



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 04:28 AM UTC

PDB ID : 2ZJQ / pdb_00002zjq
Title : Interaction of L7 with L11 induced by Micrococin binding to the Deinococcus radiodurans 50S subunit
Authors : Harms, J.M.; Wilson, D.N.; Schlutzen, F.; Connell, S.R.; Stachelhaus, T.; Zaborowska, Z.; Spahn, C.M.T.; Fucini, P.
Deposited on : 2008-03-08
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

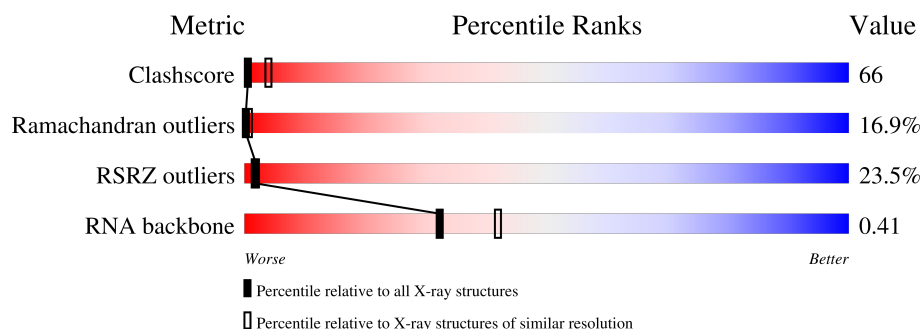
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	X	2880	18% 12% 50% 21% 11% 7%
2	Y	122	23% 16% 69% 15%
3	A	274	26% 19% 55% 13% 12%
4	B	211	20% 24% 54% 18%
5	C	205	16% 13% 53% 29%
6	D	180	23% 9% 69% 20%
7	E	185	12% 18% 60% 15% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	142	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	
30	4	37	
31	5	122	

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 84395 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ribosomal 23S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2686	Total	C	N	O	P	0	0	0
			57651	25718	10642	18606	2685			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	122	Total	C	N	O	P	0	0	0
			2598	1161	476	840	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	240	Total	C	N	O	S	0	0	0
			1826	1137	366	321	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	197	Total	C	N	O	S	0	0	0
			1506	935	287	282	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1400	892	247	254	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	144	Total	C	N	O	S	0	0	0
			1043	663	179	196	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	141	Total	C	N	O	0	0	0
			1067	655	216	196			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	MET	-	initiating methionine	UNP Q9RXJ5

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	104	Total	C	N	O		0	0	0
			779	476	161	142				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	108	Total	C	N	O		0	0	0
			871	543	172	156				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	O	94	Total	C	N	O		0	0	0
			741	465	139	137				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	93	Total	C	N	O	S	0	0	0
			726	458	136	130	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	175	Total	C	N	O	S	0	0	0
			1345	849	236	254	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	84	Total	C	N	O	S	0	0	0
			625	393	122	109	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	72	Total	C	N	O	S	0	0	0
			552	341	116	95				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	66	Total	C	N	O	S	0	0	0
			533	327	107	96	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	1	53	Total C 53 53	0	0	53

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	2	46	Total C 46 46	0	0	46

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	3	63	Total C 63 63	0	0	63

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	4	37	Total C N O S 297 179 66 47 5	0	0	0

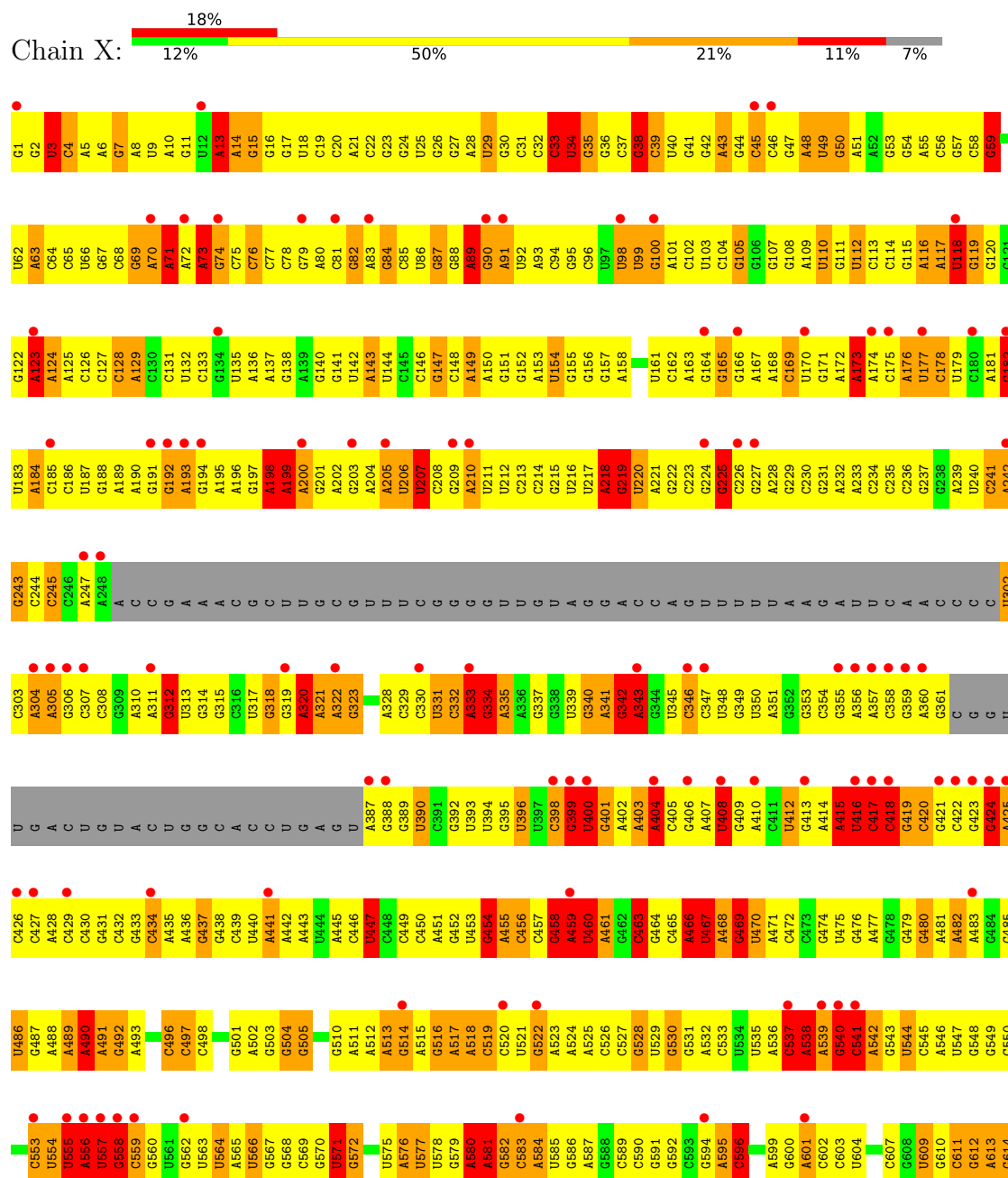
- Molecule 31 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	5	71	Total C 71 71	0	0	71

3 Residue-property plots [i](#)

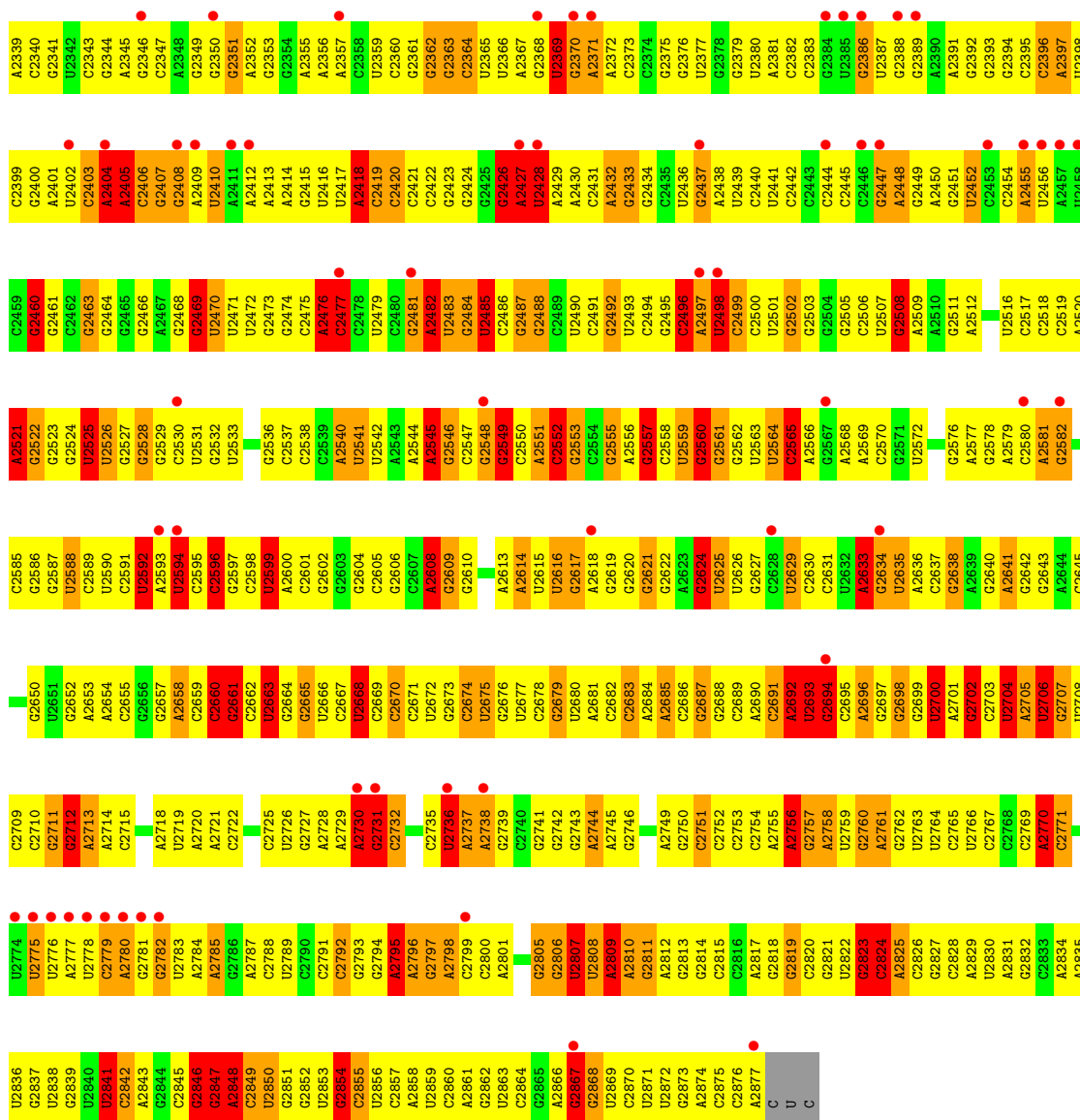
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ribosomal 23S RNA

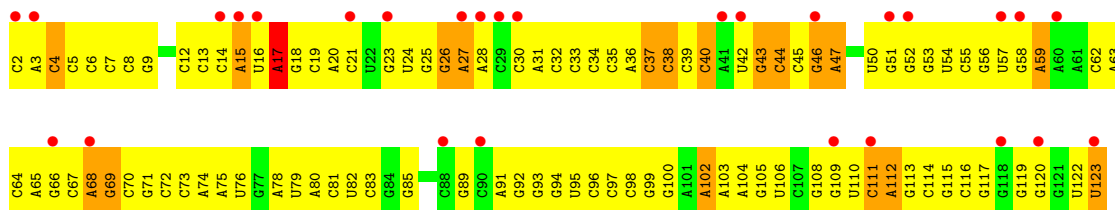


U1409	C1348	A1285	G1285	G1165	U1105	U1044	C982	U819	U859	A797	C737	C675	C615
U1410	A1349	U1286	A1226	A1166	A1106	G1045	G983	G920	U860	G798	G738	G676	U616
C1411	G1350	A1287	A1167	A1168	U1108	U1046	A984	A921	G861	G799	G739	G677	A618
C1412	G1351	A1288	G1228	G1169	U1109	U1047	G985	A922	A862	U800	A740	G678	A619
G1413	G1352	A1289	C1229	C1169	A1109	U1048	A986	A923	C863	A801	G741	G679	G620
U1414	A1353	A1290	U1170	G1110	G1110	G1049	G987	C924	C864	A802	G742	U680	U621
A1415	A1354	G1291	A1171	C1111	U1111	U1051	U895	U895	A865	C803	A743	A681	U622
A1416	A1355	A1292	U1172	U1112	U1112	C1052	C926	C927	U866	C804	C744	G682	G623
C1417	G1356	A1293	G1173	U1113	C1113	G1053	A991	G928	G867	G805	C745	A683	A624
G1418	A1357	G1294	G1174	A1114	C1114	C1054	A992	G929	U868	A806	G746	C684	G625
C1419	C1358	U1295	A1175	C1115	C993	A1055	C993	A929	C869	A807	A747	U685	A626
G1420	G1359	U1296	U1176	U1116	U1116	U1056	A984	A930	C870	C808	A748	A626	A627
U1421	G1360	G1297	U1177	U1117	U1117	A1057	A985	G931	U871	C809	C749	G687	A627
C1422	A1361	U1298	C1178	G1118	G1118	G1058	C986	G932	G872	U810	C750	A688	A628
A1423	A1362	A1299	A1179	U1119	U1119	C1059	C997	G933	U873	G811	G751	C629	C629
U1424	C1363	A1300	A1180	C1120	C1120	A1060	C998	G934	A874	G812	G752	A690	G630
G1425	C1364	U1301	G1181	A1181	C1121	G1061	A989	C935	G875	A813	U753	C691	G631
U1426	U1365	C1302	U1182	U1122	A1122	G1062	A936	A936	A876	G814	G754	A692	A632
G1427	A1366	U1303	C1183	G1123	G1123	C1063	C1001	C937	G877	U815	C755	A693	G633
A1428	A1367	U1304	G1184	U1124	U1124	C1064	C1002	G938	C878	U816	C756	G694	G634
G1429	G1368	C1305	C1185	G1125	U1125	A1065	C1003	C939	A879	A817	U757	C695	C635
U1430	C1369	U1306	G1186	A1126	C1126	G1066	A1004	G940	C880	G818	G758	U696	G636
A1431	U1370	G1307	A1187	C1127	G1127	G1067	U1005	U943	C881	C819	C759	G697	G637
G1432	C1371	U1308	G1188	A1128	G1128	A1068	C1006	U944	C882	U820	U760	A698	A638
A1433	A1372	C1311	U1189	A1129	A1129	G1069	A1007	A945	A883	A821	G761	G699	G639
U1434	G1373	G1312	C1190	U1130	U1130	G1070	G1008	G946	C884	G822	A762	C700	C640
G1436	G1374	U1313	G1191	G1131	G1131	U1071	A1011	U946	A885	U823	A763	U701	G641
U1437	C1375	A1314	A1192	C1132	C1132	U1072	A886	C947	U881	U824	A764	A702	A642
G1438	G1376	G1315	U1193	G1133	G1133	G1073	A1012	C948	G887	C818	C765	A703	A643
C1439	C1377	C1316	U1194	C1134	G1134	G1074	G1013	G949	G888	U826	A766	G704	A644
U1440	A1378	U1317	U1195	C1135	C1135	C1075	G1014	G950	C889	C827	G767	C705	G645
A1441	C1380	A1320	G1196	G1136	U1136	U1076	C951	G951	U890	C828	U768	A706	C646
C1442	G1381	A1321	U1197	A1137	A1137	U1077	A952	A952	A891	C829	U707	U707	C647
G1443	C1382	G1322	U1199	A1139	A1139	G1078	G953	G953	C830	G831	U770	A648	A648
A1444	C1383	G1323	G1200	C1139	C1139	G1079	U954	U954	G832	A832	C710	U709	U650
U1445	G1384	G1324	G1201	U1141	A1141	A1080	A955	G955	G833	A833	G773	C711	C651
U1446	C1385	U1325	U1202	G1142	G1142	G1082	C957	G957	G834	A834	A774	A712	C652
U1447	A1386	C1326	A1203	A1143	A1143	C1083	G958	G958	U835	U835	U775	G713	G653
A1448	C1389	U1327	G1204	U1144	U1144	A1084	C959	C959	C836	G776	G776	G714	A654
G1449	G1390	U1328	G1205	C1145	G1145	G1085	G1024	U960	U837	A777	A777	U715	A655
U1450	A1391	G1329	G1206	C1146	C1146	C1086	A1025	A964	A838	U778	U778	U716	U656
C1451	G1392	G1330	G1207	G1147	G1147	G1087	U1026	G965	U839	U779	U779	G717	A657
U1452	C1393	A1331	A1208	G1148	C1148	A1088	C1027	A966	U840	U780	C658	A718	C658
A1453	G1394	G1332	U1209	G1149	G1149	C1089	G1028	A967	G841	G781	G659	A719	G659
U1454	C1395	A1333	C1210	C1150	C1150	C1090	C1029	G967	A842	A782	C661	A720	C661
C1456	C1396	G1335	U1212	C1151	C1151	U1092	C1031	C968	G843	G783	C662	C721	C662
U1459	A1397	A1336	U1213	A1153	A1153	U1093	A1032	U969	G844	U784	U785	C725	C663
G1460	C1398	G1337	C1214	G1154	G1154	C1094	G1033	A971	C847	U786	G726	G726	C664
A1461	A1400	U1339	A1215	G1155	G1155	A1095	U1034	C972	A848	A787	G728	G728	A665
C1462	G1401	C1340	G1216	U1156	U1156	A1096	G1035	U973	G849	G788	G729	G729	U666
A1463	G1402	G1341	U1217	G1157	G1157	A1097	U1037	U974	C850	A729	C730	C730	A668
G1464	U1403	C1342	C1218	U1158	U1158	G1098	C1037	C975	C851	A790	G791	G791	G669
U1465	C1404	U1343	C1219	U1159	U1159	A1099	U1038	G976	U852	A731	G732	G732	U670
C1466	A1405	C1344	G1220	C1160	C1160	G1100	A1039	G977	C914	U792	G793	G793	A671
U1467	G1406	G1345	U1221	U1161	U1161	U1101	A1040	U978	G855	A794	G794	G794	C672
A1468	C1407	A1282	C1222	A1162	C1162	G1102	G1041	A979	A856	A795	G795	G795	G673
U1469	A1408	G1284	G1223	C1163	C1163	C1103	G1042	G980	G858	A796	G796	G796	U674
			A1224	C1164	C1164	G1104	A1043	C981					

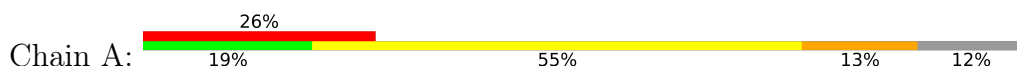


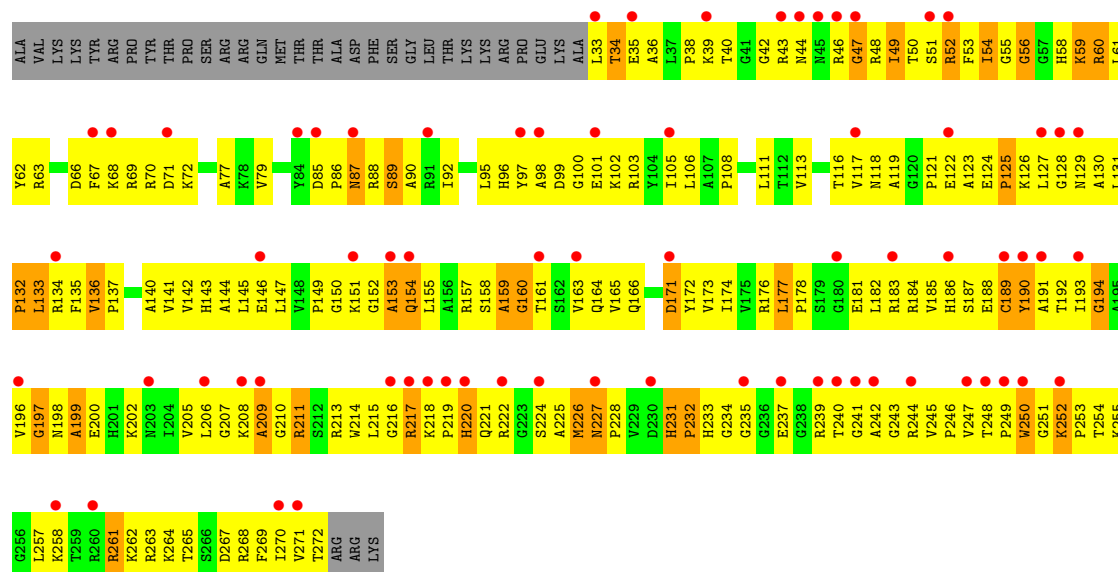


- Molecule 2: ribosomal 5S RNA

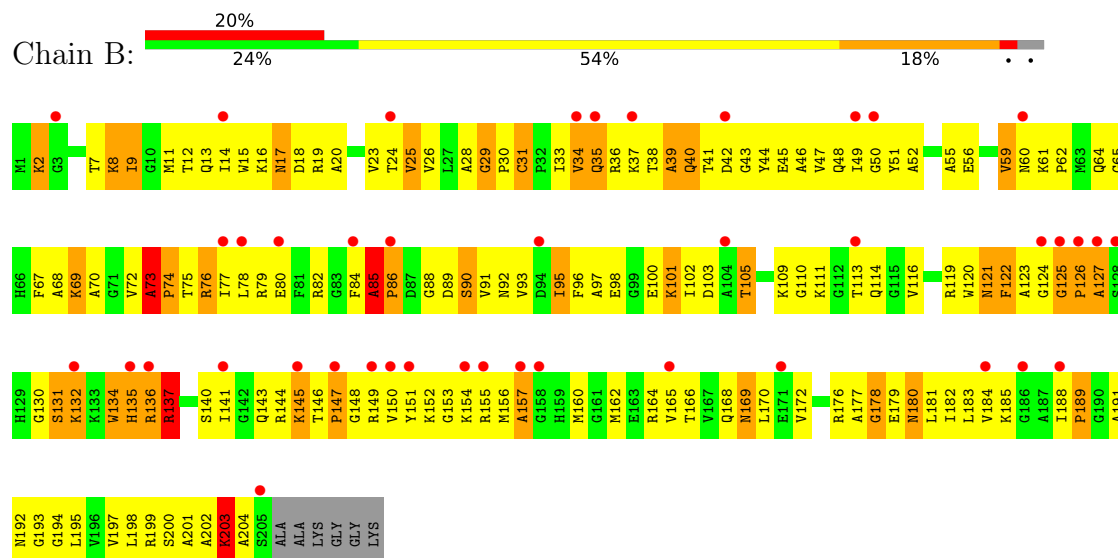


- Molecule 3: 50S ribosomal protein L2

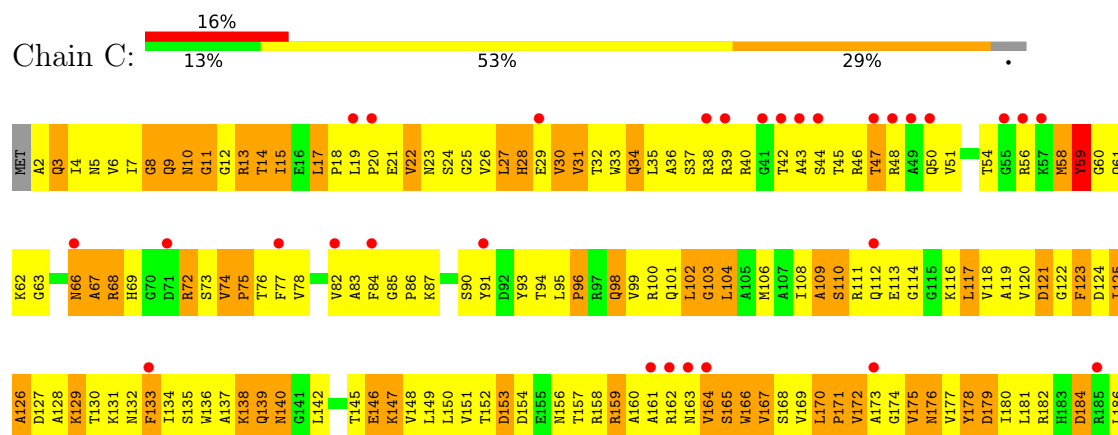


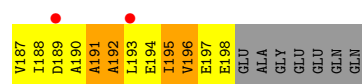


• Molecule 4: 50S ribosomal protein L3

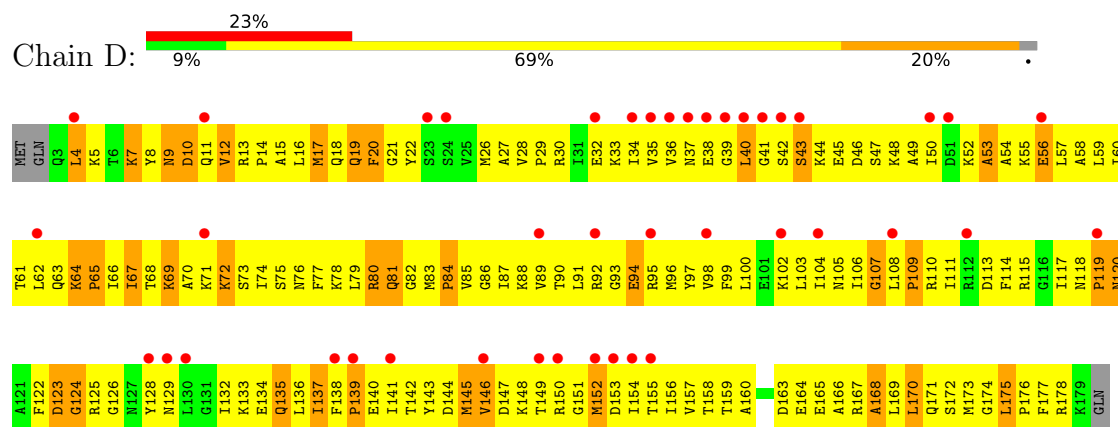


• Molecule 5: 50S ribosomal protein L4

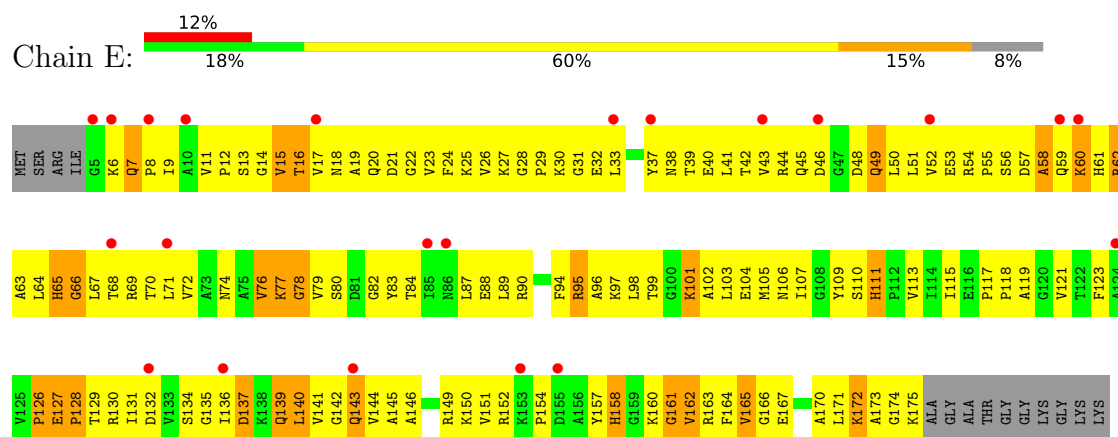




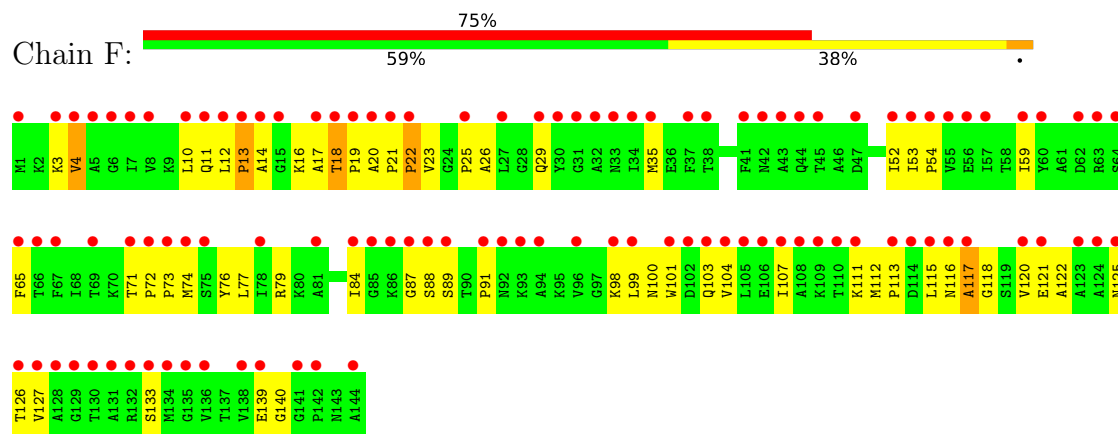
• Molecule 6: 50S ribosomal protein L5



• Molecule 7: 50S ribosomal protein L6

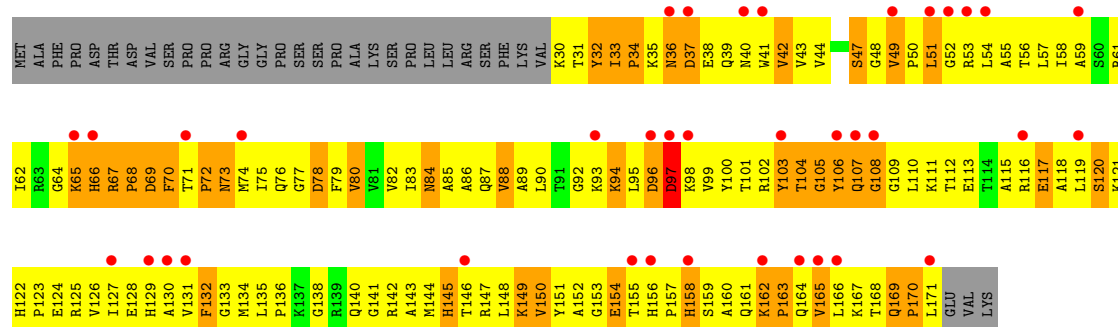


• Molecule 8: 50S ribosomal protein L11

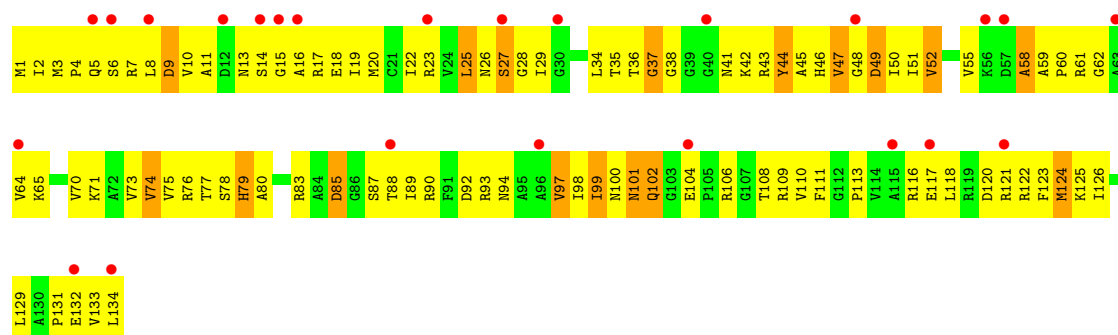


• Molecule 9: 50S ribosomal protein L13

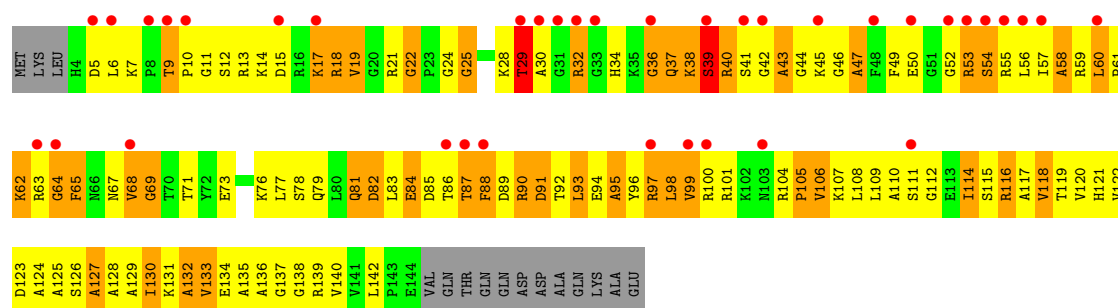
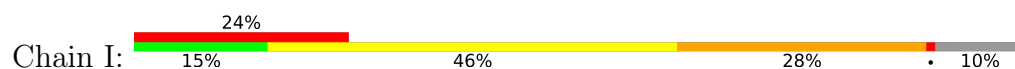




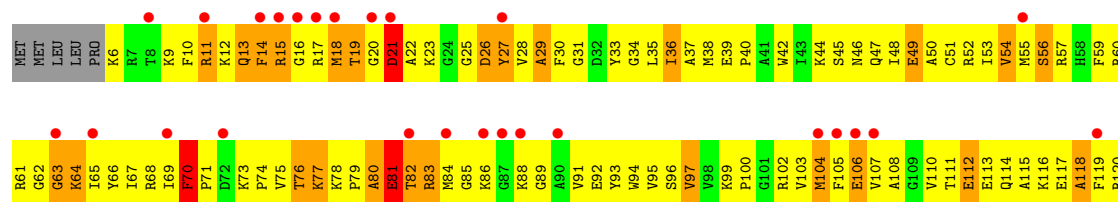
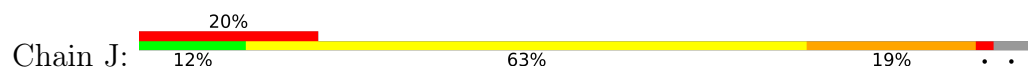
● Molecule 10: 50S ribosomal protein L14

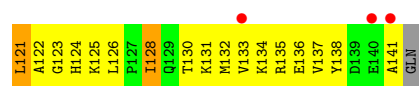


● Molecule 11: 50S ribosomal protein L15

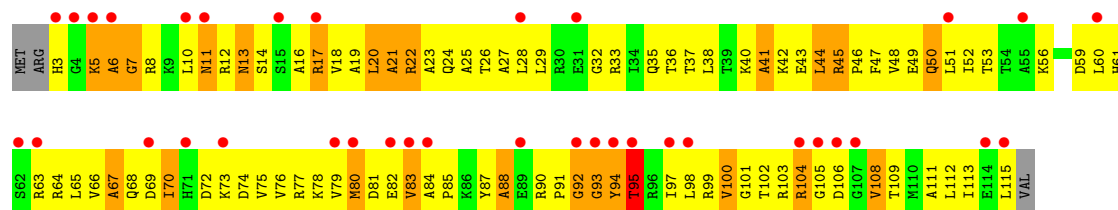
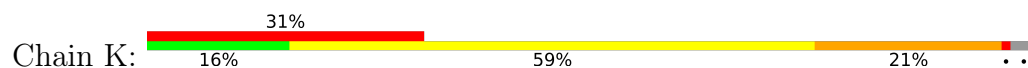


● Molecule 12: 50S ribosomal protein L16

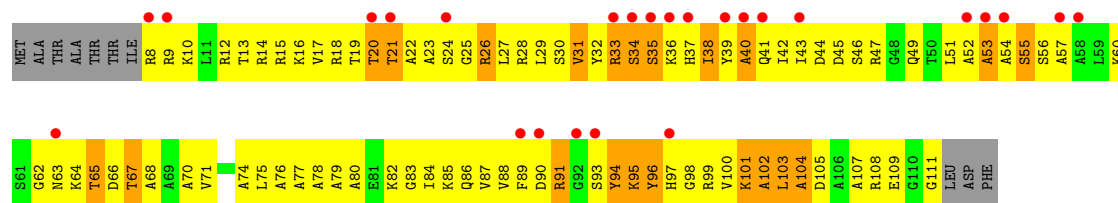
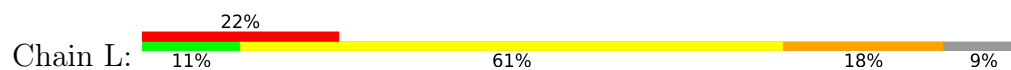




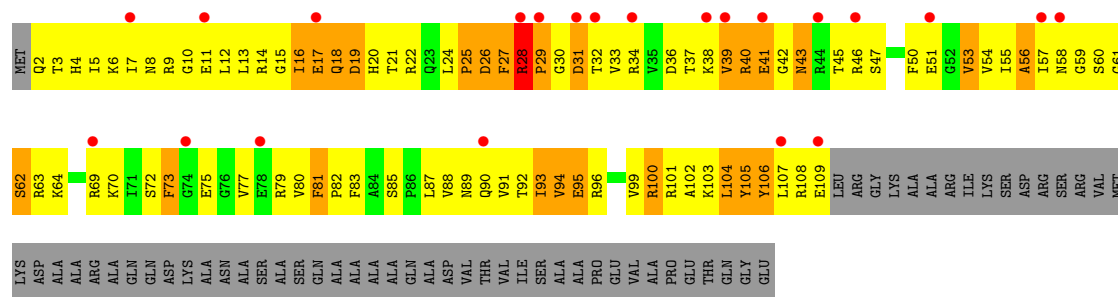
• Molecule 13: 50S ribosomal protein L17



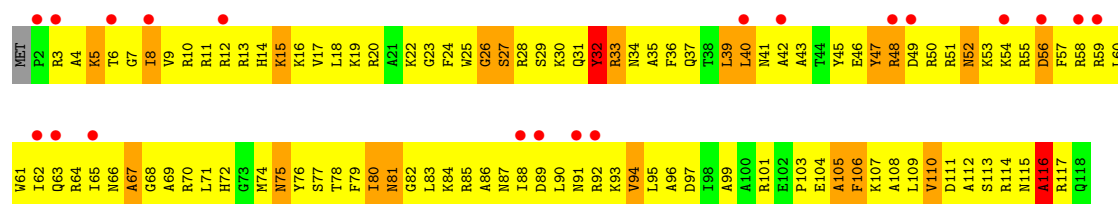
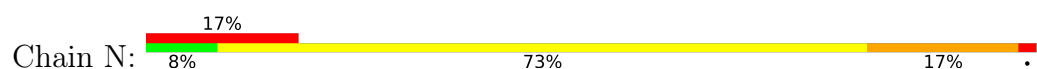
• Molecule 14: 50S ribosomal protein L18



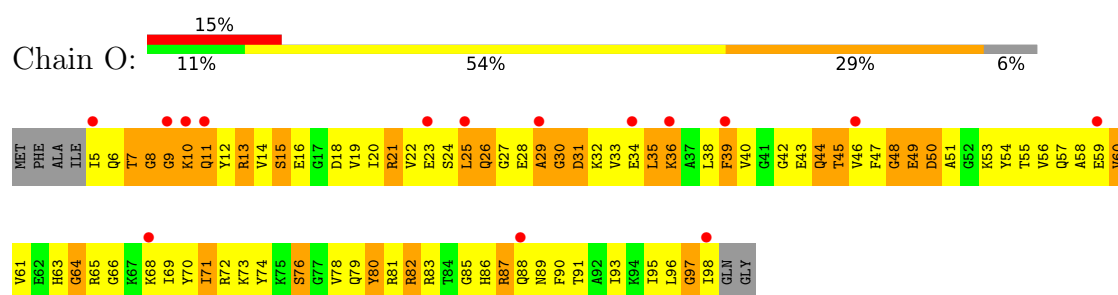
• Molecule 15: 50S ribosomal protein L19



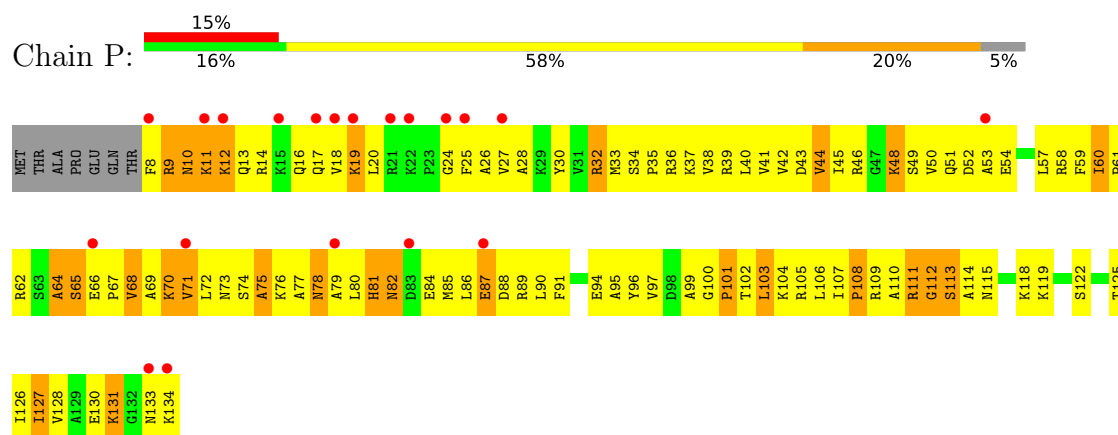
• Molecule 16: 50S ribosomal protein L20



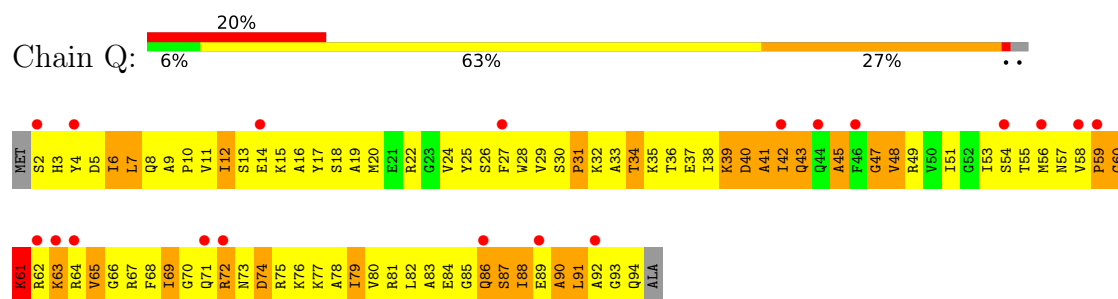
• Molecule 17: 50S ribosomal protein L21



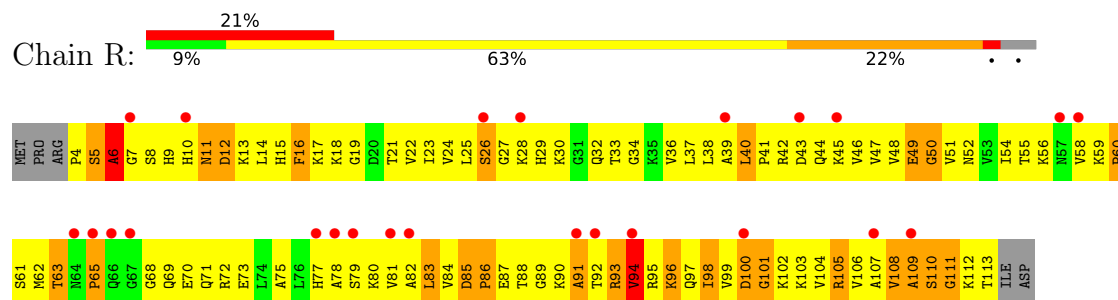
• Molecule 18: 50S ribosomal protein L22



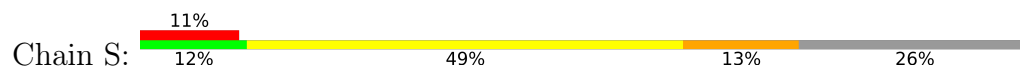
• Molecule 19: 50S ribosomal protein L23

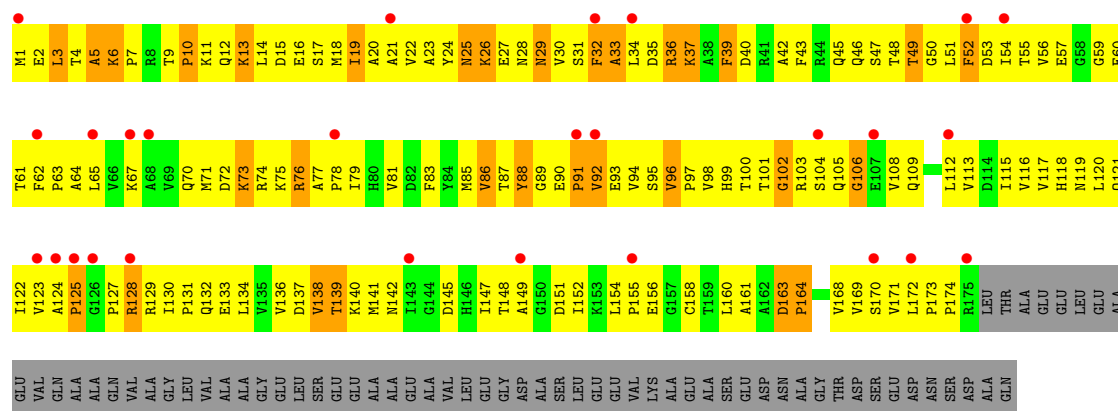


• Molecule 20: 50S ribosomal protein L24

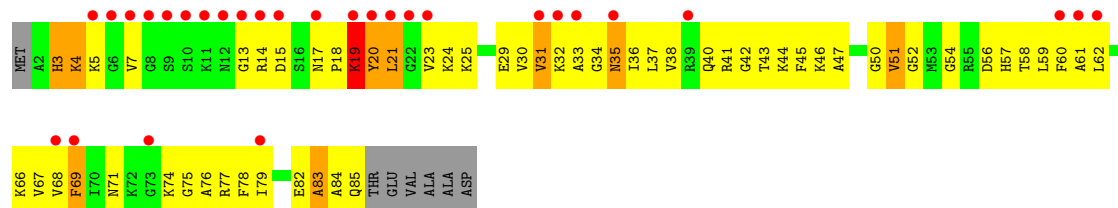


• Molecule 21: 50S ribosomal protein L25

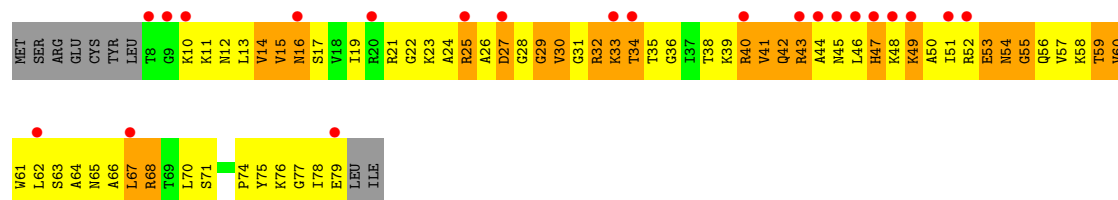
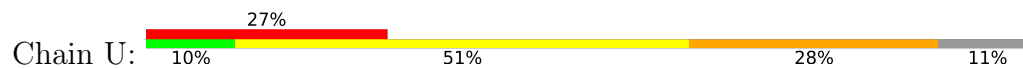




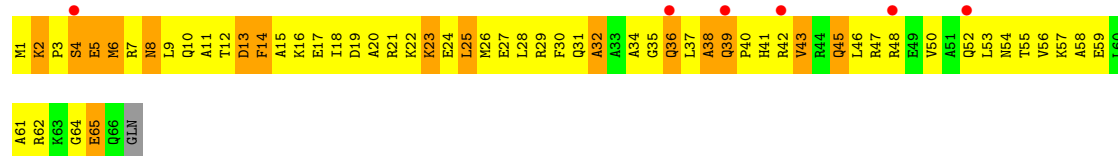
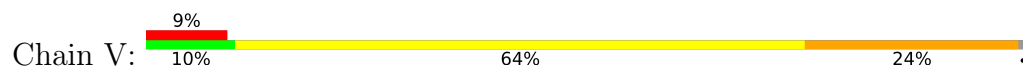
• Molecule 22: 50S ribosomal protein L27



• Molecule 23: 50S ribosomal protein L28

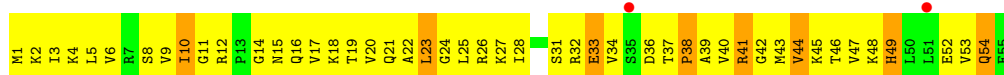


• Molecule 24: 50S ribosomal protein L29

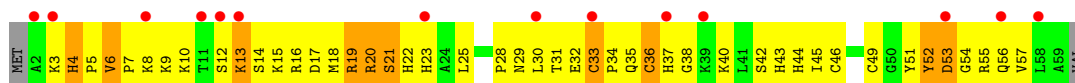


• Molecule 25: 50S ribosomal protein L30

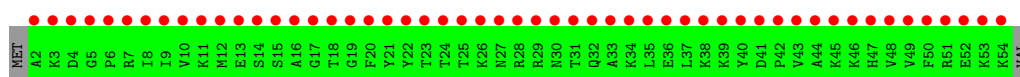




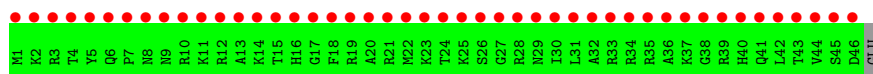
- Molecule 26: 50S ribosomal protein L32



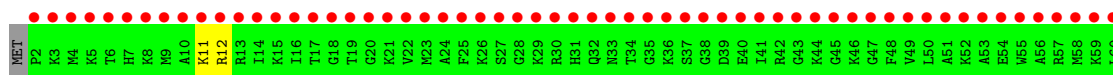
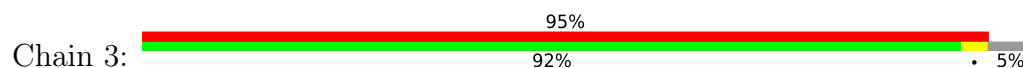
- Molecule 27: 50S ribosomal protein L33



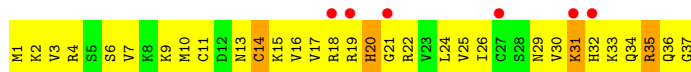
- Molecule 28: 50S ribosomal protein L34



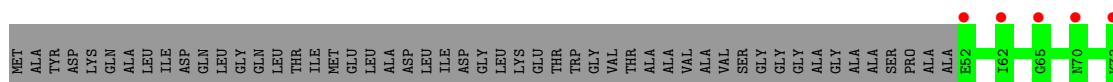
- Molecule 29: 50S ribosomal protein L35

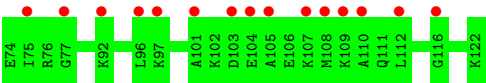


- Molecule 30: 50S ribosomal protein L36



- Molecule 31: 50S ribosomal protein L7/L12





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.90Å 408.90Å 694.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 30.00 – 3.31	Depositor EDS
% Data completeness (in resolution range)	97.8 (30.00-3.30) 97.1 (30.00-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.31Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.302 , 0.339 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	73.4	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	84395	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	X	0.61	4/64561 (0.0%)	1.05	457/100708 (0.5%)
2	Y	0.44	0/2904	0.79	2/4525 (0.0%)
3	A	0.73	1/1862 (0.1%)	1.24	17/2510 (0.7%)
4	B	0.95	0/1567	1.38	26/2105 (1.2%)
5	C	0.76	0/1529	1.27	21/2070 (1.0%)
6	D	0.69	0/1419	1.15	12/1903 (0.6%)
7	E	0.68	0/1308	1.22	9/1771 (0.5%)
8	F	0.28	0/1062	0.70	0/1440
9	G	0.79	0/1138	1.42	20/1539 (1.3%)
10	H	1.04	0/1007	1.34	13/1352 (1.0%)
11	I	0.78	1/1081 (0.1%)	1.33	12/1448 (0.8%)
12	J	0.82	1/1113 (0.1%)	1.29	18/1486 (1.2%)
13	K	1.15	2/886 (0.2%)	1.38	15/1188 (1.3%)
14	L	0.64	0/785	1.23	6/1048 (0.6%)
15	M	0.94	1/884 (0.1%)	1.44	16/1186 (1.3%)
16	N	0.76	0/994	1.18	9/1323 (0.7%)
17	O	0.71	1/750 (0.1%)	1.13	5/1000 (0.5%)
18	P	1.02	0/1027	1.36	12/1373 (0.9%)
19	Q	0.82	1/737 (0.1%)	1.30	12/988 (1.2%)
20	R	0.75	0/835	1.36	10/1121 (0.9%)
21	S	0.69	0/1370	1.17	10/1862 (0.5%)
22	T	0.72	0/633	1.15	3/838 (0.4%)
23	U	0.76	0/556	1.35	7/741 (0.9%)
24	V	0.63	0/537	1.13	6/714 (0.8%)
25	W	0.70	0/426	1.17	4/568 (0.7%)
26	Z	0.82	0/469	1.33	5/629 (0.8%)
30	4	0.68	0/298	1.08	0/390
All	All	0.66	12/91738 (0.0%)	1.10	727/137826 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	2	281
2	Y	0	2
5	C	0	1
9	G	0	1
16	N	0	1
17	O	0	1
22	T	0	1
All	All	2	288

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1056	U	O5'-C5'	6.84	1.52	1.42
13	K	80	MET	SD-CE	-6.52	1.63	1.79
1	X	557	U	C1'-N1	6.25	1.56	1.47
1	X	2322	U	O5'-C5'	6.10	1.51	1.42
13	K	94	TYR	CA-C	-6.09	1.45	1.52

The worst 5 of 727 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1055	A	N9-C1'-C2'	-26.43	72.36	112.00
1	X	557	U	N1-C1'-C2'	17.00	139.50	114.00
1	X	417	C	N1-C1'-C2'	15.49	137.24	114.00
1	X	1975	G	C2'-C3'-O3'	14.32	130.99	109.50
9	G	69	ASP	N-CA-C	-11.66	99.05	113.28

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	X	1278	A	C1'
1	X	2592	U	C1'

5 of 288 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	13	A	Sidechain
1	X	15	G	Sidechain
1	X	29	U	Sidechain
1	X	43	A	Sidechain
1	X	59	G	Sidechain

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	57651	0	29046	4361	0
2	Y	2598	0	1328	183	0
3	A	1826	0	1885	389	0
4	B	1539	0	1600	254	0
5	C	1506	0	1525	372	0
6	D	1400	0	1481	417	0
7	E	1286	0	1336	252	0
8	F	1043	0	1088	71	0
9	G	1114	0	1144	294	0
10	H	997	0	1046	174	1
11	I	1067	0	1103	296	0
12	J	1090	0	1125	279	0
13	K	878	0	930	139	1
14	L	779	0	820	234	0
15	M	871	0	894	196	0
16	N	978	0	1020	246	0
17	O	741	0	756	206	0
18	P	1014	0	1096	193	0
19	Q	726	0	753	168	0
20	R	825	0	881	274	0
21	S	1345	0	1372	286	0
22	T	625	0	655	105	0
23	U	552	0	604	211	0
24	V	533	0	558	94	0
25	W	424	0	470	87	0
26	Z	457	0	464	82	0
27	1	53	0	0	0	0
28	2	46	0	0	0	0
29	3	63	0	0	2	0
30	4	297	0	330	70	0
31	5	71	0	0	0	0
All	All	84395	0	55310	9121	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 66.

The worst 5 of 9121 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1854:G:O2'	1:X:1855:G:H5'	1.31	1.28
1:X:2195:C:C5	1:X:2196:U:C5	2.22	1.28
1:X:729:A:H2'	1:X:730:C:O4'	1.19	1.25
1:X:2196:U:H2'	1:X:2197:U:C6	1.74	1.21
1:X:731:A:H2'	1:X:732:G:O4'	1.34	1.21

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:125:LYS:NZ	13:K:82:GLU:OE2[8_555]	2.08	0.12

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	A	238/274 (87%)	150 (63%)	62 (26%)	26 (11%)	0	2
4	B	203/211 (96%)	143 (70%)	29 (14%)	31 (15%)	0	1
5	C	195/205 (95%)	89 (46%)	60 (31%)	46 (24%)	0	0
6	D	175/180 (97%)	101 (58%)	44 (25%)	30 (17%)	0	1
7	E	169/185 (91%)	98 (58%)	43 (25%)	28 (17%)	0	1
8	F	142/144 (99%)	113 (80%)	22 (16%)	7 (5%)	1	12
9	G	140/174 (80%)	76 (54%)	35 (25%)	29 (21%)	0	0
10	H	132/134 (98%)	108 (82%)	16 (12%)	8 (6%)	1	9
11	I	139/156 (89%)	63 (45%)	36 (26%)	40 (29%)	0	0
12	J	134/142 (94%)	74 (55%)	39 (29%)	21 (16%)	0	1
13	K	111/116 (96%)	75 (68%)	20 (18%)	16 (14%)	0	1
14	L	102/114 (90%)	52 (51%)	31 (30%)	19 (19%)	0	0
15	M	106/166 (64%)	57 (54%)	32 (30%)	17 (16%)	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	N	115/118 (98%)	68 (59%)	30 (26%)	17 (15%)	0	1
17	O	92/100 (92%)	53 (58%)	14 (15%)	25 (27%)	0	0
18	P	125/134 (93%)	87 (70%)	20 (16%)	18 (14%)	0	1
19	Q	91/95 (96%)	46 (50%)	23 (25%)	22 (24%)	0	0
20	R	108/115 (94%)	57 (53%)	28 (26%)	23 (21%)	0	0
21	S	173/237 (73%)	99 (57%)	43 (25%)	31 (18%)	0	0
22	T	82/91 (90%)	48 (58%)	24 (29%)	10 (12%)	0	1
23	U	70/81 (86%)	35 (50%)	18 (26%)	17 (24%)	0	0
24	V	64/67 (96%)	32 (50%)	19 (30%)	13 (20%)	0	0
25	W	53/55 (96%)	36 (68%)	11 (21%)	6 (11%)	0	2
26	Z	56/60 (93%)	35 (62%)	13 (23%)	8 (14%)	0	1
30	4	35/37 (95%)	23 (66%)	6 (17%)	6 (17%)	0	1
All	All	3050/3391 (90%)	1818 (60%)	718 (24%)	514 (17%)	0	1

5 of 514 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	54	ILE
3	A	59	LYS
3	A	60	ARG
3	A	153	ALA
3	A	154	GLN

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2680/2880 (93%)	704 (26%)	300 (11%)
2	Y	121/122 (99%)	23 (19%)	0
All	All	2801/3002 (93%)	727 (25%)	300 (10%)

5 of 727 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	4	C
1	X	13	A
1	X	14	A
1	X	34	U
1	X	35	G

5 of 300 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	2050	G
1	X	2736	U
1	X	2217	G
1	X	2428	U
1	X	955	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	X	2686/2880 (93%)	1.15	505 (18%) 3 3	11, 57, 103, 131	0
2	Y	122/122 (100%)	1.48	28 (22%) 2 2	29, 80, 102, 108	0
3	A	240/274 (87%)	1.57	71 (29%) 1 1	35, 65, 77, 90	0
4	B	205/211 (97%)	1.33	42 (20%) 2 2	30, 53, 64, 77	0
5	C	197/205 (96%)	1.20	32 (16%) 4 4	38, 60, 71, 83	0
6	D	177/180 (98%)	1.34	42 (23%) 2 1	54, 67, 76, 84	0
7	E	171/185 (92%)	0.95	22 (12%) 7 6	50, 64, 75, 80	0
8	F	144/144 (100%)	2.99	108 (75%) 0 0	0, 0, 83, 88	0
9	G	142/174 (81%)	1.38	37 (26%) 1 1	47, 59, 69, 77	0
10	H	134/134 (100%)	1.41	24 (17%) 3 3	27, 52, 62, 69	0
11	I	141/156 (90%)	1.56	37 (26%) 1 1	40, 63, 75, 83	0
12	J	136/142 (95%)	1.23	29 (21%) 2 2	45, 61, 72, 78	0
13	K	113/116 (97%)	1.57	36 (31%) 1 1	37, 50, 60, 63	0
14	L	104/114 (91%)	1.33	25 (24%) 2 1	52, 63, 73, 78	0
15	M	108/166 (65%)	1.37	22 (20%) 3 2	23, 53, 65, 73	0
16	N	117/118 (99%)	1.28	20 (17%) 4 4	39, 57, 69, 75	0
17	O	94/100 (94%)	1.10	15 (15%) 5 4	42, 61, 72, 79	0
18	P	127/134 (94%)	1.20	20 (15%) 5 4	34, 52, 66, 76	0
19	Q	93/95 (97%)	1.16	19 (20%) 3 2	47, 58, 73, 78	0
20	R	110/115 (95%)	1.31	24 (21%) 2 2	49, 62, 73, 85	0
21	S	175/237 (73%)	1.23	27 (15%) 5 4	55, 65, 76, 87	0
22	T	84/91 (92%)	1.56	29 (34%) 1 1	50, 61, 74, 80	0
23	U	72/81 (88%)	1.50	22 (30%) 1 1	52, 64, 73, 78	0
24	V	66/67 (98%)	0.82	6 (9%) 15 11	54, 63, 75, 81	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	55/55 (100%)	0.65	2 (3%) 46 31	48, 58, 70, 79	0
26	Z	58/60 (96%)	1.52	14 (24%) 2 1	35, 53, 66, 69	0
27	1	53/55 (96%)	16.64	53 (100%) 0 0	53, 61, 68, 71	0
28	2	46/47 (97%)	15.59	46 (100%) 0 0	43, 56, 62, 63	0
29	3	63/66 (95%)	14.60	63 (100%) 0 0	50, 58, 65, 67	0
30	4	37/37 (100%)	1.07	6 (16%) 4 4	52, 63, 71, 76	0
31	5	71/122 (58%)	1.50	20 (28%) 1 1	0, 0, 0, 0	0
All	All	6141/6683 (91%)	1.66	1446 (23%) 2 2	0, 60, 91, 131	0

The worst 5 of 1446 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	1	7	ARG	45.6
27	1	15	SER	32.7
27	1	5	GLY	28.8
29	3	27	SER	27.3
29	3	22	VAL	26.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.