



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 03:21 PM GMT

PDB ID : 4K0Q
Title : Crystal structure of Thermus thermophilus 70S containing tRNAs and mRNA stop codon with pseudouridine
Authors : Fernandez, I.S.; Ng, C.L.; Kelley, A.C.; Guowei, W.; Yu, Y.T.; Ramakrishnan, V.
Deposited on : 2013-04-04
Resolution : 3.30 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>

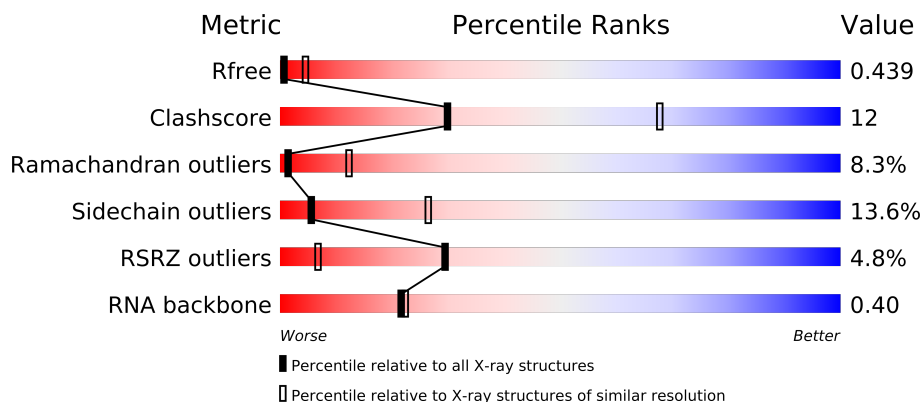
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.30 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))
R_{free}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)
RNA backbone	1838	1042 (3.90-2.70)

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.

Mol	Chain	Length	Quality of chain
1	A	2915	
2	B	119	
3	C	196	
4	D	271	
5	E	204	
6	F	207	
7	G	181	
8	H	159	
9	I	145	
10	J	130	
11	N	138	
12	O	122	

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Mol	Chain	Length	Quality of chain
13	P	146	
14	Q	141	
15	R	117	
16	S	98	
17	T	137	
18	U	117	
19	V	101	
20	W	113	
21	X	92	
22	Y	100	
23	Z	176	
24	0	84	
25	1	93	
26	2	71	
27	3	59	
28	4	30	
29	5	59	
30	6	44	
31	7	48	
32	8	63	
33	9	36	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 91380 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	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1151	A	G	CONFLICT	GB 55771382

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 3 is a protein called 50S Ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	190	Total	C	N	O	0	0	0
			1157	706	220	231			

- Molecule 4 is a protein called 50S Ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			

- Molecule 5 is a protein called 50S Ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			

- Molecule 6 is a protein called 50S Ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	207	Total	C	N	O	S	0	0	0
			1624	1035	303	283	3			

- Molecule 7 is a protein called 50S Ribosomal protein L5.

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

- Molecule 8 is a protein called 50S Ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			

- Molecule 9 is a protein called 50S Ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	145	Total	C	N	O	S	0	0	0
			1132	723	200	208	1			

- Molecule 10 is a protein called 50S Ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	130	Total	C	N	O	S	0	0	0
			651	390	130	131				

- Molecule 11 is a protein called 50S Ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	N	138	Total	C	N	O	S	0	0	0
			1105	712	206	183	4			

- Molecule 12 is a protein called 50S Ribosomal protein L14.

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

- Molecule 13 is a protein called 50S Ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	P	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 14 is a protein called 50S Ribosomal protein L16.

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

- Molecule 15 is a protein called 50S Ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	R	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 16 is a protein called 50S Ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	S	98	Total	C	N	O		0	0	0
			771	486	154	131				

- Molecule 17 is a protein called 50S Ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	T	137	Total	C	N	O	S	0	0	0
			1142	710	234	197	1			

- Molecule 18 is a protein called 50S Ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	U	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	32	ALA	PHE	CONFLICT	UNP P60491

- Molecule 19 is a protein called 50S Ribosomal protein L21.

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

- Molecule 20 is a protein called 50S Ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	W	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	113	ALA	LYS	CONFLICT	UNP Q5SHP3

- Molecule 21 is a protein called 50S Ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	X	92	Total	C	N	O	S	0	0	0
			726	471	131	124				

- Molecule 22 is a protein called 50S Ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Y	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			

- Molecule 23 is a protein called 50S Ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Z	176	Total	C	N	O	S	0	0	0
			1404	897	252	253	2			

- Molecule 24 is a protein called 50S Ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 25 is a protein called 50S Ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	1	93	Total	C	N	O	S	0	0	0
			734	460	147	126	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	81	ARG	LYS	CONFLICT	UNP P60494

- Molecule 26 is a protein called 50S Ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 27 is a protein called 50S Ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	3	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			

- Molecule 28 is a protein called 50S Ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			

- Molecule 29 is a protein called 50S Ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 30 is a protein called 50S Ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	6	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

- Molecule 31 is a protein called 50S Ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	7	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

- Molecule 32 is a protein called 50S Ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	8	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			

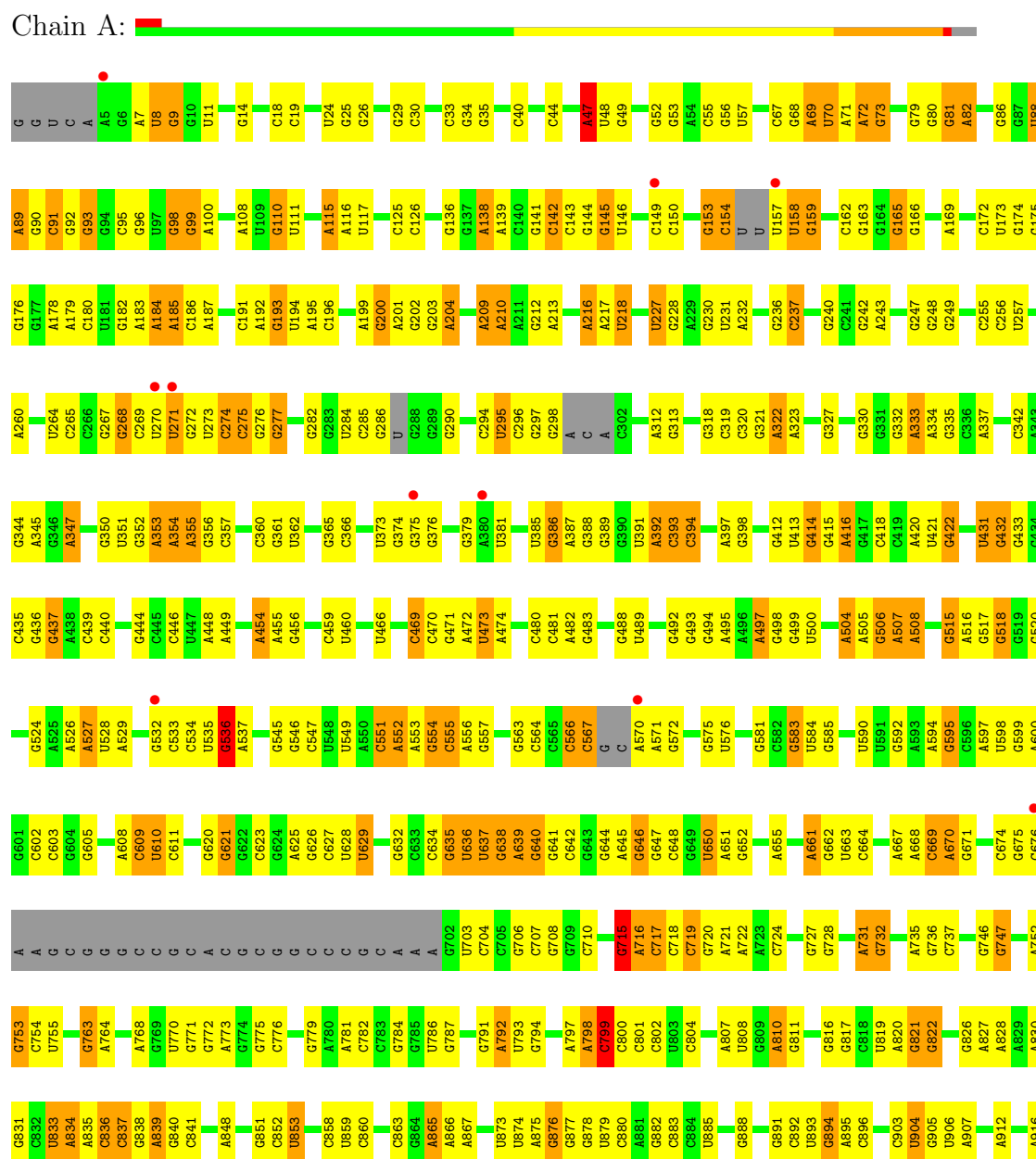
- Molecule 33 is a protein called 50S Ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

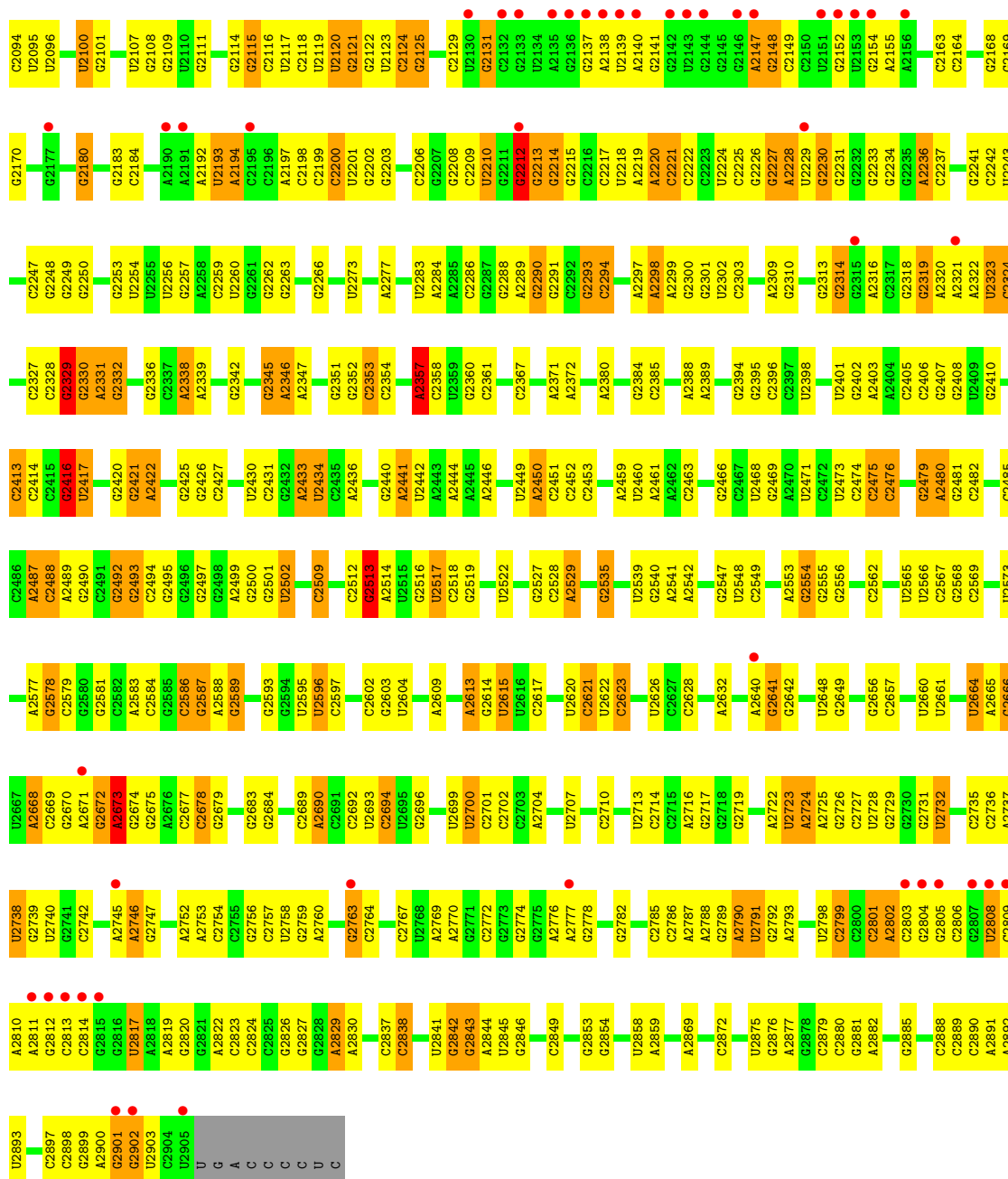
3 Residue-property plots

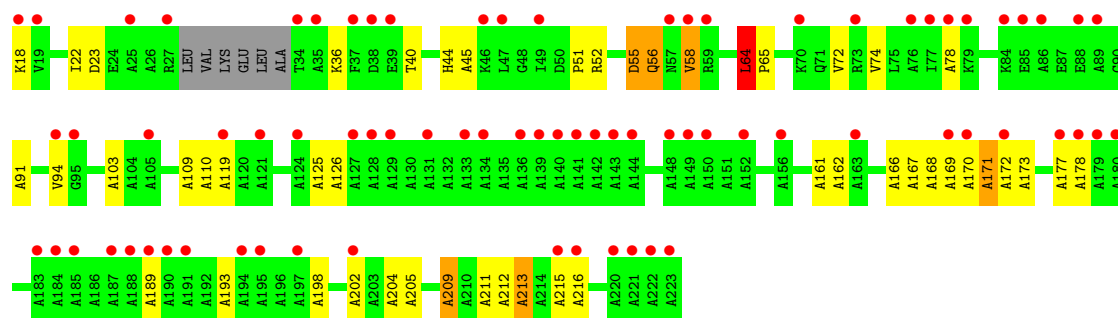
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

• Molecule 1: 23S rRNA



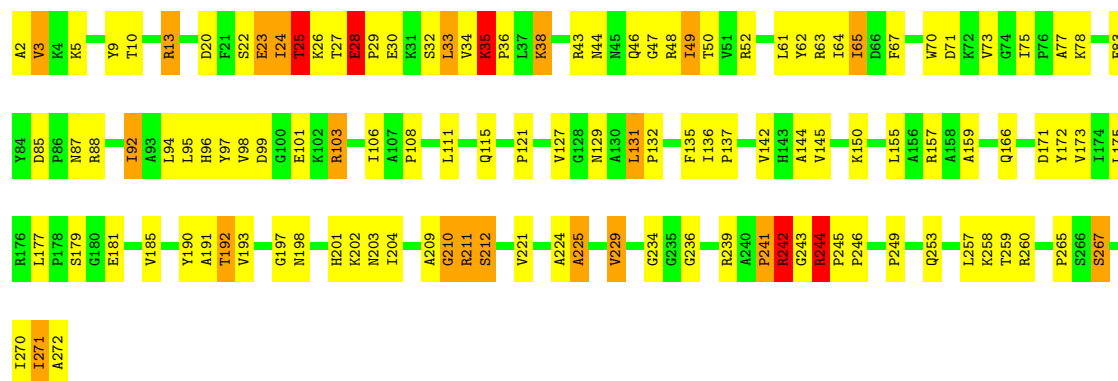
A1933	G1854	G1775	G1689	A1600	G1536	G1461	C1375	G1295	A	G1067	G992
G2018	G1855	G1776	C1690	G1601	G1537	G1462	A1376	C1296	G	U1068	G920
A1935	G1856	G1777	G1691	G1602	C1538	G1463	C1377	G1297	A	U1069	G996
C2020	C1857	A1778	A1604	G1605	A1539	G1464	C1378	A1298	U	G1070	A924
A1937	A1858	G1779	C1692	G1606	A1540	G1465	C1379	G1301	U	U1071	U1002
G1943	A1859	G1780	C1695	G1607	A1541	G1466	U1380	C1302	G	A1072	A1003
U1944	U1863		C1696	A1608	C1543	G1467	G1382	G1309	U	G1075	C930
C1946	U1864		A1698	G1609	C1544		G1383	A1310	A	U1076	C931
U1947	G1865		C1699	A1612	G1545			G1311	U	A1077	C932
U1948	U1868		A1700	A1613	C1546			U1312	A	U1078	C934
A1949	G1869		C1702	G1614	C1547			A1313	U	C1083	A936
C2032			C1703	A1615	U1548			A1314	G	U1084	G937
A2035	C1873		C1704	A1616	C1549			C1315	C	C1085	C938
A2036	G1874		U1705		C1550			G1316	U	C1086	C939
U2037	C1875			C1621	A1553			A1317	C	C1087	U940
	G1876		C1709	U1622	C1554			U1318	A	A1088	A941
A2041	A1877		G1712	C1623	A1555			A1323	U	G1089	C942
U2043	G1878		G1713	A1625	A1556			G1324	C	A1090	C943
U1960	G1879		G1713		G1557			C1325	U	A1091	A944
	A1883		G1720	A1628	C1558			G1326	G1152	G1092	A945
			C1721	A1629	U1559			U1327	A1093	A1093	
U1967	G1887		A1722	C1630	U1561			A1328	C1094	C1094	C948
C1968	A1888		G1723	A1631	C1562			G1329	A1095	A1026	C949
A1973	A1889		U1724	C1632	C1563			C1330	C1096	C1027	
G2052	U1890		U1725	C1633	G1564			A1331	C1097	A1028	
G2053	U1894		U1726		U1565			A1332	G1159	C953	
U2055	G1895		G1727	G1636	U1566			U1333	A1160	A954	A955
G2056	C1896		C1637	U1637	G1567			U1334	C1161	A	
C2057	A1897		G1728	C1638				C1335	G	G	
	C1898		C1729	G1639				A1423	C1162	C1036	
C1983	U1899		U1734		G1570			U1337	G	C1037	C959
U1984	G1900		A1735	C1643				C1338	G	G1038	C960
G1985	C1901		A1817		A1574			U1345	G	G961	
C2061	C1902		C1817		G1575			A1346	C1168	A962	
U2062	A1907		C1818		C1576			A1347	A1173	A963	
C2063	C1908		C1819		C1577			C1348	A1174	G964	
A2064	G1909		G1742		C1578				C1043	G965	
	A1905		A1821		G1579				U1175	C966	
A1991	A1906		C1743		U				G1176	U967	
C2071	C1907		A1653		A				U	U	
A2072	U1908		G1745		C				U	A1046	C968
	C1909		A1746		G				A	G1047	
C2076	U1909		A1747		A				G	C	
G2077	A1910		C1656		G				A	G	
A2078			U1765		C				G	C	
C2079	C1914		U1828		U				C	U	
A2080	G1829		C1756		G				A	A	
A2081	C1915		A1661		U				A	G	
C2082	C1916		C1662		A				A	G	
A2083	G1917		A1663		C1589				C	G1055	
C2084			C1833		A1590				U	A1056	
C2085	G1920		C1834		A1591				C	G1057	
C2086	A1921		U1835		C1592				U	U1059	
C2087	A1922				C1593				A	C	
C2088	C1923		G1846		C1594				C	G1060	
U2089					G1671				C	G1061	
G2090	C2011		A1849		U1685				C	U1062	
C2091	U2012		C1771		C1596				C	U1063	
	G2013		C1772		C1597				U	A	
	U2014		U1686		C1598				U	U1064	
	C2015		A1851		A1687				U	A1065	
			C1773		C1689				A	C1066	
			G1774		A1690					A	





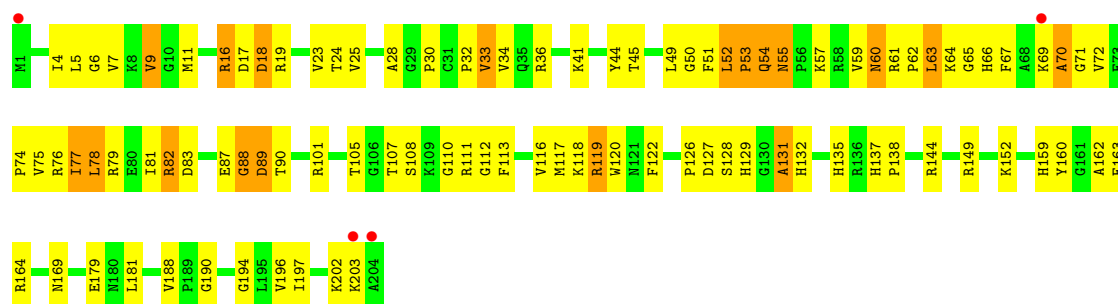
• Molecule 4: 50S Ribosomal protein L2

Chain D:



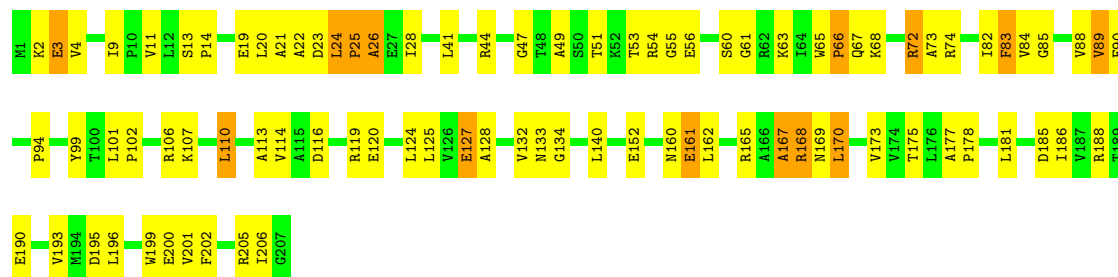
• Molecule 5: 50S Ribosomal protein L3

Chain E:



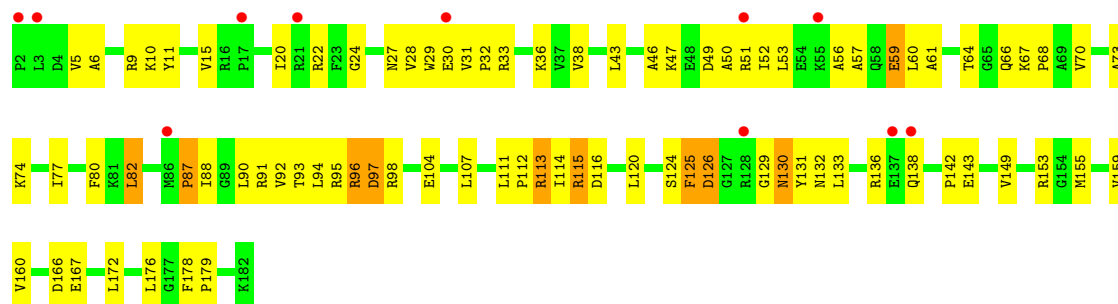
• Molecule 6: 50S Ribosomal protein L4

Chain F:



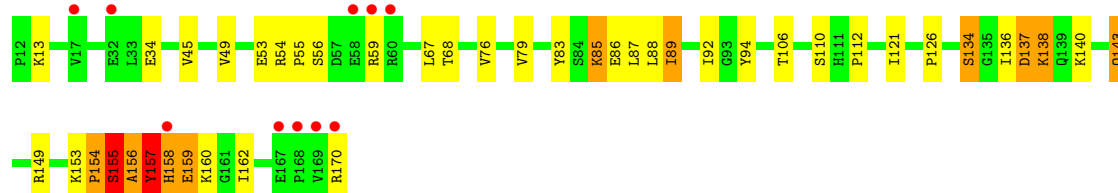
• Molecule 7: 50S Ribosomal protein L5

Chain G:



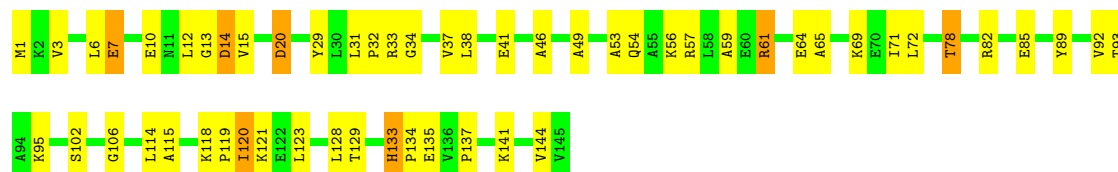
- Molecule 8: 50S Ribosomal protein L6

Chain H:



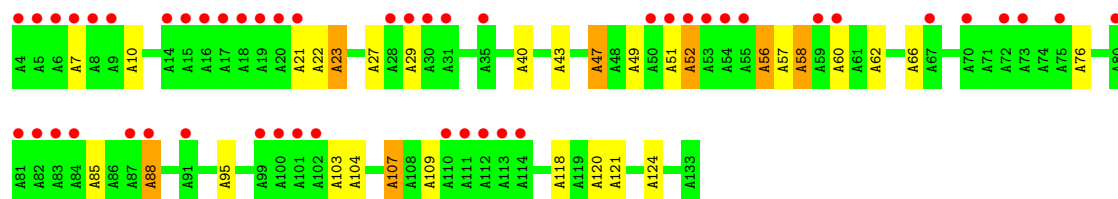
- Molecule 9: 50S Ribosomal protein L9

Chain I:



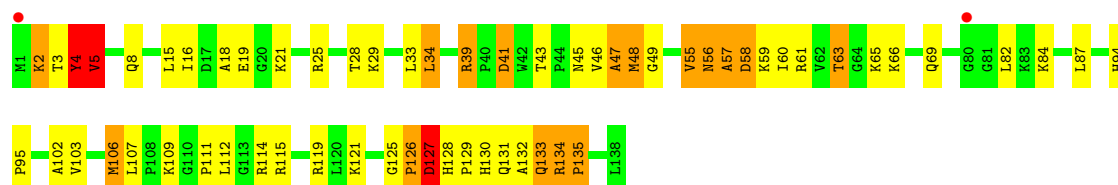
- Molecule 10: 50S Ribosomal protein L10

Chain J:



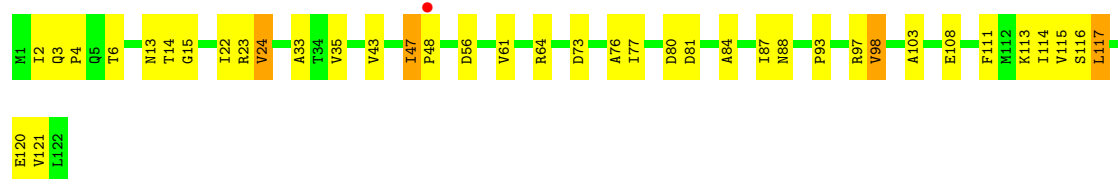
- Molecule 11: 50S Ribosomal protein L13

Chain N:



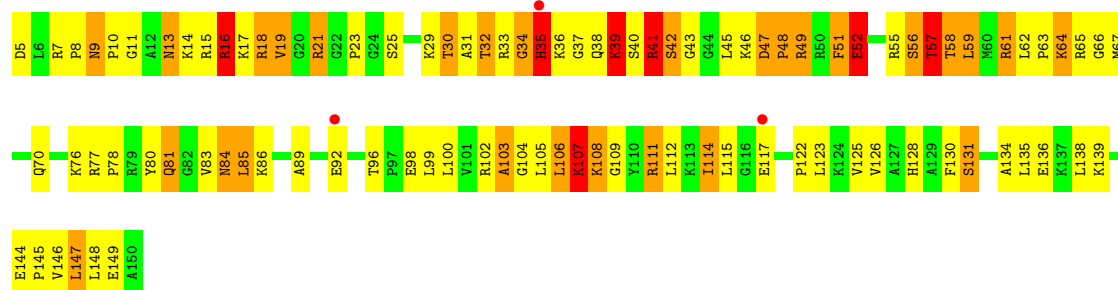
- Molecule 12: 50S Ribosomal protein L14

Chain O:



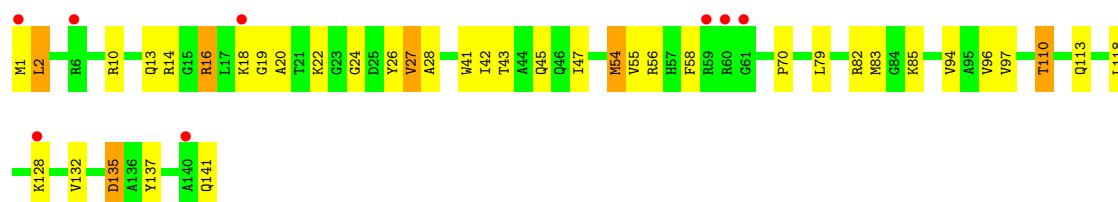
- Molecule 13: 50S Ribosomal protein L15

Chain P:



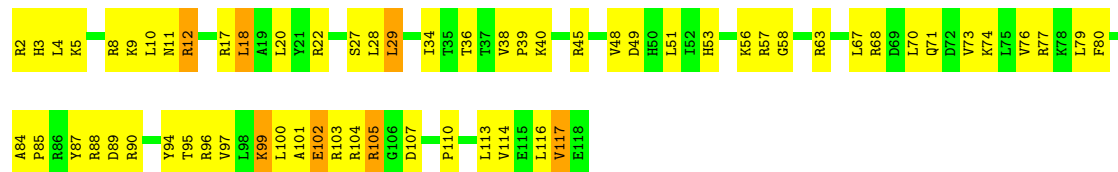
- Molecule 14: 50S Ribosomal protein L16

Chain Q:



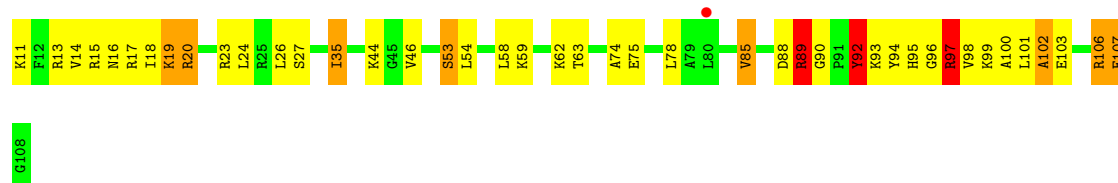
- Molecule 15: 50S Ribosomal protein L17

Chain R:



- Molecule 16: 50S Ribosomal protein L18

Chain S:



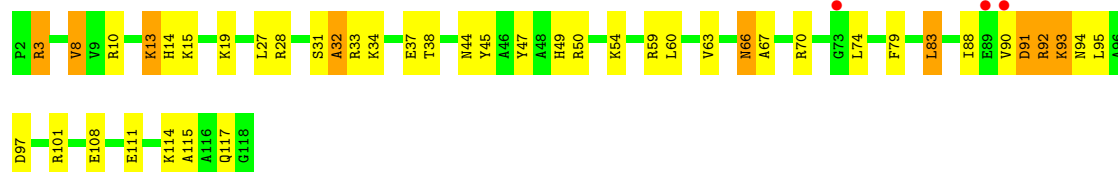
- Molecule 17: 50S Ribosomal protein L19

Chain T:



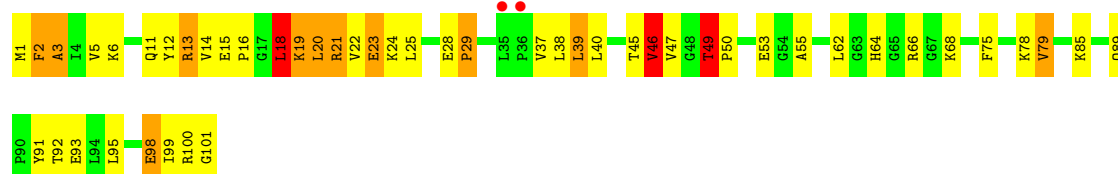
- Molecule 18: 50S Ribosomal protein L20

Chain U:



- Molecule 19: 50S Ribosomal protein L21

Chain V:



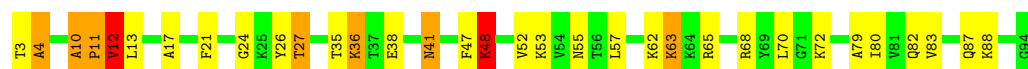
- Molecule 20: 50S Ribosomal protein L22

Chain W:



- Molecule 21: 50S Ribosomal protein L23

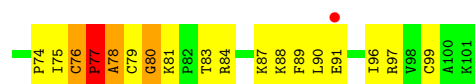
Chain X:



- Molecule 22: 50S Ribosomal protein L24

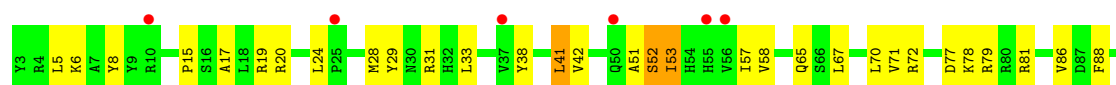
Chain Y:





- Molecule 23: 50S Ribosomal protein L25

Chain Z:



- Molecule 24: 50S Ribosomal protein L27

Chain 0:



- Molecule 25: 50S Ribosomal protein L28

Chain 1:



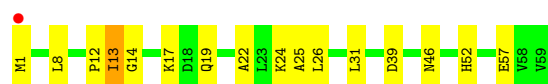
- Molecule 26: 50S Ribosomal protein L29

Chain 2:



- Molecule 27: 50S Ribosomal protein L30

Chain 3:



- Molecule 28: 50S Ribosomal protein L31

Chain 4:



- Molecule 29: 50S Ribosomal protein L32

Chain 5:



- Molecule 30: 50S Ribosomal protein L33

Chain 6: 



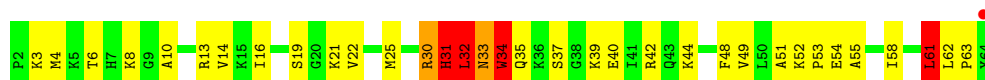
- Molecule 31: 50S Ribosomal protein L34

Chain 7: 



- Molecule 32: 50S Ribosomal protein L35

Chain 8: 



- Molecule 33: 50S Ribosomal protein L36

Chain 9: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.92Å 449.90Å 624.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.57 – 3.30 39.57 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.6 (39.57-3.30) 95.6 (39.57-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.8.0031	Depositor
R, R_{free}	0.225 , 0.279 0.436 , 0.439	Depositor DCC
R_{free} test set	41955 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 41.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 839115 reflections	Xtriage
F_o, F_c correlation	0.47	EDS
Total number of atoms	91380	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.45	5/67709 (0.0%)	0.80	93/105690 (0.1%)
2	B	0.35	0/2853	0.72	0/4451
3	C	0.48	0/1160	0.55	0/1584
4	D	0.60	0/2155	0.85	0/2905
5	E	0.56	1/1597 (0.1%)	0.83	2/2153 (0.1%)
6	F	0.52	0/1659	0.75	0/2244
7	G	0.44	0/1499	0.67	0/2016
8	H	0.47	0/1246	0.67	1/1682 (0.1%)
9	I	0.47	0/1147	0.72	0/1551
10	J	0.44	0/650	0.53	0/907
11	N	0.49	0/1132	0.77	0/1525
12	O	0.53	0/943	0.78	0/1269
13	P	0.57	0/1131	0.98	2/1504 (0.1%)
14	Q	0.46	0/1143	0.68	0/1527
15	R	0.54	0/974	0.87	0/1302
16	S	0.48	0/779	0.79	0/1036
17	T	0.58	0/1156	0.95	0/1542
18	U	0.50	0/975	0.75	0/1297
19	V	0.47	0/790	0.76	0/1057
20	W	0.52	0/907	0.77	0/1216
21	X	0.52	0/740	0.74	0/993
22	Y	0.53	0/789	0.83	0/1051
23	Z	0.44	0/1436	0.66	0/1949
24	0	0.51	0/671	0.76	0/892
25	1	0.53	0/741	0.84	1/984 (0.1%)
26	2	0.48	0/600	0.79	0/793
27	3	0.44	0/473	0.70	0/634
28	4	0.49	0/229	0.75	0/309
29	5	0.57	0/473	0.88	0/639
30	6	0.83	0/388	1.06	2/518 (0.4%)
31	7	0.58	0/427	0.85	0/561
32	8	0.54	0/516	0.88	1/679 (0.1%)
33	9	0.45	0/302	0.73	0/397
All	All	0.47	6/99390 (0.0%)	0.79	102/148857 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	20	0
4	D	0	2
5	E	0	1
13	P	0	4
15	R	0	1
30	6	0	1
All	All	20	9

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1851	A	O3'-P	-6.02	1.53	1.61
1	A	1987	A	O3'-P	-5.96	1.54	1.61
1	A	2234	G	O3'-P	-5.77	1.54	1.61
1	A	839	A	O3'-P	-5.63	1.54	1.61
5	E	127	ASP	CB-CG	5.59	1.63	1.51

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1345	U	C2'-C3'-O3'	11.83	135.53	109.50
1	A	989	A	N9-C1'-C2'	11.32	128.72	114.00
1	A	2013	G	C2'-C3'-O3'	11.20	134.14	109.50
1	A	2297	A	N9-C1'-C2'	11.08	128.41	114.00
1	A	1955	C	C2'-C3'-O3'	10.95	133.58	109.50

5 of 20 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	98	G	C1'
1	A	497	A	C3'
1	A	715	G	C4',C1',C3'
1	A	989	A	C1'
1	A	1345	U	C4',C1',C3'

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	197	GLY	Peptide
4	D	244	ARG	Peptide
5	E	131	ALA	Peptide
13	P	41	ARG	Peptide
13	P	51	PHE	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	60459	0	30488	990	0
2	B	2551	0	1295	35	0
3	C	1157	0	1160	22	0
4	D	2105	0	2182	89	0
5	E	1564	0	1629	66	0
6	F	1624	0	1677	63	0
7	G	1474	0	1535	48	0
8	H	1223	0	1282	22	0
9	I	1132	0	1218	29	0
10	J	651	0	649	14	0
11	N	1105	0	1180	42	0
12	O	933	0	996	27	0
13	P	1114	0	1187	82	0
14	Q	1122	0	1179	28	0
15	R	960	0	1021	46	0
16	S	771	0	832	33	0
17	T	1142	0	1202	67	0
18	U	958	0	1018	52	0
19	V	779	0	852	39	0
20	W	896	0	956	23	0
21	X	726	0	778	20	0
22	Y	776	0	870	45	0
23	Z	1404	0	1432	30	0
24	0	662	0	688	19	0
25	1	734	0	808	21	0
26	2	598	0	653	13	0
27	3	468	0	523	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	4	226	0	229	4	0
29	5	459	0	478	21	0
30	6	381	0	391	30	0
31	7	419	0	467	15	0
32	8	508	0	576	33	0
33	9	299	0	324	7	0
All	All	91380	0	61755	1840	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 1840 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1331:A:O2'	1:A:1333:U:OP2	1.62	1.13
1:A:1377:G:N2	1:A:1654:A:O2'	1.90	1.02
33:9:11:CYS:HB3	33:9:14:CYS:SG	1.99	1.01
1:A:1424:A:O2'	1:A:1425:G:OP1	1.78	1.00
1:A:2492:G:O2'	1:A:2493:G:OP2	1.79	0.99

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	182/196 (93%)	115 (63%)	47 (26%)	20 (11%)	1	6
4	D	269/271 (99%)	217 (81%)	31 (12%)	21 (8%)	1	14
5	E	202/204 (99%)	152 (75%)	35 (17%)	15 (7%)	2	15
6	F	205/207 (99%)	163 (80%)	28 (14%)	14 (7%)	2	18
7	G	179/181 (99%)	137 (76%)	31 (17%)	11 (6%)	2	22
8	H	157/159 (99%)	116 (74%)	25 (16%)	16 (10%)	1	7
9	I	143/145 (99%)	110 (77%)	25 (18%)	8 (6%)	3	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	128/130 (98%)	72 (56%)	42 (33%)	14 (11%)	1	6
11	N	136/138 (99%)	108 (79%)	15 (11%)	13 (10%)	1	9
12	O	120/122 (98%)	106 (88%)	13 (11%)	1 (1%)	27	78
13	P	144/146 (99%)	87 (60%)	28 (19%)	29 (20%)	0	1
14	Q	139/141 (99%)	116 (84%)	19 (14%)	4 (3%)	7	47
15	R	115/117 (98%)	92 (80%)	17 (15%)	6 (5%)	3	27
16	S	96/98 (98%)	63 (66%)	20 (21%)	13 (14%)	0	3
17	T	135/137 (98%)	89 (66%)	30 (22%)	16 (12%)	1	4
18	U	115/117 (98%)	92 (80%)	19 (16%)	4 (4%)	6	41
19	V	99/101 (98%)	72 (73%)	17 (17%)	10 (10%)	1	8
20	W	111/113 (98%)	96 (86%)	7 (6%)	8 (7%)	2	16
21	X	90/92 (98%)	75 (83%)	8 (9%)	7 (8%)	1	14
22	Y	98/100 (98%)	60 (61%)	19 (19%)	19 (19%)	0	1
23	Z	174/176 (99%)	130 (75%)	33 (19%)	11 (6%)	2	20
24	0	82/84 (98%)	72 (88%)	9 (11%)	1 (1%)	19	71
25	1	91/93 (98%)	74 (81%)	10 (11%)	7 (8%)	1	14
26	2	69/71 (97%)	54 (78%)	11 (16%)	4 (6%)	3	23
27	3	57/59 (97%)	53 (93%)	3 (5%)	1 (2%)	13	61
28	4	28/30 (93%)	20 (71%)	5 (18%)	3 (11%)	1	6
29	5	57/59 (97%)	48 (84%)	4 (7%)	5 (9%)	1	11
30	6	42/44 (96%)	23 (55%)	7 (17%)	12 (29%)	0	0
31	7	46/48 (96%)	45 (98%)	0	1 (2%)	10	55
32	8	61/63 (97%)	47 (77%)	8 (13%)	6 (10%)	1	8
33	9	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
All	All	3604/3678 (98%)	2737 (76%)	567 (16%)	300 (8%)	1	12

5 of 300 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	213	ALA
4	D	25	THR
4	D	33	LEU
4	D	242	ARG
4	D	271	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	C	61/66 (92%)	56 (92%)	5 (8%)	17	57
4	D	213/213 (100%)	176 (83%)	37 (17%)	3	14
5	E	165/165 (100%)	139 (84%)	26 (16%)	4	18
6	F	165/165 (100%)	149 (90%)	16 (10%)	12	45
7	G	155/155 (100%)	137 (88%)	18 (12%)	8	35
8	H	132/132 (100%)	120 (91%)	12 (9%)	14	49
9	I	122/122 (100%)	111 (91%)	11 (9%)	14	50
11	N	117/117 (100%)	94 (80%)	23 (20%)	2	9
12	O	100/100 (100%)	93 (93%)	7 (7%)	21	66
13	P	112/112 (100%)	86 (77%)	26 (23%)	1	5
14	Q	111/111 (100%)	101 (91%)	10 (9%)	14	50
15	R	100/100 (100%)	85 (85%)	15 (15%)	4	21
16	S	77/77 (100%)	67 (87%)	10 (13%)	6	29
17	T	120/120 (100%)	93 (78%)	27 (22%)	1	6
18	U	92/92 (100%)	82 (89%)	10 (11%)	9	38
19	V	82/82 (100%)	65 (79%)	17 (21%)	2	8
20	W	91/91 (100%)	80 (88%)	11 (12%)	7	33
21	X	74/74 (100%)	65 (88%)	9 (12%)	7	32
22	Y	84/84 (100%)	67 (80%)	17 (20%)	2	8
23	Z	155/155 (100%)	148 (96%)	7 (4%)	38	81
24	0	66/66 (100%)	60 (91%)	6 (9%)	14	49
25	1	78/78 (100%)	62 (80%)	16 (20%)	2	8
26	2	66/66 (100%)	60 (91%)	6 (9%)	14	49
27	3	51/51 (100%)	48 (94%)	3 (6%)	28	73
28	4	27/27 (100%)	24 (89%)	3 (11%)	9	37
29	5	51/51 (100%)	41 (80%)	10 (20%)	2	9
30	6	43/43 (100%)	36 (84%)	7 (16%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	7	41/41 (100%)	32 (78%)	9 (22%)	1	6
32	8	53/53 (100%)	43 (81%)	10 (19%)	2	11
33	9	33/33 (100%)	30 (91%)	3 (9%)	14	49
All	All	2837/2842 (100%)	2450 (86%)	387 (14%)	5	26

5 of 387 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	P	98	GLU
17	T	6	LEU
29	5	56	LYS
13	P	135	LEU
15	R	57	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
15	R	53	HIS
17	T	58	ASN
29	5	43	HIS
15	R	71	GLN
17	T	38	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2799/2915 (96%)	754 (26%)	122 (4%)
2	B	118/119 (99%)	27 (22%)	4 (3%)
All	All	2917/3034 (96%)	781 (26%)	126 (4%)

5 of 781 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	U
1	A	9	G
1	A	14	G
1	A	33	C
1	A	34	G

5 of 126 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1441	U
1	A	1662	C
1	A	2803	C
1	A	1472	A
1	A	1542	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2807/2915 (96%)	0.09	93 (3%) 44 10	24, 64, 168, 297	0
2	B	119/119 (100%)	0.60	6 (5%) 28 6	71, 112, 151, 191	0
3	C	190/196 (96%)	1.99	76 (40%) 1 0	109, 188, 240, 265	0
4	D	271/271 (100%)	-0.05	0 100 100	23, 56, 91, 127	0
5	E	204/204 (100%)	0.07	4 (1%) 62 19	28, 65, 120, 165	0
6	F	207/207 (100%)	0.12	0 100 100	31, 87, 149, 214	0
7	G	181/181 (100%)	0.59	11 (6%) 21 5	82, 128, 167, 210	0
8	H	159/159 (100%)	0.65	10 (6%) 19 5	70, 128, 180, 235	0
9	I	145/145 (100%)	-0.06	0 100 100	48, 101, 137, 159	0
10	J	130/130 (100%)	1.66	49 (37%) 1 0	122, 193, 233, 284	0
11	N	138/138 (100%)	0.21	2 (1%) 72 25	54, 90, 120, 133	0
12	O	122/122 (100%)	-0.00	1 (0%) 83 39	39, 64, 85, 92	0
13	P	146/146 (100%)	0.35	3 (2%) 60 17	39, 92, 134, 174	0
14	Q	141/141 (100%)	0.44	8 (5%) 23 5	58, 92, 125, 161	0
15	R	117/117 (100%)	0.06	0 100 100	40, 65, 100, 131	0
16	S	98/98 (100%)	0.47	1 (1%) 79 33	72, 110, 151, 181	0
17	T	137/137 (100%)	0.09	1 (0%) 84 42	43, 77, 135, 170	0
18	U	117/117 (100%)	0.24	3 (2%) 53 13	40, 80, 135, 155	0
19	V	101/101 (100%)	0.31	2 (1%) 62 19	61, 110, 143, 183	0
20	W	113/113 (100%)	0.03	2 (1%) 65 20	49, 66, 103, 147	0
21	X	92/92 (100%)	0.02	0 100 100	43, 77, 98, 114	0
22	Y	100/100 (100%)	0.38	2 (2%) 62 19	56, 100, 175, 209	0
23	Z	176/176 (100%)	1.24	33 (18%) 2 1	92, 149, 299, 353	0
24	0	84/84 (100%)	0.26	1 (1%) 75 29	58, 84, 105, 128	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	1	93/93 (100%)	0.07	0 100 100	39, 63, 111, 153	0
26	2	71/71 (100%)	0.05	0 100 100	60, 90, 131, 150	0
27	3	59/59 (100%)	0.36	1 (1%) 67 21	65, 101, 135, 253	0
28	4	30/30 (100%)	0.48	2 (6%) 17 4	121, 142, 163, 173	0
29	5	59/59 (100%)	0.02	2 (3%) 43 10	42, 67, 130, 179	0
30	6	44/44 (100%)	0.44	2 (4%) 32 7	51, 90, 113, 121	0
31	7	48/48 (100%)	0.07	0 100 100	31, 49, 80, 98	0
32	8	63/63 (100%)	0.22	1 (1%) 68 22	50, 77, 112, 154	0
33	9	36/36 (100%)	0.53	2 (5%) 24 5	63, 91, 115, 125	0
All	All	6598/6712 (98%)	0.27	318 (4%) 29 7	23, 78, 188, 353	0

The worst 5 of 318 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	140	ALA	10.0
8	H	170	ARG	9.7
1	A	2812	G	9.2
3	C	78	ALA	8.3
3	C	141	ALA	8.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.