



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 03:15 pm GMT

PDB ID : 2J28
EMDB ID : EMD-1261
Title : MODEL OF E. COLI SRP BOUND TO 70S RNCS
Authors : Halic, M.; Blau, M.; Becker, T.; Mielke, T.; Pool, M.R.; Wild, K.; Sinning, I.; Beckmann, R.
Deposited on : 2006-08-16
Resolution : 8.00 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

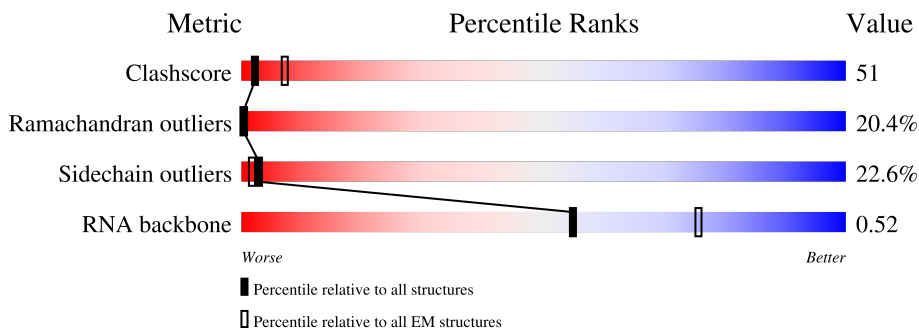
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	56	39% (Poor fit) 9% (0 outliers), 21% (1 outlier), 62% (2+ outliers)
2	1	54	33% (Poor fit) 22% (0 outliers), 43% (1 outlier), 35% (2+ outliers)
3	2	46	52% (Poor fit) 28% (0 outliers), 43% (1 outlier), 20% (2+ outliers), 9% (Not modelled)
4	3	64	52% (Poor fit) 23% (0 outliers), 48% (1 outlier), 25% (2+ outliers), . (Not modelled)
5	4	38	45% (Poor fit) 5% (0 outliers), 42% (1 outlier), 32% (2+ outliers), 21% (Not modelled)
6	7	18	22% (Poor fit) 17% (0 outliers), 83% (1 outlier)
7	8	74	5% (Poor fit) 5% (0 outliers), 73% (1 outlier), 19% (2+ outliers), 5% (Not modelled)

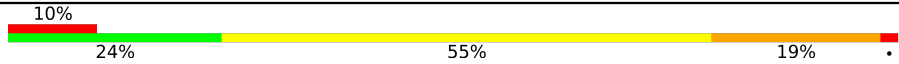
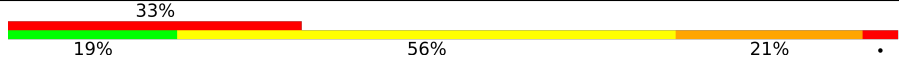
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	9	430	
9	A	117	
10	B	2904	
11	C	267	
12	D	209	
13	E	201	
14	F	178	
15	G	176	
16	H	149	
17	I	141	
18	J	140	
19	K	121	
20	L	144	
21	M	136	
22	N	127	
23	O	117	
24	P	114	
25	Q	117	
26	R	103	
27	S	110	
28	T	99	
29	U	102	
30	V	94	
31	W	84	
32	X	63	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	Y	58	
34	Z	70	

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 95358 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	1	54	441	284	81	76	0	0

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	46	377	228	90	57	2	0	0

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	64	504	323	105	74	2	0	0

- Molecule 5 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	38	302	185	65	48	4	0	0

- Molecule 6 is a protein called SIGNAL SEQUENCE.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	7	18	149	103	23	23	0	0

- Molecule 7 is a RNA chain called 4.5S SIGNAL RECOGNITION PARTICLE RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	74	Total	C	N	O	P	0	0
			1590	709	295	512	74		

- Molecule 8 is a protein called SIGNAL RECOGNITION PARTICLE 54.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	430	Total	C	N	O	S	0	0
			3306	2072	595	617	22		

- Molecule 9 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 10 is a RNA chain called 23S RIBOSOMAL RNA.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	267	Total	C	N	O	S	0	0
			2053	1271	416	359	7		

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L6.

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

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L9.

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

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L11.

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

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	J	140	1112	704	210	194	4	0	0

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	L	144	1053	654	207	190	2	0	0

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	N	127	1008	621	204	178	5	0	0

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	O	117	900	557	179	163	1	0	0

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	T	99	777	491	145	139	2	0	0

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	W	84	634	391	129	113	1	0	0

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	X	63	509	313	99	95	2	0	0

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Y	58	449	281	87	79	2	0	0

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Z	70	549	339	104	100	6	0	0

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	B	110	Total 110	Mg 110	0
35	N	1	Total 1	Mg 1	0

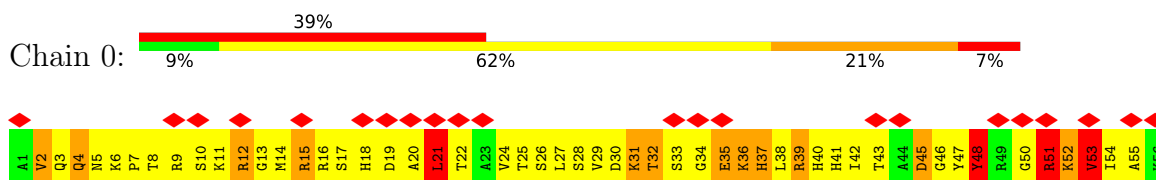
- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
36	B	506	Total 506	O 506	0
36	N	6	Total 6	O 6	0

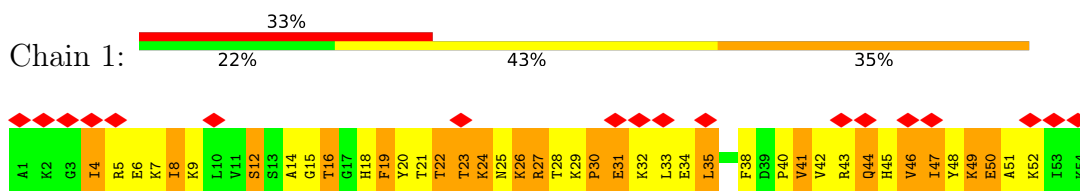
3 Residue-property plots [i](#)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

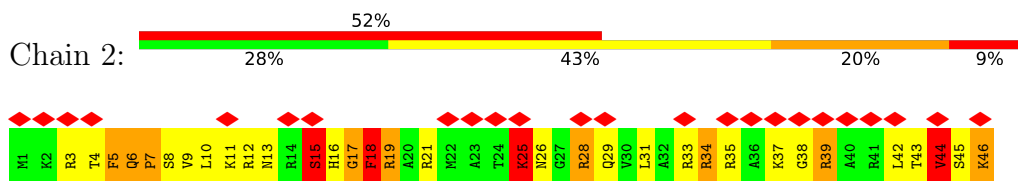
- Molecule 1: 50S RIBOSOMAL PROTEIN L32



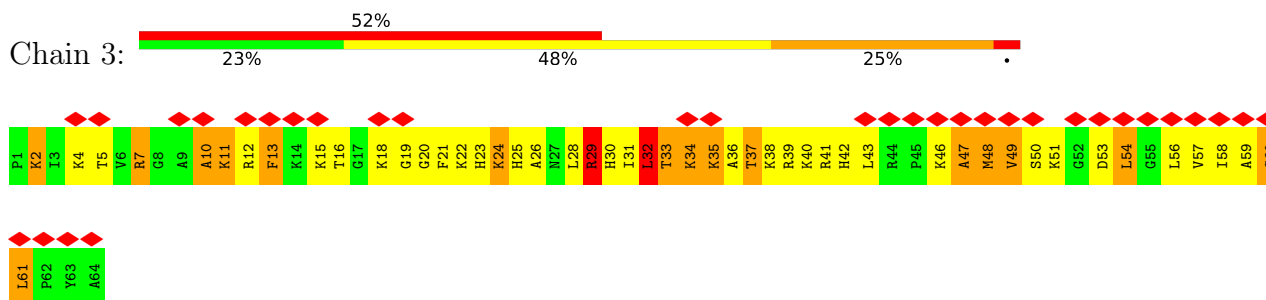
- Molecule 2: 50S RIBOSOMAL PROTEIN L33



- Molecule 3: 50S RIBOSOMAL PROTEIN L34

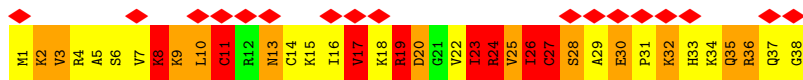


- Molecule 4: 50S RIBOSOMAL PROTEIN L35

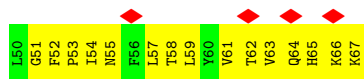


- Molecule 5: 50S RIBOSOMAL PROTEIN L36

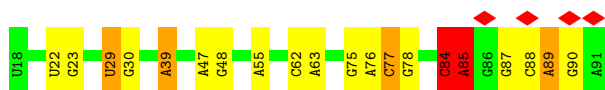




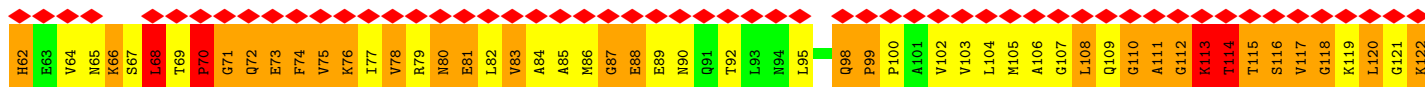
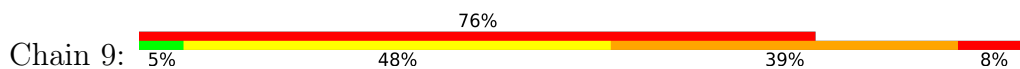
• Molecule 6: SIGNAL SEQUENCE



• Molecule 7: 4.5S SIGNAL RECOGNITION PARTICLE RNA



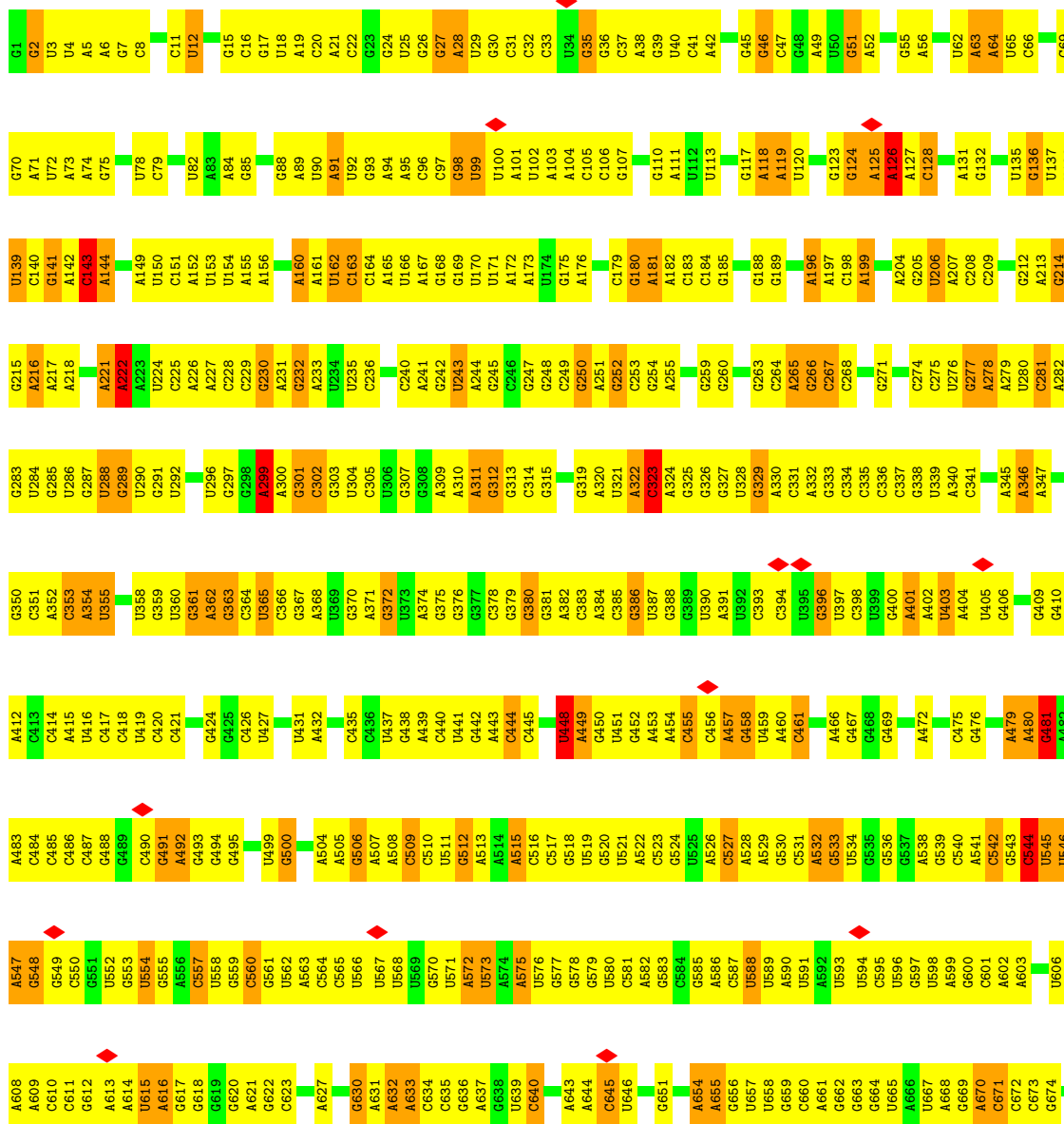
• Molecule 8: SIGNAL RECOGNITION PARTICLE 54



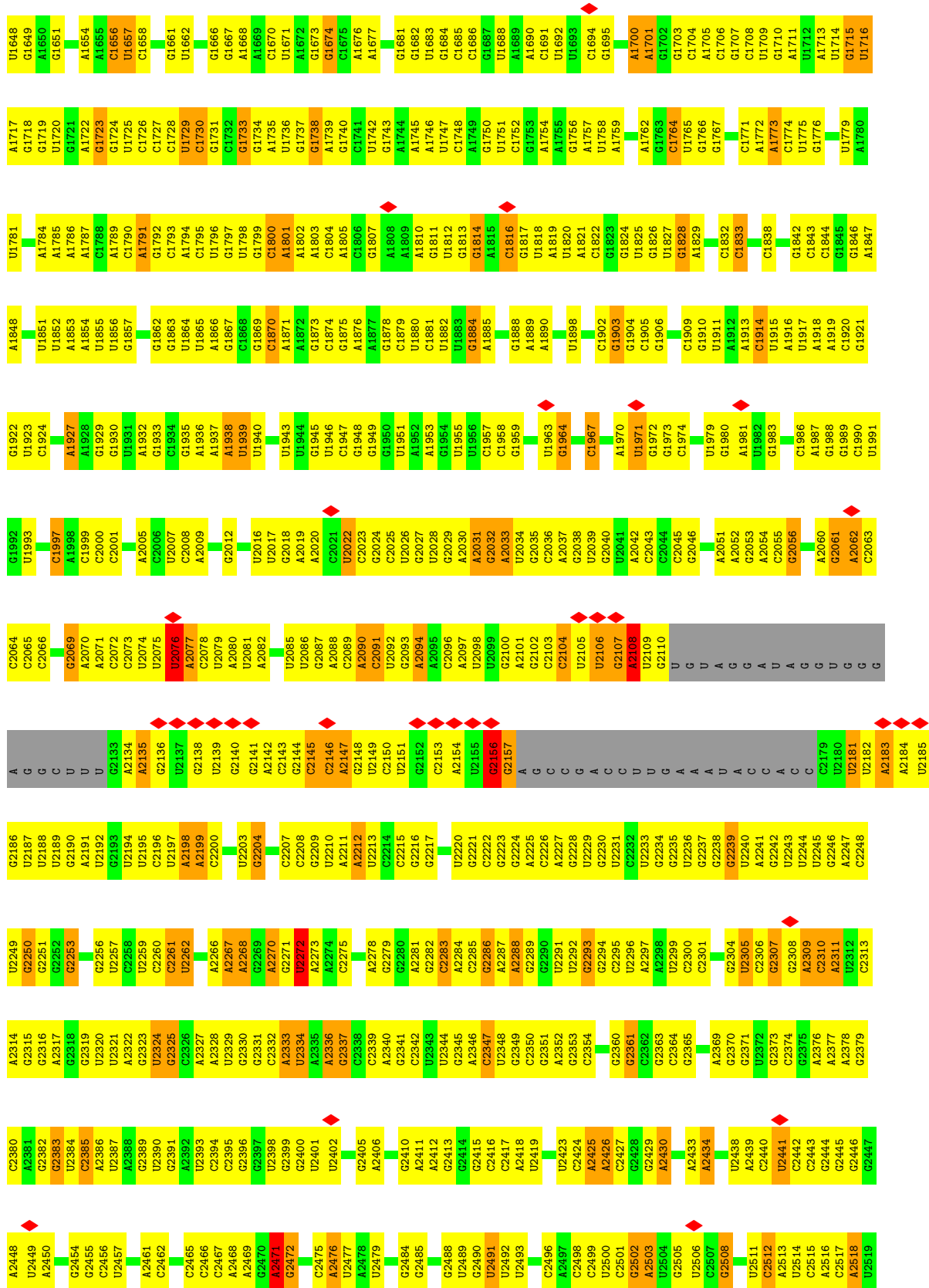
• Molecule 9: 5S RIBOSOMAL RNA

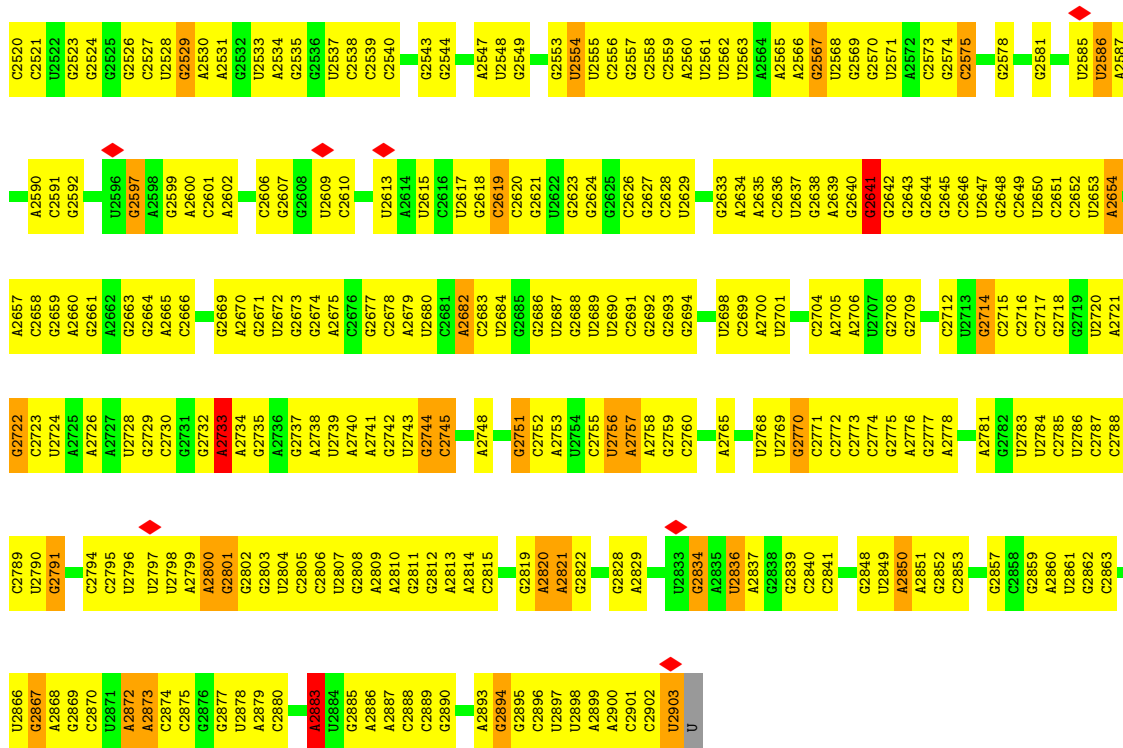


• Molecule 10: 23S RIBOSOMAL RNA

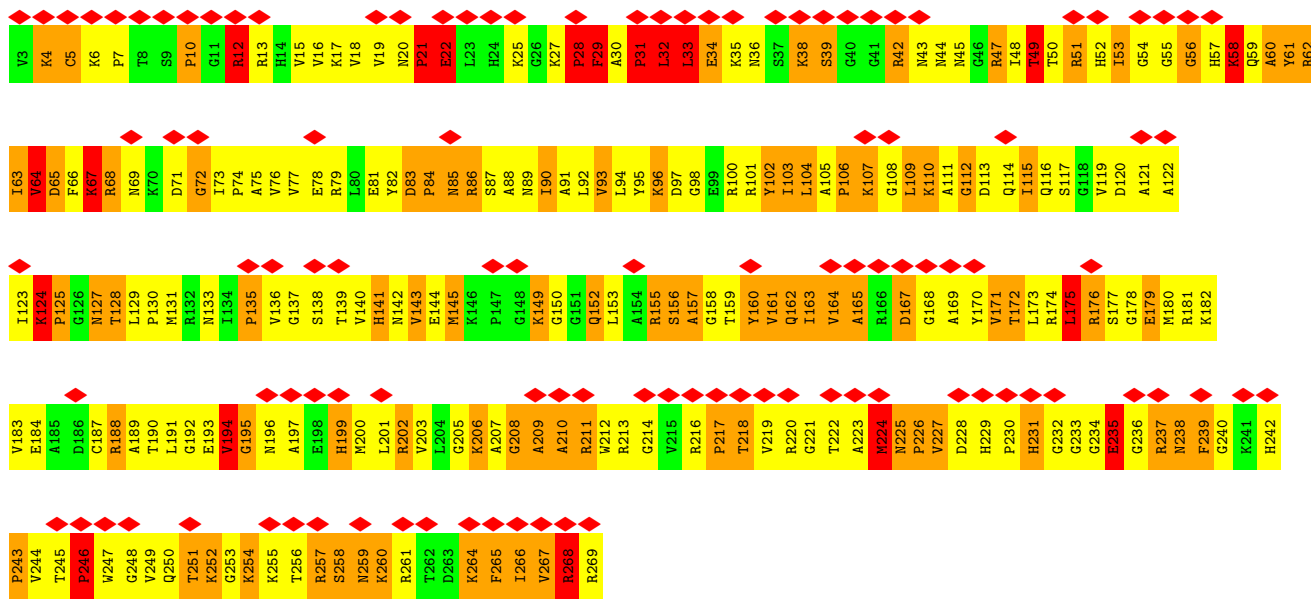


A1572	A1508	U1438	A1365	C1298	G1237	C1170	G1106	A1027	C961	A899	C838	G763	C678
G1573	A1509	A1489	G1368	G1289	G1238	G1171	G1107	A1028	G962	A900	U839	U763	C679
C1574	G1510	U1440	G1300	G1300	U1239	A1172	U1108	A1029	U963	C901	C841	A764	C680
U1578	G1511	G1441	A1301	A1301	U1240	U1173	C1109	C1030	C964	C902	G841	C765	G681
U1512	U1543	U1442	A1302	G1303	A1241	U1174	G1110	U1033	C985	G903	U843	U766	G682
G1514	G1514	G1444	A1304	A1304	U1242	A1175	A1111	G1034	G966	G904	A844	G770	A885
A1515	G1445	U1375	C1305	C1305	A1244	U1176	G1112	G1046	U967	A905	U871	G771	U886
G1516	C1446	U1376	G1309	G1309	A1245	C1177	U1113	G1042	C968	U906	A845	G772	C887
U1517	C1447	G1377	G1310	G1310	A1246	U1178	C1114	C1043	G969	G907	U846	G773	U688
C1518	G1448	G1378	U1311	U1311	A1247	U1180	G1115	U1046	U970	A908	U847	G774	U689
G1524	G1449	U1379	G1312	G1312	U1248	U1181	C1117	A1046	G971	A910	U848	G775	G690
A1525	G1380	U1380	U1312	U1312	U1249	C1182	C1118	G1047	A972	A911	U850	G776	C691
G1526	G1381	G1381	U1313	U1313	G1250	U1183	U1119	A1057	A973	C912	C851	G777	C692
A1527	A1382	G1382	C1314	C1314	C1251	U1184	U1120	U1058	G974	U913	U852	G778	A699
U1528	A1383	G1383	C1315	C1315	G1252	U1185	C1121	G1059	A975	U914	C853	U779	A699
A1529	C1384	U1384	U1316	U1316	A1253	U1186	G1122	U1060	G976	C915	C854	G780	G700
C1592	G1455	G1385	G1317	G1317	G1255	U1188	C1123	A1067	A981	G916	G855	A781	G704
U1593	C1456	U1386	U1318	U1318	G1256	U1189	G1124	U1068	C982	A917	G856	A782	A705
A1594	U1457	A1387	C1319	C1319	G1257	A1190	G1125	U1069	A983	U918	G857	A783	U709
C1595	U1488	G1388	C1320	C1320	U1258	U1191	A1126	U1070	A984	U919	G858	A784	U710
U1599	G1459	U1394	A1321	A1321	G1259	U1192	U1127	U1071	C987	A920	U859	A785	U710
U1540	U1460	A1322	U1322	U1322	A1260	U1193	A1128	U1072	A988	A921	U860	A786	G713
A1545	A1395	C1323	G1324	G1324	C1261	U1194	G1129	U1073	A989	C922	A861	A787	U714
G1601	C1462	U1325	U1325	U1325	U1262	U1195	U1130	U1074	A990	A922	G862	A788	A715
U1602	C1463	U1326	U1326	U1326	U1263	U1196	G1131	U1075	A991	A923	G863	A789	A716
A1603	G1464	U1327	U1327	U1327	U1264	U1197	U1132	U1076	A992	A924	G864	A790	C717
U1606	G1465	A1328	U1328	U1328	A1265	U1198	A1133	U1077	A993	A925	G865	A791	A718
A1608	U1470	U1329	U1329	U1329	U1266	U1199	U1134	U1078	A994	A926	G866	A792	C722
U1609	G1471	U1330	U1330	U1330	U1267	U1200	C1135	U1079	A1000	A927	G867	A793	U724
A1610	U1474	C1331	G1332	G1332	A1268	U1201	G1136	U1080	A1001	U928	G868	A794	G725
G1611	U1475	U1332	U1332	U1332	C1270	U1202	G1137	U1081	A1002	A931	U870	A795	C726
G1612	U1476	G1333	G1333	G1333	G1271	U1203	U1138	U1082	C1005	U932	U871	A796	U720
G1613	U1477	U1334	U1334	U1334	A1272	A1204	C1139	U1083	C1006	A933	C806	A797	A721
A1616	G1478	U1335	C1335	C1335	U1273	U1205	C1140	U1084	C1007	A934	C807	A798	C723
C1617	U1479	U1336	U1336	U1336	A1274	G1206	U1141	U1085	C1008	A935	U810	A799	A730
A1618	U1480	G1337	U1337	U1337	A1275	U1210	A1142	U1086	A1009	A936	G874	A819	A730
G1622	U1481	U1341	G1341	G1341	U1276	C1211	U1143	U1087	A1010	U937	G875	A819	A730
G1623	U1482	A1342	A1342	A1342	G1277	U1212	C1144	U1088	A1011	A940	G876	A819	A730
U1624	G1483	U1343	U1343	U1343	C1278	A1213	C1146	U1089	A1012	G941	G877	A819	A730
C1625	U1484	U1344	U1344	U1344	G1279	U1214	A1147	U1090	A1013	A942	G878	A819	A730
G1633	U1485	G1345	G1345	G1345	U1280	G1215	U1148	U1091	A1014	A943	G879	A819	A730
A1634	U1486	U1346	U1346	U1346	G1281	G1216	C1149	U1092	A1015	A944	G880	A819	A730
A1635	U1487	A1347	A1347	A1347	U1282	U1219	C1150	U1093	A1016	C944	G881	A819	A730
A1636	C1488	C1348	C1348	C1348	U1283	U1220	A1151	U1094	A1017	A945	G882	A819	A730
A1637	U1489	U1349	U1349	U1349	A1284	C1152	C1152	U1095	A1018	C946	G883	A819	A730
A1638	U1490	C1351	C1351	C1351	A1285	C1153	C1153	U1096	A1019	U947	G884	A819	A730
A1639	C1493	U1352	U1352	U1352	A1286	U1221	G1154	U1097	A1020	A948	G885	A819	A730
A1640	U1494	G1353	G1353	G1353	U1287	G1222	U1155	U1098	A1021	G950	G886	A819	A730
A1641	A1495	U1354	U1354	U1354	A1288	U1225	A1156	U1099	A1022	C951	G887	A819	A730
A1642	U1496	G1355	G1355	G1355	C1289	G1227	C1162	U1100	A1023	C952	G888	A819	A730
G1642	A1496	U1356	U1356	U1356	U1291	U1228	G1163	U1101	A1024	G955	G889	A819	A730
G1645	U1504	A1359	A1359	A1359	G1292	G1229	U1164	U1102	A1025	U956	G890	A819	A730
A1646	A1505	C1360	C1360	C1360	C1293	U1230	G1165	U1103	A1026	C957	G891	A819	A730
A1570	U1506	G1361	G1361	G1361	U1294	A1230	G1166	U1104	A1027	U958	G892	A819	A730
U1647	C1507	C1362	C1362	C1362	G1295	A1231	G1167	U1105	A1028	A959	G893	A819	A730
		G1363	G1363	G1363	U1296	G1232	U1168			A960	G894	A819	A730
		G1364	G1364	G1364	G1297	G1233	A1169				G895	A819	A730

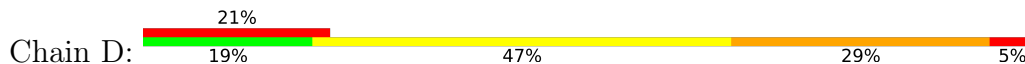


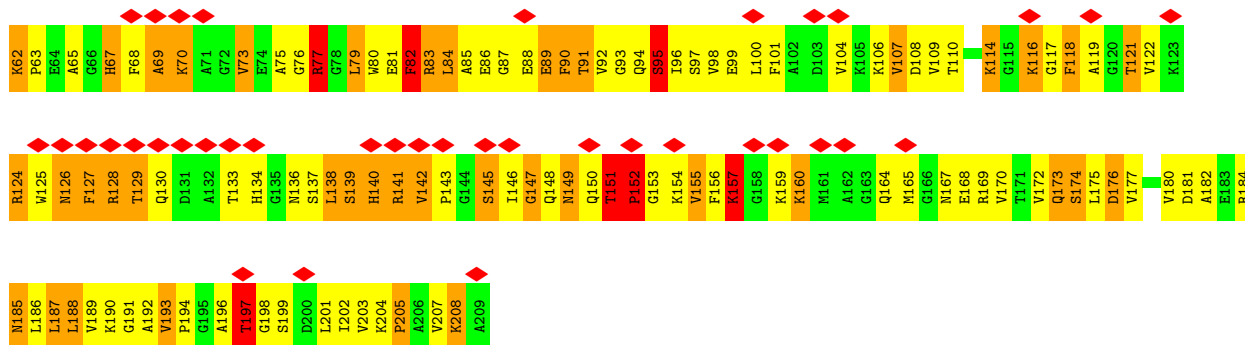


• Molecule 11: 50S RIBOSOMAL PROTEIN L2

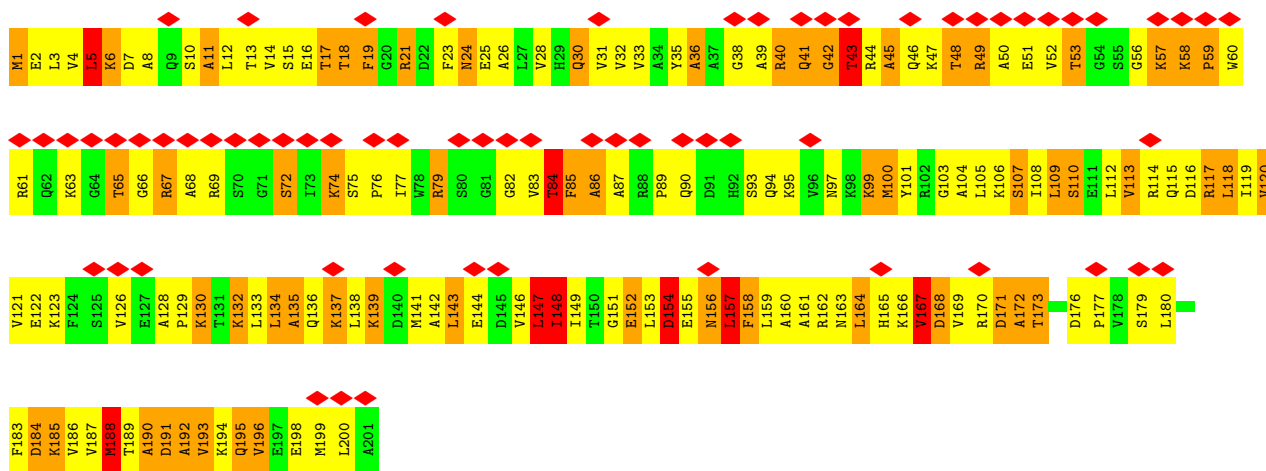
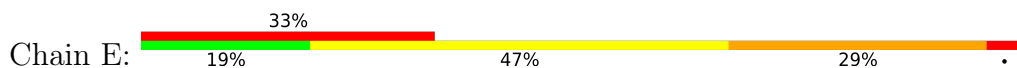


• Molecule 12: 50S RIBOSOMAL PROTEIN L3

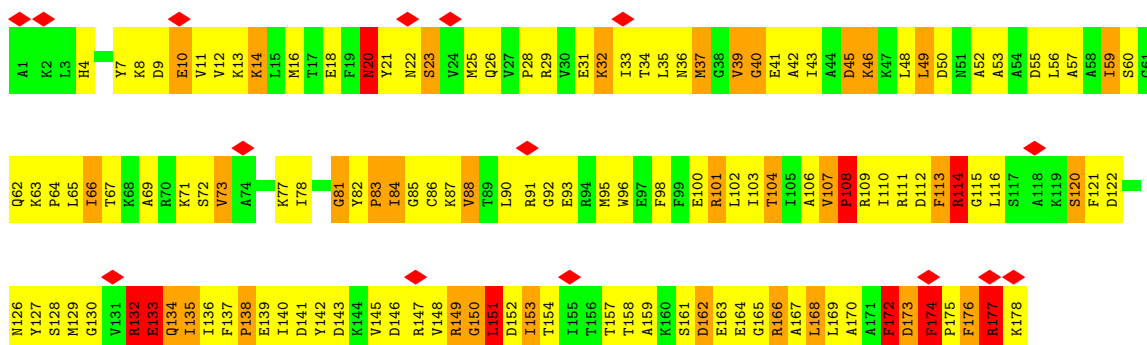




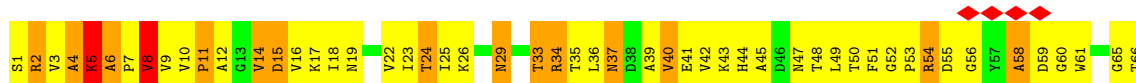
• Molecule 13: 50S RIBOSOMAL PROTEIN L4

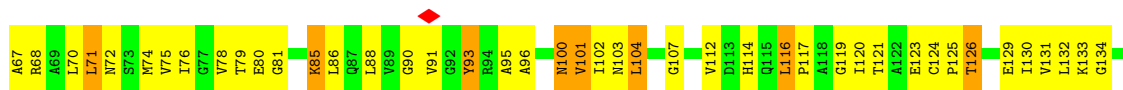


• Molecule 14: 50S RIBOSOMAL PROTEIN L5

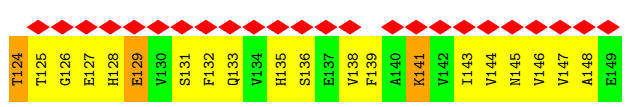
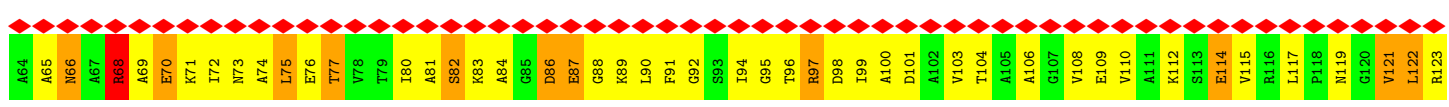
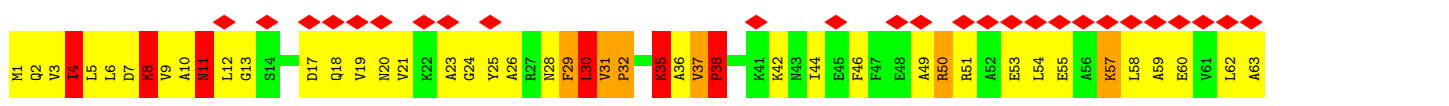
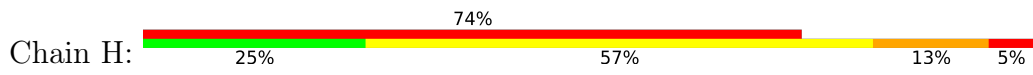


• Molecule 15: 50S RIBOSOMAL PROTEIN L6

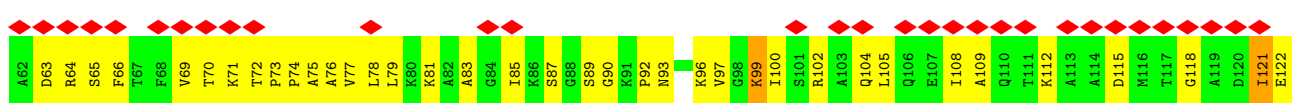
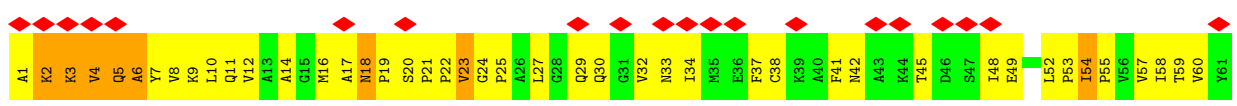




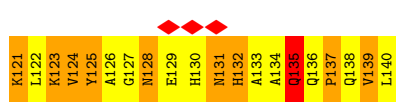
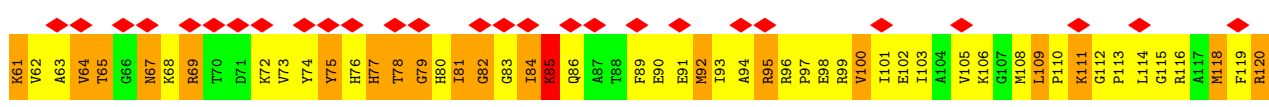
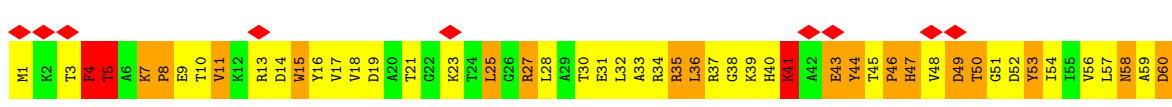
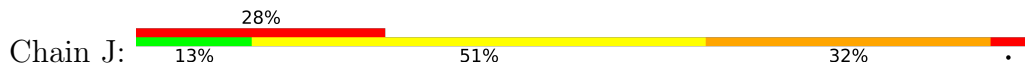
• Molecule 16: 50S RIBOSOMAL PROTEIN L9



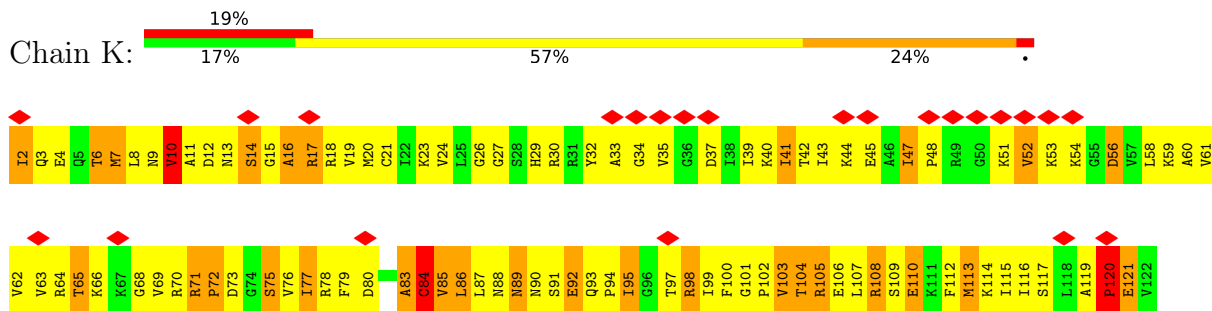
• Molecule 17: 50S RIBOSOMAL PROTEIN L11



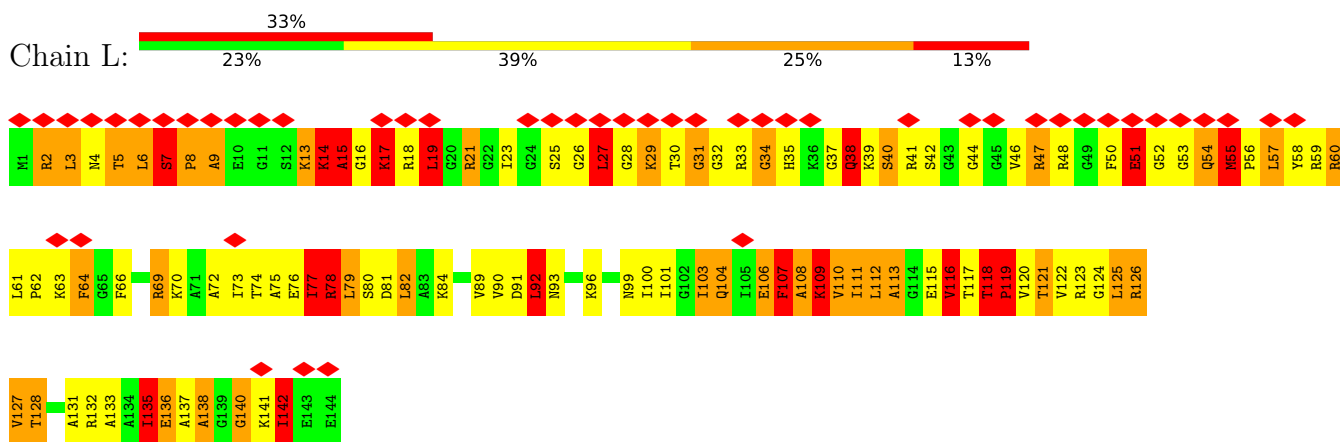
• Molecule 18: 50S RIBOSOMAL PROTEIN L13



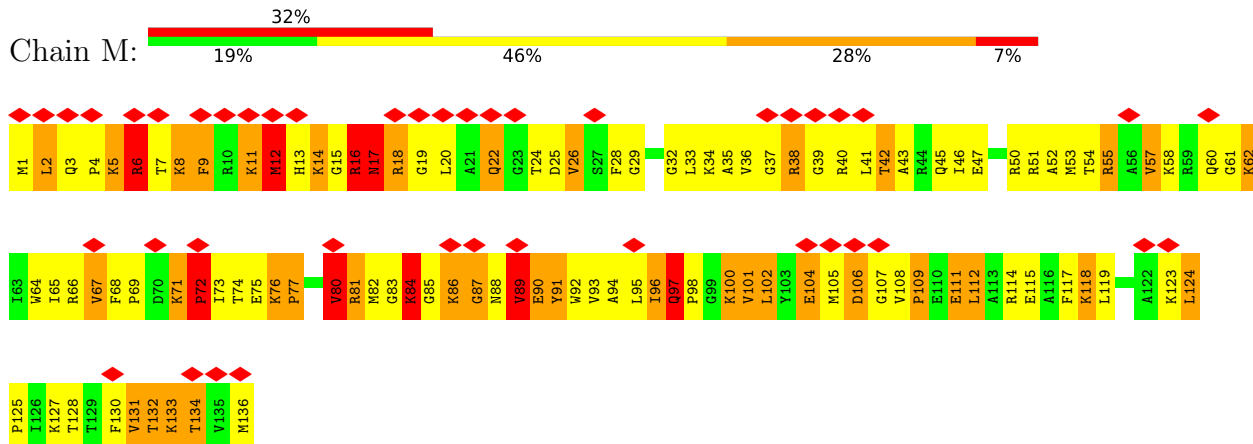
• Molecule 19: 50S RIBOSOMAL PROTEIN L14



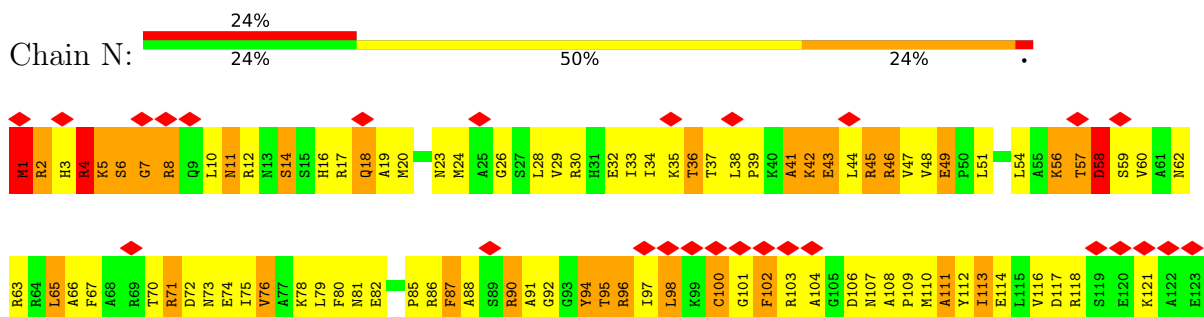
• Molecule 20: 50S RIBOSOMAL PROTEIN L15



• Molecule 21: 50S RIBOSOMAL PROTEIN L16

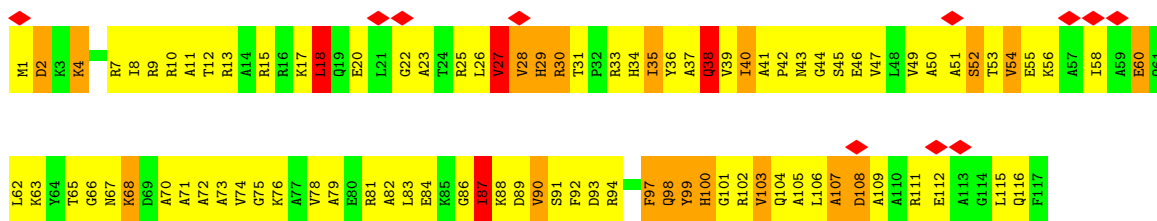


• Molecule 22: 50S RIBOSOMAL PROTEIN L17

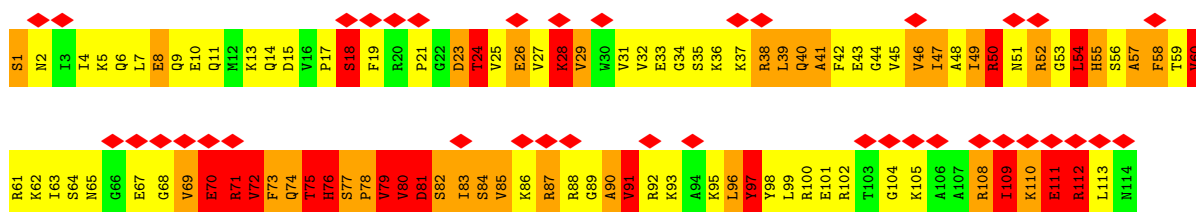




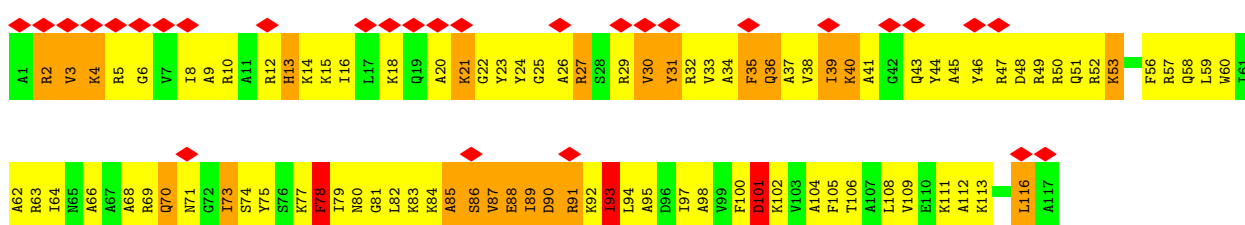
• Molecule 23: 50S RIBOSOMAL PROTEIN L18



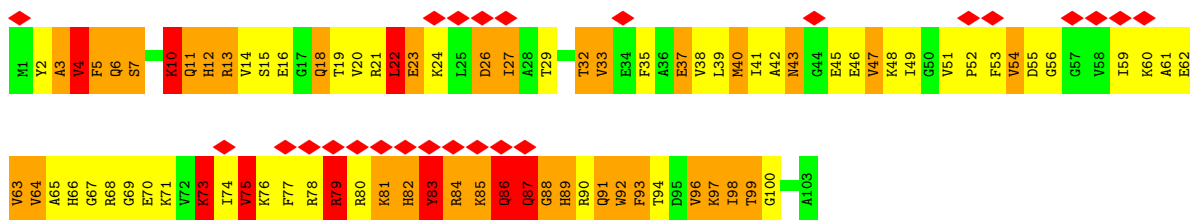
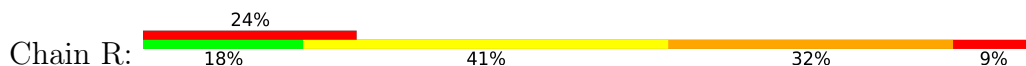
• Molecule 24: 50S RIBOSOMAL PROTEIN L19



• Molecule 25: 50S RIBOSOMAL PROTEIN L20

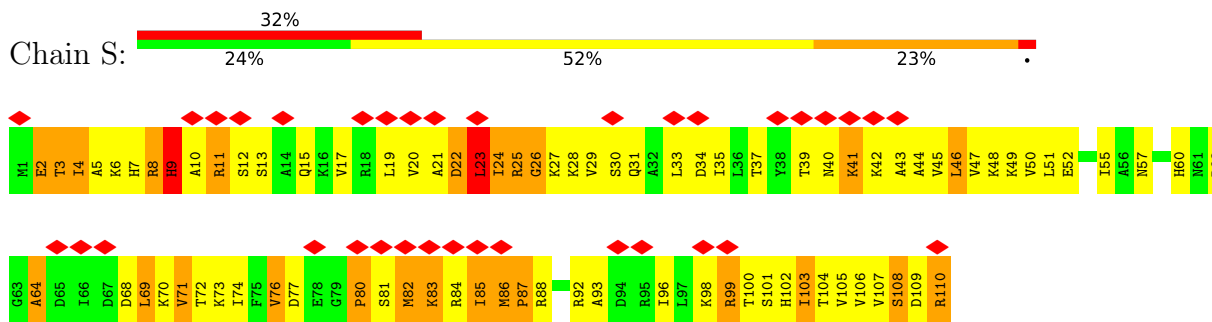


• Molecule 26: 50S RIBOSOMAL PROTEIN L21

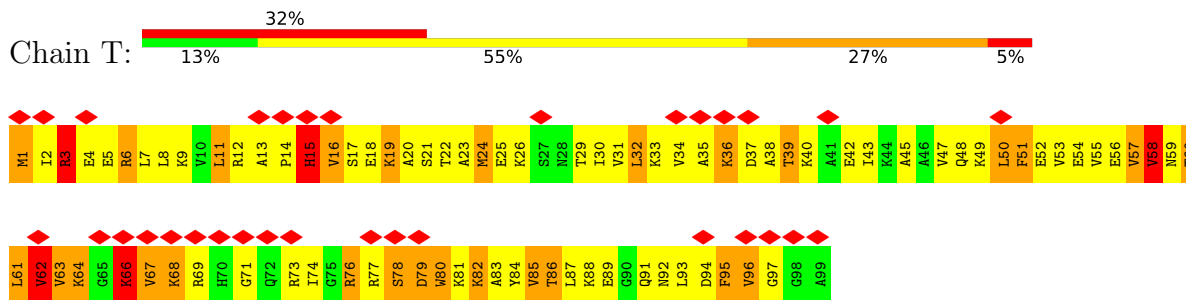


• Molecule 27: 50S RIBOSOMAL PROTEIN L22

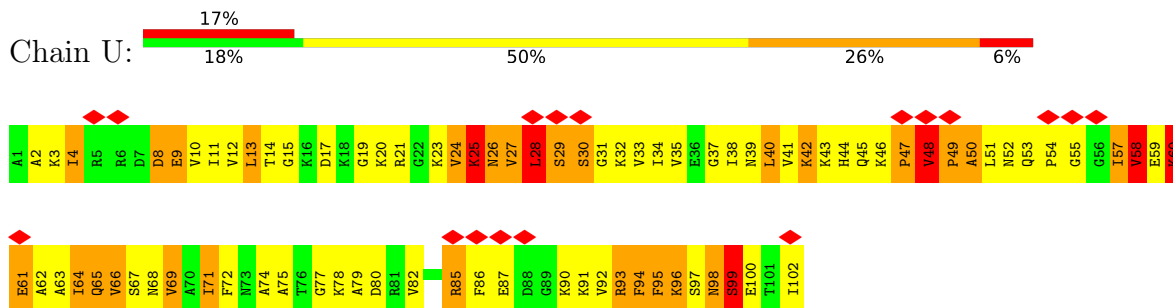




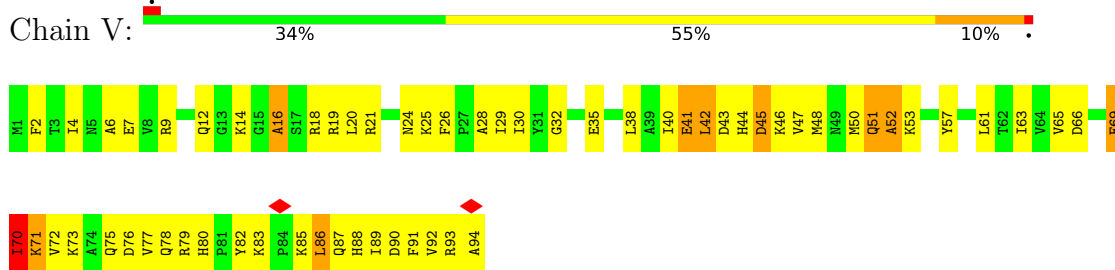
• Molecule 28: 50S RIBOSOMAL PROTEIN L23



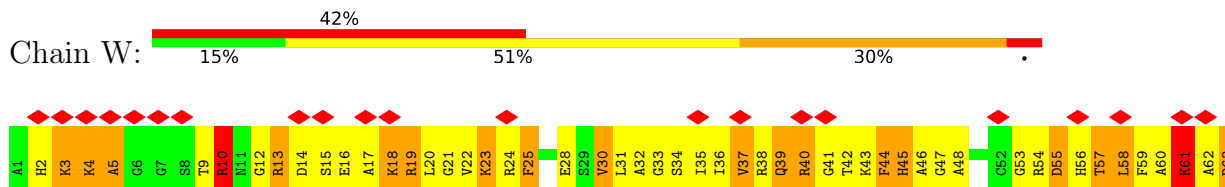
• Molecule 29: 50S RIBOSOMAL PROTEIN L24

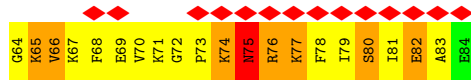


• Molecule 30: 50S RIBOSOMAL PROTEIN L25

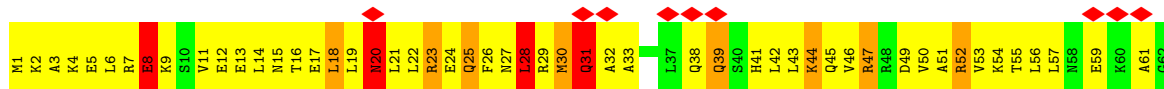


• Molecule 31: 50S RIBOSOMAL PROTEIN L27





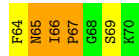
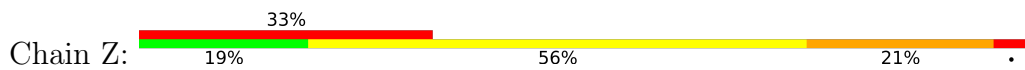
• Molecule 32: 50S RIBOSOMAL PROTEIN L29



• Molecule 33: 50S RIBOSOMAL PROTEIN L30



• Molecule 34: 50S RIBOSOMAL PROTEIN L31



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	Not provided	
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	7.522	Depositor
Minimum map value	-4.419	Depositor
Average map value	0.037	Depositor
Map value standard deviation	0.632	Depositor
Recommended contour level	0.704	Depositor
Map size (\AA)	361.62, 361.62, 361.62	wwPDB
Map dimensions	294, 294, 294	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing (\AA)	1.23, 1.23, 1.23	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0	0.41	0/450	0.97	3/599 (0.5%)
2	1	0.32	0/448	0.69	0/594
3	2	0.30	0/380	0.60	0/498
4	3	0.39	0/513	0.80	1/676 (0.1%)
5	4	0.32	0/303	0.77	0/397
6	7	0.55	0/153	0.72	0/207
7	8	1.57	10/1775 (0.6%)	1.71	18/2755 (0.7%)
8	9	4.09	56/3329 (1.7%)	2.78	80/4446 (1.8%)
9	A	0.29	0/2803	0.77	0/4371
10	B	0.34	18/68314 (0.0%)	0.79	78/106569 (0.1%)
11	C	0.40	0/2092	0.90	9/2813 (0.3%)
12	D	0.37	0/1586	0.82	4/2134 (0.2%)
13	E	0.70	4/1571 (0.3%)	0.83	5/2113 (0.2%)
14	F	0.41	1/1444 (0.1%)	1.00	10/1937 (0.5%)
15	G	0.30	0/1343	0.67	1/1816 (0.1%)
16	H	0.34	0/1122	0.71	1/1515 (0.1%)
17	I	0.60	4/1046 (0.4%)	0.76	4/1410 (0.3%)
18	J	0.32	0/1135	0.76	3/1529 (0.2%)
19	K	0.35	0/939	0.99	4/1258 (0.3%)
20	L	0.74	1/1062 (0.1%)	1.58	25/1413 (1.8%)
21	M	0.39	0/1093	0.85	5/1460 (0.3%)
22	N	0.37	0/1021	0.80	3/1364 (0.2%)
23	O	0.31	0/910	0.64	0/1219
24	P	0.58	0/929	1.40	16/1242 (1.3%)
25	Q	0.36	0/960	0.75	0/1278
26	R	0.39	0/829	0.82	3/1107 (0.3%)
27	S	0.26	0/864	0.60	0/1156
28	T	0.45	1/784 (0.1%)	0.80	1/1048 (0.1%)
29	U	0.37	0/787	0.94	7/1051 (0.7%)
30	V	0.25	0/766	0.46	0/1025
31	W	0.39	0/642	0.81	2/848 (0.2%)
32	X	0.29	0/510	0.66	0/677

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Y	0.32	0/453	0.69	1/605 (0.2%)
34	Z	0.52	0/559	0.91	1/745 (0.1%)
All	All	0.84	95/102915 (0.1%)	0.95	285/153875 (0.2%)

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	0	0	1
7	8	0	1
8	9	1	15
9	A	0	1
10	B	1	65
11	C	0	2
24	P	0	1
26	R	0	1
34	Z	0	1
All	All	2	88

The worst 5 of 95 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	9	300	VAL	CB-CG1	107.27	3.78	1.52
8	9	299	ASP	CB-CG	88.52	3.37	1.51
8	9	333	ASP	CB-CG	82.89	3.25	1.51
8	9	300	VAL	CB-CG2	75.72	3.11	1.52
8	9	370	ASP	CB-CG	68.24	2.95	1.51

The worst 5 of 285 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	9	374	VAL	O-C-N	-71.21	8.76	122.70
8	9	300	VAL	CG1-CB-CG2	-43.96	40.56	110.90
8	9	300	VAL	CA-CB-CG2	-40.13	50.71	110.90
8	9	300	VAL	CA-CB-CG1	-38.94	52.49	110.90
8	9	299	ASP	CA-CB-CG	-37.81	30.22	113.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	9	327	ASP	CA
10	B	2076	U	C3'

5 of 88 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	48	TYR	Sidechain
7	8	55	A	Sidechain
8	9	296	GLY	Peptide
8	9	299	ASP	Sidechain
8	9	319	LEU	Mainchain

5.2 Too-close contacts [i](#)

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	0	444	0	461	83	0
2	1	441	0	485	69	0
3	2	377	0	418	65	0
4	3	504	0	574	112	0
5	4	302	0	343	83	0
6	7	149	0	152	103	0
7	8	1590	0	808	81	0
8	9	3306	0	3402	1820	0
9	A	2507	0	1270	95	0
10	B	60995	0	30676	2400	0
11	C	2053	0	2122	416	0
12	D	1565	0	1616	315	0
13	E	1552	0	1619	269	0
14	F	1420	0	1460	172	0
15	G	1323	0	1374	158	0
16	H	1111	0	1148	143	0
17	I	1032	0	1088	218	0
18	J	1112	0	1147	231	0
19	K	930	0	1000	130	0
20	L	1053	0	1129	233	0
21	M	1074	0	1157	191	0
22	N	1008	0	1045	132	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	O	900	0	935	132	0
24	P	917	0	965	206	0
25	Q	947	0	1022	160	0
26	R	816	0	839	178	0
27	S	857	0	922	120	0
28	T	777	0	839	204	0
29	U	779	0	834	138	0
30	V	753	0	780	72	0
31	W	634	0	656	154	0
32	X	509	0	541	138	0
33	Y	449	0	491	64	0
34	Z	549	0	552	104	0
35	B	110	0	0	0	0
35	N	1	0	0	0	0
36	B	506	0	0	7	0
36	N	6	0	0	1	0
All	All	95358	0	63870	8126	0

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 51.

The worst 5 of 8126 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)
8:9:410:VAL:CG1	10:B:485:C:H5''	1.27	1.65
8:9:145:ILE:CD1	8:9:161:PRO:HG2	1.17	1.64
8:9:334:PHE:CE2	8:9:420:PHE:HE2	1.02	1.63
8:9:2:PHE:CZ	8:9:295:LEU:HD13	1.31	1.62
8:9:334:PHE:CZ	8:9:420:PHE:CE2	1.87	1.62

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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	
1	0	54/56 (96%)	30 (56%)	15 (28%)	9 (17%)	0	3
2	1	52/54 (96%)	21 (40%)	22 (42%)	9 (17%)	0	3
3	2	44/46 (96%)	24 (54%)	12 (27%)	8 (18%)	0	3
4	3	62/64 (97%)	35 (56%)	17 (27%)	10 (16%)	0	3
5	4	36/38 (95%)	13 (36%)	11 (31%)	12 (33%)	0	0
6	7	16/18 (89%)	14 (88%)	2 (12%)	0	100	100
8	9	403/430 (94%)	154 (38%)	100 (25%)	149 (37%)	0	0
11	C	265/267 (99%)	97 (37%)	93 (35%)	75 (28%)	0	0
12	D	207/209 (99%)	96 (46%)	67 (32%)	44 (21%)	0	2
13	E	199/201 (99%)	87 (44%)	63 (32%)	49 (25%)	0	1
14	F	176/178 (99%)	92 (52%)	52 (30%)	32 (18%)	0	3
15	G	174/176 (99%)	117 (67%)	39 (22%)	18 (10%)	0	8
16	H	147/149 (99%)	84 (57%)	44 (30%)	19 (13%)	0	5
17	I	139/141 (99%)	123 (88%)	11 (8%)	5 (4%)	3	25
18	J	138/140 (99%)	70 (51%)	36 (26%)	32 (23%)	0	1
19	K	119/121 (98%)	72 (60%)	25 (21%)	22 (18%)	0	2
20	L	142/144 (99%)	66 (46%)	37 (26%)	39 (28%)	0	0
21	M	134/136 (98%)	79 (59%)	31 (23%)	24 (18%)	0	3
22	N	125/127 (98%)	82 (66%)	32 (26%)	11 (9%)	1	11
23	O	115/117 (98%)	64 (56%)	33 (29%)	18 (16%)	0	3
24	P	112/114 (98%)	42 (38%)	38 (34%)	32 (29%)	0	0
25	Q	115/117 (98%)	79 (69%)	22 (19%)	14 (12%)	0	6
26	R	101/103 (98%)	43 (43%)	30 (30%)	28 (28%)	0	0
27	S	108/110 (98%)	67 (62%)	20 (18%)	21 (19%)	0	2
28	T	97/99 (98%)	42 (43%)	33 (34%)	22 (23%)	0	2
29	U	100/102 (98%)	46 (46%)	41 (41%)	13 (13%)	0	5
30	V	92/94 (98%)	59 (64%)	27 (29%)	6 (6%)	1	16
31	W	82/84 (98%)	31 (38%)	29 (35%)	22 (27%)	0	0
32	X	61/63 (97%)	38 (62%)	15 (25%)	8 (13%)	0	5
33	Y	56/58 (97%)	35 (62%)	18 (32%)	3 (5%)	2	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	Z	68/70 (97%)	37 (54%)	22 (32%)	9 (13%)	0	5
All	All	3739/3826 (98%)	1939 (52%)	1037 (28%)	763 (20%)	0	2

5 of 763 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	31	LYS
1	0	35	GLU
1	0	45	ASP
2	1	12	SER
2	1	23	THR

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
1	0	47/47 (100%)	33 (70%)	14 (30%)	0	2
2	1	48/48 (100%)	33 (69%)	15 (31%)	0	2
3	2	38/38 (100%)	28 (74%)	10 (26%)	0	3
4	3	51/51 (100%)	40 (78%)	11 (22%)	1	6
5	4	34/34 (100%)	17 (50%)	17 (50%)	0	0
6	7	16/17 (94%)	16 (100%)	0	100	100
8	9	357/357 (100%)	329 (92%)	28 (8%)	12	36
11	C	213/213 (100%)	150 (70%)	63 (30%)	0	2
12	D	164/164 (100%)	113 (69%)	51 (31%)	0	2
13	E	165/165 (100%)	127 (77%)	38 (23%)	1	4
14	F	149/149 (100%)	122 (82%)	27 (18%)	1	10
15	G	137/137 (100%)	111 (81%)	26 (19%)	1	8
16	H	114/114 (100%)	90 (79%)	24 (21%)	1	6
17	I	109/109 (100%)	104 (95%)	5 (5%)	27	52
18	J	114/114 (100%)	85 (75%)	29 (25%)	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	K	102/102 (100%)	81 (79%)	21 (21%)	1	7
20	L	103/103 (100%)	68 (66%)	35 (34%)	0	1
21	M	109/109 (100%)	74 (68%)	35 (32%)	0	2
22	N	103/103 (100%)	76 (74%)	27 (26%)	0	3
23	O	87/87 (100%)	69 (79%)	18 (21%)	1	6
24	P	99/99 (100%)	67 (68%)	32 (32%)	0	2
25	Q	89/89 (100%)	71 (80%)	18 (20%)	1	7
26	R	84/84 (100%)	58 (69%)	26 (31%)	0	2
27	S	93/93 (100%)	77 (83%)	16 (17%)	2	11
28	T	83/83 (100%)	60 (72%)	23 (28%)	0	3
29	U	83/83 (100%)	60 (72%)	23 (28%)	0	3
30	V	78/78 (100%)	69 (88%)	9 (12%)	5	21
31	W	62/62 (100%)	45 (73%)	17 (27%)	0	3
32	X	55/55 (100%)	43 (78%)	12 (22%)	1	6
33	Y	48/48 (100%)	33 (69%)	15 (31%)	0	2
34	Z	62/62 (100%)	46 (74%)	16 (26%)	0	3
All	All	3096/3097 (100%)	2395 (77%)	701 (23%)	3	5

5 of 701 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	N	58	ASP
27	S	19	LEU
23	O	2	ASP
22	N	57	THR
24	P	97	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
22	N	81	ASN
25	Q	80	ASN
23	O	34	HIS
24	P	11	GLN
26	R	86	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B	2837/2904 (97%)	481 (16%)	22 (0%)
7	8	68/74 (91%)	2 (2%)	1 (1%)
9	A	116/117 (99%)	20 (17%)	1 (0%)
All	All	3021/3095 (97%)	503 (16%)	24 (0%)

5 of 503 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	8	39	A
7	8	85	A
9	A	13	G
9	A	15	A
9	A	16	G

5 of 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	B	1211	C
10	B	2198	A
10	B	2076	U
10	B	2282	G
10	B	199	A

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 111 ligands modelled in this entry, 111 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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	9	34
7	8	7

The worst 5 of 41 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	8	86:G	O3'	87:G	P	10.90
1	9	315:GLN	C	316:ALA	N	5.35
1	8	22:U	O3'	23:G	P	4.45
1	9	352:GLY	C	353:LYS	N	4.18
1	9	370:ASP	C	371:LYS	N	3.83

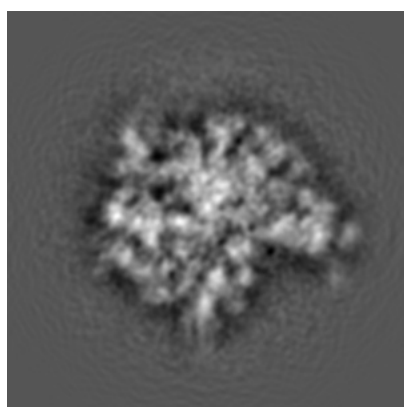
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1261. These allow visual inspection of the internal detail of the map and identification of artifacts.

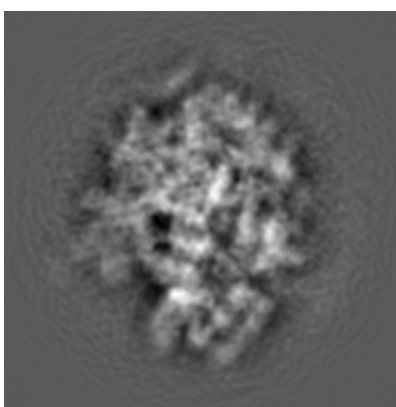
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

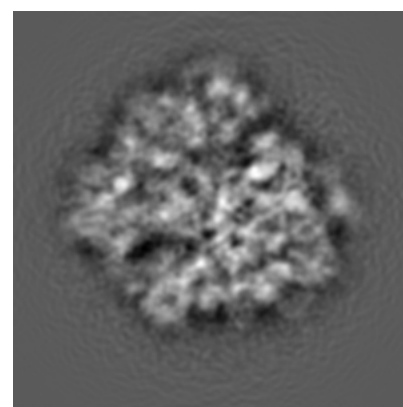
6.1.1 Primary map



X



Y

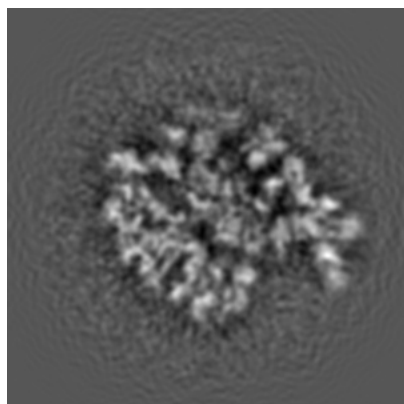


Z

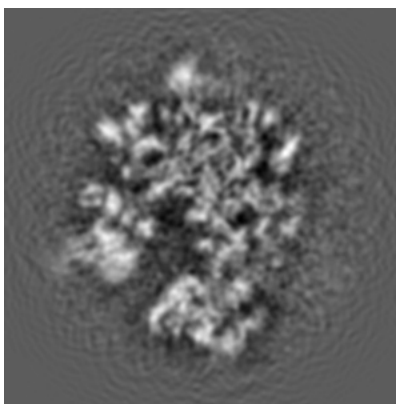
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

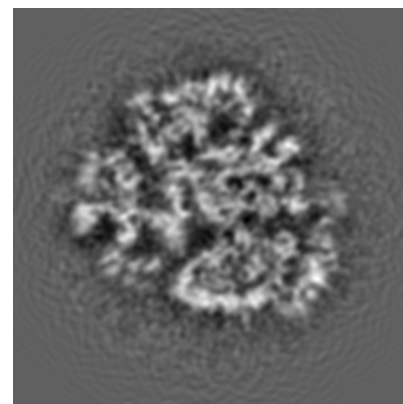
6.2.1 Primary map



X Index: 147



Y Index: 147

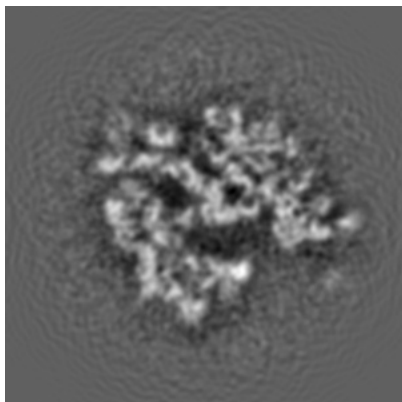


Z Index: 147

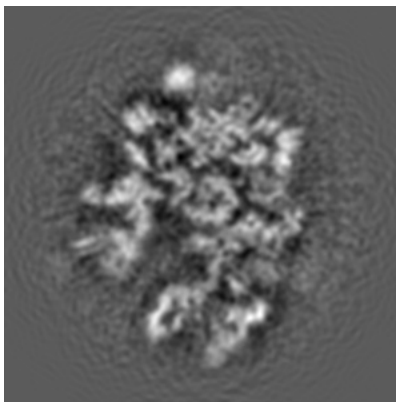
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

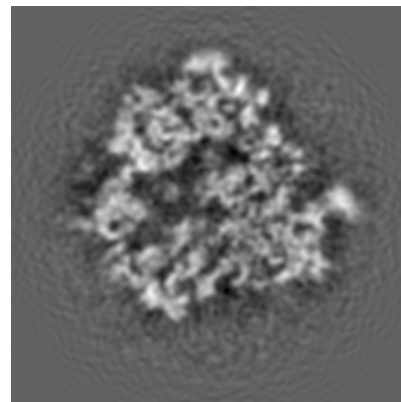
6.3.1 Primary map



X Index: 139



Y Index: 153



Z Index: 133

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.704. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

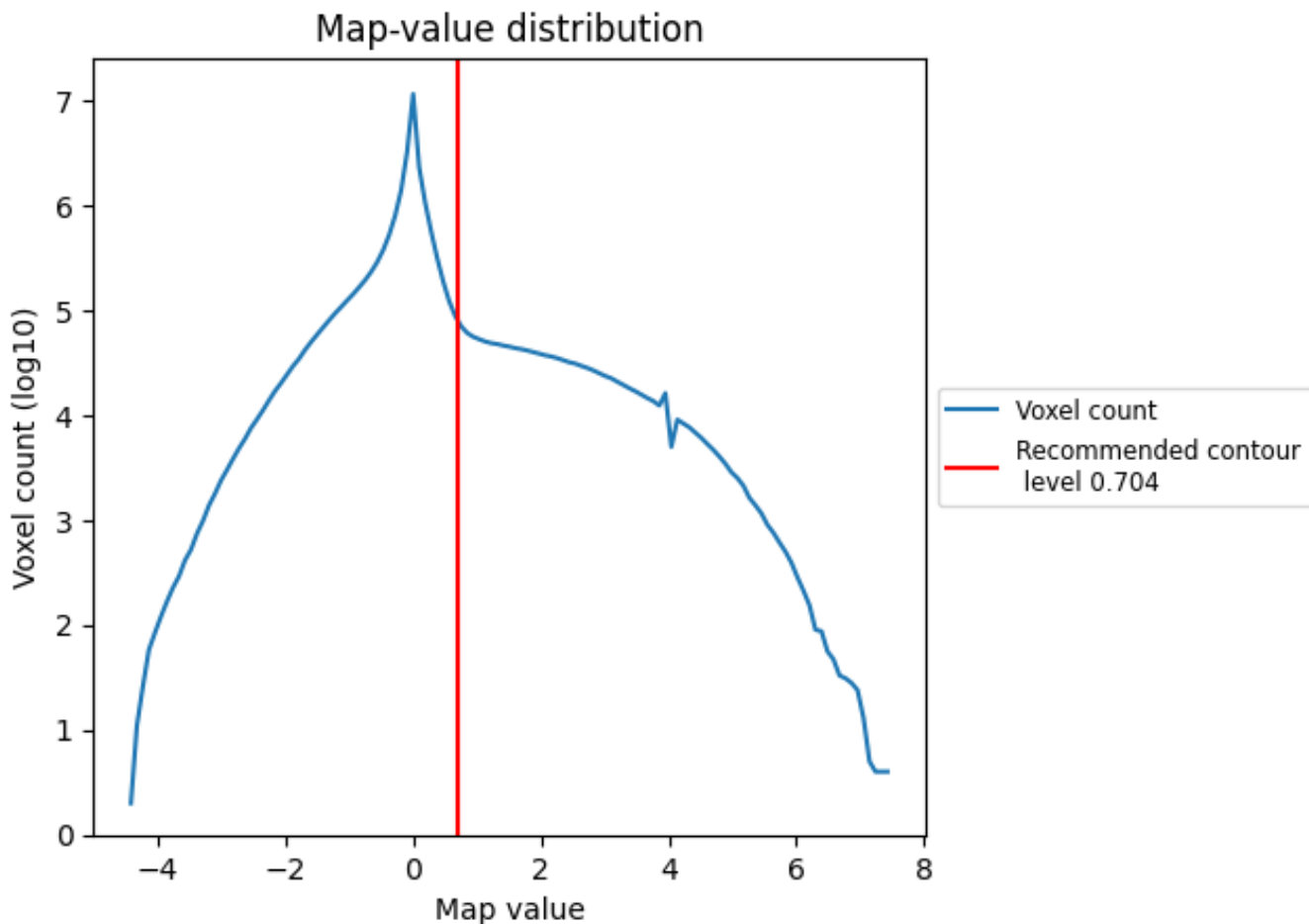
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

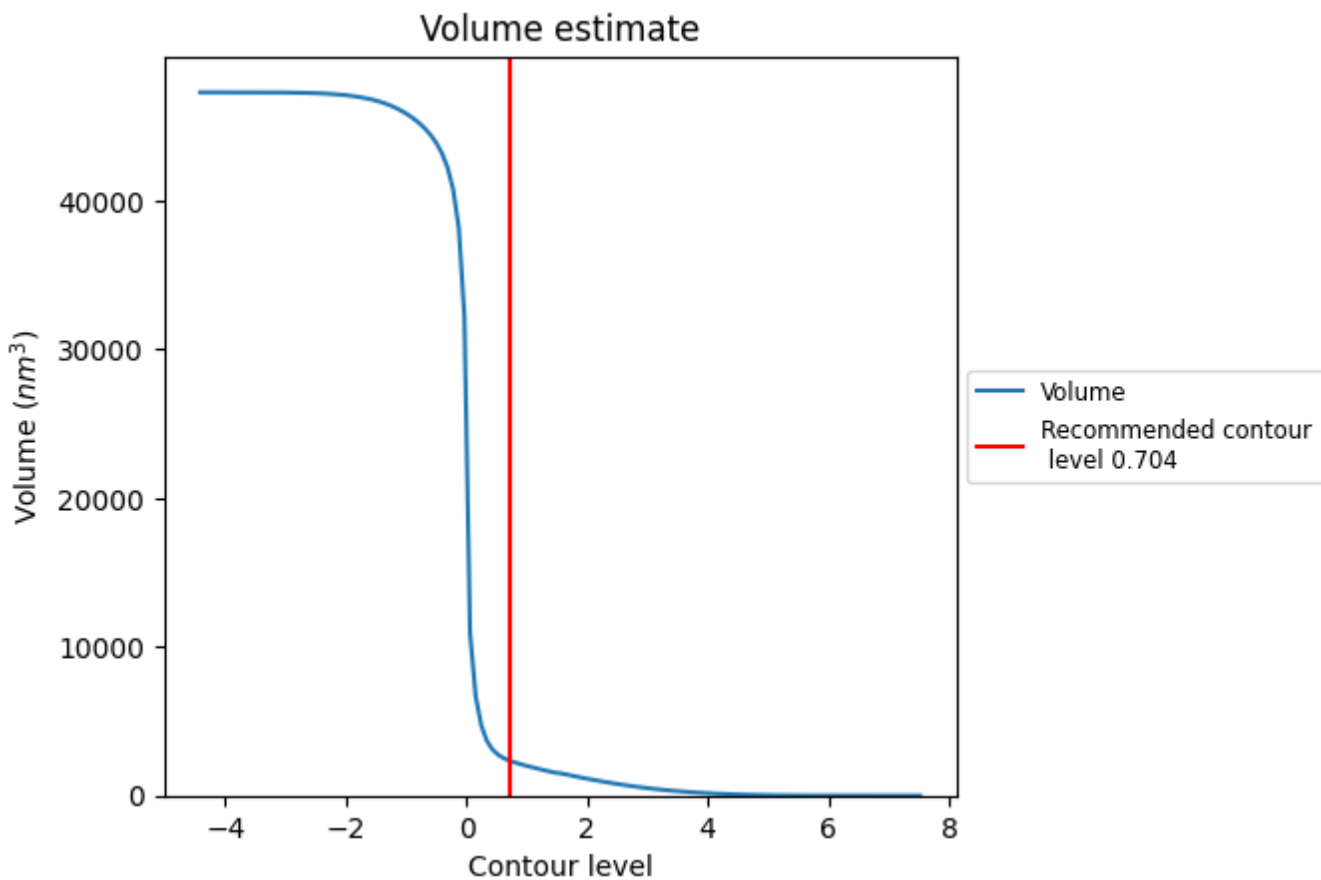
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

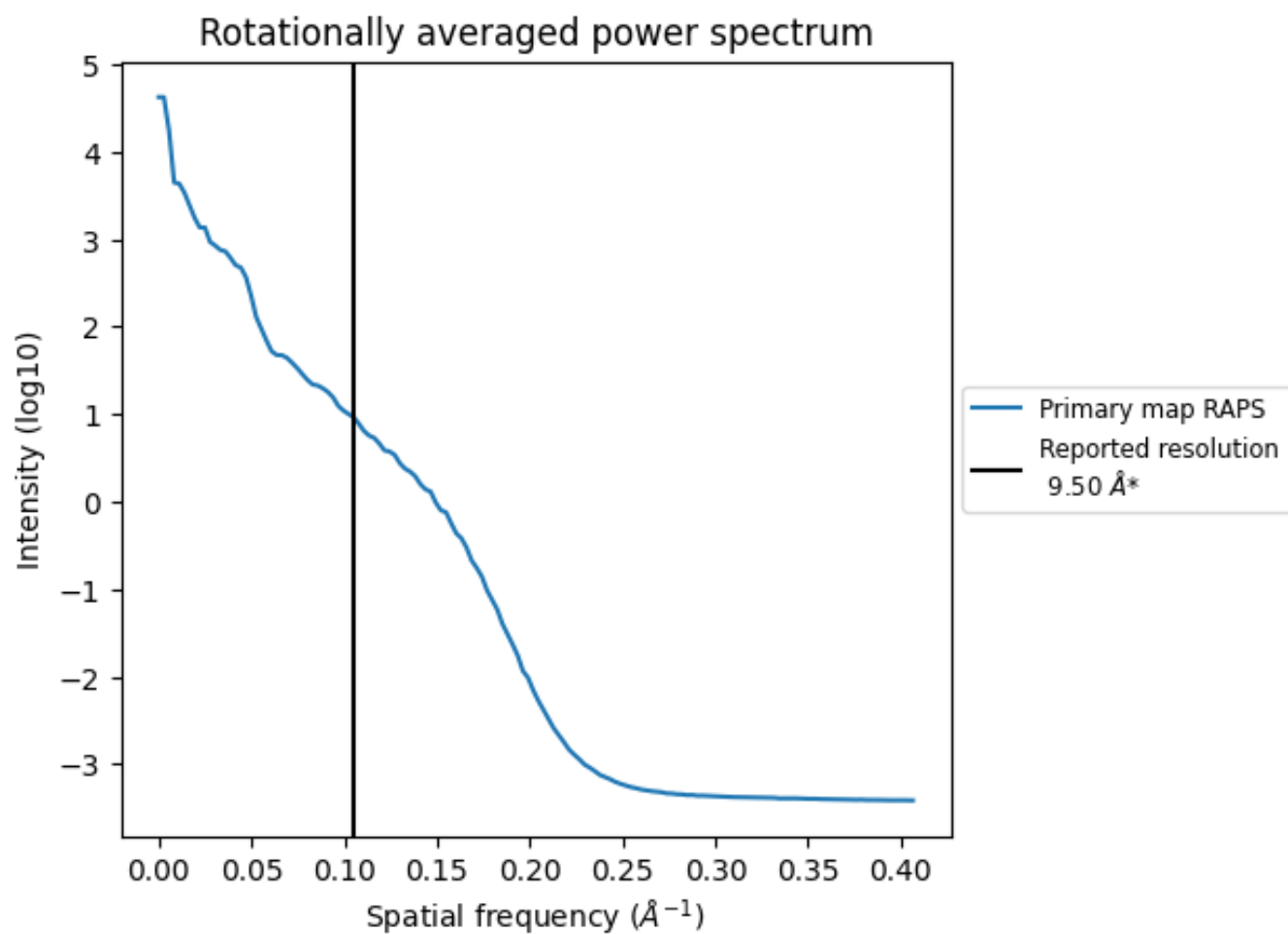
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2362 nm^3 ; this corresponds to an approximate mass of 2133 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.105 Å⁻¹

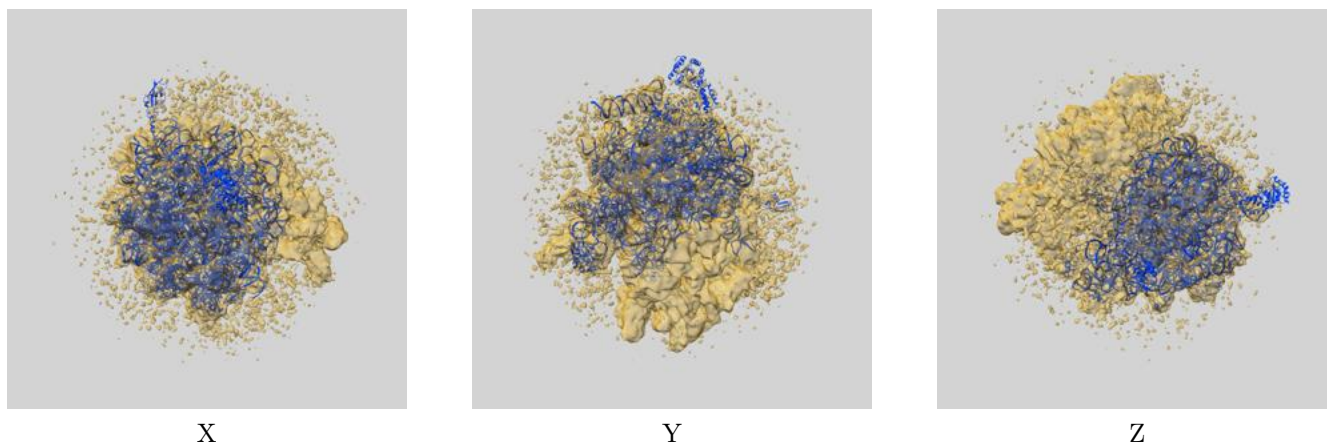
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

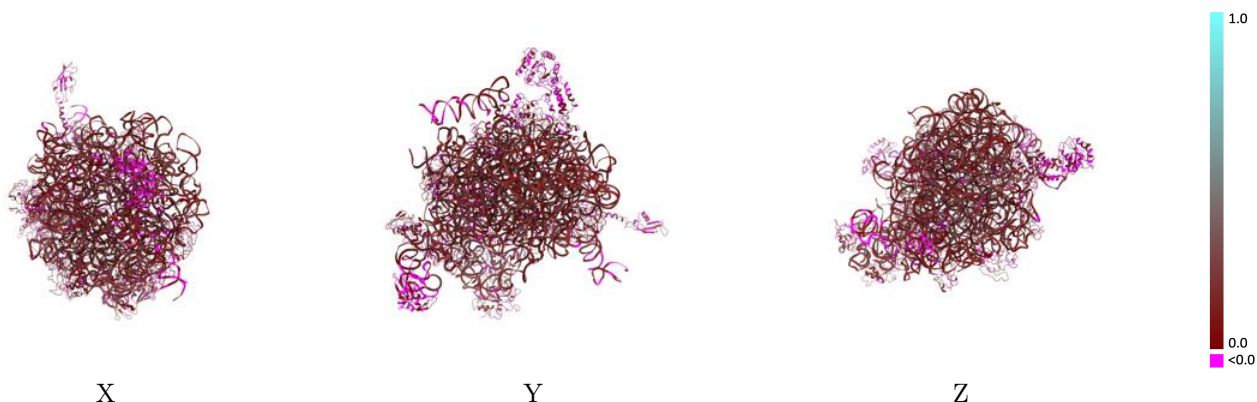
This section contains information regarding the fit between EMDB map EMD-1261 and PDB model 2J28. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



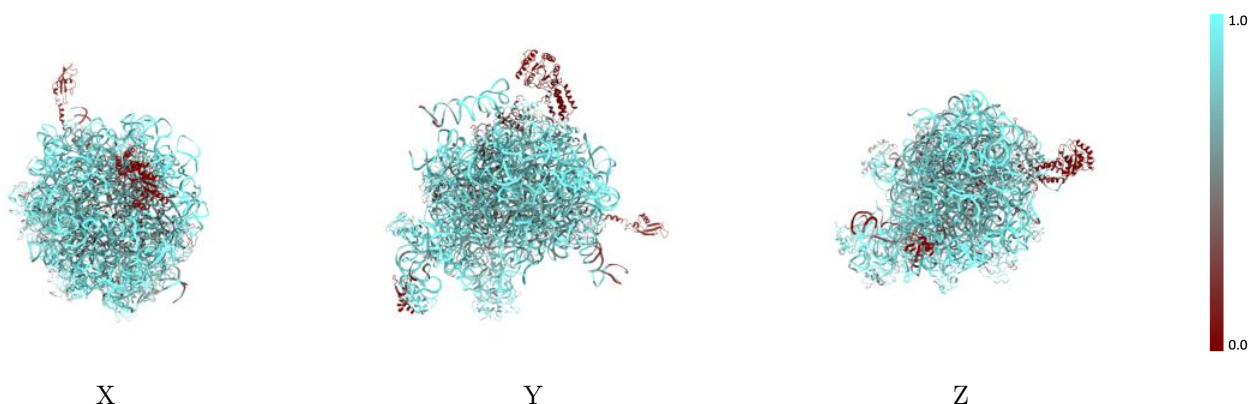
The images above show the 3D surface view of the map at the recommended contour level 0.704 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



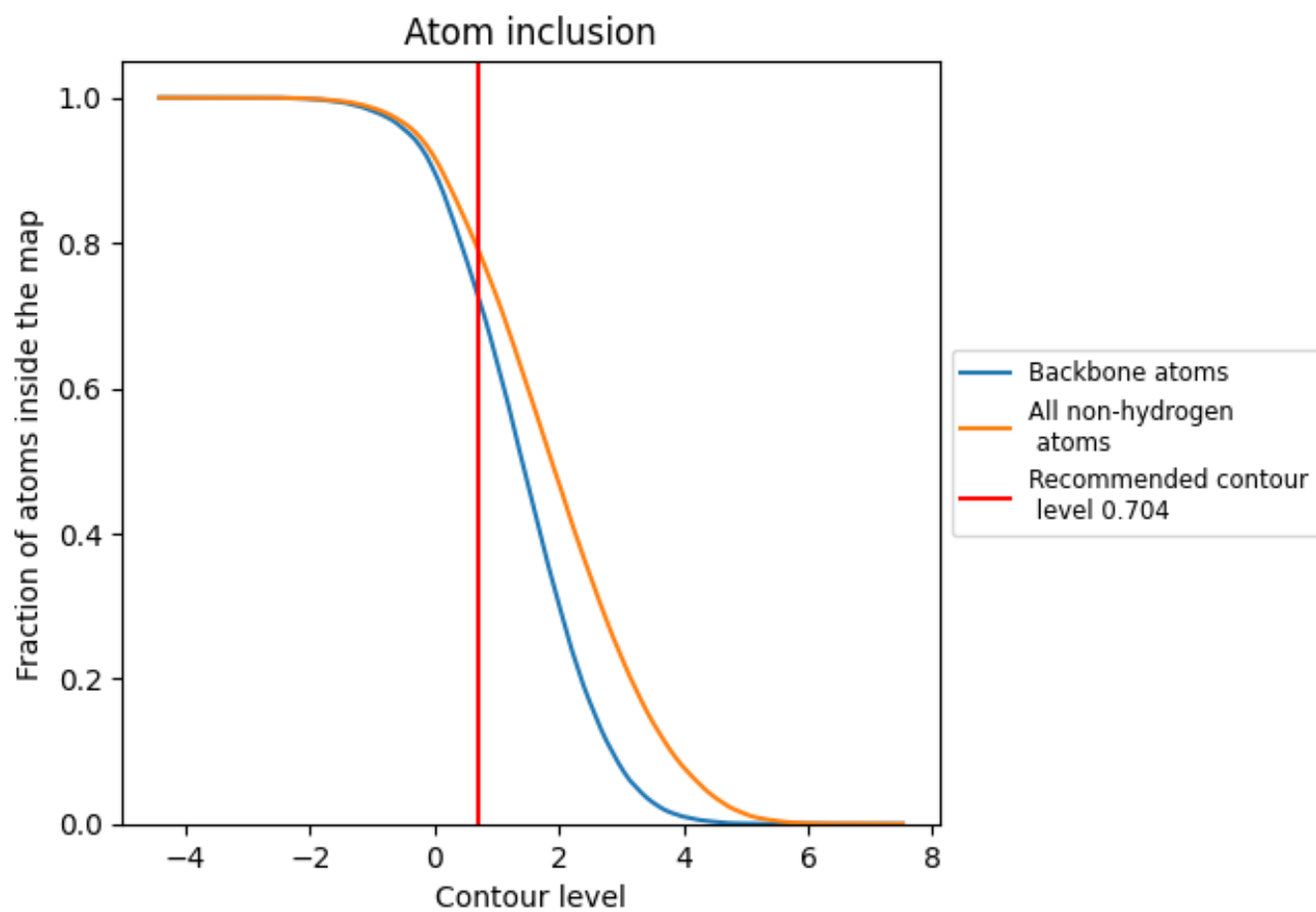
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.704).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.704) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7899	 0.1360
0	 0.5654	 0.1120
1	 0.5958	 0.0850
2	 0.4000	 0.0530
3	 0.4481	 0.0630
4	 0.4966	 0.0260
7	 0.5946	 0.0850
8	 0.8176	 0.0720
9	 0.2177	 0.0320
A	 0.9274	 0.1450
B	 0.8853	 0.1620
C	 0.5083	 0.0890
D	 0.6625	 0.1090
E	 0.6368	 0.0940
F	 0.8207	 0.0830
G	 0.8435	 0.1180
H	 0.2555	 0.0760
I	 0.5793	 0.0280
J	 0.6085	 0.1000
K	 0.6122	 0.1300
L	 0.5820	 0.0790
M	 0.5825	 0.0830
N	 0.6365	 0.1020
O	 0.7945	 0.0830
P	 0.6002	 0.1010
Q	 0.6564	 0.0990
R	 0.6913	 0.1060
S	 0.5801	 0.1180
T	 0.5926	 0.1040
U	 0.7262	 0.0880
V	 0.8862	 0.1160
W	 0.5243	 0.0560
X	 0.7284	 0.1110
Y	 0.7620	 0.1380
Z	 0.5911	 0.0890

