



wwPDB EM Validation Summary Report ⓘ

Nov 9, 2024 – 01:46 PM EST

PDB ID : 6OLI
EMDB ID : EMD-0526
Title : Structure of human ribosome nascent chain complex selectively stalled by a drug-like small molecule (USO1-RNC)
Authors : Li, W.; Cate, J.H.D.
Deposited on : 2019-04-16
Resolution : 3.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

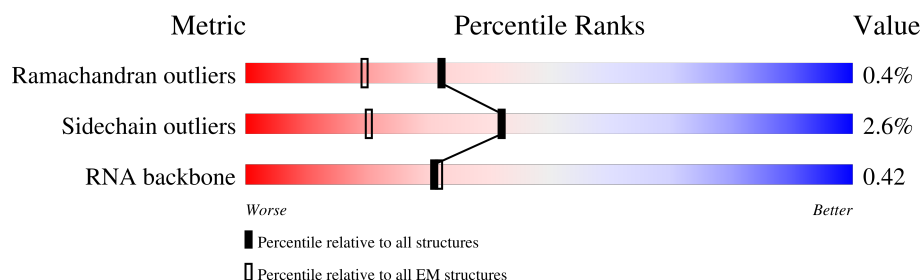
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	S2	1714	
2	SA	221	
3	SB	214	
4	SD	226	
5	SE	259	
6	SF	189	
7	SH	189	
8	SI	204	

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Mol	Chain	Length	Quality of chain
9	SK	98	
10	SL	153	
11	SP	127	
12	SQ	146	
13	SR	134	
14	SS	145	
15	ST	143	
16	SU	104	
17	SV	82	
18	SX	141	
19	Sa	102	
20	Sc	64	
21	Sd	55	
22	Sg	312	
23	SC	220	
24	SG	237	
25	SJ	185	
26	SM	118	
27	SN	150	
28	SO	137	
29	SW	129	
30	SY	131	
31	SZ	73	
32	Sb	82	
33	Se	57	

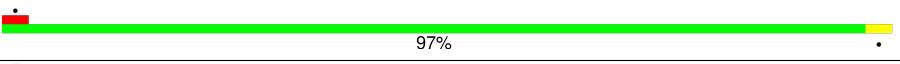
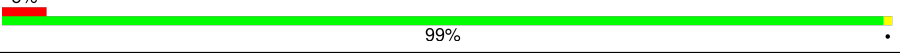
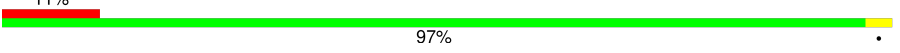
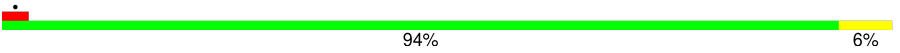

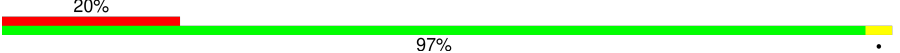
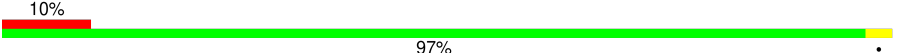
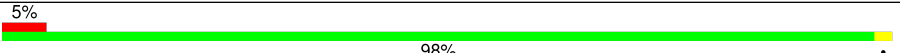

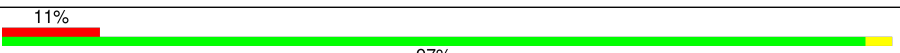
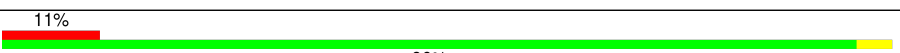
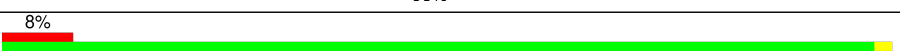
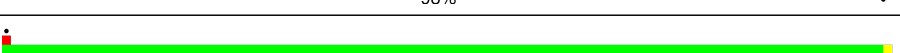
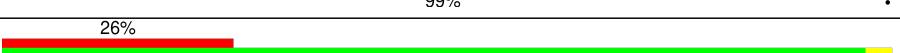
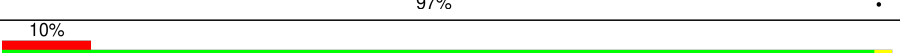
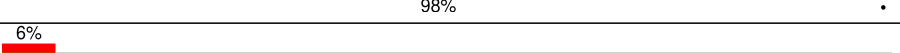
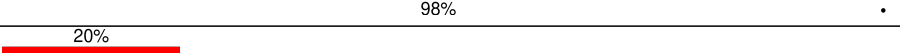
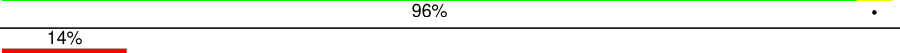

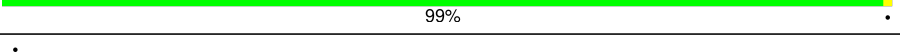
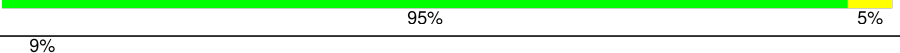


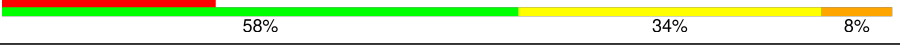

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Mol	Chain	Length	Quality of chain
34	Sf	67	96%
35	A	252	6% 97%
36	B	397	7% 96%
37	C	363	6% 96%
38	D	157	9% 71% 25%
39	E	121	77% 20%
40	F	294	12% 97%
41	G	247	18% 91%
42	H	225	5% 96%
43	I	234	19% 100%
44	J	191	14% 97%
45	K	211	11% 95%
46	L	169	14% 98%
47	M	205	13% 94% 5%
48	N	139	11% 98%
49	O	203	97%
50	P	195	95%
51	Q	153	97%
52	R	187	5% 95%
53	S	181	18% 98%
54	T	175	97%
55	U	157	6% 95% 5%
56	V	99	21% 94% 6%
57	W	129	8% 100%
58	X	61	8% 98%

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Mol	Chain	Length	Quality of chain
59	Y	117	
60	Z	134	
61	a	134	
62	b	147	
63	c	121	
64	d	103	
65	e	106	
66	f	129	
67	g	109	
68	h	114	
69	i	122	
70	j	97	
71	k	84	
72	l	69	
73	m	50	
74	n	50	
75	o	25	
76	p	105	
77	q	91	
78	r	122	
79	t	3607	
80	u	76	
81	v	76	
82	w	10	
83	y	36	

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 214867 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
1	S2	1714	Total	C	N	O	P	0	0
			36501	16306	6533	11949	1713		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
27	SN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
58	X	61	Total	C	N	O	S	0	0
			511	327	100	82	2		

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

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

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

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

- Molecule 61 is a protein called 60S ribosomal protein L27.

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

- Molecule 62 is a protein called 60S ribosomal protein L27a.

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

- Molecule 63 is a protein called 60S ribosomal protein L29.

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

- Molecule 64 is a protein called 60S ribosomal protein L30.

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

- Molecule 65 is a protein called 60S ribosomal protein L31.

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

- Molecule 66 is a protein called 60S ribosomal protein L32.

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

- Molecule 67 is a protein called 60S ribosomal protein L35a.

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

- Molecule 68 is a protein called 60S ribosomal protein L34.

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

- Molecule 69 is a protein called 60S ribosomal protein L35.

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

- Molecule 70 is a protein called 60S ribosomal protein L36.

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

- Molecule 71 is a protein called 60S ribosomal protein L37.

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

- Molecule 72 is a protein called 60S ribosomal protein L38.

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

- Molecule 73 is a protein called 60S ribosomal protein L39.

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

- Molecule 74 is a protein called 60S ribosomal protein L40.

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

- Molecule 75 is a protein called 60S ribosomal protein L41.

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

- Molecule 76 is a protein called 60S ribosomal protein L36a.

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

- Molecule 77 is a protein called 60S ribosomal protein L37a.

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

- Molecule 78 is a protein called 60S ribosomal protein L28.

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

- Molecule 79 is a RNA chain called 28S ribosomal RNA.

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

- Molecule 80 is a RNA chain called tRNA.

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

- Molecule 81 is a RNA chain called tRNA.

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

- Molecule 82 is a RNA chain called mRNA.

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

- Molecule 83 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
83	y	36	Total	C	N	O	0	0
			178	106	36	36		

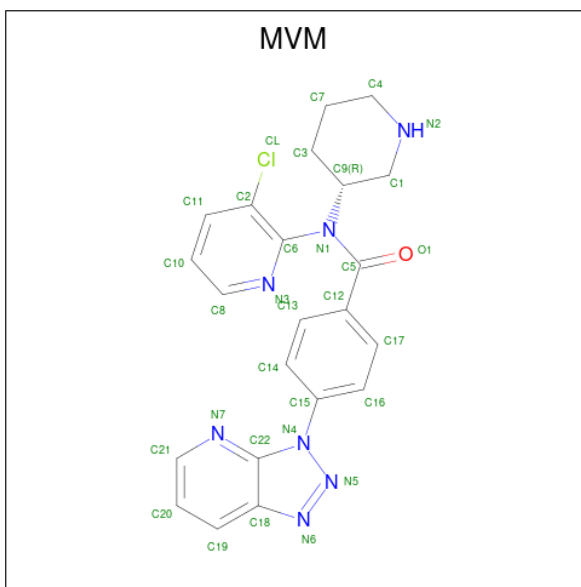
- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	S2	2	Total	Mg	0
			2	2	
84	B	1	Total	Mg	0
			1	1	
84	D	7	Total	Mg	0
			7	7	
84	E	9	Total	Mg	0
			9	9	
84	O	1	Total	Mg	0
			1	1	
84	b	1	Total	Mg	0
			1	1	
84	o	1	Total	Mg	0
			1	1	
84	t	9	Total	Mg	0
			9	9	

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- 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: C₂₂H₂₀ClN₇O).



Mol	Chain	Residues	Atoms					AltConf
86	t	1	Total	C	Cl	N	O	0
			31	22	1	7	1	

- Molecule 87 is water.

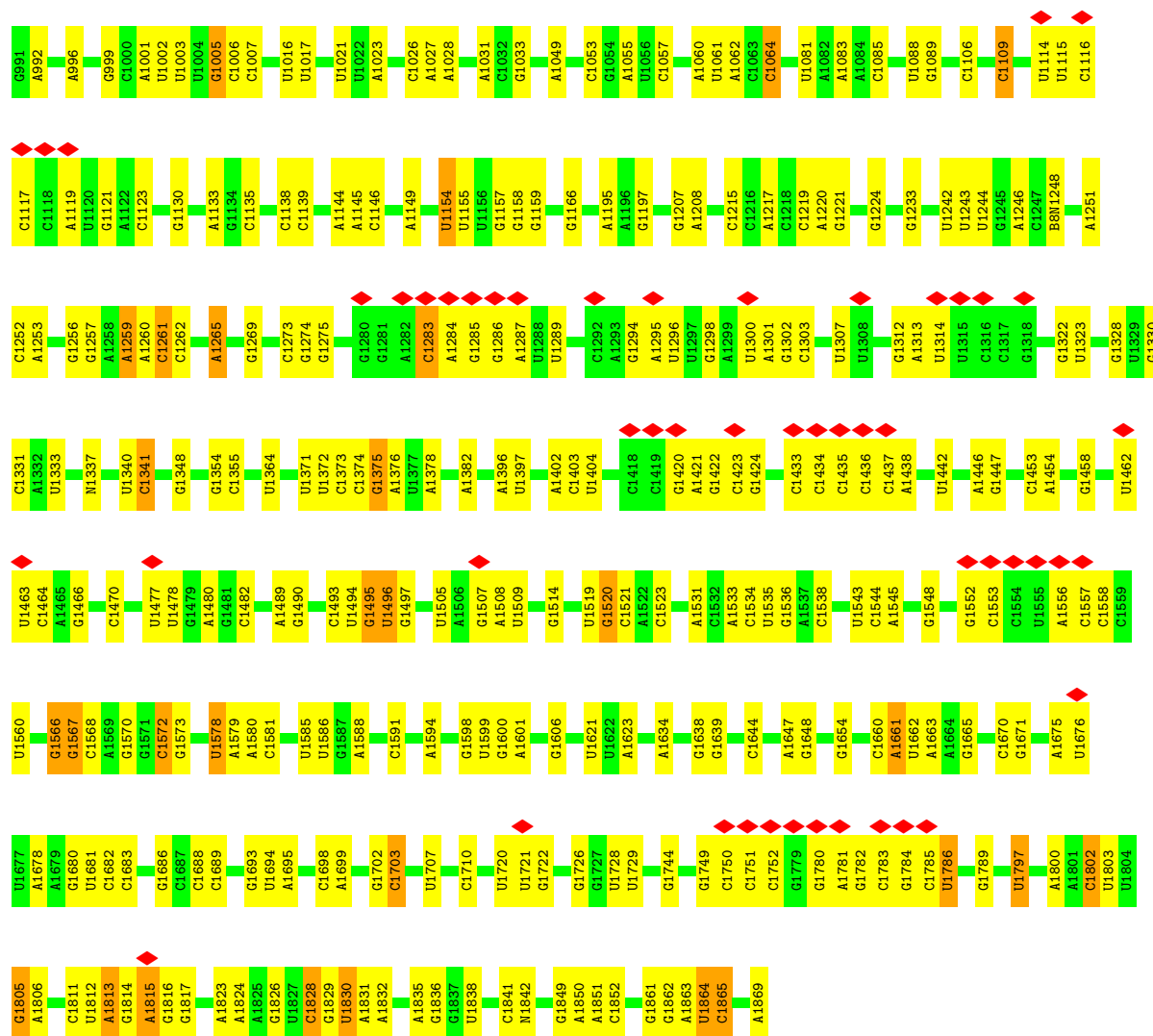
Mol	Chain	Residues	Atoms		AltConf
87	S2	5	Total	O	0
			5	5	
87	SP	1	Total	O	0
			1	1	
87	SQ	1	Total	O	0
			1	1	
87	SR	1	Total	O	0
			1	1	
87	SS	1	Total	O	0
			1	1	
87	SC	1	Total	O	0
			1	1	
87	SJ	1	Total	O	0
			1	1	
87	Sb	1	Total	O	0
			1	1	
87	Sf	1	Total	O	0
			1	1	
87	u	1	Total	O	0
			1	1	

3 Residue-property plots

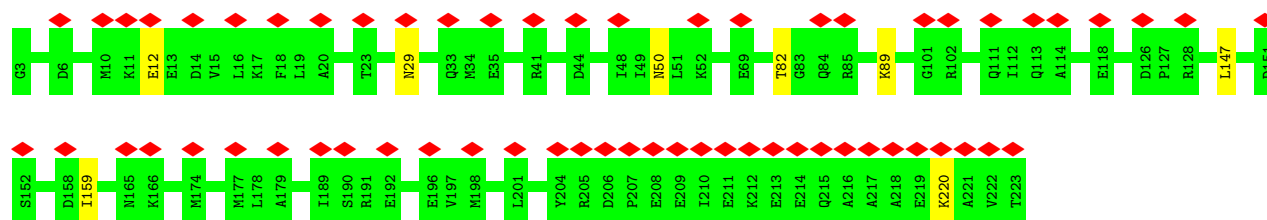
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

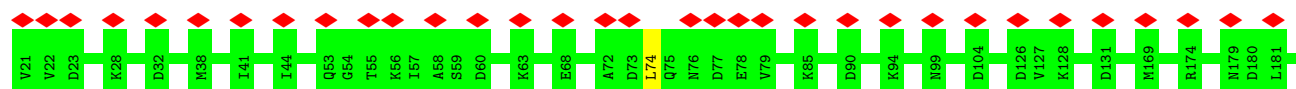


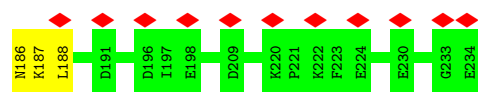


• Molecule 2: 40S ribosomal protein SA

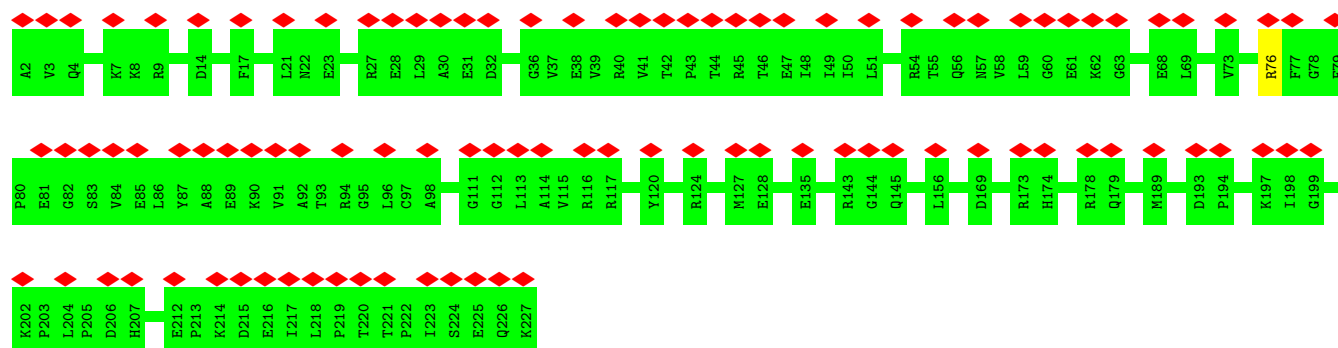


• Molecule 3: 40S ribosomal protein S3a

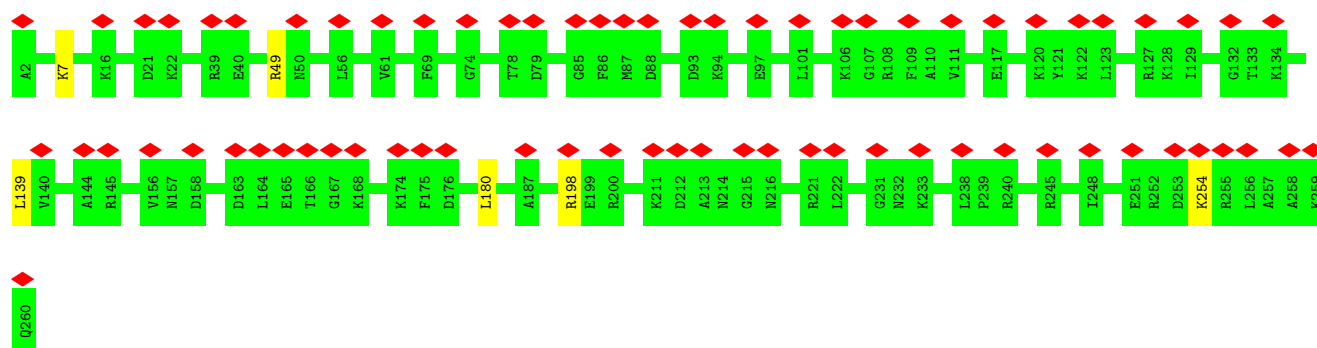




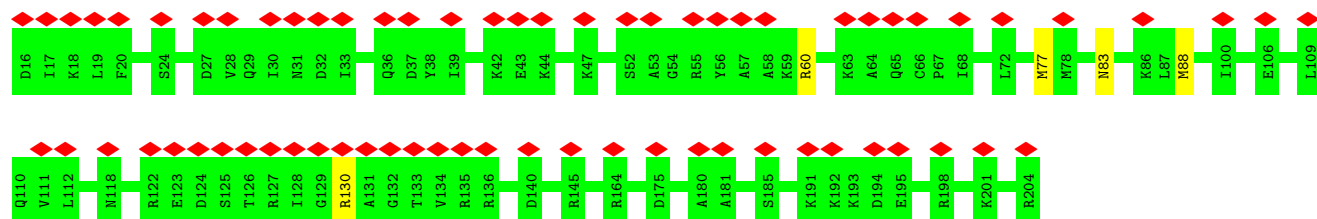
- Molecule 4: 40S ribosomal protein S3



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

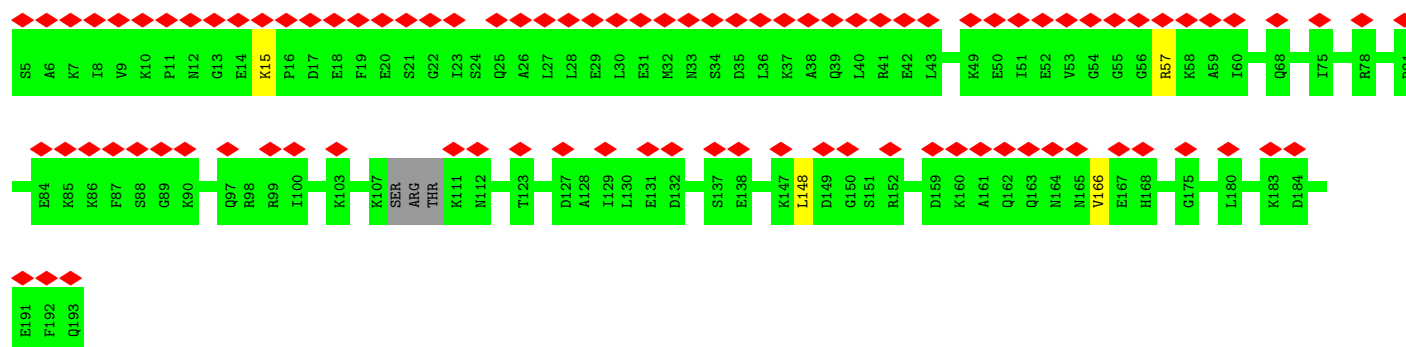


- Molecule 6: 40S ribosomal protein S5

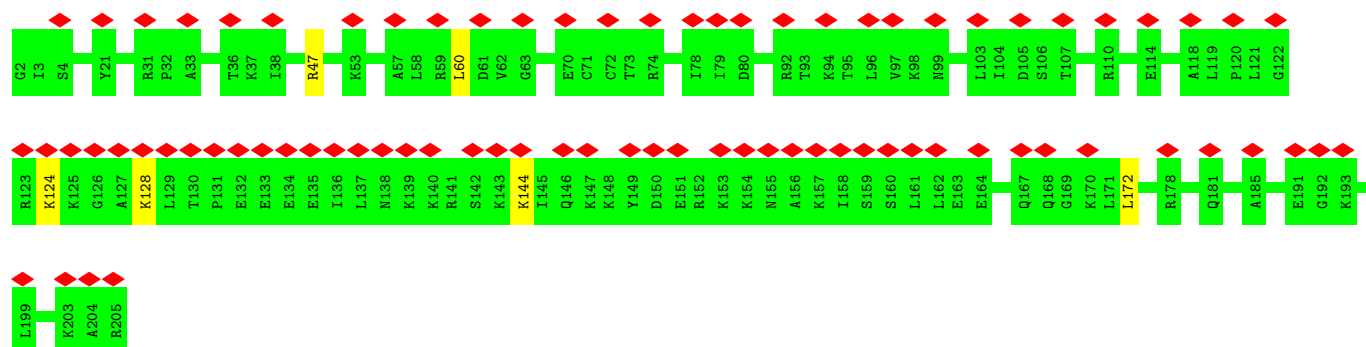
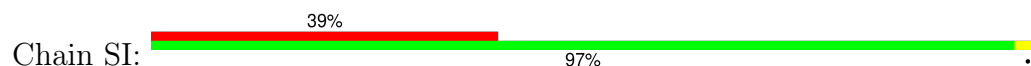


- Molecule 7: 40S ribosomal protein S7

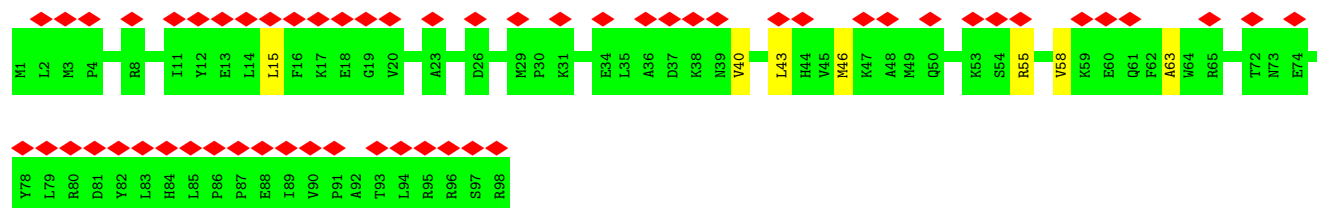




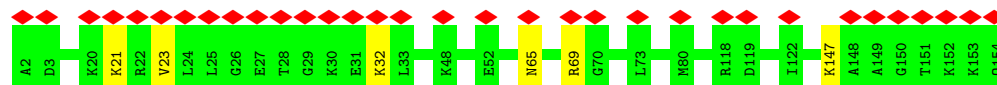
• Molecule 8: 40S ribosomal protein S8



• Molecule 9: 40S ribosomal protein S10

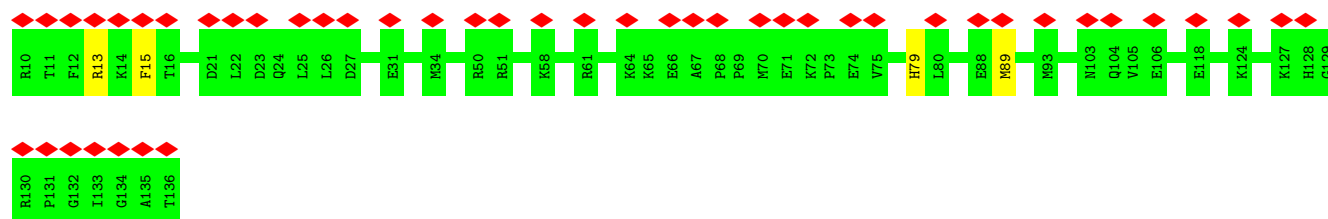


• Molecule 10: 40S ribosomal protein S11

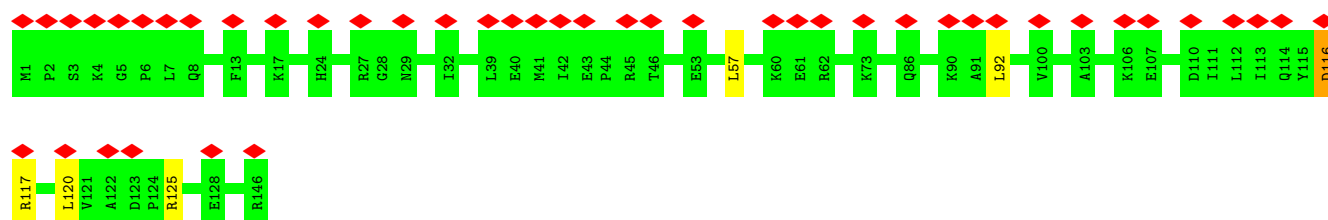


• Molecule 11: 40S ribosomal protein S15

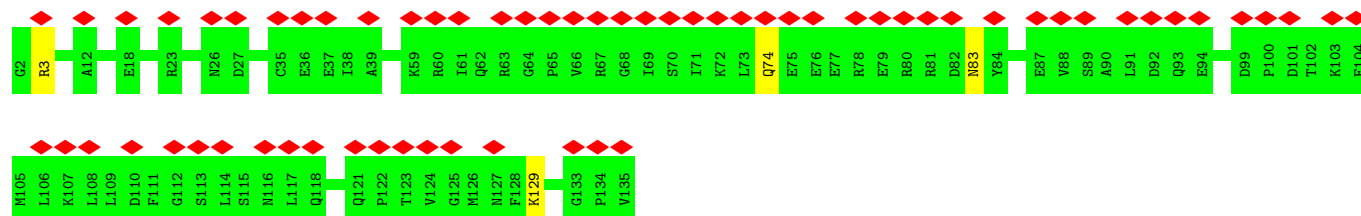




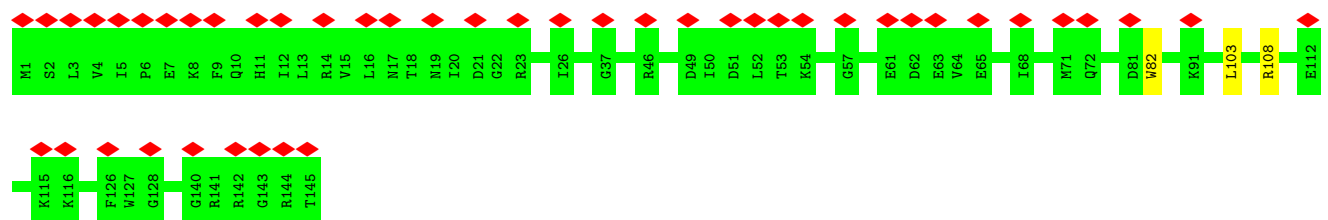
- Molecule 12: 40S ribosomal protein S16



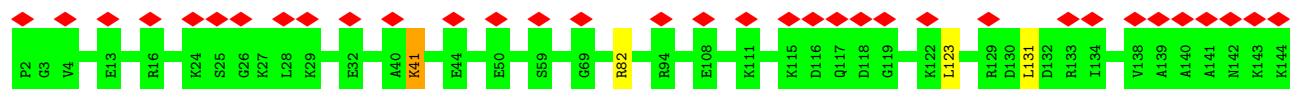
- Molecule 13: 40S ribosomal protein S17



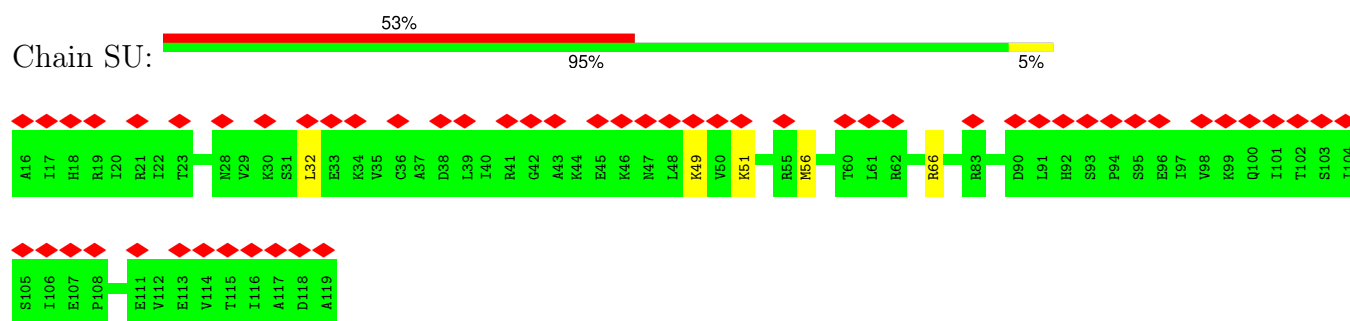
- Molecule 14: 40S ribosomal protein S18



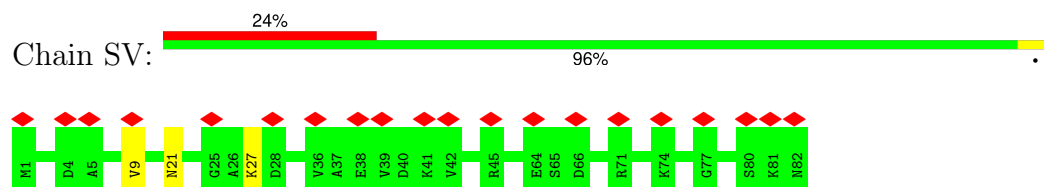
- Molecule 15: 40S ribosomal protein S19



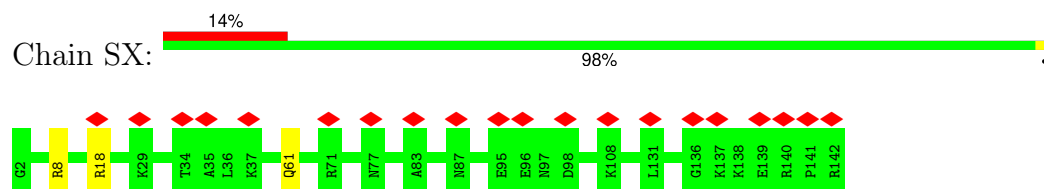
- Molecule 16: 40S ribosomal protein S20



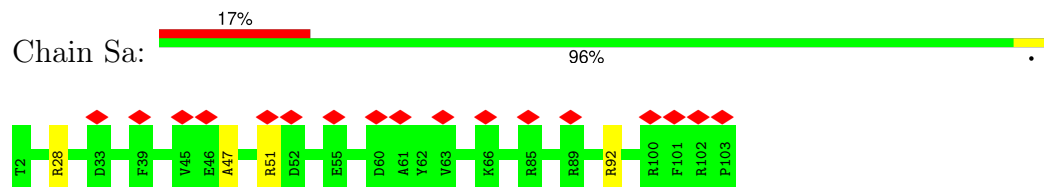
- Molecule 17: 40S ribosomal protein S21



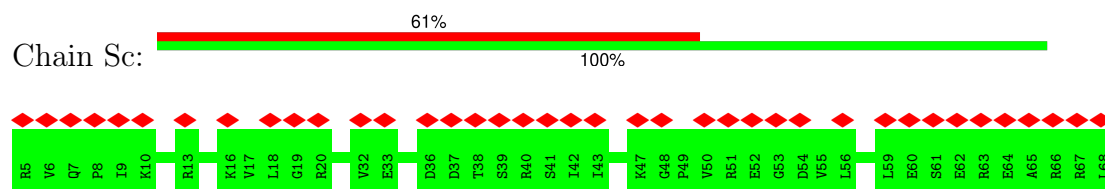
- Molecule 18: 40S ribosomal protein S23



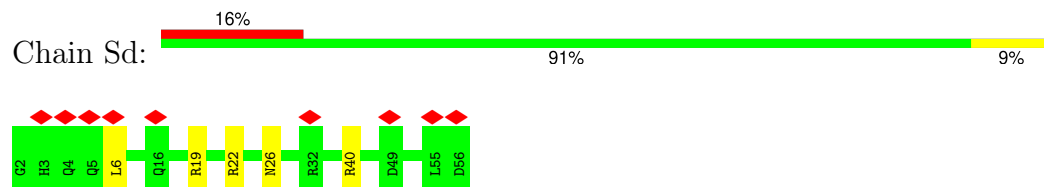
- Molecule 19: 40S ribosomal protein S26



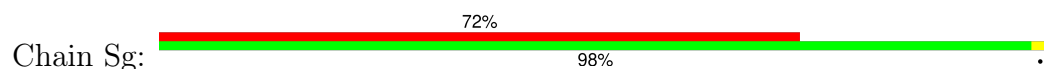
- Molecule 20: 40S ribosomal protein S28

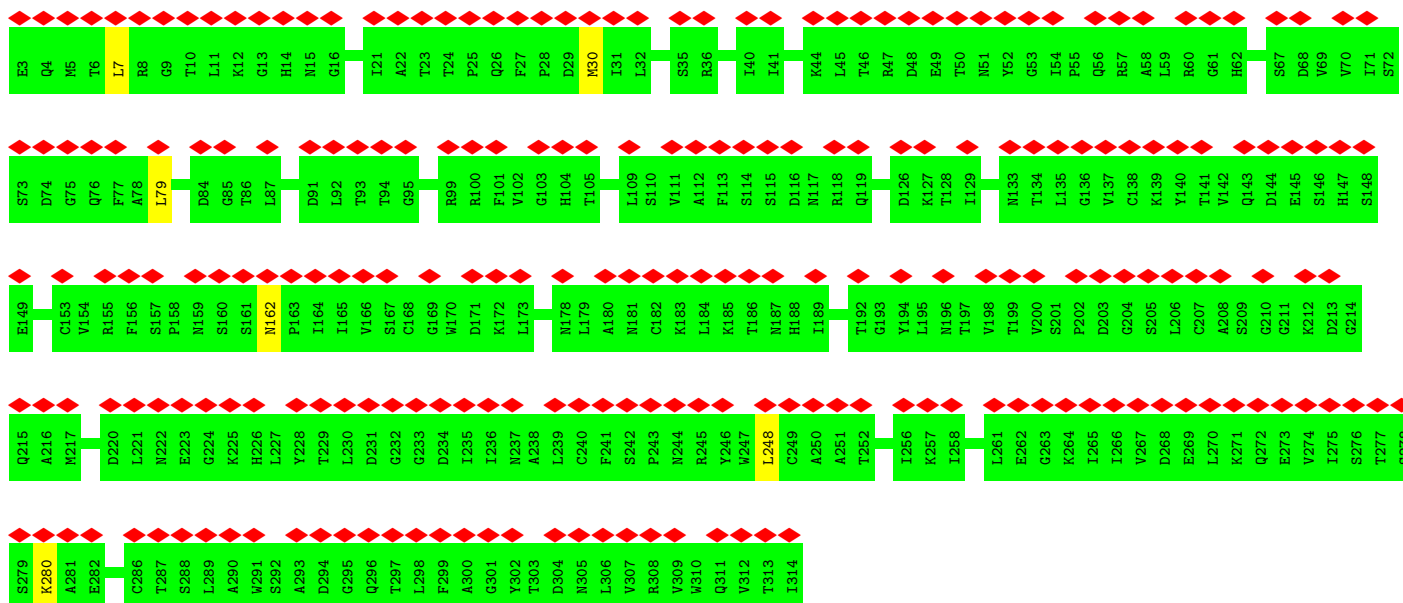


- Molecule 21: 40S ribosomal protein S29



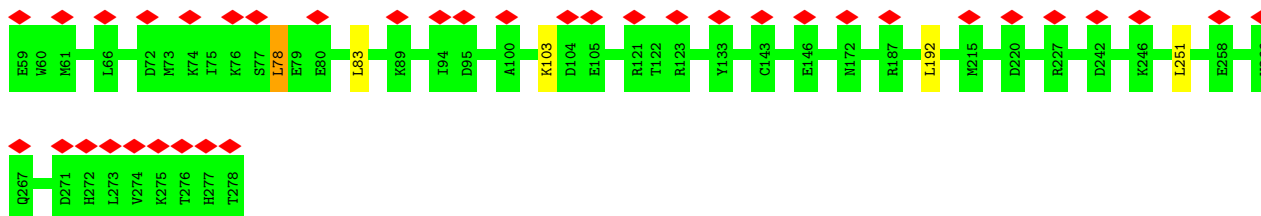
- Molecule 22: Receptor of activated protein C kinase 1





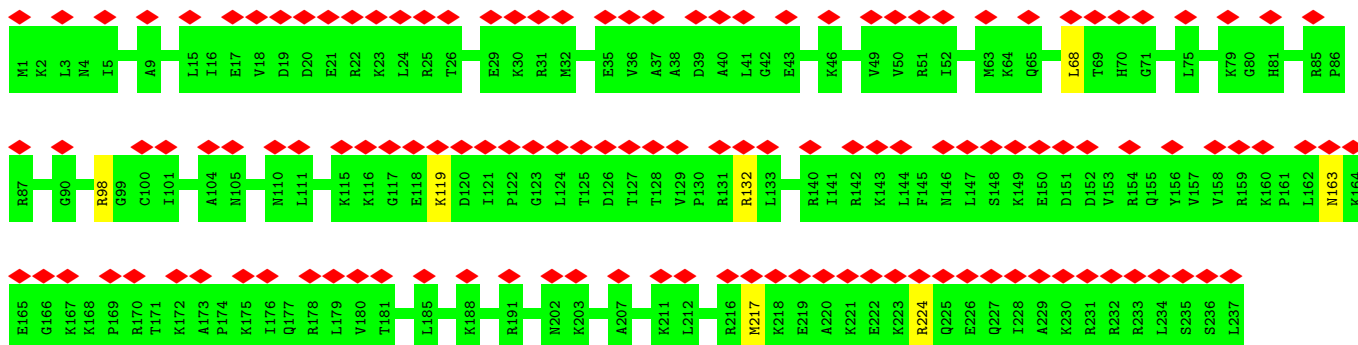
• Molecule 23: 40S ribosomal protein S2

Chain SC: 17% 98%



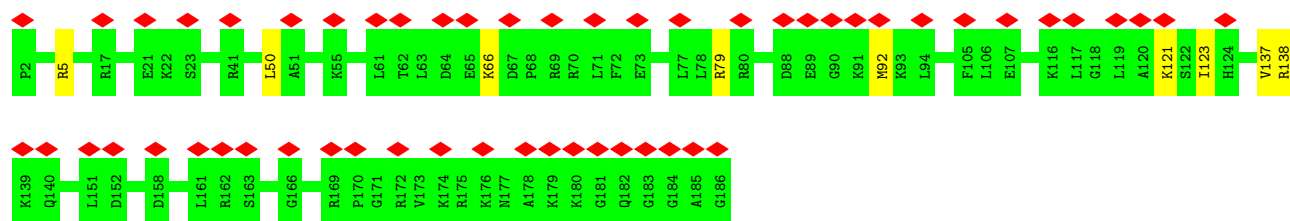
• Molecule 24: 40S ribosomal protein S6

Chain SG: 54% 97%

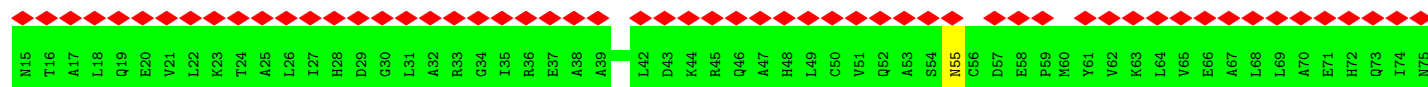


• Molecule 25: 40S ribosomal protein S9

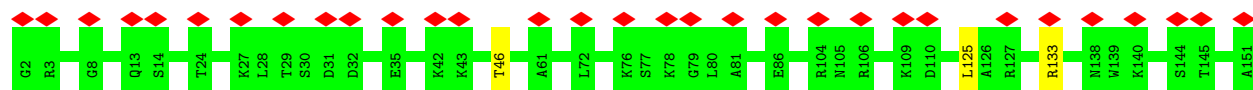
Chain SJ: 29% 95% 5%



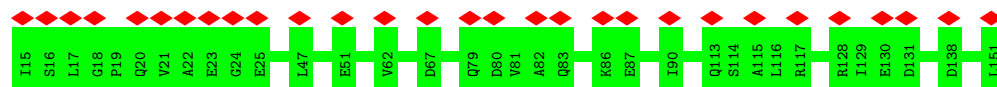
• Molecule 26: 40S ribosomal protein S12



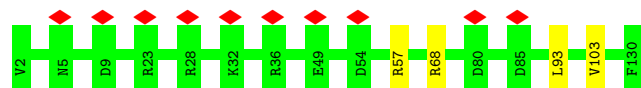
• Molecule 27: 40S ribosomal protein S13



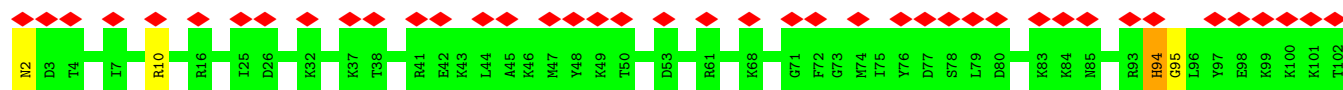
• Molecule 28: 40S ribosomal protein S14

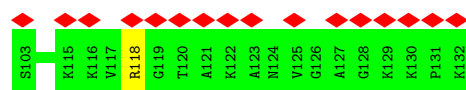


• Molecule 29: 40S ribosomal protein S15a

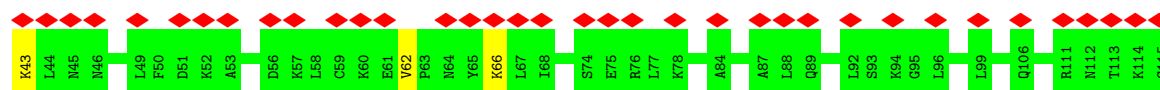


• Molecule 30: 40S ribosomal protein S24

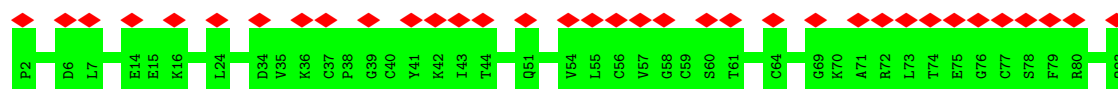




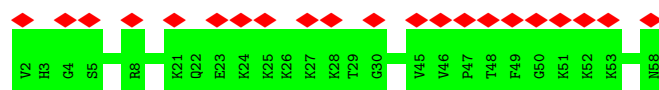
- Molecule 31: 40S ribosomal protein S25



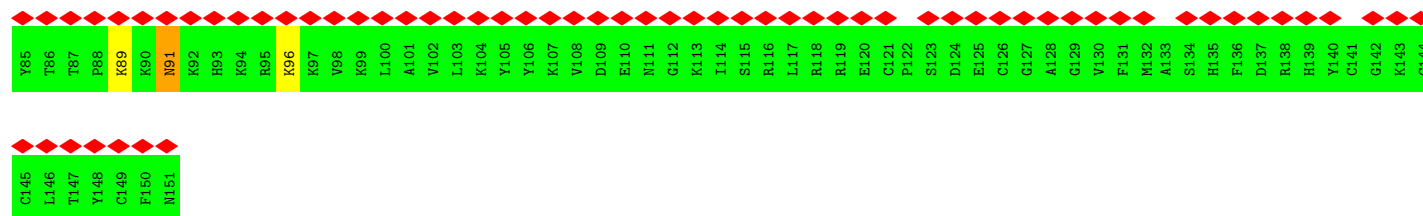
- Molecule 32: 40S ribosomal protein S27



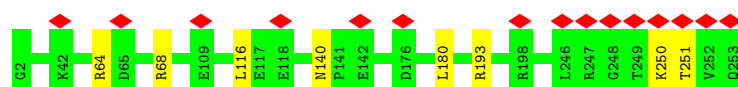
- Molecule 33: 40S ribosomal protein S30



- Molecule 34: 40S ribosomal protein S27a

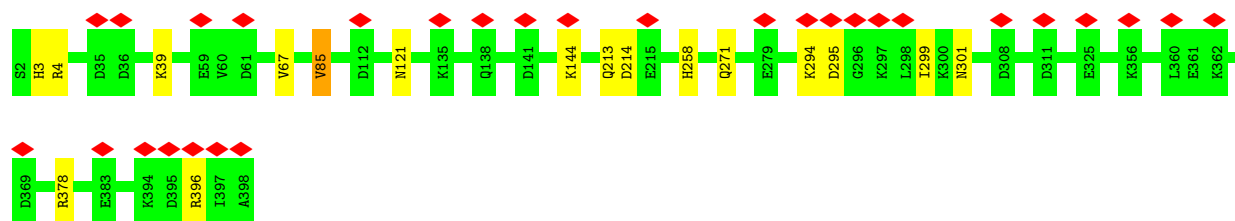


- Molecule 35: 60S ribosomal protein L8



- Molecule 36: 60S ribosomal protein L3

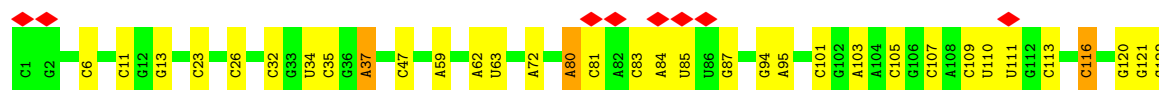




- Molecule 37: 60S ribosomal protein L4



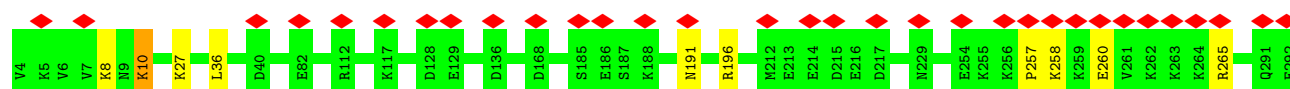
- Molecule 38: 5.8S ribosomal RNA



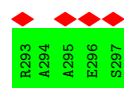
- Molecule 39: 5S ribosomal RNA

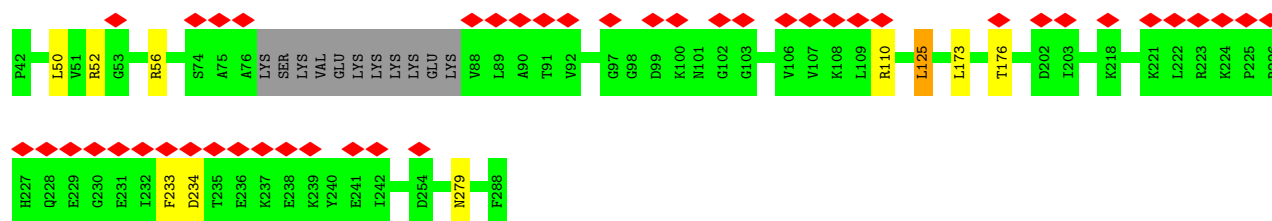


- Molecule 40: 60S ribosomal protein L5

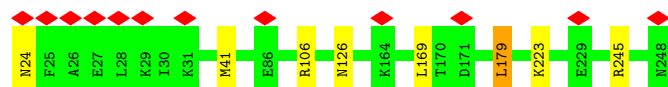


- Molecule 41: 60S ribosomal protein L6

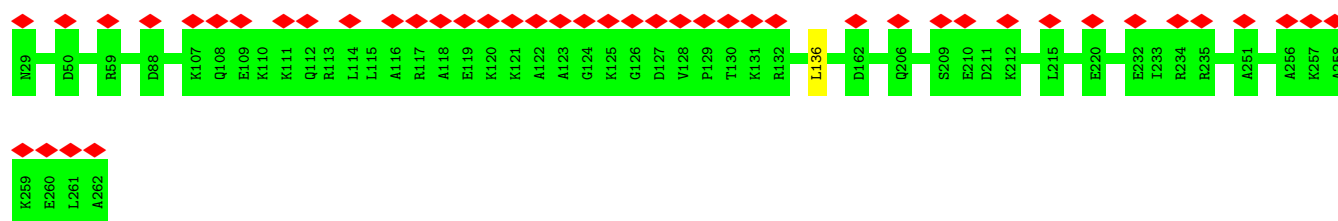




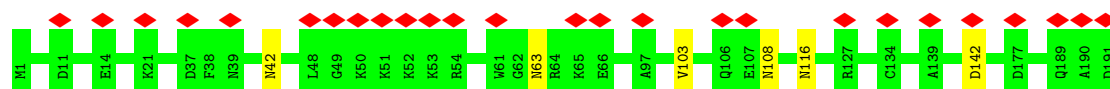
- Molecule 42: 60S ribosomal protein L7



- Molecule 43: 60S ribosomal protein L7a



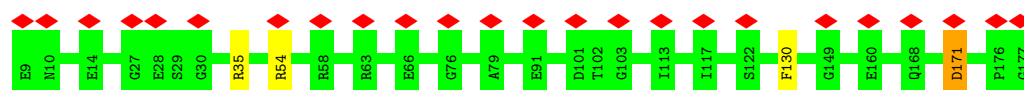
- Molecule 44: 60S ribosomal protein L9



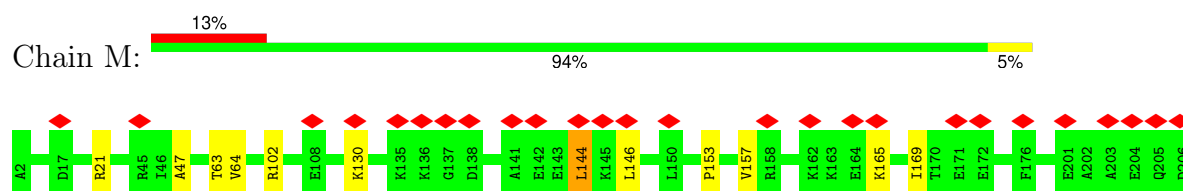
- Molecule 45: 60S ribosomal protein L10



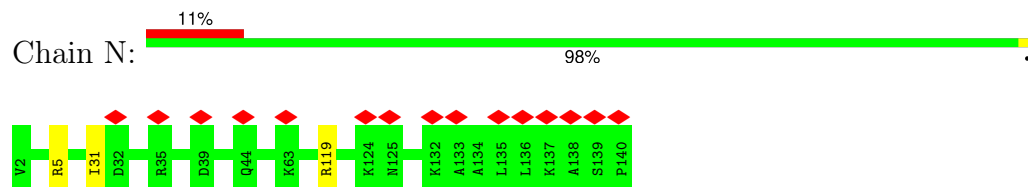
- Molecule 46: 60S ribosomal protein L11



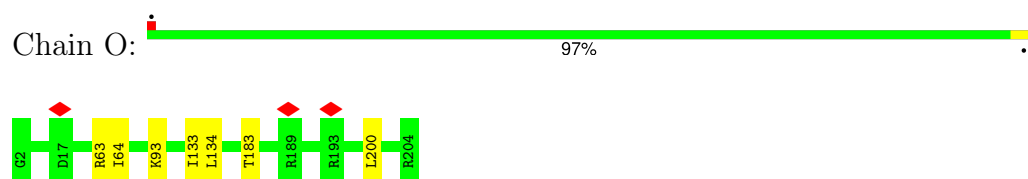
- Molecule 47: 60S ribosomal protein L13



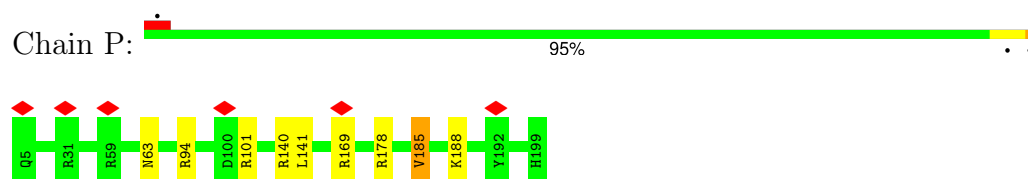
- Molecule 48: 60S ribosomal protein L14



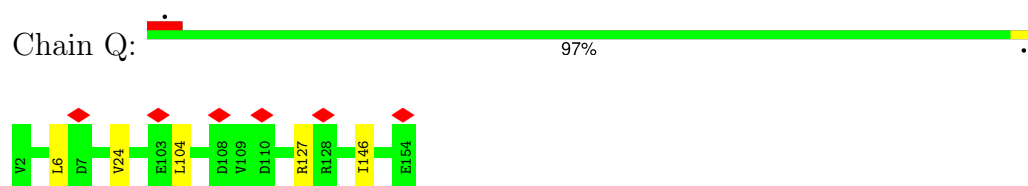
- Molecule 49: 60S ribosomal protein L15



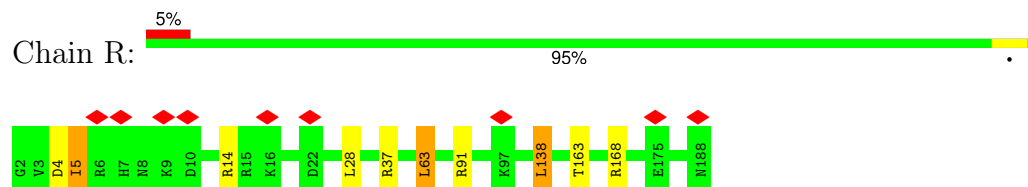
- Molecule 50: 60S ribosomal protein L13a



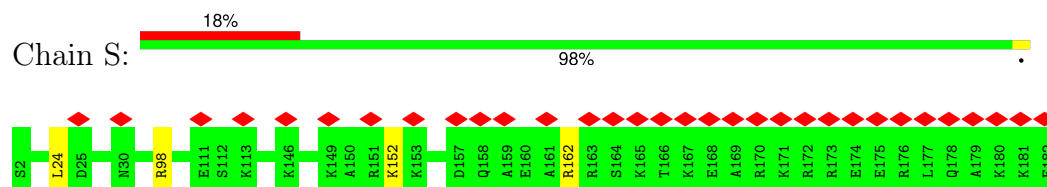
- Molecule 51: 60S ribosomal protein L17



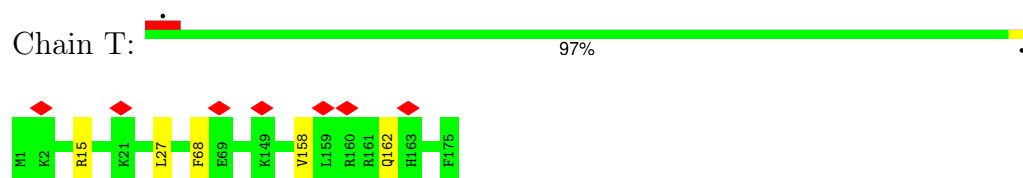
- Molecule 52: 60S ribosomal protein L18



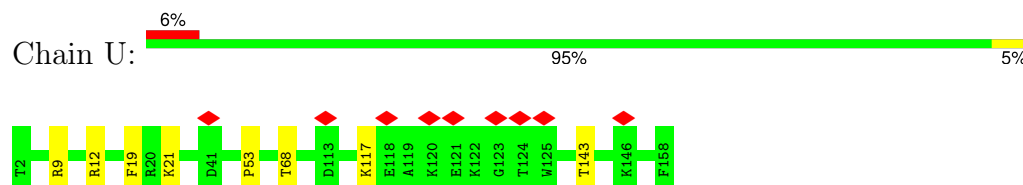
- Molecule 53: 60S ribosomal protein L19



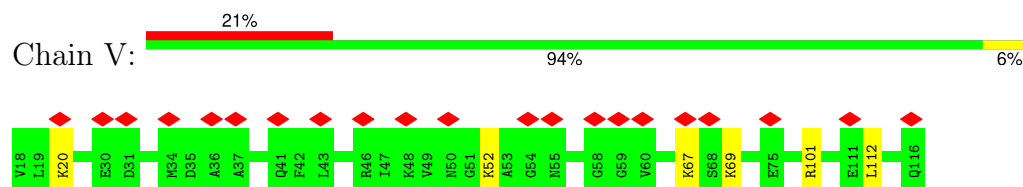
- Molecule 54: 60S ribosomal protein L18a



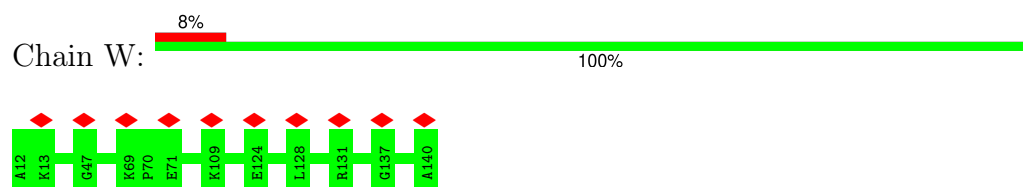
- Molecule 55: 60S ribosomal protein L21



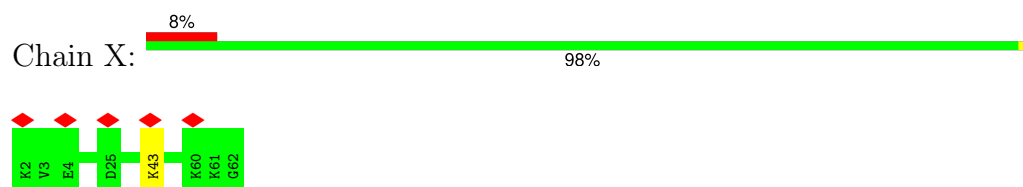
- Molecule 56: 60S ribosomal protein L22



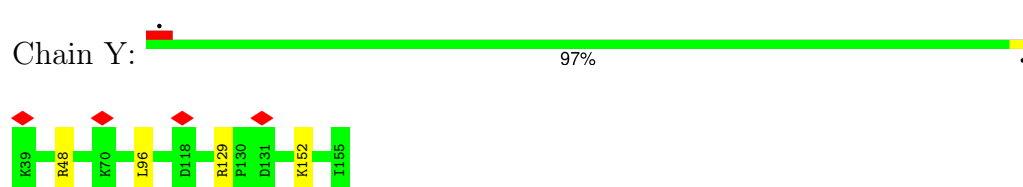
- Molecule 57: 60S ribosomal protein L23



- Molecule 58: 60S ribosomal protein L24

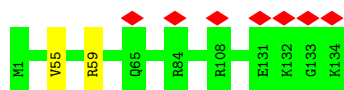


- Molecule 59: 60S ribosomal protein L23a

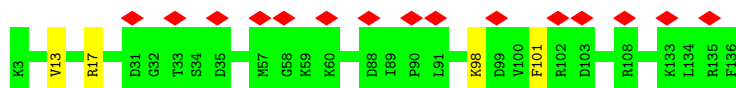


- Molecule 60: 60S ribosomal protein L26

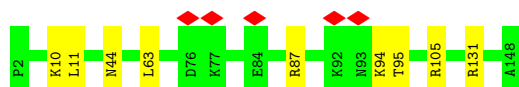




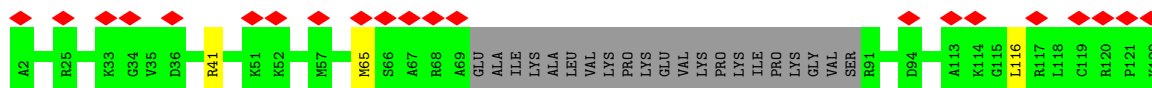
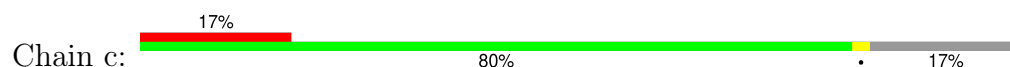
- Molecule 61: 60S ribosomal protein L27



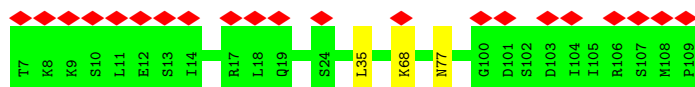
- Molecule 62: 60S ribosomal protein L27a



- Molecule 63: 60S ribosomal protein L29



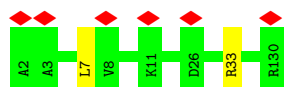
- Molecule 64: 60S ribosomal protein L30



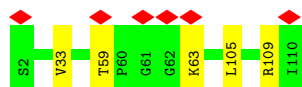
- Molecule 65: 60S ribosomal protein L31



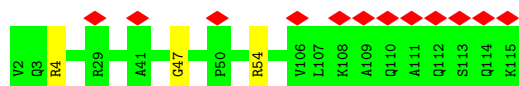
- Molecule 66: 60S ribosomal protein L32



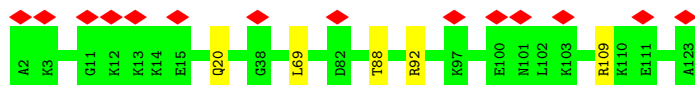
- Molecule 67: 60S ribosomal protein L35a



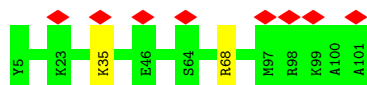
- Molecule 68: 60S ribosomal protein L34



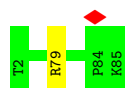
- Molecule 69: 60S ribosomal protein L35



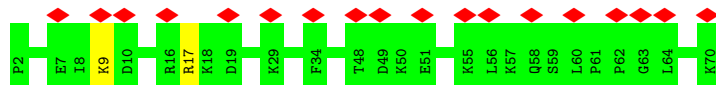
- Molecule 70: 60S ribosomal protein L36



- Molecule 71: 60S ribosomal protein L37



- Molecule 72: 60S ribosomal protein L38

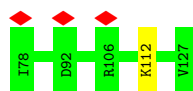


- Molecule 73: 60S ribosomal protein L39

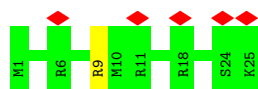




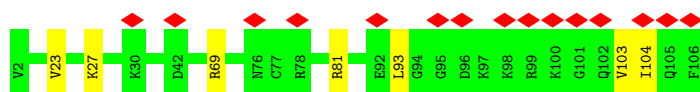
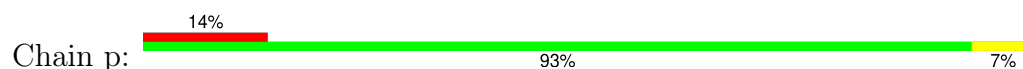
- Molecule 74: 60S ribosomal protein L40



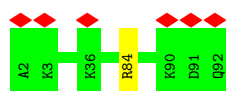
- Molecule 75: 60S ribosomal protein L41



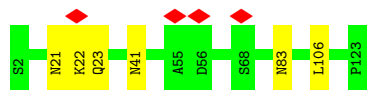
- Molecule 76: 60S ribosomal protein L36a



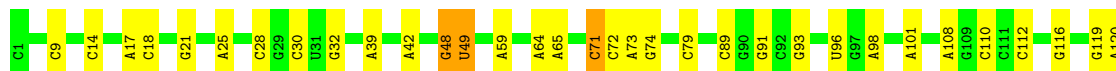
- Molecule 77: 60S ribosomal protein L37a

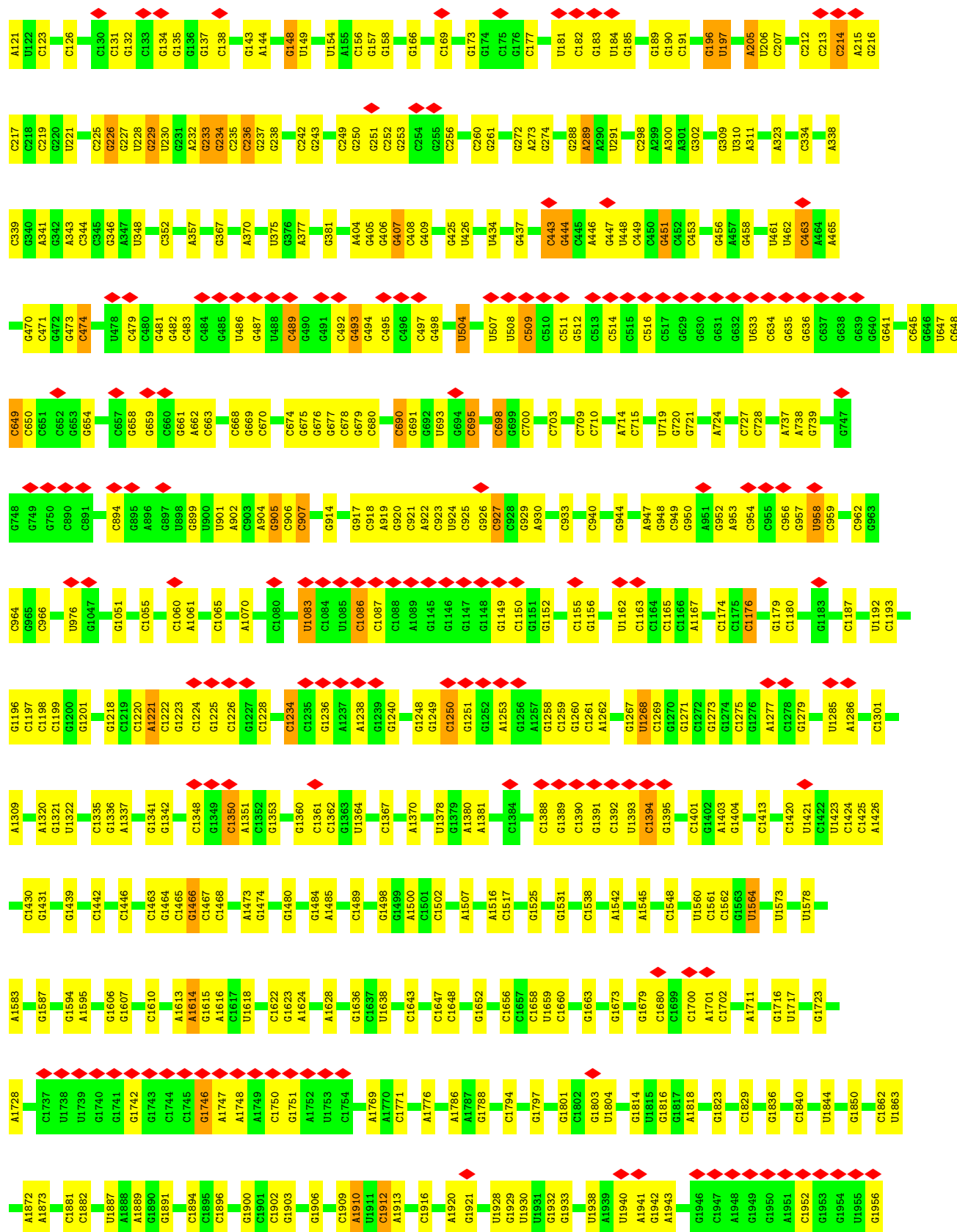


- Molecule 78: 60S ribosomal protein L28

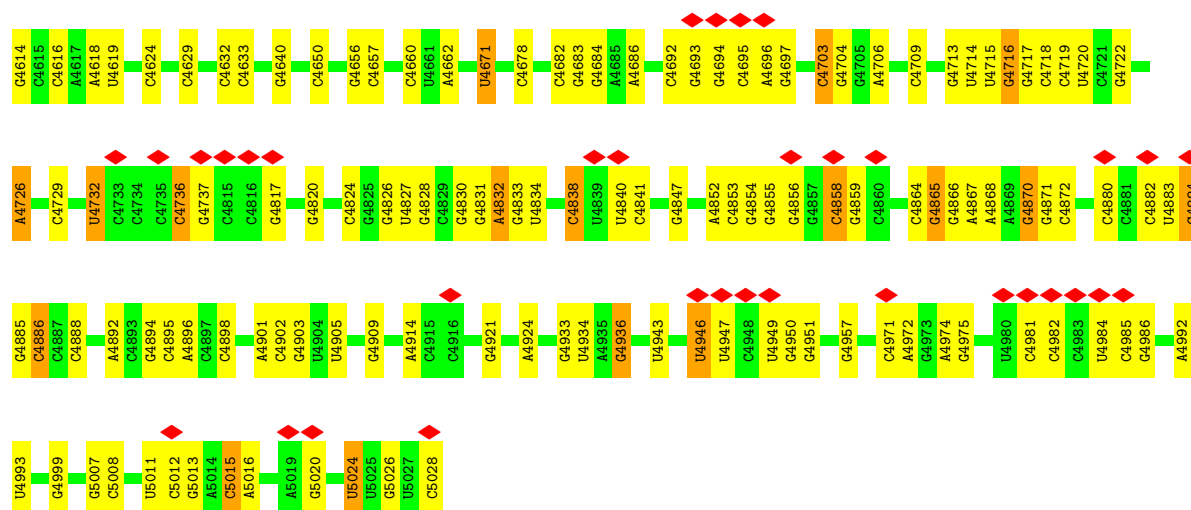


- Molecule 79: 28S ribosomal RNA

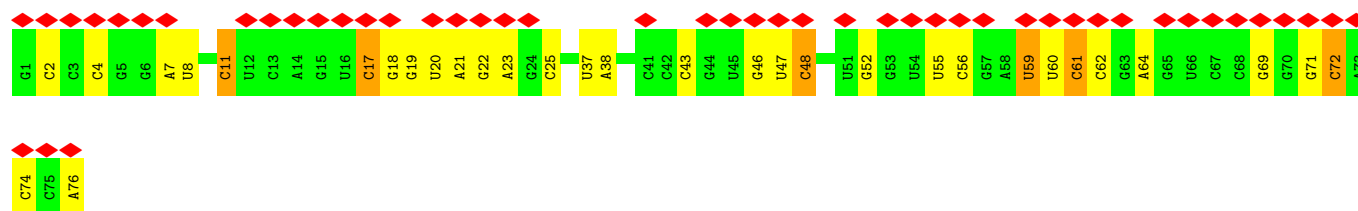




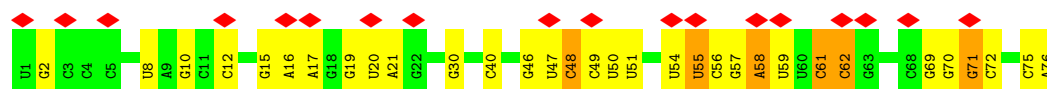
G4437	G4453	G4454	U4455	U4460	G4461	U4462	U4463	C4464	U4472	A4473	A4474	A4475	A4480	A4485	G4486	G4490	U4501	A4510	A4511	U4517	C4522	G4529	A4530	U4531	G4537	C4545	A4551	A4552	A4561	G4562	G4570	C4575	A4578	G4595	U4598	G4599	U4600	G4601																	
C4294	A4298	G4299	G4300	A4301	C4311	C4312	U4313	U4316	U4322	G4326	C4327	C4328	G4333	U4334	A4338	G4339	A4340	A4341	A4342	A4343	G4344	C4349	G4353	A4356	U4357	A4358	A4359	C4360	G4367	U4381	A4384	C4388	C4391	U4401	G4402	C4406	U4414	A4426	U4427	C4428															
C4139	G4145	C4146	C4153	C4158	A4165	C4166	A4167	A4172	A4175	A4176	C4177	C4185	A4186	A4187	A4338	G4339	U4340	A4341	A4342	A4343	G4344	C4349	G4353	A4356	U4357	A4358	A4359	C4360	G4367	U4381	A4384	C4388	C4391	U4401	G4402	C4406	U4414	A4426	U4427	C4428															
G4054	C4058	G4062	G4063	G4064	G4065	G4066	G4067	A4068	G4069	C4070	C4071	C4072	G4073	A4074	G4075	G4076	G4077	G4078	C4079	U4080	C4081	U4082	C4083	G4084	G4085	U4086	U4087	C4088	G4093	A4096	C4099	U4100	C4101	G4104	C4105	C4106	C4107	G4108	G4109	C4110	C4111	A4119	C4124	U4125	C4126	G4130	G4131	A4132							
G3790	A3795	A3796	C3797	C3798	A3799	C3805	U3809	G3810	U3811	U3822	A3838	A3847	A3848	C3849	G3850	G3851	G3852	C3858	G3859	G3860	U3863	C3864	A3865	G3866	C3867	G3868	G3869	A3872	A3876	A3877	G3878	A3879	C3880	U3886	G3887	A3894	C3897	G3909	G3917	A3918	U4037	G4046													
C3657	C3671	U3680	G3681	A3682	A3683	U3684	U3700	A3707	A3719	G3722	C3723	G3724	G3725	G3728	U3729	A3730	C3731	C3732	U3733	G3734	U3741	C3742	U3743	U3744	A3745	G3748	G3751	A3754	A3755	A3756	U3757	C3758	C3759	C3762	C3765	C3781	G3782	C3783	A3784	U3785	A3788	U3789													
A2858	U2859	A2860	G2863	C2871	U2879	G2880	G2881	C3569	A3570	G3571	C3572	C3573	U3577	U3587	G3588	C3589	G3590	A3595	G3596	G3597	A3606	C3607	U3612	U3615	C3616	A3617	A3618	A3619	A3624	A3633	A3634	G3635	C3638	G3643	C3644	U3651	C3656	U3659	G3660	U3661	G3662	A3663													
G2714	C2718	U2719	A2722	A2723	U2726	C2727	G2733	G2737	G2741	A2745	U2748	C2759	A2766	U2767	A2768	U2769	C2773	A2774	G2775	A2777	G2778	A2785	C2793	U2798	C2799	U2805	G2806	G2809	A2814	G2817	G2821	A2824	G2834	C2835	G2836	U2839	G2855																		
C2542	G2543	A2544	C2562	G2565	A2566	C2567	C2568	C2574	A2580	G2581	C2582	G2585	C2806	U2807	C2808	G2617	U2618	C2632	G2637	U2640	U2644	U2645	G2647	C2648	C2652	G2656	U2666	G2673	A2674	A2675	U2686	U2687	C2688	C2689	G2690	G2691	C2698	G2699	G2700	G2705															
G2421	U2426	G2429	A2430	G2431	A2432	G2442	U2446	U2447	C2448	C2449	C2457	G2458	C2461	G2462	A2463	U2464	G2465	G2466	C2467	C2468	U2469	C2470	A2471	G2472	U2473	U2474	G2475	C2476	G2477	G2482	C2483	C2484	G2485	A2490	A2491	A2492	C2499	G2523	U2524	G2525	G2526	U2532	U2533	C2538	G2539	C2540	G2541								
G2348	G2349	A2364	G2365	C2368	G2378	A2379	G2380	C2381	C2382	G2385	A2392	G2395	G2321	G2322	U2323	G2324	C2325	A2326	G2327	C2330	G2340	G2343	C2344	U2350	A2358	G2373	A2374	A2375	U2388	C2389	C2390	A2391	A2396	A2397	C2398	A2399	G2400	C2401	U2404	U2405	C2416														
A2028	U2029	C2032	G2036	G2037	C2043	G2043	U2051	C2054	C2064	C2065	G2066	G2067	C2068	G2069	U2070	G2072	A2073	G2075	G2076	U2077	G2078	C2081	G2082	G2083	C2087	G2088	G2089	C2090	G2091	G2092	C2093	C2228	C2229	G2230	G2231	A2232	G2233	C2234	C2237	G2238	G2239	G2240	G2241	A2242	C2245	U2246	A2247								
G1957	C1958	C1959	A1960	U1961	G1962	G1963	A1964	A1965	G1966	U1967	C1968	G1969	G1970	A1971	A1972	U1973	C1974	G1975	G1976	C1977	U1978	A1979	A1980	G1981	G1982	A1983	G1984	U1985	G1986	U1987	G1988	U1989	A1990	A1991	C1992	C1993	A1994	C1995	U1996	C1997	A1998	C2003	C2004	G2005	A2006	A2007	U2008	C2009	A2010	A2011	C2016	A2021	U2025	G2026	G2027



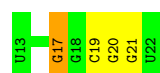
- Molecule 80: tRNA



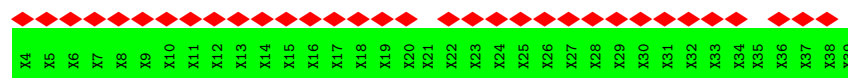
- Molecule 81: tRNA



- Molecule 82: mRNA



- Molecule 83: Nascent chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	38314	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 ($e^-/\text{\AA}^2$)	55	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	0.106	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.021	Depositor
Map size (\AA)	460.0, 460.0, 460.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.15, 1.15, 1.15	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MVM, OMU, OMC, ZN, OMG, A2M, MG, 5MC, 4AC, 6MZ, UR3, 5MU, PSU, B8Q, E3C, M7A, B8N, MA6

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	0.75	1/39959 (0.0%)	1.11	196/62253 (0.3%)
2	SA	0.45	0/1778	0.71	2/2416 (0.1%)
3	SB	0.43	0/1765	0.66	1/2362 (0.0%)
4	SD	0.41	0/1785	0.69	0/2404
5	SE	0.41	0/2101	0.66	2/2828 (0.1%)
6	SF	0.41	0/1516	0.68	0/2037
7	SH	0.41	0/1519	0.70	1/2033 (0.0%)
8	SI	0.42	0/1702	0.66	1/2271 (0.0%)
9	SK	0.43	0/851	0.70	2/1147 (0.2%)
10	SL	0.44	0/1268	0.68	0/1696
11	SP	0.43	0/1065	0.65	0/1423
12	SQ	0.43	0/1177	0.76	4/1575 (0.3%)
13	SR	0.36	0/1097	0.71	0/1474
14	SS	0.42	0/1216	0.71	2/1628 (0.1%)
15	ST	0.44	0/1131	0.68	1/1515 (0.1%)
16	SU	0.37	0/831	0.71	1/1115 (0.1%)
17	SV	0.43	0/631	0.71	0/844
18	SX	0.44	0/1116	0.72	0/1490
19	Sa	0.52	0/836	0.71	1/1121 (0.1%)
20	Sc	0.36	0/508	0.73	0/680
21	Sd	0.44	0/470	0.81	1/623 (0.2%)
22	Sg	0.40	0/2486	0.74	3/3384 (0.1%)
23	SC	0.50	0/1755	0.80	5/2371 (0.2%)
24	SG	0.36	0/1946	0.66	1/2590 (0.0%)
25	SJ	0.41	0/1561	0.77	1/2083 (0.0%)
26	SM	0.34	0/922	0.68	0/1238
27	SN	0.42	0/1232	0.66	1/1656 (0.1%)
28	SO	0.41	0/1037	0.69	0/1391
29	SW	0.50	0/1051	0.71	0/1406
30	SY	0.39	0/1094	0.68	1/1452 (0.1%)
31	SZ	0.41	0/585	0.80	0/785

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Sb	0.40	0/653	0.62	0/876
33	Se	0.36	0/458	0.69	0/604
34	Sf	0.44	1/560 (0.2%)	0.79	0/745
35	A	0.56	0/1968	0.72	2/2639 (0.1%)
36	B	0.53	0/3270	0.75	2/4377 (0.0%)
37	C	0.57	0/2942	0.77	2/3951 (0.1%)
38	D	0.96	2/3726 (0.1%)	1.17	24/5804 (0.4%)
39	E	0.90	1/2839 (0.0%)	1.05	10/4425 (0.2%)
40	F	0.50	0/2437	0.70	1/3262 (0.0%)
41	G	0.48	0/1942	0.81	5/2606 (0.2%)
42	H	0.61	0/1905	0.75	2/2539 (0.1%)
43	I	0.51	0/1913	0.71	1/2576 (0.0%)
44	J	0.46	0/1545	0.68	1/2077 (0.0%)
45	K	0.52	0/1730	0.69	2/2311 (0.1%)
46	L	0.46	0/1376	0.72	2/1841 (0.1%)
47	M	0.50	0/1688	0.75	2/2260 (0.1%)
48	N	0.51	0/1161	0.67	0/1554
49	O	0.62	0/1746	0.79	2/2338 (0.1%)
50	P	0.51	0/1638	0.71	1/2191 (0.0%)
51	Q	0.55	0/1268	0.74	2/1701 (0.1%)
52	R	0.57	0/1537	0.77	3/2052 (0.1%)
53	S	0.47	0/1533	0.72	1/2025 (0.0%)
54	T	0.55	0/1488	0.68	1/1997 (0.1%)
55	U	0.55	0/1312	0.71	0/1753
56	V	0.43	0/822	0.64	0/1103
57	W	0.54	0/983	0.66	0/1319
58	X	0.53	0/524	0.67	0/698
59	Y	0.51	0/975	0.70	0/1312
60	Z	0.55	0/1132	0.68	0/1504
61	a	0.52	0/1126	0.71	1/1502 (0.1%)
62	b	0.57	0/1191	0.80	2/1591 (0.1%)
63	c	0.44	0/826	0.70	1/1088 (0.1%)
64	d	0.50	0/812	0.75	0/1089
65	e	0.50	0/894	0.72	1/1204 (0.1%)
66	f	0.55	0/1082	0.71	0/1443
67	g	0.58	0/895	0.75	1/1198 (0.1%)
68	h	0.53	0/916	0.80	0/1220
69	i	0.48	0/1023	0.72	1/1351 (0.1%)
70	j	0.45	0/805	0.71	0/1065
71	k	0.55	0/703	0.71	0/929
72	l	0.46	0/575	0.68	0/761
73	m	0.52	0/454	0.76	0/599
74	n	0.41	0/417	0.71	0/553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	o	0.40	0/241	0.73	0/305
76	p	0.55	0/877	0.76	0/1156
77	q	0.60	0/718	0.72	0/953
78	r	0.58	0/995	0.85	1/1334 (0.1%)
79	t	0.95	10/86502 (0.0%)	1.16	539/134927 (0.4%)
80	u	0.52	0/1799	1.34	24/2800 (0.9%)
81	v	0.66	1/1802 (0.1%)	1.30	24/2797 (0.9%)
82	w	0.80	0/235	1.50	8/365 (2.2%)
All	All	0.75	16/229950 (0.0%)	1.01	896/337961 (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
25	SJ	0	1
40	F	0	1
47	M	0	1
76	p	0	1
All	All	0	4

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1495	G	C2-N3	-6.58	1.27	1.32
79	t	1221	A	N9-C4	-6.56	1.33	1.37
38	D	37	A	N9-C4	-6.53	1.33	1.37
79	t	1321	G	N9-C4	-6.51	1.32	1.38
79	t	148	G	N9-C4	-6.30	1.32	1.38

The worst 5 of 896 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	115	U	C2-N3-C4	21.07	139.65	127.00
80	u	55	U	N3-C2-O2	-14.70	111.91	122.20
81	v	61	C	C2-N1-C1'	14.12	134.33	118.80
1	S2	65	C	N1-C2-O2	14.06	127.33	118.90
81	v	61	C	N1-C2-O2	13.79	127.17	118.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
40	F	257	PRO	Peptide
47	M	130	LYS	Peptide
25	SJ	137	VAL	Peptide
76	p	103	VAL	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	SA	219/221 (99%)	192 (88%)	26 (12%)	1 (0%)	25	59
3	SB	212/214 (99%)	191 (90%)	21 (10%)	0	100	100
4	SD	224/226 (99%)	194 (87%)	30 (13%)	0	100	100
5	SE	257/259 (99%)	241 (94%)	16 (6%)	0	100	100
6	SF	187/189 (99%)	171 (91%)	16 (9%)	0	100	100
7	SH	182/189 (96%)	163 (90%)	19 (10%)	0	100	100
8	SI	202/204 (99%)	182 (90%)	20 (10%)	0	100	100
9	SK	96/98 (98%)	83 (86%)	12 (12%)	1 (1%)	13	46
10	SL	151/153 (99%)	135 (89%)	15 (10%)	1 (1%)	19	53
11	SP	125/127 (98%)	111 (89%)	14 (11%)	0	100	100
12	SQ	144/146 (99%)	127 (88%)	15 (10%)	2 (1%)	9	40
13	SR	132/134 (98%)	119 (90%)	12 (9%)	1 (1%)	16	51
14	SS	143/145 (99%)	127 (89%)	16 (11%)	0	100	100
15	ST	141/143 (99%)	130 (92%)	10 (7%)	1 (1%)	19	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	SU	102/104 (98%)	93 (91%)	9 (9%)	0	100	100
17	SV	80/82 (98%)	72 (90%)	8 (10%)	0	100	100
18	SX	139/141 (99%)	126 (91%)	13 (9%)	0	100	100
19	Sa	100/102 (98%)	88 (88%)	11 (11%)	1 (1%)	13	46
20	Sc	62/64 (97%)	51 (82%)	11 (18%)	0	100	100
21	Sd	53/55 (96%)	44 (83%)	9 (17%)	0	100	100
22	Sg	310/312 (99%)	255 (82%)	55 (18%)	0	100	100
23	SC	219/220 (100%)	201 (92%)	17 (8%)	1 (0%)	25	59
24	SG	235/237 (99%)	212 (90%)	23 (10%)	0	100	100
25	SJ	184/185 (100%)	168 (91%)	15 (8%)	1 (0%)	25	59
26	SM	116/118 (98%)	102 (88%)	14 (12%)	0	100	100
27	SN	148/150 (99%)	145 (98%)	3 (2%)	0	100	100
28	SO	135/137 (98%)	117 (87%)	18 (13%)	0	100	100
29	SW	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
30	SY	130/131 (99%)	119 (92%)	10 (8%)	1 (1%)	16	51
31	SZ	71/73 (97%)	58 (82%)	13 (18%)	0	100	100
32	Sb	80/82 (98%)	67 (84%)	13 (16%)	0	100	100
33	Se	55/57 (96%)	48 (87%)	7 (13%)	0	100	100
34	Sf	65/67 (97%)	52 (80%)	13 (20%)	0	100	100
35	A	250/252 (99%)	222 (89%)	27 (11%)	1 (0%)	30	64
36	B	395/397 (100%)	355 (90%)	37 (9%)	3 (1%)	16	51
37	C	361/363 (99%)	326 (90%)	31 (9%)	4 (1%)	12	45
40	F	292/294 (99%)	257 (88%)	32 (11%)	3 (1%)	13	46
41	G	232/247 (94%)	194 (84%)	38 (16%)	0	100	100
42	H	223/225 (99%)	209 (94%)	13 (6%)	1 (0%)	30	64
43	I	232/234 (99%)	212 (91%)	20 (9%)	0	100	100
44	J	189/191 (99%)	170 (90%)	19 (10%)	0	100	100
45	K	204/211 (97%)	179 (88%)	24 (12%)	1 (0%)	25	59
46	L	167/169 (99%)	150 (90%)	16 (10%)	1 (1%)	22	56
47	M	203/205 (99%)	168 (83%)	31 (15%)	4 (2%)	6	33
48	N	137/139 (99%)	126 (92%)	11 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	O	201/203 (99%)	181 (90%)	20 (10%)	0	100	100
50	P	193/195 (99%)	186 (96%)	6 (3%)	1 (0%)	25	59
51	Q	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
52	R	185/187 (99%)	171 (92%)	14 (8%)	0	100	100
53	S	179/181 (99%)	171 (96%)	8 (4%)	0	100	100
54	T	173/175 (99%)	158 (91%)	15 (9%)	0	100	100
55	U	155/157 (99%)	136 (88%)	17 (11%)	2 (1%)	10	41
56	V	97/99 (98%)	89 (92%)	8 (8%)	0	100	100
57	W	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
58	X	59/61 (97%)	55 (93%)	4 (7%)	0	100	100
59	Y	115/117 (98%)	107 (93%)	8 (7%)	0	100	100
60	Z	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
61	a	132/134 (98%)	118 (89%)	14 (11%)	0	100	100
62	b	145/147 (99%)	125 (86%)	19 (13%)	1 (1%)	19	53
63	c	94/121 (78%)	83 (88%)	11 (12%)	0	100	100
64	d	101/103 (98%)	86 (85%)	15 (15%)	0	100	100
65	e	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
66	f	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	51
67	g	107/109 (98%)	98 (92%)	9 (8%)	0	100	100
68	h	112/114 (98%)	101 (90%)	10 (9%)	1 (1%)	14	49
69	i	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	16	51
70	j	95/97 (98%)	88 (93%)	6 (6%)	1 (1%)	12	45
71	k	82/84 (98%)	75 (92%)	7 (8%)	0	100	100
72	l	67/69 (97%)	62 (92%)	5 (8%)	0	100	100
73	m	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
74	n	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
75	o	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
76	p	103/105 (98%)	93 (90%)	9 (9%)	1 (1%)	13	46
77	q	89/91 (98%)	83 (93%)	6 (7%)	0	100	100
78	r	120/122 (98%)	105 (88%)	12 (10%)	3 (2%)	4	29
All	All	11195/11390 (98%)	10073 (90%)	1081 (10%)	41 (0%)	32	64

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	SK	63	ALA
10	SL	23	VAL
13	SR	129	LYS
15	ST	41	LYS
23	SC	78	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	SA	183/183 (100%)	178 (97%)	5 (3%)	40	65
3	SB	195/195 (100%)	192 (98%)	3 (2%)	60	77
4	SD	189/189 (100%)	188 (100%)	1 (0%)	86	93
5	SE	222/222 (100%)	218 (98%)	4 (2%)	54	74
6	SF	159/159 (100%)	154 (97%)	5 (3%)	35	63
7	SH	166/169 (98%)	163 (98%)	3 (2%)	54	74
8	SI	177/177 (100%)	172 (97%)	5 (3%)	38	65
9	SK	89/89 (100%)	85 (96%)	4 (4%)	23	53
10	SL	137/137 (100%)	132 (96%)	5 (4%)	30	59
11	SP	113/113 (100%)	109 (96%)	4 (4%)	31	59
12	SQ	121/121 (100%)	120 (99%)	1 (1%)	79	88
13	SR	121/121 (100%)	118 (98%)	3 (2%)	42	67
14	SS	126/126 (100%)	125 (99%)	1 (1%)	79	88
15	ST	113/113 (100%)	110 (97%)	3 (3%)	40	65
16	SU	94/94 (100%)	90 (96%)	4 (4%)	25	54
17	SV	66/66 (100%)	63 (96%)	3 (4%)	23	53
18	SX	113/113 (100%)	110 (97%)	3 (3%)	40	65
19	Sa	89/89 (100%)	87 (98%)	2 (2%)	47	70
20	Sc	57/57 (100%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	Sd	48/48 (100%)	44 (92%)	4 (8%)	9	32
22	Sg	271/271 (100%)	268 (99%)	3 (1%)	70	83
23	SC	187/186 (100%)	186 (100%)	1 (0%)	86	93
24	SG	207/207 (100%)	201 (97%)	6 (3%)	37	64
25	SJ	162/161 (101%)	155 (96%)	7 (4%)	25	54
26	SM	98/100 (98%)	95 (97%)	3 (3%)	35	63
27	SN	130/130 (100%)	128 (98%)	2 (2%)	60	77
28	SO	107/107 (100%)	107 (100%)	0	100	100
29	SW	112/112 (100%)	108 (96%)	4 (4%)	30	59
30	SY	114/113 (101%)	110 (96%)	4 (4%)	31	59
31	SZ	64/64 (100%)	61 (95%)	3 (5%)	22	51
32	Sb	74/74 (100%)	74 (100%)	0	100	100
33	Se	46/46 (100%)	46 (100%)	0	100	100
34	Sf	60/60 (100%)	57 (95%)	3 (5%)	20	49
35	A	194/194 (100%)	189 (97%)	5 (3%)	41	66
36	B	345/345 (100%)	332 (96%)	13 (4%)	28	57
37	C	302/302 (100%)	293 (97%)	9 (3%)	36	63
40	F	248/248 (100%)	242 (98%)	6 (2%)	44	68
41	G	209/220 (95%)	203 (97%)	6 (3%)	37	64
42	H	194/194 (100%)	188 (97%)	6 (3%)	35	63
43	I	199/199 (100%)	199 (100%)	0	100	100
44	J	170/170 (100%)	165 (97%)	5 (3%)	37	64
45	K	178/179 (99%)	173 (97%)	5 (3%)	38	65
46	L	142/142 (100%)	140 (99%)	2 (1%)	62	79
47	M	171/171 (100%)	165 (96%)	6 (4%)	31	59
48	N	118/118 (100%)	115 (98%)	3 (2%)	42	67
49	O	171/171 (100%)	166 (97%)	5 (3%)	37	64
50	P	168/168 (100%)	160 (95%)	8 (5%)	21	50
51	Q	134/134 (100%)	131 (98%)	3 (2%)	47	70
52	R	164/164 (100%)	154 (94%)	10 (6%)	15	43
53	S	160/160 (100%)	157 (98%)	3 (2%)	52	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	T	156/156 (100%)	152 (97%)	4 (3%)	41	66
55	U	138/138 (100%)	132 (96%)	6 (4%)	25	54
56	V	89/89 (100%)	83 (93%)	6 (7%)	13	40
57	W	100/100 (100%)	100 (100%)	0	100	100
58	X	53/53 (100%)	52 (98%)	1 (2%)	52	73
59	Y	105/105 (100%)	101 (96%)	4 (4%)	28	57
60	Z	124/124 (100%)	122 (98%)	2 (2%)	58	76
61	a	117/117 (100%)	114 (97%)	3 (3%)	41	66
62	b	120/120 (100%)	114 (95%)	6 (5%)	20	49
63	c	82/101 (81%)	80 (98%)	2 (2%)	44	68
64	d	88/88 (100%)	85 (97%)	3 (3%)	32	60
65	e	97/97 (100%)	95 (98%)	2 (2%)	48	71
66	f	115/115 (100%)	114 (99%)	1 (1%)	75	86
67	g	88/88 (100%)	84 (96%)	4 (4%)	23	53
68	h	98/98 (100%)	96 (98%)	2 (2%)	50	72
69	i	109/109 (100%)	106 (97%)	3 (3%)	38	65
70	j	83/83 (100%)	82 (99%)	1 (1%)	67	82
71	k	71/71 (100%)	70 (99%)	1 (1%)	62	79
72	l	64/64 (100%)	62 (97%)	2 (3%)	35	63
73	m	47/47 (100%)	46 (98%)	1 (2%)	48	71
74	n	46/46 (100%)	45 (98%)	1 (2%)	47	70
75	o	24/24 (100%)	23 (96%)	1 (4%)	25	54
76	p	93/93 (100%)	88 (95%)	5 (5%)	18	46
77	q	74/74 (100%)	73 (99%)	1 (1%)	62	79
78	r	106/106 (100%)	104 (98%)	2 (2%)	52	73
All	All	9764/9797 (100%)	9506 (97%)	258 (3%)	42	66

5 of 258 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
65	e	93	ASN
68	h	4	ARG
34	Sf	91	ASN

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Mol	Chain	Res	Type
31	SZ	62	VAL
70	j	68	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 131 such sidechains are listed below:

Mol	Chain	Res	Type
64	d	77	ASN
66	f	107	ASN
78	r	45	HIS
35	A	50	HIS
34	Sf	91	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1690/1714 (98%)	565 (33%)	31 (1%)
38	D	156/157 (99%)	38 (24%)	0
39	E	118/121 (97%)	19 (16%)	0
79	t	3590/3607 (99%)	878 (24%)	0
80	u	74/76 (97%)	28 (37%)	0
81	v	71/76 (93%)	28 (39%)	0
82	w	9/10 (90%)	2 (22%)	0
All	All	5708/5761 (99%)	1558 (27%)	31 (0%)

5 of 1558 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	2	A
1	S2	9	U
1	S2	10	G
1	S2	11	A
1	S2	16	G

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	563	G
1	S2	1813	A
1	S2	872	A
1	S2	1815	A

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Mol	Chain	Res	Type
1	S2	1661	A

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	B8Q	S2	1219	1	18,22,23	4.74	7 (38%)	21,32,35	1.90	5 (23%)
1	UR3	S2	1830	1	19,22,23	2.79	7 (36%)	26,32,35	3.04	9 (34%)
1	A2M	S2	1678	1	18,25,26	4.29	5 (27%)	20,36,39	3.50	6 (30%)
1	4AC	S2	1842	1	21,24,25	3.23	9 (42%)	28,34,37	1.12	3 (10%)
1	PSU	S2	822	1	18,21,22	4.38	8 (44%)	21,30,33	1.92	4 (19%)
1	A2M	S2	1031	1	18,25,26	4.19	5 (27%)	20,36,39	3.68	5 (25%)
1	A2M	S2	27	1	18,25,26	4.17	5 (27%)	20,36,39	3.57	6 (30%)
1	OMC	S2	174	1	19,22,23	3.53	8 (42%)	25,31,34	0.92	1 (4%)
1	4AC	S2	1337	1	21,24,25	3.28	9 (42%)	28,34,37	1.25	3 (10%)
1	5MU	S2	814	1	19,22,23	7.59	8 (42%)	27,32,35	3.61	11 (40%)
1	PSU	S2	823	1	18,21,22	4.49	8 (44%)	21,30,33	2.18	4 (19%)
1	OMC	S2	1710	1	19,22,23	3.58	8 (42%)	25,31,34	0.65	0
1	MA6	S2	1850	1	19,26,27	1.67	2 (10%)	18,38,41	3.89	4 (22%)
1	PSU	S2	612	1	18,21,22	4.25	8 (44%)	21,30,33	2.22	6 (28%)
1	OMG	S2	683	1	19,26,27	2.37	8 (42%)	21,38,41	1.47	5 (23%)
1	B8N	S2	1248	1	25,29,30	3.15	7 (28%)	28,42,45	2.12	7 (25%)
1	A2M	S2	668	1	18,25,26	4.07	5 (27%)	20,36,39	3.84	8 (40%)
1	OMG	S2	509	1	19,26,27	2.37	8 (42%)	21,38,41	1.47	4 (19%)
1	OMC	S2	1703	1	19,22,23	3.48	8 (42%)	25,31,34	0.61	0
1	PSU	S2	1081	1	18,21,22	4.30	8 (44%)	21,30,33	1.95	4 (19%)
1	OMC	S2	517	1	19,22,23	3.39	8 (42%)	25,31,34	0.86	1 (4%)
1	6MZ	S2	1832	1	17,25,26	1.60	4 (23%)	15,36,39	2.26	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	E3C	S2	568	1	19,23,24	3.59	7 (36%)	21,33,36	2.64	6 (28%)
1	PSU	S2	119	1	18,21,22	4.45	7 (38%)	21,30,33	2.10	5 (23%)
1	OMU	S2	121	1	19,22,23	3.08	7 (36%)	25,31,34	2.00	6 (24%)
1	A2M	S2	166	1	18,25,26	4.28	6 (33%)	20,36,39	3.80	5 (25%)
1	OMU	S2	116	1	19,22,23	3.16	6 (31%)	25,31,34	1.81	4 (16%)
1	PSU	S2	1243	1	18,21,22	4.39	7 (38%)	21,30,33	1.96	4 (19%)
1	OMG	S2	644	1	19,26,27	2.44	8 (42%)	21,38,41	1.50	4 (19%)
1	A2M	S2	159	1	18,25,26	4.34	5 (27%)	20,36,39	3.63	10 (50%)
1	5MC	S2	1374	1	19,22,23	3.64	8 (42%)	26,32,35	1.05	2 (7%)
1	M7A	S2	1806	1	19,25,26	1.67	2 (10%)	25,37,40	3.74	8 (32%)
1	MA6	S2	1851	1	19,26,27	1.63	2 (10%)	18,38,41	3.88	4 (22%)
1	A2M	S2	484	1	18,25,26	4.16	6 (33%)	20,36,39	3.66	6 (30%)

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	B8Q	S2	1219	1	-	0/7/42/43	0/2/2/2
1	UR3	S2	1830	1	-	4/7/25/26	0/2/2/2
1	A2M	S2	1678	1	-	0/5/27/28	0/3/3/3
1	4AC	S2	1842	1	-	0/11/29/30	0/2/2/2
1	PSU	S2	822	1	-	4/7/25/26	0/2/2/2
1	A2M	S2	1031	1	-	1/5/27/28	0/3/3/3
1	A2M	S2	27	1	-	1/5/27/28	0/3/3/3
1	OMC	S2	174	1	-	1/9/27/28	0/2/2/2
1	4AC	S2	1337	1	-	0/11/29/30	0/2/2/2
1	5MU	S2	814	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	823	1	-	3/7/25/26	0/2/2/2
1	OMC	S2	1710	1	-	0/9/27/28	0/2/2/2
1	MA6	S2	1850	1	-	4/7/29/30	0/3/3/3
1	PSU	S2	612	1	-	2/7/25/26	0/2/2/2
1	OMG	S2	683	1	-	2/5/27/28	0/3/3/3
1	B8N	S2	1248	1	-	4/16/34/35	0/2/2/2
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	OMC	S2	1703	1	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	1081	1	-	2/7/25/26	0/2/2/2
1	OMC	S2	517	1	-	0/9/27/28	0/2/2/2
1	6MZ	S2	1832	1	-	2/5/27/28	0/3/3/3
1	E3C	S2	568	1	-	4/9/44/45	0/2/2/2
1	PSU	S2	119	1	-	2/7/25/26	0/2/2/2
1	OMU	S2	121	1	-	3/9/27/28	0/2/2/2
1	A2M	S2	166	1	-	0/5/27/28	0/3/3/3
1	OMU	S2	116	1	-	2/9/27/28	0/2/2/2
1	PSU	S2	1243	1	-	2/7/25/26	0/2/2/2
1	OMG	S2	644	1	-	1/5/27/28	0/3/3/3
1	A2M	S2	159	1	-	3/5/27/28	0/3/3/3
1	5MC	S2	1374	1	-	0/7/25/26	0/2/2/2
1	M7A	S2	1806	1	-	3/7/37/38	0/3/3/3
1	MA6	S2	1851	1	-	4/7/29/30	0/3/3/3
1	A2M	S2	484	1	-	0/5/27/28	0/3/3/3

The worst 5 of 224 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	814	5MU	C4-C5	22.49	1.81	1.44
1	S2	814	5MU	C6-N1	16.54	1.66	1.38
1	S2	159	A2M	O4'-C1'	11.96	1.56	1.40
1	S2	823	PSU	C6-C5	11.93	1.48	1.35
1	S2	166	A2M	O4'-C1'	11.89	1.56	1.40

The worst 5 of 164 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S2	1851	MA6	N1-C6-N6	-13.97	100.69	116.83
1	S2	1850	MA6	N1-C6-N6	-13.27	101.50	116.83
1	S2	1806	M7A	C5-C6-N6	11.08	142.57	123.75
1	S2	668	A2M	C1'-N9-C4	-10.11	108.88	126.64
1	S2	814	5MU	C5-C4-N3	9.88	123.91	115.32

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	S2	27	A2M	C1'-C2'-O2'-CM'

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Mol	Chain	Res	Type	Atoms
1	S2	116	OMU	O4'-C4'-C5'-O5'
1	S2	121	OMU	C3'-C4'-C5'-O5'
1	S2	121	OMU	O4'-C4'-C5'-O5'
1	S2	159	A2M	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	5110	-	32,35,35	1.68	5 (15%)	39,49,49	2.43	14 (35%)

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	5110	-	-	1/20/28/28	0/5/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	t	5110	MVM	C5-N1	5.94	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	t	5110	MVM	N5-N4	-3.74	1.31	1.37
86	t	5110	MVM	C6-N1	2.40	1.45	1.39
86	t	5110	MVM	C12-C5	2.26	1.53	1.50
86	t	5110	MVM	C7-C3	-2.01	1.48	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	t	5110	MVM	C15-N4-C22	-6.43	121.84	130.09
86	t	5110	MVM	C15-N4-N5	5.28	128.40	119.95
86	t	5110	MVM	C21-N7-C22	4.95	122.73	116.81
86	t	5110	MVM	C6-N1-C5	-4.82	117.17	122.94
86	t	5110	MVM	C1-C9-N1	-4.15	105.75	116.16

There are no chirality outliers.

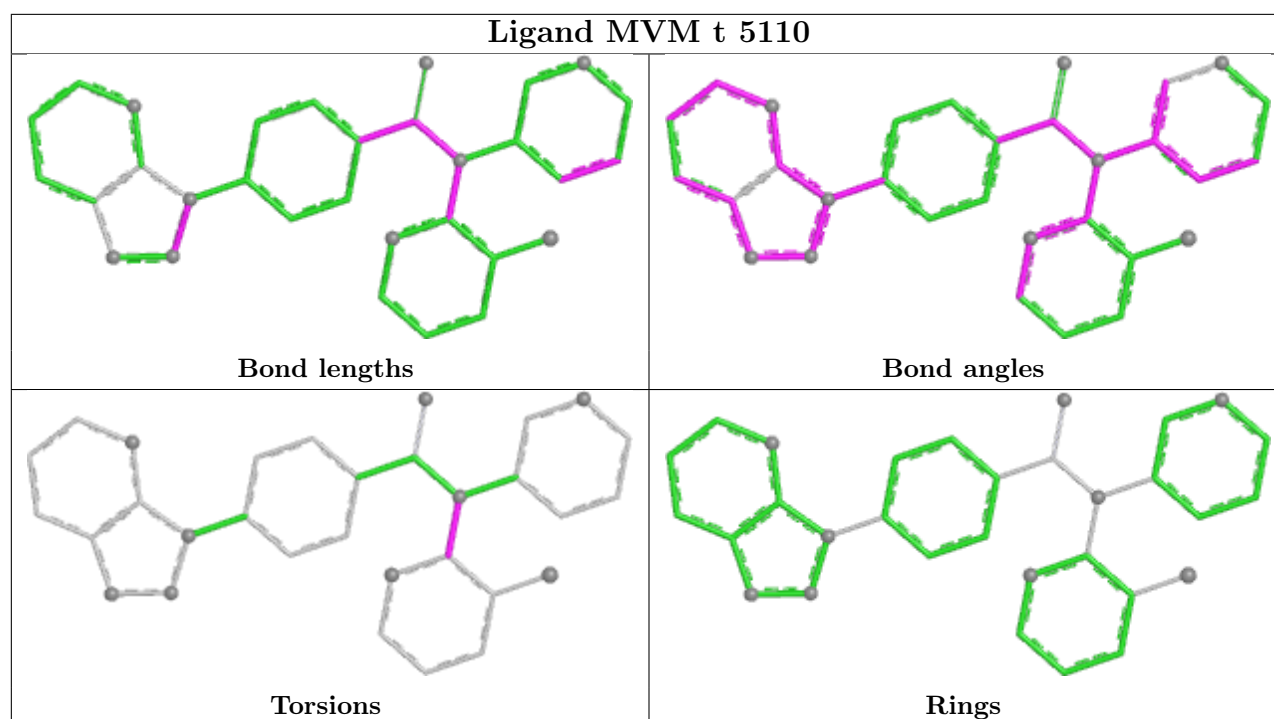
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	t	5110	MVM	C2-C6-N1-C5

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
79	t	16
1	S2	5
81	v	4
63	c	1
80	u	1

The worst 5 of 27 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	25.98
1	t	750:G	O3'	890:C	P	20.40
1	t	3919:C	O3'	4035:G	P	18.39
1	t	517:C	O3'	629:G	P	17.30
1	t	1680:C	O3'	1699:C	P	16.29

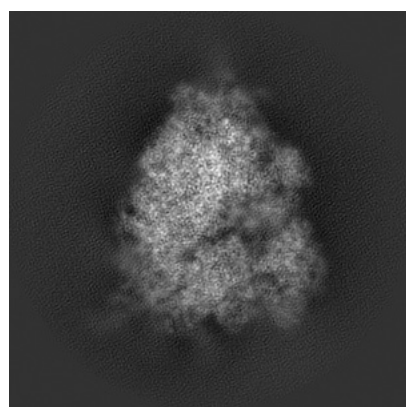
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0526. These allow visual inspection of the internal detail of the map and identification of artifacts.

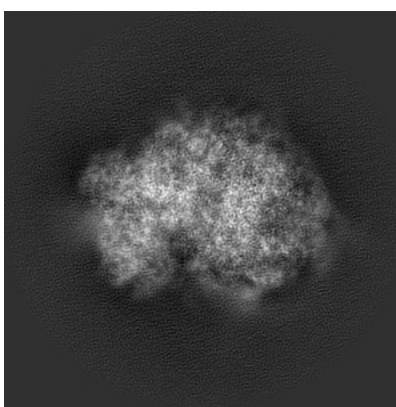
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

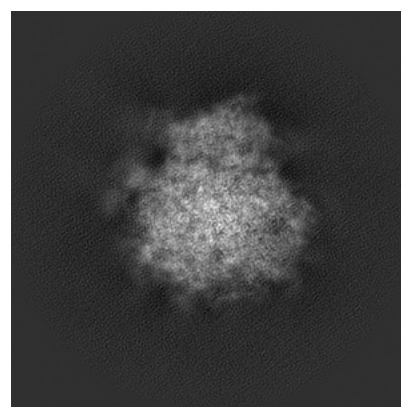
6.1.1 Primary map



X



Y

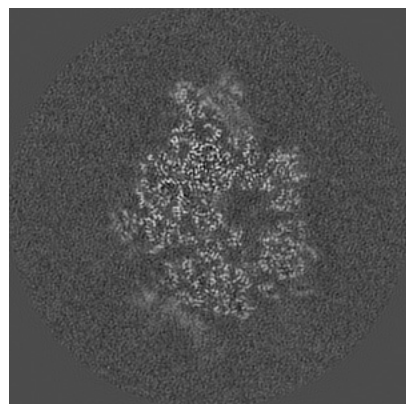


Z

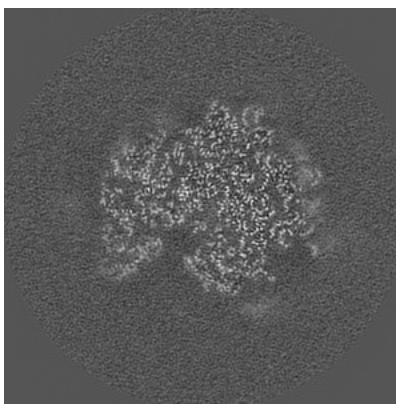
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

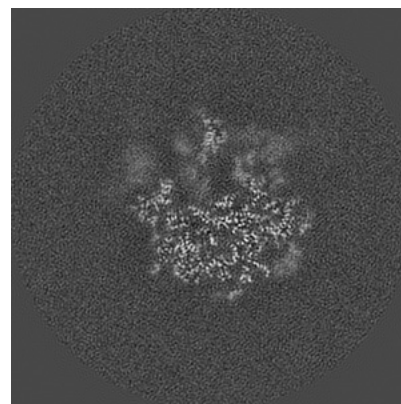
6.2.1 Primary map



X Index: 200



Y Index: 200

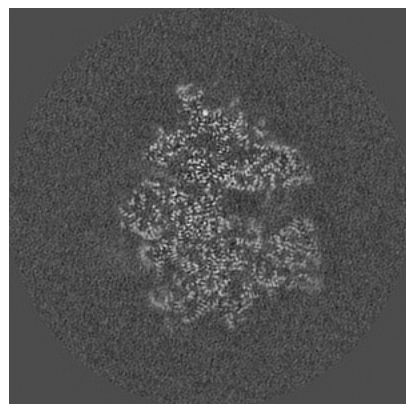


Z Index: 200

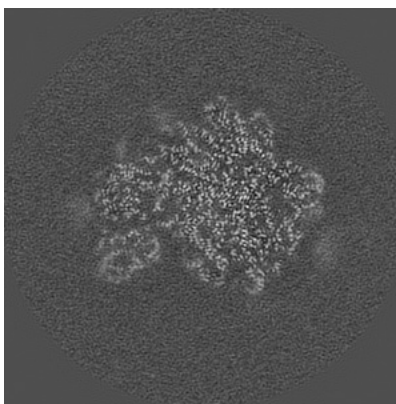
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

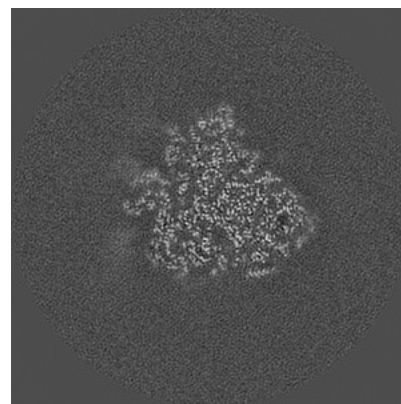
6.3.1 Primary map



X Index: 216



Y Index: 192

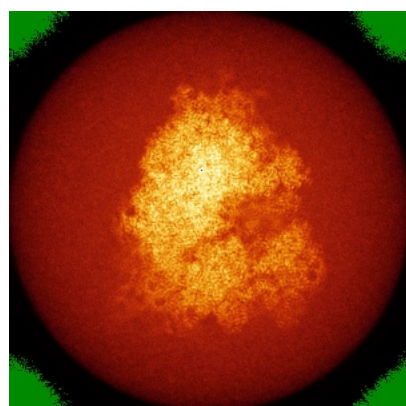


Z Index: 230

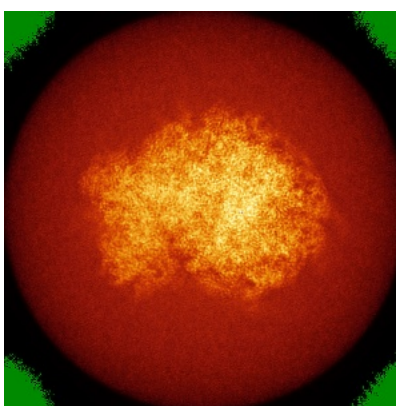
The images above show the largest variance slices of the map in three orthogonal directions.

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

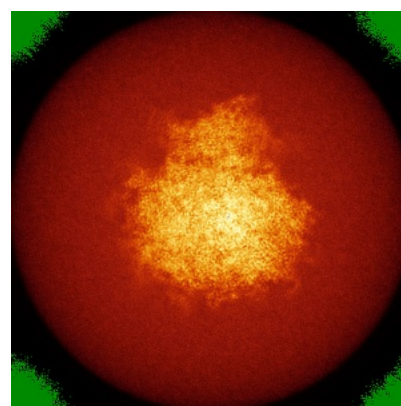
6.4.1 Primary map



X



Y

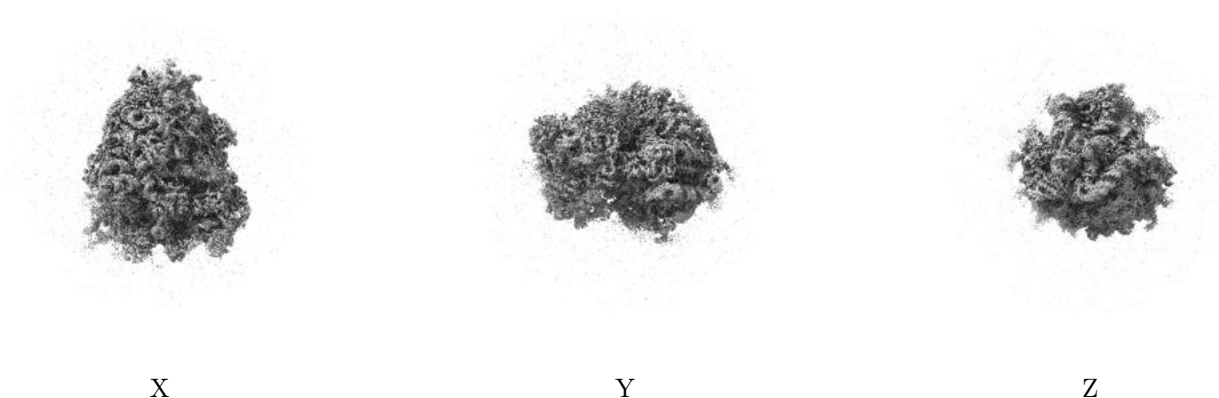


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.021. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

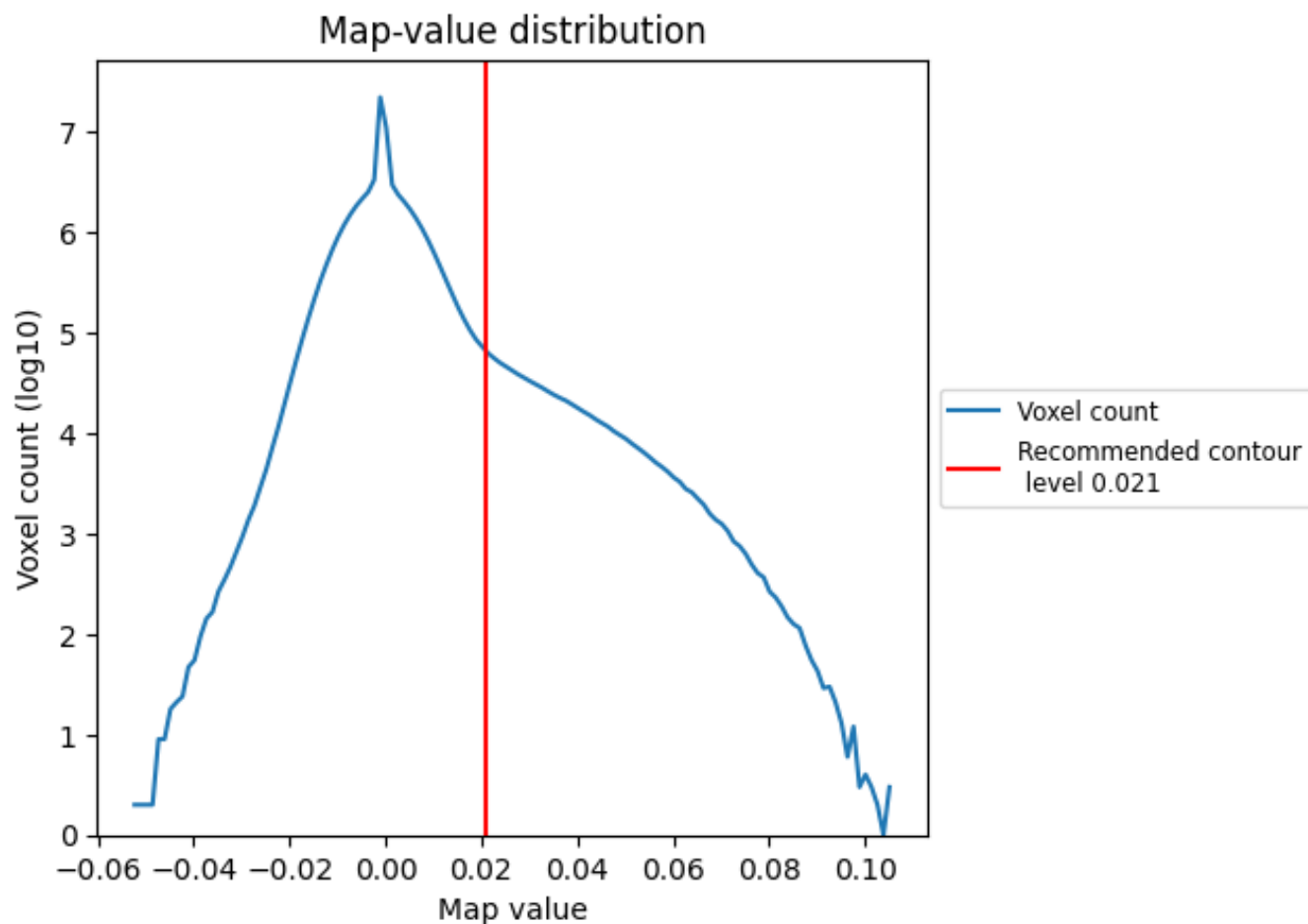
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

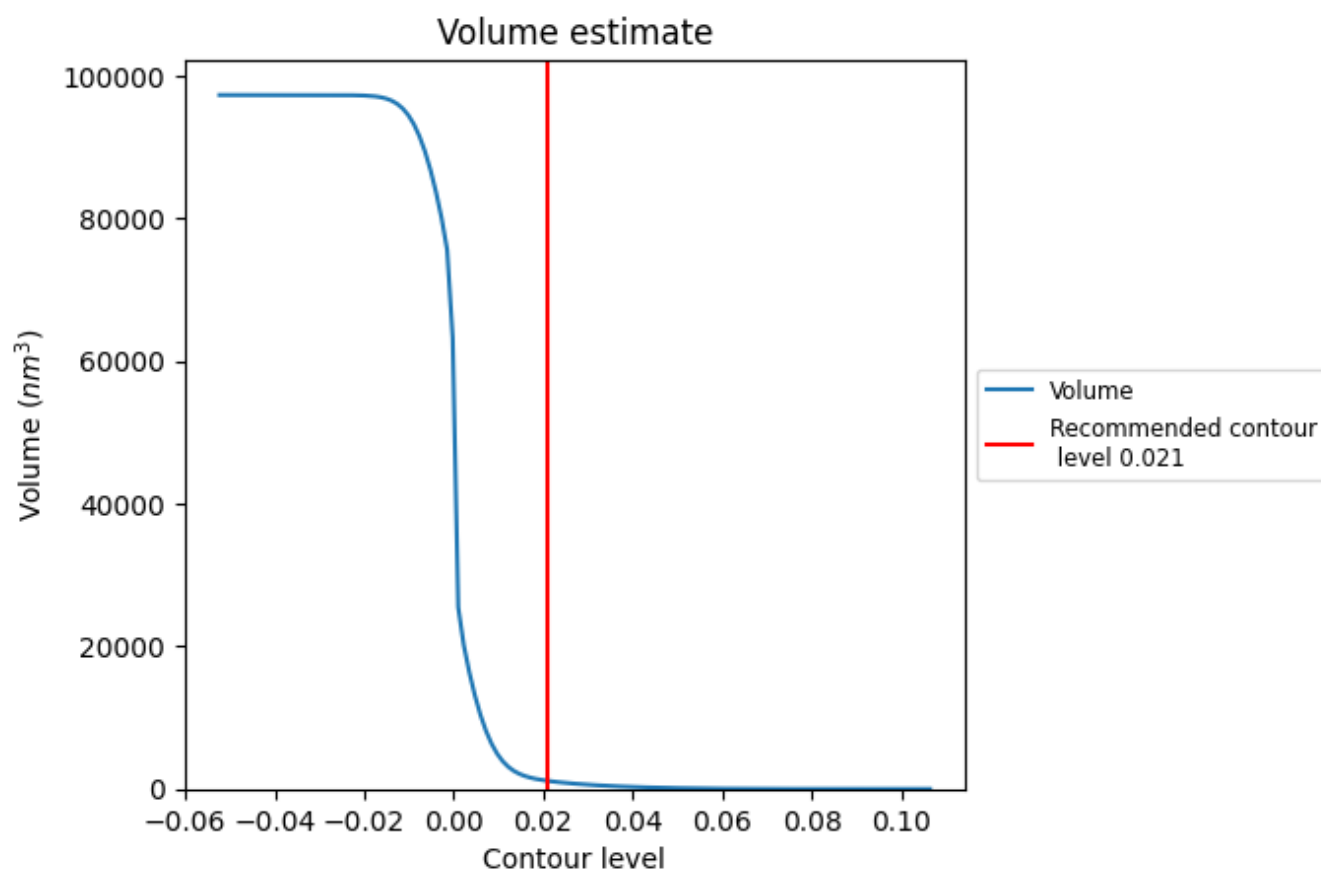
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

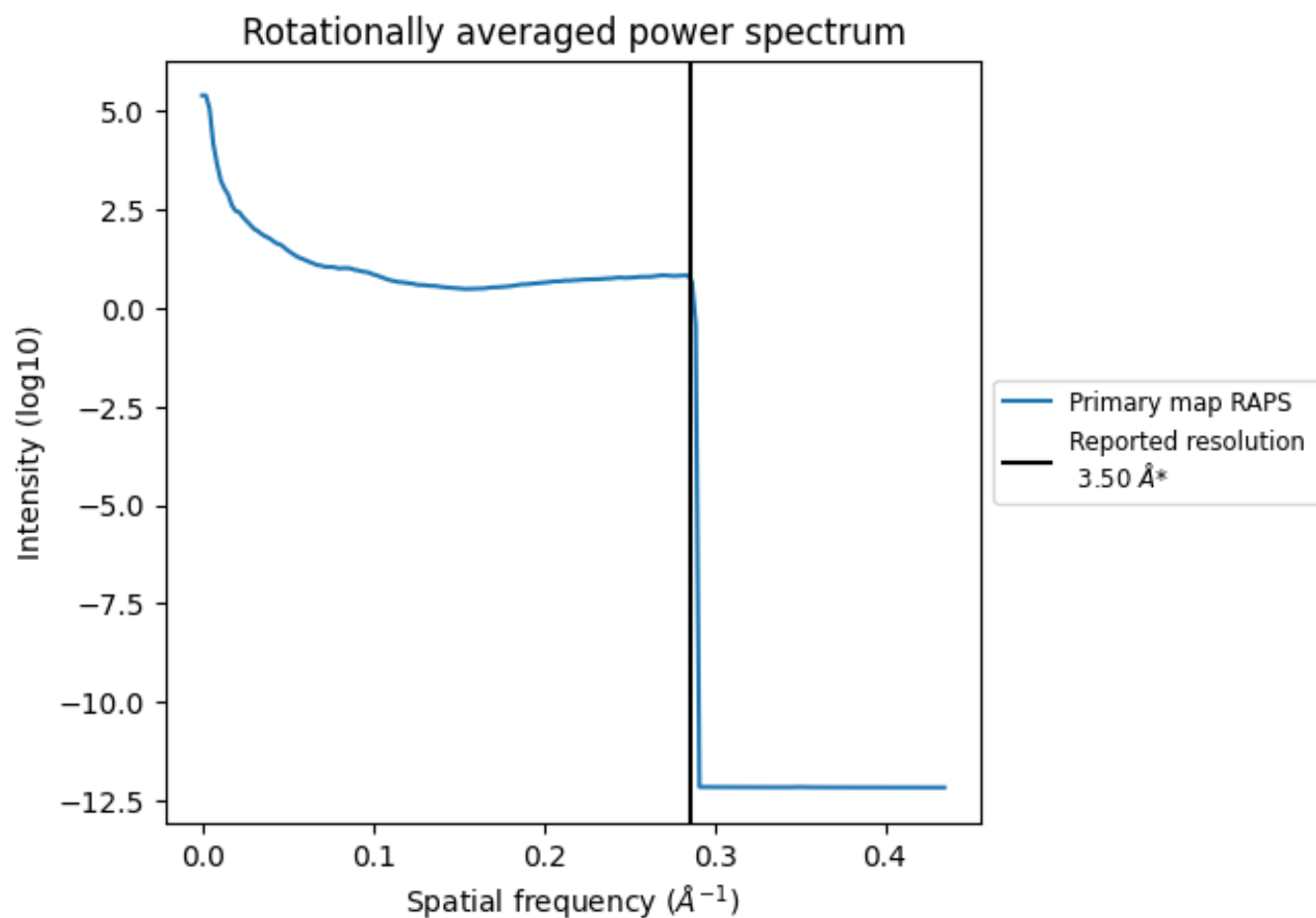
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1131 nm³; this corresponds to an approximate mass of 1022 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

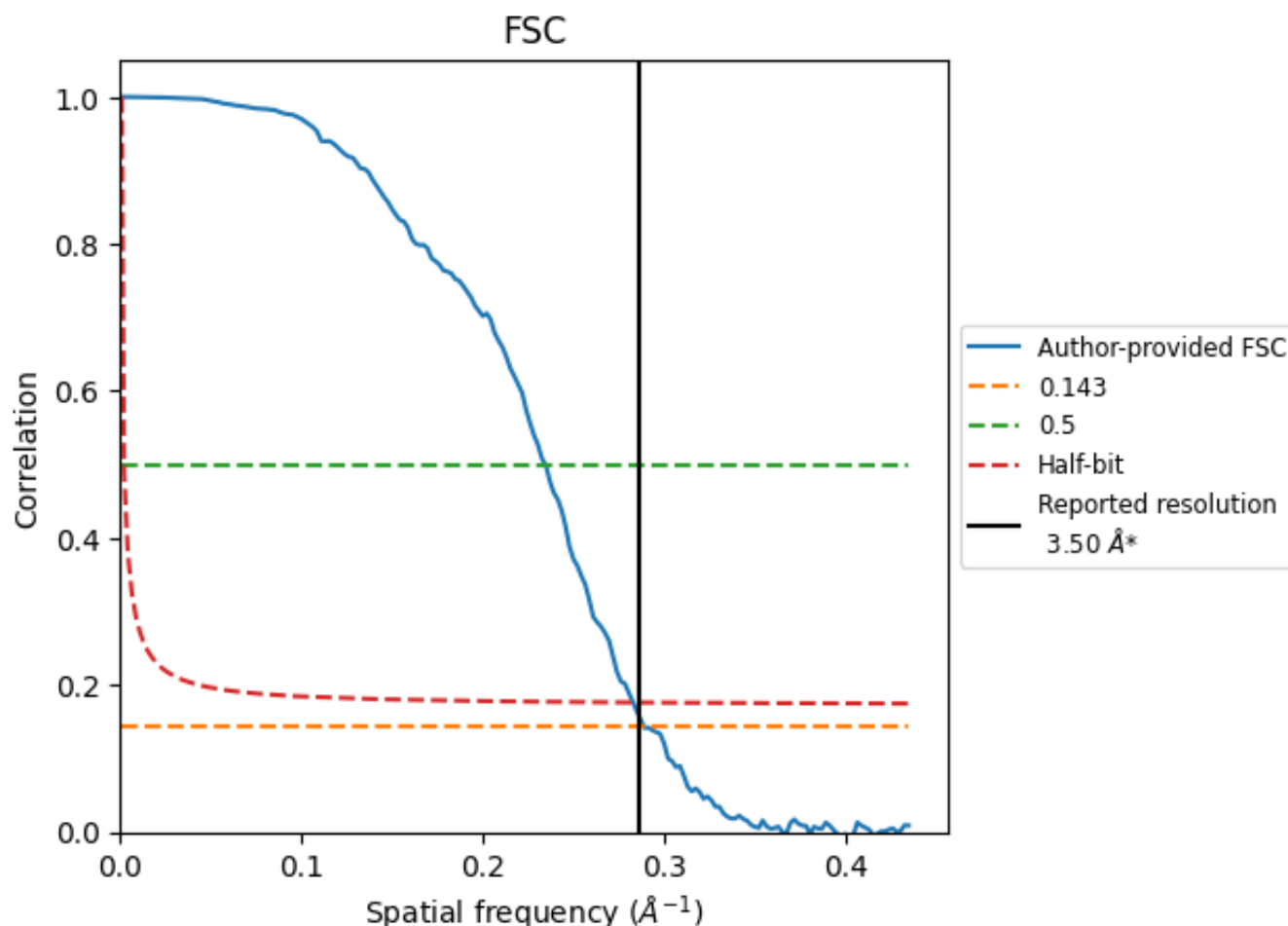


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

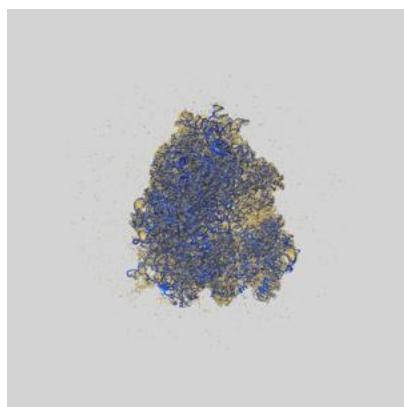
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.46	4.27	3.54
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

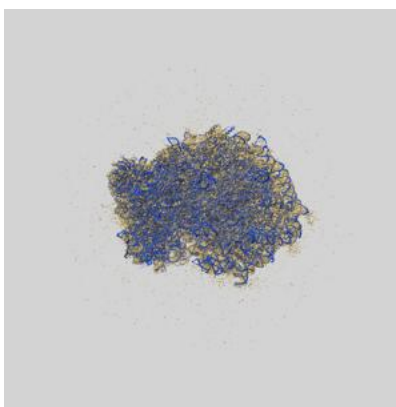
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0526 and PDB model 6OLI. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

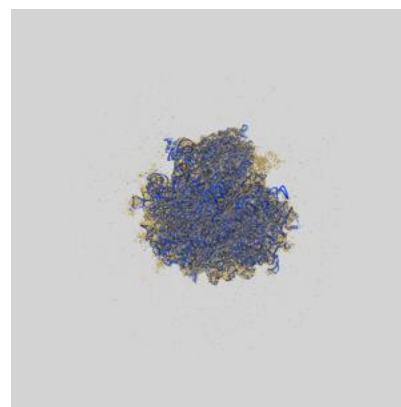
9.1 Map-model overlay [i](#)



X



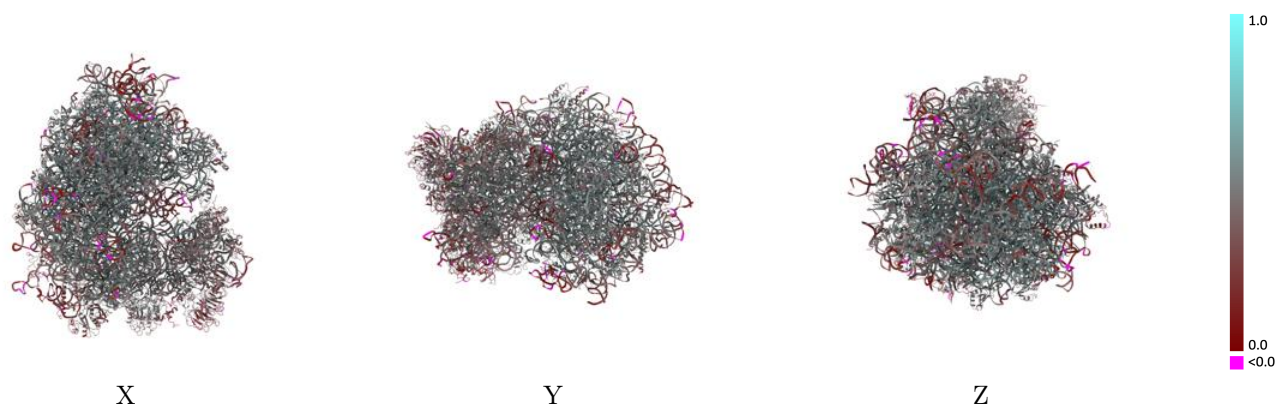
Y



Z

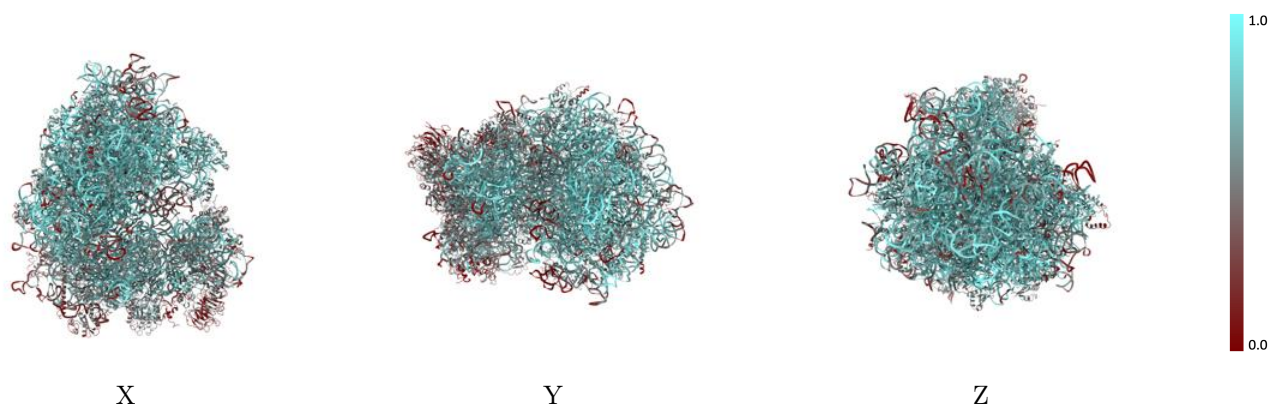
The images above show the 3D surface view of the map at the recommended contour level 0.021 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



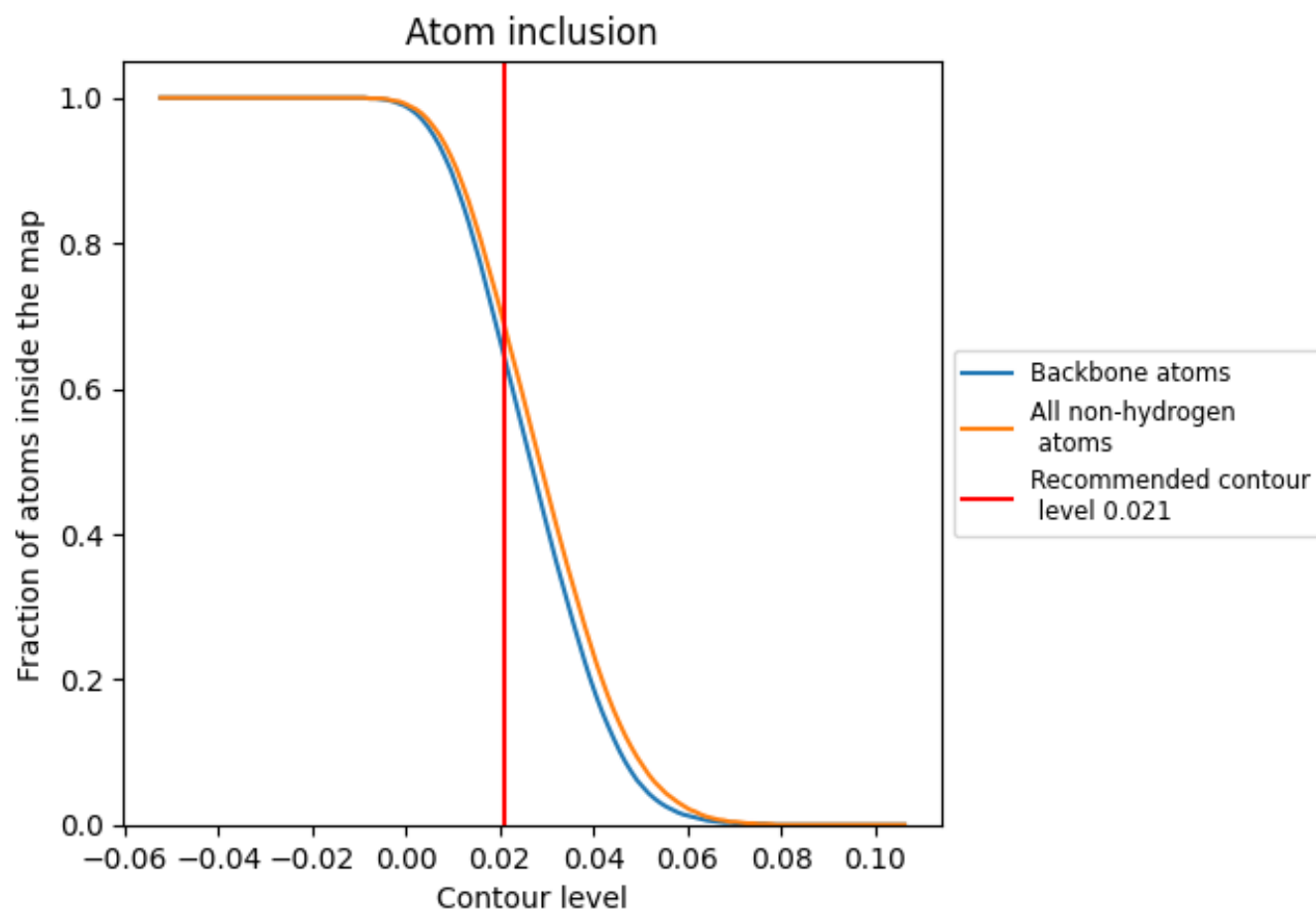
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.021).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6870	 0.4460
A	 0.7050	 0.5190
B	 0.6990	 0.4940
C	 0.7380	 0.5140
D	 0.8160	 0.4720
E	 0.9000	 0.5080
F	 0.6510	 0.4550
G	 0.6160	 0.4300
H	 0.7230	 0.5050
I	 0.5910	 0.4390
J	 0.6140	 0.4570
K	 0.6690	 0.4830
L	 0.6210	 0.4500
M	 0.6650	 0.4670
N	 0.6720	 0.4870
O	 0.7600	 0.5300
P	 0.7080	 0.5010
Q	 0.7410	 0.5120
R	 0.7090	 0.5040
S	 0.6140	 0.4470
S2	 0.7340	 0.4290
SA	 0.4960	 0.4220
SB	 0.5460	 0.4450
SC	 0.5710	 0.4530
SD	 0.4250	 0.3930
SE	 0.4950	 0.4090
SF	 0.4650	 0.3900
SG	 0.3580	 0.3210
SH	 0.3740	 0.3560
SI	 0.4570	 0.3860
SJ	 0.5280	 0.3850
SK	 0.3960	 0.3550
SL	 0.5350	 0.4160
SM	 0.0890	 0.1970
SN	 0.5730	 0.4500

















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Chain	Atom inclusion	Q-score
SO	 0.5630	 0.4530
SP	 0.5110	 0.4060
SQ	 0.4940	 0.4080
SR	 0.4050	 0.3720
SS	 0.5230	 0.3960
ST	 0.5300	 0.4170
SU	 0.3940	 0.3650
SV	 0.5250	 0.4280
SW	 0.6190	 0.4930
SX	 0.5890	 0.4600
SY	 0.4350	 0.3420
SZ	 0.4130	 0.3530
Sa	 0.6050	 0.4510
Sb	 0.4820	 0.4200
Sc	 0.3480	 0.3440
Sd	 0.6050	 0.4310
Se	 0.4530	 0.3850
Sf	 0.0810	 0.2030
Sg	 0.2720	 0.2970
T	 0.7280	 0.5090
U	 0.6790	 0.4890
V	 0.5590	 0.4190
W	 0.6740	 0.5070
X	 0.6970	 0.4850
Y	 0.6930	 0.5050
Z	 0.6960	 0.4900
a	 0.6450	 0.4660
b	 0.7440	 0.5230
c	 0.6150	 0.4490
d	 0.5820	 0.4390
e	 0.6950	 0.4720
f	 0.7520	 0.5240
g	 0.7540	 0.5210
h	 0.6810	 0.4820
i	 0.6800	 0.4830
j	 0.6500	 0.4650
k	 0.8050	 0.5360
l	 0.5460	 0.4340
m	 0.7230	 0.5010
n	 0.6930	 0.4800
o	 0.5640	 0.4820
p	 0.6660	 0.4870

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Chain	Atom inclusion	Q-score
q	 0.6820	 0.4990
r	 0.7620	 0.5120
t	 0.7940	 0.4590
u	 0.3360	 0.2860
v	 0.5480	 0.3300
w	 0.7650	 0.4830
y	 0.1290	 0.3260