wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 06:08 am GMT

PDB ID	:	6GZ3
EMDB ID	:	EMD-0098
Title	:	tRNA translocation by the eukaryotic 80S ribosome and the impact of GTP hydrolysis, Translocation-intermediate-POST-1 (TI-POST-1)
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	:	3.60 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 (1)) were used in the production of this report:

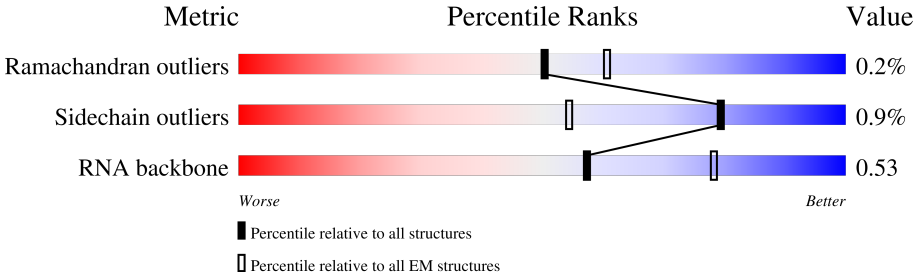
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.60 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	9% 78% 21% •
2	Bv	76	24% 82% 18%
3	Bx	12	25% 50% 50%
4	Bw	76	8% 82% 18%
5	B1	1708	12% 77% 21% •
6	BD	220	36% 100%
7	BF	190	49% 100%
8	BK	98	64% 97% •

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Mol	Chain	Length	Quality of chain
9	BM	120	98% / 100%
10	BP	120	52% / 98%
11	BQ	139	47% / 99%
12	BR	125	58% / 100%
13	BS	139	53% / 97%
14	BT	143	50% / 99%
15	BU	97	53% / 100%
16	BZ	86	79% / 99%
17	Bc	62	56% / 95%
18	Bd	51	27% / 100%
19	Bf	73	99% / 100%
20	Bg	314	84% / 100%
21	BA	215	44% / 99%
22	BB	212	37% / 99%
23	BC	222	19% / 100%
24	BE	257	26% / 97%
25	BG	232	50% / 99%
26	BH	183	67% / 100%
27	BI	207	32% / 99%
28	BJ	179	23% / 97%
29	BL	153	35% / 98%
30	BN	149	26% / 99%
31	BO	136	22% / 99%
32	BV	81	30% / 98%
33	BW	129	17% / 98%

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Mol	Chain	Length	Quality of chain
34	BX	141	22% 99%
35	BY	125	43% 99%
36	Ba	97	19% 99%
37	Bb	80	44% 100%
38	Be	55	38% 95% 5%
39	A3	157	10% 75% 22%
40	A4	119	78% 20%
41	AA	252	6% 100%
42	AB	394	10% 99%
43	AC	363	10% 98%
44	AD	294	13% 98%
45	AE	194	29% 97%
46	AF	234	10% 99%
47	AG	234	21% 100%
48	AH	191	9% 98%
49	AI	211	11% 98%
50	AJ	169	19% 99%
51	AL	205	19% 99%
52	AM	139	13% 99%
53	AN	203	100%
54	AO	195	8% 98%
55	AP	153	6% 99%
56	AQ	187	12% 98%
57	AR	181	16% 99%
58	AS	175	7% 100%

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Mol	Chain	Length	Quality of chain
59	AT	157	12% 99%
60	AU	99	23% 98%
61	AV	129	8% 100%
62	AW	121	55% 99%
63	AX	117	9% 100%
64	AY	127	10% 99%
65	AZ	134	14% 99%
66	Aa	147	10% 99%
67	Ab	68	26% 96%
68	Ac	103	21% 100%
69	Ad	106	14% 100%
70	Ae	129	5% 100%
71	Af	109	6% 98%
72	Ag	114	14% 100%
73	Ah	122	20% 96%
74	Ai	97	19% 100%
75	Aj	84	98%
76	Ak	69	29% 99%
77	Al	50	14% 94% 6%
78	Am	50	10% 98%
79	An	25	84% 100%
80	Ao	105	8% 97%
81	Ap	91	7% 99%
82	At	122	12% 96%
83	Au	217	99% 97%

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Mol	Chain	Length	Quality of chain
84	Aq	151	87% 97%
85	AK	202	76% 99%
86	Ct	853	37% 98%

2 Entry composition (i)

There are 89 unique types of molecules in this entry. The entry contains 225624 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 ap/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	12	257	115	46	84	12	0	0

- Molecule 4 is a RNA chain called pe/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 S5.

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

- Molecule 8 is a protein called ribosomal protein eS10.

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

- Molecule 9 is a protein called 40S ribosomal protein S12.

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

- Molecule 10 is a protein called ribosomal protein uS19.

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

- Molecule 11 is a protein called ribosomal protein uS9.

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

- Molecule 12 is a protein called ribosomal protein eS17.

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

- Molecule 13 is a protein called ribosomal protein uS13.

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

- Molecule 14 is a protein called ribosomal protein eS19.

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

- Molecule 15 is a protein called ribosomal protein uS10.

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

- Molecule 16 is a protein called ribosomal protein eS25.

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

- Molecule 17 is a protein called Ribosomal protein S28.

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

- Molecule 18 is a protein called ribosomal protein uS14.

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

- Molecule 19 is a protein called Ribosomal protein S27a.

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

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

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

- Molecule 21 is a protein called ribosomal protein uS2.

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

- Molecule 22 is a protein called 40S ribosomal protein S3a.

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

- Molecule 23 is a protein called ribosomal protein uS5.

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

- Molecule 24 is a protein called ribosomal protein eS4.

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

- Molecule 25 is a protein called 40S ribosomal protein S6.

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

- Molecule 26 is a protein called 40S ribosomal protein S7.

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

- Molecule 27 is a protein called ribosomal protein eS8.

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

- Molecule 28 is a protein called Ribosomal protein S9 (Predicted).

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

- Molecule 29 is a protein called Ribosomal protein S11.

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

- Molecule 30 is a protein called ribosomal protein uS15.

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

- Molecule 31 is a protein called ribosomal protein uS11.

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

- Molecule 32 is a protein called ribosomal protein eS21.

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

- Molecule 33 is a protein called Ribosomal protein S15a.

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

- Molecule 34 is a protein called Ribosomal protein S23.

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

- Molecule 35 is a protein called ribosomal protein eS24.

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

- Molecule 36 is a protein called ribosomal protein eS26.

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

- Molecule 37 is a protein called ribosomal protein eS27.

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

- Molecule 38 is a protein called ribosomal protein eS30.

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

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

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

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

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

- Molecule 41 is a protein called Ribosomal protein L8.

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

- Molecule 42 is a protein called ribosomal protein uL3.

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

- Molecule 43 is a protein called ribosomal protein uL4.

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

- Molecule 44 is a protein called ribosomal protein uL18.

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

- Molecule 45 is a protein called ribosomal protein eL6.

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

- Molecule 46 is a protein called ribosomal protein uL30.

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

- Molecule 47 is a protein called ribosomal protein eL8.

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

- Molecule 48 is a protein called ribosomal protein uL6.

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

- Molecule 49 is a protein called Ribosomal protein L10 (Predicted).

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	149	ILE	VAL	conflict	UNP B7NZQ2

- Molecule 50 is a protein called Ribosomal protein L11.

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

- Molecule 51 is a protein called ribosomal protein eL13.

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

- Molecule 52 is a protein called ribosomal protein eL14.

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

- Molecule 53 is a protein called Ribosomal protein L15.

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

- Molecule 54 is a protein called ribosomal protein uL13.

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

- Molecule 55 is a protein called ribosomal protein uL22.

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

- Molecule 56 is a protein called ribosomal protein eL18.

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

- Molecule 57 is a protein called ribosomal protein eL19.

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

- Molecule 58 is a protein called ribosomal protein eL20.

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

- Molecule 59 is a protein called ribosomal protein eL21.

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

- Molecule 60 is a protein called ribosomal protein eL22.

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

- Molecule 61 is a protein called Ribosomal protein L23.

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

- Molecule 62 is a protein called ribosomal protein eL24.

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

- Molecule 63 is a protein called ribosomal protein uL23.

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

- Molecule 64 is a protein called Ribosomal protein L26.

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

- Molecule 65 is a protein called 60S ribosomal protein L27.

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

- Molecule 66 is a protein called ribosomal protein uL15.

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

- Molecule 67 is a protein called ribosomal protein eL29.

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

- Molecule 68 is a protein called ribosomal protein eL30.

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

- Molecule 69 is a protein called ribosomal protein eL31.

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

- Molecule 70 is a protein called ribosomal protein eL32.

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

- Molecule 71 is a protein called ribosomal protein eL33.

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

- Molecule 72 is a protein called ribosomal protein eL34.

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

- Molecule 73 is a protein called ribosomal protein uL29.

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

- Molecule 74 is a protein called ribosomal protein eL36.

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

- Molecule 75 is a protein called Ribosomal protein L37.

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

- Molecule 76 is a protein called ribosomal protein eL38.

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

- Molecule 77 is a protein called ribosomal protein eL39.

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

- Molecule 78 is a protein called ribosomal protein eL40.

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

- Molecule 79 is a protein called ribosomal protein eL41.

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

- Molecule 80 is a protein called ribosomal protein eL42.

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

- Molecule 81 is a protein called ribosomal protein eL43.

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

- Molecule 82 is a protein called ribosomal protein eL28.

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

- Molecule 83 is a protein called Ribosomal protein.

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

- Molecule 84 is a protein called Ribosomal protein L12.

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

- Molecule 85 is a protein called ribosomal protein uL10.

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

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

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

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
87	A2	230	230	230	0
87	Bx	2	2	2	0
87	B1	69	69	69	0
87	BD	2	2	2	0
87	BS	1	1	1	0
87	Bd	1	1	1	0
87	Ba	1	1	1	0
87	A3	6	6	6	0
87	A4	8	8	8	0

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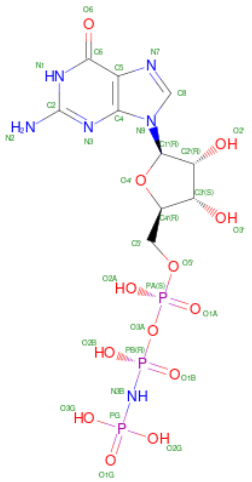
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
87	AA	1	1	1	0
87	AL	1	1	1	0
87	AN	1	1	1	0
87	AP	1	1	1	0
87	AY	1	1	1	0
87	Al	1	1	1	0
87	An	1	1	1	0

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

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

- Molecule 89 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

GNP



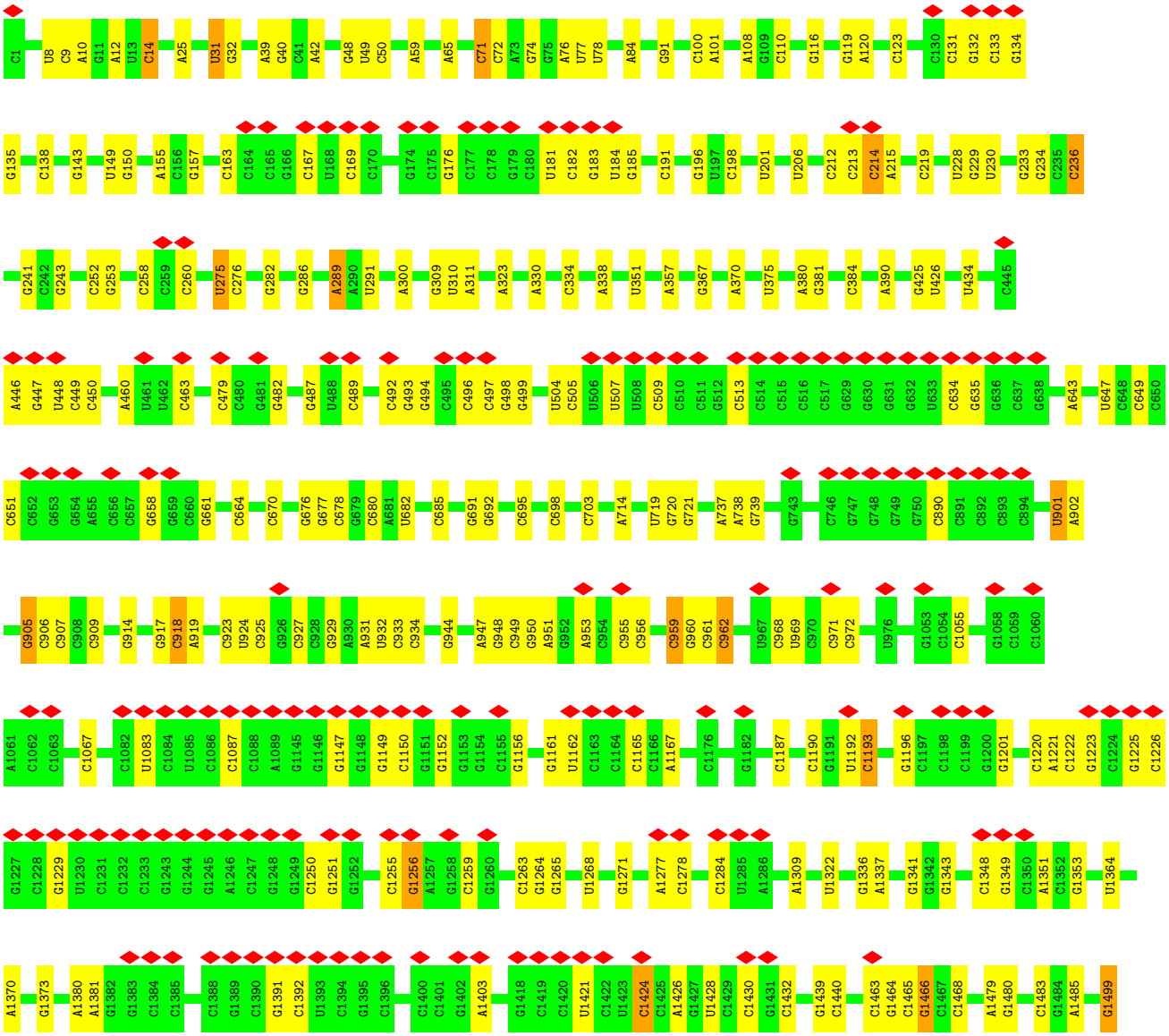
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
89	Ct	1	32	10	6	13	3	0

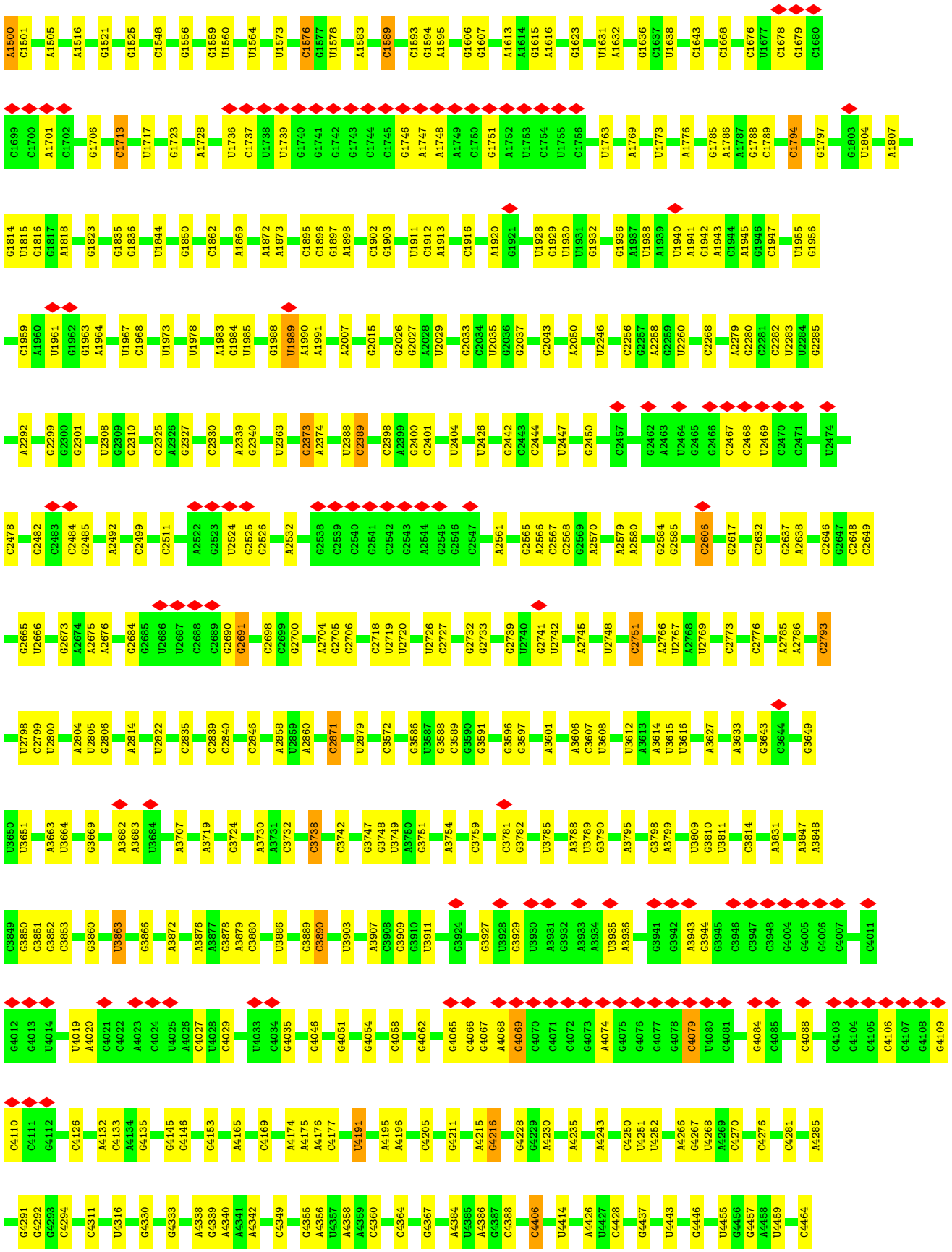
3 Residue-property plots (i)

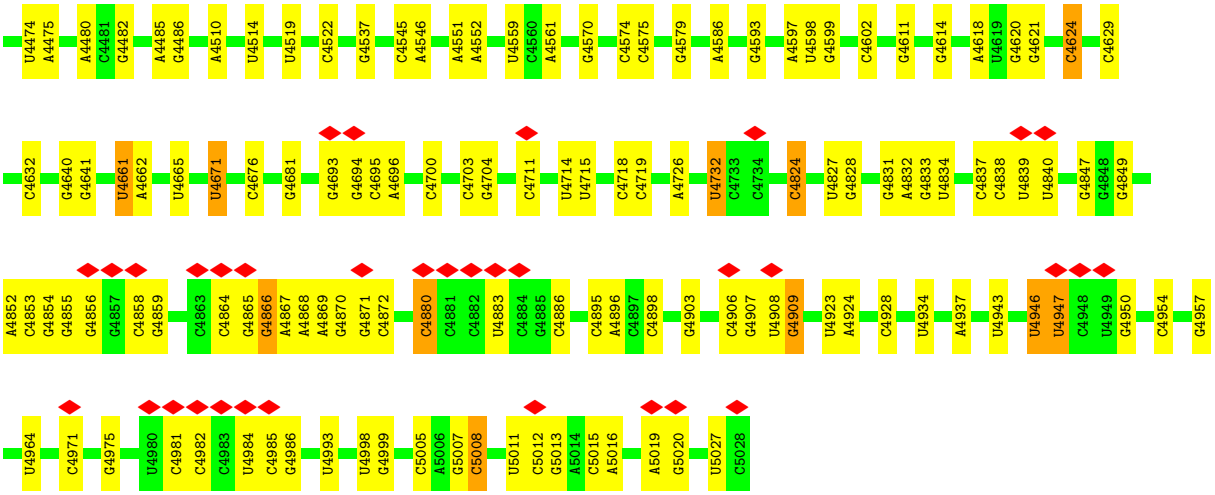
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

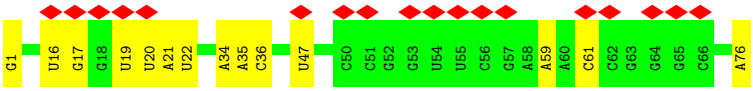



A1500 C1501 A1505 A1516 G1521 G1525 C1548 G1556 G1559 U1560 U1564 U1573 C1576 G1577 U1578 A1583 C1589 C1593 G1594 A1595 G1606 G1607 A1613 A1614 G1615 A1616 G1623 U1631 A1632 G1636 C1637 U1638 C1643 C1668 C1676 U1677 C1678 G1679 C1680
C1699 C1700 A1701 C1702 G1706 C1713 U1717 G1723 A1728 U1736 C1737 U1738 U1739 G1740 G1741 G1742 G1743 C1744 C1745 G1746 A1747 A1748 A1749 C1750 G1751 A1752 U1753 C1754 U1755 C1756 U1763 A1769 U1773 A1776 G1785 A1786 A1787 G1788 C1789 C1794 G1797 G1803 U1804 A1807
G1814 U1815 G1816 G1817 A1818 G1823 G1835 G1836 U1844 G1850 C1862 A1869 A1872 A1873 C1895 C1896 G1897 A1898 C1902 G1903 U1911 C1912 A1913 C1916 A1920 G1921 U1928 G1929 U1930 U1931 G1932 G1936 A1937 U1938 A1939 U1940 A1941 G1942 A1943 C1944 A1945 G1946 C1947 U1955 G1956
C1959 A1960 U1961 G1962 G1963 A1964 U1967 C1968 U1973 U1978 A1983 G1984 U1985 G1988 U1989 A1990 A1991 A2007 G2015 G2026 G2027 A2028 U2029 G2033 C2034 U2035 G2036 G2037 C2043 A2050 U2246 C2256 G2257 A2258 G2259 U2260 C2268 A2279 G2280 C2281 C2282 U2283 U2284 G2285
A2292 G2299 G2300 G2301 U2308 G2309 G2310 C2325 A2326 G2327 C2330 A2339 G2340 U2363 G2373 A2374 U2388 C2389 C2398 A2399 G2400 C2401 U2404 U2426 G2442 C2443 C2444 U2447 G2450 C2457 G2462 A2463 U2464 G2465 G2466 C2467 C2468 U2469 C2470 C2471 U2474
C2478 G2482 C2483 C2484 G2485 A2492 C2499 C2511 A2522 G2523 U2524 G2525 G2526 A2532 G2538 C2539 C2540 G2541 C2542 G2543 A2544 G2545 G2546 C2547 A2561 G2565 A2566 C2567 C2568 G2569 A2570 A2579 A2580 G2584 G2585 C2606 G2617 C2632 G2637 A2638 C2646 G2647 C2648 C2649
G2665 U2666 G2673 A2674 A2675 A2676 G2684 G2685 U2686 U2687 C2688 C2689 G2690 G2691 C2698 C2699 G2700 A2704 G2705 C2706 C2718 U2719 U2720 U2726 C2727 G2732 G2733 G2739 U2740 G2741 U2742 A2745 U2748 C2751 A2766 U2767 A2768 U2769 C2773 C2776 A2785 A2786 C2793
U2798 C2799 U2800 A2804 U2805 G2806 A2814 U2822 C2835 C2839 C2840 C2846 A2858 U2859 A2860 C2871 U2879 C3572 G3586 U3587 G3588 C3589 G3590 G3591 G3596 G3597 A3601 A3606 C3607 U3608 U3612 A3613 A3614 U3615 U3616 A3627 A3633 G3643 C3644 G3649
U3650 U3651 A3663 U3664 G3669 A3682 A3683 U3684 A3707 A3719 G3724 A3730 A3731 C3732 C3738 C3742 G3747 G3748 U3749 A3750 G3751 A3754 C3759 C3781 G3782 U3785 A3788 U3789 G3790 A3795 G3798 A3799 U3809 G3810 U3811 C3814 A3831 A3847 A3848
C3849 G3850 G3851 G3852 C3853 G3860 U3863 G3866 A3872 A3876 A3877 A3878 A3879 C3880 U3886 G3889 C3890 U3903 A3907 C3908 G3909 G3910 U3911 G3924 G3927 U3928 G3929 U3930 A3931 G3932 A3933 A3934 U3935 A3936 G3941 G3942 A3943 G3944 G3945 C3946 C3947 C3948 G4004 G4005 G4006 C4007 C4011
G4012 G4013 U4014 U4019 A4020 C4021 C4022 A4023 C4024 U4025 A4026 C4027 U4028 C4029 U4033 C4034 G4035 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 C4103 G4104 C4105 C4106 C4107 G4108 G4109
C4110 C4111 G4112 C4126 A4132 C4133 A4134 G4135 G4145 G4146 G4153 A4165 C4169 A4174 A4175 A4176 C4177 U4191 A4195 A4196 C4205 G4211 A4215 G4216 G4228 G4229 A4230 A4235 A4243 C4250 U4251 U4252 A4266 G4267 U4268 A4269 C4270 C4276 C4281 A4285
G4291 G4292 G4293 C4294 C4311 U4316 G4330 G4333 A4338 G4339 A4340 A4341 A4342 C4349 G4355 A4356 U4357 A4358 A4359 C4360 C4364 G4367 A4384 U4385 A4386 G4387 C4388 C4406 U4414 A4426 U4427 C4428 G4437 U4443 G4446 U4455 G4456 G4457 A4458 U4459 C4464



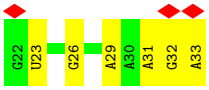
- Molecule 2: ap/P-site tRNA

Chain Bv:



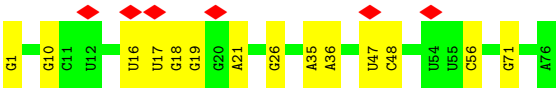
- Molecule 3: mRNA

Chain Bx:



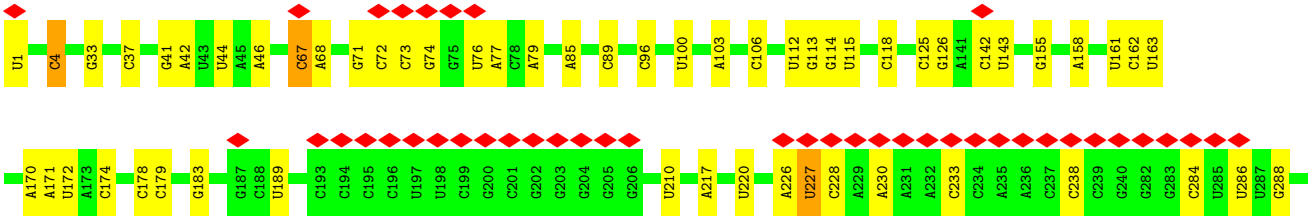
- Molecule 4: pe/E-site-tRNA

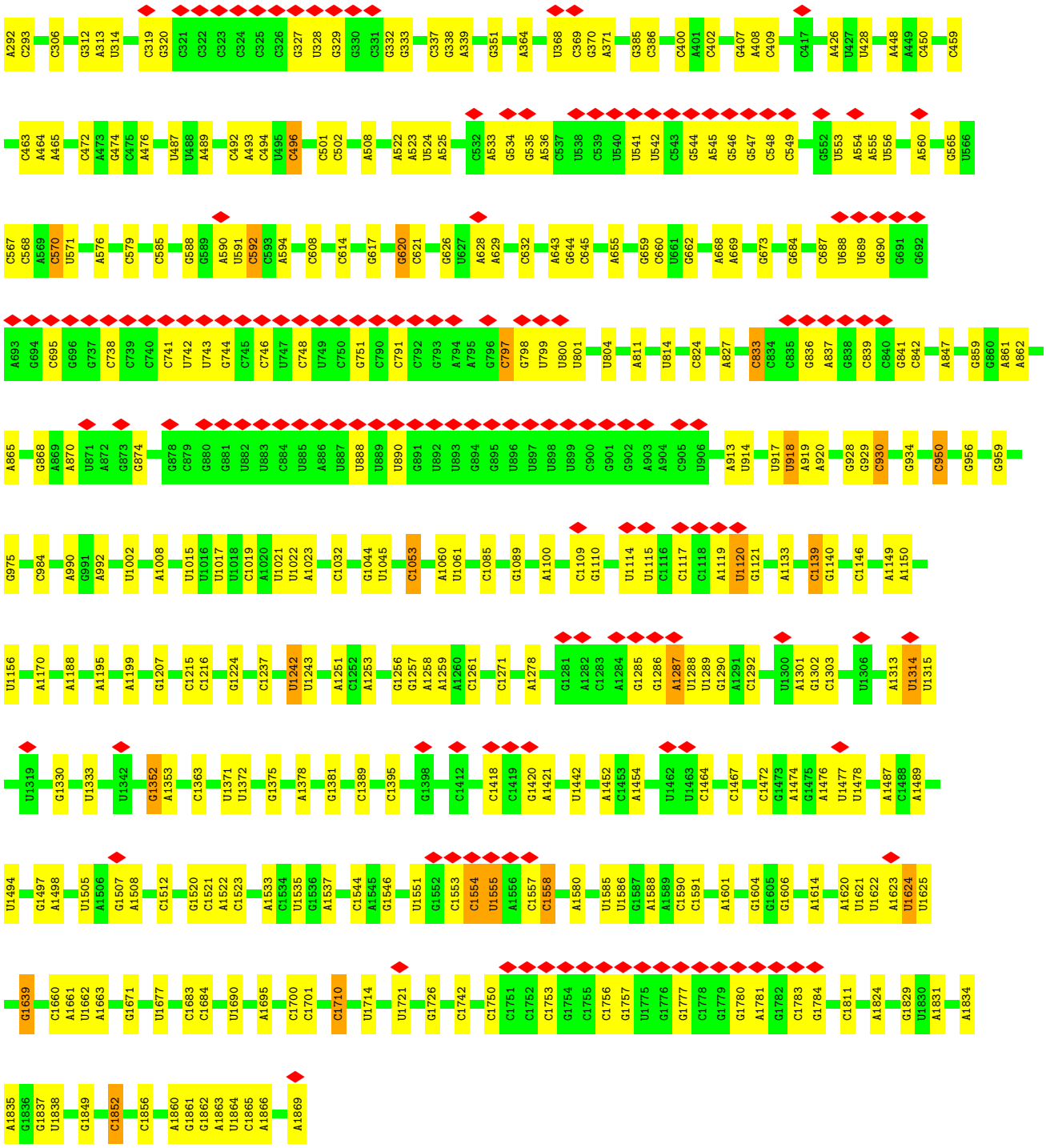
Chain Bw:



- Molecule 5: 18S ribosomal RNA

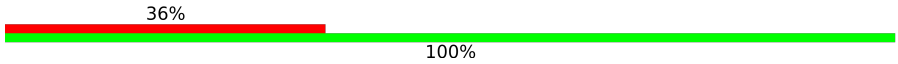
Chain B1:

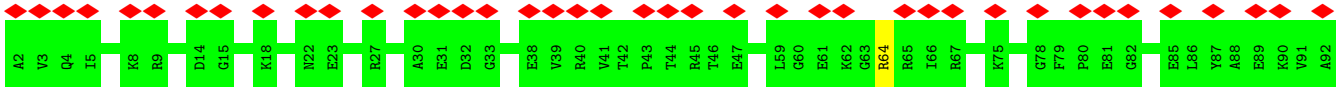


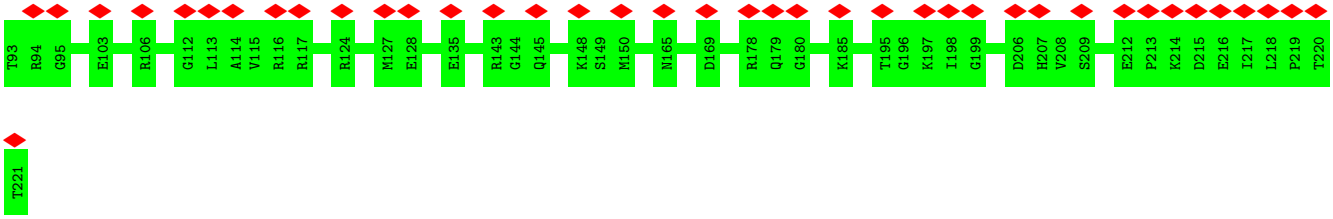


- Molecule 6: ribosomal protein uS3

Chain BD:

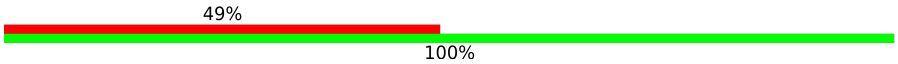


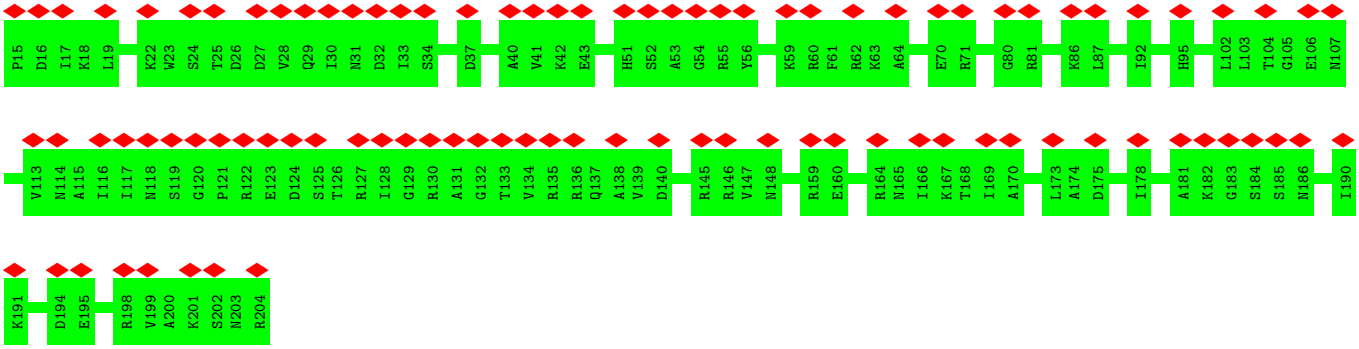




• Molecule 7: Ribosomal protein S5

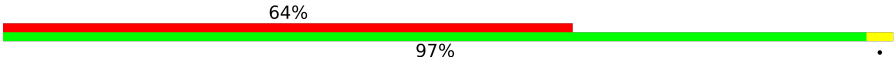
Chain BF:

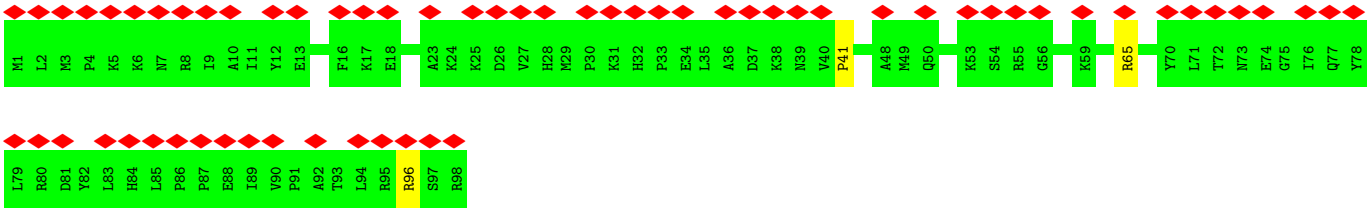




• Molecule 8: ribosomal protein eS10

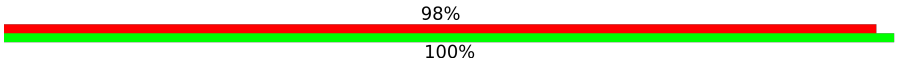
Chain BK:

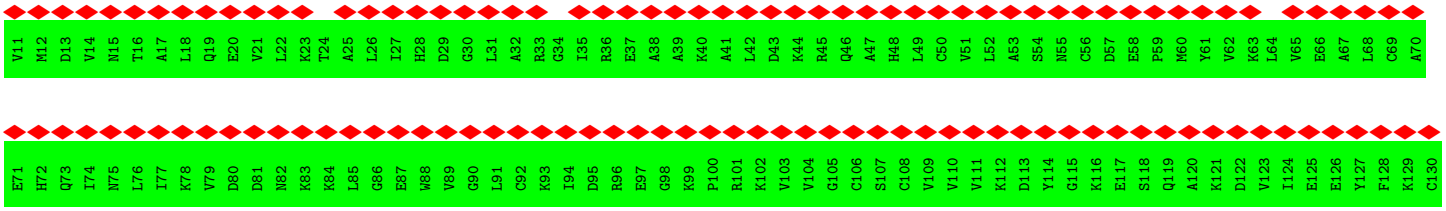




• Molecule 9: 40S ribosomal protein S12

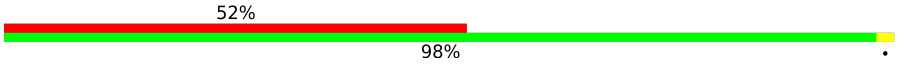
Chain BM:

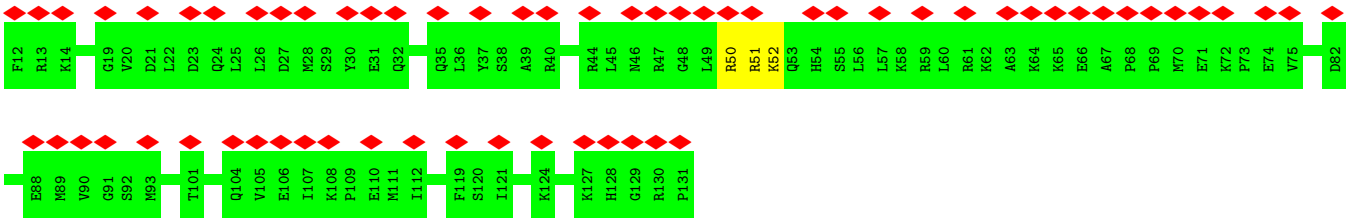




• Molecule 10: ribosomal protein uS19

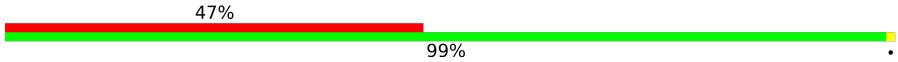
Chain BP:

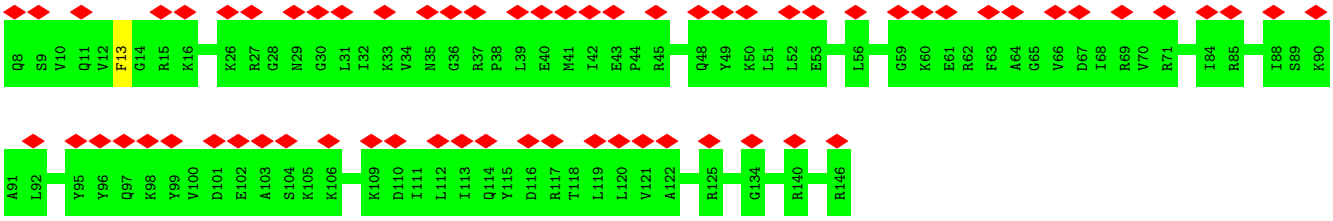




- Molecule 11: ribosomal protein uS9

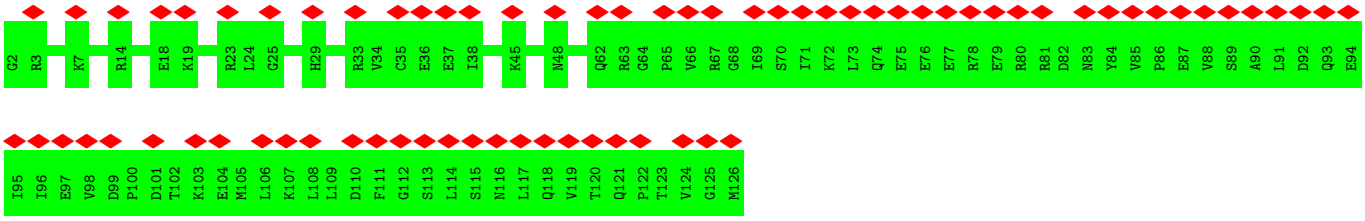
Chain BQ:





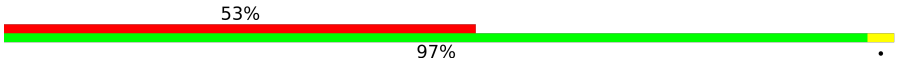
- Molecule 12: ribosomal protein eS17

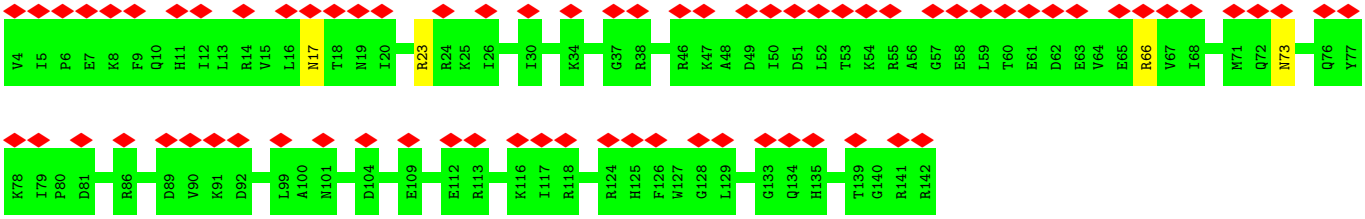
Chain BR:



- Molecule 13: ribosomal protein uS13

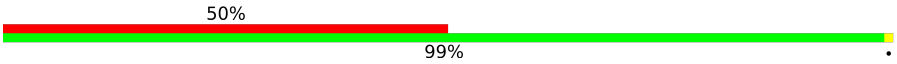
Chain BS:

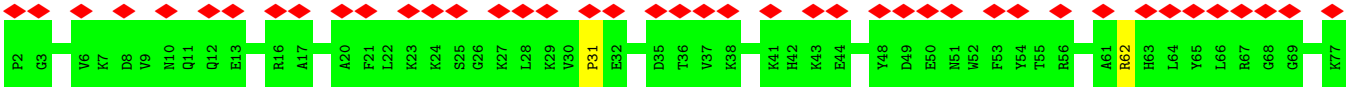


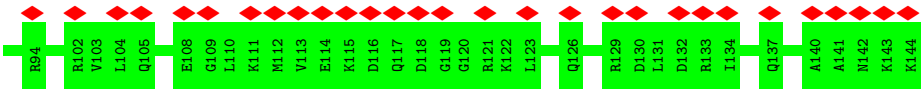


- Molecule 14: ribosomal protein eS19

Chain BT:

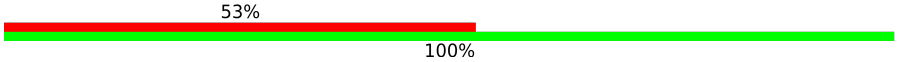


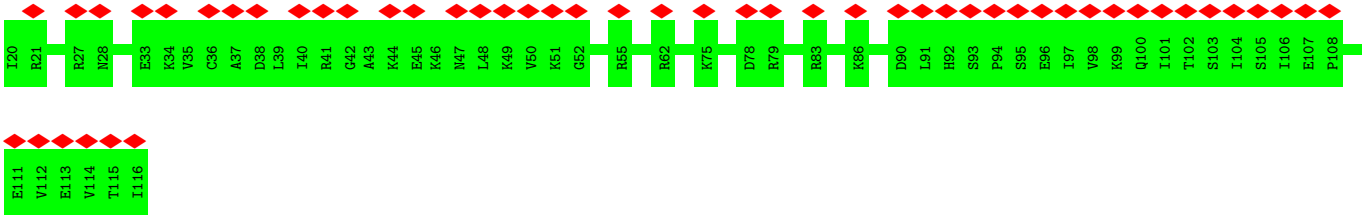




- Molecule 15: ribosomal protein uS10

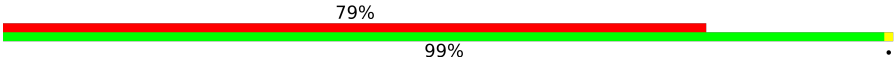
Chain BU:





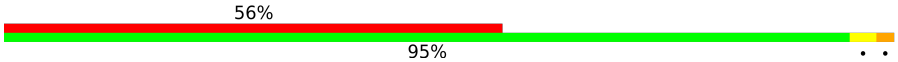
- Molecule 16: ribosomal protein eS25

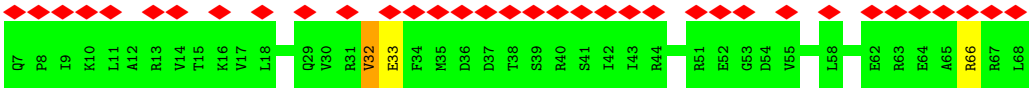
Chain BZ:



- Molecule 17: Ribosomal protein S28

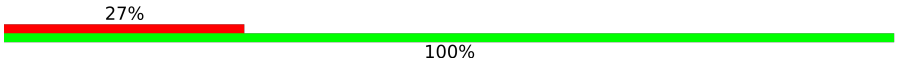
Chain Bc:

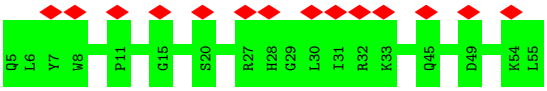




- Molecule 18: ribosomal protein uS14

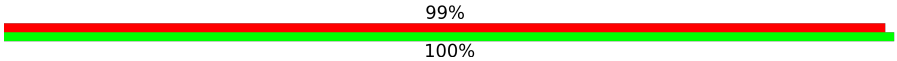
Chain Bd:

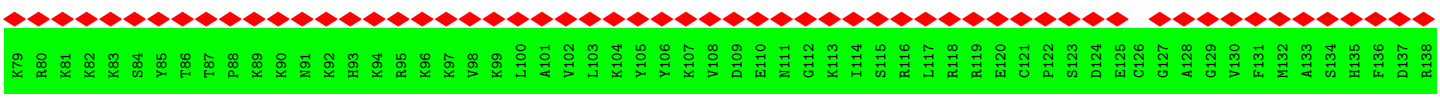


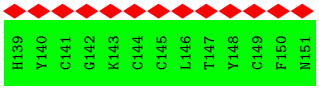


- Molecule 19: Ribosomal protein S27a

Chain Bf:

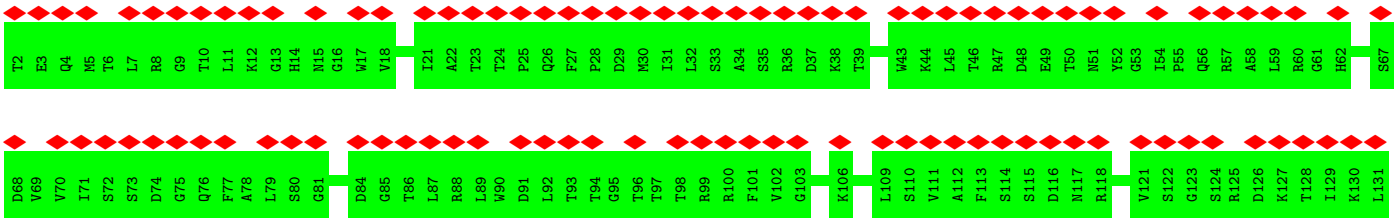


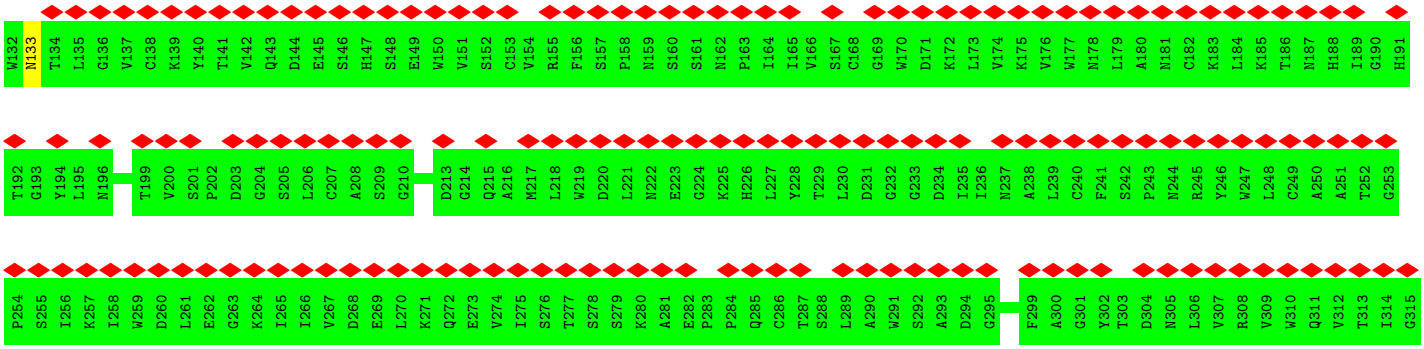




• Molecule 20: ribosomal protein RACK 1

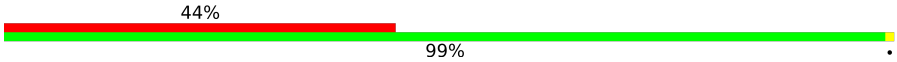
Chain Bg:

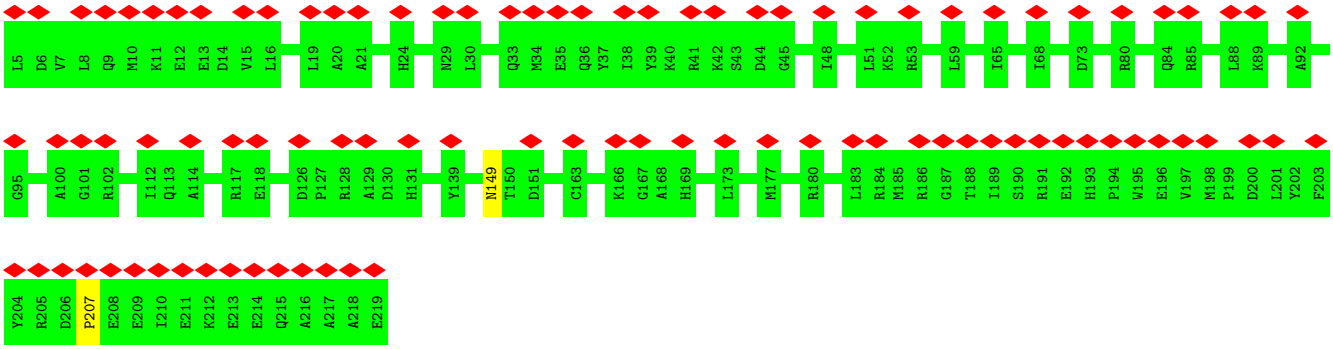




• Molecule 21: ribosomal protein uS2

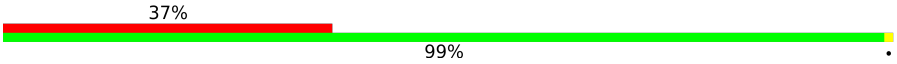
Chain BA:

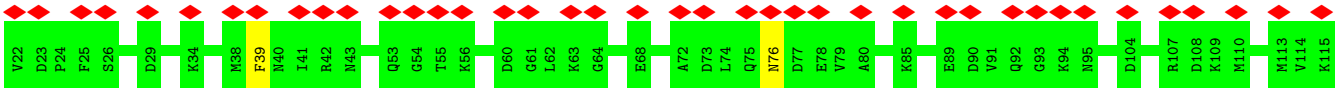


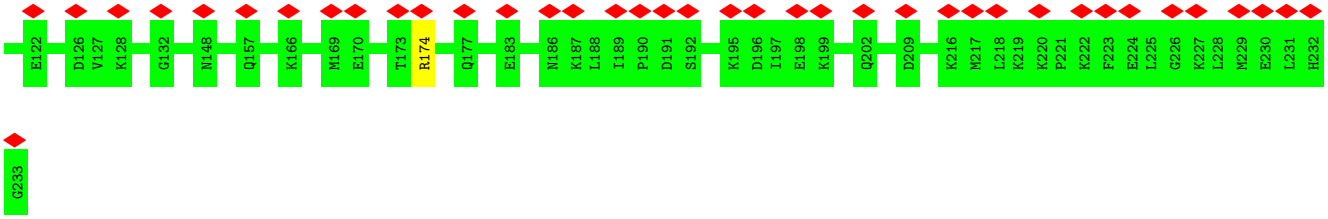


• Molecule 22: 40S ribosomal protein S3a

Chain BB:

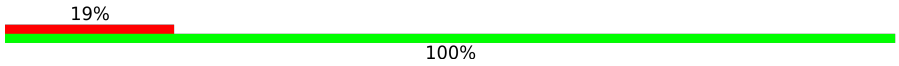


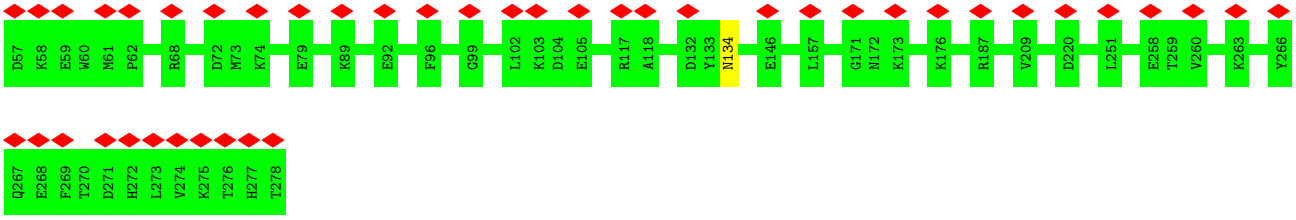




• Molecule 23: ribosomal protein uS5

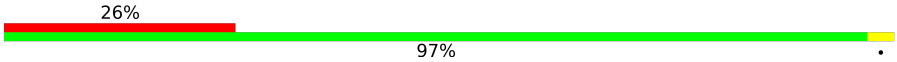
Chain BC:

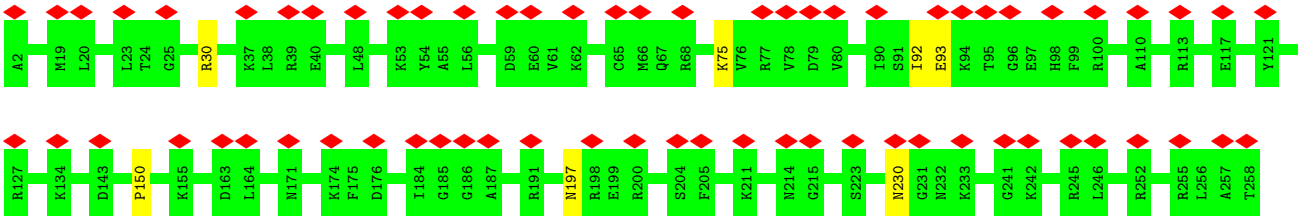




• Molecule 24: ribosomal protein eS4

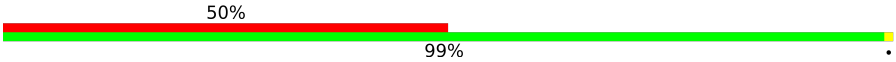
Chain BE:

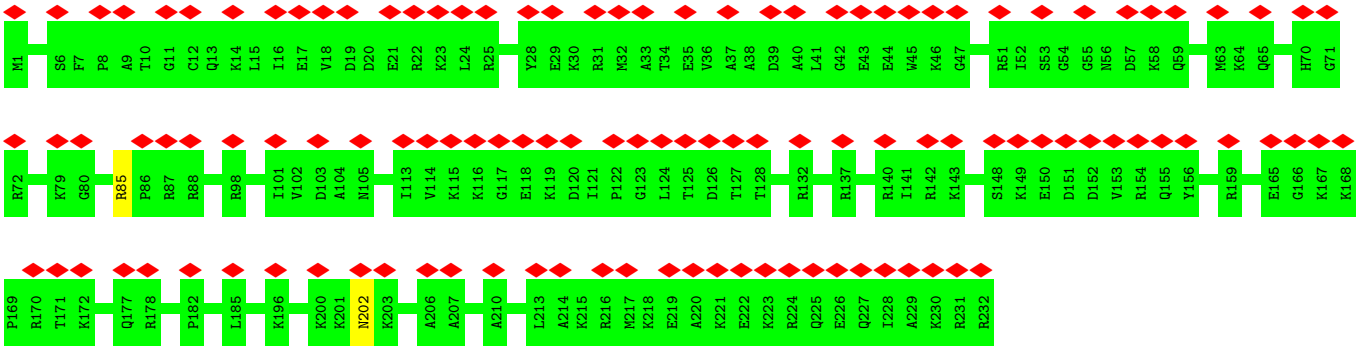




• Molecule 25: 40S ribosomal protein S6

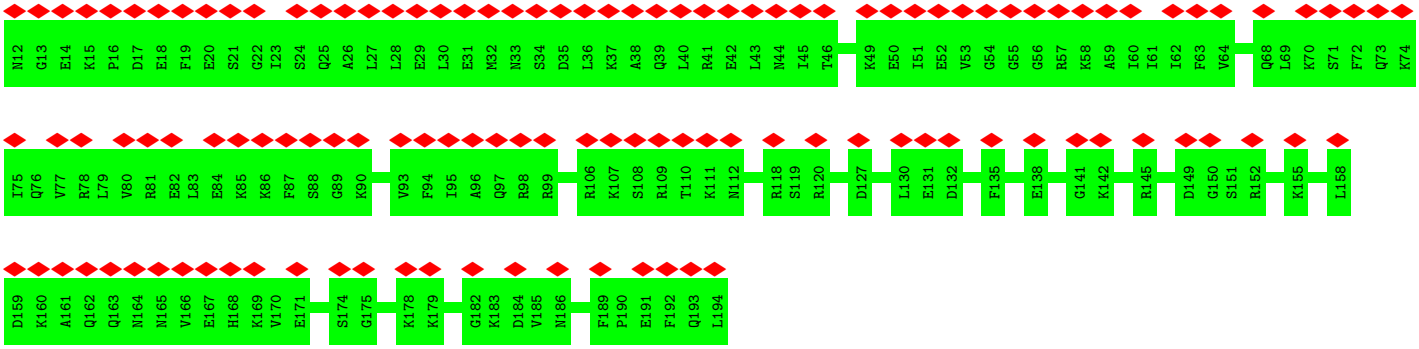
Chain BG:





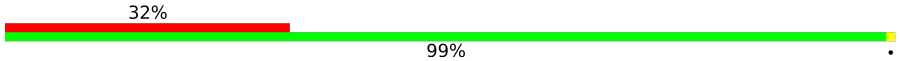
• Molecule 26: 40S ribosomal protein S7

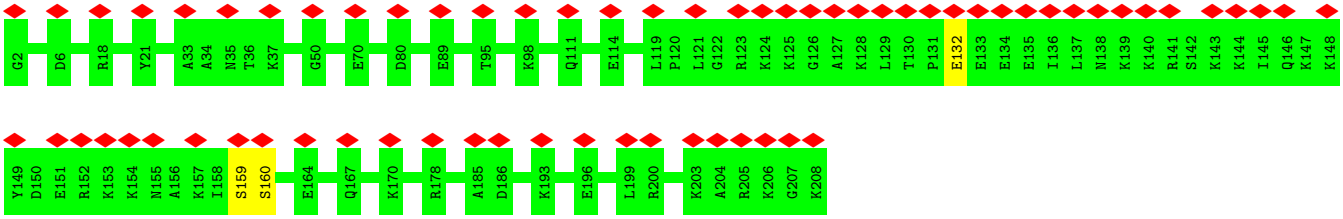
Chain BH:



• Molecule 27: ribosomal protein eS8

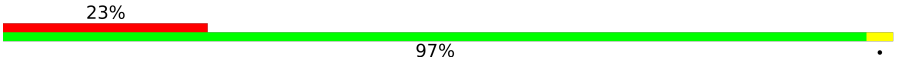
Chain BI:

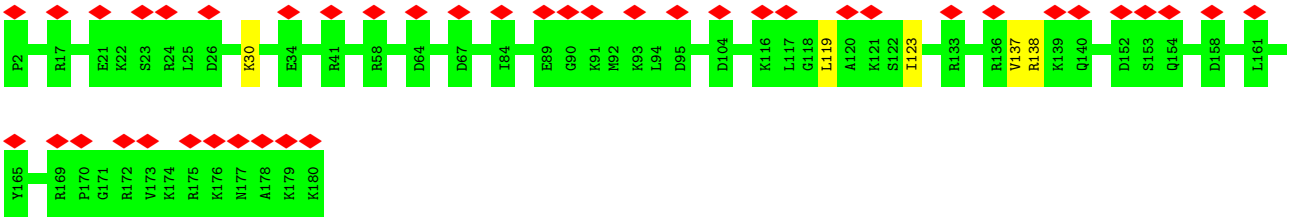




• Molecule 28: Ribosomal protein S9 (Predicted)

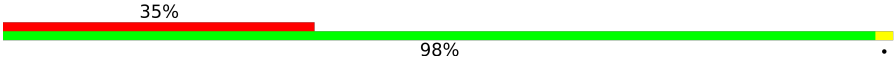
Chain BJ:

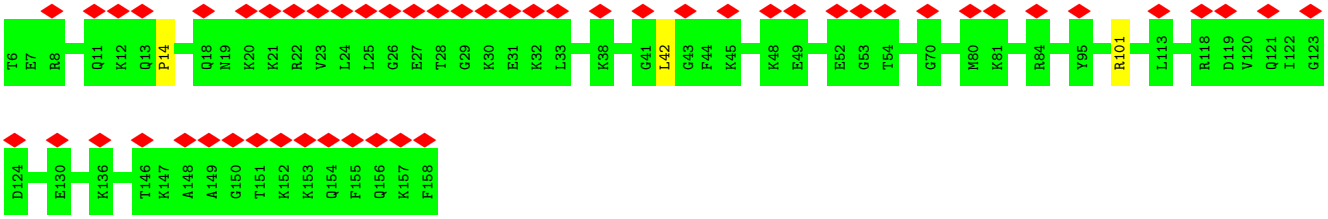




• Molecule 29: Ribosomal protein S11

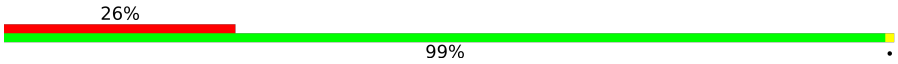
Chain BL:

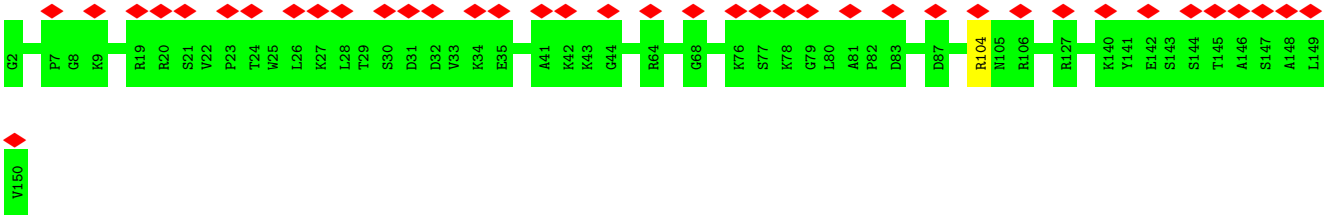




• Molecule 30: ribosomal protein uS15

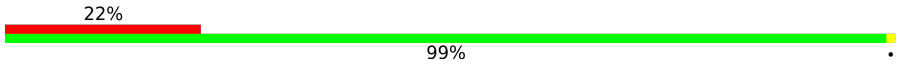
Chain BN:

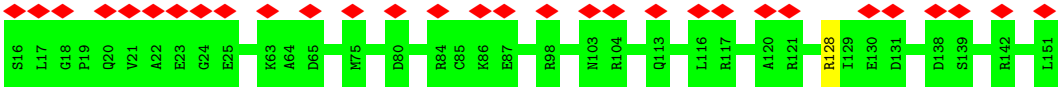




• Molecule 31: ribosomal protein uS11

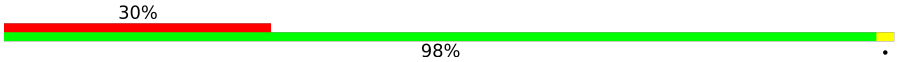
Chain BO:

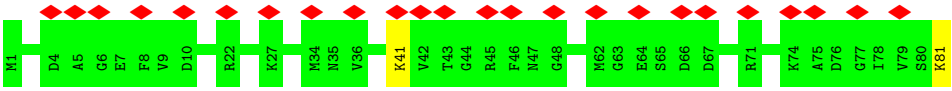




• Molecule 32: ribosomal protein eS21

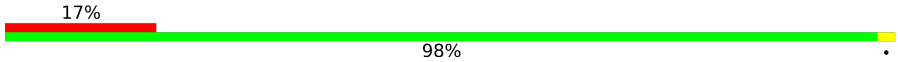
Chain BV:

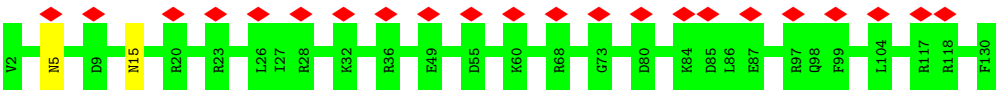




• Molecule 33: Ribosomal protein S15a

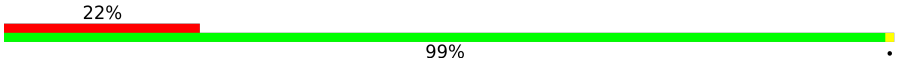
Chain BW:

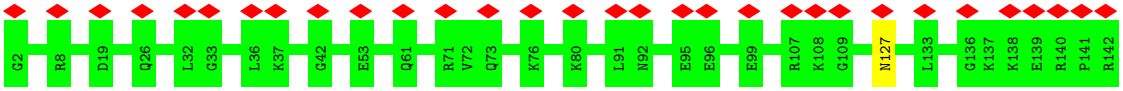




• Molecule 34: Ribosomal protein S23

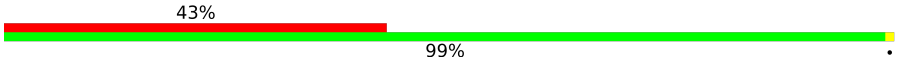
Chain BX:

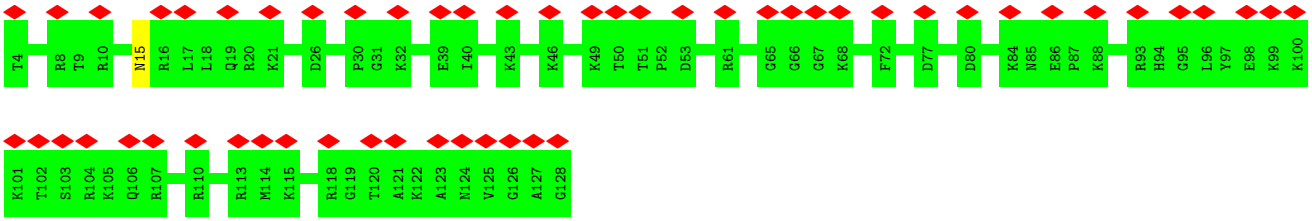




• Molecule 35: ribosomal protein eS24

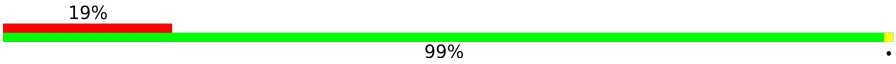
Chain BY:

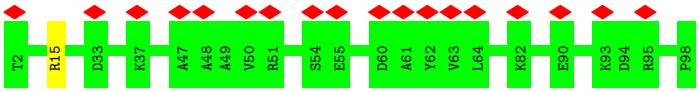




• Molecule 36: ribosomal protein eS26

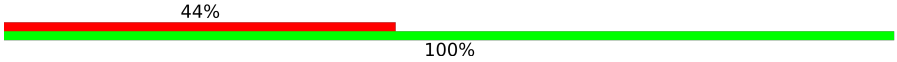
Chain Ba:

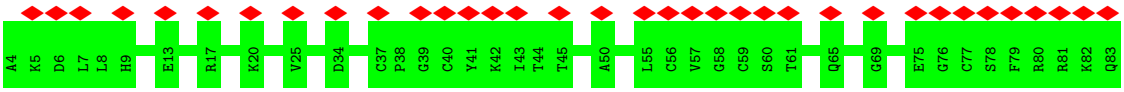




• Molecule 37: ribosomal protein eS27

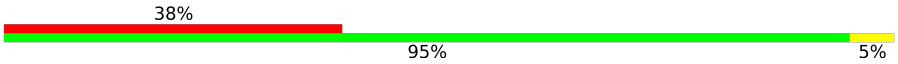
Chain Bb:

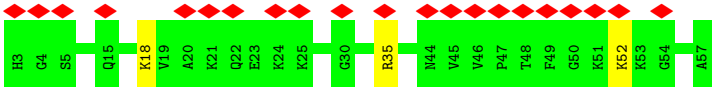




• Molecule 38: ribosomal protein eS30

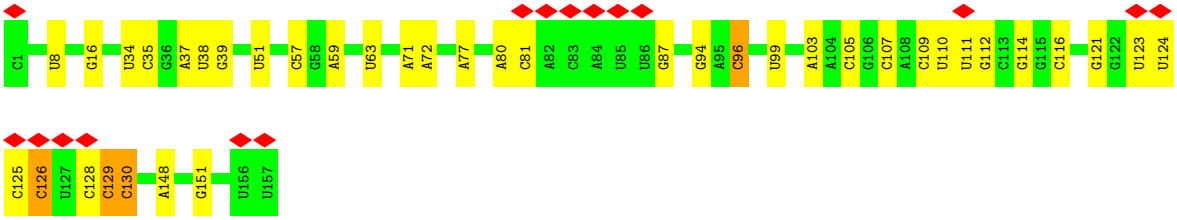
Chain Be:





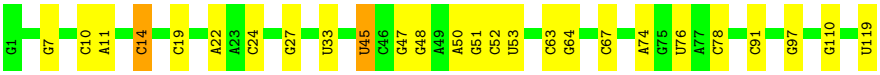
• Molecule 39: 5.8S ribosomal RNA

Chain A3:



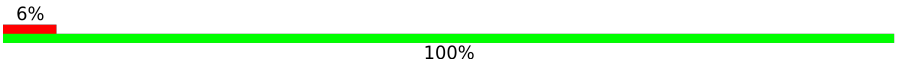
• Molecule 40: 5S ribosomal RNA

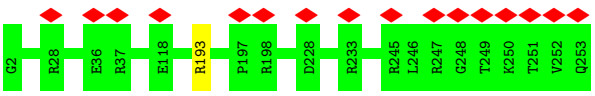
Chain A4:



• Molecule 41: Ribosomal protein L8

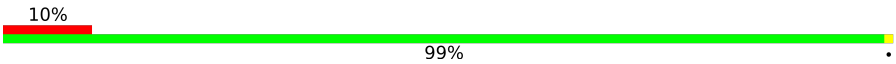
Chain AA:

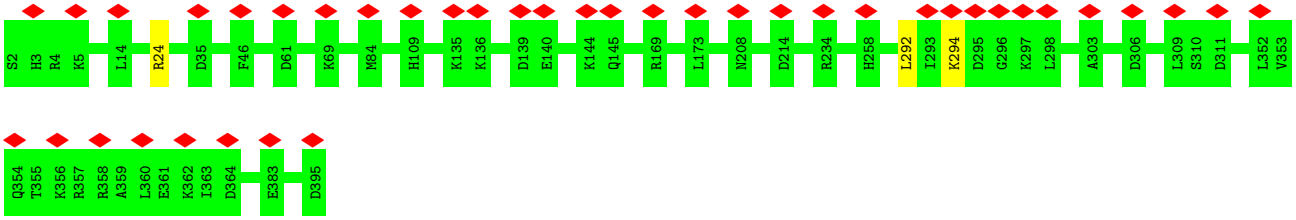




• Molecule 42: ribosomal protein uL3

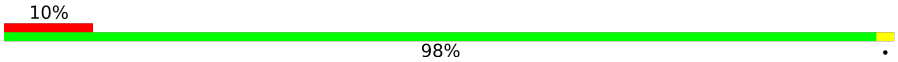
Chain AB:

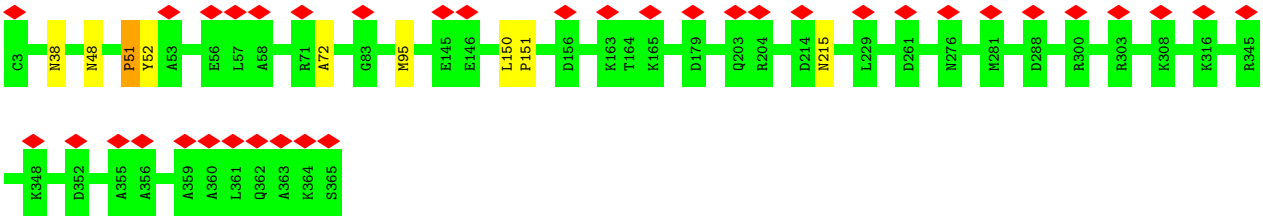




• Molecule 43: ribosomal protein uL4

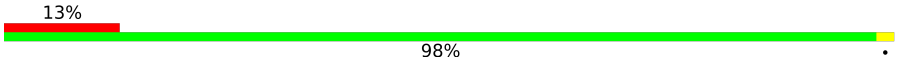
Chain AC:

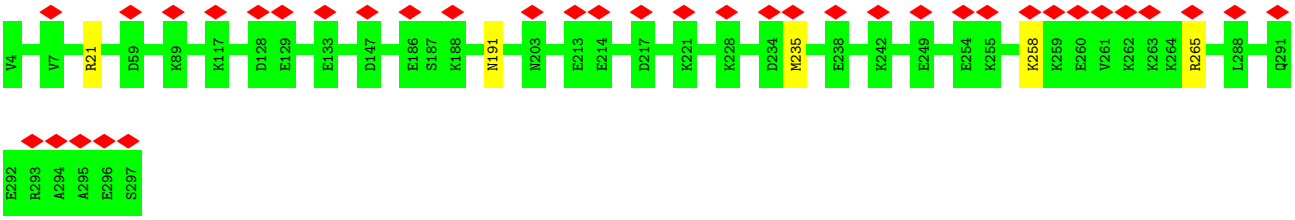




• Molecule 44: ribosomal protein uL18

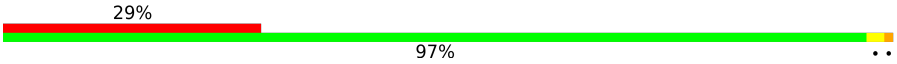
Chain AD:

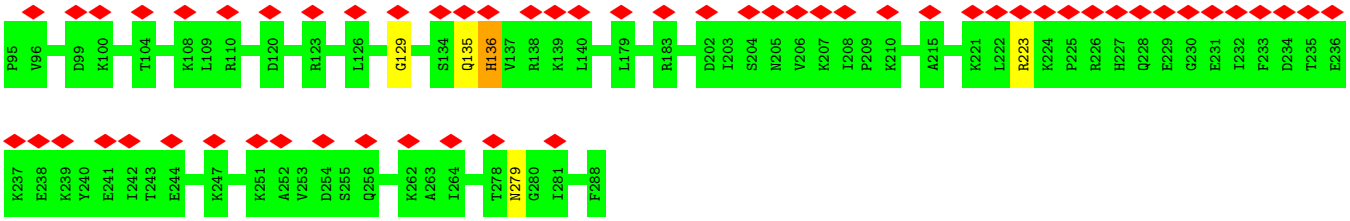




• Molecule 45: ribosomal protein eL6

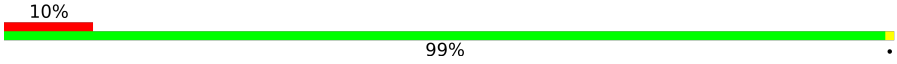
Chain AE:

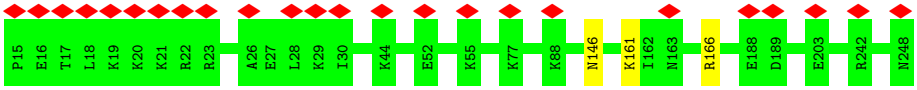




• Molecule 46: ribosomal protein uL30

Chain AF:



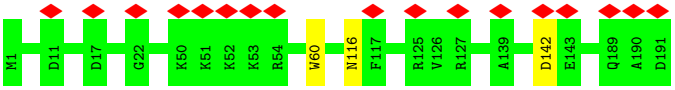


• Molecule 47: ribosomal protein eL8

Chain AG: 21% 100%

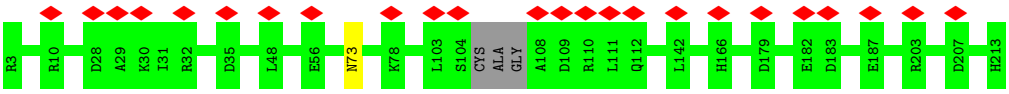
- Molecule 48: ribosomal protein uL6

Chain AH: 9% 98%



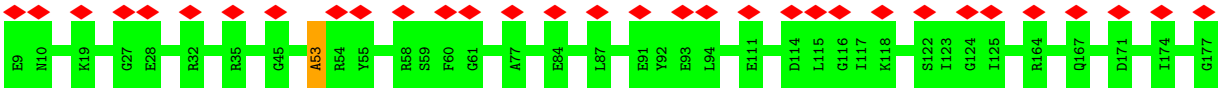
- Molecule 49: Ribosomal protein L10 (Predicted)

Chain AI: 11% 98%



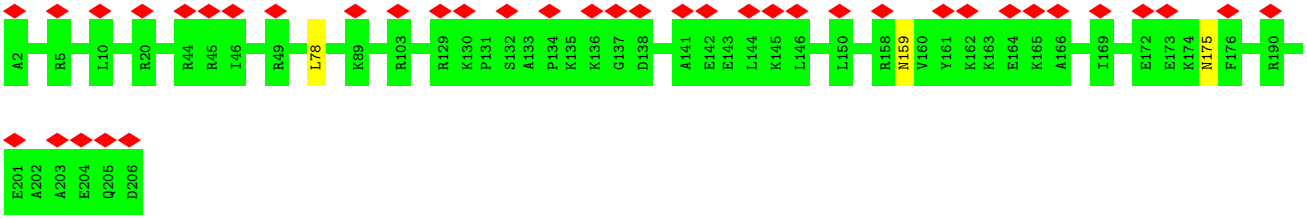
- Molecule 50: Ribosomal protein L11

Chain AJ: 19% 99%



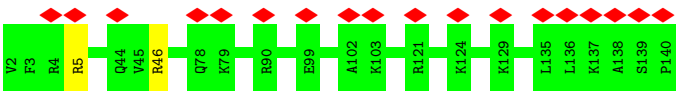
- Molecule 51: ribosomal protein eL13

Chain AL: 19% 99%



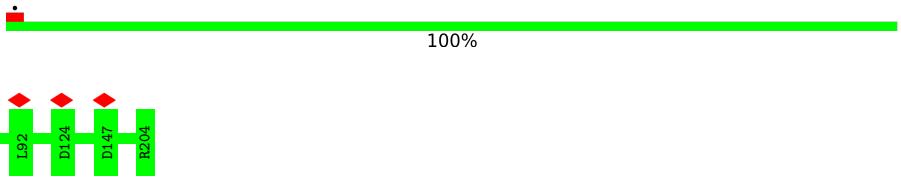
- Molecule 52: ribosomal protein eL14

Chain AM: 13% 99%



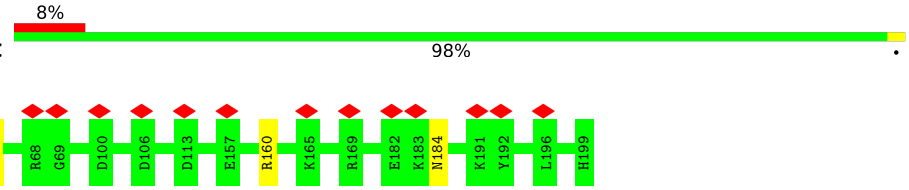
- Molecule 53: Ribosomal protein L15

Chain AN:



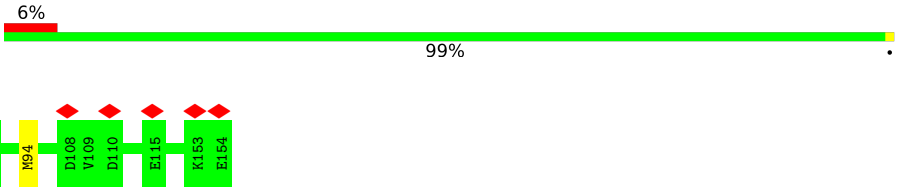
- Molecule 54: ribosomal protein uL13

Chain AO:



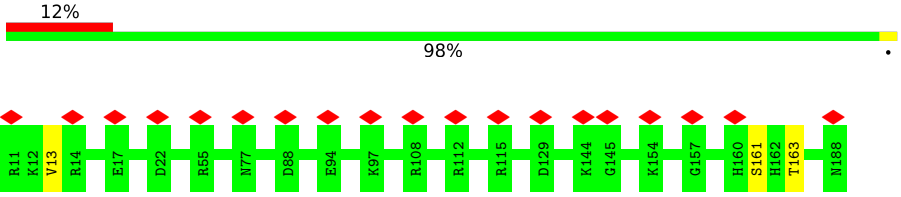
- Molecule 55: ribosomal protein uL22

Chain AP:



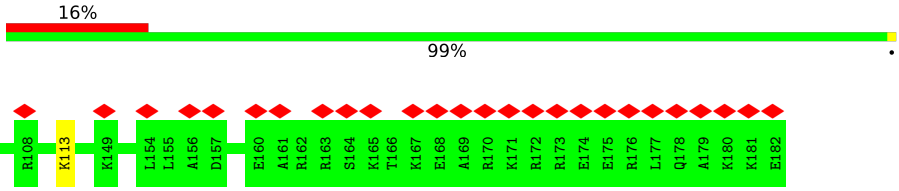
- Molecule 56: ribosomal protein eL18

Chain AQ:



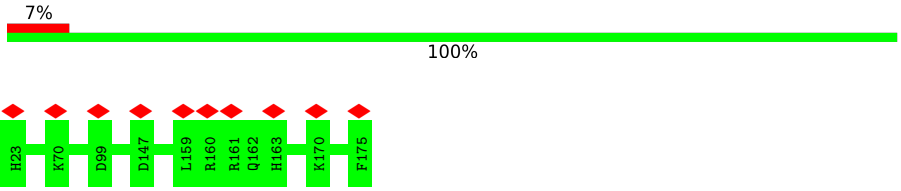
- Molecule 57: ribosomal protein eL19

Chain AR:



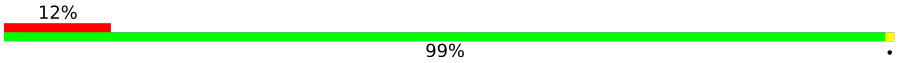
- Molecule 58: ribosomal protein eL20

Chain AS:



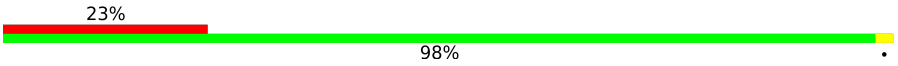
- Molecule 59: ribosomal protein eL21

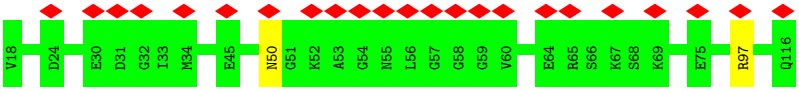
Chain AT:



• Molecule 60: ribosomal protein eL22

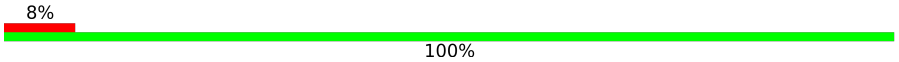
Chain AU:

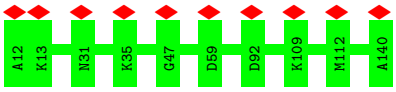




• Molecule 61: Ribosomal protein L23

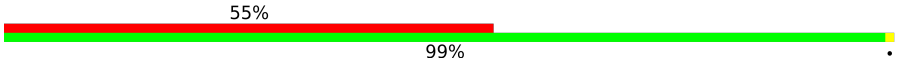
Chain AV:

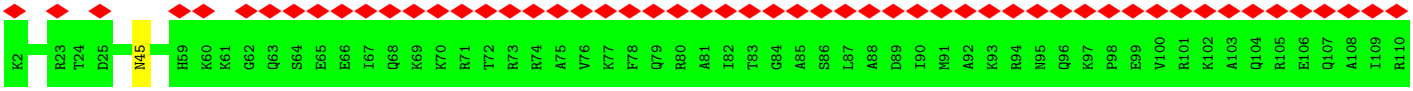


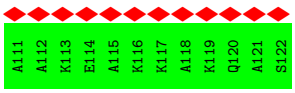


• Molecule 62: ribosomal protein eL24

Chain AW:

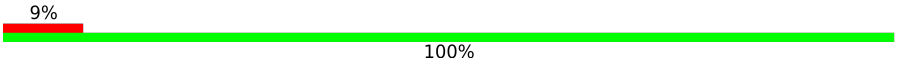


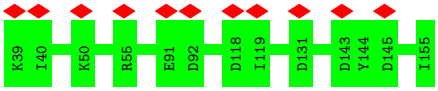




• Molecule 63: ribosomal protein uL23

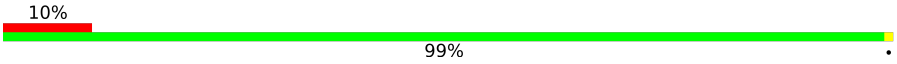
Chain AX:

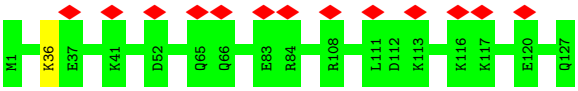




• Molecule 64: Ribosomal protein L26

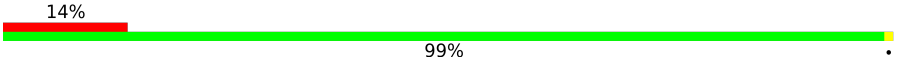
Chain AY:

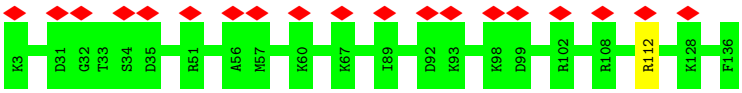




• Molecule 65: 60S ribosomal protein L27

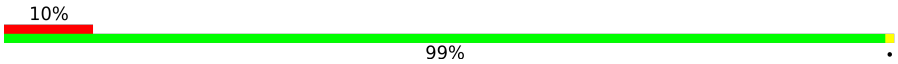
Chain AZ:

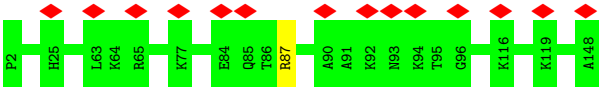




• Molecule 66: ribosomal protein uL15

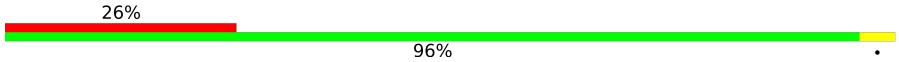
Chain Aa:

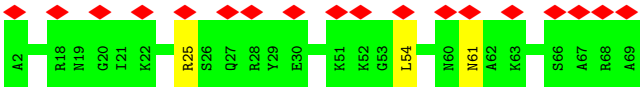




• Molecule 67: ribosomal protein eL29

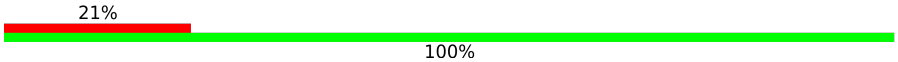
Chain Ab:

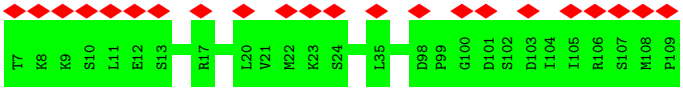




• Molecule 68: ribosomal protein eL30

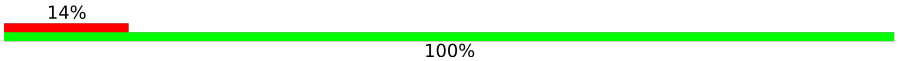
Chain Ac:

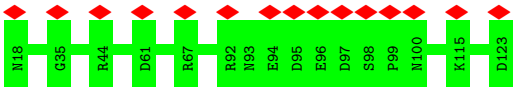




• Molecule 69: ribosomal protein eL31

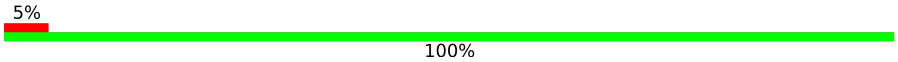
Chain Ad:

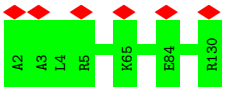




• Molecule 70: ribosomal protein eL32

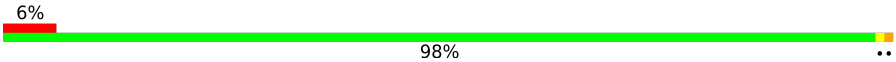
Chain Ae:

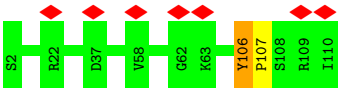




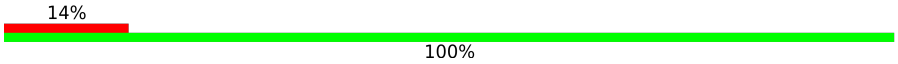
• Molecule 71: ribosomal protein eL33

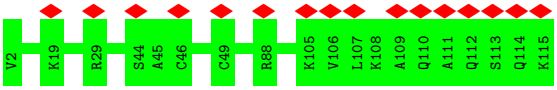
Chain Af:



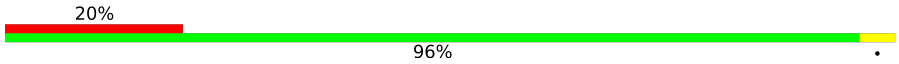


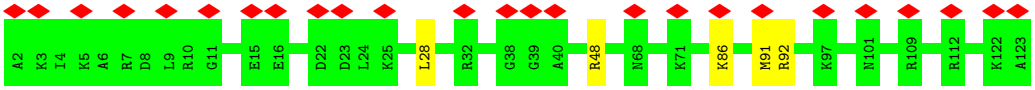
• Molecule 72: ribosomal protein eL34

Chain Ag: 

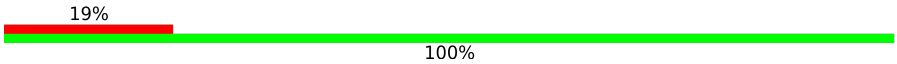


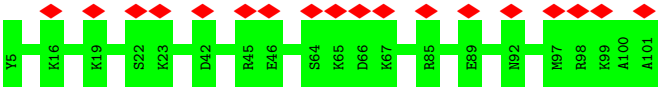
- Molecule 73: ribosomal protein uL29

Chain Ah: 

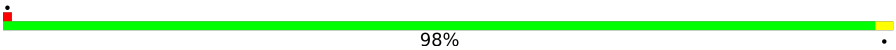


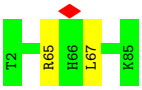
- Molecule 74: ribosomal protein eL36

Chain Ai: 

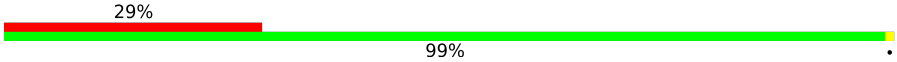


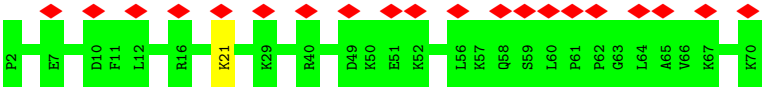
- Molecule 75: Ribosomal protein L37

Chain Aj: 

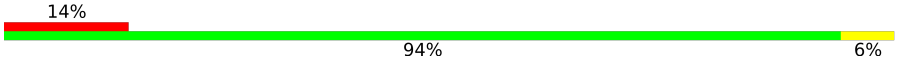


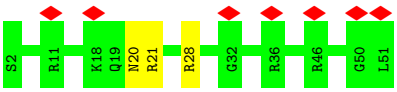
- Molecule 76: ribosomal protein eL38

Chain Ak: 

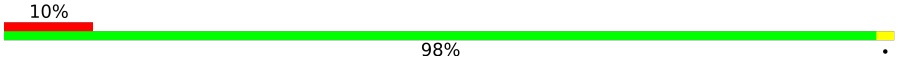


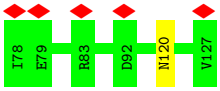
- Molecule 77: ribosomal protein eL39

Chain Al: 



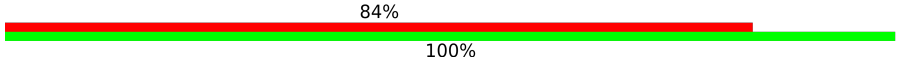
- Molecule 78: ribosomal protein eL40

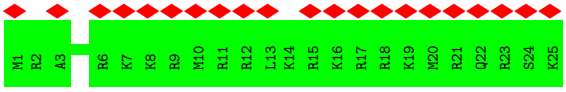
Chain Am: 



• Molecule 79: ribosomal protein eL41

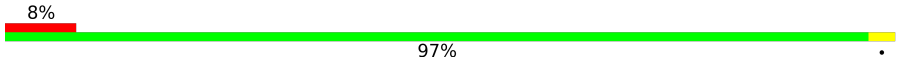
Chain An:

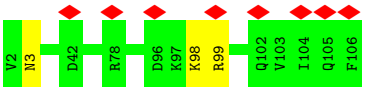




• Molecule 80: ribosomal protein eL42

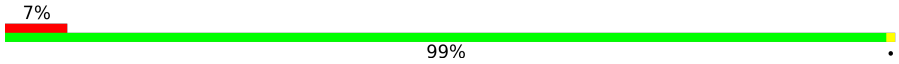
Chain Ao:

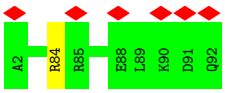




• Molecule 81: ribosomal protein eL43

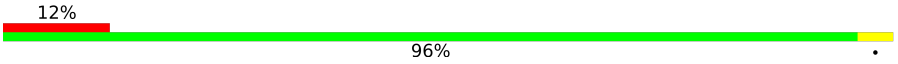
Chain Ap:

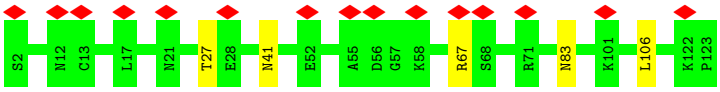




• Molecule 82: ribosomal protein eL28

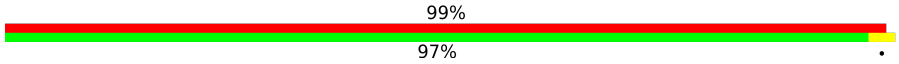
Chain At:

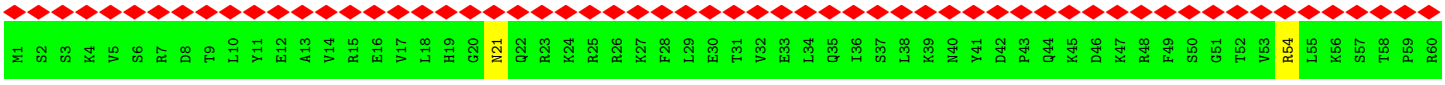


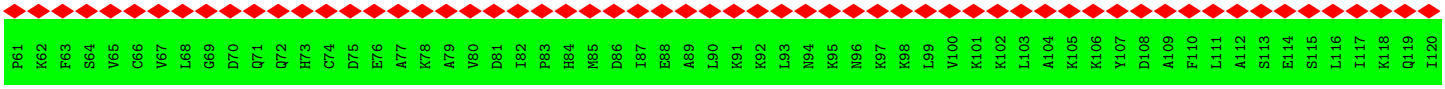


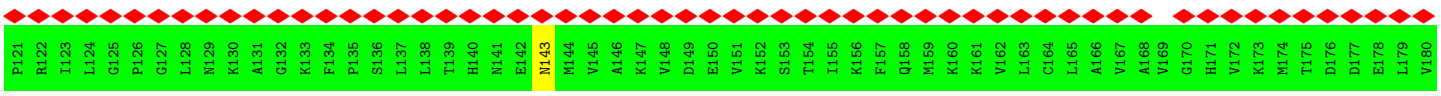
• Molecule 83: Ribosomal protein

Chain Au:









Y181 N182 I183 H184 L185 A186 V187 N188 F189 L190 V191 S192 L193 L194 K195 K196 N197 W198 Q199 N200 V201 R202 A203 L204 Y205 I206 K207 S208 T209 M210 G211 K212 P213 Q214 R215 L216 Y217

- Molecule 84: Ribosomal protein L12

Chain Aq: 87% 97%

V13 Y14 L15 R16 C17 T18 G19 G20 E21 V22 G23 A24 T25 S26 A27 L28 A29 P30 K31 I32 G33 P34 L35 G36 L37 S38 P39 K40 K41 V42 G43 D44 D45 I46 A47 K48 A49 T50 G51 D52 W53 K54 G55 L56 R57 I58 T59 V60 K61 L62 T63 I64 Q65 N66 R67 Q68 A69 Q70 I71 E72

V73 V74 P75 S76 A77 S78 A79 L80 K83 A84 L85 K86 E87 P88 P89 R90 D91 R92 K93 K94 Q95 K96 N97 T98 K99 H100 S101 G102 N103 I104 T105 F106 D107 E108 I109 V110 N111 I112 A113 R114 Q115 M116 R117 H118 R119 S120 L121 A122 R123 E124 L125 S126 G127 T128 I129 K130 E131 I132

T135 S138 V139 G140 C141 N142 V143 D144 G145 R146 H147 P148 H149 D150 I151 I152 D153 D154 I155 N156 S157 G158 A159 V160 E161 C162 P163

- Molecule 85: ribosomal protein uL10

Chain AK: 76% 99%

D5 R6 A7 T8 W9 K10 S11 N12 Y13 F14 L15 K16 I17 I18 Q19 L20 L21 D22 D23 Y24 P25 K26 C27 F28 I29 V30 G31 A32 D33 N34 K38 Q42 I43 R44 M45 S46 L47 R48 G49 K50 A51 V52 V53 L54 M55 M60 K63 A64 I65 R66 G67 H68 L69 E70 N71 N72

P73 A74 L75 E76 K77 L78 L79 P80 H81 I82 R83 G84 N85 V86 G87 F88 V89 F90 T91 K92 E93 D94 L95 T96 E97 I98 R99 D100 M101 L102 R103 A104 N105 K106 V107 P108 A109 A110 A111 R112 A113 G114 A115 I116 A117 P118 C119 E120 V121 T122 A125 Q126 N127 T128 G129 L130 G131 P132 E133

K134 F137 F138 Q139 G142 I143 T144 T145 K146 I147 S148 R149 G150 T151 I152 E153 I154 L155 S156 D157 V158 Q159 K162 T163 G164 D165 K166 V167 G168 A169 S170 E171 A172 T173 M177 L178 N179 I180 S181 P182 F183 S184 F185 G186 L187 V188 I189 Q190 F193 D194 N195 G196 S197 I198 Y199

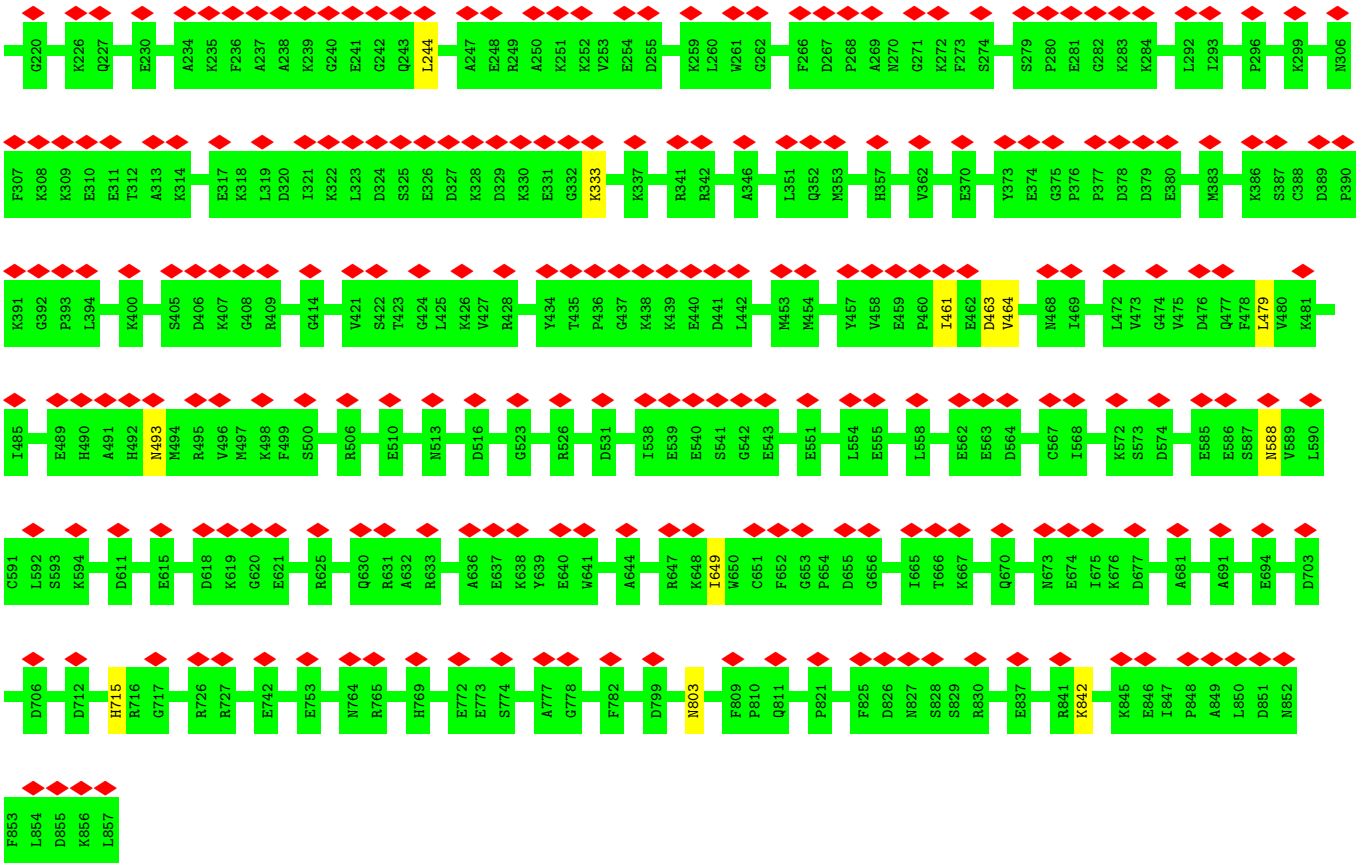
N200 P201 E202 V203 L204 D205 I206

- Molecule 86: eukaryotic elongation factor 2 (eEF2)

Chain Ct: 37% 98%

T5 V6 D7 Q8 I9 R10 A11 I12 M13 D14 K15 R20 N21 M22 S23 V24 I25 D29 C41 K42 A43 G44 I45 I46 A47 S48 A49 R50 A51 G52 E53 T54 R55 F56 T57 D58 T59 R60 K61 D62 E63 Q64 A74 F78 Y79 E80 L81 S82 E83 N84 D85 L86 N87 F88 I89

K90 Q91 S92 K93 D94 G95 A96 G97 F98 N101 L102 D110 L119 A125 D130 S133 G134 V135 E140 M156 K159 M160 D161 L165 E166 E170 E173 R180 N184 V185 N186 G193 E194 G195 E196 S197 G198 P199 N202 I203 L209 G210 T211


G220 K226 Q227 E230 A234 K235 F236 A237 A238 K239 G240 E241 G242 Q243 L244 A247 E248 R249 A250 K251 K252 V253 E254 D255 K259 L260 W261 G262 F266 D267 P268 A269 N270 G271 K272 F273 S274 S279 P280 E281 G282 K283 K284 L292 I293 P296 K299 N306
F307 K308 K309 E310 E311 T312 A313 K314 E317 K318 L319 D320 I321 K322 L323 D324 S325 E326 D327 K328 D329 K330 E331 G332 K333 K337 R341 R342 A346 L351 Q352 M353 H357 V362 E370 Y373 E374 G375 P376 P377 D378 D379 E380 M383 K386 S387 C388 D389 P390
K391 G392 P393 L394 K400 S405 D406 K407 G408 R409 G414 V421 S422 T423 G424 L425 K426 V427 R428 Y434 T435 P436 G437 K438 K439 E440 D441 L442 M453 M454 Y457 V458 E459 P460 I461 E462 D463 V464 N468 I469 L472 V473 G474 V475 D476 Q477 F478 L479 V480 K481
I485 E489 H490 A491 H492 N493 M494 R495 V496 M497 K498 F499 S500 R506 E510 N513 D516 G523 R526 D531 I538 E539 E540 S541 G542 E543 E551 L554 E555 L558 E562 E563 D564 C567 I568 K572 S573 D574 E585 E586 S587 N588 V589 L590
C591 L592 S593 K594 D611 E615 D618 K619 G620 E621 R625 Q630 R631 A632 R633 A636 E637 K638 Y639 E640 W641 A644 R647 K648 I649 W650 C651 F652 G653 P654 D655 G656 I665 T666 K667 Q670 N673 E674 I675 K676 D677 A681 A691 E694 D703
D706 D712 H715 R716 G717 R726 R727 E742 E753 N764 R765 H769 E772 E773 S774 A777 G778 F782 D799 N803 F809 P810 Q811 P821 F825 D826 N827 S828 S829 R830 E837 R841 K842 K845 E846 I847 P848 A849 L850 D851 N852
F853 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	32386	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	11.639	Depositor
Minimum map value	-3.647	Depositor
Average map value	0.347	Depositor
Map value standard deviation	0.655	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: MG, ZN, DDE, 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	1.02	277/135108 (0.2%)
2	Bv	0.37	1/1810 (0.1%)	0.98	2/2817 (0.1%)
3	Bx	0.26	0/287	0.95	0/445
4	Bw	0.36	1/1819 (0.1%)	0.91	0/2833
5	B1	0.31	1/40767 (0.0%)	1.03	200/63536 (0.3%)
6	BD	0.27	0/1736	0.51	0/2338
7	BF	0.27	0/1524	0.55	0/2048
8	BK	0.27	0/851	0.58	0/1147
9	BM	0.25	0/941	0.57	0/1264
10	BP	0.31	0/1019	0.67	1/1361 (0.1%)
11	BQ	0.26	0/1126	0.55	0/1506
12	BR	0.26	0/1023	0.52	0/1373
13	BS	0.26	0/1172	0.53	0/1570
14	BT	0.27	0/1131	0.54	0/1515
15	BU	0.25	0/778	0.52	0/1045
16	BZ	0.27	0/696	0.61	0/929
17	Bc	0.26	0/490	0.53	0/656
18	Bd	0.29	0/437	0.56	0/580
19	Bf	0.25	0/613	0.47	0/811
20	Bg	0.27	0/2497	0.53	0/3399
21	BA	0.27	0/1741	0.54	0/2366
22	BB	0.27	0/1749	0.60	0/2340
23	BC	0.28	0/1761	0.53	0/2379
24	BE	0.27	0/2072	0.53	0/2793
25	BG	0.26	0/1907	0.51	0/2538
26	BH	0.26	0/1501	0.52	0/2009
27	BI	0.27	0/1725	0.55	0/2298
28	BJ	0.26	0/1520	0.53	1/2030 (0.0%)
29	BL	0.28	0/1281	0.56	1/1710 (0.1%)
30	BN	0.26	0/1226	0.53	0/1649
31	BO	0.26	0/1029	0.51	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	0.50	0/854
38	Be	0.27	0/443	0.55	0/583
39	A3	0.32	0/3726	1.02	11/5804 (0.2%)
40	A4	0.34	0/2839	1.06	10/4425 (0.2%)
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	0.53	0/3951
44	AD	0.28	0/2437	0.53	0/3262
45	AE	0.28	0/1603	0.59	0/2153
46	AF	0.27	0/1986	0.52	0/2644
47	AG	0.28	0/1913	0.55	0/2576
48	AH	0.28	0/1545	0.58	1/2077 (0.0%)
49	AI	0.26	0/1730	0.49	0/2311
50	AJ	0.27	0/1376	0.55	1/1841 (0.1%)
51	AL	0.28	0/1688	0.56	0/2260
52	AM	0.29	0/1161	0.52	0/1554
53	AN	0.28	0/1746	0.51	0/2338
54	AO	0.27	0/1638	0.48	0/2191
55	AP	0.26	0/1268	0.48	0/1701
56	AQ	0.27	0/1537	0.61	0/2052
57	AR	0.25	0/1533	0.48	0/2025
58	AS	0.27	0/1488	0.51	0/1997
59	AT	0.27	0/1312	0.48	0/1753
60	AU	0.27	0/822	0.49	0/1103
61	AV	0.27	0/983	0.49	0/1319
62	AW	0.27	0/1004	0.51	0/1332
63	AX	0.26	0/975	0.51	0/1312
64	AY	0.26	0/1081	0.46	0/1439
65	AZ	0.27	0/1126	0.54	0/1502
66	Aa	0.27	0/1191	0.52	0/1591
67	Ab	0.27	0/569	0.64	1/750 (0.1%)
68	Ac	0.26	0/812	0.53	0/1089
69	Ad	0.26	0/894	0.53	0/1204
70	Ae	0.27	0/1082	0.53	0/1443
71	Af	0.29	0/895	0.57	0/1198
72	Ag	0.28	0/916	0.58	0/1220
73	Ah	0.25	0/1023	0.56	1/1351 (0.1%)
74	Ai	0.26	0/805	0.50	0/1065
75	Aj	0.29	0/703	0.59	1/929 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	Ak	0.26	0/575	0.57	0/761
77	Al	0.25	0/454	0.53	0/599
78	Am	0.25	0/417	0.53	0/553
79	An	0.22	0/241	0.44	0/305
80	Ao	0.28	0/877	0.53	0/1156
81	Ap	0.27	0/718	0.57	0/953
82	At	0.28	0/995	0.65	1/1334 (0.1%)
83	Au	0.27	0/1772	0.54	0/2375
84	Aq	0.29	0/1155	0.72	1/1558 (0.1%)
85	AK	0.28	0/1580	0.59	1/2133 (0.0%)
86	Ct	0.29	0/6767	0.60	3/9139 (0.0%)
All	All	0.30	3/241644 (0.0%)	0.87	515/353975 (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
8	BK	0	1
11	BQ	0	1
17	Bc	0	1
21	BA	0	1
22	BB	0	1
24	BE	0	1
27	BI	0	2
28	BJ	0	1
43	AC	0	2
44	AD	0	1
45	AE	0	3
48	AH	0	2
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	4
All	All	0	30

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Bv	1	G	OP3-P	-10.62	1.48	1.61
5	B1	1	U	OP3-P	-10.57	1.48	1.61
4	Bw	1	G	OP3-P	-10.55	1.48	1.61

The worst 5 of 515 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A2	1440	C	N1-C2-O2	10.37	125.12	118.90
1	A2	252	C	N1-C2-O2	10.20	125.02	118.90
1	A2	191	C	N3-C2-O2	-9.77	115.06	121.90
5	B1	1315	U	C2-N1-C1'	9.42	129.01	117.70
5	B1	1315	U	N1-C2-O2	9.29	129.30	122.80

There are no chirality outliers.

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	BA	207	PRO	Peptide
22	BB	39	PHE	Peptide
8	BK	65	ARG	Peptide
11	BQ	13	PHE	Peptide
17	Bc	32	VAL	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%)	209 (96%)	9 (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%)	82 (85%)	13 (14%)	1 (1%)	15	55
9	BM	118/120 (98%)	110 (93%)	8 (7%)	0	100	100
10	BP	118/120 (98%)	105 (89%)	12 (10%)	1 (1%)	19	59
11	BQ	137/139 (99%)	128 (93%)	9 (7%)	0	100	100
12	BR	123/125 (98%)	109 (89%)	14 (11%)	0	100	100
13	BS	137/139 (99%)	125 (91%)	12 (9%)	0	100	100
14	BT	141/143 (99%)	130 (92%)	10 (7%)	1 (1%)	22	61
15	BU	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
16	BZ	84/86 (98%)	74 (88%)	10 (12%)	0	100	100
17	Bc	60/62 (97%)	55 (92%)	3 (5%)	2 (3%)	4	31
18	Bd	49/51 (96%)	46 (94%)	3 (6%)	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%)	199 (93%)	14 (7%)	0	100	100
22	BB	210/212 (99%)	180 (86%)	30 (14%)	0	100	100
23	BC	220/222 (99%)	206 (94%)	14 (6%)	0	100	100
24	BE	255/257 (99%)	236 (92%)	17 (7%)	2 (1%)	19	59
25	BG	230/232 (99%)	216 (94%)	14 (6%)	0	100	100
26	BH	181/183 (99%)	166 (92%)	15 (8%)	0	100	100
27	BI	205/207 (99%)	177 (86%)	27 (13%)	1 (0%)	29	68
28	BJ	177/179 (99%)	157 (89%)	18 (10%)	2 (1%)	14	53
29	BL	151/153 (99%)	138 (91%)	12 (8%)	1 (1%)	22	61
30	BN	147/149 (99%)	131 (89%)	16 (11%)	0	100	100
31	BO	134/136 (98%)	122 (91%)	12 (9%)	0	100	100
32	BV	79/81 (98%)	76 (96%)	3 (4%)	0	100	100
33	BW	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
34	BX	139/141 (99%)	122 (88%)	17 (12%)	0	100	100
35	BY	123/125 (98%)	111 (90%)	12 (10%)	0	100	100
36	Ba	95/97 (98%)	87 (92%)	8 (8%)	0	100	100
37	Bb	78/80 (98%)	71 (91%)	7 (9%)	0	100	100
38	Be	53/55 (96%)	49 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	AA	250/252 (99%)	235 (94%)	15 (6%)	0	100	100
42	AB	392/394 (100%)	361 (92%)	31 (8%)	0	100	100
43	AC	361/363 (99%)	335 (93%)	22 (6%)	4 (1%)	14	53
44	AD	292/294 (99%)	269 (92%)	23 (8%)	0	100	100
45	AE	192/194 (99%)	161 (84%)	30 (16%)	1 (0%)	29	68
46	AF	232/234 (99%)	214 (92%)	18 (8%)	0	100	100
47	AG	232/234 (99%)	218 (94%)	14 (6%)	0	100	100
48	AH	189/191 (99%)	175 (93%)	14 (7%)	0	100	100
49	AI	204/211 (97%)	181 (89%)	23 (11%)	0	100	100
50	AJ	167/169 (99%)	152 (91%)	14 (8%)	1 (1%)	25	64
51	AL	203/205 (99%)	171 (84%)	31 (15%)	1 (0%)	29	68
52	AM	137/139 (99%)	127 (93%)	10 (7%)	0	100	100
53	AN	201/203 (99%)	185 (92%)	16 (8%)	0	100	100
54	AO	193/195 (99%)	186 (96%)	7 (4%)	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%)	163 (94%)	10 (6%)	0	100	100
59	AT	155/157 (99%)	138 (89%)	15 (10%)	2 (1%)	12	50
60	AU	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
61	AV	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
62	AW	119/121 (98%)	108 (91%)	11 (9%)	0	100	100
63	AX	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
64	AY	125/127 (98%)	119 (95%)	6 (5%)	0	100	100
65	AZ	132/134 (98%)	115 (87%)	17 (13%)	0	100	100
66	Aa	145/147 (99%)	131 (90%)	14 (10%)	0	100	100
67	Ab	66/68 (97%)	56 (85%)	10 (15%)	0	100	100
68	Ac	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
69	Ad	104/106 (98%)	101 (97%)	3 (3%)	0	100	100
70	Ae	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
71	Af	107/109 (98%)	95 (89%)	10 (9%)	2 (2%)	8	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	Ag	112/114 (98%)	100 (89%)	12 (11%)	0	100	100
73	Ah	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
74	Ai	95/97 (98%)	85 (90%)	10 (10%)	0	100	100
75	Aj	82/84 (98%)	73 (89%)	9 (11%)	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%)	44 (92%)	4 (8%)	0	100	100
79	An	23/25 (92%)	23 (100%)	0	0	100	100
80	Ao	103/105 (98%)	96 (93%)	7 (7%)	0	100	100
81	Ap	89/91 (98%)	83 (93%)	6 (7%)	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%)	112 (75%)	37 (25%)	0	100	100
85	AK	200/202 (99%)	179 (90%)	20 (10%)	1 (0%)	29	68
86	Ct	850/853 (100%)	768 (90%)	79 (9%)	3 (0%)	34	71
All	All	12538/12702 (99%)	11449 (91%)	1062 (8%)	27 (0%)	50	79

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	BP	51	ARG
28	BJ	138	ARG
71	Af	107	PRO
24	BE	93	GLU
51	AL	78	LEU

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	95

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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%)	115 (100%)	0	100	100
12	BR	113/113 (100%)	113 (100%)	0	100	100
13	BS	121/121 (100%)	117 (97%)	4 (3%)	38	69
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	97
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	95
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	71
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	50
41	AA	194/194 (100%)	193 (100%)	1 (0%)	88	95
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%)	244 (98%)	4 (2%)	62	83
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	178/179 (99%)	177 (99%)	1 (1%)	86	94
50	AJ	142/142 (100%)	142 (100%)	0	100	100
51	AL	171/171 (100%)	169 (99%)	2 (1%)	71	87
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	77
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%)	116 (99%)	1 (1%)	78	90
66	Aa	120/120 (100%)	119 (99%)	1 (1%)	81	91
67	Ab	58/58 (100%)	56 (97%)	2 (3%)	37	69
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%)	70 (99%)	1 (1%)	67	85
76	Ak	64/64 (100%)	63 (98%)	1 (2%)	62	83
77	Al	47/47 (100%)	44 (94%)	3 (6%)	17	52
78	Am	46/46 (100%)	45 (98%)	1 (2%)	52	77
79	An	24/24 (100%)	24 (100%)	0	100	100
80	Ao	93/93 (100%)	90 (97%)	3 (3%)	39	70
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	71
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	97
All	All	10924/10925 (100%)	10828 (99%)	96 (1%)	79	90

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
54	AO	65	ASN
73	Ah	92	ARG
54	AO	184	ASN
65	AZ	112	ARG
77	Al	21	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
72	Ag	73	HIS
77	Al	43	HIS
83	Au	197	ASN
33	BW	44	HIS
33	BW	16	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	3600/3612 (99%)	706 (19%)	9 (0%)
2	Bv	75/76 (98%)	12 (16%)	0
3	Bx	11/12 (91%)	6 (54%)	0
39	A3	156/157 (99%)	35 (22%)	0
4	Bw	75/76 (98%)	13 (17%)	0
40	A4	118/119 (99%)	21 (17%)	0
5	B1	1701/1708 (99%)	336 (19%)	4 (0%)
All	All	5736/5760 (99%)	1129 (19%)	13 (0%)

5 of 1129 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	8	U
1	A2	9	C
1	A2	10	A
1	A2	12	A
1	A2	14	C

5 of 13 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A2	4870	G
1	A2	4946	U
5	B1	1554	C
5	B1	369	C
5	B1	797	C

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	3,86	14,20,21	1.11	2 (14%)	14,28,30	1.52	3 (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
86	DDE	Ct	715	3,86	-	10/20/21/23	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	Ct	715	DDE	CD2-NE2	2.23	1.39	1.36
86	Ct	715	DDE	CBW-CBI	2.08	1.56	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
86	Ct	715	DDE	CBW-CBI-NAD	3.36	119.57	115.28
86	Ct	715	DDE	CB-CA-C	-2.27	107.21	111.47
86	Ct	715	DDE	CAC-NCB-CBW	2.10	115.73	110.51

There are no chirality outliers.

5 of 10 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	CBI-CBW-NCB-CAB

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	2.10	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	-	-	7/14/38/38	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	4.35	1.64	1.59
89	Ct	901	GNP	C6-N1	3.08	1.38	1.33
89	Ct	901	GNP	PG-N3B	2.81	1.70	1.63
89	Ct	901	GNP	PB-O1B	2.79	1.50	1.46
89	Ct	901	GNP	PG-O1G	2.68	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	-8.38	111.98	123.43
89	Ct	901	GNP	C2-N1-C6	5.77	125.10	115.93
89	Ct	901	GNP	N3-C2-N1	-2.75	123.55	127.22
89	Ct	901	GNP	C4-C5-C6	-2.55	118.36	120.80
89	Ct	901	GNP	C2-N3-C4	-2.16	112.89	115.36

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

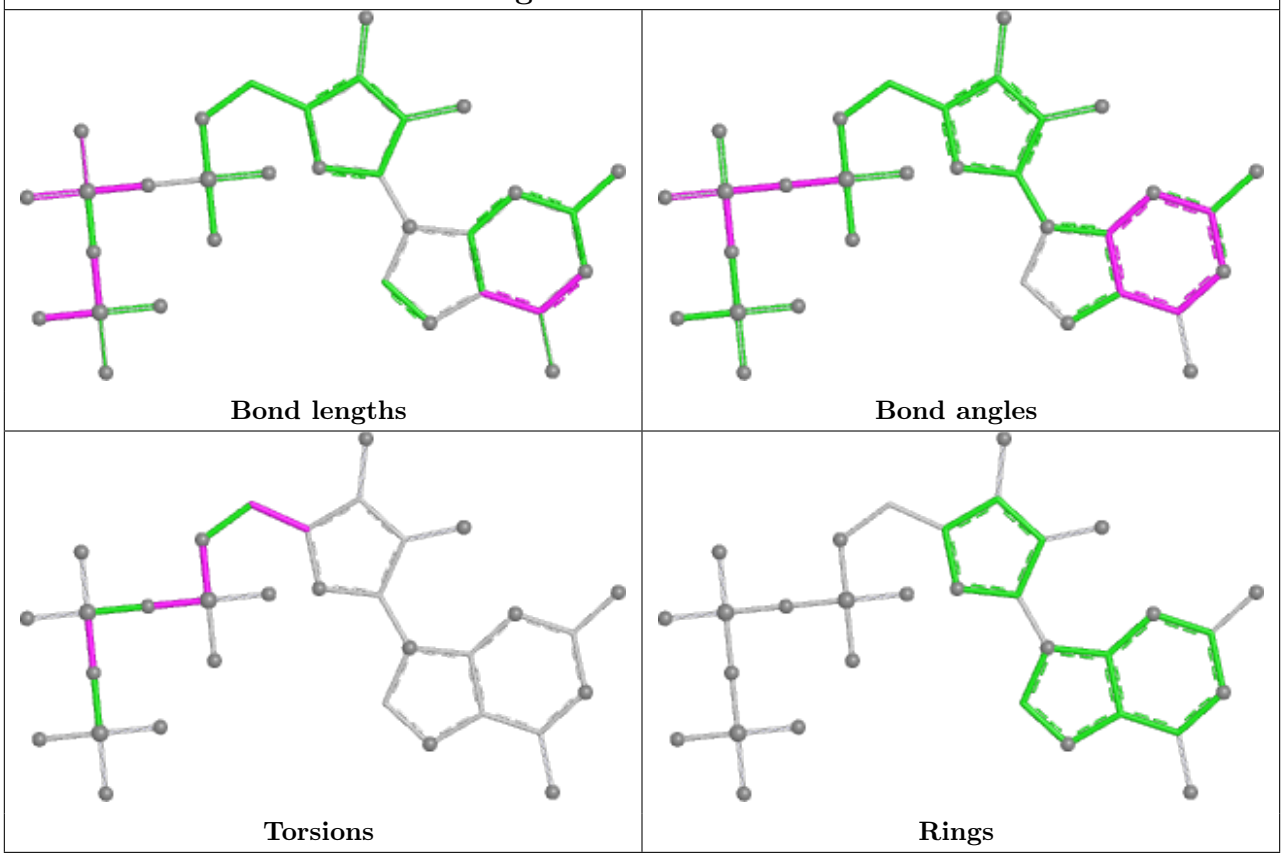
Mol	Chain	Res	Type	Atoms
89	Ct	901	GNP	PG-N3B-PB-O1B
89	Ct	901	GNP	C5'-O5'-PA-O3A
89	Ct	901	GNP	C5'-O5'-PA-O1A
89	Ct	901	GNP	C3'-C4'-C5'-O5'
89	Ct	901	GNP	O4'-C4'-C5'-O5'

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

The worst 5 of 17 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	20.66
1	B1	751:G	O3'	790:C	P	20.56
1	A2	517:C	O3'	629:G	P	18.02
1	A2	3948:C	O3'	4004:G	P	17.82
1	B1	1757:G	O3'	1775:U	P	17.75

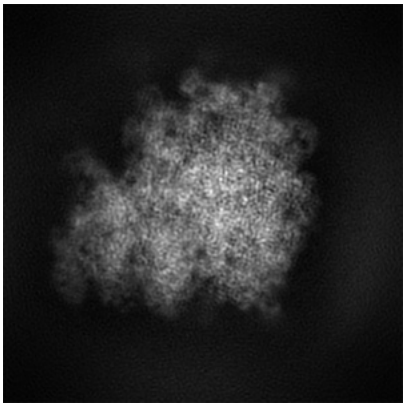
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0098. These allow visual inspection of the internal detail of the map and identification of artifacts.

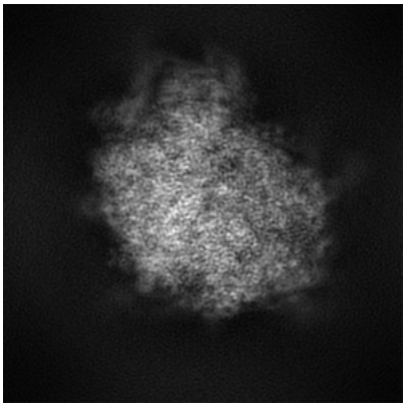
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

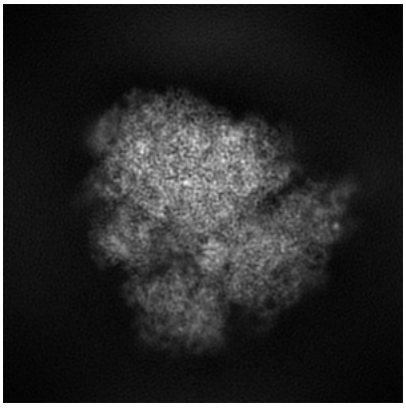
6.1.1 Primary map



X



Y

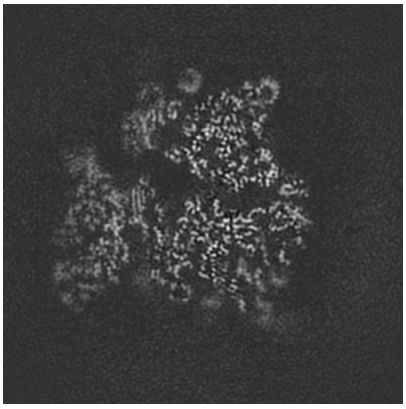


Z

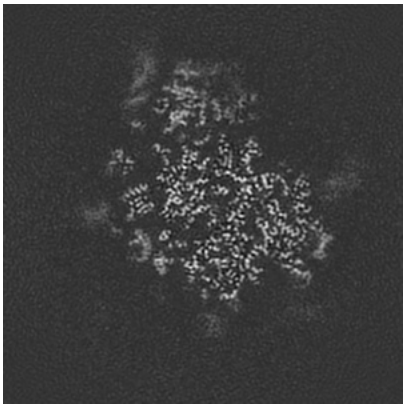
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

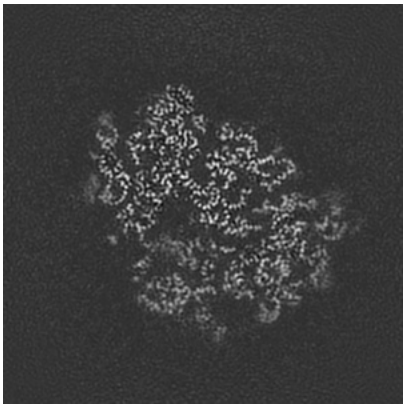
6.2.1 Primary map



X Index: 202



Y Index: 202

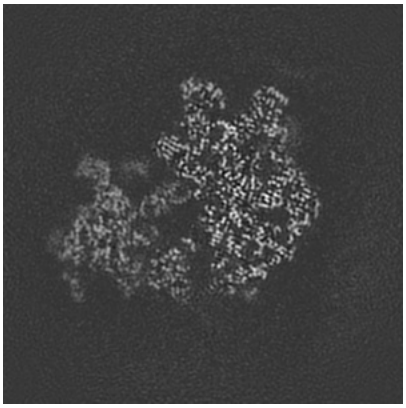


Z Index: 202

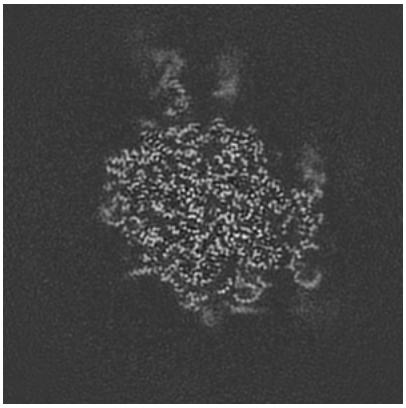
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

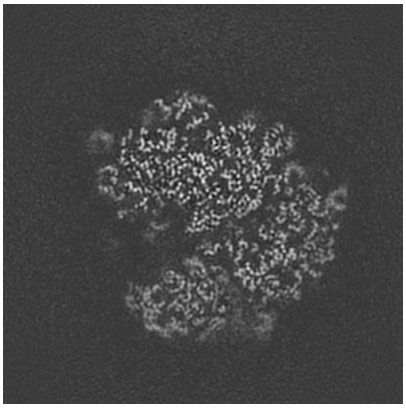
6.3.1 Primary map



X Index: 179



Y Index: 220



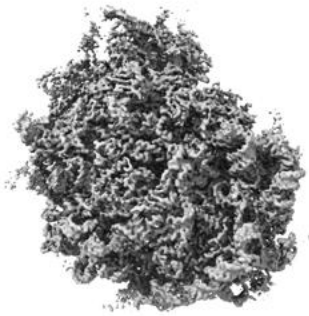
Z Index: 185

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.

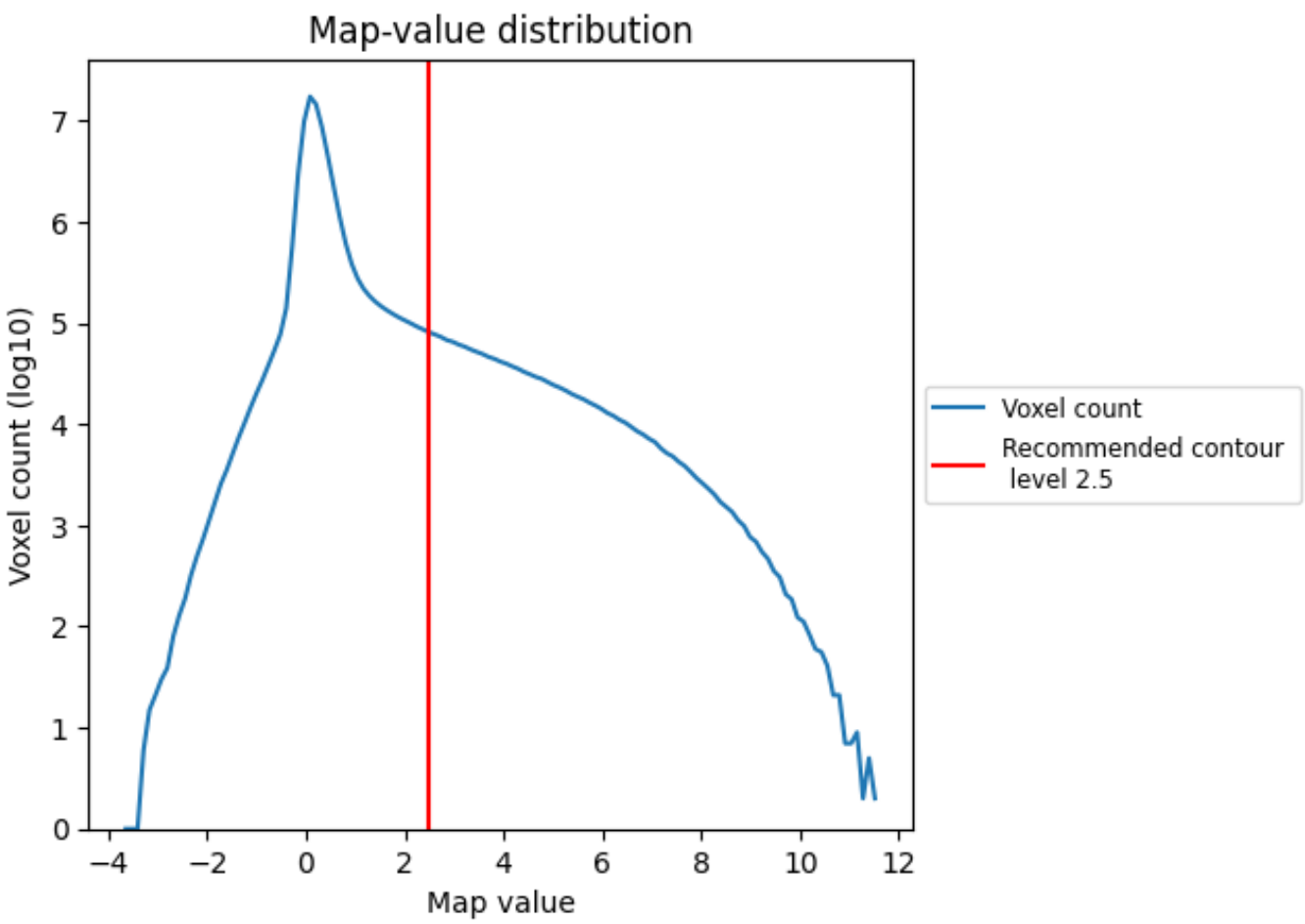
6.5 Mask visualisation (i)

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

7 Map analysis (i)

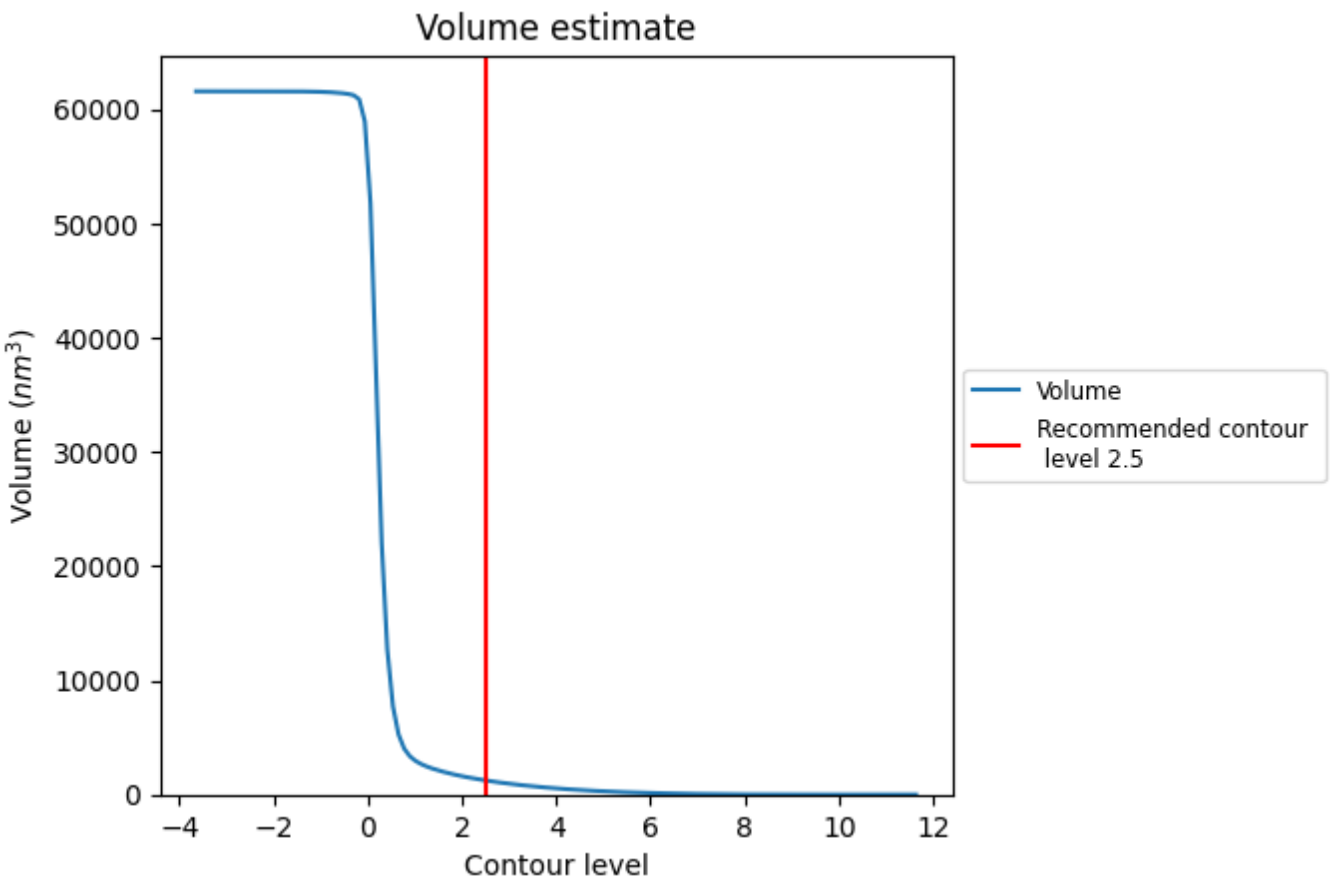
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

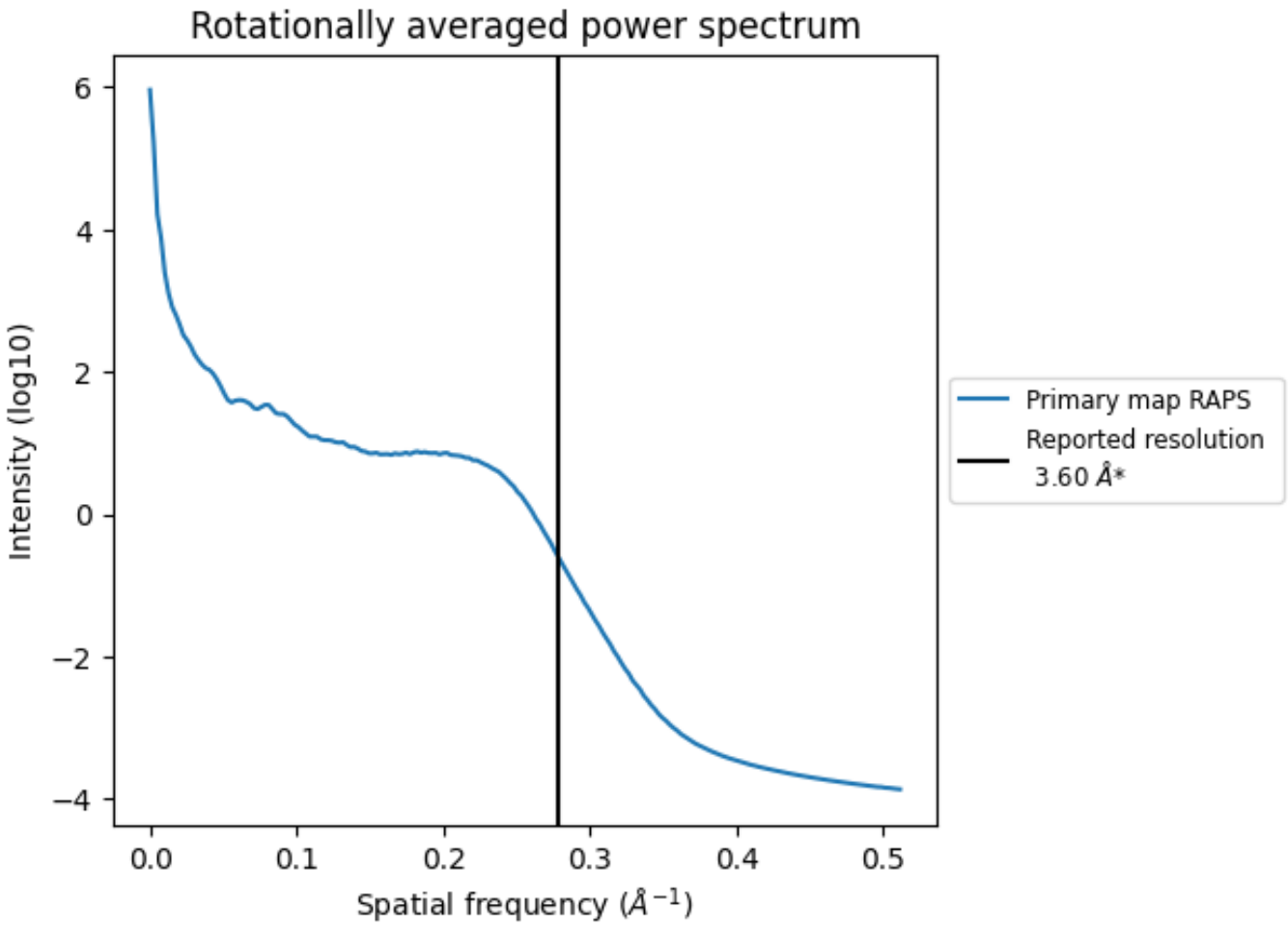
7.2 Volume estimate (i)



The volume at the recommended contour level is 1237 nm^3; this corresponds to an approximate mass of 1118 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 0.278 Å^{-1}

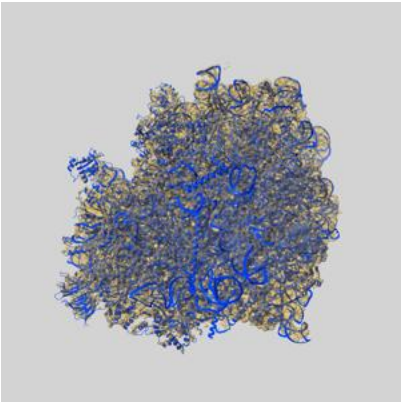
8 Fourier-Shell correlation (i)

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

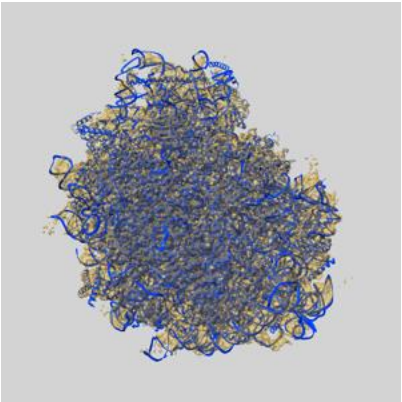
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0098 and PDB model 6GZ3. Per-residue inclusion information can be found in section 3 on page 22.

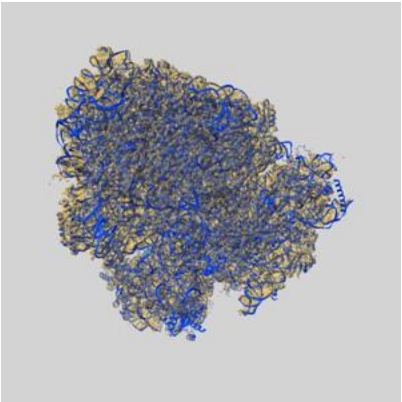
9.1 Map-model overlay (i)



X



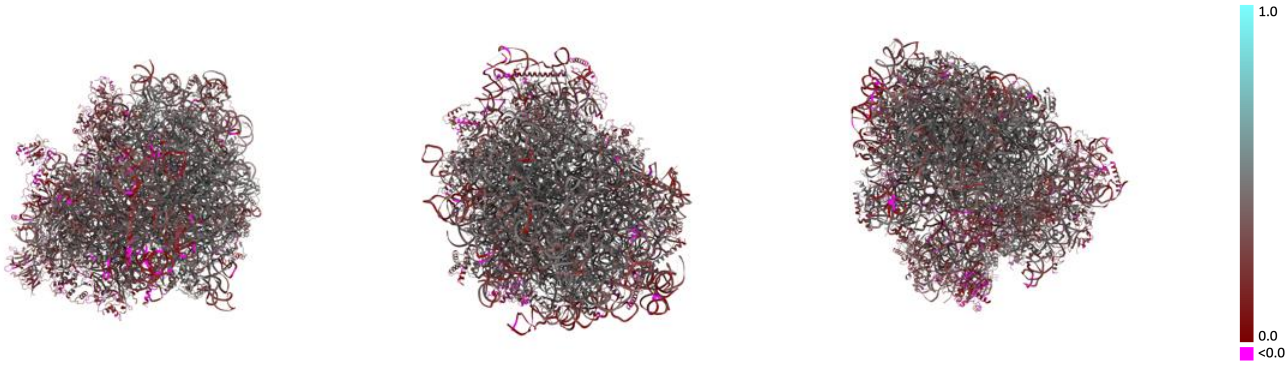
Y



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.

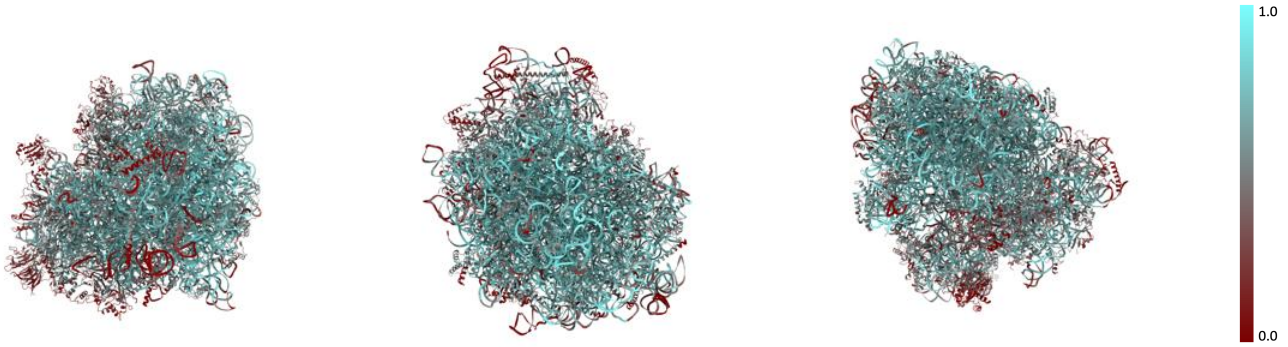
9.2 Q-score mapped to coordinate model (i)



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.

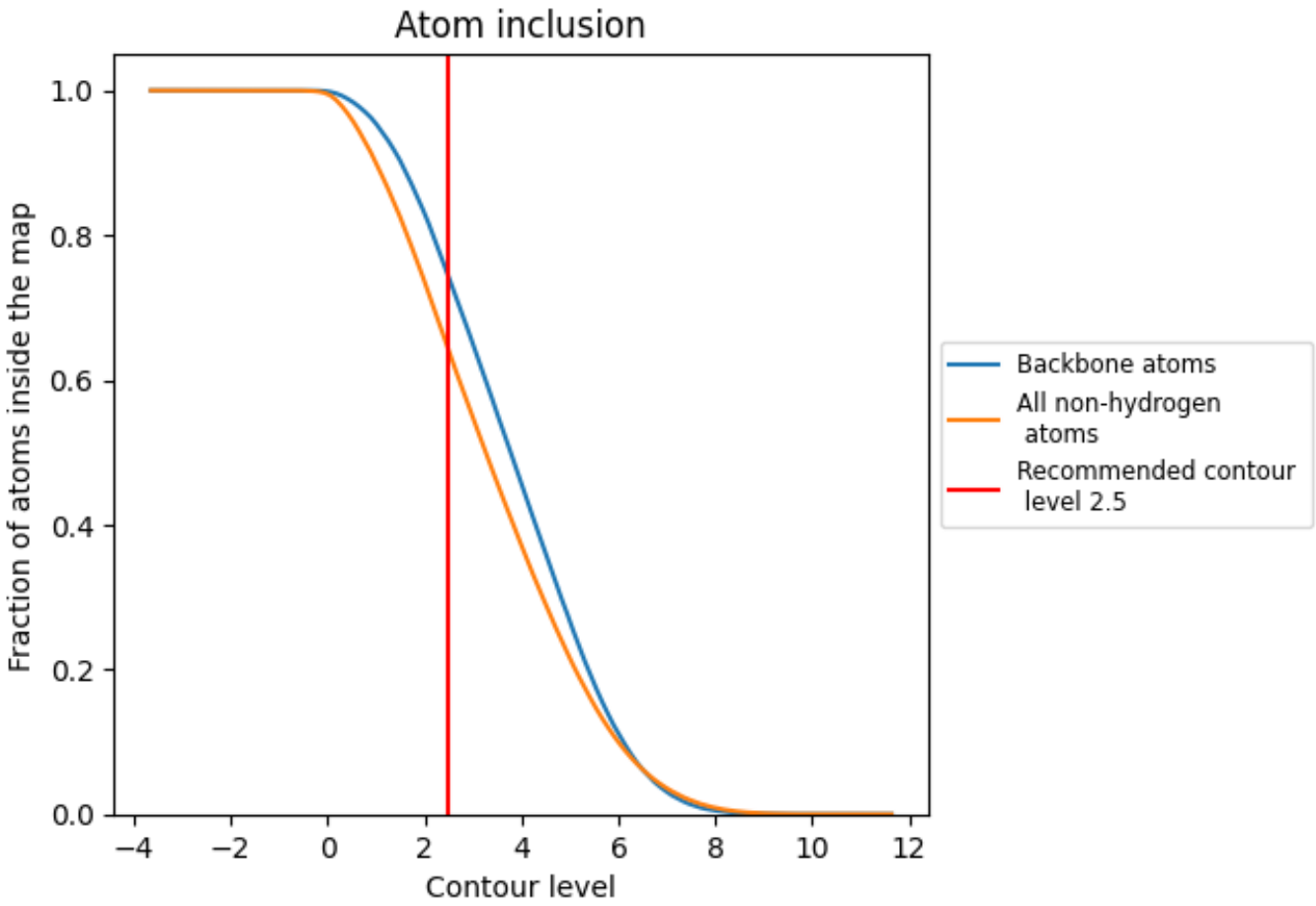
9.3 Atom inclusion mapped to coordinate model (i)



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, 74% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.6403	0.3650
A2	0.7652	0.3920
A3	0.7730	0.3970
A4	0.8501	0.4350
AA	0.6617	0.4460
AB	0.6398	0.4200
AC	0.6499	0.4150
AD	0.6158	0.3670
AE	0.5062	0.3230
AF	0.6182	0.3860
AG	0.5591	0.3630
AH	0.5847	0.4080
AI	0.6323	0.4130
AJ	0.5899	0.3710
AK	0.2461	0.2090
AL	0.5902	0.3630
AM	0.6116	0.3790
AN	0.7070	0.4320
AO	0.6430	0.4030
AP	0.6719	0.4380
AQ	0.6450	0.4010
AR	0.5690	0.3590
AS	0.6586	0.4180
AT	0.6253	0.4120
AU	0.5215	0.3620
AV	0.6399	0.4570
AW	0.3249	0.2310
AX	0.6219	0.4310
AY	0.6420	0.4130
AZ	0.6090	0.3860
Aa	0.6717	0.4210
Ab	0.5470	0.3440
Ac	0.5714	0.3640
Ad	0.6321	0.4270
Ae	0.6598	0.4260

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Chain	Atom inclusion	Q-score
Af	0.6734	0.4220
Ag	0.6076	0.3990
Ah	0.5739	0.3710
Ai	0.6181	0.3750
Aj	0.7245	0.4400
Ak	0.5009	0.3570
Al	0.6392	0.4160
Am	0.6423	0.3990
An	0.2636	0.3050
Ao	0.6337	0.4200
Ap	0.6473	0.4240
Aq	0.1342	0.1360
At	0.6536	0.3970
Au	0.0204	0.0060
B1	0.7139	0.3680
BA	0.4251	0.3060
BB	0.4746	0.3290
BC	0.5396	0.3640
BD	0.4478	0.3200
BE	0.5126	0.3390
BF	0.3860	0.2870
BG	0.3773	0.2420
BH	0.2986	0.2680
BI	0.4771	0.3280
BJ	0.5422	0.3200
BK	0.3043	0.1640
BL	0.4881	0.3470
BM	0.0643	0.1290
BN	0.5189	0.3600
BO	0.5238	0.3840
BP	0.3826	0.2500
BQ	0.4157	0.3100
BR	0.3357	0.2710
BS	0.4092	0.2540
BT	0.3845	0.2450
BU	0.3413	0.2890
BV	0.4909	0.3430
BW	0.5653	0.3820
BX	0.5640	0.4040
BY	0.4284	0.2680
BZ	0.2307	0.2110
Ba	0.5730	0.3720

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Chain	Atom inclusion	Q-score
Bb	0.4405	0.3290
Bc	0.3426	0.3010
Bd	0.5012	0.2970
Be	0.4479	0.3590
Bf	0.0634	0.1410
Bg	0.2017	0.2380
Bv	0.5302	0.3010
Bw	0.6595	0.3310
Bx	0.5058	0.2810
Ct	0.4614	0.3260