



wwPDB X-ray Structure Validation Summary Report

Nov 23, 2014 – 12:52 PM EST

PDB ID : 4W2B
Title : Crystal structure of the peptolide 12C bound to bacterial ribosome
Authors : Fagan, C.E.; Dunham, C.M.
Deposited on : 2014-03-24
Resolution : 3.60 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

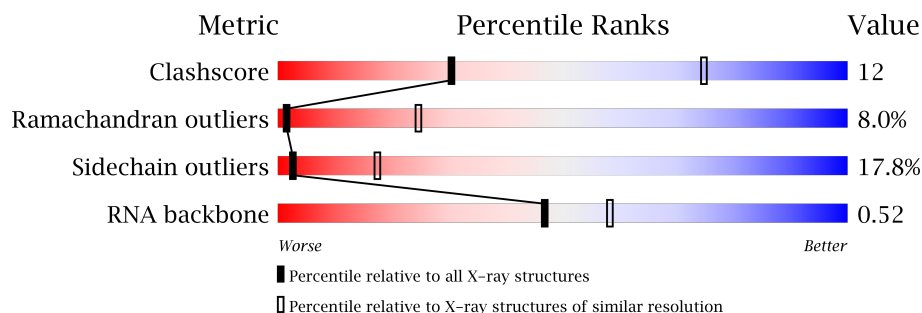
The following versions of software and data (see [references](#)) were used in the production of this report:

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) : stable24195

1 Overall quality at a glance

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1155 (3.80-3.40)
Ramachandran outliers	78287	1109 (3.80-3.40)
Sidechain outliers	78261	1108 (3.80-3.40)
RNA backbone	1838	1012 (4.40-2.76)







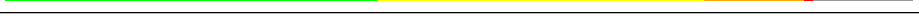

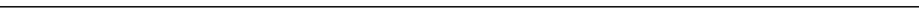
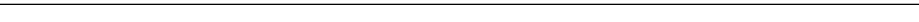








The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2915	
2	B	122	
3	C	276	
4	D	206	
5	E	210	
6	F	182	
7	G	180	
8	H	148	
9	I	140	
10	J	122	
11	K	150	
12	L	141	
13	M	118	
14	N	112	

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

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

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

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

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

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 31 is a protein called 50S ribosomal protein L36.

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	P	1	Total	Mg	0	0
			1	1		
33	D	2	Total	Mg	0	0
			2	2		
33	K	3	Total	Mg	0	0
			3	3		
33	E	1	Total	Mg	0	0
			1	1		
33	B	2	Total	Mg	0	0
			2	2		
33	C	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	V	1	Total 1	Mg 1	0	0
33	A	243	Total 243	Mg 243	0	0

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

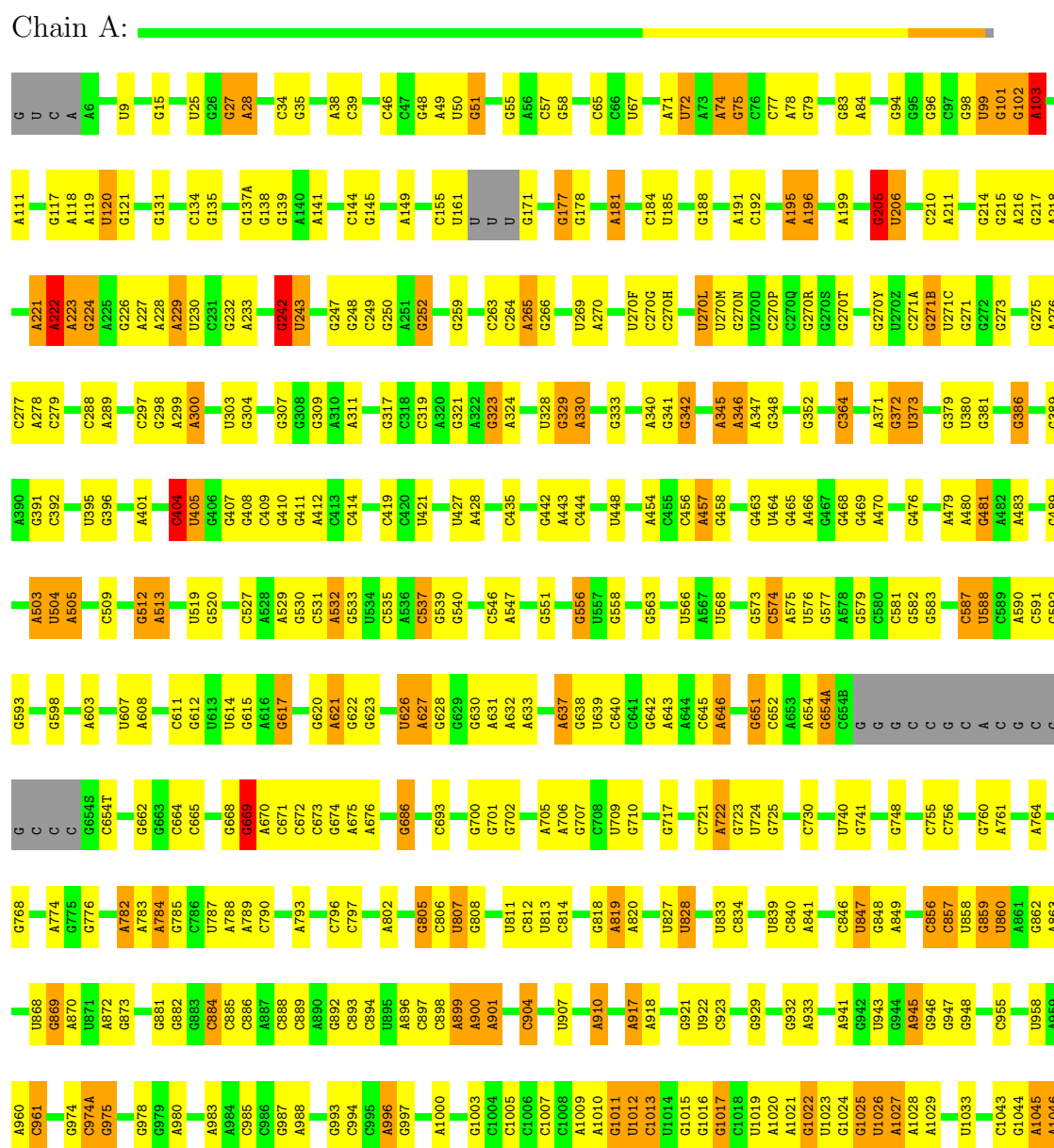
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	a	1	Total 1	Zn 1	0	0

3 Residue-property plots

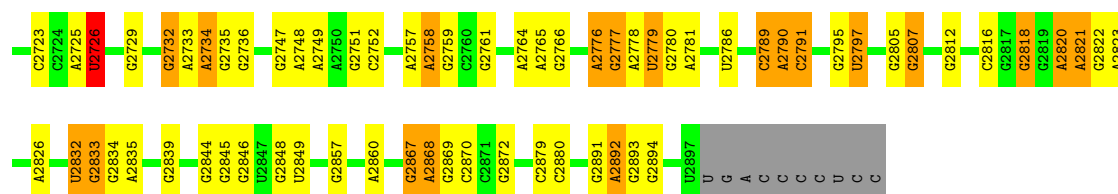
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: 23S ribosomal RNA

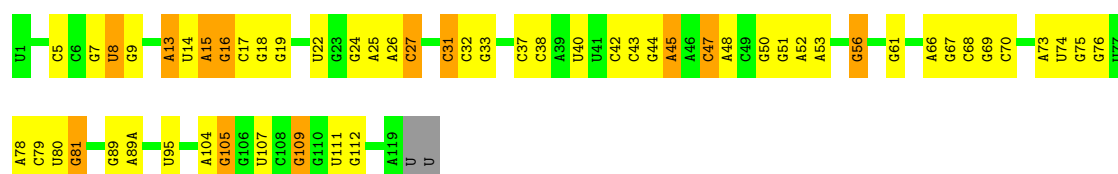


G2627	A2518	G2405	C2313	A2212	G2121	U2011	G1899	U1777	G1638	G1519	U1420	U1316	C1221	G1047
G2628	U2519	U2406	C2314	U2213	U2122	G2012	G1899	A1780	U1639	G1522	G1421	A1317	G1226	A1048
A2629	C2520		G2315	G2215	G2123	A2019	C1902	C1782	C1640	G1527	A1427	A1321	G1227	A1050
G2630			G2316	G2216	G2124				C1642		G1428	A1322	G1228	G1051
G2631	C2527	A2411	C2317	G2224	A2125	U2022	G1906	A1787	G1646	C1533	G1429	U1329	G1231	G1052
A2632	U2528	A2412	G2318	A2225	G2126	G2023	A1913		G1647	C1534	C1430	G1330	G1232	C1053
G2633	G2529	G2413	G2319	C2226	G2127				C1648	U1535	U1431	A1331	G1236	A1054
G2634		G2414	A2320	A2227	C2128	A2030	A1918	C1790	G1649	U1536	G1441	G1332	G1237	G1055
G2635	U2537	G2415	G2321				A1919	A1791	G1653	C1537	G1442	U1336	G1238	G1056
U2636	C2538		A2322	G2238	A2135	G2038	G1922	U1796	A1654	G1538	G1443	G1337		G1057
			A2323	G2239	C2136			C1797	A1664	G1542	A1444A	G1338	G1244	G1058
A2542	G2543	A2422	G2324	U2232	G2131	A2031	A1918	C1790	A1667	A1543	G1445		G1245	U1060
G2543	C2428	U2423	G2325	G2233	U2132	G2032	A1919	A1791	G1674	A1544		U1341	G1249	U1061
G2544	G2429	C2430	G2326	G2234	G2133	A2033	G1920		A1676	A1545	G1449	G1348	G1252	G1062
	A2425		C2327	G2235	A2134		G1921	U1795	A1677			U1352	G1253	G1063
	A2426		A2328		A2135		G1922	U1796	C1678	C1548	A1455	A1353	G1256	U1065
			A2329		C2136				A1678	C1549	G1458	U1357	G1259	U1066
			G2330		G2147	C2050	A1936	A1801	G1674		G1459	G1358	G1260	G1068
			G2331		C2148	A2051	A1937	G1800	C1675		A1460	G1359		A1070
					G2149	G2053	A1938	A1801	A1676		A1461		G1264	C1076
					G2150	A2054	A1939	G1801	A1677			G1364	A1265	A1077
					G2151	G2056	U1939	G1801	A1678			A1365	G1171	U1078
					G2151	G2056	U1939	G1801	A1678			A1366	G1173	C1079
					G2151	G2056	U1939	G1801	A1678			A1367	G1175	G1080
					G2151	G2056	U1939	G1801	A1678			A1368	G1176	U1081
					G2151	G2056	U1939	G1801	A1678			A1369	G1177	U1082
					G2151	G2056	U1939	G1801	A1678			A1370	G1178	U1083
					G2151	G2056	U1939	G1801	A1678			A1371	G1179	A1084
					G2151	G2056	U1939	G1801	A1678			A1372	G1180	A1085
					G2151	G2056	U1939	G1801	A1678			A1373	G1183	A1086
					G2151	G2056	U1939	G1801	A1678			A1374	G1184	A1087
					G2151	G2056	U1939	G1801	A1678			A1375	G1185	A1088
					G2151	G2056	U1939	G1801	A1678			A1376	G1186	
					G2151	G2056	U1939	G1801	A1678			A1377	G1187	G1091
					G2151	G2056	U1939	G1801	A1678			A1378	G1188	C1092
					G2151	G2056	U1939	G1801	A1678			A1379	G1189	G1093
					G2151	G2056	U1939	G1801	A1678			A1380	G1190	U1094
					G2151	G2056	U1939	G1801	A1678			A1381	G1191	A1095
					G2151	G2056	U1939	G1801	A1678			A1382	G1192	A1096
					G2151	G2056	U1939	G1801	A1678			A1383	G1193	
					G2151	G2056	U1939	G1801	A1678			A1384	G1194	U1101
					G2151	G2056	U1939	G1801	A1678			A1385	G1195	C1102
					G2151	G2056	U1939	G1801	A1678			A1386	G1196	A1103
					G2151	G2056	U1939	G1801	A1678			A1387	G1197	C1104
					G2151	G2056	U1939	G1801	A1678			A1388	G1198	
					G2151	G2056	U1939	G1801	A1678			A1389	G1199	G1110
					G2151	G2056	U1939	G1801	A1678			A1390	G1200	A1111
					G2151	G2056	U1939	G1801	A1678			A1391	G1201	G1112
					G2151	G2056	U1939	G1801	A1678			A1392	G1202	
					G2151	G2056	U1939	G1801	A1678			A1393	G1203	G1122
					G2151	G2056	U1939	G1801	A1678			A1394	G1204	
					G2151	G2056	U1939	G1801	A1678			A1395	G1205	G1125
					G2151	G2056	U1939	G1801	A1678			A1396	G1206	A1126
					G2151	G2056	U1939	G1801	A1678			A1397	G1207	
					G2151	G2056	U1939	G1801	A1678			A1398	G1208	
					G2151	G2056	U1939	G1801	A1678			A1399	G1209	
					G2151	G2056	U1939	G1801	A1678			A1400	G1210	
					G2151	G2056	U1939	G1801	A1678			A1401	G1211	
					G2151	G2056	U1939	G1801	A1678			A1402	G1212	
					G2151	G2056	U1939	G1801	A1678			A1403	G1213	
					G2151	G2056	U1939	G1801	A1678			A1404	G1214	
					G2151	G2056	U1939	G1801	A1678			A1405	G1215	
					G2151	G2056	U1939	G1801	A1678			A1406	G1216	
					G2151	G2056	U1939	G1801	A1678			A1407	G1217	
					G2151	G2056	U1939	G1801	A1678			A1408	G1218	
					G2151	G2056	U1939	G1801	A1678			A1409	G1219	
					G2151	G2056	U1939	G1801	A1678			A1410	G1220	
					G2151	G2056	U1939	G1801	A1678			A1411	G1221	
					G2151	G2056	U1939	G1801	A1678			A1412	G1222	
					G2151	G2056	U1939	G1801	A1678			A1413	G1223	
					G2151	G2056	U1939	G1801	A1678			A1414	G1224	
					G2151	G2056	U1939	G1801	A1678			A1415	G1225	
					G2151	G2056	U1939	G1801	A1678			A1416	G1226	
					G2151	G2056	U1939	G1801	A1678			A1417	G1227	
					G2151	G2056	U1939	G1801	A1678			A1418	G1228	
					G2151	G2056	U1939	G1801	A1678			A1419	G1229	
					G2151	G2056	U1939	G1801	A1678			A1420	G1230	
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					G2151	G2056	U1939	G1801	A1678			A1422	G1232	
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					G2151	G2056	U1939	G1801	A1678			A1424	G1234	
					G2151	G2056	U1939	G1801	A1678			A1425	G1235	
					G2151	G2056	U1939	G1801	A1678			A1426	G1236	
					G2151	G2056	U1939	G1801	A1678			A1427	G1237	
					G2151	G2056	U1939	G1801	A1678			A1428	G1238	
					G2151	G2056	U1939	G1801	A1678			A1429	G1239	
					G2151	G2056	U1939	G1801	A1678			A1430	G1240	
					G2151	G2056	U1939	G1801	A1678			A1431	G1241	
					G2151	G2056	U1939	G1801	A1678			A1432	G1242	
					G2151	G2056	U1939	G1801	A1678			A1433	G1243	
					G2151	G2056	U1939	G1801	A1678			A1434	G1244	
					G2151	G2056	U1939	G1801	A1678			A1435	G1245	
					G2151	G2056	U1939	G1801	A1678			A1436	G1246	
					G2151	G2056	U1939	G1801	A1678			A1437	G1247	
					G2151	G2056	U1939	G1801	A1678			A1438	G1248	
					G2151	G2056	U1939	G1801	A1678			A1439	G1249	
					G2151	G2056	U1939	G1801	A1678			A1440	G1250	
					G2151	G2056	U1939	G1801	A1678			A1441	G1251	
					G2151	G2056	U1939	G1801	A1678			A1442	G1252	
					G2151	G2056	U1939	G1801	A1678			A1443	G1253	
					G2151	G2056	U1939	G1801	A1678			A1444	G1254	
					G2151	G2056	U1939	G1801	A1678			A1445	G1255	
					G2151	G2056	U1939	G1801	A1678			A1446	G1256	
					G2151	G2056	U1939	G1801	A1678			A1447	G1257	
					G2151	G2056	U1939	G1801	A1678			A1448	G1258	
					G2151	G2056	U1939	G1801	A1678			A1449	G1259	
					G2151	G2056	U1939	G1801	A1678			A1450	G1260	
					G2151	G2056	U1939	G1801	A1678			A1451	G1261	
					G2151	G2056	U1939	G1801	A1678			A1452	G1262	
					G2151	G2056	U1939	G1801	A1678			A1453	G1263	
					G2151	G2056	U1939	G1801	A1678			A1454	G1264	
					G2151	G2056	U1939	G1801	A1678			A1455	G1265	
					G2151	G2056	U1939	G1801	A1678			A1456	G1266	
					G2151	G2056	U1939	G1801	A1678			A1457	G1267	
					G2151	G2056	U1939	G1801	A1678			A1458	G1268	
					G2151	G2056	U1939	G1801	A1678			A1459	G1269	



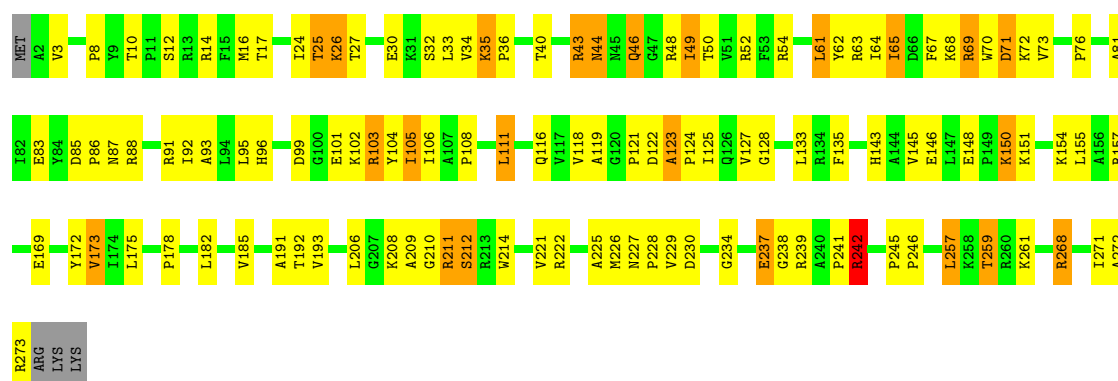
• Molecule 2: 5S ribosomal RNA

Chain B:



• Molecule 3: 50S ribosomal protein L2

Chain C:



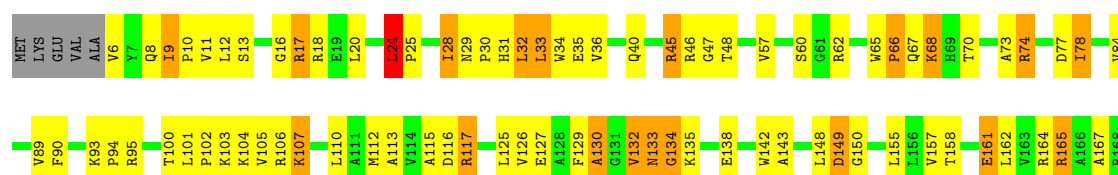
• Molecule 4: 50S ribosomal protein L3

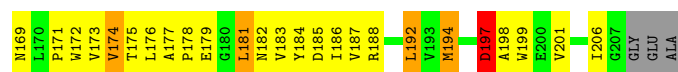
Chain D:



• Molecule 5: 50S ribosomal protein L4

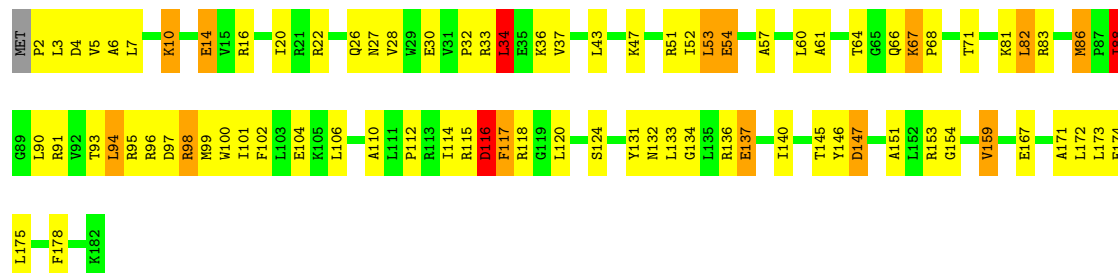
Chain E:





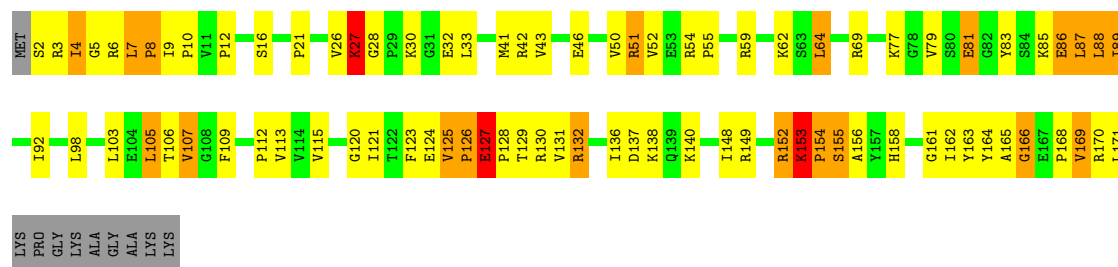
• Molecule 6: 50S ribosomal protein L5

Chain F:



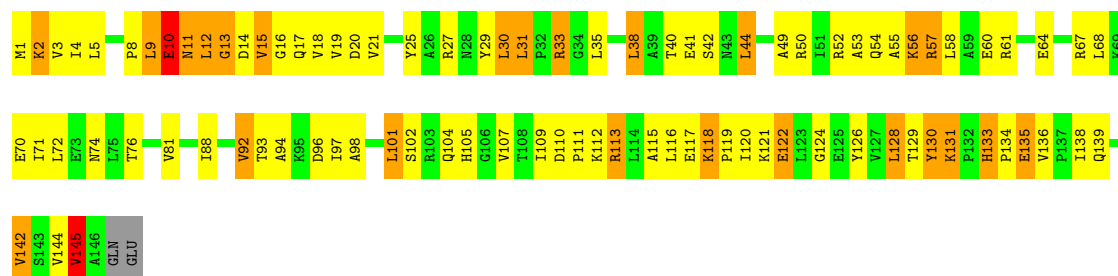
• Molecule 7: 50S ribosomal protein L6

Chain G:



• Molecule 8: 50S ribosomal protein L9

Chain H:



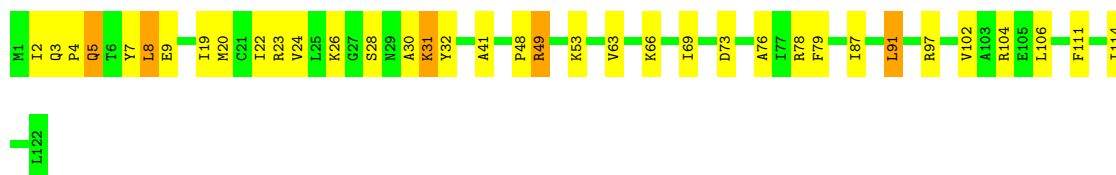
• Molecule 9: 50S ribosomal protein L13

Chain I:



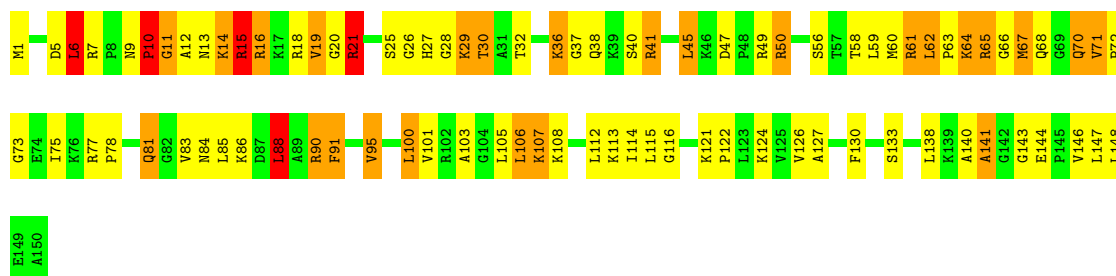
• Molecule 10: 50S ribosomal protein L14

Chain J:



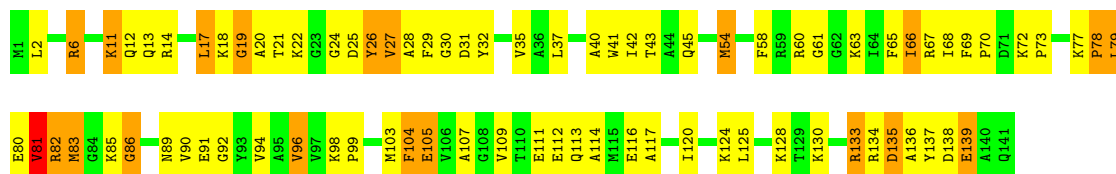
- Molecule 11: 50S ribosomal protein L15

Chain K:



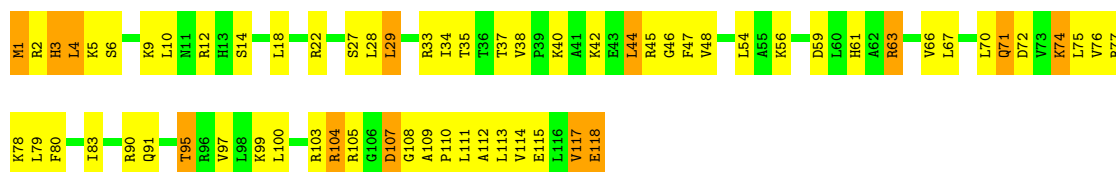
- Molecule 12: 50S ribosomal protein L16

Chain L:



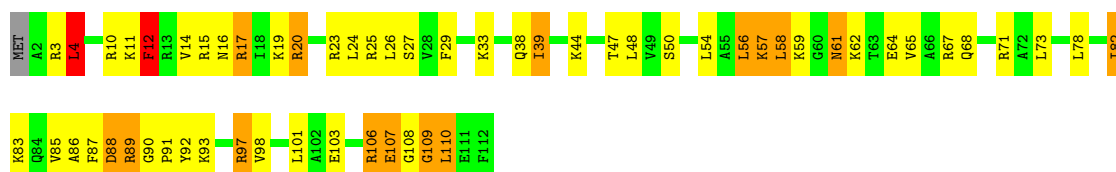
- Molecule 13: 50S ribosomal protein L17

Chain M:



- Molecule 14: 50S ribosomal protein L18

Chain N:



- Molecule 15: 50S ribosomal protein L19

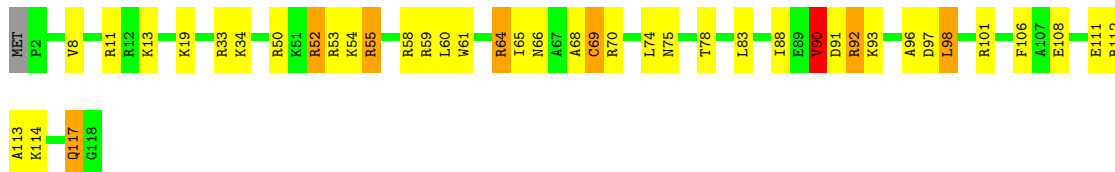
Chain O:





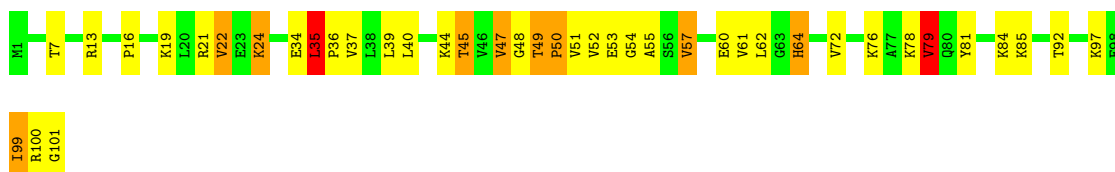
- Molecule 16: 50S ribosomal protein L20

Chain P:



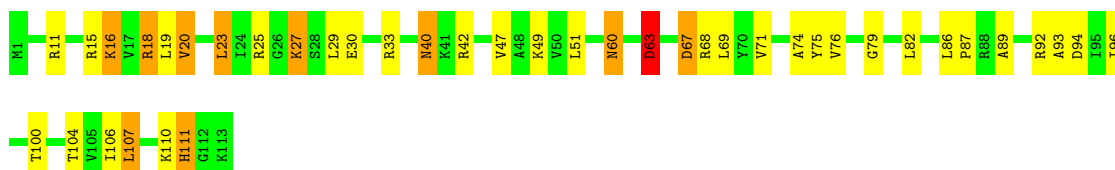
- Molecule 17: 50S ribosomal protein L21

Chain Q:



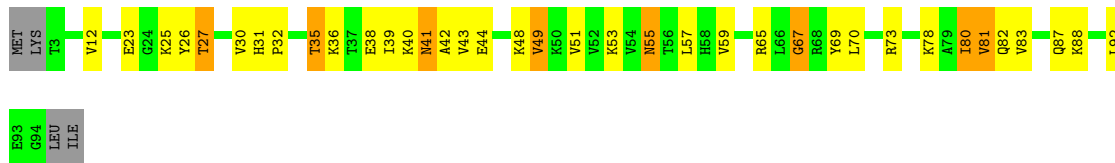
- Molecule 18: 50S ribosomal protein L22

Chain R:



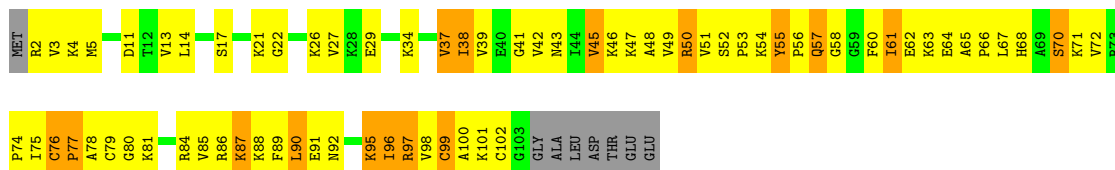
- Molecule 19: 50S ribosomal protein L23

Chain S:



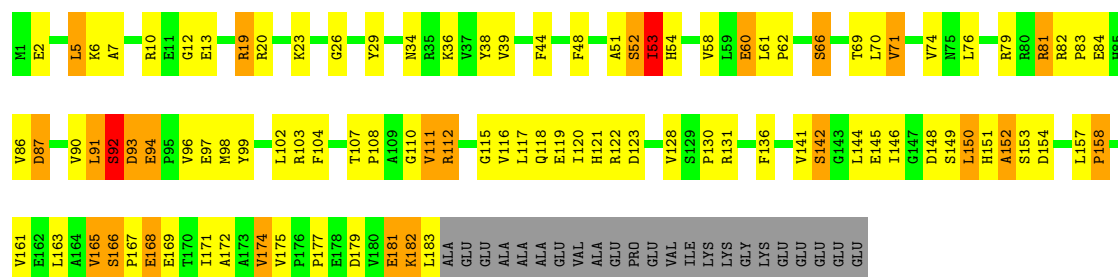
- Molecule 20: 50S ribosomal protein L24

Chain T:



- Molecule 21: 50S ribosomal protein L25

Chain U:



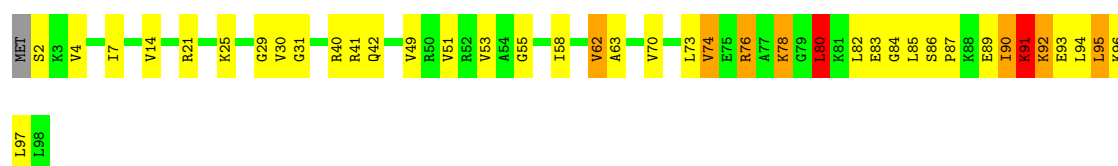
- Molecule 22: 50S ribosomal protein L27

Chain V:



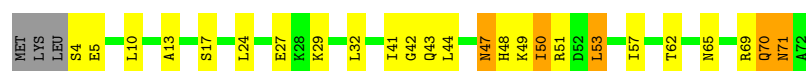
- Molecule 23: 50S ribosomal protein L28

Chain W:



- Molecule 24: 50S ribosomal protein L29

Chain X:



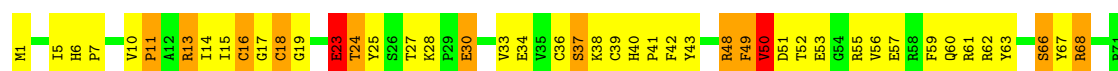
- Molecule 25: 50S ribosomal protein L30

Chain Y:



- Molecule 26: 50S ribosomal protein L31

Chain Z:



- Molecule 27: 50S ribosomal protein L32

Chain a:



- Molecule 28: 50S ribosomal protein L33

Chain b: 



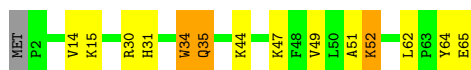
- Molecule 29: 50S ribosomal protein L34

Chain c: 



- Molecule 30: 50S ribosomal protein L35

Chain d: 



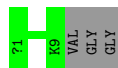
- Molecule 31: 50S ribosomal protein L36

Chain e: 



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

Chain f: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.24Å 443.46Å 618.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 3.60	Depositor
% Data completeness (in resolution range)	98.1 (49.79-3.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.222 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	92290	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, T17, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.26	0/69521	0.81	28/108529 (0.0%)
2	B	0.26	0/2878	0.88	7/4490 (0.2%)
3	C	0.51	0/2165	0.70	0/2919
4	D	0.46	1/1601 (0.1%)	0.73	3/2160 (0.1%)
5	E	0.45	1/1620 (0.1%)	0.64	1/2194 (0.0%)
6	F	0.31	0/1499	0.57	1/2016 (0.0%)
7	G	0.33	1/1332 (0.1%)	0.73	2/1802 (0.1%)
8	H	0.40	0/1151	0.75	1/1558 (0.1%)
9	I	0.41	0/1131	0.62	0/1525
10	J	0.41	0/943	0.62	1/1269 (0.1%)
11	K	0.48	1/1162 (0.1%)	0.83	1/1544 (0.1%)
12	L	0.44	0/1143	0.71	1/1527 (0.1%)
13	M	0.42	0/982	0.69	0/1312
14	N	0.36	0/892	0.64	0/1187
15	O	0.41	0/1155	0.63	0/1542
16	P	0.40	0/982	0.65	0/1306
17	Q	0.38	0/790	0.61	1/1057 (0.1%)
18	R	0.50	0/911	0.67	0/1220
19	S	0.47	0/739	0.62	0/993
20	T	0.44	0/798	0.68	0/1064
21	U	0.34	0/1493	0.60	0/2026
22	V	0.45	0/657	0.65	0/874
23	W	0.44	0/770	0.66	0/1022
24	X	0.39	0/583	0.65	0/771
25	Y	0.35	0/474	0.57	0/635
26	Z	0.33	0/594	0.68	0/795
27	a	0.43	0/473	0.78	0/639
28	b	0.35	0/431	0.69	0/575
29	c	0.49	0/438	0.68	0/575
30	d	0.55	0/525	0.79	0/691
31	e	0.26	0/310	0.45	0/407
32	f	0.22	0/56	0.45	0/70

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.31	4/100199 (0.0%)	0.78	47/150294 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1
26	Z	0	1
30	d	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	10	PRO	N-CD	5.58	1.55	1.47
4	D	22	PRO	N-CD	5.15	1.55	1.47
7	G	128	PRO	N-CD	5.10	1.54	1.47
5	E	25	PRO	N-CD	5.09	1.54	1.47

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	125	VAL	C-N-CD	-17.76	81.53	120.60
12	L	77	LYS	C-N-CD	-8.42	102.08	120.60
2	B	95	U	C5-C4-O4	7.82	130.59	125.90
1	A	2506	U	C2-N1-C1'	7.42	126.61	117.70
1	A	2702	U	C2-N1-C1'	6.85	125.92	117.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	G	153	LYS	Peptide
26	Z	38	LYS	Peptide
30	d	30	ARG	Peptide
30	d	35	GLN	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	62071	0	31284	714	0
2	B	2573	0	1306	41	0
3	C	2115	0	2195	95	0
4	D	1568	0	1634	96	0
5	E	1585	0	1632	86	0
6	F	1474	0	1535	54	0
7	G	1307	0	1382	74	0
8	H	1136	0	1223	75	0
9	I	1104	0	1180	41	0
10	J	933	0	996	21	0
11	K	1145	0	1226	78	0
12	L	1122	0	1179	57	0
13	M	968	0	1033	45	0
14	N	882	0	943	42	0
15	O	1141	0	1202	58	0
16	P	964	0	1022	31	0
17	Q	779	0	852	20	0
18	R	900	0	964	23	0
19	S	725	0	778	26	0
20	T	785	0	878	48	0
21	U	1461	0	1493	64	0
22	V	648	0	672	20	0
23	W	763	0	848	29	0
24	X	581	0	629	15	0
25	Y	469	0	518	6	0
26	Z	581	0	574	23	0
27	a	459	0	476	0	0
28	b	424	0	450	0	0
29	c	430	0	480	0	0
30	d	517	0	582	0	0
31	e	307	0	338	0	0
32	f	116	0	67	0	0
33	A	243	0	0	0	0
33	B	2	0	0	0	0
33	C	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	D	2	0	0	0	0
33	E	1	0	0	0	0
33	K	3	0	0	0	0
33	P	1	0	0	0	0
33	V	1	0	0	0	0
34	a	1	0	0	0	0
All	All	92290	0	61571	1669	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 1669 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:125:VAL:HG12	7:G:126:PRO:CD	1.64	1.25
4:D:21:VAL:HG23	4:D:22:PRO:CB	1.69	1.22
7:G:125:VAL:CG1	7:G:126:PRO:HD3	1.75	1.16
1:A:1169:G:H1	1:A:1180:C:N4	1.48	1.09
4:D:21:VAL:HG23	4:D:22:PRO:HB3	1.18	1.09

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	270/276 (98%)	226 (84%)	32 (12%)	12 (4%)	4	45
4	D	203/206 (98%)	148 (73%)	35 (17%)	20 (10%)	1	18
5	E	200/210 (95%)	170 (85%)	18 (9%)	12 (6%)	2	34
6	F	179/182 (98%)	139 (78%)	26 (14%)	14 (8%)	1	25
7	G	168/180 (93%)	116 (69%)	33 (20%)	19 (11%)	1	14
8	H	144/148 (97%)	104 (72%)	27 (19%)	13 (9%)	1	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	136/140 (97%)	104 (76%)	20 (15%)	12 (9%)	1	22
10	J	120/122 (98%)	109 (91%)	9 (8%)	2 (2%)	14	70
11	K	148/150 (99%)	106 (72%)	28 (19%)	14 (10%)	1	19
12	L	139/141 (99%)	99 (71%)	22 (16%)	18 (13%)	0	11
13	M	116/118 (98%)	106 (91%)	5 (4%)	5 (4%)	4	46
14	N	109/112 (97%)	76 (70%)	22 (20%)	11 (10%)	1	17
15	O	135/146 (92%)	107 (79%)	16 (12%)	12 (9%)	1	21
16	P	115/118 (98%)	102 (89%)	9 (8%)	4 (4%)	6	53
17	Q	99/101 (98%)	82 (83%)	11 (11%)	6 (6%)	2	34
18	R	111/113 (98%)	99 (89%)	8 (7%)	4 (4%)	5	52
19	S	90/96 (94%)	77 (86%)	11 (12%)	2 (2%)	10	64
20	T	100/110 (91%)	71 (71%)	13 (13%)	16 (16%)	0	6
21	U	181/206 (88%)	126 (70%)	34 (19%)	21 (12%)	1	13
22	V	80/85 (94%)	65 (81%)	14 (18%)	1 (1%)	18	75
23	W	95/98 (97%)	76 (80%)	10 (10%)	9 (10%)	1	19
24	X	67/72 (93%)	53 (79%)	9 (13%)	5 (8%)	2	27
25	Y	57/60 (95%)	52 (91%)	3 (5%)	2 (4%)	6	53
26	Z	69/71 (97%)	35 (51%)	18 (26%)	16 (23%)	0	2
27	a	57/60 (95%)	47 (82%)	7 (12%)	3 (5%)	3	38
28	b	47/54 (87%)	23 (49%)	13 (28%)	11 (23%)	0	1
29	c	47/49 (96%)	45 (96%)	1 (2%)	1 (2%)	11	65
30	d	62/65 (95%)	51 (82%)	6 (10%)	5 (8%)	1	24
31	e	35/37 (95%)	35 (100%)	0	0	100	100
32	f	7/12 (58%)	5 (71%)	2 (29%)	0	100	100
All	All	3386/3538 (96%)	2654 (78%)	462 (14%)	270 (8%)	1	25

5 of 270 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	26	LYS
3	C	122	ASP
3	C	242	ARG
4	D	53	PRO
4	D	63	LEU

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	214/218 (98%)	176 (82%)	38 (18%)	2	17
4	D	165/166 (99%)	126 (76%)	39 (24%)	1	8
5	E	161/166 (97%)	132 (82%)	29 (18%)	2	16
6	F	155/156 (99%)	134 (86%)	21 (14%)	6	32
7	G	142/148 (96%)	120 (84%)	22 (16%)	4	25
8	H	122/124 (98%)	98 (80%)	24 (20%)	2	12
9	I	117/119 (98%)	97 (83%)	20 (17%)	3	20
10	J	100/100 (100%)	90 (90%)	10 (10%)	11	50
11	K	116/116 (100%)	86 (74%)	30 (26%)	1	6
12	L	111/111 (100%)	94 (85%)	17 (15%)	4	26
13	M	101/101 (100%)	83 (82%)	18 (18%)	2	17
14	N	87/88 (99%)	69 (79%)	18 (21%)	2	11
15	O	120/127 (94%)	102 (85%)	18 (15%)	4	27
16	P	93/94 (99%)	79 (85%)	14 (15%)	4	27
17	Q	82/82 (100%)	66 (80%)	16 (20%)	2	13
18	R	92/92 (100%)	73 (79%)	19 (21%)	2	11
19	S	74/78 (95%)	63 (85%)	11 (15%)	4	27
20	T	85/91 (93%)	63 (74%)	22 (26%)	1	6
21	U	162/179 (90%)	132 (82%)	30 (18%)	2	15
22	V	65/67 (97%)	60 (92%)	5 (8%)	18	65
23	W	82/83 (99%)	73 (89%)	9 (11%)	9	44
24	X	64/67 (96%)	57 (89%)	7 (11%)	9	45
25	Y	51/52 (98%)	45 (88%)	6 (12%)	8	39
26	Z	63/63 (100%)	45 (71%)	18 (29%)	0	4
27	a	51/52 (98%)	36 (71%)	15 (29%)	0	4
28	b	48/52 (92%)	35 (73%)	13 (27%)	1	5
29	c	42/42 (100%)	34 (81%)	8 (19%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	d	54/55 (98%)	44 (82%)	10 (18%)	2	15
31	e	34/34 (100%)	32 (94%)	2 (6%)	28	76
32	f	5/7 (71%)	5 (100%)	0	100	100
All	All	2858/2930 (98%)	2349 (82%)	509 (18%)	2	17

5 of 509 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	138	LEU
14	N	103	GLU
27	a	46	CYS
12	L	45	GLN
13	M	71	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
14	N	34	HIS
19	S	55	ASN
27	a	22	HIS
31	e	29	ASN
31	e	32	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2879/2915 (98%)	567 (19%)	57 (1%)
2	B	119/122 (97%)	21 (17%)	1 (0%)
All	All	2998/3037 (98%)	588 (19%)	58 (1%)

5 of 588 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	15	G
1	A	28	A
1	A	34	C
1	A	35	G

5 of 58 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1026	U
1	A	1204	A
1	A	2712	U
1	A	1045	A
1	A	1085	A

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 257 ligands modelled in this entry, 257 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.