



wwPDB EM Validation Summary Report ⓘ

May 14, 2025 – 06:03 AM EDT

PDB ID : 5TCU / pdb_00005tcu
EMDB ID : EMD-8402
Title : Methicillin sensitive Staphylococcus aureus 70S ribosome
Authors : Eyal, Z.; Ahmed, T.; Belousoff, N.; Mishra, S.; Matzov, D.; Bashan, A.; Zimmermann, E.; Lithgow, T.; Bhushan, S.; Yonath, A.
Deposited on : 2016-09-15
Resolution : 3.90 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

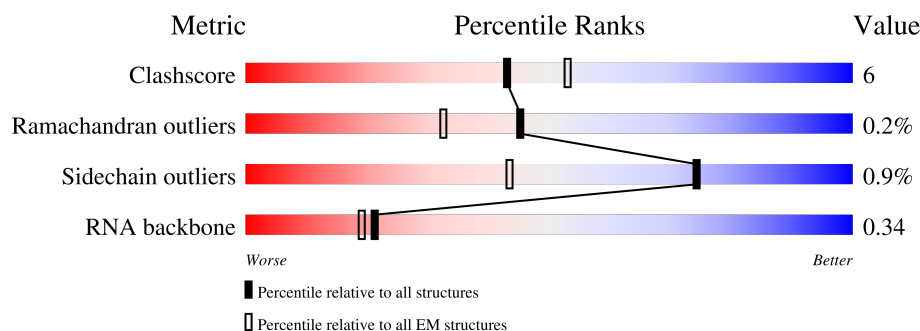
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	A	1555	<div> <div>5%</div> <div>43%</div> <div>41%</div> <div>11%</div> <div>6%</div> </div>
2	SB	202	<div> <div>44%</div> <div>77%</div> <div>23%</div> </div>
3	SC	198	<div> <div>40%</div> <div>92%</div> <div>8%</div> </div>
4	SD	156	<div> <div>9%</div> <div>81%</div> <div>19%</div> </div>
5	SE	95	<div> <div>22%</div> <div>75%</div> <div>25%</div> </div>
6	SG	155	<div> <div>50%</div> <div>83%</div> <div>17%</div> </div>
7	SF	130	<div> <div>13%</div> <div>72%</div> <div>28%</div> </div>

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Mol	Chain	Length	Quality of chain
8	SH	127	
9	S1	80	
10	S2	114	
11	S3	136	
12	S4	113	
13	S5	60	
14	S6	88	
15	S7	83	
16	S8	80	
17	S9	56	
18	SI	78	
19	SA	79	
20	X	13	
21	E	75	
22	D	76	
23	B	2923	
24	C	114	
25	L2	274	
26	LC	215	
27	LJ	205	
28	LK	166	
29	LL	174	
30	LM	145	
31	LN	122	
32	LO	145	

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Mol	Chain	Length	Quality of chain
33	LP	136	 7% 82% 18%
34	LQ	119	 77% 23%
35	LR	113	 13% 85% 14%
36	L1	109	 7% 91% 9%
37	L3	116	 6% 81% 19%
38	L4	102	 6% 84% 15%
39	L5	112	 5% 86% 13%
40	L6	89	 6% 87% 13%
41	L7	103	 17% 85% 15%
42	L8	93	 51% 96%
43	L9	82	 13% 84% 16%
44	LA	58	 24% 79% 21%
45	LB	62	 84% 16%
46	LD	57	 9% 86% 12%
47	LE	47	 94% 6%
48	LS	47	 19% 85% 15%
49	LG	43	 79% 21%
50	LH	60	 87% 13%
51	LI	37	 70% 30%
52	LF	74	 47% 93% 7%

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 133876 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 RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1464	Total	C	N	O	P	0	0
			31369	14007	5741	10159	1462		

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	SB	202	Total	C	N	O	S	0	0
			1551	979	293	278	1		

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	SC	198	Total	C	N	O	0	0
			1058	634	211	213		

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SD	156	Total	C	N	O	S	0	0
			1153	727	211	213	2		

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SE	95	Total	C	N	O	S	0	0
			785	496	138	149	2		

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SG	155	Total	C	N	O	S	0	0
			1164	724	220	217	3		

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SF	130	Total	C	N	O	S	0	0
			1007	639	180	184	4		

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SH	127	Total	C	N	O	S	0	0
			975	605	194	175	1		

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	S1	80	Total	C	N	O	0	0
			626	394	116	116		

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S2	114	Total	C	N	O	S	0	0
			826	507	158	159	2		

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S3	136	Total	C	N	O	S	0	0
			976	611	190	173	2		

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S4	113	Total	C	N	O	S	0	0
			828	510	168	149	1		

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S5	60	Total	C	N	O	S	0	0
			497	314	99	79	5		

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S6	88	Total	C	N	O	S	0	0
			713	441	148	123	1		

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S7	83	Total	C	N	O	S	0	0
			537	335	105	96	1		

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	S8	80	Total	C	N	O	0	0
			520	327	97	96		

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S9	56	Total	C	N	O	S	0	0
			458	292	88	76	2		

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SI	78	Total	C	N	O	S	0	0
			541	340	104	96	1		

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SA	78	Total	C	N	O	S	0	0
			503	303	100	99	1		

- Molecule 20 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	10	Total	C	N	O	P	0	0
			213	96	39	68	10		

- Molecule 21 is a RNA chain called P-site tRNA CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	E	75	Total	C	N	O	P	0	0
			1600	713	285	527	75		

- Molecule 22 is a RNA chain called E-site tRNA CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	D	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

- Molecule 23 is a RNA chain called 23S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B	2755	Total	C	N	O	P	0	0
			59059	26368	10814	19122	2755		

- Molecule 24 is a RNA chain called 5S rRNA CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	C	114	Total	C	N	O	P	0	0
			2430	1086	436	794	114		

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L2	274	Total	C	N	O	S	0	0
			2066	1288	414	359	5		

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LC	215	Total	C	N	O	S	0	0
			1570	987	295	283	5		

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LJ	205	Total	C	N	O	S	0	0
			1514	953	282	277	2		

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LK	166	Total	C	N	O	S	0	0
			1026	635	185	204	2		

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LL	174	Total	C	N	O	S	0	0
			1062	660	205	195	2		

- Molecule 30 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LM	145	Total	C	N	O	S	0	0
			1124	703	205	213	3		

- Molecule 31 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LN	122	Total	C	N	O	S	0	0
			918	572	174	168	4		

- Molecule 32 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	LO	145	Total	C	N	O	0	0
			1020	631	207	182		

- Molecule 33 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LP	136	Total	C	N	O	S	0	0
			1043	672	202	165	4		

- Molecule 34 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LQ	119	Total	C	N	O	S	0	0
			898	551	176	170	1		

- Molecule 35 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	LR	113	Total	C	N	O	0	0
			765	474	145	146		

- Molecule 36 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	L1	109	Total	C	N	O	0	0
			832	529	169	134		

- Molecule 37 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	L3	116	Total	C	N	O	S	0	0
			942	593	189	156	4		

- Molecule 38 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	L4	102	Total	C	N	O	S	0	0
			749	474	140	134	1		

- Molecule 39 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	L5	112	Total	C	N	O	S	0	0
			837	526	163	146	2		

- Molecule 40 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	L6	89	Total	C	N	O	S	0	0
			694	436	126	128	4		

- Molecule 41 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	L7	103	Total	C	N	O	0	0
			734	462	137	135		

- Molecule 42 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	L8	93	Total	C	N	O	0	0
			648	411	115	122		

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	L9	82	Total	C	N	O	0	0
			615	382	122	111		

- Molecule 44 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	LA	58	Total	C	N	O	0	0
			443	276	96	71		

- Molecule 45 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	LB	62	Total	C	N	O	0	0
			493	304	93	96		

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	LD	57	Total	C	N	O	0	0
			436	272	83	81		

- Molecule 47 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LE	47	Total	C	N	O	S	0	0
			356	218	77	59	2		

- Molecule 48 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LS	47	Total	C	N	O	S	0	0
			380	233	75	68	4		

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	LG	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LH	60	Total	C	N	O	S	0	0
			446	277	92	75	2		

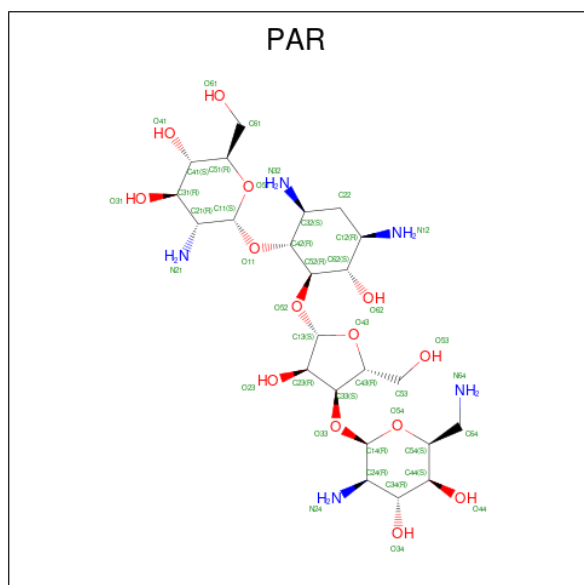
- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LI	37	Total	C	N	O	S	0	0
			272	170	57	40	5		

- Molecule 52 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LF	74	Total	C	N	O	S	0	0
			447	269	86	91	1		

- Molecule 53 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



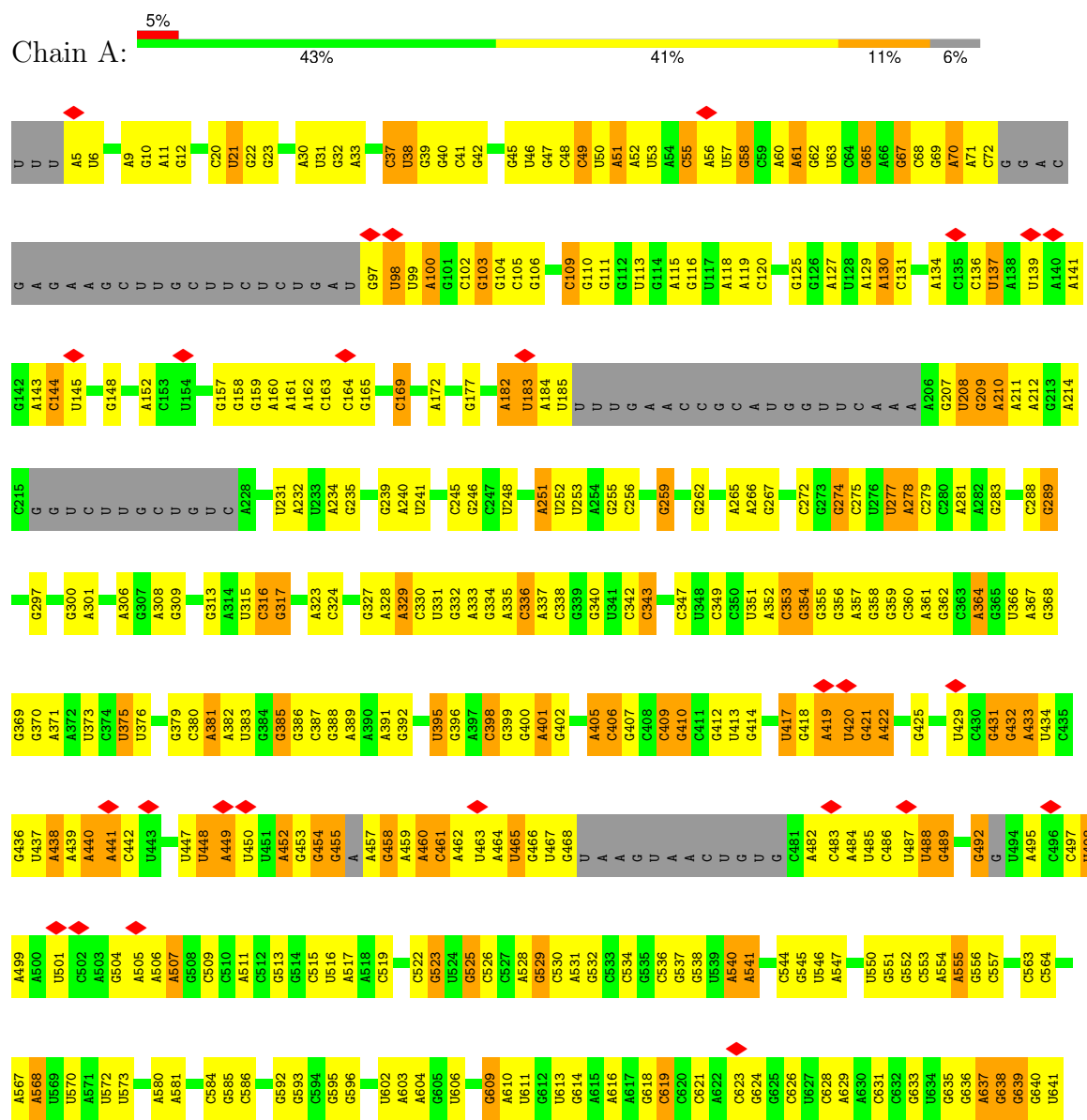
- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

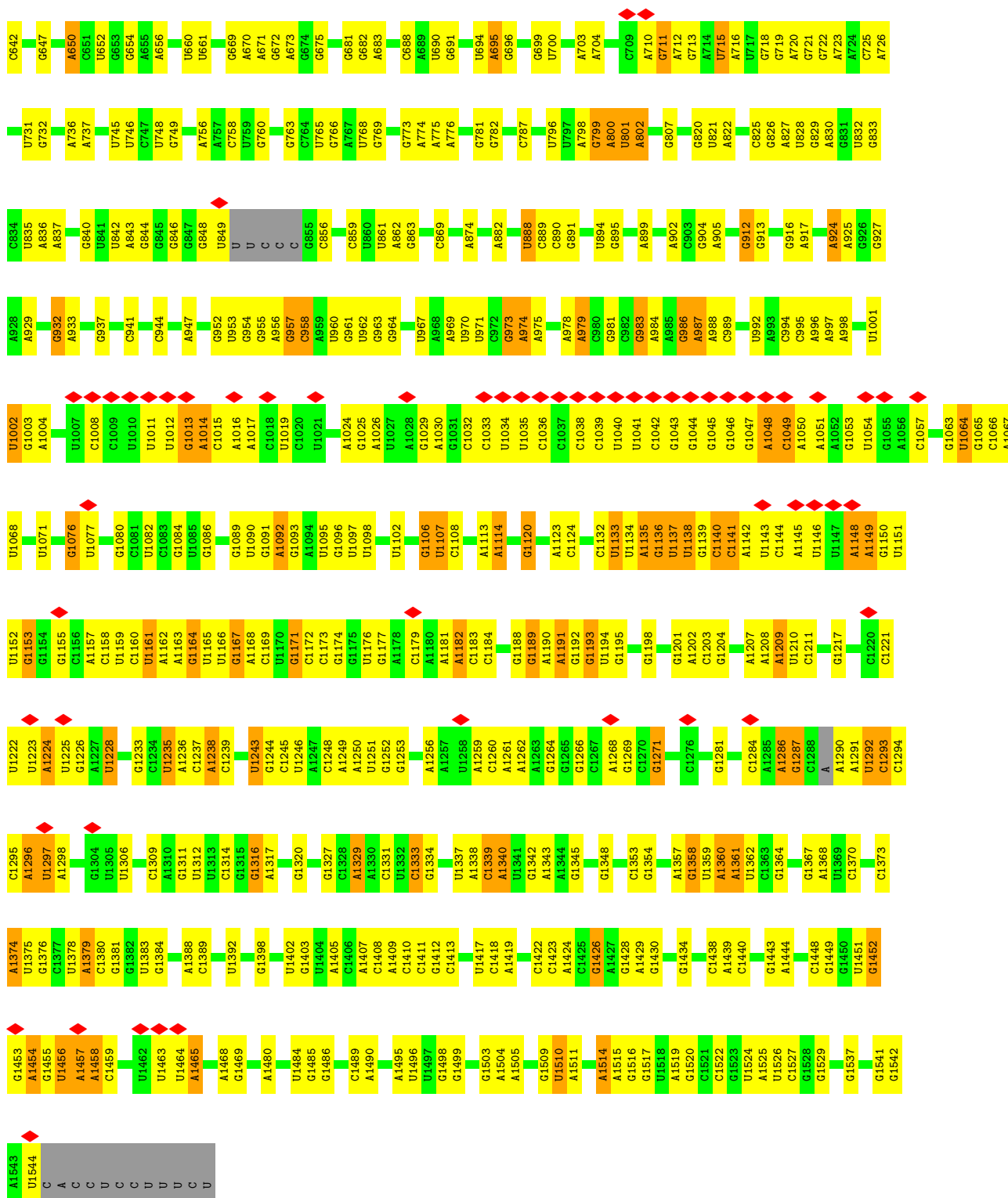
Mol	Chain	Residues	Atoms		AltConf
54	A	27	Total 27	Mg 27	0
54	SG	1	Total 1	Mg 1	0
54	B	99	Total 99	Mg 99	0
54	C	2	Total 2	Mg 2	0

3 Residue-property plots [i](#)

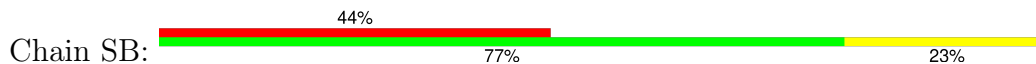
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

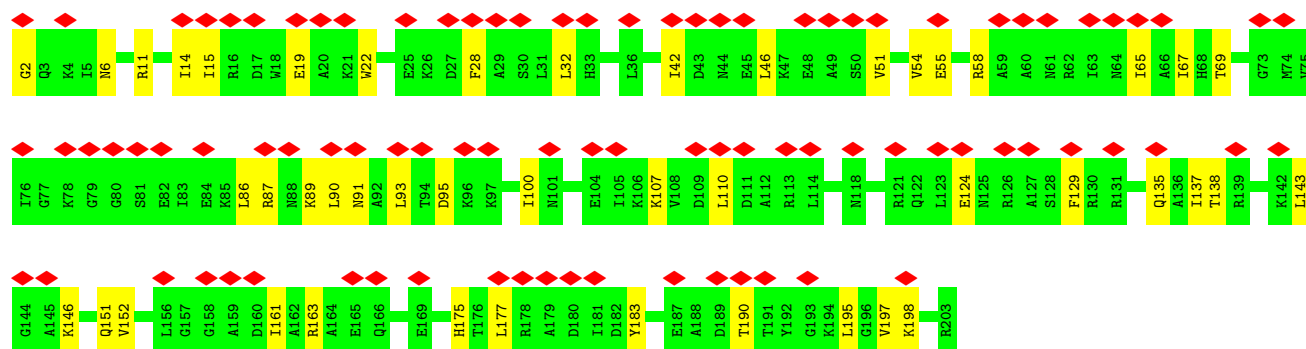
• Molecule 1: 16S rRNA



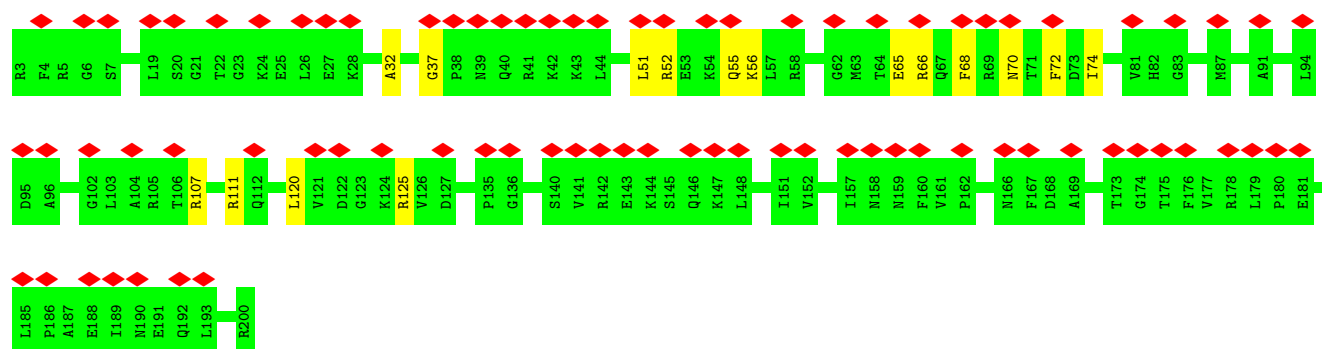
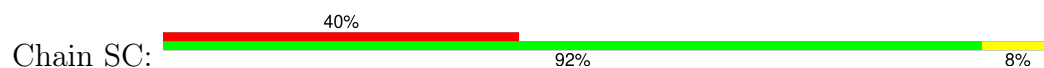


• Molecule 2: 30S ribosomal protein S3

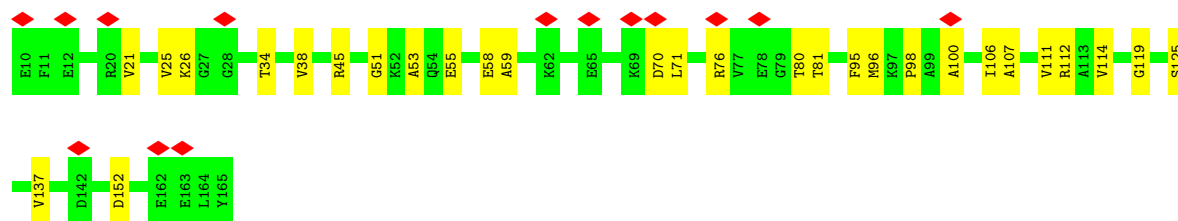
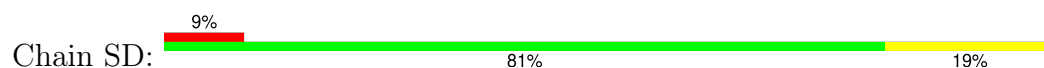




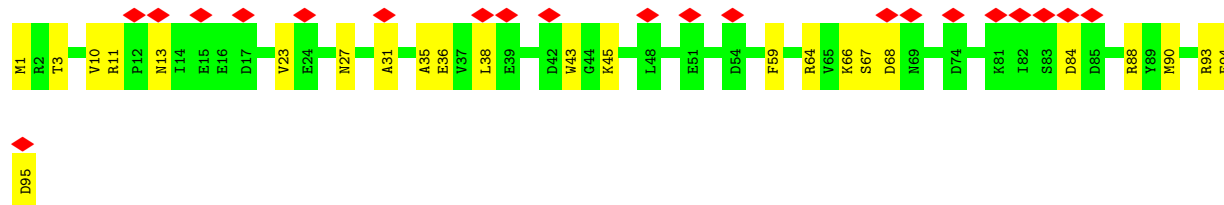
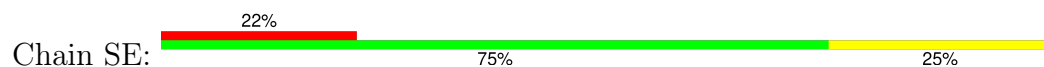
• Molecule 3: 30S ribosomal protein S4




• Molecule 4: 30S ribosomal protein S5

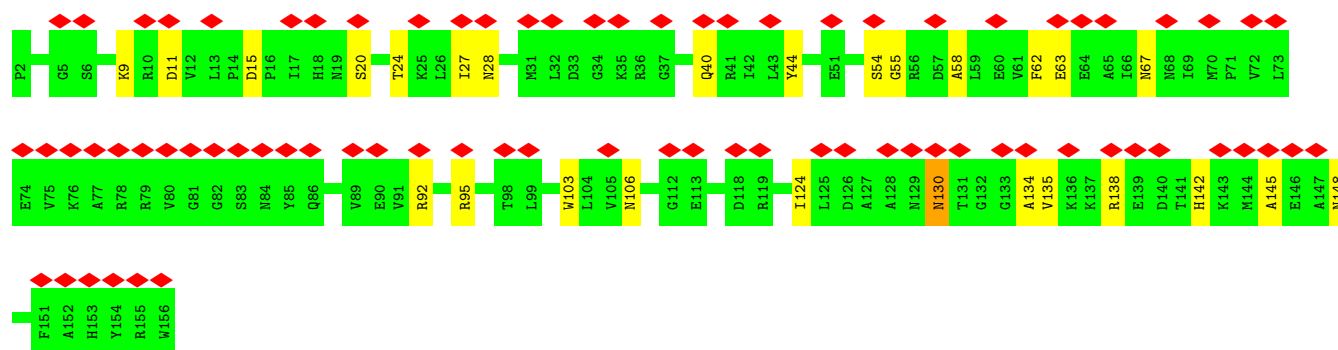


• Molecule 5: 30S ribosomal protein S6



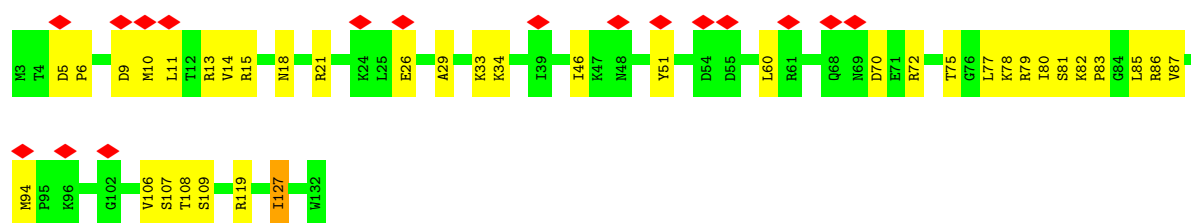
• Molecule 6: 30S ribosomal protein S7

Chain SG: 



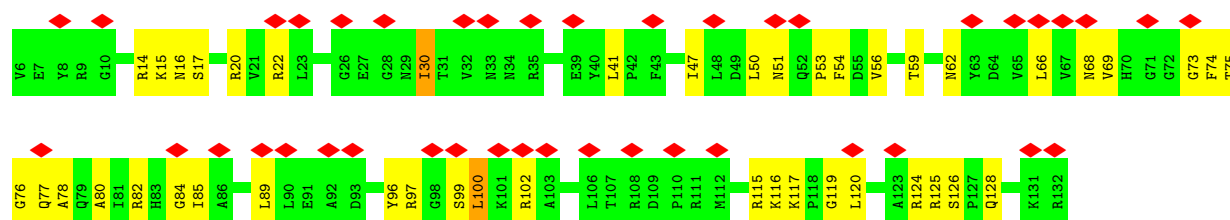
• Molecule 7: 30S ribosomal protein S8

Chain SF: 




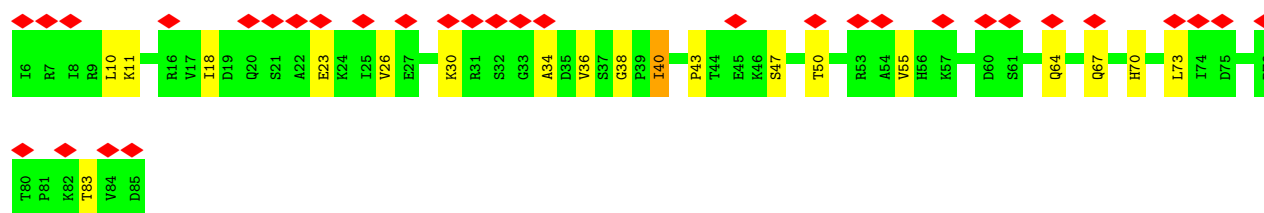
• Molecule 8: 30S ribosomal protein S9

Chain SH: 




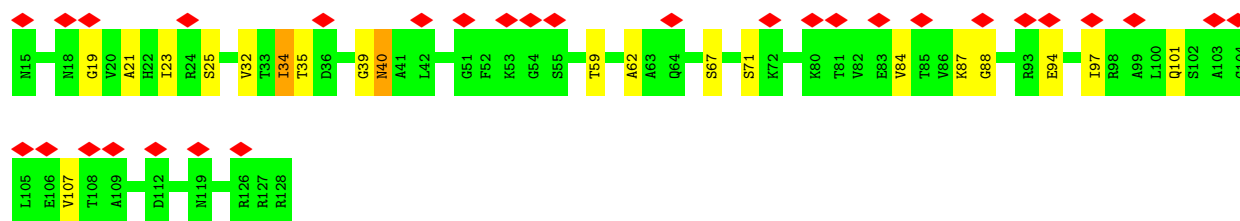
• Molecule 9: 30S ribosomal protein S10

Chain S1: 

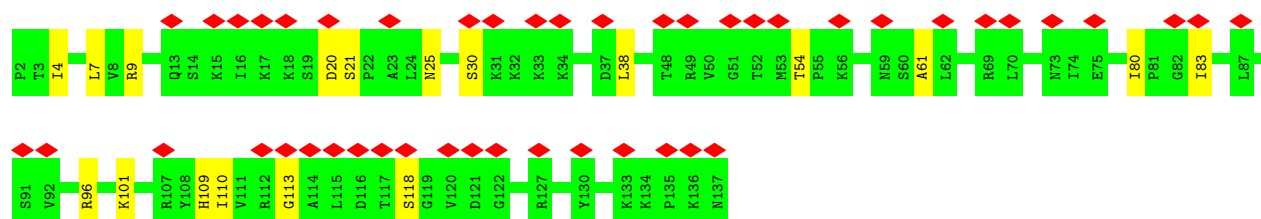
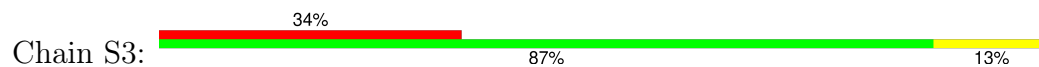


• Molecule 10: 30S ribosomal protein S11

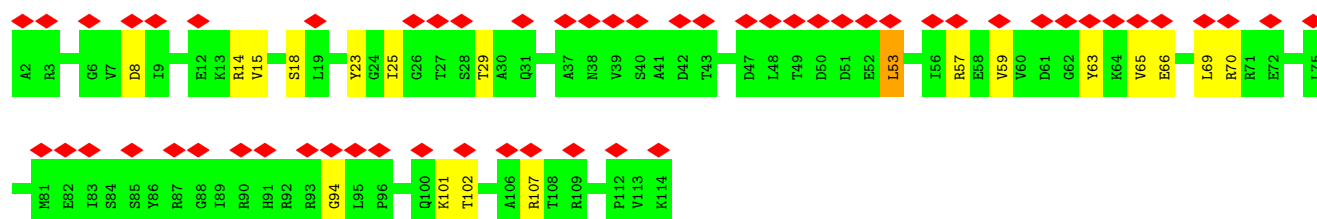
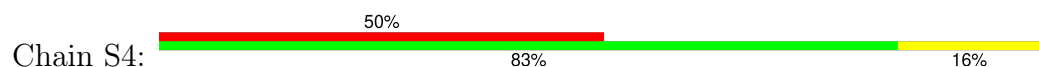
Chain S2: 



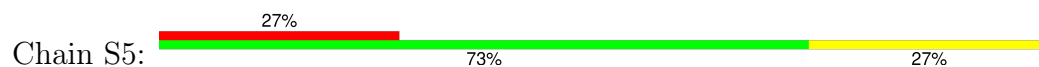
- Molecule 11: 30S ribosomal protein S12



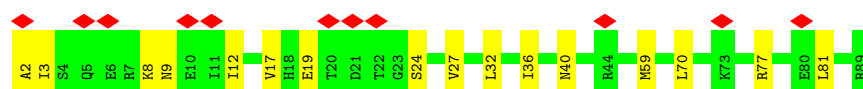
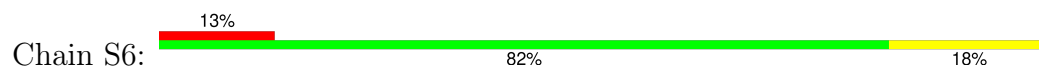
- Molecule 12: 30S ribosomal protein S13



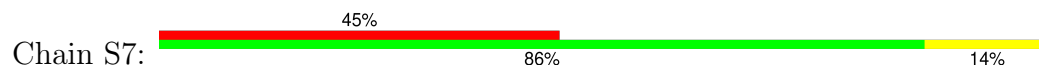
- Molecule 13: 30S ribosomal protein S14 type Z

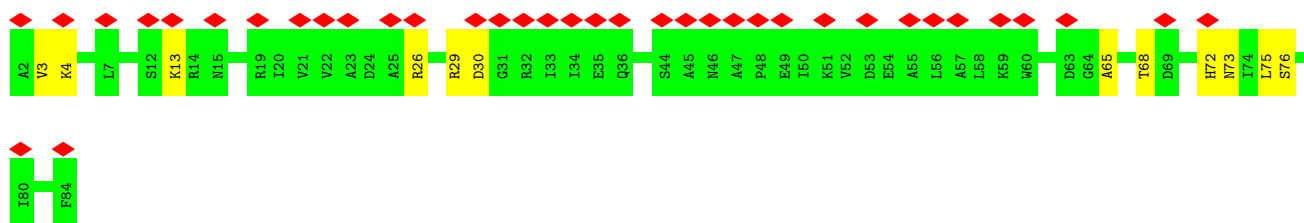


- Molecule 14: 30S ribosomal protein S15

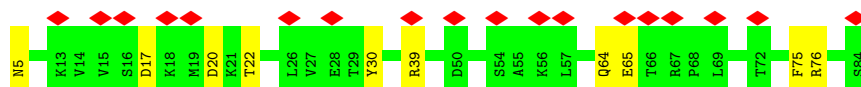
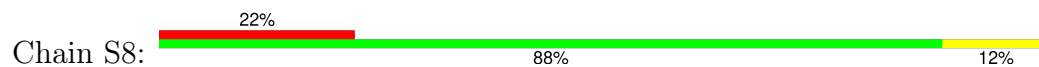


- Molecule 15: 30S ribosomal protein S16

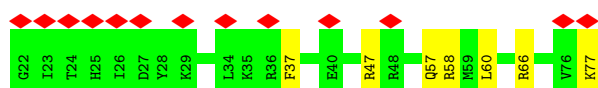
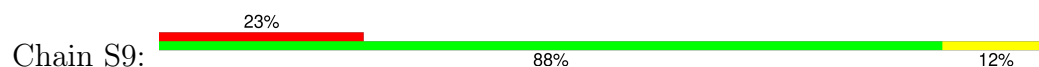




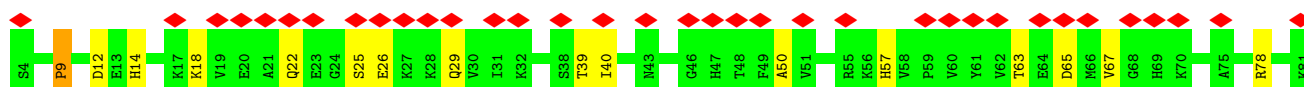
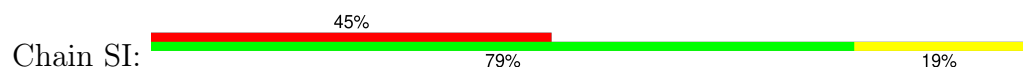
- Molecule 16: 30S ribosomal protein S17



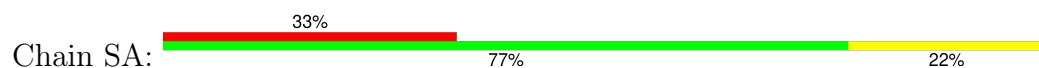
- Molecule 17: 30S ribosomal protein S18



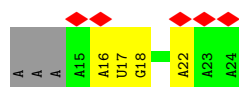
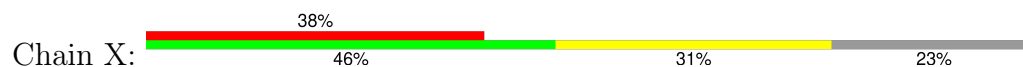
- Molecule 18: 30S ribosomal protein S19



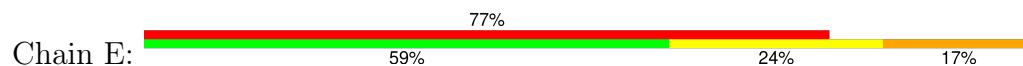
- Molecule 19: 30S ribosomal protein S20

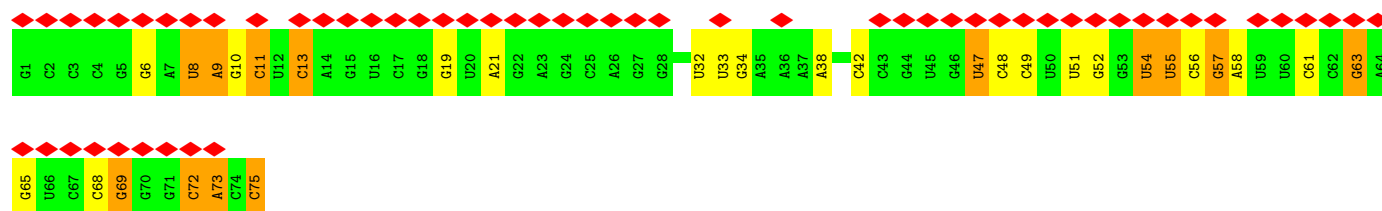


- Molecule 20: mRNA

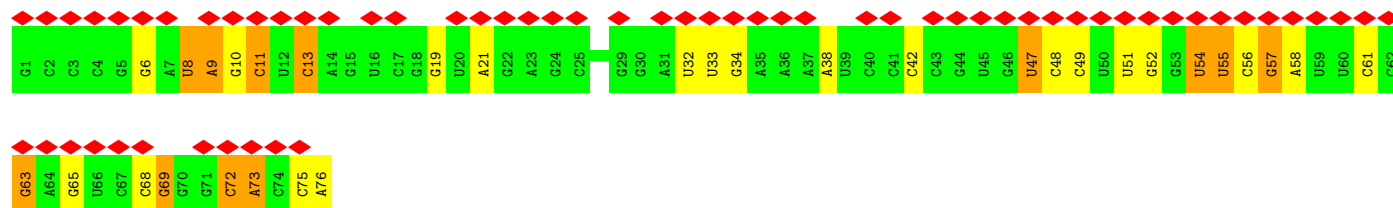
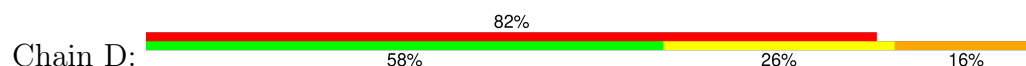


- Molecule 21: P-site tRNA CHAIN

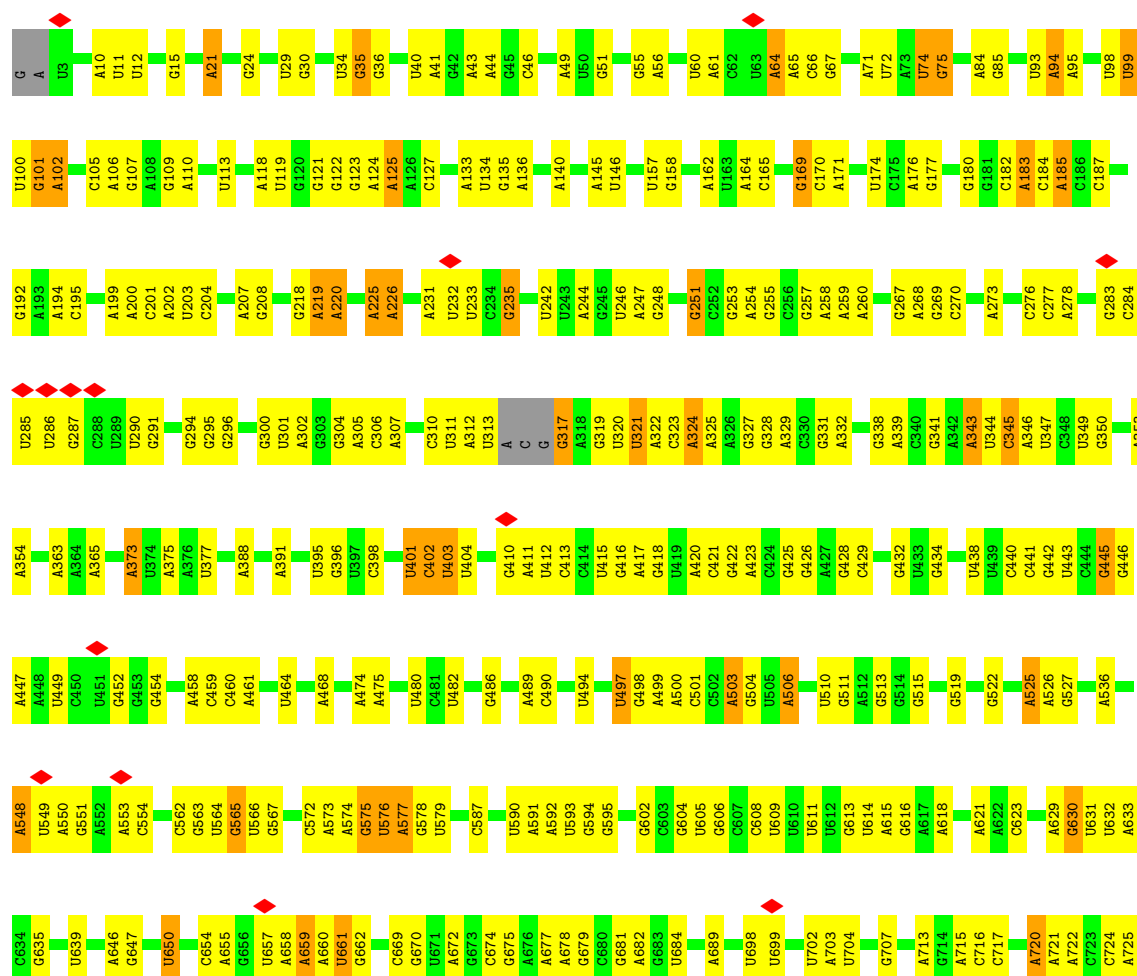




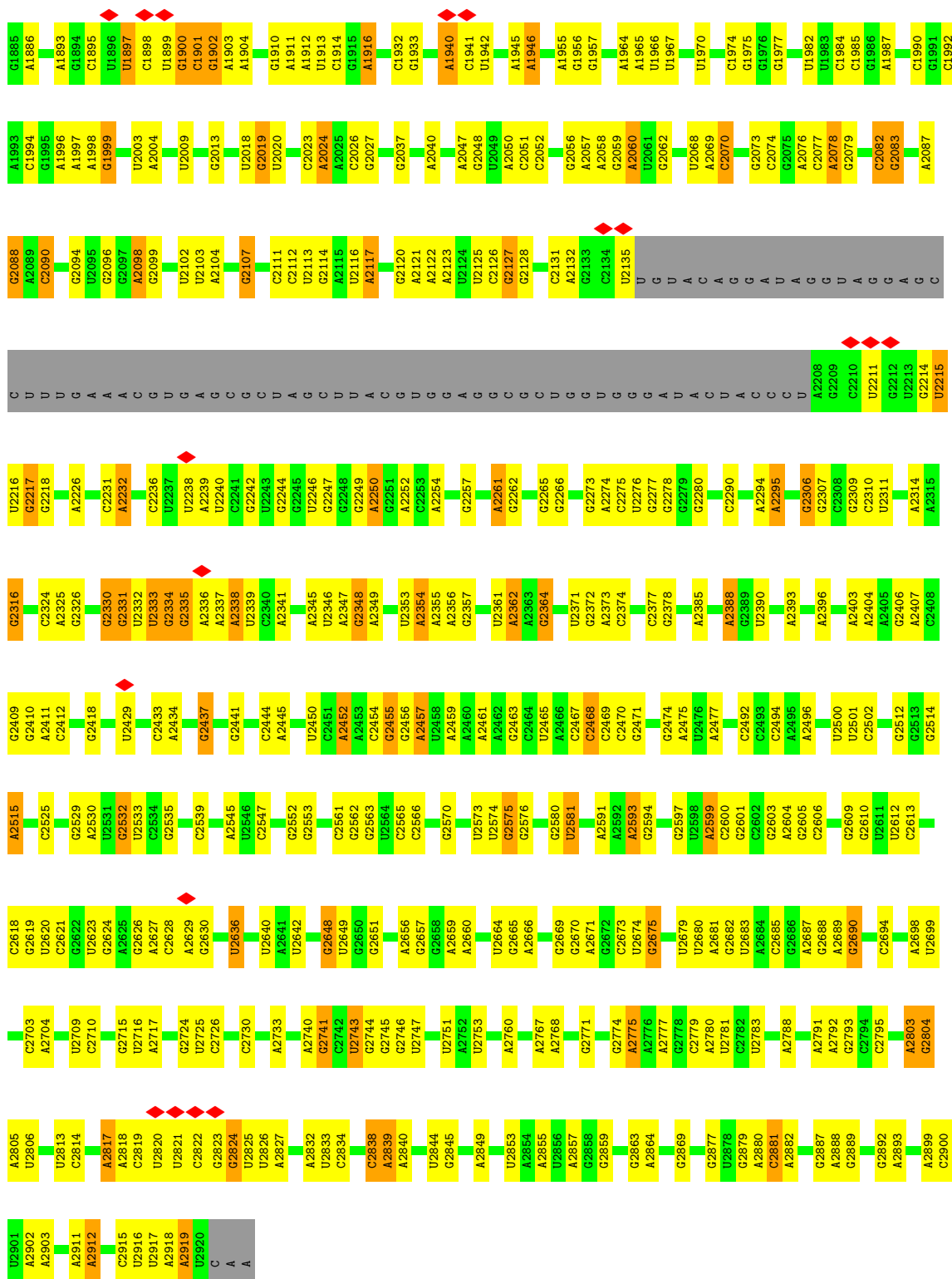
• Molecule 22: E-site tRNA CHAIN



• Molecule 23: 23S RRNA

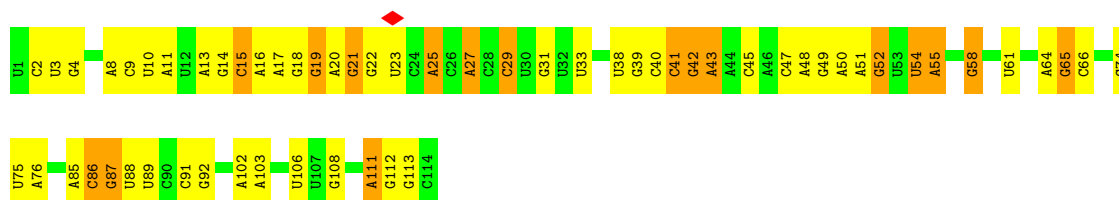


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A1800	G1697	G1596	A1530	A1463	G1383	U1194	C	U1060	G982	A908	A834	U731
A1698	A1698	U1597	U	U1464	G1384	U1195	A	U1063	G983	U916	A835	G736
G1803	U1599	G1465	A	G1466	U1389	C1197	U	A1065	A985	G919	G837	C737
U1806	U1703	A1600	G	G1467	G1392	G1206	U	G1066	G986	G922	A838	G741
A1807	U1707	U1602	C	G1468	G1397	G1207	A	U1067	C988	G923	C841	G752
U1808	U1603	U1603	A	A1471	G1398	A1208	A	G1068	A989	G924	U842	G752
C1809	G1710	C1604	A	C1472	G1399	U1209	G	G1069	G990	G925	G845	C755
A1810	G1711	A1605	A1539	G1473	G1401	U1210	A	A1070	A991	G	A846	A760
A1811	A1712	C1606	U1540	U1477	A1402	G1211	G	A1071	A992	C	A847	A761
A1818	A1713	C1612	C1541	A1478	A1406	U1212	U	G1074	C993	G	A848	A762
U1821	C1716	G1613	G1543	U1482	G1406	C1213	G	U1077	A994	C	U849	A763
C1822	A1720	A1614	G1544	A1483	G1407	U1215	C	U1078	C997	C	G850	C764
U1823	A1720	G1615	U1545	G1484	G1408	U1216	U	G1079	A1001	C	G854	U765
C1824	U1737	A1616	A1546	U1487	U1409	U1217	A	U1080	U1002	C	U855	G766
U1825	G1738	C1622	C1547	A1488	A1410	A1218	U	G1081	A1003	U	U856	A767
G1826	G1739	U1625	U1548	A1489	U1415	G1219	A	C1082	U1004	C	C857	A768
C1827	G1740	G1626	G1550	G1490	U1416	C1221	G	U1083	G1005	G	A864	G774
U1828	G1741	A1826	U	U1491	U1417	U1222	U	U1085	G1012	G	A865	A775
A1742	A1742	G1627	A	G1492	U1420	A1225	C	U1086	G1016	U	A866	A779
G1747	G1747	U1628	A1556	U1493	A1421	G1226	C	C1087	A1017	U	U867	A780
G1748	G1748	A1630	G1557	G1494	A1422	U1227	A	C1088	A1018	A	A868	C781
U1755	U1755	G1631	C1557	G1495	C1423	A1228	U	G1089	A1019	C942	U871	G782
U1755	U1755	A1635	U1558	G1496	A1424	G1234	A	U1090	G1020	C943	U872	G783
U1755	U1755	U1636	U1559	U1497	G1425	C1235	A	G1091	A1024	G944	U873	G783
A1758	G1759	A1637	G1560	U1498	U1426	G1235	A	A1092	A1025	A945	U874	U787
G1759	G1760	G1638	G1561	U1499	U1427	A1241	C	C1093	A1026	A946	U875	A788
U1842	G1761	U1640	A1567	G1500	U1428	A1242	U	G1094	A1027	U947	G876	U787
G1844	U1845	G1641	U1568	G1501	A1432	A1243	U	A1095	G1028	G951	C877	U792
U1845	U1762	G1641	U1568	A1502	U1433	A1244	U	C1096	A1031	A952	U879	G793
A1846	U1763	C1651	G1569	U1503	U1434	U1248	U	U1097	A1032	G	A880	U797
U1763	U1763	A1652	U1570	U1504	A1435	U1249	U	U1098	A1032	A955	A797	A797
A1764	A1764	A1652	G1574	G1505	A1440	C1254	G	G1099	A1032	A956	C883	G802
A1765	A1765	A1653	G1574	C1506	C1440	A1255	A	U	C1035	C957	U884	G802
U1853	U1766	A1654	A1575	A1507	C1441	G1265	U	U	C1036	C957	C885	G805
U1854	G1767	G1657	A1576	C1508	C1442	U1267	U	C1038	C1037	C960	G888	A809
A1855	G1768	G1657	G1577	G1509	A1443	G1268	U	U	C1038	C961	A809	A810
C1857	C1769	A1660	C1579	U1510	U1446	A1269	U	C1039	A1040	A962	C811	U812
C1860	C1770	C1661	A	C1511	A1447	C1271	U	G	G1041	U964	U892	G813
U1861	A1771	A1662	U	U1512	A1448	U1270	C	U	U1042	C967	G883	G813
A1773	A1773	G1663	U	A1514	A1449	G1271	U	U	A1044	A894	A894	A814
C1781	C1781	A1666	G	G1515	A1450	C1274	U	A	A1045	A968	U895	G815
U1784	G1785	G1675	A	C1516	U1451	A1275	A	G	G1046	A969	A897	G816
G1785	A1786	C1682	U1586	A1517	C1452	G1276	U	U	U1047	U970	G900	G820
U1786	U1786	U1682	C1587	G1518	G1453	C1277	A	A	U1048	U971	G901	G822
G1877	G1877	G1686	U1588	A1520	U	G1278	C	C	C1049	A972	G904	A826
U1878	U1878	U1686	U1589	A1521	U	A1285	U	U	C1050	A973	U905	A827
U1879	U1879	C1690	C1590	C1524	A	A1288	A	A	G1051	U974	G906	A906
A1880	G1790	G1691	G1591	U1525	A1459	G1289	C	C	A1057	U976	U905	A827
A1881	G1791	U1592	A1592	G1526	U1460	A1289	C	C	U1058	A977	A828	A828
G1884	C1794	G1692	U1594	A1527	C1461	G1290	A	A				

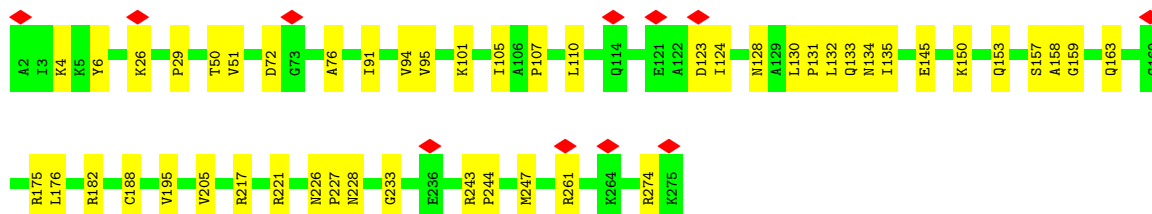
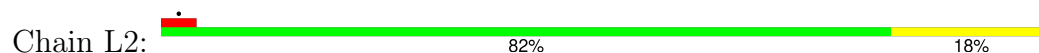


• Molecule 24: 5S rRNA CHAIN

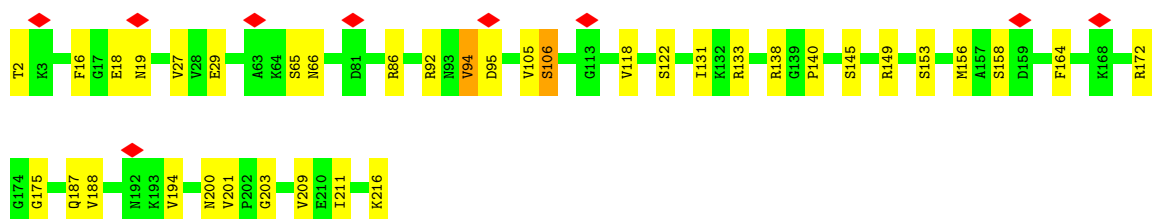
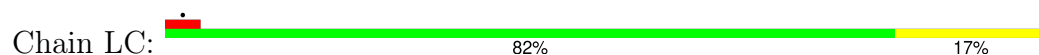




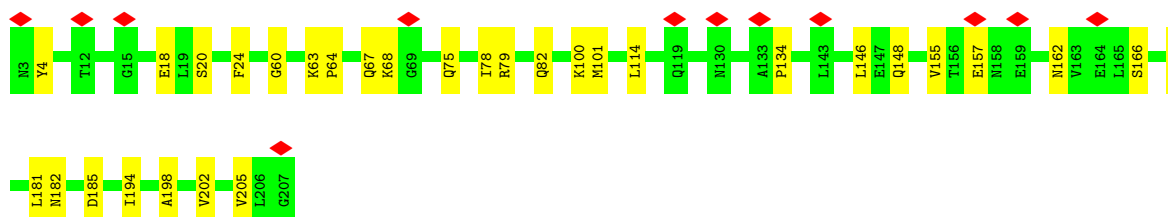
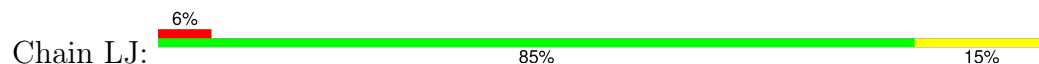
- Molecule 25: 50S ribosomal protein L2



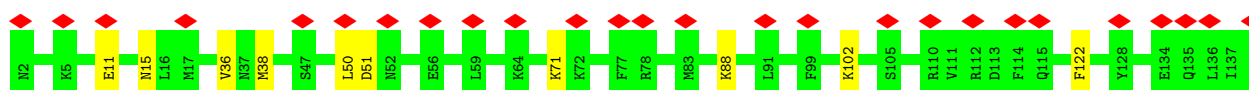
- Molecule 26: 50S ribosomal protein L3

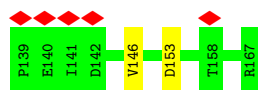


- Molecule 27: 50S ribosomal protein L4

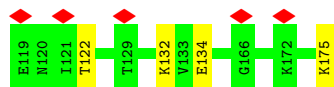
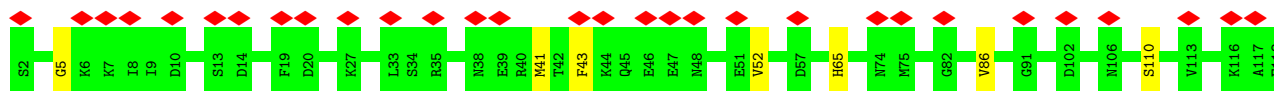


- Molecule 28: 50S ribosomal protein L5

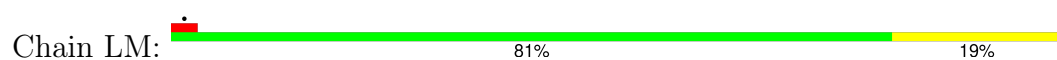




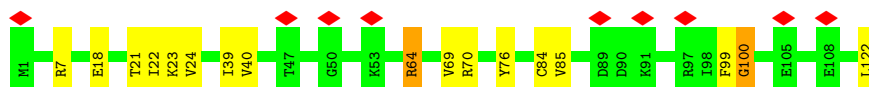
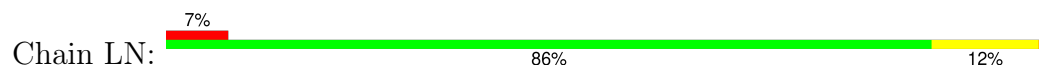
- Molecule 29: 50S ribosomal protein L6



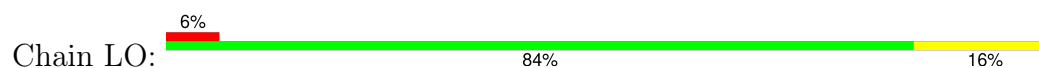
- Molecule 30: 50S ribosomal protein L13



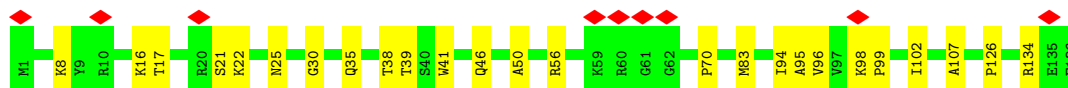
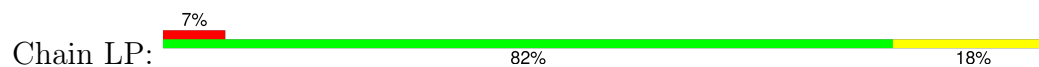
- Molecule 31: 50S ribosomal protein L14



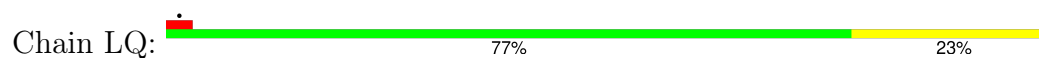
- Molecule 32: 50S ribosomal protein L15

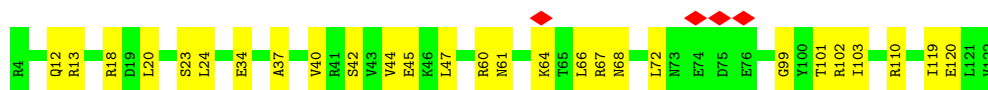


- Molecule 33: 50S ribosomal protein L16

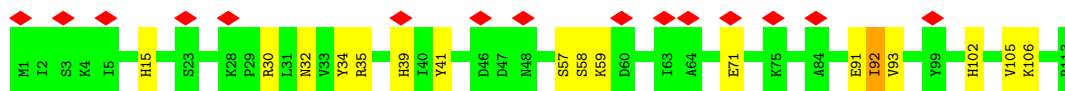
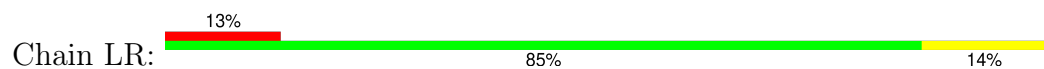


- Molecule 34: 50S ribosomal protein L17

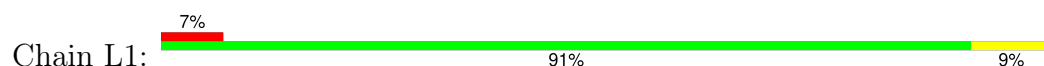




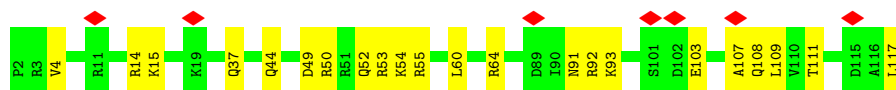
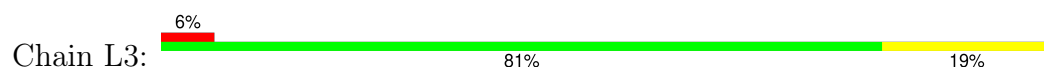
- Molecule 35: 50S ribosomal protein L18



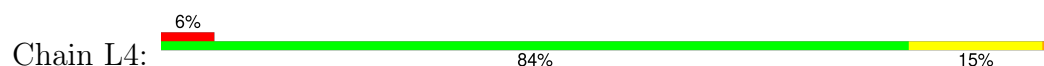
- Molecule 36: 50S ribosomal protein L19



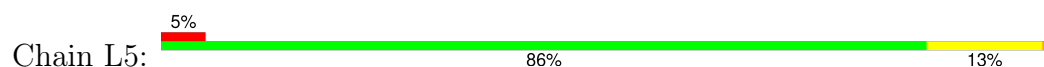
- Molecule 37: 50S ribosomal protein L20



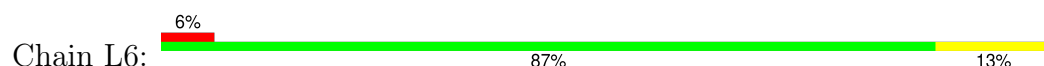
- Molecule 38: 50S ribosomal protein L21



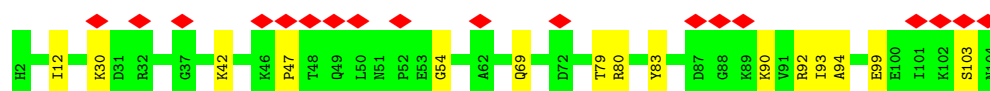
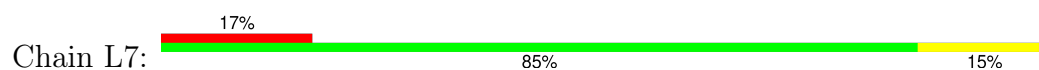
- Molecule 39: 50S ribosomal protein L22



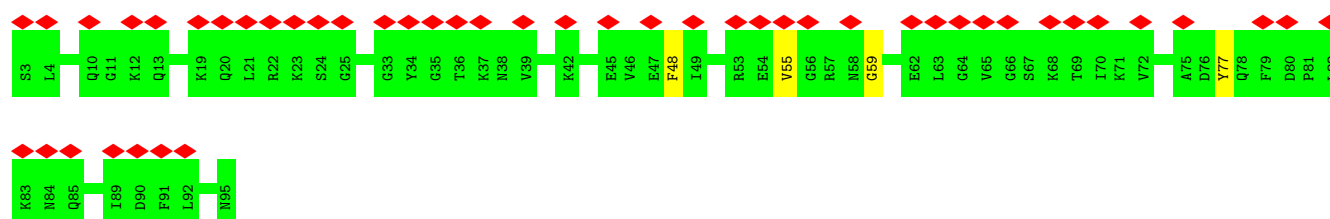
- Molecule 40: 50S ribosomal protein L23



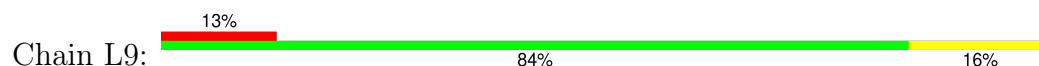
- Molecule 41: 50S ribosomal protein L24



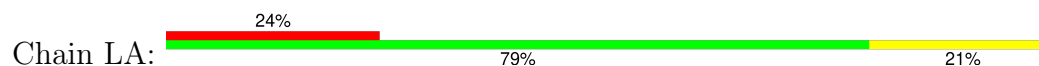
- Molecule 42: 50S ribosomal protein L25



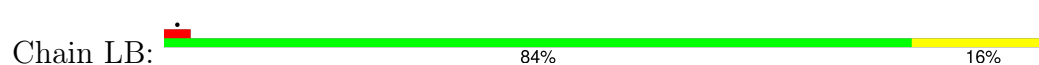
- Molecule 43: 50S ribosomal protein L27



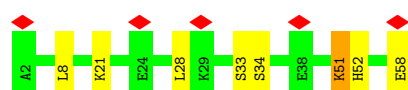
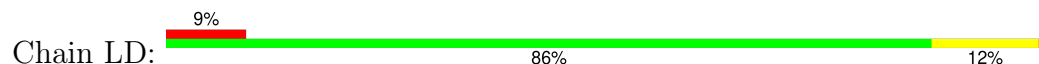
- Molecule 44: 50S ribosomal protein L28



- Molecule 45: 50S ribosomal protein L29

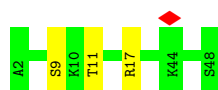


- Molecule 46: 50S ribosomal protein L30

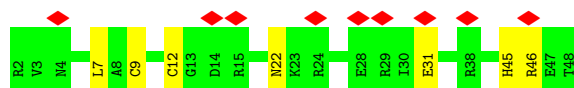
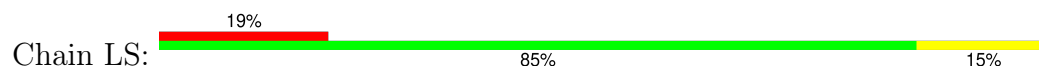


- Molecule 47: 50S ribosomal protein L32

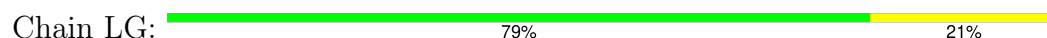




- Molecule 48: 50S ribosomal protein L33 1



- Molecule 49: 50S ribosomal protein L34



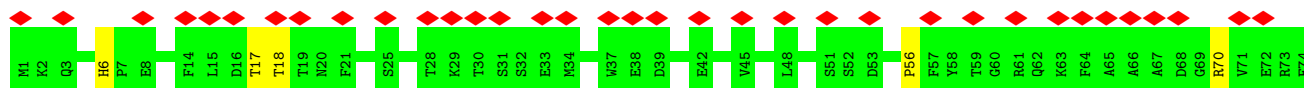
- Molecule 50: 50S ribosomal protein L35



- Molecule 51: 50S ribosomal protein L36



- Molecule 52: 50S ribosomal protein L31 type B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	126000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.370	Depositor
Minimum map value	-0.205	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.065	Depositor
Map size (\AA)	393.6, 393.6, 393.6	wwPDB
Map dimensions	410, 410, 410	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.96000004, 0.96000004, 0.96000004	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PAR, 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	0.45	0/35118	0.55	6/54749 (0.0%)
2	SB	0.38	0/1573	0.72	0/2121
3	SC	0.29	0/1062	0.67	2/1465 (0.1%)
4	SD	0.46	0/1167	0.71	0/1576
5	SE	0.39	0/796	0.65	0/1069
6	SG	0.34	0/1180	0.69	0/1595
7	SF	0.47	0/1019	0.79	0/1371
8	SH	0.35	0/990	0.84	1/1332 (0.1%)
9	S1	0.40	0/637	0.69	1/865 (0.1%)
10	S2	0.39	0/840	0.68	0/1137
11	S3	0.41	0/991	0.80	0/1337
12	S4	0.36	0/835	0.89	4/1123 (0.4%)
13	S5	0.40	0/507	0.78	0/674
14	S6	0.44	0/721	0.70	0/964
15	S7	0.32	0/541	0.69	0/733
16	S8	0.31	0/527	0.61	0/721
17	S9	0.37	0/465	0.68	0/620
18	SI	0.31	0/551	0.76	0/747
19	SA	0.29	0/502	0.52	0/679
20	X	0.39	0/238	0.54	0/368
21	E	0.27	0/1787	0.51	0/2784
22	D	0.28	0/1809	0.51	0/2819
23	B	0.62	0/66138	0.56	7/103134 (0.0%)
24	C	0.46	0/2717	0.54	1/4232 (0.0%)
25	L2	0.63	0/2101	0.71	0/2823
26	LC	0.56	0/1593	0.79	0/2143
27	LJ	0.56	0/1536	0.75	0/2078
28	LK	0.35	0/1033	0.69	0/1412
29	LL	0.29	0/1074	0.54	0/1467
30	LM	0.51	0/1146	0.73	0/1546
31	LN	0.58	0/925	0.85	1/1242 (0.1%)
32	LO	0.56	0/1034	0.79	0/1388

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	LP	0.52	0/1067	0.70	0/1436
34	LQ	0.54	0/900	0.76	0/1205
35	LR	0.41	0/770	0.70	0/1044
36	L1	0.50	0/844	0.66	0/1134
37	L3	0.61	0/954	0.74	0/1264
38	L4	0.51	0/758	0.70	0/1014
39	L5	0.60	0/845	0.74	0/1140
40	L6	0.56	0/701	0.72	0/939
41	L7	0.38	0/742	0.71	2/1001 (0.2%)
42	L8	0.31	0/655	0.65	0/888
43	L9	0.54	0/621	0.75	0/824
44	LA	0.48	0/449	0.71	0/600
45	LB	0.44	0/494	0.70	0/660
46	LD	0.50	0/438	0.74	0/591
47	LE	0.56	0/361	0.71	0/481
48	LS	0.43	0/385	0.72	0/518
49	LG	0.67	0/371	0.79	0/484
50	LH	0.51	0/450	0.84	2/597 (0.3%)
51	LI	0.49	0/275	0.70	0/366
52	LF	0.25	0/454	0.58	0/624
All	All	0.53	0/145687	0.60	27/219124 (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
5	SE	0	1
6	SG	0	1
10	S2	0	1
11	S3	0	1
13	S5	0	1
15	S7	0	1
18	SI	0	1
25	L2	0	1
26	LC	0	3
28	LK	0	1
30	LM	0	1
31	LN	0	1
33	LP	0	1
34	LQ	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
38	L4	0	2
42	L8	0	2
43	L9	0	1
48	LS	0	1
50	LH	0	1
All	All	0	23

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	317	G	OP1-P-O3'	-9.59	79.22	108.00
12	S4	8	ASP	CA-C-N	6.40	126.58	120.43
12	S4	8	ASP	C-N-CA	6.40	126.58	120.43
23	B	317	G	OP2-P-O3'	-5.89	90.33	108.00
12	S4	94	GLY	CA-C-N	5.74	129.03	122.83

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	S2	40	ASN	Peptide
11	S3	54	THR	Peptide
13	S5	15	LYS	Peptide
5	SE	43	TRP	Peptide
6	SG	124	ILE	Peptide

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	A	31369	0	15803	351	0
2	SB	1551	0	1570	31	0
3	SC	1058	0	568	8	0
4	SD	1153	0	1210	19	0
5	SE	785	0	781	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	SG	1164	0	1146	20	0
7	SF	1007	0	1050	22	0
8	SH	975	0	970	37	0
9	S1	626	0	628	12	0
10	S2	826	0	817	13	0
11	S3	976	0	966	11	0
12	S4	828	0	809	10	0
13	S5	497	0	512	13	0
14	S6	713	0	733	12	0
15	S7	537	0	462	9	0
16	S8	520	0	415	6	0
17	S9	458	0	496	7	0
18	SI	541	0	482	10	0
19	SA	503	0	451	13	0
20	X	213	0	108	0	0
21	E	1600	0	810	15	0
22	D	1619	0	822	14	0
23	B	59059	0	29695	460	0
24	C	2430	0	1229	28	0
25	L2	2066	0	2161	32	0
26	LC	1570	0	1593	22	0
27	LJ	1514	0	1540	21	0
28	LK	1026	0	797	8	0
29	LL	1062	0	808	6	0
30	LM	1124	0	1101	17	0
31	LN	918	0	981	8	0
32	LO	1020	0	998	18	0
33	LP	1043	0	1084	16	0
34	LQ	898	0	932	19	0
35	LR	765	0	720	11	0
36	L1	832	0	875	10	0
37	L3	942	0	1014	20	0
38	L4	749	0	730	10	0
39	L5	837	0	893	13	0
40	L6	694	0	705	7	0
41	L7	734	0	731	11	0
42	L8	648	0	598	1	0
43	L9	615	0	637	9	0
44	LA	443	0	461	8	0
45	LB	493	0	503	6	0
46	LD	436	0	474	5	0
47	LE	356	0	354	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	LS	380	0	379	3	0
49	LG	367	0	415	8	0
50	LH	446	0	465	4	0
51	LI	272	0	290	9	0
52	LF	447	0	289	4	0
53	A	42	0	44	0	0
54	A	27	0	0	0	0
54	B	99	0	0	0	0
54	C	2	0	0	0	0
54	SG	1	0	0	0	0
All	All	133876	0	85105	1269	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 6.

The worst 5 of 1269 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)
23:B:1037:A:N7	23:B:1206:G:N1	2.02	1.08
23:B:1037:A:C5	23:B:1206:G:N1	2.22	1.07
1:A:251:A:C5	1:A:289:G:N2	2.26	1.03
23:B:497:U:C2	23:B:499:A:N7	2.27	1.02
23:B:420:A:H62	23:B:446:G:N2	1.62	0.98

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	
2	SB	200/202 (99%)	165 (82%)	34 (17%)	1 (0%)	25	60
3	SC	196/198 (99%)	151 (77%)	45 (23%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	SD	154/156 (99%)	135 (88%)	19 (12%)	0	100	100
5	SE	93/95 (98%)	87 (94%)	6 (6%)	0	100	100
6	SG	153/155 (99%)	134 (88%)	19 (12%)	0	100	100
7	SF	128/130 (98%)	110 (86%)	18 (14%)	0	100	100
8	SH	125/127 (98%)	101 (81%)	24 (19%)	0	100	100
9	S1	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
10	S2	112/114 (98%)	85 (76%)	27 (24%)	0	100	100
11	S3	134/136 (98%)	98 (73%)	36 (27%)	0	100	100
12	S4	111/113 (98%)	87 (78%)	24 (22%)	0	100	100
13	S5	58/60 (97%)	49 (84%)	9 (16%)	0	100	100
14	S6	86/88 (98%)	77 (90%)	9 (10%)	0	100	100
15	S7	81/83 (98%)	60 (74%)	21 (26%)	0	100	100
16	S8	78/80 (98%)	58 (74%)	20 (26%)	0	100	100
17	S9	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
18	SI	76/78 (97%)	54 (71%)	21 (28%)	1 (1%)	10	41
19	SA	76/79 (96%)	74 (97%)	2 (3%)	0	100	100
25	L2	272/274 (99%)	230 (85%)	42 (15%)	0	100	100
26	LC	213/215 (99%)	164 (77%)	46 (22%)	3 (1%)	9	39
27	LJ	203/205 (99%)	174 (86%)	27 (13%)	2 (1%)	13	46
28	LK	164/166 (99%)	120 (73%)	44 (27%)	0	100	100
29	LL	172/174 (99%)	136 (79%)	36 (21%)	0	100	100
30	LM	143/145 (99%)	118 (82%)	24 (17%)	1 (1%)	19	54
31	LN	120/122 (98%)	97 (81%)	22 (18%)	1 (1%)	16	51
32	LO	143/145 (99%)	107 (75%)	36 (25%)	0	100	100
33	LP	134/136 (98%)	114 (85%)	19 (14%)	1 (1%)	19	54
34	LQ	117/119 (98%)	98 (84%)	19 (16%)	0	100	100
35	LR	111/113 (98%)	85 (77%)	25 (22%)	1 (1%)	14	48
36	L1	107/109 (98%)	95 (89%)	12 (11%)	0	100	100
37	L3	114/116 (98%)	107 (94%)	7 (6%)	0	100	100
38	L4	100/102 (98%)	83 (83%)	16 (16%)	1 (1%)	13	46
39	L5	110/112 (98%)	97 (88%)	13 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	L6	87/89 (98%)	75 (86%)	12 (14%)	0	100	100
41	L7	101/103 (98%)	80 (79%)	21 (21%)	0	100	100
42	L8	91/93 (98%)	78 (86%)	13 (14%)	0	100	100
43	L9	80/82 (98%)	67 (84%)	13 (16%)	0	100	100
44	LA	56/58 (97%)	47 (84%)	9 (16%)	0	100	100
45	LB	60/62 (97%)	53 (88%)	7 (12%)	0	100	100
46	LD	55/57 (96%)	48 (87%)	7 (13%)	0	100	100
47	LE	45/47 (96%)	37 (82%)	8 (18%)	0	100	100
48	LS	45/47 (96%)	39 (87%)	6 (13%)	0	100	100
49	LG	41/43 (95%)	38 (93%)	3 (7%)	0	100	100
50	LH	58/60 (97%)	46 (79%)	12 (21%)	0	100	100
51	LI	35/37 (95%)	27 (77%)	8 (23%)	0	100	100
52	LF	72/74 (97%)	46 (64%)	26 (36%)	0	100	100
All	All	5042/5135 (98%)	4153 (82%)	877 (17%)	12 (0%)	45	75

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	LR	71	GLU
2	SB	129	PHE
18	SI	9	PRO
27	LJ	67	GLN
26	LC	19	ASN

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 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	
2	SB	151/164 (92%)	149 (99%)	2 (1%)	65	76
3	SC	23/174 (13%)	23 (100%)	0	100	100
4	SD	120/122 (98%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	SE	82/83 (99%)	82 (100%)	0	100	100
6	SG	115/131 (88%)	114 (99%)	1 (1%)	75	83
7	SF	107/111 (96%)	104 (97%)	3 (3%)	38	59
8	SH	96/105 (91%)	95 (99%)	1 (1%)	73	81
9	S1	67/73 (92%)	67 (100%)	0	100	100
10	S2	85/90 (94%)	84 (99%)	1 (1%)	67	78
11	S3	95/118 (80%)	94 (99%)	1 (1%)	70	79
12	S4	75/97 (77%)	73 (97%)	2 (3%)	40	60
13	S5	51/52 (98%)	51 (100%)	0	100	100
14	S6	74/80 (92%)	74 (100%)	0	100	100
15	S7	36/70 (51%)	36 (100%)	0	100	100
16	S8	35/75 (47%)	35 (100%)	0	100	100
17	S9	49/50 (98%)	49 (100%)	0	100	100
18	SI	45/69 (65%)	45 (100%)	0	100	100
19	SA	37/66 (56%)	37 (100%)	0	100	100
25	L2	212/221 (96%)	212 (100%)	0	100	100
26	LC	158/173 (91%)	155 (98%)	3 (2%)	52	70
27	LJ	154/168 (92%)	153 (99%)	1 (1%)	84	88
28	LK	67/147 (46%)	67 (100%)	0	100	100
29	LL	61/152 (40%)	60 (98%)	1 (2%)	58	73
30	LM	117/123 (95%)	114 (97%)	3 (3%)	41	61
31	LN	100/100 (100%)	98 (98%)	2 (2%)	50	68
32	LO	91/111 (82%)	91 (100%)	0	100	100
33	LP	101/113 (89%)	101 (100%)	0	100	100
34	LQ	90/100 (90%)	90 (100%)	0	100	100
35	LR	63/90 (70%)	62 (98%)	1 (2%)	58	73
36	L1	83/95 (87%)	83 (100%)	0	100	100
37	L3	96/96 (100%)	93 (97%)	3 (3%)	35	56
38	L4	68/86 (79%)	68 (100%)	0	100	100
39	L5	84/91 (92%)	83 (99%)	1 (1%)	67	78
40	L6	72/80 (90%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	L7	71/88 (81%)	71 (100%)	0	100	100
42	L8	58/82 (71%)	58 (100%)	0	100	100
43	L9	61/64 (95%)	61 (100%)	0	100	100
44	LA	43/49 (88%)	42 (98%)	1 (2%)	45	64
45	LB	52/57 (91%)	51 (98%)	1 (2%)	52	70
46	LD	50/51 (98%)	48 (96%)	2 (4%)	27	51
47	LE	35/43 (81%)	35 (100%)	0	100	100
48	LS	42/45 (93%)	42 (100%)	0	100	100
49	LG	39/39 (100%)	39 (100%)	0	100	100
50	LH	44/52 (85%)	43 (98%)	1 (2%)	45	64
51	LI	29/35 (83%)	29 (100%)	0	100	100
52	LF	23/66 (35%)	23 (100%)	0	100	100
All	All	3507/4347 (81%)	3476 (99%)	31 (1%)	74	83

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	LJ	114	LEU
45	LB	66	LYS
30	LM	58	ILE
46	LD	58	GLU
37	L3	117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
40	L6	73	ASN
42	L8	84	ASN
47	LE	40	HIS
11	S3	42	GLN
11	S3	13	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1455/1555 (93%)	523 (35%)	24 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	X	9/13 (69%)	4 (44%)	1 (11%)
21	E	74/75 (98%)	25 (33%)	1 (1%)
22	D	75/76 (98%)	26 (34%)	1 (1%)
23	B	2746/2923 (93%)	817 (29%)	28 (1%)
24	C	113/114 (99%)	37 (32%)	1 (0%)
All	All	4472/4756 (94%)	1432 (32%)	56 (1%)

5 of 1432 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	U
1	A	9	A
1	A	10	G
1	A	21	U
1	A	23	G

5 of 56 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	B	267	G
24	C	40	C
23	B	850	G
23	B	2709	U
23	B	1940	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 130 ligands modelled in this entry, 129 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
53	PAR	A	1601	-	44,45,45	0.28	0	63,67,67	1.09	6 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	PAR	A	1601	-	-	3/18/94/94	0/4/4/4

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A	1601	PAR	O52-C13-O43	-3.60	107.69	111.37
53	A	1601	PAR	C13-C23-C33	-3.23	98.21	102.10
53	A	1601	PAR	O33-C14-C24	-2.96	103.24	108.08
53	A	1601	PAR	C32-C22-C12	-2.57	106.61	111.02
53	A	1601	PAR	O11-C42-C32	-2.21	103.90	109.18

There are no chirality outliers.

All (3) torsion outliers are listed below:

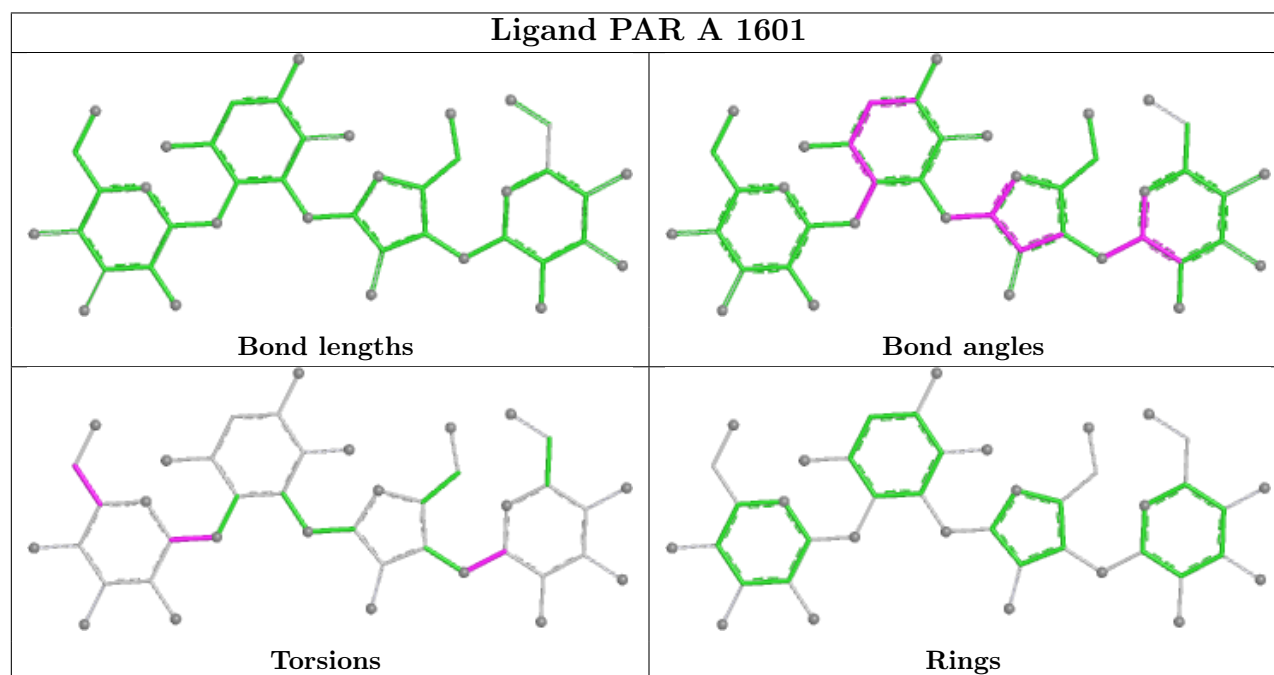
Mol	Chain	Res	Type	Atoms
53	A	1601	PAR	O54-C14-O33-C33
53	A	1601	PAR	O51-C11-O11-C42
53	A	1601	PAR	O51-C51-C61-O61

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1460:C	O3'	1461:U	P	4.77

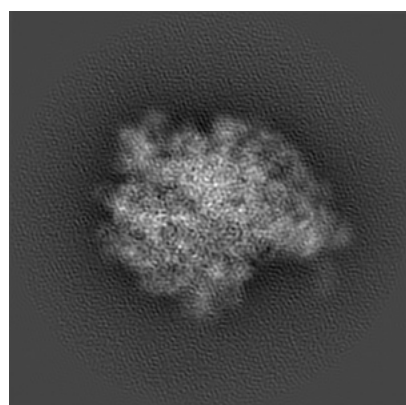
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8402. These allow visual inspection of the internal detail of the map and identification of artifacts.

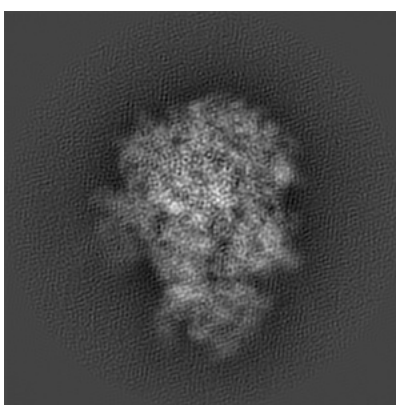
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

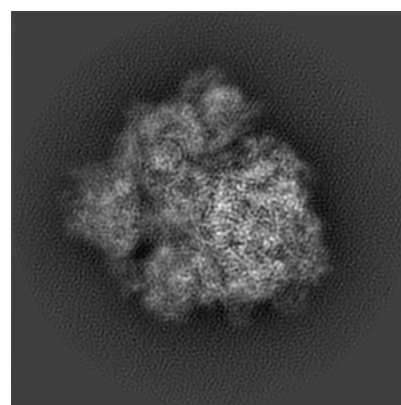
6.1.1 Primary map



X



Y

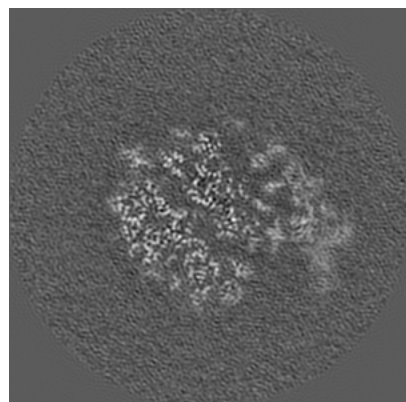


Z

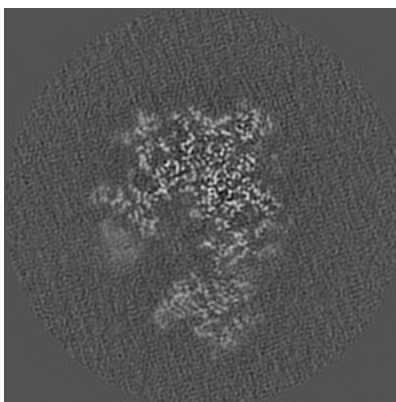
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

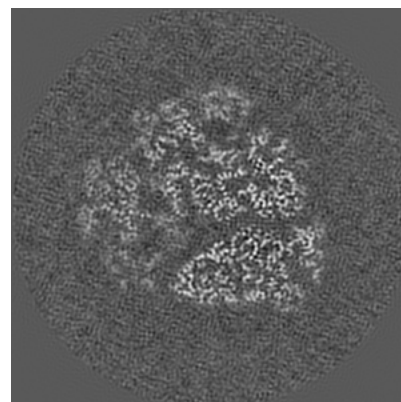
6.2.1 Primary map



X Index: 205



Y Index: 205

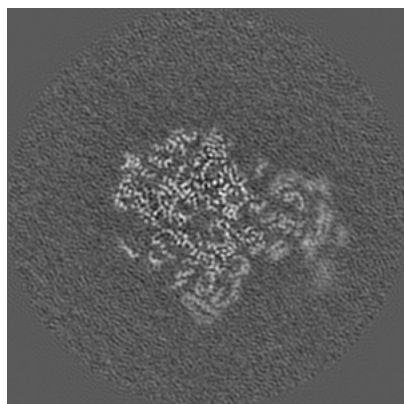


Z Index: 205

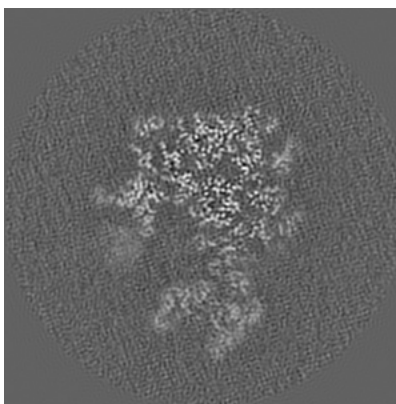
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

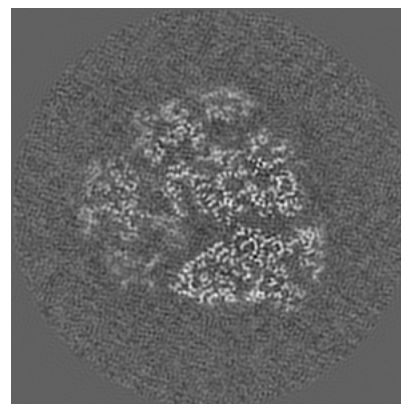
6.3.1 Primary map



X Index: 215



Y Index: 211

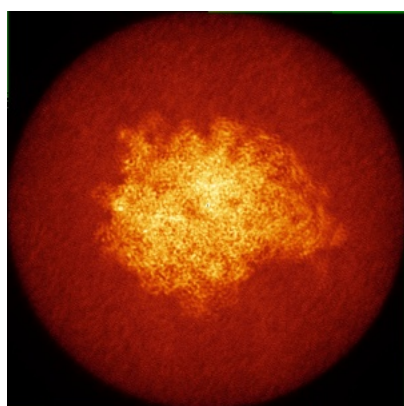


Z Index: 206

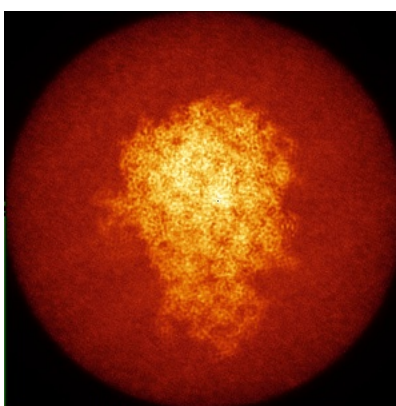
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

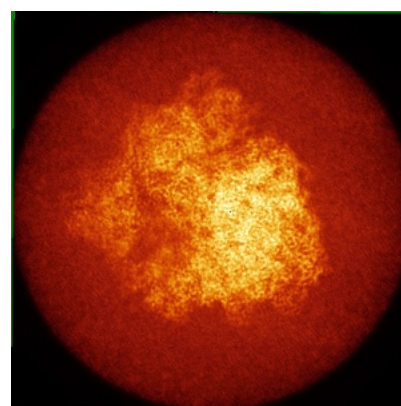
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.065. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

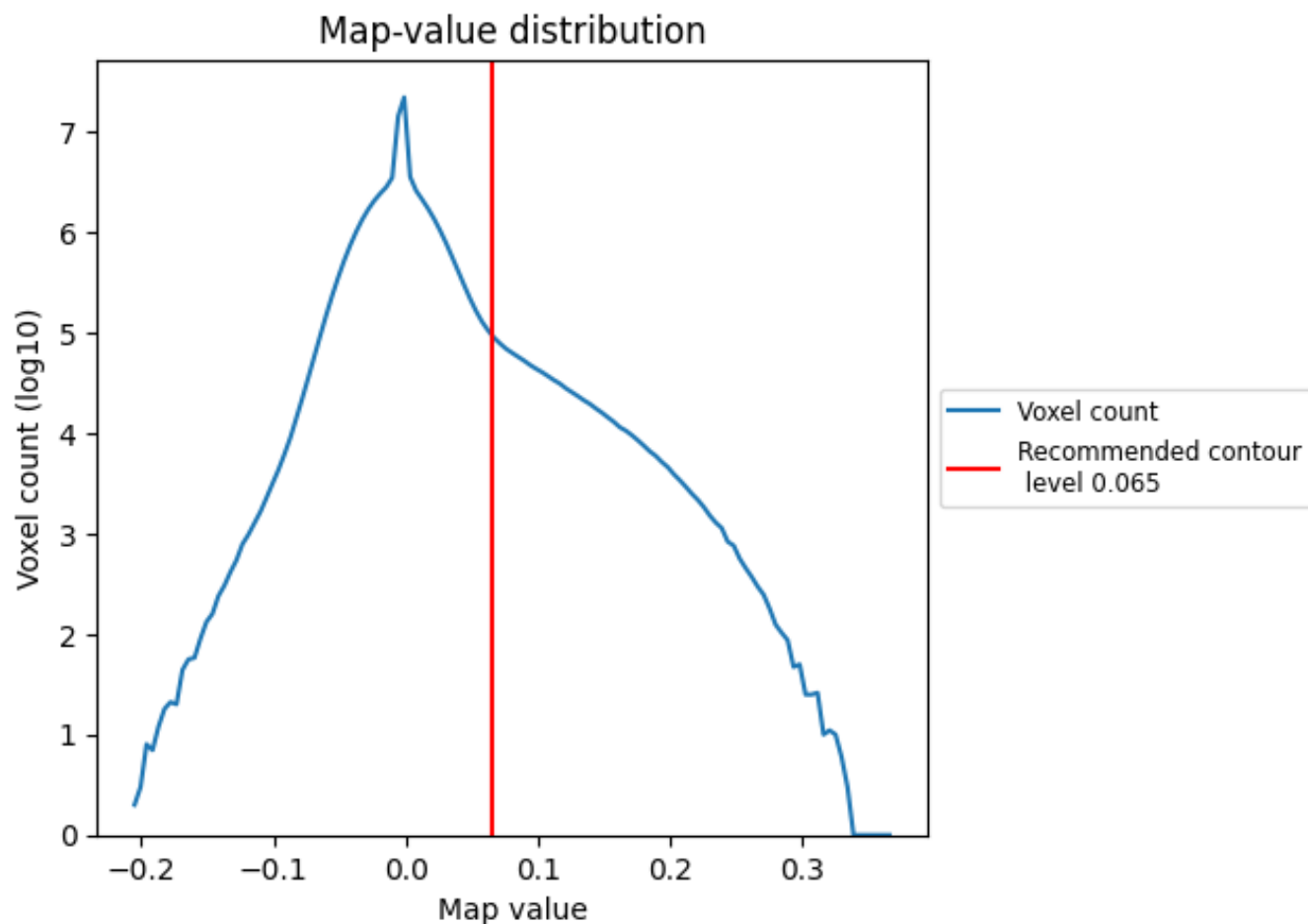
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

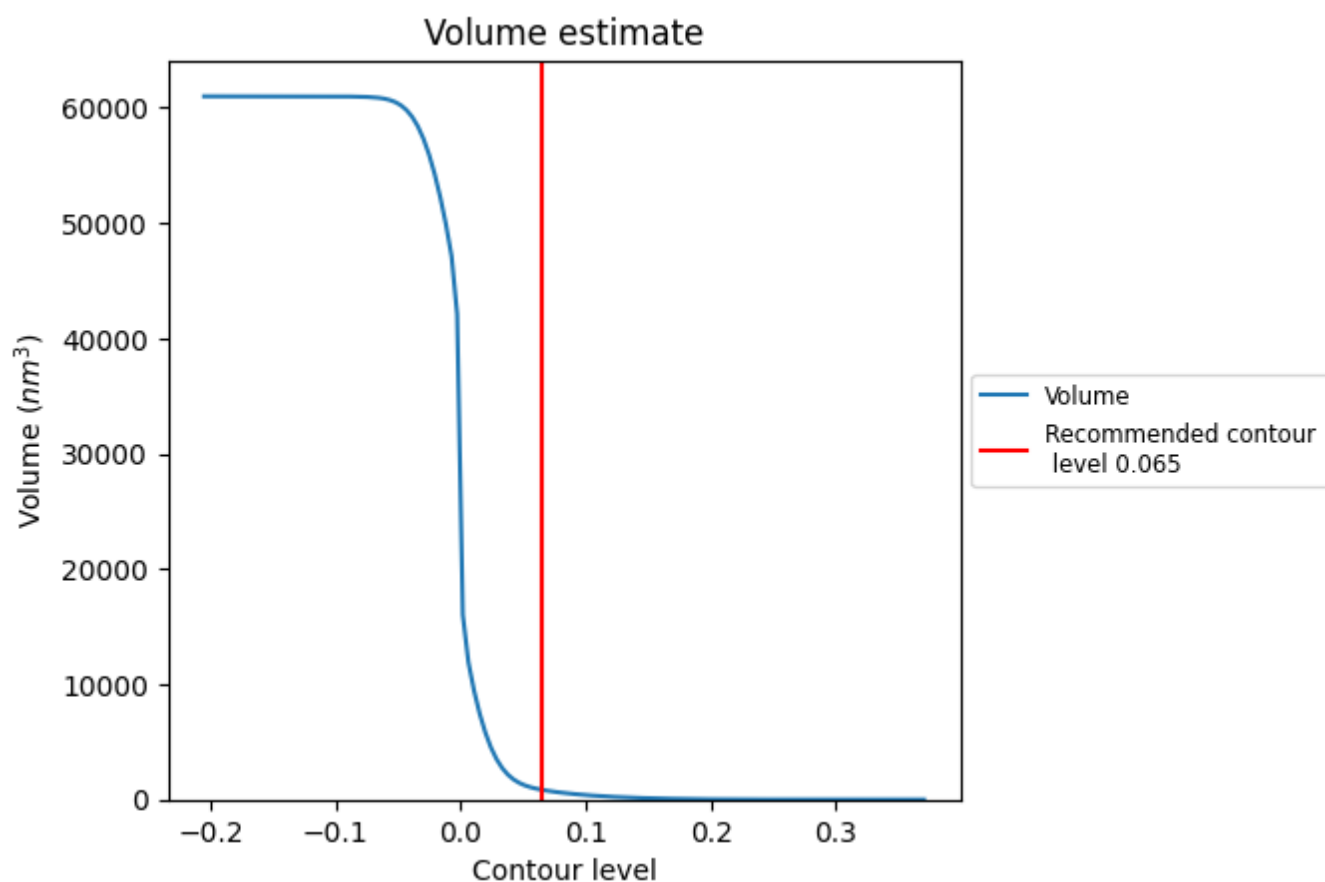
This section contains the results of statistical analysis of the map.

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.

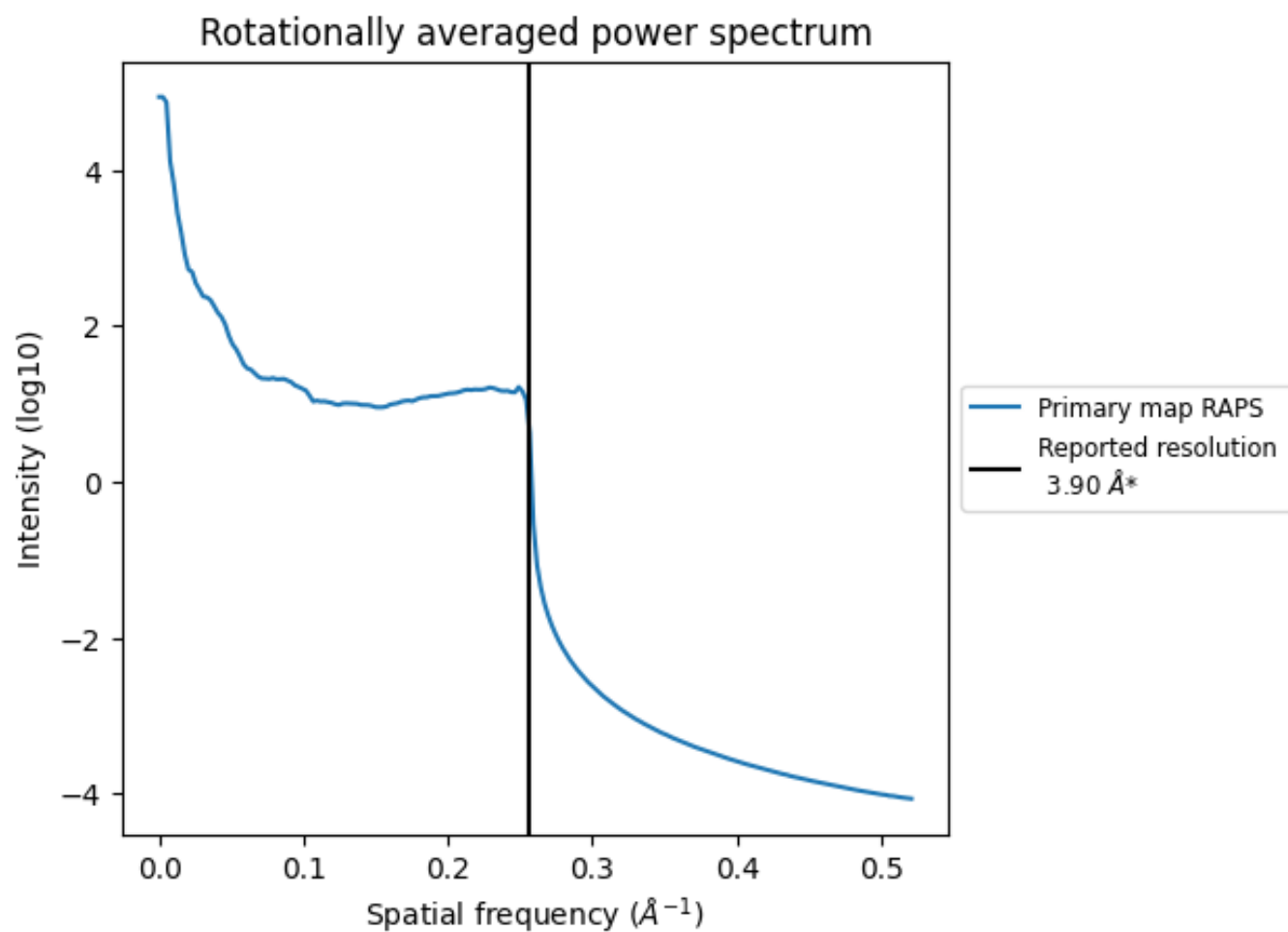
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 844 nm³; this corresponds to an approximate mass of 762 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

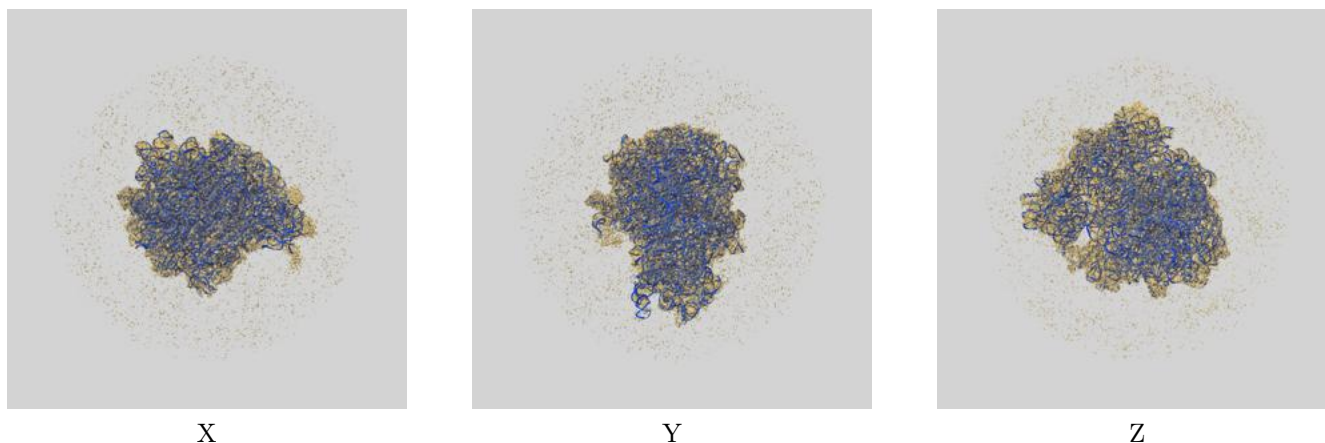
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

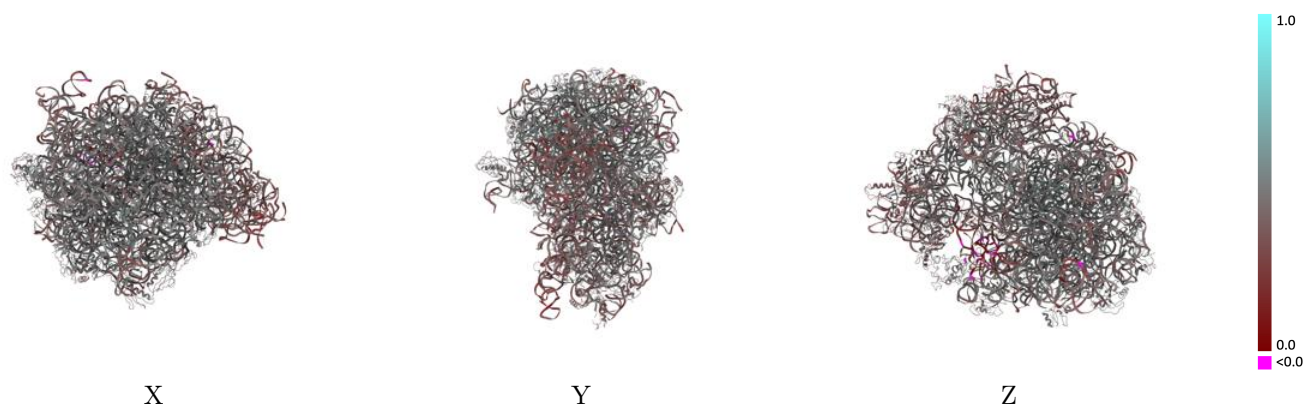
This section contains information regarding the fit between EMDB map EMD-8402 and PDB model 5TCU. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



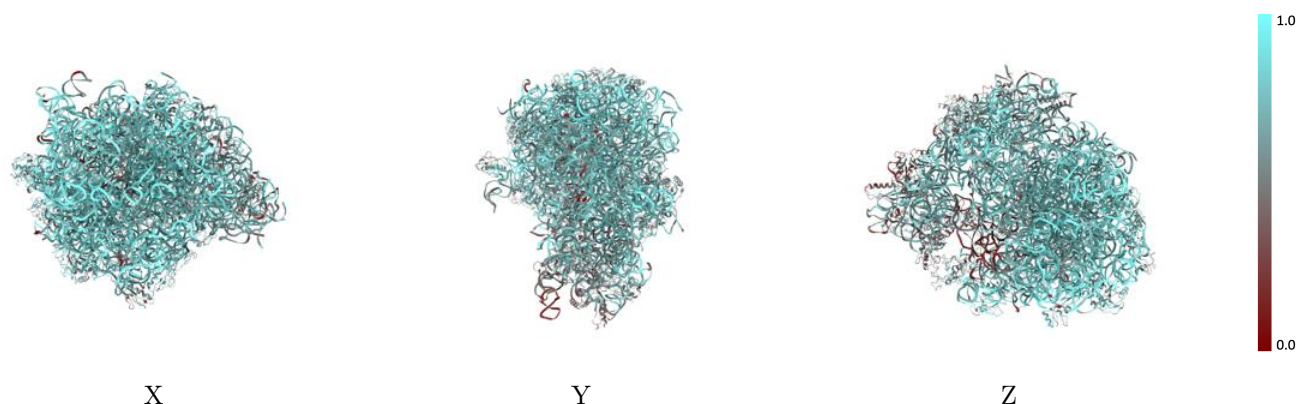
The images above show the 3D surface view of the map at the recommended contour level 0.065 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



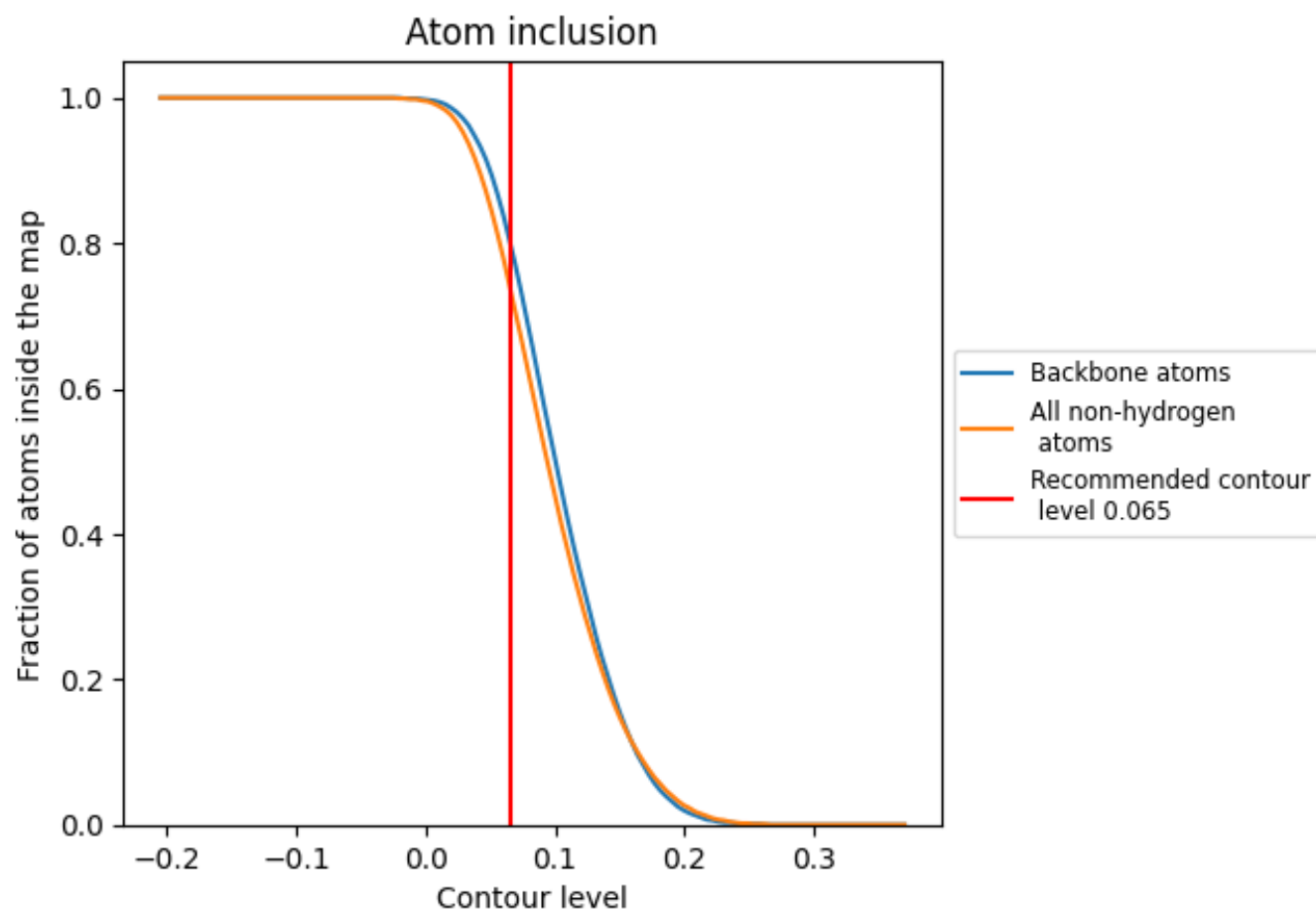
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.065).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 74% 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 (0.065) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7410	 0.4310
A	 0.7350	 0.3970
B	 0.8450	 0.4480
C	 0.8290	 0.4150
D	 0.2460	 0.1320
E	 0.2540	 0.2870
L1	 0.7020	 0.4910
L2	 0.7320	 0.5000
L3	 0.7290	 0.4710
L4	 0.7310	 0.4780
L5	 0.6950	 0.4870
L6	 0.6930	 0.4630
L7	 0.5790	 0.4400
L8	 0.4020	 0.4390
L9	 0.6830	 0.4890
LA	 0.5790	 0.4600
LB	 0.7060	 0.4520
LC	 0.7330	 0.4820
LD	 0.6780	 0.4860
LE	 0.7230	 0.4860
LF	 0.4920	 0.4100
LG	 0.7430	 0.4970
LH	 0.7980	 0.5100
LI	 0.6960	 0.4930
LJ	 0.7140	 0.4740
LK	 0.6300	 0.4380
LL	 0.6320	 0.4390
LM	 0.6810	 0.4750
LN	 0.6460	 0.4900
LO	 0.7360	 0.4800
LP	 0.6850	 0.4890
LQ	 0.7160	 0.4820
LR	 0.6780	 0.4310
LS	 0.6100	 0.4690
S1	 0.4910	 0.4130



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Chain	Atom inclusion	Q-score
S2	 0.5280	 0.4240
S3	 0.5180	 0.4320
S4	 0.4080	 0.3840
S5	 0.5190	 0.4440
S6	 0.6410	 0.4290
S7	 0.5020	 0.3830
S8	 0.5750	 0.4260
S9	 0.5600	 0.4390
SA	 0.5170	 0.3590
SB	 0.4450	 0.4140
SC	 0.5110	 0.3810
SD	 0.6060	 0.4600
SE	 0.5760	 0.4280
SF	 0.6220	 0.4430
SG	 0.4270	 0.4130
SH	 0.5130	 0.4010
SI	 0.4160	 0.3940
X	 0.4550	 0.4080