wwPDB EM Validation Summary Report (i)

Nov 27, 2022 – 09:15 AM EST

PDB ID	:	6OLF
EMDB ID	:	EMD-0599
Title	:	Human ribosome nascent chain complex (CDH1-RNC) stalled by a drug-like molecule with AA and PE tRNAs
Authors	:	Li, W.; Cate, J.H.D.
Deposited on	:	2019-04-16
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:

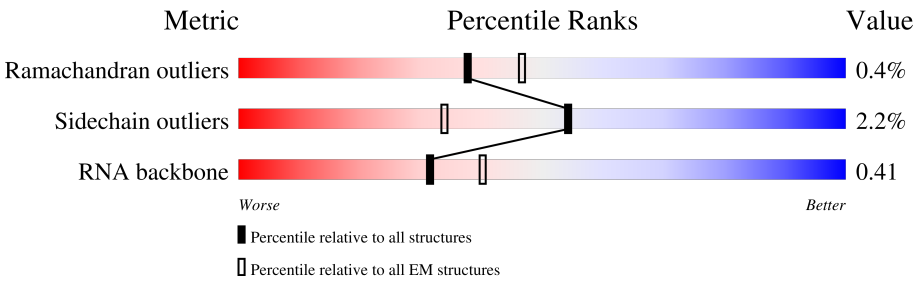
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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	S2	1714	13% 59% 37% •
2	SA	221	39% 96% •
3	SB	214	47% 97% •
4	SD	226	60% 99% •
5	SE	259	47% 98% •
6	SF	189	65% 98% •
7	SH	189	54% 97% • •
8	SI	204	43% 98% •

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Mol	Chain	Length	Quality of chain
9	SK	98	67% 97%
10	SL	153	39% 95% 5%
11	SP	127	43% 98%
12	SQ	146	54% 97%
13	SR	134	66% 99%
14	SS	145	54% 99%
15	ST	143	53% 97%
16	SU	104	61% 94% 6%
17	SV	82	37% 96%
18	SX	141	30% 98%
19	Sa	102	25% 97%
20	Sc	64	67% 100%
21	Sd	55	27% 89% 11%
22	Sg	312	78% 98%
23	SC	220	33% 98%
24	SG	237	63% 97%
25	SJ	185	50% 95% 5%
26	SM	118	97% 97%
27	SN	150	29% 99%
28	SO	137	45% 100%
29	SW	129	23% 98%
30	SY	131	44% 98%
31	SZ	73	77% 95% 5%
32	Sb	82	54% 100%
33	Se	57	54% 98%

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Mol	Chain	Length	Quality of chain
34	Sf	67	93% 96%
35	A	252	8% 98%
36	B	397	14% 98%
37	C	363	11% 96%
38	D	157	11% 71% 26%
39	E	119	80% 20%
40	F	294	17% 97%
41	G	247	26% 92%
42	H	225	8% 97%
43	I	234	24% 100%
44	J	191	24% 97%
45	K	211	18% 96%
46	L	169	21% 99%
47	M	205	20% 97%
48	N	139	12% 99%
49	O	203	6% 98%
50	P	195	8% 96%
51	Q	153	5% 97%
52	R	187	11% 96%
53	S	181	22% 97%
54	T	175	12% 98%
55	U	157	12% 97%
56	V	99	23% 94% 6%
57	W	129	18% 100%
58	X	121	56% 98%

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Mol	Chain	Length	Quality of chain
59	Y	117	16% 97%
60	Z	134	14% 99%
61	b	147	7% 96%
62	c	121	21% 80% 17%
63	d	103	21% 99%
64	e	106	15% 94% 6%
65	f	129	9% 98%
66	g	109	7% 96%
67	h	114	13% 95% 5%
68	i	122	14% 95% 5%
69	j	97	21% 98%
70	k	84	98%
71	l	69	41% 99%
72	m	50	16% 96%
73	n	50	20% 100%
74	o	25	28% 96%
75	p	105	23% 95% 5%
76	q	91	11% 99%
77	r	122	7% 97%
78	t	3607	9% 68% 29%
79	v	76	50% 49% 45% 7%
80	w	10	10% 60% 40%
81	y	39	95% 95% 5%
82	u	76	62% 37% 50% 13%
83	a	134	16% 98%

2 Entry composition (i)

There are 87 unique types of molecules in this entry. The entry contains 215429 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	S2	1714	36501	16306	6533	11949	1713	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	SA	221	1741	1106	305	322	8	0	0

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	SB	214	1738	1103	310	311	14	0	0

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SD	226	1757	1120	316	314	7	0	0

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SE	259	2059	1316	383	352	8	0	0

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	SF	189	1495	934	284	270	7	0	0

- Molecule 7 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	SH	186	1497	956	274	266	1	0	0

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	SI	204	1673	1050	329	289	5	0	0

- Molecule 9 is a protein called 40S ribosomal protein S10.

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

- Molecule 10 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	SL	153	1247	793	234	214	6	0	0

- Molecule 11 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	SP	127	1045	663	198	177	7	0	0

- Molecule 12 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	SQ	146	1158	736	218	200	4	0	0

- Molecule 13 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	SR	134	1082	680	201	197	4	0	0

- Molecule 14 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	SS	145	1198	751	242	203	2	0	0

- Molecule 15 is a protein called 40S ribosomal protein S19.

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

- Molecule 16 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	SU	104	821	514	155	148	4	0	0

- Molecule 17 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	SV	82	625	384	116	120	5	0	0

- Molecule 18 is a protein called 40S ribosomal protein S23.

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

- Molecule 19 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Sa	102	821	512	171	133	5	0	0

- Molecule 20 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Sc	64	506	308	102	94	2	0	0

- Molecule 21 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Sd	55	459	286	94	74	5	0	0

- Molecule 22 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Sg	312	2429	1531	423	463	12	0	0

- Molecule 23 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	SC	220	1715	1109	296	300	10	1	0

- Molecule 24 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	SG	237	1923	1200	387	329	7	0	0

- Molecule 25 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	SJ	185	1533	974	309	248	2	1	0

- Molecule 26 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	SM	118	912	571	161	173	7	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SM	52	GLN	LEU	conflict	UNP P25398
SM	69	LEU	CYS	conflict	UNP P25398
SM	99	ASN	LYS	conflict	UNP P25398

- Molecule 27 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	SN	150	1208	773	229	205	1	0	0

- Molecule 28 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	SO	137	1024	627	200	191	6	0	0

- Molecule 29 is a protein called 40S ribosomal protein S15a.

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

- Molecule 30 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	SY	131	1073	678	212	178	5	1	0

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	SZ	73	579	372	106	100	1	0	0

- Molecule 32 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Sb	82	640	402	118	113	7	0	0

- Molecule 33 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Se	57	452	281	99	71	1	0	0

- Molecule 34 is a protein called 40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Sf	67	548	346	102	93	7	0	0

- Molecule 35 is a protein called 60S ribosomal protein L8.

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

- Molecule 36 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	B	397	3202	2039	602	547	14	0	0

- Molecule 37 is a protein called 60S ribosomal protein L4.

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

- Molecule 38 is a RNA chain called 5.8S ribosomal RNA.

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

- Molecule 39 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 40 is a protein called 60S ribosomal protein L5.

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

- Molecule 41 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	G	236	1904	1222	361	317	4	0	0

- Molecule 42 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	H	225	1870	1202	358	301	9	0	0

- Molecule 43 is a protein called 60S ribosomal protein L7a.

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

- Molecule 44 is a protein called 60S ribosomal protein L9.

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

- Molecule 45 is a protein called 60S ribosomal protein L10.

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

- Molecule 46 is a protein called 60S ribosomal protein L11.

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

- Molecule 47 is a protein called 60S ribosomal protein L13.

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

- Molecule 48 is a protein called 60S ribosomal protein L14.

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

- Molecule 49 is a protein called 60S ribosomal protein L15.

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

- Molecule 50 is a protein called 60S ribosomal protein L13a.

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

- Molecule 51 is a protein called 60S ribosomal protein L17.

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

- Molecule 52 is a protein called 60S ribosomal protein L18.

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

- Molecule 53 is a protein called 60S ribosomal protein L19.

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

- Molecule 54 is a protein called 60S ribosomal protein L18a.

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

- Molecule 55 is a protein called 60S ribosomal protein L21.

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

- Molecule 56 is a protein called 60S ribosomal protein L22.

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

- Molecule 57 is a protein called 60S ribosomal protein L23.

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

- Molecule 58 is a protein called 60S ribosomal protein L24.

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

- Molecule 59 is a protein called 60S ribosomal protein L23a.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	Z	134	1115	700	226	186	3	0	0

- Molecule 61 is a protein called 60S ribosomal protein L27a.

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

- Molecule 62 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	c	100	814	506	179	125	4	0	0

- Molecule 63 is a protein called 60S ribosomal protein L30.

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

- Molecule 64 is a protein called 60S ribosomal protein L31.

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

- Molecule 65 is a protein called 60S ribosomal protein L32.

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

- Molecule 66 is a protein called 60S ribosomal protein L35a.

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

- Molecule 67 is a protein called 60S ribosomal protein L34.

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

- Molecule 68 is a protein called 60S ribosomal protein L35.

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

- Molecule 69 is a protein called 60S ribosomal protein L36.

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

- Molecule 70 is a protein called 60S ribosomal protein L37.

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

- Molecule 71 is a protein called 60S ribosomal protein L38.

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

- Molecule 72 is a protein called 60S ribosomal protein L39.

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

- Molecule 73 is a protein called 60S ribosomal protein L40.

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

- Molecule 74 is a protein called 60S ribosomal protein L41.

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

- Molecule 75 is a protein called 60S ribosomal protein L36a.

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

- Molecule 76 is a protein called 60S ribosomal protein L37a.

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

- Molecule 77 is a protein called 60S ribosomal protein L28.

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

- Molecule 78 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
78	t	3607	77332	34436	14150	25139	3607	0	0

- Molecule 79 is a RNA chain called AA tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
79	v	76	1618	721	287	534	76	0	0

- Molecule 80 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
80	w	10	213	95	37	72	9	0	0

- Molecule 81 is a protein called Cadherin-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
81	y	39	262	180	40	42	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	6	ALA	-	insertion	UNP P12830

- Molecule 82 is a RNA chain called PE tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
82	u	76	1613	720	283	535	75	0	0

- Molecule 83 is a protein called 60S ribosomal protein L27.

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

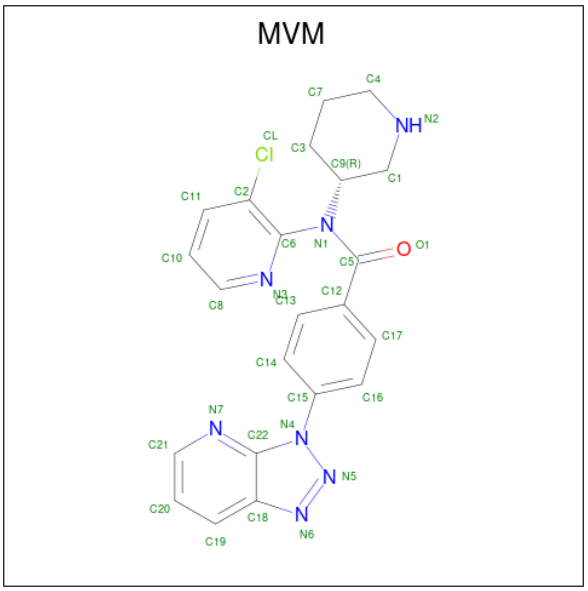
- Molecule 84 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
84	S2	1	1	1	0
84	Sa	1	1	1	0
84	Sf	1	1	1	0
84	k	1	1	1	0
84	p	1	1	1	0
84	q	1	1	1	0

- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
85	S2	3	3	3	0
85	D	6	6	6	0
85	E	9	9	9	0
85	b	2	2	2	0
85	t	11	11	11	0

- Molecule 86 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
86	t	1	Total 31	C 22	Cl 1	N 7	O 1	0

- Molecule 87 is water.

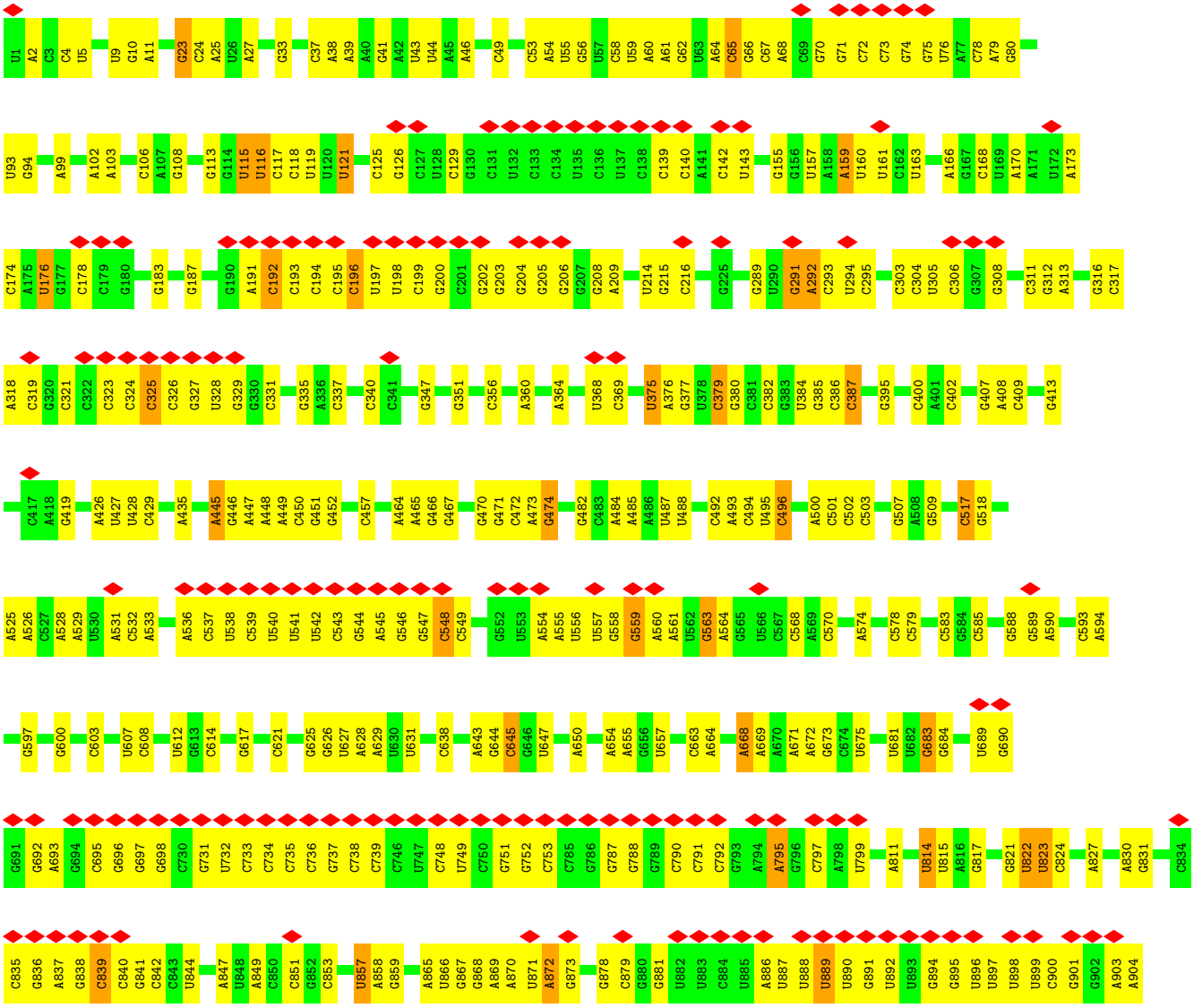
Mol	Chain	Residues	Atoms		AltConf
87	S2	5	Total 5	O 5	0
87	SP	1	Total 1	O 1	0
87	SQ	1	Total 1	O 1	0
87	SR	1	Total 1	O 1	0
87	SS	2	Total 2	O 2	0
87	SV	1	Total 1	O 1	0
87	SN	1	Total 1	O 1	0
87	Sf	1	Total 1	O 1	0
87	u	1	Total 1	O 1	0

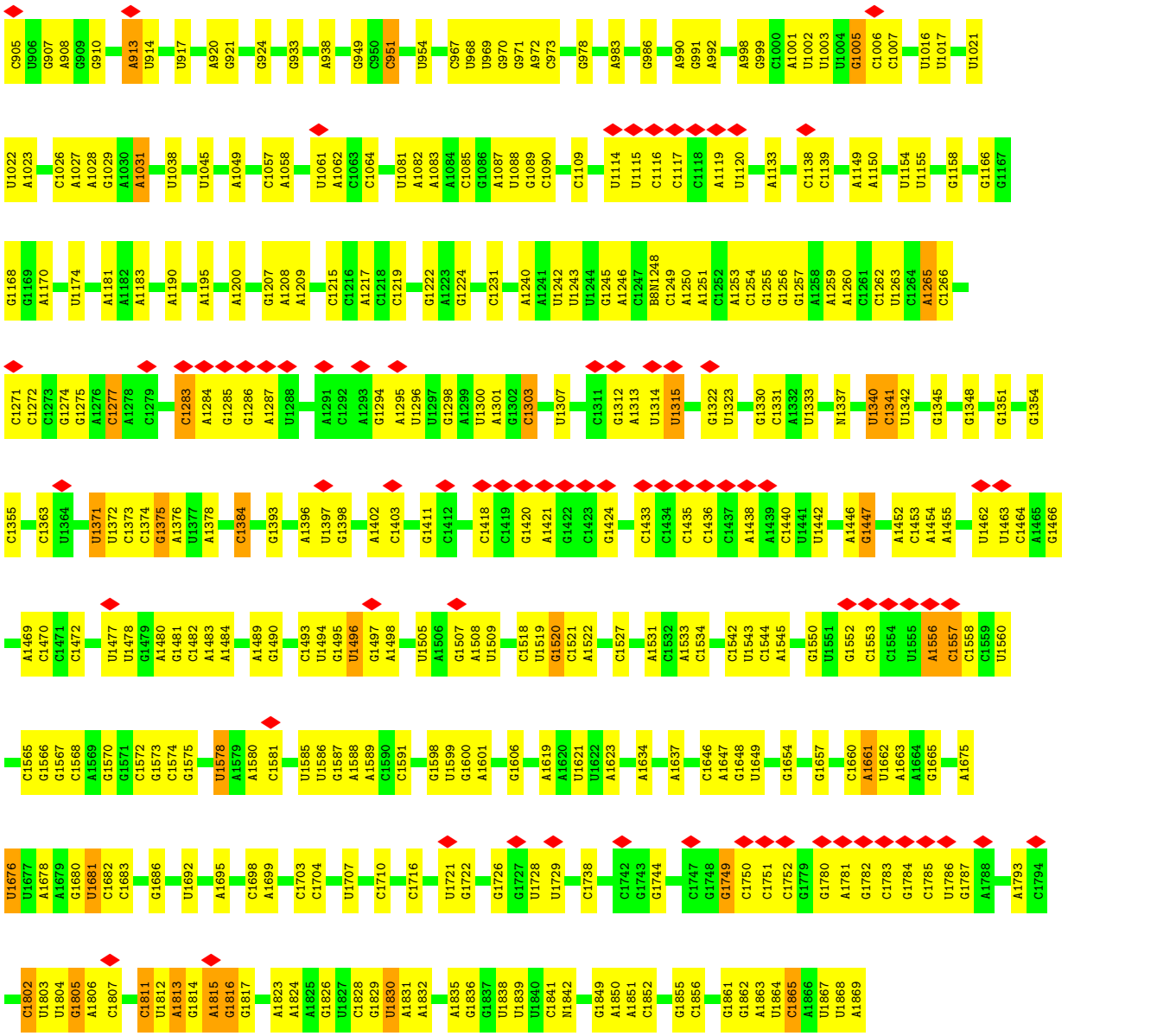
3 Residue-property plots (i)

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: 18S ribosomal RNA

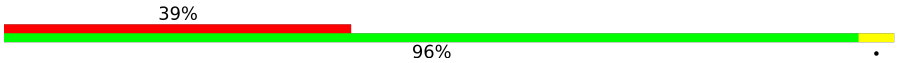
Chain S2:

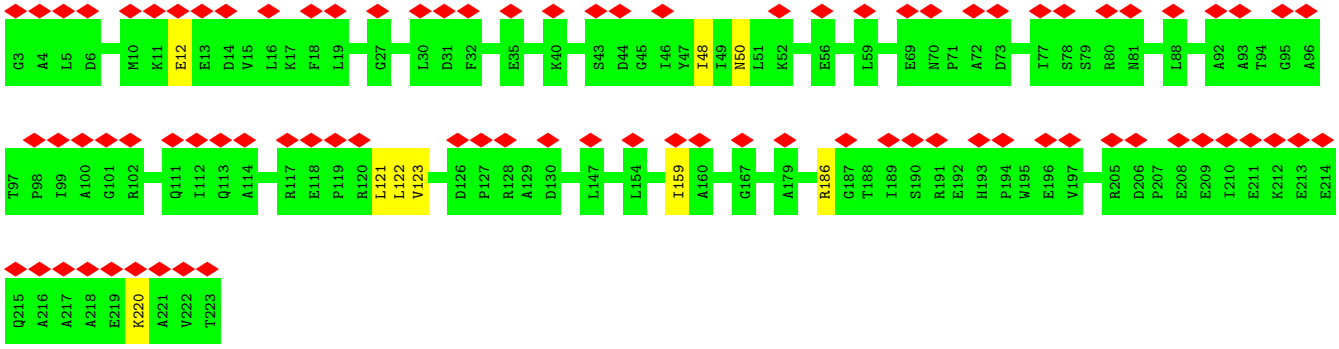




- Molecule 2: 40S ribosomal protein SA

Chain SA:





- Molecule 3: 40S ribosomal protein S3a

Chain SB: 47% 97%

V21 V22 D23 P24 F25 S26 D29 W30 Y31 D32 P36 A37 M38 F39 M40 I41 R42 N43 I44 G45 K46 T47 R51 T52 Q53 G54 T55 K56 I57 A58 S59 D60 G61 L62 K63 G64 R65 V66 F67 E68 A72 D73 L74 Q75 N76 D77 E78 V79 A80 F81 L86 I87 D90

K94 N95 C96 L97 T98 N99 F100 H101 G102 M103 D104 R107 D108 K116 M120 I121 E122 D126 V127 K128 T129 T130 D131 G132 Y133 L134 N147 N148 R151 R162 K167 M168 M169 M172 T173 R174 E175 V176 Q177 T178 N179 D180 N186 K187 L188 I189 P190 D191 S192 I193

G194 K195 D196 I197 E198 K199 I204 D209 V210 F211 L218 K219 K220 P221 K222 F223 E224 K227 E230 L231 H232 G233 E234

- Molecule 4: 40S ribosomal protein S3

Chain SD: 60% 99%

A2 V3 K7 D14 K18 A19 E20 L21 N22 E23 F24 A30 E31 D32 G33 Y34 S35 G36 V37 E38 V39 R40 V41 T42 P43 T44 R45 T46 E47 I48 I49 I50 L51 A52 T53 R54 T55 Q56 N57 V58 L59 G60 E61 K62 G63 R64 R65 I66 R67 T70 A71 V72 K75 R76

F77 G78 F79 P80 E81 G82 S83 V84 E85 L86 Y87 A88 E89 K90 V91 A92 T93 R94 G95 L96 C97 A98 E103 S104 Y107 K108 L109 L110 G111 G112 L113 A114 V115 R116 R117 A118 C119 Y120 G121 V122 L123 R124 F125 I126 M127 E128 V136 S139 G140 K141 L142 R143 G144 Q145 K148

S149 V153 D154 G155 L156 M157 I158 G161 N165 D169 T170 L177 R178 Q179 G180 G183 I184 K185 V192 D193 P194 T195 G196 K197 I198 G199 P200 K201 K202 P203 L204 P205 D206 H207 V208 S209 I210 V211 E212 P213 K214 D215 E216 I217 L218 P219 T220 T221 P222 I223 S224 E225 Q226

K227

- Molecule 5: 40S ribosomal protein S4, X isoform

Chain SE: 47% 98%

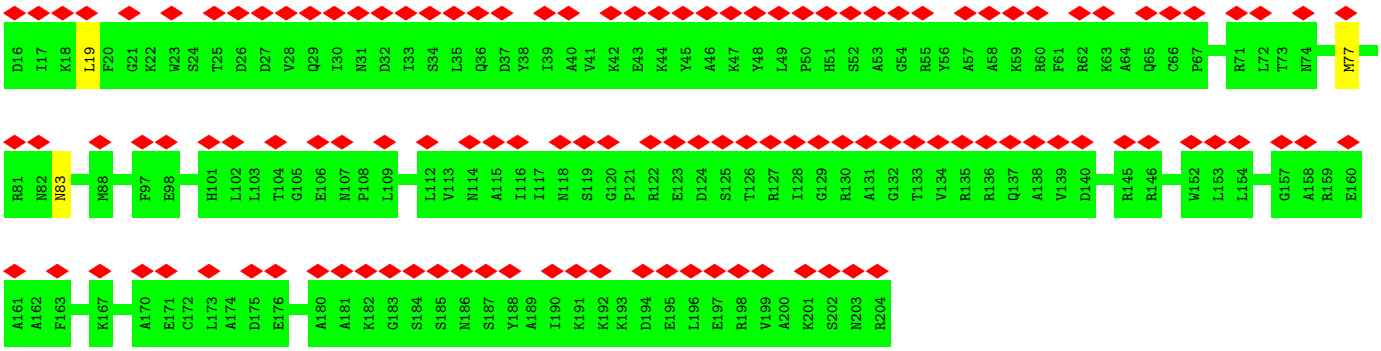
A2 R3 G4 K7 K16 L20 D21 K22 L23 T24 G34 P35 H36 K37 L38 R39 E40 C41 L42 I46 R49 N50 R51 L52 K53 L56 T57 G58 D59 E60 K63 I64 Q67 R68 K71 I72 D73 G74 R77 T78 D79 I80 G85 D88 V89 I90 S91

I92 D93 G96 E97 K106 A110 V111 H112 R113 I114 T115 P116 E117 E118 K122 L123 C124 R127 H142 D143 A144 R145 T146 I147 R148 Y149 P150 D151 P152 L153 I154 K155 V156 N157 D158 T159 I160 L164 E165 I169 T170 D171 F172 I173 D176 T177 G178 N179 L180 C181 M182

V183 T184 G185 G186 A187 N188 I192 N197 R198 E199 S204 F205 D206 H209 D212 A213 N214 G215 A219 N224 I228 S237 L238 P239 R240 G241 K242 G243 I244 R245 I248 A249 E250 E251 R252 D253 K254 R255 L256 A257 A258 K259 Q260

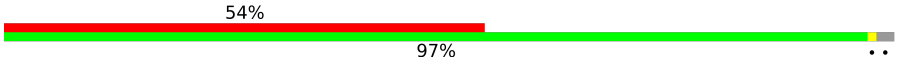
- Molecule 6: 40S ribosomal protein S5

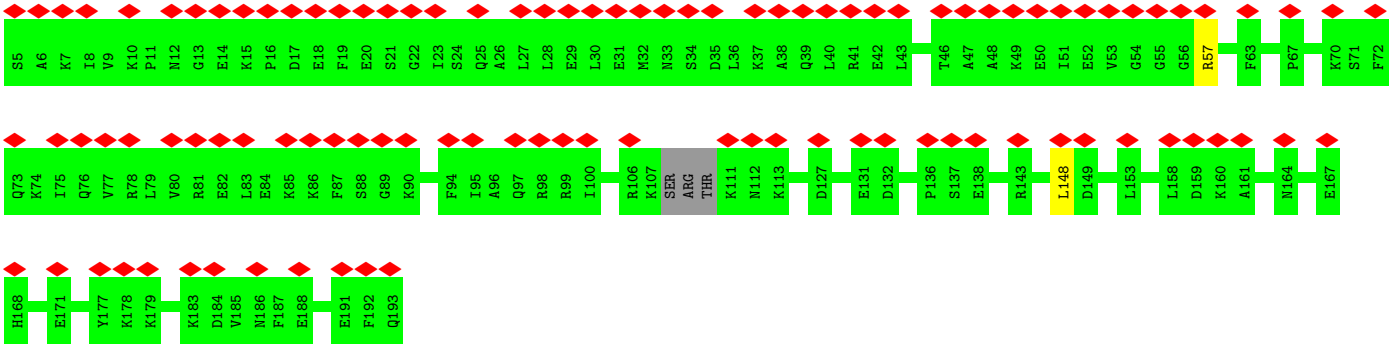
Chain SF: 65% 98%



- Molecule 7: 40S ribosomal protein S7

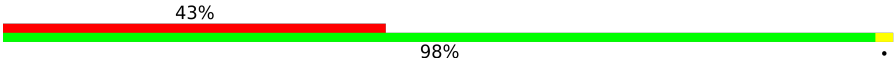
Chain SH:

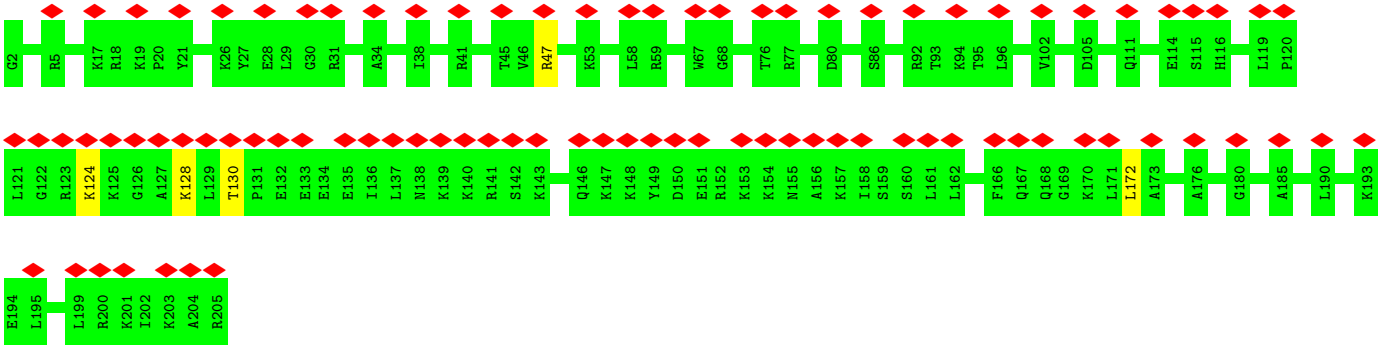




- Molecule 8: 40S ribosomal protein S8

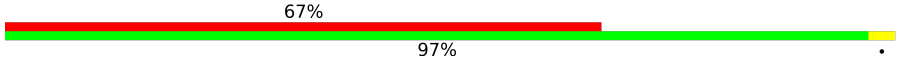
Chain SI:

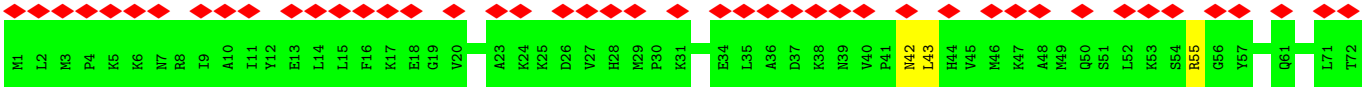


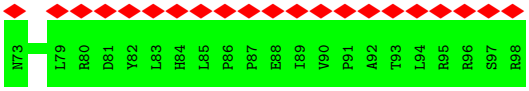


- Molecule 9: 40S ribosomal protein S10

Chain SK:

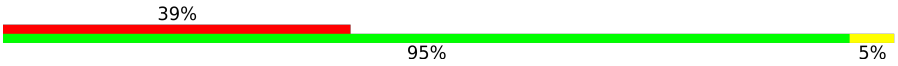


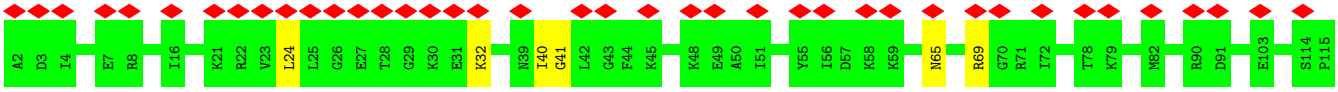


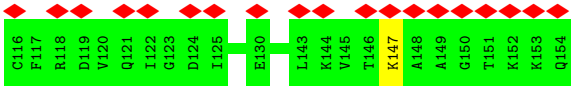


- Molecule 10: 40S ribosomal protein S11

Chain SL:

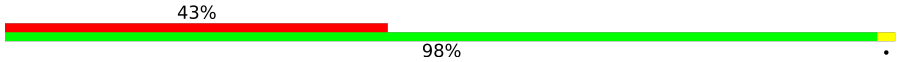


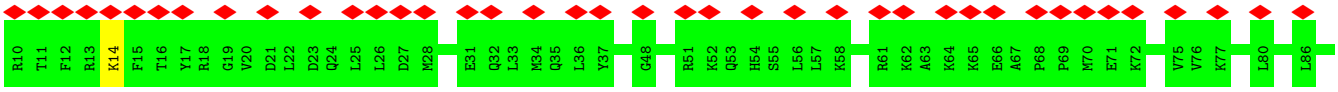


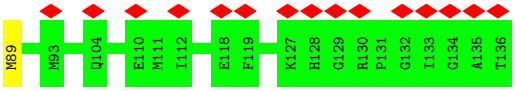


- Molecule 11: 40S ribosomal protein S15

Chain SP:

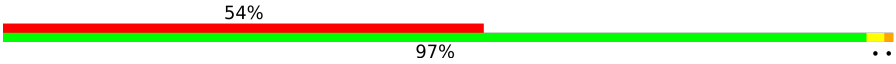


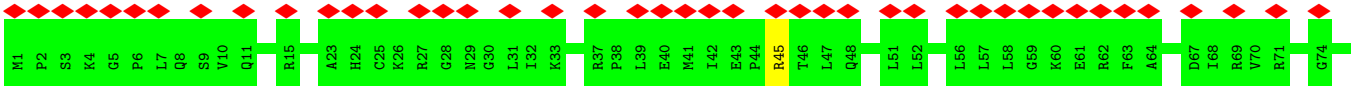


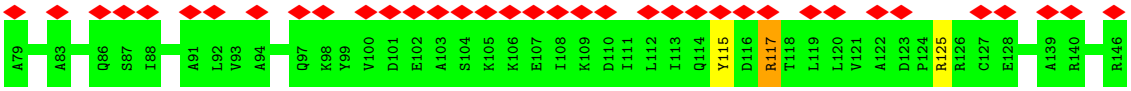


- Molecule 12: 40S ribosomal protein S16

Chain SQ:

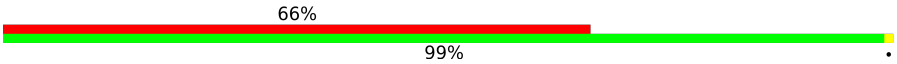


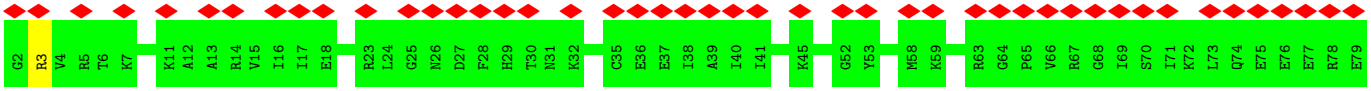


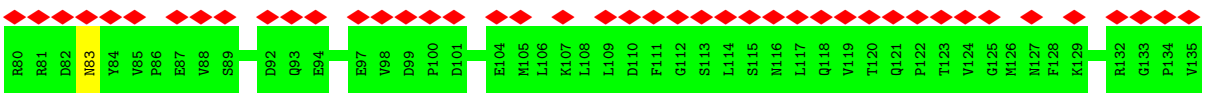


- Molecule 13: 40S ribosomal protein S17

Chain SR:

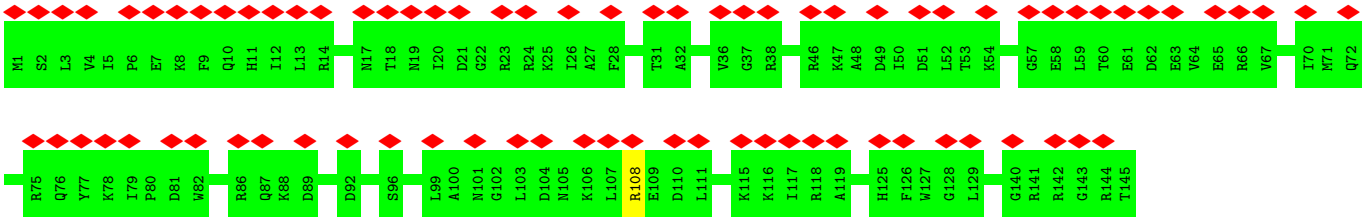






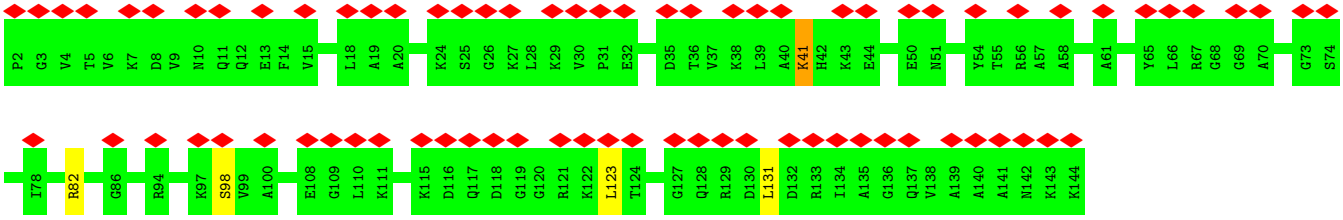
- Molecule 14: 40S ribosomal protein S18

Chain SS: 54% 99%



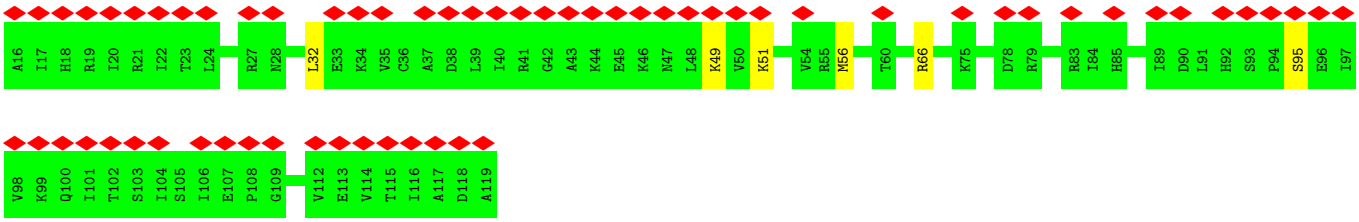
- Molecule 15: 40S ribosomal protein S19

Chain ST: 53% 97%



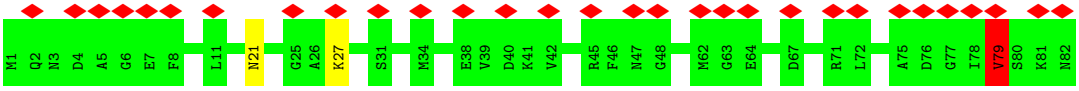
- Molecule 16: 40S ribosomal protein S20

Chain SU: 61% 94% 6%



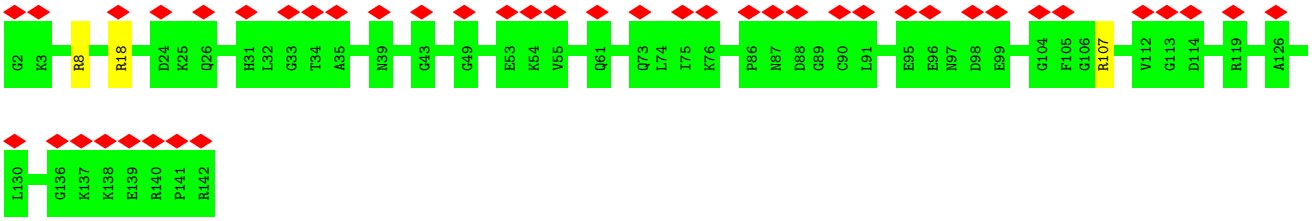
- Molecule 17: 40S ribosomal protein S21

Chain SV: 37% 96%



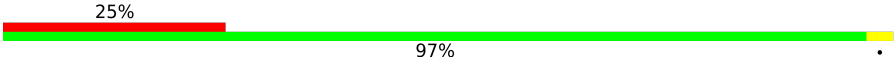
- Molecule 18: 40S ribosomal protein S23

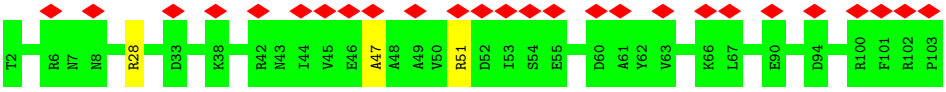
Chain SX: 30% 98%



• Molecule 19: 40S ribosomal protein S26

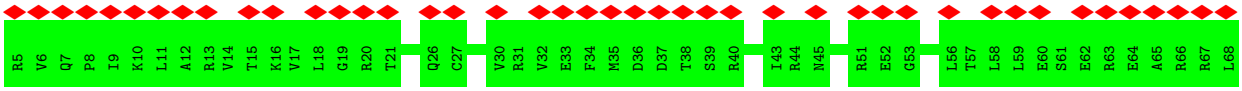
Chain Sa:





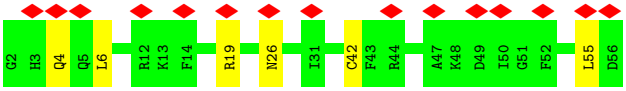
• Molecule 20: 40S ribosomal protein S28

Chain Sc:



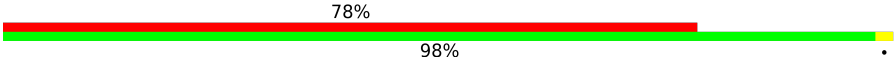
• Molecule 21: 40S ribosomal protein S29

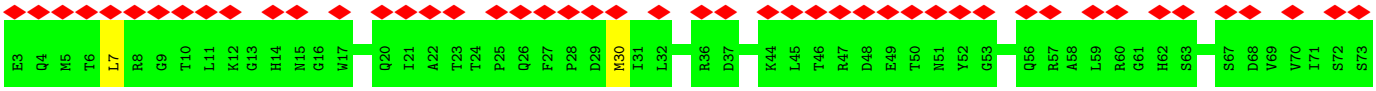
Chain Sd:

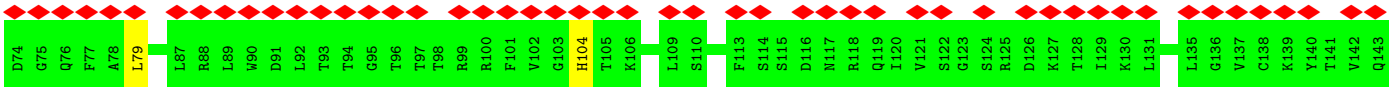


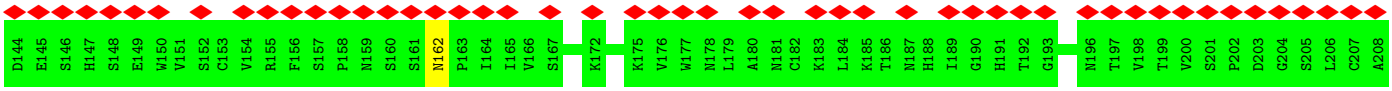
• Molecule 22: Receptor of activated protein C kinase 1

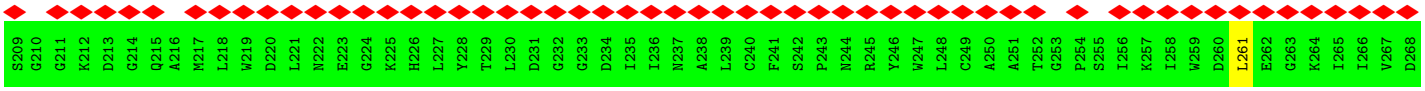
Chain Sg:

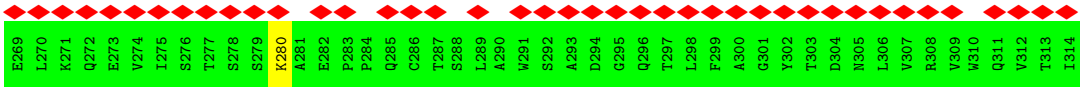






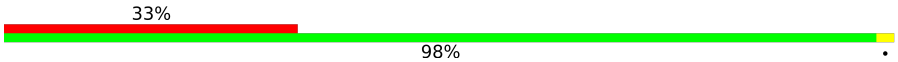


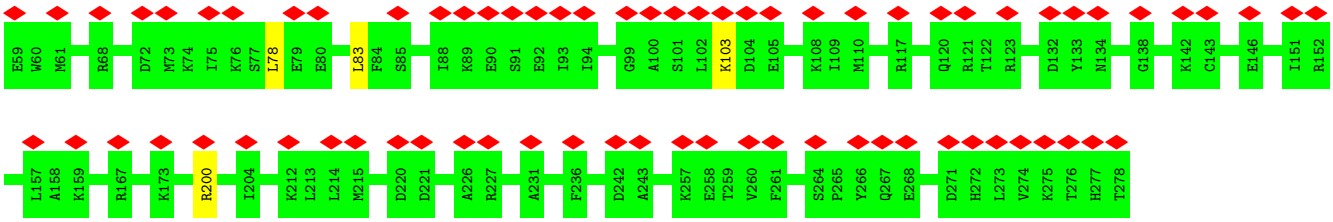




• Molecule 23: 40S ribosomal protein S2

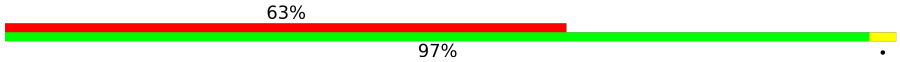
Chain SC:

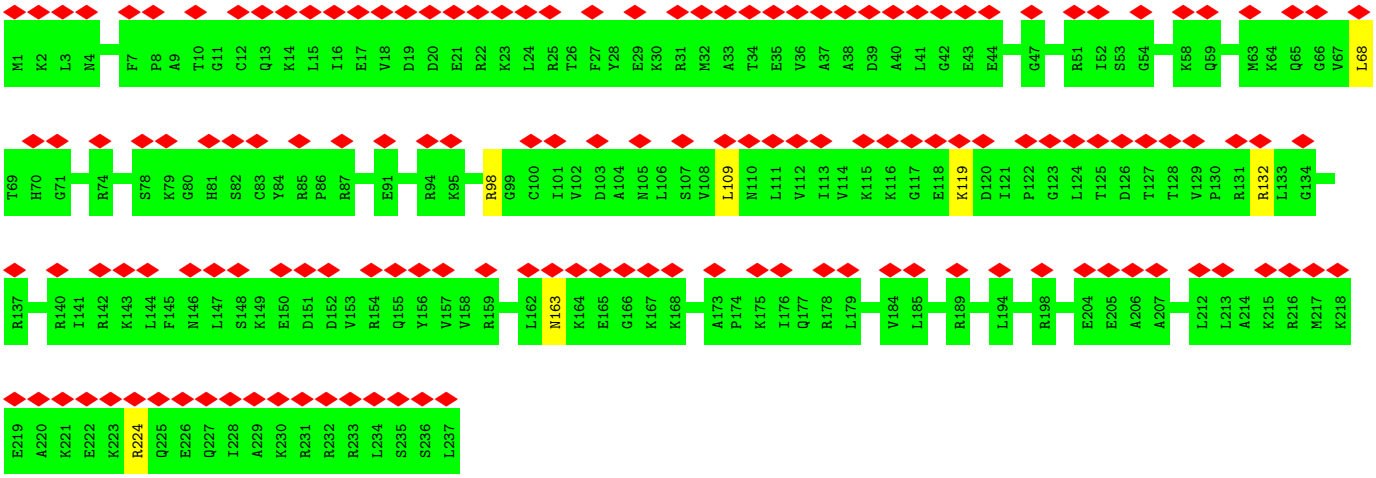




- Molecule 24: 40S ribosomal protein S6

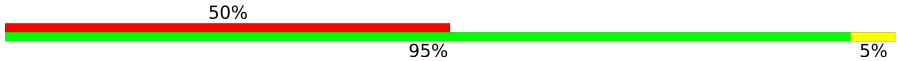
Chain SG:

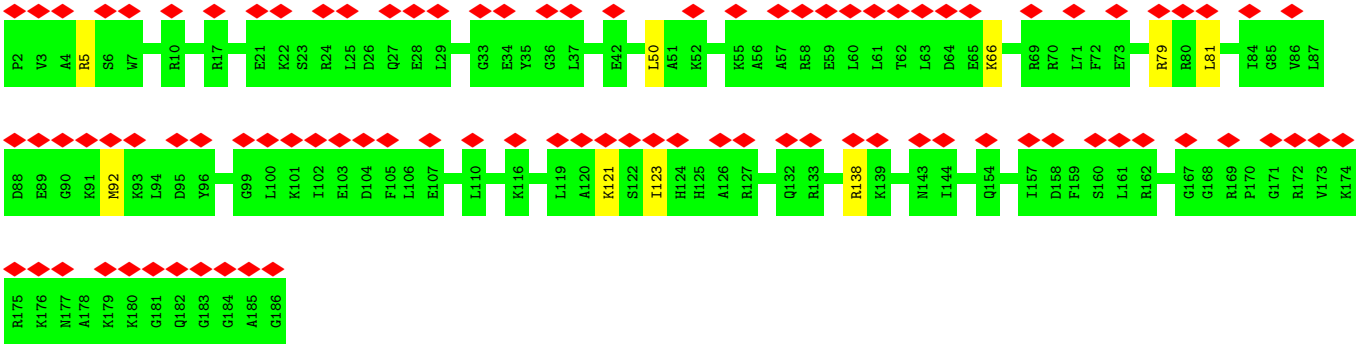




- Molecule 25: 40S ribosomal protein S9

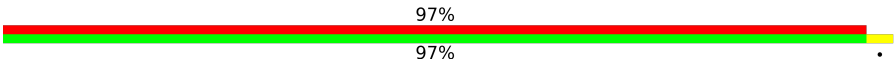
Chain SJ:

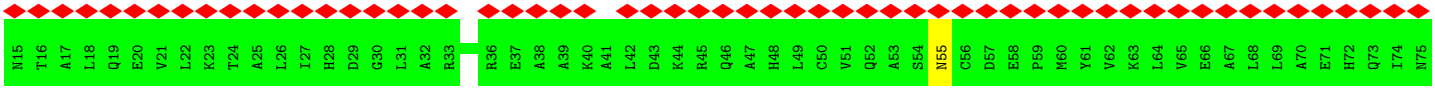


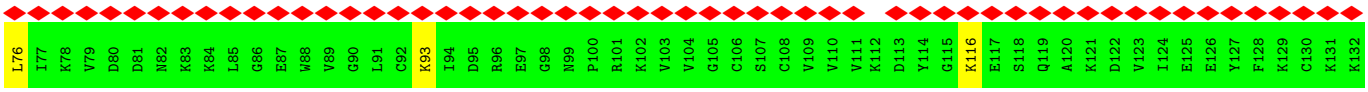


- Molecule 26: 40S ribosomal protein S12

Chain SM:

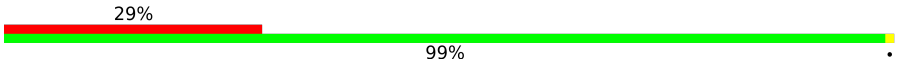


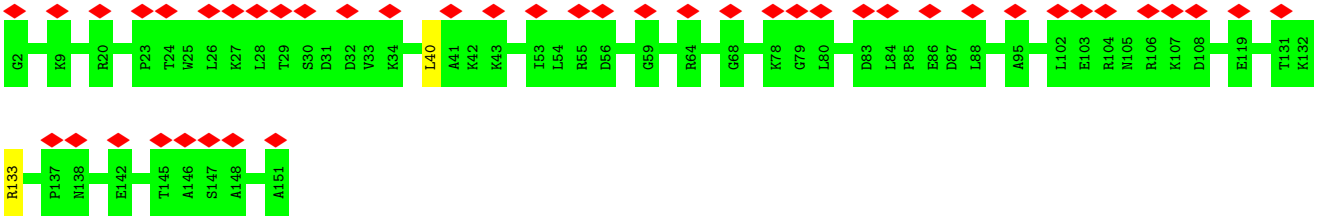




• Molecule 27: 40S ribosomal protein S13

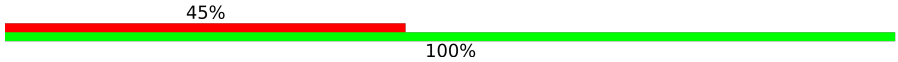
Chain SN:

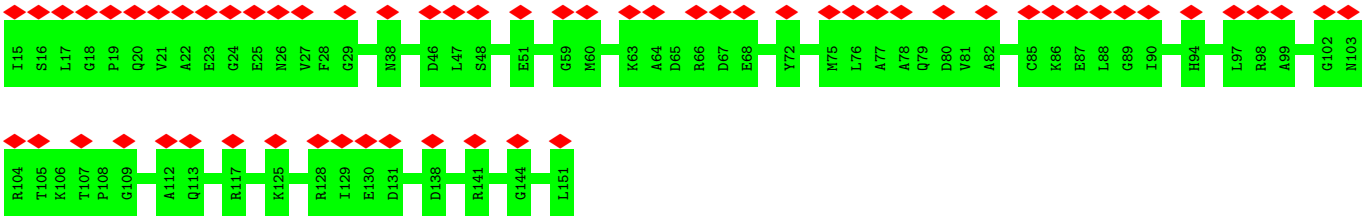




• Molecule 28: 40S ribosomal protein S14

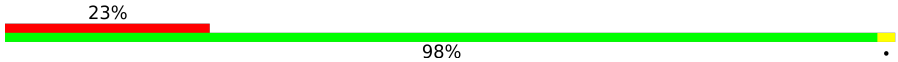
Chain SO:

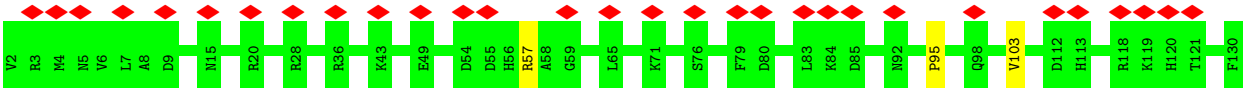




• Molecule 29: 40S ribosomal protein S15a

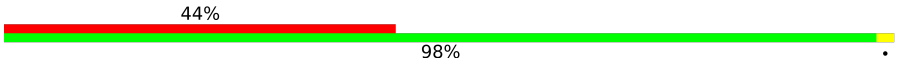
Chain SW:

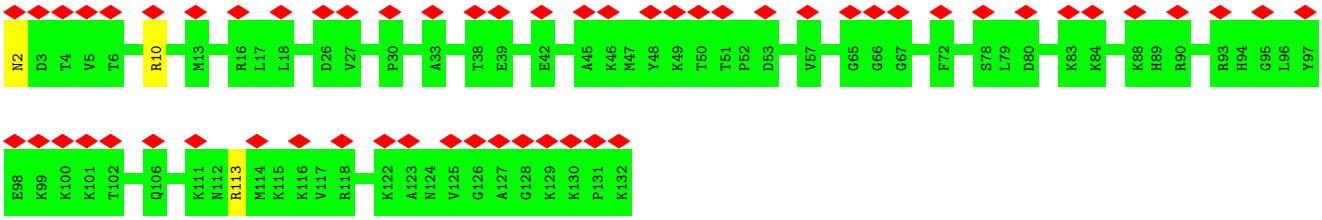




• Molecule 30: 40S ribosomal protein S24

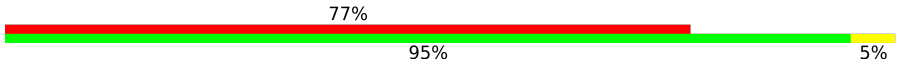
Chain SY:

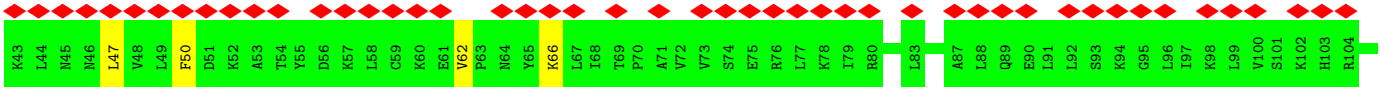


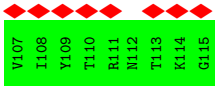


• Molecule 31: 40S ribosomal protein S25

Chain SZ:

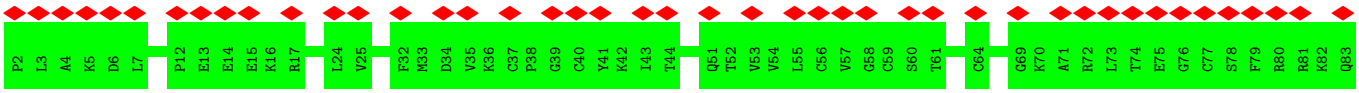






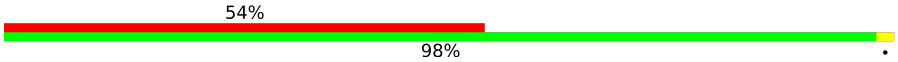
- Molecule 32: 40S ribosomal protein S27

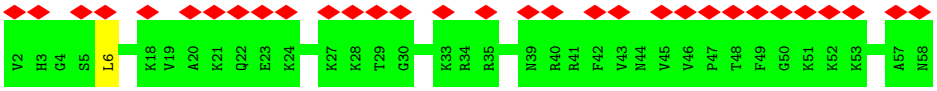
Chain Sb:



- Molecule 33: 40S ribosomal protein S30

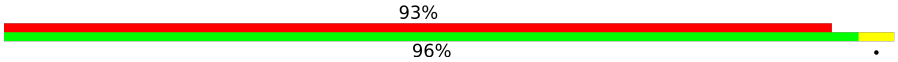
Chain Se:

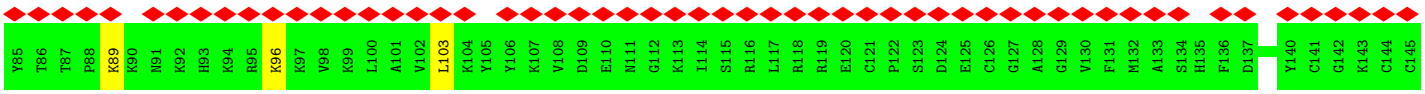


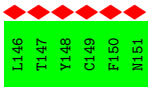


- Molecule 34: 40S ribosomal protein S27a

Chain Sf:

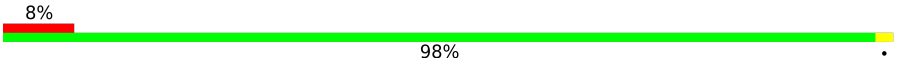


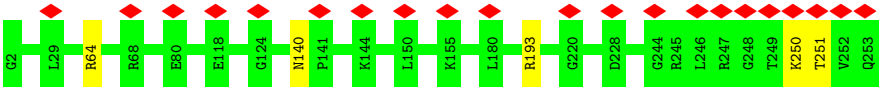




- Molecule 35: 60S ribosomal protein L8

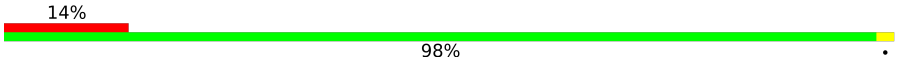
Chain A:

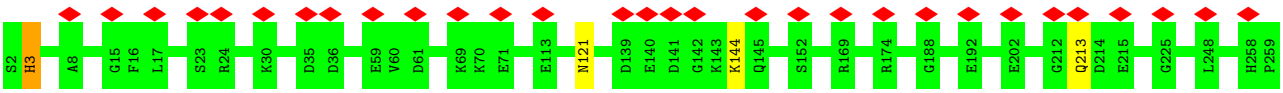


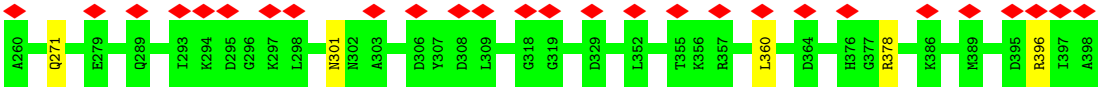


- Molecule 36: 60S ribosomal protein L3

Chain B:

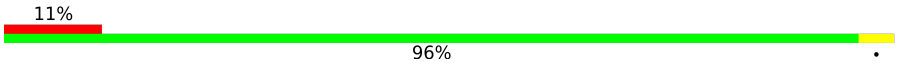


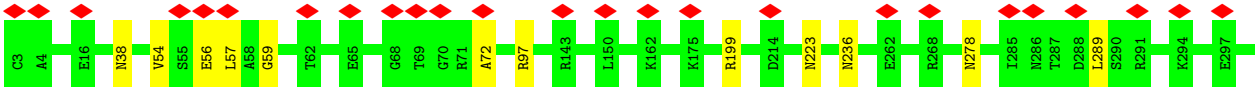


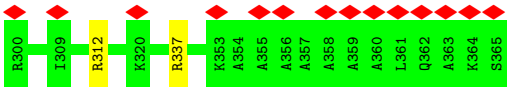


- Molecule 37: 60S ribosomal protein L4

Chain C:

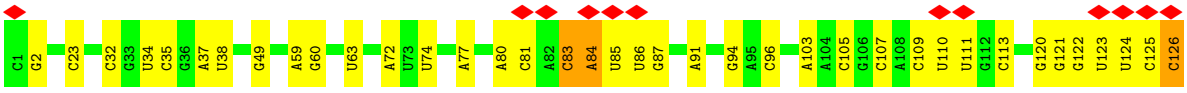


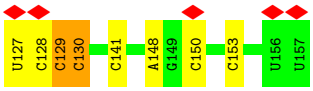




- Molecule 38: 5.8S ribosomal RNA

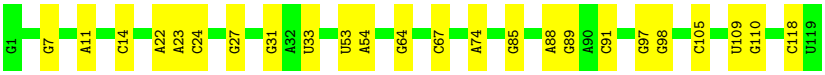
Chain D:





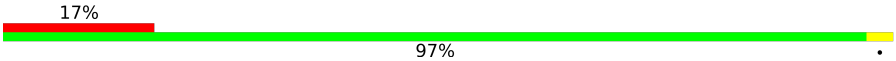
- Molecule 39: 5S ribosomal RNA

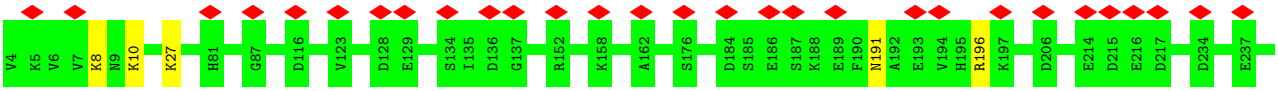
Chain E:

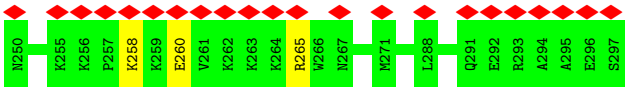


- Molecule 40: 60S ribosomal protein L5

Chain F:

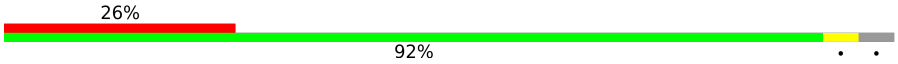


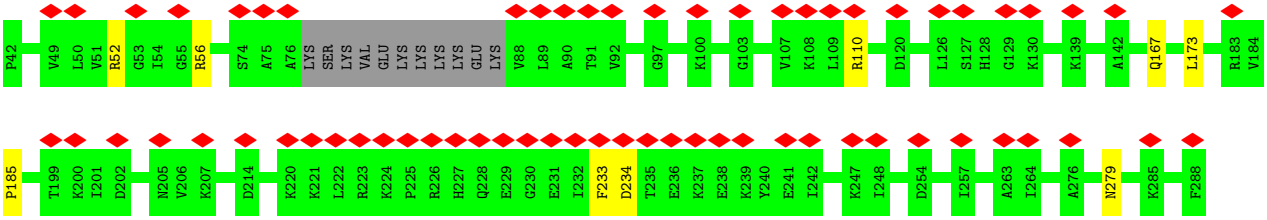




- Molecule 41: 60S ribosomal protein L6

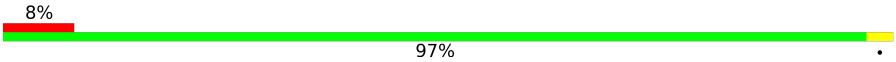
Chain G:

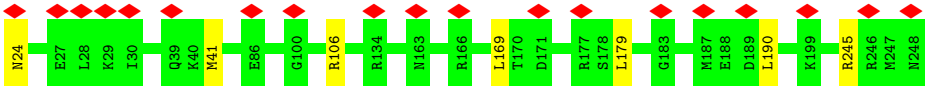




• Molecule 42: 60S ribosomal protein L7

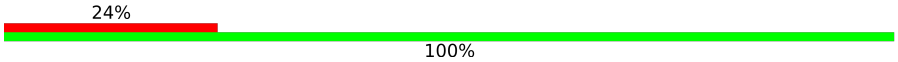
Chain H:

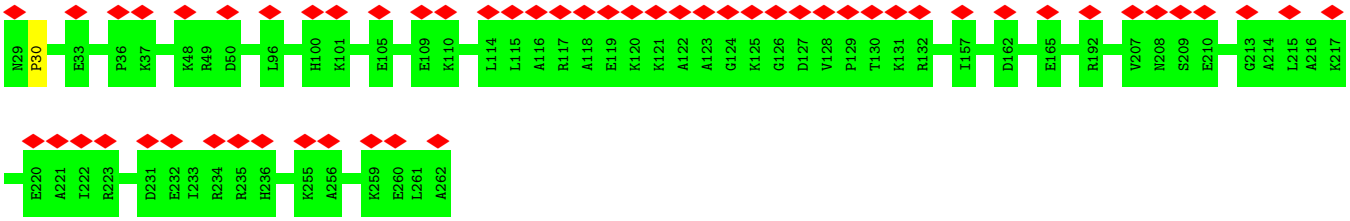




• Molecule 43: 60S ribosomal protein L7a

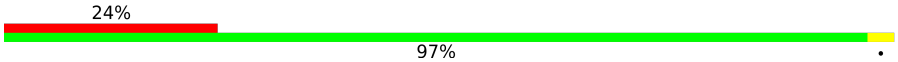
Chain I:

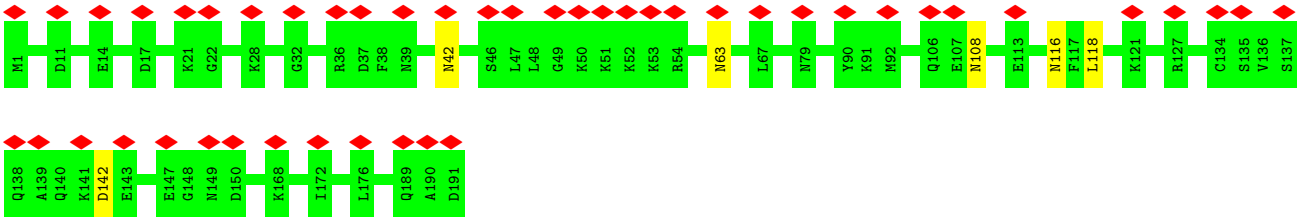




• Molecule 44: 60S ribosomal protein L9

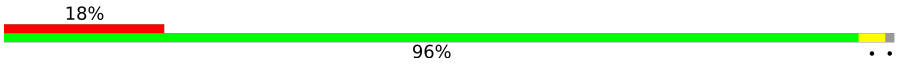
Chain J:

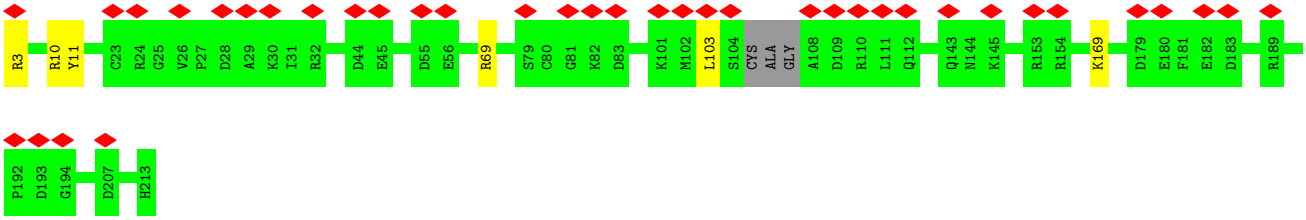




• Molecule 45: 60S ribosomal protein L10

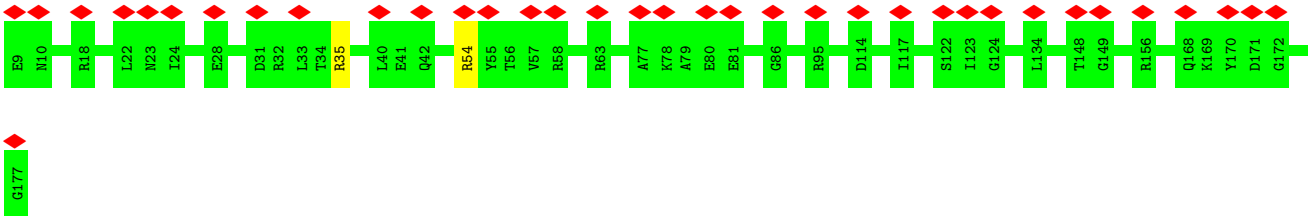
Chain K:





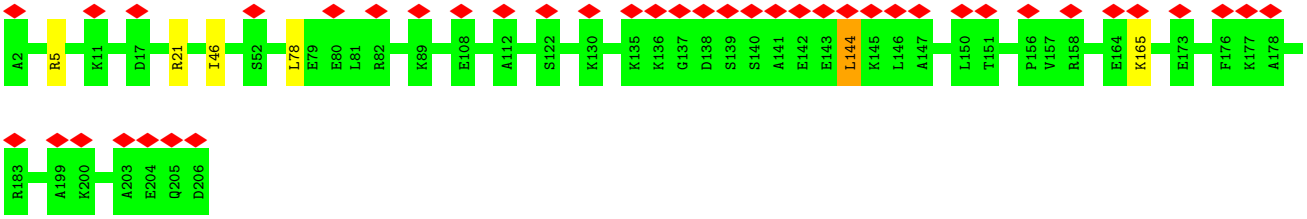
• Molecule 46: 60S ribosomal protein L11

Chain L: 21% 99%



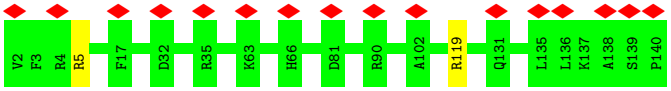
- Molecule 47: 60S ribosomal protein L13

Chain M: 20% 97%



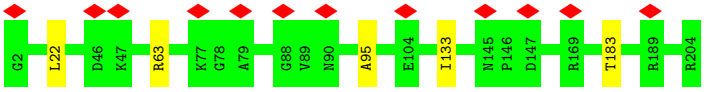
- Molecule 48: 60S ribosomal protein L14

Chain N: 12% 99%



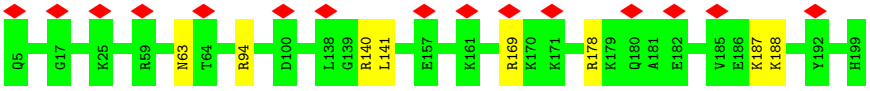
- Molecule 49: 60S ribosomal protein L15

Chain O: 6% 98%



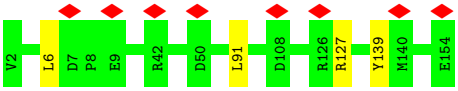
- Molecule 50: 60S ribosomal protein L13a

Chain P: 8% 96%



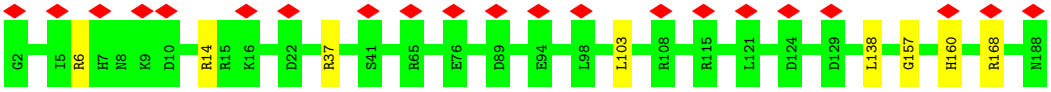
- Molecule 51: 60S ribosomal protein L17

Chain Q: 5% 97%



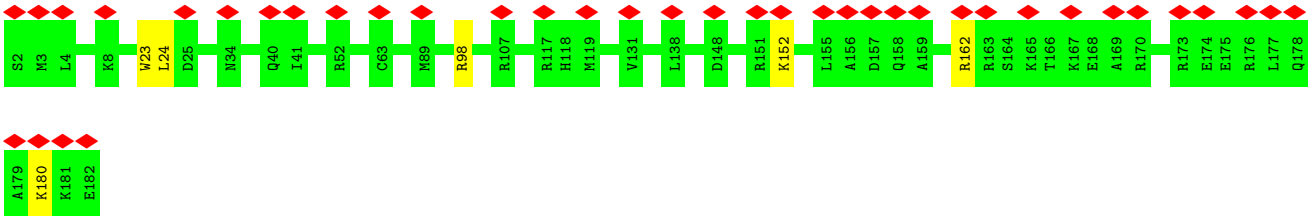
• Molecule 52: 60S ribosomal protein L18

Chain R: 11% 96%



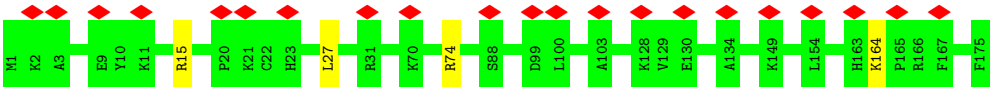
• Molecule 53: 60S ribosomal protein L19

Chain S: 22% 97%



• Molecule 54: 60S ribosomal protein L18a

Chain T: 12% 98%

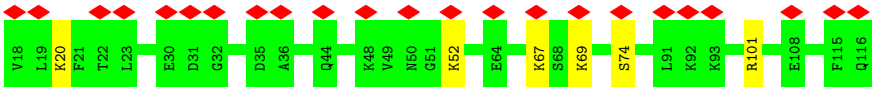


• Molecule 55: 60S ribosomal protein L21

Chain U: 12% 97%

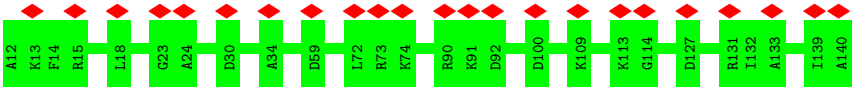
• Molecule 56: 60S ribosomal protein L22

Chain V: 23% 94% 6%



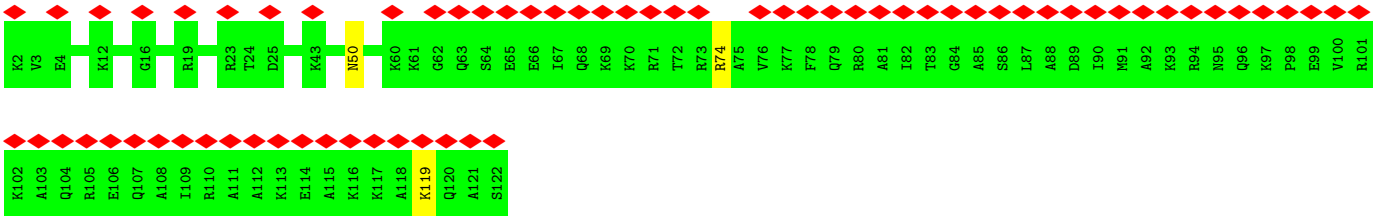
• Molecule 57: 60S ribosomal protein L23

Chain W: 18% 100%



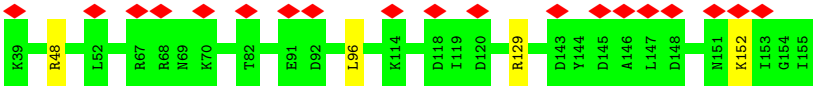
• Molecule 58: 60S ribosomal protein L24

Chain X: 56% 98%



- Molecule 59: 60S ribosomal protein L23a

Chain Y: 16% 97%

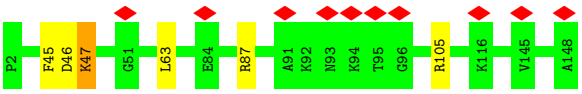


- Molecule 60: 60S ribosomal protein L26

Chain Z: 14% 99%

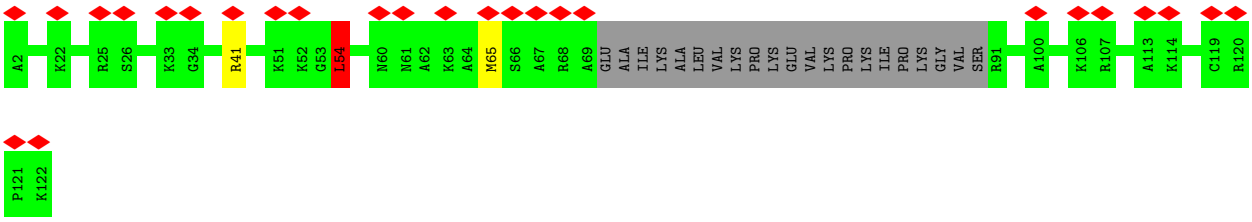
- Molecule 61: 60S ribosomal protein L27a

Chain b: 7% 96%



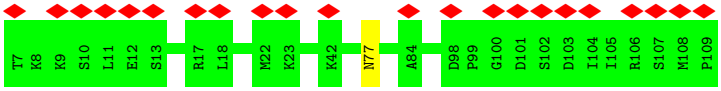
- Molecule 62: 60S ribosomal protein L29

Chain c: 21% 80% 17%



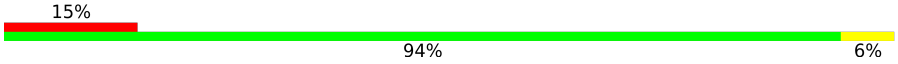
- Molecule 63: 60S ribosomal protein L30

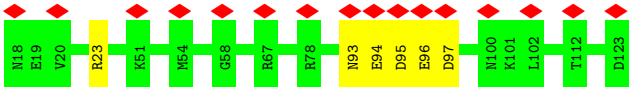
Chain d: 21% 99%



- Molecule 64: 60S ribosomal protein L31

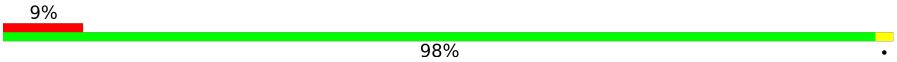
Chain e:

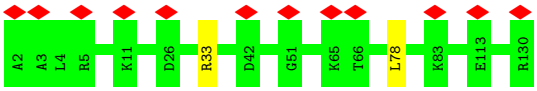




- Molecule 65: 60S ribosomal protein L32

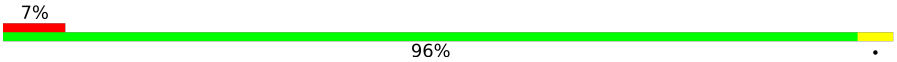
Chain f:

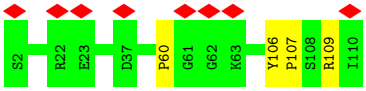




- Molecule 66: 60S ribosomal protein L35a

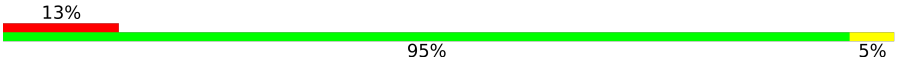
Chain g:

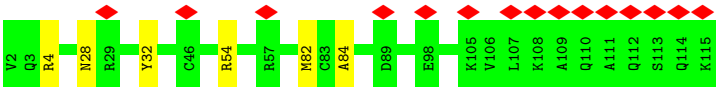




- Molecule 67: 60S ribosomal protein L34

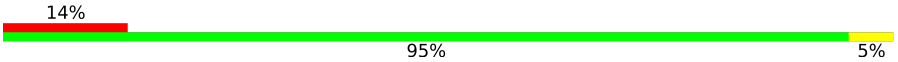
Chain h:

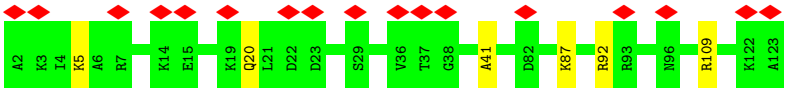




- Molecule 68: 60S ribosomal protein L35

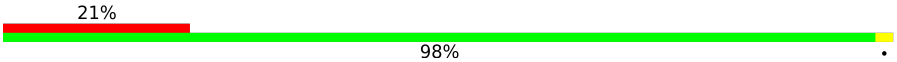
Chain i:

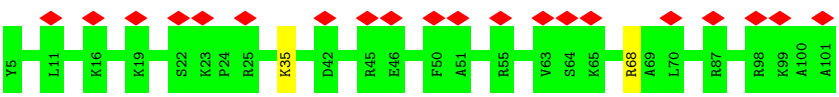




- Molecule 69: 60S ribosomal protein L36

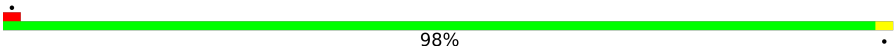
Chain j:

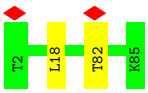




- Molecule 70: 60S ribosomal protein L37

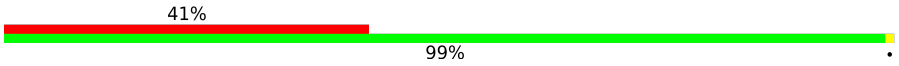
Chain k:

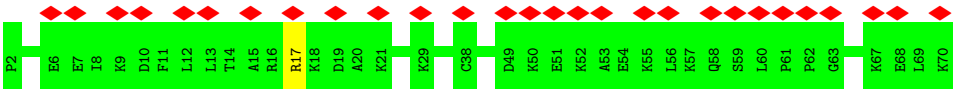




• Molecule 71: 60S ribosomal protein L38

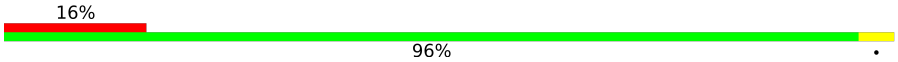
Chain l:

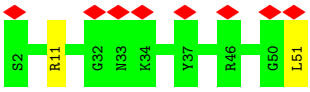




• Molecule 72: 60S ribosomal protein L39

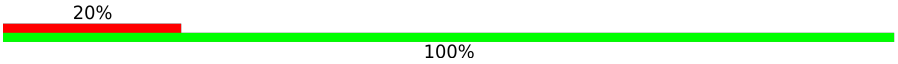
Chain m:

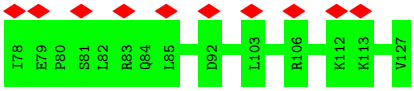




• Molecule 73: 60S ribosomal protein L40

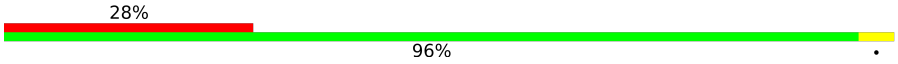
Chain n:

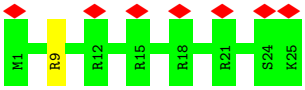




• Molecule 74: 60S ribosomal protein L41

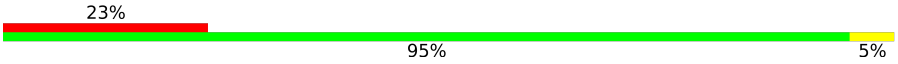
Chain o:

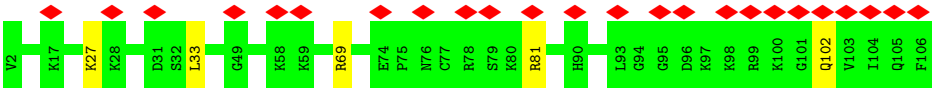




• Molecule 75: 60S ribosomal protein L36a

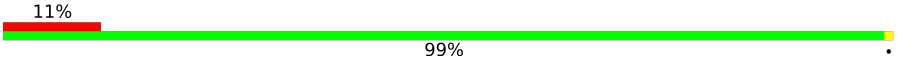
Chain p:

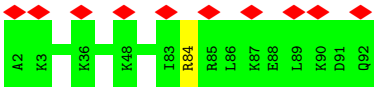




• Molecule 76: 60S ribosomal protein L37a

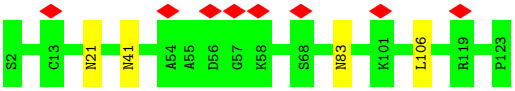
Chain q:





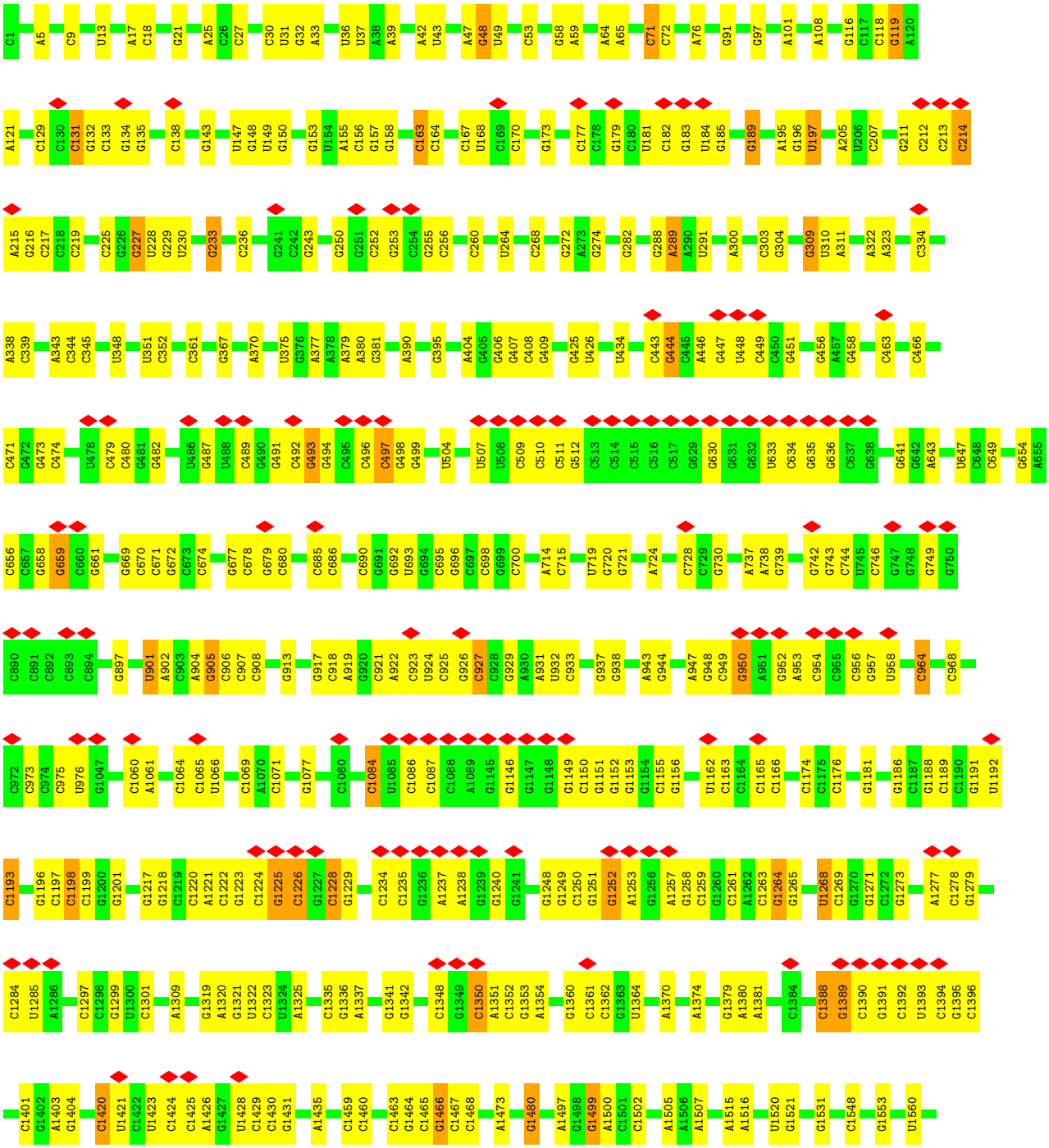
• Molecule 77: 60S ribosomal protein L28

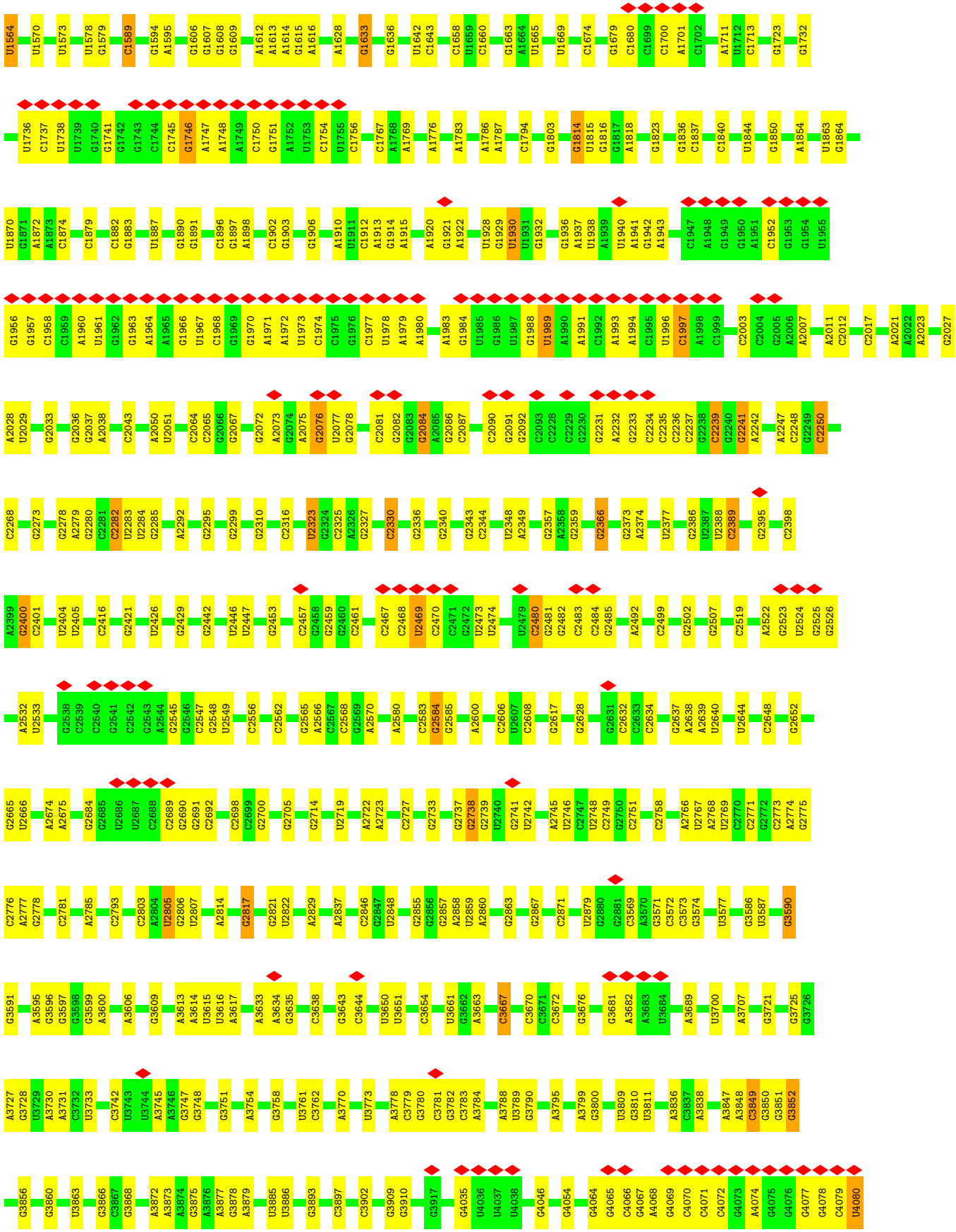
Chain r: 7% 97%

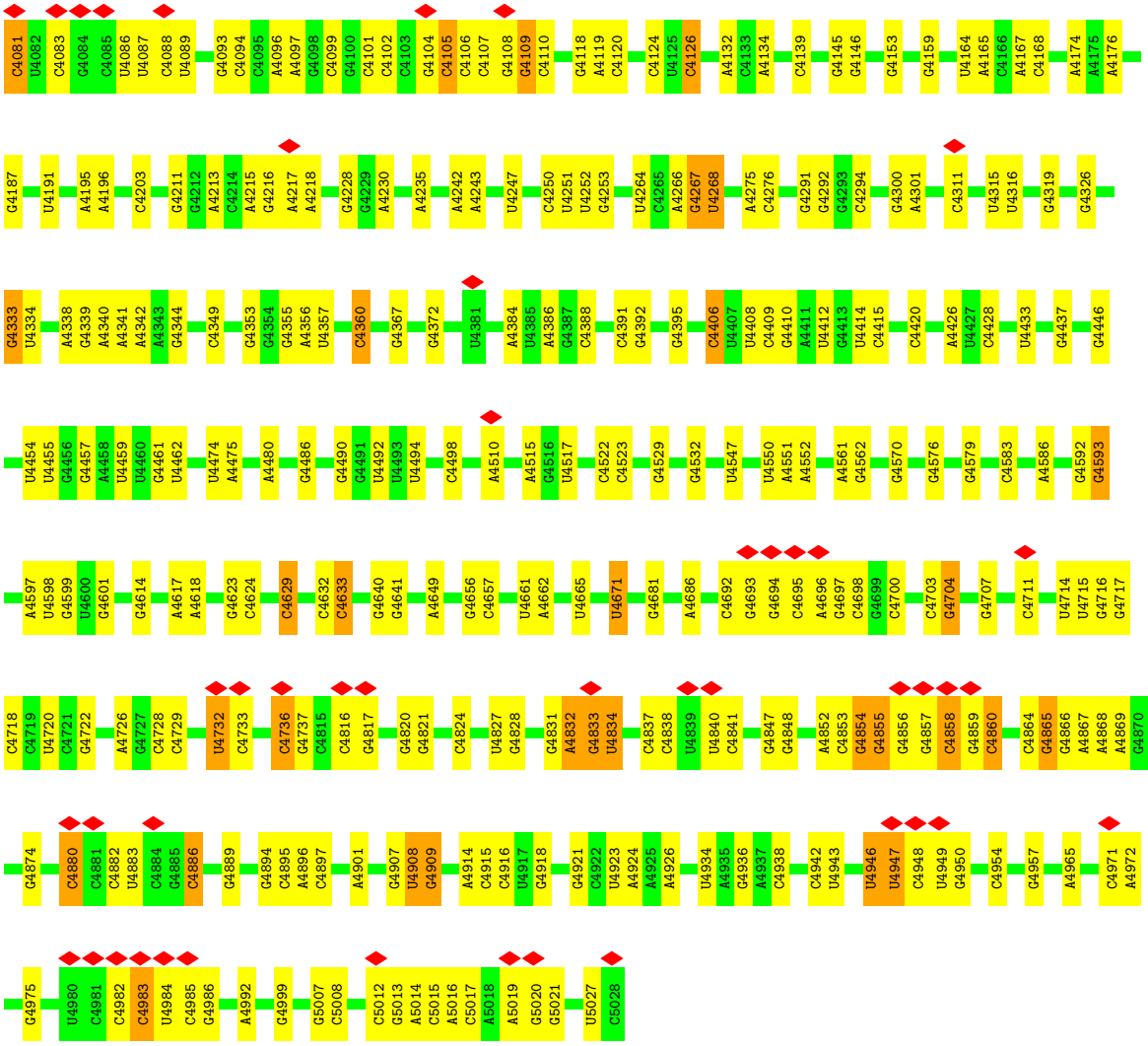


• Molecule 78: 28S ribosomal RNA

Chain t: 9% 68% 29%

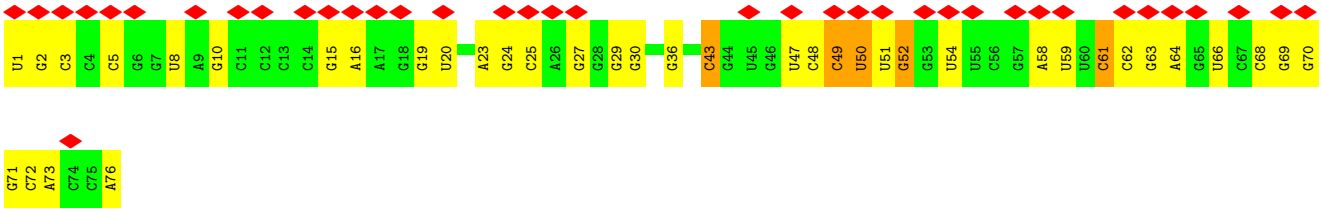



U1564 U1570 U1573 U1578 G1579 C1589 G1594 A1595 G1606 G1607 G1608 G1609 A1612 A1613 A1614 G1615 A1616 A1628 G1633 G1636 U1642 C1643 C1658 U1659 C1660 G1663 A1664 U1665 U1669 C1674 G1679 C1680 C1699 C1700 A1701 C1702 A1711 U1712 C1713 G1723 G1732
U1736 C1737 U1738 U1739 G1740 G1741 G1742 G1743 C1744 C1745 G1746 A1747 A1748 A1749 C1750 G1751 A1752 U1753 C1754 U1755 C1756 C1767 A1768 A1769 A1776 A1783 A1786 A1787 C1794 G1803 G1814 U1815 G1816 G1817 A1818 G1823 G1836 C1837 C1840 U1844 G1850 A1854 U1863 G1864
U1870 G1871 A1872 A1873 C1874 C1879 C1882 G1883 U1887 G1890 G1891 C1896 G1897 A1898 C1902 G1903 G1906 A1910 U1911 C1912 A1913 G1914 A1915 A1920 G1921 A1922 U1928 G1929 U1930 U1931 G1932 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 U1973 C1974 C1975 G1976 C1977 U1978 A1979 A1980 A1983 G1984 U1985 G1986 U1987 G1988 U1989 A1990 A1991 C1992 A1993 A1994 C1995 U1996 C1997 A1998 C1999 C2003 C2004 G2005 A2006 A2007 A2011 C2012 C2017 A2021 A2022 A2023 G2027
A2028 U2029 G2033 G2036 G2037 A2038 C2043 A2050 U2051 C2064 C2065 G2066 G2067 G2072 A2073 G2074 A2075 G2076 U2077 G2078 C2081 G2082 G2083 G2084 A2085 G2086 C2087 C2090 G2091 G2092 C2093 C2228 C2229 G2230 G2231 A2232 G2233 C2234 C2235 C2236 C2237 G2238 C2239 G2240 G2241 A2242 A2247 C2248 G2249 C2250
C2268 G2273 G2278 A2279 G2280 C2281 C2282 U2283 U2284 G2285 A2292 G2295 G2299 G2310 C2316 U2323 G2324 C2325 A2326 G2327 C2330 G2336 G2340 G2343 C2344 U2348 A2349 G2357 A2358 G2359 G2366 G2373 A2374 U2377 G2386 U2387 U2388 C2389 G2395 C2398
A2399 G2400 C2401 U2404 U2405 C2416 G2421 U2426 G2429 G2442 U2446 U2447 G2453 C2457 G2458 G2459 G2460 C2461 C2467 C2468 U2469 C2470 C2471 G2472 U2473 U2474 U2479 C2480 G2481 G2482 C2483 C2484 G2485 A2492 C2499 G2502 G2507 C2519 A2522 G2523 U2524 G2525 G2526
A2532 U2533 G2538 C2539 C2540 G2541 C2542 G2543 A2544 G2545 G2546 C2547 G2548 U2549 C2556 C2562 G2565 A2566 C2567 C2568 G2569 A2570 A2580 C2583 G2584 G2585 A2600 C2606 U2607 C2608 G2617 G2628 G2631 C2632 C2633 C2634 G2637 A2638 A2639 U2640 U2644 C2648 G2652
G2665 U2666 A2674 A2675 G2684 G2685 U2686 U2687 C2688 C2689 G2690 G2691 C2692 C2698 C2699 G2700 G2705 G2714 U2719 A2722 A2723 C2727 G2733 G2737 G2738 G2739 U2740 G2741 U2742 A2745 U2746 C2747 U2748 C2749 G2750 C2751 C2758 A2766 U2767 A2768 U2769 C2770 C2771 G2772 C2773 A2774 G2775
C2776 A2777 G2778 C2781 A2785 C2793 C2803 A2804 U2805 G2806 U2807 A2814 G2817 G2821 U2822 A2829 A2837 C2846 G2847 U2848 G2855 G2856 G2857 A2858 U2859 A2860 G2863 G2867 C2871 U2879 G2880 G2881 C3569 A3570 G3571 C3572 C3573 G3574 U3577 G3586 U3587 G3590
G3591 A3595 G3596 G3597 G3598 G3599 A3600 A3606 G3609 A3613 A3614 U3615 U3616 A3617 A3633 A3634 G3635 C3638 G3643 C3644 U3650 U3651 C3654 U3661 G3662 A3663 C3667 C3670 C3671 C3672 G3676 G3681 A3682 A3683 U3684 A3689 U3700 A3707 G3721 G3725 G3726
A3727 G3728 U3729 A3730 A3731 C3732 U3733 C3742 U3743 U3744 A3745 A3746 G3747 G3748 G3751 A3754 G3758 U3761 C3762 A3770 U3773 A3778 C3779 G3780 C3781 G3782 C3783 A3784 A3788 U3789 G3790 A3795 A3799 G3800 U3809 G3810 U3811 A3836 C3837 A3838 A3847 A3848 C3849 G3850 G3851 G3852
G3856 G3860 U3863 G3866 C3867 G3868 A3872 A3873 A3874 G3875 A3876 A3877 G3878 A3879 U3885 U3886 G3893 C3897 C3902 G3909 G3910 G3917 G4035 U4036 U4037 U4038 G4046 G4054 G4064 G4065 C4066 G4067 A4068 G4069 C4070 C4071 C4072 G4073 A4074 G4075 G4076 G4077 G4078 C4079 U4080



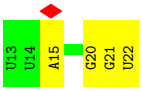
- Molecule 79: AA tRNA

Chain v:



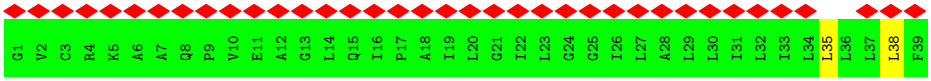
- Molecule 80: mRNA

Chain w:



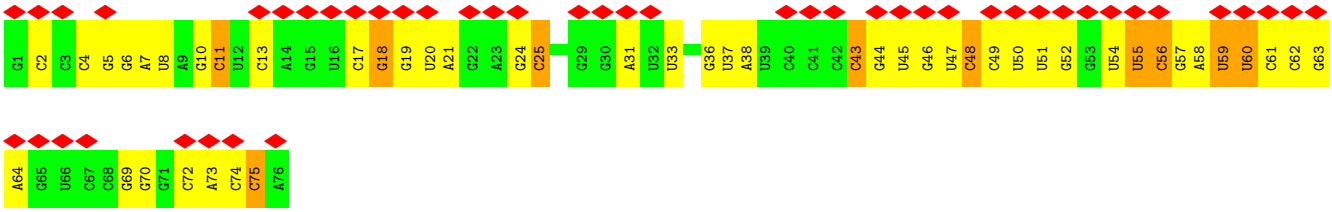
- Molecule 81: Cadherin-1

Chain y: 95% 95% 5%



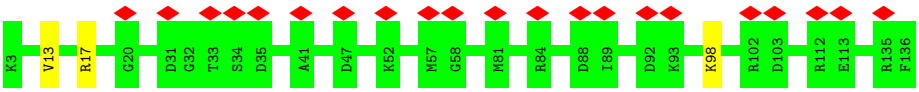
- Molecule 82: PE tRNA

Chain u: 62% 37% 50% 13%



- Molecule 83: 60S ribosomal protein L27

Chain a: 16% 98%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10350	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	0.096	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	460.0, 460.0, 460.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	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: B8Q, M7A, MG, MA6, 5MC, ZN, OMG, E3C, 4AC, PSU, B8N, OMU, OMC, MVM, 5MU, A2M, 6MZ, UR3

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	S2	2.35	14/39959 (0.0%)	1.15	217/62253 (0.3%)
2	SA	0.42	0/1778	0.67	1/2416 (0.0%)
3	SB	0.39	0/1765	0.63	2/2362 (0.1%)
4	SD	0.38	0/1785	0.68	0/2404
5	SE	0.37	0/2101	0.65	0/2828
6	SF	0.36	0/1516	0.64	1/2037 (0.0%)
7	SH	0.40	0/1519	0.69	1/2033 (0.0%)
8	SI	0.38	0/1702	0.69	2/2271 (0.1%)
9	SK	0.42	0/851	0.67	0/1147
10	SL	1.36	1/1268 (0.1%)	0.82	5/1696 (0.3%)
11	SP	0.37	0/1065	0.65	0/1423
12	SQ	0.40	0/1177	0.66	0/1575
13	SR	0.35	0/1097	0.68	0/1474
14	SS	0.36	0/1216	0.66	0/1628
15	ST	0.34	0/1131	0.63	1/1515 (0.1%)
16	SU	0.33	0/831	0.68	1/1115 (0.1%)
17	SV	0.42	0/631	0.73	1/844 (0.1%)
18	SX	0.43	0/1116	0.69	0/1490
19	Sa	0.45	0/836	0.67	0/1121
20	Sc	0.38	0/508	0.68	0/680
21	Sd	0.50	1/470 (0.2%)	0.80	2/623 (0.3%)
22	Sg	0.35	0/2486	0.73	4/3384 (0.1%)
23	SC	0.47	0/1755	0.74	1/2371 (0.0%)
24	SG	0.34	0/1946	0.66	2/2590 (0.1%)
25	SJ	0.38	0/1561	0.73	2/2083 (0.1%)
26	SM	0.32	0/922	0.69	1/1238 (0.1%)
27	SN	0.37	0/1232	0.64	1/1656 (0.1%)
28	SO	0.38	0/1037	0.66	0/1391
29	SW	0.43	0/1051	0.63	0/1406
30	SY	0.35	0/1094	0.60	0/1452
31	SZ	0.36	0/585	0.85	1/785 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Sb	0.37	0/653	0.63	0/876
33	Se	0.34	0/458	0.65	0/604
34	Sf	0.35	0/560	0.72	1/745 (0.1%)
35	A	0.52	0/1968	0.67	0/2639
36	B	0.48	0/3270	0.70	2/4377 (0.0%)
37	C	0.49	0/2942	0.68	1/3951 (0.0%)
38	D	0.91	1/3726 (0.0%)	1.13	20/5804 (0.3%)
39	E	0.86	0/2839	1.07	7/4425 (0.2%)
40	F	0.44	0/2437	0.65	0/3262
41	G	0.43	0/1942	0.74	3/2606 (0.1%)
42	H	0.53	0/1905	0.71	3/2539 (0.1%)
43	I	0.45	0/1913	0.68	0/2576
44	J	0.43	0/1545	0.69	2/2077 (0.1%)
45	K	0.45	0/1730	0.66	1/2311 (0.0%)
46	L	0.42	0/1376	0.68	0/1841
47	M	0.47	0/1688	0.71	1/2260 (0.0%)
48	N	0.45	0/1161	0.62	0/1554
49	O	0.57	0/1746	0.71	0/2338
50	P	0.47	0/1638	0.65	1/2191 (0.0%)
51	Q	0.49	0/1268	0.65	2/1701 (0.1%)
52	R	0.50	0/1537	0.69	2/2052 (0.1%)
53	S	0.46	0/1533	0.71	1/2025 (0.0%)
54	T	0.51	0/1488	0.66	1/1997 (0.1%)
55	U	0.48	0/1312	0.67	0/1753
56	V	0.44	0/822	0.68	0/1103
57	W	0.45	0/983	0.62	0/1319
58	X	4.12	1/1004 (0.1%)	0.74	1/1332 (0.1%)
59	Y	0.45	0/975	0.65	0/1312
60	Z	0.48	0/1132	0.64	0/1504
61	b	0.52	0/1191	0.69	0/1591
62	c	0.39	0/826	0.70	1/1088 (0.1%)
63	d	0.49	0/812	0.72	0/1089
64	e	0.45	0/894	0.67	0/1204
65	f	0.48	0/1082	0.64	1/1443 (0.1%)
66	g	0.53	0/895	0.72	1/1198 (0.1%)
67	h	0.53	1/916 (0.1%)	0.73	0/1220
68	i	0.42	0/1023	0.70	0/1351
69	j	0.38	0/805	0.66	0/1065
70	k	0.51	0/703	0.71	1/929 (0.1%)
71	l	0.37	0/575	0.67	0/761
72	m	0.42	0/454	0.71	1/599 (0.2%)
73	n	0.40	0/417	0.69	0/553
74	o	0.42	0/241	0.72	0/305

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
75	p	0.46	0/877	0.71	1/1156 (0.1%)
76	q	0.54	0/718	0.74	0/953
77	r	0.53	0/995	0.74	1/1334 (0.1%)
78	t	0.91	4/86502 (0.0%)	1.17	508/134927 (0.4%)
79	v	0.58	0/1802	1.23	14/2797 (0.5%)
80	w	0.70	0/235	1.25	2/365 (0.5%)
81	y	0.35	0/263	1.02	1/359 (0.3%)
82	u	0.56	0/1800	1.39	34/2804 (1.2%)
83	a	0.47	0/1126	0.69	0/1502
All	All	1.21	23/230694 (0.0%)	1.01	861/338958 (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
11	SP	0	1
15	ST	0	1
16	SU	0	1
56	V	0	1
62	c	0	1
All	All	0	5

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	291	G	N7-C5	229.25	2.76	1.39
1	S2	291	G	C8-N7	214.07	2.59	1.30
1	S2	291	G	N9-C8	184.78	2.67	1.37
1	S2	291	G	N9-C4	174.09	2.77	1.38
1	S2	291	G	C5-C4	160.98	2.51	1.38

The worst 5 of 861 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	291	G	C6-N1-C2	25.90	140.64	125.10
1	S2	291	G	N3-C4-C5	-25.47	115.87	128.60
1	S2	291	G	C6-C5-N7	23.18	144.31	130.40
1	S2	115	U	C2-N3-C4	21.35	139.81	127.00
1	S2	291	G	N1-C2-N3	19.64	135.68	123.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	SP	14	LYS	Peptide
15	ST	98	SER	Peptide
16	SU	95	SER	Peptide
56	V	74	SER	Mainchain
62	c	54	LEU	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	
2	SA	219/221 (99%)	185 (84%)	33 (15%)	1 (0%)	29	67
3	SB	212/214 (99%)	183 (86%)	28 (13%)	1 (0%)	29	67
4	SD	224/226 (99%)	191 (85%)	33 (15%)	0	100	100
5	SE	257/259 (99%)	223 (87%)	34 (13%)	0	100	100
6	SF	187/189 (99%)	161 (86%)	26 (14%)	0	100	100
7	SH	182/189 (96%)	159 (87%)	23 (13%)	0	100	100
8	SI	202/204 (99%)	171 (85%)	31 (15%)	0	100	100
9	SK	96/98 (98%)	83 (86%)	13 (14%)	0	100	100
10	SL	151/153 (99%)	134 (89%)	17 (11%)	0	100	100
11	SP	125/127 (98%)	109 (87%)	16 (13%)	0	100	100
12	SQ	144/146 (99%)	123 (85%)	19 (13%)	2 (1%)	11	46
13	SR	132/134 (98%)	107 (81%)	25 (19%)	0	100	100
14	SS	143/145 (99%)	126 (88%)	17 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	ST	141/143 (99%)	127 (90%)	13 (9%)	1 (1%)	22	60
16	SU	102/104 (98%)	91 (89%)	11 (11%)	0	100	100
17	SV	80/82 (98%)	68 (85%)	11 (14%)	1 (1%)	12	48
18	SX	139/141 (99%)	120 (86%)	19 (14%)	0	100	100
19	Sa	100/102 (98%)	84 (84%)	15 (15%)	1 (1%)	15	52
20	Sc	62/64 (97%)	48 (77%)	14 (23%)	0	100	100
21	Sd	53/55 (96%)	39 (74%)	13 (24%)	1 (2%)	8	41
22	Sg	310/312 (99%)	245 (79%)	65 (21%)	0	100	100
23	SC	219/220 (100%)	191 (87%)	27 (12%)	1 (0%)	29	67
24	SG	235/237 (99%)	207 (88%)	28 (12%)	0	100	100
25	SJ	184/185 (100%)	163 (89%)	20 (11%)	1 (0%)	29	67
26	SM	116/118 (98%)	97 (84%)	19 (16%)	0	100	100
27	SN	148/150 (99%)	142 (96%)	6 (4%)	0	100	100
28	SO	135/137 (98%)	116 (86%)	19 (14%)	0	100	100
29	SW	127/129 (98%)	115 (91%)	11 (9%)	1 (1%)	19	57
30	SY	130/131 (99%)	118 (91%)	12 (9%)	0	100	100
31	SZ	71/73 (97%)	58 (82%)	12 (17%)	1 (1%)	11	46
32	Sb	80/82 (98%)	68 (85%)	12 (15%)	0	100	100
33	Se	55/57 (96%)	45 (82%)	10 (18%)	0	100	100
34	Sf	65/67 (97%)	51 (78%)	14 (22%)	0	100	100
35	A	250/252 (99%)	219 (88%)	30 (12%)	1 (0%)	34	71
36	B	395/397 (100%)	342 (87%)	52 (13%)	1 (0%)	41	75
37	C	361/363 (99%)	326 (90%)	32 (9%)	3 (1%)	19	57
40	F	292/294 (99%)	253 (87%)	38 (13%)	1 (0%)	41	75
41	G	232/247 (94%)	188 (81%)	43 (18%)	1 (0%)	34	71
42	H	223/225 (99%)	202 (91%)	21 (9%)	0	100	100
43	I	232/234 (99%)	213 (92%)	18 (8%)	1 (0%)	34	71
44	J	189/191 (99%)	162 (86%)	27 (14%)	0	100	100
45	K	204/211 (97%)	183 (90%)	19 (9%)	2 (1%)	15	52
46	L	167/169 (99%)	143 (86%)	24 (14%)	0	100	100
47	M	203/205 (99%)	166 (82%)	36 (18%)	1 (0%)	29	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	N	137/139 (99%)	122 (89%)	15 (11%)	0	100	100
49	O	201/203 (99%)	174 (87%)	26 (13%)	1 (0%)	29	67
50	P	193/195 (99%)	183 (95%)	10 (5%)	0	100	100
51	Q	151/153 (99%)	142 (94%)	9 (6%)	0	100	100
52	R	185/187 (99%)	163 (88%)	21 (11%)	1 (0%)	29	67
53	S	179/181 (99%)	164 (92%)	15 (8%)	0	100	100
54	T	173/175 (99%)	153 (88%)	19 (11%)	1 (1%)	25	63
55	U	155/157 (99%)	130 (84%)	23 (15%)	2 (1%)	12	48
56	V	97/99 (98%)	89 (92%)	8 (8%)	0	100	100
57	W	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
58	X	119/121 (98%)	101 (85%)	17 (14%)	1 (1%)	19	57
59	Y	115/117 (98%)	106 (92%)	9 (8%)	0	100	100
60	Z	132/134 (98%)	118 (89%)	14 (11%)	0	100	100
61	b	145/147 (99%)	124 (86%)	20 (14%)	1 (1%)	22	60
62	c	94/121 (78%)	82 (87%)	12 (13%)	0	100	100
63	d	101/103 (98%)	87 (86%)	14 (14%)	0	100	100
64	e	104/106 (98%)	94 (90%)	8 (8%)	2 (2%)	8	41
65	f	127/129 (98%)	111 (87%)	16 (13%)	0	100	100
66	g	107/109 (98%)	93 (87%)	12 (11%)	2 (2%)	8	41
67	h	112/114 (98%)	98 (88%)	12 (11%)	2 (2%)	8	42
68	i	120/122 (98%)	110 (92%)	8 (7%)	2 (2%)	9	43
69	j	95/97 (98%)	88 (93%)	6 (6%)	1 (1%)	14	51
70	k	82/84 (98%)	72 (88%)	10 (12%)	0	100	100
71	l	67/69 (97%)	62 (92%)	5 (8%)	0	100	100
72	m	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
73	n	48/50 (96%)	39 (81%)	9 (19%)	0	100	100
74	o	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
75	p	103/105 (98%)	89 (86%)	14 (14%)	0	100	100
76	q	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
77	r	120/122 (98%)	104 (87%)	15 (12%)	1 (1%)	19	57
81	y	37/39 (95%)	18 (49%)	19 (51%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
83	a	132/134 (98%)	113 (86%)	19 (14%)	0	100	100
All	All	11292/11489 (98%)	9844 (87%)	1408 (12%)	40 (0%)	38	71

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	SB	86	LEU
12	SQ	117	ARG
17	SV	79	VAL
23	SC	78	LEU
37	C	59	GLY

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	
2	SA	183/183 (100%)	176 (96%)	7 (4%)	33	59
3	SB	195/195 (100%)	191 (98%)	4 (2%)	53	73
4	SD	189/189 (100%)	187 (99%)	2 (1%)	73	84
5	SE	222/222 (100%)	216 (97%)	6 (3%)	44	67
6	SF	159/159 (100%)	157 (99%)	2 (1%)	69	82
7	SH	166/169 (98%)	165 (99%)	1 (1%)	86	91
8	SI	177/177 (100%)	174 (98%)	3 (2%)	60	78
9	SK	89/89 (100%)	86 (97%)	3 (3%)	37	62
10	SL	137/137 (100%)	132 (96%)	5 (4%)	35	61
11	SP	113/113 (100%)	112 (99%)	1 (1%)	78	87
12	SQ	121/121 (100%)	118 (98%)	3 (2%)	47	69
13	SR	121/121 (100%)	119 (98%)	2 (2%)	60	78
14	SS	126/126 (100%)	125 (99%)	1 (1%)	81	89
15	ST	113/113 (100%)	110 (97%)	3 (3%)	44	67
16	SU	94/94 (100%)	90 (96%)	4 (4%)	29	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	SV	66/66 (100%)	63 (96%)	3 (4%)	27	56
18	SX	113/113 (100%)	110 (97%)	3 (3%)	44	67
19	Sa	89/89 (100%)	87 (98%)	2 (2%)	52	71
20	Sc	57/57 (100%)	57 (100%)	0	100	100
21	Sd	48/48 (100%)	46 (96%)	2 (4%)	30	57
22	Sg	271/271 (100%)	268 (99%)	3 (1%)	73	84
23	SC	187/186 (100%)	184 (98%)	3 (2%)	62	79
24	SG	207/207 (100%)	202 (98%)	5 (2%)	49	69
25	SJ	162/161 (101%)	155 (96%)	7 (4%)	29	57
26	SM	98/100 (98%)	95 (97%)	3 (3%)	40	64
27	SN	130/130 (100%)	129 (99%)	1 (1%)	81	89
28	SO	107/107 (100%)	107 (100%)	0	100	100
29	SW	112/112 (100%)	110 (98%)	2 (2%)	59	77
30	SY	114/113 (101%)	110 (96%)	4 (4%)	36	62
31	SZ	64/64 (100%)	62 (97%)	2 (3%)	40	64
32	Sb	74/74 (100%)	74 (100%)	0	100	100
33	Se	46/46 (100%)	45 (98%)	1 (2%)	52	71
34	Sf	60/60 (100%)	58 (97%)	2 (3%)	38	63
35	A	194/194 (100%)	190 (98%)	4 (2%)	53	73
36	B	345/345 (100%)	338 (98%)	7 (2%)	55	74
37	C	302/302 (100%)	292 (97%)	10 (3%)	38	63
40	F	248/248 (100%)	241 (97%)	7 (3%)	43	66
41	G	209/220 (95%)	204 (98%)	5 (2%)	49	69
42	H	194/194 (100%)	190 (98%)	4 (2%)	53	73
43	I	199/199 (100%)	199 (100%)	0	100	100
44	J	170/170 (100%)	166 (98%)	4 (2%)	49	69
45	K	178/179 (99%)	175 (98%)	3 (2%)	60	78
46	L	142/142 (100%)	140 (99%)	2 (1%)	67	81
47	M	171/171 (100%)	166 (97%)	5 (3%)	42	65
48	N	118/118 (100%)	116 (98%)	2 (2%)	60	78
49	O	171/171 (100%)	167 (98%)	4 (2%)	50	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	P	168/168 (100%)	161 (96%)	7 (4%)	30	57
51	Q	134/134 (100%)	132 (98%)	2 (2%)	65	80
52	R	164/164 (100%)	159 (97%)	5 (3%)	41	64
53	S	160/160 (100%)	155 (97%)	5 (3%)	40	64
54	T	156/156 (100%)	154 (99%)	2 (1%)	69	82
55	U	138/138 (100%)	135 (98%)	3 (2%)	52	71
56	V	89/89 (100%)	84 (94%)	5 (6%)	21	51
57	W	100/100 (100%)	100 (100%)	0	100	100
58	X	100/100 (100%)	100 (100%)	0	100	100
59	Y	105/105 (100%)	101 (96%)	4 (4%)	33	59
60	Z	124/124 (100%)	123 (99%)	1 (1%)	81	89
61	b	120/120 (100%)	114 (95%)	6 (5%)	24	53
62	c	82/101 (81%)	79 (96%)	3 (4%)	34	60
63	d	88/88 (100%)	87 (99%)	1 (1%)	73	84
64	e	97/97 (100%)	93 (96%)	4 (4%)	30	58
65	f	115/115 (100%)	114 (99%)	1 (1%)	78	87
66	g	88/88 (100%)	87 (99%)	1 (1%)	73	84
67	h	98/98 (100%)	95 (97%)	3 (3%)	40	64
68	i	109/109 (100%)	105 (96%)	4 (4%)	34	60
69	j	83/83 (100%)	82 (99%)	1 (1%)	71	83
70	k	71/71 (100%)	70 (99%)	1 (1%)	67	81
71	l	64/64 (100%)	63 (98%)	1 (2%)	62	79
72	m	47/47 (100%)	46 (98%)	1 (2%)	53	73
73	n	46/46 (100%)	46 (100%)	0	100	100
74	o	24/24 (100%)	23 (96%)	1 (4%)	30	57
75	p	93/93 (100%)	89 (96%)	4 (4%)	29	57
76	q	74/74 (100%)	73 (99%)	1 (1%)	67	81
77	r	106/106 (100%)	104 (98%)	2 (2%)	57	75
81	y	23/29 (79%)	22 (96%)	1 (4%)	29	57
83	a	117/117 (100%)	114 (97%)	3 (3%)	46	68
All	All	9834/9873 (100%)	9614 (98%)	220 (2%)	54	71

5 of 220 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	F	196	ARG
49	O	22	LEU
83	a	98	LYS
67	h	82	MET
41	G	56	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 134 such sidechains are listed below:

Mol	Chain	Res	Type
63	d	77	ASN
66	g	55	ASN
77	r	12	ASN
25	SJ	140	GLN
25	SJ	111	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1690/1714 (98%)	617 (36%)	26 (1%)
38	D	156/157 (99%)	40 (25%)	0
39	E	118/119 (99%)	20 (16%)	0
78	t	3590/3607 (99%)	1000 (27%)	0
79	v	71/76 (93%)	37 (52%)	0
80	w	9/10 (90%)	3 (33%)	0
82	u	75/76 (98%)	43 (57%)	0
All	All	5709/5759 (99%)	1760 (30%)	26 (0%)

5 of 1760 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	2	A
1	S2	4	C
1	S2	5	U
1	S2	9	U
1	S2	10	G

5 of 26 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	1375	G
1	S2	1572	C
1	S2	1815	A
1	S2	1567	G
1	S2	1600	G

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

34 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OMC	S2	1710	1	19,22,23	3.57	8 (42%)	26,31,34	0.71	0
1	PSU	S2	822	1	18,21,22	4.30	8 (44%)	22,30,33	1.83	4 (18%)
1	4AC	S2	1337	1	21,24,25	3.37	9 (42%)	29,34,37	1.23	4 (13%)
1	PSU	S2	1243	1	18,21,22	4.26	8 (44%)	22,30,33	1.63	4 (18%)
1	B8N	S2	1248	1	24,29,30	2.81	5 (20%)	29,42,45	1.91	6 (20%)
1	5MU	S2	814	1	19,22,23	7.54	8 (42%)	28,32,35	3.50	11 (39%)
1	MA6	S2	1851	1	19,26,27	1.08	1 (5%)	18,38,41	3.81	3 (16%)
1	A2M	S2	159	1	18,25,26	4.15	6 (33%)	18,36,39	3.56	7 (38%)
1	6MZ	S2	1832	1	18,25,26	2.01	4 (22%)	16,36,39	1.67	2 (12%)
1	A2M	S2	27	1	18,25,26	4.13	6 (33%)	18,36,39	3.49	4 (22%)
1	5MC	S2	1374	1	18,22,23	3.42	7 (38%)	26,32,35	1.13	2 (7%)
1	PSU	S2	612	1	18,21,22	4.28	8 (44%)	22,30,33	1.97	6 (27%)
1	UR3	S2	1830	1	19,22,23	2.56	5 (26%)	26,32,35	2.57	7 (26%)
1	OMC	S2	1703	1	19,22,23	3.49	8 (42%)	26,31,34	0.78	0
1	OMC	S2	517	1	19,22,23	3.54	8 (42%)	26,31,34	0.84	0
1	PSU	S2	823	1	18,21,22	4.29	8 (44%)	22,30,33	1.98	5 (22%)
1	MA6	S2	1850	1	19,26,27	1.07	1 (5%)	18,38,41	3.97	3 (16%)
1	A2M	S2	668	1	18,25,26	4.00	6 (33%)	18,36,39	4.01	7 (38%)
1	OMG	S2	509	1	18,26,27	2.52	8 (44%)	19,38,41	1.47	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	E3C	S2	568	1	18,23,24	3.50	6 (33%)	21,33,36	2.55	5 (23%)
1	A2M	S2	1031	1	18,25,26	4.03	6 (33%)	18,36,39	3.53	5 (27%)
1	M7A	S2	1806	1	20,25,26	2.03	3 (15%)	28,37,40	3.52	8 (28%)
1	OMU	S2	121	1	19,22,23	3.05	7 (36%)	26,31,34	1.88	5 (19%)
1	OMU	S2	116	1	19,22,23	3.10	6 (31%)	26,31,34	1.77	5 (19%)
1	A2M	S2	166	1	18,25,26	4.19	7 (38%)	18,36,39	3.37	5 (27%)
1	PSU	S2	1081	1	18,21,22	4.23	8 (44%)	22,30,33	1.85	5 (22%)
1	4AC	S2	1842	1,85	21,24,25	3.33	9 (42%)	29,34,37	1.21	5 (17%)
1	PSU	S2	119	1	18,21,22	4.39	7 (38%)	22,30,33	1.79	4 (18%)
1	OMC	S2	174	1	19,22,23	3.59	8 (42%)	26,31,34	0.79	0
1	A2M	S2	1678	1	18,25,26	4.18	7 (38%)	18,36,39	3.19	5 (27%)
1	OMG	S2	683	1	18,26,27	2.47	8 (44%)	19,38,41	1.45	4 (21%)
1	A2M	S2	484	1	18,25,26	4.13	7 (38%)	18,36,39	3.48	4 (22%)
1	OMG	S2	644	1	18,26,27	2.56	8 (44%)	19,38,41	1.48	4 (21%)
1	B8Q	S2	1219	1	17,22,23	4.67	6 (35%)	22,32,35	1.93	5 (22%)

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
1	OMC	S2	1710	1	-	0/9/27/28	0/2/2/2
1	PSU	S2	822	1	-	2/7/25/26	0/2/2/2
1	4AC	S2	1337	1	-	0/11/29/30	0/2/2/2
1	PSU	S2	1243	1	-	2/7/25/26	0/2/2/2
1	B8N	S2	1248	1	-	0/16/34/35	0/2/2/2
1	5MU	S2	814	1	-	0/7/25/26	0/2/2/2
1	MA6	S2	1851	1	-	5/7/29/30	0/3/3/3
1	A2M	S2	159	1	-	4/5/27/28	0/3/3/3
1	6MZ	S2	1832	1	-	2/5/27/28	0/3/3/3
1	A2M	S2	27	1	-	1/5/27/28	0/3/3/3
1	5MC	S2	1374	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	612	1	-	1/7/25/26	0/2/2/2
1	UR3	S2	1830	1	-	7/7/25/26	0/2/2/2
1	OMC	S2	1703	1	-	2/9/27/28	0/2/2/2
1	OMC	S2	517	1	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	823	1	-	4/7/25/26	0/2/2/2
1	MA6	S2	1850	1	-	5/7/29/30	0/3/3/3
1	A2M	S2	668	1	-	2/5/27/28	0/3/3/3
1	OMG	S2	509	1	-	1/5/27/28	0/3/3/3
1	E3C	S2	568	1	-	4/9/44/45	0/2/2/2
1	A2M	S2	1031	1	-	3/5/27/28	0/3/3/3
1	M7A	S2	1806	1	-	3/7/37/38	0/3/3/3
1	OMU	S2	121	1	-	3/9/27/28	0/2/2/2
1	OMU	S2	116	1	-	2/9/27/28	0/2/2/2
1	A2M	S2	166	1	-	0/5/27/28	0/3/3/3
1	PSU	S2	1081	1	-	2/7/25/26	0/2/2/2
1	4AC	S2	1842	1,85	-	0/11/29/30	0/2/2/2
1	PSU	S2	119	1	-	1/7/25/26	0/2/2/2
1	OMC	S2	174	1	-	0/9/27/28	0/2/2/2
1	A2M	S2	1678	1	-	0/5/27/28	0/3/3/3
1	OMG	S2	683	1	-	2/5/27/28	0/3/3/3
1	A2M	S2	484	1	-	1/5/27/28	0/3/3/3
1	OMG	S2	644	1	-	2/5/27/28	0/3/3/3
1	B8Q	S2	1219	1	-	0/7/42/43	0/2/2/2

The worst 5 of 225 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	814	5MU	C4-C5	22.08	1.81	1.44
1	S2	814	5MU	C6-N1	16.66	1.66	1.38
1	S2	814	5MU	C6-C5	-11.74	1.15	1.34
1	S2	1219	B8Q	C4-N3	11.60	1.66	1.48
1	S2	119	PSU	C6-C5	11.31	1.48	1.35

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	1850	MA6	N1-C6-N6	-14.99	101.28	117.06
1	S2	1851	MA6	N1-C6-N6	-14.44	101.85	117.06
1	S2	1806	M7A	C5-C6-N6	10.86	142.30	123.74
1	S2	668	A2M	C1'-N9-C4	-10.43	108.31	126.64
1	S2	1806	M7A	N6-C6-N1	-9.47	97.62	118.35

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	S2	27	A2M	C1'-C2'-O2'-CM'
1	S2	116	OMU	C3'-C4'-C5'-O5'
1	S2	116	OMU	O4'-C4'-C5'-O5'
1	S2	159	A2M	O4'-C4'-C5'-O5'
1	S2	159	A2M	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 37 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	$\#\|Z\| > 2$
86	MVM	t	5112	-	33,35,35	1.77	4 (12%)	36,49,49	2.24	13 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	MVM	t	5112	-	-	0/20/28/28	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	t	5112	MVM	C5-N1	6.44	1.46	1.37
86	t	5112	MVM	N5-N4	-4.43	1.30	1.37
86	t	5112	MVM	C6-N1	2.54	1.45	1.39
86	t	5112	MVM	C12-C5	2.47	1.54	1.50

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
86	t	5112	MVM	C15-N4-C22	-5.46	124.10	129.98
86	t	5112	MVM	C21-N7-C22	4.70	122.60	116.77
86	t	5112	MVM	C7-C3-C9	4.33	119.43	110.82
86	t	5112	MVM	N3-C6-N1	3.86	120.41	116.33
86	t	5112	MVM	C1-C9-N1	-3.67	106.93	116.16

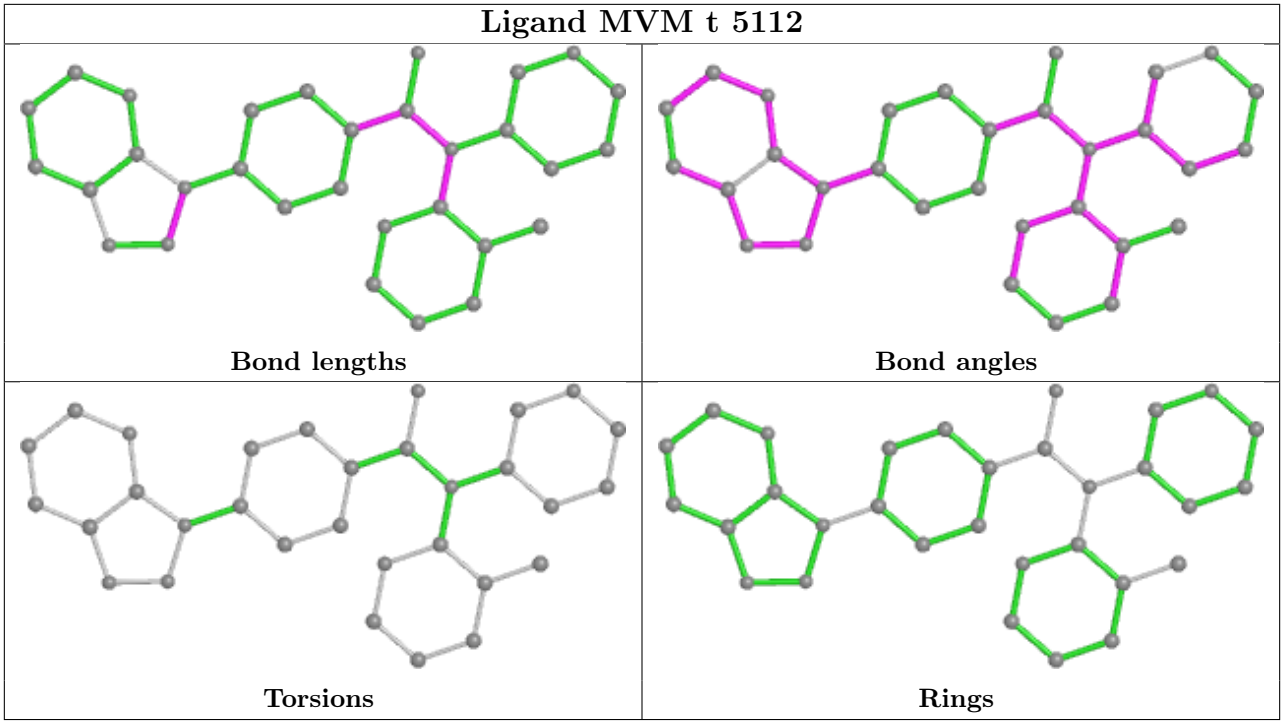
There are no chirality outliers.

There are no torsion outliers.

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.



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
78	t	16
1	S2	5
79	v	4
62	c	1

The worst 5 of 26 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S2	753:C	O3'	785:C	P	26.21
1	t	750:G	O3'	890:C	P	19.49
1	t	3919:C	O3'	4035:G	P	17.88
1	t	1680:C	O3'	1699:C	P	17.58
1	t	517:C	O3'	629:G	P	17.45

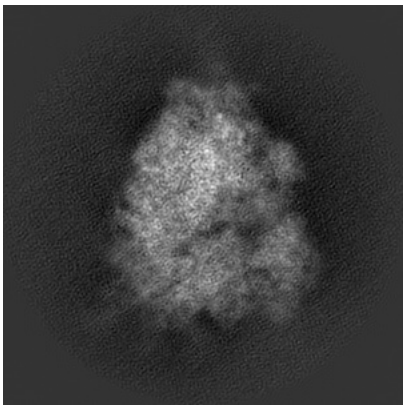
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0599. These allow visual inspection of the internal detail of the map and identification of artifacts.

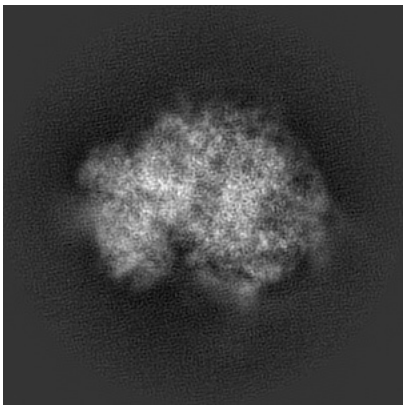
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

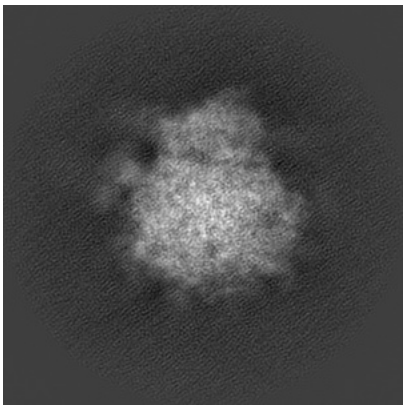
6.1.1 Primary map



X

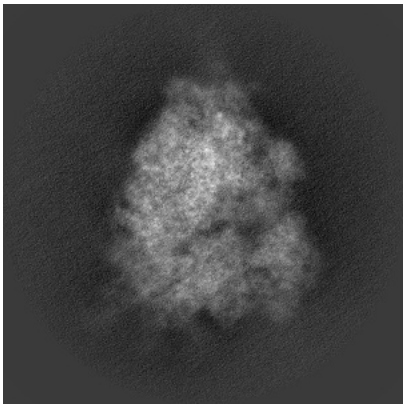


Y

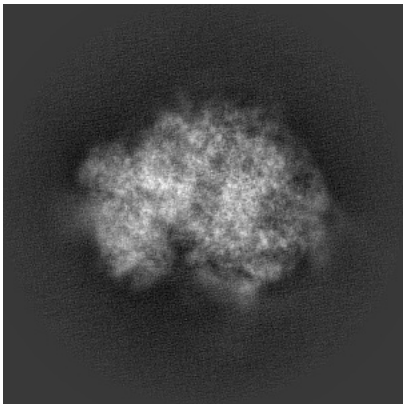


Z

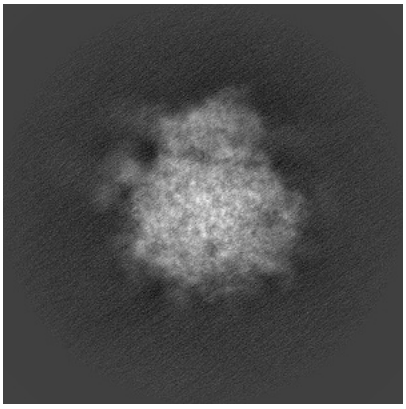
6.1.2 Raw map



X



Y

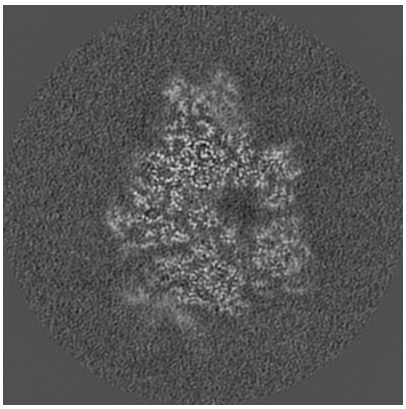


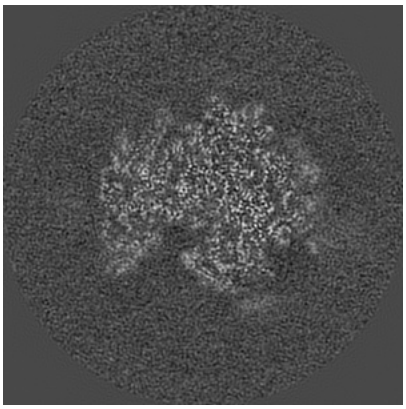
Z

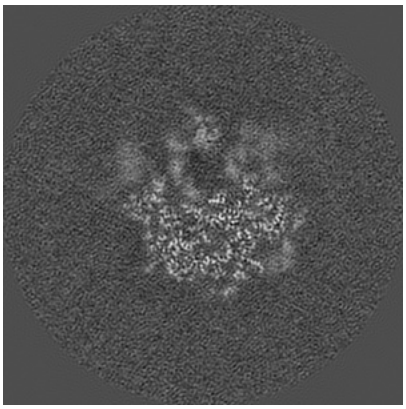
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

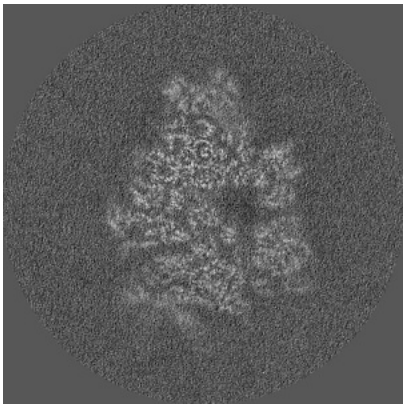
6.2.1 Primary map

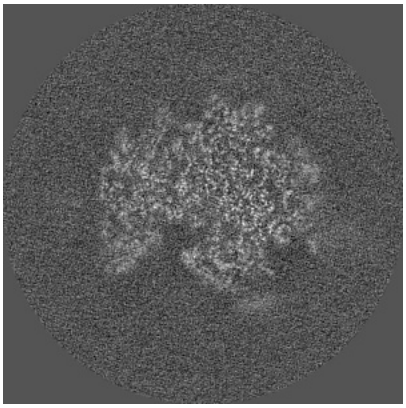

X Index: 200

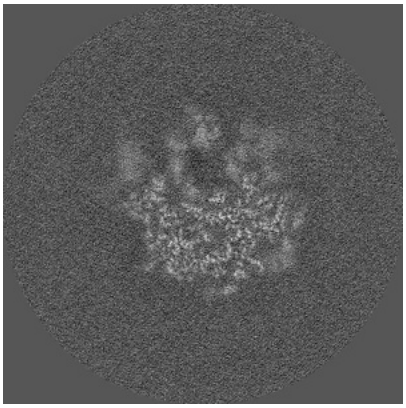

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

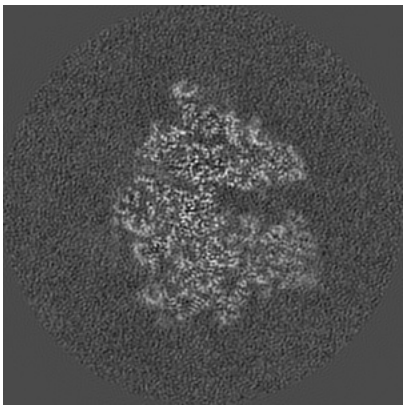

Y Index: 200

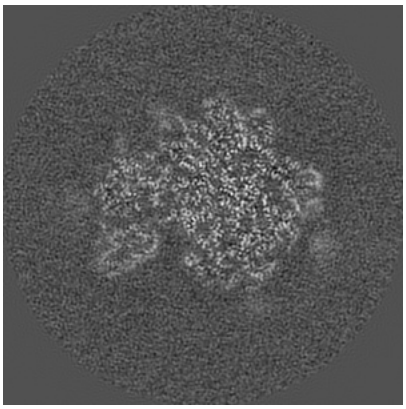

Z Index: 200

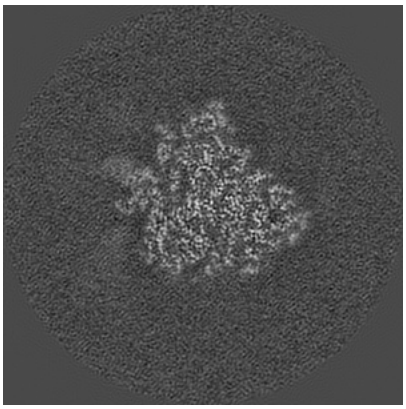
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

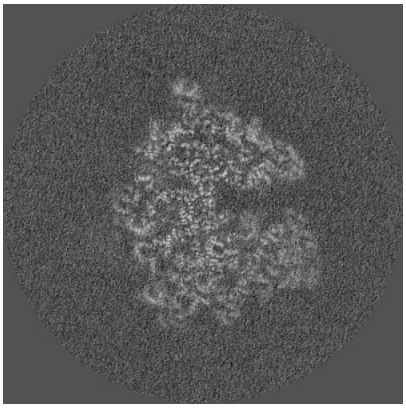
6.3.1 Primary map

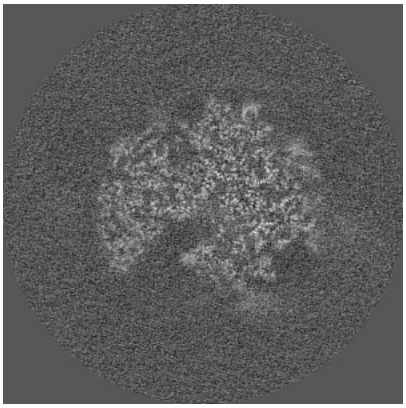

X Index: 218

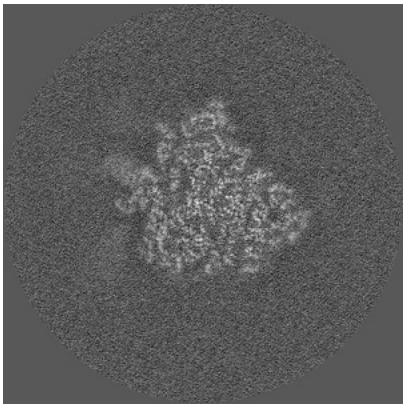

Y Index: 193


Z Index: 229

6.3.2 Raw map


X Index: 219


Y Index: 204


Z Index: 229

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 0.02. 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.

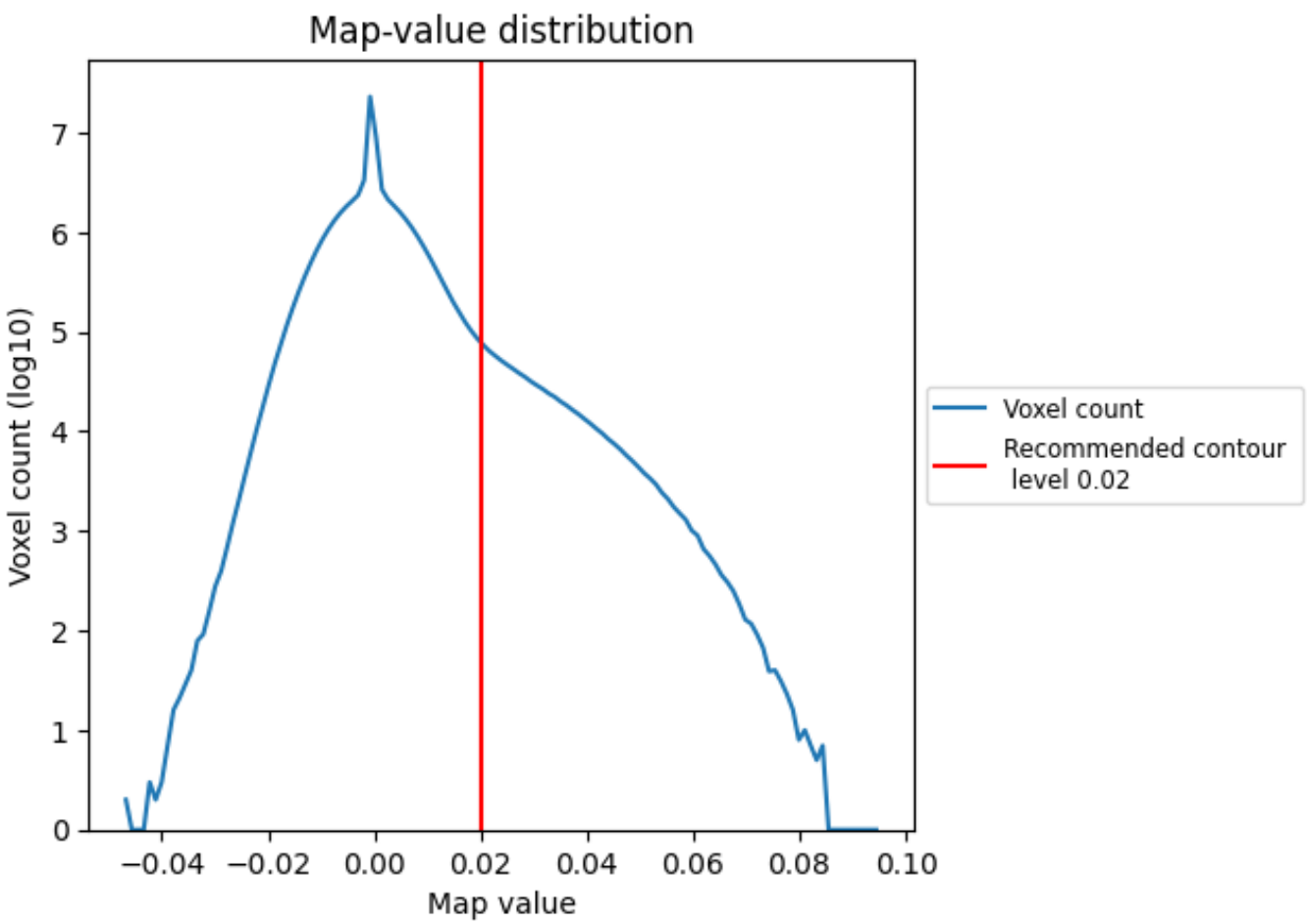
6.5 Mask visualisation (i)

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

7 Map analysis (i)

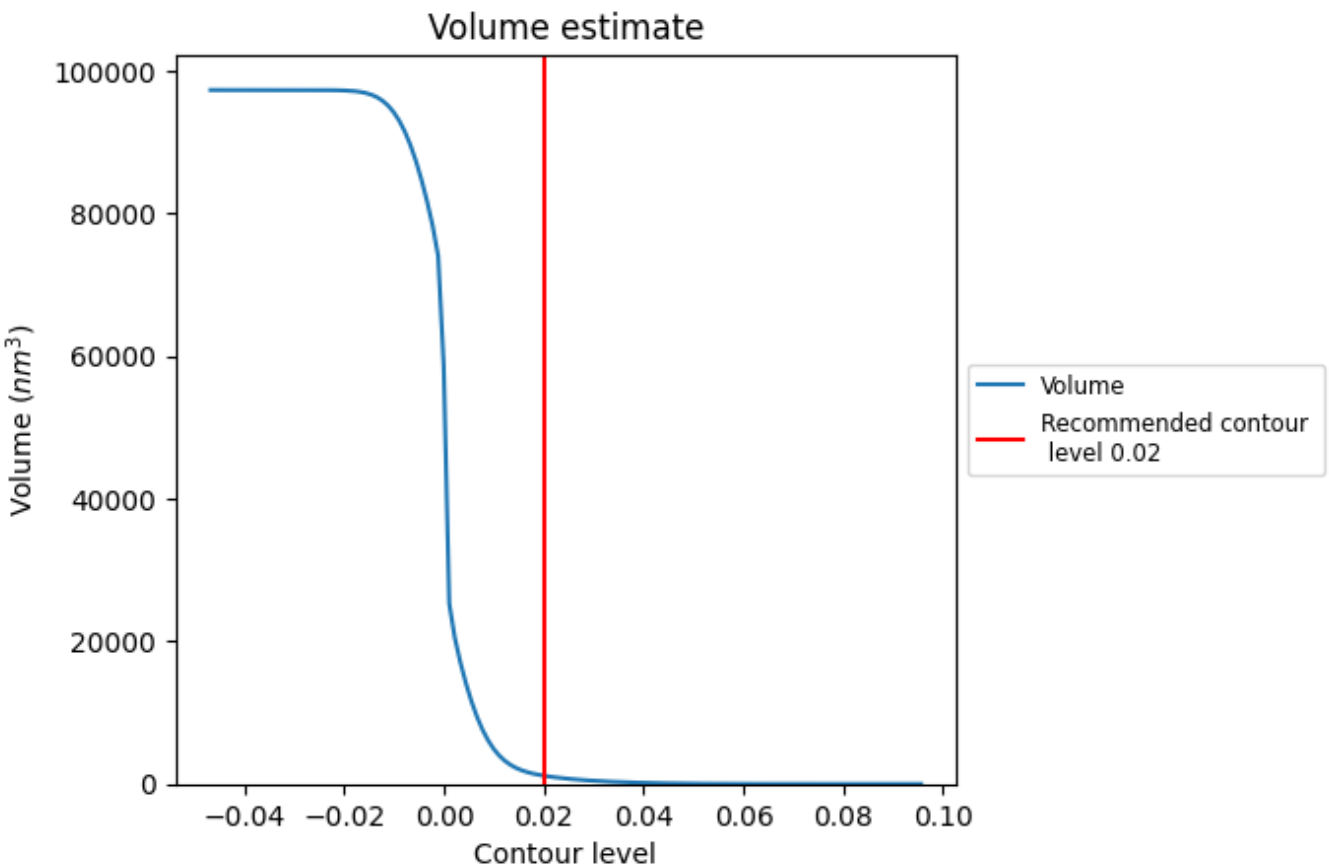
This section contains the results of statistical analysis of the map.

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.

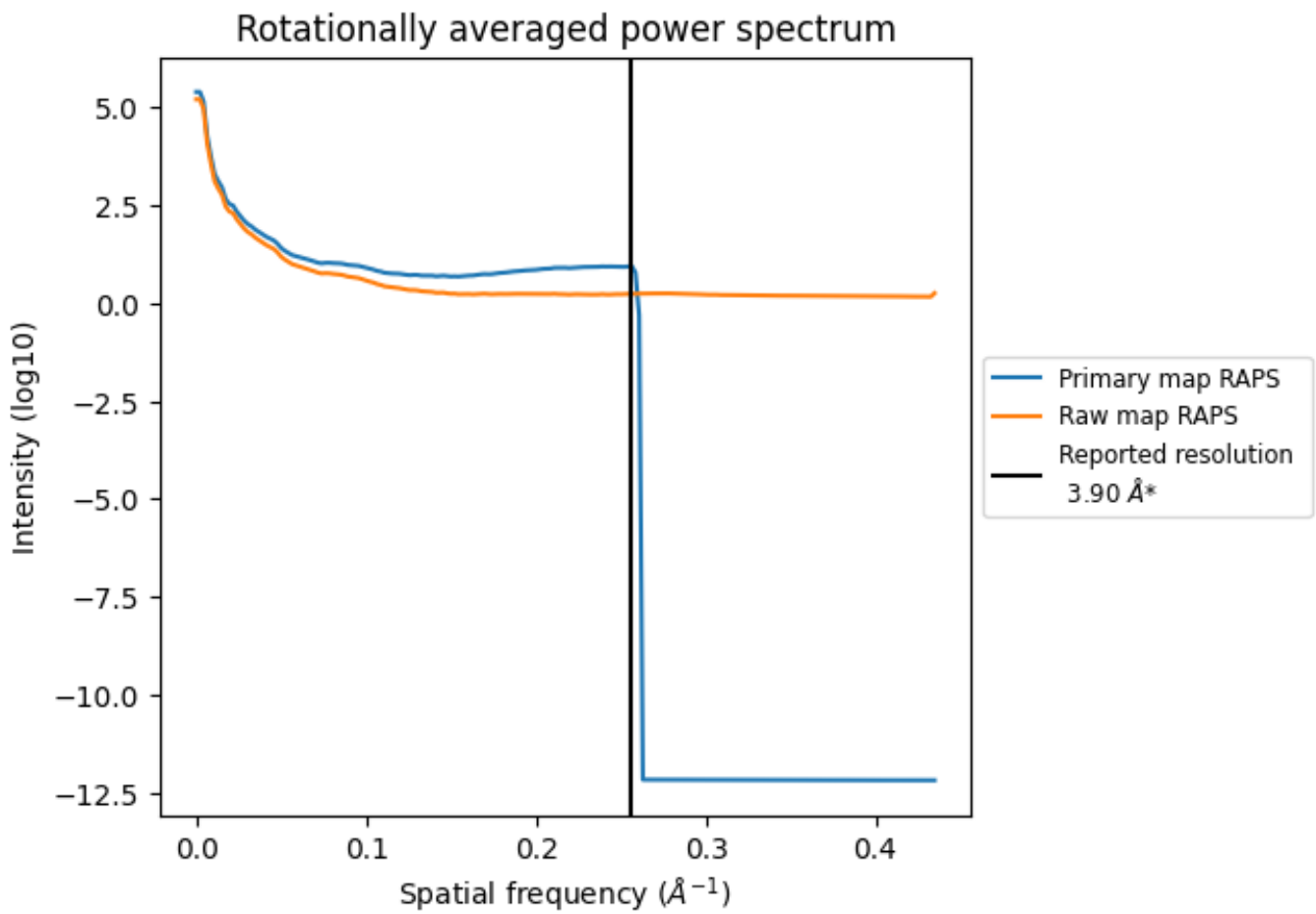
7.2 Volume estimate (i)



The volume at the recommended contour level is 1153 nm^3; this corresponds to an approximate mass of 1042 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)

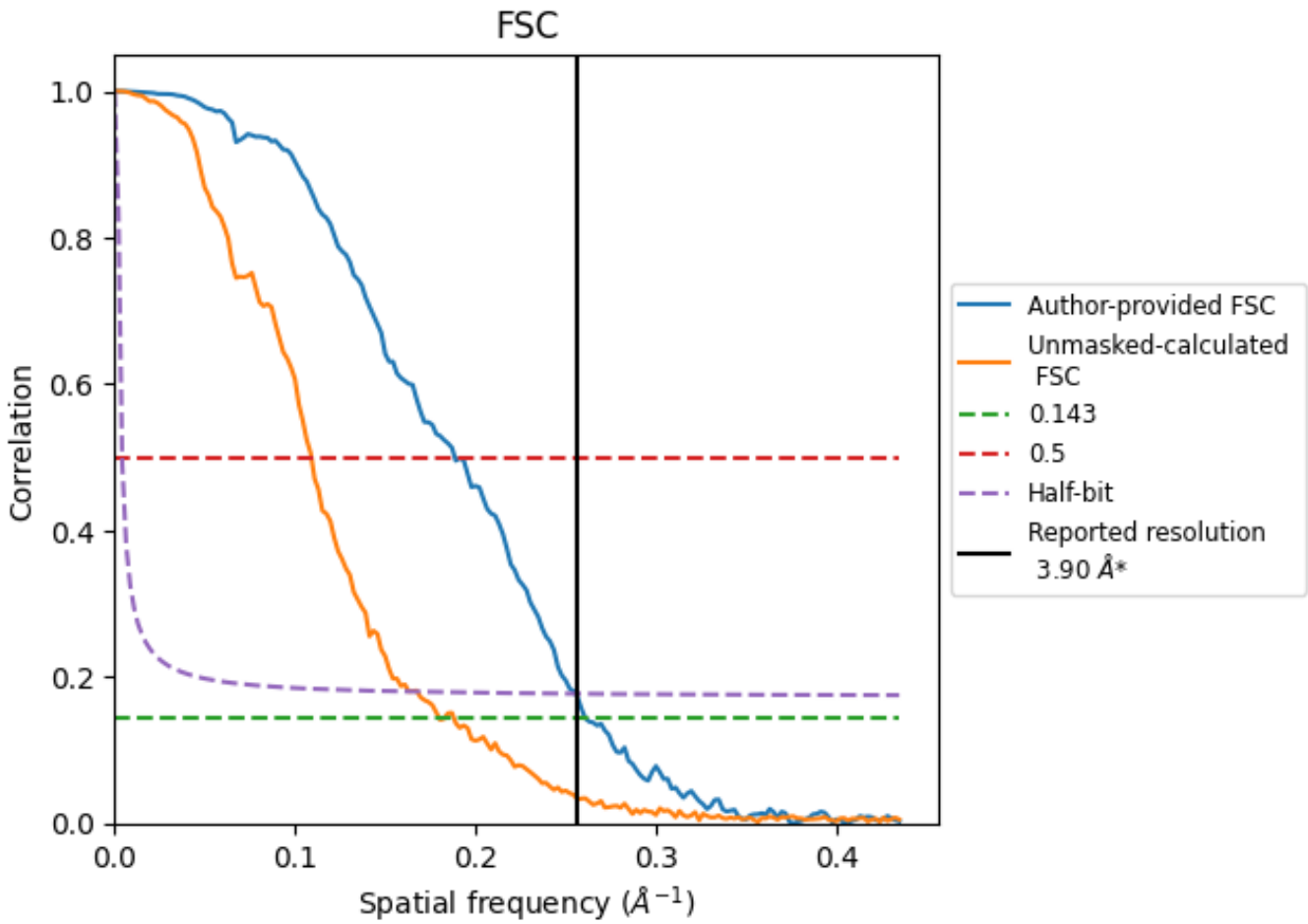


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

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)

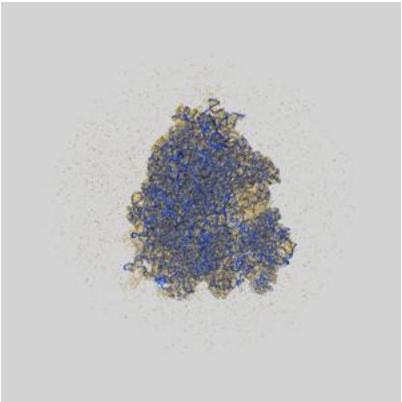
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.83	5.31	3.92
Unmasked-calculated*	5.56	9.17	5.96

*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 5.56 differs from the reported value 3.9 by more than 10 %

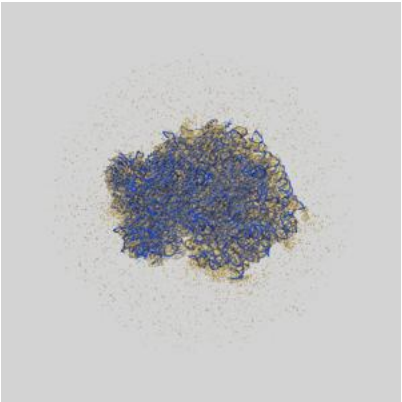
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0599 and PDB model 6OLF. Per-residue inclusion information can be found in section 3 on page 20.

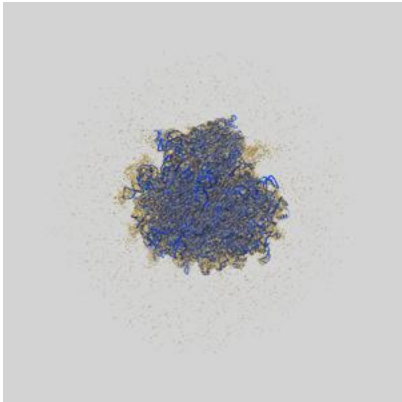
9.1 Map-model overlay (i)



X



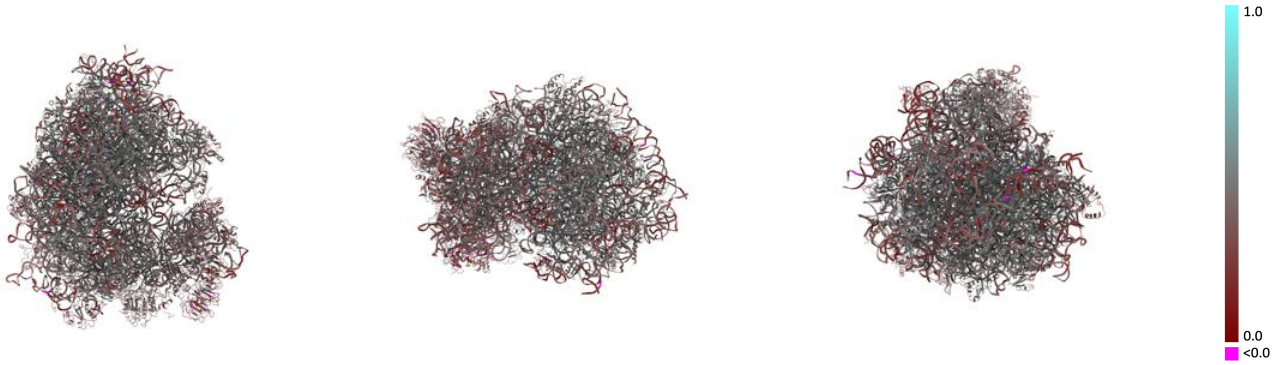
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

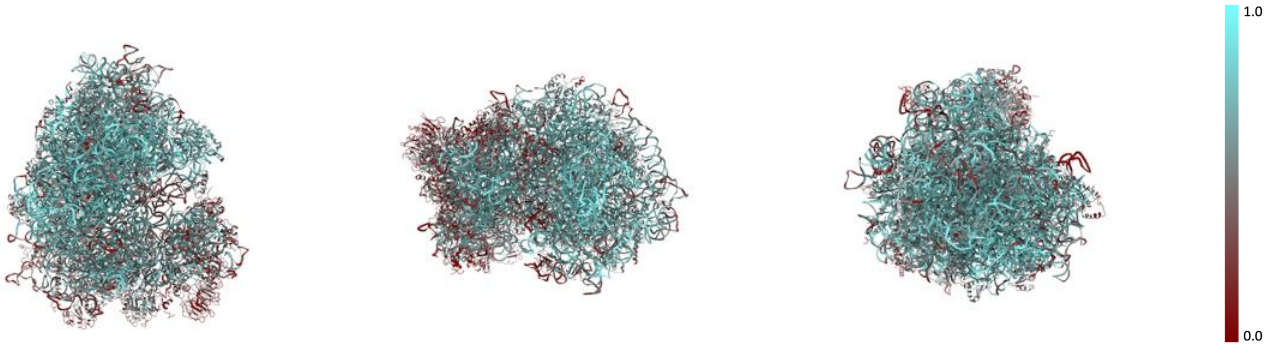
9.2 Q-score mapped to coordinate model (i)



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.

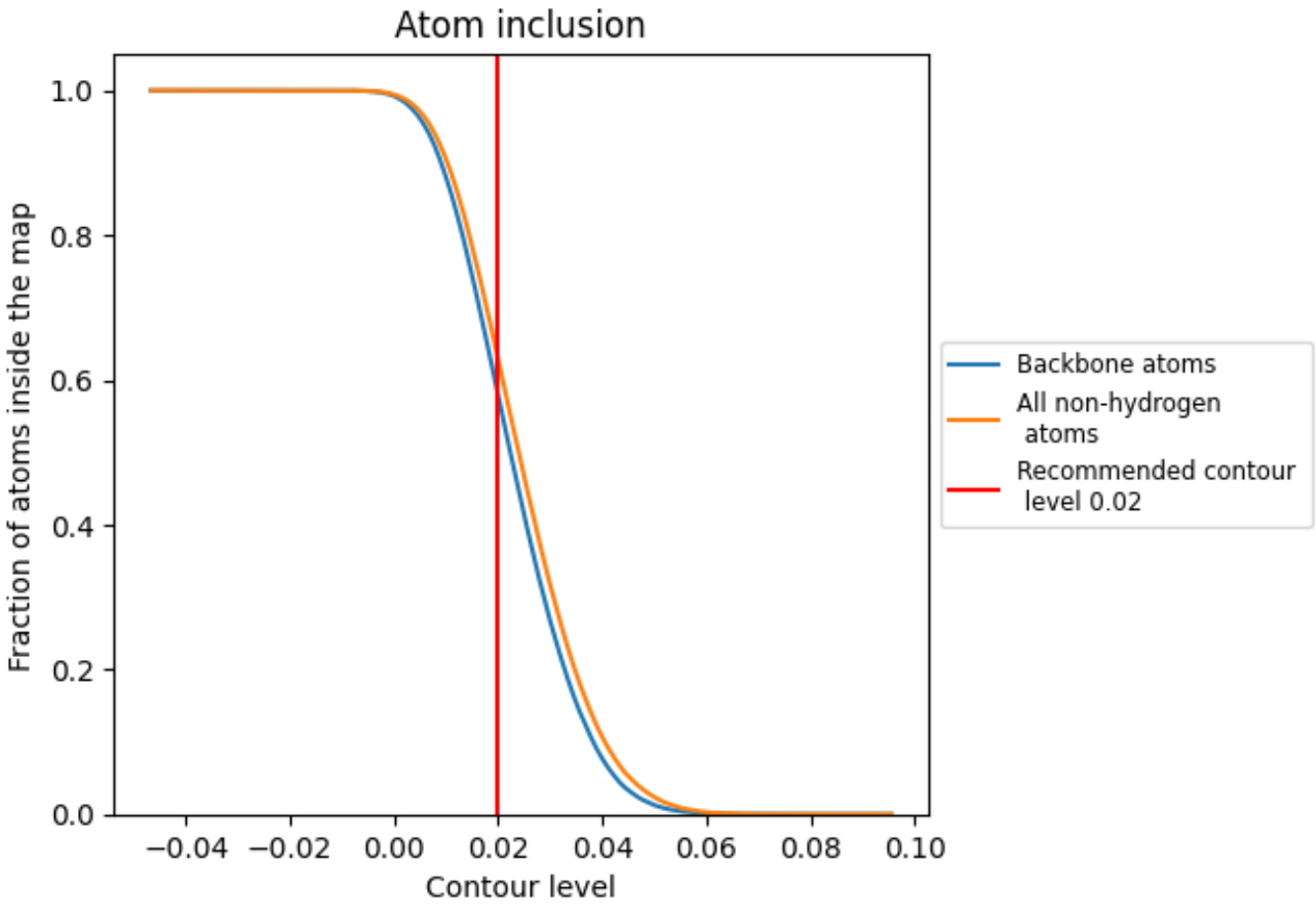
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 58% of all backbone atoms, 63% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6276	0.4070
A	0.6385	0.4810
B	0.6075	0.4550
C	0.6370	0.4590
D	0.7643	0.4230
E	0.8514	0.4420
F	0.5973	0.4180
G	0.5384	0.4070
H	0.6464	0.4600
I	0.5586	0.4220
J	0.5329	0.4310
K	0.6049	0.4520
L	0.5518	0.4140
M	0.5969	0.4250
N	0.6116	0.4410
O	0.6907	0.4830
P	0.6418	0.4600
Q	0.6501	0.4620
R	0.6257	0.4660
S	0.5683	0.4300
S2	0.6707	0.3900
SA	0.4588	0.4080
SB	0.4139	0.3990
SC	0.5063	0.4180
SD	0.3396	0.3550
SE	0.4153	0.3680
SF	0.3308	0.3550
SG	0.3353	0.3370
SH	0.3599	0.3410
SI	0.4257	0.3780
SJ	0.4294	0.3710
SK	0.3130	0.3370
SL	0.4604	0.3950
SM	0.1022	0.2340
SN	0.5068	0.4250

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Chain	Atom inclusion	Q-score
SO	0.4352	0.4040
SP	0.4303	0.3590
SQ	0.3806	0.3640
SR	0.3356	0.3670
SS	0.3859	0.3620
ST	0.3956	0.3630
SU	0.3387	0.3470
SV	0.4779	0.3850
SW	0.5475	0.4430
SX	0.5070	0.4150
SY	0.4087	0.3570
SZ	0.2827	0.3230
Sa	0.5311	0.4160
Sb	0.3838	0.3790
Sc	0.2716	0.3370
Sd	0.5351	0.4090
Se	0.3753	0.3740
Sf	0.1442	0.2410
Sg	0.2307	0.3030
T	0.6178	0.4550
U	0.6069	0.4540
V	0.5380	0.3890
W	0.5787	0.4650
X	0.3396	0.3120
Y	0.6047	0.4440
Z	0.6169	0.4420
a	0.5959	0.4350
b	0.6670	0.4700
c	0.5580	0.4300
d	0.5625	0.4200
e	0.5943	0.4400
f	0.6511	0.4670
g	0.6888	0.4790
h	0.6099	0.4630
i	0.5892	0.4170
j	0.5840	0.4220
k	0.7275	0.4870
l	0.4883	0.3950
m	0.6147	0.4560
n	0.6020	0.4420
o	0.5571	0.4410
p	0.5442	0.4490

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Chain	Atom inclusion	Q-score
q	0.6270	0.4670
r	0.6621	0.4560
t	0.7557	0.4140
u	0.3391	0.2500
v	0.4061	0.3060
w	0.5915	0.4150
y	0.1145	0.2570