



wwPDB X-ray Structure Validation Summary Report

Sep 15, 2014 – 12:24 PM EDT

PDB ID : 1VVY
Title : Crystal Structure of Frameshift Suppressor tRNA SufA6 Bound to Codon CCC-U in the Absence of Paromomycin
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-06-27
Resolution : 3.92 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>

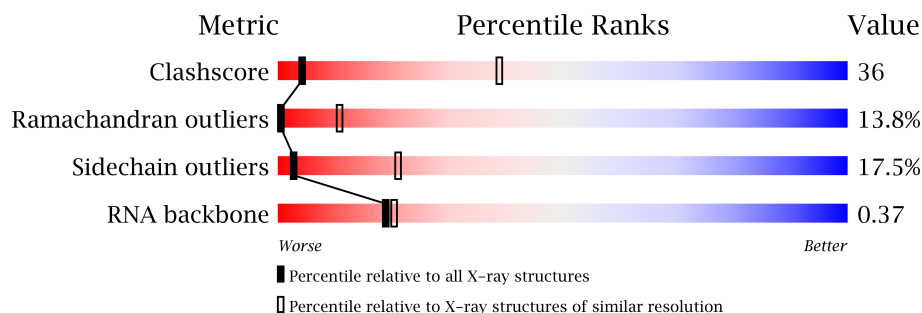
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.92 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	1180 (4.34-3.50)
Ramachandran outliers	78287	1124 (4.34-3.50)
Sidechain outliers	78261	1112 (4.34-3.50)
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 92243 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	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			

- 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	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called tRNA acceptor end mimic.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	P	1	Total	Mg	0	0
			1	1		
33	0	1	Total	Mg	0	0
			1	1		
33	D	1	Total	Mg	0	0
			1	1		
33	E	2	Total	Mg	0	0
			2	2		
33	B	2	Total	Mg	0	0
			2	2		
33	A	239	Total	Mg	0	0
			239	239		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	5	1	Total 1	Mg 1	0	0
33	8	1	Total 1	Mg 1	0	0
33	R	2	Total 2	Mg 2	0	0
33	F	1	Total 1	Mg 1	0	0

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

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

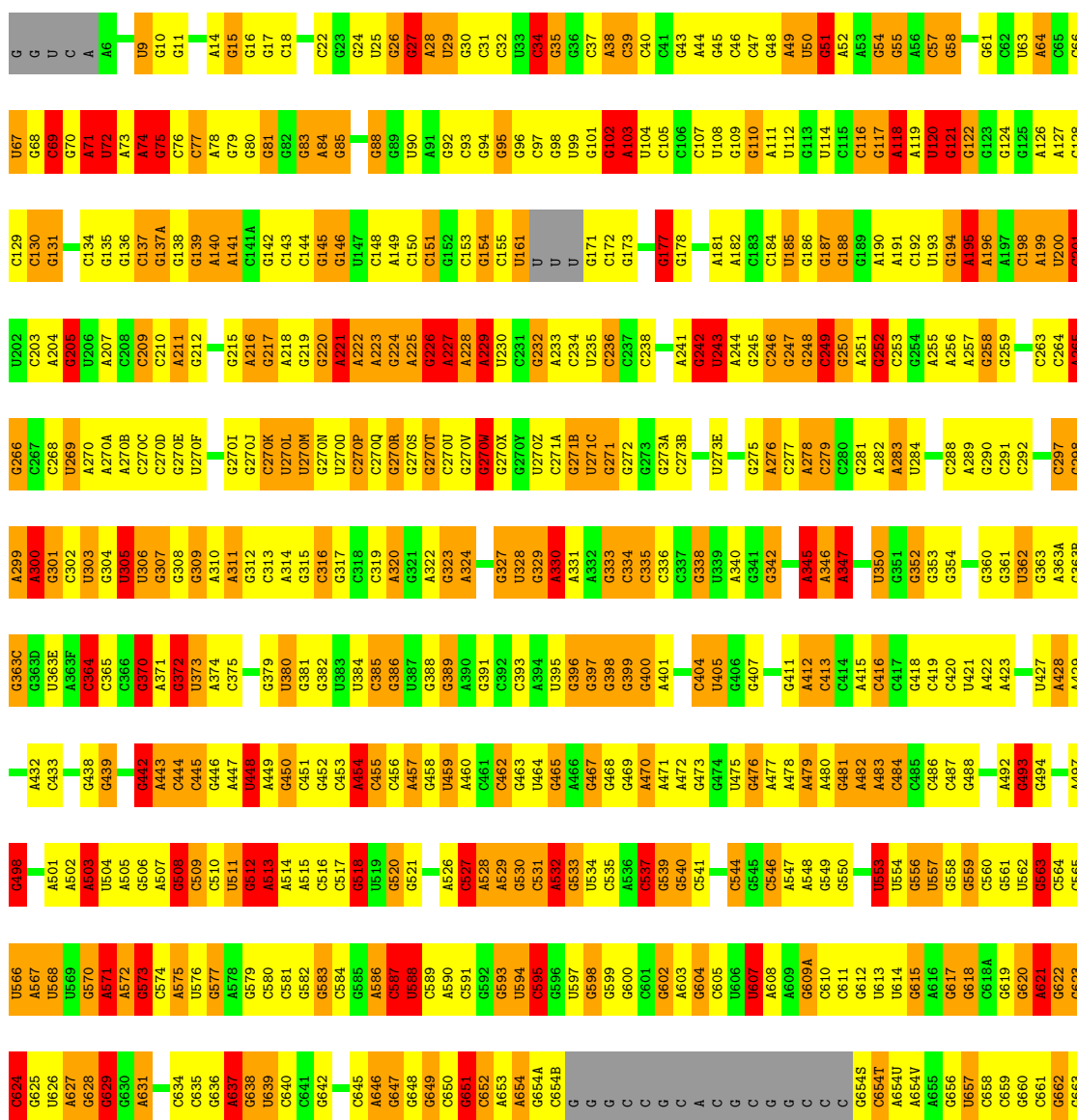
3 Residue-property plots

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.

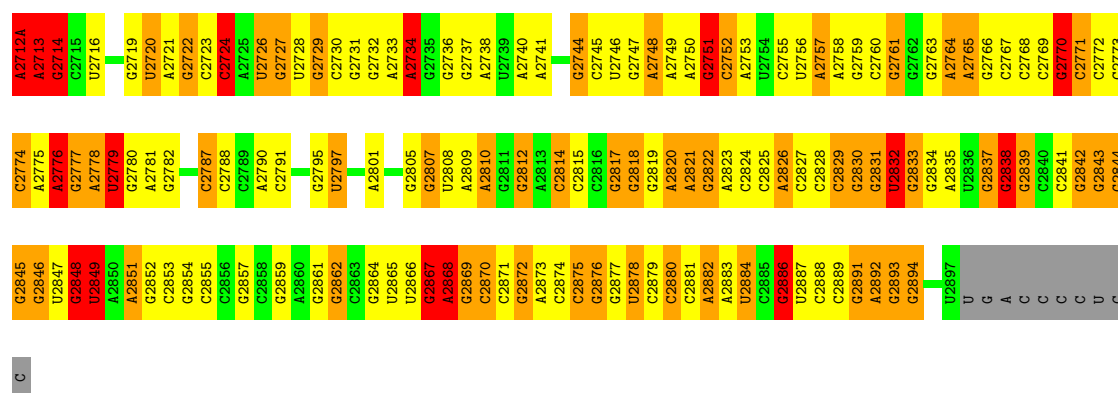
• Molecule 1: 23S rRNA

Chain A:



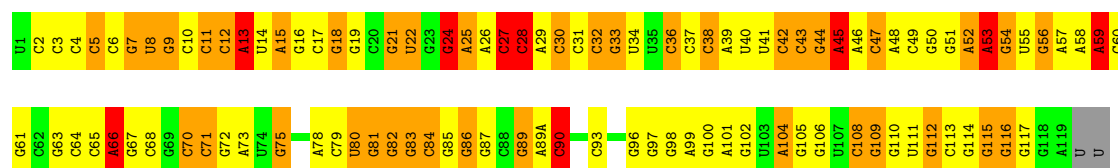
A1603	C1537	G1475	G1413	C1290	C1230	U1165	G1099	G1037	C974A	U913	U851	A189	G725	C664
C1604	G1538	C1476	G1414	C1291	G1231	C1166	G1099	G1038	G975	C914	G852	C790	G726	C665
C1605	G1539	A1477	G1415	U1292	G1232	U1167	G1100	C1038	G976	C915	G853	C791	A727	G666
G1606	C1283	A1354	G1416	C1293	C1233	G1168	U1101	C1037	G977	G916	G854	G792	G728	U667
C1607	G1479	G1355	G1417	U1294	C1234	G1169	C1102	G1041	G978	A917	G855	A793	G729	G668
A1608	G1542	G1418	G1418	C1295	G1235	G1356	A1103	G1042	G979	A918	G856	C796	G730	G669
A1609	A1943	U1357	A1419	G1296	G1236	U1357	C1104	C1043	A980	G919	C857	C796	C731	A670
A1610	G1421	G1358	G1420	C1297	A1237	G1173	G1104	G1044	A981	G920	U858	C797	G732	C671
A1611	G1483	A1359	G1421	C1298	G1238	U1174	G1106	A1045	A982	G921	G859	C798	G733	C672
C1612	G1485	A1360	G1422	G1299	G1239	U1175	U1107	A1046	A983	G922	U860	C799	G734	C673
G1613	A1486	G1361	G1423	U1300	A1240	A1177	U1108	G1047	A984	C923	A861	G801	A735	G674
A1614	G1487	C1362	G1424	A1301	A1241	C1178	C1109	G1048	C985	C924	G862	A802	C736	A675
C1615	A1488	A1363	A1425	G1302	A1242	C1179	G1110	C1049	C986	C925	A863	U803	C737	A676
A1616	G1429	G1364	C1428	G1303	G1243	C1180	A1111	A1050	G987	A926	G864	A804	G738	A677
C1617	G1430	A1365	C1429	C1304	G1244	C1181	G1112	G1051	A988	G928	C865	G905	G739	C678
A1618	U1431	A1366	G1430	C1305	G1245	A1182	U1113	C1052	G989	G929	A866	C906	U740	C679
C1619	A1494	A1367	U1431	C1306	A1246	G1183	G1114	C1053	A990	U930	G867	U807	G741	G680
G1620	A1559	G1368	C1432	A1307	G1247	G1184	G1115	A1054	C991	G931	U868	G808	G742	G681
U1621	A1495	C1369	U1433	A1308	G1248	C1185	C1116	G1055	C992	G932	G869	G809	G743	G682
G1622	A1496	G1370	A1434	G1309	U1249	G1186	C1123	G1056	G993	A933	A870	U810	G744	C683
G1623	U1497	G1371	G1435	G1310	G1250	G1187	C1124	A1057	G994	G934	A871	U811	G745	G684
G1624	C1498	U1372	G1436	G1311	C1251	U1188	G1125	G1058	C995	C935	A872	C812	G746	A685
C1625	C1499	A1373	C1437	U1312	G1252	A1189	G1126	G1059	A996	C936	G873	U813	U747	G686
G1626	G1500	U1374	U1438	U1313	A1253	G1190	A1127	U1060	G997	U937	G874	C814	G747	G687
G1627	C1564	C1375	A1439	C1314	A1254	G1191	C1127	U1061	C998	G938	G875	C815	A751	U688
G1628	C1565	G1376	G1440	C1315	U1255	G1192	A1128	G1062	U999	C816	C876	C817	A752	A689
U1629	A1567	G1377	G1441	U1316	G1256	G1193	A1129	G1063	A1000	C941	U877	C818	C753	G690
G1630	C1503	U1378	G1442	C1317	G1257	A1194	U1130	C1064	A1001	G942	A878	C819	C754	
A1632	C1504	A1379	G1443	G1320	C1258	G1195	G1131	U1065	A1002	U943	G879	A819	C755	C693
G1633	C1506	G1380	G1444	C1321	G1259	C1196	A1132	U1066	G1003	G944	G880	A820	C756	U694
C1634	A1507	U1444A	U1444A	A1321	G1260	G1197	U1133	A1067	C1004	A945	G881	A821	U757	G695
A1635	A1508	C1445	C1445	A1322	G1261	U1198	C1135	G1068	C1005	G946	G882	U822	C758	G696
G1636	C1509	G1446	G1446	U1323	A1262	U1199	G1136	A1069	G1006	G947	G883	G823	C759	C697
A1637	U1576	G1447	G1448	G1324	G1263	C1200	G1137	A1070	C1007	G948	G884	A824	G760	C698
C1638	C1577	G1448	A1449	G1325	G1264	C1201	G1138	G1071	C1008	C949	C885	C825	A761	A699
U1639	U1578	G1449	G1449A	U1326	A1265	G1202	G1139	G1072	A1009	G950	C886	U826	U762	G700
C1640	A1579	U1390	C1450	G1327	G1266	G1203	C1140	A1073	A887	C951	U887	U827	G765	G701
A1641	A1580	U1391	C1451	U1328	U1267	A1204	U1141	G1074	G1011	G952	C888	U828	G766	G702
G1642	U1516	A1392	A1453	U1329	A1268	U1205	U1142	C1075	U1012	A953	C889	A829	U767	U703
G1643	G1517	A1393	C1454	C1330	A1269	G1206	A1142A	G1076	G1013	G954	C890	G830	G768	G704
C1644	C1518	U1394	G1455	A1331	C1270	C1207	A1143	A1077	U1014	C955	G892	G831	G769	A706
G1645	C1585	G1395	G1455	G1332	G1271	C1208	G1144	U1078	G1015	G956	C893	G832	G770	G707
C1646	U1519	A1396	G1456	C1333	A1272	G1209	C1145	C1079	G1016	A957	U896	U833	G770	G708
G1647	U1520	U1396	G1458	G1334	U1273	A1210	G1146	C1080	G1017	U958	C894	C834	U773	U709
C1648	G1521	U1397	G1459	U1335	A1274	U1211	G1149	U1081	C1018	A959	A896	A835	A774	G710
U1649	U1522	C1398	A1460	A1336	A1275	A1212	C1150	U1082	U1019	A960	C897	G836	G775	G711
G1650	U1523	C1399	G1461	G1337	A1276	A1213	G1151	U1083	C1020	C961	C898	C837	G776	G712
G1651	G1524	G1400	C1462	G1338	G1277	A1214	C1152	A1084	A1021	G962	A899	C838	A777	G713
G1652	G1525	G1401	C1463	G1339	A1278	G1215	G1153	A1085	G1022	U963	A900	U839	G778	U714
A1653	U1526	C1402	C1464	U1340	G1279	G1216	C1154	A1086	U1023	C964	A901	C840	U779	G715
G1654	G1527	C1403	G1465	U1341	G1280	G1280	G1155	G1087	G1024	C965	C902	A841	G780	A716
C1655	A1528	A1404	G1466	A1342	U1281	A1220	A1156	A1088	G1025	G966	G903	G842	A781	A717
A1656	A1529	U1405	C1467	G1343	U1282	C1221	U1157	G1089	U1026	C967	C904	G843	A782	G718
C1657	G1530	U1406	C1468	G1344	G1283	C1222	G1157	U1090	A1027	G968	C944	C844	A783	A719
C1658	C1531	A1469	C1470	G1345	G1284	C1223	C1158	G1091	A1028	U969	C908	G845	A784	C720
U1659	C1532	C1408	G1470	C1346	G1285	G1224	C1161	C1092	A1029	C970	A909	C846	G785	G721
C1660	C1533	G1409	A1471	G1347	A1286	C1225	G1162	G1093	G1030	C971	A910	G847	C786	A722
G1661	U1534	C1410	A1472	G1348	A1287	G1226	G1163	U1094	G1031	G972	A911	G848	G787	G723
C1662	U1602	C1411	C1473	A1349	U1288	G1227	G1164	A1095	A1032	C974	C912	C850	U788	U724

C2646	U2647	U2648	U2649	U2650	U2651	U2652	U2653	U2654	U2655	U2656	U2657	U2658	U2659	U2660	U2661	U2662	U2663	U2664	U2665	U2666	U2667	U2668	U2669	U2670	U2671	U2672	U2673	U2674	U2675	U2676	U2677	U2678	U2679	U2680	U2681	U2682	U2683	U2684	U2685	U2686	U2687	U2688	U2689	U2690	U2691	U2692	U2693	U2694	U2695	U2696	U2697	U2698	U2699	U2700	U2701	U2702	U2703	U2704	U2705	U2706	U2707	U2708	U2709	U2710	U2711	U2712																																																																																																																																																																																																																																																							
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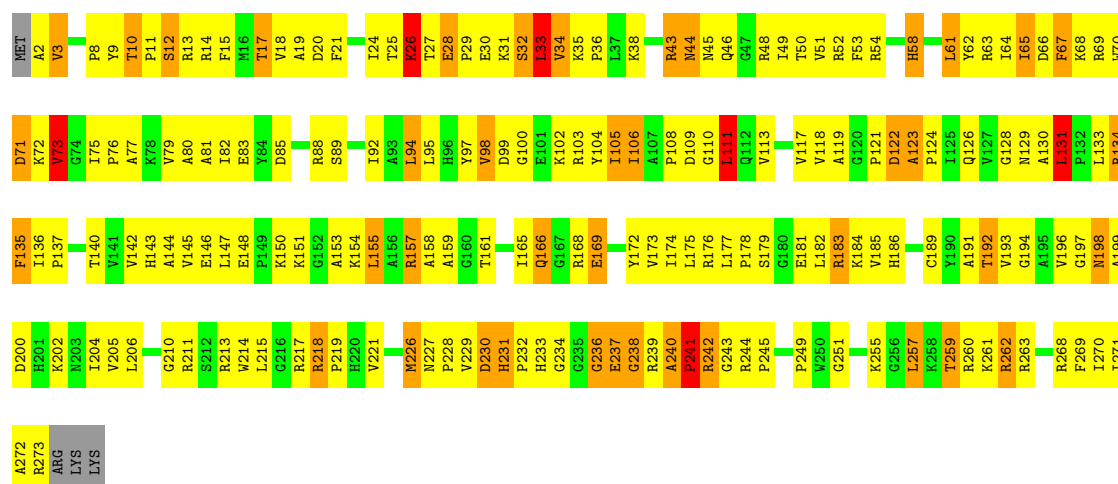
- Molecule 2: 5S rRNA

Chain B:



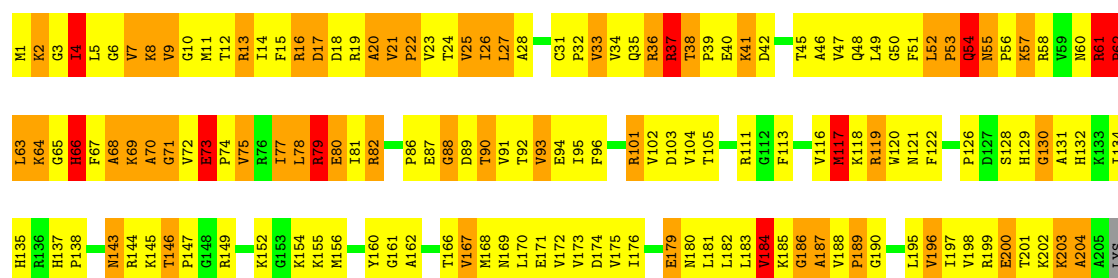
- Molecule 3: 50S ribosomal protein L2

Chain D:



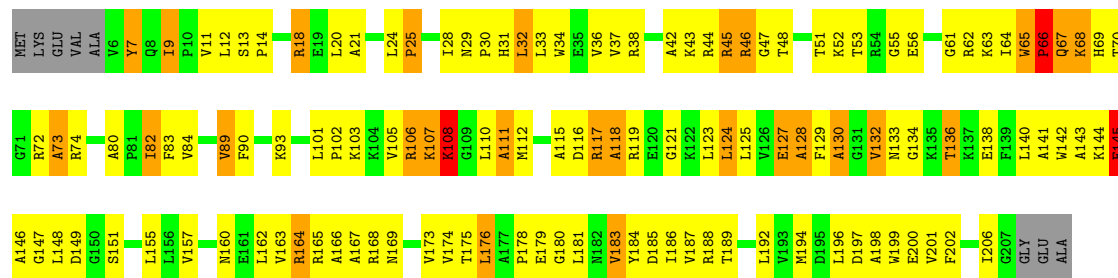
- Molecule 4: 50S ribosomal protein L3

Chain E:



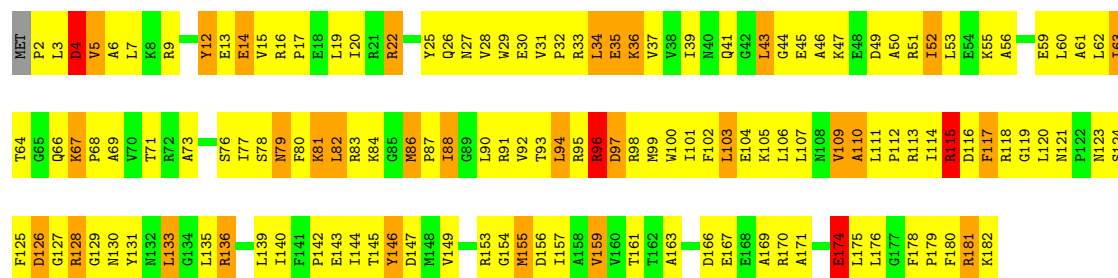
- Molecule 5: 50S ribosomal protein L4

Chain F:



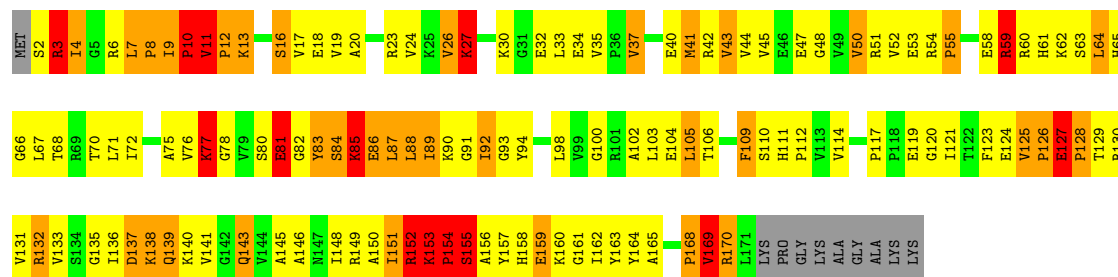
- Molecule 6: 50S ribosomal protein L5

Chain G:



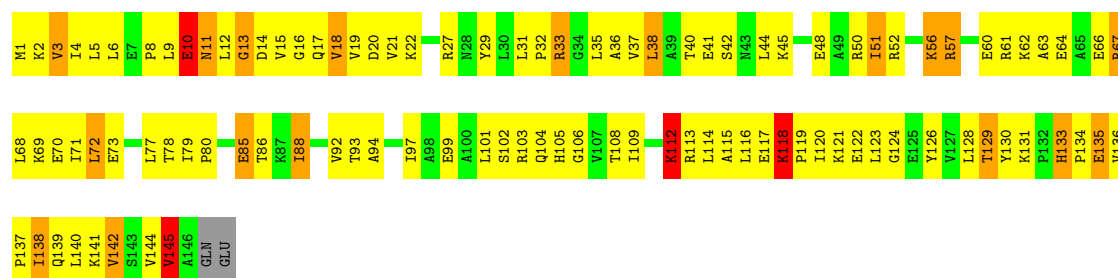
- Molecule 7: 50S ribosomal protein L6

Chain H:



- Molecule 8: 50S ribosomal protein L9

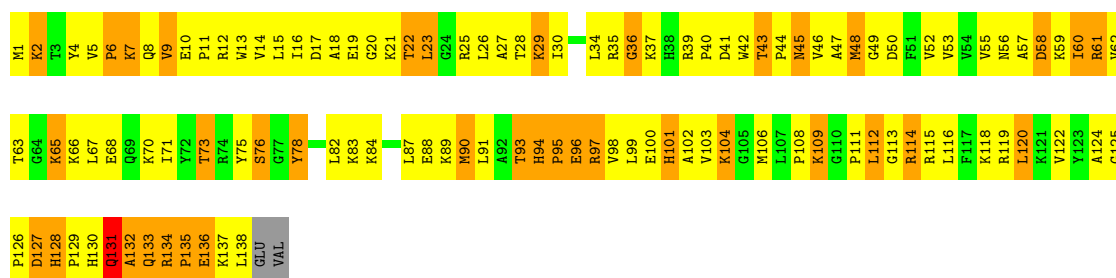
Chain I:



- Molecule 9: 50S ribosomal protein L13

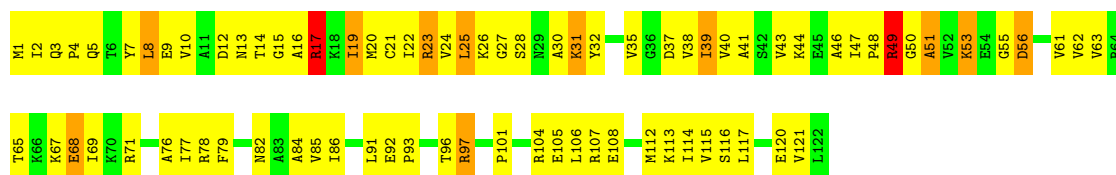
Chain N:





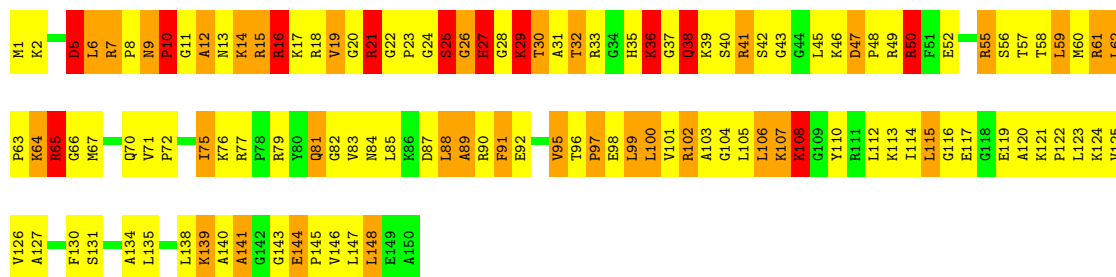
• Molecule 10: 50S ribosomal protein L14

Chain O:



• Molecule 11: 50S ribosomal protein L15

Chain P:



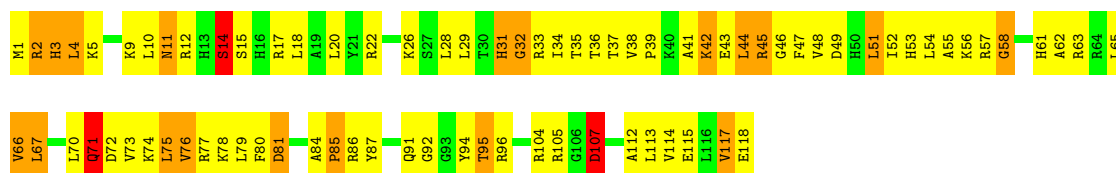
• Molecule 12: 50S ribosomal protein L16

Chain Q:



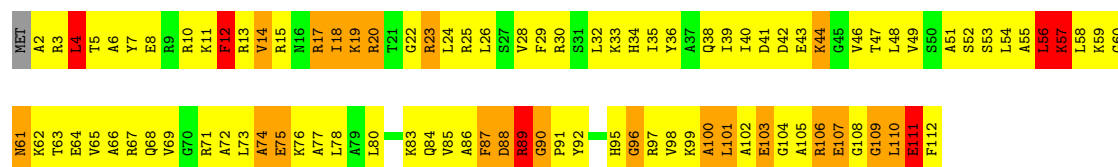
• Molecule 13: 50S ribosomal protein L17

Chain R:



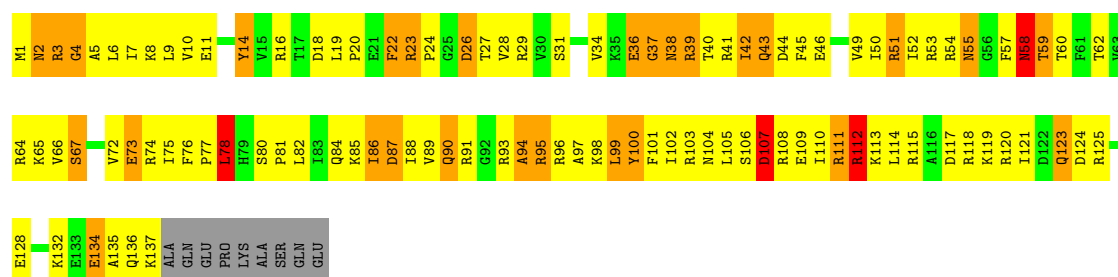
- Molecule 14: 50S ribosomal protein L18

Chain S:



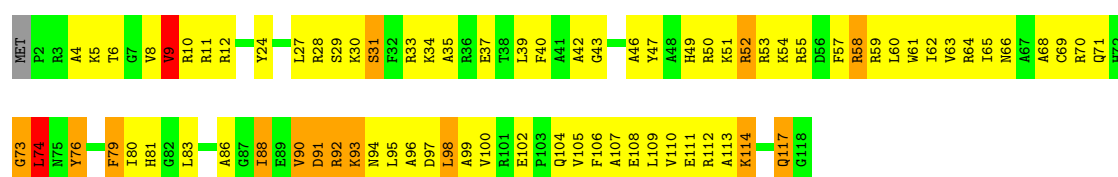
- Molecule 15: 50S ribosomal protein L19

Chain T:



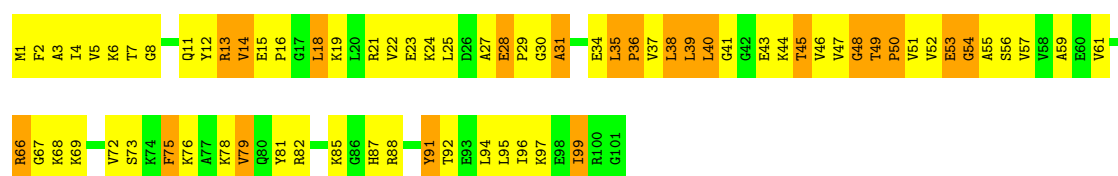
- Molecule 16: 50S ribosomal protein L20

Chain U:



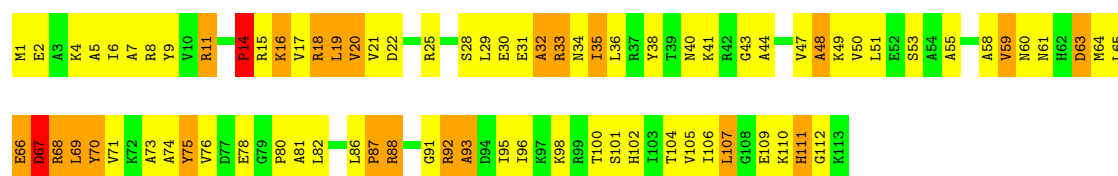
- Molecule 17: 50S ribosomal protein L21

Chain V:



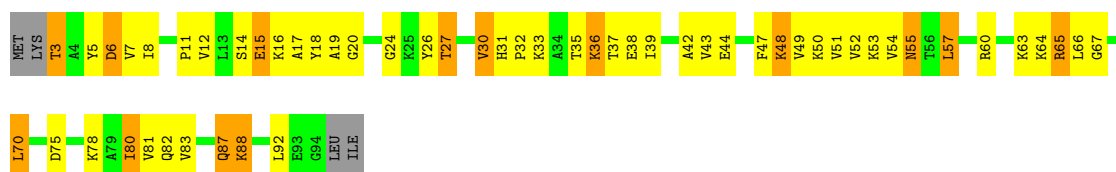
- Molecule 18: 50S ribosomal protein L22

Chain W:



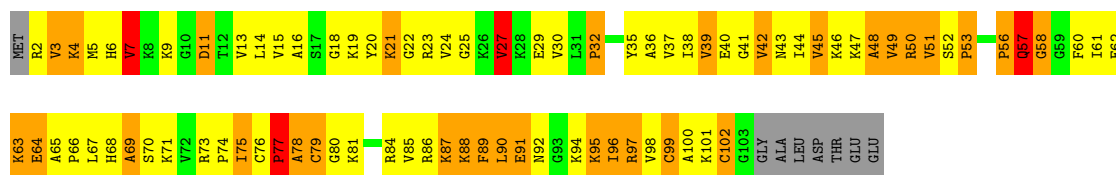
- Molecule 19: 50S ribosomal protein L23

Chain X:



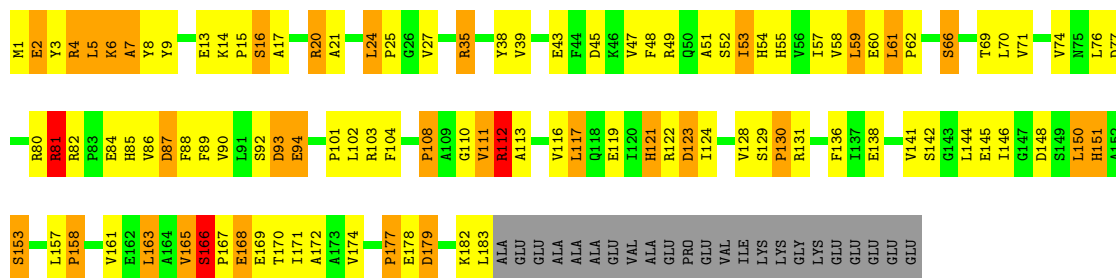
- Molecule 20: 50S ribosomal protein L24

Chain Y:



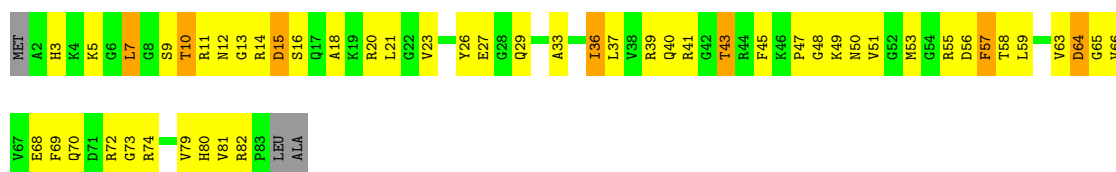
- Molecule 21: 50S ribosomal protein L25

Chain Z:



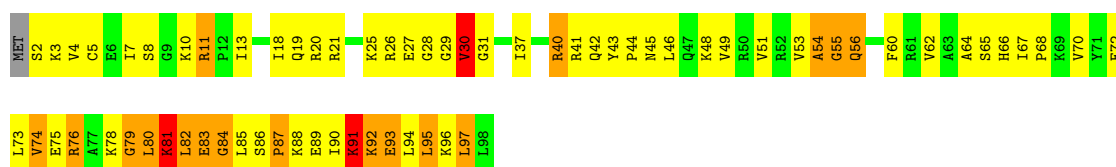
- Molecule 22: 50S ribosomal protein L27

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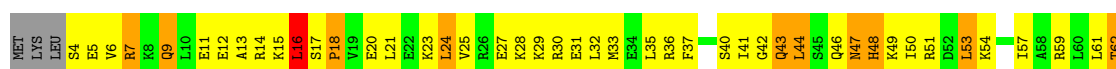
- Molecule 23: 50S ribosomal protein L28

Chain 1:



- Molecule 24: 50S ribosomal protein L29

Chain 2:





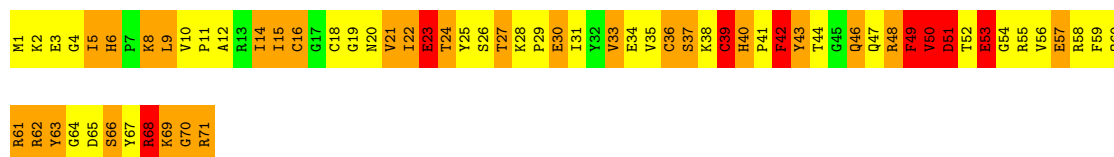
- Molecule 25: 50S ribosomal protein L30

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:



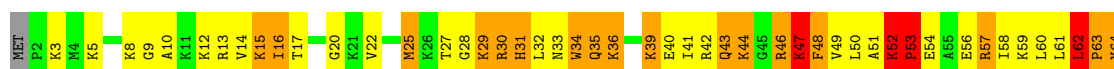
- Molecule 29: 50S ribosomal protein L34

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	210.38Å 451.02Å 621.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.77 – 3.92	Depositor
% Data completeness (in resolution range)	99.7 (34.77-3.92)	Depositor
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX	Depositor
R, R_{free}	0.208 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	92243	wwPDB-VP
Average B, all atoms (Å ²)	53.0	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	1.03	104/69521 (0.1%)	1.85	2693/108529 (2.5%)
2	B	0.82	1/2878 (0.0%)	1.59	60/4490 (1.3%)
3	D	0.60	2/2165 (0.1%)	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	3/1802 (0.2%)
8	I	0.44	0/1151	0.77	1/1558 (0.1%)
9	N	0.46	0/1131	0.78	1/1525 (0.1%)
10	O	0.54	0/943	0.71	0/1269
11	P	0.50	0/1162	0.95	3/1544 (0.2%)
12	Q	0.54	0/1143	0.91	3/1527 (0.2%)
13	R	0.45	0/982	0.80	1/1312 (0.1%)
14	S	0.46	0/892	0.82	1/1187 (0.1%)
15	T	0.47	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	0.44	0/1493	0.70	0/2026
22	0	0.52	0/657	0.73	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	0.47	0/474	0.71	0/635
26	4	0.38	0/594	0.78	1/795 (0.1%)
27	5	0.51	0/473	0.74	0/639
28	6	0.42	0/431	0.76	0/575
29	7	0.56	0/438	0.76	0/575
30	8	0.62	0/525	0.93	1/691 (0.1%)
31	9	0.35	0/310	0.59	0/407
32	a	0.78	0/40	1.78	1/60 (1.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.91	107/100183 (0.1%)	1.64	2779/150284 (1.8%)

The worst 5 of 107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	783	A	N7-C5	-10.47	1.32	1.39
1	A	783	A	C5-C6	-9.29	1.32	1.41
3	D	236	GLY	C-N	8.54	1.53	1.34
1	A	1142(A)	A	N9-C4	-8.29	1.32	1.37
1	A	1274	A	N9-C4	-8.09	1.32	1.37

The worst 5 of 2779 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2490	G	C6-C5-N7	-18.87	119.08	130.40
1	A	783	A	C6-C5-N7	-17.19	120.27	132.30
1	A	783	A	N1-C6-N6	16.89	128.74	118.60
1	A	2490	G	C4-C5-N7	16.43	117.37	110.80
1	A	2490	G	N3-C4-N9	15.10	135.06	126.00

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	62071	0	31285	1905	0
2	B	2573	0	1306	121	0
3	D	2115	0	2195	324	0
4	E	1568	0	1634	270	0
5	F	1585	0	1632	178	0
6	G	1474	0	1535	199	0
7	H	1307	0	1382	226	0
8	I	1136	0	1223	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	N	1104	0	1180	200	0
10	O	933	0	996	125	0
11	P	1145	0	1228	256	0
12	Q	1122	0	1179	157	0
13	R	968	0	1033	115	0
14	S	882	0	943	166	0
15	T	1141	0	1202	148	0
16	U	964	0	1022	130	0
17	V	779	0	852	130	0
18	W	900	0	964	100	0
19	X	725	0	778	70	0
20	Y	785	0	878	167	0
21	Z	1461	0	1493	81	0
22	0	648	0	671	48	0
23	1	763	0	848	142	0
24	2	581	0	629	83	0
25	3	469	0	518	41	0
26	4	581	0	574	132	0
27	5	459	0	480	73	0
28	6	424	0	450	90	0
29	7	430	0	480	42	0
30	8	517	0	582	104	0
31	9	307	0	335	23	0
32	a	74	0	51	0	0
33	0	1	0	0	0	0
33	5	1	0	0	0	0
33	8	1	0	0	0	0
33	A	239	0	0	0	0
33	B	2	0	0	0	0
33	D	1	0	0	0	0
33	E	2	0	0	0	0
33	F	1	0	0	0	0
33	P	1	0	0	0	0
33	R	2	0	0	0	0
34	9	1	0	0	0	0
All	All	92243	0	61558	5410	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 36.

The worst 5 of 5410 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	1.53
23:1:81:LYS:NZ	23:1:81:LYS:HA	1.43	1.34
23:1:81:LYS:HE2	23:1:81:LYS:N	1.50	1.26
12:Q:59:ARG:O	12:Q:60:ARG:HD2	1.38	1.22
7:H:127:GLU:HG2	7:H:128:PRO:CD	1.70	1.20

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	D	270/276 (98%)	203 (75%)	48 (18%)	19 (7%)	2	33
4	E	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	3
5	F	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	20
6	G	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	1	15
7	H	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	2
8	I	144/148 (97%)	99 (69%)	32 (22%)	13 (9%)	1	24
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%)	95 (68%)	30 (22%)	14 (10%)	1	20
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%)	87 (76%)	19 (16%)	9 (8%)	1	29
17	V	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	20
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	Y	100/110 (91%)	58 (58%)	16 (16%)	26 (26%)	0	2
21	Z	181/206 (88%)	113 (62%)	46 (25%)	22 (12%)	1	14
22	0	80/85 (94%)	66 (82%)	10 (12%)	4 (5%)	3	43
23	1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	1	15
24	2	67/72 (93%)	47 (70%)	11 (16%)	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	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	2
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	3379/3526 (96%)	2252 (67%)	662 (20%)	465 (14%)	0	11

5 of 465 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	214/218 (98%)	177 (83%)	37 (17%)	3	21
4	E	165/166 (99%)	128 (78%)	37 (22%)	1	11
5	F	161/166 (97%)	140 (87%)	21 (13%)	6	38
6	G	155/156 (99%)	130 (84%)	25 (16%)	3	27
7	H	142/148 (96%)	114 (80%)	28 (20%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	122/124 (98%)	94 (77%)	28 (23%)	1	9
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	30
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	30
20	Y	85/91 (93%)	70 (82%)	15 (18%)	3	21
21	Z	162/179 (90%)	133 (82%)	29 (18%)	2	20
22	0	65/67 (97%)	58 (89%)	7 (11%)	9	48
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	51/52 (98%)	39 (76%)	12 (24%)	1	9
28	6	48/52 (92%)	38 (79%)	10 (21%)	2	13
29	7	42/42 (100%)	39 (93%)	3 (7%)	21	68
30	8	54/55 (98%)	39 (72%)	15 (28%)	0	6
31	9	34/34 (100%)	32 (94%)	2 (6%)	28	75
All	All	2853/2923 (98%)	2355 (82%)	498 (18%)	3	21

5 of 498 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	P	88	LEU
14	S	106	ARG
27	5	19	ARG
11	P	146	VAL
13	R	37	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
11	P	84	ASN
15	T	58	ASN
25	3	19	GLN
12	Q	123	HIS
13	R	3	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2879/2916 (98%)	835 (29%)	82 (2%)
2	B	119/122 (97%)	32 (26%)	3 (2%)
32	a	1/3 (33%)	0	0
All	All	2999/3041 (98%)	867 (28%)	85 (2%)

5 of 867 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	10	G
1	A	11	G
1	A	15	G
1	A	27	G

5 of 85 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1130	U
1	A	1312	U
1	A	2776	A
1	A	1141	U
1	A	1220	A

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	2.43	9 (23%)	54,57,60	2.62	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	9.20	1.41	1.23
32	a	76	PPU	C-N3'	5.46	1.46	1.34
32	a	76	PPU	C9-N6	-5.39	1.32	1.45
32	a	76	PPU	C10-N6	-5.14	1.32	1.45
32	a	76	PPU	C8-N9	-3.09	1.32	1.36

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	-8.53	121.39	128.89
32	a	76	PPU	C3'-N3'-C	-8.18	110.17	123.19
32	a	76	PPU	C5-C4-N3	-6.38	119.76	125.98
32	a	76	PPU	C2'-C1'-N9	-5.44	98.53	113.35
32	a	76	PPU	C2'-C3'-N3'	5.17	125.08	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 252 ligands modelled in this entry, 252 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.