wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 06:30 am GMT

PDB ID	:	6GZ5
EMDB ID	:	EMD-0100
Title	:	tRNA translocation by the eukaryotic 80S ribosome and the impact of GTP hydrolysis, Translocation-intermediate-POST-3 (TI-POST-3)
Authors	:	Flis, J.; Holm, M.; Rundlet, E.J.; Loerke, J.; Hilal, T.; Dabrowski, M.; Buerger, J.; Mielke, T.; Blanchard, S.C.; Spahn, C.M.T.; Budkevich, T.V.
Deposited on	:	2018-07-03
Resolution	:	3.50 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 (i) 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 (i)) were used in the production of this report:

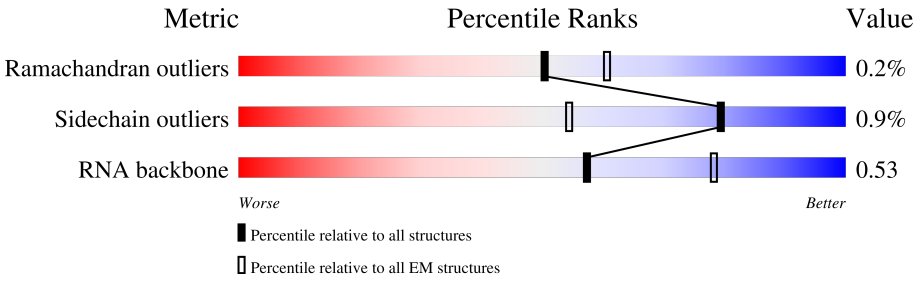
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.50 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)
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 <=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	A2	3612	8% 78% 21%
2	Bv	76	11% 82% 18%
3	Bx	11	36% 82% 18%
4	Bw	76	21% 80% 20%
5	B1	1708	11% 77% 22%
6	BD	220	50% 100%
7	BF	190	49% 100%
8	BK	98	73% 98%

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Mol	Chain	Length	Quality of chain
9	BM	120	100% 100%
10	BP	120	69% 98%
11	BQ	139	47% 99%
12	BR	125	58% 100%
13	BS	139	55% 96%
14	BT	143	55% 99%
15	BU	97	66% 100%
16	BZ	86	72% 98%
17	Bc	62	52% 95% 5%
18	Bd	51	35% 100%
19	Bf	73	100% 100%
20	Bg	314	95% 100%
21	BA	215	27% 100%
22	BB	212	20% 99%
23	BC	222	18% 100%
24	BE	257	13% 97%
25	BG	232	34% 99%
26	BH	183	48% 100%
27	BI	207	22% 99%
28	BJ	179	19% 98%
29	BL	153	23% 98%
30	BN	149	17% 99%
31	BO	136	14% 99%
32	BV	81	25% 98%
33	BW	129	9% 98%

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Mol	Chain	Length	Quality of chain
34	BX	141	16% 99%
35	BY	125	34% 99%
36	Ba	97	16% 99%
37	Bb	80	26% 100%
38	Be	55	29% 95% 5%
39	A3	157	10% 75% 22%
40	A4	119	80% 18%
41	AA	252	6% 100%
42	AB	394	8% 99%
43	AC	363	8% 98%
44	AD	294	12% 98%
45	AE	194	27% 97%
46	AF	234	9% 99%
47	AG	234	18% 100%
48	AH	191	10% 98%
49	AI	208	11% 99%
50	AJ	169	14% 99%
51	AL	205	17% 98%
52	AM	139	9% 99%
53	AN	203	100%
54	AO	195	5% 98%
55	AP	153	5% 99%
56	AQ	187	10% 98%
57	AR	181	13% 99%
58	AS	175	6% 100%

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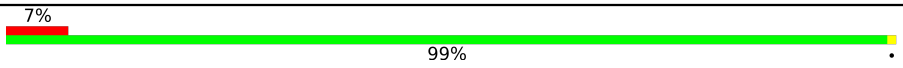
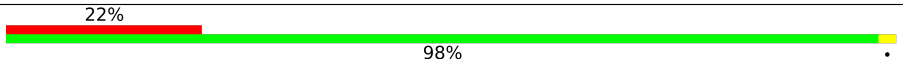
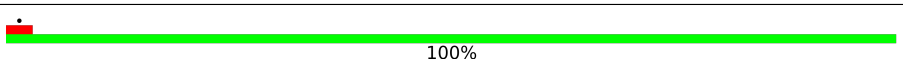
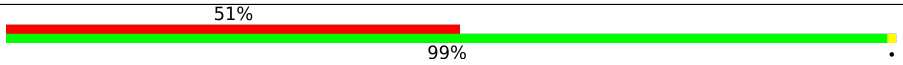
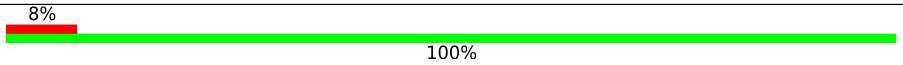
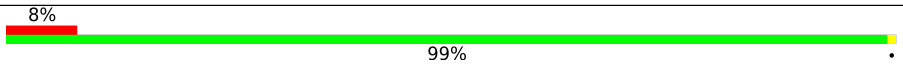
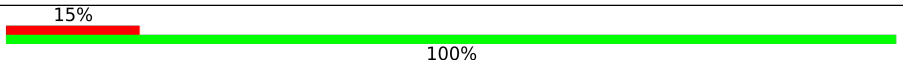
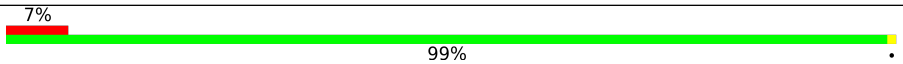
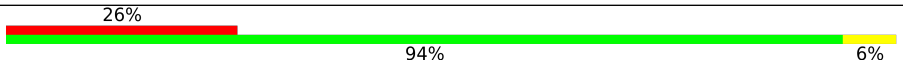
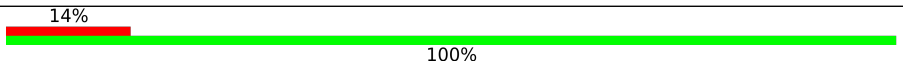
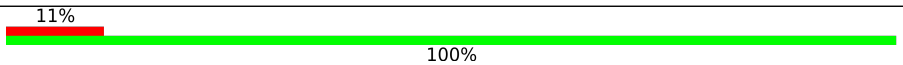
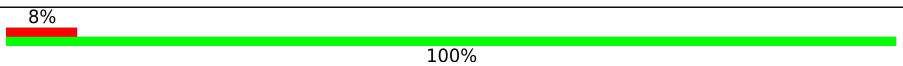
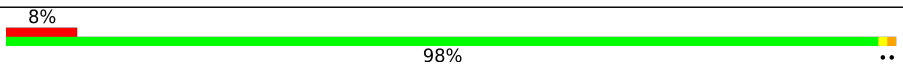
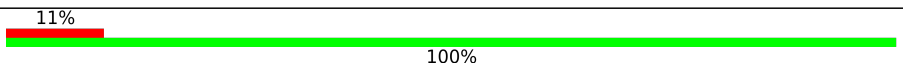
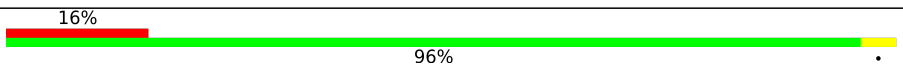
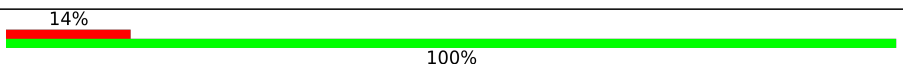
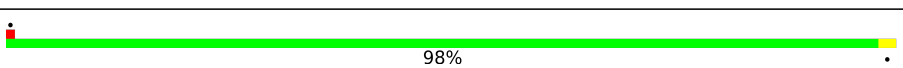
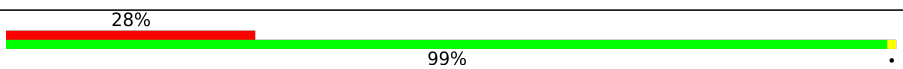
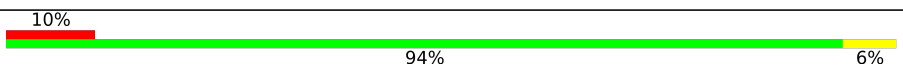
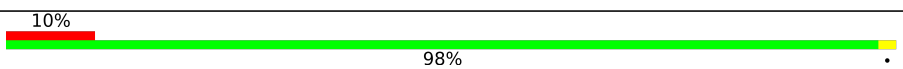
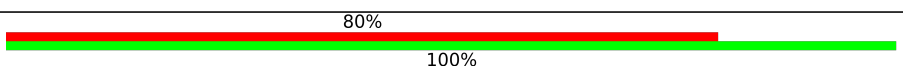
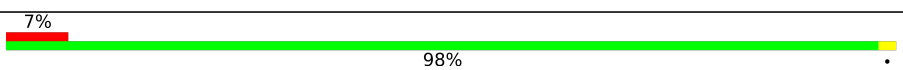
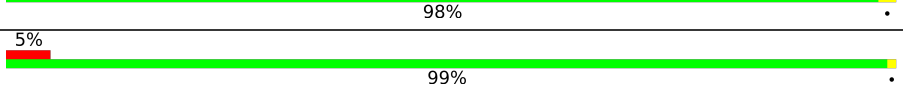
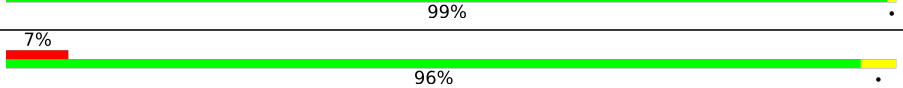
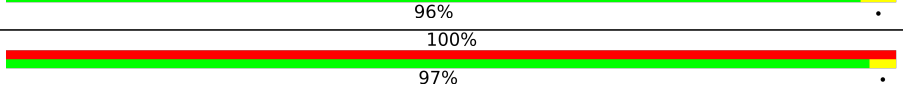
Mol	Chain	Length	Quality of chain
59	AT	157	
60	AU	99	
61	AV	129	
62	AW	121	
63	AX	117	
64	AY	127	
65	AZ	134	
66	Aa	147	
67	Ab	68	
68	Ac	103	
69	Ad	106	
70	Ae	129	
71	Af	109	
72	Ag	114	
73	Ah	122	
74	Ai	97	
75	Aj	84	
76	Ak	69	
77	Al	50	
78	Am	50	
79	An	25	
80	Ao	105	
81	Ap	91	
82	At	122	
83	Au	217	

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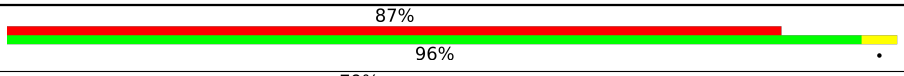
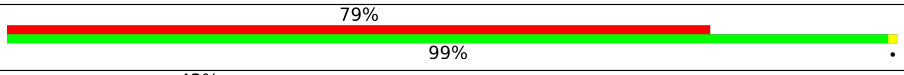
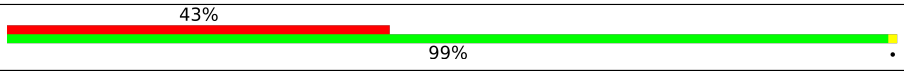
Mol	Chain	Length	Quality of chain
84	Aq	151	
85	AK	202	
86	Ct	853	

2 Entry composition (i)

There are 89 unique types of molecules in this entry. The entry contains 225601 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 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A2	3612	77427	34482	14158	25175	3612	0	0

- Molecule 2 is a RNA chain called P/P-site-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	Bv	76	1620	723	290	531	76	0	0

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	Bx	11	234	105	41	77	11	0	0

- Molecule 4 is a RNA chain called E/E-site-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	Bw	76	1627	725	294	532	76	0	0

- Molecule 5 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	B1	1708	36456	16274	6546	11928	1708	0	0

- Molecule 6 is a protein called ribosomal protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	BD	220	1709	1090	308	304	7	0	0

- Molecule 7 is a protein called ribosomal protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BF	190	Total	C	N	O	S	0	0
			1502	939	285	271	7		

- Molecule 8 is a protein called ribosomal protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 9 is a protein called ribosomal protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BM	120	Total	C	N	O	S	0	0
			931	584	164	174	9		

- Molecule 10 is a protein called ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BP	120	Total	C	N	O	S	0	0
			999	636	188	168	7		

- Molecule 11 is a protein called ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BQ	139	Total	C	N	O	S	0	0
			1109	704	210	192	3		

- Molecule 12 is a protein called ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BR	125	Total	C	N	O	S	0	0
			1011	634	187	186	4		

- Molecule 13 is a protein called ribosomal protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BS	139	Total	C	N	O	S	0	0
			1154	725	233	195	1		

- Molecule 14 is a protein called ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BT	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 15 is a protein called ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BU	97	Total	C	N	O	S	0	0
			769	483	144	138	4		

- Molecule 16 is a protein called ribosomal protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BZ	86	Total	C	N	O	S	0	0
			688	442	129	116	1		

- Molecule 17 is a protein called ribosomal protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Bc	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 18 is a protein called ribosomal protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Bd	51	Total	C	N	O	S	0	0
			427	269	87	66	5		

- Molecule 19 is a protein called ribosomal protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Bf	73	Total	C	N	O	S	0	0
			601	379	115	100	7		

- Molecule 20 is a protein called ribosomal protein RACK 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Bg	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

- Molecule 21 is a protein called ribosomal protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BA	215	Total	C	N	O	S	0	0
			1704	1083	298	315	8		

- Molecule 22 is a protein called ribosomal protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BB	212	Total	C	N	O	S	0	0
			1722	1093	308	307	14		

- Molecule 23 is a protein called ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BC	222	Total	C	N	O	S	0	0
			1724	1114	296	304	10		

- Molecule 24 is a protein called ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BE	257	Total	C	N	O	S	0	0
			2031	1298	381	344	8		

- Molecule 25 is a protein called ribosomal protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BG	232	Total	C	N	O	S	0	0
			1884	1176	379	322	7		

- Molecule 26 is a protein called ribosomal protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BH	183	Total	C	N	O	S	0	0
			1479	941	272	265	1		

- Molecule 27 is a protein called ribosomal protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BI	207	Total	C	N	O	S	0	0
			1696	1064	334	293	5		

- Molecule 28 is a protein called ribosomal protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BJ	179	Total	C	N	O	S	0	0
			1495	953	299	241	2		

- Molecule 29 is a protein called ribosomal protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BL	153	Total	C	N	O	S	0	0
			1258	804	235	213	6		

- Molecule 30 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BN	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 31 is a protein called ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BO	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 32 is a protein called ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BV	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

- Molecule 33 is a protein called ribosomal protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 34 is a protein called ribosomal protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 35 is a protein called ribosomal protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BY	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 36 is a protein called ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ba	97	Total	C	N	O	S	0	0
			774	481	160	128	5		

- Molecule 37 is a protein called ribosomal protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Bb	80	Total	C	N	O	S	0	0
			625	391	116	111	7		

- Molecule 38 is a protein called ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Be	55	Total	C	N	O	S	0	0
			437	272	96	68	1		

- Molecule 39 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	A3	157	Total	C	N	O	P	0	0
			3337	1489	587	1104	157		

- Molecule 40 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A4	119	Total	C	N	O	P	0	0
			2541	1132	454	836	119		

- Molecule 41 is a protein called ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AA	252	Total	C	N	O	S	0	0
			1930	1209	395	320	6		

- Molecule 42 is a protein called ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AB	394	Total	C	N	O	S	0	0
			3178	2024	596	544	14		

- Molecule 43 is a protein called ribosomal protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AC	363	Total	C	N	O	S	0	0
			2888	1817	577	480	14		

- Molecule 44 is a protein called ribosomal protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AD	294	Total	C	N	O	S	0	0
			2392	1510	436	432	14		

- Molecule 45 is a protein called ribosomal protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AE	194	Total	C	N	O	S	0	0
			1571	1013	294	263	1		

- Molecule 46 is a protein called ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AF	234	Total	C	N	O	S	0	0
			1950	1252	376	313	9		

- Molecule 47 is a protein called ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AG	234	Total	C	N	O	S	0	0
			1880	1197	362	317	4		

- Molecule 48 is a protein called ribosomal protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AH	191	Total	C	N	O	S	0	0
			1526	960	285	275	6		

- Molecule 49 is a protein called ribosomal protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AI	208	Total	C	N	O	S	0	0
			1692	1074	327	278	13		

- Molecule 50 is a protein called ribosomal protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AJ	169	Total	C	N	O	S	0	0
			1353	855	252	240	6		

- Molecule 51 is a protein called ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AL	205	Total	C	N	O	S	0	0
			1657	1036	344	273	4		

- Molecule 52 is a protein called ribosomal protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 53 is a protein called ribosomal protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 54 is a protein called ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	AO	195	Total	C	N	O	S	0	0
			1606	1034	315	252	5		

- Molecule 55 is a protein called ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 56 is a protein called ribosomal protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 57 is a protein called ribosomal protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AR	181	Total	C	N	O	S	0	0
			1517	938	329	241	9		

- Molecule 58 is a protein called ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AS	175	Total	C	N	O	S	0	0
			1449	921	283	234	11		

- Molecule 59 is a protein called ribosomal protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AT	157	Total	C	N	O	S	0	0
			1284	815	250	214	5		

- Molecule 60 is a protein called ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AU	99	Total	C	N	O	S	0	0
			808	518	141	147	2		

- Molecule 61 is a protein called ribosomal protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AV	129	Total	C	N	O	S	0	0
			969	613	182	169	5		

- Molecule 62 is a protein called ribosomal protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AW	121	Total	C	N	O	S	0	0
			989	617	202	167	3		

- Molecule 63 is a protein called ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AX	117	Total	C	N	O	S	0	0
			958	612	180	165	1		

- Molecule 64 is a protein called ribosomal protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AY	127	Total	C	N	O	S	0	0
			1064	668	216	177	3		

- Molecule 65 is a protein called ribosomal protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AZ	134	Total	C	N	O	S	0	0
			1103	712	207	181	3		

- Molecule 66 is a protein called ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Aa	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 67 is a protein called ribosomal protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Ab	68	Total	C	N	O	S	0	0
			559	344	122	90	3		

- Molecule 68 is a protein called ribosomal protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Ac	103	Total	C	N	O	S	0	0
			801	508	141	145	7		

- Molecule 69 is a protein called ribosomal protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ad	106	Total	C	N	O	S	0	0
			879	555	170	152	2		

- Molecule 70 is a protein called ribosomal protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Ae	129	Total	C	N	O	S	0	0
			1064	673	220	166	5		

- Molecule 71 is a protein called ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Af	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 72 is a protein called ribosomal protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Ag	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 73 is a protein called ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Ah	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 74 is a protein called ribosomal protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Ai	97	Total	C	N	O	S	0	0
			794	497	168	124	5		

- Molecule 75 is a protein called ribosomal protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Aj	84	Total	C	N	O	S	0	0
			689	423	152	109	5		

- Molecule 76 is a protein called ribosomal protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Ak	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 77 is a protein called ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Al	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 78 is a protein called ribosomal protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Am	50	Total	C	N	O	S	0	0
			411	254	87	64	6		

- Molecule 79 is a protein called ribosomal protein eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	An	25	Total	C	N	O	S	0	0
			240	145	64	28	3		

- Molecule 80 is a protein called ribosomal protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Ao	105	Total	C	N	O	S	0	0
			863	542	175	140	6		

- Molecule 81 is a protein called ribosomal protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Ap	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 82 is a protein called ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	At	122	Total	C	N	O	S	0	0
			980	607	204	165	4		

- Molecule 83 is a protein called ribosomal protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Au	217	Total	C	N	O	S	0	0
			1744	1114	314	307	9		

- Molecule 84 is a protein called ribosomal protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Aq	151	Total	C	N	O	S	0	0
			1140	708	215	213	4		

- Molecule 85 is a protein called ribosomal protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	AK	202	Total	C	N	O	S	0	0
			1556	989	272	286	9		

- Molecule 86 is a protein called eukaryotic elongation factor 2 (eEF2).

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Ct	853	Total	C	N	O	S	0	0
			6659	4226	1146	1243	44		

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	A2	229	Total	Mg	0
			229	229	
87	Bx	1	Total	Mg	0
			1	1	
87	B1	73	Total	Mg	0
			73	73	
87	BD	1	Total	Mg	0
			1	1	
87	Ba	1	Total	Mg	0
			1	1	
87	A3	7	Total	Mg	0
			7	7	
87	A4	8	Total	Mg	0
			8	8	
87	AA	1	Total	Mg	0
			1	1	
87	AC	1	Total	Mg	0
			1	1	
87	AL	1	Total	Mg	0
			1	1	
87	AO	1	Total	Mg	0
			1	1	
87	AP	1	Total	Mg	0
			1	1	

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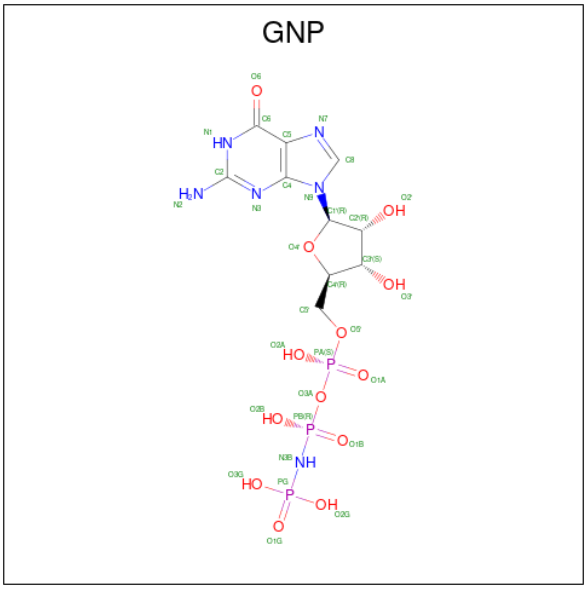
Mol	Chain	Residues	Atoms	AltConf
87	AY	1	Total Mg 1 1	0
87	An	1	Total Mg 1 1	0

- Molecule 88 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
88	Bd	1	Total Zn 1 1	0
88	Ba	1	Total Zn 1 1	0
88	Aj	1	Total Zn 1 1	0
88	Ao	1	Total Zn 1 1	0
88	Ap	1	Total Zn 1 1	0

- Molecule 89 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



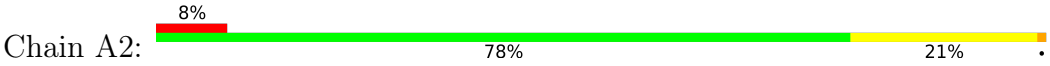
Mol	Chain	Residues	Atoms	AltConf
89	Ct	1	Total C N O P 32 10 6 13 3	0

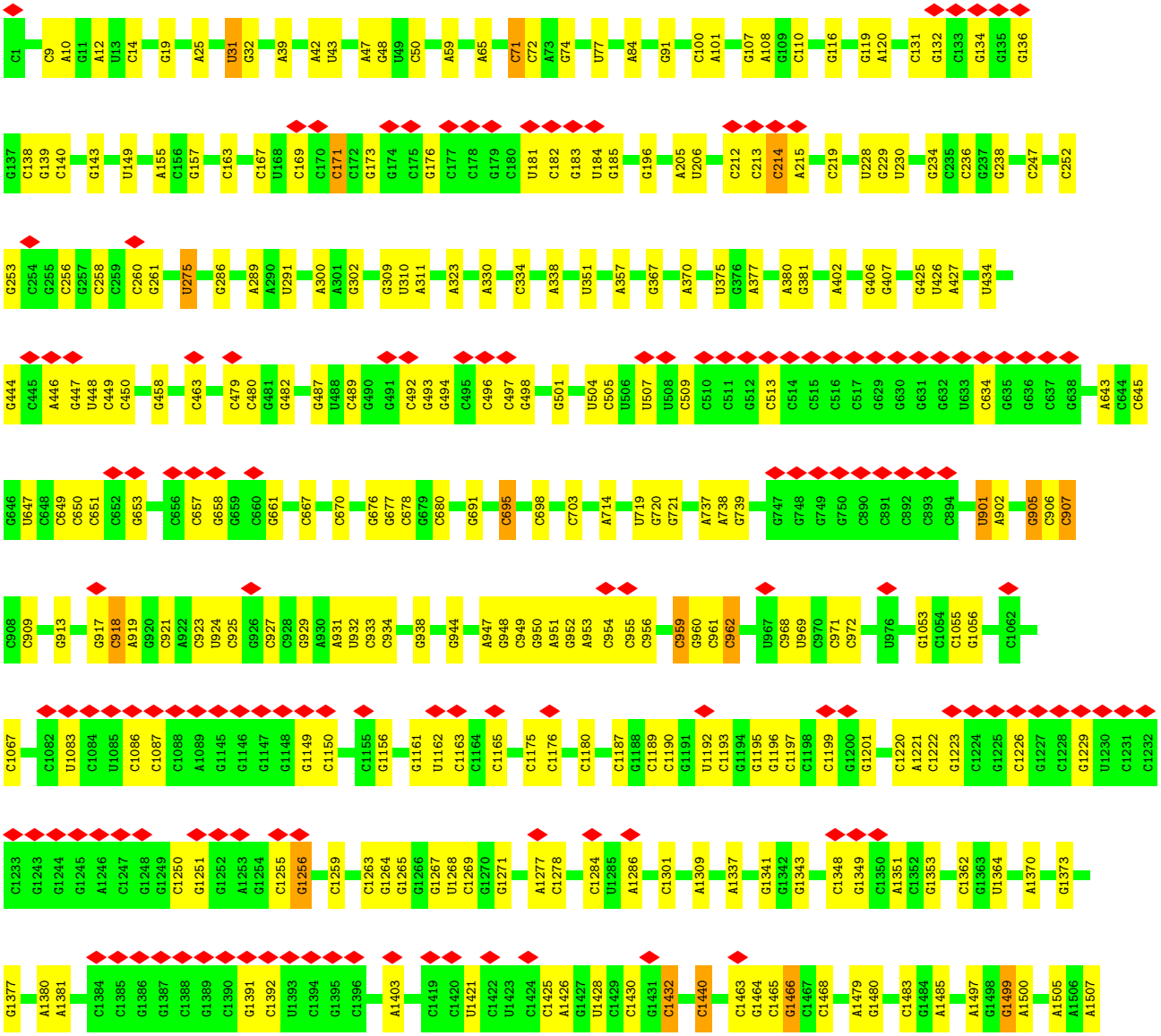
3 Residue-property plots (i)

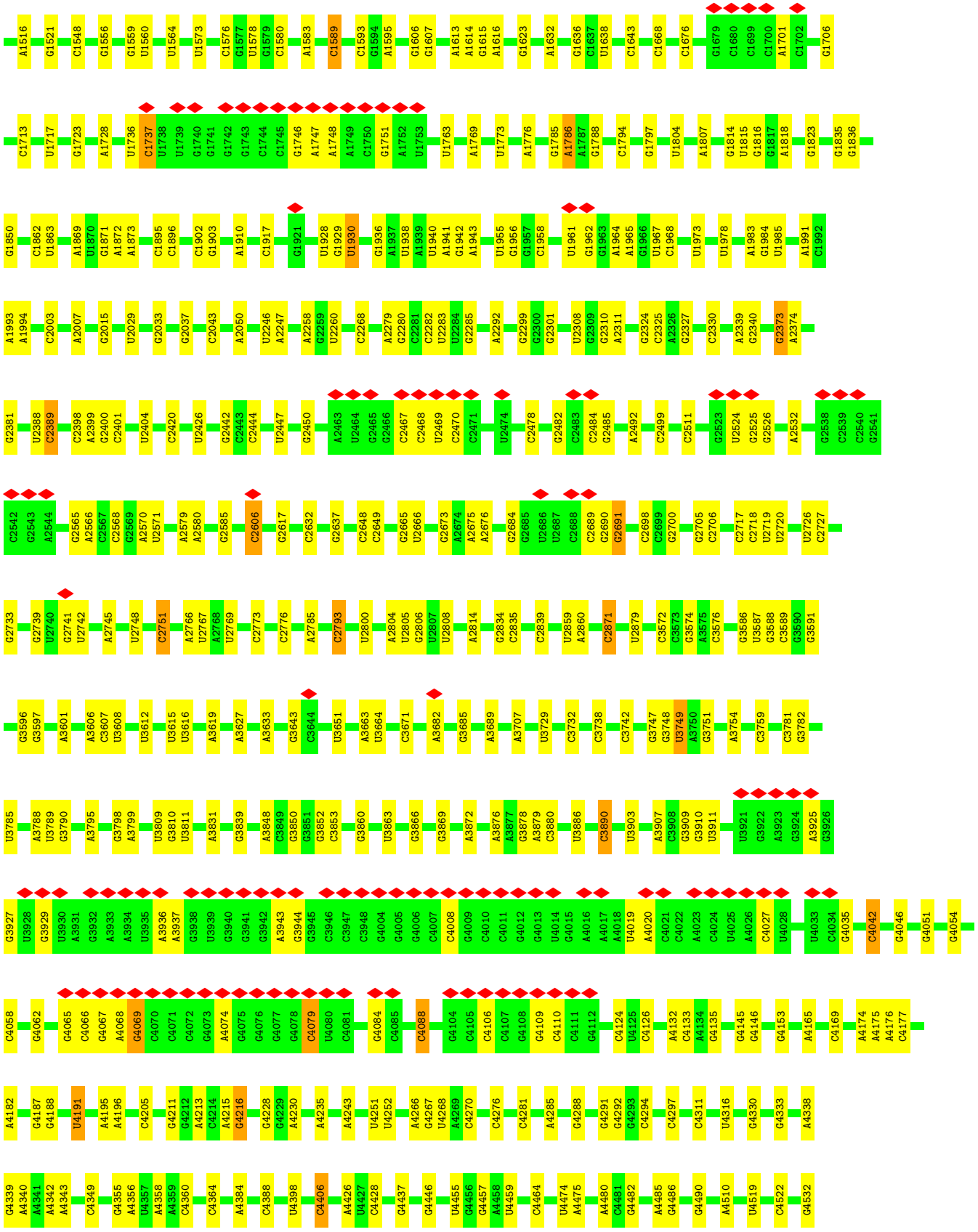
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

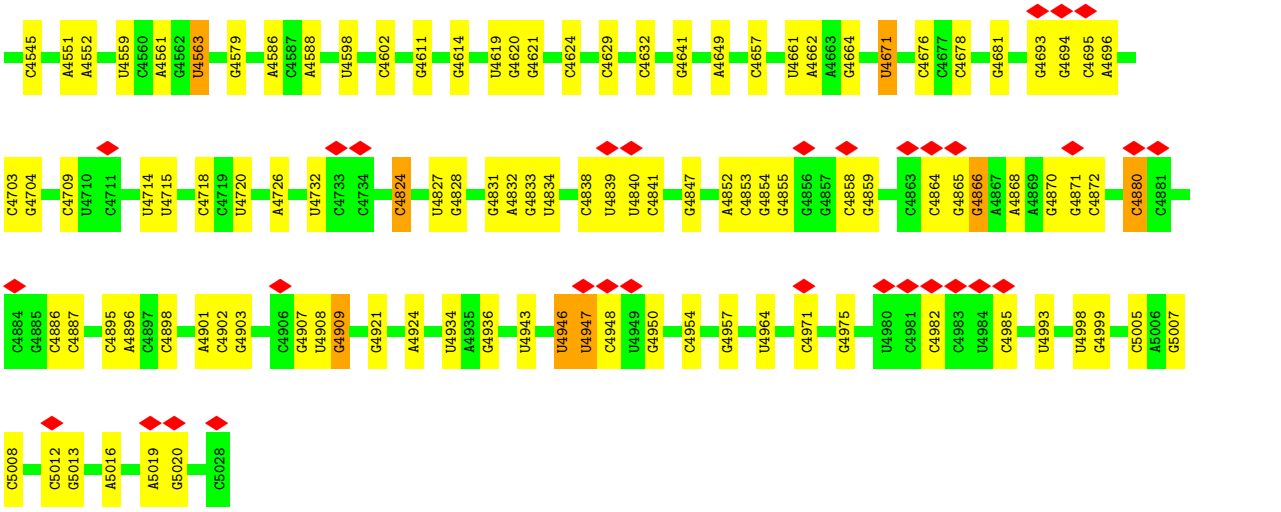
- Molecule 1: 28S ribosomal RNA

Chain A2:

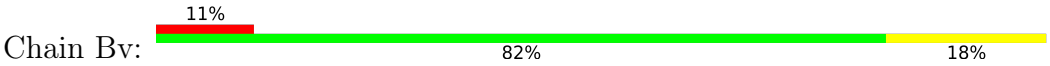


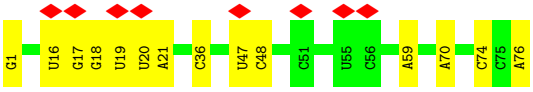



A1516 G1521 C1548 G1556 G1559 U1560 U1564 U1573 C1576 G1577 U1578 G1579 C1580 A1583 C1589 C1593 G1594 A1595 G1606 G1607 A1613 A1614 G1615 A1616 G1623 A1632 G1636 C1637 U1638 C1643 C1668 C1676 G1679 C1680 C1699 C1700 A1701 C1702 G1706
C1713 U1717 G1723 A1728 U1736 C1737 U1738 U1739 G1740 G1741 G1742 G1743 C1744 C1745 G1746 A1747 A1748 A1749 C1750 G1751 A1752 U1753 U1763 A1769 U1773 A1776 G1785 A1786 A1787 G1788 C1794 G1797 U1804 A1807 G1814 U1815 G1816 G1817 A1818 G1823 G1835 G1836
G1850 C1862 U1863 A1869 U1870 G1871 A1872 A1873 C1895 C1896 C1902 G1903 A1910 C1917 G1921 U1928 G1929 U1930 G1936 A1937 U1938 A1939 U1940 A1941 G1942 A1943 U1955 G1956 G1957 C1958 U1961 G1962 G1963 A1964 A1965 G1966 U1967 C1968 U1973 U1978 A1983 G1984 U1985 A1991 C1992
A1993 A1994 C2003 A2007 G2015 U2029 G2033 G2037 C2043 A2050 U2246 A2247 A2258 G2259 U2260 C2268 A2279 G2280 C2281 C2282 U2283 U2284 G2285 A2292 G2299 G2300 G2301 U2308 G2309 G2310 A2311 G2324 C2325 A2326 G2327 C2330 A2339 G2340 G2373 A2374
G2381 U2388 C2389 C2398 A2399 G2400 C2401 U2404 C2420 U2426 G2442 C2443 C2444 U2447 G2450 A2463 U2464 G2465 G2466 C2467 C2468 U2469 C2470 C2471 U2474 C2478 G2482 C2483 C2484 G2485 A2492 C2499 C2511 G2523 U2524 G2525 G2526 A2532 G2538 C2539 C2540 G2541
C2542 G2543 A2544 G2565 A2566 C2567 C2568 G2569 A2570 U2571 A2579 A2580 G2585 C2606 G2617 C2632 G2637 C2648 C2649 G2665 U2666 G2673 A2674 A2675 A2676 G2684 G2685 U2686 U2687 C2688 C2689 G2690 G2691 C2698 C2699 G2700 G2705 C2706 C2717 C2718 U2719 U2720 U2726 C2727
G2733 G2739 U2740 G2741 U2742 A2745 U2748 C2751 A2766 U2767 A2768 U2769 C2773 C2776 A2785 C2793 U2800 A2804 U2805 G2806 U2807 U2808 A2814 G2834 C2835 C2839 U2859 A2860 C2871 U2879 C3572 C3573 G3574 A3575 C3576 G3586 U3587 G3588 C3589 G3590 G3591
G3596 G3597 A3601 A3606 C3607 U3608 U3612 U3615 U3616 A3619 A3627 A3633 G3643 C3644 U3651 A3663 U3664 C3671 A3682 G3685 A3689 A3707 U3729 C3732 C3738 C3742 G3747 G3748 U3749 A3750 G3751 A3754 C3759 C3781 G3782
U3785 A3788 U3789 G3790 A3795 G3798 A3799 U3809 G3810 U3811 A3831 G3839 A3848 C3849 G3850 G3851 G3852 C3853 G3860 U3863 G3866 G3869 A3872 A3876 A3877 G3878 A3879 C3880 U3886 C3890 U3903 A3907 C3908 G3909 G3910 U3911 U3921 G3922 A3923 G3924 A3925 G3926
G3927 U3928 G3929 U3930 A3931 G3932 A3933 A3934 U3935 A3936 A3937 G3938 U3939 G3940 G3941 G3942 A3943 G3944 G3945 C3946 C3947 C3948 G4004 G4005 G4006 C4007 C4008 C4009 C4010 C4011 G4012 G4013 U4014 G4015 A4016 A4017 A4018 U4019 A4020 C4021 C4022 A4023 C4024 U4025 A4026 C4027 U4028 U4033 C4034 G4035 C4042 G4046 G4051 G4054
C4058 G4062 G4065 C4066 G4067 A4068 G4069 C4070 C4071 C4072 G4073 A4074 G4075 G4076 G4077 G4078 C4079 U4080 C4081 G4084 C4085 C4088 G4104 C4105 C4106 C4107 G4108 C4109 C4110 C4111 G4112 C4124 U4125 C4126 A4132 C4133 A4134 G4135 G4145 G4146 G4153 A4165 C4169 A4174 A4175 A4176 C4177
A4182 G4187 G4188 U4191 A4195 A4196 C4205 G4211 G4212 A4213 C4214 A4215 G4216 G4228 G4229 A4230 A4235 A4243 U4251 U4252 A4266 G4267 U4268 A4269 C4270 C4276 C4281 A4285 G4288 G4291 G4292 G4293 C4294 C4297 C4311 U4316 G4330 G4333 A4338
G4339 A4340 A4341 A4342 A4343 C4349 G4355 A4356 U4357 A4358 A4369 C4360 C4364 A4384 C4388 U4398 C4406 A4426 U4427 C4428 G4437 G4446 U4455 G4456 G4457 A4458 U4459 C4464 U4474 A4475 A4480 C4481 G4482 A4485 G4486 G4490 A4510 U4519 C4522 G4532

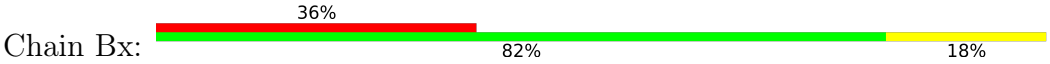


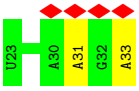
• Molecule 2: P/P-site-tRNA



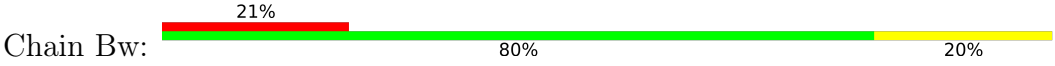


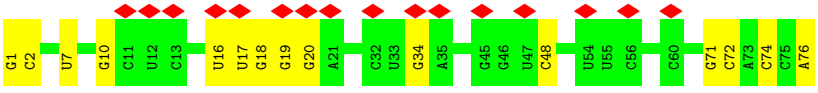
• Molecule 3: mRNA



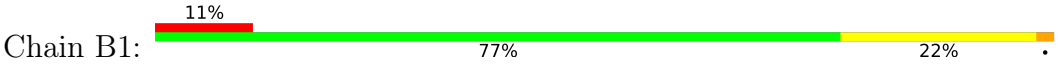


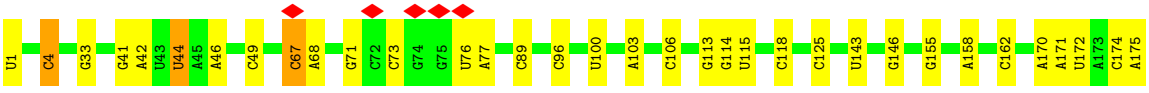
• Molecule 4: E/E-site-tRNA

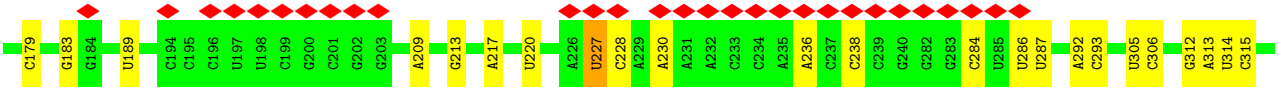


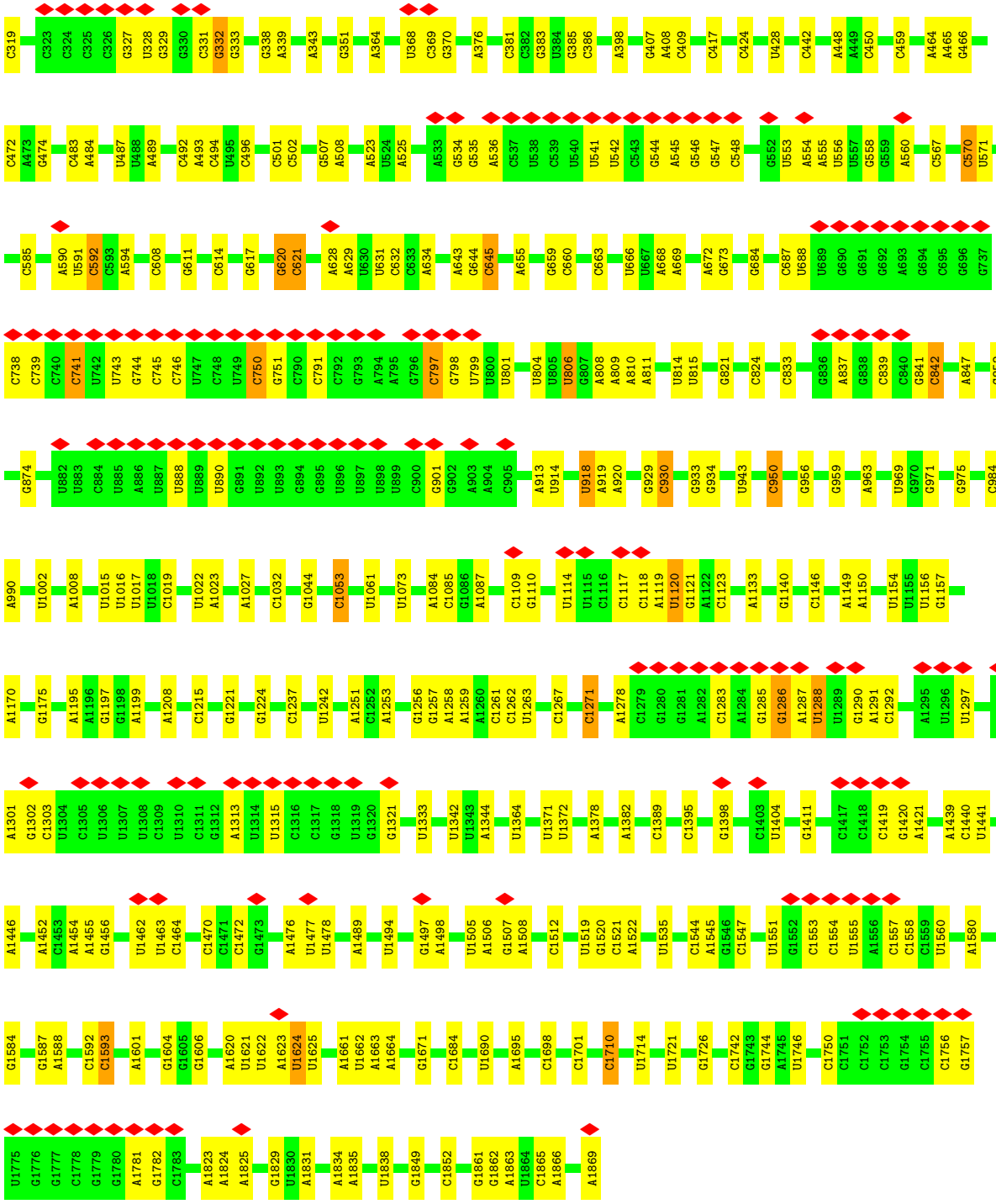


• Molecule 5: 18S ribosomal RNA



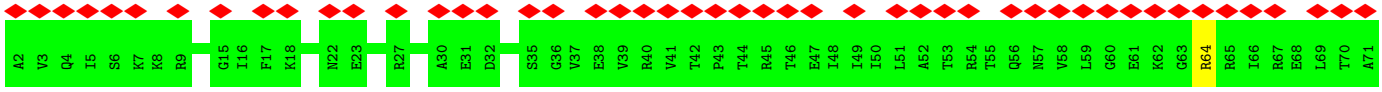


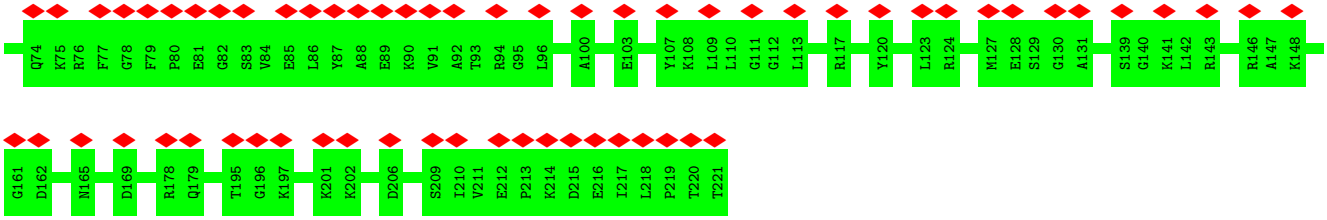




• Molecule 6: ribosomal protein uS3

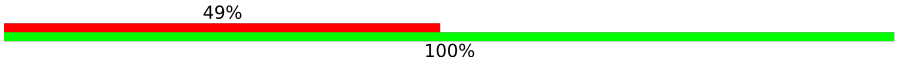
Chain BD:

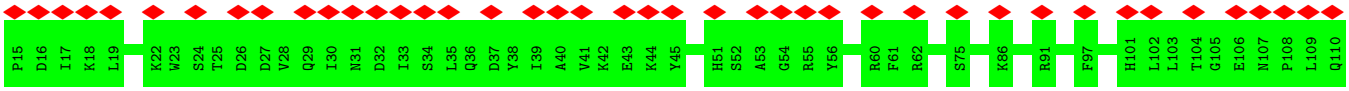




• Molecule 7: ribosomal protein uS7

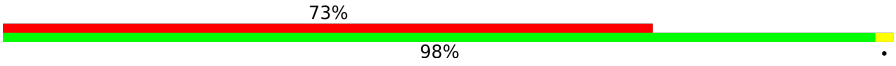
Chain BF:

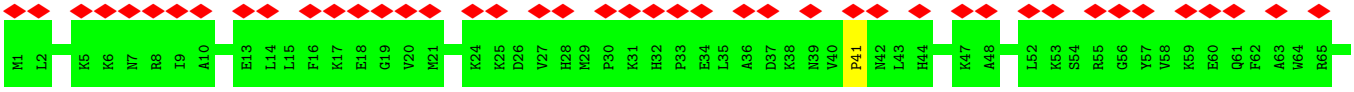




• Molecule 8: ribosomal protein eS10

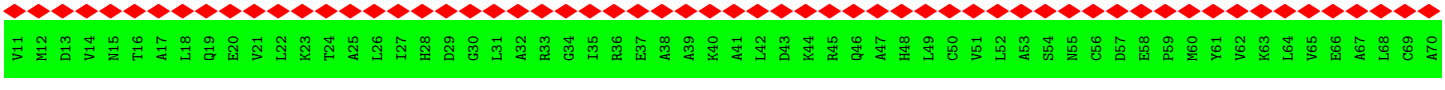
Chain BK:





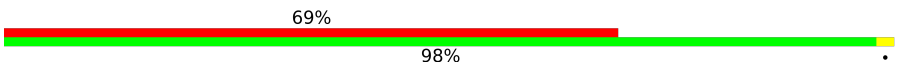
• Molecule 9: ribosomal protein eS12

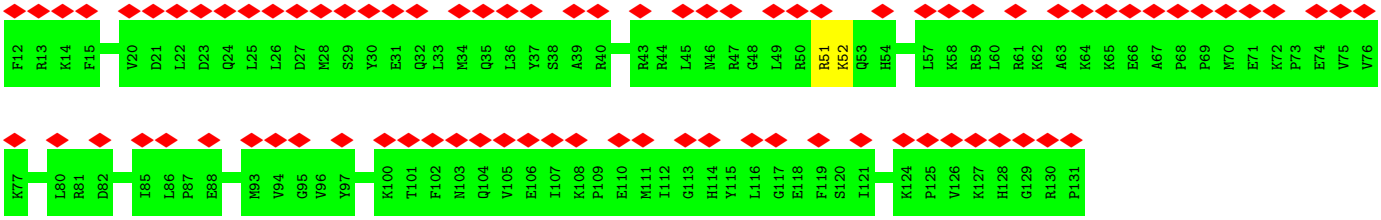
Chain BM:



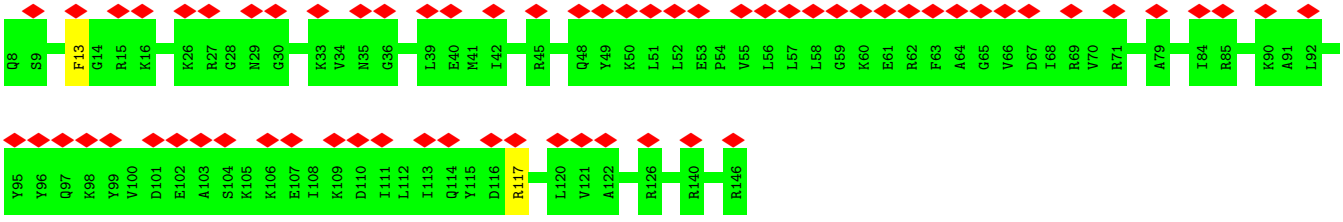
• Molecule 10: ribosomal protein uS19

Chain BP:

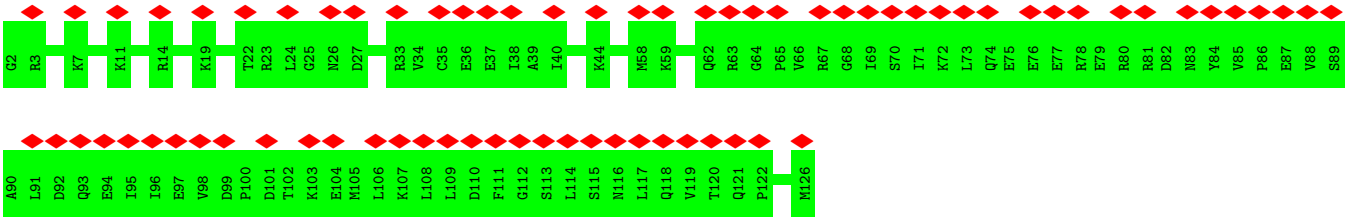




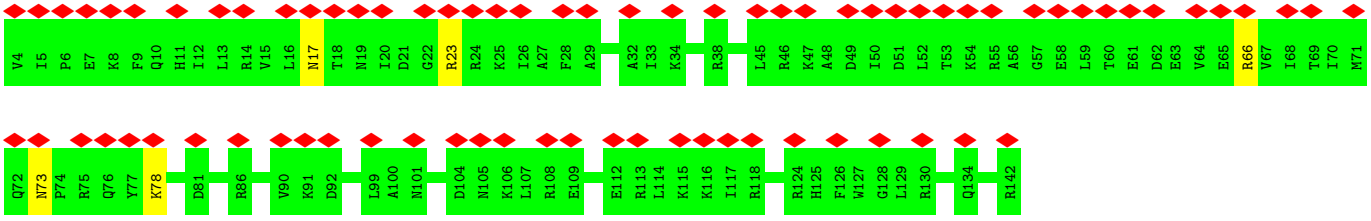
• Molecule 11: ribosomal protein uS9



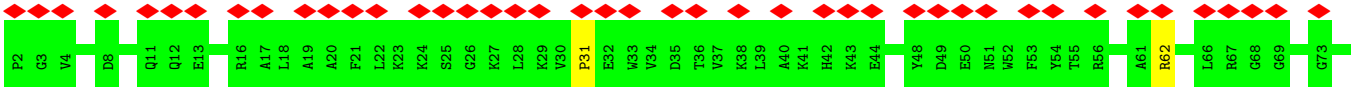
• Molecule 12: ribosomal protein eS17

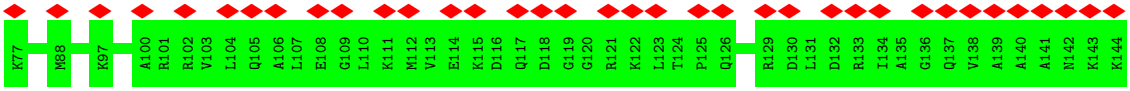


• Molecule 13: ribosomal protein uS13



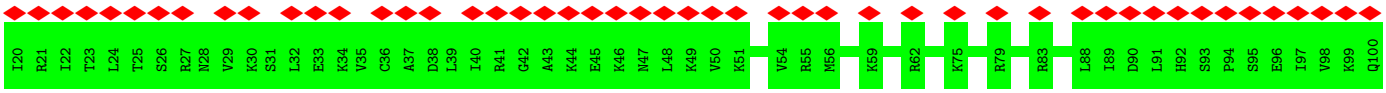
• Molecule 14: ribosomal protein eS19

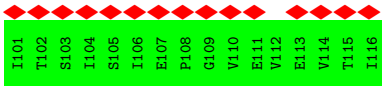




• Molecule 15: ribosomal protein uS10

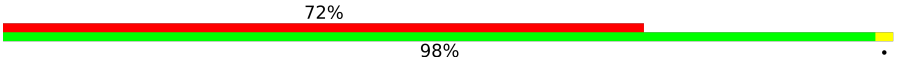
Chain BU:

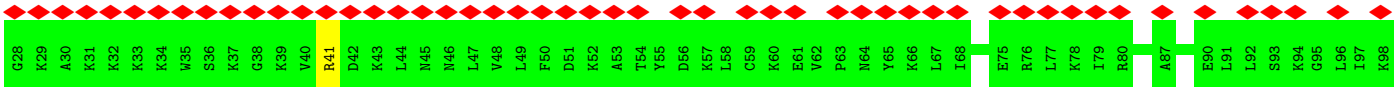


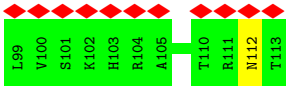


• Molecule 16: ribosomal protein eS25

Chain BZ:

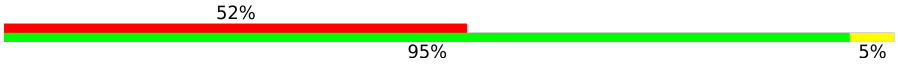


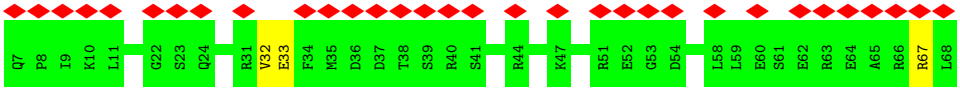




• Molecule 17: ribosomal protein eS28

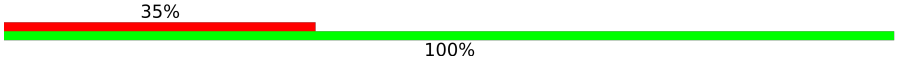
Chain Bc:

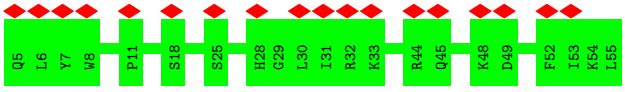




• Molecule 18: ribosomal protein uS14

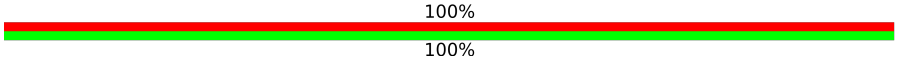
Chain Bd:

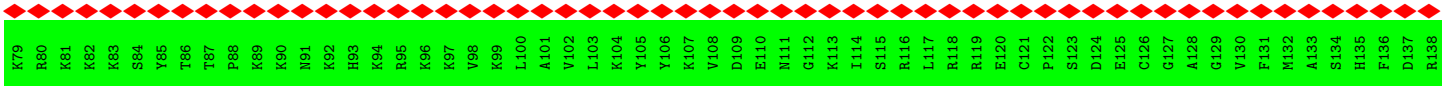


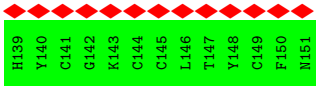


• Molecule 19: ribosomal protein eS31

Chain Bf:

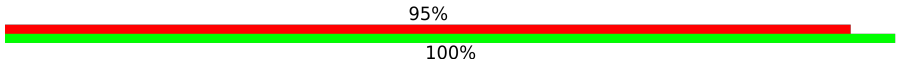


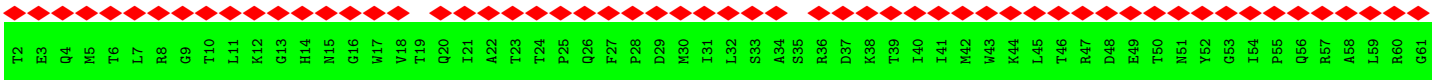


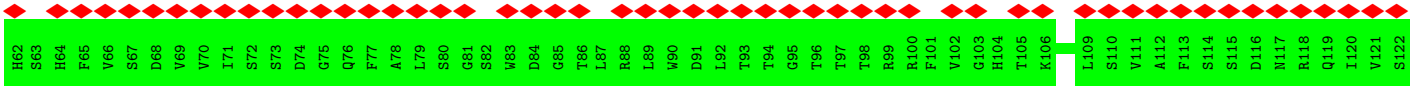


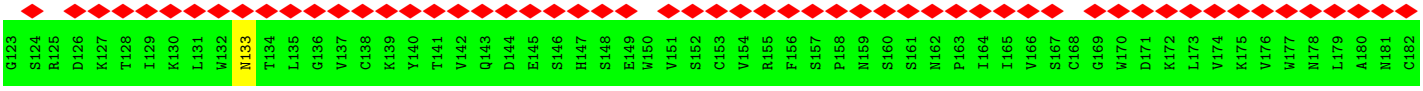
• Molecule 20: ribosomal protein RACK 1

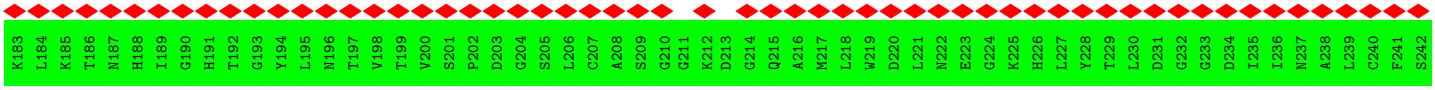
Chain Bg:

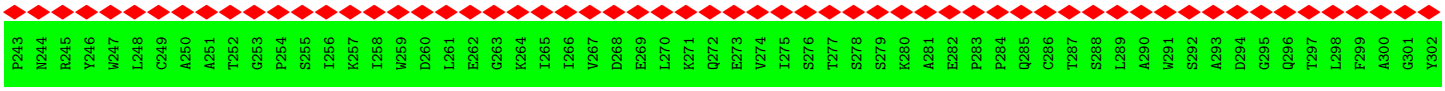


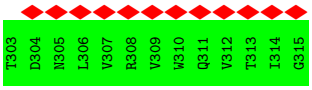






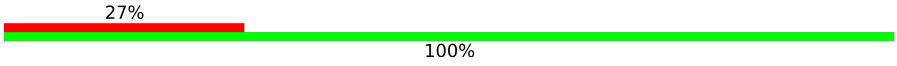


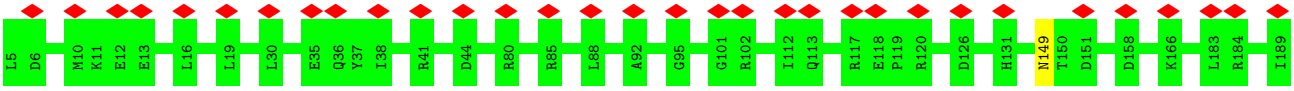


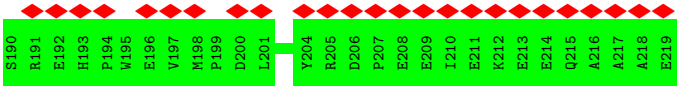


• Molecule 21: ribosomal protein uS2

Chain BA:

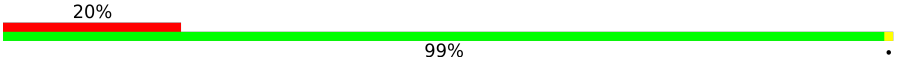


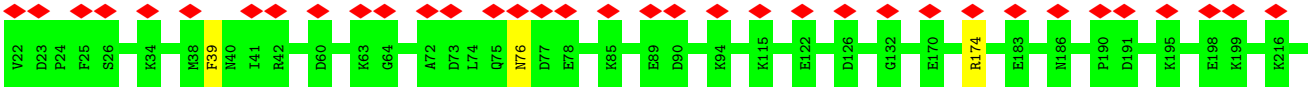


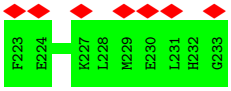


• Molecule 22: ribosomal protein eS1

Chain BB:

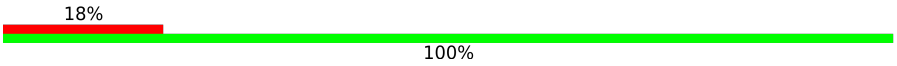


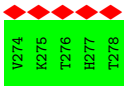




• Molecule 23: ribosomal protein uS5

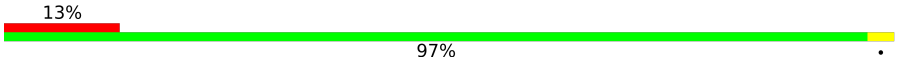
Chain BC:

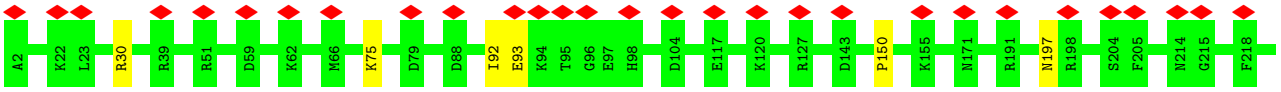


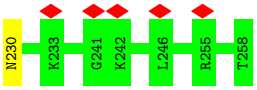


• Molecule 24: ribosomal protein eS4

Chain BE:

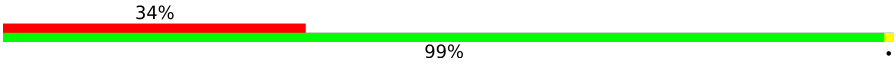


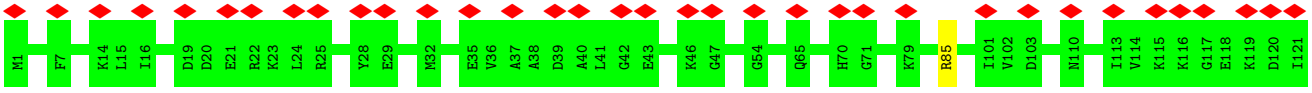


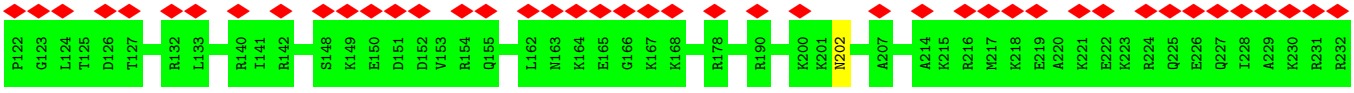


• Molecule 25: ribosomal protein eS6

Chain BG:

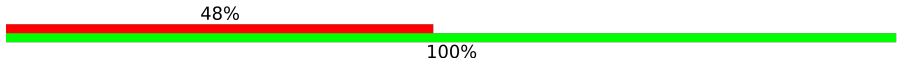


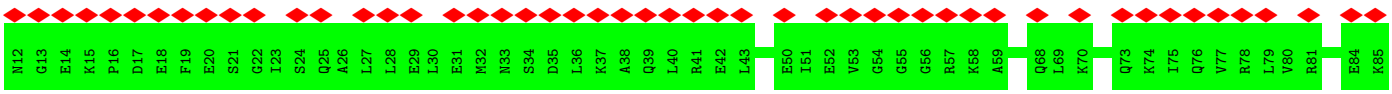


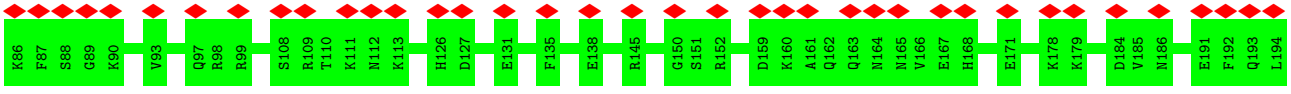


• Molecule 26: ribosomal protein eS7

Chain BH:

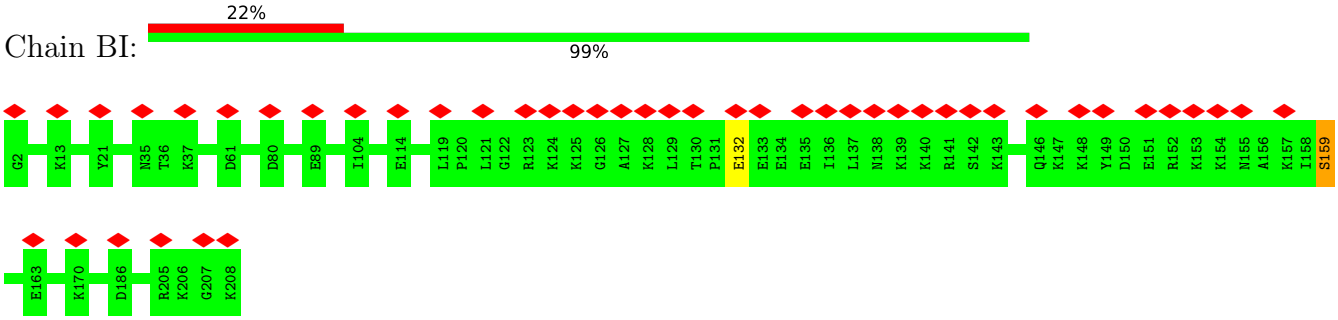






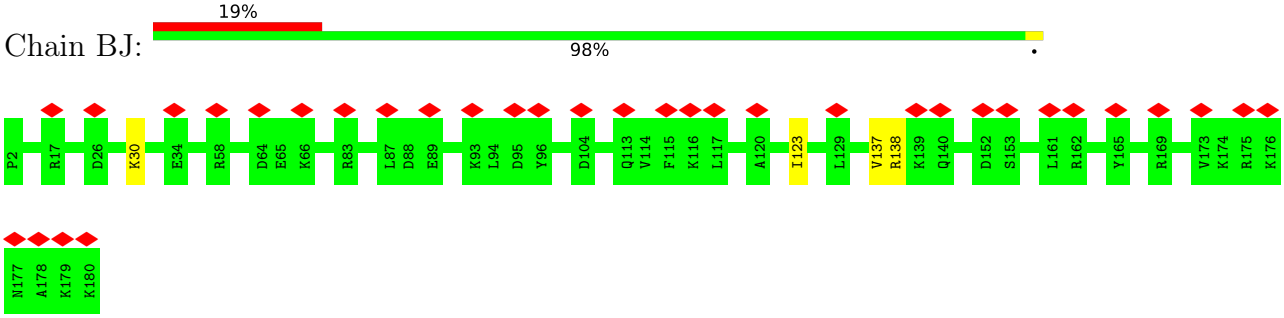
• Molecule 27: ribosomal protein eS8

Chain BI:



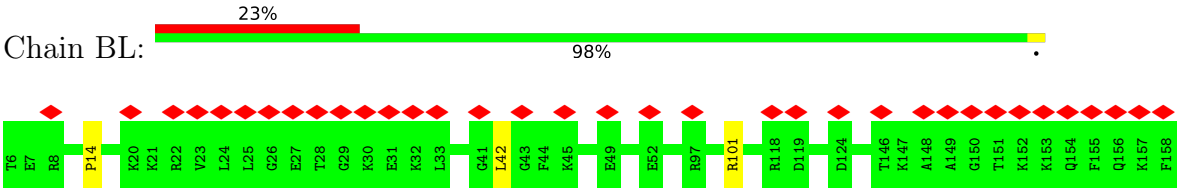
• Molecule 28: ribosomal protein uS4

Chain BJ:



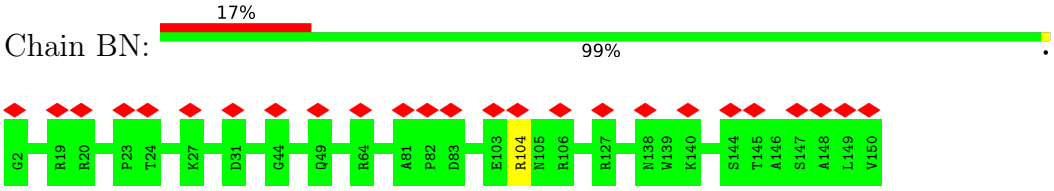
• Molecule 29: ribosomal protein uS17

Chain BL:



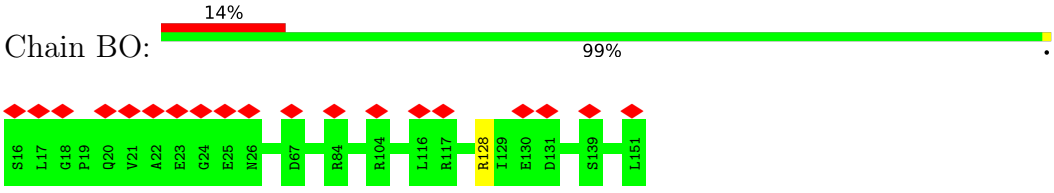
• Molecule 30: ribosomal protein uS15

Chain BN:



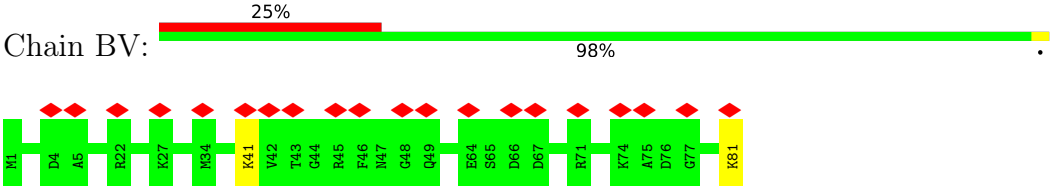
• Molecule 31: ribosomal protein uS11

Chain BO:



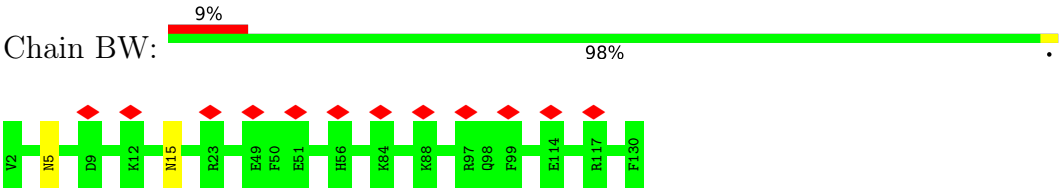
• Molecule 32: ribosomal protein eS21

Chain BV:



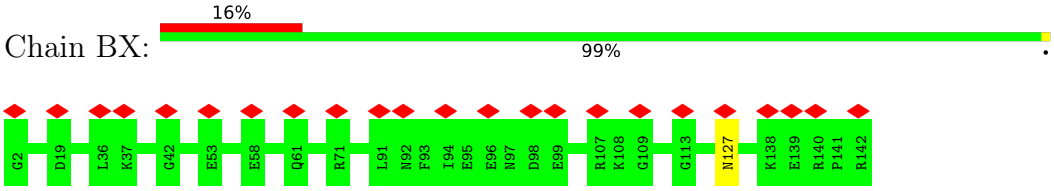
• Molecule 33: ribosomal protein uS8

Chain BW:



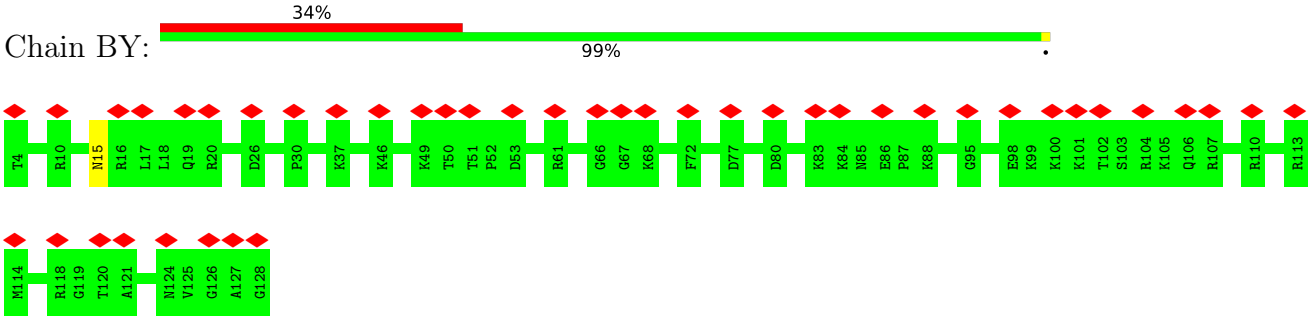
• Molecule 34: ribosomal protein uS12

Chain BX:



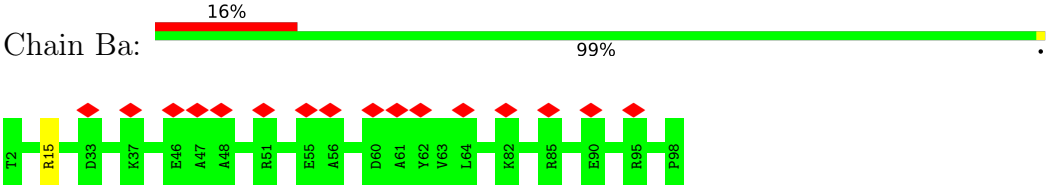
• Molecule 35: ribosomal protein eS24

Chain BY:



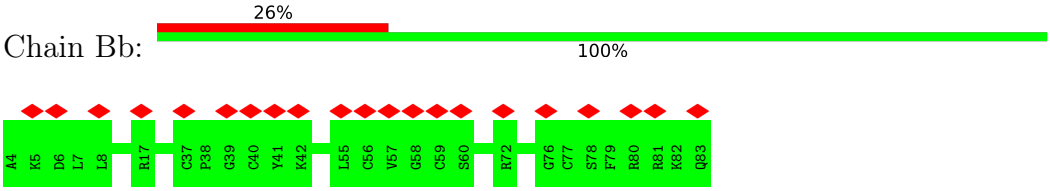
• Molecule 36: ribosomal protein eS26

Chain Ba:



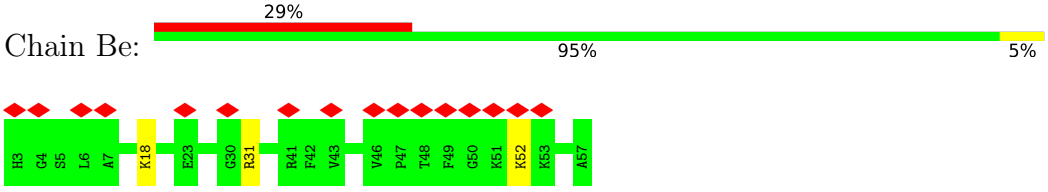
• Molecule 37: ribosomal protein eS27

Chain Bb:



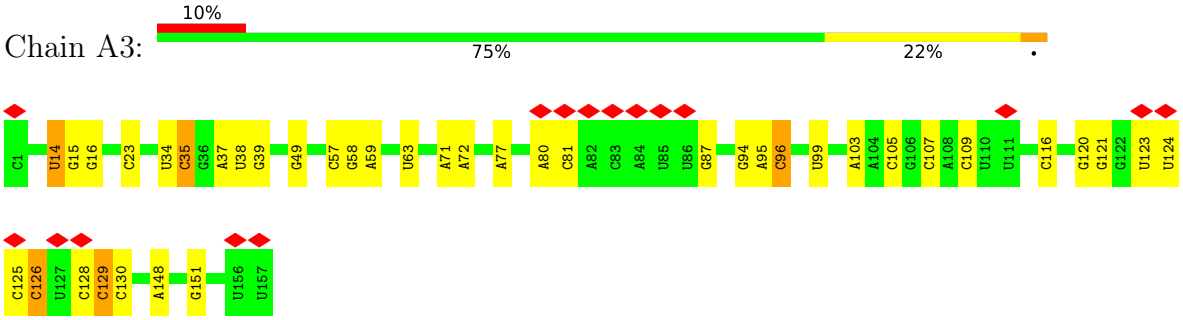
• Molecule 38: ribosomal protein eS30

Chain Be:



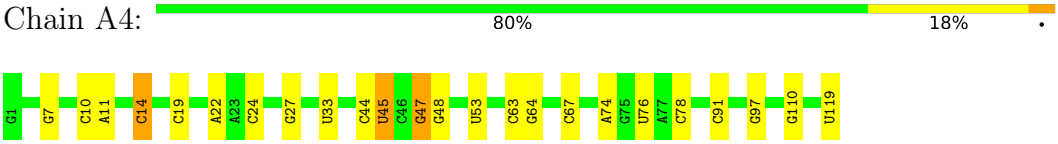
• Molecule 39: 5.8S ribosomal RNA

Chain A3:



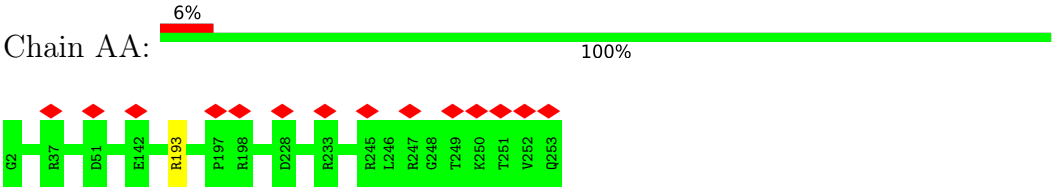
• Molecule 40: 5S ribosomal RNA

Chain A4:



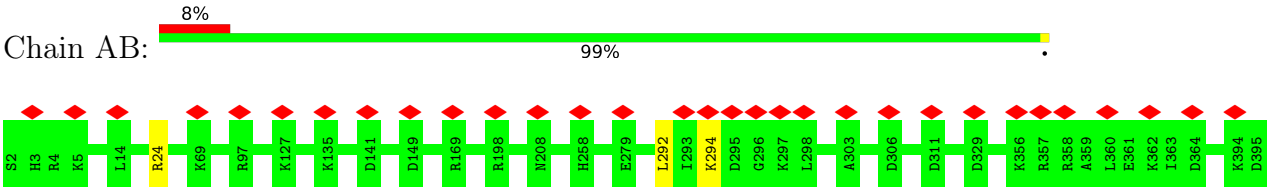
• Molecule 41: ribosomal protein uL2

Chain AA:



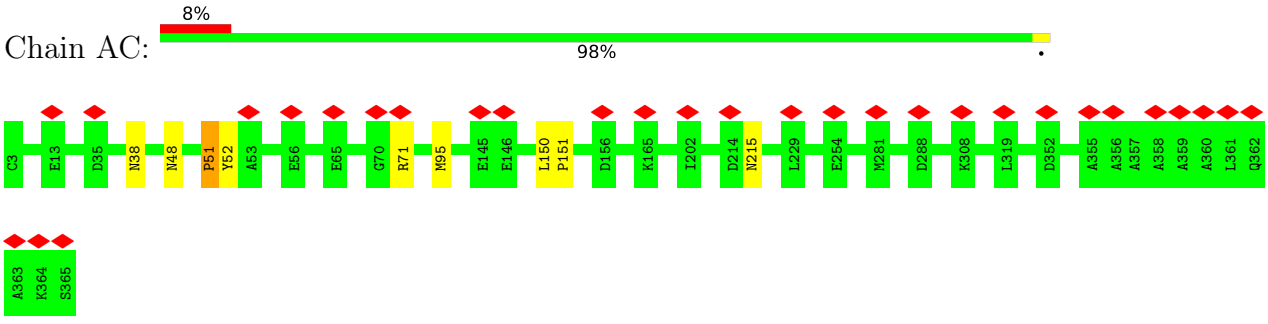
• Molecule 42: ribosomal protein uL3

Chain AB:



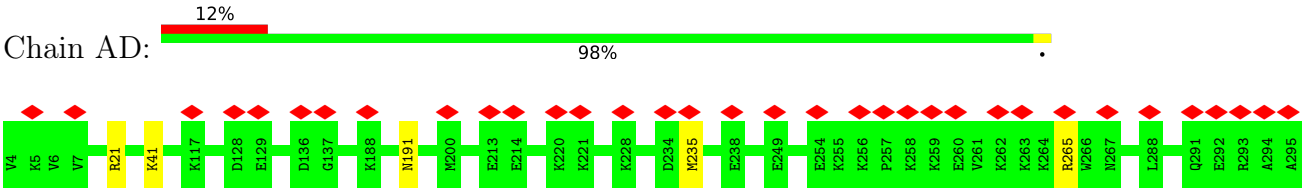
• Molecule 43: ribosomal protein uL4

Chain AC:



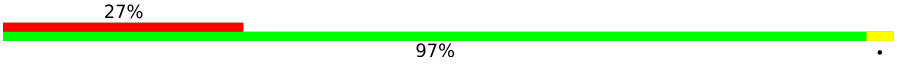
• Molecule 44: ribosomal protein uL18

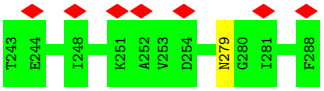
Chain AD:



• Molecule 45: ribosomal protein eL6

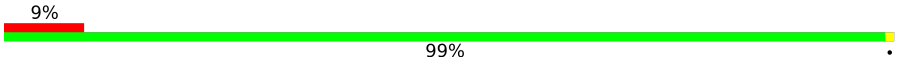
Chain AE:

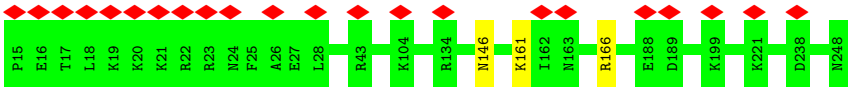




• Molecule 46: ribosomal protein uL30

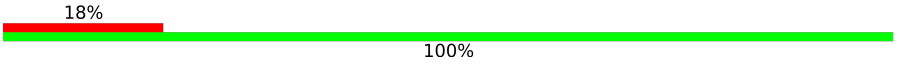
Chain AF:

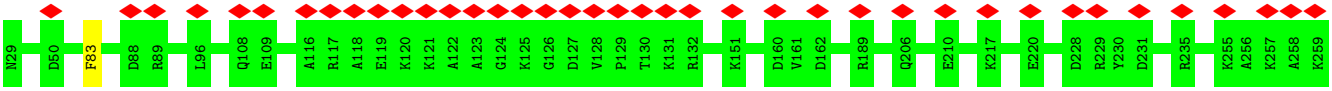




• Molecule 47: ribosomal protein eL8

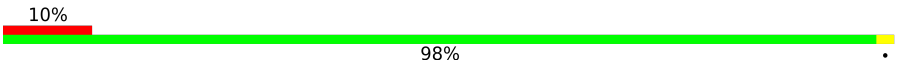
Chain AG:

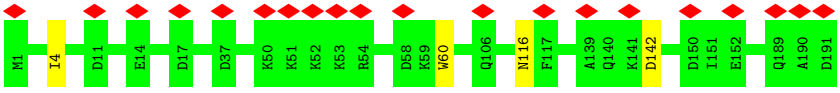




• Molecule 48: ribosomal protein uL6

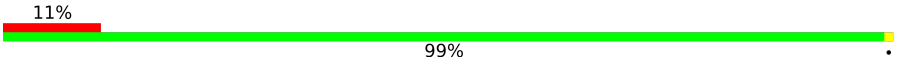
Chain AH:

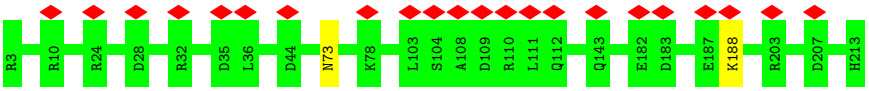




• Molecule 49: ribosomal protein uL16

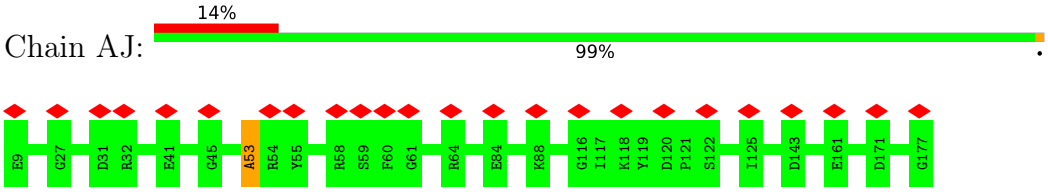
Chain AI:





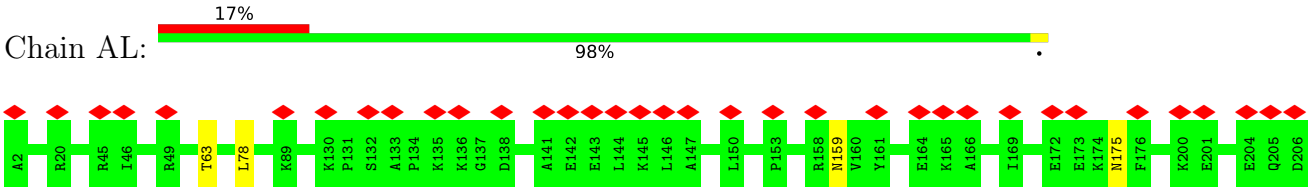
• Molecule 50: ribosomal protein uL5

Chain AJ:



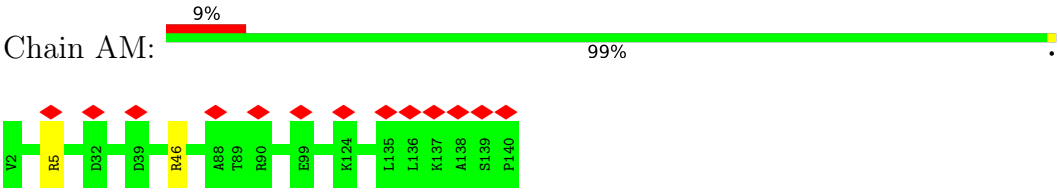
• Molecule 51: ribosomal protein eL13

Chain AL:



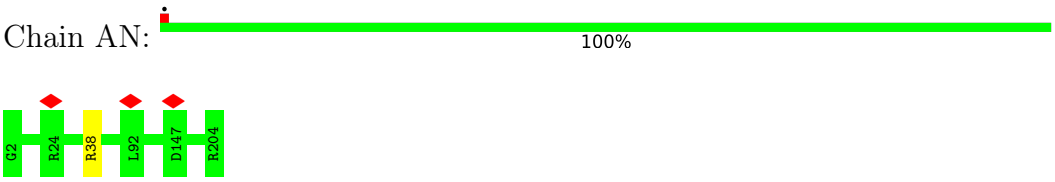
• Molecule 52: ribosomal protein eL14

Chain AM:



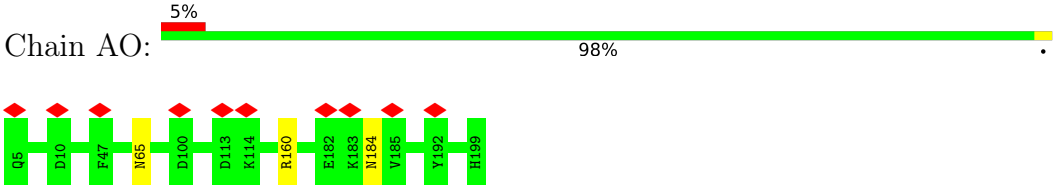
• Molecule 53: ribosomal protein eL15

Chain AN:



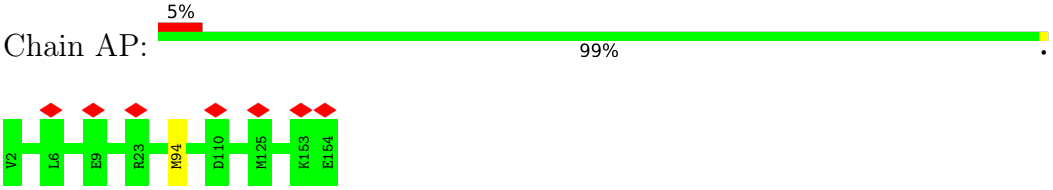
• Molecule 54: ribosomal protein uL13

Chain AO:



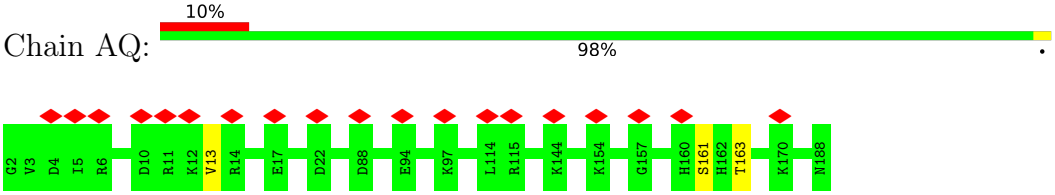
• Molecule 55: ribosomal protein uL22

Chain AP:



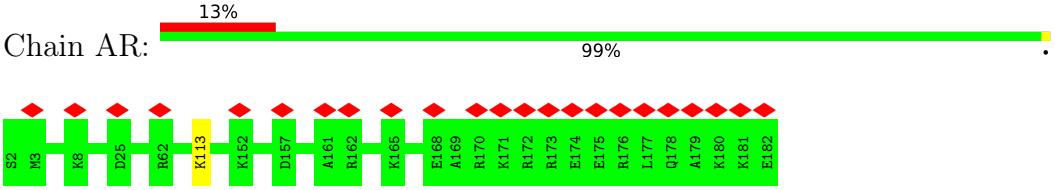
• Molecule 56: ribosomal protein eL18

Chain AQ:



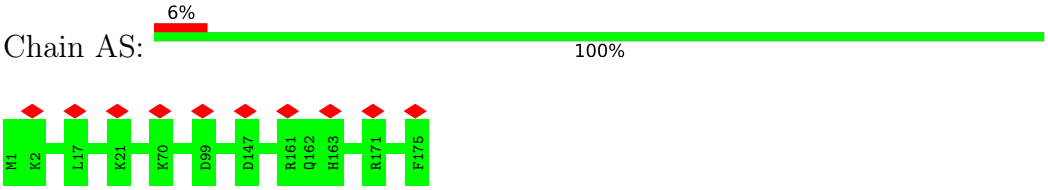
• Molecule 57: ribosomal protein eL19

Chain AR:



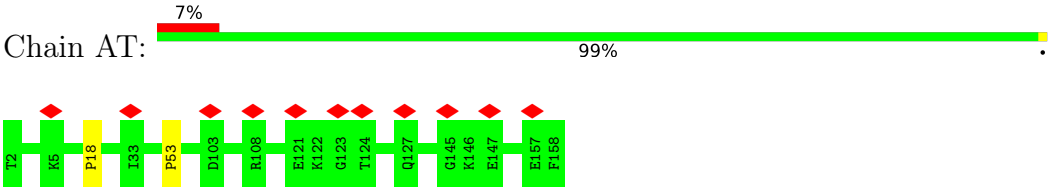
• Molecule 58: ribosomal protein eL20

Chain AS:



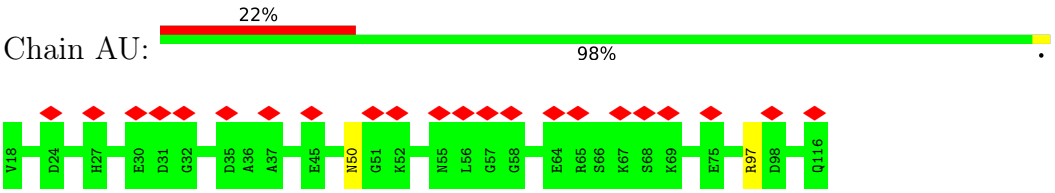
• Molecule 59: ribosomal protein eL21

Chain AT:



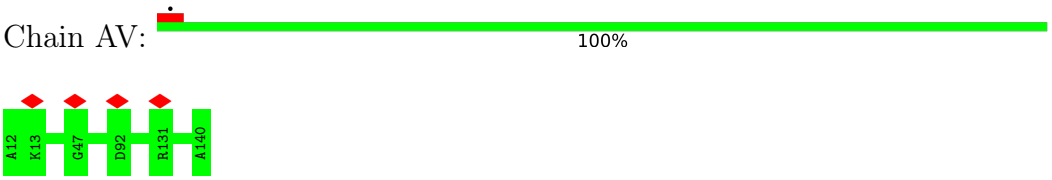
• Molecule 60: ribosomal protein eL22

Chain AU:



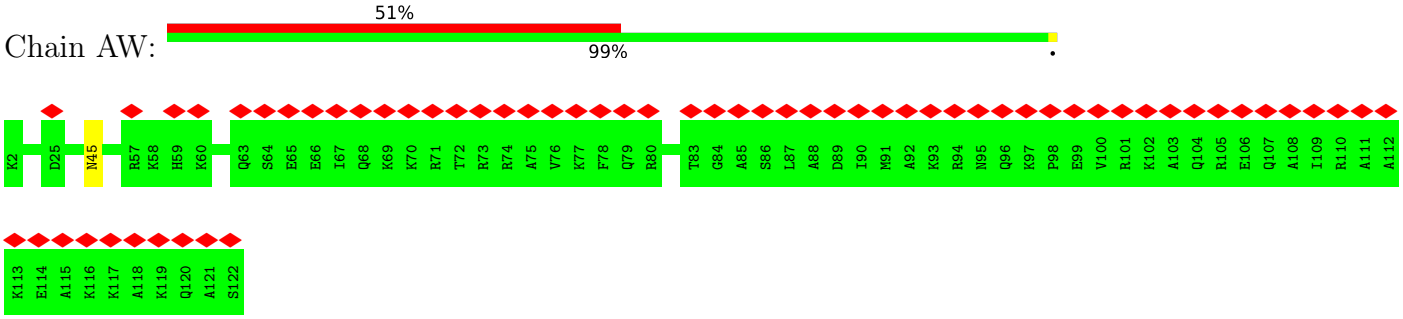
• Molecule 61: ribosomal protein uL14

Chain AV:



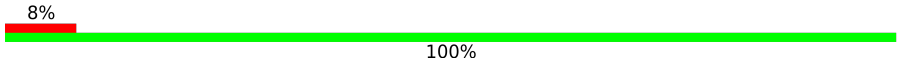
• Molecule 62: ribosomal protein eL24

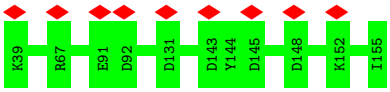
Chain AW:



• Molecule 63: ribosomal protein uL23

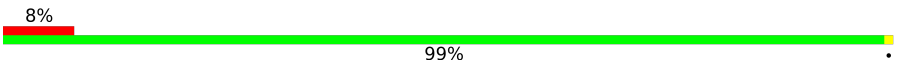
Chain AX:

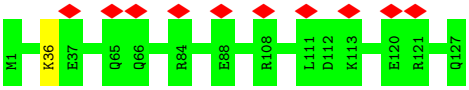




• Molecule 64: ribosomal protein uL24

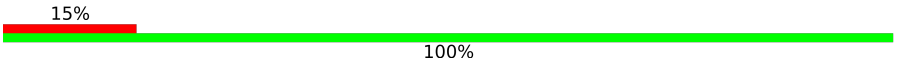
Chain AY:

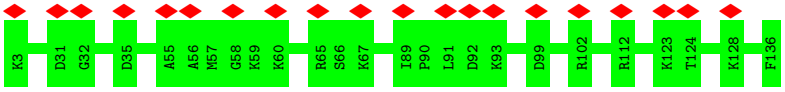




• Molecule 65: ribosomal protein eL27

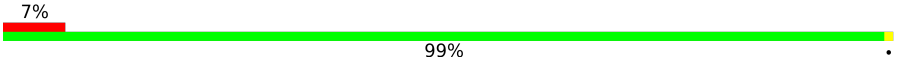
Chain AZ:

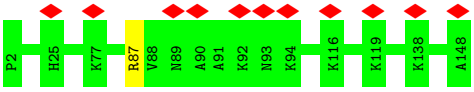




• Molecule 66: ribosomal protein uL15

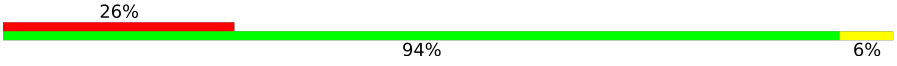
Chain Aa:

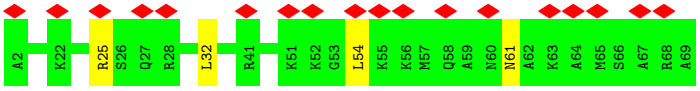




• Molecule 67: ribosomal protein eL29

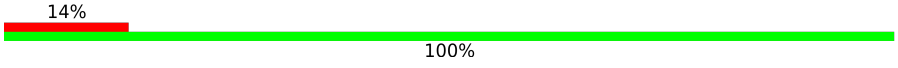
Chain Ab:

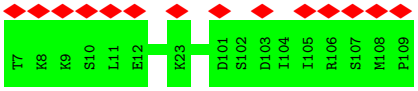




• Molecule 68: ribosomal protein eL30

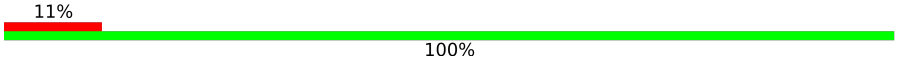
Chain Ac:

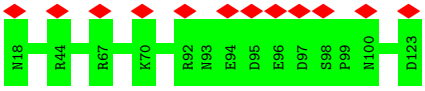




• Molecule 69: ribosomal protein eL31

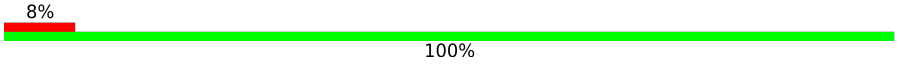
Chain Ad:

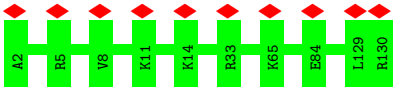




• Molecule 70: ribosomal protein eL32

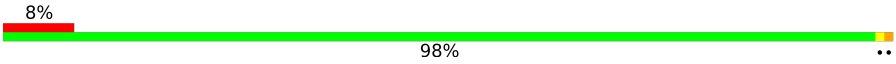
Chain Ae:





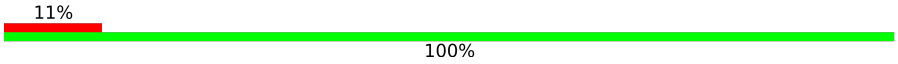
• Molecule 71: ribosomal protein eL33

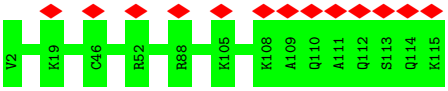
Chain Af:



• Molecule 72: ribosomal protein eL34

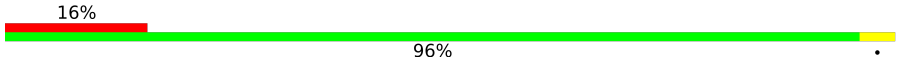
Chain Ag:

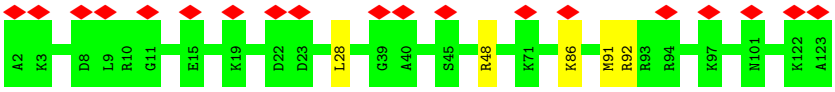




• Molecule 73: ribosomal protein uL29

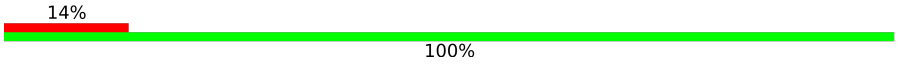
Chain Ah:

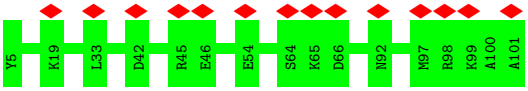




• Molecule 74: ribosomal protein eL36

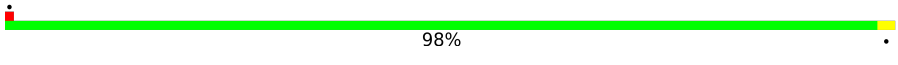
Chain Ai:

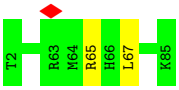




• Molecule 75: ribosomal protein eL37

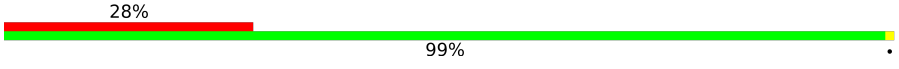
Chain Aj:

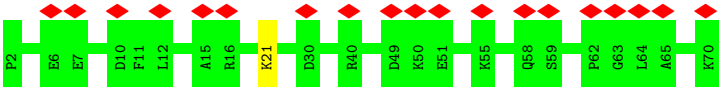




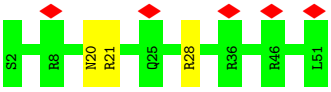
• Molecule 76: ribosomal protein eL38

Chain Ak:

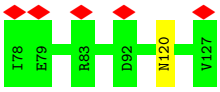




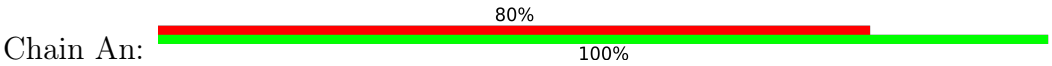
• Molecule 77: ribosomal protein eL39

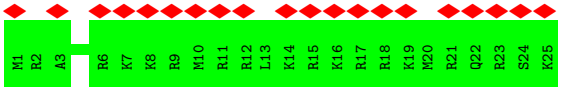


• Molecule 78: ribosomal protein eL40

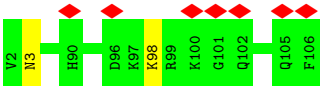


• Molecule 79: ribosomal protein eL41

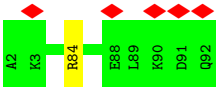




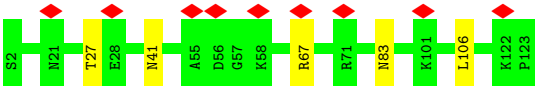
• Molecule 80: ribosomal protein eL42



• Molecule 81: ribosomal protein eL43

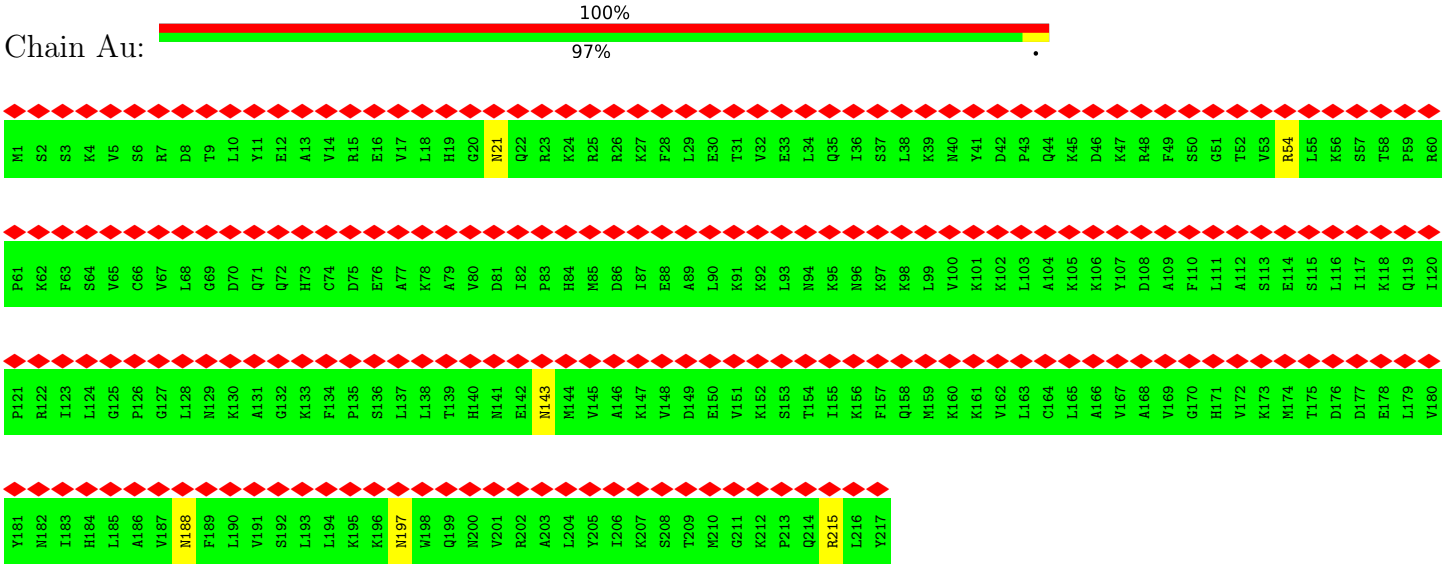


• Molecule 82: ribosomal protein eL28



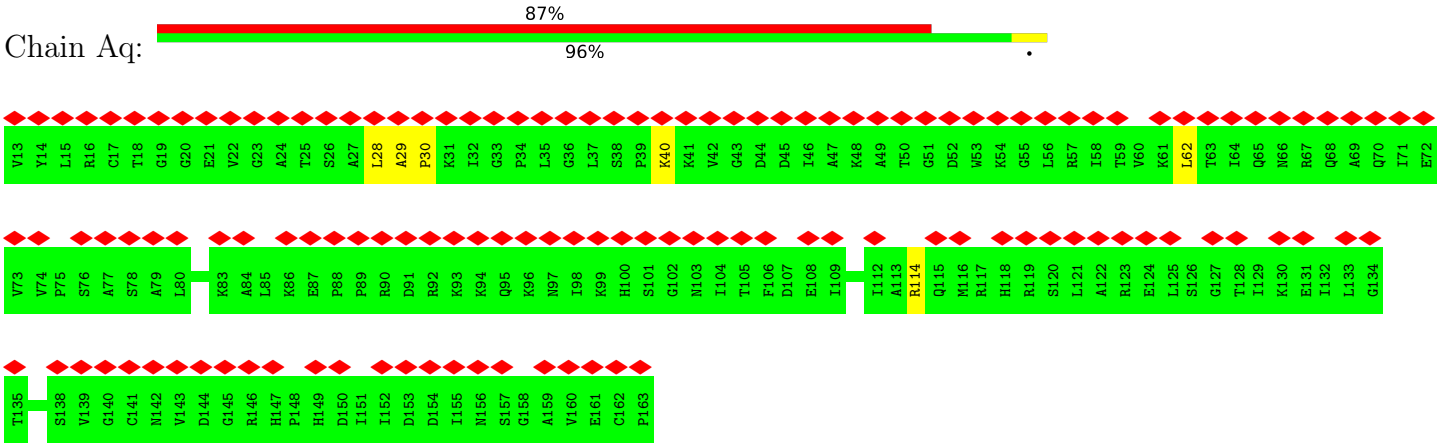
• Molecule 83: ribosomal protein uL1

Chain Au:



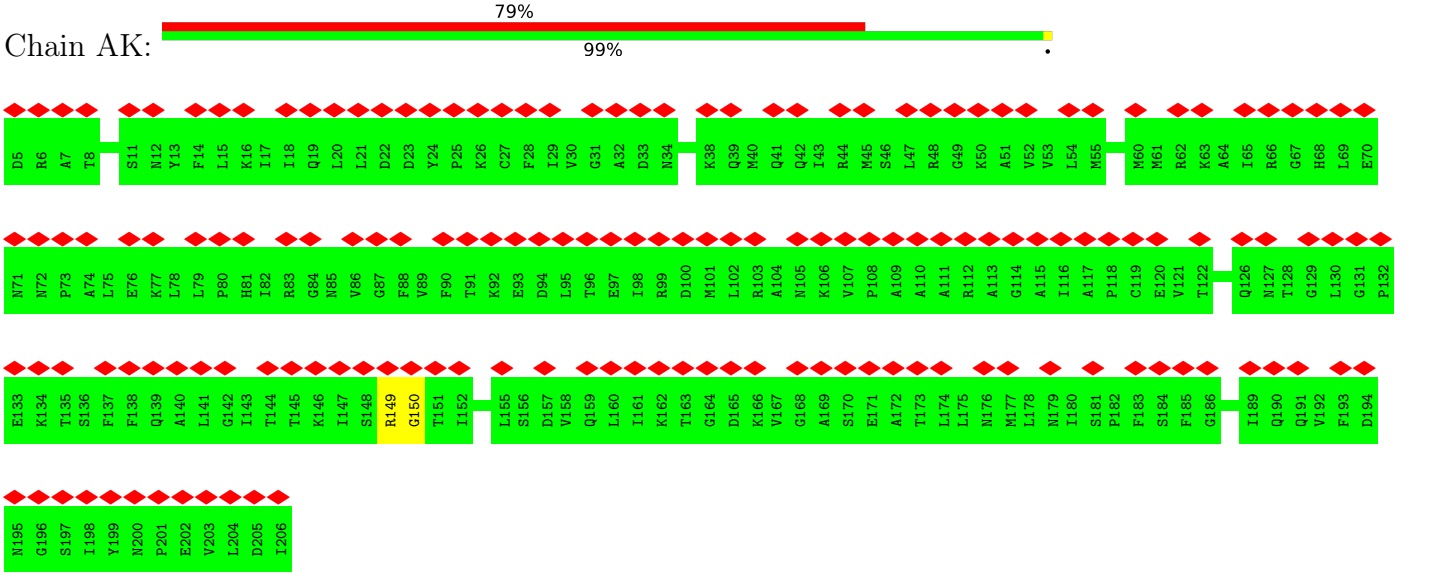
• Molecule 84: ribosomal protein uL11

Chain Aq:



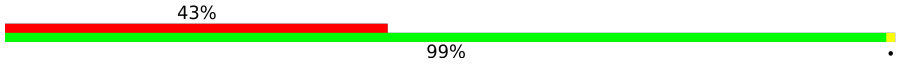
• Molecule 85: ribosomal protein uL10

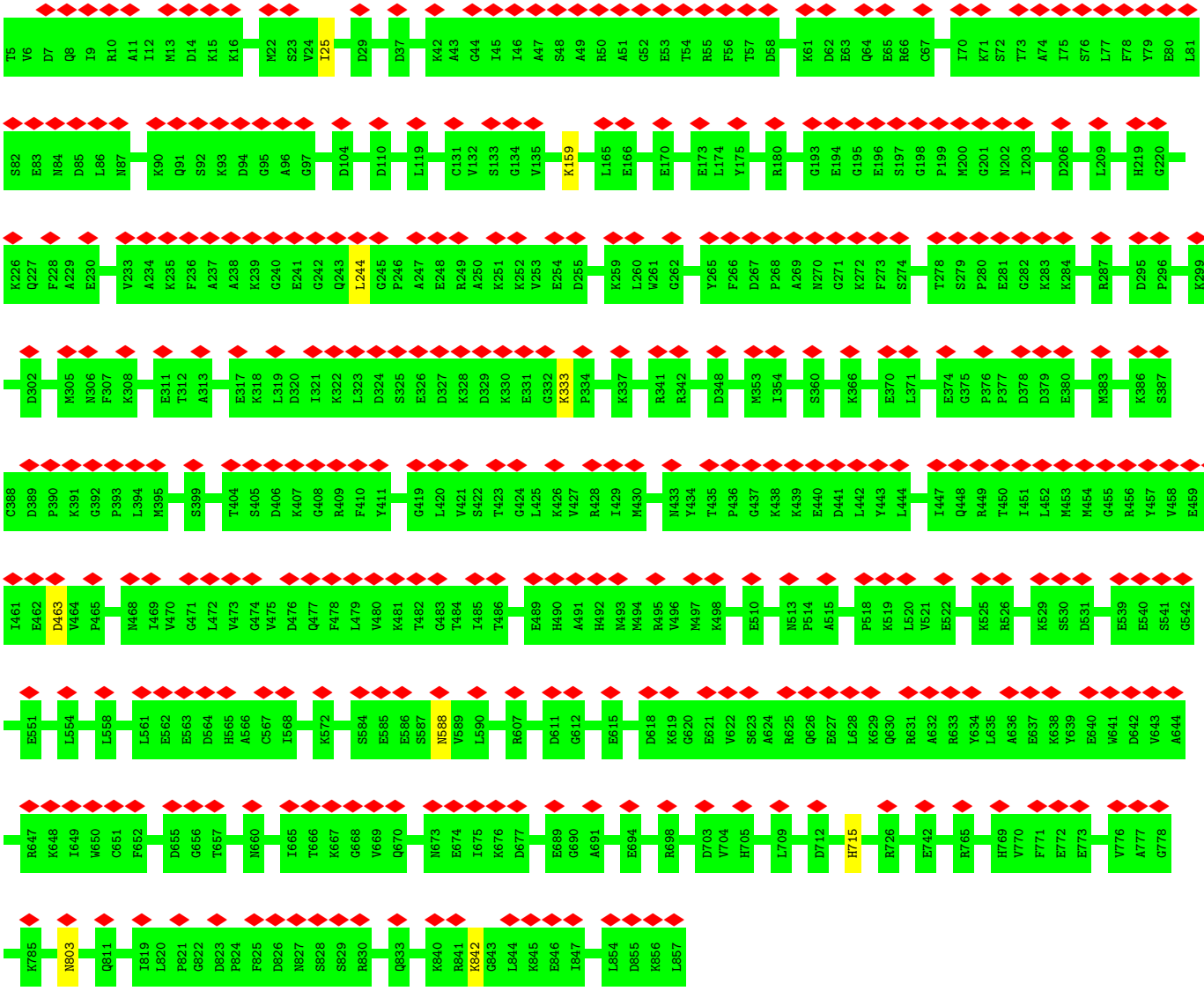
Chain AK:



• Molecule 86: eukaryotic elongation factor 2 (eEF2)

Chain Ct:


43%
99%


T5 V6 D7 Q8 I9 R10 A11 I12 M13 D14 K15 K16 M22 S23 V24 I25 D29 D37 K42 A43 G44 I45 I46 A47 S48 A49 R50 A51 G52 E53 T54 R55 F56 T57 D58 K61 D62 E63 Q64 E65 R66 C67 I70 K71 S72 T73 A74 I75 S76 L77 F78 Y79 E80 L81
S82 E83 N84 D85 L86 N87 K90 Q91 S92 K93 D94 G95 A96 G97 D104 D110 L119 C131 V132 S133 G134 V135 K159 L165 E166 E170 E173 L174 Y175 R180 G193 E194 G195 E196 S197 G198 P199 M200 G201 N202 I203 D206 L209 H219 G220
K226 Q227 F228 A229 E230 V233 A234 K235 F236 A237 A238 K239 G240 E241 G242 Q243 L244 G245 P246 A247 E248 R249 A250 K251 K252 V253 E254 D255 K259 L260 W261 G262 Y265 F266 D267 P268 A269 N270 G271 K272 F273 S274 T278 S279 P280 E281 G282 K283 K284 R287 D295 P296 K299
D302 M305 N306 F307 K308 E311 T312 A313 E317 K318 L319 D320 I321 K322 L323 D324 S325 E326 D327 K328 D329 K330 E331 G332 K333 P334 K337 R341 R342 D348 M353 I354 S360 K366 E370 L371 E374 G375 P376 P377 D378 D379 E380 M383 K386 S387
C388 D389 P390 K391 G392 P393 L394 M395 S399 T404 S405 D406 K407 G408 R409 F410 Y411 G419 L420 V421 S422 T423 G424 L425 K426 V427 R428 I429 M430 N433 Y434 T435 P436 G437 K438 K439 E440 D441 L442 Y443 L444 I447 Q448 R449 T450 I451 L452 M453 M454 G455 R456 Y457 V458 E459 P460
I461 E462 D463 V464 P465 N468 I469 V470 G471 L472 V473 G474 V475 D476 Q477 F478 L479 V480 K481 T482 G483 T484 I485 T486 E489 H490 A491 H492 N493 M494 R495 V496 M497 K498 E510 N513 P514 A515 P518 K519 L520 V521 E522 K525 R526 K529 S530 D531 E539 E540 S541 G542
E551 L554 L558 L561 E562 E563 D564 H565 A566 C567 I568 K572 S584 E585 E586 S587 N588 V589 L590 R607 D611 G612 E615 D618 K619 G620 E621 V622 S623 A624 R625 Q626 E627 L628 K629 Q630 R631 A632 R633 Y634 L635 A636 E637 K638 Y639 E640 W641 D642 V643 A644
R647 K648 I649 W650 C651 F652 D655 G656 T657 N660 I665 T666 K667 G668 V669 Q670 N673 E674 I675 K676 D677 E689 G690 A691 E694 R698 D703 V704 H705 L709 D712 H715 R726 E742 R765 H769 V770 F771 E772 E773 V776 A777 G778
K785 N803 Q811 I819 L820 P821 G822 D823 P824 F825 D826 N827 S828 S829 R830 Q833 K840 R841 K842 G843 L844 K845 E846 I847 L854 D855 K856 L857

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	44522	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	13.064	Depositor
Minimum map value	-4.149	Depositor
Average map value	0.343	Depositor
Map value standard deviation	0.691	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	394.875, 394.875, 394.875	wwPDB
Map dimensions	405, 405, 405	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.975, 0.975, 0.975	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: DDE, MG, ZN, GNP

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	A2	0.32	0/86613	1.01	274/135108 (0.2%)
2	Bv	0.36	1/1810 (0.1%)	0.96	1/2817 (0.0%)
3	Bx	0.23	0/261	0.86	0/404
4	Bw	0.38	1/1819 (0.1%)	1.00	6/2833 (0.2%)
5	B1	0.31	1/40767 (0.0%)	1.04	204/63536 (0.3%)
6	BD	0.26	0/1736	0.51	0/2338
7	BF	0.27	0/1524	0.55	0/2048
8	BK	0.27	0/851	0.55	0/1147
9	BM	0.25	0/941	0.55	0/1264
10	BP	0.30	0/1019	0.63	0/1361
11	BQ	0.26	0/1126	0.55	0/1506
12	BR	0.25	0/1023	0.50	0/1373
13	BS	0.26	0/1172	0.51	0/1570
14	BT	0.27	0/1131	0.54	0/1515
15	BU	0.24	0/778	0.53	0/1045
16	BZ	0.27	0/696	0.59	0/929
17	Bc	0.25	0/490	0.54	0/656
18	Bd	0.28	0/437	0.60	0/580
19	Bf	0.25	0/613	0.50	0/811
20	Bg	0.26	0/2497	0.52	0/3399
21	BA	0.27	0/1741	0.54	0/2366
22	BB	0.27	0/1749	0.61	0/2340
23	BC	0.28	0/1761	0.53	0/2379
24	BE	0.27	0/2072	0.54	0/2793
25	BG	0.26	0/1907	0.52	0/2538
26	BH	0.26	0/1501	0.50	0/2009
27	BI	0.27	0/1725	0.55	0/2298
28	BJ	0.27	0/1520	0.52	0/2030
29	BL	0.28	0/1281	0.57	1/1710 (0.1%)
30	BN	0.26	0/1226	0.52	0/1649
31	BO	0.26	0/1029	0.50	0/1380
32	BV	0.27	0/623	0.50	0/833

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	BW	0.28	0/1051	0.53	0/1406
34	BX	0.28	0/1116	0.53	0/1490
35	BY	0.26	0/1032	0.50	0/1371
36	Ba	0.26	0/786	0.53	0/1053
37	Bb	0.26	0/637	0.51	0/854
38	Be	0.28	0/443	0.54	0/583
39	A3	0.32	0/3726	1.03	15/5804 (0.3%)
40	A4	0.32	0/2839	1.02	13/4425 (0.3%)
41	AA	0.28	0/1968	0.54	0/2639
42	AB	0.28	0/3246	0.54	1/4345 (0.0%)
43	AC	0.27	0/2942	0.52	0/3951
44	AD	0.28	0/2437	0.51	0/3262
45	AE	0.28	0/1603	0.58	0/2153
46	AF	0.28	0/1986	0.51	0/2644
47	AG	0.28	0/1913	0.54	1/2576 (0.0%)
48	AH	0.28	0/1545	0.59	1/2077 (0.0%)
49	AI	0.27	0/1730	0.50	0/2311
50	AJ	0.27	0/1376	0.56	1/1841 (0.1%)
51	AL	0.28	0/1688	0.56	0/2260
52	AM	0.28	0/1161	0.50	0/1554
53	AN	0.28	0/1746	0.51	0/2338
54	AO	0.28	0/1638	0.49	0/2191
55	AP	0.26	0/1268	0.49	0/1701
56	AQ	0.27	0/1537	0.60	0/2052
57	AR	0.25	0/1533	0.48	0/2025
58	AS	0.27	0/1488	0.52	0/1997
59	AT	0.27	0/1312	0.49	0/1753
60	AU	0.28	0/822	0.50	0/1103
61	AV	0.27	0/983	0.49	0/1319
62	AW	0.26	0/1004	0.47	0/1332
63	AX	0.26	0/975	0.51	0/1312
64	AY	0.25	0/1081	0.45	0/1439
65	AZ	0.27	0/1126	0.53	0/1502
66	Aa	0.27	0/1191	0.52	0/1591
67	Ab	0.27	0/569	0.65	2/750 (0.3%)
68	Ac	0.27	0/812	0.53	0/1089
69	Ad	0.26	0/894	0.52	0/1204
70	Ae	0.26	0/1082	0.55	0/1443
71	Af	0.28	0/895	0.57	0/1198
72	Ag	0.28	0/916	0.57	0/1220
73	Ah	0.25	0/1023	0.55	1/1351 (0.1%)
74	Ai	0.25	0/805	0.50	0/1065
75	Aj	0.29	0/703	0.58	0/929

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	Ak	0.26	0/575	0.53	0/761
77	Al	0.26	0/454	0.53	0/599
78	Am	0.25	0/417	0.52	0/553
79	An	0.22	0/241	0.42	0/305
80	Ao	0.28	0/877	0.52	0/1156
81	Ap	0.28	0/718	0.55	0/953
82	At	0.28	0/995	0.65	1/1334 (0.1%)
83	Au	0.26	0/1772	0.53	0/2375
84	Aq	0.30	0/1155	0.69	2/1558 (0.1%)
85	AK	0.28	0/1580	0.60	0/2133
86	Ct	0.28	0/6767	0.57	2/9139 (0.0%)
All	All	0.30	3/241618 (0.0%)	0.86	526/353934 (0.1%)

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
11	BQ	0	1
16	BZ	0	1
22	BB	0	1
24	BE	0	1
27	BI	0	2
28	BJ	0	1
43	AC	0	3
45	AE	0	2
48	AH	0	3
49	AI	0	1
56	AQ	0	2
57	AR	0	1
71	Af	0	1
73	Ah	0	1
82	At	0	1
84	Aq	0	2
85	AK	0	1
86	Ct	0	2
All	All	0	27

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B1	1	U	OP3-P	-10.61	1.48	1.61
4	Bw	1	G	OP3-P	-10.60	1.48	1.61
2	Bv	1	G	OP3-P	-10.57	1.48	1.61

The worst 5 of 526 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B1	496	C	N1-C2-O2	10.70	125.32	118.90
5	B1	621	C	N1-C2-O2	10.09	124.95	118.90
5	B1	797	C	C2-N1-C1'	10.06	129.87	118.80
1	A2	252	C	N1-C2-O2	9.62	124.67	118.90
5	B1	1271	C	N1-C2-O2	9.56	124.64	118.90

There are no chirality outliers.

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	BB	39	PHE	Peptide
24	BE	92	ILE	Peptide
27	BI	132	GLU	Peptide
11	BQ	13	PHE	Peptide
16	BZ	41	ARG	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
6	BD	218/220 (99%)	210 (96%)	8 (4%)	0	100	100
7	BF	188/190 (99%)	173 (92%)	15 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	BK	96/98 (98%)	81 (84%)	14 (15%)	1 (1%)	15 54
9	BM	118/120 (98%)	109 (92%)	9 (8%)	0	100 100
10	BP	118/120 (98%)	102 (86%)	15 (13%)	1 (1%)	19 58
11	BQ	137/139 (99%)	131 (96%)	6 (4%)	0	100 100
12	BR	123/125 (98%)	107 (87%)	16 (13%)	0	100 100
13	BS	137/139 (99%)	126 (92%)	11 (8%)	0	100 100
14	BT	141/143 (99%)	129 (92%)	11 (8%)	1 (1%)	22 61
15	BU	95/97 (98%)	92 (97%)	3 (3%)	0	100 100
16	BZ	84/86 (98%)	74 (88%)	10 (12%)	0	100 100
17	Bc	60/62 (97%)	54 (90%)	4 (7%)	2 (3%)	4 28
18	Bd	49/51 (96%)	45 (92%)	4 (8%)	0	100 100
19	Bf	71/73 (97%)	63 (89%)	8 (11%)	0	100 100
20	Bg	312/314 (99%)	283 (91%)	29 (9%)	0	100 100
21	BA	213/215 (99%)	201 (94%)	12 (6%)	0	100 100
22	BB	210/212 (99%)	179 (85%)	31 (15%)	0	100 100
23	BC	220/222 (99%)	208 (94%)	12 (6%)	0	100 100
24	BE	255/257 (99%)	236 (92%)	17 (7%)	2 (1%)	19 58
25	BG	230/232 (99%)	213 (93%)	17 (7%)	0	100 100
26	BH	181/183 (99%)	172 (95%)	9 (5%)	0	100 100
27	BI	205/207 (99%)	176 (86%)	28 (14%)	1 (0%)	29 68
28	BJ	177/179 (99%)	153 (86%)	22 (12%)	2 (1%)	14 52
29	BL	151/153 (99%)	137 (91%)	13 (9%)	1 (1%)	22 61
30	BN	147/149 (99%)	133 (90%)	14 (10%)	0	100 100
31	BO	134/136 (98%)	123 (92%)	11 (8%)	0	100 100
32	BV	79/81 (98%)	76 (96%)	3 (4%)	0	100 100
33	BW	127/129 (98%)	121 (95%)	6 (5%)	0	100 100
34	BX	139/141 (99%)	126 (91%)	13 (9%)	0	100 100
35	BY	123/125 (98%)	108 (88%)	15 (12%)	0	100 100
36	Ba	95/97 (98%)	86 (90%)	9 (10%)	0	100 100
37	Bb	78/80 (98%)	71 (91%)	7 (9%)	0	100 100
38	Be	53/55 (96%)	48 (91%)	5 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	AA	250/252 (99%)	233 (93%)	17 (7%)	0	100	100
42	AB	392/394 (100%)	358 (91%)	34 (9%)	0	100	100
43	AC	361/363 (99%)	325 (90%)	33 (9%)	3 (1%)	19	58
44	AD	292/294 (99%)	268 (92%)	24 (8%)	0	100	100
45	AE	192/194 (99%)	161 (84%)	30 (16%)	1 (0%)	29	68
46	AF	232/234 (99%)	215 (93%)	17 (7%)	0	100	100
47	AG	232/234 (99%)	219 (94%)	13 (6%)	0	100	100
48	AH	189/191 (99%)	174 (92%)	15 (8%)	0	100	100
49	AI	204/208 (98%)	187 (92%)	17 (8%)	0	100	100
50	AJ	167/169 (99%)	151 (90%)	15 (9%)	1 (1%)	25	64
51	AL	203/205 (99%)	171 (84%)	31 (15%)	1 (0%)	29	68
52	AM	137/139 (99%)	126 (92%)	11 (8%)	0	100	100
53	AN	201/203 (99%)	182 (90%)	19 (10%)	0	100	100
54	AO	193/195 (99%)	184 (95%)	9 (5%)	0	100	100
55	AP	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
56	AQ	185/187 (99%)	163 (88%)	21 (11%)	1 (0%)	29	68
57	AR	179/181 (99%)	168 (94%)	11 (6%)	0	100	100
58	AS	173/175 (99%)	162 (94%)	11 (6%)	0	100	100
59	AT	155/157 (99%)	138 (89%)	15 (10%)	2 (1%)	12	48
60	AU	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
61	AV	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
62	AW	119/121 (98%)	110 (92%)	9 (8%)	0	100	100
63	AX	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
64	AY	125/127 (98%)	119 (95%)	6 (5%)	0	100	100
65	AZ	132/134 (98%)	117 (89%)	15 (11%)	0	100	100
66	Aa	145/147 (99%)	129 (89%)	16 (11%)	0	100	100
67	Ab	66/68 (97%)	55 (83%)	11 (17%)	0	100	100
68	Ac	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
69	Ad	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
70	Ae	127/129 (98%)	115 (91%)	12 (9%)	0	100	100
71	Af	107/109 (98%)	97 (91%)	8 (8%)	2 (2%)	8	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	Ag	112/114 (98%)	101 (90%)	11 (10%)	0	100	100
73	Ah	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
74	Ai	95/97 (98%)	85 (90%)	10 (10%)	0	100	100
75	Aj	82/84 (98%)	75 (92%)	7 (8%)	0	100	100
76	Ak	67/69 (97%)	64 (96%)	3 (4%)	0	100	100
77	Al	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
78	Am	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
79	An	23/25 (92%)	23 (100%)	0	0	100	100
80	Ao	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
81	Ap	89/91 (98%)	82 (92%)	7 (8%)	0	100	100
82	At	120/122 (98%)	105 (88%)	15 (12%)	0	100	100
83	Au	215/217 (99%)	197 (92%)	18 (8%)	0	100	100
84	Aq	149/151 (99%)	115 (77%)	34 (23%)	0	100	100
85	AK	200/202 (99%)	179 (90%)	20 (10%)	1 (0%)	29	68
86	Ct	850/853 (100%)	758 (89%)	91 (11%)	1 (0%)	51	84
All	All	12538/12699 (99%)	11430 (91%)	1084 (9%)	24 (0%)	50	81

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	BE	93	GLU
28	BJ	138	ARG
71	Af	107	PRO
10	BP	51	ARG
43	AC	51	PRO

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	
6	BD	183/183 (100%)	182 (100%)	1 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	BF	160/160 (100%)	160 (100%)	0	100	100
8	BK	89/89 (100%)	88 (99%)	1 (1%)	73	88
9	BM	102/102 (100%)	102 (100%)	0	100	100
10	BP	109/109 (100%)	108 (99%)	1 (1%)	78	90
11	BQ	115/115 (100%)	114 (99%)	1 (1%)	78	90
12	BR	113/113 (100%)	113 (100%)	0	100	100
13	BS	121/121 (100%)	116 (96%)	5 (4%)	30	63
14	BT	113/113 (100%)	112 (99%)	1 (1%)	78	90
15	BU	90/90 (100%)	90 (100%)	0	100	100
16	BZ	75/75 (100%)	74 (99%)	1 (1%)	69	86
17	Bc	55/55 (100%)	54 (98%)	1 (2%)	59	81
18	Bd	45/45 (100%)	45 (100%)	0	100	100
19	Bf	66/66 (100%)	66 (100%)	0	100	100
20	Bg	272/272 (100%)	271 (100%)	1 (0%)	91	96
21	BA	180/180 (100%)	179 (99%)	1 (1%)	86	94
22	BB	193/193 (100%)	191 (99%)	2 (1%)	76	88
23	BC	188/188 (100%)	187 (100%)	1 (0%)	88	94
24	BE	220/220 (100%)	216 (98%)	4 (2%)	59	81
25	BG	202/202 (100%)	200 (99%)	2 (1%)	76	88
26	BH	164/164 (100%)	164 (100%)	0	100	100
27	BI	179/179 (100%)	179 (100%)	0	100	100
28	BJ	160/160 (100%)	159 (99%)	1 (1%)	86	94
29	BL	138/138 (100%)	137 (99%)	1 (1%)	84	93
30	BN	130/130 (100%)	129 (99%)	1 (1%)	81	91
31	BO	106/106 (100%)	105 (99%)	1 (1%)	78	90
32	BV	65/65 (100%)	63 (97%)	2 (3%)	40	70
33	BW	112/112 (100%)	110 (98%)	2 (2%)	59	81
34	BX	113/113 (100%)	112 (99%)	1 (1%)	78	90
35	BY	107/107 (100%)	106 (99%)	1 (1%)	78	90
36	Ba	84/84 (100%)	83 (99%)	1 (1%)	71	87
37	Bb	72/72 (100%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
38	Be	44/44 (100%)	41 (93%)	3 (7%)	16 48
41	AA	194/194 (100%)	193 (100%)	1 (0%)	88 94
42	AB	343/343 (100%)	341 (99%)	2 (1%)	86 94
43	AC	302/302 (100%)	298 (99%)	4 (1%)	69 86
44	AD	248/248 (100%)	243 (98%)	5 (2%)	55 79
45	AE	174/174 (100%)	172 (99%)	2 (1%)	73 88
46	AF	203/203 (100%)	200 (98%)	3 (2%)	65 84
47	AG	199/199 (100%)	199 (100%)	0	100 100
48	AH	170/170 (100%)	170 (100%)	0	100 100
49	AI	178/178 (100%)	177 (99%)	1 (1%)	86 94
50	AJ	142/142 (100%)	142 (100%)	0	100 100
51	AL	171/171 (100%)	168 (98%)	3 (2%)	59 81
52	AM	118/118 (100%)	116 (98%)	2 (2%)	60 82
53	AN	171/171 (100%)	170 (99%)	1 (1%)	86 94
54	AO	168/168 (100%)	165 (98%)	3 (2%)	59 81
55	AP	134/134 (100%)	133 (99%)	1 (1%)	84 93
56	AQ	164/164 (100%)	164 (100%)	0	100 100
57	AR	160/160 (100%)	160 (100%)	0	100 100
58	AS	156/156 (100%)	156 (100%)	0	100 100
59	AT	138/138 (100%)	138 (100%)	0	100 100
60	AU	89/89 (100%)	87 (98%)	2 (2%)	52 78
61	AV	100/100 (100%)	100 (100%)	0	100 100
62	AW	100/100 (100%)	99 (99%)	1 (1%)	76 88
63	AX	105/105 (100%)	105 (100%)	0	100 100
64	AY	119/119 (100%)	118 (99%)	1 (1%)	81 91
65	AZ	117/117 (100%)	117 (100%)	0	100 100
66	Aa	120/120 (100%)	119 (99%)	1 (1%)	81 91
67	Ab	58/58 (100%)	56 (97%)	2 (3%)	37 68
68	Ac	88/88 (100%)	88 (100%)	0	100 100
69	Ad	97/97 (100%)	97 (100%)	0	100 100
70	Ae	115/115 (100%)	115 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	Af	88/88 (100%)	88 (100%)	0	100	100
72	Ag	98/98 (100%)	98 (100%)	0	100	100
73	Ah	109/109 (100%)	106 (97%)	3 (3%)	43	72
74	Ai	83/83 (100%)	83 (100%)	0	100	100
75	Aj	71/71 (100%)	69 (97%)	2 (3%)	43	72
76	Ak	64/64 (100%)	63 (98%)	1 (2%)	62	83
77	Al	47/47 (100%)	44 (94%)	3 (6%)	17	50
78	Am	46/46 (100%)	45 (98%)	1 (2%)	52	78
79	An	24/24 (100%)	24 (100%)	0	100	100
80	Ao	93/93 (100%)	91 (98%)	2 (2%)	52	78
81	Ap	74/74 (100%)	73 (99%)	1 (1%)	67	85
82	At	106/106 (100%)	103 (97%)	3 (3%)	43	72
83	Au	196/196 (100%)	190 (97%)	6 (3%)	40	70
84	Aq	124/124 (100%)	122 (98%)	2 (2%)	62	83
85	AK	170/170 (100%)	170 (100%)	0	100	100
86	Ct	725/725 (100%)	722 (100%)	3 (0%)	91	96
All	All	10924/10924 (100%)	10825 (99%)	99 (1%)	79	90

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
51	AL	175	ASN
67	Ab	61	ASN
52	AM	46	ARG
60	AU	50	ASN
75	Aj	65	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 138 such sidechains are listed below:

Mol	Chain	Res	Type
73	Ah	63	GLN
78	Am	120	ASN
83	Au	197	ASN
34	BX	127	ASN
34	BX	61	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	3600/3612 (99%)	701 (19%)	8 (0%)
2	Bv	75/76 (98%)	12 (16%)	0
3	Bx	10/11 (90%)	2 (20%)	0
39	A3	156/157 (99%)	37 (23%)	0
4	Bw	75/76 (98%)	12 (16%)	0
40	A4	118/119 (99%)	19 (16%)	0
5	B1	1701/1708 (99%)	339 (19%)	3 (0%)
All	All	5735/5759 (99%)	1122 (19%)	11 (0%)

5 of 1122 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	9	C
1	A2	10	A
1	A2	12	A
1	A2	14	C
1	A2	19	G

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A2	4946	U
5	B1	227	U
5	B1	797	C
5	B1	369	C
1	A2	4661	U

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
86	DDE	Ct	715	86	14,20,21	1.08	1 (7%)	14,28,30	1.43	2 (14%)

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
86	DDE	Ct	715	86	-	9/20/21/23	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	Ct	715	DDE	CD2-NE2	2.25	1.39	1.36

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
86	Ct	715	DDE	CBW-CBI-NAD	3.11	119.24	115.28
86	Ct	715	DDE	CAU-CBW-CBI	-2.46	106.32	111.20

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	Ct	715	DDE	CA-CB-CG-ND1
86	Ct	715	DDE	CA-CB-CG-CD2
86	Ct	715	DDE	NAD-CBI-CBW-NCB
86	Ct	715	DDE	OAG-CBI-CBW-NCB
86	Ct	715	DDE	CE1-CAT-CAU-CBW

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 333 ligands modelled in this entry, 332 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	$\#\|Z\| > 2$
89	GNP	Ct	901	-	29,34,34	1.58	7 (24%)	33,54,54	2.13	7 (21%)

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
89	GNP	Ct	901	-	-	4/14/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	Ct	901	GNP	PB-O3A	4.43	1.64	1.59
89	Ct	901	GNP	C6-N1	3.03	1.38	1.33
89	Ct	901	GNP	PG-N3B	2.89	1.70	1.63
89	Ct	901	GNP	PB-O1B	2.71	1.50	1.46
89	Ct	901	GNP	PG-O1G	2.66	1.50	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
89	Ct	901	GNP	C5-C6-N1	-8.37	111.99	123.43
89	Ct	901	GNP	C2-N1-C6	5.81	125.16	115.93
89	Ct	901	GNP	N3-C2-N1	-2.77	123.53	127.22
89	Ct	901	GNP	C4-C5-C6	-2.59	118.32	120.80
89	Ct	901	GNP	PB-O3A-PA	-2.43	124.07	132.62

There are no chirality outliers.

All (4) torsion outliers are listed below:

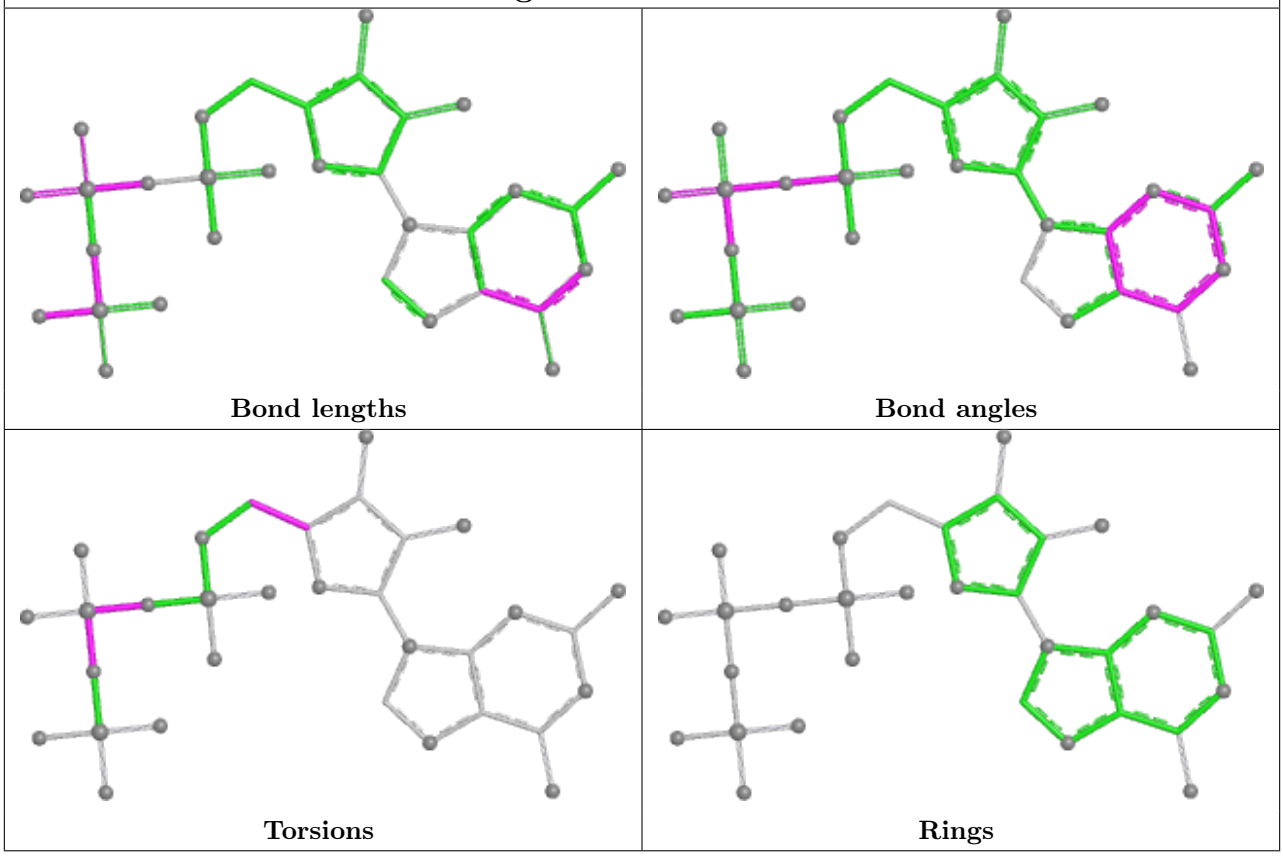
Mol	Chain	Res	Type	Atoms
89	Ct	901	GNP	PG-N3B-PB-O1B
89	Ct	901	GNP	PA-O3A-PB-O1B
89	Ct	901	GNP	O4'-C4'-C5'-O5'
89	Ct	901	GNP	C3'-C4'-C5'-O5'

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 then 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.

Ligand GNP Ct 901



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	A2	11
5	B1	6
49	AI	1

The worst 5 of 18 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B1	126:G	O3'	141:A	P	20.96
1	B1	751:G	O3'	790:C	P	20.10
1	A2	517:C	O3'	629:G	P	18.31
1	B1	1757:G	O3'	1775:U	P	18.01
1	A2	3948:C	O3'	4004:G	P	17.65

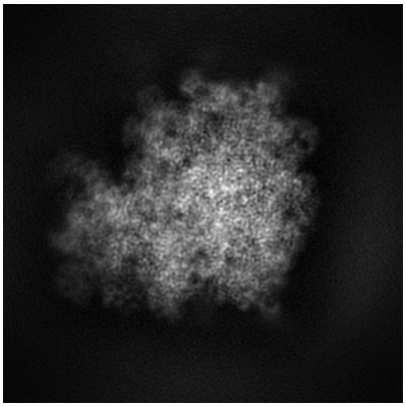
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0100. These allow visual inspection of the internal detail of the map and identification of artifacts.

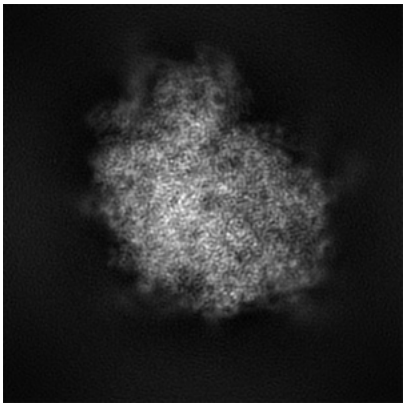
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

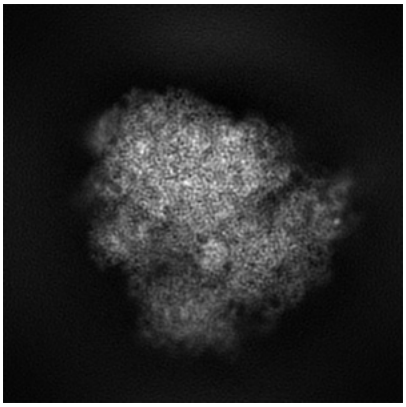
6.1.1 Primary map



X



Y

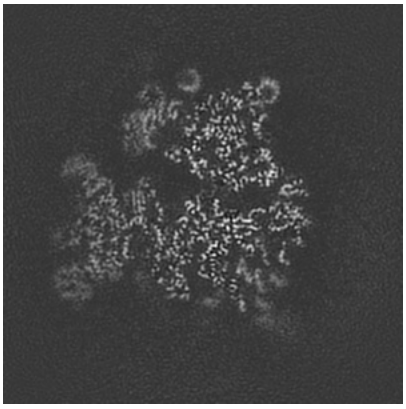


Z

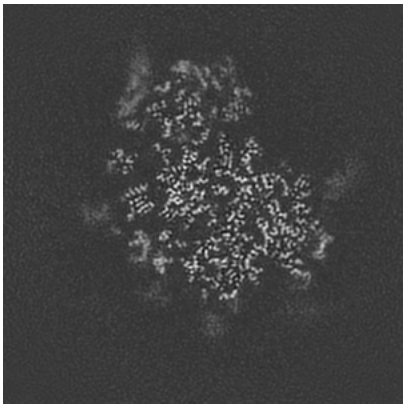
The images above show the map projected in three orthogonal directions.

6.2 Central slices

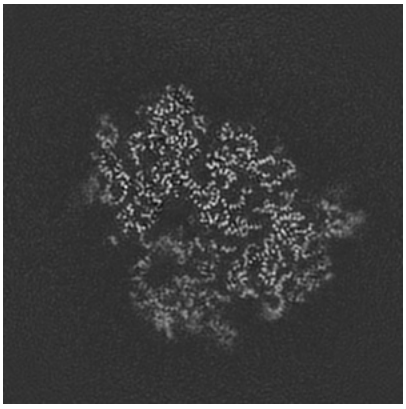
6.2.1 Primary map



X Index: 202



Y Index: 202

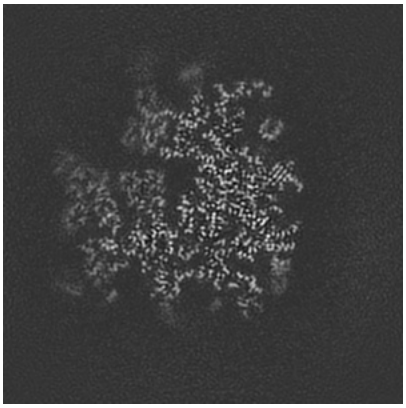


Z Index: 202

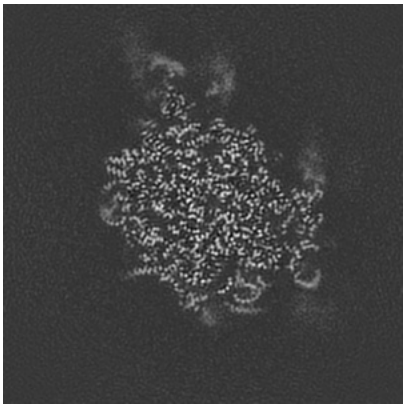
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

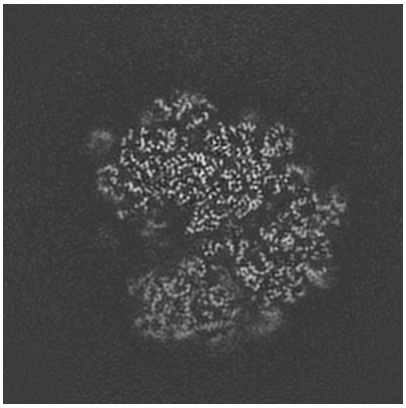
6.3.1 Primary map



X Index: 214



Y Index: 220

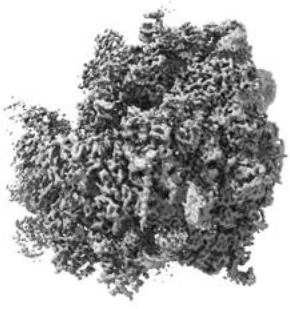


Z Index: 185

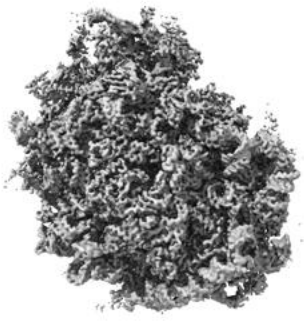
The images above show the largest variance slices of the map in three orthogonal directions.

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 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

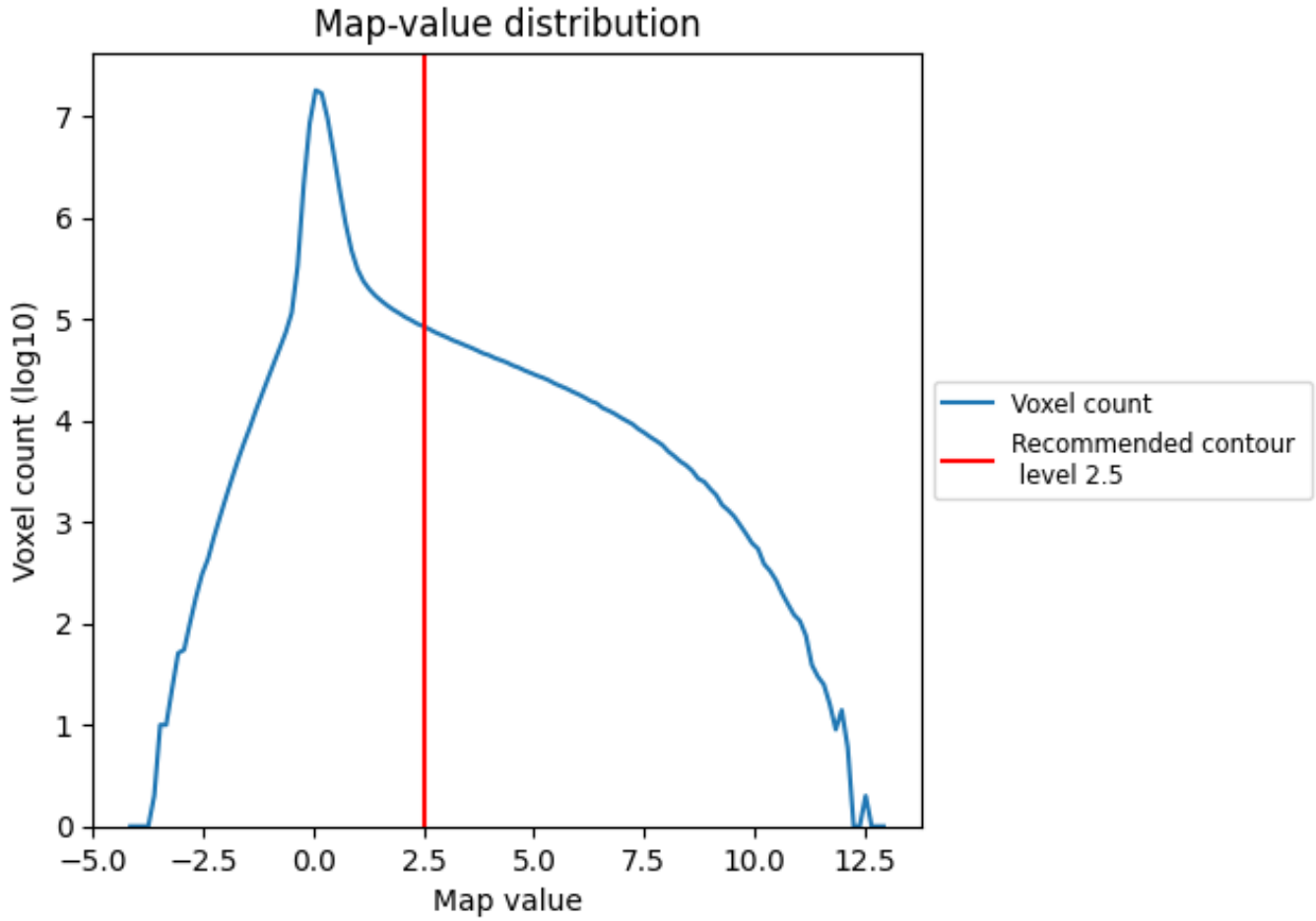
6.5 Mask visualisation (i)

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

7 Map analysis

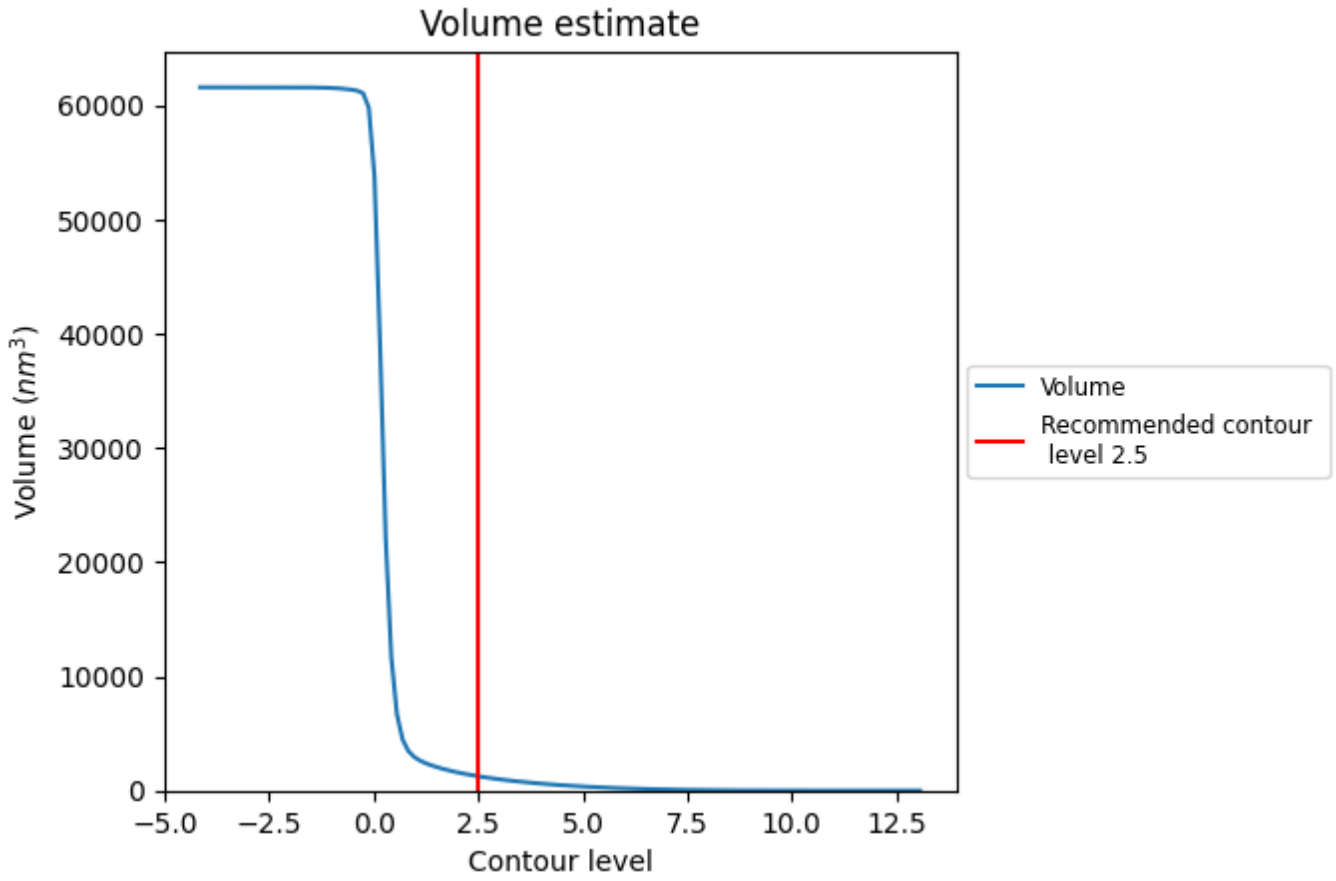
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

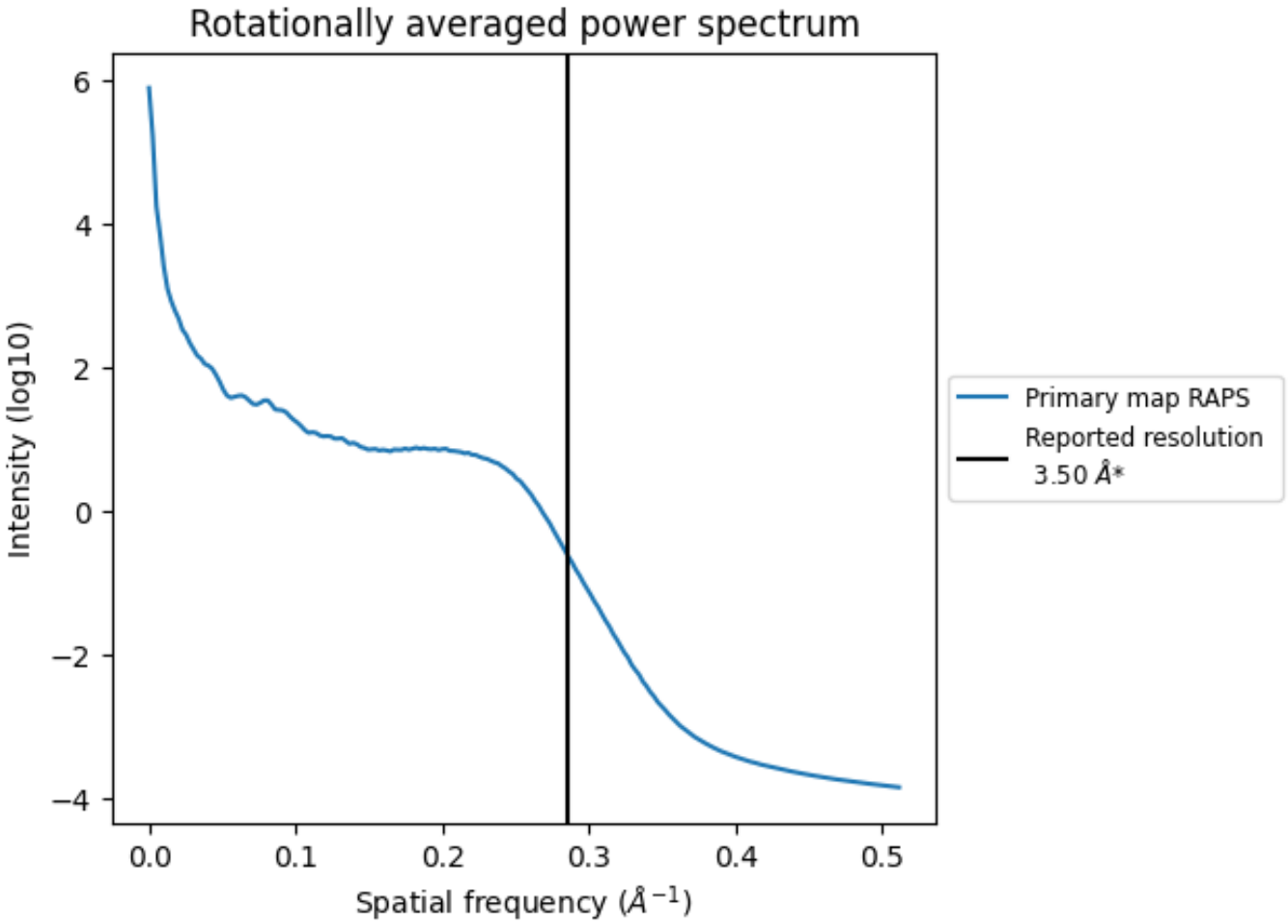
7.2 Volume estimate (i)



The volume at the recommended contour level is 1254 nm^3; this corresponds to an approximate mass of 1133 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 0.286 Å^{-1}

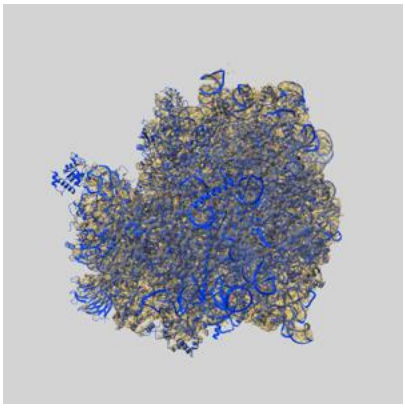
8 Fourier-Shell correlation (i)

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

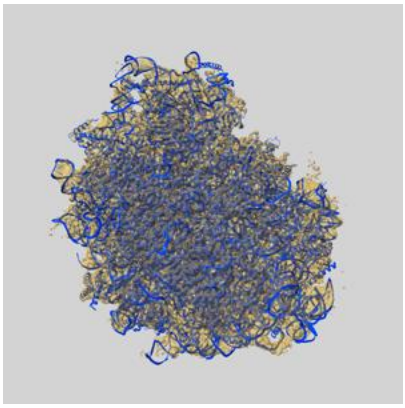
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0100 and PDB model 6GZ5. Per-residue inclusion information can be found in section 3 on page 21.

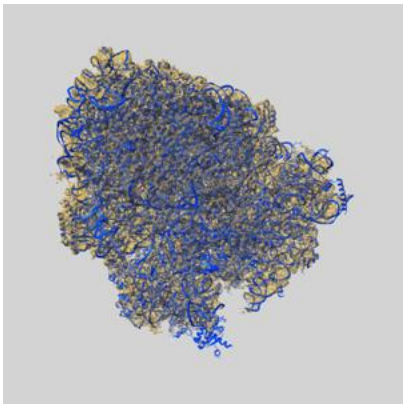
9.1 Map-model overlay



X



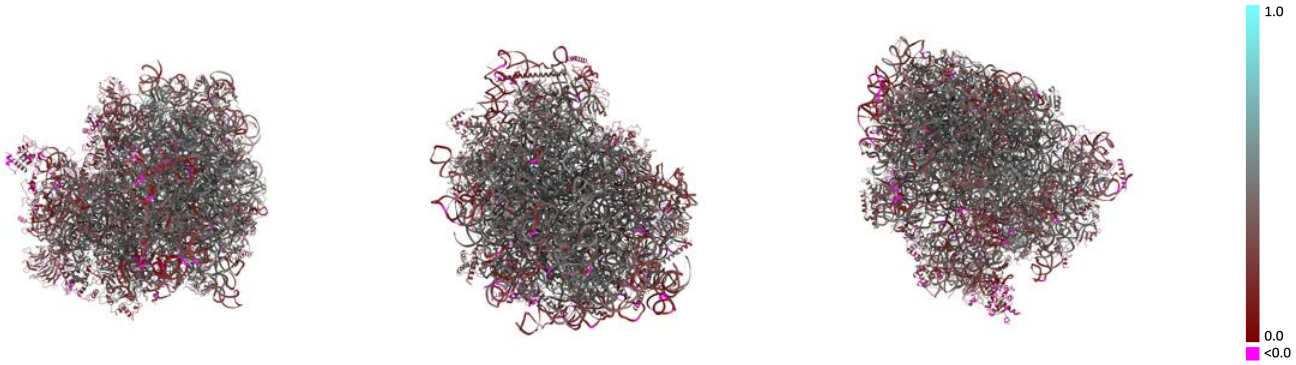
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5 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.

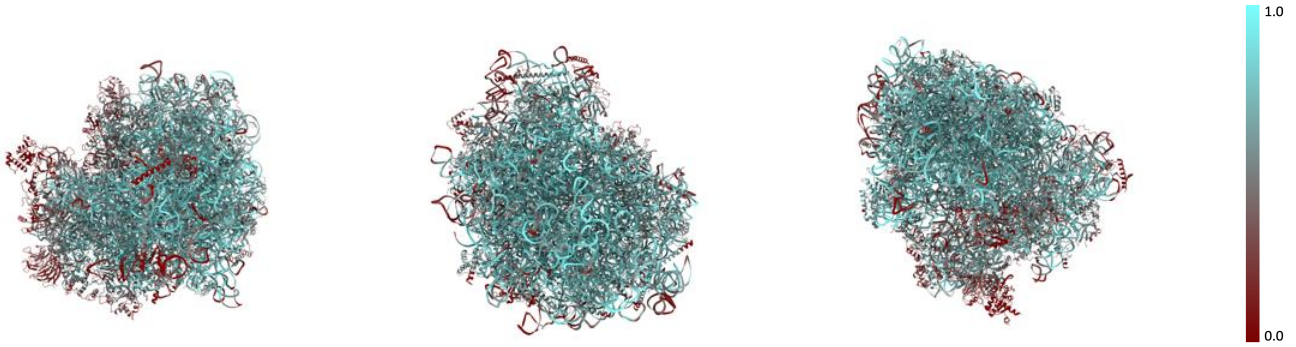
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

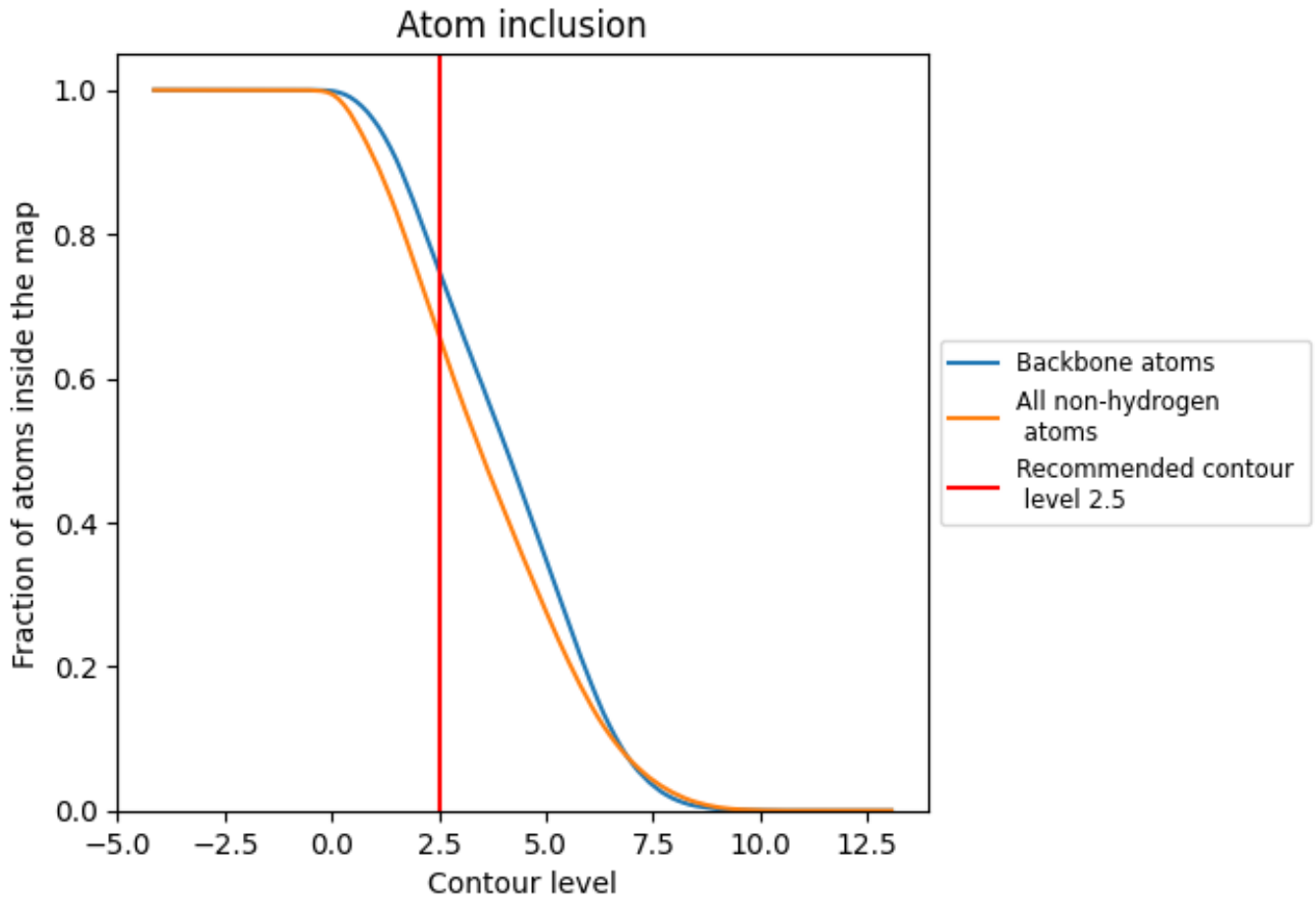
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (2.5).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 66% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6587	0.3800
A2	0.7811	0.4050
A3	0.7841	0.4080
A4	0.8678	0.4500
AA	0.6954	0.4590
AB	0.6601	0.4290
AC	0.6773	0.4270
AD	0.6404	0.3830
AE	0.5303	0.3270
AF	0.6479	0.3960
AG	0.5849	0.3840
AH	0.6136	0.4210
AI	0.6433	0.4220
AJ	0.6014	0.3840
AK	0.2402	0.2380
AL	0.6065	0.3680
AM	0.6287	0.3990
AN	0.7327	0.4440
AO	0.6587	0.4090
AP	0.7059	0.4470
AQ	0.6733	0.4200
AR	0.6221	0.4020
AS	0.6743	0.4360
AT	0.6725	0.4260
AU	0.5532	0.3730
AV	0.6758	0.4690
AW	0.3637	0.2890
AX	0.6541	0.4360
AY	0.6673	0.4220
AZ	0.6445	0.3990
Aa	0.7044	0.4350
Ab	0.5912	0.3520
Ac	0.6110	0.4040
Ad	0.6663	0.4400
Ae	0.6598	0.4370

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Chain	Atom inclusion	Q-score
Af	0.6865	0.4210
Ag	0.6318	0.4160
Ah	0.6116	0.3860
Ai	0.6181	0.3730
Aj	0.7595	0.4580
Ak	0.5224	0.3650
Al	0.6761	0.4360
Am	0.6826	0.4150
An	0.3818	0.3300
Ao	0.6706	0.4430
Ap	0.6589	0.4310
Aq	0.1377	0.1370
At	0.6876	0.4000
Au	0.0163	0.0650
B1	0.7341	0.3890
BA	0.5093	0.3400
BB	0.5626	0.3700
BC	0.5691	0.3920
BD	0.3713	0.3110
BE	0.5768	0.3810
BF	0.4175	0.3130
BG	0.4774	0.2990
BH	0.3897	0.2870
BI	0.5553	0.3640
BJ	0.5659	0.3220
BK	0.2410	0.1910
BL	0.5626	0.3700
BM	0.0131	0.1000
BN	0.5969	0.3960
BO	0.5927	0.4050
BP	0.3247	0.2610
BQ	0.3905	0.3010
BR	0.3499	0.2690
BS	0.3681	0.2680
BT	0.3669	0.2370
BU	0.2813	0.2680
BV	0.5390	0.3690
BW	0.6158	0.3980
BX	0.5994	0.4060
BY	0.4995	0.3120
BZ	0.2411	0.2450
Ba	0.6198	0.3960

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Chain	Atom inclusion	Q-score
Bb	0.5220	0.3620
Bc	0.3638	0.3350
Bd	0.4805	0.2810
Be	0.4976	0.3380
Bf	0.0223	0.1160
Bg	0.1177	0.2480
Bv	0.6444	0.3670
Bw	0.5335	0.2810
Bx	0.5404	0.3780
Ct	0.4278	0.3080