wwPDB EM Validation Summary Report (i)

Oct 28, 2024 – 07:54 pm GMT

PDB ID	:	7NWG
EMDB ID	:	EMD-12631
Title	:	Mammalian pre-termination 80S ribosome with Hybrid P/E- and A/P-site tRNA's bound by Blasticidin S.
Authors	:	Powers, K.T.; Yadav, S.K.N.; Bufton, J.C.; Schaffitzel, C.
Deposited on	:	2021-03-16
Resolution	:	3.80 Å(reported)
Based on initial model	:	6HCJ

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

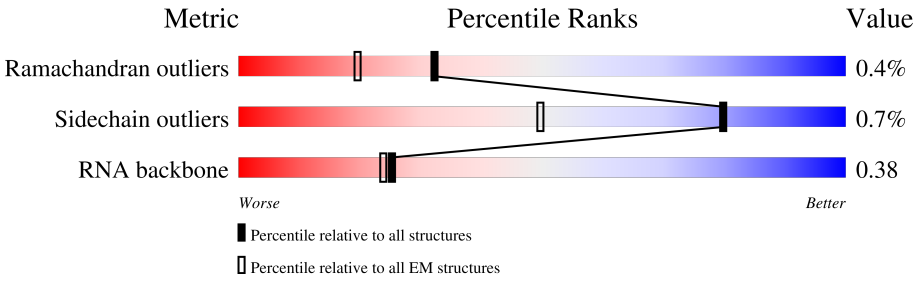
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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 <=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	51	3788	56% 35% 5%
2	71	120	60% 32% 8%
3	81	151	65% 30% 5%
4	A2	1818	56% 35%
5	B2	295	73% 26%
6	C2	264	80% 19%
7	D2	259	85% 15%
8	E2	281	81% 19%

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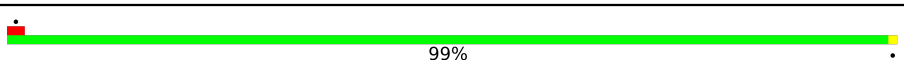
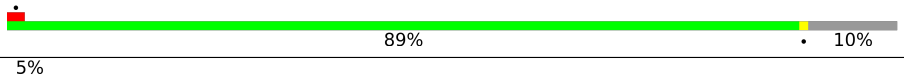
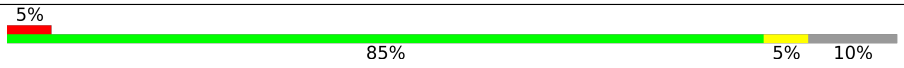
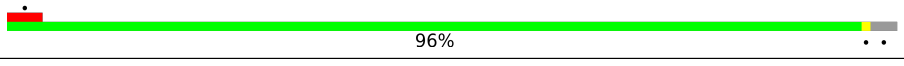
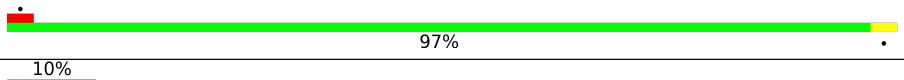
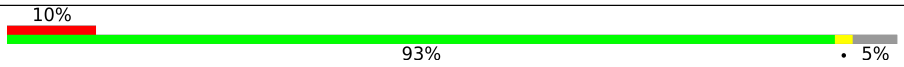
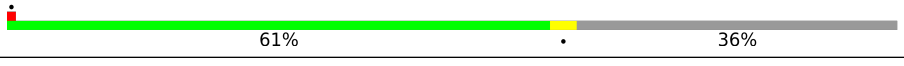
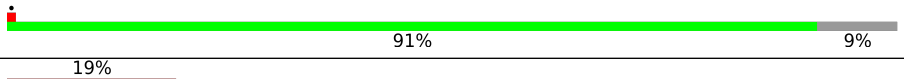
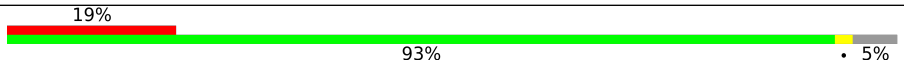
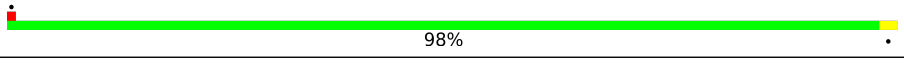
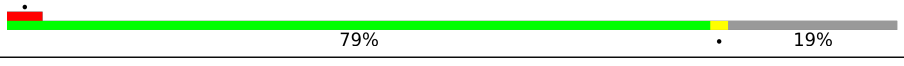
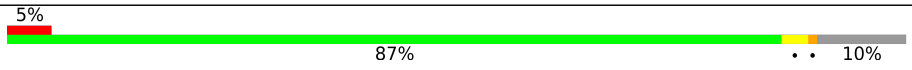
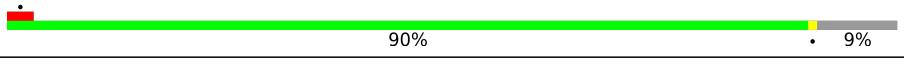
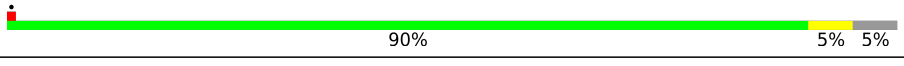
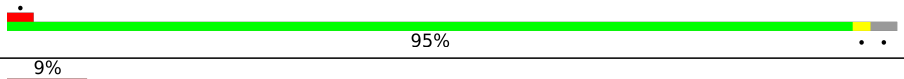
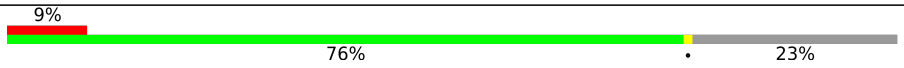
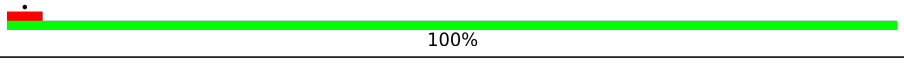
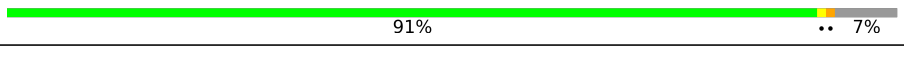
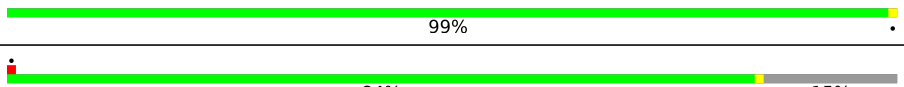
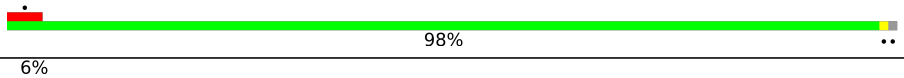
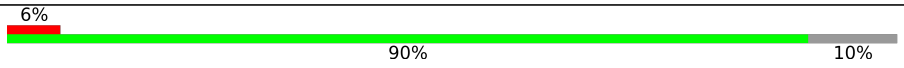
Mol	Chain	Length	Quality of chain
9	F2	262	
10	G2	205	
11	H2	262	
12	I2	190	
13	J2	206	
14	K2	194	
15	L2	151	
16	M2	158	
17	N2	123	
18	O2	149	
19	P2	168	
20	Q2	145	
21	R2	157	
22	S2	145	
23	T2	152	
24	U2	145	
25	V2	130	
26	W2	83	
27	X2	139	
28	Y2	141	
29	Z2	146	
30	a2	198	
31	b2	117	
32	c2	84	
33	d2	69	

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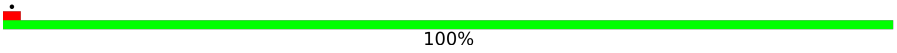
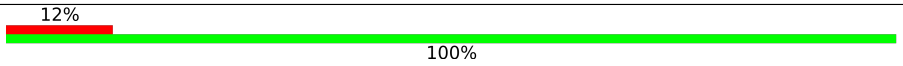
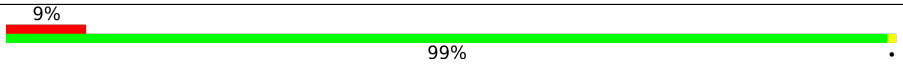
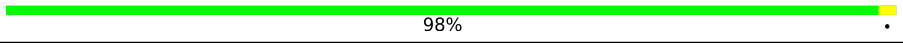
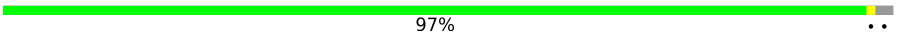
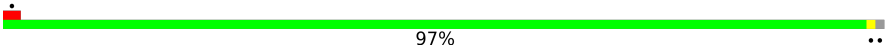
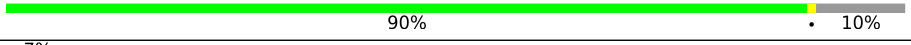
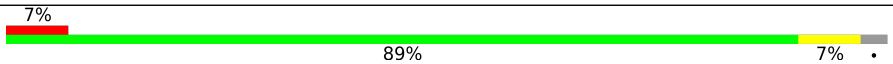
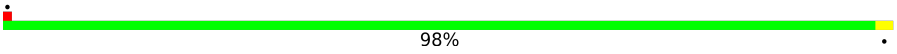
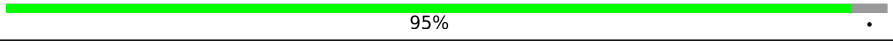
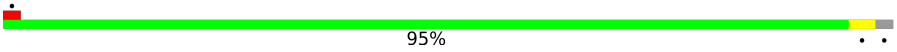
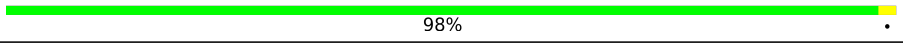
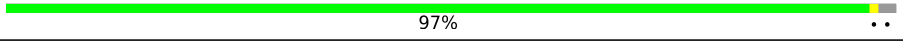
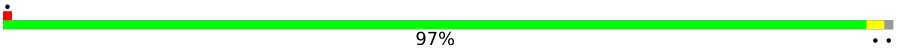
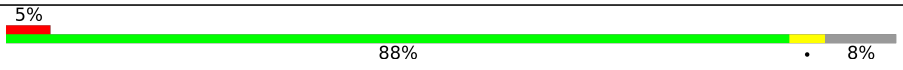
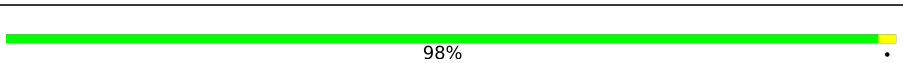
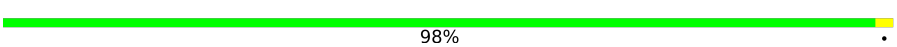
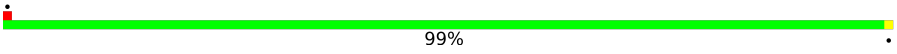
Mol	Chain	Length	Quality of chain
34	e2	55	
35	f2	133	
36	g2	68	
37	h2	313	
38	A3	246	
39	B3	403	
40	C3	425	
41	D3	297	
42	E3	291	
43	F3	249	
44	G3	241	
45	H3	190	
46	I3	214	
47	J3	181	
48	L3	211	
49	M3	218	
50	N3	203	
51	O3	203	
52	P3	199	
53	Q3	188	
54	R3	196	
55	S3	176	
56	T3	159	
57	U3	128	
58	V3	131	

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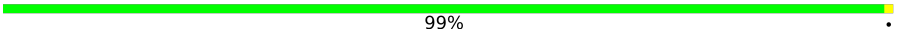
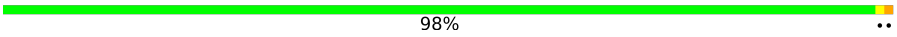
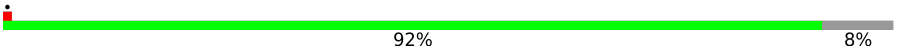
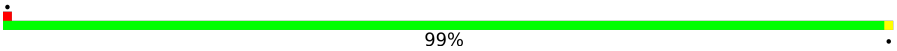
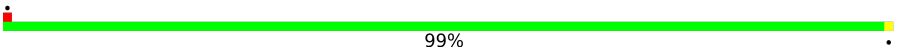
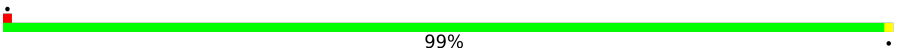
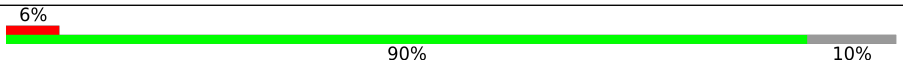
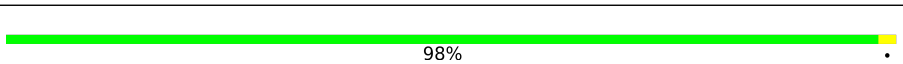
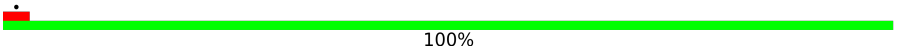
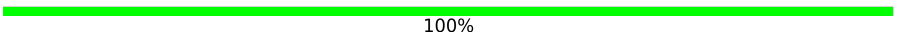
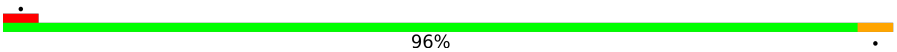
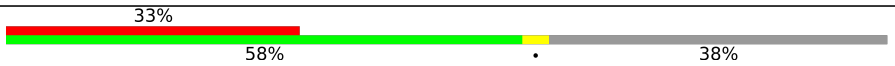
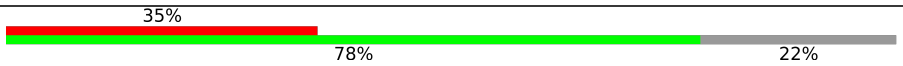
Mol	Chain	Length	Quality of chain
59	X3	156	
60	Y3	132	
61	Z3	135	
62	a3	160	
63	b3	245	
64	c3	115	
65	d3	107	
66	e3	128	
67	f3	109	
68	g3	126	
69	h3	122	
70	i3	117	
71	j3	97	
72	k3	69	
73	l3	50	
74	m3	128	
75	n3	25	
76	o3	142	
77	p3	109	
78	r3	137	
79	q3	74	
80	t3	318	
81	u3	195	
82	v3	18	
83	33	75	

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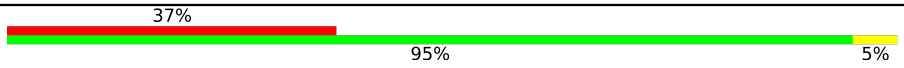
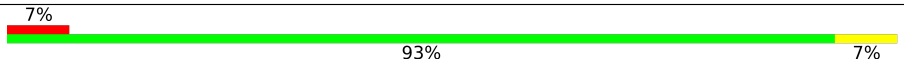
Mol	Chain	Length	Quality of chain
84	w3	217	
85	1	15	
86	W	134	

2 Entry composition (i)

There are 89 unique types of molecules in this entry. The entry contains 383415 atoms, of which 163452 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 28S Ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
1	51	3626	116849	34571	39208	14211	25233	3626	0	0

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
2	71	120	3853	1141	1295	456	842	119	0	0

- Molecule 3 is a RNA chain called 5.8S Ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
3	81	151	4835	1432	1627	564	1062	150	0	0

- Molecule 4 is a RNA chain called 18S Ribosomal RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
4	A2	1740	55909	16578	18768	6668	12156	1739	0	0

- Molecule 5 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	B2	217	3418	1086	1708	300	316	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B2	114	THR	ALA	conflict	UNP G1TLT8

- Molecule 6 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	C2	213	Total	C	H	N	O	S	0	0
			3532	1098	1803	309	308	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C2	236	GLY	SER	conflict	UNP G1SS70
C2	242	ALA	THR	conflict	UNP G1SS70

- Molecule 7 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	D2	221	Total	C	H	N	O	S	0	0
			3522	1111	1806	295	301	9		

- Molecule 8 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	E2	228	Total	C	H	N	O	S	0	0
			3624	1125	1859	316	316	8		

- Molecule 9 is a protein called S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	F2	262	Total	C	H	N	O	S	0	0
			4252	1324	2176	386	358	8		

- Molecule 10 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	G2	185	Total	C	H	N	O	S	0	0
			2993	921	1522	277	266	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G2	0	MET	-	initiating methionine	UNP G1TFM5

- Molecule 11 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	H2	237	Total	C	H	N	O	S	0	0
			4008	1200	2085	387	329	7		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H2	-12	LEU	-	expression tag	UNP A0A5K1UJS7
H2	-11	PHE	-	expression tag	UNP A0A5K1UJS7
H2	-10	ARG	-	expression tag	UNP A0A5K1UJS7
H2	-9	GLY	-	expression tag	UNP A0A5K1UJS7
H2	-8	ALA	-	expression tag	UNP A0A5K1UJS7
H2	-7	SER	-	expression tag	UNP A0A5K1UJS7
H2	-6	GLU	-	expression tag	UNP A0A5K1UJS7
H2	-5	ALA	-	expression tag	UNP A0A5K1UJS7
H2	-4	VAL	-	expression tag	UNP A0A5K1UJS7
H2	-3	GLY	-	expression tag	UNP A0A5K1UJS7
H2	-2	SER	-	expression tag	UNP A0A5K1UJS7
H2	-1	LEU	-	expression tag	UNP A0A5K1UJS7
H2	0	LYS	-	expression tag	UNP A0A5K1UJS7

- Molecule 12 is a protein called ribosomal protein eS7.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	I2	185	Total	C	H	N	O	S	0	0
			3070	952	1582	271	264	1		

- Molecule 13 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	J2	206	Total	C	H	N	O	S	0	0
			3457	1058	1771	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J2	47	ARG	GLY	variant	UNP G1TJW1

- Molecule 14 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	K2	185	Total	C	H	N	O	S	0	0
			3165	969	1640	306	248	2		

- Molecule 15 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	L2	96	Total	C	H	N	O	S	0	0
			1646	530	836	143	131	6		

- Molecule 16 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	M2	143	Total	C	H	N	O	S	0	0
			2424	749	1249	222	198	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M2	25	GLN	LEU	conflict	UNP G1TRM4
M2	29	SER	GLY	conflict	UNP G1TRM4

- Molecule 17 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	N2	117	Total	C	H	N	O	S	0	0
			1847	570	939	161	169	8		

- Molecule 18 is a protein called ribosomal protein uS15.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	O2	149	Total	C	H	N	O	S	0	0
			2491	770	1289	228	203	1		

- Molecule 19 is a protein called uS11.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	P2	136	Total	C	H	N	O	S	0	0
			2055	621	1039	199	190	6		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P2	-16	MET	-	initiating methionine	UNP G1T1F0
P2	-15	LYS	-	expression tag	UNP G1T1F0
P2	-14	ALA	-	expression tag	UNP G1T1F0
P2	-13	ARG	-	expression tag	UNP G1T1F0

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Chain	Residue	Modelled	Actual	Comment	Reference
P2	-12	ALA	-	expression tag	UNP G1T1F0
P2	-11	LEU	-	expression tag	UNP G1T1F0
P2	-10	SER	-	expression tag	UNP G1T1F0
P2	-9	GLY	-	expression tag	UNP G1T1F0
P2	-8	SER	-	expression tag	UNP G1T1F0
P2	-7	GLY	-	expression tag	UNP G1T1F0
P2	-6	VAL	-	expression tag	UNP G1T1F0
P2	-5	ARG	-	expression tag	UNP G1T1F0

- Molecule 20 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	Q2	120	Total	C	H	N	O	S	0	0
			2042	635	1045	187	168	7		

- Molecule 21 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	R2	142	Total	C	H	N	O	S	0	0
			2323	717	1195	213	195	3		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R2	-8	VAL	GLU	conflict	UNP G1SGX4
R2	-7	GLU	ASP	conflict	UNP G1SGX4
R2	-6	LEU	ARG	conflict	UNP G1SGX4
R2	-5	VAL	HIS	conflict	UNP G1SGX4
R2	-4	LEU	SER	conflict	UNP G1SGX4
R2	-3	VAL	SER	conflict	UNP G1SGX4
R2	-2	LEU	ALA	conflict	UNP G1SGX4
R2	-1	GLY	ALA	conflict	UNP G1SGX4

- Molecule 22 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	S2	132	Total	C	H	N	O	S	0	0
			2189	670	1121	199	195	4		

- Molecule 23 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	T2	144	Total	C	H	N	O	S	0	0
			2439	746	1249	241	202	1		

- Molecule 24 is a protein called S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	U2	141	Total	C	H	N	O	S	0	0
			2227	688	1130	211	195	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U2	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 25 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	V2	100	Total	C	H	N	O	S	0	0
			1657	498	862	152	141	4		

- Molecule 26 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	W2	83	Total	C	H	N	O	S	0	0
			1273	393	637	117	121	5		

- Molecule 27 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	X2	129	Total	C	H	N	O	S	0	0
			2114	659	1080	193	176	6		

- Molecule 28 is a protein called Ribosomal protein S23.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	Y2	141	Total	C	H	N	O	S	0	0
			2263	693	1165	219	183	3		

- Molecule 29 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	Z2	124	Total	C	H	N	O	S	0	0
			2094	640	1083	198	168	5		

- Molecule 30 is a protein called ribosomal protein eS25.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	a2	75	Total	C	H	N	O	S	0	0
			1254	382	656	111	104	1		

- Molecule 31 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	b2	101	Total	C	H	N	O	S	0	0
			1678	507	864	170	132	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
32	c2	83	Total	C	H	N	O	S	0	0
			1323	408	672	121	115	7		

- Molecule 33 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	d2	62	Total	C	H	N	O	S	0	0
			1002	297	514	97	92	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d2	5	HIS	ARG	conflict	UNP G1TIB4

- Molecule 34 is a protein called uS14.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	e2	55	Total	C	H	N	O	S	0	0
			911	286	452	94	74	5		

- Molecule 35 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	f2	55	Total	C	H	N	O	S	0	0
			935	274	492	97	71	1		

- Molecule 36 is a protein called eS31.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	g2	68	Total	C	H	N	O	S	0	0
			1122	351	567	103	94	7		

- Molecule 37 is a protein called ribosomal protein RACK1.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	h2	313	Total	C	H	N	O	S	0	0
			4829	1535	2393	424	465	12		

- Molecule 38 is a protein called L8.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	A3	246	Total	C	H	N	O	S	0	0
			3870	1183	1983	387	311	6		

- Molecule 39 is a protein called uL3.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	B3	394	Total	C	H	N	O	S	0	0
			6482	2020	3310	597	542	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B3	1	MET	-	initiating methionine	UNP G1TL06

- Molecule 40 is a protein called uL4.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	C3	362	Total	C	H	N	O	S	0	0
			5937	1812	3054	577	480	14		

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C3	379	VAL	-	expression tag	UNP G1SVW5

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Chain	Residue	Modelled	Actual	Comment	Reference
C3	380	LYS	-	expression tag	UNP G1SVW5
C3	381	LYS	-	expression tag	UNP G1SVW5
C3	382	PRO	-	expression tag	UNP G1SVW5
C3	383	ARG	-	expression tag	UNP G1SVW5
C3	384	ALA	-	expression tag	UNP G1SVW5
C3	385	VAL	-	expression tag	UNP G1SVW5
C3	386	GLY	-	expression tag	UNP G1SVW5
C3	387	ILE	-	expression tag	UNP G1SVW5
C3	388	LYS	-	expression tag	UNP G1SVW5
C3	389	GLN	-	expression tag	UNP G1SVW5
C3	390	LYS	-	expression tag	UNP G1SVW5
C3	391	LYS	-	expression tag	UNP G1SVW5
C3	392	LYS	-	expression tag	UNP G1SVW5
C3	393	PRO	-	expression tag	UNP G1SVW5
C3	394	VAL	-	expression tag	UNP G1SVW5
C3	395	VAL	-	expression tag	UNP G1SVW5
C3	396	GLY	-	expression tag	UNP G1SVW5
C3	397	ARG	-	expression tag	UNP G1SVW5
C3	398	LYS	-	expression tag	UNP G1SVW5
C3	399	ALA	-	expression tag	UNP G1SVW5
C3	400	ALA	-	expression tag	UNP G1SVW5
C3	401	ALA	-	expression tag	UNP G1SVW5
C3	402	ALA	-	expression tag	UNP G1SVW5
C3	403	LYS	-	expression tag	UNP G1SVW5
C3	404	LYS	-	expression tag	UNP G1SVW5
C3	405	PRO	-	expression tag	UNP G1SVW5
C3	406	ALA	-	expression tag	UNP G1SVW5
C3	407	ALA	-	expression tag	UNP G1SVW5
C3	408	ASP	-	expression tag	UNP G1SVW5
C3	409	LYS	-	expression tag	UNP G1SVW5
C3	410	LYS	-	expression tag	UNP G1SVW5
C3	411	ALA	-	expression tag	UNP G1SVW5
C3	412	ALA	-	expression tag	UNP G1SVW5
C3	413	ASP	-	expression tag	UNP G1SVW5
C3	414	LYS	-	expression tag	UNP G1SVW5
C3	415	ARG	-	expression tag	UNP G1SVW5
C3	416	ALA	-	expression tag	UNP G1SVW5
C3	417	GLY	-	expression tag	UNP G1SVW5
C3	418	PRO	-	expression tag	UNP G1SVW5
C3	419	GLU	-	expression tag	UNP G1SVW5
C3	420	ASP	-	expression tag	UNP G1SVW5
C3	421	LYS	-	expression tag	UNP G1SVW5

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Chain	Residue	Modelled	Actual	Comment	Reference
C3	422	LYS	-	expression tag	UNP G1SVW5
C3	423	PRO	-	expression tag	UNP G1SVW5
C3	424	ALA	-	expression tag	UNP G1SVW5
C3	425	ALA	-	expression tag	UNP G1SVW5

- Molecule 41 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	D3	293	Total	C	H	N	O	S	0	0
			4815	1512	2424	438	427	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D3	1	MET	-	initiating methionine	UNP G1SYJ6

- Molecule 42 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	E3	216	Total	C	H	N	O	S	0	0
			3616	1115	1887	329	282	3		

- Molecule 43 is a protein called uL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	F3	225	Total	C	H	N	O	S	0	0
			3870	1205	1995	358	303	9		

- Molecule 44 is a protein called L7a.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	G3	233	Total	C	H	N	O	S	0	0
			3905	1199	2026	361	315	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G3	244	GLY	CYS	conflict	UNP G1STW0

- Molecule 45 is a protein called L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	H3	190	Total	C	H	N	O	S	0	0
			3113	954	1597	284	272	6		

- Molecule 46 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	I3	205	Total	C	H	N	O	S	0	0
			3376	1056	1712	321	274	13		

- Molecule 47 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	J3	170	Total	C	H	N	O	S	0	0
			2761	861	1399	254	241	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J3	0	GLN	-	insertion	UNP G1TUB8
J3	1	ARG	-	insertion	UNP G1TUB8
J3	2	PRO	-	insertion	UNP G1TUB8

- Molecule 48 is a protein called L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	L3	207	Total	C	H	N	O	S	0	0
			3455	1047	1781	348	275	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L3	74	ARG	HIS	conflict	UNP G1TKB3
L3	190	ARG	HIS	conflict	UNP G1TKB3

- Molecule 49 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	M3	138	Total	C	H	N	O	S	0	0
			2348	727	1211	221	182	7		

- Molecule 50 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	N3	203	Total	C	H	N	O	S	0	0
			3450	1072	1749	359	266	4		

- Molecule 51 is a protein called 60S RIBOSOMAL PROTEIN UL13.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	O3	199	Total	C	H	N	O	S	0	0
			3408	1051	1778	319	255	5		

- Molecule 52 is a protein called uL22.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	P3	153	Total	C	H	N	O	S	0	0
			2516	777	1274	241	215	9		

- Molecule 53 is a protein called L18.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	Q3	187	Total	C	H	N	O	S	0	0
			3149	946	1634	315	250	4		

- Molecule 54 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	R3	180	Total	C	H	N	O	S	0	0
			3172	933	1664	328	238	9		

- Molecule 55 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	S3	176	Total	C	H	N	O	S	0	0
			2970	930	1508	285	236	11		

- Molecule 56 is a protein called eL21.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	T3	159	Total	C	H	N	O	S	0	0
			2664	823	1366	252	217	6		

- Molecule 57 is a protein called L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	U3	99	Total	C	H	N	O	S	0	0
			1642	519	833	141	147	2		

- Molecule 58 is a protein called eL14.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	V3	131	Total	C	H	N	O	S	0	0
			2018	618	1039	184	172	5		

- Molecule 59 is a protein called uL23.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	X3	118	Total	C	H	N	O	S	0	0
			2003	618	1036	181	167	1		

- Molecule 60 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	Y3	132	Total	C	H	N	O	S	0	0
			2291	692	1189	223	184	3		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
61	Z3	135	Total	C	H	N	O	S	0	0
			2289	714	1182	208	182	3		

- Molecule 62 is a protein called uL15.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	a3	147	Total	C	H	N	O	S	0	0
			2372	734	1210	239	185	4		

- Molecule 63 is a protein called eL29.

Mol	Chain	Residues	Atoms						AltConf	Trace
63	b3	104	Total	C	H	N	O	S	0	0
			1768	527	920	189	129	3		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b3	227	ALA	-	expression tag	UNP G1SGR6
b3	228	PRO	-	expression tag	UNP G1SGR6
b3	229	VAL	-	expression tag	UNP G1SGR6
b3	230	PRO	-	expression tag	UNP G1SGR6
b3	231	ALA	-	expression tag	UNP G1SGR6
b3	232	GLN	-	expression tag	UNP G1SGR6
b3	233	ALA	-	expression tag	UNP G1SGR6
b3	234	PRO	-	expression tag	UNP G1SGR6
b3	235	PRO	-	expression tag	UNP G1SGR6
b3	236	LYS	-	expression tag	UNP G1SGR6
b3	237	GLY	-	expression tag	UNP G1SGR6
b3	238	ALA	-	expression tag	UNP G1SGR6
b3	239	GLN	-	expression tag	UNP G1SGR6
b3	240	PRO	-	expression tag	UNP G1SGR6
b3	241	PRO	-	expression tag	UNP G1SGR6
b3	242	ALA	-	expression tag	UNP G1SGR6
b3	243	LYS	-	expression tag	UNP G1SGR6
b3	244	ALA	-	expression tag	UNP G1SGR6
b3	245	PRO	-	expression tag	UNP G1SGR6

- Molecule 64 is a protein called eL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
64	c3	98	Total	C	H	N	O	S	0	0
			1555	481	794	134	140	6		

- Molecule 65 is a protein called eL31.

Mol	Chain	Residues	Atoms						AltConf	Trace
65	d3	107	Total	C	H	N	O	S	0	0
			1818	560	930	171	155	2		

- Molecule 66 is a protein called eL32.

Mol	Chain	Residues	Atoms						AltConf	Trace
66	e3	128	Total	C	H	N	O	S	0	0
			2200	667	1147	216	165	5		

- Molecule 67 is a protein called eL33.

Mol	Chain	Residues	Atoms						AltConf	Trace
67	f3	109	Total	C	H	N	O	S	0	0
			1788	555	912	174	143	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
68	g3	114	Total	C	H	N	O	S	0	0
			1905	566	999	187	147	6		

- Molecule 69 is a protein called uL29.

Mol	Chain	Residues	Atoms						AltConf	Trace
69	h3	122	Total	C	H	N	O	S	0	0
			2160	640	1147	204	168	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
70	i3	102	Total	C	H	N	O	S	0	0
			1746	520	916	176	129	5		

- Molecule 71 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms						AltConf	Trace
71	j3	86	Total	C	H	N	O	S	0	0
			1442	434	737	155	111	5		

- Molecule 72 is a protein called L38.

Mol	Chain	Residues	Atoms						AltConf	Trace
72	k3	69	Total	C	H	N	O	S	0	0
			1206	366	637	103	99	1		

- Molecule 73 is a protein called eL39.

Mol	Chain	Residues	Atoms						AltConf	Trace
73	l3	50	Total	C	H	N	O	S	0	0
			927	286	480	96	64	1		

- Molecule 74 is a protein called 60S RIBOSOMAL PROTEIN EL40.

Mol	Chain	Residues	Atoms						AltConf	Trace
74	m3	52	Total	C	H	N	O	S	0	0
			895	266	466	90	67	6		

- Molecule 75 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms						AltConf	Trace
75	n3	25	Total	C	H	N	O	S	0	0
			528	145	289	64	27	3		

- Molecule 76 is a protein called eL42.

Mol	Chain	Residues	Atoms						AltConf	Trace
76	o3	104	Total	C	H	N	O	S	0	0
			1775	533	924	174	138	6		

- Molecule 77 is a protein called ribosomal protein eL43.

Mol	Chain	Residues	Atoms						AltConf	Trace
77	p3	91	Total	C	H	N	O	S	0	0
			1466	445	758	136	120	7		

- Molecule 78 is a protein called eL28.

Mol	Chain	Residues	Atoms						AltConf	Trace
78	r3	124	Total	C	H	N	O	S	0	0
			2045	616	1051	205	167	6		

- Molecule 79 is a RNA chain called A/P-Site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
79	q3	74	Total	C	H	N	O	P	0	0
			2381	705	805	286	512	73		

- Molecule 80 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms						AltConf	Trace
80	t3	196	Total	C	H	N	O	S	0	0
			3071	959	1564	263	276	9		

- Molecule 81 is a protein called uL12.

Mol	Chain	Residues	Atoms						AltConf	Trace
81	u3	153	Total	C	H	N	O	S	0	0
			2378	722	1218	218	217	3		

- Molecule 82 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
82	v3	18	Total	C	H	N	O	P	0	0
			573	171	192	65	127	18		

- Molecule 83 is a RNA chain called P/E-Site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
83	33	75	Total	C	H	N	O	P	0	0
			2403	712	809	281	527	74		

- Molecule 84 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
84	w3	217	Total	C	H	N	O	S	0	0
			3595	1113	1854	312	307	9		

- Molecule 85 is a protein called Sec61Beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	1	15	Total	C	H	N	O	S	0	0
			242	82	117	20	22	1		

- Molecule 86 is a protein called 60S ribosomal protein L24-like protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
86	W	63	Total	C	H	N	O	S	0	0
			1069	337	541	103	85	3		

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

Mol	Chain	Residues	Atoms		AltConf
87	51	193	Total	Mg	0
			193	193	
87	71	6	Total	Mg	0
			6	6	
87	81	7	Total	Mg	0
			7	7	
87	A2	74	Total	Mg	0
			74	74	
87	F2	1	Total	Mg	0
			1	1	
87	K2	1	Total	Mg	0
			1	1	

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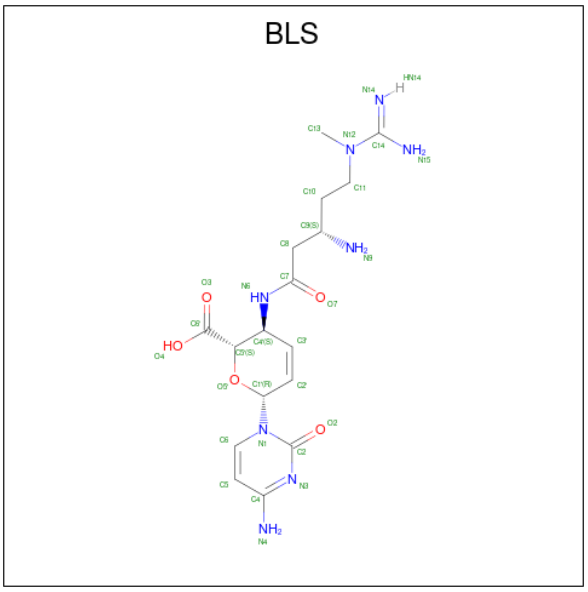
Mol	Chain	Residues	Atoms	AltConf
87	M2	1	Total Mg 1 1	0
87	b2	1	Total Mg 1 1	0
87	g2	1	Total Mg 1 1	0
87	B3	3	Total Mg 3 3	0
87	J3	1	Total Mg 1 1	0
87	N3	1	Total Mg 1 1	0
87	P3	2	Total Mg 2 2	0
87	R3	1	Total Mg 1 1	0
87	V3	2	Total Mg 2 2	0
87	a3	1	Total Mg 1 1	0
87	e3	1	Total Mg 1 1	0
87	g3	1	Total Mg 1 1	0
87	33	1	Total Mg 1 1	0

- Molecule 88 is BLASTICIDIN S (three-letter code: BLS) (formula: $C_{17}H_{26}N_8O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
88	51	1	Total	C	H	N	O	0
			55	17	25	8	5	

- Molecule 89 is ZINC ION (three-letter code: ZN) (formula: Zn).

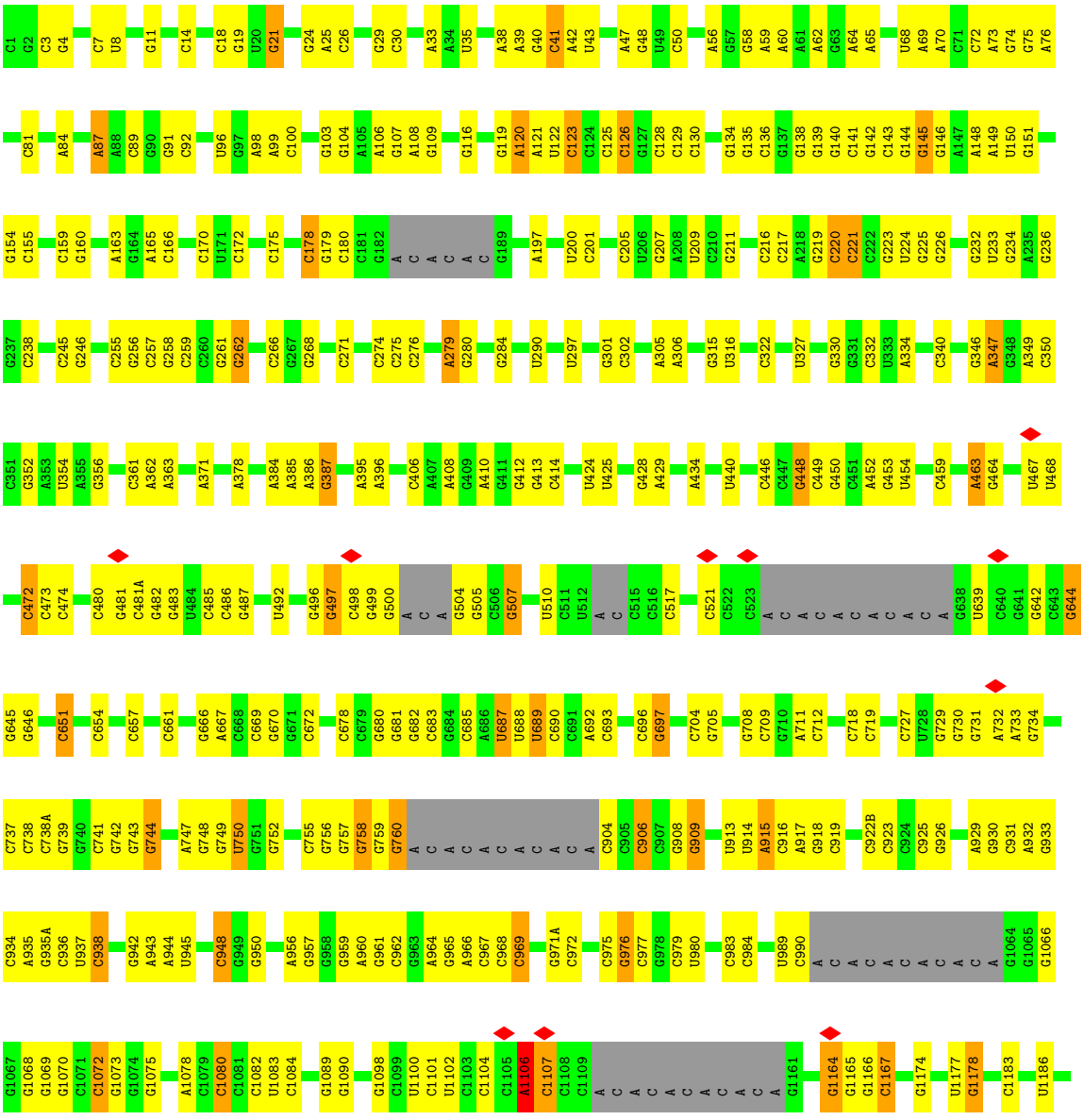
Mol	Chain	Residues	Atoms		AltConf
89	A2	2	Total	Zn	0
			2	2	
89	b2	1	Total	Zn	0
			1	1	
89	g3	1	Total	Zn	0
			1	1	
89	j3	1	Total	Zn	0
			1	1	
89	m3	1	Total	Zn	0
			1	1	
89	o3	1	Total	Zn	0
			1	1	
89	p3	1	Total	Zn	0
			1	1	

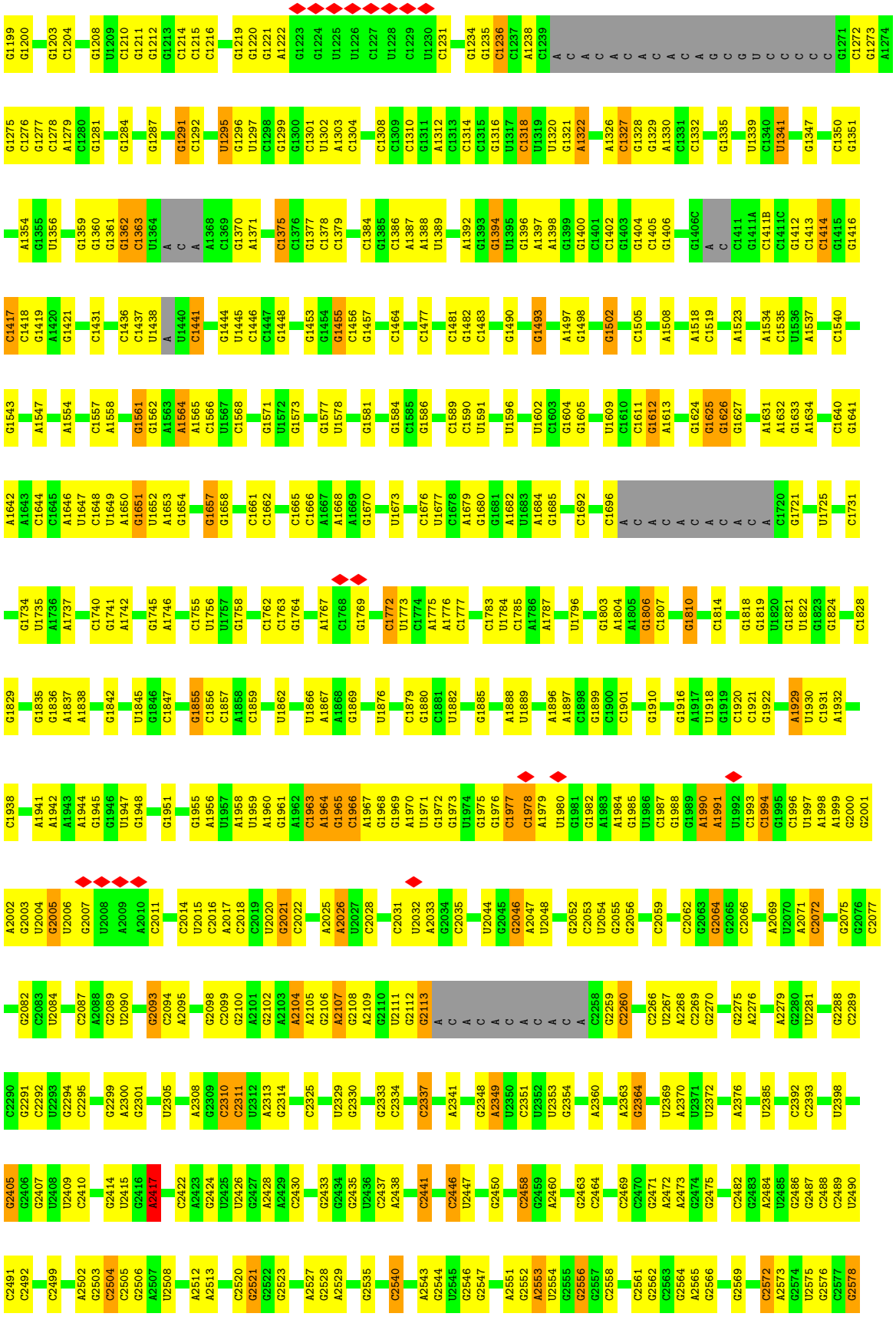
3 Residue-property plots (i)

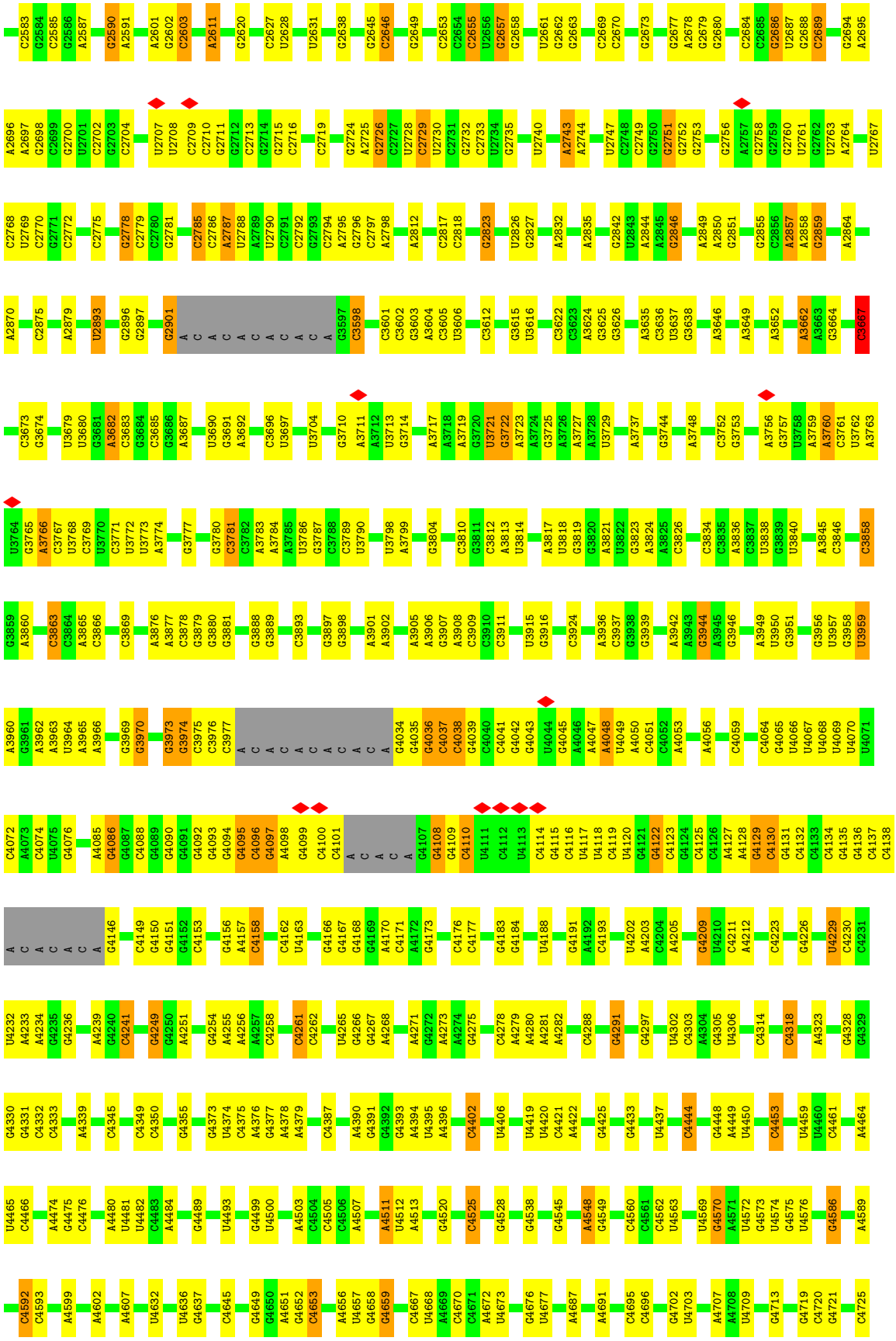
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

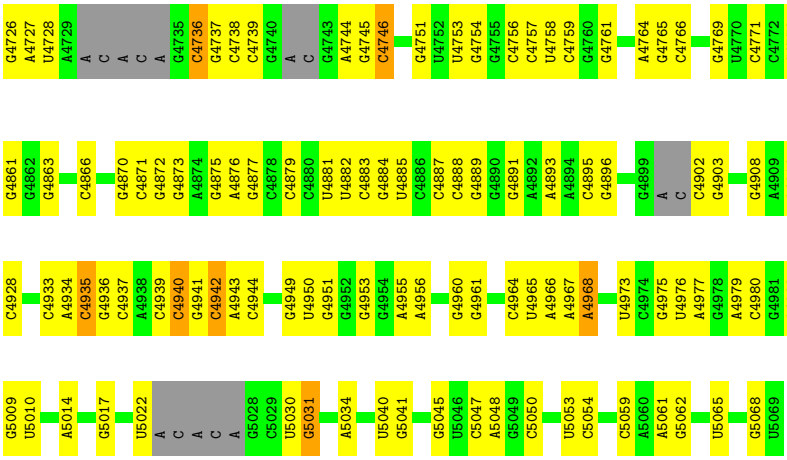
- Molecule 1: 28S Ribosomal RNA

Chain 51:



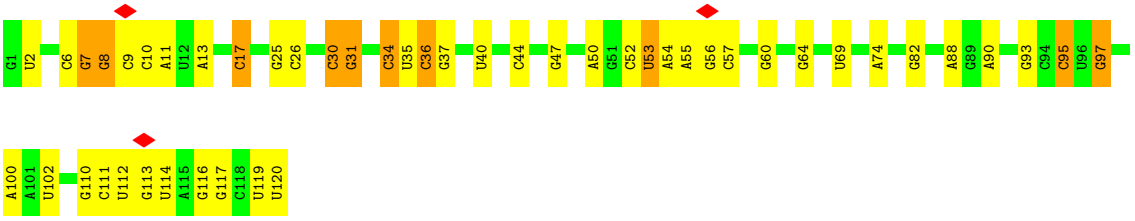






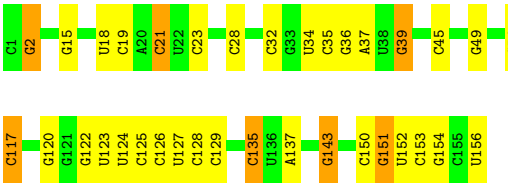
• Molecule 2: 5S Ribosomal RNA

Chain 71:



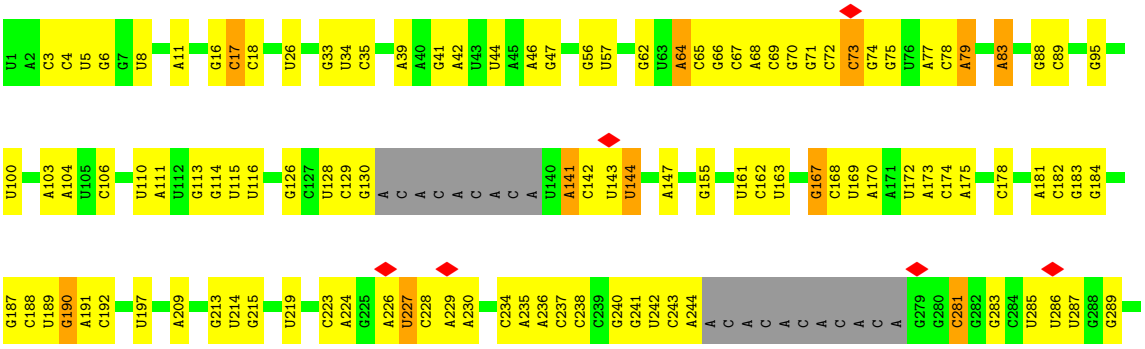
• Molecule 3: 5.8S Ribosomal RNA

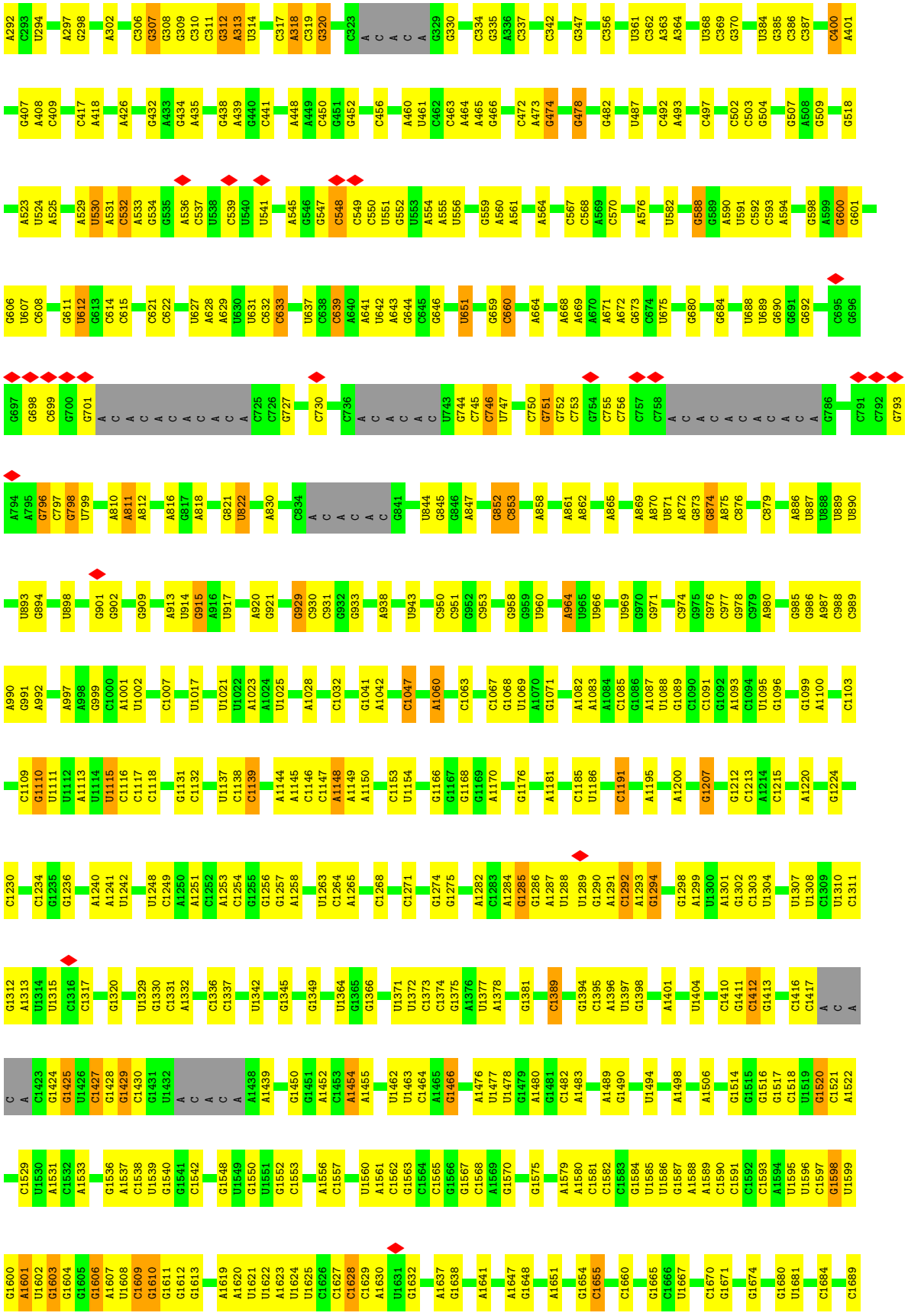
Chain 81:



• Molecule 4: 18S Ribosomal RNA

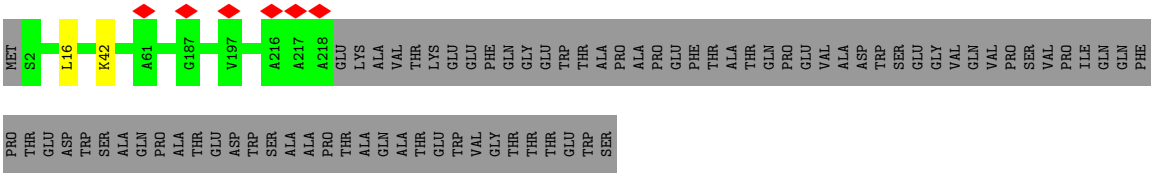
Chain A2:





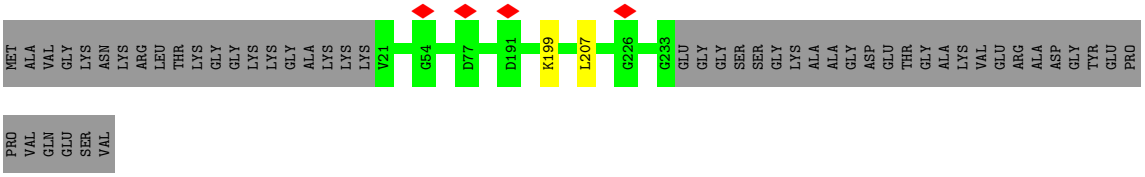
• Molecule 5: 40S ribosomal protein SA

Chain B2:



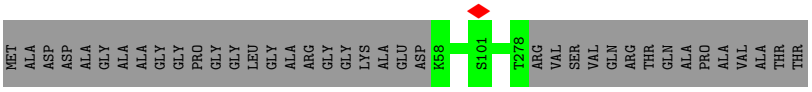
• Molecule 6: 40S ribosomal protein S3a

Chain C2:



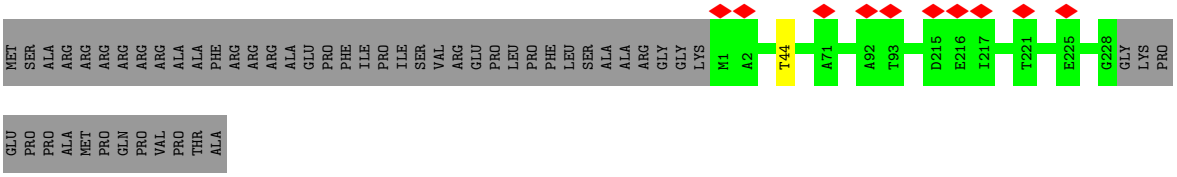
• Molecule 7: 40S ribosomal protein S2

Chain D2:



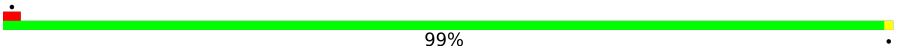
• Molecule 8: 40S ribosomal protein S3

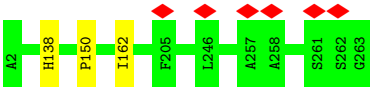
Chain E2:



• Molecule 9: S4

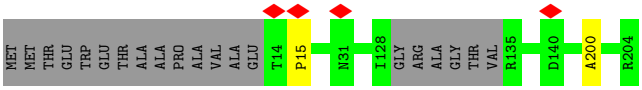
Chain F2:





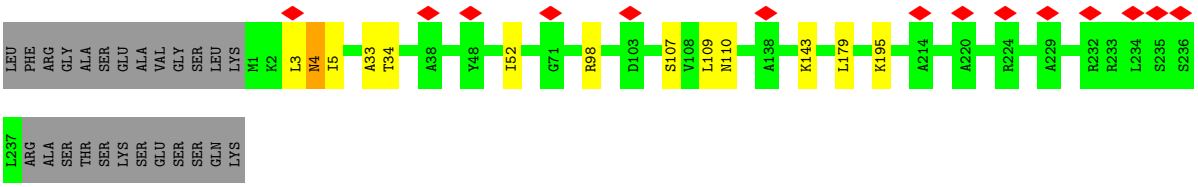
• Molecule 10: Ribosomal protein S5

Chain G2:



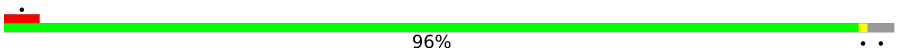
• Molecule 11: 40S ribosomal protein S6

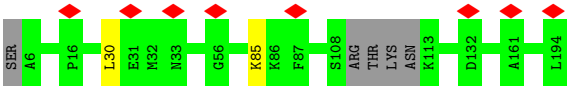
Chain H2:



• Molecule 12: ribosomal protein eS7

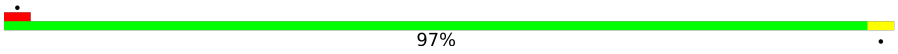
Chain I2:

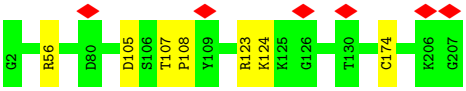




• Molecule 13: 40S ribosomal protein S8

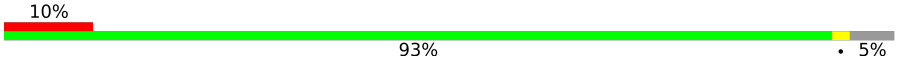
Chain J2:

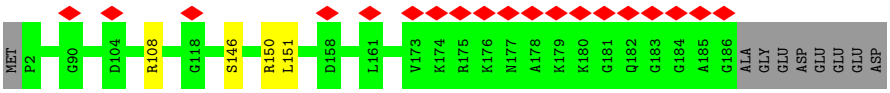




• Molecule 14: 40S ribosomal protein S9

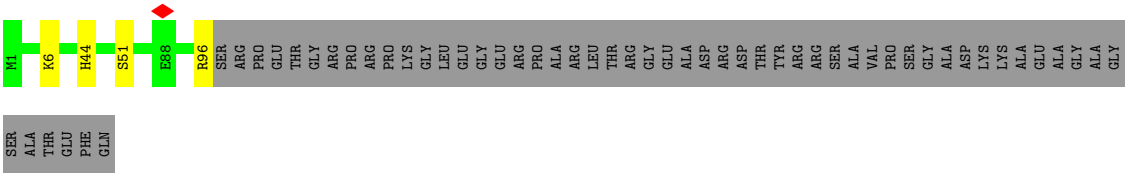
Chain K2:





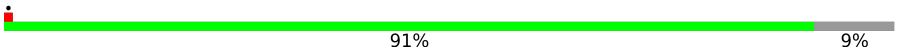
• Molecule 15: 40S ribosomal protein S10

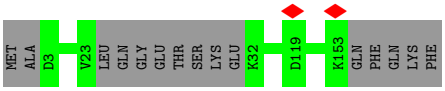
Chain L2:



• Molecule 16: 40S ribosomal protein S11

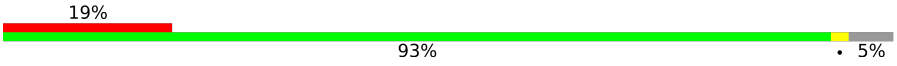
Chain M2:

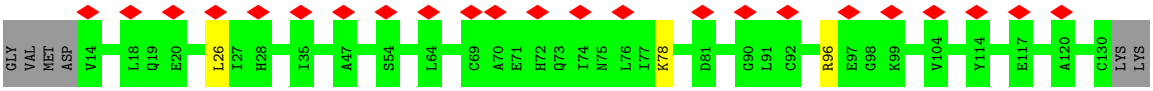




• Molecule 17: 40S ribosomal protein S12

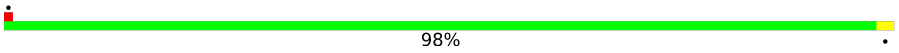
Chain N2:

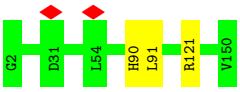




• Molecule 18: ribosomal protein uS15

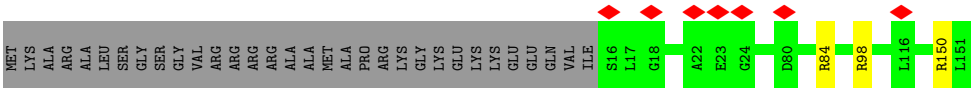
Chain O2:





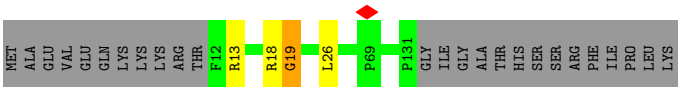
• Molecule 19: uS11

Chain P2:



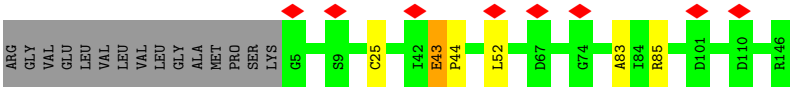
• Molecule 20: 40S ribosomal protein uS19

Chain Q2:



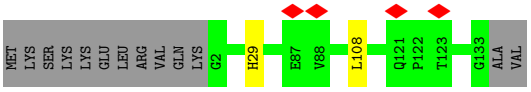
• Molecule 21: Ribosomal protein S16

Chain R2:



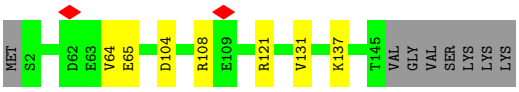
• Molecule 22: 40S ribosomal protein S17

Chain S2:



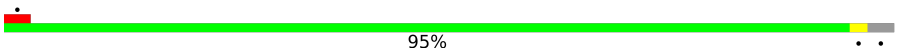
• Molecule 23: 40S ribosomal protein uS13

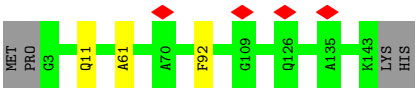
Chain T2:



• Molecule 24: S19

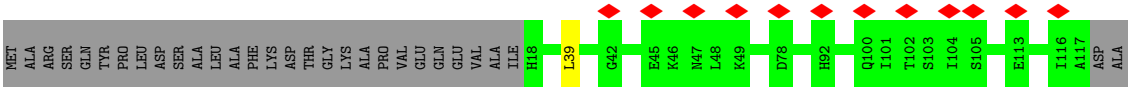
Chain U2:





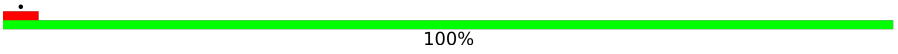
• Molecule 25: 40S ribosomal protein S20

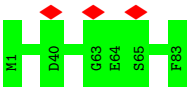
Chain V2:



• Molecule 26: 40S ribosomal protein S21

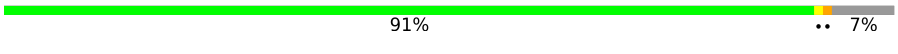
Chain W2:

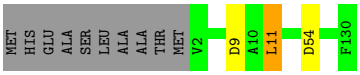




• Molecule 27: Ribosomal protein S15a

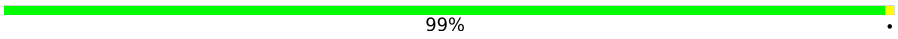
Chain X2:

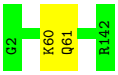




• Molecule 28: Ribosomal protein S23

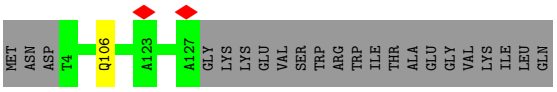
Chain Y2:





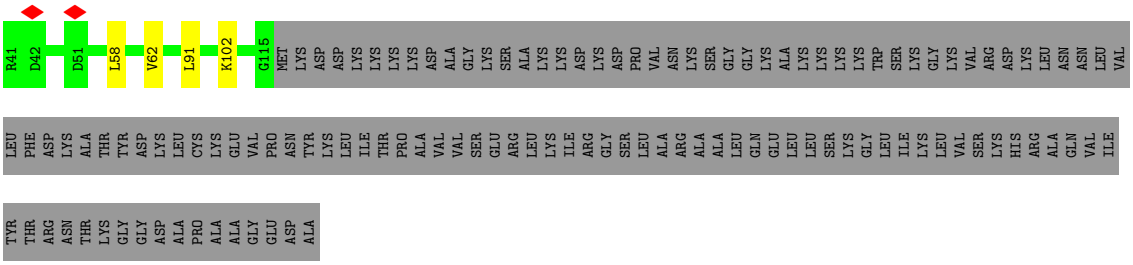
• Molecule 29: 40S ribosomal protein S24

Chain Z2:



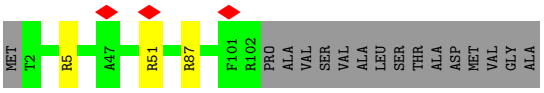
• Molecule 30: ribosomal protein eS25

Chain a2:



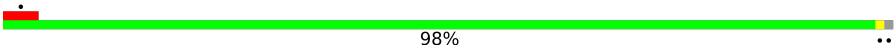
• Molecule 31: 40S ribosomal protein S26

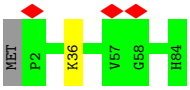
Chain b2:



• Molecule 32: 40S ribosomal protein S27

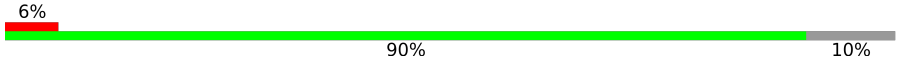
Chain c2:

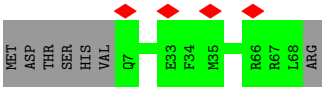




• Molecule 33: 40S ribosomal protein S28

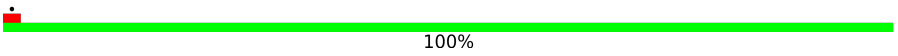
Chain d2:





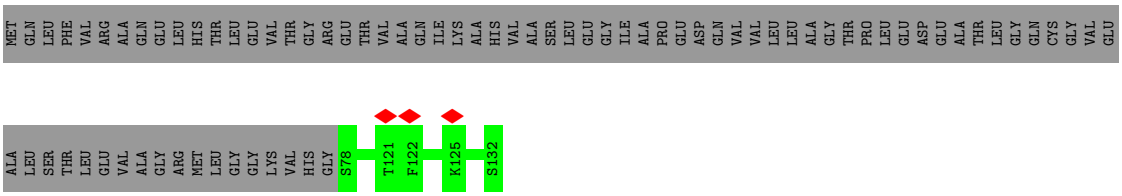
• Molecule 34: uS14

Chain e2:



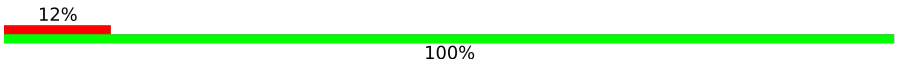
• Molecule 35: 40S ribosomal protein S30

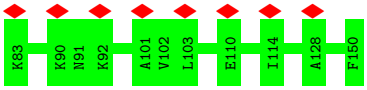
Chain f2:



• Molecule 36: eS31

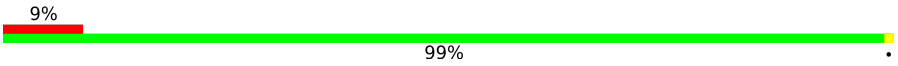
Chain g2:

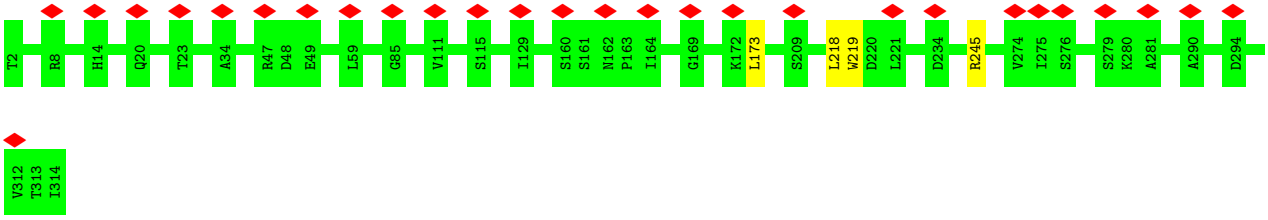




• Molecule 37: ribosomal protein RACK1

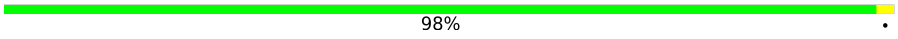
Chain h2:

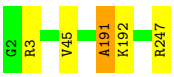




• Molecule 38: L8

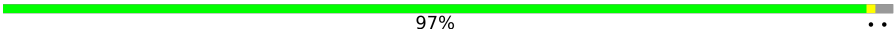
Chain A3:

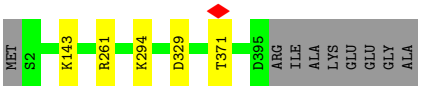




• Molecule 39: uL3

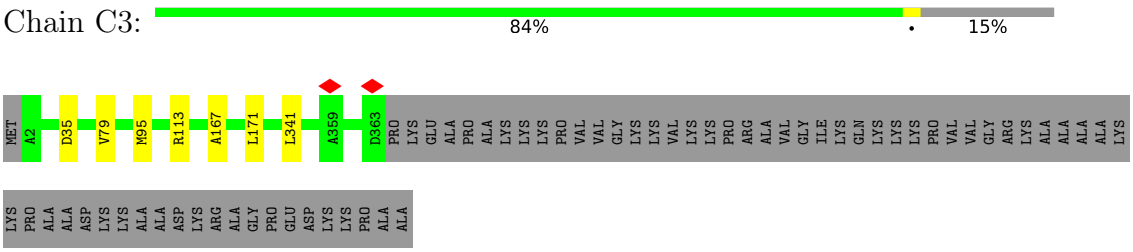
Chain B3:





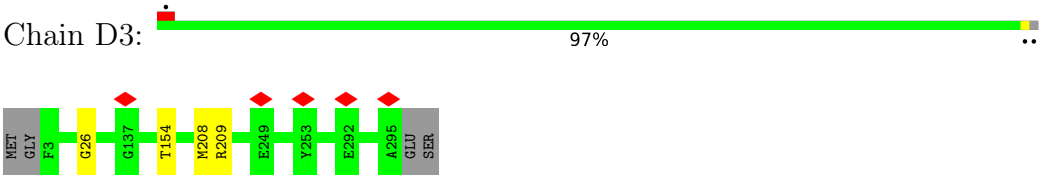
• Molecule 40: uL4

Chain C3:



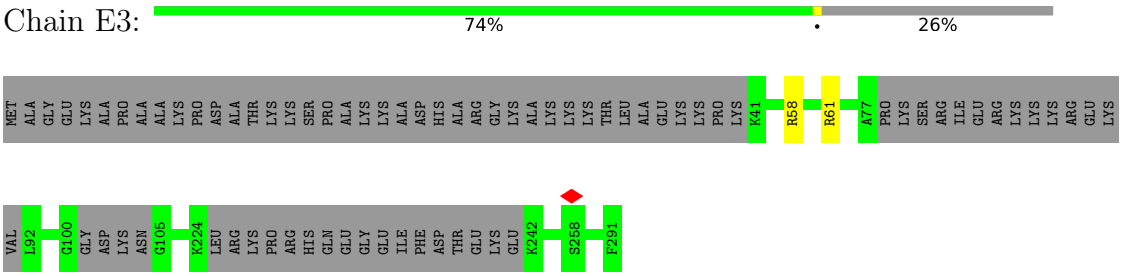
• Molecule 41: 60S ribosomal protein L5

Chain D3:



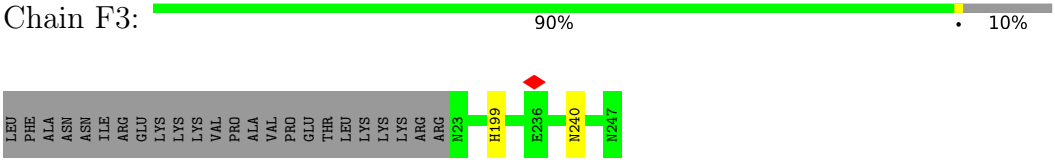
• Molecule 42: 60S ribosomal protein L6

Chain E3:



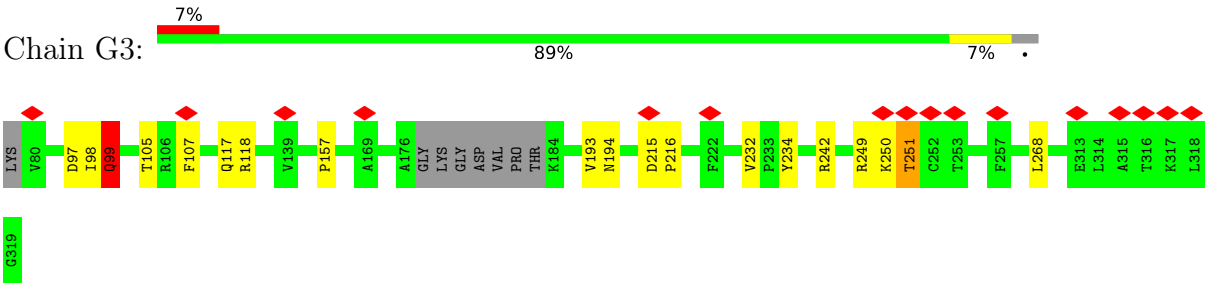
• Molecule 43: uL30

Chain F3:



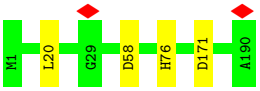
• Molecule 44: L7a

Chain G3:



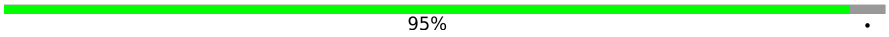
• Molecule 45: L9

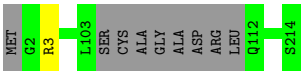
Chain H3:



• Molecule 46: 60S ribosomal protein L10

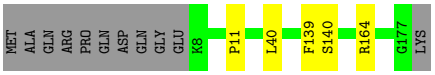
Chain I3:





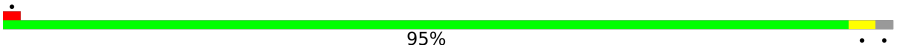
• Molecule 47: 60S ribosomal protein L11

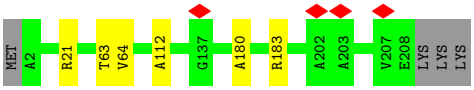
Chain J3:



• Molecule 48: L13

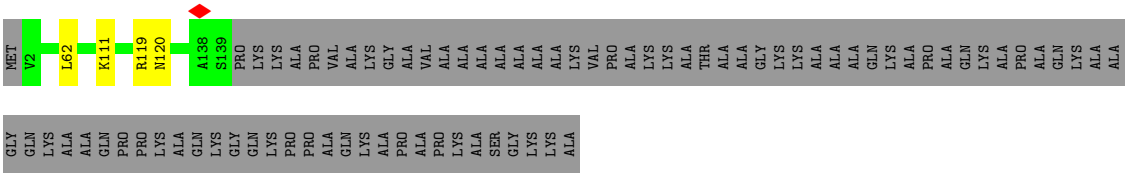
Chain L3:





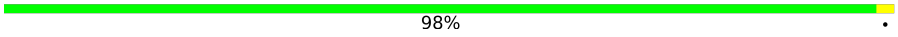
• Molecule 49: Ribosomal protein L14

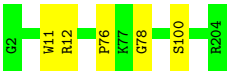
Chain M3:



• Molecule 50: Ribosomal protein L15

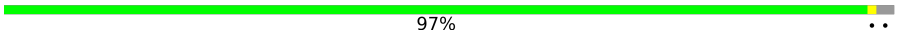
Chain N3:





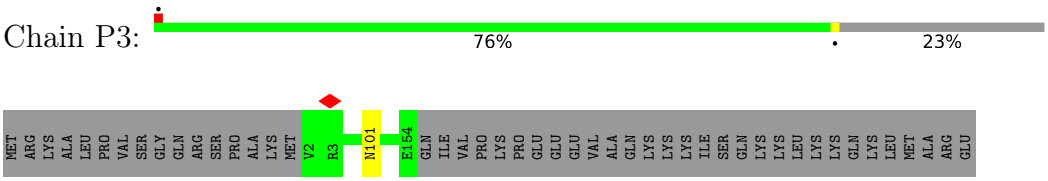
• Molecule 51: 60S RIBOSOMAL PROTEIN UL13

Chain O3:



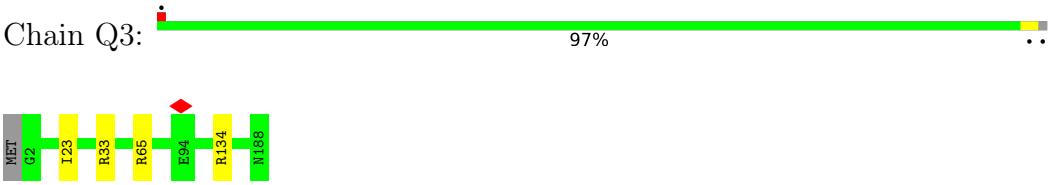
• Molecule 52: uL22

Chain P3:



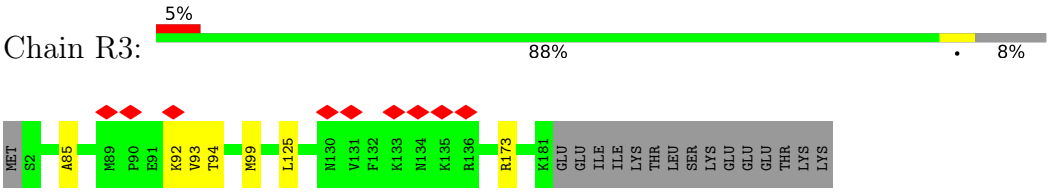
• Molecule 53: L18

Chain Q3:



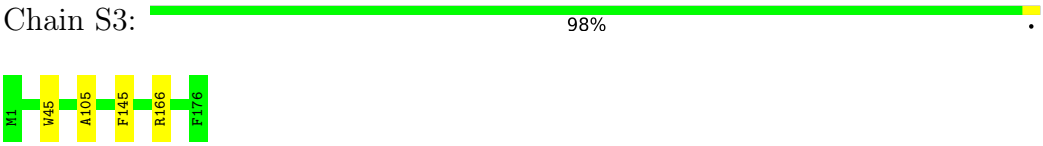
• Molecule 54: 60S ribosomal protein L19

Chain R3:



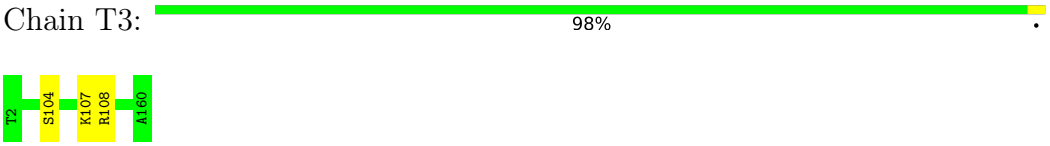
• Molecule 55: 60S ribosomal protein L18a

Chain S3:



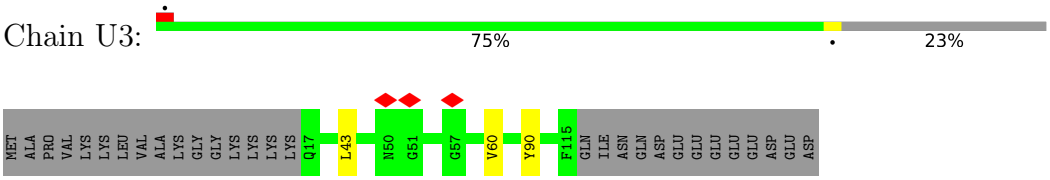
• Molecule 56: eL21

Chain T3:



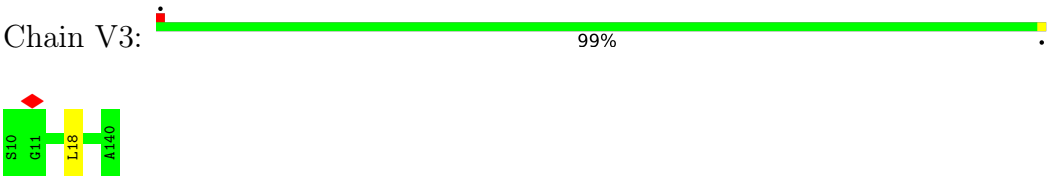
• Molecule 57: L22

Chain U3:



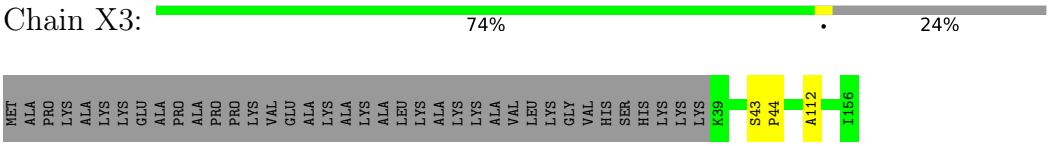
• Molecule 58: eL14

Chain V3:



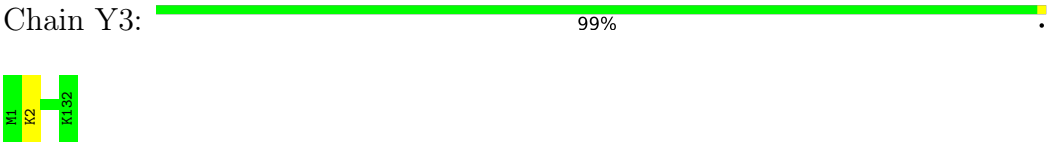
• Molecule 59: uL23

Chain X3:



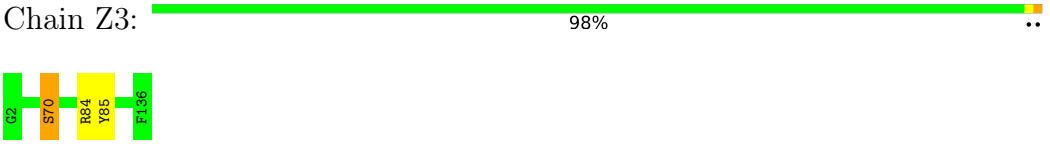
• Molecule 60: Ribosomal protein L26

Chain Y3:



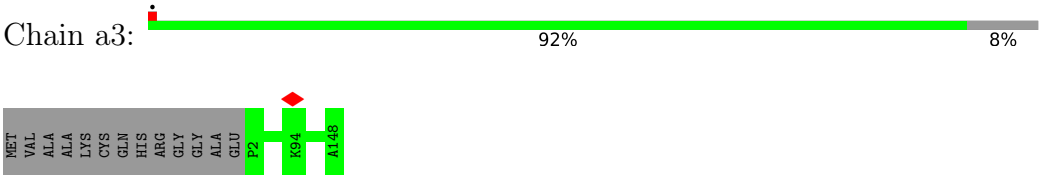
• Molecule 61: 60S ribosomal protein L27

Chain Z3:



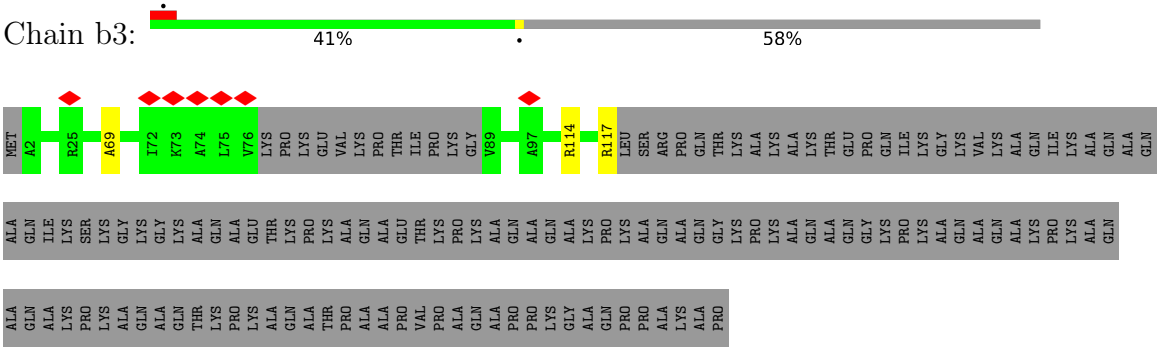
• Molecule 62: uL15

Chain a3:



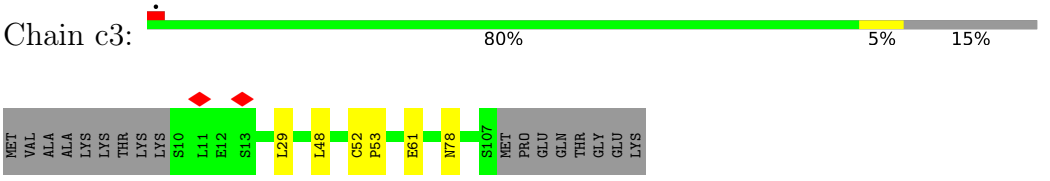
• Molecule 63: eL29

Chain b3:



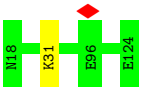
• Molecule 64: eL30

Chain c3:



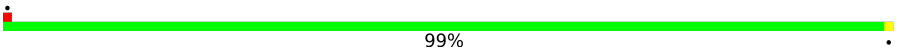
• Molecule 65: eL31

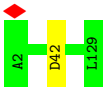
Chain d3:



• Molecule 66: eL32

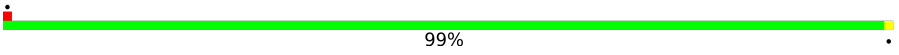
Chain e3:

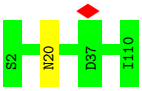




• Molecule 67: eL33

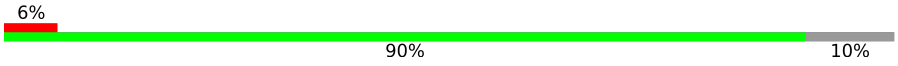
Chain f3:

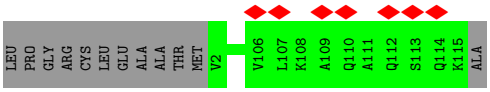




• Molecule 68: 60S ribosomal protein L34

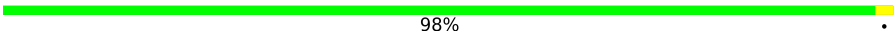
Chain g3:





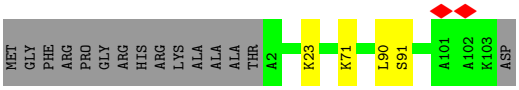
• Molecule 69: uL29

Chain h3:



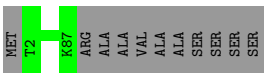
• Molecule 70: 60S ribosomal protein L36

Chain i3:



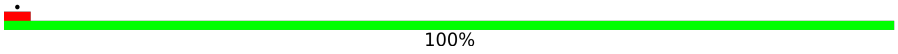
• Molecule 71: Ribosomal protein L37

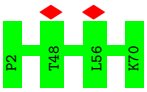
Chain j3:



• Molecule 72: L38

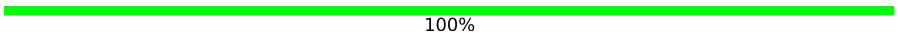
Chain k3:





• Molecule 73: eL39

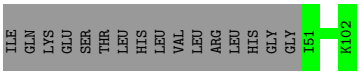
Chain l3:



There are no outlier residues recorded for this chain.

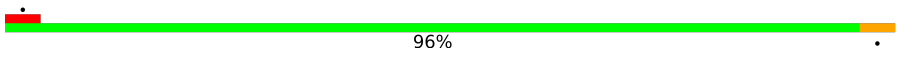
• Molecule 74: 60S RIBOSOMAL PROTEIN EL40

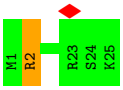
Chain m3:



• Molecule 75: 60s ribosomal protein l41

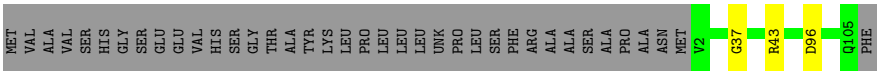
Chain n3:





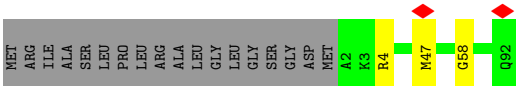
• Molecule 76: eL42

Chain o3:



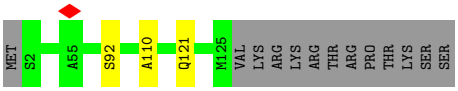
• Molecule 77: ribosomal protein eL43

Chain p3:



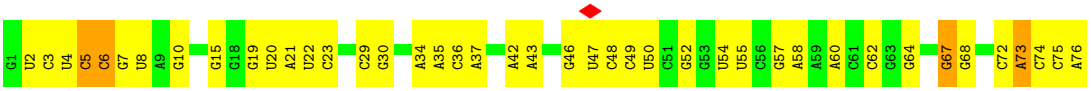
• Molecule 78: eL28

Chain r3:



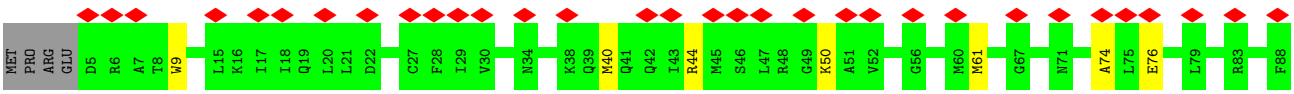
• Molecule 79: A/P-Site tRNA

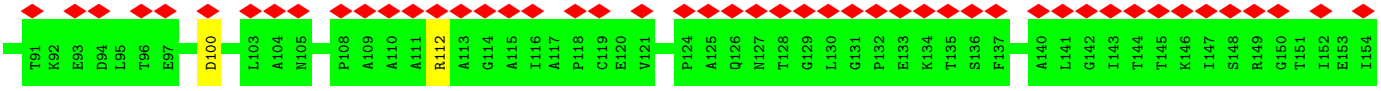
Chain q3:

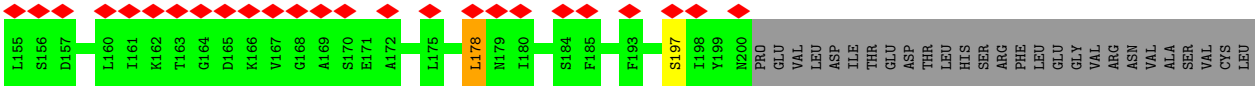


• Molecule 80: 60S acidic ribosomal protein P0

Chain t3:

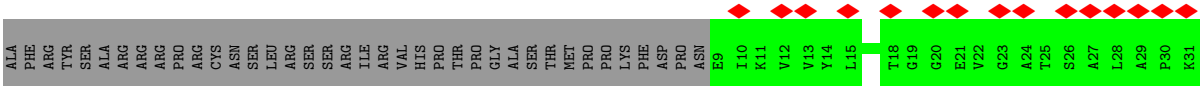


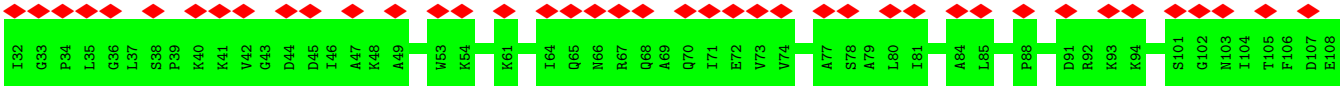


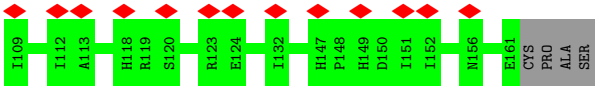


• Molecule 81: uL12

Chain u3:

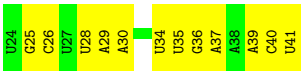






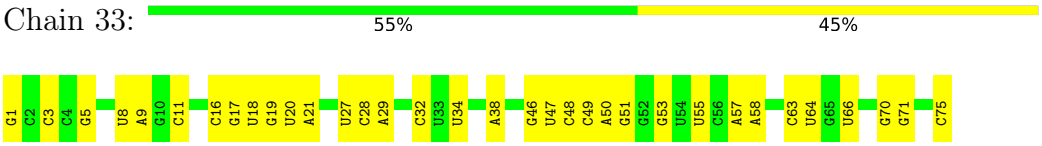
• Molecule 82: mRNA

Chain v3:



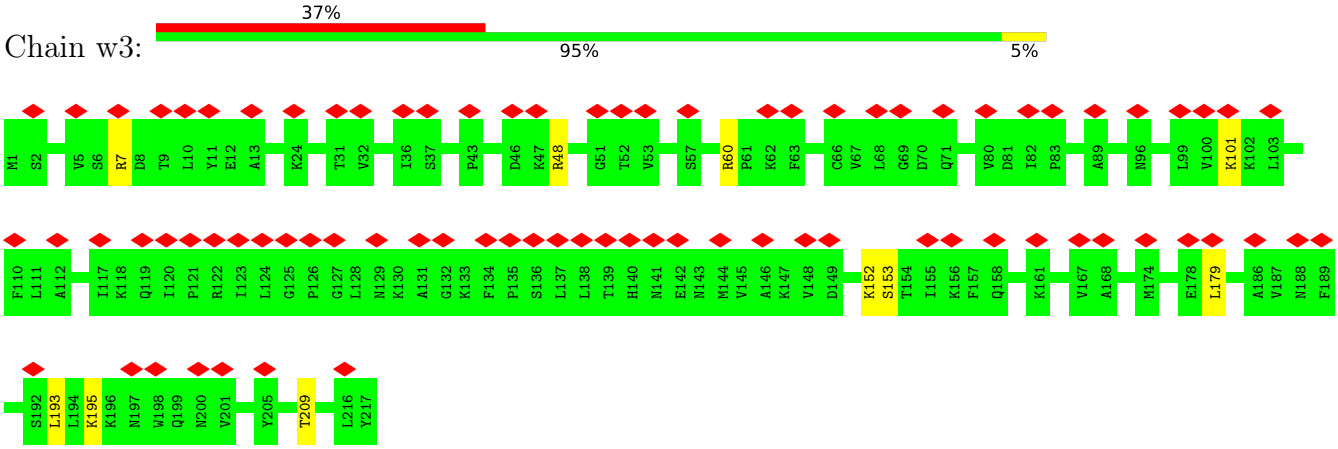
• Molecule 83: P/E-Site tRNA

Chain 33:



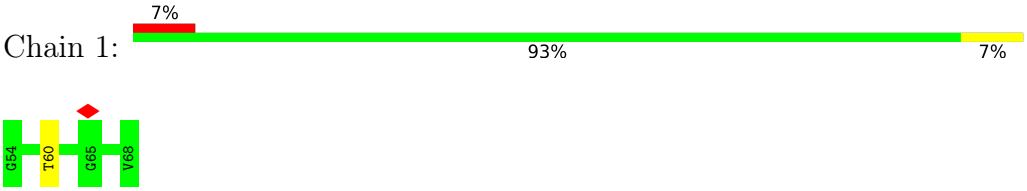
• Molecule 84: Ribosomal protein

Chain w3:



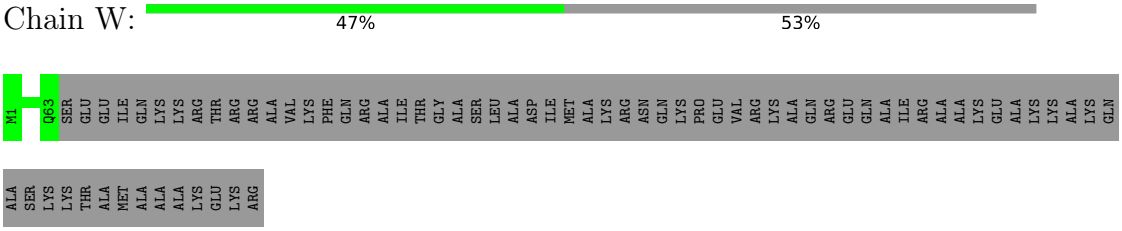
• Molecule 85: Sec61Beta

Chain 1:



• Molecule 86: 60S ribosomal protein L24-like protein

Chain W:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29879	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	41.9	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	79000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.172	Depositor
Minimum map value	-0.107	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	405.0, 405.0, 405.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, BLS

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	51	1.13	47/86836 (0.1%)	1.56	873/135406 (0.6%)
2	71	1.03	1/2858 (0.0%)	1.31	19/4455 (0.4%)
3	81	1.43	6/3581 (0.2%)	1.32	23/5577 (0.4%)
4	A2	0.94	4/41517 (0.0%)	1.33	306/64674 (0.5%)
5	B2	0.58	0/1747	0.77	0/2374
6	C2	0.63	0/1756	0.78	0/2350
7	D2	0.69	0/1753	0.74	0/2369
8	E2	0.54	0/1793	0.72	0/2413
9	F2	0.55	0/2118	0.70	0/2849
10	G2	0.53	0/1492	0.77	0/2005
11	H2	0.51	0/1946	0.82	0/2590
12	I2	0.53	0/1510	0.77	0/2022
13	J2	0.56	0/1715	0.80	0/2287
14	K2	0.58	1/1550 (0.1%)	0.83	1/2069 (0.0%)
15	L2	0.54	0/834	0.79	0/1125
16	M2	0.68	0/1195	0.73	0/1597
17	N2	0.46	0/918	0.80	1/1233 (0.1%)
18	O2	0.65	0/1226	0.74	0/1649
19	P2	0.60	0/1029	0.74	0/1380
20	Q2	0.61	0/1017	0.80	1/1358 (0.1%)
21	R2	0.57	0/1146	0.76	0/1534
22	S2	0.53	0/1082	0.73	0/1452
23	T2	0.55	0/1208	0.79	0/1618
24	U2	0.56	0/1115	0.78	0/1493
25	V2	0.53	0/805	0.80	1/1081 (0.1%)
26	W2	0.56	0/643	0.73	0/860
27	X2	0.70	0/1051	0.78	1/1406 (0.1%)
28	Y2	0.71	0/1116	0.76	0/1490
29	Z2	0.53	0/1028	0.78	0/1366
30	a2	0.51	0/604	0.82	0/810
31	b2	0.67	0/828	0.74	0/1109
32	c2	0.54	0/665	0.68	0/891

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	d2	0.51	0/490	0.84	0/656
34	e2	0.64	0/470	0.72	0/623
35	f2	0.50	0/447	0.78	0/587
36	g2	0.49	0/567	0.80	0/753
37	h2	0.47	0/2493	0.75	1/3394 (0.0%)
38	A3	0.86	0/1925	0.79	0/2581
39	B3	0.76	0/3240	0.73	0/4339
40	C3	0.82	1/2937 (0.0%)	0.79	0/3946
41	D3	0.67	0/2437	0.76	1/3264 (0.0%)
42	E3	0.67	0/1762	0.77	0/2362
43	F3	0.87	1/1911 (0.1%)	0.78	0/2549
44	G3	1.57	1/1909 (0.1%)	0.90	5/2566 (0.2%)
45	H3	0.70	0/1535	0.78	0/2063
46	I3	0.76	0/1702	0.74	0/2272
47	J3	0.70	1/1385 (0.1%)	0.78	0/1852
48	L3	0.69	0/1705	0.76	0/2283
49	M3	0.76	0/1158	0.81	0/1547
50	N3	0.83	0/1746	0.78	0/2338
51	O3	0.83	0/1662	0.76	0/2222
52	P3	0.82	0/1268	0.75	0/1700
53	Q3	0.84	0/1539	0.80	0/2054
54	R3	0.69	0/1524	0.90	0/2013
55	S3	0.81	1/1501 (0.1%)	0.75	0/2012
56	T3	0.79	0/1326	0.74	0/1770
57	U3	0.59	0/823	0.80	1/1104 (0.1%)
58	V3	0.80	0/993	0.76	0/1332
59	X3	0.73	0/984	0.76	0/1323
60	Y3	0.78	0/1119	0.75	0/1488
61	Z3	0.67	0/1130	0.77	0/1507
62	a3	0.81	0/1191	0.73	0/1590
63	b3	0.57	0/861	0.78	0/1138
64	c3	0.68	0/771	0.77	1/1034 (0.1%)
65	d3	0.71	0/903	0.73	0/1216
66	e3	0.81	0/1071	0.78	0/1429
67	f3	0.88	0/895	0.80	0/1198
68	g3	0.72	0/916	0.82	0/1220
69	h3	0.71	0/1021	0.76	0/1348
70	i3	0.65	0/841	0.76	0/1112
71	j3	0.85	0/720	0.78	0/952
72	k3	0.62	0/575	0.82	0/761
73	l3	0.74	0/459	0.77	0/608
74	m3	0.62	0/435	0.76	0/575
75	n3	0.65	0/240	1.05	0/305

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	o3	0.70	0/864	0.75	0/1140
77	p3	0.87	0/718	0.86	0/953
78	r3	0.80	2/1010 (0.2%)	0.78	0/1354
79	q3	0.69	0/1759	1.16	12/2733 (0.4%)
80	t3	0.38	0/1530	0.83	2/2064 (0.1%)
81	u3	0.39	0/1174	0.81	0/1582
82	v3	0.59	0/425	0.89	0/659
83	33	0.73	0/1780	1.11	6/2773 (0.2%)
84	w3	0.41	0/1769	0.85	2/2371 (0.1%)
85	1	0.42	0/129	0.63	0/173
86	W	0.71	0/541	0.54	0/720
All	All	0.94	66/235968 (0.0%)	1.26	1257/346400 (0.4%)

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
1	51	0	14
2	71	0	1
3	81	0	1
4	A2	0	4
5	B2	0	1
8	E2	0	1
9	F2	0	1
10	G2	0	1
11	H2	0	7
12	I2	0	1
13	J2	0	4
15	L2	0	2
18	O2	0	3
20	Q2	0	2
21	R2	0	2
22	S2	0	1
23	T2	0	3
24	U2	0	1
27	X2	0	2
29	Z2	0	1
30	a2	0	1
37	h2	0	1
38	A3	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
39	B3	0	1
40	C3	0	4
42	E3	0	1
43	F3	0	1
44	G3	0	11
45	H3	0	2
47	J3	0	2
48	L3	0	3
49	M3	0	2
50	N3	0	5
51	O3	0	3
52	P3	0	1
53	Q3	0	2
54	R3	0	2
55	S3	0	2
56	T3	0	2
57	U3	0	2
59	X3	0	1
61	Z3	0	2
63	b3	0	2
64	c3	0	3
66	e3	0	1
67	f3	0	1
69	h3	0	2
70	i3	0	3
75	n3	0	1
76	o3	0	1
77	p3	0	1
78	r3	0	1
80	t3	0	6
84	w3	0	2
All	All	0	129

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	G3	117	GLN	CB-CG	62.24	3.20	1.52
1	51	1966	C	N1-C6	41.23	1.61	1.37
3	81	151	G	C6-N1	29.84	1.60	1.39
3	81	151	G	N1-C2	25.61	1.58	1.37
3	81	151	G	N3-C4	22.98	1.51	1.35

The worst 5 of 1257 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	51	1966	C	C6-N1-C2	-187.56	45.27	120.30
1	51	1966	C	N1-C2-N3	-136.00	24.00	119.20
1	51	1966	C	N3-C4-C5	-65.39	95.74	121.90
1	51	1966	C	C4-C5-C6	-57.09	88.85	117.40
1	51	1966	C	C6-N1-C1'	29.32	155.99	120.80

There are no chirality outliers.

5 of 129 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	51	1106	A	Sidechain
1	51	221	C	Sidechain
1	51	41	C	Sidechain
1	51	497	G	Sidechain
1	51	727	C	Sidechain

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	
5	B2	215/295 (73%)	189 (88%)	26 (12%)	0	100	100
6	C2	211/264 (80%)	192 (91%)	19 (9%)	0	100	100
7	D2	219/259 (85%)	205 (94%)	14 (6%)	0	100	100
8	E2	226/281 (80%)	209 (92%)	17 (8%)	0	100	100
9	F2	260/262 (99%)	232 (89%)	27 (10%)	1 (0%)	30	63
10	G2	181/205 (88%)	162 (90%)	18 (10%)	1 (1%)	22	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	H2	235/262 (90%)	184 (78%)	47 (20%)	4 (2%)	7 34
12	I2	181/190 (95%)	169 (93%)	12 (7%)	0	100 100
13	J2	204/206 (99%)	168 (82%)	33 (16%)	3 (2%)	8 37
14	K2	183/194 (94%)	157 (86%)	26 (14%)	0	100 100
15	L2	94/151 (62%)	86 (92%)	8 (8%)	0	100 100
16	M2	139/158 (88%)	129 (93%)	10 (7%)	0	100 100
17	N2	115/123 (94%)	96 (84%)	19 (16%)	0	100 100
18	O2	147/149 (99%)	136 (92%)	11 (8%)	0	100 100
19	P2	134/168 (80%)	122 (91%)	12 (9%)	0	100 100
20	Q2	118/145 (81%)	106 (90%)	11 (9%)	1 (1%)	16 49
21	R2	140/157 (89%)	126 (90%)	12 (9%)	2 (1%)	9 37
22	S2	130/145 (90%)	122 (94%)	8 (6%)	0	100 100
23	T2	142/152 (93%)	119 (84%)	22 (16%)	1 (1%)	19 52
24	U2	139/145 (96%)	125 (90%)	12 (9%)	2 (1%)	9 37
25	V2	98/130 (75%)	92 (94%)	6 (6%)	0	100 100
26	W2	81/83 (98%)	72 (89%)	9 (11%)	0	100 100
27	X2	127/139 (91%)	117 (92%)	10 (8%)	0	100 100
28	Y2	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	9 37
29	Z2	122/146 (84%)	109 (89%)	13 (11%)	0	100 100
30	a2	73/198 (37%)	65 (89%)	8 (11%)	0	100 100
31	b2	99/117 (85%)	89 (90%)	10 (10%)	0	100 100
32	c2	81/84 (96%)	76 (94%)	5 (6%)	0	100 100
33	d2	60/69 (87%)	58 (97%)	2 (3%)	0	100 100
34	e2	53/55 (96%)	50 (94%)	3 (6%)	0	100 100
35	f2	53/133 (40%)	49 (92%)	4 (8%)	0	100 100
36	g2	66/68 (97%)	53 (80%)	13 (20%)	0	100 100
37	h2	311/313 (99%)	261 (84%)	50 (16%)	0	100 100
38	A3	244/246 (99%)	205 (84%)	36 (15%)	3 (1%)	11 40
39	B3	392/403 (97%)	354 (90%)	38 (10%)	0	100 100
40	C3	360/425 (85%)	330 (92%)	30 (8%)	0	100 100
41	D3	291/297 (98%)	257 (88%)	32 (11%)	2 (1%)	19 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	E3	208/291 (72%)	189 (91%)	19 (9%)	0	100	100
43	F3	223/249 (90%)	208 (93%)	15 (7%)	0	100	100
44	G3	227/241 (94%)	188 (83%)	35 (15%)	4 (2%)	7	34
45	H3	188/190 (99%)	175 (93%)	13 (7%)	0	100	100
46	I3	201/214 (94%)	178 (89%)	23 (11%)	0	100	100
47	J3	168/181 (93%)	150 (89%)	17 (10%)	1 (1%)	22	55
48	L3	205/211 (97%)	185 (90%)	18 (9%)	2 (1%)	13	44
49	M3	136/218 (62%)	123 (90%)	13 (10%)	0	100	100
50	N3	201/203 (99%)	179 (89%)	22 (11%)	0	100	100
51	O3	197/203 (97%)	182 (92%)	15 (8%)	0	100	100
52	P3	151/199 (76%)	143 (95%)	8 (5%)	0	100	100
53	Q3	185/188 (98%)	170 (92%)	15 (8%)	0	100	100
54	R3	178/196 (91%)	156 (88%)	19 (11%)	3 (2%)	7	34
55	S3	174/176 (99%)	157 (90%)	16 (9%)	1 (1%)	22	55
56	T3	157/159 (99%)	146 (93%)	11 (7%)	0	100	100
57	U3	97/128 (76%)	77 (79%)	20 (21%)	0	100	100
58	V3	129/131 (98%)	117 (91%)	12 (9%)	0	100	100
59	X3	116/156 (74%)	99 (85%)	15 (13%)	2 (2%)	7	34
60	Y3	130/132 (98%)	121 (93%)	9 (7%)	0	100	100
61	Z3	133/135 (98%)	113 (85%)	18 (14%)	2 (2%)	8	37
62	a3	145/160 (91%)	133 (92%)	12 (8%)	0	100	100
63	b3	100/245 (41%)	95 (95%)	5 (5%)	0	100	100
64	c3	96/115 (84%)	87 (91%)	8 (8%)	1 (1%)	13	44
65	d3	105/107 (98%)	93 (89%)	12 (11%)	0	100	100
66	e3	126/128 (98%)	116 (92%)	10 (8%)	0	100	100
67	f3	107/109 (98%)	94 (88%)	13 (12%)	0	100	100
68	g3	112/126 (89%)	100 (89%)	12 (11%)	0	100	100
69	h3	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
70	i3	100/117 (86%)	93 (93%)	7 (7%)	0	100	100
71	j3	84/97 (87%)	74 (88%)	10 (12%)	0	100	100
72	k3	67/69 (97%)	54 (81%)	13 (19%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
73	l3	48/50 (96%)	41 (85%)	7 (15%)	0	100 100
74	m3	50/128 (39%)	46 (92%)	4 (8%)	0	100 100
75	n3	23/25 (92%)	20 (87%)	2 (9%)	1 (4%)	2 20
76	o3	102/142 (72%)	93 (91%)	9 (9%)	0	100 100
77	p3	89/109 (82%)	72 (81%)	16 (18%)	1 (1%)	12 42
78	r3	122/137 (89%)	111 (91%)	11 (9%)	0	100 100
80	t3	194/318 (61%)	152 (78%)	41 (21%)	1 (0%)	25 58
81	u3	151/195 (77%)	127 (84%)	24 (16%)	0	100 100
84	w3	215/217 (99%)	181 (84%)	31 (14%)	3 (1%)	9 37
85	1	13/15 (87%)	7 (54%)	5 (38%)	1 (8%)	1 11
86	W	61/134 (46%)	50 (82%)	11 (18%)	0	100 100
All	All	11697/13624 (86%)	10406 (89%)	1246 (11%)	45 (0%)	32 63

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	H2	34	THR
13	J2	105	ASP
23	T2	137	LYS
28	Y2	61	GLN
54	R3	85	ALA

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
5	B2	180/245 (74%)	179 (99%)	1 (1%)	84 88
6	C2	194/229 (85%)	192 (99%)	2 (1%)	73 80
7	D2	187/208 (90%)	187 (100%)	0	100 100
8	E2	189/232 (82%)	189 (100%)	0	100 100
9	F2	224/224 (100%)	223 (100%)	1 (0%)	89 91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	G2	158/171 (92%)	158 (100%)	0	100	100
11	H2	207/227 (91%)	204 (99%)	3 (1%)	62	75
12	I2	165/170 (97%)	164 (99%)	1 (1%)	84	88
13	J2	178/178 (100%)	178 (100%)	0	100	100
14	K2	161/168 (96%)	159 (99%)	2 (1%)	67	77
15	L2	87/127 (68%)	85 (98%)	2 (2%)	45	63
16	M2	130/143 (91%)	130 (100%)	0	100	100
17	N2	99/104 (95%)	97 (98%)	2 (2%)	50	68
18	O2	130/130 (100%)	130 (100%)	0	100	100
19	P2	106/130 (82%)	103 (97%)	3 (3%)	38	59
20	Q2	109/130 (84%)	108 (99%)	1 (1%)	75	82
21	R2	117/129 (91%)	114 (97%)	3 (3%)	41	61
22	S2	119/131 (91%)	118 (99%)	1 (1%)	79	84
23	T2	125/132 (95%)	122 (98%)	3 (2%)	44	62
24	U2	111/115 (96%)	111 (100%)	0	100	100
25	V2	92/115 (80%)	92 (100%)	0	100	100
26	W2	67/67 (100%)	67 (100%)	0	100	100
27	X2	112/119 (94%)	111 (99%)	1 (1%)	75	82
28	Y2	113/113 (100%)	113 (100%)	0	100	100
29	Z2	107/126 (85%)	107 (100%)	0	100	100
30	a2	66/167 (40%)	63 (96%)	3 (4%)	23	47
31	b2	88/99 (89%)	85 (97%)	3 (3%)	32	55
32	c2	75/76 (99%)	74 (99%)	1 (1%)	65	76
33	d2	55/62 (89%)	55 (100%)	0	100	100
34	e2	48/48 (100%)	48 (100%)	0	100	100
35	f2	46/106 (43%)	46 (100%)	0	100	100
36	g2	61/61 (100%)	61 (100%)	0	100	100
37	h2	272/272 (100%)	270 (99%)	2 (1%)	81	86
38	A3	189/189 (100%)	187 (99%)	2 (1%)	70	79
39	B3	342/348 (98%)	338 (99%)	4 (1%)	67	77
40	C3	302/347 (87%)	300 (99%)	2 (1%)	81	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
41	D3	247/250 (99%)	246 (100%)	1 (0%)	89 91
42	E3	190/251 (76%)	189 (100%)	1 (0%)	86 90
43	F3	196/218 (90%)	196 (100%)	0	100 100
44	G3	200/206 (97%)	198 (99%)	2 (1%)	73 80
45	H3	169/169 (100%)	167 (99%)	2 (1%)	67 77
46	I3	175/181 (97%)	174 (99%)	1 (1%)	84 88
47	J3	143/152 (94%)	142 (99%)	1 (1%)	81 86
48	L3	172/176 (98%)	171 (99%)	1 (1%)	84 88
49	M3	117/161 (73%)	115 (98%)	2 (2%)	56 72
50	N3	171/171 (100%)	171 (100%)	0	100 100
51	O3	171/173 (99%)	171 (100%)	0	100 100
52	P3	134/175 (77%)	134 (100%)	0	100 100
53	Q3	164/165 (99%)	162 (99%)	2 (1%)	67 77
54	R3	159/175 (91%)	157 (99%)	2 (1%)	65 76
55	S3	157/157 (100%)	157 (100%)	0	100 100
56	T3	139/139 (100%)	138 (99%)	1 (1%)	81 86
57	U3	89/114 (78%)	89 (100%)	0	100 100
58	V3	101/101 (100%)	100 (99%)	1 (1%)	73 80
59	X3	106/134 (79%)	106 (100%)	0	100 100
60	Y3	123/123 (100%)	122 (99%)	1 (1%)	79 84
61	Z3	117/117 (100%)	117 (100%)	0	100 100
62	a3	119/127 (94%)	119 (100%)	0	100 100
63	b3	84/184 (46%)	83 (99%)	1 (1%)	67 77
64	c3	84/98 (86%)	83 (99%)	1 (1%)	67 77
65	d3	98/98 (100%)	97 (99%)	1 (1%)	73 80
66	e3	114/114 (100%)	114 (100%)	0	100 100
67	f3	88/88 (100%)	88 (100%)	0	100 100
68	g3	98/106 (92%)	98 (100%)	0	100 100
69	h3	109/109 (100%)	108 (99%)	1 (1%)	75 82
70	i3	86/96 (90%)	85 (99%)	1 (1%)	67 77
71	j3	73/80 (91%)	73 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
72	k3	64/64 (100%)	64 (100%)	0	100 100
73	l3	47/47 (100%)	47 (100%)	0	100 100
74	m3	48/116 (41%)	48 (100%)	0	100 100
75	n3	24/24 (100%)	24 (100%)	0	100 100
76	o3	92/121 (76%)	90 (98%)	2 (2%)	47 64
77	p3	74/87 (85%)	73 (99%)	1 (1%)	62 75
78	r3	108/121 (89%)	108 (100%)	0	100 100
80	t3	164/258 (64%)	161 (98%)	3 (2%)	54 71
81	u3	126/163 (77%)	126 (100%)	0	100 100
84	w3	195/196 (100%)	192 (98%)	3 (2%)	60 74
85	1	13/13 (100%)	13 (100%)	0	100 100
86	W	55/109 (50%)	55 (100%)	0	100 100
All	All	10214/11565 (88%)	10139 (99%)	75 (1%)	80 86

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
54	R3	173	ARG
80	t3	197	SER
58	V3	18	LEU
70	i3	23	LYS
23	T2	121	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
45	H3	79	ASN
54	R3	130	ASN
84	w3	40	ASN
47	J3	112	HIS
51	O3	50	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	51	3589/3788 (94%)	1190 (33%)	53 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	71	119/120 (99%)	43 (36%)	0
3	81	149/151 (98%)	45 (30%)	0
4	A2	1718/1818 (94%)	607 (35%)	31 (1%)
79	q3	70/74 (94%)	40 (57%)	0
82	v3	17/18 (94%)	12 (70%)	0
83	33	74/75 (98%)	29 (39%)	2 (2%)
All	All	5736/6044 (94%)	1966 (34%)	86 (1%)

5 of 1966 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	51	4	G
1	51	7	C
1	51	8	U
1	51	14	C
1	51	18	C

5 of 86 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	A2	241	G
4	A2	870	A
4	A2	434	G
4	A2	688	U
4	A2	1253	A

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 308 ligands modelled in this entry, 307 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	$\#\|Z\| > 2$
88	BLS	51	5294	-	28,31,31	0.83	0	28,43,43	1.72	4 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
88	BLS	51	5294	-	-	9/21/38/38	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
88	51	5294	BLS	O5'-C1'-C2'	-5.95	109.92	113.13
88	51	5294	BLS	C4-N3-C2	3.74	120.13	116.34
88	51	5294	BLS	C10-C11-N12	-3.21	106.98	112.15
88	51	5294	BLS	N4-C4-N3	2.34	120.19	116.49

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	51	5294	BLS	C4'-C5'-C6'-O4
88	51	5294	BLS	C4'-C5'-C6'-O3
88	51	5294	BLS	C11-C10-C9-C8
88	51	5294	BLS	C11-C10-C9-N9
88	51	5294	BLS	O7-C7-C8-C9

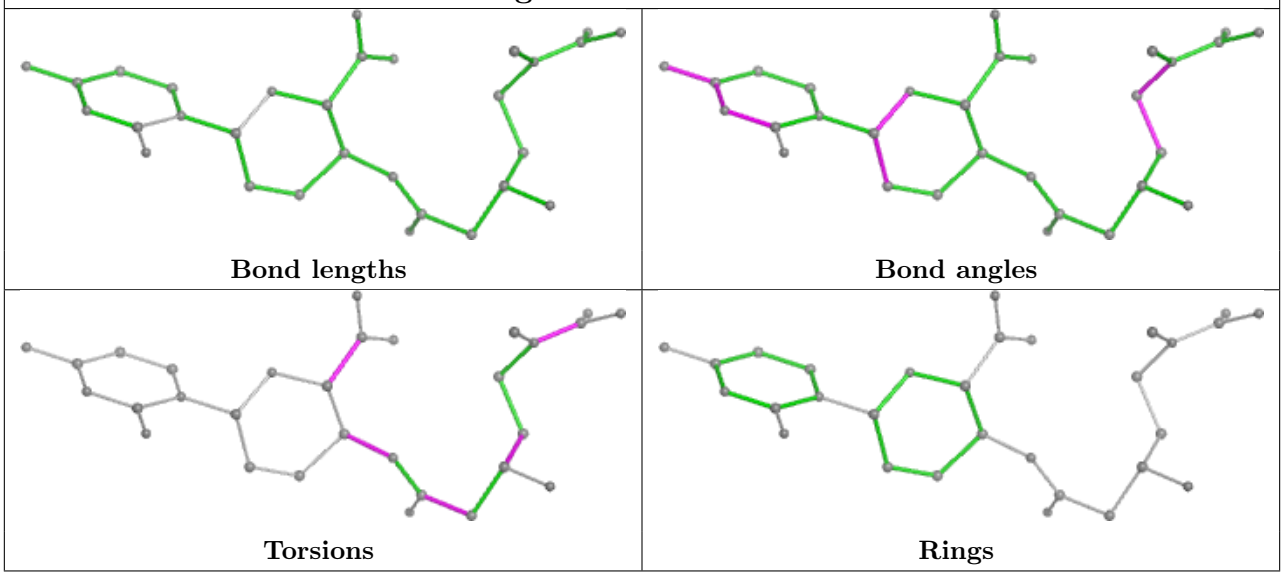
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand BLS 51 5294



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
4	A2	11
1	51	7
79	q3	3
3	81	1
44	G3	1

The worst 5 of 23 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	81	79:G	O3'	85:U	P	13.18

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A2	201:C	O3'	202:G	P	8.18
1	q3	15:G	O3'	18:G	P	7.28
1	A2	747:U	O3'	748:C	P	6.91
1	51	1232:G	O3'	1233:G	P	5.66

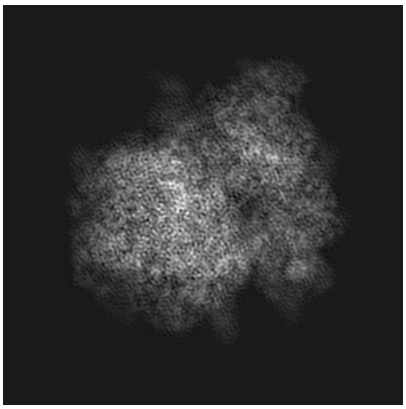
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12631. These allow visual inspection of the internal detail of the map and identification of artifacts.

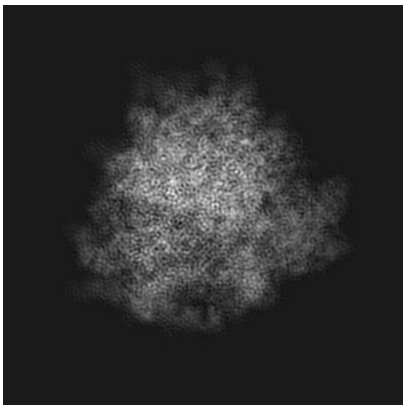
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

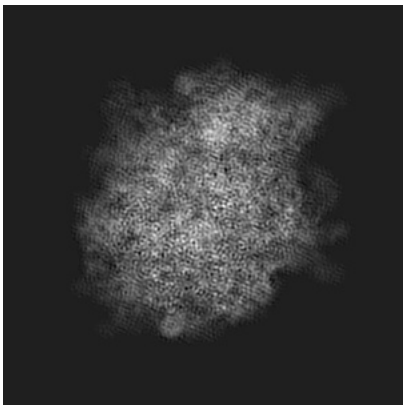
6.1.1 Primary map



X

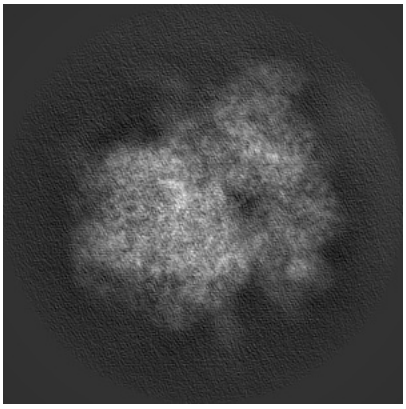


Y

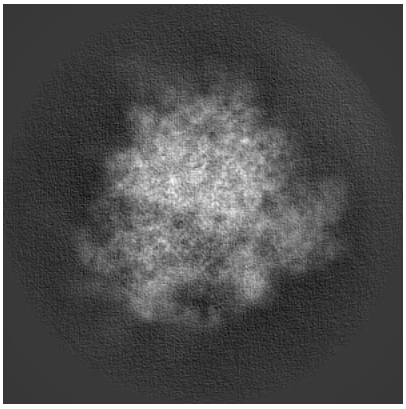


Z

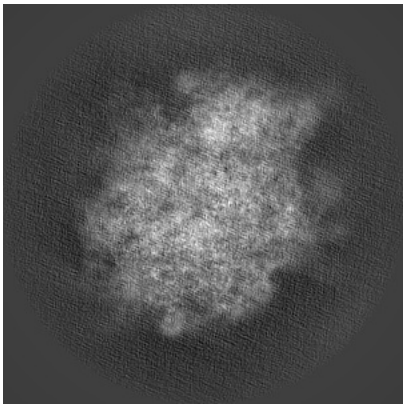
6.1.2 Raw map



X



Y

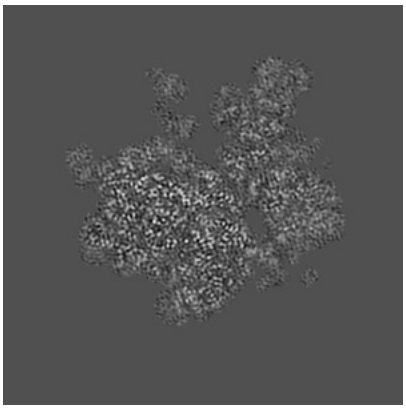


Z

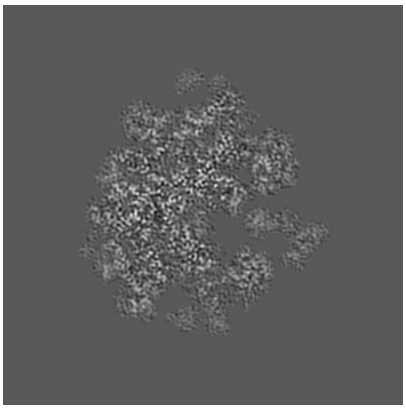
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

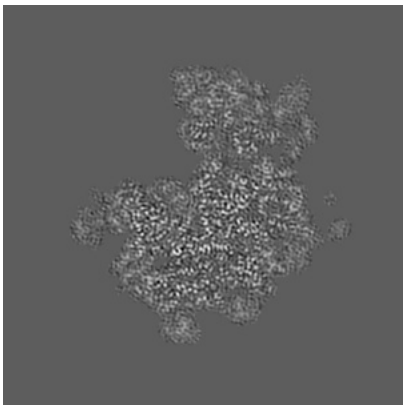
6.2.1 Primary map



X Index: 150

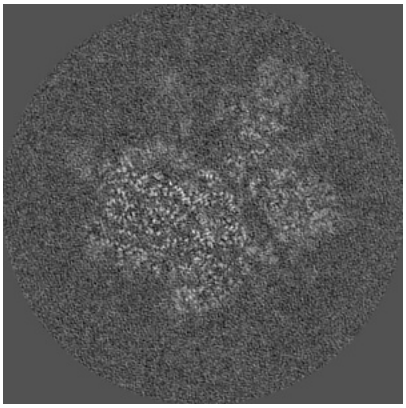


Y Index: 150

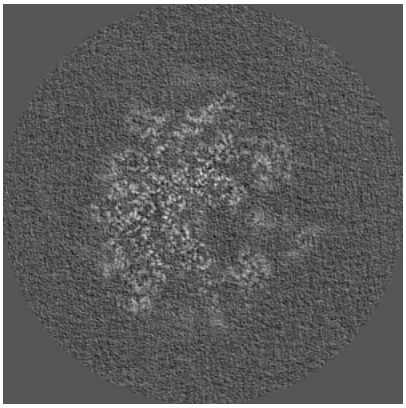


Z Index: 150

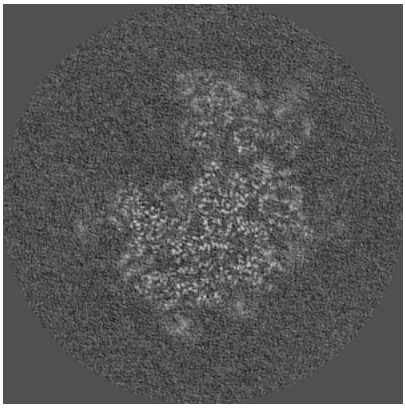
6.2.2 Raw map



X Index: 150



Y Index: 150

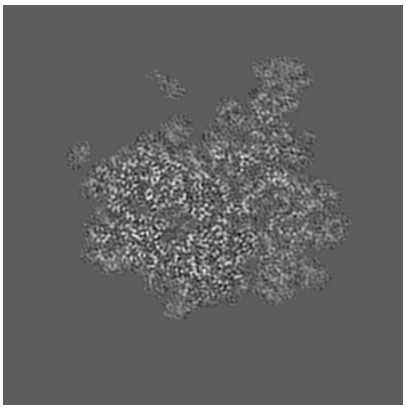


Z Index: 150

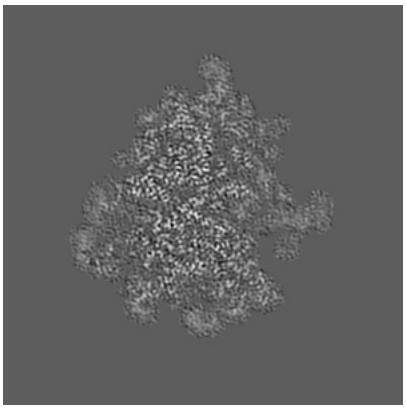
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

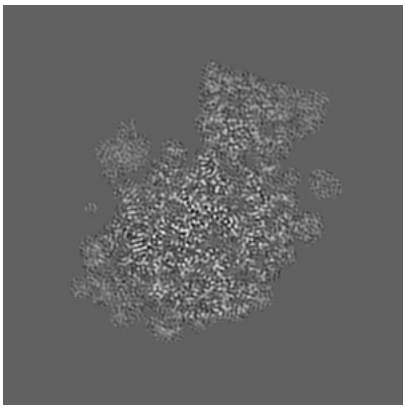
6.3.1 Primary map



X Index: 158

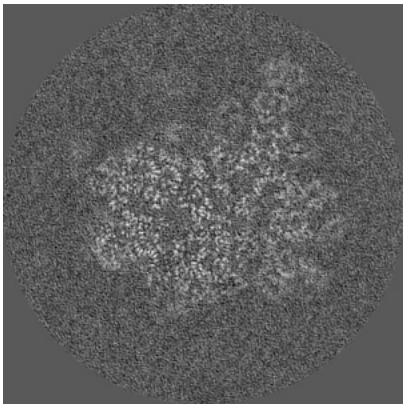


Y Index: 130

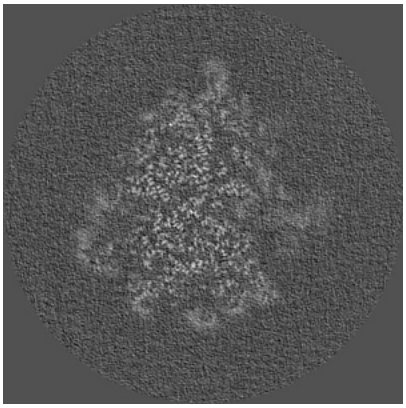


Z Index: 124

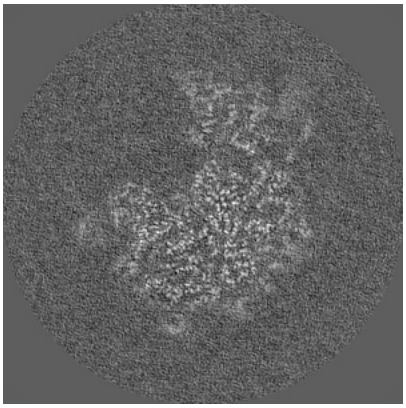
6.3.2 Raw map



X Index: 159



Y Index: 130

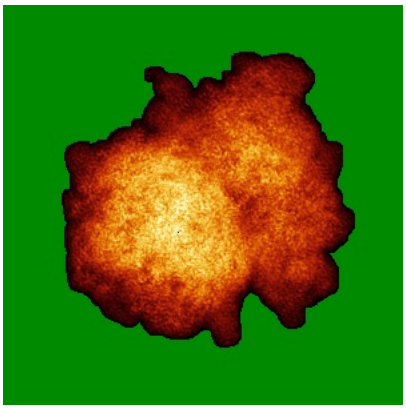


Z Index: 148

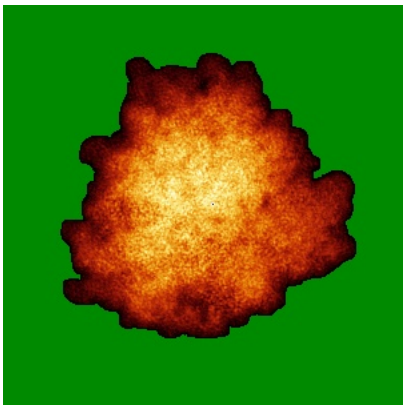
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

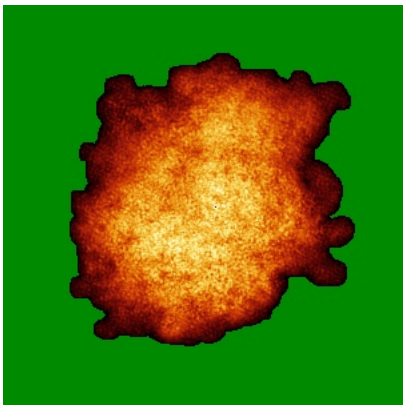
6.4.1 Primary map



X

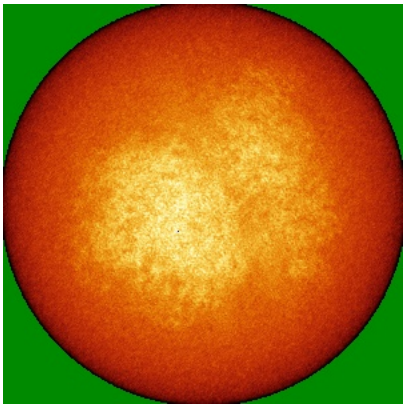


Y

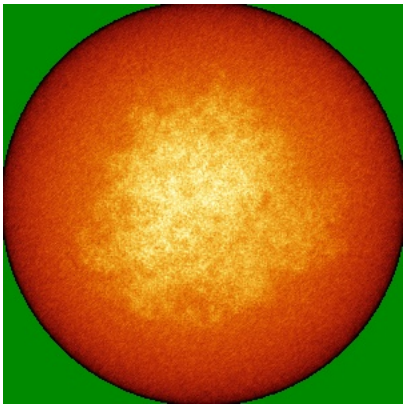


Z

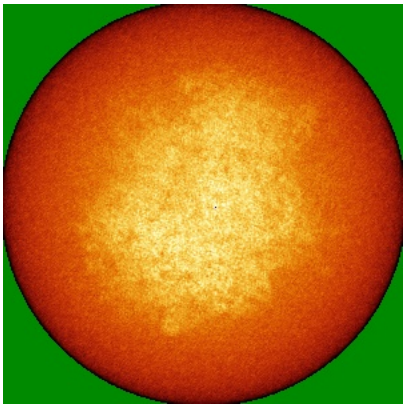
6.4.2 Raw map



X



Y

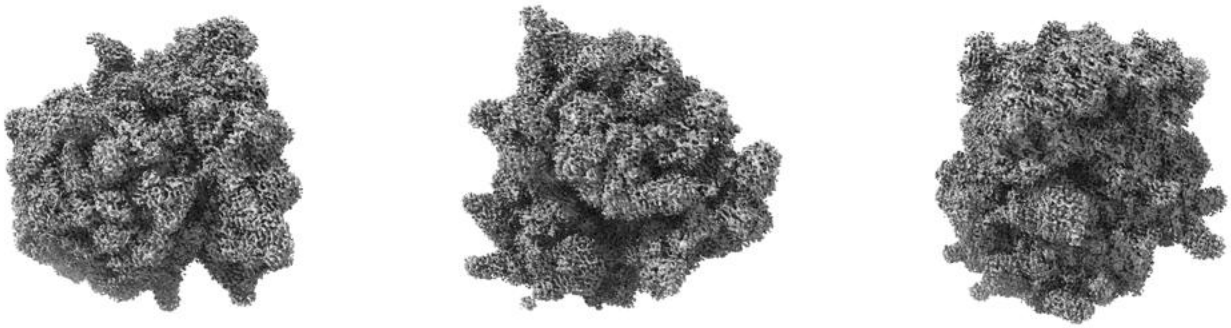


Z

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)

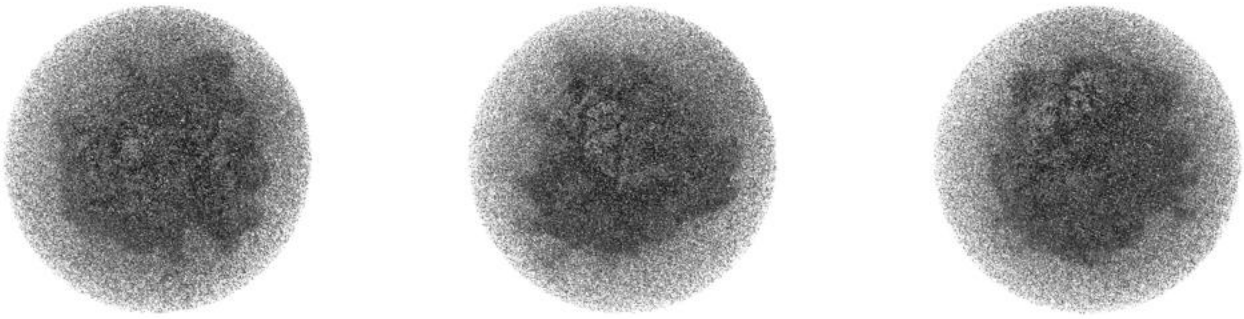
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

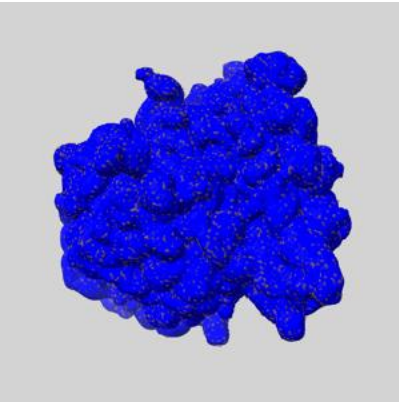
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

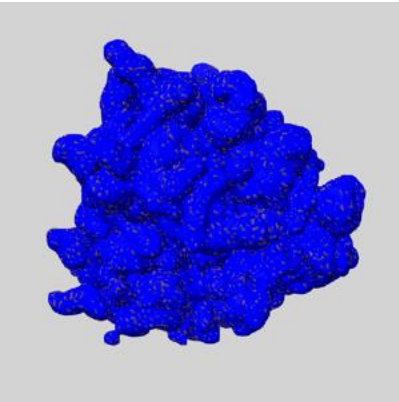
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

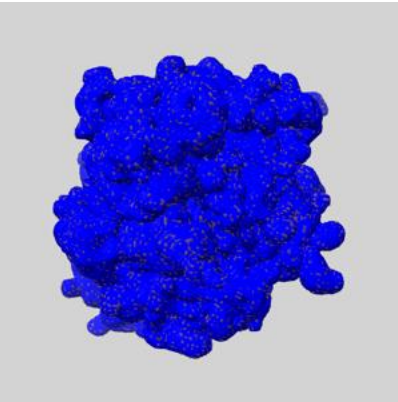
6.6.1 emd_12631_msk_1.map (i)



X



Y

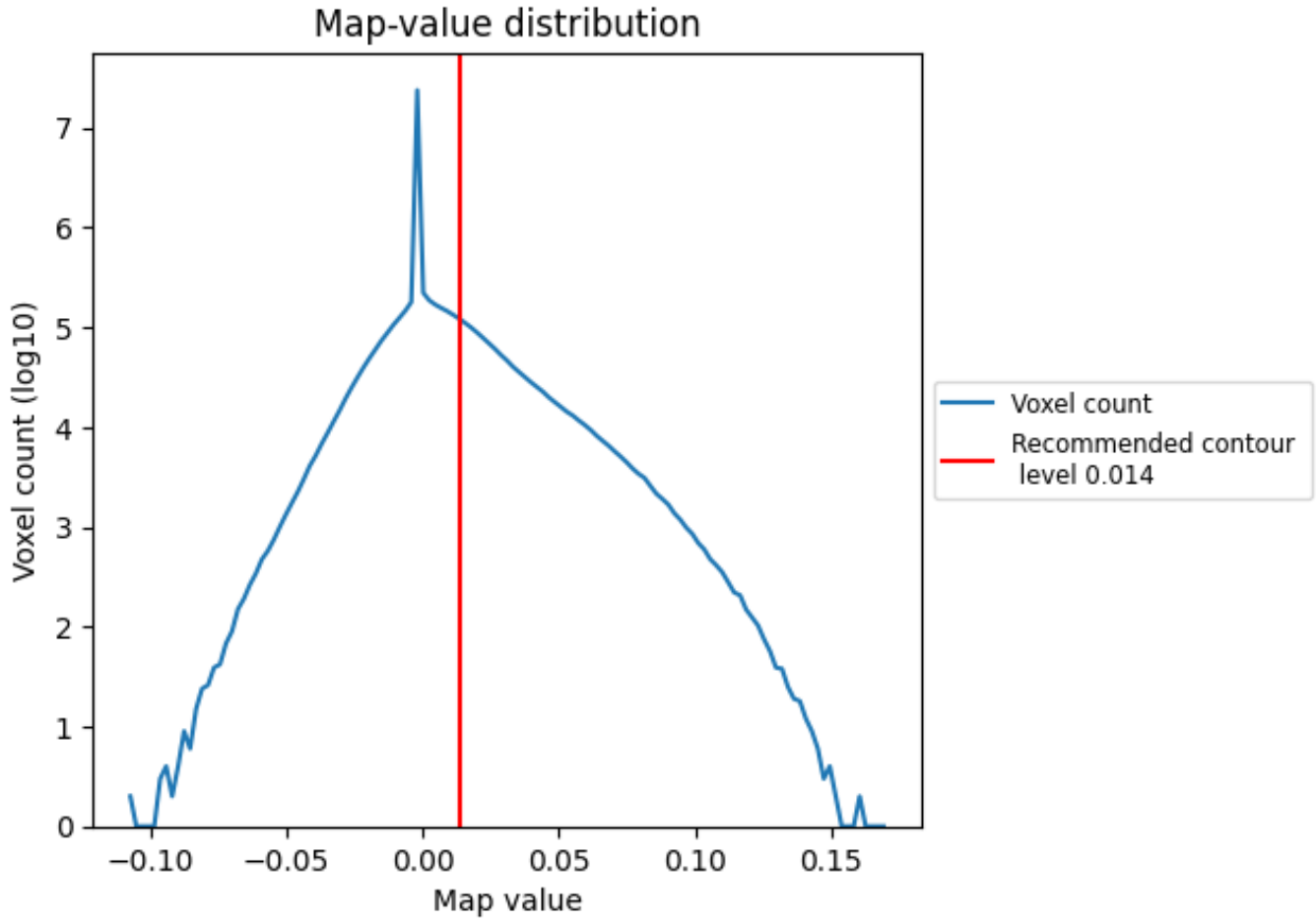


Z

7 Map analysis

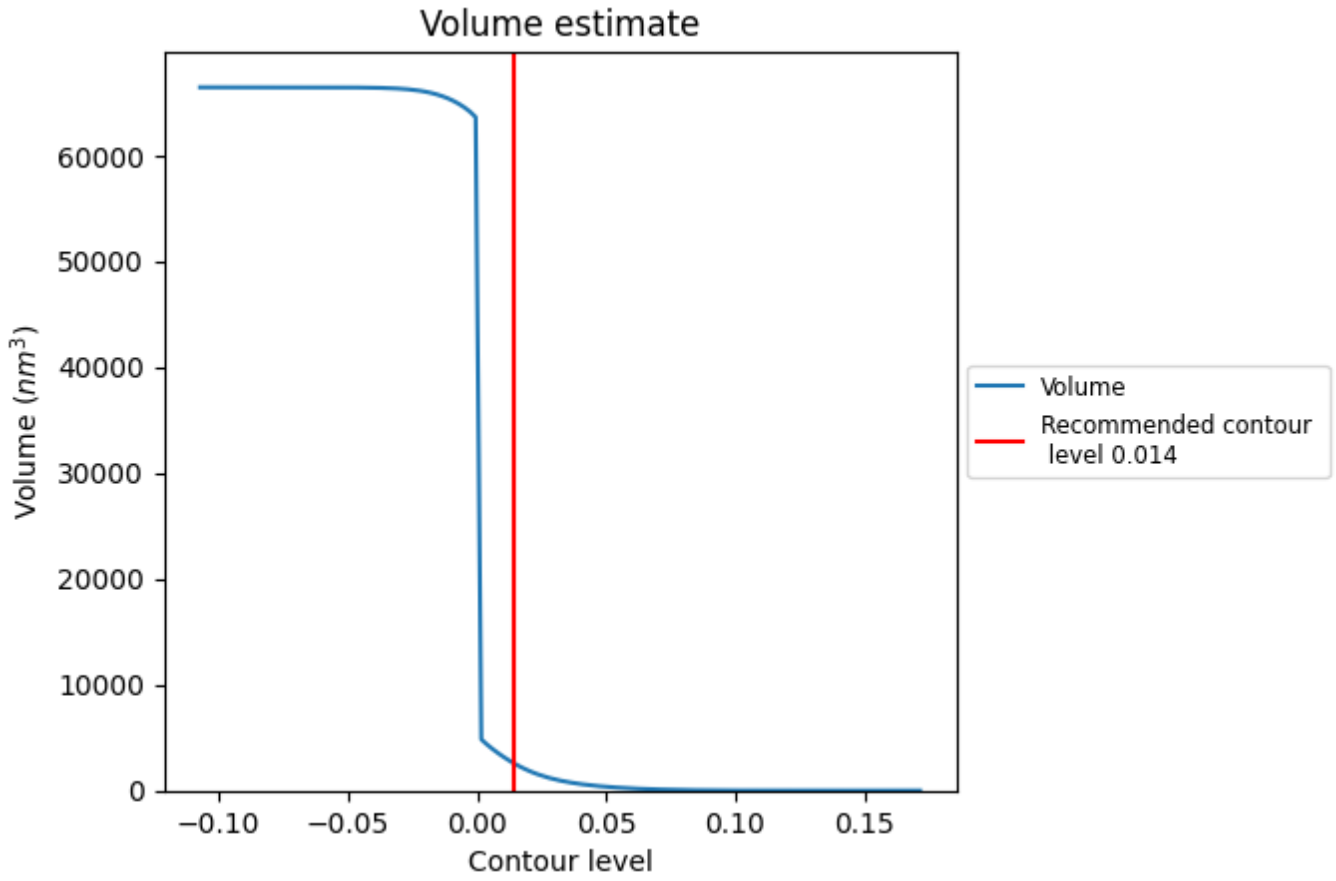
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

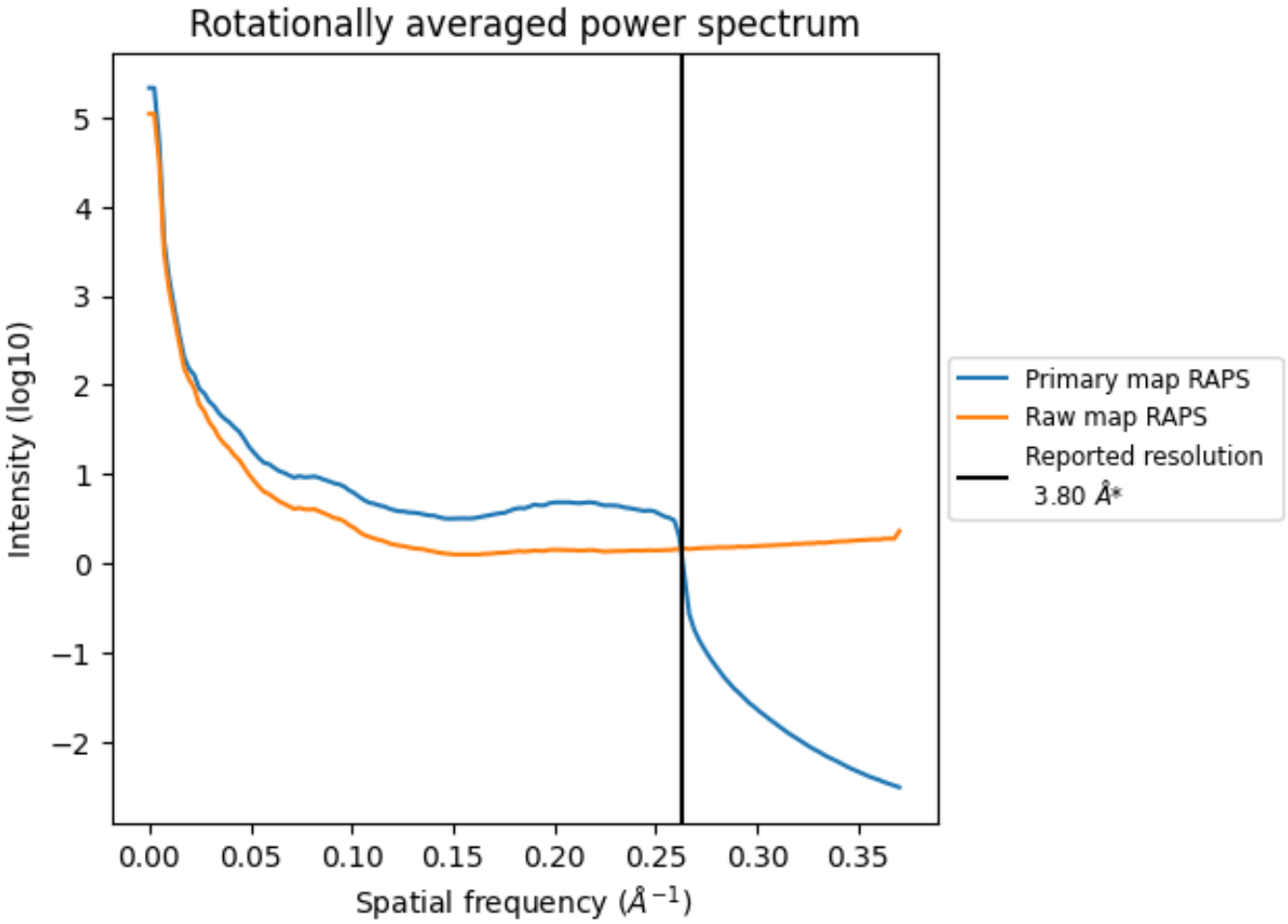
7.2 Volume estimate (i)



The volume at the recommended contour level is 2614 nm^3; this corresponds to an approximate mass of 2362 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)

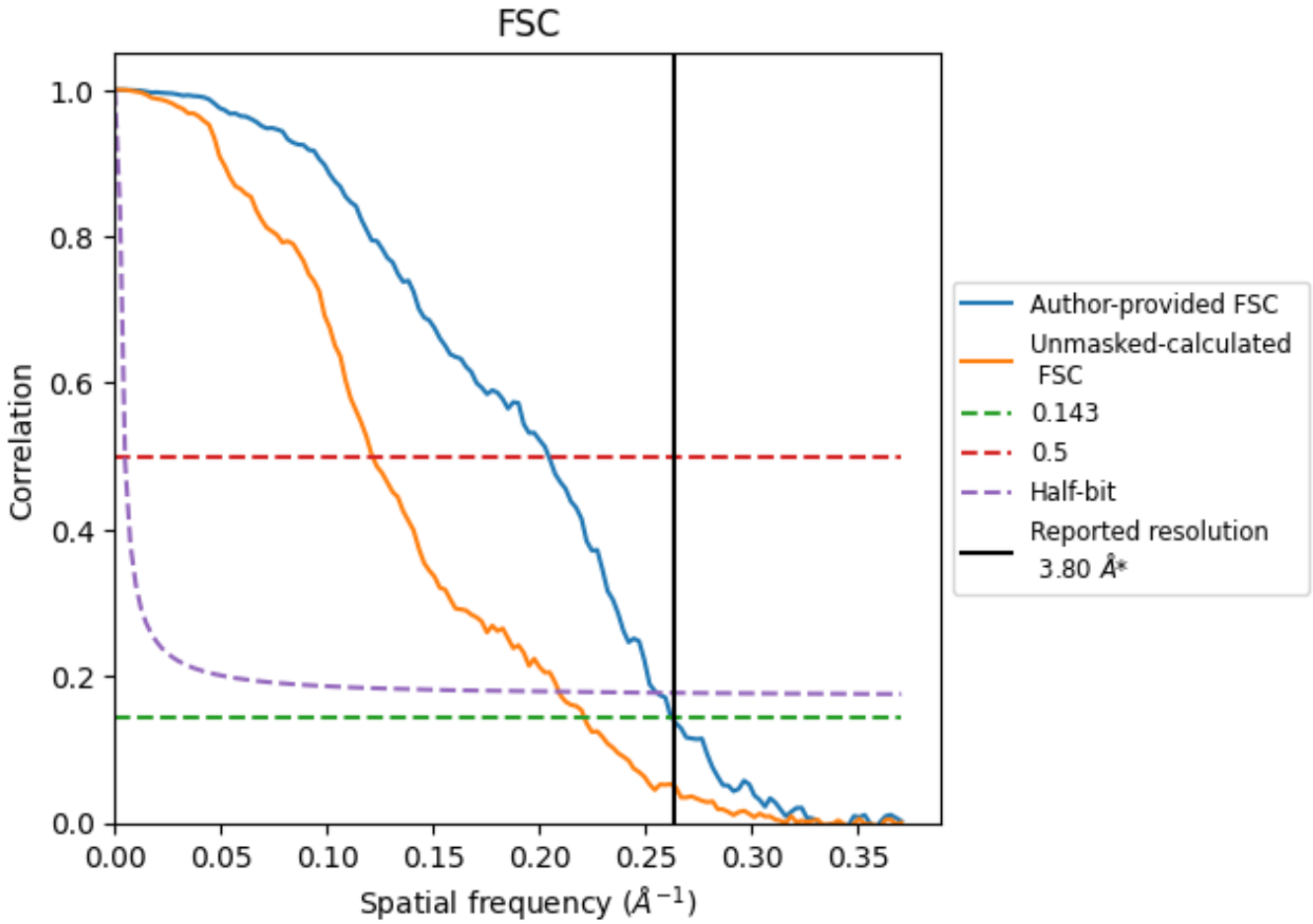


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8.2 Resolution estimates (i)

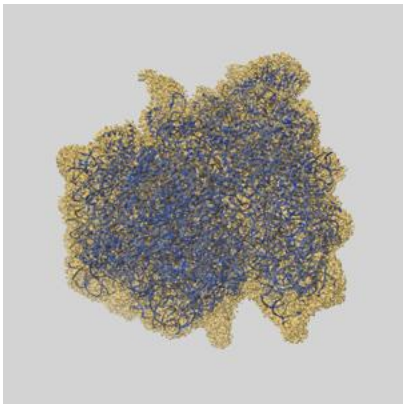
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.81	4.89	3.92
Unmasked-calculated*	4.52	8.24	4.78

*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 4.52 differs from the reported value 3.8 by more than 10 %

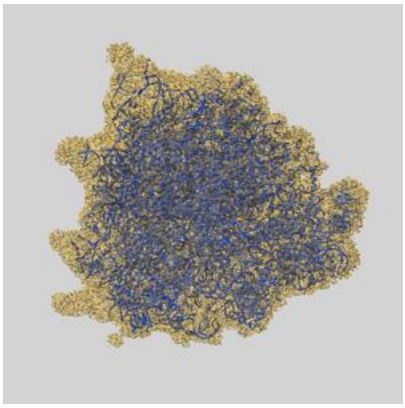
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12631 and PDB model 7NWG. Per-residue inclusion information can be found in section 3 on page 26.

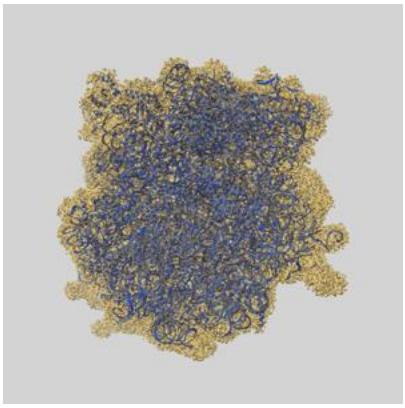
9.1 Map-model overlay



X



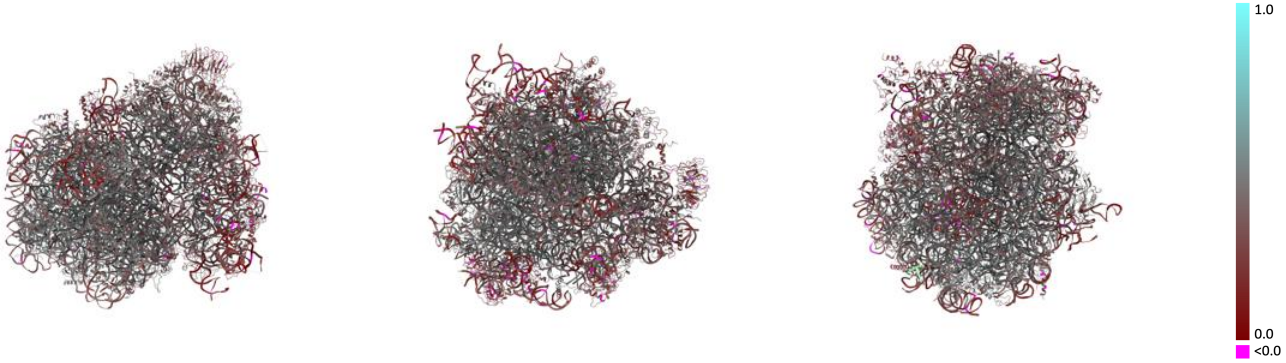
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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.

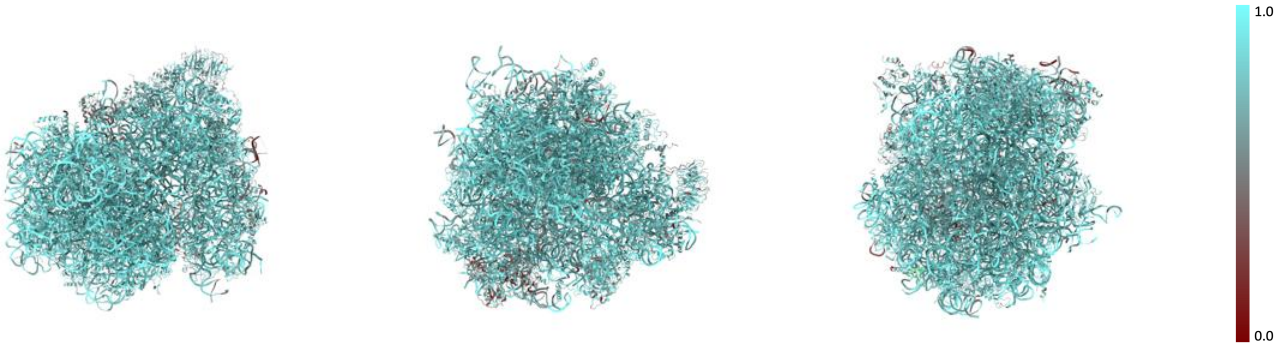
9.2 Q-score mapped to coordinate model (i)



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.

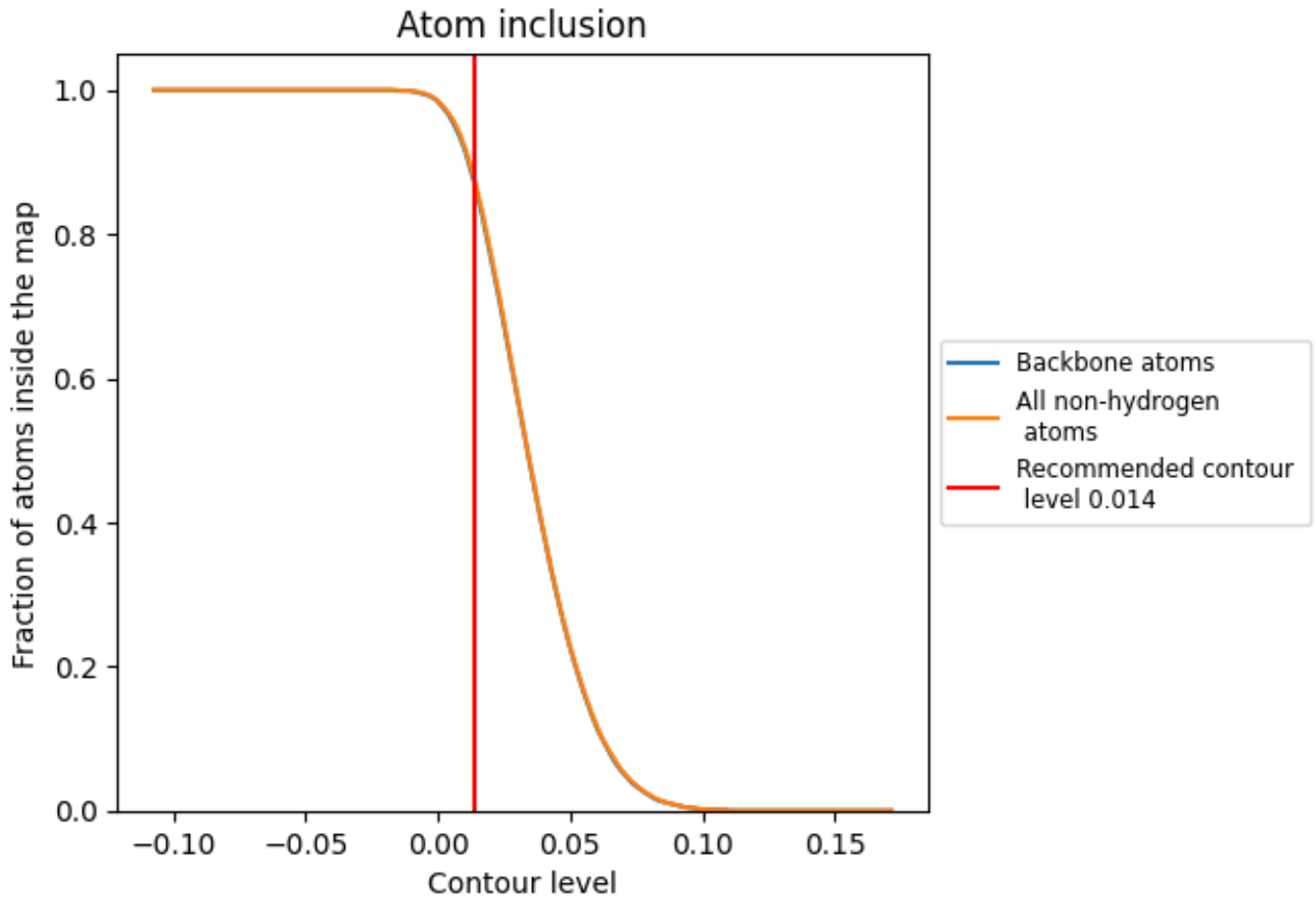
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.014).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8740	0.4060
1	0.6860	0.3610
33	0.9050	0.3580
51	0.9180	0.4110
71	0.9300	0.4220
81	0.9390	0.4300
A2	0.8970	0.3760
A3	0.8880	0.4770
B2	0.8090	0.3910
B3	0.8830	0.4690
C2	0.8350	0.4220
C3	0.8890	0.4760
D2	0.8340	0.4300
D3	0.8580	0.4190
E2	0.7640	0.3760
E3	0.8800	0.4330
F2	0.8190	0.3980
F3	0.8730	0.4680
G2	0.7980	0.3780
G3	0.7890	0.3830
H2	0.7680	0.3290
H3	0.8580	0.4320
I2	0.7690	0.3580
I3	0.8790	0.4660
J2	0.7960	0.3770
J3	0.8660	0.4220
K2	0.7720	0.3610
L2	0.8250	0.3680
L3	0.8660	0.4520
M2	0.8550	0.4460
M3	0.8580	0.4290
N2	0.6400	0.2720
N3	0.9090	0.4930
O2	0.8440	0.4200
O3	0.8830	0.4770

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Chain	Atom inclusion	Q-score
P2	0.8090	0.4110
P3	0.8920	0.4810
Q2	0.8740	0.4130
Q3	0.8970	0.4880
R2	0.7920	0.3860
R3	0.8420	0.4200
S2	0.7750	0.3610
S3	0.8920	0.4630
T2	0.8460	0.3890
T3	0.8810	0.4690
U2	0.8240	0.3670
U3	0.8390	0.3840
V2	0.7200	0.3400
V3	0.8770	0.4820
W	0.9020	0.4820
W2	0.8100	0.3940
X2	0.8550	0.4380
X3	0.8610	0.4430
Y2	0.8610	0.4590
Y3	0.8970	0.4750
Z2	0.8180	0.3680
Z3	0.8390	0.4200
a2	0.7580	0.3490
a3	0.9060	0.4900
b2	0.8600	0.4570
b3	0.8060	0.4070
c2	0.7900	0.4040
c3	0.8320	0.4270
d2	0.7530	0.3530
d3	0.8500	0.4450
e2	0.8930	0.4270
e3	0.8770	0.4870
f2	0.8070	0.3960
f3	0.8880	0.4840
g2	0.7260	0.2860
g3	0.8510	0.4460
h2	0.7100	0.2930
h3	0.8810	0.4460
i3	0.8590	0.4390
j3	0.9200	0.5020
k3	0.7900	0.3770
l3	0.9020	0.4820

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Chain	Atom inclusion	Q-score
m3	0.8970	0.4580
n3	0.8390	0.4600
o3	0.8910	0.4680
p3	0.8480	0.4630
q3	0.8730	0.3480
r3	0.8920	0.4740
t3	0.4090	0.2180
u3	0.4240	0.2080
v3	0.8320	0.4020
w3	0.4850	0.2100