wwPDB EM Validation Summary Report (i)

Apr 22, 2024 – 04:54 pm BST

PDB ID	:	7NHN
EMDB ID	:	EMD-12334
Title	:	VgaL, an antibiotic resistance ABCF, in complex with 70S ribosome from Listeria monocytogenes
Authors	:	Crowe-McAuliffe, C.; Turnbull, K.J.; Hauryliuk, V.; Wilson, D.N.
Deposited on	:	2021-02-10
Resolution	:	2.90 Å(reported)

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

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

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

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

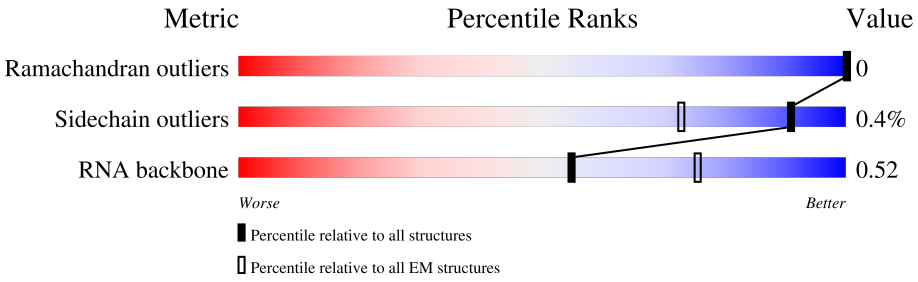
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	0	567	27% 81% · 19%
2	D	77	· 73% 22% · ·
3	b	14	36% 36% 21% 43%
4	A	2928	10% 74% 23% · ·
5	a	1542	19% 78% 19% ·
6	G	277	· 97% · ·
7	H	209	· 97% · ·
8	I	207	9% 98% ·

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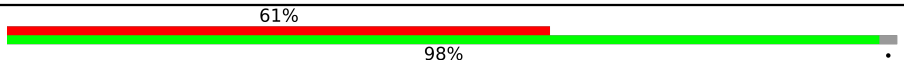
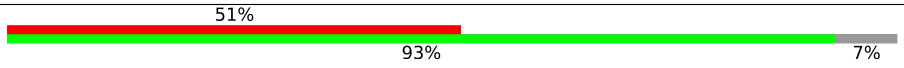
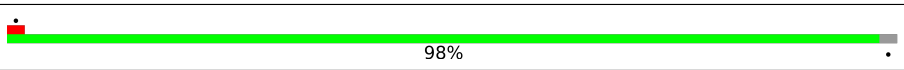
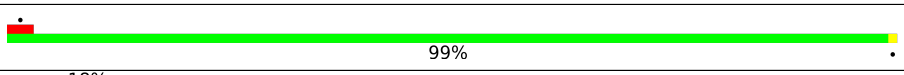
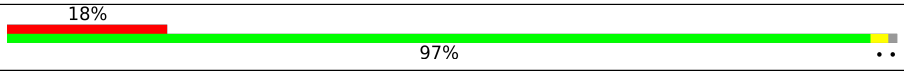
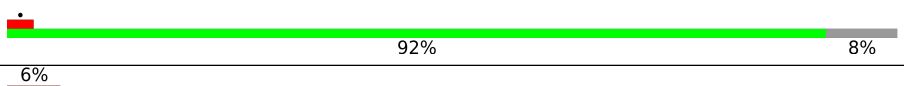
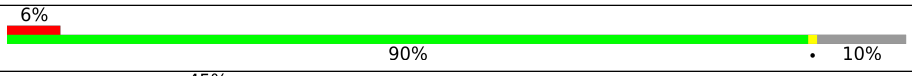
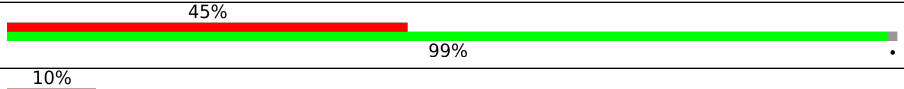
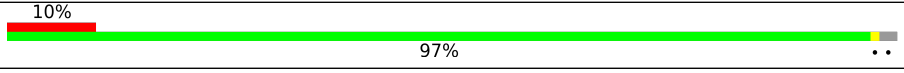
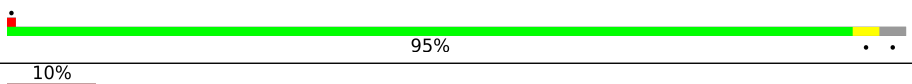
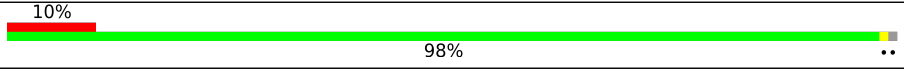
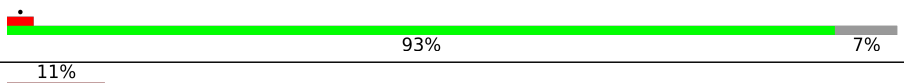
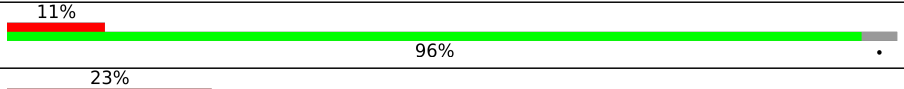
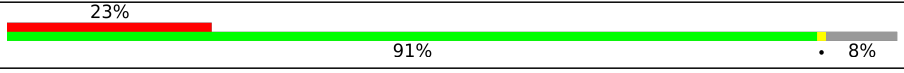
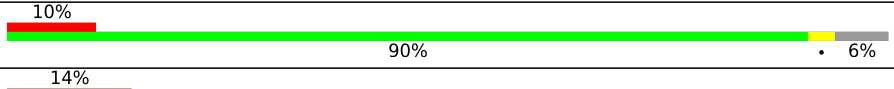
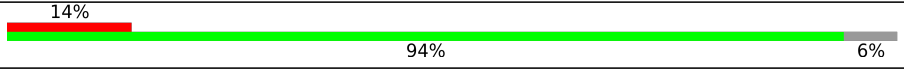
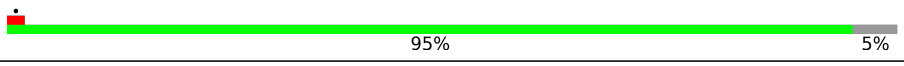
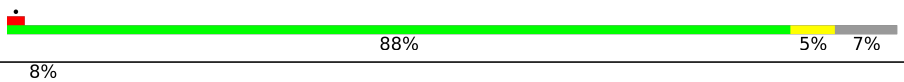
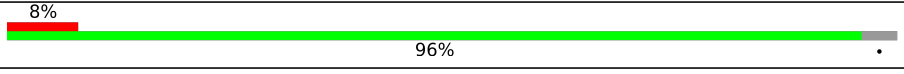
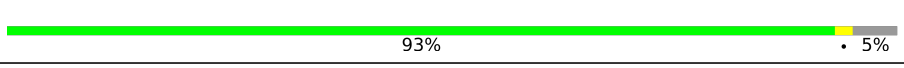
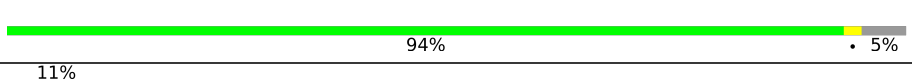
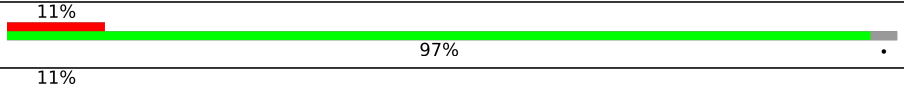
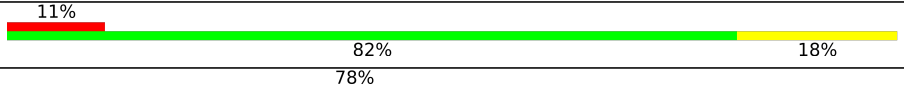
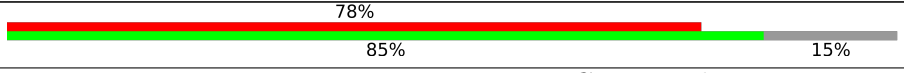
Mol	Chain	Length	Quality of chain
9	J	179	
10	K	178	
11	M	145	
12	N	122	
13	O	146	
14	P	144	
15	Q	135	
16	R	119	
17	S	114	
18	T	119	
19	U	102	
20	V	118	
21	W	94	
22	X	103	
23	Z	96	
24	1	62	
25	2	63	
26	3	59	
27	5	57	
28	6	49	
29	7	44	
30	8	66	
31	9	37	
32	B	114	
33	c	249	

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Mol	Chain	Length	Quality of chain
34	d	218	58% 93% 6%
35	e	200	80% 100%
36	f	167	40% 96%
37	g	97	92% 96%
38	h	156	63% 90% 10%
39	i	132	56% 98%
40	j	130	67% 95%
41	k	102	69% 94% 6%
42	l	129	75% 88% 12%
43	m	137	34% 96%
44	n	121	69% 93% 6%
45	o	61	21% 98%
46	p	89	54% 96%
47	q	90	52% 98%
48	r	87	64% 92% 8%
49	s	79	67% 78% 22%
50	t	92	57% 88% 12%
51	u	84	50% 94% 5%
52	4	81	84% 95%

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 144375 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Lmo0919 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	461	3647	2298	650	689	10	0	0

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	104	GLN	GLU	engineered mutation	UNP Q8Y8I3
0	408	GLN	GLU	engineered mutation	UNP Q8Y8I3
0	524	GLY	-	expression tag	UNP Q8Y8I3
0	525	GLY	-	expression tag	UNP Q8Y8I3
0	526	HIS	-	expression tag	UNP Q8Y8I3
0	527	HIS	-	expression tag	UNP Q8Y8I3
0	528	HIS	-	expression tag	UNP Q8Y8I3
0	529	HIS	-	expression tag	UNP Q8Y8I3
0	530	HIS	-	expression tag	UNP Q8Y8I3
0	531	HIS	-	expression tag	UNP Q8Y8I3
0	532	ALA	-	expression tag	UNP Q8Y8I3
0	533	LYS	-	expression tag	UNP Q8Y8I3
0	534	GLY	-	expression tag	UNP Q8Y8I3
0	535	GLY	-	expression tag	UNP Q8Y8I3
0	536	GLU	-	expression tag	UNP Q8Y8I3
0	537	ASN	-	expression tag	UNP Q8Y8I3
0	538	LEU	-	expression tag	UNP Q8Y8I3
0	539	TYR	-	expression tag	UNP Q8Y8I3
0	540	PHE	-	expression tag	UNP Q8Y8I3
0	541	GLN	-	expression tag	UNP Q8Y8I3
0	542	GLY	-	expression tag	UNP Q8Y8I3
0	543	VAL	-	expression tag	UNP Q8Y8I3
0	544	ALA	-	expression tag	UNP Q8Y8I3
0	545	ASP	-	expression tag	UNP Q8Y8I3
0	546	TYR	-	expression tag	UNP Q8Y8I3
0	547	LYS	-	expression tag	UNP Q8Y8I3
0	548	ASP	-	expression tag	UNP Q8Y8I3
0	549	HIS	-	expression tag	UNP Q8Y8I3

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Chain	Residue	Modelled	Actual	Comment	Reference
0	550	ASP	-	expression tag	UNP Q8Y8I3
0	551	GLY	-	expression tag	UNP Q8Y8I3
0	552	ASP	-	expression tag	UNP Q8Y8I3
0	553	TYR	-	expression tag	UNP Q8Y8I3
0	554	LYS	-	expression tag	UNP Q8Y8I3
0	555	ASP	-	expression tag	UNP Q8Y8I3
0	556	HIS	-	expression tag	UNP Q8Y8I3
0	557	ASP	-	expression tag	UNP Q8Y8I3
0	558	ILE	-	expression tag	UNP Q8Y8I3
0	559	ASP	-	expression tag	UNP Q8Y8I3
0	560	TYR	-	expression tag	UNP Q8Y8I3
0	561	LYS	-	expression tag	UNP Q8Y8I3
0	562	ASP	-	expression tag	UNP Q8Y8I3
0	563	ASP	-	expression tag	UNP Q8Y8I3
0	564	ASP	-	expression tag	UNP Q8Y8I3
0	565	ASP	-	expression tag	UNP Q8Y8I3
0	566	LYS	-	expression tag	UNP Q8Y8I3
0	567	GLY	-	expression tag	UNP Q8Y8I3

- Molecule 2 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	74	Total	C	N	O	P	0	0
			1580	704	284	518	74		

- Molecule 3 is a RNA chain called RNA (5'-R(P*GP*AP*GP*GP*UP*NP*NP*NP*NP*NP *NP*AP*UP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	8	Total	C	N	O	P	0	0
			176	78	34	56	8		

- Molecule 4 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	2908	Total	C	N	O	P	0	0
			62459	27874	11545	20132	2908		

- Molecule 5 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	1513	Total	C	N	O	P	0	0
			32445	14473	5939	10520	1513		

- Molecule 6 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	273	Total	C	N	O	S	0	0
			2108	1307	415	379	7		

- Molecule 7 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	206	Total	C	N	O	S	0	0
			1582	995	291	292	4		

- Molecule 8 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	I	203	Total	C	N	O	0	0
			1563	987	286	290		

- Molecule 9 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	175	Total	C	N	O	S	0	0
			1365	865	236	258	6		

- Molecule 10 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	165	Total	C	N	O	S	0	0
			1271	801	232	237	1		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	142	Total	C	N	O	S	0	0
			1117	708	201	205	3		

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	122	Total 925	C 573	N 175	O 172	S 5	0	0

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	O	144	Total 1094	C 675	N 214	O 205	0	0

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	133	Total 1055	C 675	N 205	O 170	S 5	0	0

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	122	Total 983	C 619	N 191	O 172	S 1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	R	118	Total 914	C 564	N 176	O 174	0	0

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	S	112	Total 905	C 570	N 181	O 154	0	0

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	116	Total 939	C 596	N 185	O 154	S 4	0	0

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	101	Total	C	N	O	S	0	0
			786	507	134	144	1		

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	V	110	Total	C	N	O	0	0
			848	534	160	154		

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	90	Total	C	N	O	S	0	0
			731	462	129	138	2		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	95	Total	C	N	O	S	0	0
			723	459	134	127	3		

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	73	Total	C	N	O	S	0	0
			563	345	111	106	1		

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1	58	Total	C	N	O	S	0	0
			457	283	96	76	2		

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	2	59	Total	C	N	O	S	0	0
			487	298	94	94	1		

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	3	56	Total	C	N	O	S	0	0
			433	272	82	78	1		

- Molecule 27 is a protein called 50S ribosomal protein L32-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	53	Total	C	N	O	S	0	0
			425	259	87	74	5		

- Molecule 28 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	47	Total	C	N	O	S	0	0
			400	243	81	73	3		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7	42	Total	C	N	O	S	0	0
			357	217	87	52	1		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	8	63	Total	C	N	O	S	0	0
			512	317	113	78	4		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	9	36	Total	C	N	O	S	0	0
			292	183	59	44	6		

- Molecule 32 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B	114	Total	C	N	O	P	0	0
			2428	1082	428	804	114		

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	212	Total	C	N	O	S	0	0
			1720	1096	306	312	6		

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	204	Total	C	N	O	S	0	0
			1624	1013	311	297	3		

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	199	Total	C	N	O	S	0	0
			1596	999	302	293	2		

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	161	Total	C	N	O	S	0	0
			1180	738	217	223	2		

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	93	Total	C	N	O	S	0	0
			782	495	136	149	2		

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	141	Total	C	N	O	S	0	0
			1114	695	209	202	8		

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	130	Total	C	N	O	S	0	0
			1015	646	179	188	2		

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	126	Total	C	N	O	S	0	0
			985	618	194	172	1		

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	96	Total	C	N	O	S	0	0
			771	485	141	143	2		

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	114	Total	C	N	O	S	0	0
			837	516	161	157	3		

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	134	Total	C	N	O	S	0	0
			1040	645	209	184	2		

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	114	Total	C	N	O	S	0	0
			906	557	180	168	1		

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	60	Total	C	N	O	S	0	0
			490	313	97	75	5		

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	86	Total	C	N	O	S	0	0
			722	448	145	127	2		

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	88	Total	C	N	O	S	0	0
			711	451	132	126	2		

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	80	Total	C	N	O	S	0	0
			656	413	123	119	1		

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	62	Total	C	N	O	S	0	0
			504	325	92	85	2		

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	81	Total	C	N	O	S	0	0
			655	418	120	115	2		

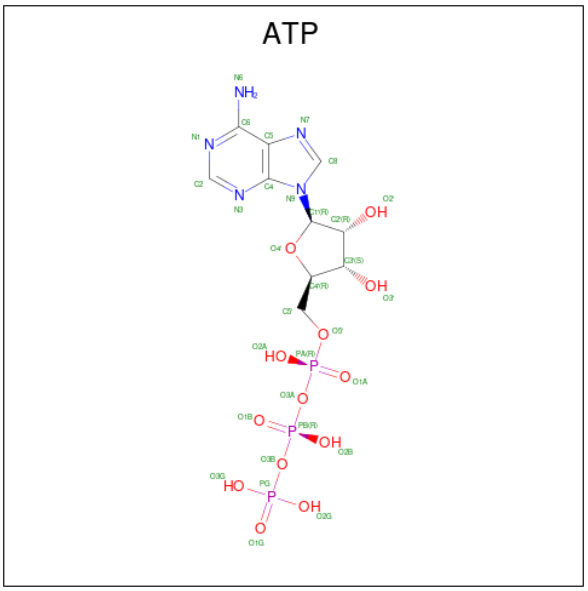
- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	80	Total	C	N	O	S	0	0
			611	369	125	116	1		

- Molecule 52 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	4	79	Total	C	N	O	S	0	0
			637	403	109	124	1		

- Molecule 53 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

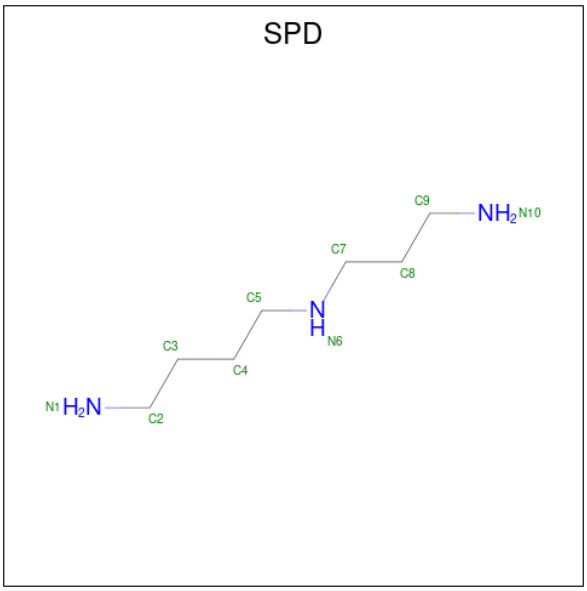


Mol	Chain	Residues	Atoms					AltConf
53	0	1	Total 31	C 10	N 5	O 13	P 3	0
53	0	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	0	2	Total 2	Mg 2	0
54	D	1	Total 1	Mg 1	0
54	b	1	Total 1	Mg 1	0
54	A	114	Total 114	Mg 114	0
54	a	21	Total 21	Mg 21	0
54	G	1	Total 1	Mg 1	0
54	H	1	Total 1	Mg 1	0
54	O	1	Total 1	Mg 1	0
54	o	1	Total 1	Mg 1	0

- Molecule 55 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms	AltConf
55	A	1	Total C N 10 7 3	0
55	a	1	Total C N 10 7 3	0

- Molecule 56 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
56	A	17	Total K 17 17	0
56	a	3	Total K 3 3	0
56	P	1	Total K 1 1	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

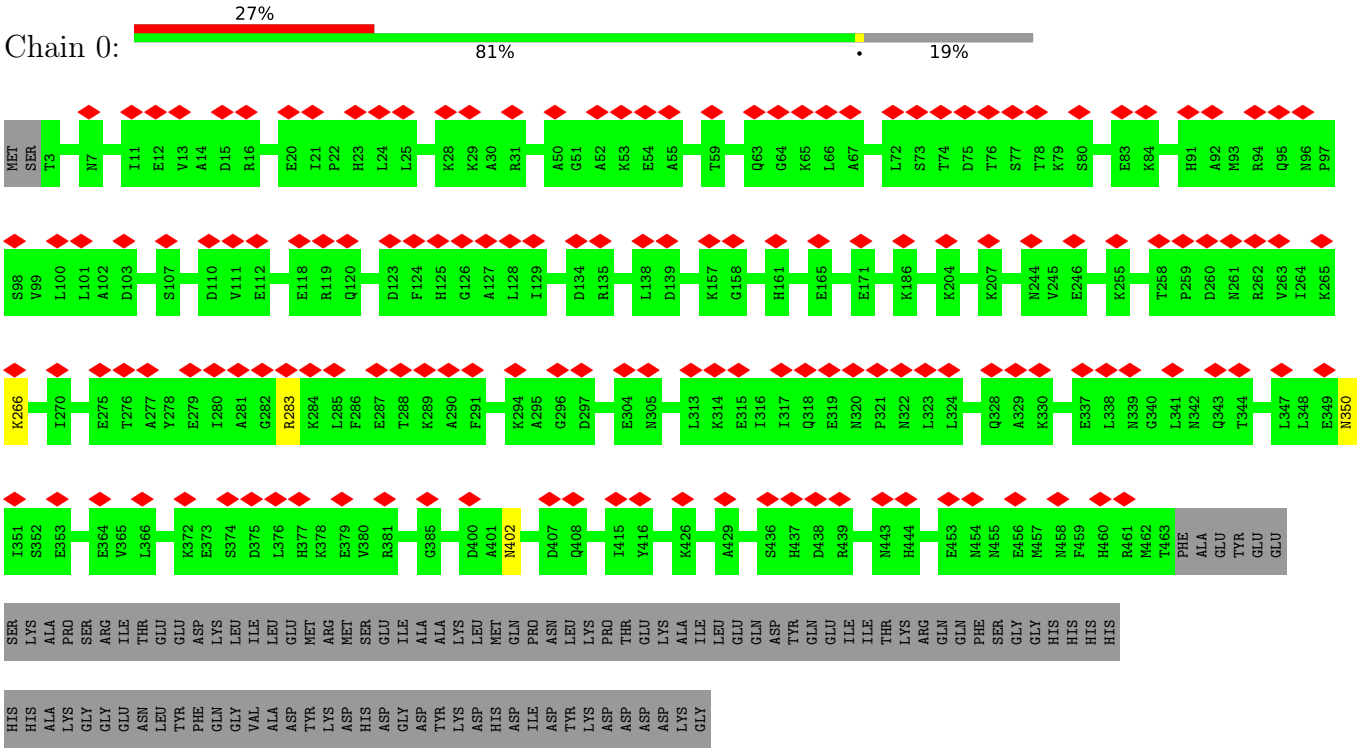
Mol	Chain	Residues	Atoms	AltConf
57	5	1	Total Zn 1 1	0
57	9	1	Total Zn 1 1	0
57	o	1	Total Zn 1 1	0

3 Residue-property plots (i)

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

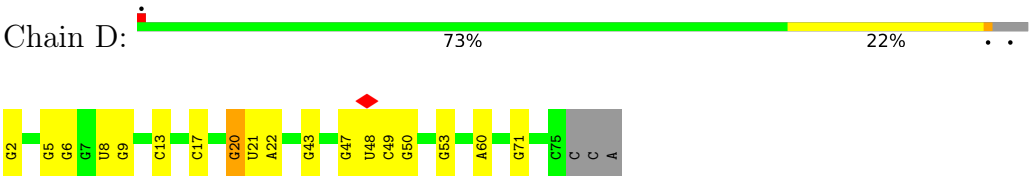
• Molecule 1: Lmo0919 protein

Chain 0:



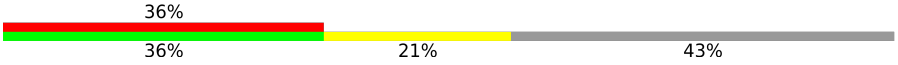
• Molecule 2: tRNA-fMet

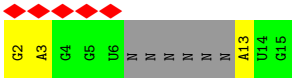
Chain D:



• Molecule 3: RNA (5'-R(P*GP*AP*GP*GP*UP*NP*NP*NP*NP*NP*NP*AP*UP*G)-3')

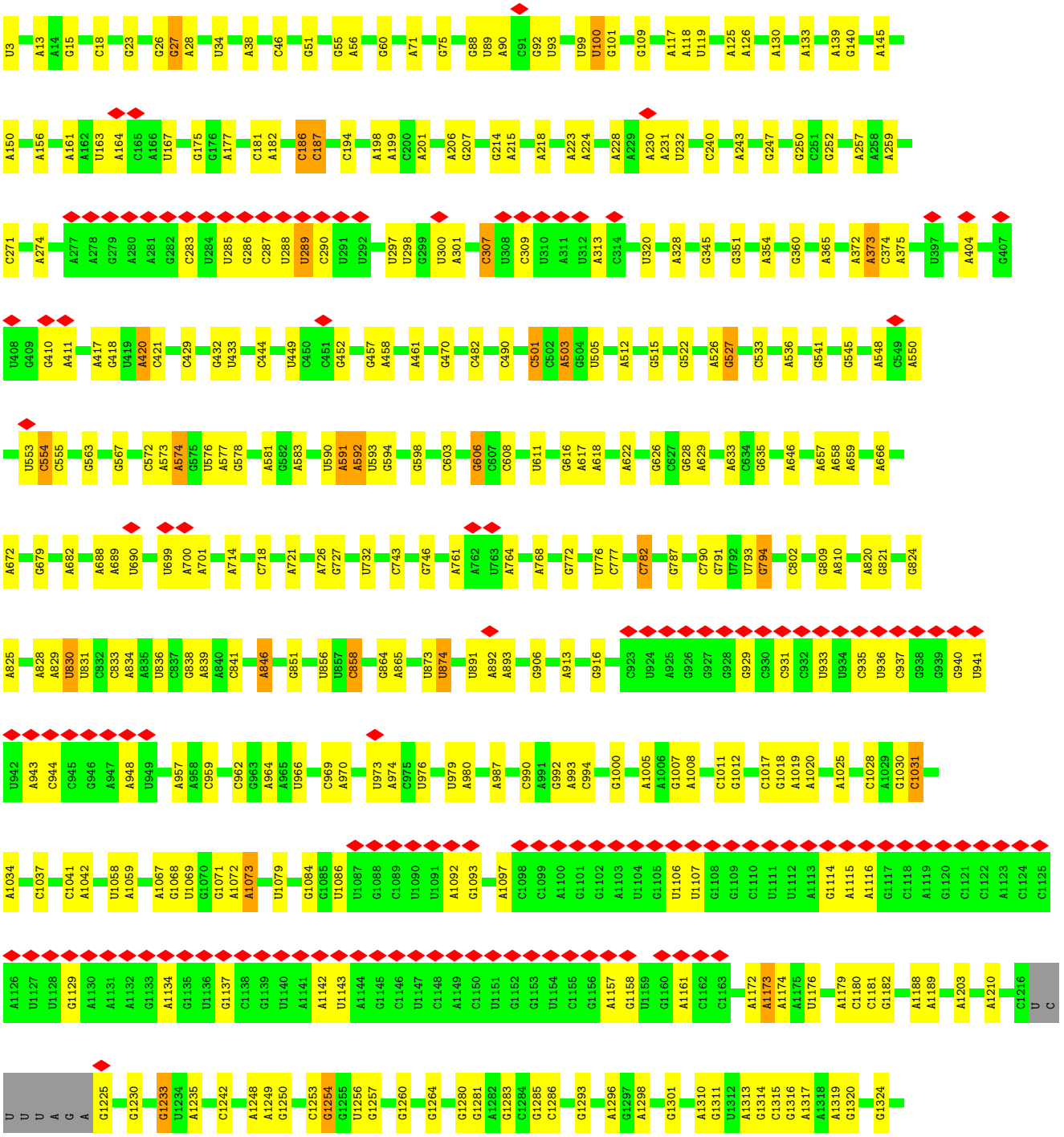
Chain b:

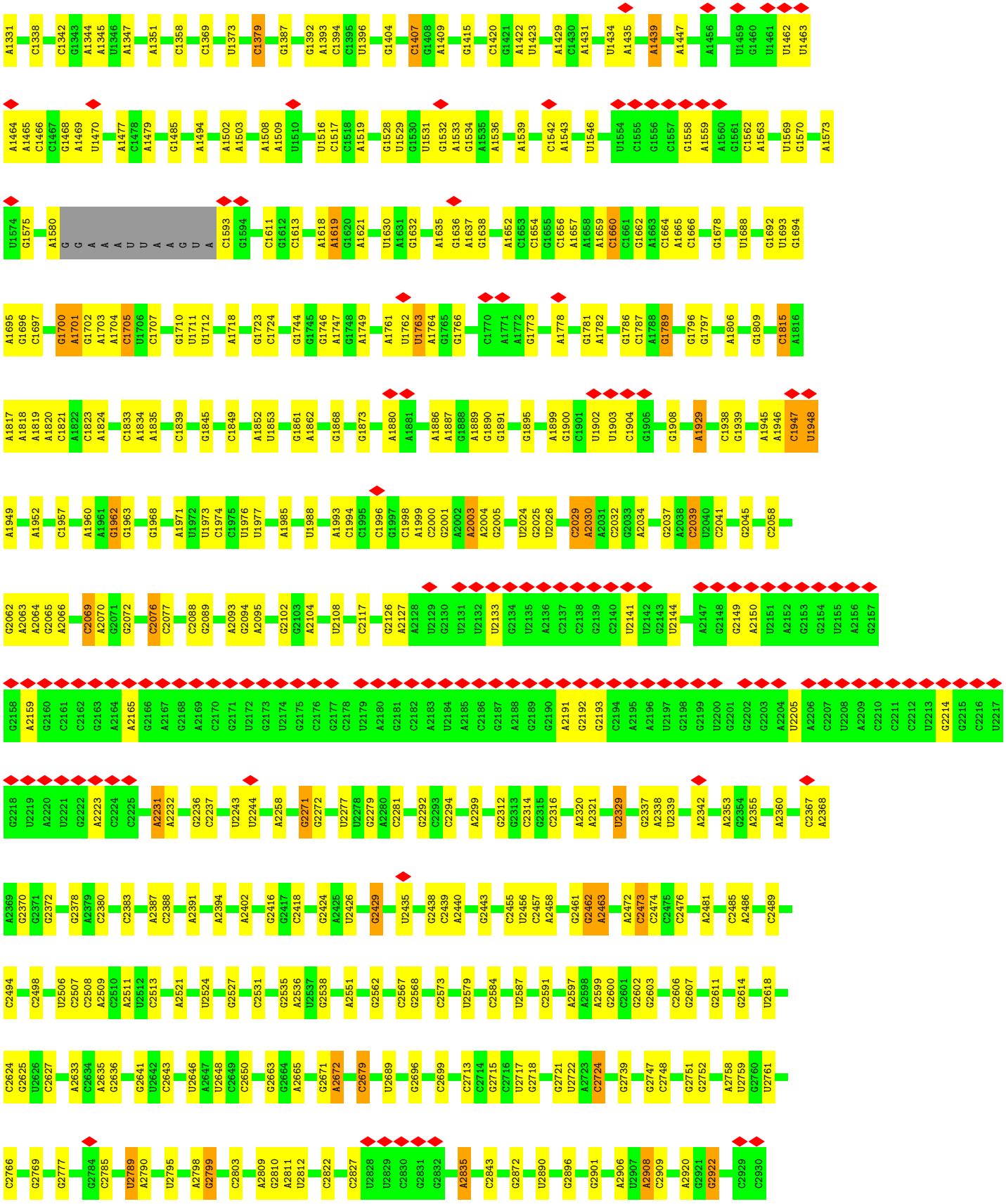




• Molecule 4: 23S rRNA

Chain A:



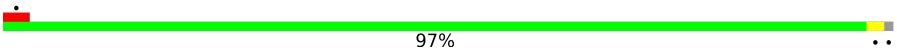


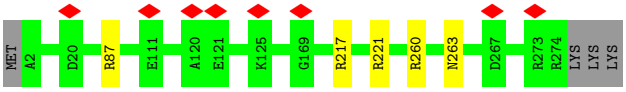
• Molecule 5: 16S rRNA

Chain a:

• Molecule 6: 50S ribosomal protein L2

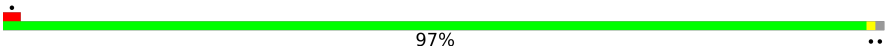
Chain G:

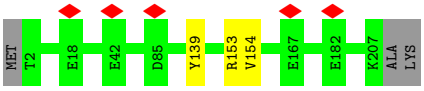




• Molecule 7: 50S ribosomal protein L3

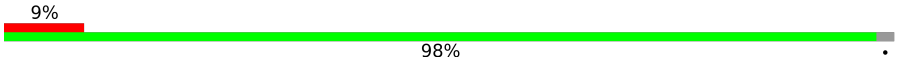
Chain H:

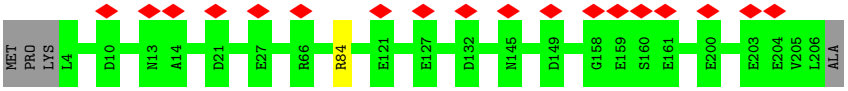




• Molecule 8: 50S ribosomal protein L4

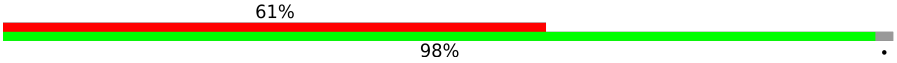
Chain I:

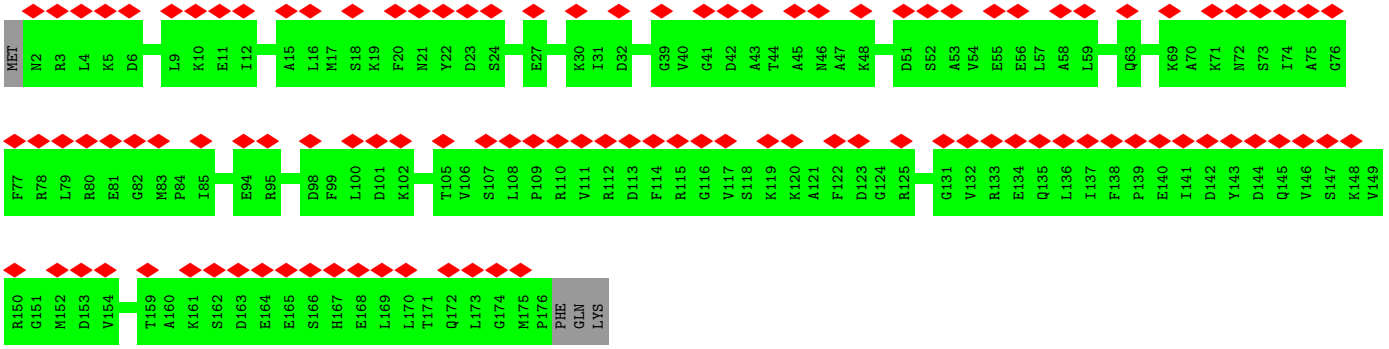




• Molecule 9: 50S ribosomal protein L5

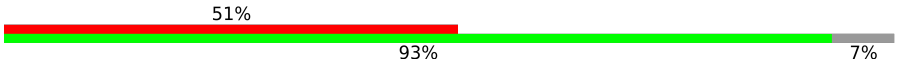
Chain J:

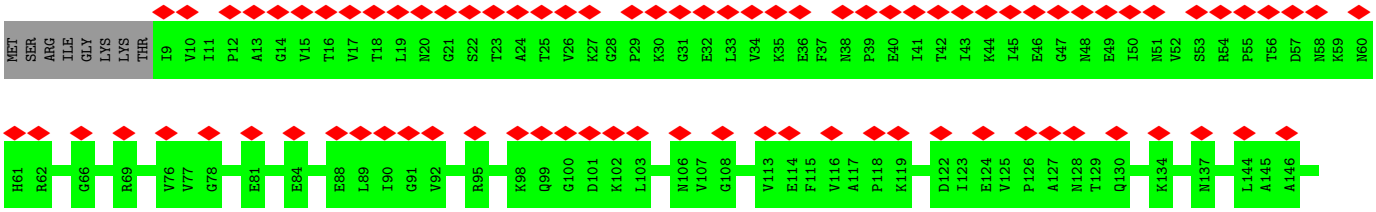


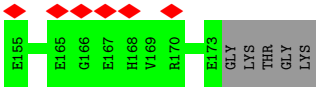


• Molecule 10: 50S ribosomal protein L6

Chain K:

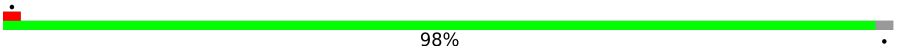


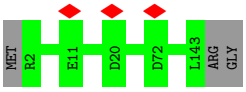




• Molecule 11: 50S ribosomal protein L13

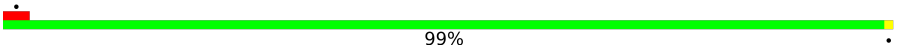
Chain M:

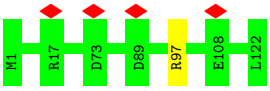




• Molecule 12: 50S ribosomal protein L14

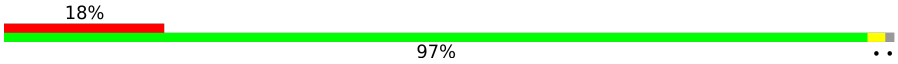
Chain N:

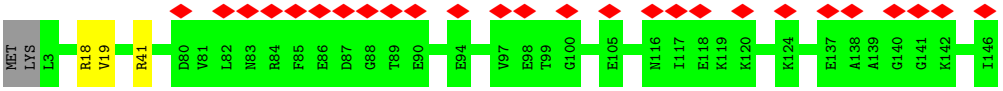




• Molecule 13: 50S ribosomal protein L15

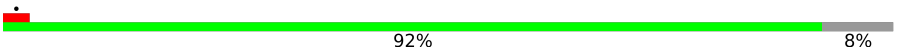
Chain O:

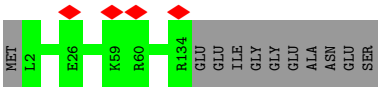




• Molecule 14: 50S ribosomal protein L16

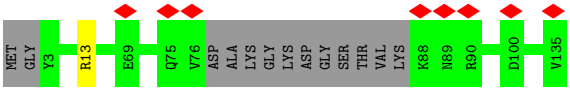
Chain P:





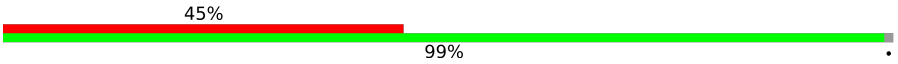
• Molecule 15: 50S ribosomal protein L17

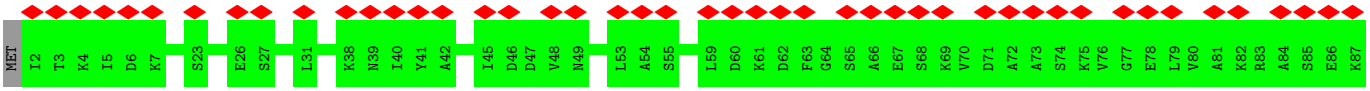
Chain Q:

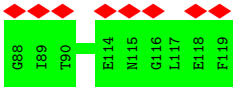


• Molecule 16: 50S ribosomal protein L18

Chain R:

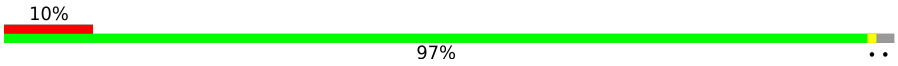


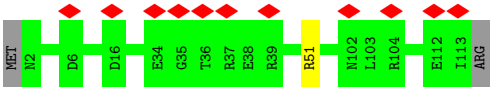




• Molecule 17: 50S ribosomal protein L19

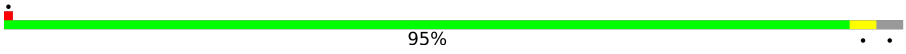
Chain S:

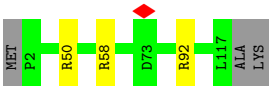




• Molecule 18: 50S ribosomal protein L20

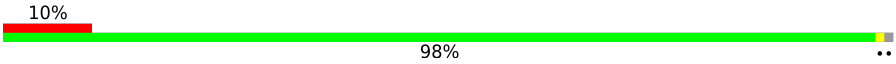
Chain T:

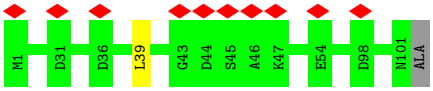




• Molecule 19: 50S ribosomal protein L21

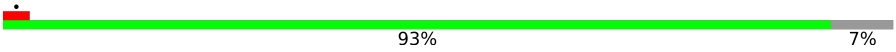
Chain U:

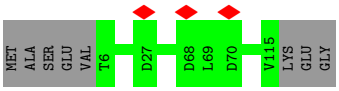




• Molecule 20: 50S ribosomal protein L22

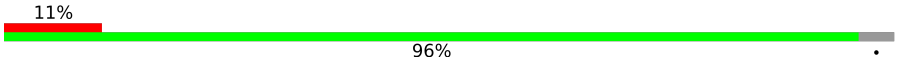
Chain V:

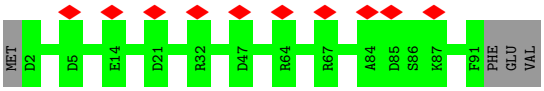




• Molecule 21: 50S ribosomal protein L23

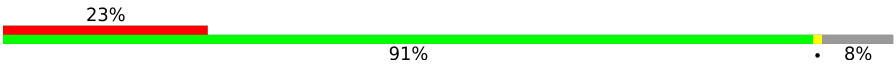
Chain W:

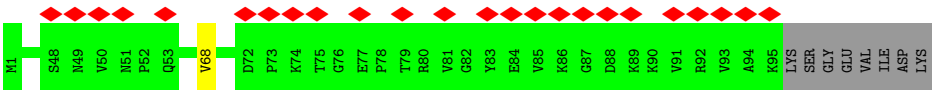




• Molecule 22: 50S ribosomal protein L24

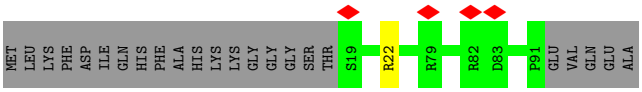
Chain X:





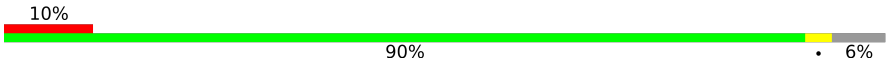
• Molecule 23: 50S ribosomal protein L27

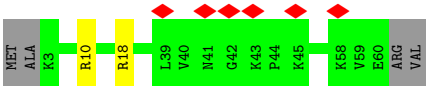
Chain Z:



• Molecule 24: 50S ribosomal protein L28

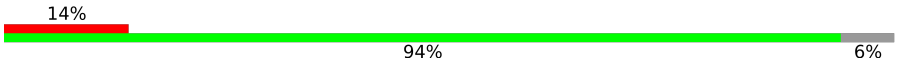
Chain 1:

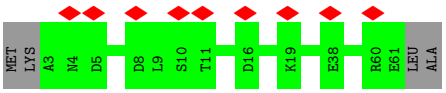




• Molecule 25: 50S ribosomal protein L29

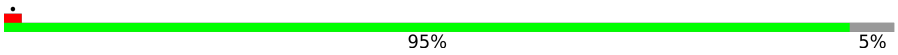
Chain 2:

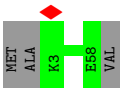




• Molecule 26: 50S ribosomal protein L30

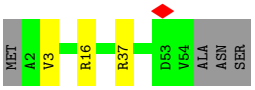
Chain 3:





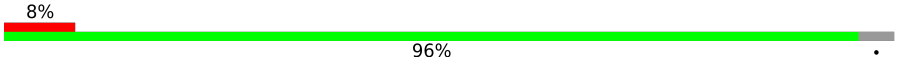
• Molecule 27: 50S ribosomal protein L32-2

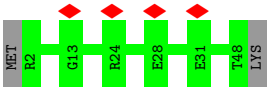
Chain 5:



• Molecule 28: 50S ribosomal protein L33 1

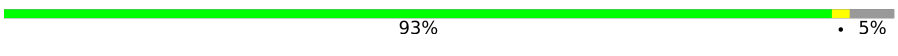
Chain 6:

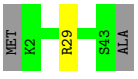




• Molecule 29: 50S ribosomal protein L34

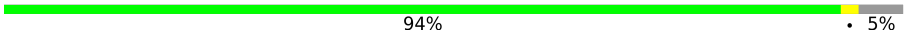
Chain 7:





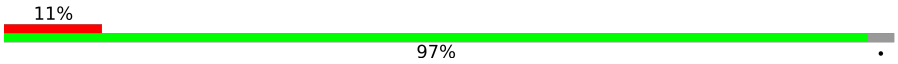
• Molecule 30: 50S ribosomal protein L35

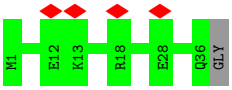
Chain 8:



• Molecule 31: 50S ribosomal protein L36

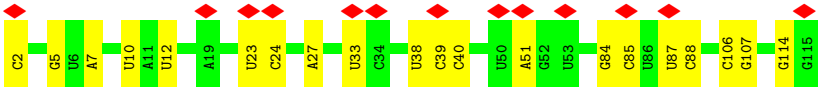
Chain 9:





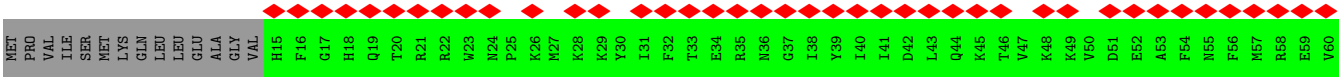
• Molecule 32: 5S rRNA

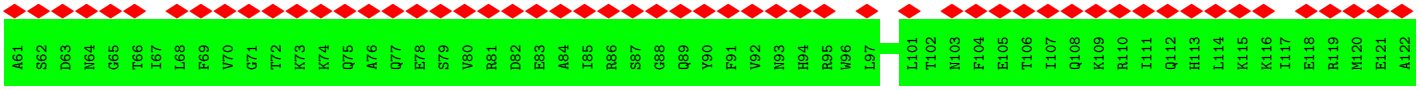
Chain B:

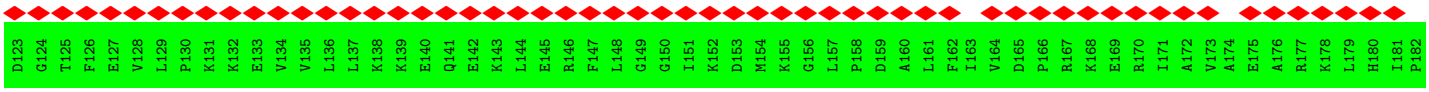


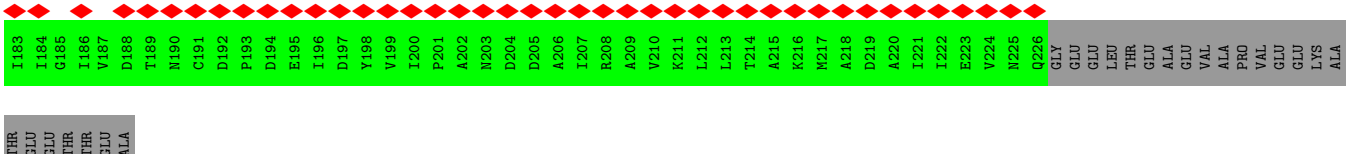
• Molecule 33: 30S ribosomal protein S2

Chain c:



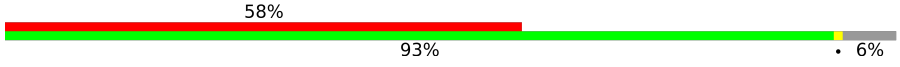


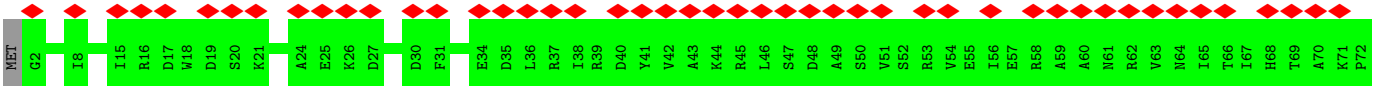


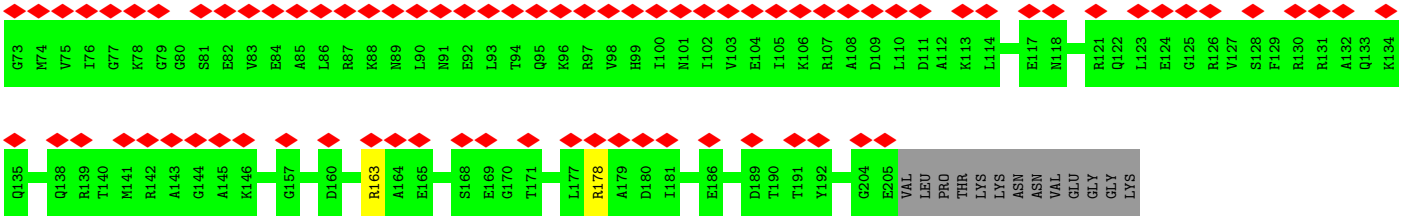


• Molecule 34: 30S ribosomal protein S3

Chain d:

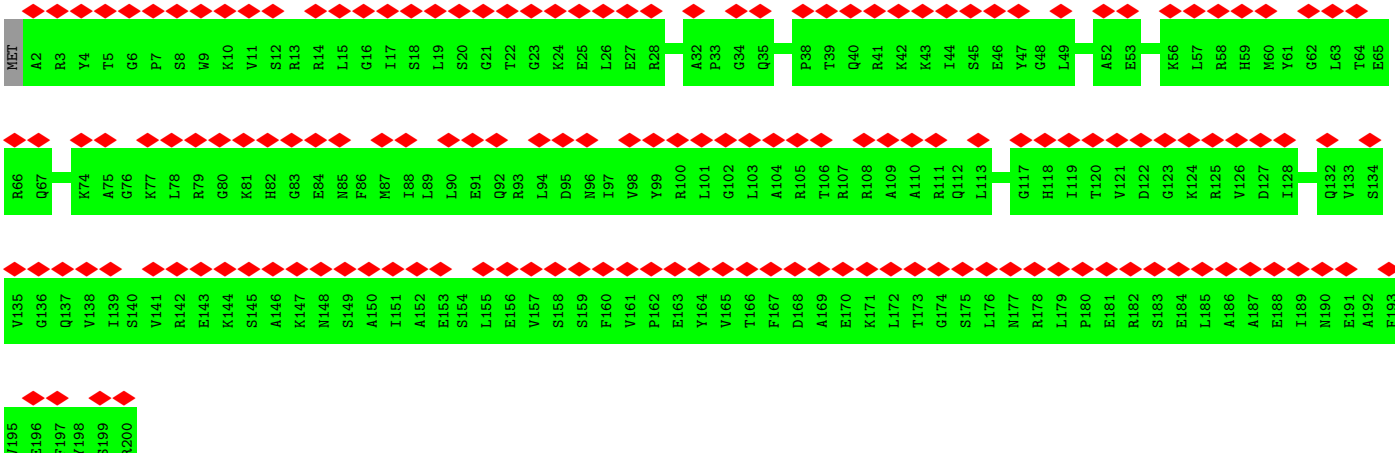






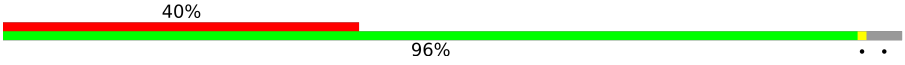
• Molecule 35: 30S ribosomal protein S4

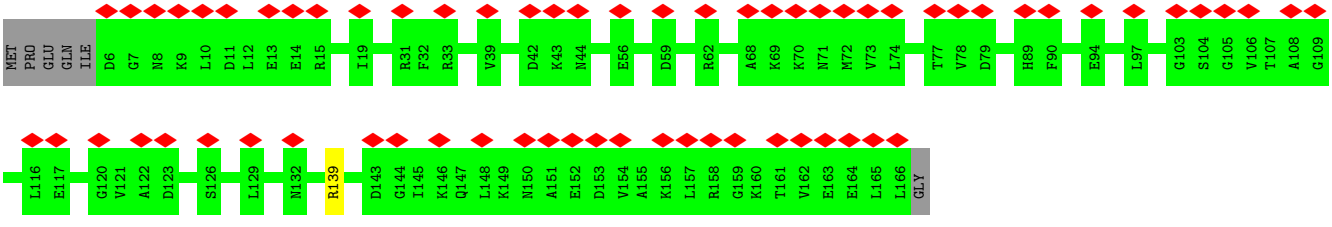
Chain e:



• Molecule 36: 30S ribosomal protein S5

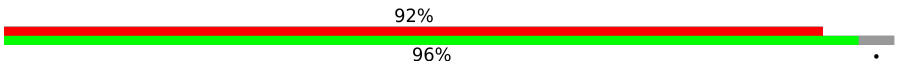
Chain f:

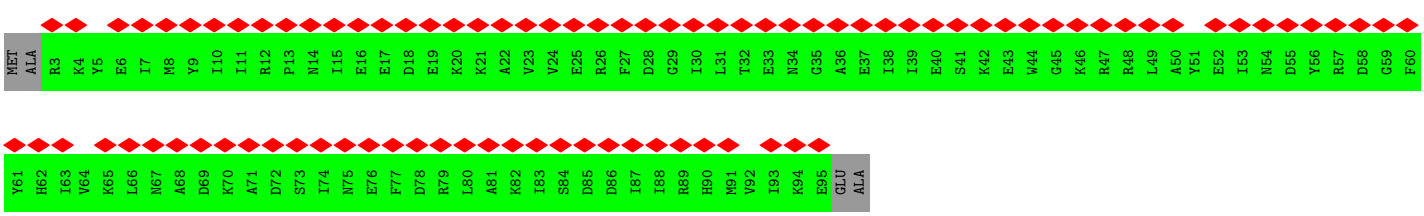




• Molecule 37: 30S ribosomal protein S6

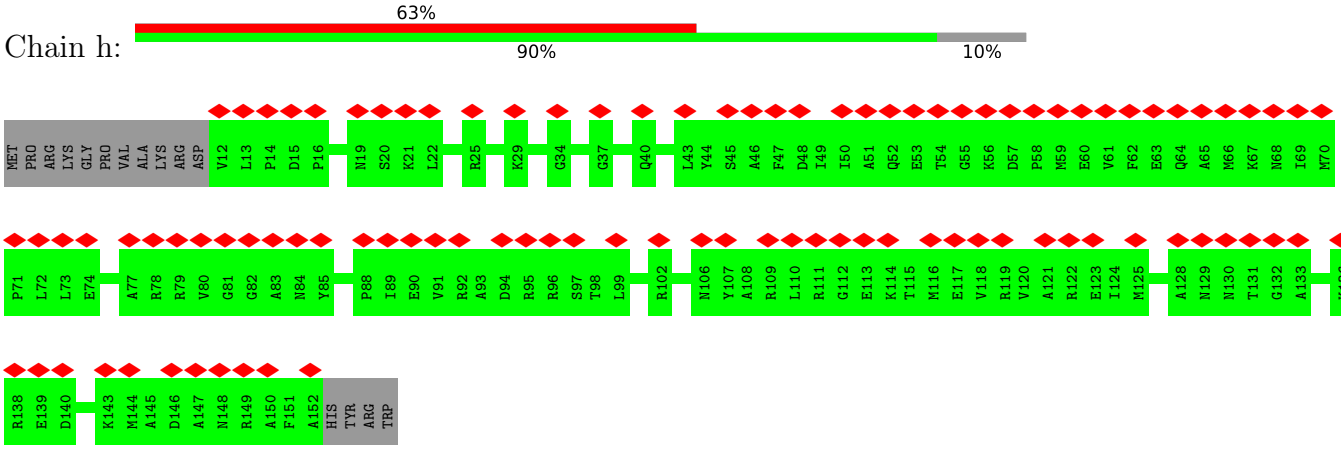
Chain g:





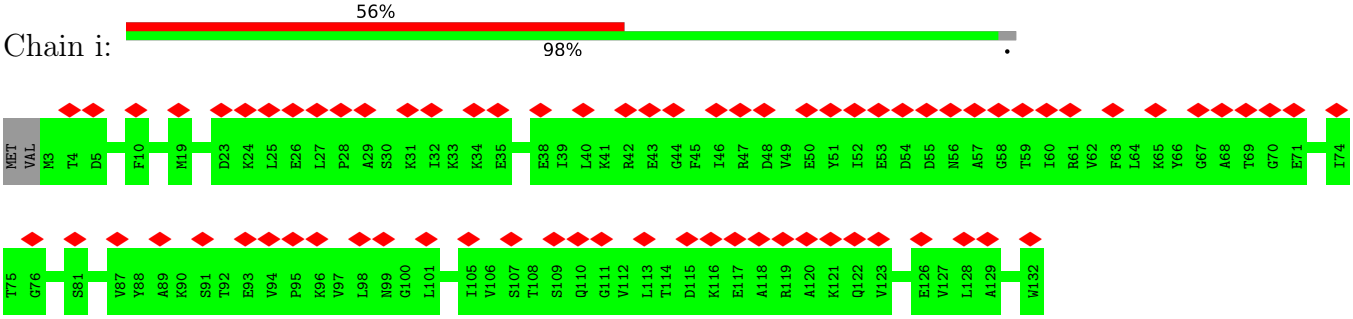
• Molecule 38: 30S ribosomal protein S7

Chain h:



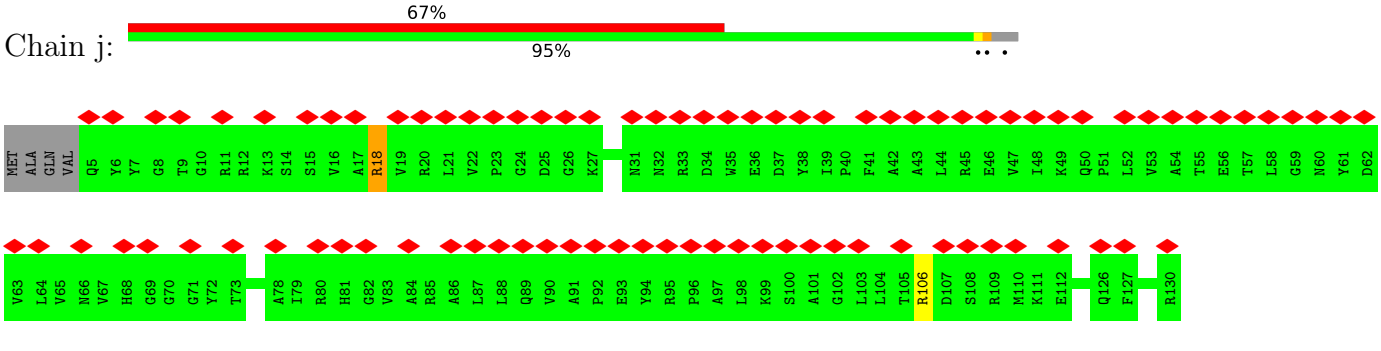
• Molecule 39: 30S ribosomal protein S8

Chain i:



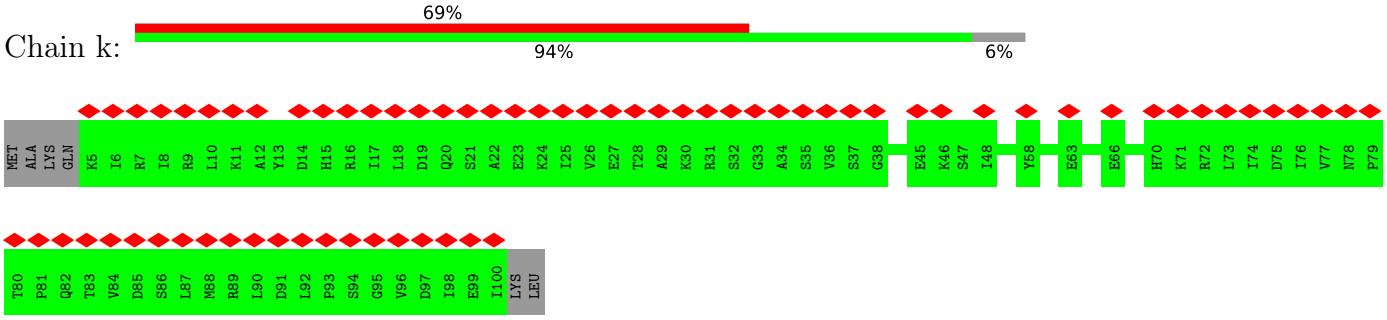
• Molecule 40: 30S ribosomal protein S9

Chain j:



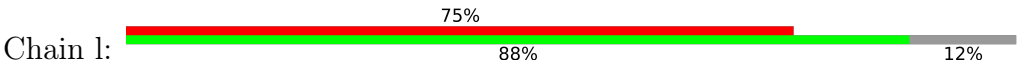
• Molecule 41: 30S ribosomal protein S10

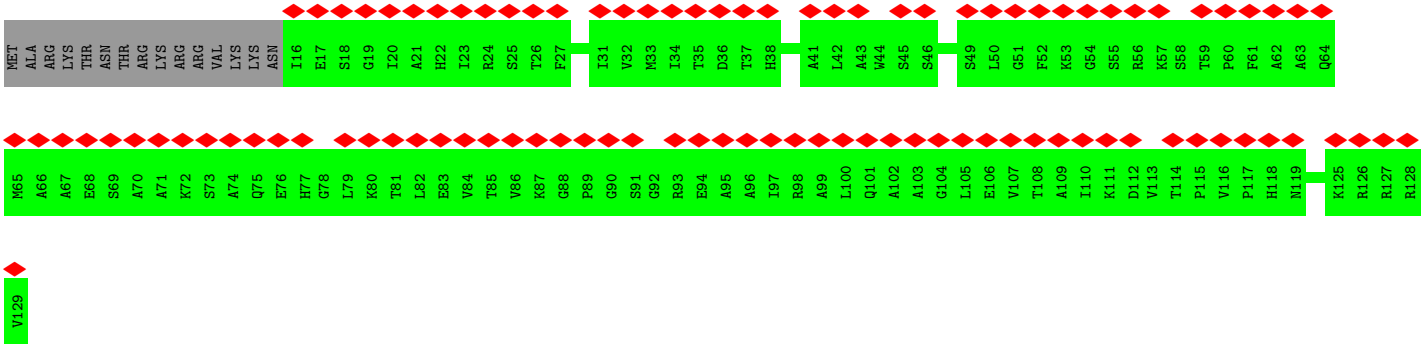
Chain k:



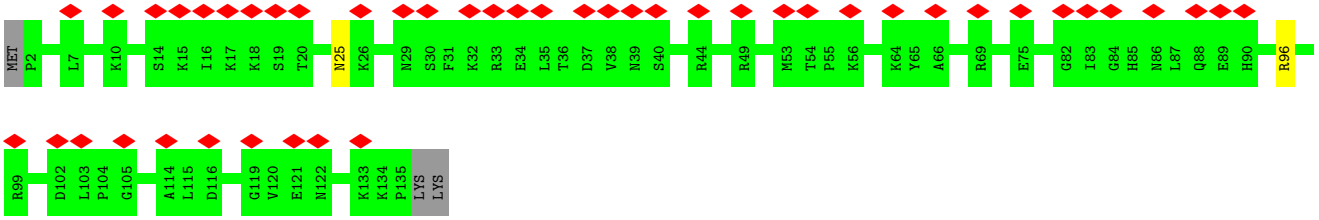
• Molecule 42: 30S ribosomal protein S11

Chain l:

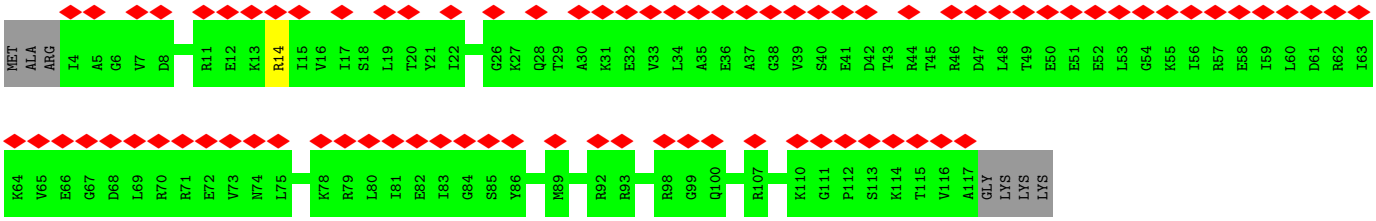




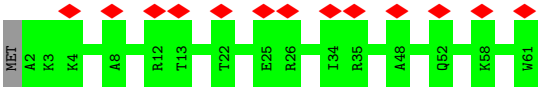
• Molecule 43: 30S ribosomal protein S12



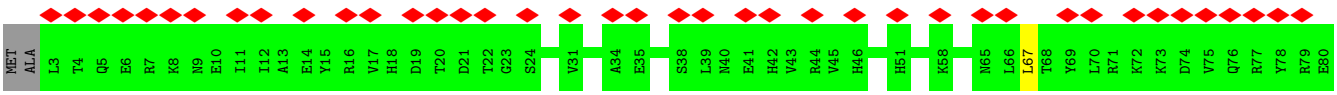
• Molecule 44: 30S ribosomal protein S13

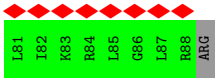


• Molecule 45: 30S ribosomal protein S14 type Z



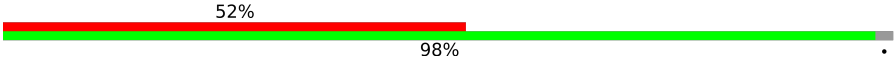
• Molecule 46: 30S ribosomal protein S15

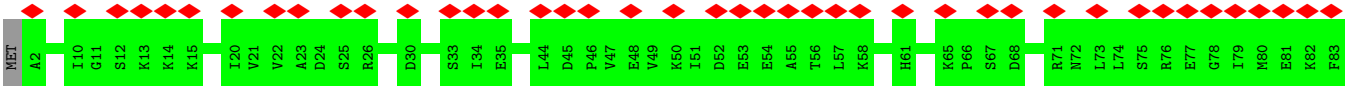


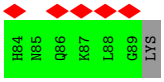


• Molecule 47: 30S ribosomal protein S16

Chain q:

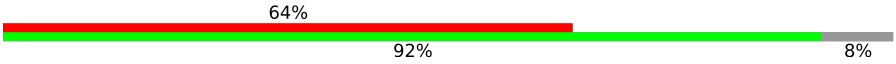


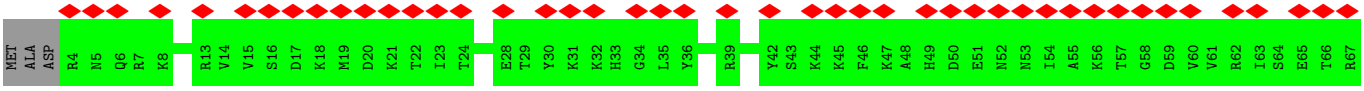


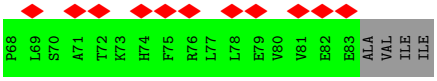


• Molecule 48: 30S ribosomal protein S17

Chain r:

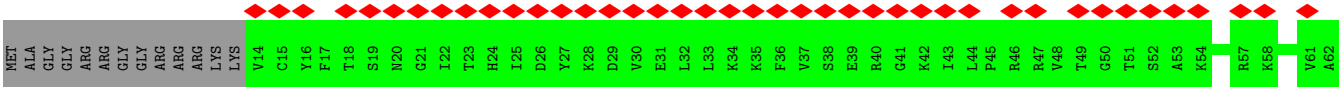


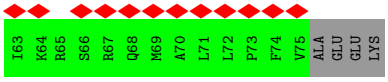




• Molecule 49: 30S ribosomal protein S18

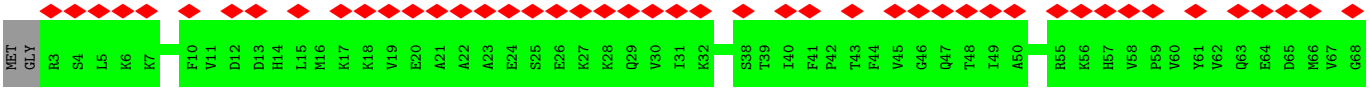
Chain s:

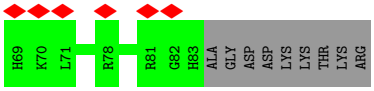




• Molecule 50: 30S ribosomal protein S19

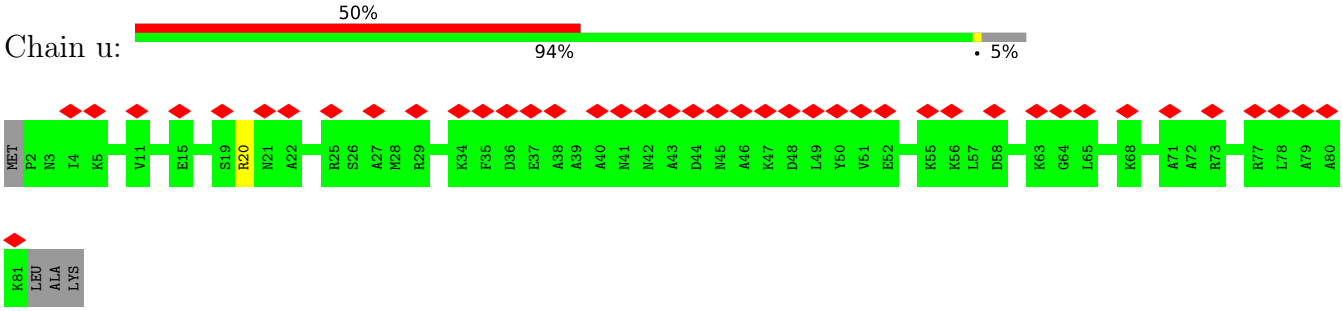
Chain t:





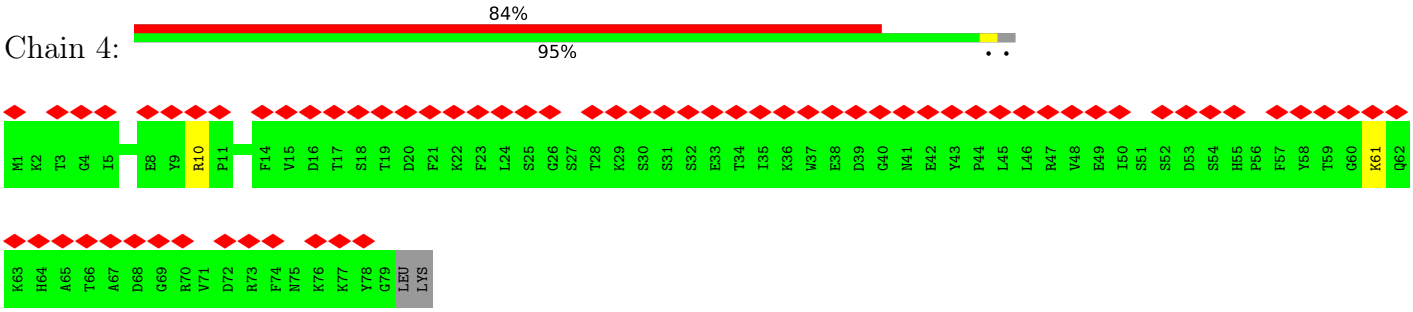
• Molecule 51: 30S ribosomal protein S20

Chain u:



• Molecule 52: 50S ribosomal protein L31 type B

Chain 4:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45548	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	26.3	Depositor
Minimum defocus (nm)	-700	Depositor
Maximum defocus (nm)	-1900	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.096	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	366.432, 366.432, 366.432	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.041, 1.041, 1.041	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: K, SPD, ZN, ATP, MG

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	0	0.53	0/3699	0.63	0/4976
2	D	0.96	0/1765	1.12	3/2750 (0.1%)
3	b	0.69	0/196	1.13	2/302 (0.7%)
4	A	1.36	55/69974 (0.1%)	1.26	295/109160 (0.3%)
5	a	0.85	0/36323	1.06	32/56652 (0.1%)
6	G	0.81	0/2144	0.78	5/2875 (0.2%)
7	H	0.91	2/1604 (0.1%)	0.73	0/2156
8	I	0.83	0/1583	0.73	0/2133
9	J	0.46	0/1383	0.69	0/1863
10	K	0.44	0/1293	0.61	0/1749
11	M	0.81	0/1140	0.68	0/1533
12	N	0.83	0/932	0.76	1/1248 (0.1%)
13	O	0.75	1/1105 (0.1%)	0.78	2/1470 (0.1%)
14	P	0.79	0/1077	0.75	0/1439
15	Q	0.80	0/994	0.82	1/1329 (0.1%)
16	R	0.51	0/923	0.70	0/1232
17	S	0.81	0/917	0.82	0/1230
18	T	0.94	0/952	0.85	4/1266 (0.3%)
19	U	0.95	0/799	0.71	1/1072 (0.1%)
20	V	0.83	0/858	0.82	0/1160
21	W	0.78	0/739	0.77	0/990
22	X	0.65	1/733 (0.1%)	0.68	0/980
23	Z	0.85	0/570	0.86	0/758
24	1	0.69	0/462	0.87	3/612 (0.5%)
25	2	0.56	0/488	0.73	0/651
26	3	0.71	0/436	0.73	0/585
27	5	0.94	1/433 (0.2%)	0.85	1/577 (0.2%)
28	6	0.70	0/404	0.76	0/541
29	7	1.01	0/360	0.96	1/469 (0.2%)
30	8	0.86	0/519	0.85	1/675 (0.1%)
31	9	0.78	0/295	0.69	0/387
32	B	0.82	0/2711	1.07	2/4224 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	c	0.38	0/1749	0.64	0/2351
34	d	0.47	0/1649	0.68	1/2218 (0.0%)
35	e	0.44	0/1624	0.66	0/2179
36	f	0.53	0/1192	0.71	2/1609 (0.1%)
37	g	0.39	0/794	0.61	0/1063
38	h	0.42	0/1128	0.65	0/1514
39	i	0.48	0/1028	0.69	0/1382
40	j	0.49	0/1003	0.71	1/1349 (0.1%)
41	k	0.47	0/783	0.68	0/1056
42	l	0.38	0/851	0.66	0/1148
43	m	0.57	0/1056	0.80	0/1418
44	n	0.46	0/912	0.76	2/1220 (0.2%)
45	o	0.61	0/500	0.73	0/664
46	p	0.42	0/732	0.73	1/980 (0.1%)
47	q	0.47	0/724	0.71	0/971
48	r	0.45	0/665	0.68	0/889
49	s	0.41	0/512	0.68	0/686
50	t	0.47	0/671	0.63	0/902
51	u	0.43	0/614	0.71	1/817 (0.1%)
52	4	0.41	0/654	0.63	0/881
All	All	1.07	60/156652 (0.0%)	1.09	362/234341 (0.2%)

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1067	A	N9-C4	-6.93	1.33	1.37
4	A	628	G	N9-C4	-6.37	1.32	1.38
4	A	554	C	C4-C5	-6.19	1.38	1.43
4	A	846	A	N9-C4	-5.98	1.34	1.37
4	A	1705	C	C4-C5	-5.83	1.38	1.43

The worst 5 of 362 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	554	C	C6-N1-C2	-10.30	116.18	120.30
4	A	2507	C	C6-N1-C2	-8.88	116.75	120.30
4	A	1823	C	C5-C4-N4	-8.61	114.17	120.20
4	A	1666	C	C5-C4-N4	-8.57	114.20	120.20
4	A	2699	C	N3-C2-O2	-8.39	116.03	121.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	459/567 (81%)	430 (94%)	29 (6%)	0	100	100
6	G	271/277 (98%)	256 (94%)	15 (6%)	0	100	100
7	H	204/209 (98%)	191 (94%)	13 (6%)	0	100	100
8	I	201/207 (97%)	190 (94%)	11 (6%)	0	100	100
9	J	173/179 (97%)	163 (94%)	10 (6%)	0	100	100
10	K	163/178 (92%)	155 (95%)	8 (5%)	0	100	100
11	M	140/145 (97%)	136 (97%)	4 (3%)	0	100	100
12	N	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
13	O	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
14	P	131/144 (91%)	126 (96%)	5 (4%)	0	100	100
15	Q	118/135 (87%)	113 (96%)	5 (4%)	0	100	100
16	R	116/119 (98%)	106 (91%)	10 (9%)	0	100	100
17	S	110/114 (96%)	103 (94%)	7 (6%)	0	100	100
18	T	114/119 (96%)	107 (94%)	7 (6%)	0	100	100
19	U	99/102 (97%)	93 (94%)	6 (6%)	0	100	100
20	V	108/118 (92%)	106 (98%)	2 (2%)	0	100	100
21	W	88/94 (94%)	82 (93%)	6 (7%)	0	100	100
22	X	93/103 (90%)	91 (98%)	2 (2%)	0	100	100
23	Z	71/96 (74%)	67 (94%)	4 (6%)	0	100	100
24	1	56/62 (90%)	51 (91%)	5 (9%)	0	100	100
25	2	57/63 (90%)	54 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	3	54/59 (92%)	51 (94%)	3 (6%)	0	100	100
27	5	51/57 (90%)	49 (96%)	2 (4%)	0	100	100
28	6	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
29	7	40/44 (91%)	39 (98%)	1 (2%)	0	100	100
30	8	61/66 (92%)	53 (87%)	8 (13%)	0	100	100
31	9	34/37 (92%)	30 (88%)	4 (12%)	0	100	100
33	c	210/249 (84%)	188 (90%)	22 (10%)	0	100	100
34	d	202/218 (93%)	185 (92%)	17 (8%)	0	100	100
35	e	197/200 (98%)	182 (92%)	15 (8%)	0	100	100
36	f	159/167 (95%)	149 (94%)	10 (6%)	0	100	100
37	g	91/97 (94%)	83 (91%)	8 (9%)	0	100	100
38	h	139/156 (89%)	130 (94%)	9 (6%)	0	100	100
39	i	128/132 (97%)	116 (91%)	12 (9%)	0	100	100
40	j	124/130 (95%)	114 (92%)	10 (8%)	0	100	100
41	k	94/102 (92%)	87 (93%)	7 (7%)	0	100	100
42	l	112/129 (87%)	100 (89%)	12 (11%)	0	100	100
43	m	132/137 (96%)	120 (91%)	12 (9%)	0	100	100
44	n	112/121 (93%)	103 (92%)	9 (8%)	0	100	100
45	o	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
46	p	84/89 (94%)	81 (96%)	3 (4%)	0	100	100
47	q	86/90 (96%)	81 (94%)	5 (6%)	0	100	100
48	r	78/87 (90%)	73 (94%)	5 (6%)	0	100	100
49	s	60/79 (76%)	59 (98%)	1 (2%)	0	100	100
50	t	79/92 (86%)	75 (95%)	4 (5%)	0	100	100
51	u	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
52	4	77/81 (95%)	59 (77%)	18 (23%)	0	100	100
All	All	5619/6112 (92%)	5249 (93%)	370 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	400/492 (81%)	396 (99%)	4 (1%)	76 92
6	G	221/225 (98%)	220 (100%)	1 (0%)	88 96
7	H	169/171 (99%)	168 (99%)	1 (1%)	86 96
8	I	171/174 (98%)	170 (99%)	1 (1%)	86 96
9	J	151/155 (97%)	151 (100%)	0	100 100
10	K	137/147 (93%)	137 (100%)	0	100 100
11	M	119/121 (98%)	119 (100%)	0	100 100
12	N	101/101 (100%)	101 (100%)	0	100 100
13	O	113/115 (98%)	113 (100%)	0	100 100
14	P	105/113 (93%)	105 (100%)	0	100 100
15	Q	102/111 (92%)	102 (100%)	0	100 100
16	R	96/97 (99%)	96 (100%)	0	100 100
17	S	98/100 (98%)	97 (99%)	1 (1%)	76 92
18	T	95/97 (98%)	95 (100%)	0	100 100
19	U	82/82 (100%)	82 (100%)	0	100 100
20	V	91/97 (94%)	91 (100%)	0	100 100
21	W	80/84 (95%)	80 (100%)	0	100 100
22	X	81/88 (92%)	81 (100%)	0	100 100
23	Z	58/76 (76%)	57 (98%)	1 (2%)	60 86
24	1	50/53 (94%)	50 (100%)	0	100 100
25	2	52/55 (94%)	52 (100%)	0	100 100
26	3	50/52 (96%)	50 (100%)	0	100 100
27	5	47/50 (94%)	46 (98%)	1 (2%)	53 81
28	6	46/48 (96%)	46 (100%)	0	100 100
29	7	38/39 (97%)	38 (100%)	0	100 100
30	8	53/56 (95%)	53 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	9	35/35 (100%)	35 (100%)	0	100	100
33	c	185/215 (86%)	185 (100%)	0	100	100
34	d	165/177 (93%)	164 (99%)	1 (1%)	86	96
35	e	169/170 (99%)	169 (100%)	0	100	100
36	f	126/131 (96%)	126 (100%)	0	100	100
37	g	83/85 (98%)	83 (100%)	0	100	100
38	h	117/130 (90%)	117 (100%)	0	100	100
39	i	108/110 (98%)	108 (100%)	0	100	100
40	j	99/102 (97%)	97 (98%)	2 (2%)	55	82
41	k	88/93 (95%)	88 (100%)	0	100	100
42	l	86/100 (86%)	86 (100%)	0	100	100
43	m	115/118 (98%)	113 (98%)	2 (2%)	60	86
44	n	97/102 (95%)	97 (100%)	0	100	100
45	o	51/52 (98%)	51 (100%)	0	100	100
46	p	79/81 (98%)	79 (100%)	0	100	100
47	q	78/80 (98%)	78 (100%)	0	100	100
48	r	73/78 (94%)	73 (100%)	0	100	100
49	s	56/67 (84%)	56 (100%)	0	100	100
50	t	70/78 (90%)	70 (100%)	0	100	100
51	u	63/66 (96%)	63 (100%)	0	100	100
52	4	71/73 (97%)	69 (97%)	2 (3%)	43	76
All	All	4820/5142 (94%)	4803 (100%)	17 (0%)	91	97

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	m	96	ARG
52	4	61	LYS
17	S	51	ARG
23	Z	22	ARG
27	5	37	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
34	d	175	HIS
38	h	68	ASN
46	p	62	HIS
43	m	25	ASN
46	p	37	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	D	73/77 (94%)	16 (21%)	0
3	b	6/14 (42%)	1 (16%)	0
32	B	113/114 (99%)	18 (15%)	1 (0%)
4	A	2905/2928 (99%)	571 (19%)	48 (1%)
5	a	1509/1542 (97%)	294 (19%)	0
All	All	4606/4675 (98%)	900 (19%)	49 (1%)

5 of 900 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	5	G
2	D	6	G
2	D	8	U
2	D	9	G
2	D	13	C

5 of 49 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	A	1533	A
4	A	1946	A
4	A	1569	U
4	A	1880	A
4	A	2320	A

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 171 ligands modelled in this entry, 167 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
53	ATP	0	602	54	26,33,33	0.73	0	31,52,52	0.74	2 (6%)
55	SPD	A	3001	-	9,9,9	0.49	0	8,8,8	1.36	2 (25%)
53	ATP	0	601	54	26,33,33	0.68	0	31,52,52	0.73	2 (6%)
55	SPD	a	1601	-	9,9,9	0.28	0	8,8,8	0.86	0

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
53	ATP	0	602	54	-	7/18/38/38	0/3/3/3
55	SPD	A	3001	-	-	4/7/7/7	-
53	ATP	0	601	54	-	7/18/38/38	0/3/3/3
55	SPD	a	1601	-	-	2/7/7/7	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	A	3001	SPD	C4-C5-N6	-2.76	104.68	112.14
55	A	3001	SPD	C8-C7-N6	-2.38	105.71	112.14
53	0	602	ATP	C5-C6-N6	2.32	123.87	120.35
53	0	601	ATP	C5-C6-N6	2.27	123.81	120.35
53	0	602	ATP	PB-O3B-PG	2.03	139.78	132.83

There are no chirality outliers.

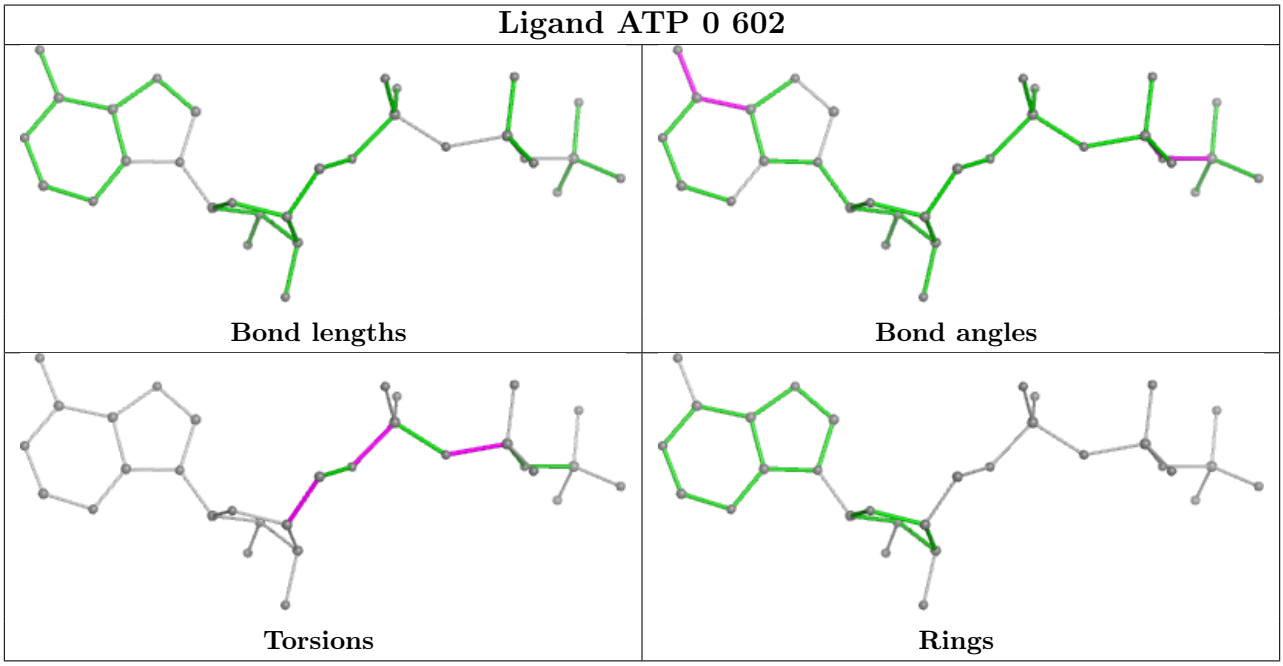
5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	0	601	ATP	C5'-O5'-PA-O1A
53	0	601	ATP	C5'-O5'-PA-O2A
53	0	601	ATP	C5'-O5'-PA-O3A
53	0	602	ATP	C5'-O5'-PA-O2A
53	0	602	ATP	C3'-C4'-C5'-O5'

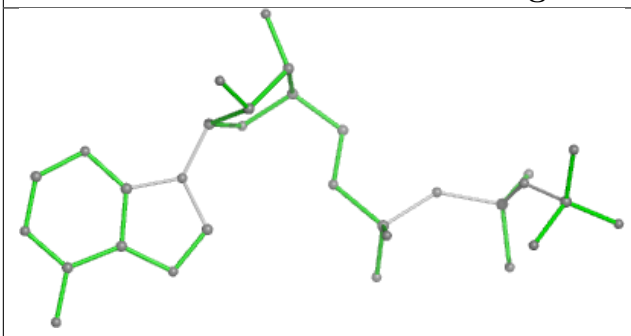
There are no ring outliers.

No monomer is involved in short contacts.

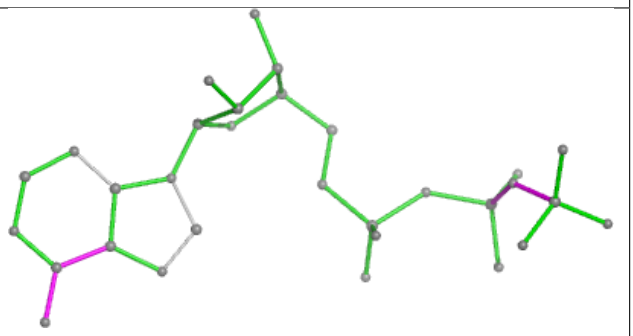
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



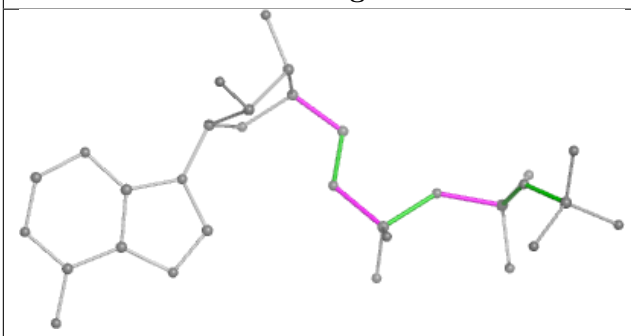
Ligand ATP 0 601



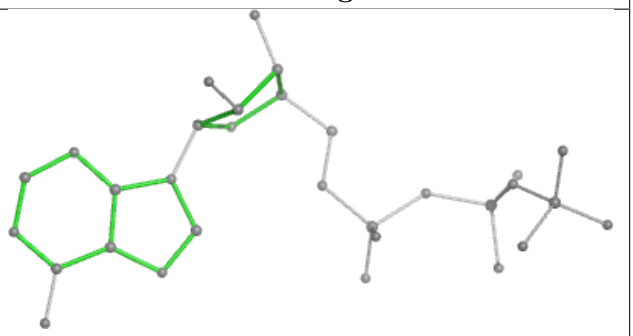
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

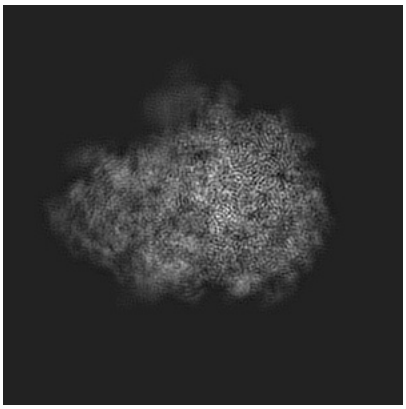
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12334. These allow visual inspection of the internal detail of the map and identification of artifacts.

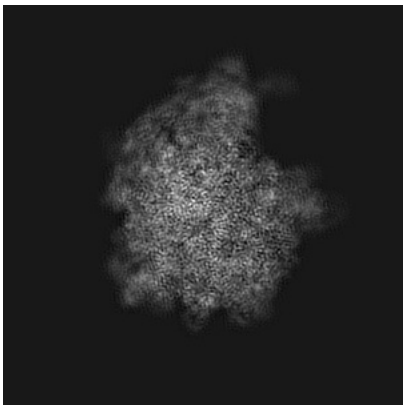
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

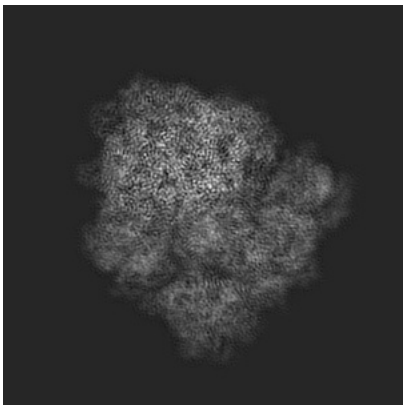
6.1.1 Primary map



X

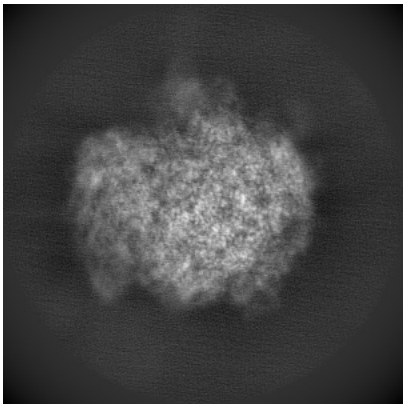


Y

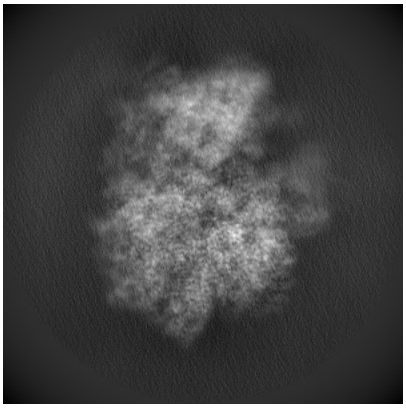


Z

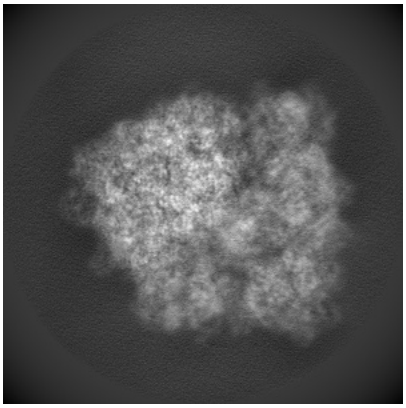
6.1.2 Raw map



X



Y

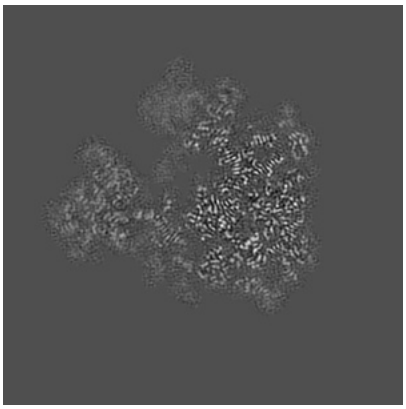


Z

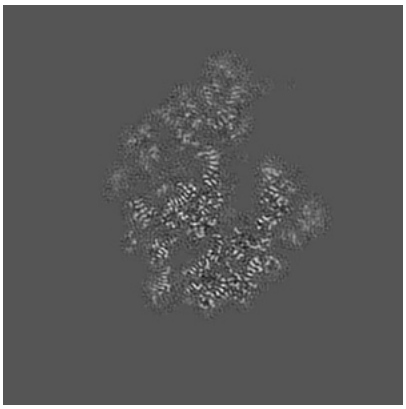
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

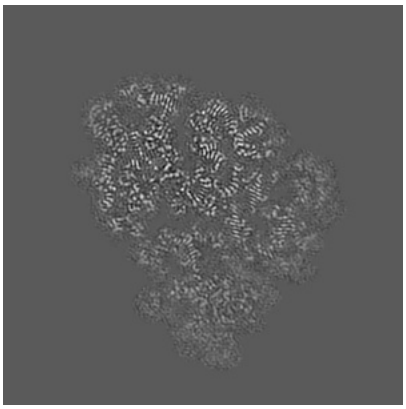
6.2.1 Primary map



X Index: 176

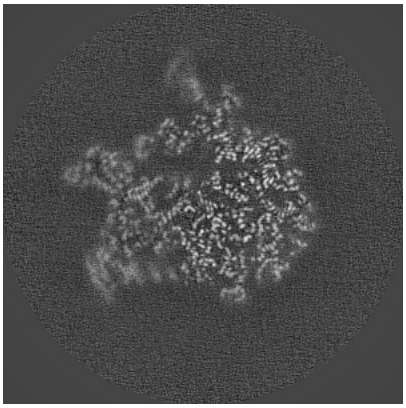


Y Index: 176

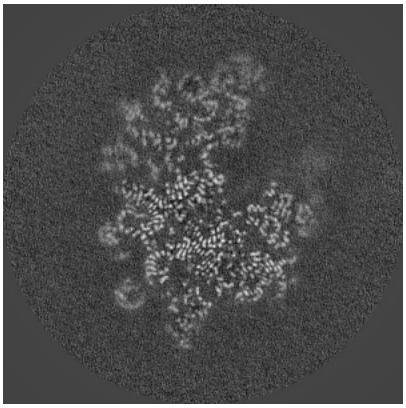


Z Index: 176

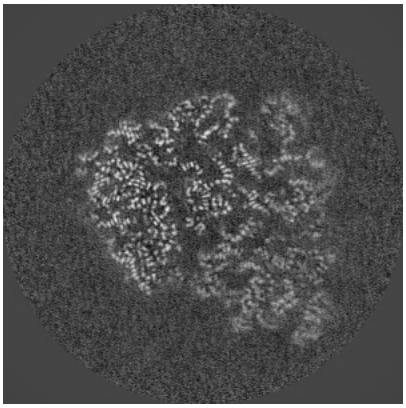
6.2.2 Raw map



X Index: 210



Y Index: 210

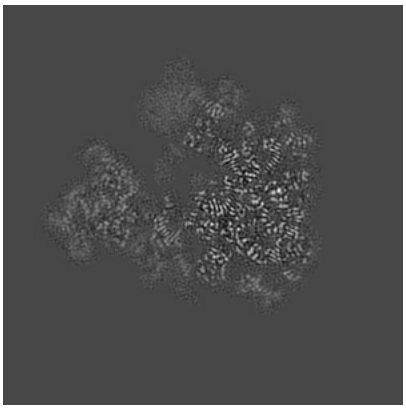


Z Index: 210

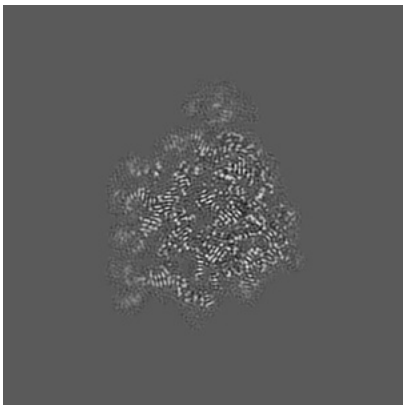
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

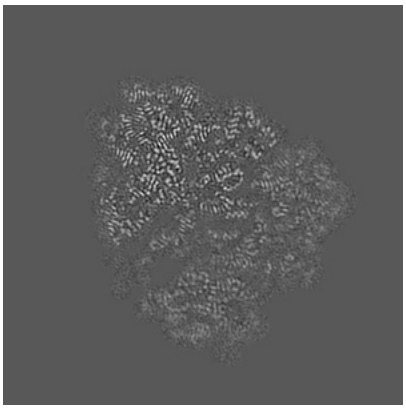
6.3.1 Primary map



X Index: 174

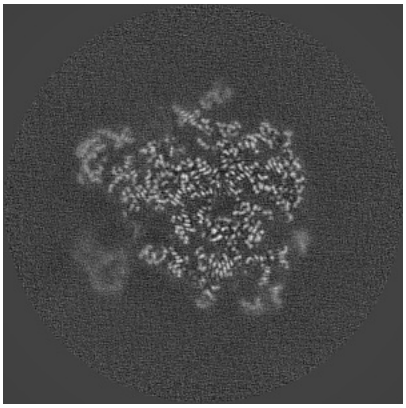


Y Index: 218

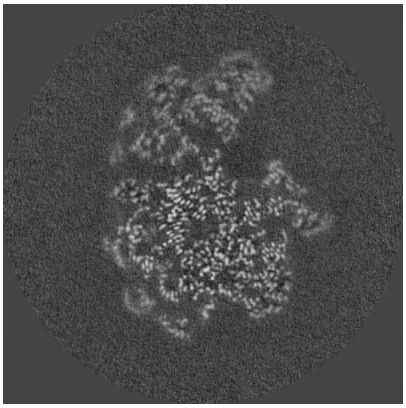


Z Index: 186

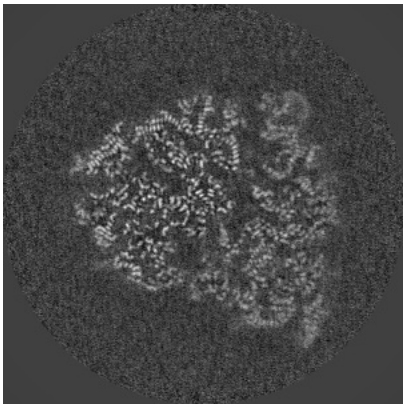
6.3.2 Raw map



X Index: 180



Y Index: 225

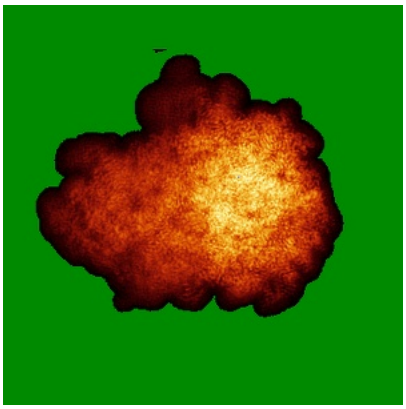


Z Index: 203

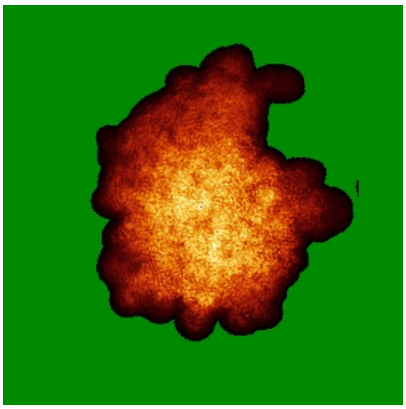
The images above show the largest variance slices of the map in three orthogonal directions.

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

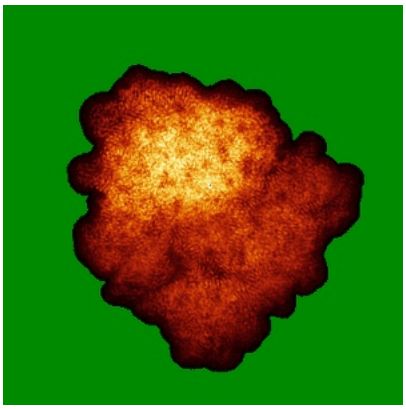
6.4.1 Primary map



X

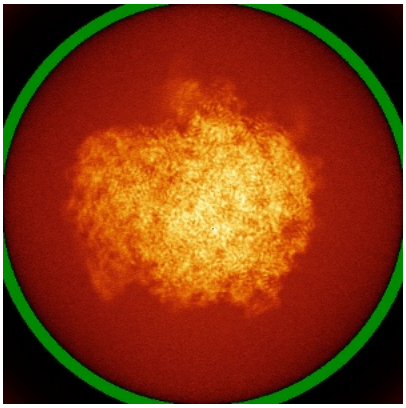


Y

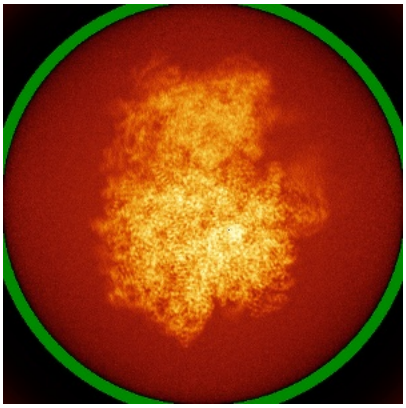


Z

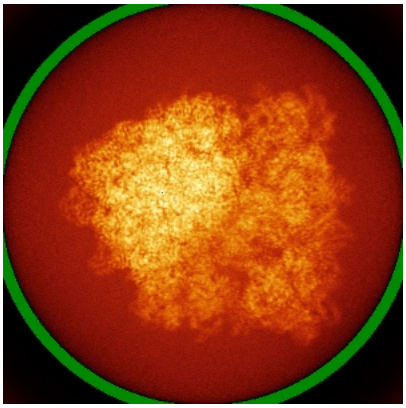
6.4.2 Raw map



X



Y

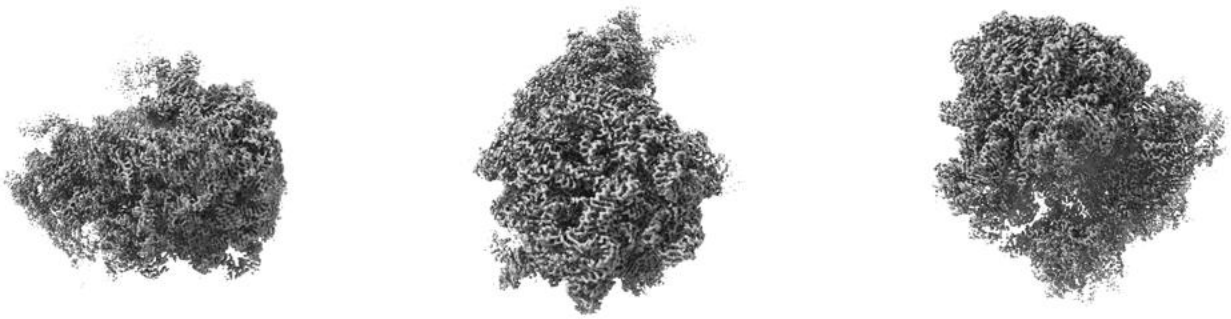


Z

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 0.025. 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.

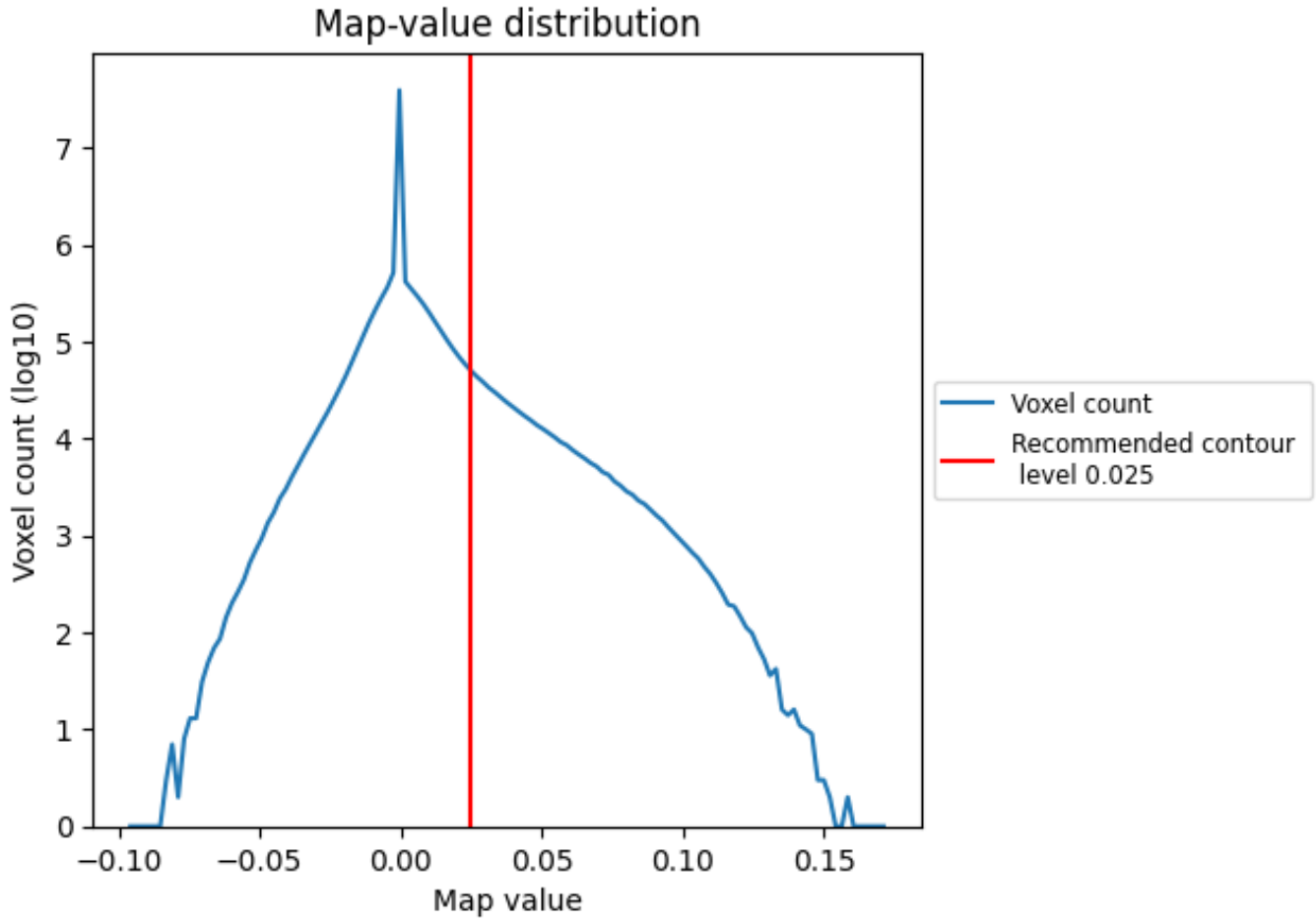
6.6 Mask visualisation (i)

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

7 Map analysis

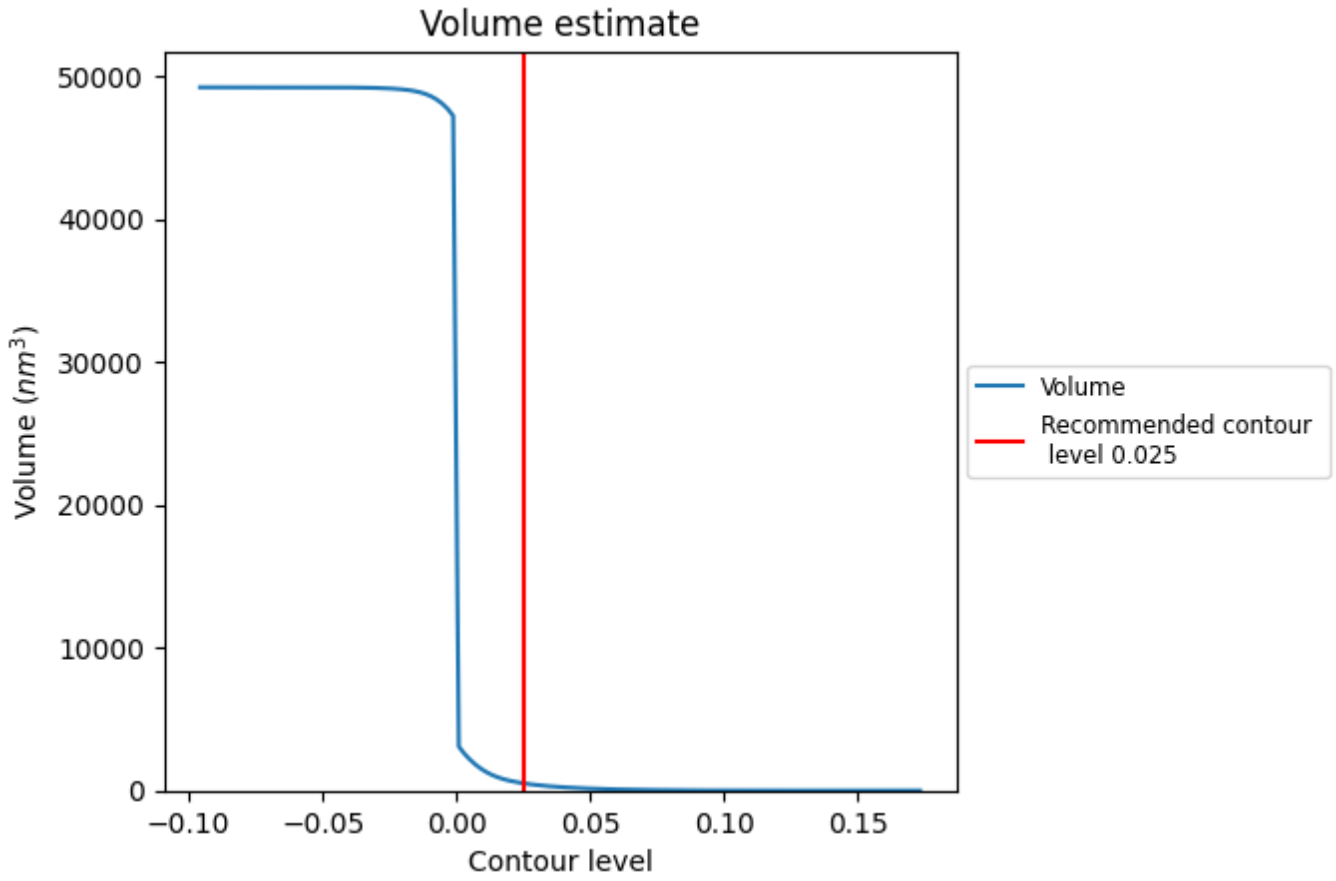
This section contains the results of statistical analysis of the map.

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.

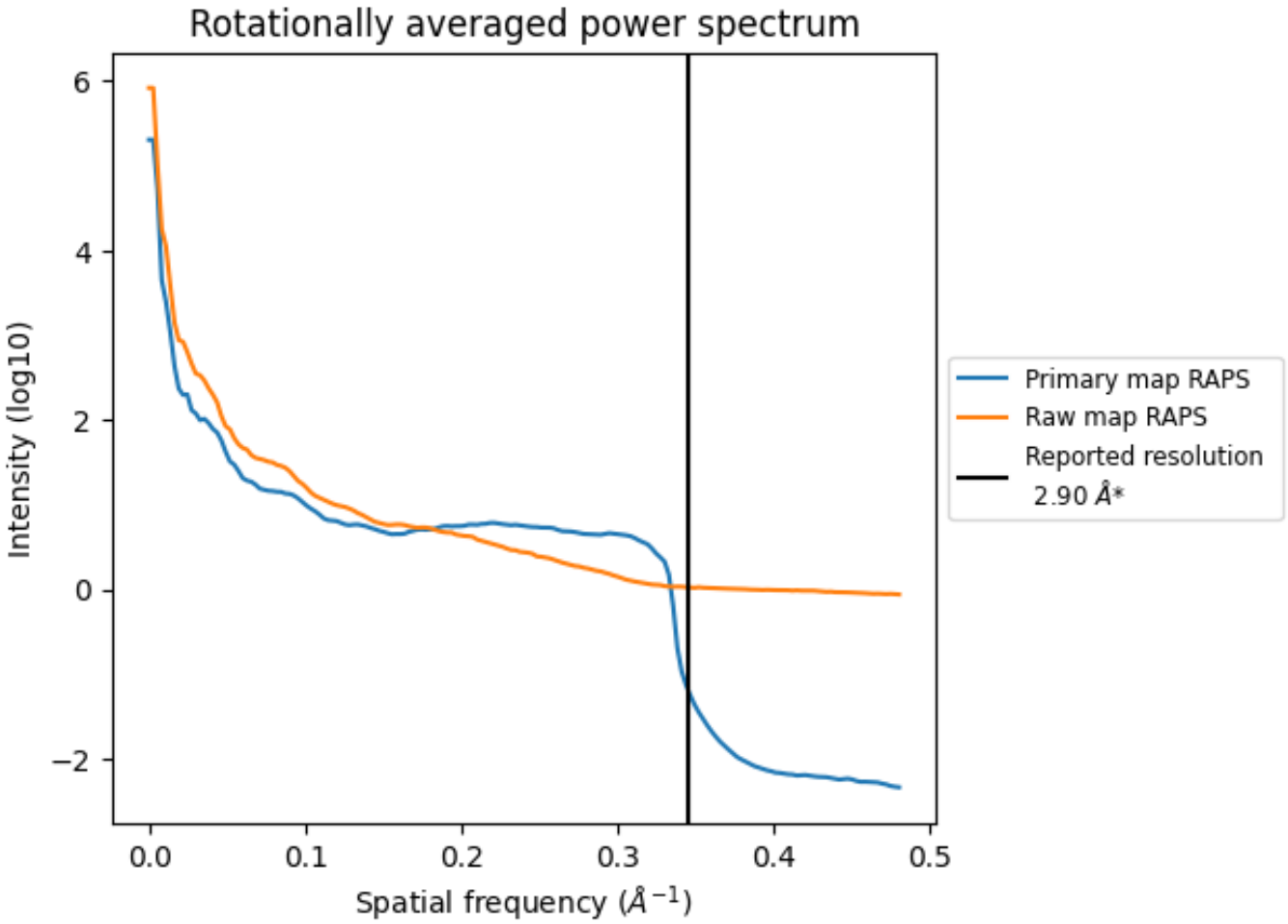
7.2 Volume estimate (i)



The volume at the recommended contour level is 510 nm^3; this corresponds to an approximate mass of 461 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)

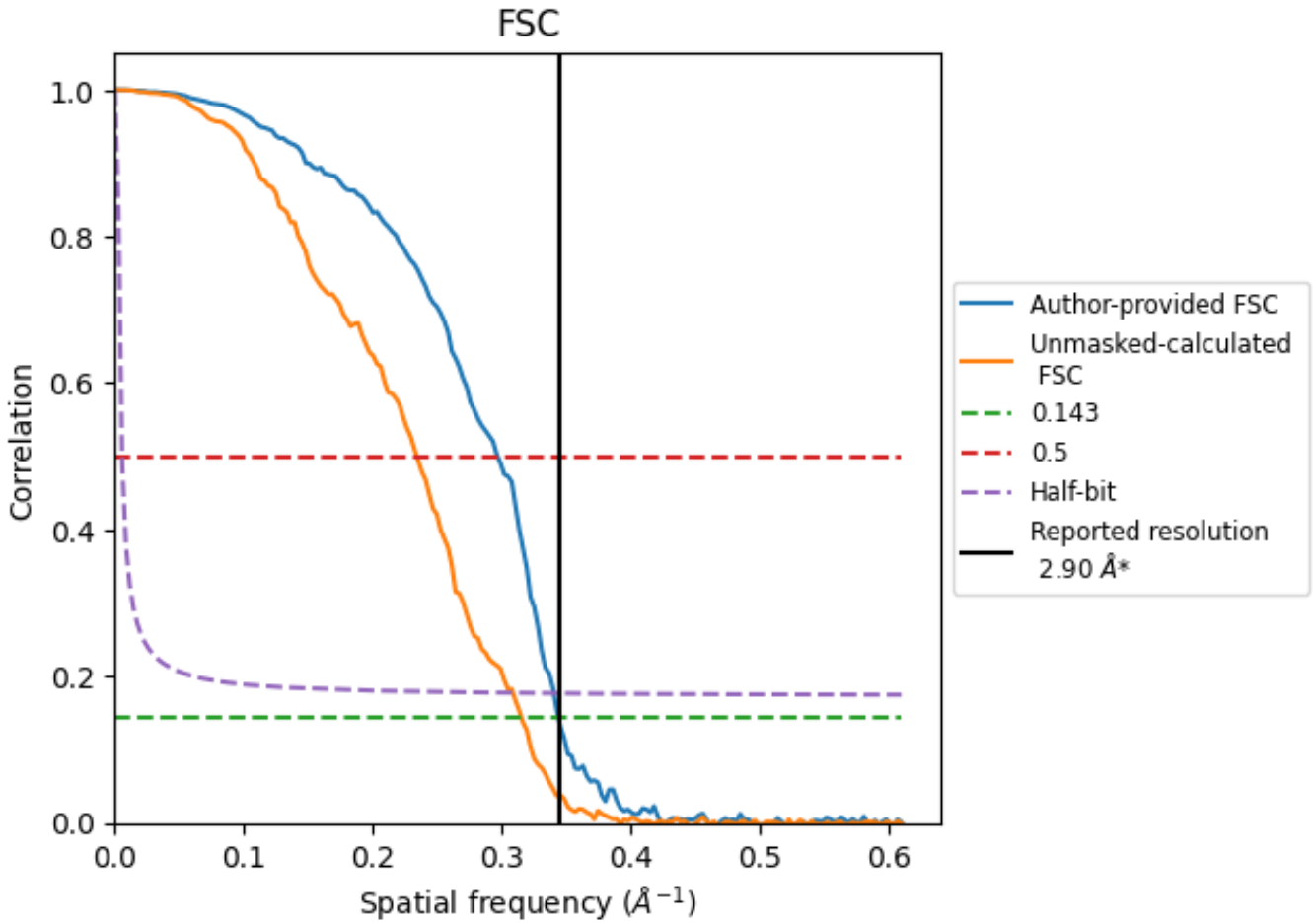


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

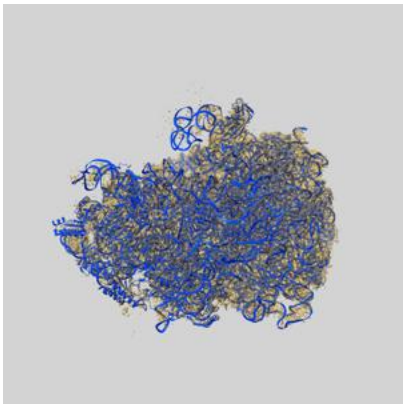
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.91	3.37	2.94
Unmasked-calculated*	3.17	4.27	3.24

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

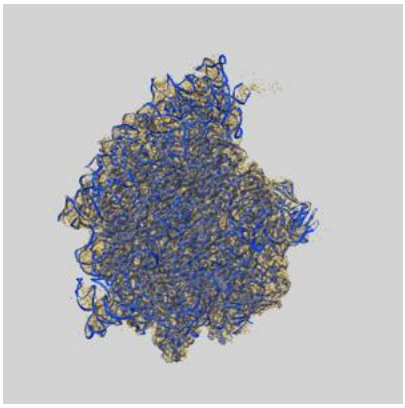
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12334 and PDB model 7NHN. Per-residue inclusion information can be found in section 3 on page 16.

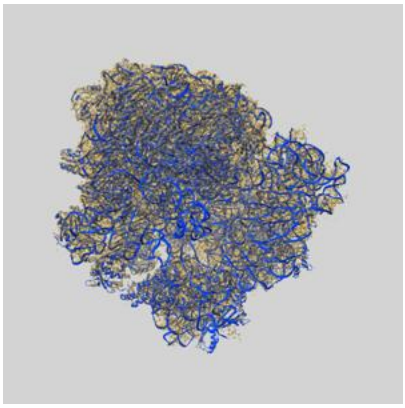
9.1 Map-model overlay



X



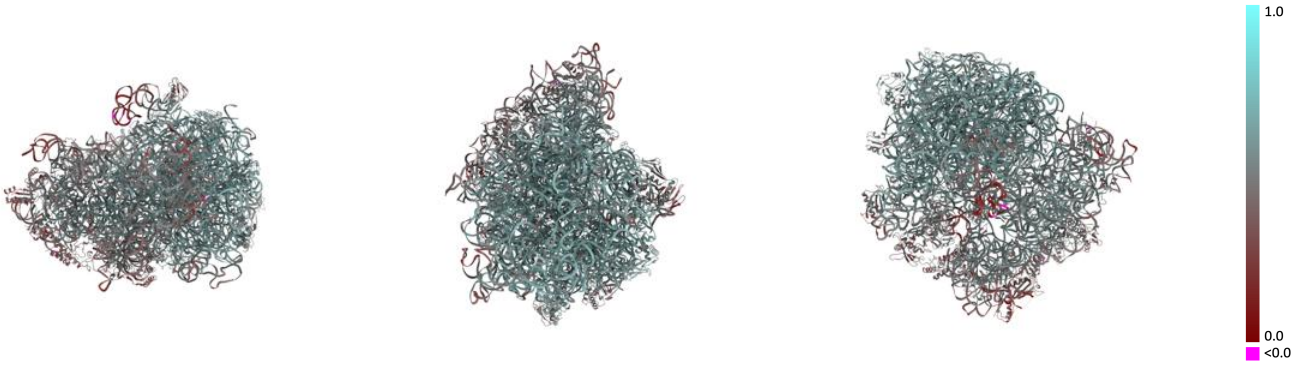
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

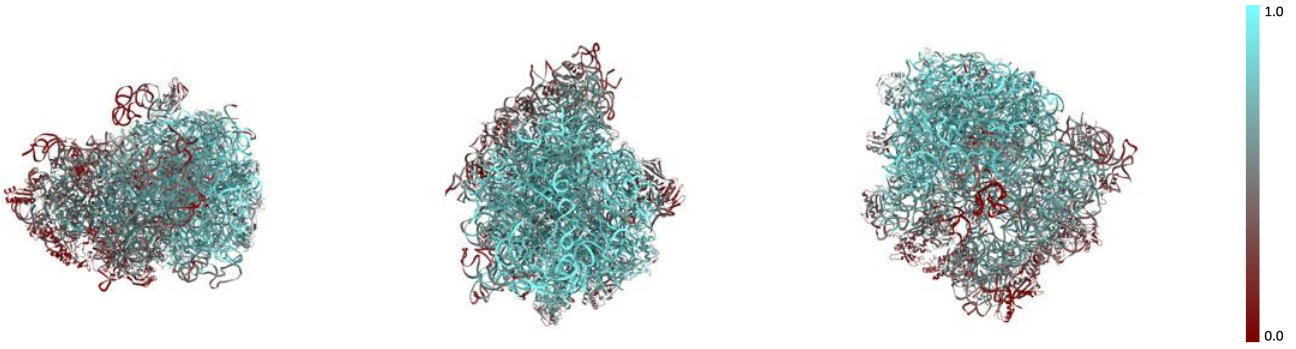
9.2 Q-score mapped to coordinate model (i)



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.

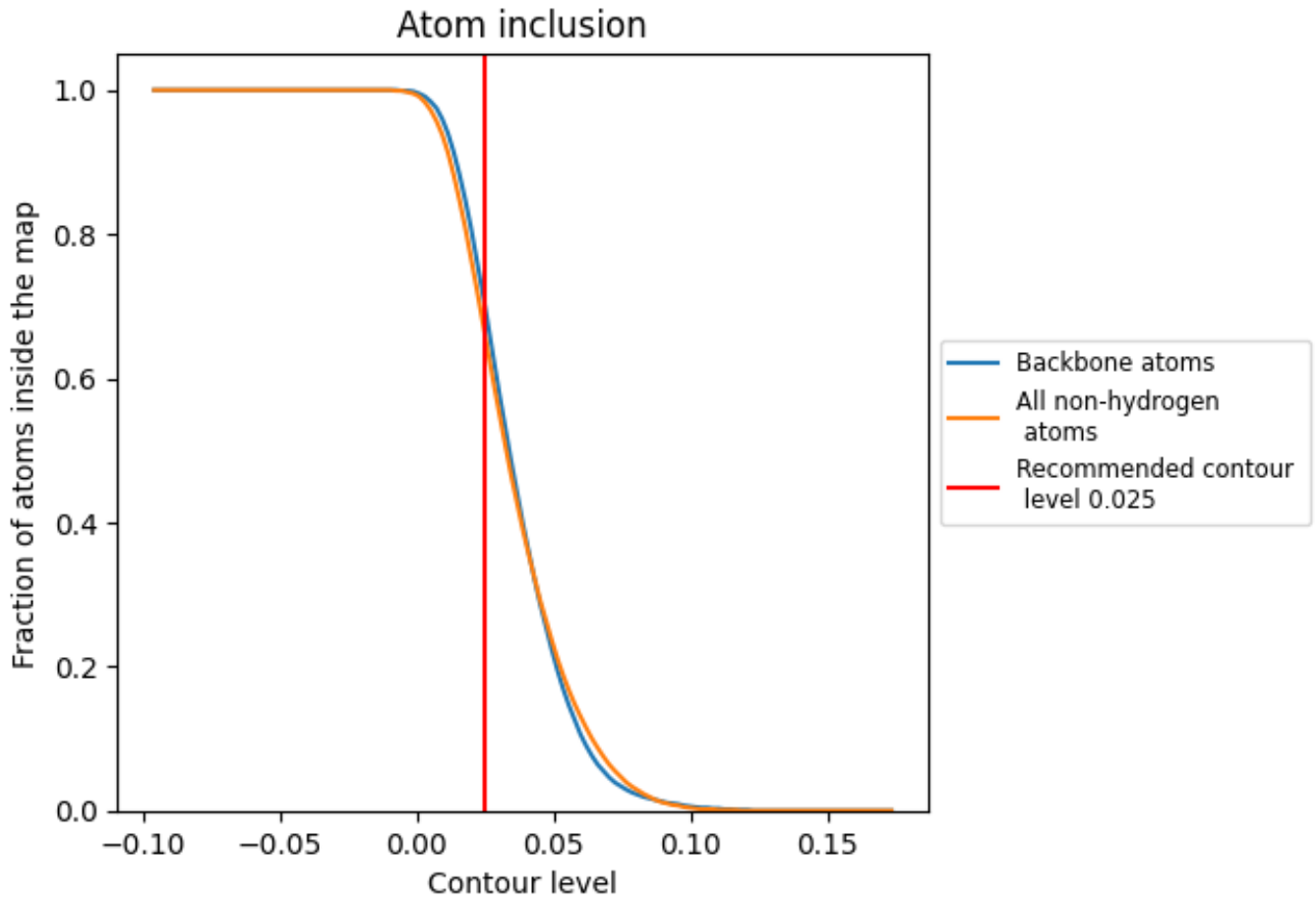
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6580	0.5340
0	0.4960	0.5080
1	0.6680	0.5450
2	0.5900	0.5190
3	0.6890	0.5490
4	0.1590	0.3490
5	0.7690	0.5920
6	0.6670	0.5580
7	0.8050	0.6050
8	0.7950	0.5970
9	0.6790	0.5630
A	0.8020	0.5750
B	0.6380	0.5140
D	0.6980	0.5650
G	0.7450	0.5870
H	0.7660	0.5900
I	0.6670	0.5530
J	0.3340	0.4490
K	0.3660	0.4460
M	0.7530	0.5880
N	0.7130	0.5730
O	0.6250	0.5350
P	0.7110	0.5620
Q	0.7370	0.5750
R	0.4380	0.4590
S	0.7160	0.5630
T	0.7580	0.5830
U	0.7170	0.5770
V	0.7460	0.5790
W	0.6640	0.5460
X	0.5380	0.5250
Z	0.7360	0.5810
a	0.5980	0.5070
b	0.3050	0.4010
c	0.1630	0.3880

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Chain	Atom inclusion	Q-score
d	0.3690	0.4470
e	0.2500	0.4260
f	0.4360	0.4920
g	0.1370	0.3280
h	0.2870	0.4300
i	0.3660	0.4630
j	0.3230	0.4270
k	0.2470	0.4010
l	0.2080	0.3950
m	0.4650	0.5100
n	0.2820	0.4100
o	0.5100	0.4980
p	0.3580	0.4250
q	0.4020	0.4740
r	0.3280	0.4650
s	0.2390	0.4010
t	0.3110	0.4380
u	0.3960	0.4520