



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 12:47 PM GMT

PDB ID : 2I2V
Title : Crystal Structure of Ribosome with messenger RNA and the Anticodon stem-loop of P-site tRNA. This file contains the 50s subunit of one 70s ribosome. The entire crystal structure contains two 70s ribosomes and is described in remark 400.
Authors : Berk, V.; Zhang, W.; Pai, R.D.; Cate, J.H.D.
Deposited on : 2006-08-16
Resolution : 3.22 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

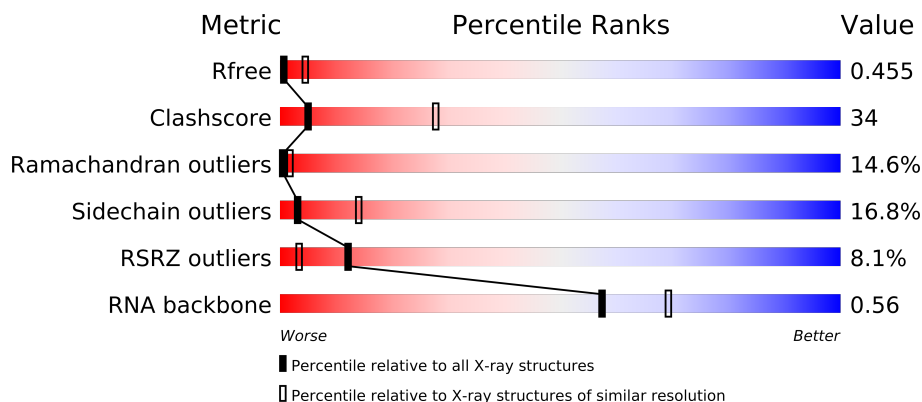
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 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 3.22 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1205 (3.30-3.14)
Clashscore	79885	1072 (3.28-3.16)
Ramachandran outliers	78287	1052 (3.28-3.16)
Sidechain outliers	78261	1051 (3.28-3.16)
RSRZ outliers	66119	1206 (3.30-3.14)
RNA backbone	1838	1004 (3.74-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	120	
2	B	2904	
3	C	272	
4	D	209	
5	E	201	
6	F	178	
7	G	176	
8	H	149	
9	I	141	
10	J	142	
11	K	123	
12	L	144	

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Mol	Chain	Length	Quality of chain
13	M	136	
14	N	127	
15	O	117	
16	P	114	
17	Q	117	
18	R	103	
19	S	110	
20	T	100	
21	U	103	
22	V	94	
23	W	84	
24	X	77	
25	Y	63	
26	Z	58	
27	0	56	
28	1	54	
29	2	46	
30	3	64	
31	4	38	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
33	MG	B	2933	-	X
33	MG	B	2936	-	X
33	MG	B	2941	-	X
33	MG	B	2945	-	X
33	MG	B	2956	-	X
33	MG	B	2981	-	X
33	MG	B	2993	-	X

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 90315 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 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	116	Total	C	N	O		0	0	0
			892	552	178	162				

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	102	Total	C	N	O			
			779	492	146	141	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	94	Total	C	N	O	S			
			753	479	137	134	3	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	79	Total	C	N	O	S			
			596	367	120	108	1	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	77	Total	C	N	O	S			
			625	388	129	106	2	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	63	Total	C	N	O	S			
			509	313	99	95	2	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	58	Total	C	N	O	S			
			449	281	87	79	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	0	56	Total	C	N	O	S			
			444	269	94	80	1	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	1	50	Total	C	N	O	0	0	0
			409	263	75	71			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	4	1	Total	Zn	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	B	119	Total	Mg	0	0
			119	119		

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	2	1	Total	O	0	0
			1	1		
34	4	4	Total	O	0	0
			4	4		
34	B	532	Total	O	0	0
			532	532		

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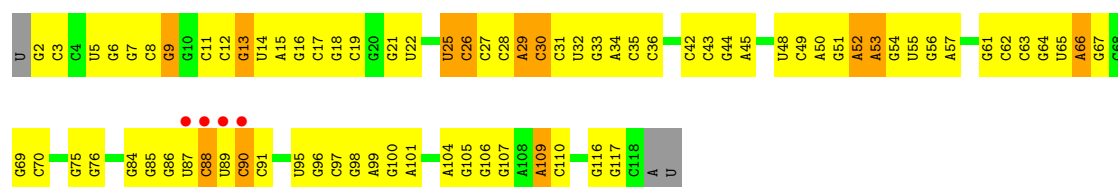
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	C	8	Total 8	O 8	0	0
34	D	1	Total 1	O 1	0	0
34	E	2	Total 2	O 2	0	0
34	J	2	Total 2	O 2	0	0
34	L	3	Total 3	O 3	0	0
34	N	2	Total 2	O 2	0	0
34	T	1	Total 1	O 1	0	0

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.

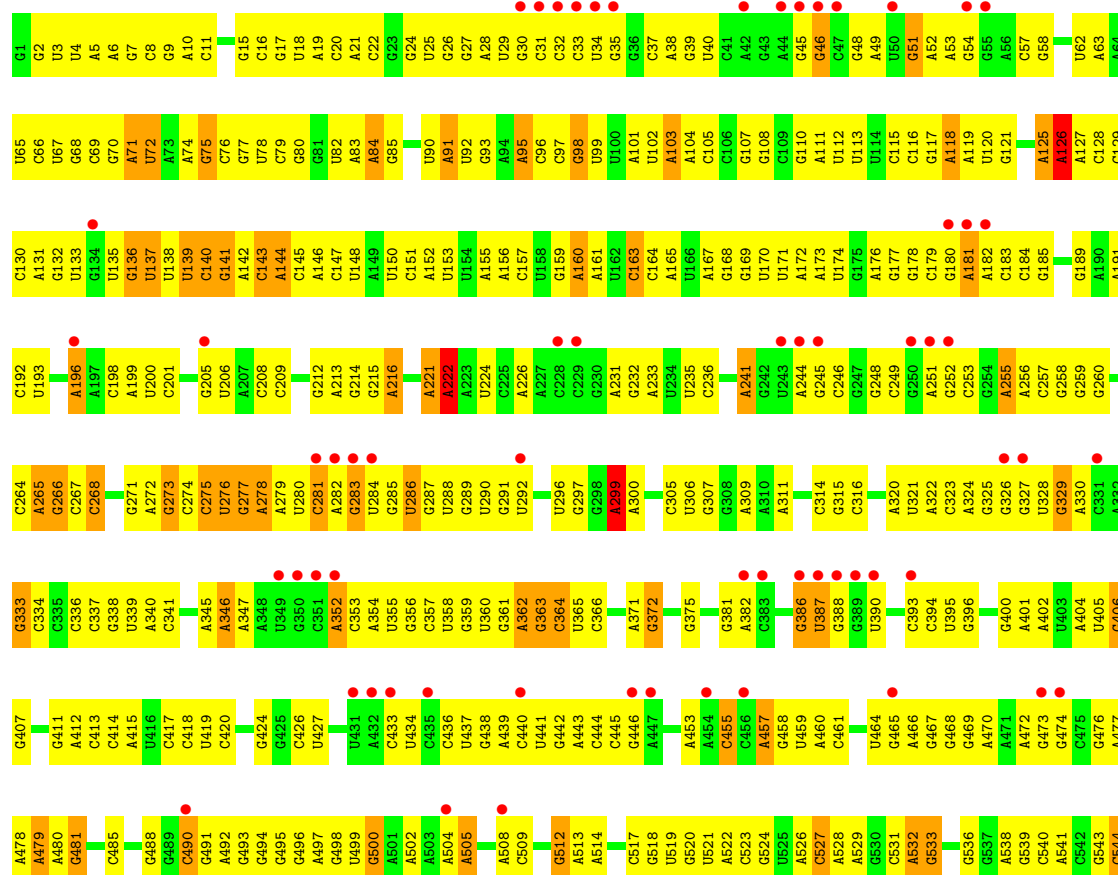
• Molecule 1: 5S ribosomal RNA

Chain A: 



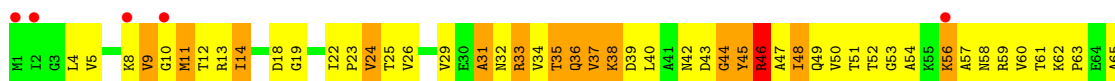
• Molecule 2: 23S ribosomal RNA

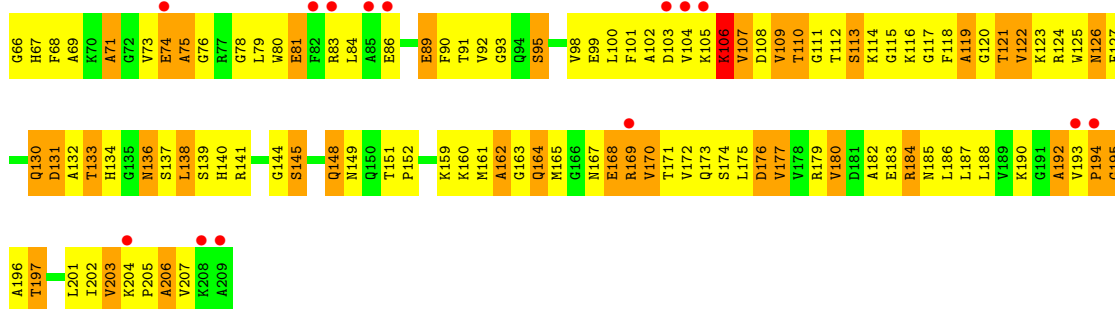
Chain B: 



U1476	G1410	G1279	G1211	A1144	A1077	A1010	U934	C873	U741	G674	A608	U545
A1477	U1411	G1280	G1212	C1445	A1080	G1011	C935	G874	A742	A675	A609	U546
G1478	A1412	G1281	A1213	C1446	U1081	U1012	A941	C875	A676	A677	C610	G547
G1482	A1413	U1282	A1214	C1447	U1082	G1013	G942	C876	C678	G611	G548	G549
G1483	C1414	U1283	G1215	U1448	U1083	A1014	A943	A877	C679	G612	G550	C550
U1484	U1415	A1284	G1216	C1449	U1084	U1015	C944	A878	C680	A613	G551	G552
U1485	G1416	A1285	U1219	C1450	A1085	G1017	A945	G	C681	A614	U615	U553
U1486	U1210	A1286	U1220	C1451	A1086	U1018	C946	G	G682	U615	G620	U554
U1487	A1237	A1287	C1221	C1452	A1088	U1019	A947	G	G683	U615	G620	U555
U1488	A1420	G1288	C1221	C1453	A1089	A1020	C948	G	G684	U615	G620	U556
U1489	G1421	U1291	U1224	A1454	A1090	A1021	G949	U	G685	U615	G620	U557
A1490	G1426	G1292	U1225	G1455	A1091	G1022	C950	C	G686	U615	G620	U558
G1491	A1427	C1293	A1286	C1456	G1092	U1023	C951	A	G687	U615	G620	U559
G1492	C1428	U1294	G1227	C1457	G1093	G1024	C952	U	G688	U615	G620	C560
A1493	A1429	C1295	G1228	C1458	G1094	G1025	G953	C	G689	U615	G620	G561
A1494	G1430	G1296	C1229	C1459	U1095	G1026	G954	C	G690	U615	G620	U562
A1495	A1431	C1297	G1230	C1460	U1096	A1027	G955	C	G691	U615	G620	U563
A1496	A1432	G1298	U1231	A1461	U1097	A1028	C956	G	G692	U615	G620	C564
U1497	A1433	G1299	G1232	C1462	A1098	A1029	U958	A	G693	U615	G620	C565
C1498	A1434	A1301	U1233	C1463	C1100	G1030	A959	C	G694	U615	G620	U566
A1504	G1437	A1302	G1235	C1464	C1101	A1031	C961	U	G695	U615	G620	U567
A1505	C1370	G1306	G1236	C1465	C1102	U1033	C962	A	G696	U615	G620	U568
U1506	G1371	U1307	A1237	C1466	C1103	G1034	U963	C	G697	U615	G620	U569
C1507	U1372	G1308	G1238	C1467	G1104	G1037	C964	C898	G698	U615	G620	G570
A1508	A1373	U1309	U1239	C1468	U1105	G1038	C965	A899	G699	U615	G620	U571
A1509	G1374	G1310	U1240	C1469	C1106	U1039	G966	A900	G700	U615	G620	A572
G1510	U1375	G1311	G1241	C1470	C1107	G1041	U967	C901	G701	U615	G620	U573
G1511	U1376	U1312	A1242	C1471	G1108	G1042	C968	C902	G702	U615	G620	A574
C1512	U1377	G1313	U1243	C1472	G1109	C1043	G969	C903	G703	U615	G620	A575
U1513	G1380	U1314	C1244	C1473	G1110	A1046	U970	G904	G704	U615	G620	A576
G1514	G1381	C1315	G1245	C1474	A1111	A1047	C971	A905	G705	U615	G620	U580
G1515	G1382	U1316	A1246	C1475	G1112	G1047	A972	U906	U709	U615	G620	C581
A1516	A1383	C1317	A1247	C1476	U1113	U1047	G974	U907	U710	U615	G620	A582
G1517	A1384	U1318	U1248	C1477	C1114	A1050	A975	C908	G711	U615	G620	G583
U1524	A1385	G1319	U1249	C1478	G1115	G1051	A981	A909	G712	U615	G620	G584
A1525	C1386	C1320	G1250	C1479	G1116	G1052	C982	A910	G713	U615	G620	G585
C1526	G1387	A1321	A1253	C1480	G1117	C1053	C983	A911	G714	U615	G620	A586
G1527	U1388	C1322	A1254	C1481	G1118	A1054	A984	C912	G715	U615	G620	C587
A1528	U1389	C1323	U1255	C1482	U1119	G1055	C985	C913	G716	U615	G620	U588
G1529	A1392	U1325	G1256	C1483	G1120	G1056	C986	U914	G717	U615	G620	U589
U1530	A1393	U1326	U1257	C1484	G1121	A1057	C987	A915	G718	U615	G620	A590
C1531	U1394	A1327	U1258	C1485	G1122	G1058	A988	G916	G719	U615	G620	A591
A1532	A1395	G1331	G1259	C1486	U1130	U1060	C989	A917	G720	U615	G620	A592
U1533	U1396	G1332	A1260	C1487	U1131	U1061	A990	A918	G721	U615	G620	A593
U1534	U1397	G1333	G1261	C1488	U1132	G1062	C991	U919	G722	U615	G620	U594
A1535	C1398	G1334	U1262	C1489	U1133	G1063	C992	A920	G723	U615	G620	C595
C1536	U1400	C1335	U1263	C1490	A1134	C1064	C993	A921	G724	U615	G620	U596
G1537	G1401	A1336	A1264	C1491	G1135	U1065	C994	G923	G725	U615	G620	G597
U1538	U1402	G1337	U1265	C1492	C1136	U1066	A996	A924	G726	U615	G620	U598
G1539	U1403	G1338	G1270	C1493	G1137	U1067	A997	A925	G727	U615	G620	U599
A1540	A1404	G1339	C1271	C1494	U1138	G1068	C998	G926	G728	U615	G620	G600
U1541	U1405	U1340	A1272	C1495	A1069	G1069	U999	A927	G729	U615	G620	C601
U1542	U1406	G1341	U1273	C1496	G1139	A1070	A1000	A928	G730	U615	G620	A602
G1543	G1407	U1342	A1274	C1497	C1140	G1071	A1001	U929	G731	U615	G620	G603
A1544	U1408	U1343	A1275	C1498	U1141	C1072	C1005	U930	G732	U615	G620	G604
G1546	U1409	C1344	A1276	C1499	A1142	U1072	C1006	U931	G733	U615	G620	G605
		C1345	G1210		A1143	C1076		A933	G734	U615	G620	U607

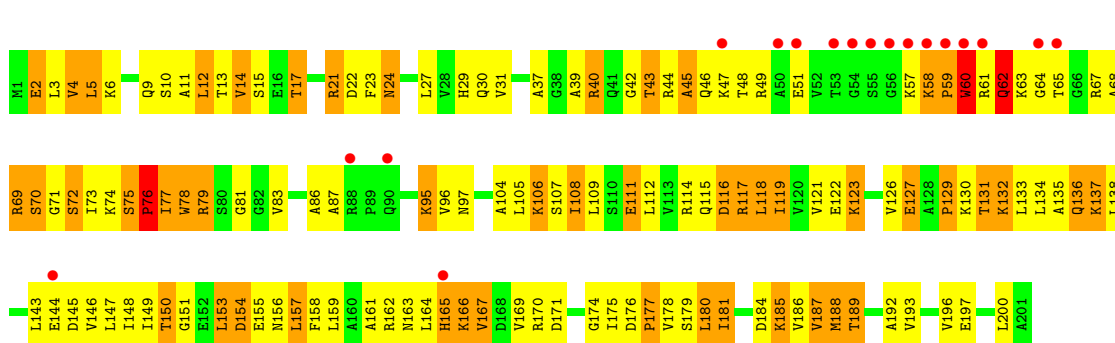
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U2356	G2357	G2358	G2359	G2360	G2361	G2362	G2363	G2364	G2365	G2366	G2367	G2368	G2369	G2370	G2371	G2372	G2373	G2374	G2375	G2376	G2377	G2378	G2379	G2380	G2381	G2382	G2383	G2384	G2385	G2386	G2387	G2388	G2389	G2390	G2391	G2392	G2393	G2394	G2395	G2396	G2400	U2401	U2402	C2403	U2404	G2405	A2406	U2407	U2408	G2409	G2410	A2411	A2412	G2413	G2414	G2415	C2416	C2417	C2418	A2419	G2420	G2421	C2422	U2423
G2293	G2294	C2295	U2296	A2297	G2298	U2299	C2300	C2301	G2304	U2305	C2306	G2307	G2308	A2309	C2310	A2311	U2312	C2313	A2314	G2315	G2316	A2317	G2318	G2319	U2320	A2321	A2322	G2323	U2324	G2325	G2326	A2327	U2328	G2329	G2330	G2331	C2332	A2333	U2334	G2335	A2336	G2337	C2338	G2339	A2340	G2341	C2342	U2343	U2344	G2345	A2346	C2347	U2348	A2352	G2353	U2354	G2355							
G2232	U2233	G2234	G2235	U2236	G2237	G2238	G2239	U2240	A2241	G2242	U2243	U2244	U2245	G2246	A2247	G2248	G2249	G2250	G2251	G2252	G2253	G2254	G2255	G2256	U2257	G2258	G2261	U2262	G2263	G2264	U2265	A2266	G2267	G2268	G2269	A2270	G2271	G2272	A2273	A2274	G2275	G2276	G2277	A2278	G2279	G2280	G2281	G2282	A2283	A2284	C2285	G2286	A2287	A2288	G2289	G2290	U2291	U2292						
A	A	U	A	C	C	A	C	C	U2179	U2180	U2181	U2182	A2183	U2184	U2185	G2186	U2187	U2188	U2189	U2190	U2191	U2192	G2193	U2194	U2195	U2196	U2197	U2198	A2199	C2200	U2203	G2204	C2205	C2206	C2207	C2208	G2209	U2210	A2211	A2212	U2213	C2214	C2215	G2216	G2217	G2218	U2219	U2220	G2221	C2222	A2225	C2226	A2227	G2228	G2229	U2230	U2231							
U2109	G2110	U	G	U	U	A	G	G	A	U	G	G	U	G	G	A	A	G	C	C	U	U	U	G2133	A2134	A2135	G2136	U2137	G2138	G2139	G2141	A2142	G2143	G2144	C2145	C2146	A2147	G2148	U2149	C2150	U2151	G2152	C2153	A2154	U2155	G2156	G2157	A	G	C	C	A	C	U	U	A								
A2042	C2043	C2044	C2045	G2046	C2047	G2048	G2049	C2050	A2051	A2052	C2055	G2056	A2059	A2060	G2061	A2062	C2063	C2064	C2065	C2066	C2067	G2068	G2069	A2070	A2071	C2072	C2073	U2074	U2075	U2076	U2077	U2078	U2079	U2080	U2081	U2082	C2083	C2084	U2085	U2086	G2087	A2088	C2089	A2090	C2091	U2092	G2093	A2094	A2095	C2096	G2100	A2101	G2102	G2103	C2104	U2105	U2106	G2107	A2108					
G1968	A1969	U1970	U1971	G1972	G1973	C1974	G1985	A1986	A1987	G1988	G1989	U1991	U1992	U1993	C1994	C1997	A1998	C1999	C2000	C2001	G2002	C2008	A2009	G2010	U2011	G2012	A2013	A2014	U2015	U2016	U2017	G2018	A2019	A2020	C2021	U2022	C2023	C2024	G2025	U2026	G2027	U2028	A2029	U2030	A2031	G2032	A2033	A2034	G2035	C2036	A2037	G2038	U2039	G2040	U2041									
A1899	C1902	G1903	G1904	G1905	G1906	G1907	C1908	C1909	C1913	A1914	U1915	A1916	U1917	A1918	G1921	U1922	C1923	C1924	C1925	U1926	A1927	A1928	G1929	G1930	U1931	G1935	A1936	A1937	U1938	U1939	U1940	U1943	U1944	G1945	U1946	C1947	G1948	G1949	G1950	U1951	U1955	U1956	C1957	C1958	G1959	C1961	G1962	C1963	G1964	C1965	A1966	C1967												
U1834	C1837	C1838	G1839	G1842	C1843	C1844	G1845	A1847	A1848	G1849	G1850	A1853	A1854	U1855	U1856	G1857	G1862	U1863	U1864	U1865	A1866	G1867	G1868	G1869	G1870	A1871	A1872	A1873	C1874	G1875	A1876	A1877	G1878	C1879	U1880	C1881	U1882	U1883	G1884	A1885	U1886	C1887	G1888	A1889	A1890	U1891	G1892	C1893	U1894	G1895	G1896	U1897	U1898											
G1767	A1773	G1776	U1777	U1778	U1779	U1780	U1781	U1782	A1783	A1784	A1785	A1786	A1787	G1788	A1789	C1790	A1791	A1794	C1795	U1796	G1797	U1798	G1799	C1800	A1801	A1802	G1803	A1804	A1805	C1806	G1807	A1808	A1809	A1810	G1811	G1812	G1813	G1814	A1815	G1816	G1817	U1818	A1819	U1820	A1821	C1822	G1823	A1824	U1825	G1826	U1827	U1828	A1829	C1830	C1833									
G1613	A1616	C1617	A1618	G1623	U1624	C1625	A1634	A1635	U1636	G1637	C1638	C1639	A1640	G1642	G1643	U1647	U1648	U1649	A1650	G1651	A1652	C1653	A1654	A1655	C1656	U1657	C1658	G1661	U1662	A1665	G1666	G1667	A1668	A1669	G1674	U1680	G1681	G1682	U1683	G1684	C1685	C1686	G1687	U1688	A1689	A1690	U1691	G1696																
G1595	A1700	C1704	U1709	G1710	A1711	U1712	A1713	U1714	G1715	U1716	A1717	U1720	G1721	A1722	G1723	G1724	C1725	U1726	C1727	G1728	U1729	C1730	G1731	C1732	A1733	G1734	A1735	U1736	G1737	G1738	A1739	G1740	A1745	A1746	U1747	C1748	A1749	G1750	U1751	C1752	G1753	A1754	A1755	G1756	A1757	U1758	A1759	C1760	G1761	G1762	G1763	C1764	U1765	G1766										
C1547	A1548	C1549	C1550	A1551	A1552	A1553	C1556	C1557	U1558	U1559	G1560	C1561	C1562	U1563	C1564	C1565	A1566	A1567	A1570	A1571	A1572	G1573	C1574	C1575	A1576	C1577	U1578	A1579	A1580	C1581	C1582	A1583	U1584	C1585	A1586	A1590	A1591	C1592	A1593	U1594	C1595	U1599	C1600	G1601	U1602	U1603	C1604	C1605	G1606	C1607	A1608	A1609	A1610											





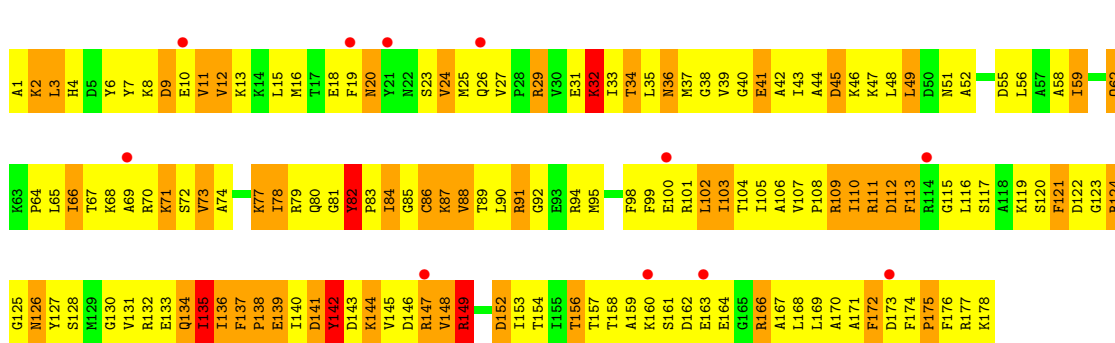
- Molecule 5: 50S ribosomal protein L4

Chain E:



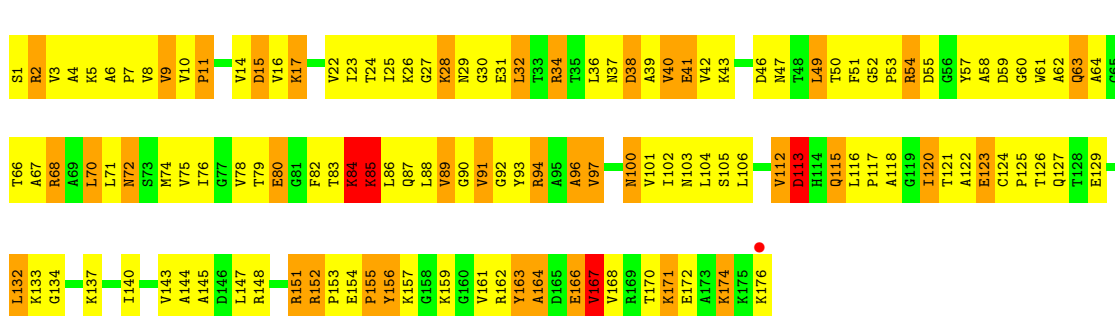
- Molecule 6: 50S ribosomal protein L5

Chain F:



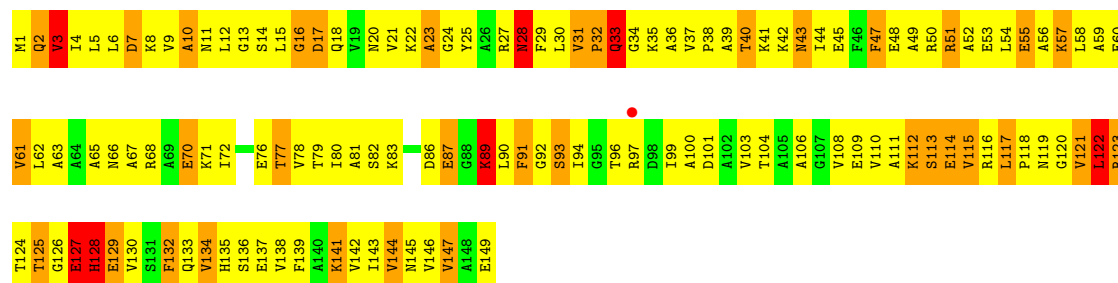
- Molecule 7: 50S ribosomal protein L6

Chain G:



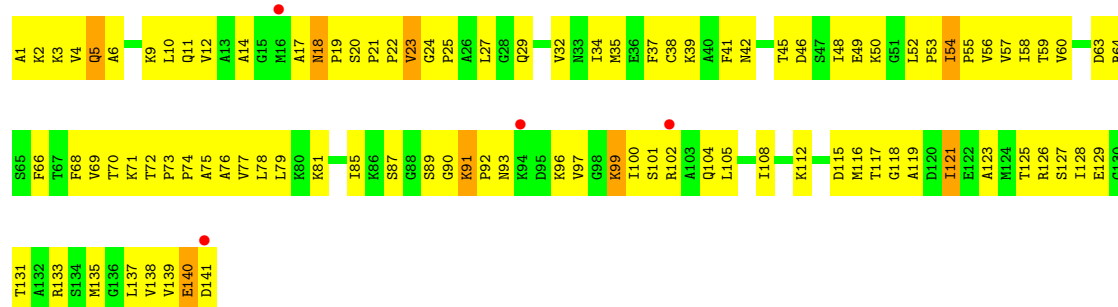
- Molecule 8: 50S ribosomal protein L9

Chain H: 



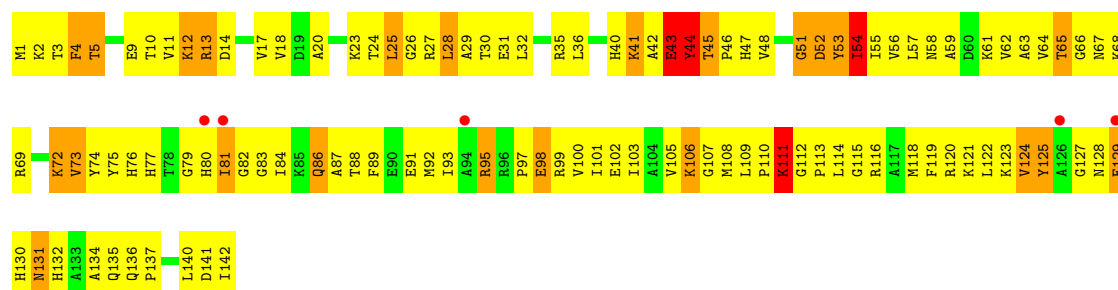
- Molecule 9: 50S ribosomal protein L11

Chain I: 



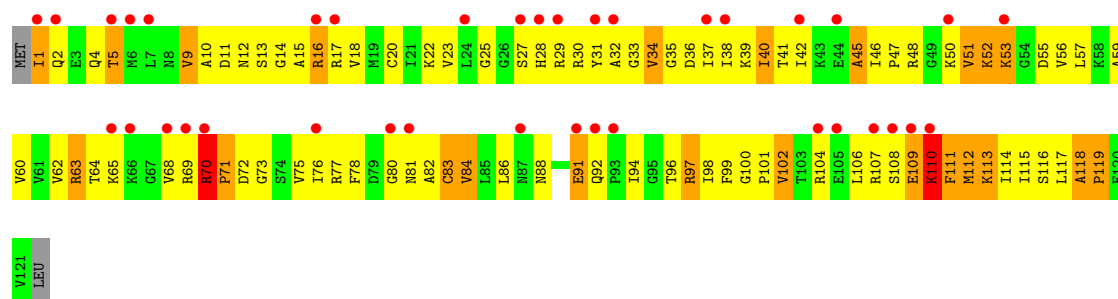
- Molecule 10: 50S ribosomal protein L13

Chain J: 

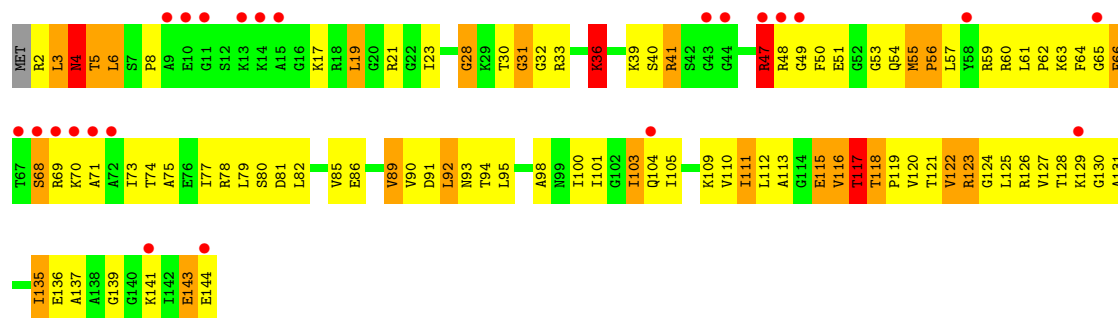


- Molecule 11: 50S ribosomal protein L14

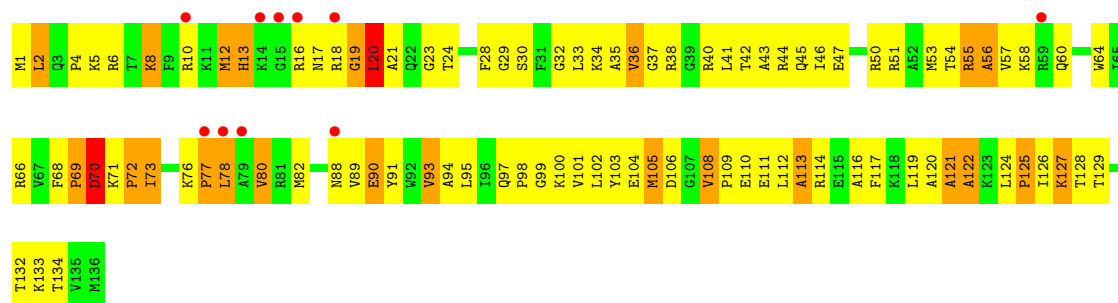
Chain K: 



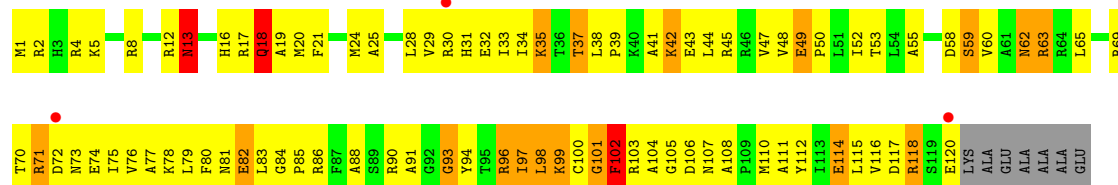
- Molecule 12: 50S ribosomal protein L15

Chain L: 

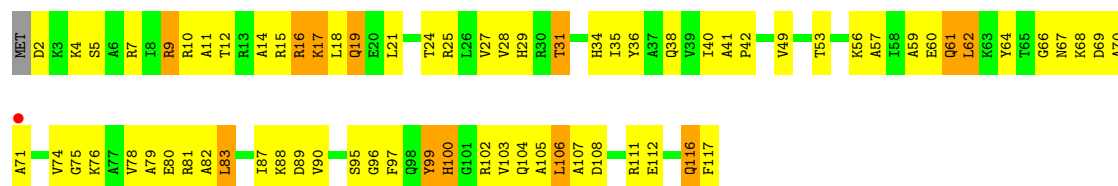
- Molecule 13: 50S ribosomal protein L16

Chain M: 

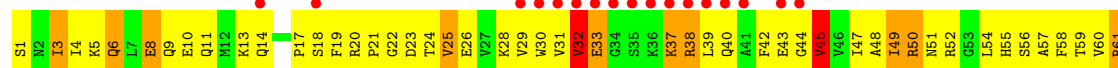
- Molecule 14: 50S ribosomal protein L17

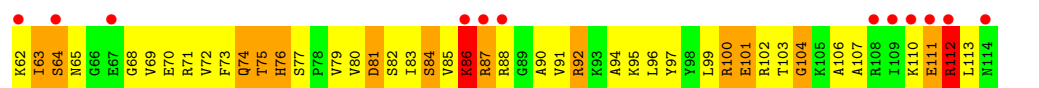
Chain N: 

- Molecule 15: 50S ribosomal protein L18

Chain O: 

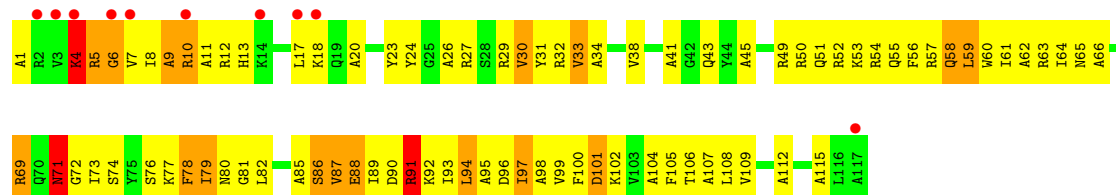
- Molecule 16: 50S ribosomal protein L19

Chain P: 



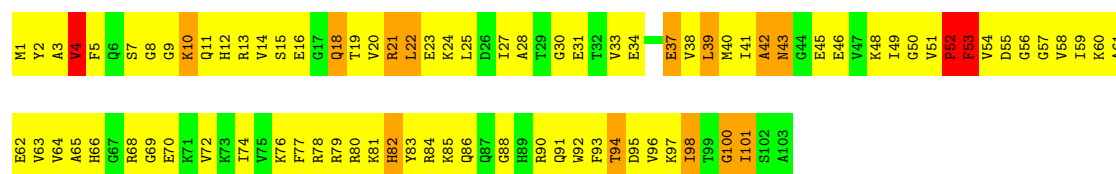
- Molecule 17: 50S ribosomal protein L20

Chain Q:



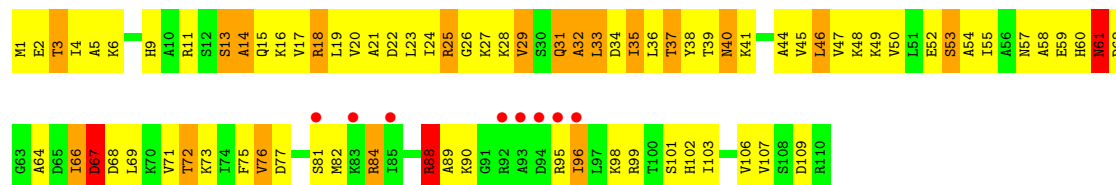
- Molecule 18: 50S ribosomal protein L21

Chain R:



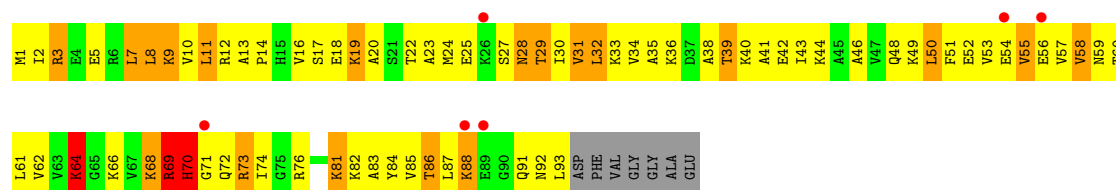
- Molecule 19: 50S ribosomal protein L22

Chain S:



- Molecule 20: 50S ribosomal protein L23

Chain T:

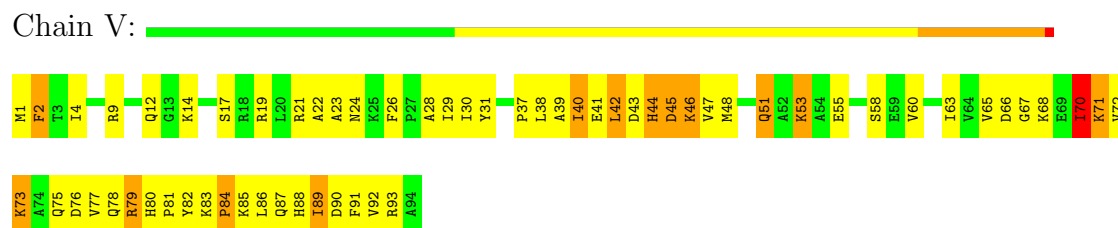


- Molecule 21: 50S ribosomal protein L24

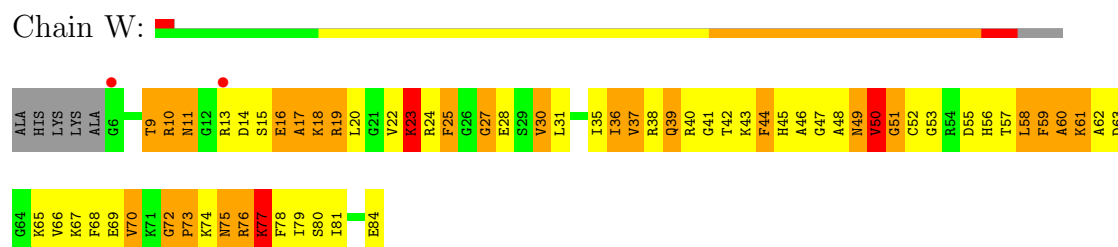
Chain U:



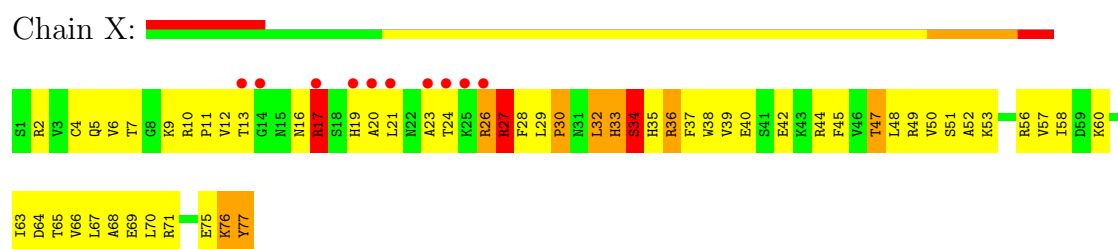
- Molecule 22: 50S ribosomal protein L25



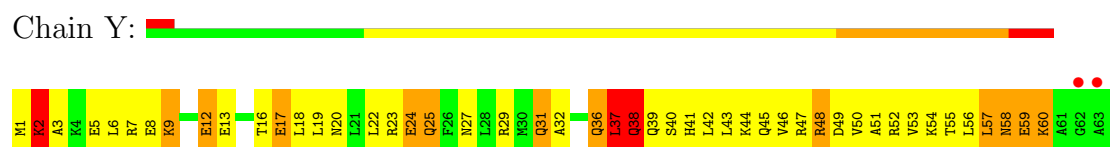
- Molecule 23: 50S ribosomal protein L27



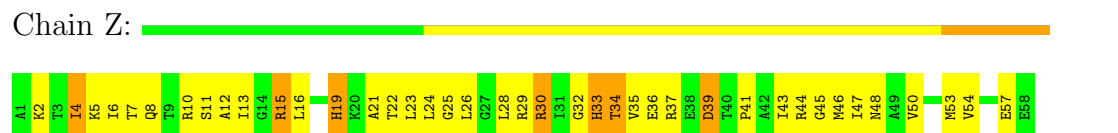
- Molecule 24: 50S ribosomal protein L28



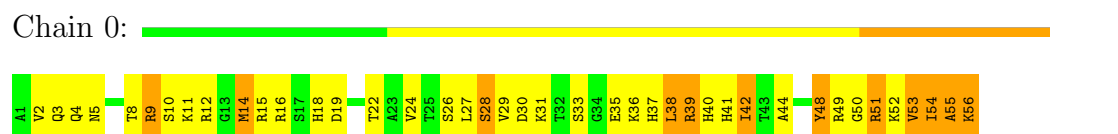
- Molecule 25: 50S ribosomal protein L29



- Molecule 26: 50S ribosomal protein L30



- Molecule 27: 50S ribosomal protein L32



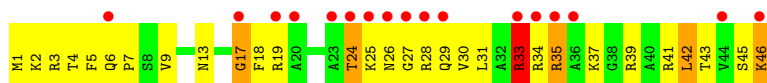
- Molecule 28: 50S ribosomal protein L33





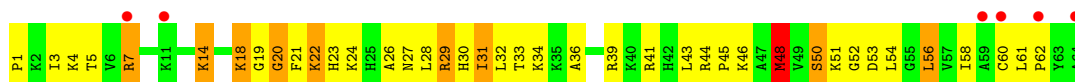
- Molecule 29: 50S ribosomal protein L34

Chain 2:



- Molecule 30: 50S ribosomal protein L35

Chain 3:



- Molecule 31: 50S ribosomal protein L36

Chain 4:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.78Å 395.22Å 744.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.22 184.07 – 3.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.22) 75.7 (184.07-3.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.287 , 0.320 0.450 , 0.455	Depositor DCC
R_{free} test set	37267 reflections (4.95%)	DCC
Wilson B-factor (Å ²)	80.0	Xtriage
Anisotropy	0.720	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 2.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 753156 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.62	EDS
Total number of atoms	90315	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

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	0.24	0/2803	0.73	0/4371
2	B	0.28	7/68314 (0.0%)	0.77	62/106569 (0.1%)
3	C	0.22	0/2121	0.52	0/2852
4	D	0.25	0/1586	0.60	0/2134
5	E	0.24	0/1571	0.61	2/2113 (0.1%)
6	F	0.27	0/1444	0.59	0/1937
7	G	0.23	0/1343	0.52	0/1816
8	H	0.26	0/1122	0.52	0/1515
9	I	0.24	0/1046	0.46	0/1410
10	J	0.24	0/1152	0.59	0/1551
11	K	0.25	0/939	0.81	2/1258 (0.2%)
12	L	0.23	0/1054	0.58	0/1403
13	M	0.26	0/1093	0.56	0/1460
14	N	0.25	0/973	0.62	0/1301
15	O	0.23	0/902	0.55	0/1209
16	P	0.25	0/929	0.60	0/1242
17	Q	0.26	0/960	0.65	0/1278
18	R	0.26	0/829	0.58	0/1107
19	S	0.23	0/864	0.61	1/1156 (0.1%)
20	T	0.23	0/744	0.73	2/994 (0.2%)
21	U	0.26	0/787	0.56	0/1051
22	V	0.25	0/766	0.46	0/1025
23	W	0.31	0/603	0.65	0/797
24	X	0.25	0/635	0.58	0/848
25	Y	0.25	0/510	0.64	0/677
26	Z	0.23	0/453	0.55	0/605
27	0	0.22	0/450	0.65	0/599
28	1	0.27	0/416	0.55	0/554
29	2	0.26	0/380	0.58	0/498
30	3	0.26	0/513	0.66	2/676 (0.3%)
31	4	0.23	0/303	0.54	0/397
All	All	0.27	7/97605 (0.0%)	0.73	71/146403 (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
2	B	0	36

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1086	A	C5-C6	-16.20	1.26	1.41
2	B	1088	A	C6-N1	-10.54	1.28	1.35
2	B	1060	U	C2-N3	7.83	1.43	1.37
2	B	1086	A	N3-C4	-6.81	1.30	1.34
2	B	1086	A	N7-C5	-6.47	1.35	1.39

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2204	G	O5'-P-OP1	-29.28	75.56	110.70
2	B	2791	G	O5'-P-OP2	-29.23	75.63	110.70
2	B	2204	G	O5'-P-OP2	18.17	132.50	110.70
2	B	2791	G	O5'-P-OP1	17.21	131.35	110.70
2	B	2203	U	OP1-P-O3'	14.86	137.90	105.20

There are no chirality outliers.

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	221	A	Sidechain
2	B	222	A	Sidechain
2	B	299	A	Sidechain
2	B	500	G	Sidechain
2	B	51	G	Sidechain

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	2507	0	1270	76	0
2	B	60995	0	30678	2146	0
3	C	2082	0	2157	215	0
4	D	1565	0	1616	215	0
5	E	1552	0	1619	165	0
6	F	1420	0	1460	241	0
7	G	1323	0	1374	175	0
8	H	1111	0	1148	174	0
9	I	1032	0	1088	184	0
10	J	1129	0	1162	167	0
11	K	930	0	1003	95	0
12	L	1045	0	1117	123	0
13	M	1074	0	1157	105	0
14	N	960	0	1000	102	0
15	O	892	0	923	73	0
16	P	917	0	965	109	0
17	Q	947	0	1022	140	0
18	R	816	0	839	114	0
19	S	857	0	922	96	0
20	T	738	0	807	118	0
21	U	779	0	834	105	0
22	V	753	0	780	71	0
23	W	596	0	610	146	0
24	X	625	0	655	78	0
25	Y	509	0	543	75	0
26	Z	449	0	491	40	0
27	0	444	0	461	48	0
28	1	409	0	440	32	0
29	2	377	0	418	29	0
30	3	504	0	574	48	0
31	4	302	0	340	28	0
32	4	1	0	0	0	0
33	B	119	0	0	0	0
34	2	1	0	0	0	0
34	4	4	0	0	0	0
34	B	532	0	0	5	0
34	C	8	0	0	0	0
34	D	1	0	0	0	0
34	E	2	0	0	0	0
34	J	2	0	0	0	0
34	L	3	0	0	0	0
34	N	2	0	0	0	0

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Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	T	1	0	0	0	0
All	All	90315	0	59473	5011	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 34.

The worst 5 of 5011 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:101:GLY:HA2	14:N:110:MET:H	1.04	1.18
5:E:46:GLN:HG3	5:E:87:ALA:HB3	1.31	1.12
11:K:70:ARG:HB3	11:K:71:PRO:CD	1.76	1.12
2:B:855:G:H21	23:W:23:LYS:HG2	1.04	1.11
4:D:148:GLN:HG3	4:D:152:PRO:HG2	1.27	1.08

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	269/272 (99%)	168 (62%)	63 (23%)	38 (14%)	0	2
4	D	207/209 (99%)	110 (53%)	56 (27%)	41 (20%)	0	0
5	E	199/201 (99%)	127 (64%)	42 (21%)	30 (15%)	0	1
6	F	176/178 (99%)	95 (54%)	43 (24%)	38 (22%)	0	0
7	G	174/176 (99%)	93 (53%)	55 (32%)	26 (15%)	0	1
8	H	147/149 (99%)	68 (46%)	54 (37%)	25 (17%)	0	1
9	I	139/141 (99%)	114 (82%)	21 (15%)	4 (3%)	7	43
10	J	140/142 (99%)	88 (63%)	30 (21%)	22 (16%)	0	1
11	K	119/123 (97%)	75 (63%)	26 (22%)	18 (15%)	0	1
12	L	141/144 (98%)	81 (57%)	37 (26%)	23 (16%)	0	1
13	M	134/136 (98%)	77 (58%)	33 (25%)	24 (18%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	N	118/127 (93%)	75 (64%)	27 (23%)	16 (14%)	0	2
15	O	114/117 (97%)	85 (75%)	24 (21%)	5 (4%)	4	29
16	P	112/114 (98%)	71 (63%)	20 (18%)	21 (19%)	0	0
17	Q	115/117 (98%)	74 (64%)	28 (24%)	13 (11%)	1	4
18	R	101/103 (98%)	64 (63%)	24 (24%)	13 (13%)	0	3
19	S	108/110 (98%)	66 (61%)	26 (24%)	16 (15%)	0	1
20	T	91/100 (91%)	52 (57%)	25 (28%)	14 (15%)	0	1
21	U	100/103 (97%)	57 (57%)	28 (28%)	15 (15%)	0	1
22	V	92/94 (98%)	73 (79%)	12 (13%)	7 (8%)	2	12
23	W	77/84 (92%)	29 (38%)	22 (29%)	26 (34%)	0	0
24	X	75/77 (97%)	41 (55%)	27 (36%)	7 (9%)	1	8
25	Y	61/63 (97%)	34 (56%)	21 (34%)	6 (10%)	1	7
26	Z	56/58 (97%)	42 (75%)	11 (20%)	3 (5%)	3	24
27	0	54/56 (96%)	34 (63%)	10 (18%)	10 (18%)	0	1
28	1	48/54 (89%)	33 (69%)	6 (12%)	9 (19%)	0	0
29	2	44/46 (96%)	26 (59%)	14 (32%)	4 (9%)	1	8
30	3	62/64 (97%)	41 (66%)	17 (27%)	4 (6%)	2	17
31	4	36/38 (95%)	21 (58%)	11 (31%)	4 (11%)	1	5
All	All	3309/3396 (97%)	2014 (61%)	813 (25%)	482 (15%)	0	2

5 of 482 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	35	LYS
3	C	53	ILE
3	C	77	VAL
3	C	140	VAL
3	C	184	GLU

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	216/217 (100%)	182 (84%)	34 (16%)	4	17
4	D	164/164 (100%)	137 (84%)	27 (16%)	3	14
5	E	165/165 (100%)	130 (79%)	35 (21%)	1	8
6	F	149/149 (100%)	117 (78%)	32 (22%)	1	7
7	G	137/137 (100%)	110 (80%)	27 (20%)	2	9
8	H	114/114 (100%)	86 (75%)	28 (25%)	1	3
9	I	109/109 (100%)	104 (95%)	5 (5%)	37	80
10	J	116/116 (100%)	100 (86%)	16 (14%)	5	24
11	K	102/104 (98%)	83 (81%)	19 (19%)	2	11
12	L	102/103 (99%)	88 (86%)	14 (14%)	5	25
13	M	109/109 (100%)	93 (85%)	16 (15%)	4	21
14	N	100/103 (97%)	84 (84%)	16 (16%)	3	16
15	O	86/87 (99%)	76 (88%)	10 (12%)	8	35
16	P	99/99 (100%)	77 (78%)	22 (22%)	1	6
17	Q	89/89 (100%)	73 (82%)	16 (18%)	2	12
18	R	84/84 (100%)	67 (80%)	17 (20%)	2	9
19	S	93/93 (100%)	79 (85%)	14 (15%)	4	19
20	T	80/84 (95%)	64 (80%)	16 (20%)	2	9
21	U	83/84 (99%)	70 (84%)	13 (16%)	4	17
22	V	78/78 (100%)	67 (86%)	11 (14%)	5	23
23	W	59/62 (95%)	48 (81%)	11 (19%)	2	11
24	X	67/67 (100%)	57 (85%)	10 (15%)	4	20
25	Y	55/55 (100%)	43 (78%)	12 (22%)	1	7
26	Z	48/48 (100%)	43 (90%)	5 (10%)	10	39
27	0	47/47 (100%)	40 (85%)	7 (15%)	4	20
28	1	45/48 (94%)	38 (84%)	7 (16%)	4	17
29	2	38/38 (100%)	33 (87%)	5 (13%)	6	27
30	3	51/51 (100%)	43 (84%)	8 (16%)	4	17
31	4	34/34 (100%)	29 (85%)	5 (15%)	4	21
All	All	2719/2738 (99%)	2261 (83%)	458 (17%)	3	14

5 of 458 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	31	TYR
14	N	21	PHE
26	Z	30	ARG
11	K	64	THR
12	L	117	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 101 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	136	GLN
14	N	62	ASN
25	Y	38	GLN
11	K	4	GLN
12	L	54	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	116/120 (96%)	19 (16%)	2 (1%)
2	B	2837/2904 (97%)	420 (14%)	17 (0%)
All	All	2953/3024 (97%)	439 (14%)	19 (0%)

5 of 439 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	13	G
1	A	15	A
1	A	16	G
1	A	25	U

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1210	G
2	B	1930	G
2	B	2425	A
2	B	973	A
2	B	2430	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 120 ligands modelled in this entry, 120 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 ⓘ

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	117/120 (97%)	-0.13	4 (3%) 43 9	33, 66, 105, 180	0
2	B	2841/2904 (97%)	0.17	271 (9%) 8 2	12, 55, 149, 180	0
3	C	271/272 (99%)	0.23	21 (7%) 13 4	9, 52, 97, 153	0
4	D	209/209 (100%)	0.40	19 (9%) 9 2	20, 59, 119, 166	0
5	E	201/201 (100%)	0.22	18 (8%) 10 2	11, 76, 143, 178	0
6	F	178/178 (100%)	0.15	11 (6%) 20 4	49, 110, 166, 180	0
7	G	176/176 (100%)	-0.39	1 (0%) 86 43	38, 88, 155, 174	0
8	H	149/149 (100%)	-0.41	1 (0%) 84 40	35, 109, 150, 180	0
9	I	141/141 (100%)	-0.20	4 (2%) 50 11	105, 179, 180, 180	0
10	J	142/142 (100%)	-0.04	5 (3%) 42 9	19, 53, 108, 175	0
11	K	121/123 (98%)	1.71	37 (30%) 1 1	27, 64, 130, 163	0
12	L	143/144 (99%)	0.62	23 (16%) 2 1	17, 64, 115, 180	0
13	M	136/136 (100%)	0.09	10 (7%) 14 4	11, 56, 109, 176	0
14	N	120/127 (94%)	-0.05	3 (2%) 54 13	19, 57, 97, 180	0
15	O	116/117 (99%)	-0.29	1 (0%) 81 35	28, 71, 129, 157	0
16	P	114/114 (100%)	1.22	29 (25%) 1 1	26, 73, 123, 174	0
17	Q	117/117 (100%)	0.09	10 (8%) 11 3	22, 53, 104, 158	0
18	R	103/103 (100%)	-0.26	0 100 100	23, 72, 131, 156	0
19	S	110/110 (100%)	0.11	8 (7%) 15 4	18, 53, 108, 152	0
20	T	93/100 (93%)	0.12	6 (6%) 18 4	35, 72, 141, 178	0
21	U	102/103 (99%)	-0.28	0 100 100	41, 94, 154, 180	0
22	V	94/94 (100%)	-0.36	0 100 100	31, 70, 138, 156	0
23	W	79/84 (94%)	-0.14	2 (2%) 54 13	7, 42, 103, 180	0
24	X	77/77 (100%)	0.13	10 (12%) 4 1	23, 60, 112, 152	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	63/63 (100%)	-0.30	2 (3%) 45 10	34, 92, 158, 180	0
26	Z	58/58 (100%)	-0.33	0 100 100	22, 58, 110, 114	0
27	0	56/56 (100%)	-0.07	0 100 100	19, 56, 118, 135	0
28	1	50/54 (92%)	-0.30	1 (2%) 62 18	26, 76, 119, 163	0
29	2	46/46 (100%)	2.01	17 (36%) 1 0	17, 47, 97, 131	0
30	3	64/64 (100%)	0.64	6 (9%) 9 2	27, 49, 85, 105	0
31	4	38/38 (100%)	-0.58	0 100 100	44, 68, 126, 165	0
All	All	6325/6420 (98%)	0.15	520 (8%) 12 3	7, 62, 154, 180	0

The worst 5 of 520 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1537	G	22.0
2	B	1535	A	20.7
2	B	1536	C	18.7
2	B	1539	U	17.3
1	A	88	C	15.2

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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
33	MG	B	2936	1/1	0.48	4.94	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	B	2993	1/1	0.85	4.26	51,51,51,51	0
33	MG	B	2945	1/1	0.24	3.98	32,32,32,32	0
33	MG	B	2933	1/1	1.12	3.83	92,92,92,92	0
33	MG	B	2956	1/1	0.49	3.74	137,137,137,137	0
33	MG	B	2941	1/1	0.44	3.34	32,32,32,32	0
33	MG	B	2981	1/1	0.62	2.16	57,57,57,57	0
33	MG	B	2965	1/1	0.18	1.79	97,97,97,97	0
33	MG	B	2990	1/1	0.22	1.53	57,57,57,57	0
33	MG	B	2927	1/1	0.14	1.17	46,46,46,46	0
33	MG	B	2938	1/1	0.20	1.15	87,87,87,87	0
33	MG	B	3000	1/1	0.19	1.06	46,46,46,46	0
33	MG	B	2975	1/1	0.22	1.02	30,30,30,30	0
33	MG	B	2998	1/1	0.46	1.02	77,77,77,77	0
33	MG	B	2970	1/1	0.28	0.84	30,30,30,30	0
33	MG	B	2971	1/1	0.41	0.83	33,33,33,33	0
33	MG	B	2915	1/1	0.19	0.52	16,16,16,16	0
33	MG	B	2932	1/1	0.29	0.41	42,42,42,42	0
33	MG	B	2939	1/1	0.43	0.40	27,27,27,27	0
33	MG	B	2973	1/1	0.28	0.29	48,48,48,48	0
33	MG	B	3018	1/1	0.42	0.24	43,43,43,43	0
33	MG	B	2931	1/1	0.35	0.17	43,43,43,43	0
33	MG	B	2911	1/1	0.14	0.14	49,49,49,49	0
33	MG	B	2923	1/1	0.20	-0.19	43,43,43,43	0
33	MG	B	3006	1/1	0.47	-0.28	67,67,67,67	0
33	MG	B	2906	1/1	0.18	-0.30	44,44,44,44	0
33	MG	B	2952	1/1	0.23	-0.35	45,45,45,45	0
33	MG	B	2969	1/1	0.11	-0.42	67,67,67,67	0
33	MG	B	3003	1/1	0.17	-0.45	19,19,19,19	0
33	MG	B	2921	1/1	0.17	-0.48	34,34,34,34	0
33	MG	B	2947	1/1	0.13	-0.68	49,49,49,49	0
33	MG	B	2986	1/1	0.16	-0.69	104,104,104,104	0
33	MG	B	2913	1/1	0.14	-0.74	48,48,48,48	0
33	MG	B	2995	1/1	0.13	-0.76	39,39,39,39	0
33	MG	B	3014	1/1	0.17	-0.79	41,41,41,41	0
33	MG	B	2934	1/1	0.21	-0.81	46,46,46,46	0
33	MG	B	2950	1/1	0.15	-0.87	47,47,47,47	0
32	ZN	4	401	1/1	0.10	-0.87	72,72,72,72	0
33	MG	B	3001	1/1	0.13	-0.91	39,39,39,39	0
33	MG	B	3017	1/1	0.19	-0.98	27,27,27,27	0
33	MG	B	2997	1/1	0.13	-1.08	54,54,54,54	0
33	MG	B	2992	1/1	0.15	-1.14	83,83,83,83	0
33	MG	B	2951	1/1	0.14	-1.15	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	B	2984	1/1	0.10	-1.16	29,29,29,29	0
33	MG	B	2937	1/1	0.08	-1.20	43,43,43,43	0
33	MG	B	2991	1/1	0.10	-1.28	28,28,28,28	0
33	MG	B	2980	1/1	0.15	-1.34	49,49,49,49	0
33	MG	B	2960	1/1	0.06	-1.34	28,28,28,28	0
33	MG	B	2935	1/1	0.17	-1.35	16,16,16,16	0
33	MG	B	2907	1/1	0.07	-1.36	24,24,24,24	0
33	MG	B	3008	1/1	0.11	-1.39	50,50,50,50	0
33	MG	B	2963	1/1	0.10	-1.40	110,110,110,110	0
33	MG	B	2954	1/1	0.06	-1.42	51,51,51,51	0
33	MG	B	3021	1/1	0.07	-1.44	26,26,26,26	0
33	MG	B	3012	1/1	0.13	-1.50	36,36,36,36	0
33	MG	B	2926	1/1	0.12	-1.55	42,42,42,42	0
33	MG	B	3020	1/1	0.09	-1.58	54,54,54,54	0
33	MG	B	2966	1/1	0.07	-1.58	54,54,54,54	0
33	MG	B	2959	1/1	0.08	-1.63	30,30,30,30	0
33	MG	B	2908	1/1	0.09	-1.67	21,21,21,21	0
33	MG	B	2910	1/1	0.07	-1.67	38,38,38,38	0
33	MG	B	2972	1/1	0.06	-1.67	35,35,35,35	0
33	MG	B	2989	1/1	0.09	-1.70	21,21,21,21	0
33	MG	B	2914	1/1	0.09	-1.73	20,20,20,20	0
33	MG	B	2916	1/1	0.09	-1.73	37,37,37,37	0
33	MG	B	2987	1/1	0.09	-1.73	31,31,31,31	0
33	MG	B	3023	1/1	0.06	-1.77	64,64,64,64	0
33	MG	B	2929	1/1	0.13	-1.79	40,40,40,40	0
33	MG	B	2996	1/1	0.10	-1.80	44,44,44,44	0
33	MG	B	2922	1/1	0.17	-1.89	32,32,32,32	0
33	MG	B	3007	1/1	0.06	-1.91	46,46,46,46	0
33	MG	B	3015	1/1	0.03	-1.93	38,38,38,38	0
33	MG	B	2976	1/1	0.13	-1.95	39,39,39,39	0
33	MG	B	2919	1/1	0.14	-2.00	49,49,49,49	0
33	MG	B	2942	1/1	0.13	-2.01	19,19,19,19	0
33	MG	B	2982	1/1	0.19	-2.02	28,28,28,28	0
33	MG	B	3002	1/1	0.12	-2.03	42,42,42,42	0
33	MG	B	2944	1/1	0.12	-2.04	41,41,41,41	0
33	MG	B	2968	1/1	0.13	-2.06	32,32,32,32	0
33	MG	B	3010	1/1	0.11	-2.08	29,29,29,29	0
33	MG	B	2925	1/1	0.14	-2.17	50,50,50,50	0
33	MG	B	2930	1/1	0.05	-2.18	38,38,38,38	0
33	MG	B	2918	1/1	0.10	-2.25	32,32,32,32	0
33	MG	B	3016	1/1	0.11	-2.27	52,52,52,52	0
33	MG	B	2974	1/1	0.15	-2.28	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	B	3013	1/1	0.08	-2.31	28,28,28,28	0
33	MG	B	2977	1/1	0.15	-2.42	7,7,7,7	0
33	MG	B	2943	1/1	0.10	-2.51	95,95,95,95	0
33	MG	B	2988	1/1	0.08	-2.53	26,26,26,26	0
33	MG	B	2964	1/1	0.09	-2.58	35,35,35,35	0
33	MG	B	2917	1/1	0.09	-2.64	62,62,62,62	0
33	MG	B	2994	1/1	0.12	-2.69	62,62,62,62	0
33	MG	B	3011	1/1	0.06	-2.74	24,24,24,24	0
33	MG	B	2999	1/1	0.05	-2.82	26,26,26,26	0
33	MG	B	2958	1/1	0.11	-2.86	53,53,53,53	0
33	MG	B	3005	1/1	0.05	-2.87	44,44,44,44	0
33	MG	B	2983	1/1	0.07	-2.93	18,18,18,18	0
33	MG	B	2924	1/1	0.08	-2.95	25,25,25,25	0
33	MG	B	3022	1/1	0.05	-2.96	35,35,35,35	0
33	MG	B	2912	1/1	0.07	-2.96	55,55,55,55	0
33	MG	B	2940	1/1	0.08	-2.97	36,36,36,36	0
33	MG	B	2928	1/1	0.08	-2.97	22,22,22,22	0
33	MG	B	2961	1/1	0.05	-2.99	63,63,63,63	0
33	MG	B	2920	1/1	0.07	-3.19	43,43,43,43	0
33	MG	B	2978	1/1	0.06	-3.29	9,9,9,9	0
33	MG	B	2955	1/1	0.07	-3.37	48,48,48,48	0
33	MG	B	2957	1/1	0.06	-3.73	37,37,37,37	0
33	MG	B	2949	1/1	0.07	-3.86	140,140,140,140	0
33	MG	B	2962	1/1	0.08	-3.93	136,136,136,136	0
33	MG	B	2905	1/1	0.07	-4.20	14,14,14,14	0
33	MG	B	3009	1/1	0.04	-4.20	18,18,18,18	0
33	MG	B	2948	1/1	0.07	-4.35	20,20,20,20	0
33	MG	B	3004	1/1	0.04	-5.35	10,10,10,10	0
33	MG	B	2946	1/1	0.04	-5.42	56,56,56,56	0
33	MG	B	2985	1/1	0.07	-5.66	36,36,36,36	0
33	MG	B	2979	1/1	0.06	-6.42	46,46,46,46	0
33	MG	B	2967	1/1	0.04	-6.68	45,45,45,45	0
33	MG	B	2953	1/1	0.07	-7.21	42,42,42,42	0
33	MG	B	2909	1/1	0.08	-13.11	66,66,66,66	0
33	MG	B	3019	1/1	0.34	-	132,132,132,132	0

6.5 Other polymers ⓘ

There are no such residues in this entry.