



wwPDB X-ray Structure Validation Summary Report

Sep 15, 2014 – 01:29 PM EDT

PDB ID : 1VVS
Title : Crystal Structure of Frameshift Suppressor tRNA SufA6 Bound to Codon CCC-A on the Ribosome
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-06-13
Resolution : 3.90 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>

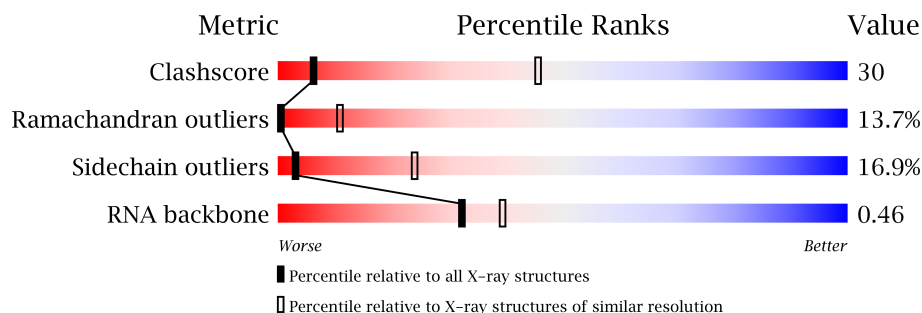
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.90 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	1173 (4.30-3.50)
Ramachandran outliers	78287	1118 (4.30-3.50)
Sidechain outliers	78261	1107 (4.30-3.50)
RNA backbone	1838	1018 (5.00-2.80)

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	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 92279 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	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	T	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	U	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	V	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	W	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	X	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	Y	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	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	58	Total	C	N	O	S	0	0	0
			451	283	89	74	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	P	2	Total	Mg	0	0
			2	2		
33	Q	1	Total	Mg	0	0
			1	1		
33	E	1	Total	Mg	0	0
			1	1		
33	B	3	Total	Mg	0	0
			3	3		
33	7	1	Total	Mg	0	0
			1	1		
33	A	265	Total	Mg	0	0
			265	265		

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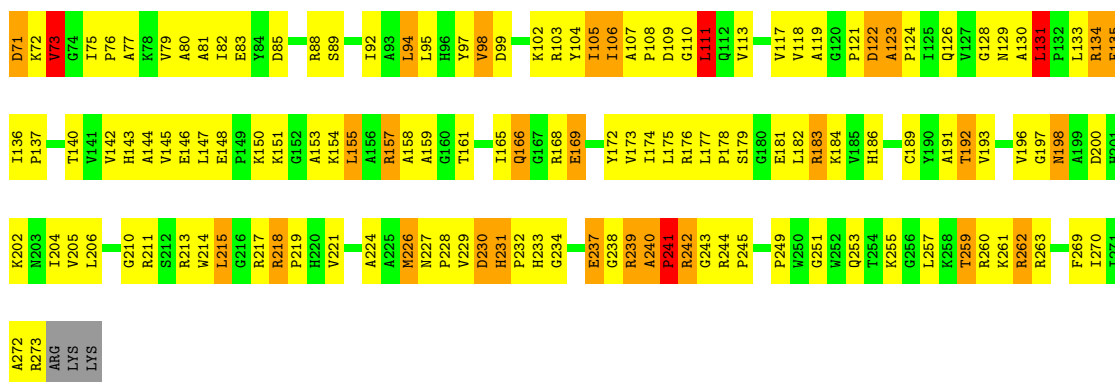
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	5	1	Total	Mg	0	0
			1	1		
33	X	1	Total	Mg	0	0
			1	1		

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

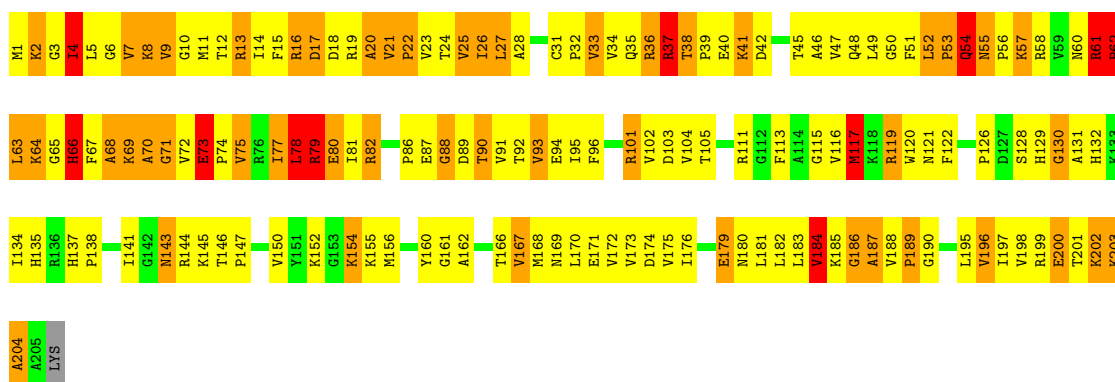
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	9	1	Total	Zn	0	0
			1	1		

C1965	C1892	C1804	A1729	C1636	A1543	A1471	C1403	G1332	C1258	G1190	A1111	G1042	C964	A820
A1966	C1893	U1805	U1730	C1637	A1544	A1472	C1404	C1333	C1259	G1191	U1113	C1043	C965	A821
C1967	C1894	U1806	U1731	C1638	A1545	G1473	U1405	C1334	G1260	G1113	U1112	G1044	A896	U822
G1968	C1895	A1812	A1732	C1639		G1474	U1406	U1335	G1261	A1194	G1114	A1045	C971	
A1969	C1896	G1813	G1733	U1638	C1547	G1475	C1407	A1336	A1262	G1195		A1046	C897	U827
A1970		G1814	C1734	C1640	C1548	C1476	C1408	G1337	U1263	C1196		G1047	A973	U828
A1971	C1899	A1815		A1641	C1549		C1409	G1338	U1264	C1197		A1048	A899	U829
A1972	A1972	G1816	C1742	C1642	C1550	G1479	G1410	C1339	A1265	U1198		C1049	A900	A829
G1973	C1902	U1817	G1743	C1643	C1551	U1482	C1411	U1340	U1266	U1199		A1050	C974A	G830
C1974	G1903	U1818		C1646		U1483	A1412	U1341	U1267	C1200	C1124		C975	G831
A1975		A1819	G1750	C1647	A1558	G1484			A1268	C1201		C1053		G832
G1976	G1906	U1820	C1751	C1648	G1559	G1485	G1416		A1269	C1202	G1125	A1054	C904	U833
A1977	G1907	A1821	C1752				C1417	U1344	C1270	G1203	A1126	A1055		
C1978	C1908	G1822	G1753	C1651	C1564		A1418	A1349	U1271	A1127		G1056	U907	U839
C1979	A1913	G1823	C1754	C1652	C1565	G1488	A1419	A1419	A1272	U1205	A1128	A1057	A891	C940
G1980		A1824	G1755	U1653	A1566	U1489	U1420	G1351	U1273	U1206	A1130	G1058	A909	C941
A1981		A1825	A1756	C1654	A1567	A1490	G1421	U1352	A1274	C1207	G1131	G1059	A983	G842
A1916		G1826	U1757	A1655	G1568		G1422	A1353	A1275	C1208		U1060	A984	G843
U1917	A1917	C1827	A1856	C1656	A1569	C1493	G1423	A1354	U1276	G1209	C1135	U1061	C985	C844
A1918	A1918	G1828	A1759	C1657	A1570	A1494	G1424	A1354	G1277	A1210	G1136	G1062		C946
A1919	A1919	A1829		C1658	A1571	A1496	G1425	U1357	U1278	U1211	G1137	G1063	A988	C947
C1920		A1762	G1763		A1572	U1497	A1426	G1358	G1279	G1212	G1138		C915	C948
		G1764	G1765	C1662	G1573		A1427	A1359	U1282	A1213	G1139	U1066	A990	G848
U1923	U1923	U1834	C1766				C1428	A1360		A1214	U1141	A1067	C991	A849
C1924		G1835	C1765	G1666	U1576	U1503	G1429	A1361	U1286	C1217	U1142	G1068	C992	A917
		C1836		C1667	C1577	C1504	A1430	G1364	A1287		A1143	A1069	A989	A849
A1927	A1927	C1837	G1769	A1668	U1578	C1505	U1431	A1365	U1288	C1221	G1151	U1077	C993	C850
A1928		G1838	G1770	U1669	A1579	C1506	A1432	U1366		A1142A		A1078	C994	G852
G1929	G1929	U1839	C1771	A1507	A1580	A1507	U1433	G1368		G1221		G1079	A996	
G1930			G1772	C1672		A1508	A1434	G1369	C1291	C1222		C1076	C997	G855
U1931	U1931	C1843	A1773	U1673	C1585	C1509	G1435	C1370	U1292	C1223	A1155	U1077	A1000	C857
A1932	A1932	C1844	C1774	C1674	A1586	A1510	A1436	G1371	C1293			U1078	G928	U858
G1933	G1933	G1845	U1775	C1675	A1597	A1511	U1437	U1372		A1156	G1003	C1079	G929	U860
C1934	C1934	G1846	G1776	U1676	C1592	G1512	A1438	A1373	U1300	G1227	G1157		G1004	A861
G1935	A1947	A1847	U1777	A1677	G1593	C1513	A1439	G1374	A1301	A1228	C1158	U1082	C1005	G862
A1936	A1948	G1848	U1778		G1594	U1514	G1440	C1375		C1230		U1083	C1006	A863
A1937	C1949	G1849	U1779	G1681	G1595	C1515	G1441	C1376	C1304	G1231	C1161	U1084	C1007	G864
A1938	G1850	C1850	A1780	C1682	A1596	U1516	G1442	G1377	C1305			A1085	C1008	G865
U1939	U1939	G1851	C1781	C1683	A1597	G1517	G1443	C1378		C1232	G1164	U1086	G937	A866
U1940		A1853	G1782	C1678	C1598	G1518	A1444	A1379	A1308	U1234	U1165	G1087	G1011	G867
C1941			A1783	A1689	C1598	G1519	G1444A	C1379	U1012	U1235	C1166	A1088	U1012	U868
					C1600	U1520	C1445	G1381	G1310	G1236		G1089	C1013	
G1944	G1857		A1784			G1521		G1382	G1311	A1237	G1169	U1090	U943	A870
U1945	G1858		A1785	U1693	A1603	G1522	A1449	C1383	U1312	A1238	G1170		U1019	U871
G1946	A1859		A1786	C1694	C1694	G1523	G1449A	A1384	C1313	G1239	G1171	G1093	G944	A872
			A1787	C1695	C1695	C1533		C1385	C1314	U1240	A1021	A1094	A945	A873
G1949	U1864		C1788	G1696	C1607	U1528		C1386	C1315	U1249	G1173	U1095	G946	G872
G1969	G1869		A1789	A1698	A1608	A1529	U1454	C1387	C1316	A1241	G1174	A1096	G1022	
C1950	C1870		C1790	C1699	A1609	C1530	G1455	C1387	U1317		U1175	U1097	G947	
U1951	A1871		A1791	G1699	C1531			G1388	G1317	G1244	U1176	U1023	U1024	
A1952	C1872			A1700	C1532	G1522		G1389	C1318			A1098	G950	A878
U2034	G1878		U1794		A1614	G1523	G1458	U1390	C1318	G1248	A1177	G1099	G951	G879
G2035	C1882		C1795	G1705	C1615	C1533	G1459	C1391	C1319	U1249	G1178	U1025	C951	G880
C2036	U1955		U1796	C1706	A1616	U1534	A1460	U1391	C1320	A1249	U1026	G952	G952	G881
G2037	C1883		C1797	G1707	C1617	U1535	A1461		C1321	G1250	A1027	G956	G956	G882
C1958	A1884		C1798	C1708	A1618	A1536		U1394	A1322	C1251	C1102	A1029	A957	C884
G1959	C1885		G1799	C1709	G1622	C1537	G1465	A1395	C1324	U1252	G1184	A1103	U1033	C885
A1960	C1886		C1800	G1725	C1623	U1538	G1466	U1396	G1324	A1253	G1185	C1104	G1030	C886
U2041			G1801	G1726	G1624	G1539	C1467	U1397		G1186	A1029	G1106		A887
			A1802	U1727	C1625	G1540	C1468	C1398	G1328	U1255	G1187	G1106		C888
C2042	U1963		A1803	U1728	C1626	U1541	A1469		U1329	U1256	G1188	C1109	U1033	C889
	C1964		A1804	C1729	C1627	A1542	A1470	C1402	C1257	G1257	A1189	C1109	G1036	C890



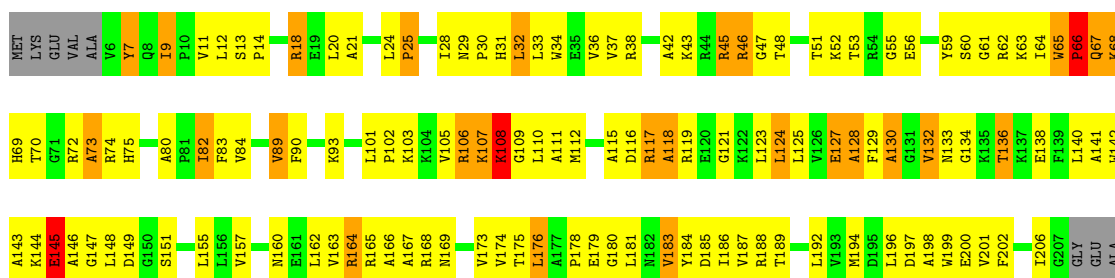
• Molecule 4: 50S ribosomal protein L3

Chain E:



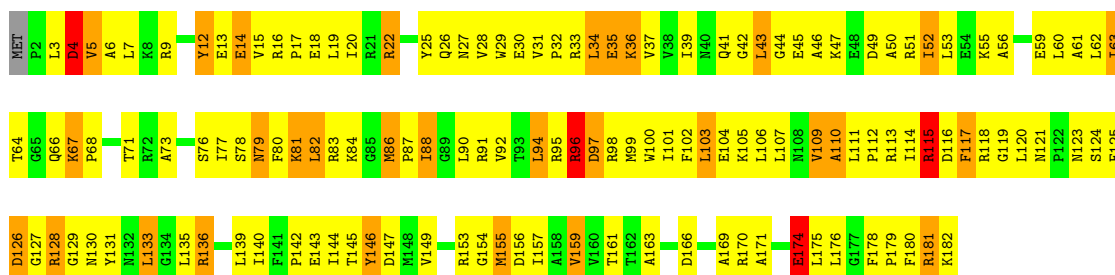
• Molecule 5: 50S ribosomal protein L4

Chain F:



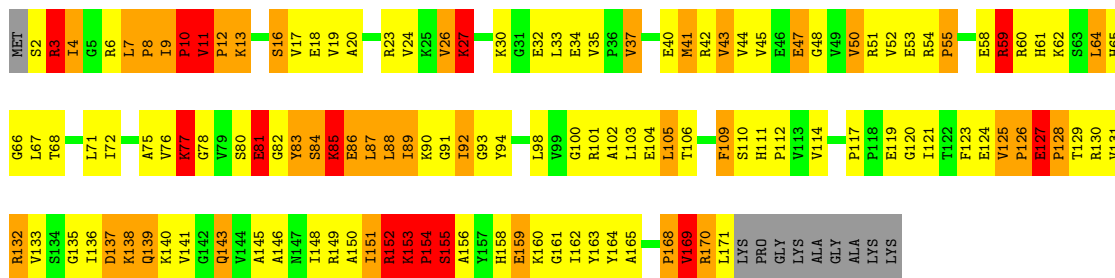
• Molecule 6: 50S ribosomal protein L5

Chain G:



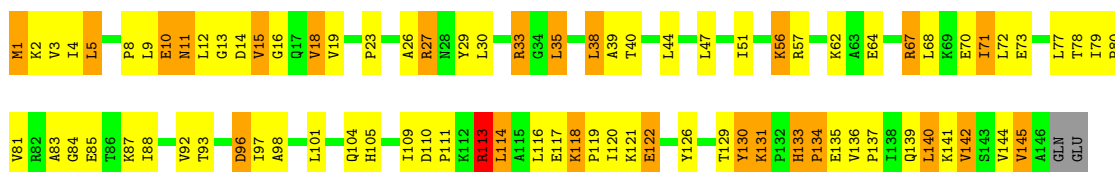
- Molecule 7: 50S ribosomal protein L6

Chain H:



- Molecule 8: 50S ribosomal protein L9

Chain I:



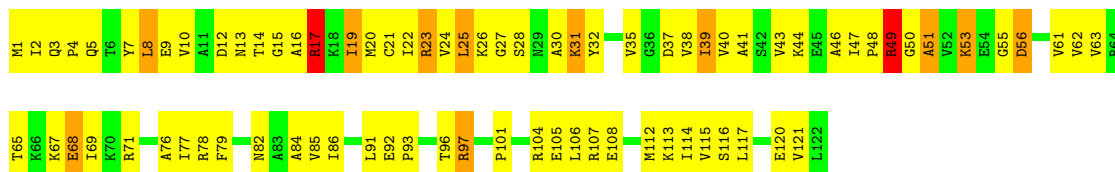
- Molecule 9: 50S ribosomal protein L13

Chain N:



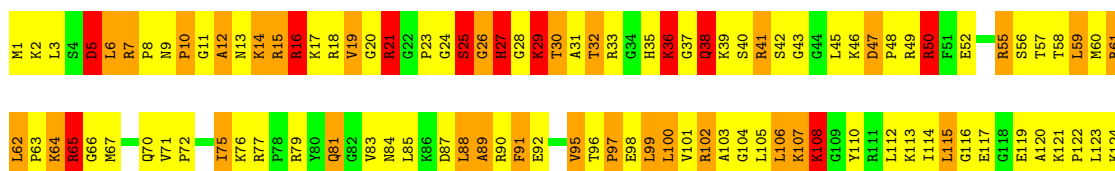
- Molecule 10: 50S ribosomal protein L14

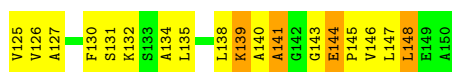
Chain O:



- Molecule 11: 50S ribosomal protein L15

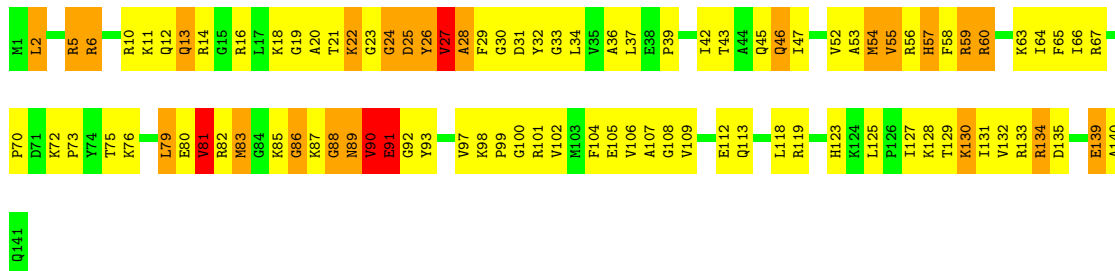
Chain P:





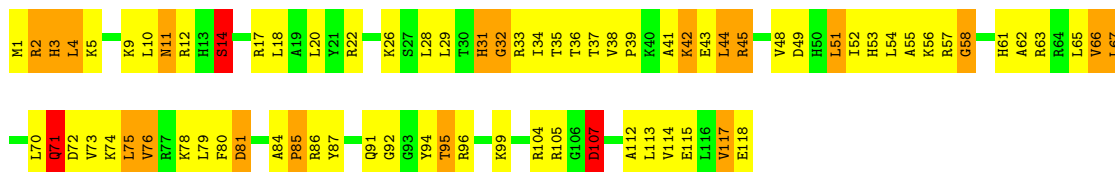
- Molecule 12: 50S ribosomal protein L16

Chain Q:



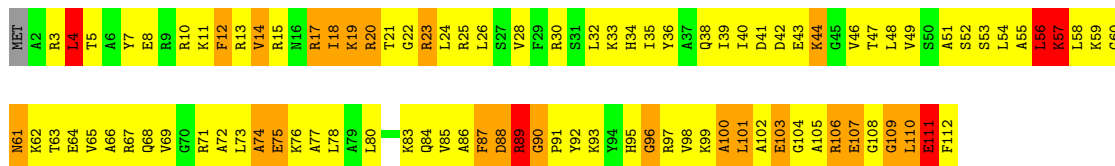
- Molecule 13: 50S ribosomal protein L17

Chain R:



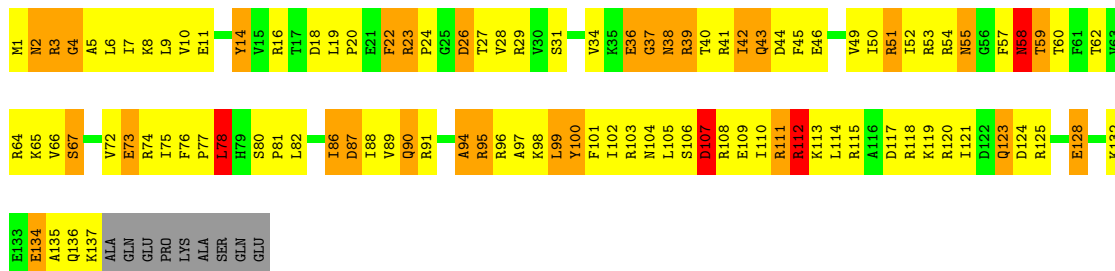
- Molecule 14: 50S ribosomal protein L18

Chain S:



- Molecule 15: 50S ribosomal protein L19

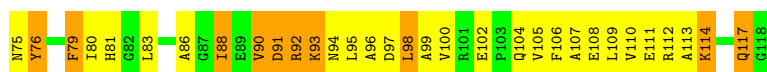
Chain T:



- Molecule 16: 50S ribosomal protein L20

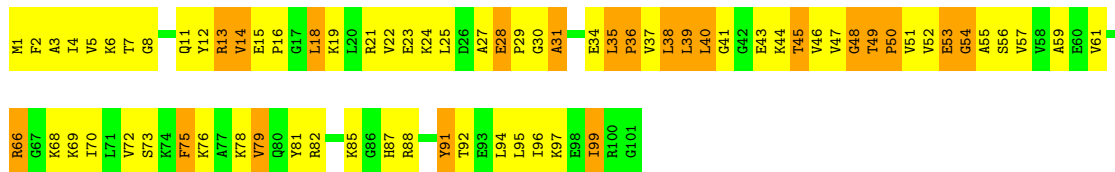
Chain U:





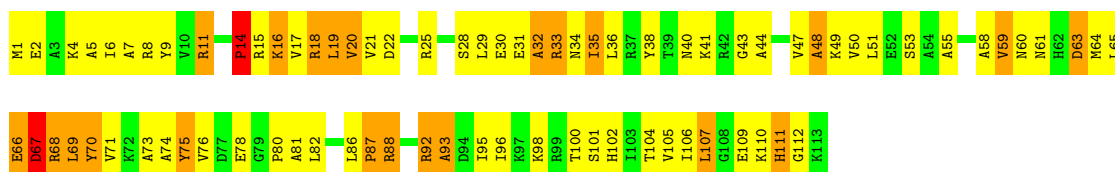
- Molecule 17: 50S ribosomal protein L21

Chain V:



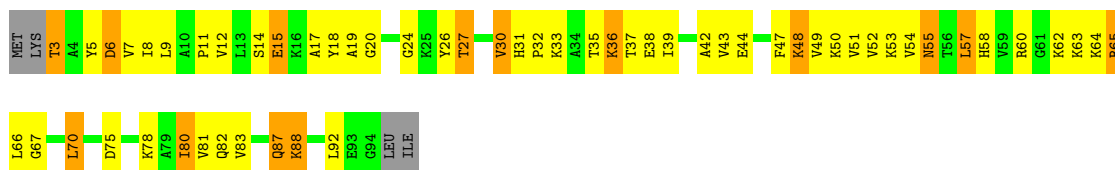
- Molecule 18: 50S ribosomal protein L22

Chain W:



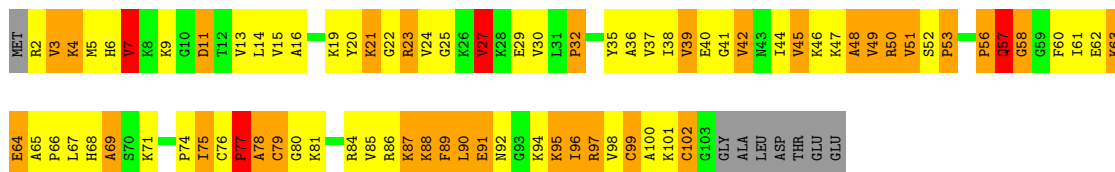
- Molecule 19: 50S ribosomal protein L23

Chain X:



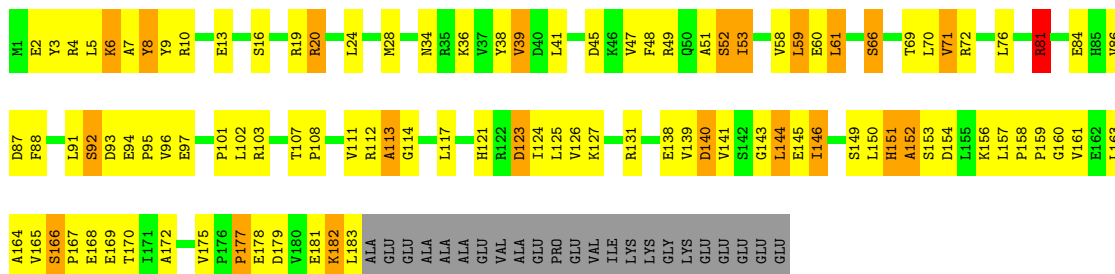
- Molecule 20: 50S ribosomal protein L24

Chain Y:



- Molecule 21: 50S ribosomal protein L25

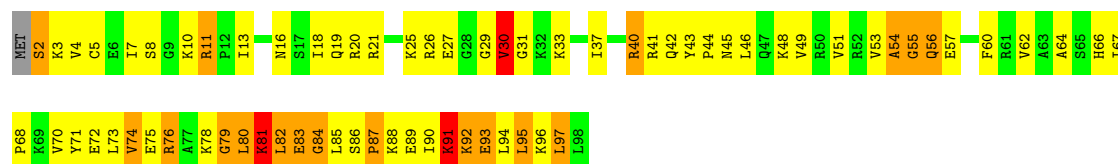
Chain Z:



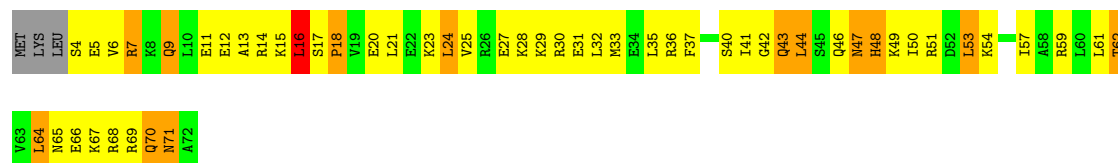
- Molecule 22: 50S ribosomal protein L27

Chain 0: 

- Molecule 23: 50S ribosomal protein L28

Chain 1: 

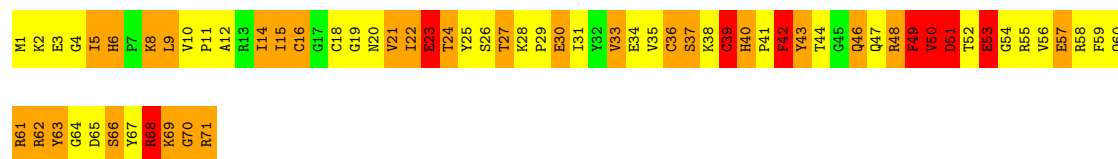
- Molecule 24: 50S ribosomal protein L29

Chain 2: 

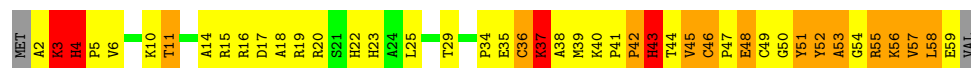
- Molecule 25: 50S ribosomal protein L30

Chain 3: 

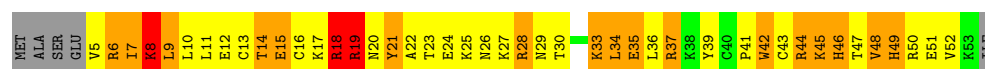
- Molecule 26: 50S ribosomal protein L31

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	210.24Å 446.10Å 623.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.68 – 3.90	Depositor
% Data completeness (in resolution range)	99.0 (49.68-3.90)	Depositor
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX	Depositor
R, R_{free}	0.235 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	92279	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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	0.59	2/69543 (0.0%)	1.12	219/108563 (0.2%)
2	B	0.49	0/2878	1.04	4/4490 (0.1%)
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	0.34	0/1151	0.61	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	0.50	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	0.83	1/1187 (0.1%)
15	T	0.46	0/1155	0.73	2/1542 (0.1%)
16	U	0.48	0/982	0.78	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	0.36	0/1493	0.62	0/2026
22	0	0.42	0/657	0.65	0/874
23	1	0.49	0/770	0.85	1/1022 (0.1%)
24	2	0.51	0/583	0.84	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	0.50	0/465	0.74	0/629
28	6	0.43	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	0.79	0/40	1.83	1/60 (1.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.56	3/100197 (0.0%)	1.05	249/150308 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1142(A)	A	N9-C4	-6.45	1.33	1.37
1	A	1378	A	N9-C4	-5.14	1.34	1.37
3	D	241	PRO	N-CD	5.05	1.54	1.47

The worst 5 of 249 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	761	A	N1-C6-N6	11.29	125.37	118.60
4	E	21	VAL	C-N-CD	-10.09	98.39	120.60
1	A	196	A	N1-C6-N6	9.24	124.14	118.60
12	Q	81	VAL	CB-CA-C	-8.71	94.84	111.40
1	A	2506	U	N3-C2-O2	-8.58	116.20	122.20

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	31295	1254	0
2	B	2573	0	1306	57	0
3	D	2115	0	2195	316	0
4	E	1568	0	1634	272	0
5	F	1585	0	1632	179	0
6	G	1474	0	1535	184	0
7	H	1307	0	1382	227	3
8	I	1136	0	1223	56	0
9	N	1104	0	1180	186	0
10	O	933	0	996	129	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	P	1145	0	1228	239	0
12	Q	1122	0	1178	149	0
13	R	968	0	1033	114	0
14	S	882	0	943	159	0
15	T	1141	0	1202	150	0
16	U	964	0	1022	134	0
17	V	779	0	852	128	0
18	W	900	0	964	102	0
19	X	725	0	778	67	0
20	Y	785	0	878	154	3
21	Z	1461	0	1493	70	0
22	0	648	0	672	39	0
23	1	763	0	848	140	0
24	2	581	0	629	79	0
25	3	469	0	518	44	0
26	4	581	0	574	133	0
27	5	451	0	471	68	0
28	6	424	0	450	90	0
29	7	430	0	480	44	0
30	8	517	0	582	102	0
31	9	307	0	336	20	0
32	a	74	0	51	0	0
33	5	1	0	0	0	0
33	7	1	0	0	0	0
33	A	265	0	0	0	0
33	B	3	0	0	0	0
33	E	1	0	0	0	0
33	P	2	0	0	0	0
33	Q	1	0	0	0	0
33	X	1	0	0	0	0
34	9	1	0	0	0	0
All	All	92279	0	61560	4640	3

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 30.

The worst 5 of 4640 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	1.35	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	1.69	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	1.21

All (3) 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)
7:H:45:VAL:O	20:Y:24:VAL:N[4.445]	1.97	0.23
7:H:44:VAL:CG2	20:Y:23:ARG:CD[4.445]	2.08	0.12
7:H:47:GLU:OE2	20:Y:79:CYS:CB[4.445]	2.18	0.02

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	33
4	E	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	3
5	F	200/210 (95%)	143 (72%)	37 (18%)	20 (10%)	1	20
6	G	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	1	14
7	H	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	2
8	I	144/148 (97%)	100 (69%)	27 (19%)	17 (12%)	1	14
9	N	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	7
10	O	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	2	30
11	P	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	3
12	Q	139/141 (99%)	97 (70%)	28 (20%)	14 (10%)	1	19
13	R	116/118 (98%)	82 (71%)	20 (17%)	14 (12%)	1	14
14	S	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	6
15	T	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	9
16	U	115/118 (98%)	86 (75%)	20 (17%)	9 (8%)	1	29
17	V	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	W	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	13
19	X	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	3	40
20	Y	100/110 (91%)	57 (57%)	17 (17%)	26 (26%)	0	2
21	Z	181/206 (88%)	128 (71%)	35 (19%)	18 (10%)	1	20
22	0	80/85 (94%)	67 (84%)	11 (14%)	2 (2%)	9	62
23	1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	1	15
24	2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	11
25	3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	3	41
26	4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
27	5	56/60 (93%)	32 (57%)	9 (16%)	15 (27%)	0	1
28	6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	1
29	7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	36
30	8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	5
31	9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	3378/3526 (96%)	2267 (67%)	648 (19%)	463 (14%)	0	11

5 of 463 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%)	178 (83%)	36 (17%)	3	24
4	E	165/166 (99%)	127 (77%)	38 (23%)	1	10
5	F	161/166 (97%)	140 (87%)	21 (13%)	6	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	155/156 (99%)	131 (84%)	24 (16%)	4	28
7	H	142/148 (96%)	114 (80%)	28 (20%)	2	15
8	I	122/124 (98%)	101 (83%)	21 (17%)	3	22
9	N	117/119 (98%)	98 (84%)	19 (16%)	3	26
10	O	100/100 (100%)	90 (90%)	10 (10%)	11	52
11	P	116/116 (100%)	89 (77%)	27 (23%)	1	9
12	Q	111/111 (100%)	93 (84%)	18 (16%)	3	26
13	R	101/101 (100%)	84 (83%)	17 (17%)	3	24
14	S	87/88 (99%)	74 (85%)	13 (15%)	4	31
15	T	120/127 (94%)	97 (81%)	23 (19%)	2	16
16	U	93/94 (99%)	80 (86%)	13 (14%)	5	34
17	V	82/82 (100%)	71 (87%)	11 (13%)	6	36
18	W	92/92 (100%)	77 (84%)	15 (16%)	3	26
19	X	74/78 (95%)	63 (85%)	11 (15%)	4	31
20	Y	85/91 (93%)	70 (82%)	15 (18%)	3	21
21	Z	162/179 (90%)	139 (86%)	23 (14%)	5	34
22	0	65/67 (97%)	60 (92%)	5 (8%)	18	65
23	1	82/83 (99%)	67 (82%)	15 (18%)	2	18
24	2	64/67 (96%)	57 (89%)	7 (11%)	9	47
25	3	51/52 (98%)	40 (78%)	11 (22%)	1	11
26	4	63/63 (100%)	44 (70%)	19 (30%)	0	5
27	5	50/52 (96%)	38 (76%)	12 (24%)	1	8
28	6	48/52 (92%)	38 (79%)	10 (21%)	2	13
29	7	42/42 (100%)	39 (93%)	3 (7%)	21	69
30	8	54/55 (98%)	39 (72%)	15 (28%)	0	6
31	9	34/34 (100%)	32 (94%)	2 (6%)	28	75
All	All	2852/2923 (98%)	2370 (83%)	482 (17%)	3	24

5 of 482 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	P	91	PHE
14	S	103	GLU

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Mol	Chain	Res	Type
27	5	25	LEU
12	Q	2	LEU
13	R	37	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
11	P	84	ASN
15	T	58	ASN
25	3	19	GLN
15	T	55	ASN
16	U	94	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2880/2916 (98%)	639 (22%)	65 (2%)
2	B	119/122 (97%)	25 (21%)	1 (0%)
32	a	1/3 (33%)	0	0
All	All	3000/3041 (98%)	664 (22%)	66 (2%)

5 of 664 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	11	G
1	A	15	G
1	A	27	G
1	A	34	C

5 of 66 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1026	U
1	A	1210	A
1	A	2712	U
1	A	1045	A
1	A	1109	C

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	9.22	1.41	1.23
32	a	76	PPU	C9-N6	-5.43	1.32	1.45
32	a	76	PPU	C-N3'	5.36	1.46	1.34
32	a	76	PPU	C10-N6	-5.14	1.32	1.45
32	a	76	PPU	C4-N9	-3.13	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	-8.58	121.34	128.89
32	a	76	PPU	C3'-N3'-C	-8.12	110.25	123.19
32	a	76	PPU	C5-C4-N3	-6.29	119.85	125.98
32	a	76	PPU	C2'-C1'-N9	-5.43	98.56	113.35
32	a	76	PPU	C2'-C3'-N3'	5.18	125.10	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 276 ligands modelled in this entry, 276 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.