	0
21	Z	181/206 (88%)	130 (72%)	34 (19%)	17 (9%)	1	8
22	0	80/85 (94%)	70 (88%)	9 (11%)	1 (1%)	18	68
23	1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	1	4
24	2	67/72 (93%)	47 (70%)	11 (16%)	9 (13%)	0	2
25	3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	3	24
26	4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
27	5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	0
28	6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
29	7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	17
30	8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	1
31	9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	3379/3526 (96%)	2278 (67%)	640 (19%)	461 (14%)	0	2

5 of 461 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	26	LYS
3	D	28	GLU
3	D	123	ALA
3	D	231	HIS
4	E	4	ILE

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	214/218 (98%)	177 (83%)	37 (17%)	3	13
4	E	165/166 (99%)	127 (77%)	38 (23%)	1	5
5	F	161/166 (97%)	140 (87%)	21 (13%)	6	28
6	G	155/156 (99%)	130 (84%)	25 (16%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	142/148 (96%)	114 (80%)	28 (20%)	2	9
8	I	122/124 (98%)	93 (76%)	29 (24%)	1	4
9	N	117/119 (98%)	98 (84%)	19 (16%)	3	15
10	O	100/100 (100%)	90 (90%)	10 (10%)	11	41
11	P	116/116 (100%)	89 (77%)	27 (23%)	1	5
12	Q	111/111 (100%)	93 (84%)	18 (16%)	3	15
13	R	101/101 (100%)	84 (83%)	17 (17%)	3	14
14	S	87/88 (99%)	74 (85%)	13 (15%)	4	20
15	T	120/127 (94%)	97 (81%)	23 (19%)	2	10
16	U	93/94 (99%)	80 (86%)	13 (14%)	5	24
17	V	82/82 (100%)	71 (87%)	11 (13%)	6	26
18	W	92/92 (100%)	77 (84%)	15 (16%)	3	15
19	X	74/78 (95%)	63 (85%)	11 (15%)	4	20
20	Y	85/91 (93%)	70 (82%)	15 (18%)	3	13
21	Z	162/179 (90%)	140 (86%)	22 (14%)	5	26
22	0	65/67 (97%)	61 (94%)	4 (6%)	26	70
23	1	82/83 (99%)	67 (82%)	15 (18%)	2	12
24	2	64/67 (96%)	57 (89%)	7 (11%)	9	37
25	3	51/52 (98%)	40 (78%)	11 (22%)	1	7
26	4	63/63 (100%)	44 (70%)	19 (30%)	0	1
27	5	51/52 (98%)	39 (76%)	12 (24%)	1	4
28	6	48/52 (92%)	38 (79%)	10 (21%)	2	8
29	7	42/42 (100%)	39 (93%)	3 (7%)	21	63
30	8	54/55 (98%)	39 (72%)	15 (28%)	0	2
31	9	34/34 (100%)	32 (94%)	2 (6%)	28	72
All	All	2853/2923 (98%)	2363 (83%)	490 (17%)	3	14

5 of 490 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	P	61	ARG
14	S	44	LYS
27	5	19	ARG

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Mol	Chain	Res	Type
11	P	91	PHE
12	Q	91	GLU

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	81	GLN
15	T	55	ASN
24	2	9	GLN
11	P	84	ASN
15	T	58	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2880/2916 (98%)	626 (21%)	70 (2%)
2	B	119/122 (97%)	30 (25%)	1 (0%)
32	a	1/3 (33%)	0	0
All	All	3000/3041 (98%)	656 (21%)	71 (2%)

5 of 656 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	15	G
1	A	27	G
1	A	34	C
1	A	46	C

5 of 71 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1045	A
1	A	1210	A
1	A	2726	U
1	A	1078	U
1	A	1130	U

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	PPU	a	76	1,32	38,40,41	2.42	9 (23%)	54,57,60	2.61	14 (25%)

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	PPU	a	76	1,32	-	0/26/43/44	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	76	PPU	O-C	9.19	1.41	1.23
32	a	76	PPU	C9-N6	-5.43	1.32	1.45
32	a	76	PPU	C-N3'	5.37	1.46	1.34
32	a	76	PPU	C10-N6	-5.13	1.32	1.45
32	a	76	PPU	C4-N9	-3.10	1.33	1.37

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	76	PPU	N3-C2-N1	-8.55	121.37	128.89
32	a	76	PPU	C3'-N3'-C	-8.14	110.23	123.19
32	a	76	PPU	C5-C4-N3	-6.30	119.84	125.98
32	a	76	PPU	C2'-C1'-N9	-5.45	98.50	113.35
32	a	76	PPU	C2'-C3'-N3'	5.17	125.09	113.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 279 ligands modelled in this entry, 279 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.