wwPDB EM Validation Summary Report (i)

Nov 27, 2022 – 09:34 AM EST

PDB ID	:	6OLZ
EMDB ID	:	EMD-0598
Title	:	Human ribosome nascent chain complex (PCSK9-RNC) stalled by a drug-like molecule with PP tRNA
Authors	:	Li, W.; Cate, J.H.D.
Deposited on	:	2019-04-17
Resolution	:	3.90 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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:

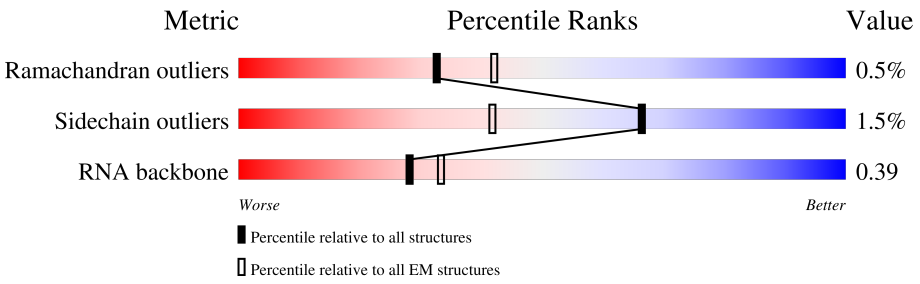
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	AA	248	8% 98%
2	BA	215	36% 99%
3	AB	394	12% 99%
4	BB	212	43% 98%
5	AC	363	12% 94%
6	BC	222	32% 99%
7	A3	157	9% 62% 33% 5%
8	A4	119	72% 27%

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Mol	Chain	Length	Quality of chain
9	AD	294	19% 97%
10	AE	247	21% 88% 9%
11	AF	234	9% 97%
12	AG	234	26% 99%
13	AH	191	19% 99%
14	AI	211	17% 95%
15	AJ	169	30% 99%
16	AL	205	19% 95%
17	AM	139	12% 99%
18	AN	203	5% 98%
19	AO	195	9% 97%
20	AP	153	5% 100%
21	AQ	187	13% 99%
22	AR	181	17% 98%
23	AS	175	8% 99%
24	AT	157	13% 99%
25	AU	99	34% 99%
26	AV	129	11% 99%
27	AW	121	55% 98%
28	AX	117	10% 100%
29	AY	127	7% 98%
30	AZ	134	15% 99%
31	Aa	147	10% 99%
32	Ab	118	27% 76% 5% 18%
33	Ac	103	20% 98%

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Mol	Chain	Length	Quality of chain
34	Ad	106	10% 100%
35	Ae	129	11% 98%
36	Af	109	10% 98%
37	Ag	114	14% 100%
38	Ah	122	11% 97%
39	Ai	97	18% 99%
40	Aj	84	5% 98%
41	Ak	69	29% 97%
42	Al	50	20% 94% 6%
43	Am	50	8% 96%
44	An	25	36% 100%
45	Ao	105	21% 98%
46	Ap	91	13% 98%
47	At	122	7% 97%
48	A2	3643	9% 66% 30%
49	B1	1708	17% 63% 33%
50	BD	220	77% 98%
51	BE	257	39% 97%
52	BF	190	70% 97%
53	BG	232	57% 99%
54	BH	183	61% 98%
55	BI	207	30% 99%
56	BJ	179	41% 98%
57	BK	98	88% 98%
58	BL	153	36% 99%

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Mol	Chain	Length	Quality of chain
59	BM	120	99% 98%
60	BN	149	37% 99%
61	BO	136	31% 99%
62	BP	120	67% 97%
63	BQ	139	68% 100%
64	BR	125	68% 98%
65	BS	139	65% 96%
66	BT	143	69% 97%
67	BU	97	70% 100%
68	BV	81	41% 98%
69	BW	129	26% 98%
70	BX	139	30% 99%
71	BY	125	46% 98%
72	BZ	86	72% 95% 5%
73	Ba	97	32% 99%
74	Bb	80	41% 99%
75	Bc	62	73% 97%
76	Bd	51	59% 98%
77	Be	55	47% 93% 7%
78	Bf	73	93% 99%
79	Bg	314	92% 99%
80	Bv	76	91% 58% 39%
81	Bx	16	88% 44% 56%
82	A	26	92% 81% 19%

2 Entry composition (i)

There are 85 unique types of molecules in this entry. The entry contains 214215 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AA	248	1898	1189	389	314	6	0	0

- Molecule 2 is a protein called 40S ribosomal protein SA.

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

- Molecule 3 is a protein called 60S ribosomal protein L3.

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

- Molecule 4 is a protein called 40S ribosomal protein S3a.

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

- Molecule 5 is a protein called 60S ribosomal protein L4.

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

- Molecule 6 is a protein called 40S ribosomal protein S2.

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

- Molecule 7 is a RNA chain called 5.8S ribosomal RNA.

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

- Molecule 8 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 9 is a protein called 60S ribosomal protein L5.

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

- Molecule 10 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	AE	226	1838	1180	350	304	4	0	0

- Molecule 11 is a protein called 60S ribosomal protein L7.

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

- Molecule 12 is a protein called 60S ribosomal protein L7a.

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

- Molecule 13 is a protein called 60S ribosomal protein L9.

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

- Molecule 14 is a protein called 60S ribosomal protein L10.

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

- Molecule 15 is a protein called 60S ribosomal protein L11.

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

- Molecule 16 is a protein called 60S ribosomal protein L13.

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

- Molecule 17 is a protein called 60S ribosomal protein L14.

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

- Molecule 18 is a protein called 60S ribosomal protein L15.

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

- Molecule 19 is a protein called 60S ribosomal protein L13a.

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

- Molecule 20 is a protein called 60S ribosomal protein L17.

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

- Molecule 21 is a protein called 60S ribosomal protein L18.

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

- Molecule 22 is a protein called 60S ribosomal protein L19.

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

- Molecule 23 is a protein called 60S ribosomal protein L18a.

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

- Molecule 24 is a protein called 60S ribosomal protein L21.

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

- Molecule 25 is a protein called 60S ribosomal protein L22.

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

- Molecule 26 is a protein called 60S ribosomal protein L23.

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

- Molecule 27 is a protein called 60S ribosomal protein L24.

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

- Molecule 28 is a protein called 60S ribosomal protein L23a.

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

- Molecule 29 is a protein called 60S ribosomal protein L26.

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

- Molecule 30 is a protein called 60S ribosomal protein L27.

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

- Molecule 31 is a protein called 60S ribosomal protein L27a.

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

- Molecule 32 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Ab	97	792	492	175	122	3	0	0

- Molecule 33 is a protein called 60S ribosomal protein L30.

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

- Molecule 34 is a protein called 60S ribosomal protein L31.

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

- Molecule 35 is a protein called 60S ribosomal protein L32.

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

- Molecule 36 is a protein called 60S ribosomal protein L35a.

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

- Molecule 37 is a protein called 60S ribosomal protein L34.

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

- Molecule 38 is a protein called 60S ribosomal protein L35.

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

- Molecule 39 is a protein called 60S ribosomal protein L36.

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

- Molecule 40 is a protein called 60S ribosomal protein L37.

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

- Molecule 41 is a protein called 60S ribosomal protein L38.

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

- Molecule 42 is a protein called 60S ribosomal protein L39.

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

- Molecule 43 is a protein called 60S ribosomal protein L40.

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

- Molecule 44 is a protein called 60S ribosomal protein L41.

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

- Molecule 45 is a protein called 60S ribosomal protein L36a.

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

- Molecule 46 is a protein called 60S ribosomal protein L37a.

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

- Molecule 47 is a protein called 60S ribosomal protein L28.

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

- Molecule 48 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
48	A2	3643	78102	34781	14290	25388	3643	0	0

- Molecule 49 is a RNA chain called 18S ribosomal RNA.

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

- Molecule 50 is a protein called 40S ribosomal protein S3.

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

- Molecule 51 is a protein called 40S ribosomal protein S4, Y isoform 1.

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

- Molecule 52 is a protein called 40S ribosomal protein S5.

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

- Molecule 53 is a protein called 40S ribosomal protein S6.

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

- Molecule 54 is a protein called 40S ribosomal protein S7.

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

- Molecule 55 is a protein called 40S ribosomal protein S8.

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

- Molecule 56 is a protein called 40S ribosomal protein S9.

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

- Molecule 57 is a protein called 40S ribosomal protein S10.

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

- Molecule 58 is a protein called 40S ribosomal protein S11.

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

- Molecule 59 is a protein called 40S ribosomal protein S12.

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

- Molecule 60 is a protein called 40S ribosomal protein S13.

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

- Molecule 61 is a protein called 40S ribosomal protein S14.

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

- Molecule 62 is a protein called 40S ribosomal protein S15.

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

- Molecule 63 is a protein called 40S ribosomal protein S16.

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

- Molecule 64 is a protein called 40S ribosomal protein S17.

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

- Molecule 65 is a protein called 40S ribosomal protein S18.

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

- Molecule 66 is a protein called 40S ribosomal protein S19.

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

- Molecule 67 is a protein called 40S ribosomal protein S20.

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

- Molecule 68 is a protein called 40S ribosomal protein S21.

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

- Molecule 69 is a protein called 40S ribosomal protein S15a.

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

- Molecule 70 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	BX	139	1080	682	214	181	3	0	0

- Molecule 71 is a protein called 40S ribosomal protein S24.

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

- Molecule 72 is a protein called 40S ribosomal protein S25.

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

- Molecule 73 is a protein called 40S ribosomal protein S26.

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

- Molecule 74 is a protein called 40S ribosomal protein S27.

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

- Molecule 75 is a protein called 40S ribosomal protein S28.

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

- Molecule 76 is a protein called 40S ribosomal protein S29.

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

- Molecule 77 is a protein called 40S ribosomal protein S30.

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

- Molecule 78 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 79 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 80 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
80	Bv	76	1623	723	290	534	76	0	0

- Molecule 81 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
81	Bx	16	320	144	32	128	16	0	0

- Molecule 82 is a protein called Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
82	A	26	128	76	26	26	0	0

- Molecule 83 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
83	AA	1	1	1	0
83	AB	2	2	2	0
83	BC	1	1	1	0

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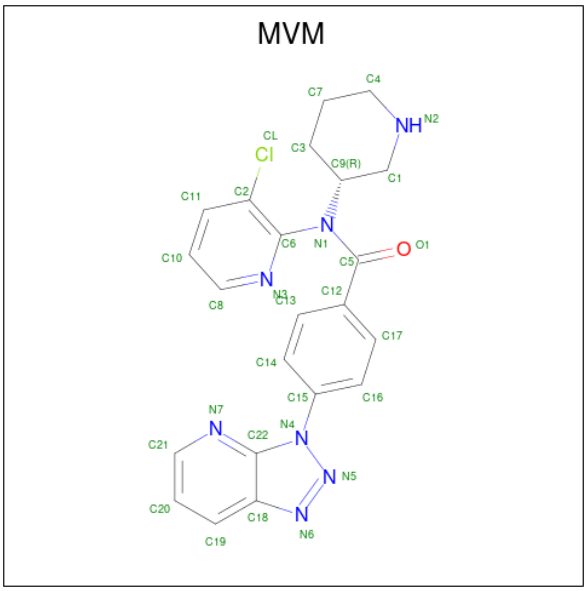
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
83	A3	8	8	8	0
83	A4	9	9	9	0
83	AN	1	1	1	0
83	AP	2	2	2	0
83	Aa	2	2	2	0
83	Ae	1	1	1	0
83	Aj	1	1	1	0
83	Al	1	1	1	0
83	An	1	1	1	0
83	A2	220	220	220	0
83	B1	73	73	73	0
83	BI	1	1	1	0
83	Bv	2	2	2	0

- Molecule 84 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 85 is N-(3-chloropyridin-2-yl)-N-[(3R)-piperidin-3-yl]-4-(3H-[1,2,3]triazolo[4,5-b]pyridin-3-yl)benzamide (three-letter code: MVM) (formula: $C_{22}H_{20}ClN_7O$).



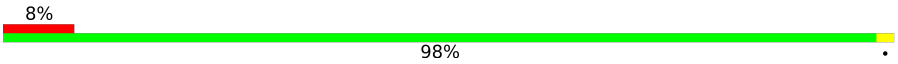
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Cl	N	O	
85	A	1	31	22	1	7	1	0

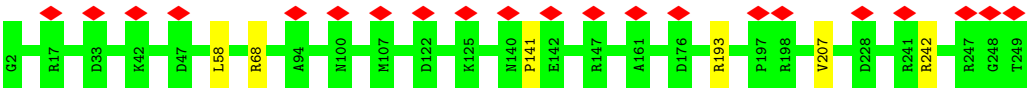
3 Residue-property plots (i)

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: 60S ribosomal protein L8

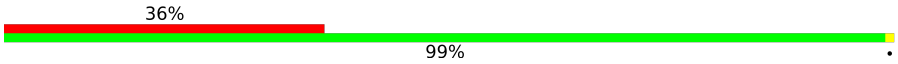
Chain AA:

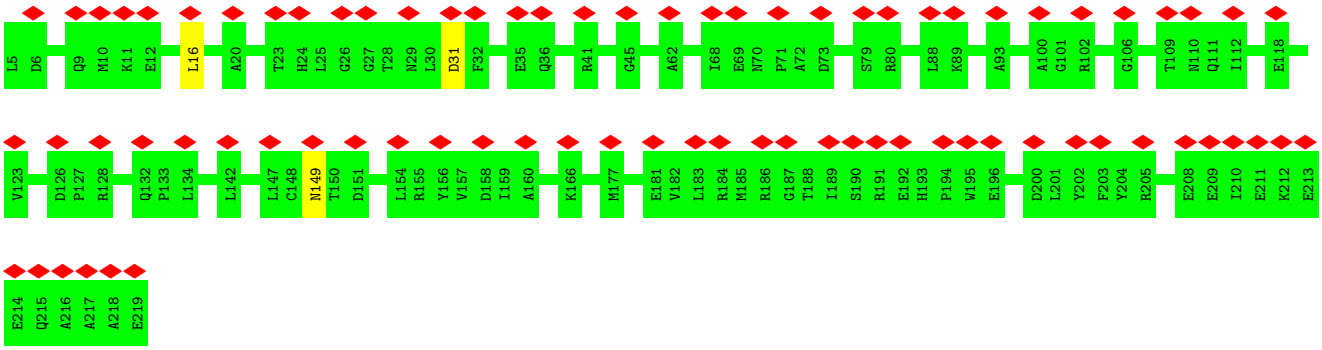




- Molecule 2: 40S ribosomal protein SA

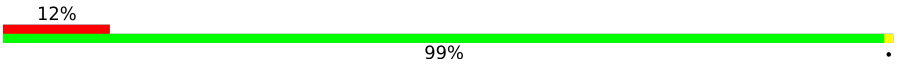
Chain BA:

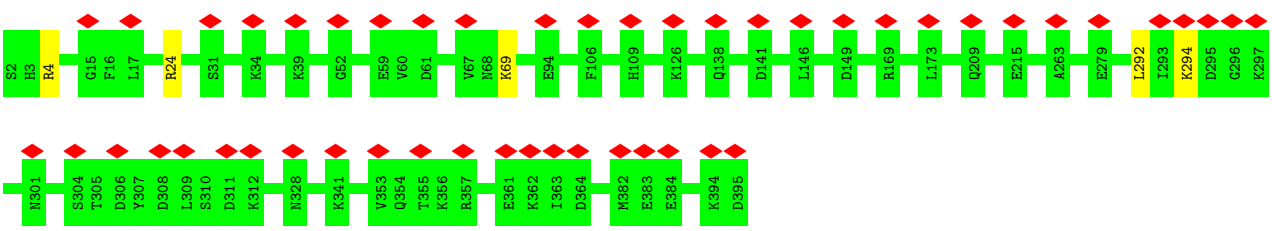




- Molecule 3: 60S ribosomal protein L3

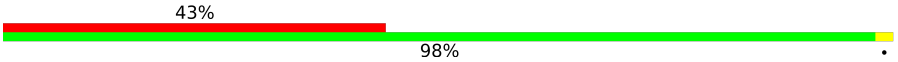
Chain AB:

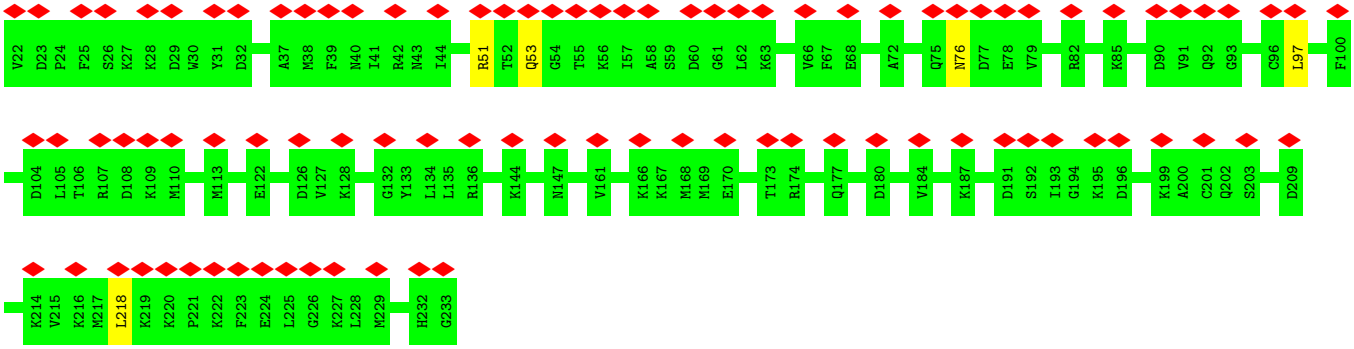




- Molecule 4: 40S ribosomal protein S3a

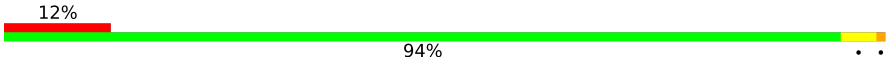
Chain BB:

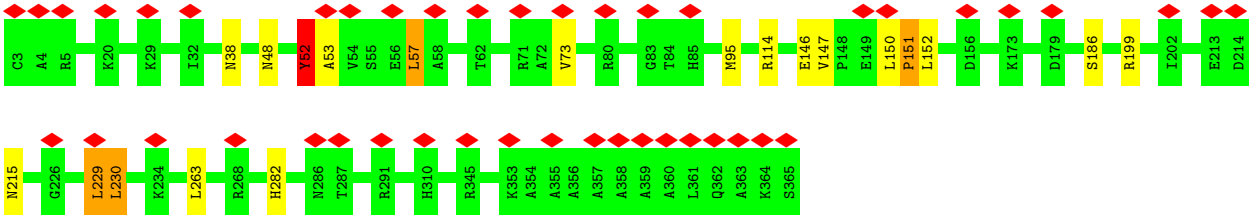




- Molecule 5: 60S ribosomal protein L4

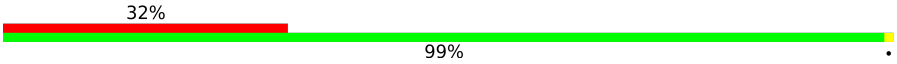
Chain AC:

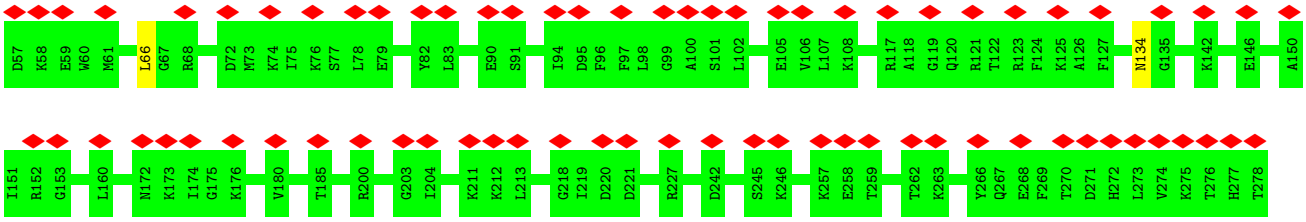




- Molecule 6: 40S ribosomal protein S2

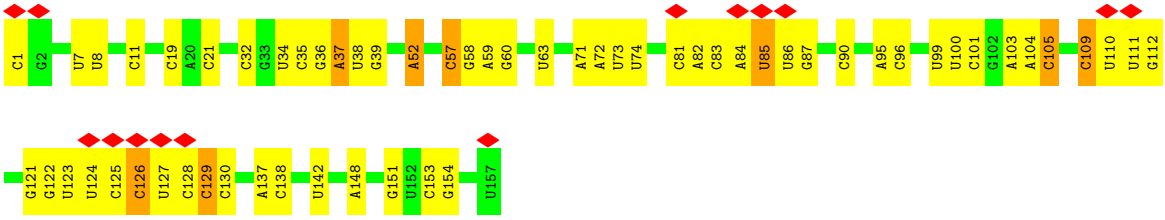
Chain BC:





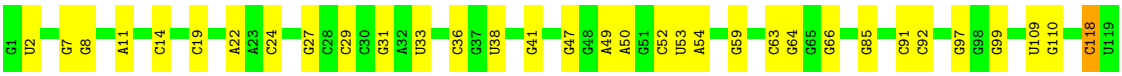
- Molecule 7: 5.8S ribosomal RNA

Chain A3:



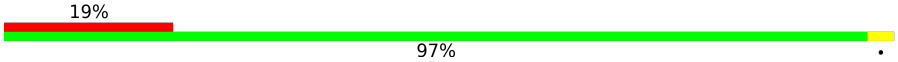
- Molecule 8: 5S ribosomal RNA

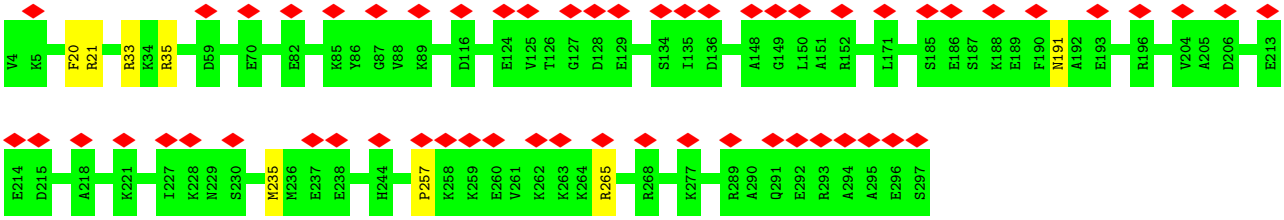
Chain A4:



• Molecule 9: 60S ribosomal protein L5

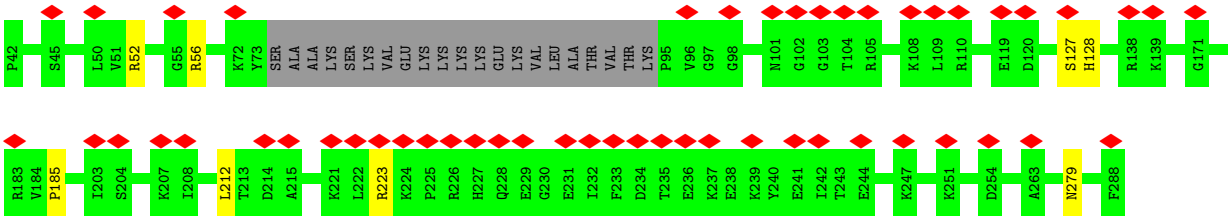
Chain AD:





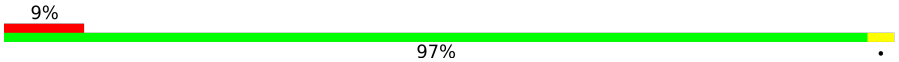
• Molecule 10: 60S ribosomal protein L6

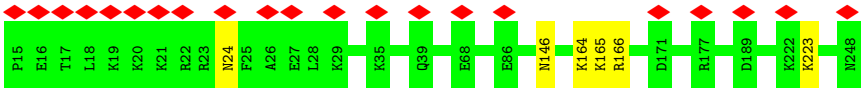
Chain AE:



• Molecule 11: 60S ribosomal protein L7

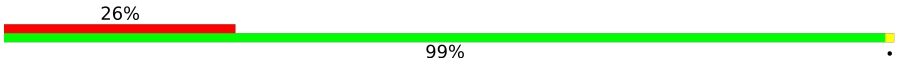
Chain AF:

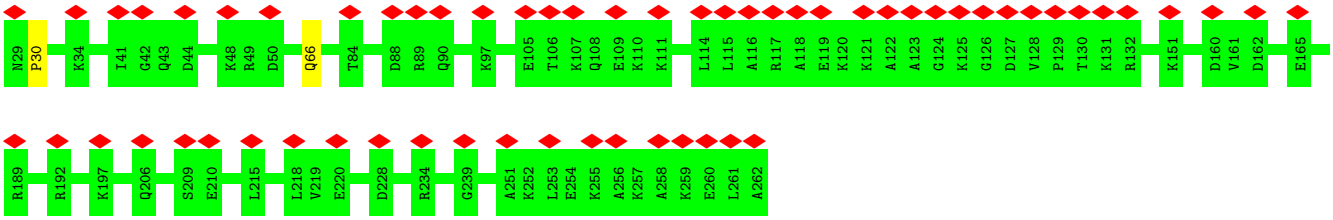




• Molecule 12: 60S ribosomal protein L7a

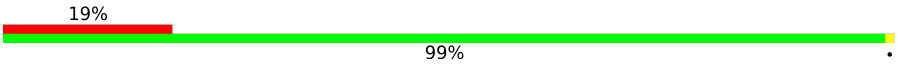
Chain AG:

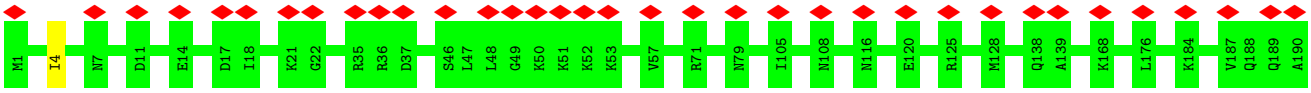




• Molecule 13: 60S ribosomal protein L9

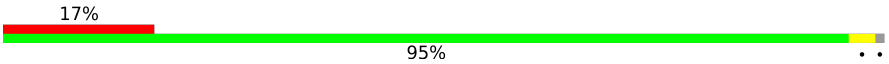
Chain AH:

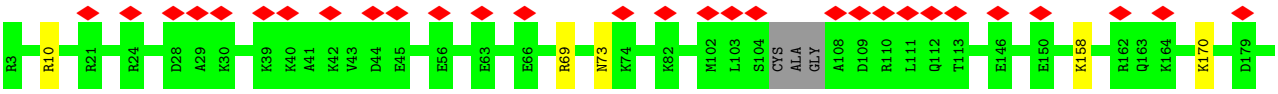


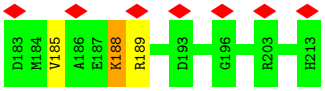


• Molecule 14: 60S ribosomal protein L10

Chain AI:

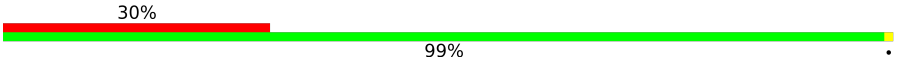


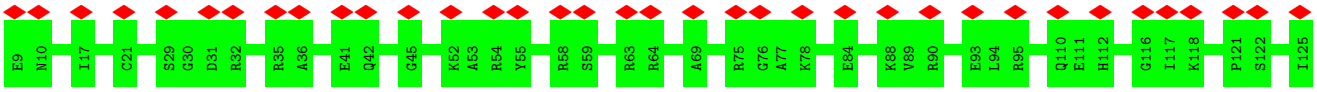


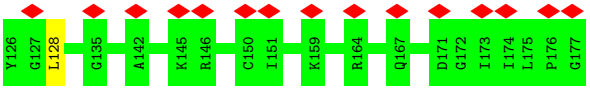


• Molecule 15: 60S ribosomal protein L11

Chain AJ:

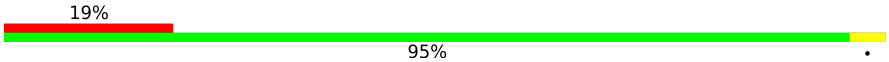


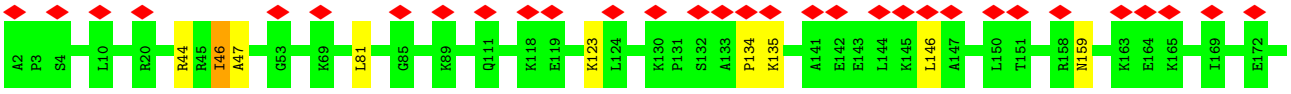


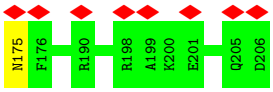


• Molecule 16: 60S ribosomal protein L13

Chain AL:

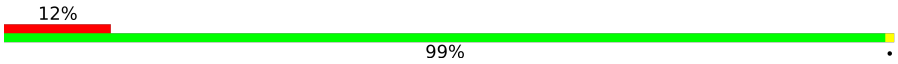


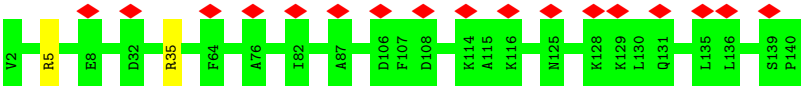




• Molecule 17: 60S ribosomal protein L14

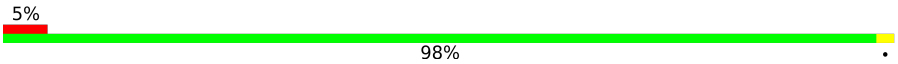
Chain AM:

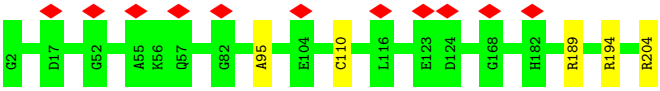




• Molecule 18: 60S ribosomal protein L15

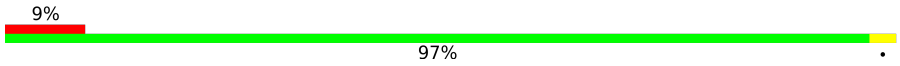
Chain AN:

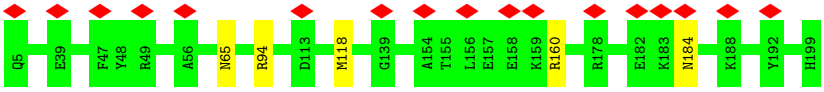




• Molecule 19: 60S ribosomal protein L13a

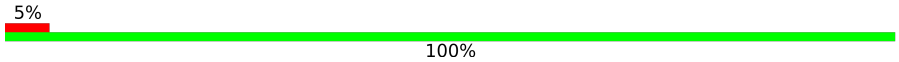
Chain AO:

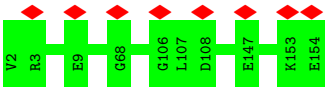




• Molecule 20: 60S ribosomal protein L17

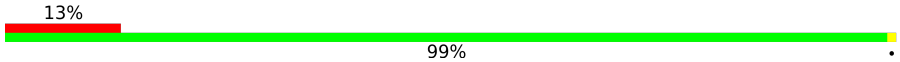
Chain AP:

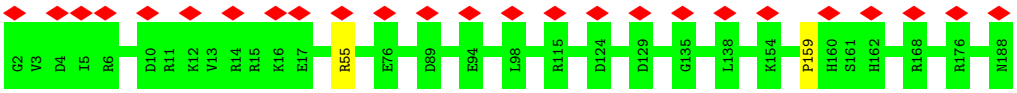




• Molecule 21: 60S ribosomal protein L18

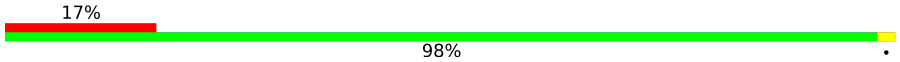
Chain AQ:

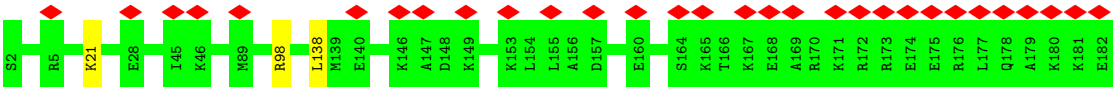




• Molecule 22: 60S ribosomal protein L19

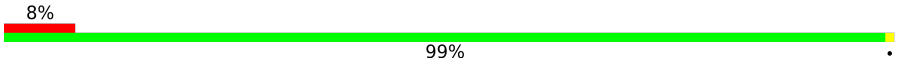
Chain AR:

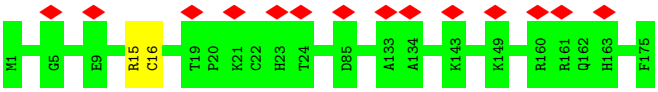




• Molecule 23: 60S ribosomal protein L18a

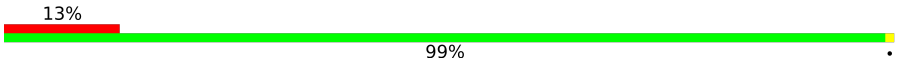
Chain AS:

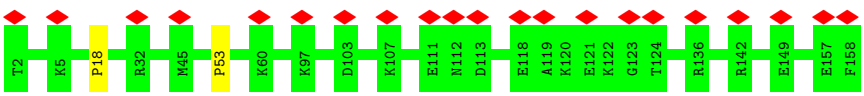




• Molecule 24: 60S ribosomal protein L21

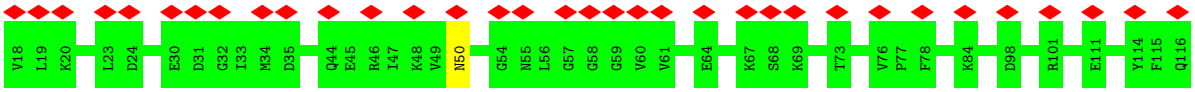
Chain AT:





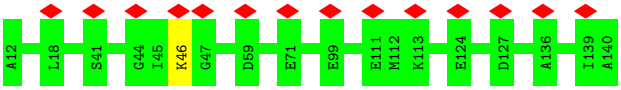
• Molecule 25: 60S ribosomal protein L22

Chain AU: 34% 99%



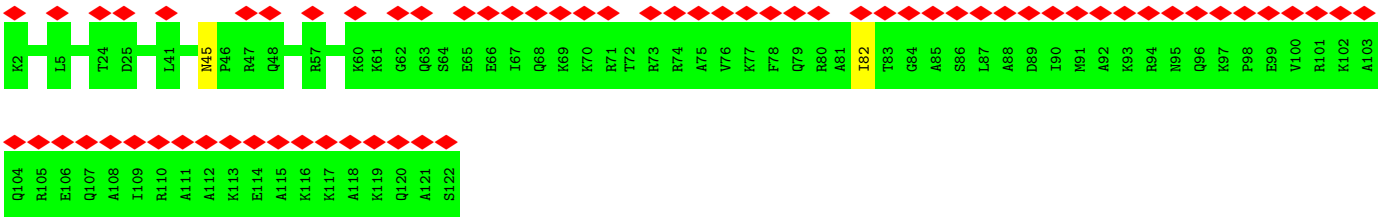
• Molecule 26: 60S ribosomal protein L23

Chain AV: 11% 99%



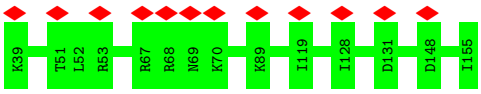
• Molecule 27: 60S ribosomal protein L24

Chain AW: 55% 98%



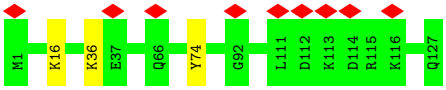
• Molecule 28: 60S ribosomal protein L23a

Chain AX: 10% 100%



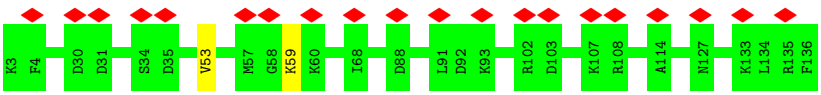
• Molecule 29: 60S ribosomal protein L26

Chain AY: 7% 98%



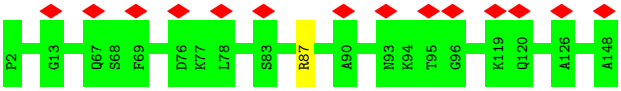
• Molecule 30: 60S ribosomal protein L27

Chain AZ: 15% 99%



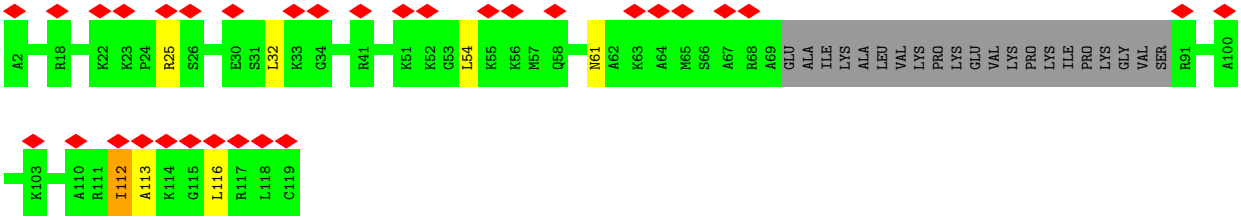
• Molecule 31: 60S ribosomal protein L27a

Chain Aa: 10% 99%



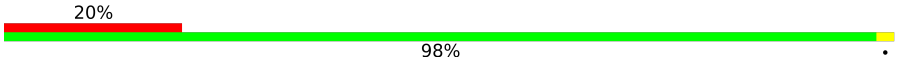
- Molecule 32: 60S ribosomal protein L29

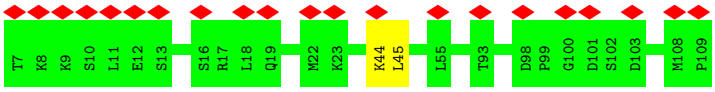
Chain Ab:



- Molecule 33: 60S ribosomal protein L30

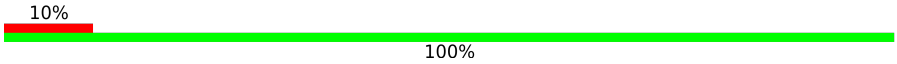
Chain Ac:

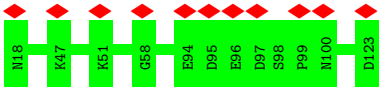




- Molecule 34: 60S ribosomal protein L31

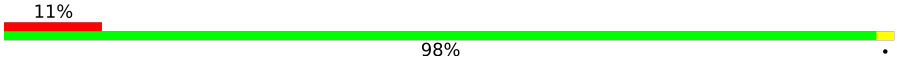
Chain Ad:

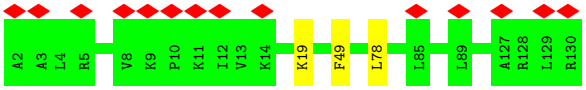




- Molecule 35: 60S ribosomal protein L32

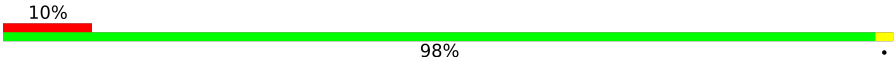
Chain Ae:

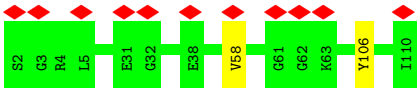




- Molecule 36: 60S ribosomal protein L35a

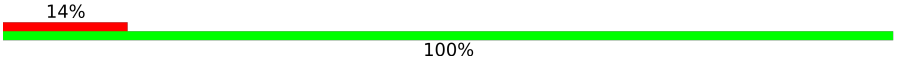
Chain Af:

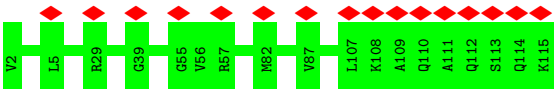




- Molecule 37: 60S ribosomal protein L34

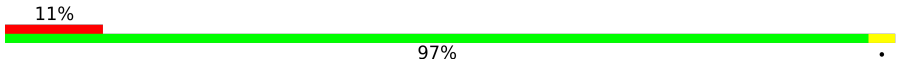
Chain Ag:

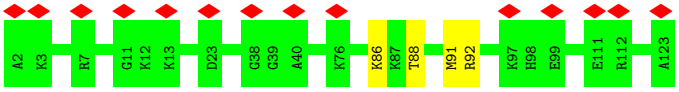




• Molecule 38: 60S ribosomal protein L35

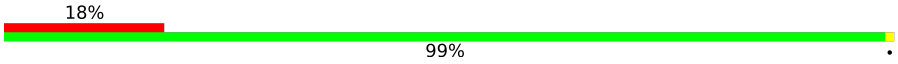
Chain Ah:

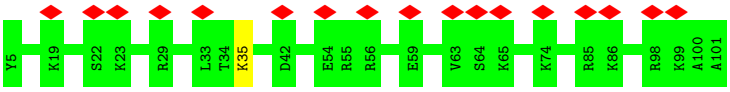




• Molecule 39: 60S ribosomal protein L36

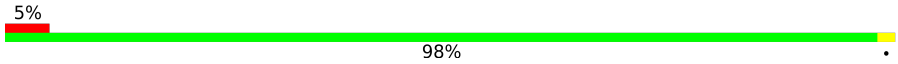
Chain Ai:

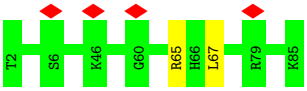




• Molecule 40: 60S ribosomal protein L37

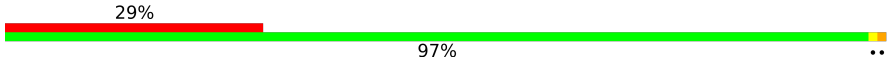
Chain Aj:

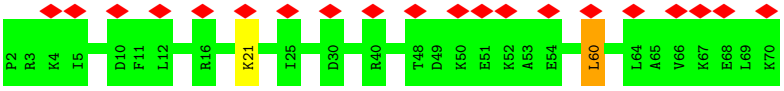




• Molecule 41: 60S ribosomal protein L38

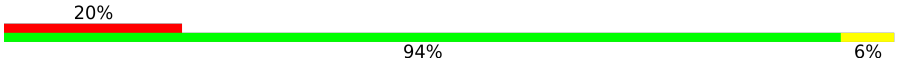
Chain Ak:

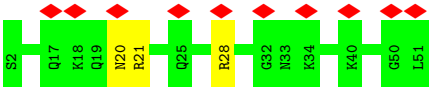




• Molecule 42: 60S ribosomal protein L39

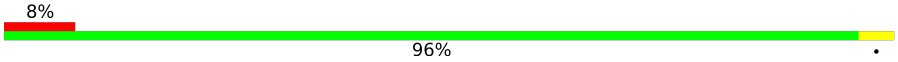
Chain Al:

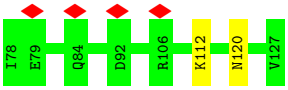




• Molecule 43: 60S ribosomal protein L40

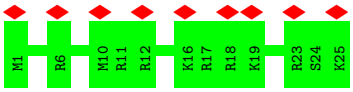
Chain Am:





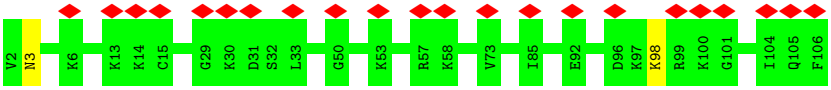
• Molecule 44: 60S ribosomal protein L41

Chain An: 36% 100%



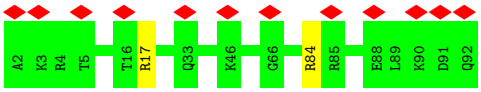
• Molecule 45: 60S ribosomal protein L36a

Chain Ao: 21% 98%



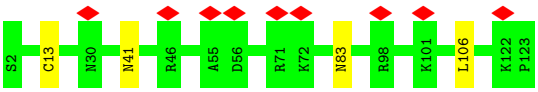
• Molecule 46: 60S ribosomal protein L37a

Chain Ap: 13% 98%



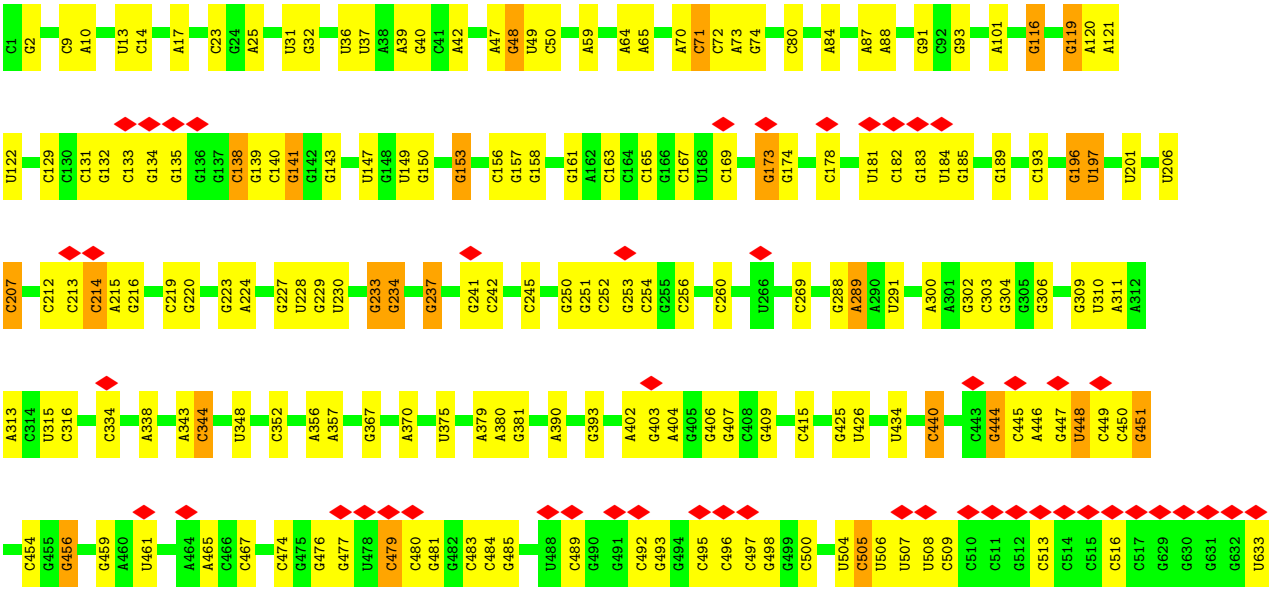
• Molecule 47: 60S ribosomal protein L28

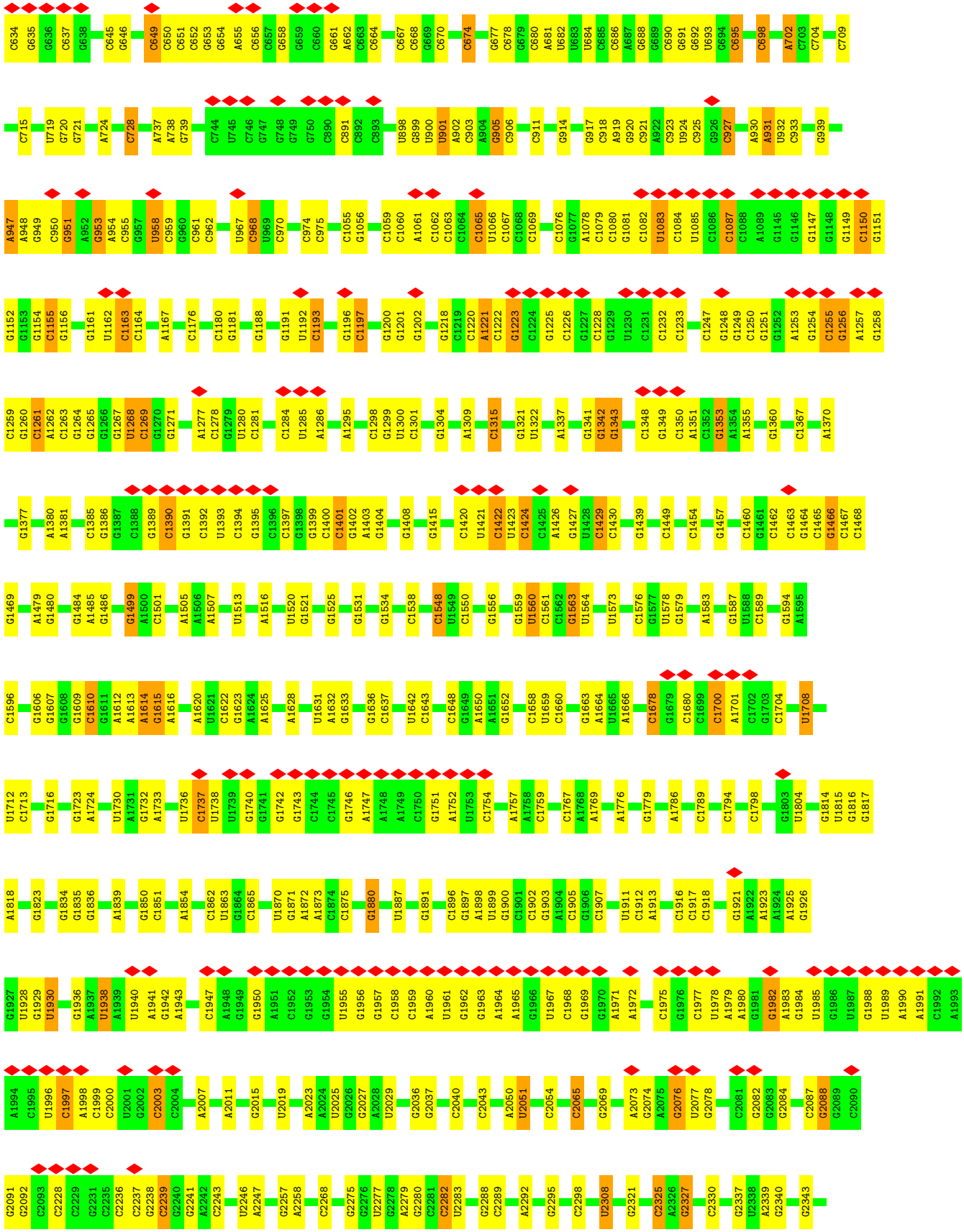
Chain At: 7% 97%



• Molecule 48: 28S ribosomal RNA

Chain A2: 9% 66% 30%




C634 G635 G636 C637 G638 C645 G646 C649 C650 C651 C652 G653 G654 A655 C656 C657 G658 G659 C660 G661 A662 C663 C664 C667 C668 G669 C670 C674 G677 C678 G679 C680 A681 U682 U683 U684 C685 C686 A687 G688 G689 C690 G691 G692 U693 G694 C695 C698 A702 C703 C704 C709
C715 U719 G720 G721 A724 C728 A737 A738 G739 C744 U745 C746 G747 G748 G749 G750 C890 C891 C892 C893 U898 G899 U900 U901 A902 C903 A904 G905 C906 C911 G914 G917 C918 A919 G920 C921 A922 C923 U924 C925 G926 C927 A930 A931 U932 C933 G939
A947 A948 G949 C950 G951 A952 G953 A954 C955 G957 U958 C959 G960 C961 C962 U967 C968 U969 C970 C974 C975 C1055 G1056 C1059 C1060 A1061 C1062 C1063 C1064 C1065 U1066 C1067 C1068 C1069 C1076 G1077 A1078 C1079 C1080 G1081 C1082 U1083 C1084 U1085 C1086 C1087 C1088 A1089 G1145 G1146 G1147 G1148 G1149 C1150 G1151
G1152 G1153 G1154 C1155 G1156 G1161 U1162 C1163 C1164 A1167 C1176 C1180 G1181 G1188 G1191 U1192 C1193 G1196 C1197 G1200 G1201 G1202 G1218 C1219 C1220 A1221 C1222 G1223 C1224 G1225 C1226 G1227 C1228 G1229 U1230 C1231 C1232 C1233 C1247 G1248 G1249 C1250 G1251 G1252 A1253 G1254 C1255 G1256 A1257 G1258
C1259 G1260 C1261 A1262 C1263 G1264 G1265 G1266 G1267 U1268 C1269 G1270 G1271 A1277 C1278 G1279 U1280 C1281 C1284 U1285 A1286 A1295 C1298 G1299 U1300 C1301 G1304 A1309 C1315 G1321 U1322 A1337 G1341 G1342 G1343 C1348 G1349 C1350 A1351 C1352 G1353 A1354 A1355 G1360 C1367 A1370
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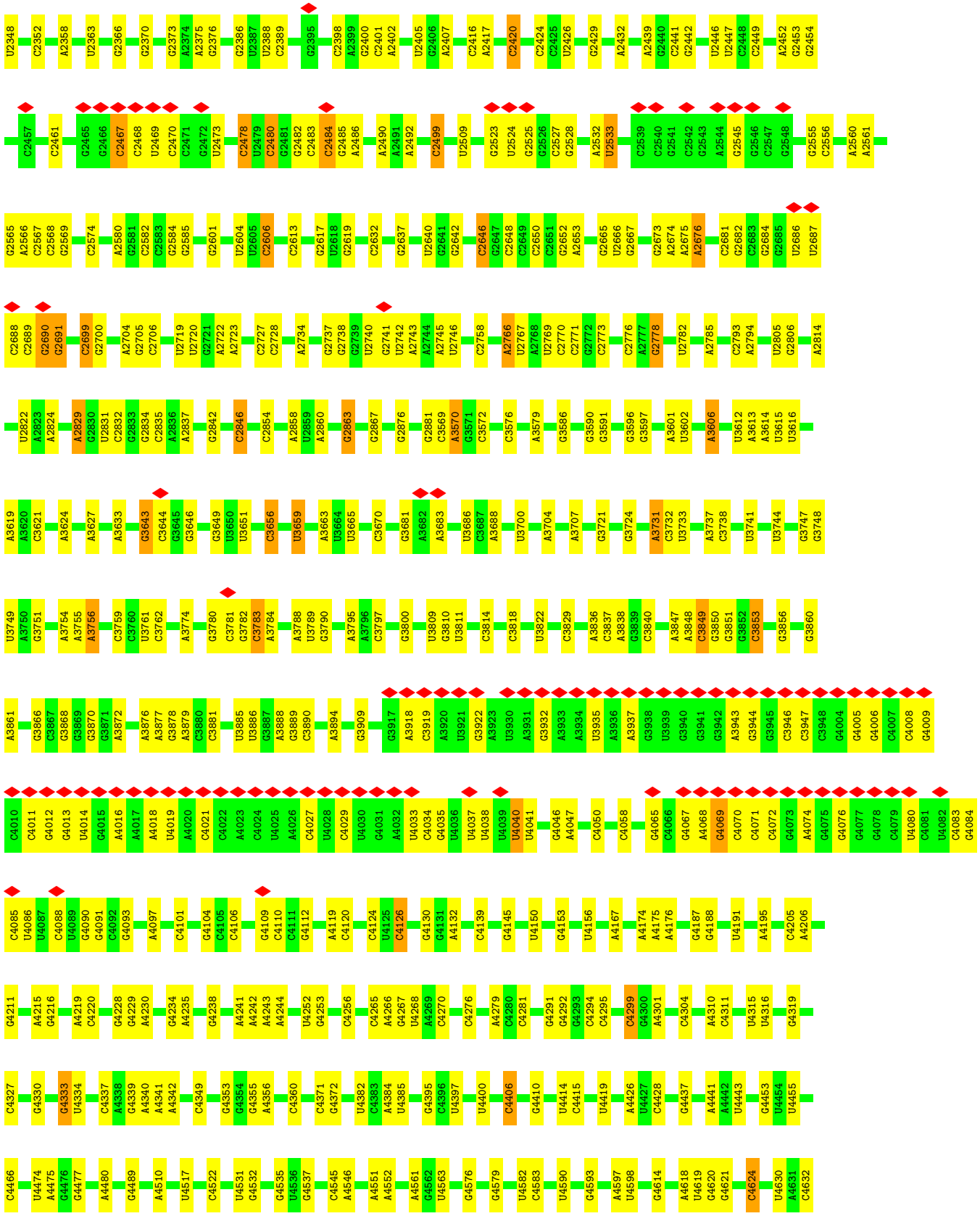
C1596 G1606 G1607 G1608 G1609 C1610 G1611 A1612 A1613 A1614 G1615 A1616 A1620 U1621 C1622 G1623 A1624 A1625 A1628 U1631 A1632 G1633 G1636 C1637 U1642 C1643 C1648 G1649 A1650 A1651 G1652 C1658 U1659 C1660 G1663 A1664 U1665 A1666 C1678 G1679 C1680 C1699 C1700 A1701 C1702 G1703 C1704 U1708
U1712 C1713 G1716 G1723 A1724 U1730 A1731 G1732 A1733 U1736 C1737 U1738 U1739 G1740 G1741 G1742 G1743 C1744 C1745 G1746 A1747 A1748 A1749 C1750 G1751 A1752 U1753 C1754 A1757 A1758 C1759 C1767 A1768 A1769 A1776 G1779 A1786 C1789 C1794 C1798 G1803 U1804 G1814 U1815 G1816 G1817
A1818 G1823 G1834 G1835 G1836 A1839 G1850 C1851 A1854 C1862 U1863 G1864 C1865 U1870 G1871 A1872 A1873 C1874 C1875 G1880 U1887 G1891 C1896 G1897 A1898 U1899 G1900 C1901 C1902 G1903 A1904 C1905 G1906 C1907 U1911 C1912 A1913 C1916 C1917 C1918 G1921 A1922 A1923 A1924 A1925 G1926
G1927 U1928 G1929 U1930 G1936 A1937 U1938 A1939 U1940 A1941 G1942 A1943 C1947 A1948 G1949 G1950 A1951 C1952 G1953 G1954 U1955 G1956 G1957 C1958 C1959 A1960 U1961 G1962 G1963 A1964 A1965 G1966 U1967 C1968 G1969 G1970 A1971 A1972 C1975 G1976 C1977 U1978 A1979 A1980 G1981 G1982 A1983 G1984 U1985 G1986 U1987 G1988 U1989 A1990 A1991 C1992 A1993
A1994 C1995 U1996 C1997 A1998 C1999 C2000 U2001 G2002 C2003 C2004 A2007 A2011 G2015 U2019 A2023 A2024 U2025 G2026 G2027 A2028 U2029 G2036 G2037 C2040 C2043 A2050 U2051 C2054 C2065 G2069 A2073 G2074 A2075 G2076 U2077 G2078 C2081 G2082 G2083 G2084 C2087 G2088 G2089 C2090
G2091 G2092 C2093 C2228 C2229 G2231 C2235 C2236 C2237 G2238 C2239 G2240 G2241 A2242 C2243 U2246 A2247 G2257 A2258 C2268 G2275 G2276 U2277 G2278 A2279 G2280 C2281 C2282 U2283 G2288 C2289 A2292 G2295 C2298 U2308 G2321 C2325 A2326 G2327 C2330 G2337 U2338 A2339 G2340 G2343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C2457 C2461 G2465 G2466 C2467 C2468 U2469 C2470 C2471 G2472 U2473 C2478 U2479 C2480 G2481 G2482 C2483 C2484 G2485 A2486 A2490 A2491 A2492 C2499 U2509 G2523 U2524 G2525 G2526 C2527 G2528 A2532 U2533 C2539 C2540 G2541 C2542 G2543 A2544 G2545 G2546 C2547 G2548 G2555 C2556 A2560 A2561
G2565 A2566 C2567 C2568 G2569 C2574 A2580 G2581 C2582 C2583 G2584 G2585 G2601 U2604 U2605 C2606 C2613 G2617 U2618 G2619 C2632 G2637 U2640 C2641 G2642 C2646 G2647 C2648 C2649 C2650 C2651 G2652 A2653 G2665 U2666 G2667 G2673 A2674 A2675 A2676 C2681 G2682 C2683 G2684 G2685 U2686 U2687
C2688 C2689 G2690 G2691 C2699 G2700 A2704 G2705 C2706 U2719 U2720 G2721 A2722 A2723 C2727 C2728 A2734 G2737 G2738 G2739 U2740 G2741 U2742 A2743 A2744 A2745 U2746 C2758 A2766 U2767 A2768 U2769 C2770 C2771 G2772 C2773 C2776 A2777 G2778 U2782 A2785 C2793 A2794 U2805 G2806 A2814
U2822 A2823 A2824 A2829 G2830 U2831 C2832 G2833 G2834 C2835 A2836 A2837 G2842 C2846 C2854 A2858 U2859 A2860 G2863 G2867 G2876 G2881 C3569 A3570 G3571 C3572 C3576 A3579 G3586 G3590 G3591 G3596 G3597 A3601 U3602 A3606 U3612 A3613 A3614 U3615 U3616
A3619 A3620 C3621 A3624 A3627 A3633 G3643 C3644 G3645 G3646 G3649 U3650 U3651 C3656 U3659 A3663 U3664 U3665 C3670 G3681 A3682 A3683 U3686 C3687 A3688 U3700 A3704 A3707 G3721 G3724 A3731 C3732 U3733 A3737 C3738 U3741 U3744 G3747 G3748
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A3861 G3866 C3867 G3868 G3869 G3870 G3871 A3872 A3876 A3877 G3878 A3879 C3880 C3881 U3885 U3886 G3887 A3888 G3889 C3890 A3894 G3909 G3917 A3918 C3919 A3920 U3921 G3922 A3923 U3930 A3931 G3932 A3933 A3934 U3935 A3936 A3937 G3938 U3939 G3940 G3941 G3942 A3943 G3944 G3945 C3946 C3947 C3948 G4004 G4005 G4006 C4007 C4008 G4009
C4010 C4011 G4012 G4013 U4014 G4015 A4016 A4017 A4018 U4019 A4020 C4021 C4022 A4023 C4024 U4025 A4026 C4027 U4028 C4029 U4030 G4031 A4032 U4033 C4034 G4035 U4036 U4037 U4038 U4039 U4040 U4041 G4046 A4047 C4050 C4058 G4065 C4066 G4067 A4068 G4069 C4070 C4071 C4072 G4073 A4074 G4075 G4076 G4077 G4078 C4079 U4080 C4081 U4082 C4083 G4084
C4085 U4086 U4087 C4088 U4089 G4090 G4091 C4092 G4093 A4097 C4101 G4104 C4105 C4106 G4109 C4110 C4111 G4112 A4119 C4120 C4124 U4125 C4126 G4130 G4131 A4132 C4139 G4145 U4150 G4153 U4156 A4167 A4174 A4175 A4176 G4187 G4188 U4191 A4195 C4205 A4206
G4211 A4215 G4216 A4219 C4220 G4228 G4229 A4230 G4234 A4235 G4238 A4241 A4242 A4243 A4244 U4252 G4253 C4256 C4265 A4266 G4267 U4268 A4269 C4270 C4276 A4279 C4280 C4281 G4291 G4292 G4293 C4294 C4295 C4299 G4300 A4301 C4304 A4310 C4311 U4315 U4316 G4319
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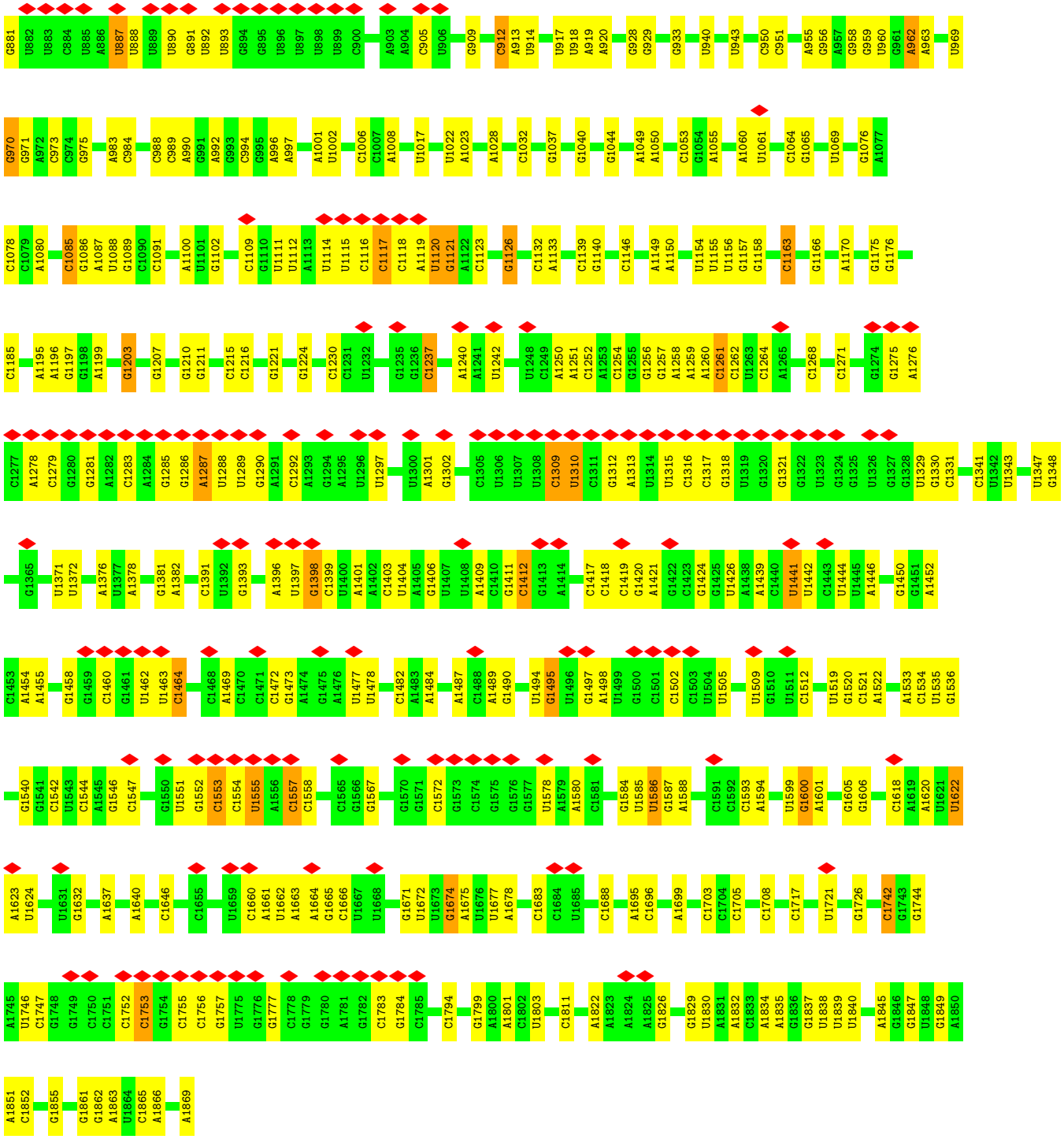
C4466 U4474 A4475 G4476 G4477 A4480 G4489 A4510 U4517 C4522 U4531 G4532 G4535 U4536 G4537 C4545 A4546 A4551 A4552 A4561 G4562 U4563 G4576 G4579 U4582 C4583 U4590 G4593 A4597 U4598 G4614 A4618 U4619 G4620 G4621 C4624 U4630 A4631 C4632

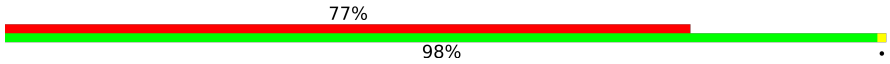
- Molecule 49: 18S ribosomal RNA

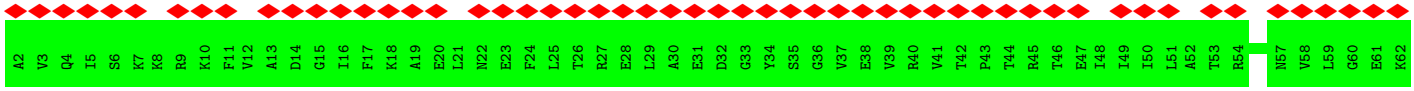
Chain B1:

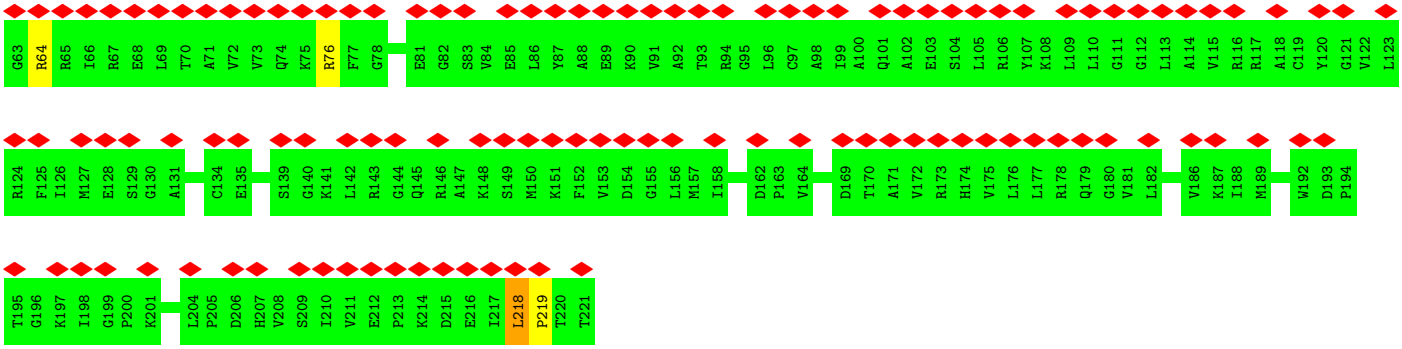


- Molecule 50: 40S ribosomal protein S3

Chain BD:

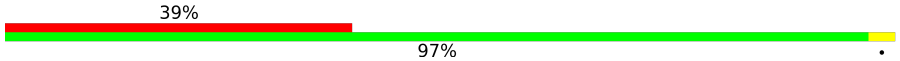


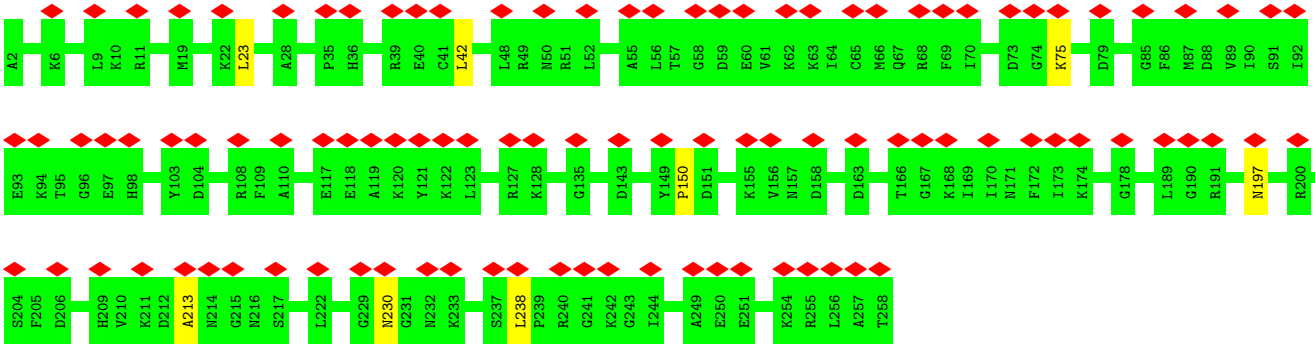




- Molecule 51: 40S ribosomal protein S4, Y isoform 1

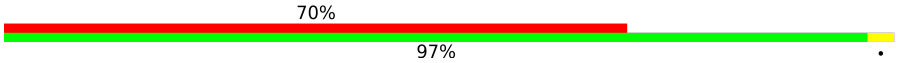
Chain BE:

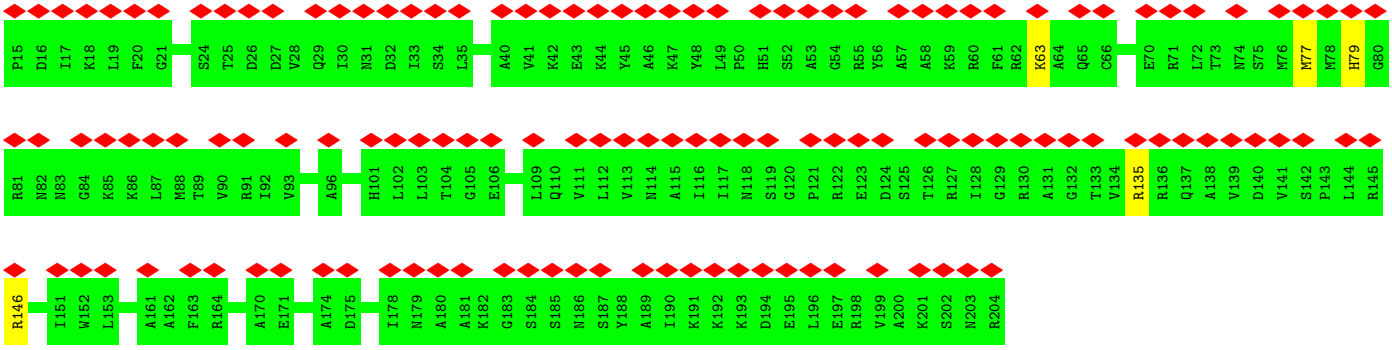




- Molecule 52: 40S ribosomal protein S5

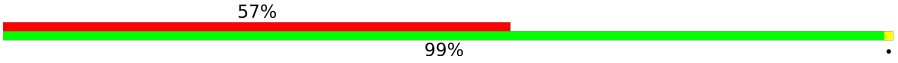
Chain BF:

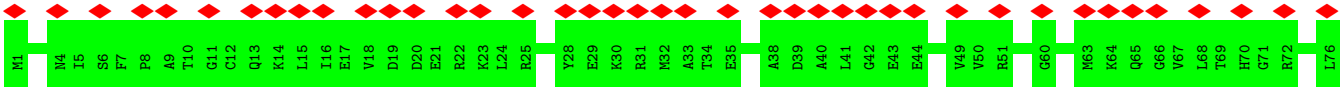


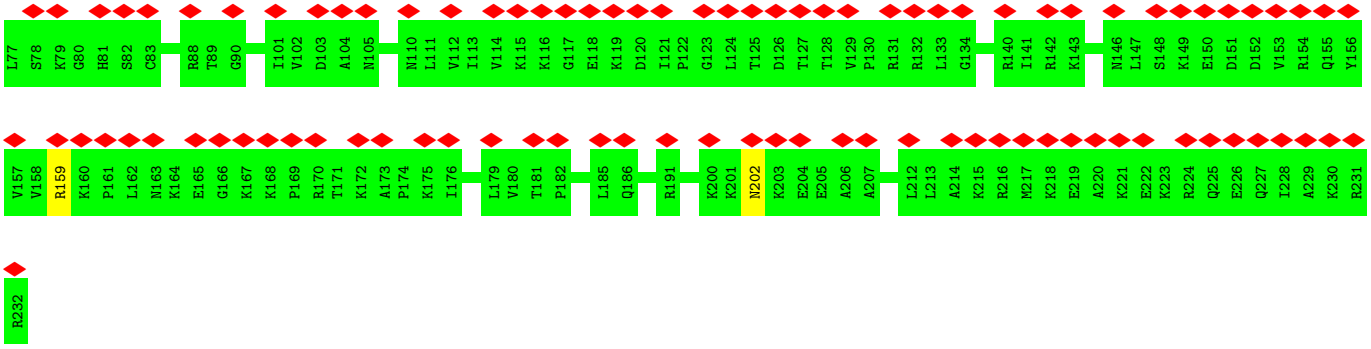


- Molecule 53: 40S ribosomal protein S6

Chain BG:

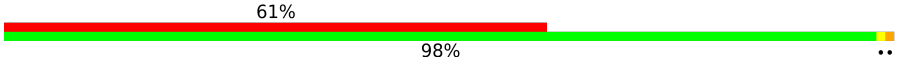






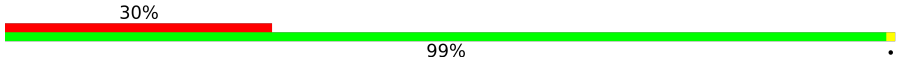
- Molecule 54: 40S ribosomal protein S7

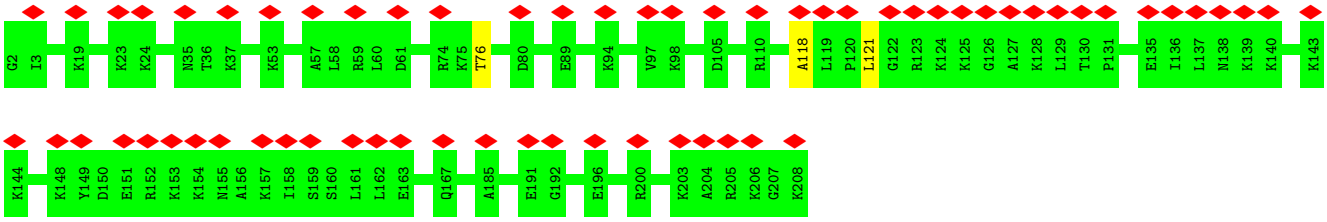
Chain BH:



- Molecule 55: 40S ribosomal protein S8

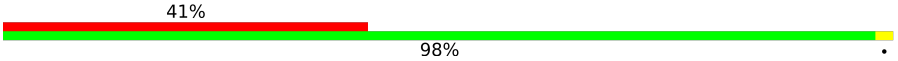
Chain BI:

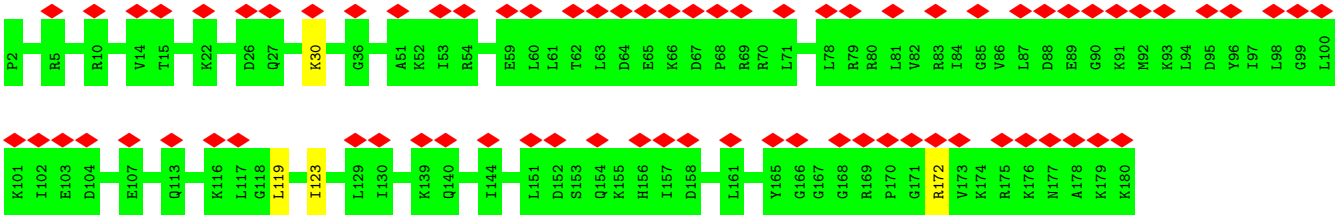




- Molecule 56: 40S ribosomal protein S9

Chain BJ:





- Molecule 57: 40S ribosomal protein S10

Chain BK: 88% 98%

M1 L2 M3 P4 K5 R8 I9 A10 I11 Y12 E13 L14 L15 F16 K17 E18 G19 V20 M21 V22 A23 K24 K25 D26 V27 H28 M29 P30 K31 H32 P33 E34 L35 A36 D37 K38 N39 V40 P41 N42 L43 H44 K47 A48 M49 Q50 S51 L52 K53 S54 R55 G56 Y57 V58 K59 E60 Q61 F62

A63 W64 R65 H66 F67 Y70 L71 T72 N73 E74 G75 I76 Q77 Y78 L79 R80 D81 Y82 L83 H84 L85 P86 P87 E88 I89 V90 P91 A92 T93 L94 R95 R96 S97 R98

- Molecule 58: 40S ribosomal protein S11

Chain BL: 36% 99%

T6 E7 R8 Q13 P14 F17 Q18 N19 K20 K21 R22 V23 L24 L25 G26 E27 T28 G29 K30 E31 K32 L33 P34 N39 L42 K45 E52 K59 R71 I72 L73 S74 G75 K81 D91 R97 K104 L113 R118 D119 V120 Q121 I122 G123 D124

E130 T137 L143 T146 K147 A148 A149 G150 T151 K152 K153 Q154 F155 Q156 K157 F158

- Molecule 59: 40S ribosomal protein S12

Chain BM: 99% 98%

V11 M12 D13 V14 N15 T16 A17 L18 Q19 E20 V21 L22 K23 T24 A25 L26 I27 H28 D29 G30 L31 A32 R33 G34 I35 R36 E37 A38 A39 K40 A41 L42 D43 K44 R45 Q46 A47 H48 L49 C50 V51 L52 A53 S54 N55 C56 D57 E58 P59 M60 Y61 V62 K63 L64 V65 E66 A67 L68 C69 A70

E71 H72 Q73 I74 N75 L76 I77 K78 V79 D80 D81 N82 K83 K84 L85 G86 E87 W88 V89 G90 L91 C92 K93 I94 D95 R96 E97 G98 K99 P100 R101 K102 V103 V104 G105 C106 S107 C108 V109 V110 V111 K112 D113 Y114 G115 K116 E117 S118 Q119 A120 K121 D122 V123 I124 E125 E126 Y127 F128 K129 C130

- Molecule 60: 40S ribosomal protein S13

Chain BN: 37% 99%

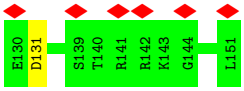
G2 R3 M4 H5 A6 S14 A15 L16 R19 R20 S21 V22 P23 L26 K27 L28 D31 E35 K39 L40 A41 K42 K43 G44 L45 T46 P47 S48 Q49 G59 R64 G68 N69 K70 I74 L75 K76 S77 K78 A81 P82 D83 L84 K93 K100 E103

R104 N105 R106 K107 D108 K109 D110 L117 I118 E119 R127 N138 W139 K140 Y141 E142 S143 S144 T145 A146 V150

- Molecule 61: 40S ribosomal protein S14

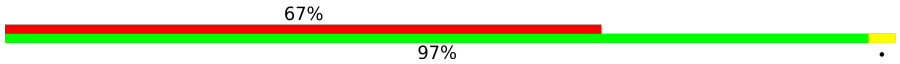
Chain BO: 31% 99%

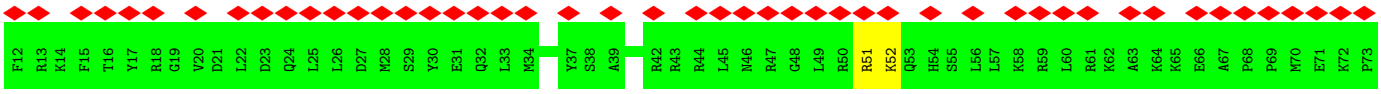
S16 L17 G18 P19 Q20 V21 A22 E23 G24 E25 G29 F34 D39 G59 M60 A64 D65 R66 D67 Y72 M75 L76 A77 A82 Q83 R84 C85 K86 E87 L88 G89 A92 A99 T100 G101 G102 N103 R104 L116 R117 A118 L119 S122 G123 M124 R128 I129

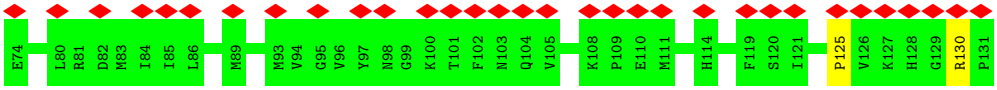


- Molecule 62: 40S ribosomal protein S15

Chain BP:

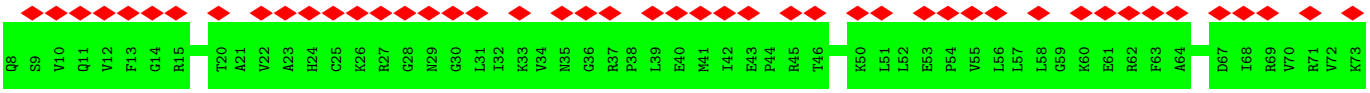


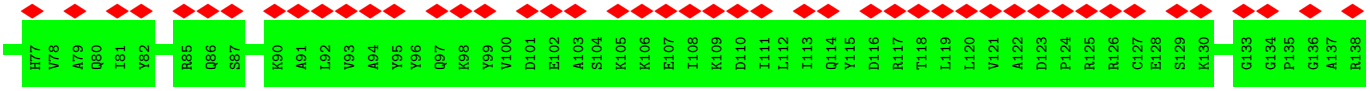




- Molecule 63: 40S ribosomal protein S16

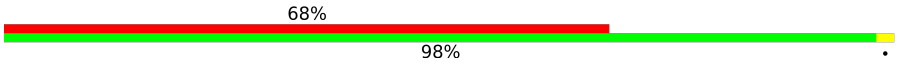
Chain BQ:

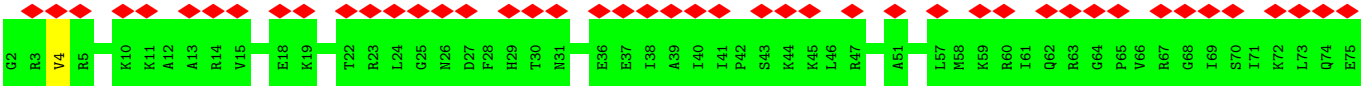


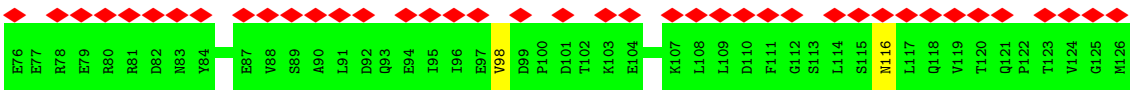


- Molecule 64: 40S ribosomal protein S17

Chain BR:

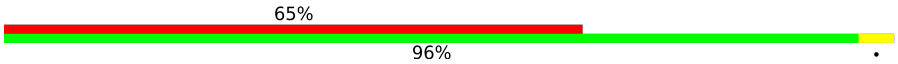


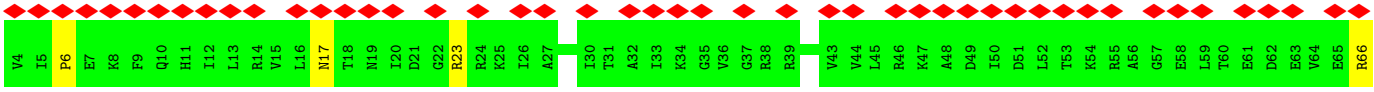


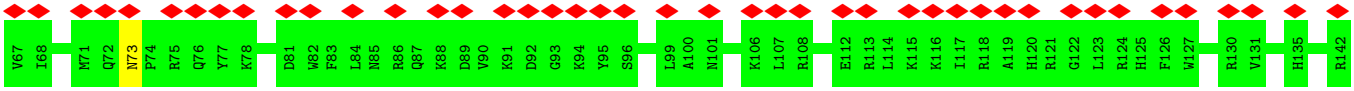


- Molecule 65: 40S ribosomal protein S18

Chain BS:

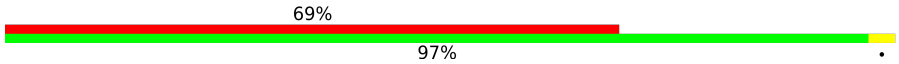


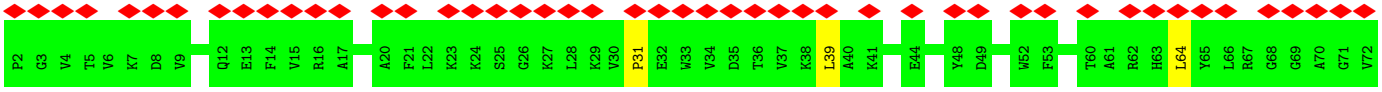


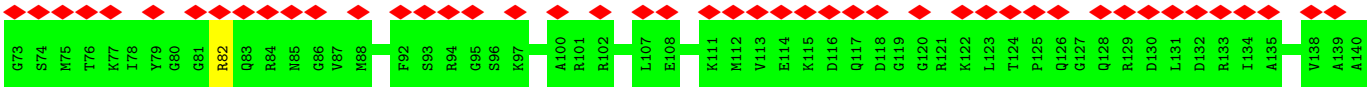


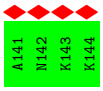
- Molecule 66: 40S ribosomal protein S19

Chain BT:



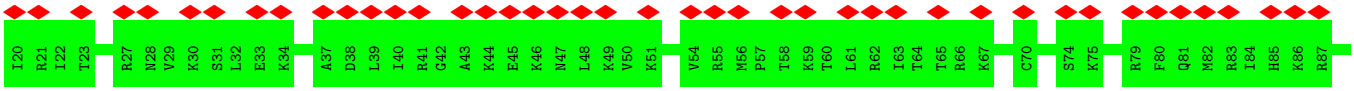


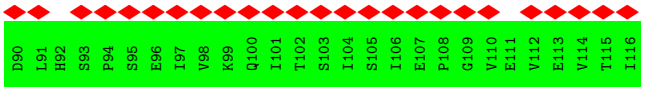




- Molecule 67: 40S ribosomal protein S20

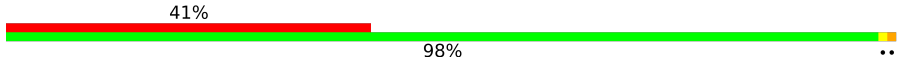
Chain BU:

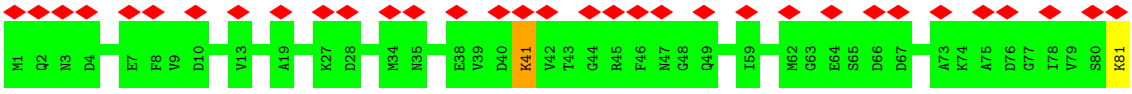




- Molecule 68: 40S ribosomal protein S21

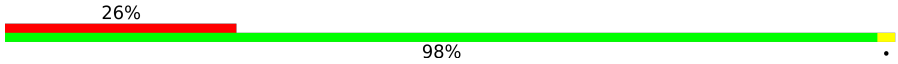
Chain BV:

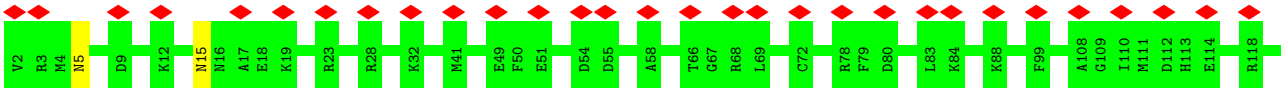


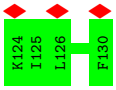


- Molecule 69: 40S ribosomal protein S15a

Chain BW:

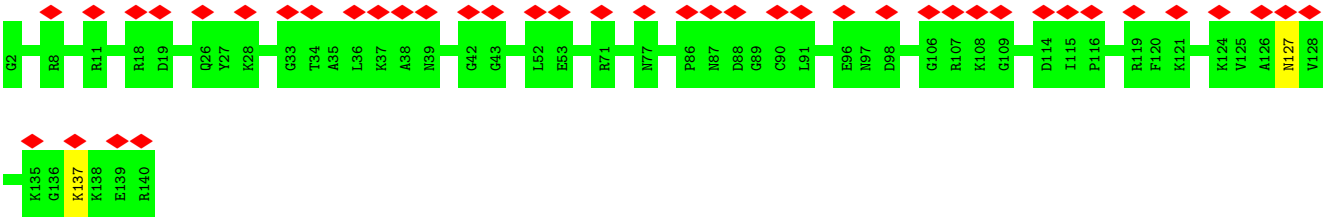






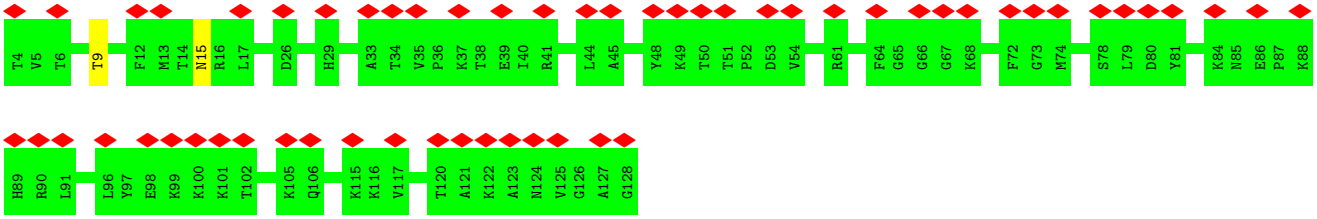
- Molecule 70: 40S ribosomal protein S23

Chain BX: 30% 99%



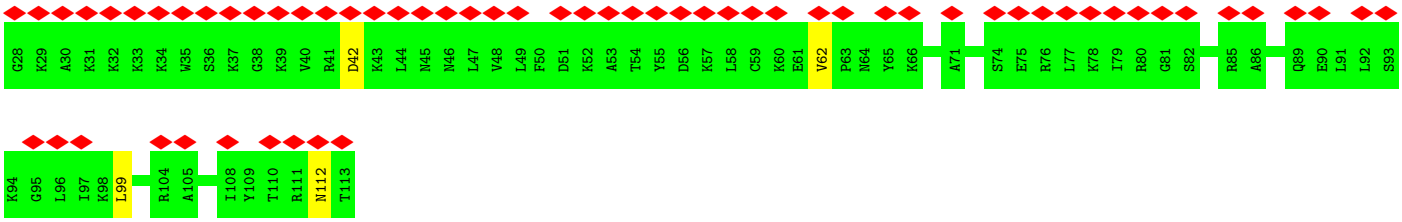
- Molecule 71: 40S ribosomal protein S24

Chain BY: 46% 98%



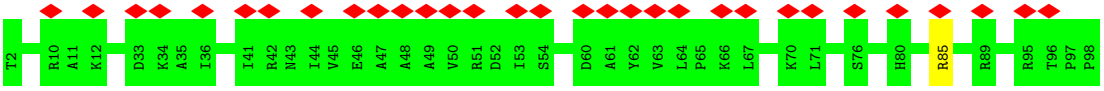
- Molecule 72: 40S ribosomal protein S25

Chain BZ: 72% 95% 5%



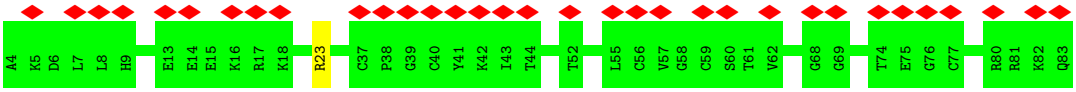
- Molecule 73: 40S ribosomal protein S26

Chain Ba: 32% 99%



- Molecule 74: 40S ribosomal protein S27

Chain Bb: 41% 99%



- Molecule 75: 40S ribosomal protein S28

Chain Bc: 73% 97%

Q7 P8 I9 K10 L11 A12 R13 V14 V17 R20 Q24 G25 Q26 Q29 V30 R31 V32 E33 F34 M35 D36 D37 T38 S39 R40 S41 I42 I43 R44 N45 V46 K47 G48 R51 E52 G53 D54 V55 L56 T57 L58 L59 E60 S61 E62 R63 E64 A65 R66 R67 L68

- Molecule 76: 40S ribosomal protein S29

Chain Bd: 59% 98%

Q5 L6 Y7 W8 S9 H10 P11 R12 G15 Q16 R19 C24 S25 N26 R27 H28 G29 L30 I31 R32 K33 Y34 G35 L36 N37 M38 C39 C42 F43 R44 Q45 K48 D49 F52 I53 K54 L55

- Molecule 77: 40S ribosomal protein S30

Chain Be: 47% 93% 7%

H3 G4 S5 L6 A7 R8 A9 G10 G14 K18 V19 A20 K21 Q22 E23 K24 K27 K28 T29 G30 R31 A32 R35 N39 R40 R41 F42 V46 P47 T48 F49 G50 K51 K52 K53 G54 A57

- Molecule 78: Ubiquitin-40S ribosomal protein S27a

Chain Bf: 93% 99%

K79 R80 K81 K82 K83 S84 Y85 T86 T87 P88 K89 K90 N91 K92 H93 K94 R95 K96 K97 V98 K99 L100 A101 V102 L103 K104 Y105 Y106 K107 V108 D109 E110 N111 G112 K113 I114 S115 R116 L117 R118 R119 E120 C121 P122 S123 D124 E125 C126 G127 A128 G129 V130 F131 M132 A133 S134 H135 F136 D137 R138

H139 Y140 C141 G142 K143 C144 C145 L146 T147 Y148 C149 F150 N151

- Molecule 79: Receptor of activated protein C kinase 1

Chain Bg: 92% 99%

T2 E3 Q4 M5 T6 L7 R8 G9 T10 L11 K12 G13 H14 N15 G16 W17 V18 T19 Q20 I21 A22 T23 T24 P25 Q26 F27 P28 D29 M30 I31 L32 S33 A34 S35 R36 D37 K38 T39 I40 I41 M42 W43 K44 L45 T46 R47 D48 E49 T50 N51 Y52 G53 I54 P55 Q56 R57 A58 L59 R60 G61

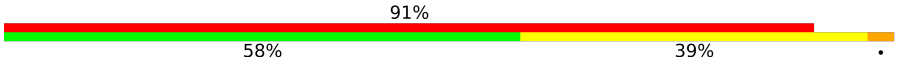
H62 S63 H64 F65 V66 S67 D68 V69 V70 I71 S72 S73 D74 G75 Q76 F77 A78 L79 S80 G81 S82 W83 D84 G85 T86 L87 R88 L89 W90 D91 L92 T93 T94 G95 T96 T97 T98 R99 R100 F101 V102 G103 H104 T105 K106 D107 V108 L109 S110 V111 A112 F113 S114 S115 D116 N117 R118 Q119 I120 V121

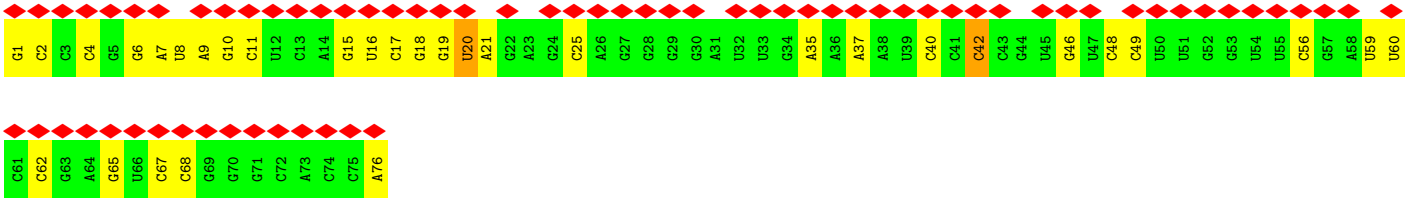
S122 G123 S124 R125 D126 K127 T128 I129 K130 L131 W132 N133 T134 L135 G136 V137 C138 K139 Y140 T141 V142 Q143 D144 E145 S146 H147 S148 E149 W150 V151 S152 C153 V154 R155 F156 S157 P158 N159 S160 S161 N162 P163 I164 I165 V166 S167 C168 G169 W170 D171 K172 L173 V174 K175 V176 W177 N178 L179 A180 N181

C182 K183 L184 K185 T186 N187 H188 I189 G190 H191 T192 G193 Y194 L195 N196 T197 V198 T199 V200 S201 P202 D203 G204 S205 L206 C207 A208 S209 G210 G211 K212 D213 G214 Q215 A216 M217 L218 W219 D220 L221 N222 E223 G224 K225 H226 L227 Y228 T229 L230 D231 G232 G233 D234 I235 I236 N237 A238 L239 C240 F241

- Molecule 80: tRNA

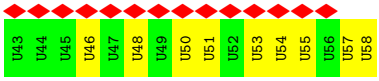
Chain Bv:





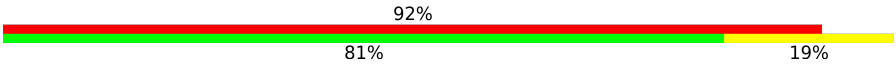
- Molecule 81: mRNA

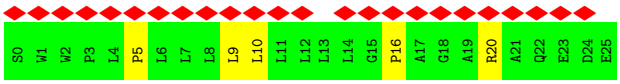
Chain Bx:



- Molecule 82: Proprotein convertase subtilisin/kexin type 9

Chain A:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7214	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	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	0.104	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	488.0, 488.0, 488.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.22, 1.22, 1.22	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: ZN, MG, MVM

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	AA	0.55	0/1936	0.67	0/2596
2	BA	0.44	0/1741	0.71	1/2366 (0.0%)
3	AB	0.54	0/3246	0.71	1/4345 (0.0%)
4	BB	0.41	0/1749	0.71	1/2340 (0.0%)
5	AC	0.58	1/2942 (0.0%)	0.82	7/3951 (0.2%)
6	BC	0.46	0/1761	0.66	0/2379
7	A3	0.98	1/3726 (0.0%)	1.29	46/5804 (0.8%)
8	A4	0.91	0/2839	1.14	7/4425 (0.2%)
9	AD	0.46	0/2437	0.66	0/3262
10	AE	0.45	0/1876	0.75	1/2514 (0.0%)
11	AF	0.57	0/1986	0.72	2/2644 (0.1%)
12	AG	0.45	0/1913	0.68	0/2576
13	AH	0.46	0/1545	0.71	1/2077 (0.0%)
14	AI	0.50	0/1730	0.68	0/2311
15	AJ	0.44	0/1376	0.69	1/1841 (0.1%)
16	AL	0.53	0/1688	0.76	2/2260 (0.1%)
17	AM	0.47	0/1161	0.65	0/1554
18	AN	0.61	1/1746 (0.1%)	0.70	0/2338
19	AO	0.51	0/1638	0.70	0/2191
20	AP	0.50	0/1268	0.61	0/1701
21	AQ	0.58	0/1537	0.79	0/2052
22	AR	0.43	0/1533	0.68	1/2025 (0.0%)
23	AS	0.53	1/1488 (0.1%)	0.68	0/1997
24	AT	0.55	0/1312	0.69	0/1753
25	AU	0.43	0/822	0.65	0/1103
26	AV	0.48	0/983	0.68	0/1319
27	AW	0.46	0/1004	0.68	1/1332 (0.1%)
28	AX	0.45	0/975	0.67	0/1312
29	AY	0.48	0/1081	0.67	0/1439
30	AZ	0.52	0/1126	0.71	0/1502
31	Aa	0.55	0/1191	0.68	0/1591
32	Ab	2.58	2/804 (0.2%)	0.78	2/1060 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Ac	0.48	0/812	0.64	0/1089
34	Ad	0.51	0/894	0.68	0/1204
35	Ae	0.55	0/1082	0.70	2/1443 (0.1%)
36	Af	0.56	0/895	0.73	0/1198
37	Ag	0.51	0/916	0.76	0/1220
38	Ah	0.55	1/1023 (0.1%)	0.73	0/1351
39	Ai	0.45	0/805	0.69	0/1065
40	Aj	0.55	0/703	0.76	1/929 (0.1%)
41	Ak	0.44	0/575	0.70	1/761 (0.1%)
42	Al	0.45	0/454	0.68	0/599
43	Am	0.45	0/417	0.67	0/553
44	An	0.49	0/241	0.85	0/305
45	Ao	0.51	0/877	0.69	0/1156
46	Ap	0.54	0/718	0.71	0/953
47	At	0.51	0/995	0.77	2/1334 (0.1%)
48	A2	1.27	17/87365 (0.0%)	1.27	737/136272 (0.5%)
49	B1	0.76	1/40767 (0.0%)	1.24	314/63536 (0.5%)
50	BD	0.40	0/1736	0.68	1/2338 (0.0%)
51	BE	0.41	0/2072	0.71	3/2793 (0.1%)
52	BF	0.39	0/1524	0.70	1/2048 (0.0%)
53	BG	0.38	0/1907	0.71	0/2538
54	BH	0.39	0/1501	0.70	1/2009 (0.0%)
55	BI	0.44	0/1725	0.70	0/2298
56	BJ	0.41	0/1520	0.70	1/2030 (0.0%)
57	BK	0.40	0/851	0.71	0/1147
58	BL	0.46	0/1281	0.74	1/1710 (0.1%)
59	BM	0.37	0/941	0.71	2/1264 (0.2%)
60	BN	0.40	0/1226	0.69	1/1649 (0.1%)
61	BO	0.45	1/1029 (0.1%)	0.70	0/1380
62	BP	0.41	0/1019	0.80	0/1361
63	BQ	0.37	0/1126	0.70	0/1506
64	BR	0.36	0/1023	0.68	0/1373
65	BS	0.39	0/1172	0.69	0/1570
66	BT	0.40	0/1131	0.70	1/1515 (0.1%)
67	BU	0.35	0/778	0.68	0/1045
68	BV	0.38	0/623	0.68	0/833
69	BW	0.44	0/1051	0.71	0/1406
70	BX	0.46	0/1097	0.69	0/1464
71	BY	0.37	0/1032	0.65	0/1371
72	BZ	0.36	0/696	0.77	1/929 (0.1%)
73	Ba	0.44	0/786	0.66	0/1053
74	Bb	0.46	0/637	0.72	0/854
75	Bc	0.32	0/490	0.70	0/656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	Bd	0.43	0/437	0.79	1/580 (0.2%)
77	Be	0.38	0/443	0.71	0/583
78	Bf	0.35	0/613	0.66	0/811
79	Bg	0.35	0/2497	0.68	1/3399 (0.0%)
80	Bv	0.56	1/1813 (0.1%)	1.16	7/2823 (0.2%)
81	Bx	0.40	0/351	1.05	0/540
82	A	0.19	0/127	0.56	0/175
All	All	0.92	27/229954 (0.0%)	1.09	1153/337979 (0.3%)

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
22	AR	0	1
52	BF	0	1
All	All	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	A2	1254	G	N3-C4	132.95	2.28	1.35
48	A2	1254	G	C2-N3	109.51	2.20	1.32
48	A2	1254	G	C6-N1	99.11	2.08	1.39
48	A2	1254	G	N1-C2	89.30	2.09	1.37
48	A2	1254	G	C5-C4	82.35	1.96	1.38

The worst 5 of 1153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A2	1254	G	C2-N3-C4	39.26	131.53	111.90
48	A2	1254	G	C4-C5-N7	-37.76	95.70	110.80
48	A2	1254	G	N3-C4-C5	-34.88	111.16	128.60
48	A2	1254	G	N3-C4-N9	33.78	146.27	126.00
48	A2	1254	G	N1-C2-N3	-29.77	106.04	123.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	AR	21	LYS	Peptide
52	BF	79	HIS	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	
1	AA	246/248 (99%)	216 (88%)	29 (12%)	1 (0%)	34	71
2	BA	213/215 (99%)	193 (91%)	20 (9%)	0	100	100
3	AB	392/394 (100%)	352 (90%)	39 (10%)	1 (0%)	41	75
4	BB	210/212 (99%)	175 (83%)	34 (16%)	1 (0%)	29	67
5	AC	361/363 (99%)	323 (90%)	32 (9%)	6 (2%)	9	43
6	BC	220/222 (99%)	196 (89%)	24 (11%)	0	100	100
9	AD	292/294 (99%)	261 (89%)	30 (10%)	1 (0%)	41	75
10	AE	222/247 (90%)	184 (83%)	35 (16%)	3 (1%)	11	46
11	AF	232/234 (99%)	201 (87%)	30 (13%)	1 (0%)	34	71
12	AG	232/234 (99%)	208 (90%)	23 (10%)	1 (0%)	34	71
13	AH	189/191 (99%)	172 (91%)	17 (9%)	0	100	100
14	AI	204/211 (97%)	181 (89%)	21 (10%)	2 (1%)	15	52
15	AJ	167/169 (99%)	146 (87%)	21 (13%)	0	100	100
16	AL	203/205 (99%)	174 (86%)	26 (13%)	3 (2%)	10	45
17	AM	137/139 (99%)	119 (87%)	18 (13%)	0	100	100
18	AN	201/203 (99%)	172 (86%)	28 (14%)	1 (0%)	29	67
19	AO	193/195 (99%)	183 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	AP	151/153 (99%)	142 (94%)	9 (6%)	0	100	100
21	AQ	185/187 (99%)	165 (89%)	19 (10%)	1 (0%)	29	67
22	AR	179/181 (99%)	170 (95%)	9 (5%)	0	100	100
23	AS	173/175 (99%)	153 (88%)	20 (12%)	0	100	100
24	AT	155/157 (99%)	131 (84%)	22 (14%)	2 (1%)	12	48
25	AU	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
26	AV	127/129 (98%)	123 (97%)	4 (3%)	0	100	100
27	AW	119/121 (98%)	103 (87%)	16 (13%)	0	100	100
28	AX	115/117 (98%)	104 (90%)	11 (10%)	0	100	100
29	AY	125/127 (98%)	116 (93%)	9 (7%)	0	100	100
30	AZ	132/134 (98%)	116 (88%)	16 (12%)	0	100	100
31	Aa	145/147 (99%)	124 (86%)	21 (14%)	0	100	100
32	Ab	93/118 (79%)	81 (87%)	9 (10%)	3 (3%)	4	32
33	Ac	101/103 (98%)	94 (93%)	7 (7%)	0	100	100
34	Ad	104/106 (98%)	91 (88%)	13 (12%)	0	100	100
35	Ae	127/129 (98%)	107 (84%)	20 (16%)	0	100	100
36	Af	107/109 (98%)	96 (90%)	11 (10%)	0	100	100
37	Ag	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
38	Ah	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
39	Ai	95/97 (98%)	81 (85%)	13 (14%)	1 (1%)	14	51
40	Aj	82/84 (98%)	75 (92%)	7 (8%)	0	100	100
41	Ak	67/69 (97%)	62 (92%)	5 (8%)	0	100	100
42	Al	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
43	Am	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
44	An	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
45	Ao	103/105 (98%)	92 (89%)	11 (11%)	0	100	100
46	Ap	89/91 (98%)	78 (88%)	11 (12%)	0	100	100
47	At	120/122 (98%)	106 (88%)	14 (12%)	0	100	100
50	BD	218/220 (99%)	193 (88%)	23 (11%)	2 (1%)	17	54
51	BE	255/257 (99%)	231 (91%)	23 (9%)	1 (0%)	34	71
52	BF	188/190 (99%)	163 (87%)	25 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	BG	230/232 (99%)	197 (86%)	33 (14%)	0	100	100
54	BH	181/183 (99%)	158 (87%)	22 (12%)	1 (1%)	25	63
55	BI	205/207 (99%)	170 (83%)	34 (17%)	1 (0%)	29	67
56	BJ	177/179 (99%)	157 (89%)	19 (11%)	1 (1%)	25	63
57	BK	96/98 (98%)	77 (80%)	18 (19%)	1 (1%)	15	52
58	BL	151/153 (99%)	131 (87%)	19 (13%)	1 (1%)	22	60
59	BM	118/120 (98%)	110 (93%)	8 (7%)	0	100	100
60	BN	147/149 (99%)	129 (88%)	18 (12%)	0	100	100
61	BO	134/136 (98%)	116 (87%)	18 (13%)	0	100	100
62	BP	118/120 (98%)	100 (85%)	16 (14%)	2 (2%)	9	43
63	BQ	137/139 (99%)	121 (88%)	16 (12%)	0	100	100
64	BR	123/125 (98%)	107 (87%)	15 (12%)	1 (1%)	19	57
65	BS	137/139 (99%)	117 (85%)	19 (14%)	1 (1%)	22	60
66	BT	141/143 (99%)	126 (89%)	14 (10%)	1 (1%)	22	60
67	BU	95/97 (98%)	87 (92%)	8 (8%)	0	100	100
68	BV	79/81 (98%)	72 (91%)	6 (8%)	1 (1%)	12	48
69	BW	127/129 (98%)	117 (92%)	10 (8%)	0	100	100
70	BX	137/139 (99%)	124 (90%)	13 (10%)	0	100	100
71	BY	123/125 (98%)	113 (92%)	10 (8%)	0	100	100
72	BZ	84/86 (98%)	71 (84%)	12 (14%)	1 (1%)	13	49
73	Ba	95/97 (98%)	84 (88%)	10 (10%)	1 (1%)	14	51
74	Bb	78/80 (98%)	68 (87%)	10 (13%)	0	100	100
75	Bc	60/62 (97%)	52 (87%)	6 (10%)	2 (3%)	4	31
76	Bd	49/51 (96%)	38 (78%)	11 (22%)	0	100	100
77	Be	53/55 (96%)	45 (85%)	8 (15%)	0	100	100
78	Bf	71/73 (97%)	61 (86%)	9 (13%)	1 (1%)	11	46
79	Bg	312/314 (99%)	273 (88%)	39 (12%)	0	100	100
82	A	24/26 (92%)	16 (67%)	3 (12%)	5 (21%)	0	2
All	All	11199/11402 (98%)	9901 (88%)	1246 (11%)	52 (0%)	32	67

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AB	4	ARG
5	AC	53	ALA
5	AC	151	PRO
14	AI	189	ARG
16	AL	46	ILE

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AA	190/190 (100%)	185 (97%)	5 (3%)	46	68
2	BA	180/180 (100%)	178 (99%)	2 (1%)	73	84
3	AB	343/343 (100%)	340 (99%)	3 (1%)	78	87
4	BB	193/193 (100%)	190 (98%)	3 (2%)	62	79
5	AC	302/302 (100%)	289 (96%)	13 (4%)	29	57
6	BC	188/188 (100%)	186 (99%)	2 (1%)	73	84
9	AD	248/248 (100%)	241 (97%)	7 (3%)	43	66
10	AE	202/220 (92%)	198 (98%)	4 (2%)	55	74
11	AF	203/203 (100%)	200 (98%)	3 (2%)	65	80
12	AG	199/199 (100%)	198 (100%)	1 (0%)	88	93
13	AH	170/170 (100%)	170 (100%)	0	100	100
14	AI	178/179 (99%)	171 (96%)	7 (4%)	32	59
15	AJ	142/142 (100%)	142 (100%)	0	100	100
16	AL	171/171 (100%)	165 (96%)	6 (4%)	36	62
17	AM	118/118 (100%)	116 (98%)	2 (2%)	60	78
18	AN	171/171 (100%)	168 (98%)	3 (2%)	59	77
19	AO	168/168 (100%)	163 (97%)	5 (3%)	41	64
20	AP	134/134 (100%)	134 (100%)	0	100	100
21	AQ	164/164 (100%)	163 (99%)	1 (1%)	86	91
22	AR	160/160 (100%)	159 (99%)	1 (1%)	86	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	AS	156/156 (100%)	155 (99%)	1 (1%)	86	91
24	AT	138/138 (100%)	138 (100%)	0	100	100
25	AU	89/89 (100%)	88 (99%)	1 (1%)	73	84
26	AV	100/100 (100%)	99 (99%)	1 (1%)	76	86
27	AW	100/100 (100%)	99 (99%)	1 (1%)	76	86
28	AX	105/105 (100%)	105 (100%)	0	100	100
29	AY	119/119 (100%)	116 (98%)	3 (2%)	47	69
30	AZ	117/117 (100%)	115 (98%)	2 (2%)	60	78
31	Aa	120/120 (100%)	119 (99%)	1 (1%)	81	89
32	Ab	79/98 (81%)	75 (95%)	4 (5%)	24	53
33	Ac	88/88 (100%)	86 (98%)	2 (2%)	50	71
34	Ad	97/97 (100%)	97 (100%)	0	100	100
35	Ae	115/115 (100%)	114 (99%)	1 (1%)	78	87
36	Af	88/88 (100%)	86 (98%)	2 (2%)	50	71
37	Ag	98/98 (100%)	98 (100%)	0	100	100
38	Ah	109/109 (100%)	106 (97%)	3 (3%)	43	66
39	Ai	83/83 (100%)	83 (100%)	0	100	100
40	Aj	71/71 (100%)	70 (99%)	1 (1%)	67	81
41	Ak	64/64 (100%)	62 (97%)	2 (3%)	40	64
42	Al	47/47 (100%)	44 (94%)	3 (6%)	17	47
43	Am	46/46 (100%)	44 (96%)	2 (4%)	29	57
44	An	24/24 (100%)	24 (100%)	0	100	100
45	Ao	93/93 (100%)	91 (98%)	2 (2%)	52	71
46	Ap	74/74 (100%)	72 (97%)	2 (3%)	44	67
47	At	106/106 (100%)	104 (98%)	2 (2%)	57	75
50	BD	183/183 (100%)	181 (99%)	2 (1%)	73	84
51	BE	220/220 (100%)	216 (98%)	4 (2%)	59	77
52	BF	160/160 (100%)	157 (98%)	3 (2%)	57	75
53	BG	202/202 (100%)	200 (99%)	2 (1%)	76	86
54	BH	164/164 (100%)	162 (99%)	2 (1%)	71	83
55	BI	179/179 (100%)	177 (99%)	2 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	BJ	160/160 (100%)	158 (99%)	2 (1%)	69	82
57	BK	89/89 (100%)	88 (99%)	1 (1%)	73	84
58	BL	138/138 (100%)	138 (100%)	0	100	100
59	BM	102/102 (100%)	101 (99%)	1 (1%)	76	86
60	BN	130/130 (100%)	129 (99%)	1 (1%)	81	89
61	BO	106/106 (100%)	105 (99%)	1 (1%)	78	87
62	BP	109/109 (100%)	107 (98%)	2 (2%)	59	77
63	BQ	115/115 (100%)	115 (100%)	0	100	100
64	BR	113/113 (100%)	111 (98%)	2 (2%)	59	77
65	BS	121/121 (100%)	117 (97%)	4 (3%)	38	63
66	BT	113/113 (100%)	111 (98%)	2 (2%)	59	77
67	BU	90/90 (100%)	90 (100%)	0	100	100
68	BV	65/65 (100%)	63 (97%)	2 (3%)	40	64
69	BW	112/112 (100%)	110 (98%)	2 (2%)	59	77
70	BX	111/111 (100%)	109 (98%)	2 (2%)	59	77
71	BY	107/107 (100%)	105 (98%)	2 (2%)	57	75
72	BZ	75/75 (100%)	73 (97%)	2 (3%)	44	67
73	Ba	84/84 (100%)	84 (100%)	0	100	100
74	Bb	72/72 (100%)	71 (99%)	1 (1%)	67	81
75	Bc	55/55 (100%)	55 (100%)	0	100	100
76	Bd	45/45 (100%)	45 (100%)	0	100	100
77	Be	44/44 (100%)	40 (91%)	4 (9%)	9	35
78	Bf	66/66 (100%)	66 (100%)	0	100	100
79	Bg	272/272 (100%)	271 (100%)	1 (0%)	91	94
All	All	9752/9790 (100%)	9601 (98%)	151 (2%)	66	80

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
54	BH	152	ARG
72	BZ	62	VAL
56	BJ	30	LYS
65	BS	23	ARG
79	Bg	133	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 127 such sidechains are listed below:

Mol	Chain	Res	Type
21	AQ	44	ASN
69	BW	5	ASN
32	Ab	60	ASN
65	BS	19	ASN
72	BZ	89	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
48	A2	3626/3643 (99%)	1021 (28%)	12 (0%)
49	B1	1701/1708 (99%)	533 (31%)	6 (0%)
7	A3	156/157 (99%)	49 (31%)	1 (0%)
8	A4	118/119 (99%)	29 (24%)	0
80	Bv	75/76 (98%)	28 (37%)	0
81	Bx	15/16 (93%)	9 (60%)	0
All	All	5691/5719 (99%)	1669 (29%)	19 (0%)

5 of 1669 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A3	8	U
7	A3	32	C
7	A3	34	U
7	A3	35	C
7	A3	36	G

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
49	B1	216	C
49	B1	869	A
49	B1	1398	G
49	B1	797	C
48	A2	3755	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 332 ligands modelled in this entry, 331 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	$\#\|Z\| > 2$
85	MVM	A	101	-	33,35,35	1.75	6 (18%)	36,49,49	2.50	14 (38%)

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
85	MVM	A	101	-	-	3/20/28/28	0/5/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	A	101	MVM	C5-N1	5.88	1.45	1.37
85	A	101	MVM	N5-N4	-4.53	1.30	1.37
85	A	101	MVM	C6-N1	2.72	1.45	1.39
85	A	101	MVM	O1-C5	-2.28	1.18	1.22
85	A	101	MVM	C2-CL	2.07	1.78	1.73

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	A	101	MVM	C15-N4-C22	-8.27	121.07	129.98
85	A	101	MVM	C15-N4-N5	4.81	127.66	119.95
85	A	101	MVM	N3-C6-N1	4.32	120.91	116.33
85	A	101	MVM	C21-N7-C22	3.93	121.65	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	A	101	MVM	C7-C3-C9	3.66	118.09	110.82

There are no chirality outliers.

All (3) torsion outliers are listed below:

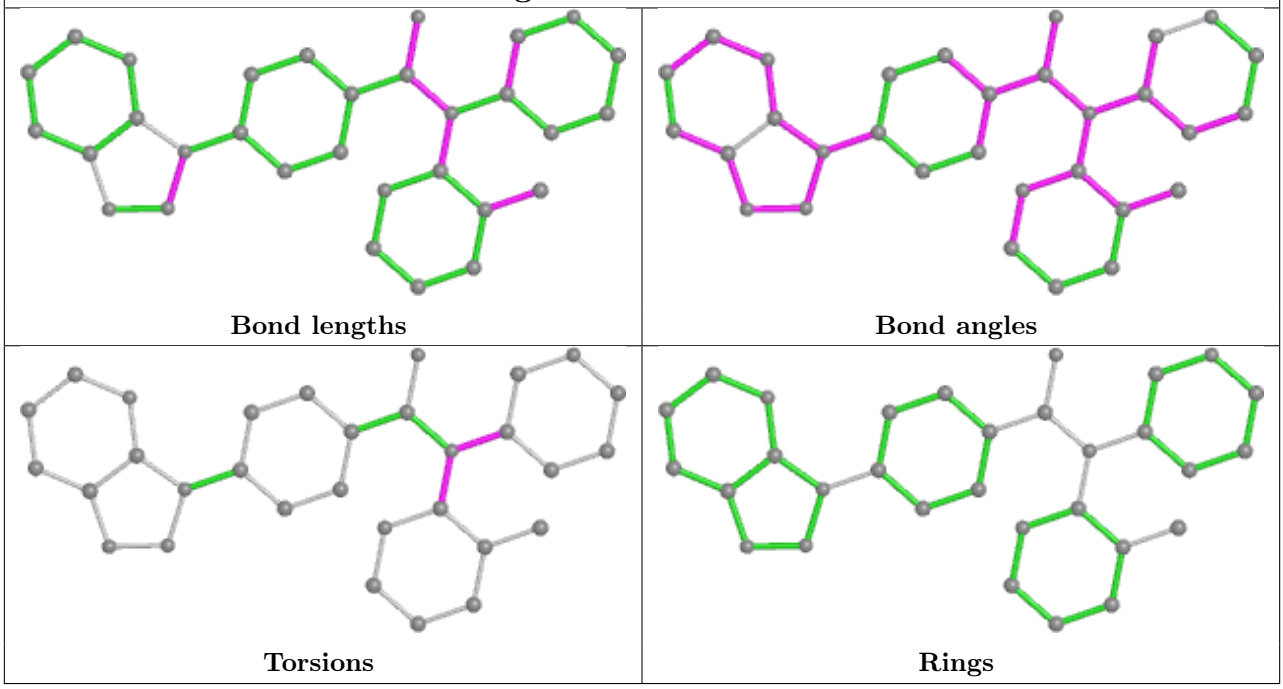
Mol	Chain	Res	Type	Atoms
85	A	101	MVM	C3-C9-N1-C5
85	A	101	MVM	C3-C9-N1-C6
85	A	101	MVM	N3-C6-N1-C5

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 MVM A 101



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
48	A2	16
49	B1	6

The worst 5 of 22 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A2	3923:A	O3'	3930:U	P	31.28
1	B1	126:G	O3'	141:A	P	22.59
1	A2	2231:G	O3'	2235:C	P	21.97
1	A2	3948:C	O3'	4004:G	P	18.85
1	B1	1426:U	O3'	1438:A	P	18.66

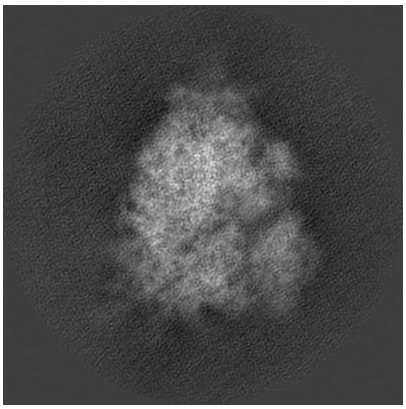
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0598. These allow visual inspection of the internal detail of the map and identification of artifacts.

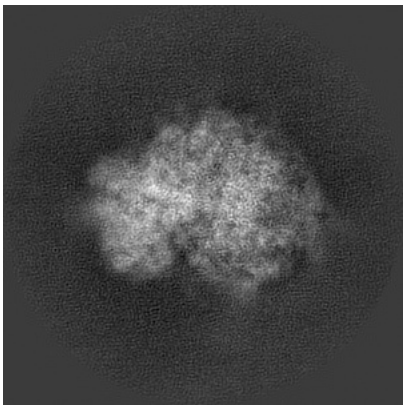
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

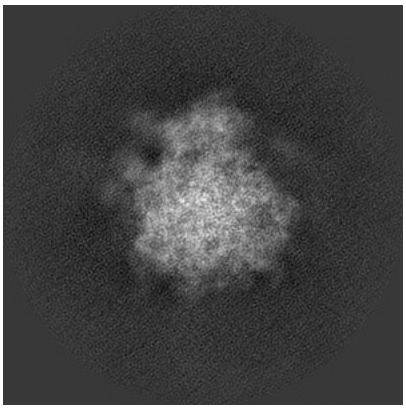
6.1.1 Primary map



X

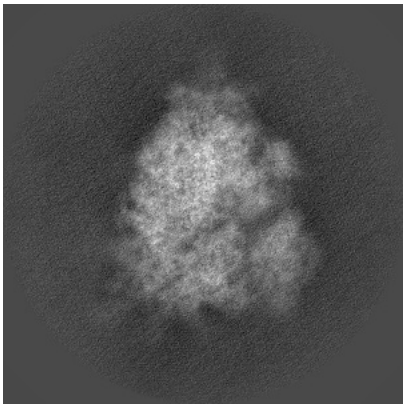


Y

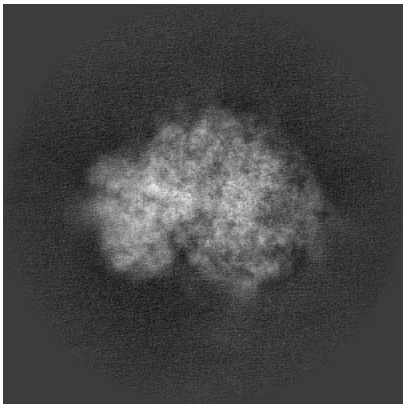


Z

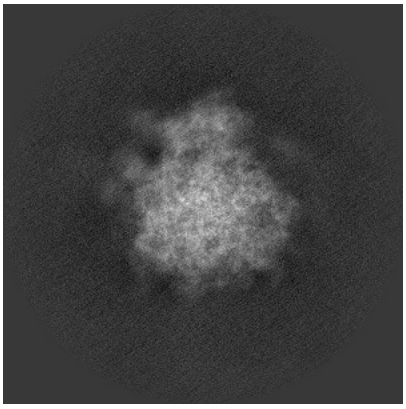
6.1.2 Raw map



X



Y

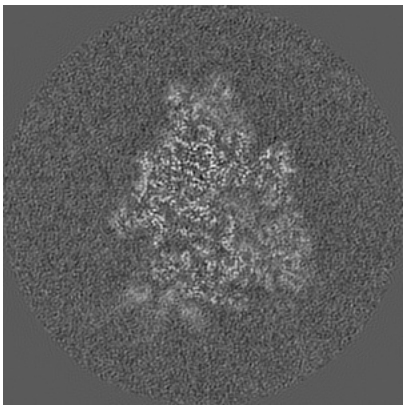


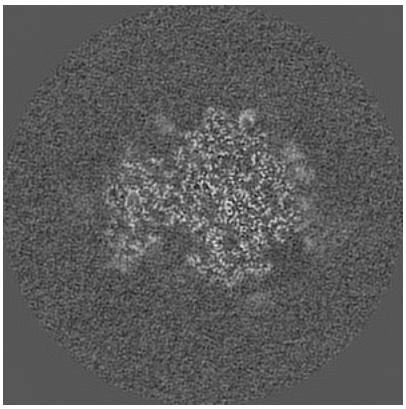
Z

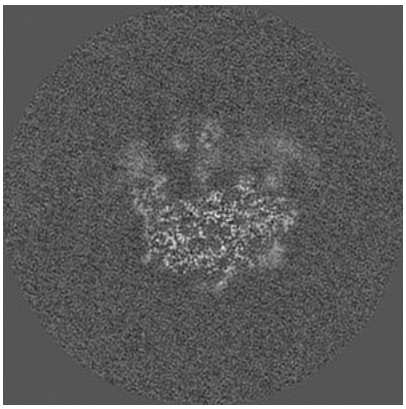
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

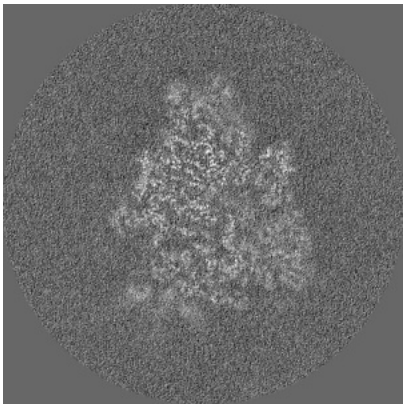
6.2.1 Primary map

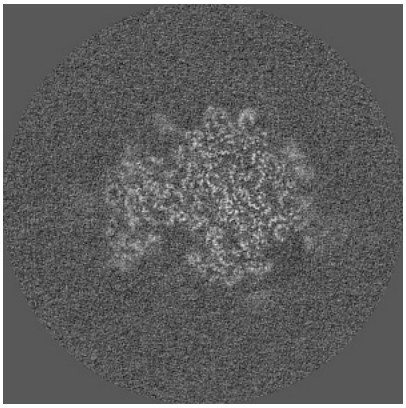

X Index: 200

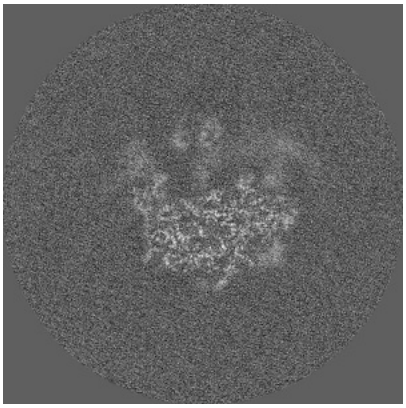

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

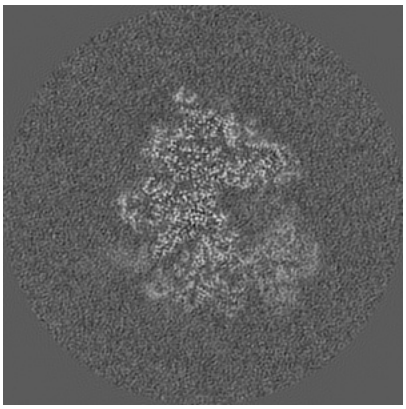

Y Index: 200

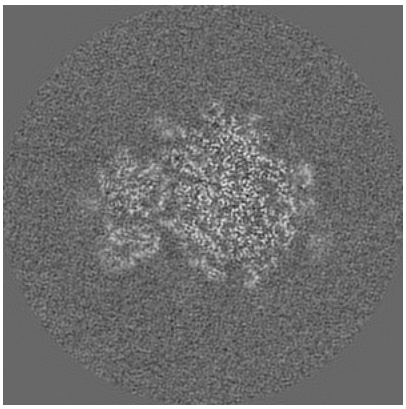

Z Index: 200

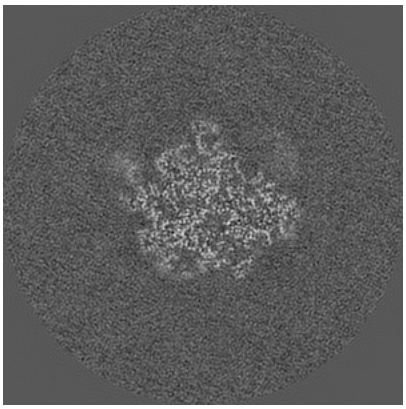
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

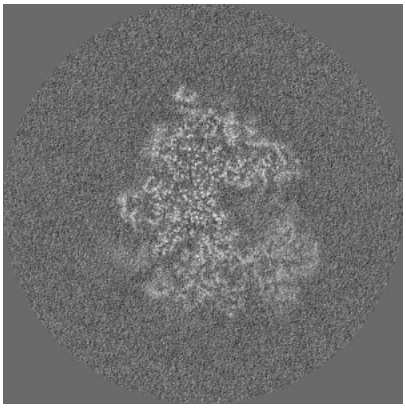
6.3.1 Primary map

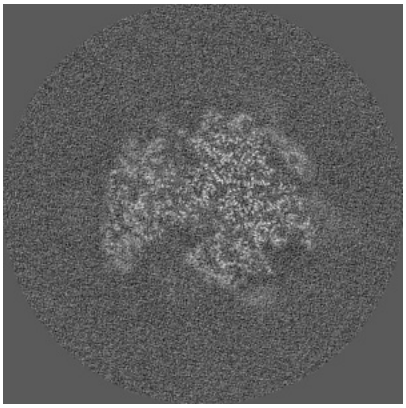

X Index: 217

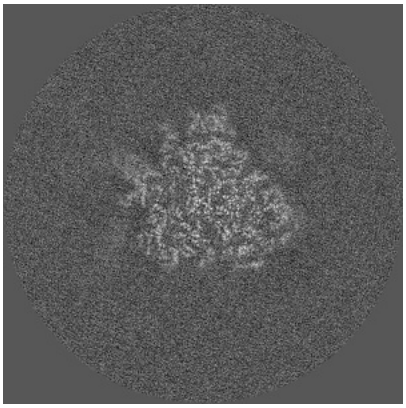

Y Index: 194


Z Index: 220

6.3.2 Raw map


X Index: 217

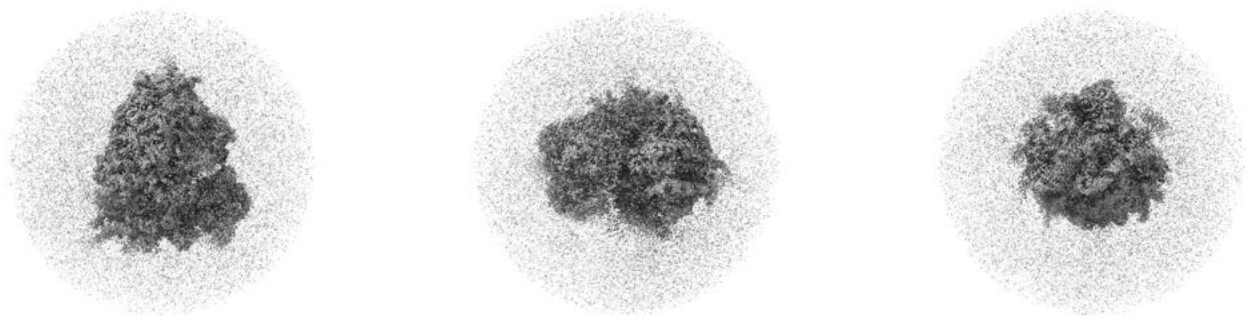

Y Index: 205


Z Index: 228

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

6.4 Orthogonal surface views (i)

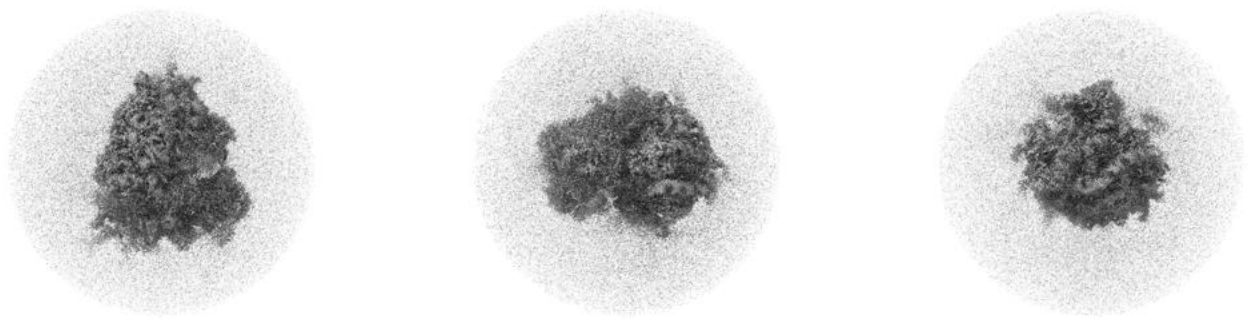
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

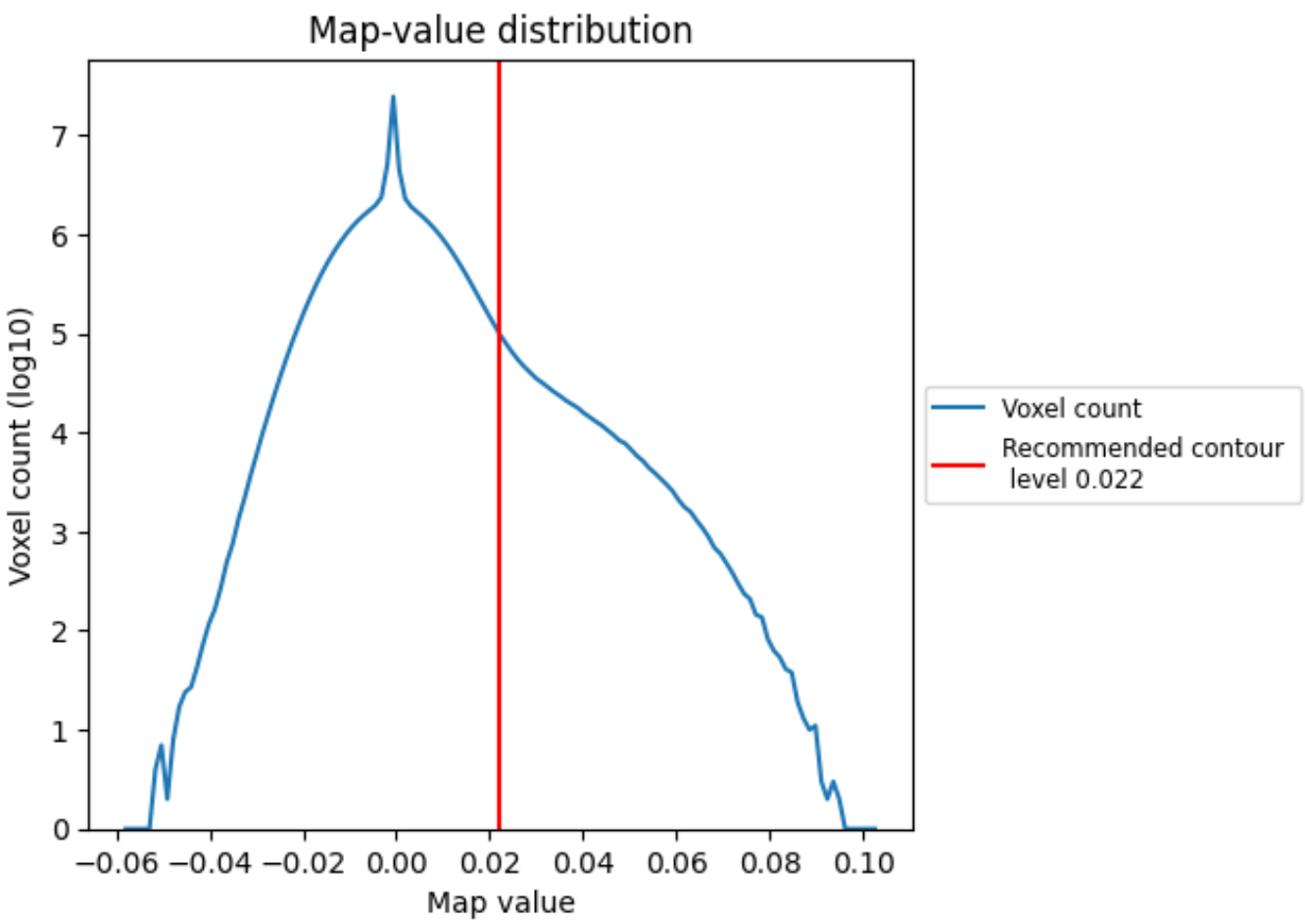
6.5 Mask visualisation (i)

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

7 Map analysis (i)

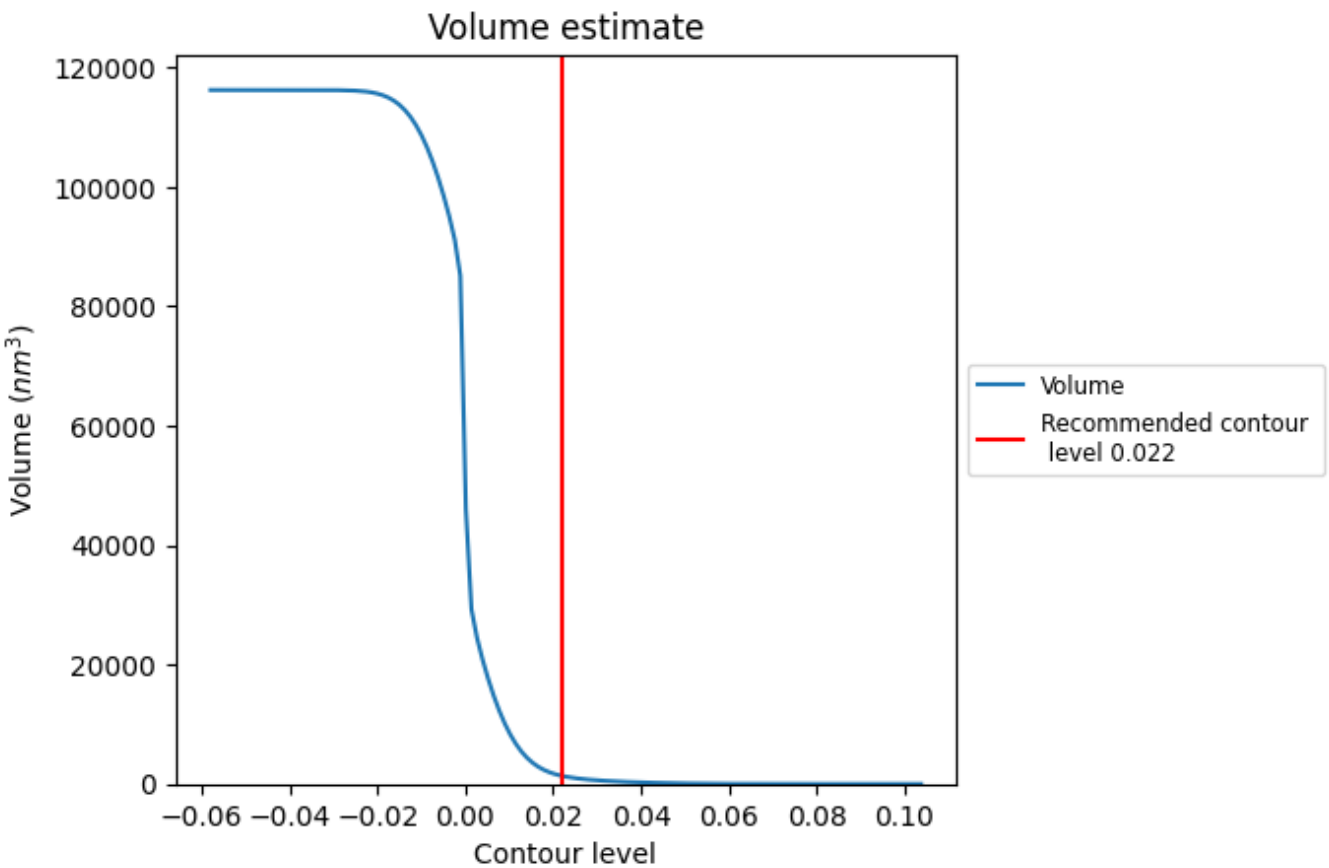
This section contains the results of statistical analysis of the map.

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.

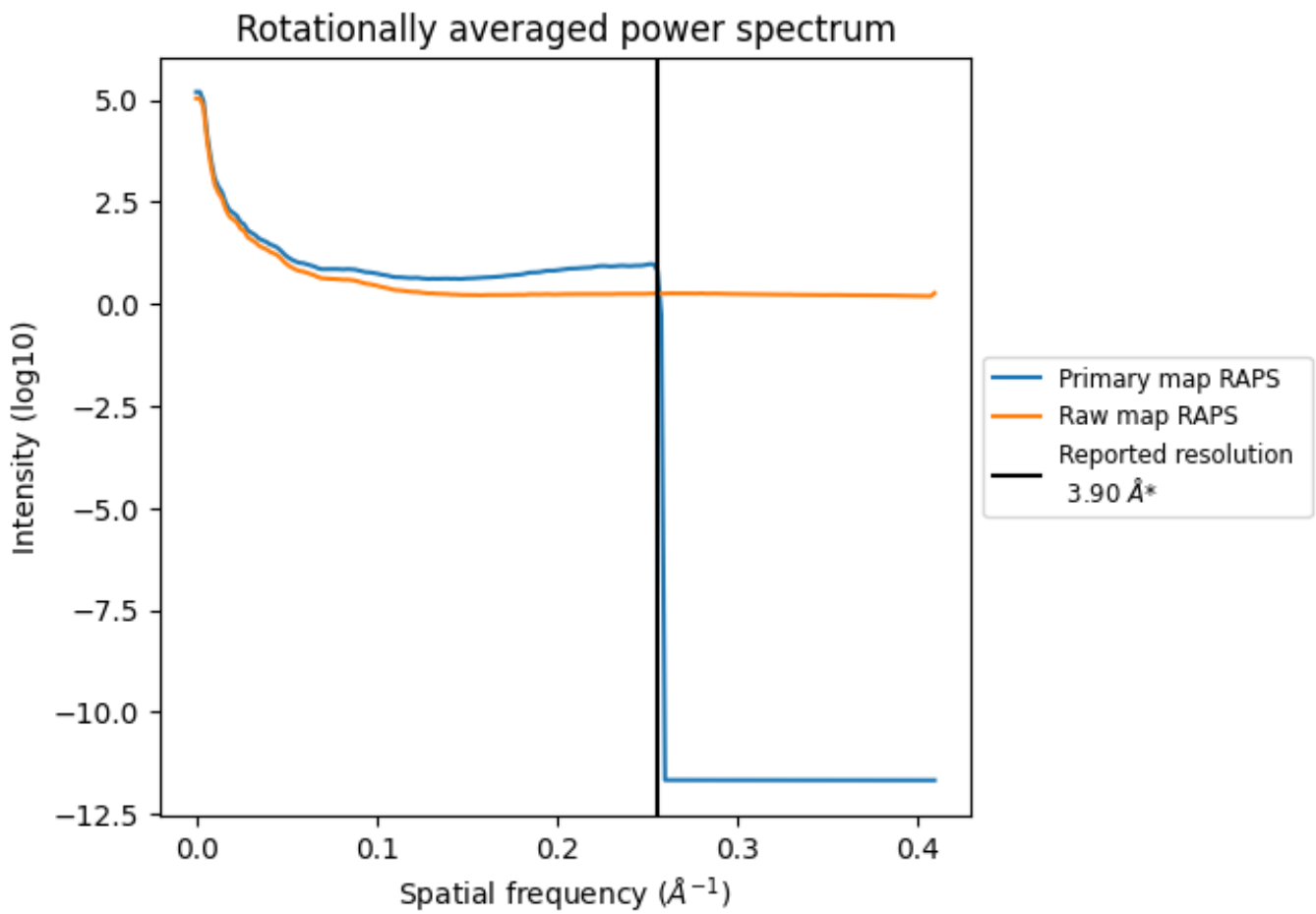
7.2 Volume estimate (i)



The volume at the recommended contour level is 1361 nm^3; this corresponds to an approximate mass of 1230 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)

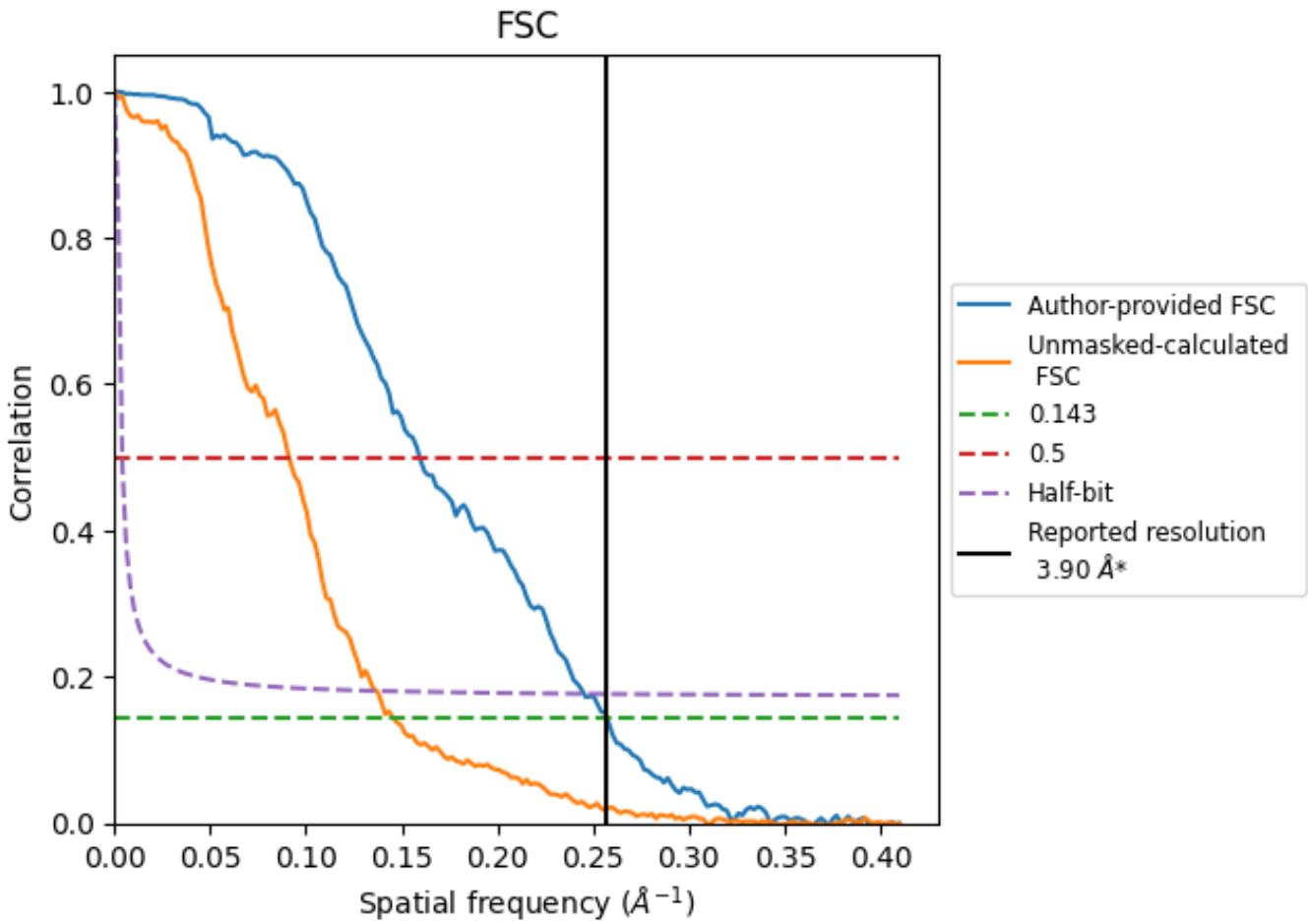


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

8.2 Resolution estimates (i)

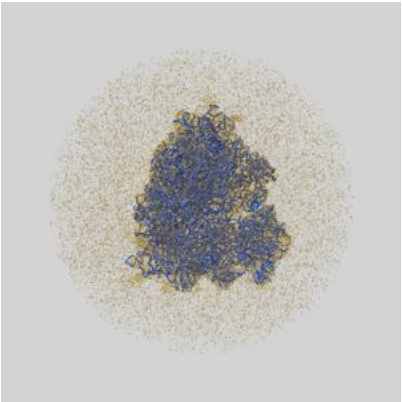
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.89	6.27	4.08
Unmasked-calculated*	6.86	10.96	7.30

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.86 differs from the reported value 3.9 by more than 10 %

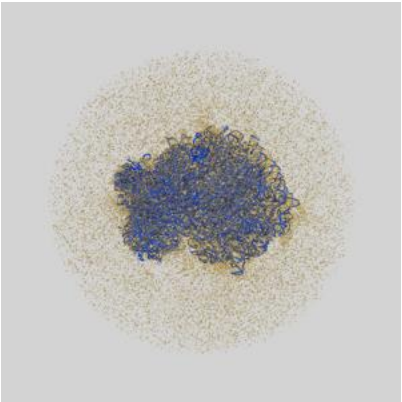
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0598 and PDB model 6OLZ. Per-residue inclusion information can be found in section 3 on page 20.

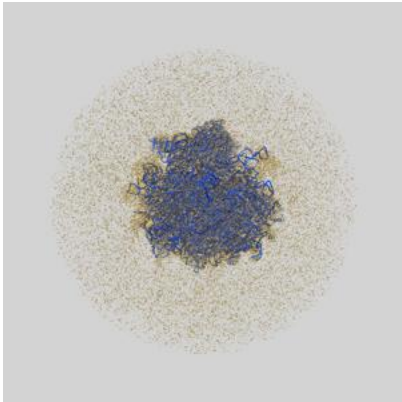
9.1 Map-model overlay (i)



X



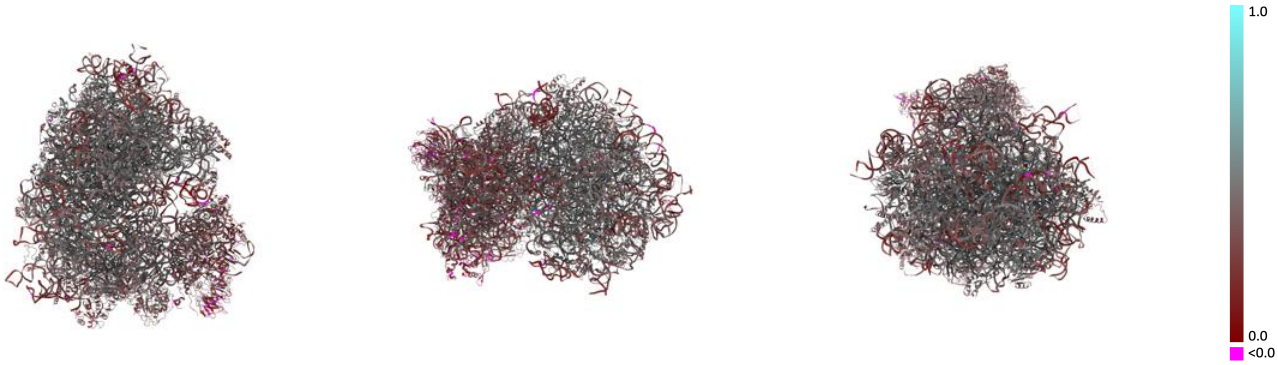
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022 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.

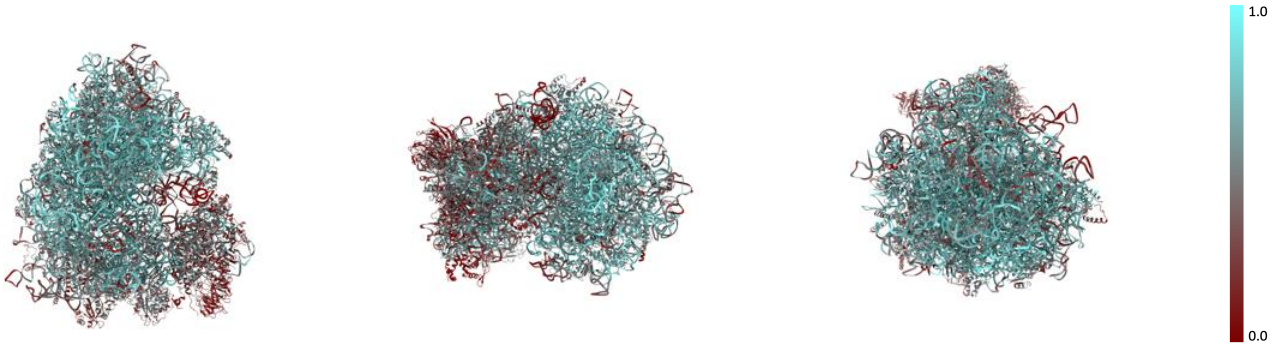
9.2 Q-score mapped to coordinate model (i)



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.

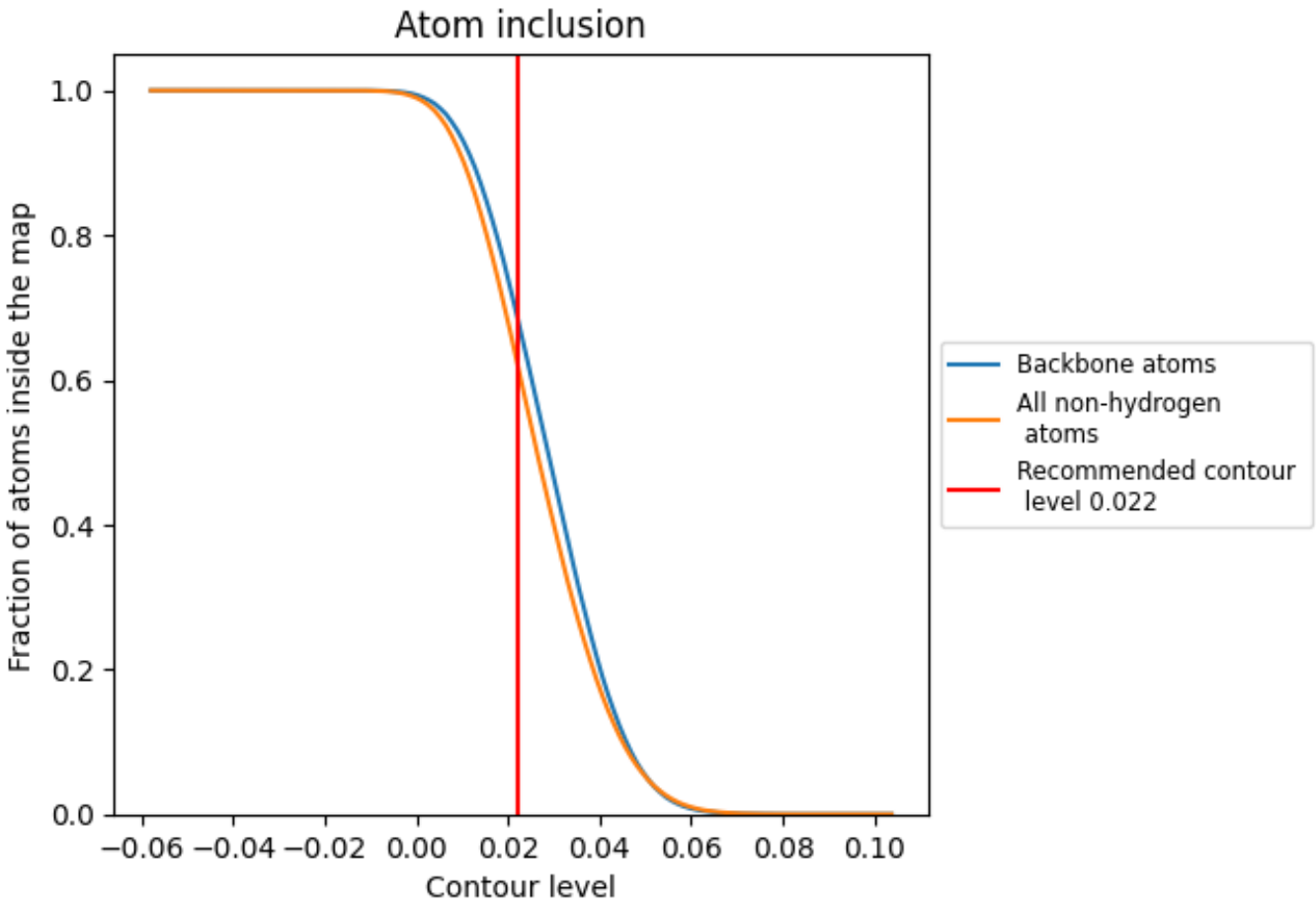
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.022).

9.4 Atom inclusion (i)



At the recommended contour level, 69% of all backbone atoms, 62% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6244	0.3940
A	0.2516	0.3170
A2	0.7482	0.4090
A3	0.7584	0.4190
A4	0.8396	0.4390
AA	0.6536	0.4800
AB	0.6307	0.4530
AC	0.6539	0.4610
AD	0.5624	0.3920
AE	0.5303	0.3990
AF	0.6219	0.4410
AG	0.5416	0.4000
AH	0.5625	0.4300
AI	0.5915	0.4410
AJ	0.5137	0.3780
AL	0.5931	0.4140
AM	0.6251	0.4380
AN	0.6915	0.4760
AO	0.6334	0.4560
AP	0.6656	0.4730
AQ	0.6436	0.4640
AR	0.5938	0.4170
AS	0.6478	0.4620
AT	0.6093	0.4610
AU	0.5114	0.3850
AV	0.6177	0.4720
AW	0.3679	0.3430
AX	0.6284	0.4480
AY	0.6485	0.4620
AZ	0.6006	0.4220
Aa	0.6749	0.4650
Ab	0.5334	0.3850
Ac	0.5536	0.4100
Ad	0.6215	0.4460
Ae	0.6573	0.4720

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Chain	Atom inclusion	Q-score
Af	0.6401	0.4720
Ag	0.6110	0.4530
Ah	0.6106	0.4220
Ai	0.6024	0.4130
Aj	0.7158	0.4890
Ak	0.5081	0.3880
Al	0.5849	0.4380
Am	0.6373	0.4520
An	0.5273	0.4190
Ao	0.6229	0.4480
Ap	0.6096	0.4430
At	0.6578	0.4510
B1	0.6445	0.3640
BA	0.4474	0.3730
BB	0.4622	0.3870
BC	0.4956	0.3990
BD	0.2437	0.2790
BE	0.4566	0.3800
BF	0.3025	0.3080
BG	0.3636	0.3210
BH	0.3393	0.3290
BI	0.5159	0.4110
BJ	0.4446	0.3500
BK	0.2025	0.2460
BL	0.4873	0.4030
BM	0.0436	0.1750
BN	0.4889	0.3940
BO	0.4965	0.4110
BP	0.2916	0.2920
BQ	0.3178	0.2950
BR	0.2879	0.2990
BS	0.3141	0.2870
BT	0.2930	0.2630
BU	0.2853	0.2960
BV	0.4328	0.3670
BW	0.5257	0.4170
BX	0.5185	0.4040
BY	0.4193	0.3250
BZ	0.2396	0.2770
Ba	0.5188	0.4030
Bb	0.4796	0.4030
Bc	0.2532	0.3040

Continued on next page...

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Chain	Atom inclusion	Q-score
Bd	0.3439	0.3100
Be	0.4242	0.3860
Bf	0.1096	0.2150
Bg	0.1365	0.2190
Bv	0.2000	0.2750
Bx	0.1250	0.2270