Full wwPDB EM Validation Report (i)

Jul 3, 2024 – 04:34 am BST

PDB ID	:	7NHK
EMDB ID	:	EMD-12331
Title	:	LsaA, an antibiotic resistance ABCF, in complex with 70S ribosome from Enterococcus faecalis
Authors	:	Crowe-McAuliffe, C.; Kasari, M.; Hauryliuk, V.H.; Wilson, D.N.
Deposited on	:	2021-02-10
Resolution	:	2.90 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

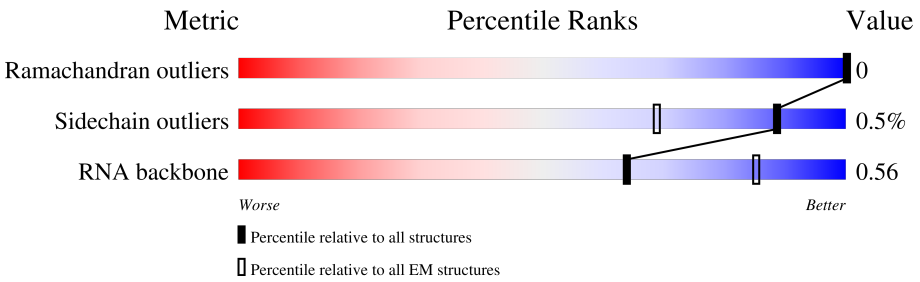
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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	541	32% 91% 9%
2	1	62	31% 95% 5%
3	2	59	15% 97% •
4	4	59	• 90% 10%
5	5	49	8% 98% •
6	6	44	11% 98% •
7	7	66	• 95% • •
8	8	38	13% 100%

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Mol	Chain	Length	Quality of chain
9	A	2912	10% 79% 20%
10	B	116	6% 74% 23%
11	G	276	11% 98%
12	H	209	11% 99%
13	I	207	18% 99%
14	J	179	77% 97%
15	K	178	51% 97%
16	M	147	14% 99%
17	N	122	17% 99%
18	O	146	21% 100%
19	P	144	8% 93% 7%
20	Q	127	16% 98%
21	R	118	31% 98%
22	S	115	20% 98%
23	T	119	8% 97%
24	U	102	17% 99%
25	V	115	9% 96%
26	W	96	14% 95% 5%
27	X	103	34% 98%
28	Y	95	78% 22%
29	Z	62	21% 97%
30	a	1558	10% 79% 18%
31	c	261	59% 85% 15%
32	d	218	40% 94% 6%
33	e	203	50% 97%

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Mol	Chain	Length	Quality of chain
34	f	166	39% 98%
35	g	100	92% 97%
36	h	156	47% 97%
37	i	132	43% 99%
38	j	130	35% 96%
39	k	102	53% 93% 6%
40	l	129	59% 88% 10%
41	m	137	25% 98%
42	n	121	50% 94% 6%
43	o	61	10% 97%
44	p	89	51% 96%
45	q	91	40% 96%
46	r	88	35% 92% 8%
47	s	79	63% 81% 16%
48	t	92	40% 88% 12%
49	u	83	27% 96%
50	D	77	18% 79% 17%
51	b	20	30% 50% 15% 35%
52	F	229	58% 58% 42%
53	3	89	55% 61% 38%

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 146150 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 ABC-F type ribosomal protection protein Lsa(A).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	495	4018	2557	688	764	9	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	142	GLN	GLU	engineered mutation	UNP A0A4U4C430
0	452	GLN	GLU	engineered mutation	UNP A0A4U4C430
0	499	GLY	-	expression tag	UNP A0A4U4C430
0	500	HIS	-	expression tag	UNP A0A4U4C430
0	501	HIS	-	expression tag	UNP A0A4U4C430
0	502	HIS	-	expression tag	UNP A0A4U4C430
0	503	HIS	-	expression tag	UNP A0A4U4C430
0	504	HIS	-	expression tag	UNP A0A4U4C430
0	505	HIS	-	expression tag	UNP A0A4U4C430
0	506	ALA	-	expression tag	UNP A0A4U4C430
0	507	LYS	-	expression tag	UNP A0A4U4C430
0	508	GLY	-	expression tag	UNP A0A4U4C430
0	509	GLY	-	expression tag	UNP A0A4U4C430
0	510	GLU	-	expression tag	UNP A0A4U4C430
0	511	ASN	-	expression tag	UNP A0A4U4C430
0	512	LEU	-	expression tag	UNP A0A4U4C430
0	513	TYR	-	expression tag	UNP A0A4U4C430
0	514	PHE	-	expression tag	UNP A0A4U4C430
0	515	GLN	-	expression tag	UNP A0A4U4C430
0	516	GLY	-	expression tag	UNP A0A4U4C430
0	517	VAL	-	expression tag	UNP A0A4U4C430
0	518	ALA	-	expression tag	UNP A0A4U4C430
0	519	ASP	-	expression tag	UNP A0A4U4C430
0	520	TYR	-	expression tag	UNP A0A4U4C430
0	521	LYS	-	expression tag	UNP A0A4U4C430
0	522	ASP	-	expression tag	UNP A0A4U4C430
0	523	HIS	-	expression tag	UNP A0A4U4C430

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Chain	Residue	Modelled	Actual	Comment	Reference
0	524	ASP	-	expression tag	UNP A0A4U4C430
0	525	GLY	-	expression tag	UNP A0A4U4C430
0	526	ASP	-	expression tag	UNP A0A4U4C430
0	527	TYR	-	expression tag	UNP A0A4U4C430
0	528	LYS	-	expression tag	UNP A0A4U4C430
0	529	ASP	-	expression tag	UNP A0A4U4C430
0	530	HIS	-	expression tag	UNP A0A4U4C430
0	531	ASP	-	expression tag	UNP A0A4U4C430
0	532	ILE	-	expression tag	UNP A0A4U4C430
0	533	ASP	-	expression tag	UNP A0A4U4C430
0	534	TYR	-	expression tag	UNP A0A4U4C430
0	535	LYS	-	expression tag	UNP A0A4U4C430
0	536	ASP	-	expression tag	UNP A0A4U4C430
0	537	ASP	-	expression tag	UNP A0A4U4C430
0	538	ASP	-	expression tag	UNP A0A4U4C430
0	539	ASP	-	expression tag	UNP A0A4U4C430
0	540	LYS	-	expression tag	UNP A0A4U4C430
0	541	GLY	-	expression tag	UNP A0A4U4C430

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	59	491	307	91	92	1	0	0

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	57	428	266	80	81	1	0	0

- Molecule 4 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	53	406	248	84	69	5	0	0

- Molecule 5 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	48	410	247	84	75	4	0	0

- Molecule 6 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	43	369	224	90	53	2	0	0

- Molecule 7 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	7	64	522	320	122	78	2	0	0

- Molecule 8 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	8	38	305	188	66	45	6	0	0

- Molecule 9 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	A	2905	62352	27832	11466	20149	2905	0	0

- Molecule 10 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	B	114	2439	1088	439	798	114	0	0

- Molecule 11 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	G	274	2106	1305	414	380	7	0	0

- Molecule 12 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	H	207	1579	994	292	289	4	0	0

- Molecule 13 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	205	1572	984	289	297	2	0	0

- Molecule 14 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	J	176	1383	882	237	258	6	0	0

- Molecule 15 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	K	174	1335	838	242	251	4	0	0

- Molecule 16 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	M	145	1130	715	205	207	3	0	0

- Molecule 17 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	N	122	923	574	176	171	2	0	0

- Molecule 18 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	O	146	1096	677	212	206	1	0	0

- Molecule 19 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	P	134	1070	683	209	173	5	0	0

- Molecule 20 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Q	125	997	615	192	187	3	0	0

- Molecule 21 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	R	117	900	556	175	168	1	0	0

- Molecule 22 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	S	114	925	582	185	158	0	0

- Molecule 23 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	T	116	935	593	181	157	4	0	0

- Molecule 24 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	U	101	779	497	138	142	2	0	0

- Molecule 25 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	V	111	841	527	154	158	2	0	0

- Molecule 26 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	W	91	736	469	129	134	4	0	0

- Molecule 27 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	X	101	763	486	135	140	2	0	0

- Molecule 28 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	Y	74	559	344	107	108	0	0

- Molecule 29 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Z	60	473	294	96	81	2	0	0

- Molecule 30 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
30	a	1517	32512	14505	5942	10548	1517	0	0

- Molecule 31 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	c	222	1773	1126	312	326	9	0	0

- Molecule 32 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	d	206	1626	1024	305	294	3	0	0

- Molecule 33 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	e	200	1611	1010	301	296	4	0	0

- Molecule 34 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	f	163	1197	752	222	221	2	0	0

- Molecule 35 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	g	97	795	501	137	154	3	0	0

- Molecule 36 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	h	153	1218	759	232	221	6	0	0

- Molecule 37 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	i	131	1041	662	184	193	2	0	0

- Molecule 38 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	j	128	989	615	197	176	1	0	0

- Molecule 39 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	k	96	773	487	142	142	2	0	0

- Molecule 40 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	l	116	854	527	163	160	4	0	0

- Molecule 41 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	m	135	1060	658	213	187	2	0	0

- Molecule 42 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	n	114	902	552	183	166	1	0	0

- Molecule 43 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	o	60	492	310	100	77	5	0	0

- Molecule 44 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	p	85	716	440	146	129	1	0	0

- Molecule 45 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	q	87	692	437	128	125	2	0	0

- Molecule 46 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	r	81	669	419	125	122	3	0	0

- Molecule 47 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	s	66	542	346	105	90	1	0	0

- Molecule 48 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	t	81	659	424	121	112	2	0	0

- Molecule 49 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	u	80	603	368	117	116	2	0	0

- Molecule 50 is a RNA chain called tRNA-fMETi.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
50	D	74	1582	705	287	516	74	0	0

- Molecule 51 is a RNA chain called RNA (5'-R(P*GP*GP*AP*GP*GP*UP*AP*UP*GP*AP*CP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
51	b	13	285	127	57	88	13	0	0

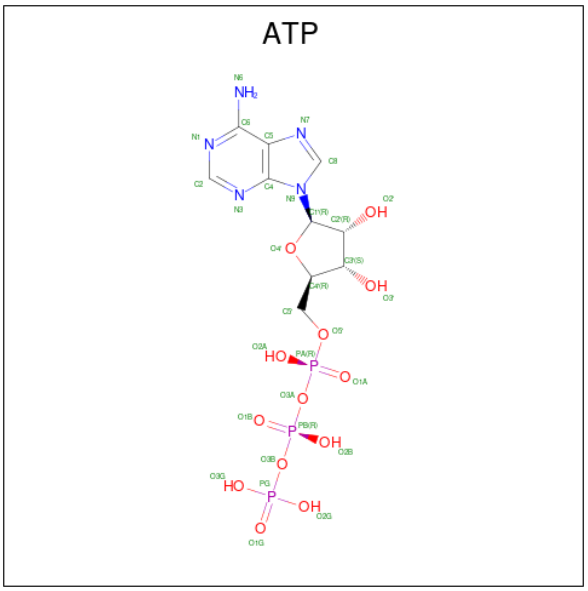
- Molecule 52 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	F	132	1004	635	172	197	0	0

- Molecule 53 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	3	55	448	289	76	81	2	0	0

- Molecule 54 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
54	0	1	Total	C	N	O	P	0
			31	10	5	13	3	
54	0	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	0	2	Total	Mg	0
			2	2	
55	A	117	Total	Mg	0
			117	117	
55	B	1	Total	Mg	0
			1	1	
55	O	1	Total	Mg	0
			1	1	
55	a	25	Total	Mg	0
			25	25	
55	D	1	Total	Mg	0
			1	1	

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	4	1	Total	Zn	0
			1	1	

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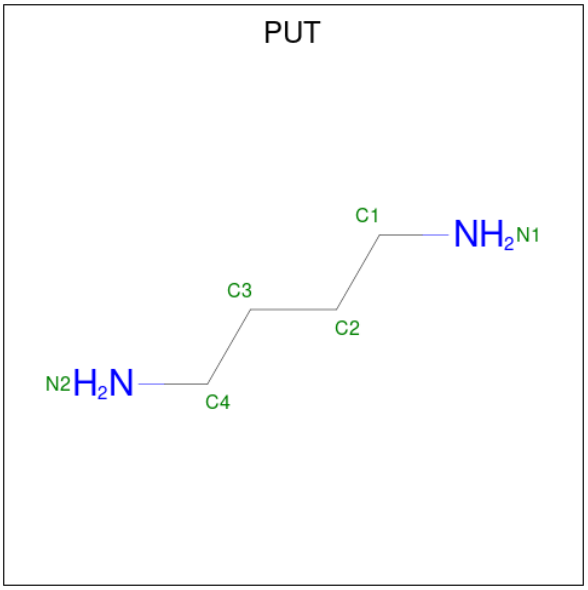
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
56	8	1	1	1	0
			Total	Zn	
56	o	1	1	1	0

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
57	A	21	21	21	0
			Total	K	
57	P	1	1	1	0
			Total	K	
57	a	7	7	7	0

- Molecule 58 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



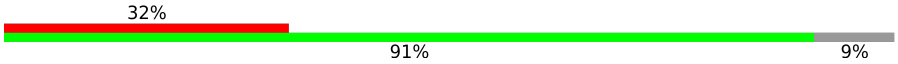
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
58	A	1	6	4	2	0
			Total	C	N	
58	A	1	6	4	2	0
			Total	C	N	
58	a	1	6	4	2	0
			Total	C	N	
58	a	1	6	4	2	0

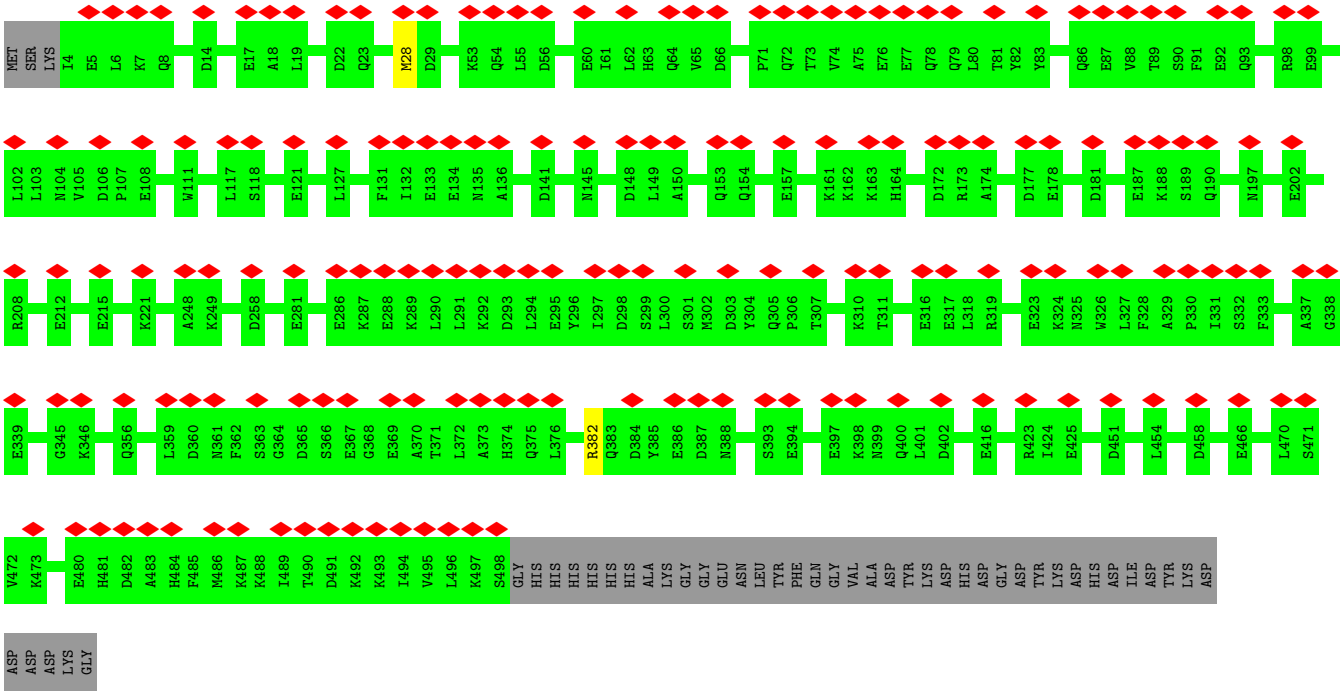
3 Residue-property plots (i)

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: ABC-F type ribosomal protection protein Lsa(A)

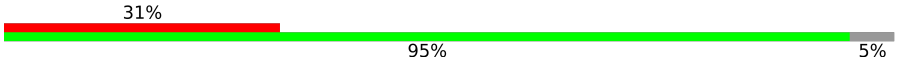
Chain 0:

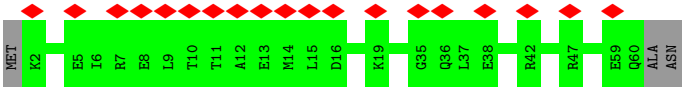




- Molecule 2: 50S ribosomal protein L29

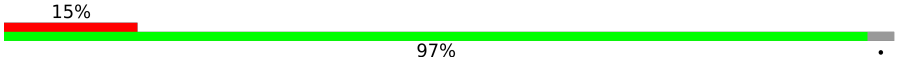
Chain 1:

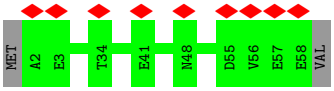




- Molecule 3: 50S ribosomal protein L30

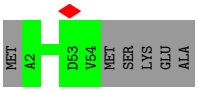
Chain 2:





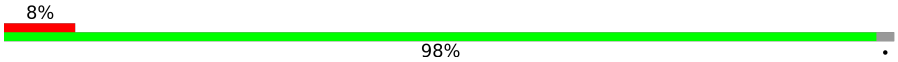
• Molecule 4: 50S ribosomal protein L32

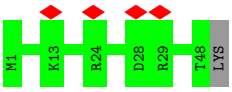
Chain 4:



• Molecule 5: 50S ribosomal protein L33

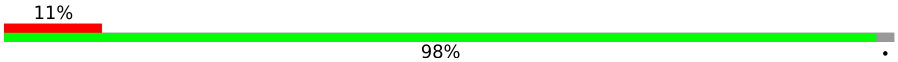
Chain 5:

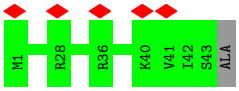




• Molecule 6: 50S ribosomal protein L34

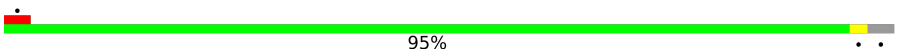
Chain 6:

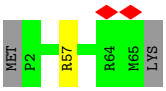




• Molecule 7: 50S ribosomal protein L35

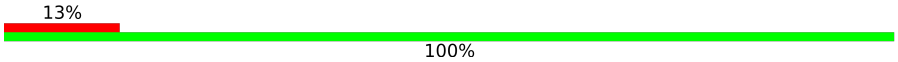
Chain 7:

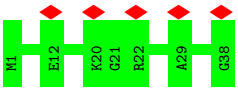




• Molecule 8: 50S ribosomal protein L36

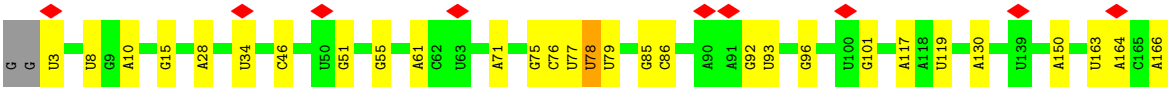
Chain 8:

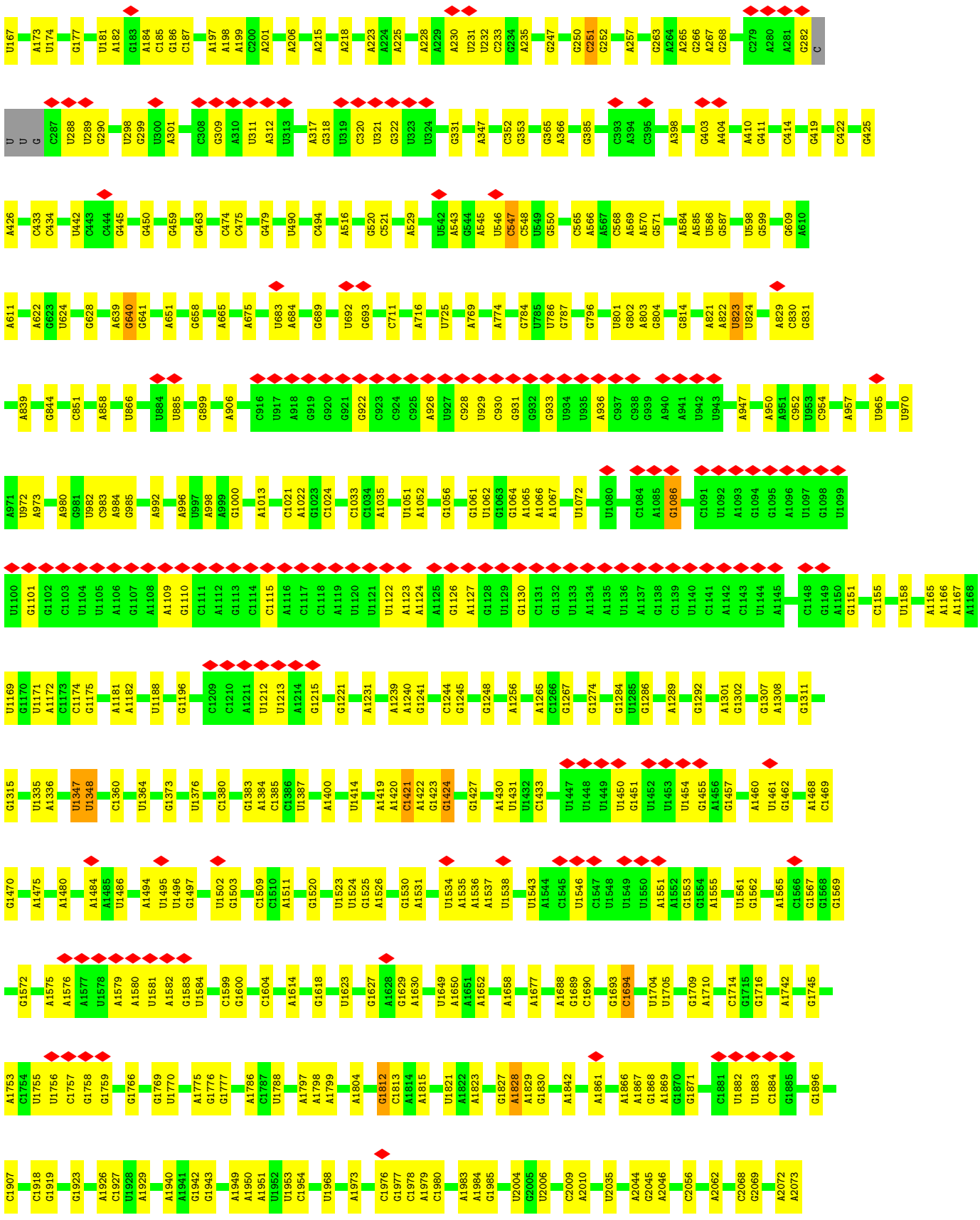




• Molecule 9: 23S rRNA

Chain A:

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U U G C287 U288 U289 G290 U298 G299 U300 A301 C308 G309 A310 U311 A312 U313 A317 G318 U319 C320 U321 G322 U323 U324 G331 A347 C352 G353 G365 A366 G385 C393 A394 C395 A398 G403 A404 A410 G411 C414 G419 C422 G425
A426 C433 C434 U442 C443 C444 G445 G450 G459 G463 C474 C475 G479 U490 G494 A516 G520 C521 A529 U542 A543 G544 A545 U546 C547 C548 U549 G550 C565 A566 A567 C568 A569 A570 G571 A584 A585 U586 G587 U598 G599 G609 A610
A611 A622 G623 U624 G628 A639 G640 G641 A651 G658 A665 A675 U683 A684 G689 U692 G693 C711 A716 U725 A769 A774 G784 U785 U786 G787 G796 U801 G802 A803 G804 G814 A821 A822 U823 U824 A829 C830 G831
A839 G844 C851 A858 U866 U884 U885 G899 A906 C916 U917 A918 G919 G920 G921 G922 C923 C924 C925 A926 U927 C928 U929 C930 G931 G932 G933 U934 U935 A936 C937 C938 G939 A940 A941 U942 U943 A947 A950 A951 C952 U953 C954 A957 U965 U970
A971 U972 A973 A980 G981 U982 C983 A984 G985 A992 A996 U997 A998 A999 G1000 A1013 C1021 A1022 G1023 C1024 C1033 C1034 A1035 U1051 A1052 G1056 G1061 U1062 G1063 G1064 A1065 A1066 A1067 U1072 U1080 C1084 A1085 G1086 C1091 U1092 A1093 G1094 G1095 A1096 U1097 G1098 U1099
U1100 G1101 G1102 C1103 U1104 U1105 A1106 G1107 A1108 A1109 G1110 C1111 A1112 G1113 C1114 C1115 A1116 C1117 C1118 A1119 U1120 U1121 U1122 A1123 A1124 A1125 G1126 A1127 G1128 U1129 G1130 C1131 G1132 U1133 A1134 A1135 U1136 A1137 G1138 C1139 U1140 C1141 A1142 C1143 U1144 A1145 C1148 G1149 A1150 G1151 C1155 U1158 A1165 A1166 A1167 A1168
U1169 G1170 U1171 A1172 C1173 C1174 G1175 A1181 A1182 U1188 G1196 C1209 C1210 A1211 U1212 U1213 A1214 G1215 G1221 A1231 A1239 A1240 G1241 C1244 G1245 G1248 A1256 A1265 C1266 G1267 G1274 G1284 U1285 G1286 A1289 G1292 A1301 G1302 G1307 A1308 G1311
G1315 U1335 A1336 U1347 U1348 C1360 U1364 G1373 U1376 C1380 G1383 A1384 C1385 C1386 U1387 A1400 U1414 A1419 A1420 C1421 A1422 G1423 G1424 G1427 A1430 U1431 U1432 C1433 U1447 U1448 U1449 U1450 G1451 U1452 U1453 U1454 G1455 A1456 G1457 A1460 U1461 G1462 A1468 C1469
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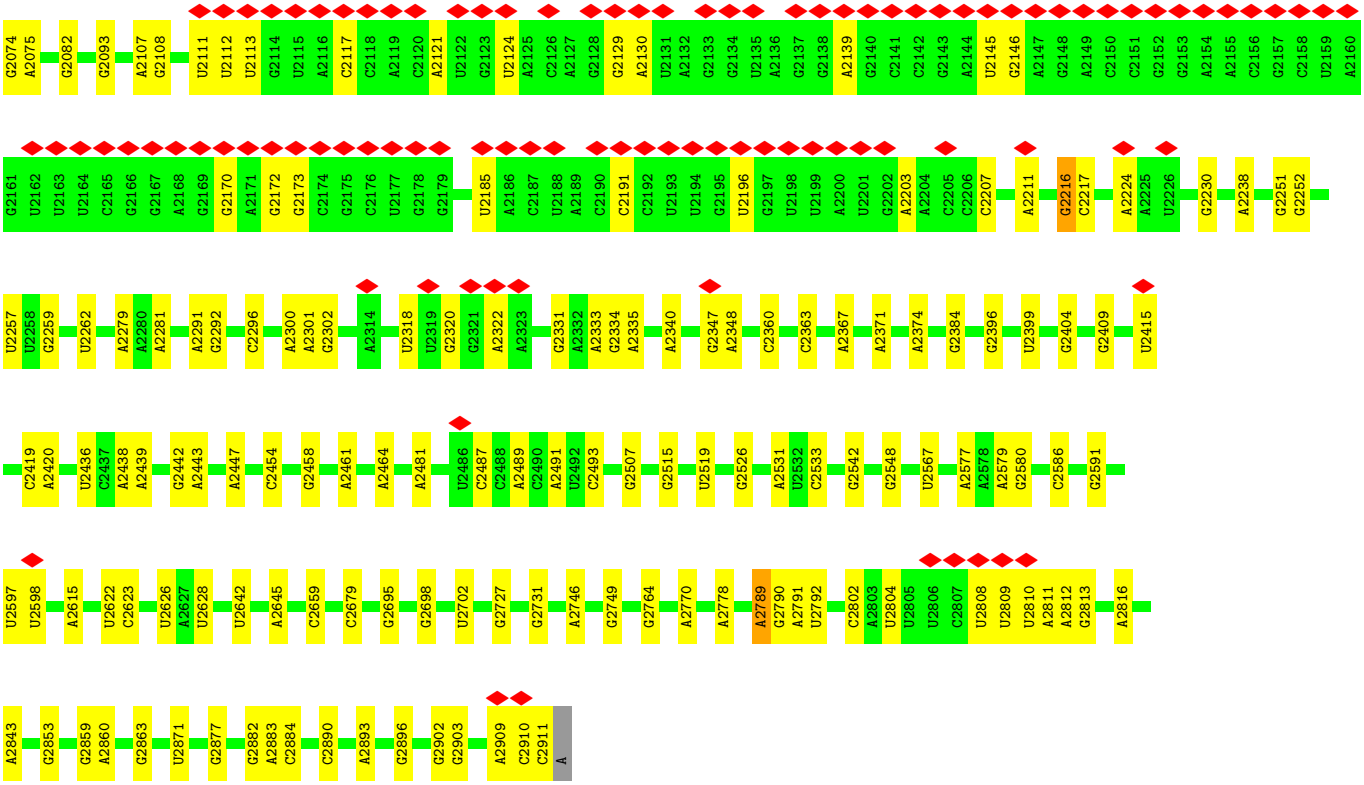
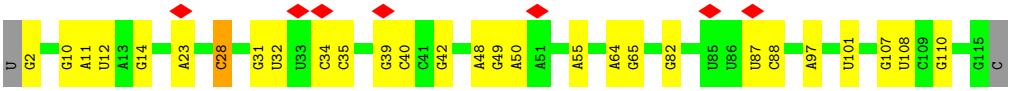
C1907 C1918 G1919 G1923 A1926 C1927 U1928 A1929 A1940 A1941 G1942 G1943 A1949 A1950 A1951 U1952 U1953 C1954 U1968 A1973 C1976 G1977 C1978 A1979 C1980 A1983 A1984 G1985 U2004 G2005 U2006 C2009 A2010 U2035 A2044 G2045 A2046 C2056 A2062 C2068 G2069 A2072 A2073



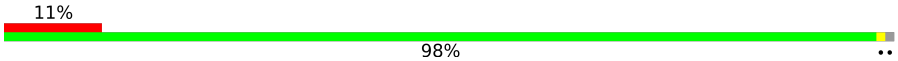
- Molecule 10: 5S rRNA

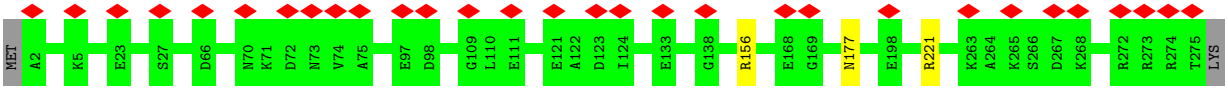
Chain B:



- Molecule 11: 50S ribosomal protein L2

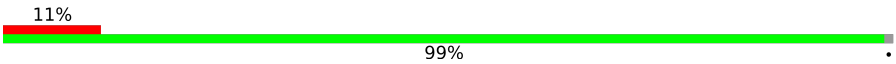
Chain G:

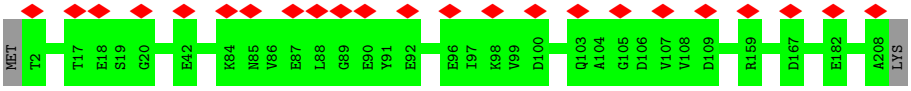




- Molecule 12: 50S ribosomal protein L3

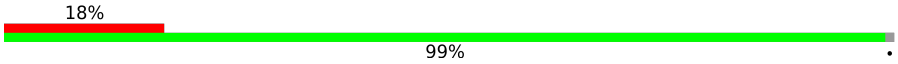
Chain H:

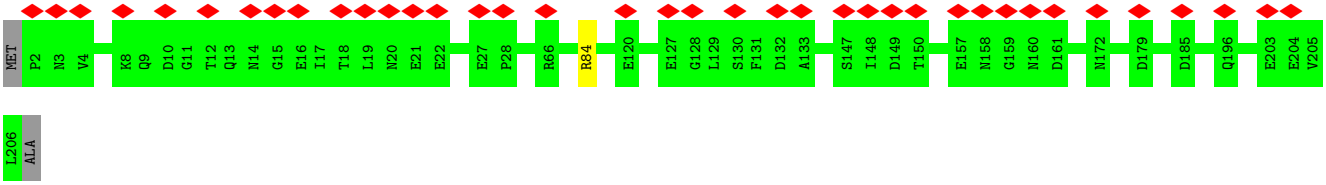




- Molecule 13: 50S ribosomal protein L4

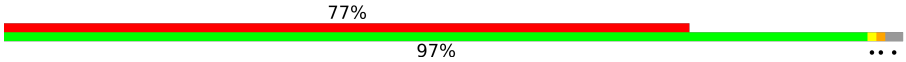
Chain I:

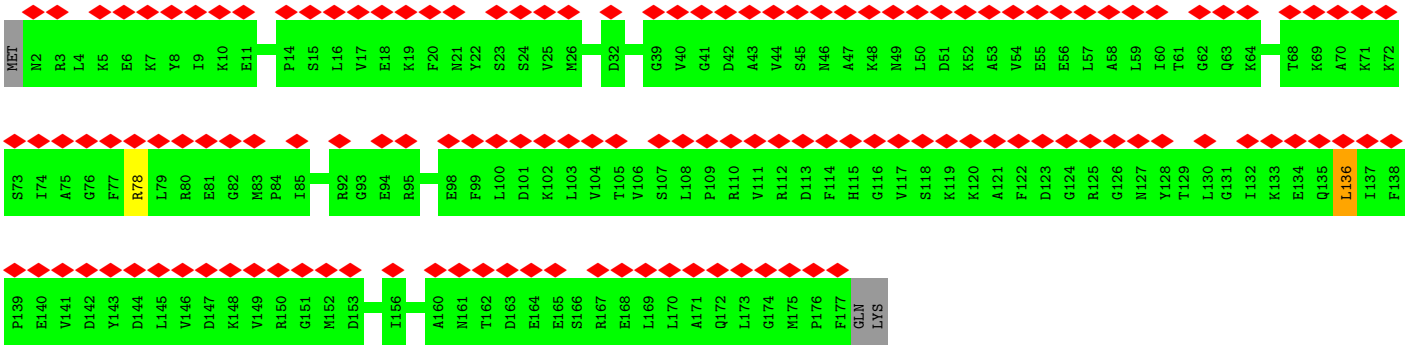




• Molecule 14: 50S ribosomal protein L5

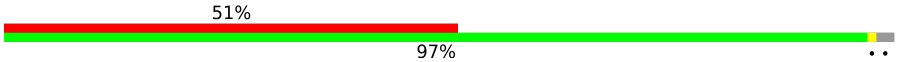
Chain J:

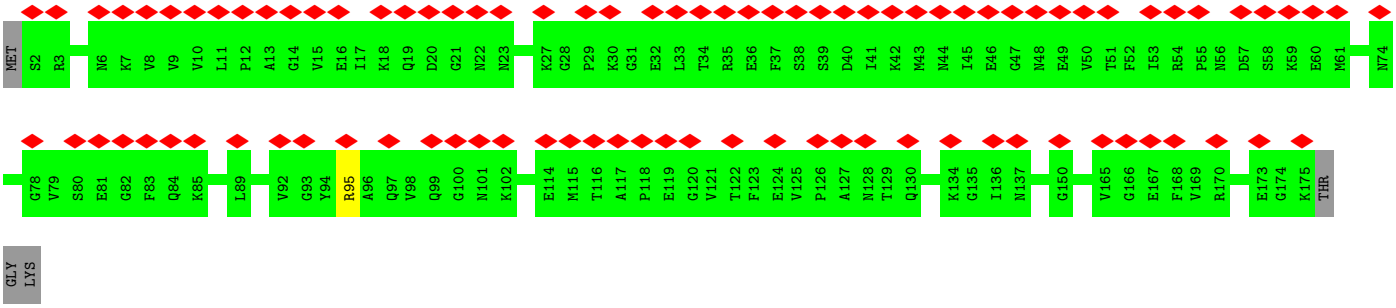




• Molecule 15: 50S ribosomal protein L6

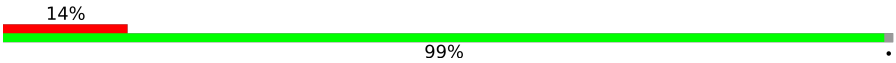
Chain K:

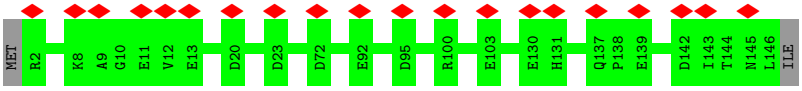




• Molecule 16: 50S ribosomal protein L13

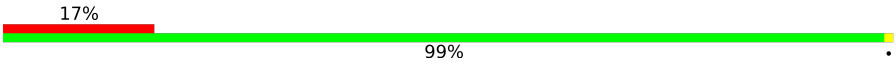
Chain M:

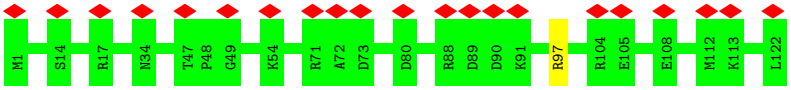




• Molecule 17: 50S ribosomal protein L14

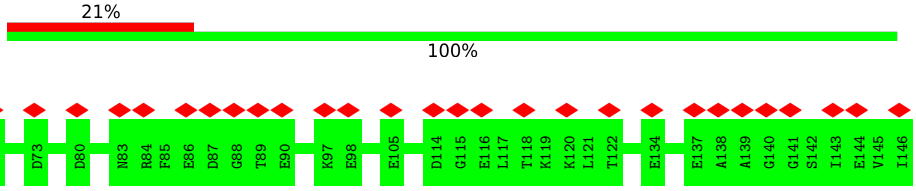
Chain N:





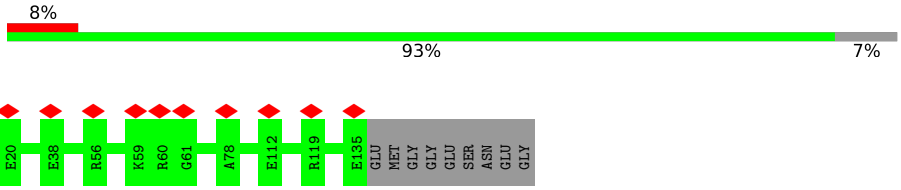
- Molecule 18: 50S ribosomal protein L15

Chain O:



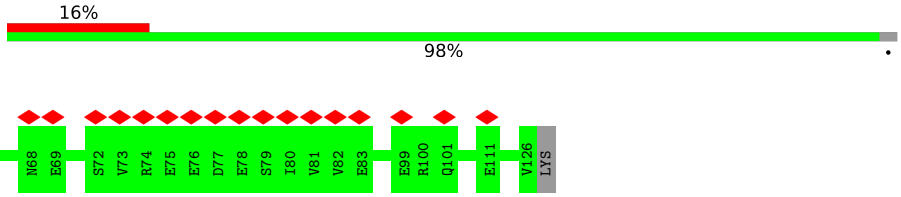
- Molecule 19: 50S ribosomal protein L16

Chain P:



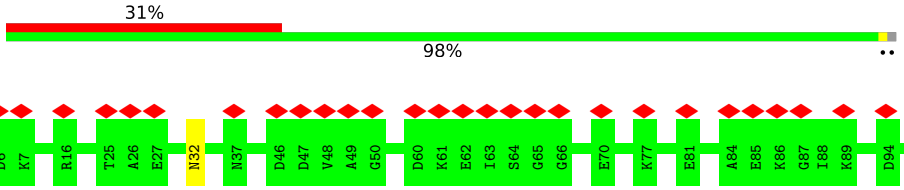
- Molecule 20: 50S ribosomal protein L17

Chain Q:



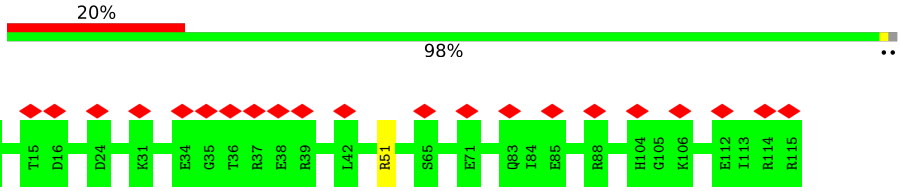
- Molecule 21: 50S ribosomal protein L18

Chain R:



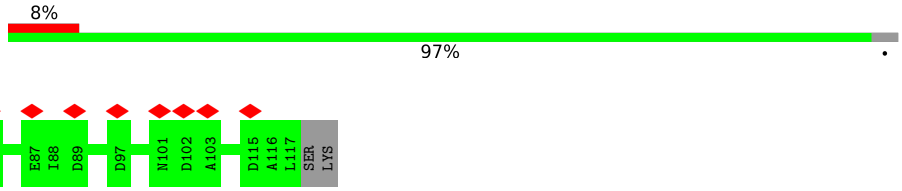
- Molecule 22: 50S ribosomal protein L19

Chain S:



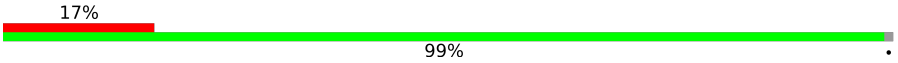
- Molecule 23: 50S ribosomal protein L20

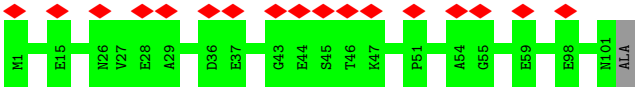
Chain T:



- Molecule 24: 50S ribosomal protein L21

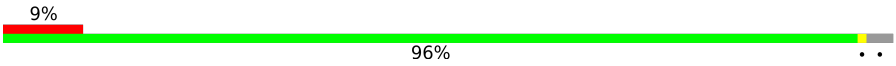
Chain U:

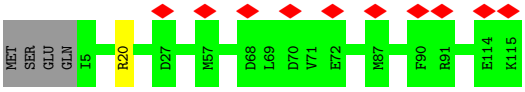




• Molecule 25: 50S ribosomal protein L22

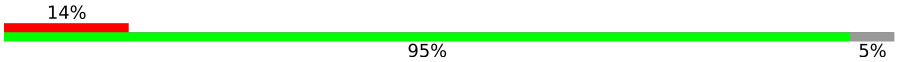
Chain V:

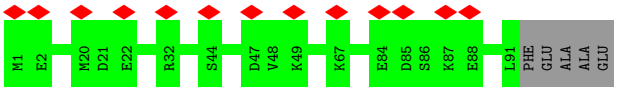




• Molecule 26: 50S ribosomal protein L23

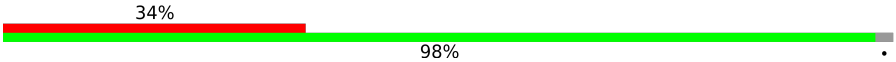
Chain W:

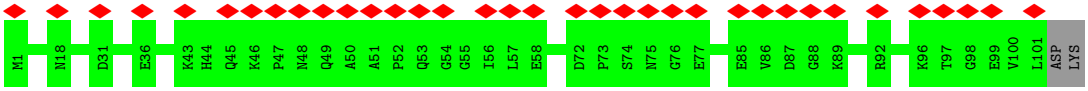




• Molecule 27: 50S ribosomal protein L24

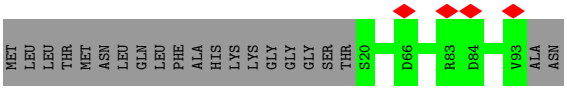
Chain X:





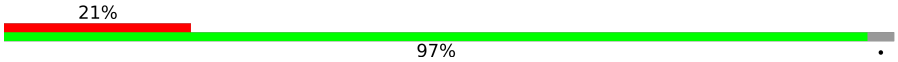
• Molecule 28: 50S ribosomal protein L27

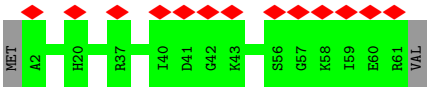
Chain Y:



• Molecule 29: 50S ribosomal protein L28

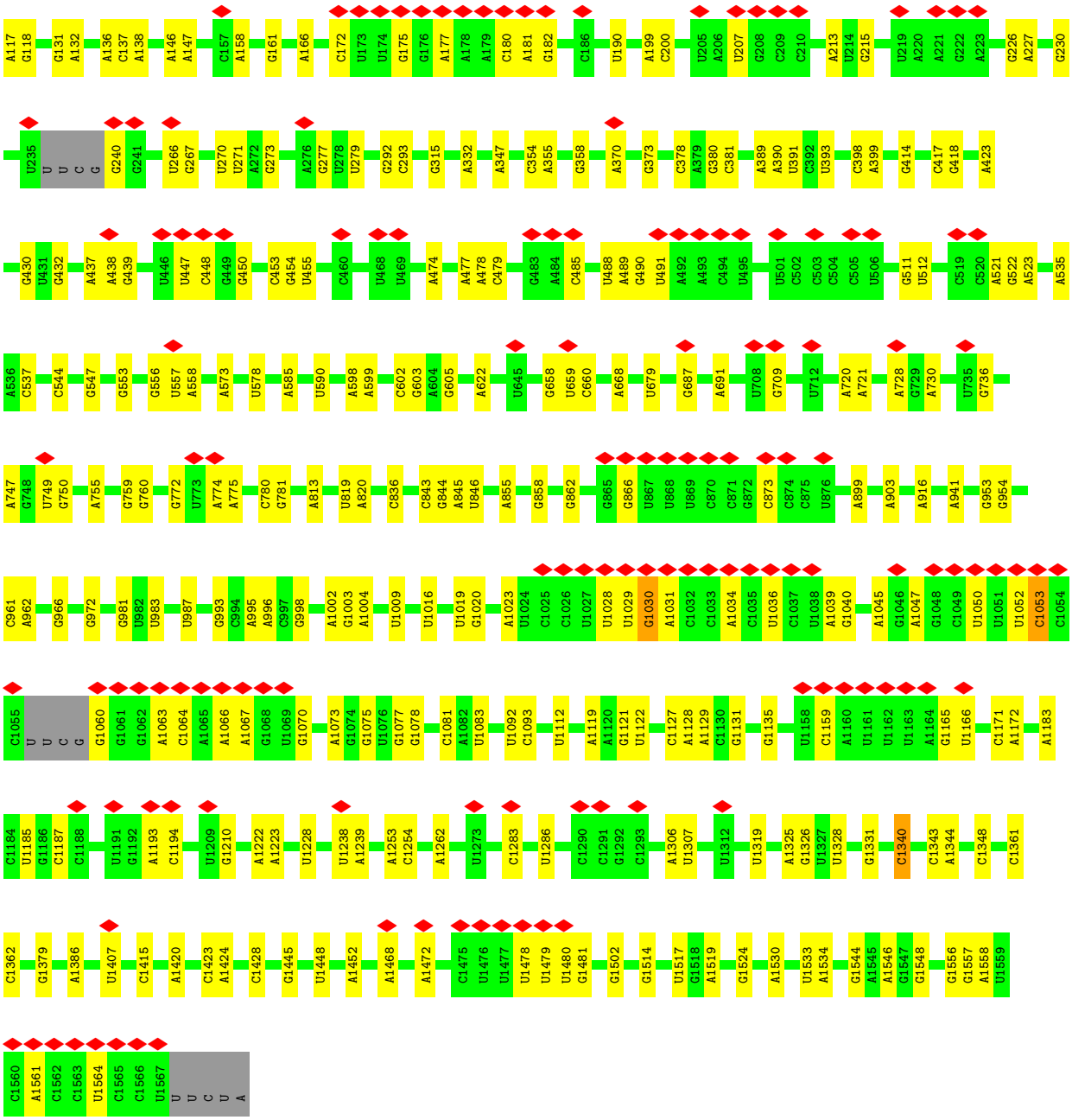
Chain Z:





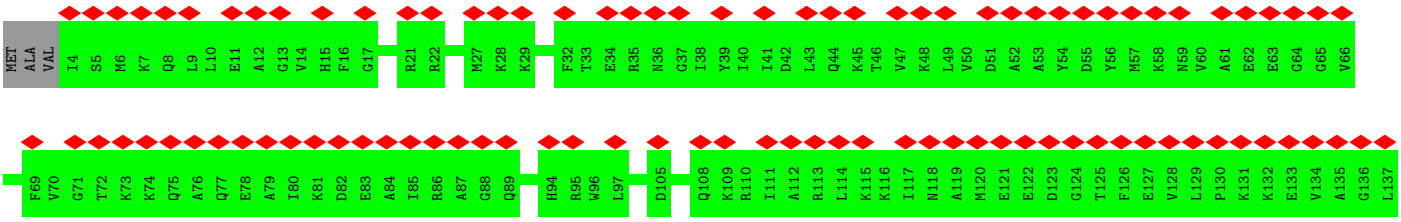
• Molecule 30: 16S rRNA

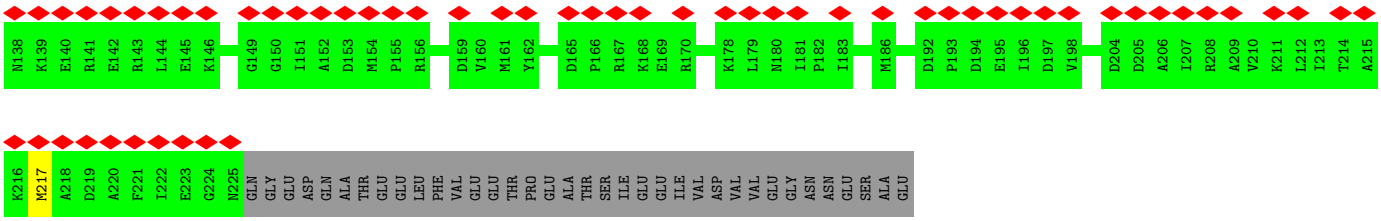
Chain a:



• Molecule 31: 30S ribosomal protein S2

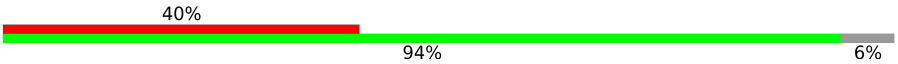
Chain c: 59% 85% 15%

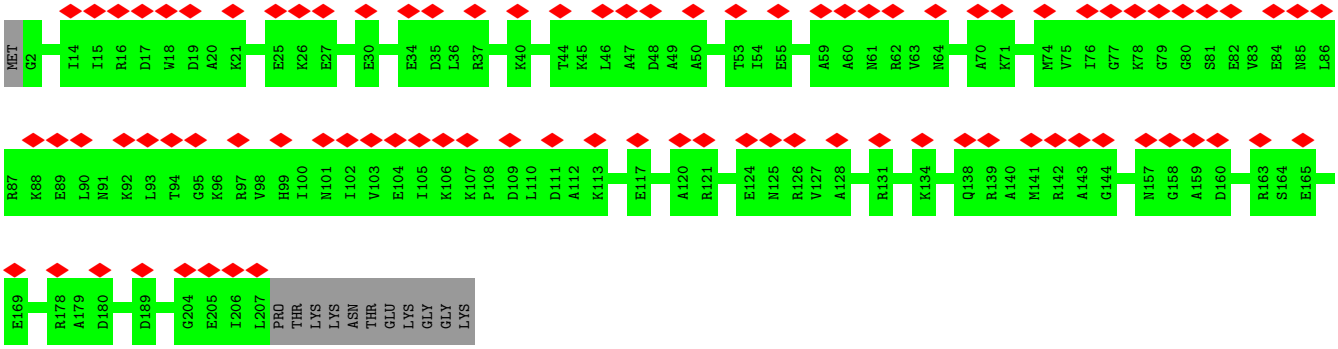




• Molecule 32: 30S ribosomal protein S3

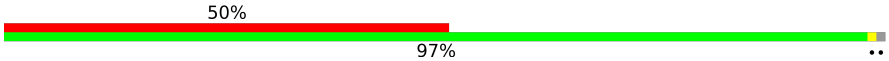
Chain d:

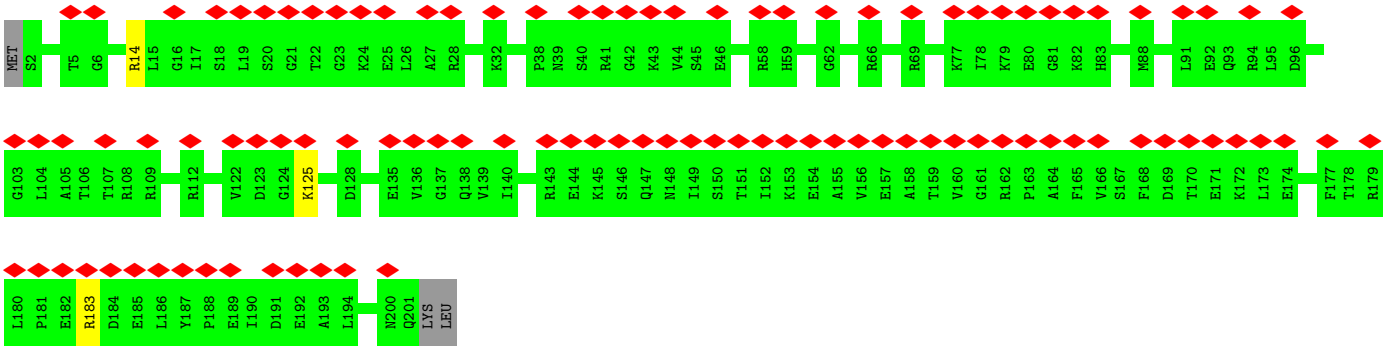




• Molecule 33: 30S ribosomal protein S4

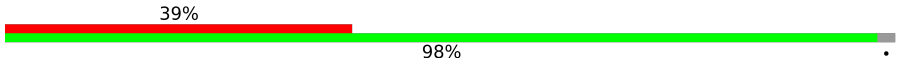
Chain e:

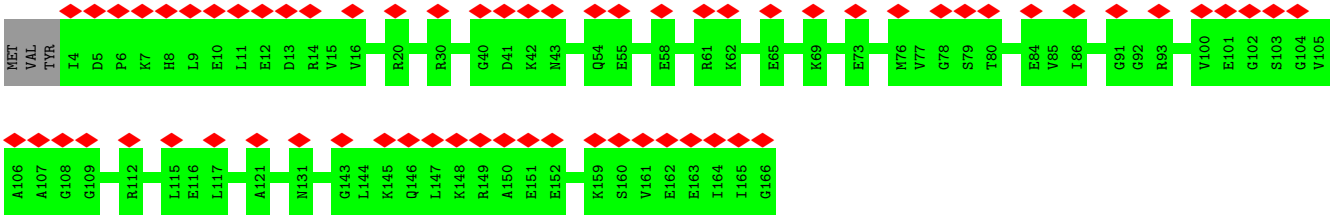




• Molecule 34: 30S ribosomal protein S5

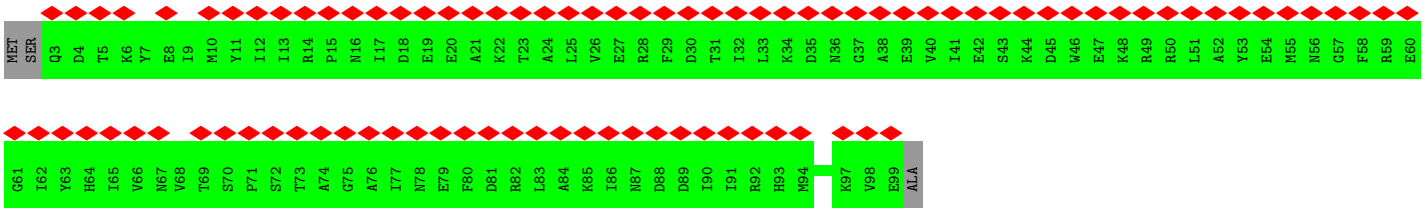
Chain f:





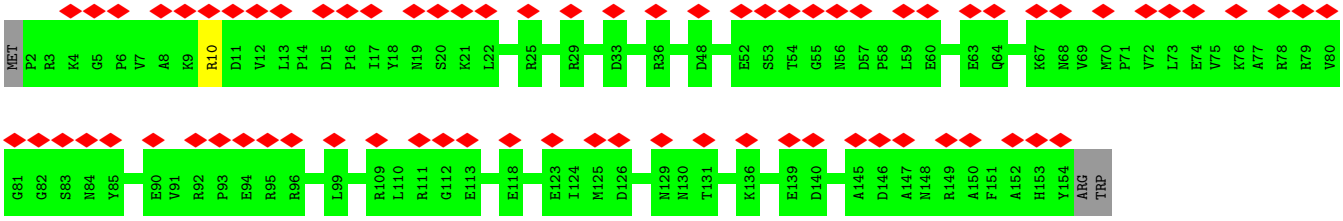
• Molecule 35: 30S ribosomal protein S6

Chain g: 92% 97%



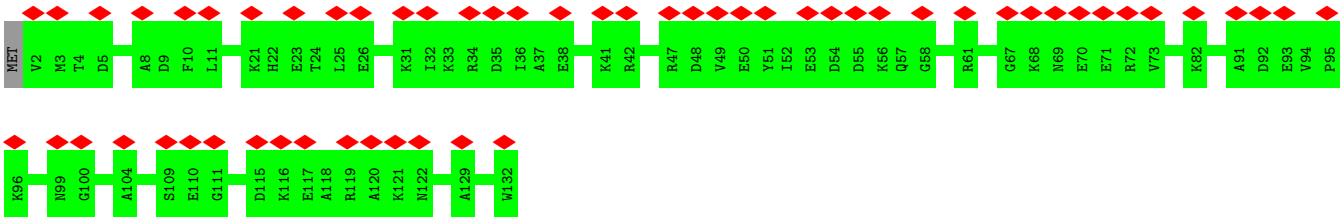
- Molecule 36: 30S ribosomal protein S7

Chain h: 47% 97%



- Molecule 37: 30S ribosomal protein S8

Chain i: 43% 99%

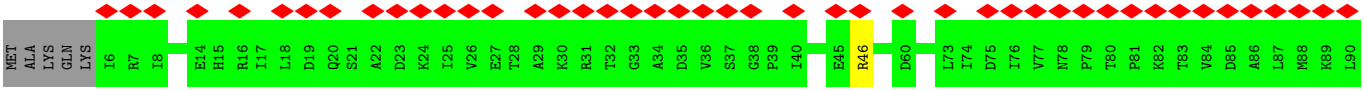


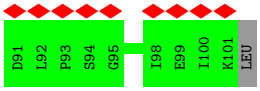
- Molecule 38: 30S ribosomal protein S9

Chain j: 35% 96%

- Molecule 39: 30S ribosomal protein S10

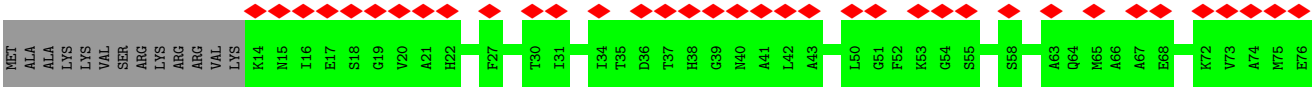
Chain k: 53% 93% 6%

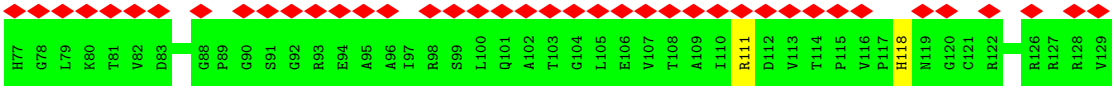




- Molecule 40: 30S ribosomal protein S11

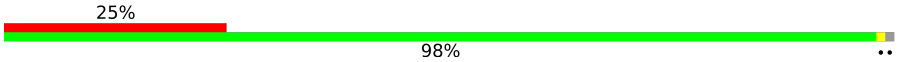
Chain l:

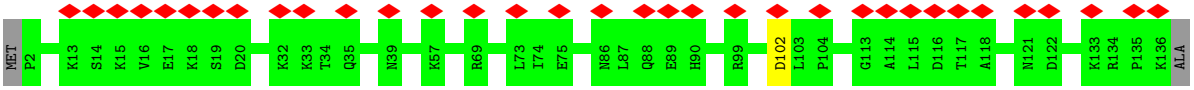




- Molecule 41: 30S ribosomal protein S12

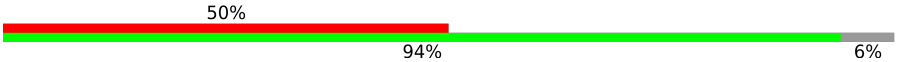
Chain m:

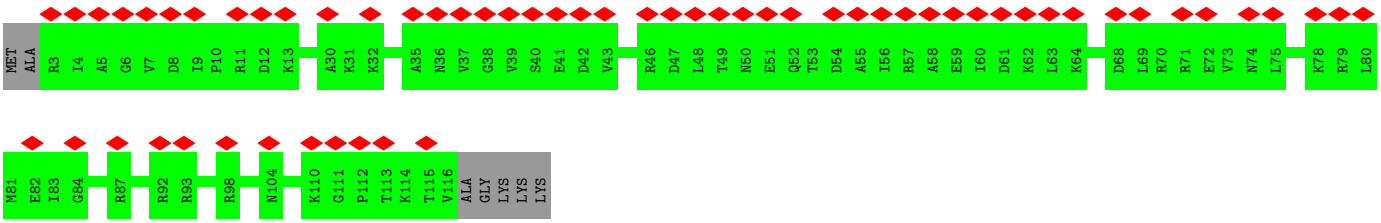




- Molecule 42: 30S ribosomal protein S13

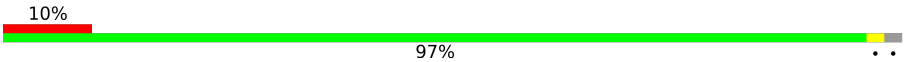
Chain n:

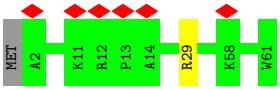




- Molecule 43: 30S ribosomal protein S14 type Z

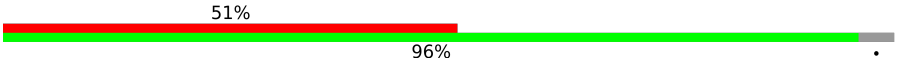
Chain o:

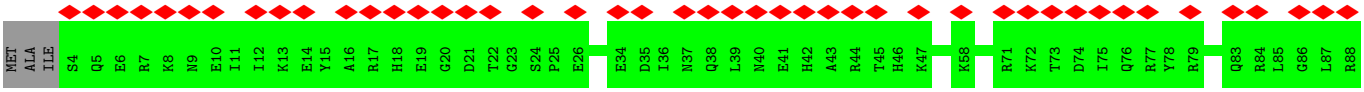




- Molecule 44: 30S ribosomal protein S15

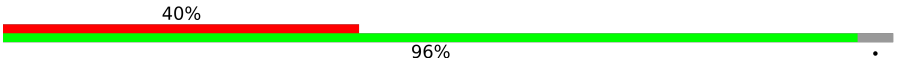
Chain p:

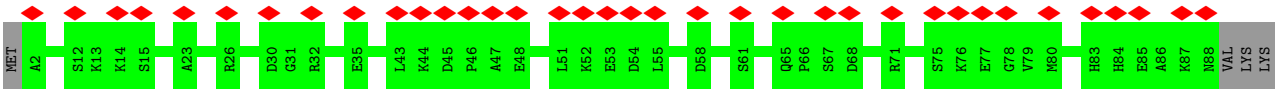




• Molecule 45: 30S ribosomal protein S16

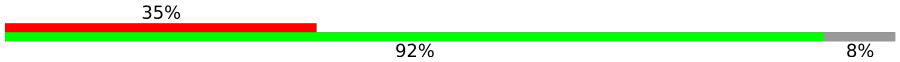
Chain q:

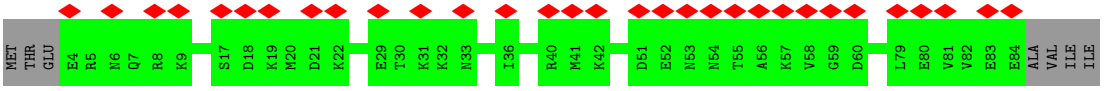




• Molecule 46: 30S ribosomal protein S17

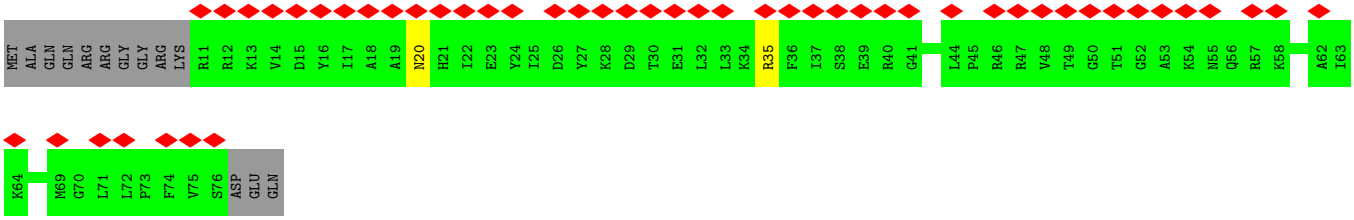
Chain r:





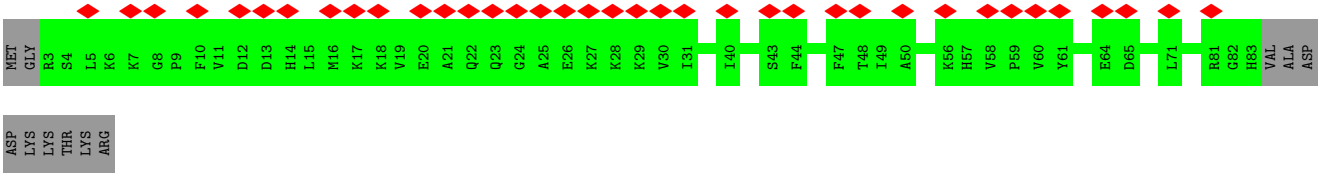
• Molecule 47: 30S ribosomal protein S18

Chain s:



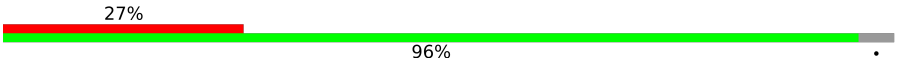
• Molecule 48: 30S ribosomal protein S19

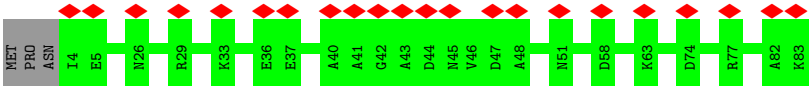
Chain t:



• Molecule 49: 30S ribosomal protein S20

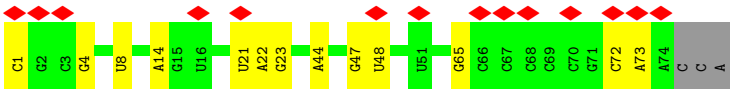
Chain u:





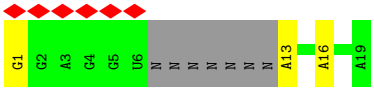
• Molecule 50: tRNA-fMETi

Chain D:



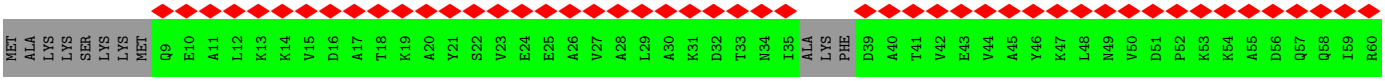
• Molecule 51: RNA (5'-R(P*GP*GP*AP*GP*GP*UP*AP*UP*GP*AP*CP*AP*A)-3')

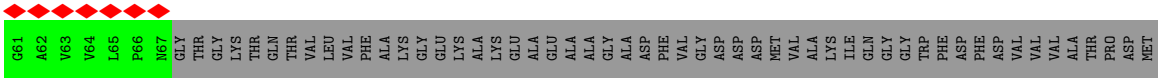
Chain b:

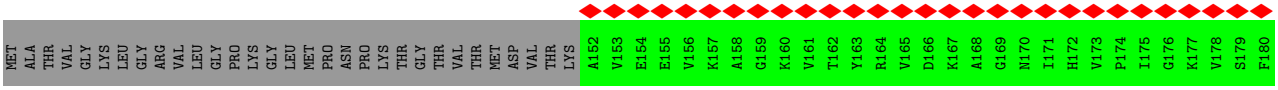


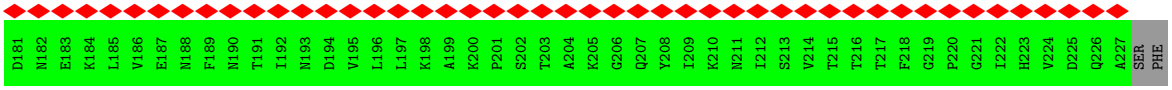
• Molecule 52: 50S ribosomal protein L1

Chain F:



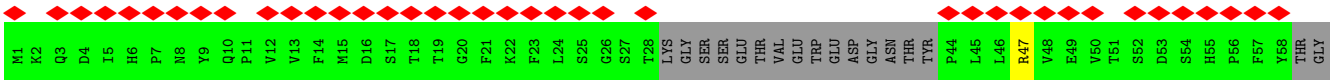


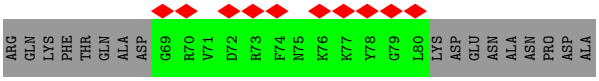




• Molecule 53: 50S ribosomal protein L31 type B

Chain 3:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59262	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 ($e^-/Å^2$)	38	Depositor
Minimum defocus (nm)	-700	Depositor
Maximum defocus (nm)	-2200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.110	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	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: PUT, ATP, MG, ZN, K

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	0.37	0/4089	0.56	0/5506
2	1	0.35	0/492	0.67	0/654
3	2	0.36	0/430	0.59	0/579
4	4	0.49	0/413	0.65	0/549
5	5	0.45	0/414	0.67	0/552
6	6	0.46	0/372	0.79	0/484
7	7	0.46	0/528	0.75	1/689 (0.1%)
8	8	0.46	0/310	0.58	0/409
9	A	0.76	0/69847	0.99	48/108953 (0.0%)
10	B	0.51	0/2728	0.89	2/4252 (0.0%)
11	G	0.45	0/2141	0.66	1/2881 (0.0%)
12	H	0.50	0/1601	0.62	0/2150
13	I	0.49	0/1595	0.60	0/2157
14	J	0.33	0/1402	0.61	1/1885 (0.1%)
15	K	0.34	0/1355	0.58	0/1825
16	M	0.47	0/1151	0.61	0/1555
17	N	0.46	0/930	0.69	1/1247 (0.1%)
18	O	0.46	0/1106	0.68	0/1474
19	P	0.45	0/1093	0.63	0/1457
20	Q	0.43	0/1006	0.65	0/1349
21	R	0.37	0/909	0.63	0/1216
22	S	0.46	0/939	0.73	0/1262
23	T	0.51	0/948	0.65	0/1261
24	U	0.46	0/791	0.59	0/1061
25	V	0.44	0/850	0.66	2/1145 (0.2%)
26	W	0.44	0/743	0.62	0/993
27	X	0.37	0/772	0.57	0/1035
28	Y	0.48	0/565	0.65	0/755
29	Z	0.40	0/479	0.67	0/638
30	a	0.59	0/36394	0.93	20/56758 (0.0%)
31	c	0.30	0/1803	0.53	0/2430
32	d	0.37	0/1651	0.58	0/2219

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	e	0.36	0/1641	0.58	0/2206
34	f	0.36	0/1209	0.57	0/1628
35	g	0.30	0/807	0.60	0/1087
36	h	0.34	0/1238	0.61	0/1668
37	i	0.35	0/1054	0.64	0/1417
38	j	0.37	0/1002	0.63	0/1343
39	k	0.37	0/785	0.62	0/1059
40	l	0.34	0/869	0.58	0/1174
41	m	0.45	1/1077 (0.1%)	0.72	1/1446 (0.1%)
42	n	0.32	0/908	0.60	0/1219
43	o	0.43	0/504	0.66	0/669
44	p	0.32	0/726	0.60	0/969
45	q	0.37	0/704	0.58	0/945
46	r	0.37	0/677	0.58	0/903
47	s	0.31	0/549	0.64	1/733 (0.1%)
48	t	0.35	0/676	0.59	0/906
49	u	0.31	0/605	0.56	0/807
50	D	0.55	0/1768	0.90	1/2755 (0.0%)
51	b	0.50	0/319	1.00	2/494 (0.4%)
52	F	0.28	0/1015	0.51	0/1373
53	3	0.35	0/459	0.53	0/615
All	All	0.62	1/158439 (0.0%)	0.89	81/236796 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	m	102	ASP	C-N	5.02	1.45	1.34

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	2487	C	C6-N1-C2	-9.23	116.61	120.30
9	A	1086	G	O4'-C1'-N9	8.88	115.30	108.20
9	A	547	C	C6-N1-C2	-8.65	116.84	120.30
9	A	2679	C	C6-N1-C2	-8.62	116.85	120.30
9	A	2883	A	N1-C6-N6	-8.54	113.47	118.60
9	A	822	A	N1-C6-N6	7.67	123.20	118.60
9	A	2679	C	N3-C2-O2	-7.31	116.78	121.90
9	A	1828	A	OP1-P-OP2	-7.06	109.01	119.60
30	a	1060	G	OP1-P-OP2	-7.03	109.05	119.60
30	a	111	A	OP1-P-OP2	-7.01	109.08	119.60
50	D	1	C	OP1-P-OP2	-6.92	109.22	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2679	C	N1-C2-O2	6.90	123.04	118.90
9	A	1815	A	N7-C8-N9	6.87	117.23	113.80
10	B	2	G	OP1-P-OP2	-6.86	109.31	119.60
51	b	13	A	OP1-P-OP2	-6.86	109.31	119.60
30	a	845	A	OP1-P-OP2	-6.86	109.32	119.60
51	b	1	G	OP1-P-OP2	-6.78	109.42	119.60
9	A	3	U	OP1-P-OP2	-6.73	109.50	119.60
30	a	780	C	C2-N1-C1'	6.47	125.92	118.80
30	a	240	G	OP1-P-OP2	-6.43	109.95	119.60
9	A	2487	C	N3-C2-O2	-6.42	117.40	121.90
9	A	550	G	O4'-C1'-N9	6.35	113.28	108.20
25	V	20	ARG	NE-CZ-NH2	-6.30	117.15	120.30
30	a	131	G	OP1-P-OP2	-6.30	110.15	119.60
30	a	1548	G	OP1-P-OP2	-6.23	110.25	119.60
9	A	1348	U	C2-N1-C1'	6.21	125.15	117.70
9	A	2216	G	OP1-P-OP2	-6.20	110.30	119.60
9	A	640	G	O4'-C1'-N9	6.18	113.14	108.20
9	A	2009	C	N1-C2-O2	6.11	122.56	118.90
9	A	1812	G	C8-N9-C4	-6.08	103.97	106.40
30	a	9	G	OP1-P-OP2	-6.05	110.53	119.60
9	A	547	C	C5-C6-N1	6.03	124.01	121.00
10	B	28	C	C6-N1-C2	-6.00	117.90	120.30
9	A	2384	G	OP1-P-OP2	-6.00	110.61	119.60
30	a	844	G	OP1-P-O3'	5.99	118.37	105.20
9	A	197	A	OP1-P-OP2	-5.94	110.69	119.60
9	A	823	U	N3-C2-O2	-5.93	118.05	122.20
9	A	2487	C	N1-C2-O2	5.85	122.41	118.90
9	A	822	A	C5-C6-N6	-5.83	119.04	123.70
30	a	57	A	O5'-P-OP1	-5.80	100.48	105.70
30	a	981	G	C6-C5-N7	-5.67	127.00	130.40
17	N	97	ARG	NE-CZ-NH1	5.66	123.13	120.30
30	a	981	G	N3-C4-N9	5.65	129.39	126.00
9	A	1694	C	O4'-C1'-N1	5.55	112.64	108.20
9	A	1424	G	C6-C5-N7	-5.51	127.10	130.40
9	A	1827	G	OP1-P-O3'	5.46	117.20	105.20
11	G	221	ARG	NE-CZ-NH1	5.45	123.03	120.30
30	a	9	G	O4'-C1'-N9	5.45	112.56	108.20
30	a	1030	G	N3-C4-C5	-5.42	125.89	128.60
9	A	185	C	C6-N1-C2	-5.42	118.13	120.30
9	A	1815	A	C5-N7-C8	-5.40	101.20	103.90
9	A	1421	C	O4'-C1'-N1	5.39	112.51	108.20
9	A	1424	G	N3-C4-N9	5.38	129.23	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	78	U	C5-C6-N1	5.38	125.39	122.70
9	A	1347	U	P-O3'-C3'	5.37	126.14	119.70
25	V	20	ARG	NE-CZ-NH1	5.37	122.98	120.30
14	J	136	LEU	CA-CB-CG	5.36	127.62	115.30
9	A	1788	U	C5-C4-O4	-5.30	122.72	125.90
30	a	774	A	P-O3'-C3'	5.27	126.02	119.70
9	A	1433	C	N1-C2-O2	5.23	122.04	118.90
30	a	780	C	C6-N1-C1'	-5.23	114.52	120.80
9	A	2789	A	P-O3'-C3'	5.19	125.93	119.70
41	m	102	ASP	CB-CG-OD2	5.19	122.97	118.30
9	A	2257	U	N3-C4-O4	5.19	123.03	119.40
30	a	1030	G	C4-N9-C1'	5.17	133.22	126.50
30	a	1053	C	C6-N1-C2	-5.15	118.24	120.30
9	A	1424	G	C4-N9-C1'	5.15	133.19	126.50
9	A	823	U	C2-N1-C1'	5.15	123.88	117.70
9	A	2009	C	N3-C2-O2	-5.14	118.30	121.90
30	a	1030	G	C2-N3-C4	5.13	114.47	111.90
9	A	1421	C	C6-N1-C2	-5.13	118.25	120.30
9	A	1424	G	C4-C5-N7	5.12	112.85	110.80
47	s	35	ARG	NE-CZ-NH1	5.11	122.86	120.30
9	A	251	C	P-O3'-C3'	5.10	125.82	119.70
7	7	57	ARG	NE-CZ-NH1	5.09	122.85	120.30
9	A	822	A	C4-C5-N7	5.06	113.23	110.70
9	A	822	A	C6-C5-N7	-5.05	128.76	132.30
9	A	1907	C	N1-C2-O2	5.04	121.93	118.90
9	A	822	A	C5-N7-C8	-5.03	101.39	103.90
30	a	1340	C	C6-N1-C2	-5.01	118.30	120.30
9	A	414	C	C6-N1-C2	-5.01	118.30	120.30

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	493/541 (91%)	468 (95%)	25 (5%)	0	100	100
2	1	57/62 (92%)	57 (100%)	0	0	100	100
3	2	55/59 (93%)	53 (96%)	2 (4%)	0	100	100
4	4	51/59 (86%)	46 (90%)	5 (10%)	0	100	100
5	5	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
6	6	41/44 (93%)	41 (100%)	0	0	100	100
7	7	62/66 (94%)	56 (90%)	6 (10%)	0	100	100
8	8	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	G	272/276 (99%)	252 (93%)	20 (7%)	0	100	100
12	H	205/209 (98%)	193 (94%)	12 (6%)	0	100	100
13	I	203/207 (98%)	188 (93%)	15 (7%)	0	100	100
14	J	174/179 (97%)	163 (94%)	11 (6%)	0	100	100
15	K	172/178 (97%)	160 (93%)	12 (7%)	0	100	100
16	M	143/147 (97%)	134 (94%)	9 (6%)	0	100	100
17	N	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
18	O	144/146 (99%)	130 (90%)	14 (10%)	0	100	100
19	P	132/144 (92%)	128 (97%)	4 (3%)	0	100	100
20	Q	123/127 (97%)	114 (93%)	9 (7%)	0	100	100
21	R	115/118 (98%)	106 (92%)	9 (8%)	0	100	100
22	S	112/115 (97%)	106 (95%)	6 (5%)	0	100	100
23	T	114/119 (96%)	110 (96%)	4 (4%)	0	100	100
24	U	99/102 (97%)	94 (95%)	5 (5%)	0	100	100
25	V	109/115 (95%)	104 (95%)	5 (5%)	0	100	100
26	W	89/96 (93%)	87 (98%)	2 (2%)	0	100	100
27	X	99/103 (96%)	91 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Y	72/95 (76%)	68 (94%)	4 (6%)	0	100	100
29	Z	58/62 (94%)	52 (90%)	6 (10%)	0	100	100
31	c	220/261 (84%)	209 (95%)	11 (5%)	0	100	100
32	d	204/218 (94%)	189 (93%)	15 (7%)	0	100	100
33	e	198/203 (98%)	187 (94%)	11 (6%)	0	100	100
34	f	161/166 (97%)	149 (92%)	12 (8%)	0	100	100
35	g	95/100 (95%)	91 (96%)	4 (4%)	0	100	100
36	h	151/156 (97%)	145 (96%)	6 (4%)	0	100	100
37	i	129/132 (98%)	116 (90%)	13 (10%)	0	100	100
38	j	126/130 (97%)	114 (90%)	12 (10%)	0	100	100
39	k	94/102 (92%)	90 (96%)	4 (4%)	0	100	100
40	l	114/129 (88%)	109 (96%)	5 (4%)	0	100	100
41	m	133/137 (97%)	117 (88%)	16 (12%)	0	100	100
42	n	112/121 (93%)	102 (91%)	10 (9%)	0	100	100
43	o	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
44	p	83/89 (93%)	81 (98%)	2 (2%)	0	100	100
45	q	85/91 (93%)	79 (93%)	6 (7%)	0	100	100
46	r	79/88 (90%)	68 (86%)	11 (14%)	0	100	100
47	s	64/79 (81%)	60 (94%)	4 (6%)	0	100	100
48	t	79/92 (86%)	72 (91%)	7 (9%)	0	100	100
49	u	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
52	F	126/229 (55%)	119 (94%)	7 (6%)	0	100	100
53	3	49/89 (55%)	48 (98%)	1 (2%)	0	100	100
All	All	5834/6334 (92%)	5463 (94%)	371 (6%)	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	435/473 (92%)	433 (100%)	2 (0%)	88	96
2	1	54/56 (96%)	54 (100%)	0	100	100
3	2	48/50 (96%)	48 (100%)	0	100	100
4	4	43/48 (90%)	43 (100%)	0	100	100
5	5	48/49 (98%)	48 (100%)	0	100	100
6	6	39/39 (100%)	39 (100%)	0	100	100
7	7	51/53 (96%)	51 (100%)	0	100	100
8	8	35/35 (100%)	35 (100%)	0	100	100
11	G	224/226 (99%)	222 (99%)	2 (1%)	78	93
12	H	170/172 (99%)	170 (100%)	0	100	100
13	I	172/173 (99%)	171 (99%)	1 (1%)	86	96
14	J	153/156 (98%)	151 (99%)	2 (1%)	69	90
15	K	145/148 (98%)	144 (99%)	1 (1%)	84	95
16	M	122/124 (98%)	122 (100%)	0	100	100
17	N	98/98 (100%)	98 (100%)	0	100	100
18	O	112/112 (100%)	112 (100%)	0	100	100
19	P	107/114 (94%)	107 (100%)	0	100	100
20	Q	107/109 (98%)	107 (100%)	0	100	100
21	R	91/92 (99%)	90 (99%)	1 (1%)	73	92
22	S	97/98 (99%)	96 (99%)	1 (1%)	76	92
23	T	92/95 (97%)	92 (100%)	0	100	100
24	U	83/83 (100%)	83 (100%)	0	100	100
25	V	94/98 (96%)	94 (100%)	0	100	100
26	W	82/85 (96%)	82 (100%)	0	100	100
27	X	85/87 (98%)	85 (100%)	0	100	100
28	Y	59/75 (79%)	59 (100%)	0	100	100
29	Z	53/55 (96%)	53 (100%)	0	100	100
31	c	187/220 (85%)	186 (100%)	1 (0%)	88	96
32	d	164/174 (94%)	164 (100%)	0	100	100
33	e	174/177 (98%)	171 (98%)	3 (2%)	60	86
34	f	125/128 (98%)	125 (100%)	0	100	100
35	g	86/88 (98%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	h	130/133 (98%)	129 (99%)	1 (1%)	81	94
37	i	112/113 (99%)	112 (100%)	0	100	100
38	j	101/102 (99%)	98 (97%)	3 (3%)	41	75
39	k	87/92 (95%)	86 (99%)	1 (1%)	73	92
40	l	90/101 (89%)	88 (98%)	2 (2%)	52	81
41	m	118/119 (99%)	118 (100%)	0	100	100
42	n	98/102 (96%)	98 (100%)	0	100	100
43	o	51/52 (98%)	50 (98%)	1 (2%)	55	82
44	p	76/79 (96%)	76 (100%)	0	100	100
45	q	77/81 (95%)	77 (100%)	0	100	100
46	r	75/81 (93%)	75 (100%)	0	100	100
47	s	57/67 (85%)	56 (98%)	1 (2%)	59	85
48	t	70/79 (89%)	70 (100%)	0	100	100
49	u	61/64 (95%)	61 (100%)	0	100	100
52	F	109/183 (60%)	109 (100%)	0	100	100
53	3	51/79 (65%)	50 (98%)	1 (2%)	55	82
All	All	4998/5317 (94%)	4974 (100%)	24 (0%)	89	96

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	28	MET
1	0	382	ARG
11	G	156	ARG
11	G	177	ASN
13	I	84	ARG
14	J	78	ARG
14	J	136	LEU
15	K	95	ARG
21	R	32	ASN
22	S	51	ARG
31	c	217	MET
33	e	14	ARG
33	e	125	LYS
33	e	183	ARG
36	h	10	ARG

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Mol	Chain	Res	Type
38	j	14	ASN
38	j	106	ARG
38	j	130	ARG
39	k	46	ARG
40	l	111	ARG
40	l	118	HIS
43	o	29	ARG
47	s	20	ASN
53	3	47	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	146	HIS
16	M	145	ASN
20	Q	57	HIS
24	U	75	GLN
49	u	21	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B	113/116 (97%)	25 (22%)	3 (2%)
30	a	1513/1558 (97%)	271 (17%)	0
50	D	73/77 (94%)	12 (16%)	1 (1%)
51	b	11/20 (55%)	1 (9%)	0
9	A	2903/2912 (99%)	560 (19%)	39 (1%)
All	All	4613/4683 (98%)	869 (18%)	43 (0%)

All (869) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A	8	U
9	A	10	A
9	A	15	G
9	A	28	A
9	A	34	U
9	A	46	C
9	A	51	G
9	A	55	G

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Mol	Chain	Res	Type
9	A	61	A
9	A	71	A
9	A	75	G
9	A	76	C
9	A	77	U
9	A	78	U
9	A	79	U
9	A	85	G
9	A	86	C
9	A	93	U
9	A	96	G
9	A	101	G
9	A	117	A
9	A	119	U
9	A	130	A
9	A	150	A
9	A	163	U
9	A	164	A
9	A	166	A
9	A	167	U
9	A	173	A
9	A	177	G
9	A	181	U
9	A	182	A
9	A	184	A
9	A	186	G
9	A	187	C
9	A	198	A
9	A	199	A
9	A	201	A
9	A	206	A
9	A	215	A
9	A	218	A
9	A	223	A
9	A	225	A
9	A	228	A
9	A	230	A
9	A	231	U
9	A	232	U
9	A	233	C
9	A	235	A
9	A	247	G

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Mol	Chain	Res	Type
9	A	250	G
9	A	251	C
9	A	252	G
9	A	257	A
9	A	263	G
9	A	265	A
9	A	266	G
9	A	267	A
9	A	268	G
9	A	282	G
9	A	289	U
9	A	290	G
9	A	298	U
9	A	299	G
9	A	301	A
9	A	309	G
9	A	311	U
9	A	312	A
9	A	317	A
9	A	318	G
9	A	320	C
9	A	321	U
9	A	322	G
9	A	331	G
9	A	347	A
9	A	352	C
9	A	353	G
9	A	365	G
9	A	366	A
9	A	385	G
9	A	398	A
9	A	403	G
9	A	404	A
9	A	410	A
9	A	411	G
9	A	419	G
9	A	422	C
9	A	425	G
9	A	426	A
9	A	434	C
9	A	442	U
9	A	445	G

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Mol	Chain	Res	Type
9	A	450	G
9	A	459	G
9	A	463	G
9	A	474	C
9	A	475	C
9	A	479	G
9	A	490	U
9	A	494	C
9	A	516	A
9	A	520	G
9	A	521	C
9	A	529	A
9	A	543	A
9	A	545	A
9	A	546	U
9	A	547	C
9	A	548	C
9	A	565	C
9	A	566	A
9	A	568	C
9	A	569	A
9	A	570	A
9	A	571	G
9	A	584	A
9	A	585	A
9	A	586	U
9	A	587	G
9	A	598	U
9	A	599	G
9	A	609	G
9	A	611	A
9	A	622	A
9	A	624	U
9	A	628	G
9	A	639	A
9	A	640	G
9	A	641	G
9	A	651	A
9	A	665	A
9	A	675	A
9	A	683	U
9	A	684	A

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Mol	Chain	Res	Type
9	A	689	G
9	A	692	U
9	A	693	G
9	A	711	C
9	A	716	A
9	A	725	U
9	A	769	A
9	A	784	G
9	A	786	U
9	A	787	G
9	A	796	G
9	A	801	U
9	A	803	A
9	A	804	G
9	A	814	G
9	A	821	A
9	A	823	U
9	A	824	U
9	A	829	A
9	A	830	C
9	A	831	G
9	A	839	A
9	A	844	G
9	A	851	C
9	A	858	A
9	A	866	U
9	A	885	U
9	A	899	G
9	A	906	A
9	A	922	G
9	A	926	A
9	A	928	C
9	A	929	U
9	A	930	C
9	A	931	G
9	A	933	G
9	A	936	A
9	A	947	A
9	A	950	A
9	A	952	C
9	A	954	C
9	A	957	A

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Mol	Chain	Res	Type
9	A	965	U
9	A	970	U
9	A	972	U
9	A	973	A
9	A	980	A
9	A	983	C
9	A	984	A
9	A	985	G
9	A	992	A
9	A	996	A
9	A	998	A
9	A	1000	G
9	A	1013	A
9	A	1021	C
9	A	1022	A
9	A	1024	C
9	A	1035	A
9	A	1051	U
9	A	1052	A
9	A	1056	G
9	A	1061	G
9	A	1062	U
9	A	1064	G
9	A	1065	A
9	A	1066	A
9	A	1067	A
9	A	1072	U
9	A	1086	G
9	A	1101	G
9	A	1109	A
9	A	1110	G
9	A	1115	C
9	A	1122	U
9	A	1123	A
9	A	1124	A
9	A	1126	G
9	A	1127	A
9	A	1130	G
9	A	1151	G
9	A	1155	C
9	A	1158	U
9	A	1165	A

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Mol	Chain	Res	Type
9	A	1166	A
9	A	1167	A
9	A	1169	U
9	A	1171	U
9	A	1172	A
9	A	1174	C
9	A	1175	G
9	A	1181	A
9	A	1182	A
9	A	1188	U
9	A	1196	G
9	A	1212	U
9	A	1213	U
9	A	1215	G
9	A	1221	G
9	A	1231	A
9	A	1240	A
9	A	1241	G
9	A	1244	C
9	A	1245	G
9	A	1248	G
9	A	1256	A
9	A	1265	A
9	A	1267	G
9	A	1274	G
9	A	1284	G
9	A	1286	G
9	A	1289	A
9	A	1292	G
9	A	1302	G
9	A	1307	G
9	A	1308	A
9	A	1311	G
9	A	1315	G
9	A	1335	U
9	A	1336	A
9	A	1347	U
9	A	1348	U
9	A	1360	C
9	A	1364	U
9	A	1373	G
9	A	1376	U

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Mol	Chain	Res	Type
9	A	1380	C
9	A	1383	G
9	A	1384	A
9	A	1385	C
9	A	1387	U
9	A	1400	A
9	A	1414	U
9	A	1419	A
9	A	1420	A
9	A	1421	C
9	A	1422	A
9	A	1423	G
9	A	1424	G
9	A	1427	G
9	A	1430	A
9	A	1431	U
9	A	1451	G
9	A	1454	U
9	A	1455	G
9	A	1457	G
9	A	1460	A
9	A	1461	U
9	A	1462	G
9	A	1468	A
9	A	1469	C
9	A	1470	G
9	A	1475	A
9	A	1480	A
9	A	1484	A
9	A	1486	U
9	A	1494	A
9	A	1495	U
9	A	1496	U
9	A	1497	G
9	A	1502	U
9	A	1503	G
9	A	1509	C
9	A	1511	A
9	A	1520	G
9	A	1523	U
9	A	1524	U
9	A	1526	A

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Mol	Chain	Res	Type
9	A	1530	G
9	A	1531	A
9	A	1534	U
9	A	1535	A
9	A	1537	A
9	A	1538	U
9	A	1543	U
9	A	1546	U
9	A	1551	A
9	A	1553	G
9	A	1555	A
9	A	1562	G
9	A	1565	A
9	A	1567	G
9	A	1569	G
9	A	1572	G
9	A	1575	A
9	A	1576	A
9	A	1579	A
9	A	1580	A
9	A	1581	U
9	A	1582	A
9	A	1583	G
9	A	1584	U
9	A	1599	C
9	A	1600	G
9	A	1604	C
9	A	1614	A
9	A	1618	G
9	A	1623	U
9	A	1627	G
9	A	1629	G
9	A	1630	A
9	A	1649	U
9	A	1650	A
9	A	1652	A
9	A	1658	A
9	A	1677	A
9	A	1688	A
9	A	1689	G
9	A	1690	C
9	A	1694	C

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Mol	Chain	Res	Type
9	A	1704	U
9	A	1705	U
9	A	1709	G
9	A	1710	A
9	A	1714	C
9	A	1716	G
9	A	1742	A
9	A	1745	G
9	A	1753	A
9	A	1755	U
9	A	1756	U
9	A	1757	C
9	A	1758	G
9	A	1759	G
9	A	1766	G
9	A	1769	G
9	A	1770	U
9	A	1775	A
9	A	1776	G
9	A	1777	G
9	A	1786	A
9	A	1798	A
9	A	1799	A
9	A	1804	A
9	A	1812	G
9	A	1813	C
9	A	1821	U
9	A	1823	A
9	A	1828	A
9	A	1829	A
9	A	1830	G
9	A	1842	A
9	A	1861	A
9	A	1867	A
9	A	1869	A
9	A	1871	G
9	A	1882	U
9	A	1883	U
9	A	1884	C
9	A	1896	G
9	A	1918	C
9	A	1919	G

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Mol	Chain	Res	Type
9	A	1923	G
9	A	1927	C
9	A	1929	A
9	A	1940	A
9	A	1942	G
9	A	1943	G
9	A	1949	A
9	A	1950	A
9	A	1951	A
9	A	1953	U
9	A	1954	C
9	A	1968	U
9	A	1973	A
9	A	1976	C
9	A	1977	G
9	A	1978	C
9	A	1979	A
9	A	1980	C
9	A	1983	A
9	A	1984	A
9	A	1985	G
9	A	2004	U
9	A	2006	U
9	A	2010	A
9	A	2035	U
9	A	2044	A
9	A	2045	G
9	A	2046	A
9	A	2056	C
9	A	2062	A
9	A	2068	C
9	A	2069	G
9	A	2072	A
9	A	2073	A
9	A	2074	G
9	A	2075	A
9	A	2082	G
9	A	2093	G
9	A	2107	A
9	A	2108	G
9	A	2112	U
9	A	2113	U

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Mol	Chain	Res	Type
9	A	2117	C
9	A	2121	A
9	A	2124	U
9	A	2129	G
9	A	2130	A
9	A	2139	A
9	A	2145	U
9	A	2146	G
9	A	2170	G
9	A	2172	G
9	A	2173	G
9	A	2185	U
9	A	2191	C
9	A	2196	U
9	A	2203	A
9	A	2207	C
9	A	2211	A
9	A	2216	G
9	A	2217	C
9	A	2224	A
9	A	2230	G
9	A	2238	A
9	A	2251	G
9	A	2252	G
9	A	2259	G
9	A	2262	U
9	A	2279	A
9	A	2281	A
9	A	2291	A
9	A	2292	G
9	A	2296	C
9	A	2300	A
9	A	2301	A
9	A	2302	G
9	A	2318	U
9	A	2320	G
9	A	2322	A
9	A	2331	G
9	A	2333	A
9	A	2334	G
9	A	2335	A
9	A	2340	A

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Mol	Chain	Res	Type
9	A	2347	G
9	A	2348	A
9	A	2360	C
9	A	2363	C
9	A	2367	A
9	A	2371	A
9	A	2374	A
9	A	2396	G
9	A	2399	U
9	A	2404	G
9	A	2409	G
9	A	2415	U
9	A	2420	A
9	A	2436	U
9	A	2438	A
9	A	2439	A
9	A	2442	G
9	A	2443	A
9	A	2447	A
9	A	2454	C
9	A	2458	G
9	A	2461	A
9	A	2464	A
9	A	2481	A
9	A	2489	A
9	A	2491	A
9	A	2493	C
9	A	2507	G
9	A	2515	G
9	A	2519	U
9	A	2526	G
9	A	2531	A
9	A	2533	C
9	A	2542	G
9	A	2548	G
9	A	2567	U
9	A	2577	A
9	A	2579	A
9	A	2580	G
9	A	2586	C
9	A	2591	G
9	A	2597	U

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Mol	Chain	Res	Type
9	A	2598	U
9	A	2615	A
9	A	2622	U
9	A	2623	C
9	A	2626	U
9	A	2628	U
9	A	2642	U
9	A	2645	A
9	A	2659	C
9	A	2695	G
9	A	2698	G
9	A	2702	U
9	A	2727	G
9	A	2731	G
9	A	2746	A
9	A	2749	G
9	A	2764	G
9	A	2770	A
9	A	2778	A
9	A	2790	G
9	A	2791	A
9	A	2792	U
9	A	2802	C
9	A	2804	U
9	A	2808	U
9	A	2809	U
9	A	2810	U
9	A	2811	A
9	A	2812	A
9	A	2813	G
9	A	2816	A
9	A	2843	A
9	A	2853	G
9	A	2859	G
9	A	2860	A
9	A	2863	G
9	A	2871	U
9	A	2877	G
9	A	2882	G
9	A	2884	C
9	A	2890	C
9	A	2893	A

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Mol	Chain	Res	Type
9	A	2896	G
9	A	2902	G
9	A	2903	G
9	A	2909	A
9	A	2910	C
9	A	2911	C
10	B	10	G
10	B	11	A
10	B	12	U
10	B	14	G
10	B	23	A
10	B	28	C
10	B	32	U
10	B	34	C
10	B	35	C
10	B	39	G
10	B	40	C
10	B	42	G
10	B	49	G
10	B	50	A
10	B	55	A
10	B	64	A
10	B	65	G
10	B	82	G
10	B	87	U
10	B	88	C
10	B	97	A
10	B	101	U
10	B	107	G
10	B	108	U
10	B	110	G
30	a	10	A
30	a	11	G
30	a	24	G
30	a	33	G
30	a	34	A
30	a	41	G
30	a	46	G
30	a	49	C
30	a	50	C
30	a	51	U
30	a	53	A

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Mol	Chain	Res	Type
30	a	56	C
30	a	57	A
30	a	116	G
30	a	117	A
30	a	118	G
30	a	132	A
30	a	136	A
30	a	137	C
30	a	138	A
30	a	146	A
30	a	147	A
30	a	158	A
30	a	161	G
30	a	166	A
30	a	172	C
30	a	175	G
30	a	177	A
30	a	180	C
30	a	181	A
30	a	182	G
30	a	190	U
30	a	199	A
30	a	200	C
30	a	207	U
30	a	213	A
30	a	215	G
30	a	226	G
30	a	227	A
30	a	230	G
30	a	266	U
30	a	267	G
30	a	270	U
30	a	271	U
30	a	273	G
30	a	277	G
30	a	279	U
30	a	292	G
30	a	293	C
30	a	315	G
30	a	332	A
30	a	347	A
30	a	354	C

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Mol	Chain	Res	Type
30	a	355	A
30	a	358	G
30	a	370	A
30	a	373	G
30	a	378	C
30	a	380	G
30	a	381	C
30	a	389	A
30	a	390	A
30	a	391	U
30	a	393	U
30	a	398	C
30	a	399	A
30	a	414	G
30	a	417	C
30	a	418	G
30	a	423	A
30	a	430	G
30	a	432	G
30	a	437	A
30	a	438	A
30	a	439	G
30	a	447	U
30	a	448	C
30	a	450	G
30	a	453	C
30	a	454	G
30	a	455	U
30	a	474	A
30	a	477	A
30	a	478	A
30	a	479	C
30	a	485	C
30	a	488	U
30	a	489	A
30	a	490	G
30	a	491	U
30	a	511	G
30	a	512	U
30	a	521	A
30	a	522	G
30	a	523	A

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Mol	Chain	Res	Type
30	a	535	A
30	a	537	C
30	a	544	C
30	a	547	G
30	a	553	G
30	a	556	G
30	a	557	U
30	a	558	A
30	a	573	A
30	a	578	U
30	a	585	A
30	a	590	U
30	a	598	A
30	a	599	A
30	a	602	C
30	a	603	G
30	a	605	G
30	a	622	A
30	a	658	G
30	a	659	U
30	a	660	C
30	a	668	A
30	a	679	U
30	a	687	G
30	a	691	A
30	a	709	G
30	a	720	A
30	a	721	A
30	a	728	A
30	a	730	A
30	a	736	G
30	a	747	A
30	a	749	U
30	a	750	G
30	a	755	A
30	a	759	G
30	a	760	G
30	a	772	G
30	a	775	A
30	a	781	G
30	a	813	A
30	a	819	U

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Mol	Chain	Res	Type
30	a	820	A
30	a	836	C
30	a	843	C
30	a	846	U
30	a	855	A
30	a	858	G
30	a	862	G
30	a	866	G
30	a	873	C
30	a	899	A
30	a	903	A
30	a	916	A
30	a	941	A
30	a	953	G
30	a	954	G
30	a	961	C
30	a	962	A
30	a	966	G
30	a	972	G
30	a	983	U
30	a	987	U
30	a	993	G
30	a	995	A
30	a	996	A
30	a	998	G
30	a	1002	A
30	a	1003	G
30	a	1004	A
30	a	1009	U
30	a	1016	U
30	a	1019	U
30	a	1020	G
30	a	1023	A
30	a	1028	U
30	a	1029	U
30	a	1030	G
30	a	1031	A
30	a	1034	A
30	a	1036	U
30	a	1039	A
30	a	1040	G
30	a	1045	A

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Mol	Chain	Res	Type
30	a	1047	A
30	a	1050	U
30	a	1052	U
30	a	1053	C
30	a	1063	A
30	a	1064	C
30	a	1066	A
30	a	1067	A
30	a	1070	G
30	a	1073	A
30	a	1075	G
30	a	1077	G
30	a	1078	G
30	a	1081	C
30	a	1083	U
30	a	1092	U
30	a	1093	C
30	a	1112	U
30	a	1119	A
30	a	1121	G
30	a	1122	U
30	a	1127	C
30	a	1128	A
30	a	1129	A
30	a	1131	G
30	a	1135	G
30	a	1159	C
30	a	1165	G
30	a	1166	U
30	a	1171	C
30	a	1172	A
30	a	1183	A
30	a	1185	U
30	a	1187	C
30	a	1193	A
30	a	1194	C
30	a	1210	G
30	a	1222	A
30	a	1223	A
30	a	1228	U
30	a	1238	U
30	a	1239	A

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Mol	Chain	Res	Type
30	a	1253	A
30	a	1254	C
30	a	1262	A
30	a	1283	C
30	a	1286	U
30	a	1306	A
30	a	1307	U
30	a	1319	U
30	a	1325	A
30	a	1326	G
30	a	1328	U
30	a	1331	G
30	a	1340	C
30	a	1343	C
30	a	1344	A
30	a	1348	C
30	a	1361	C
30	a	1362	C
30	a	1379	G
30	a	1386	A
30	a	1407	U
30	a	1415	C
30	a	1420	A
30	a	1423	C
30	a	1424	A
30	a	1428	C
30	a	1445	G
30	a	1448	U
30	a	1452	A
30	a	1468	A
30	a	1472	A
30	a	1478	U
30	a	1479	U
30	a	1480	U
30	a	1481	G
30	a	1502	G
30	a	1514	G
30	a	1517	U
30	a	1519	A
30	a	1524	G
30	a	1530	A
30	a	1533	U

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Mol	Chain	Res	Type
30	a	1534	A
30	a	1544	G
30	a	1546	A
30	a	1556	G
30	a	1557	G
30	a	1558	A
30	a	1561	A
30	a	1564	U
50	D	4	G
50	D	8	U
50	D	14	A
50	D	21	U
50	D	22	A
50	D	23	G
50	D	44	A
50	D	47	G
50	D	48	U
50	D	65	G
50	D	72	C
50	D	73	A
51	b	16	A

All (43) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	92	G
9	A	174	U
9	A	199	A
9	A	231	U
9	A	251	C
9	A	288	U
9	A	433	C
9	A	520	G
9	A	658	G
9	A	774	A
9	A	802	G
9	A	823	U
9	A	982	U
9	A	1033	C
9	A	1239	A
9	A	1240	A
9	A	1301	A

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Mol	Chain	Res	Type
9	A	1335	U
9	A	1347	U
9	A	1450	U
9	A	1525	G
9	A	1530	G
9	A	1536	A
9	A	1561	U
9	A	1583	G
9	A	1693	G
9	A	1797	A
9	A	1812	G
9	A	1828	A
9	A	1866	A
9	A	1868	G
9	A	1926	A
9	A	2111	U
9	A	2300	A
9	A	2419	C
9	A	2438	A
9	A	2789	A
9	A	2808	U
9	A	2810	U
10	B	31	G
10	B	48	A
10	B	49	G
50	D	22	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 185 ligands modelled in this entry, 179 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
58	PUT	a	1634	-	5,5,5	0.20	0	4,4,4	0.48	0
58	PUT	A	3138	-	5,5,5	0.25	0	4,4,4	0.37	0
58	PUT	a	1633	-	5,5,5	0.24	0	4,4,4	0.44	0
54	ATP	0	602	55	26,33,33	0.69	0	31,52,52	0.74	2 (6%)
58	PUT	A	3139	-	5,5,5	0.23	0	4,4,4	0.49	0
54	ATP	0	601	55	26,33,33	0.65	0	31,52,52	0.75	1 (3%)

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
58	PUT	a	1634	-	-	1/3/3/3	-
58	PUT	A	3138	-	-	1/3/3/3	-
58	PUT	a	1633	-	-	0/3/3/3	-
54	ATP	0	602	55	-	4/18/38/38	0/3/3/3
58	PUT	A	3139	-	-	1/3/3/3	-
54	ATP	0	601	55	-	3/18/38/38	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	0	602	ATP	C5-C6-N6	2.27	123.80	120.35
54	0	601	ATP	C5-C6-N6	2.24	123.76	120.35
54	0	602	ATP	PB-O3B-PG	2.04	139.83	132.83

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	0	602	ATP	PB-O3B-PG-O2G
58	A	3138	PUT	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

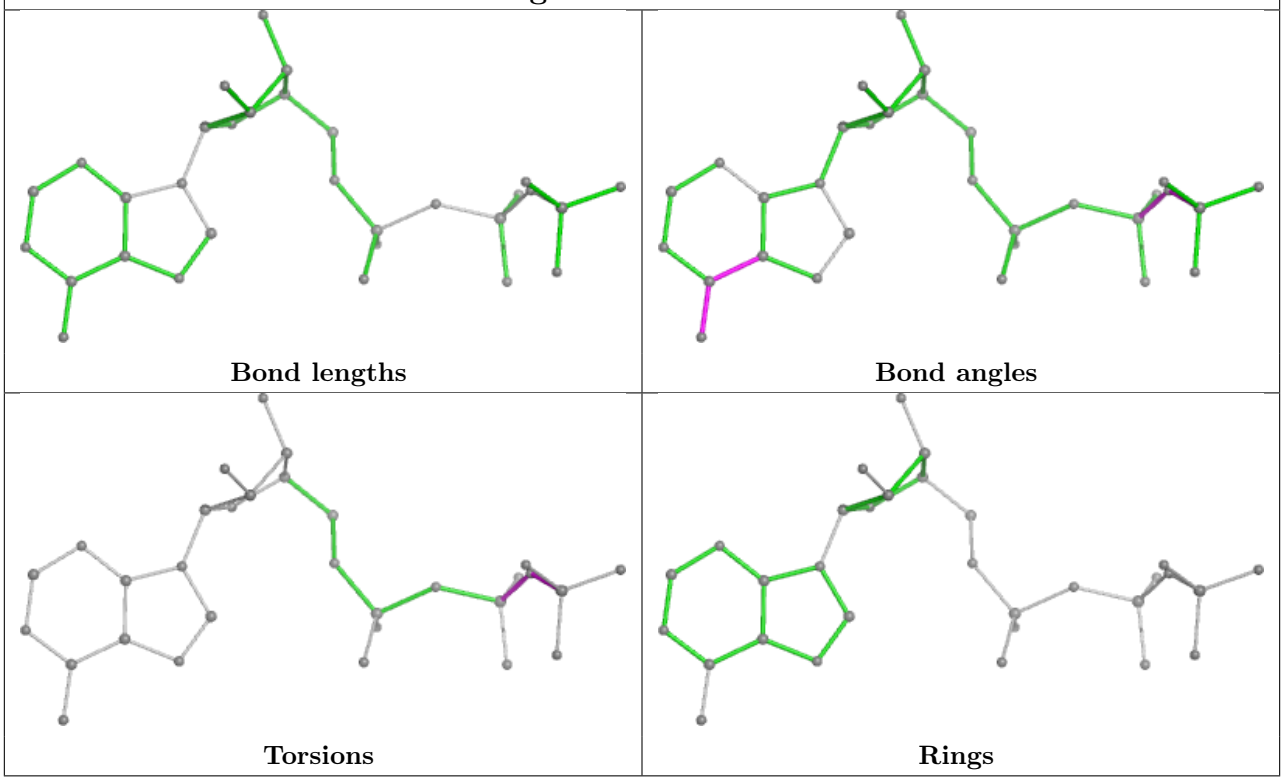
Mol	Chain	Res	Type	Atoms
54	0	602	ATP	PG-O3B-PB-O2B
54	0	601	ATP	O4'-C4'-C5'-O5'
54	0	602	ATP	PG-O3B-PB-O1B
54	0	601	ATP	C3'-C4'-C5'-O5'
54	0	601	ATP	PB-O3B-PG-O3G
54	0	602	ATP	PB-O3B-PG-O3G
58	A	3139	PUT	C2-C3-C4-N2
58	a	1634	PUT	C2-C3-C4-N2

There are no ring outliers.

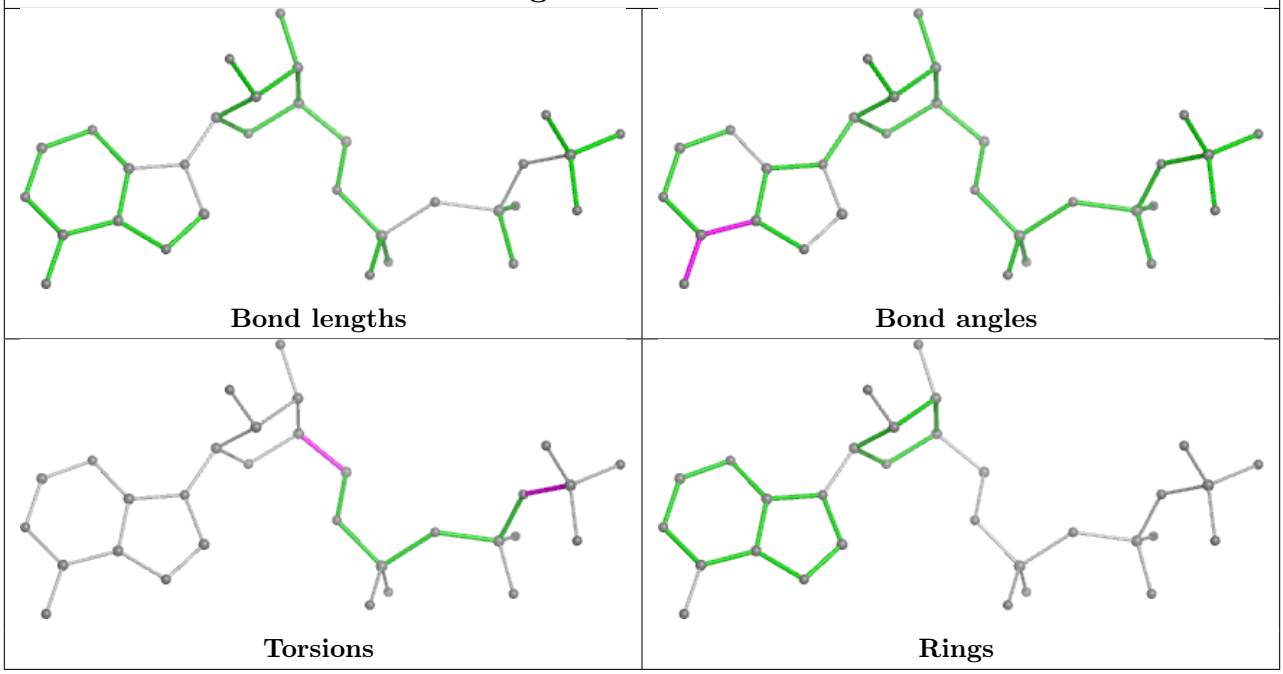
No monomer is involved in short contacts.

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 0 602



Ligand ATP 0 601



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.

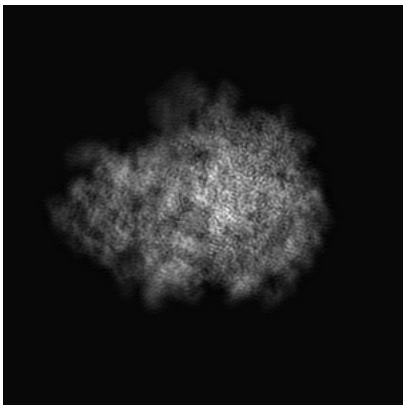
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12331. These allow visual inspection of the internal detail of the map and identification of artifacts.

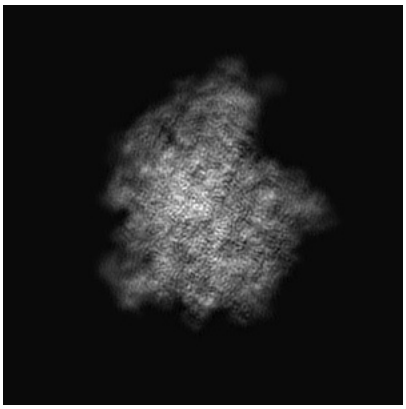
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

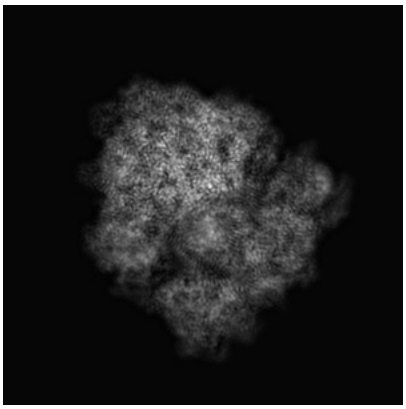
6.1.1 Primary map



X

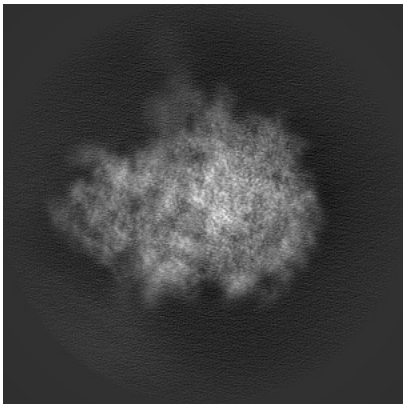


Y

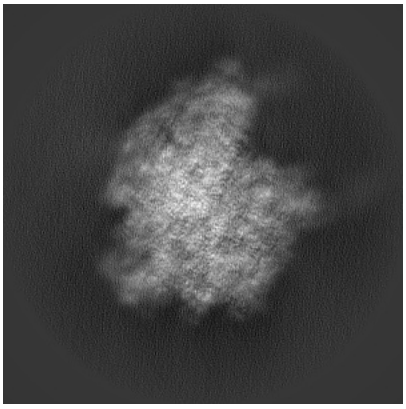


Z

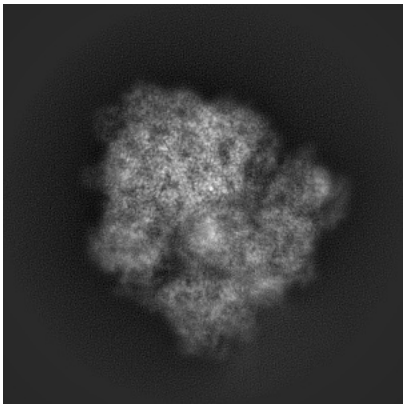
6.1.2 Raw map



X



Y

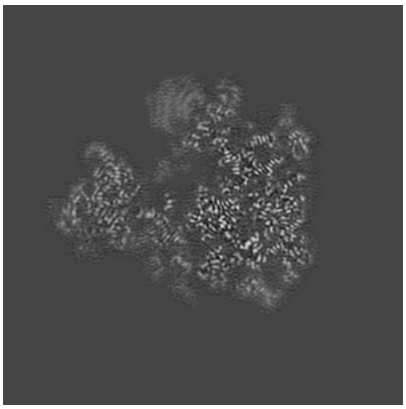


Z

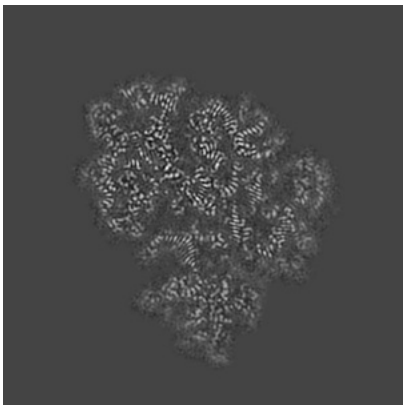
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

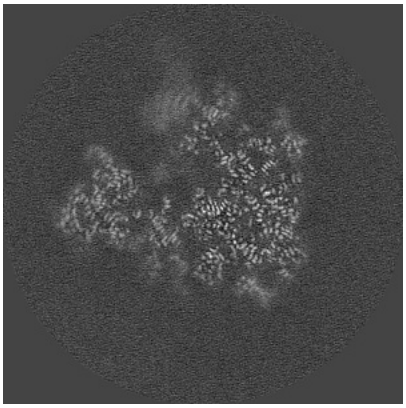
6.2.1 Primary map

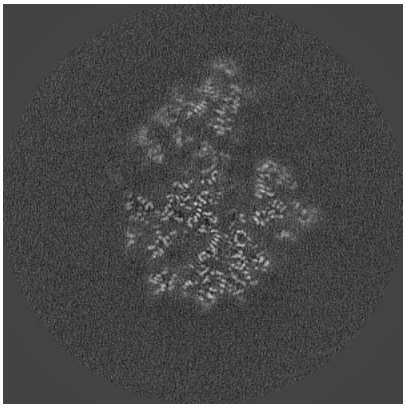

X Index: 176

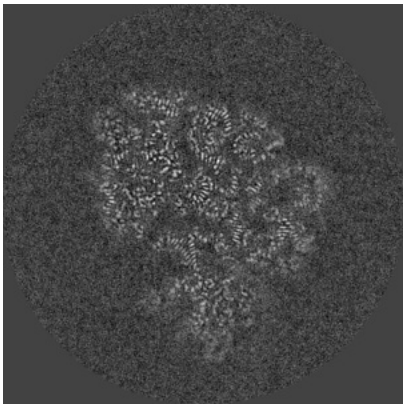
Y Index: 176


Z Index: 176

6.2.2 Raw map


X Index: 180

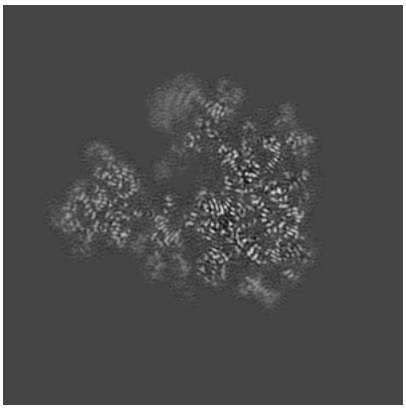

Y Index: 180


Z Index: 180

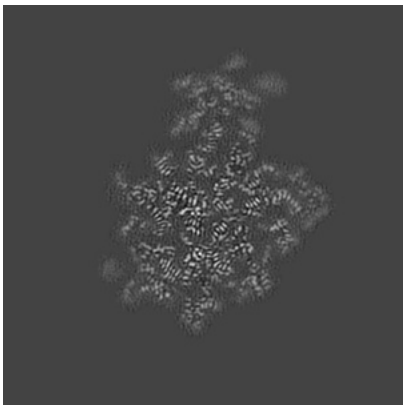
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

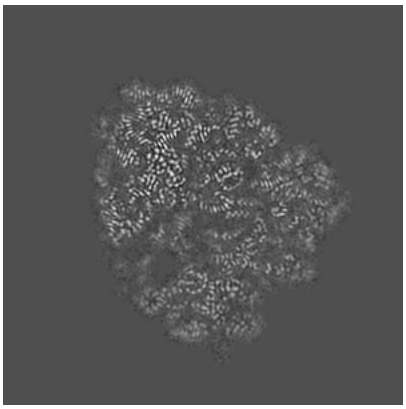
6.3.1 Primary map



X Index: 174

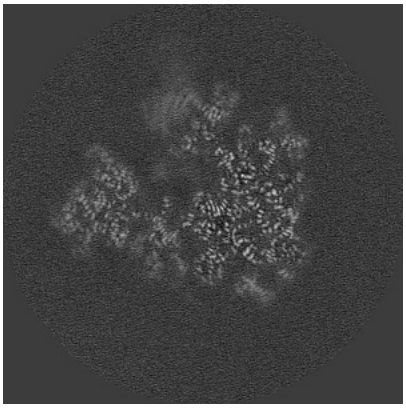


Y Index: 197

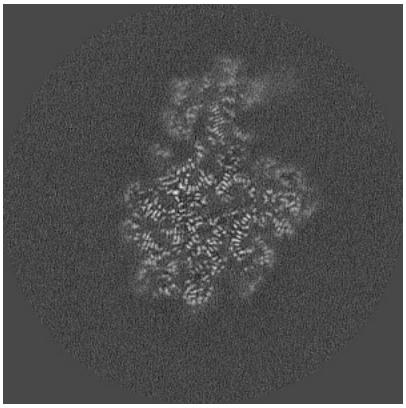


Z Index: 186

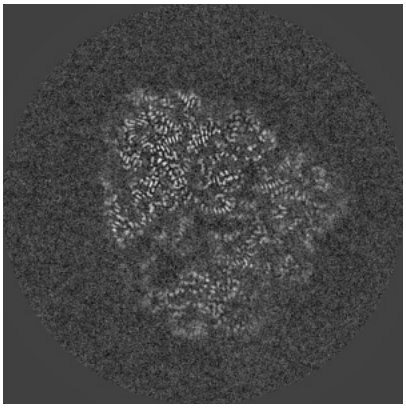
6.3.2 Raw map



X Index: 179



Y Index: 190

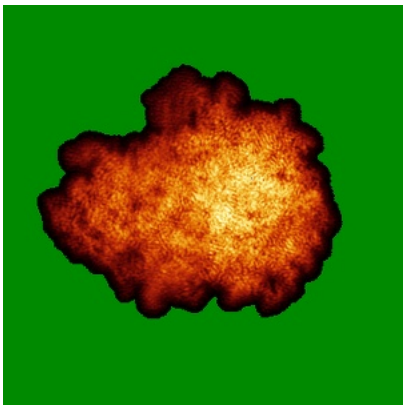


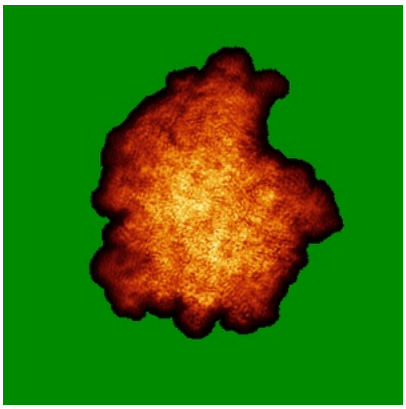
Z Index: 189

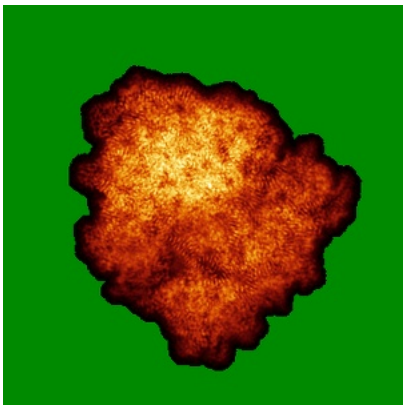
The images above show the largest variance slices of the map in three orthogonal directions.

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

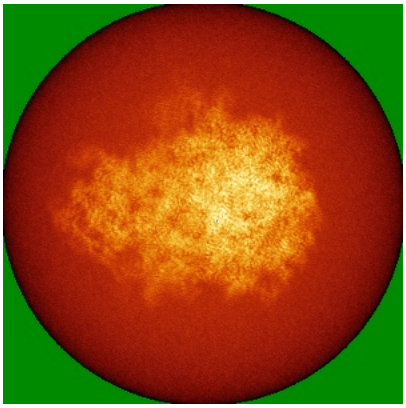
6.4.1 Primary map

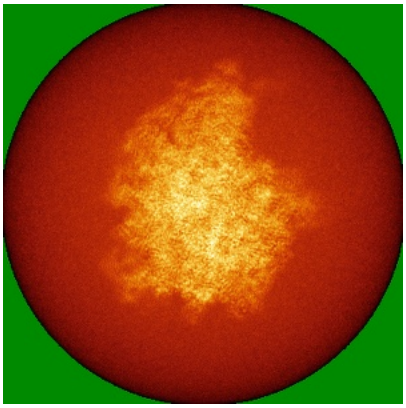

X

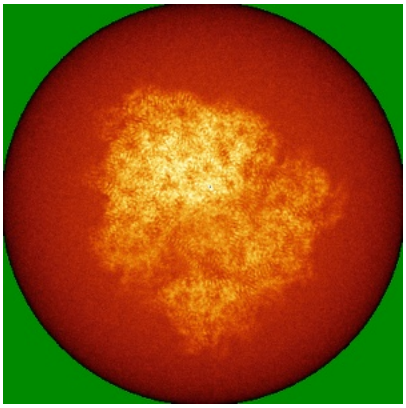

Y


Z

6.4.2 Raw map


X

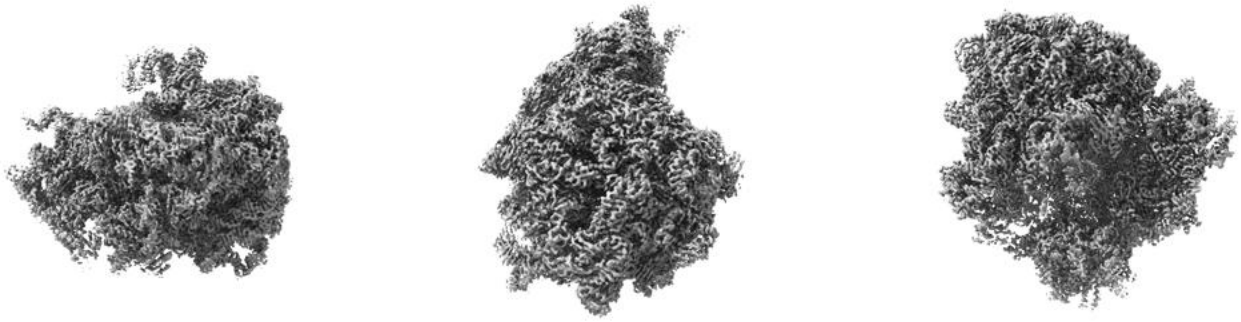

Y


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 0.02. 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.

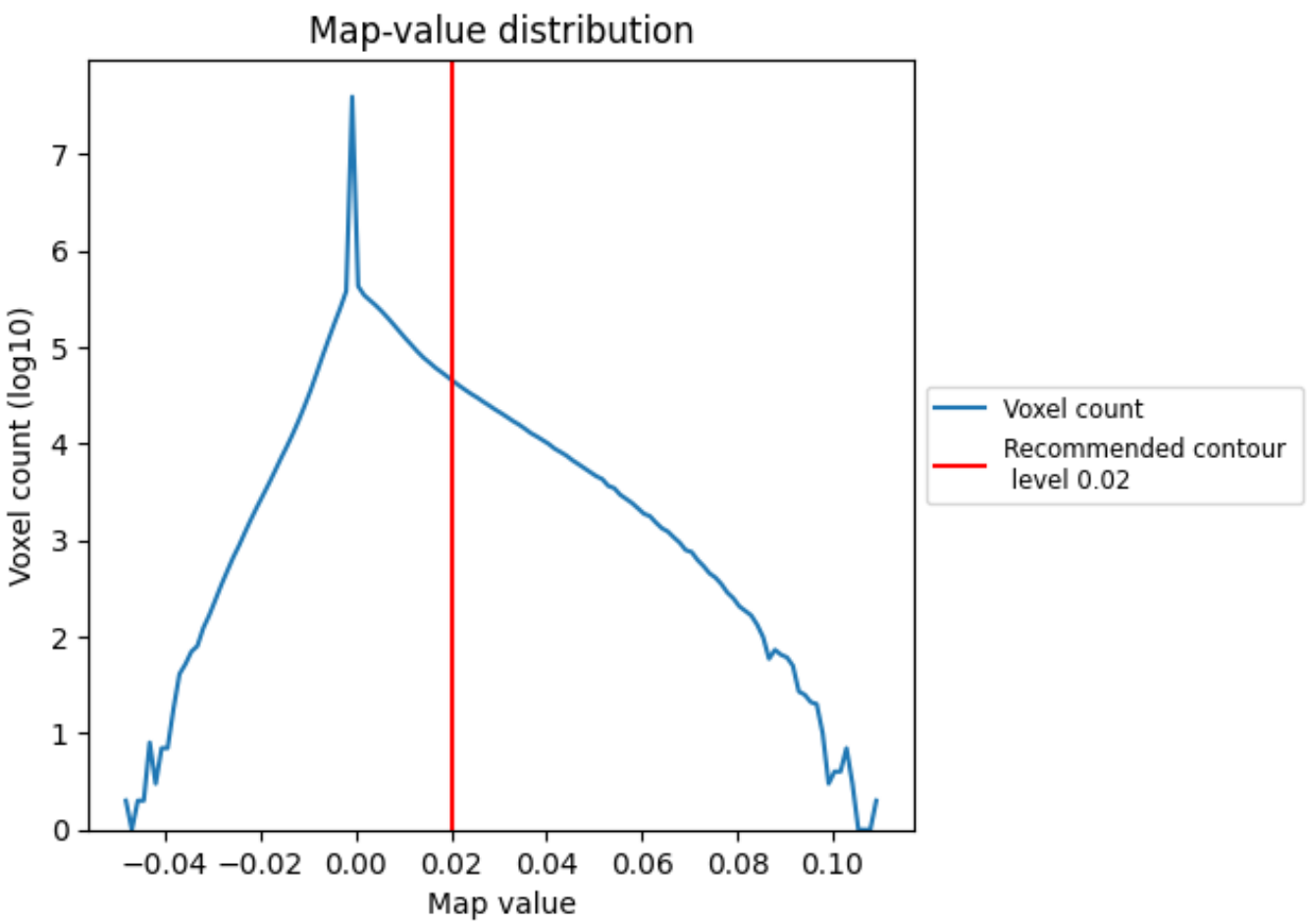
6.6 Mask visualisation (i)

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

7 Map analysis (i)

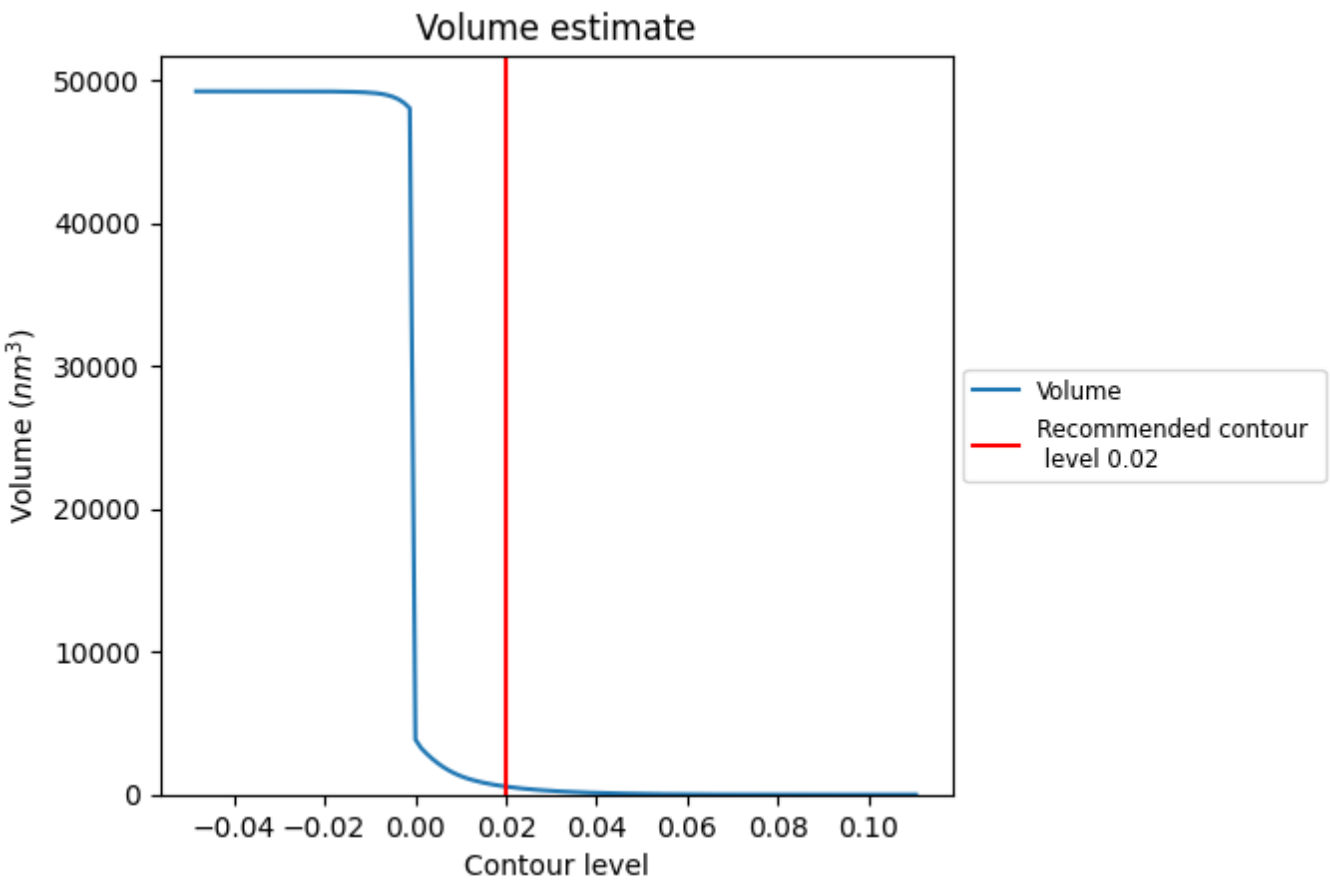
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

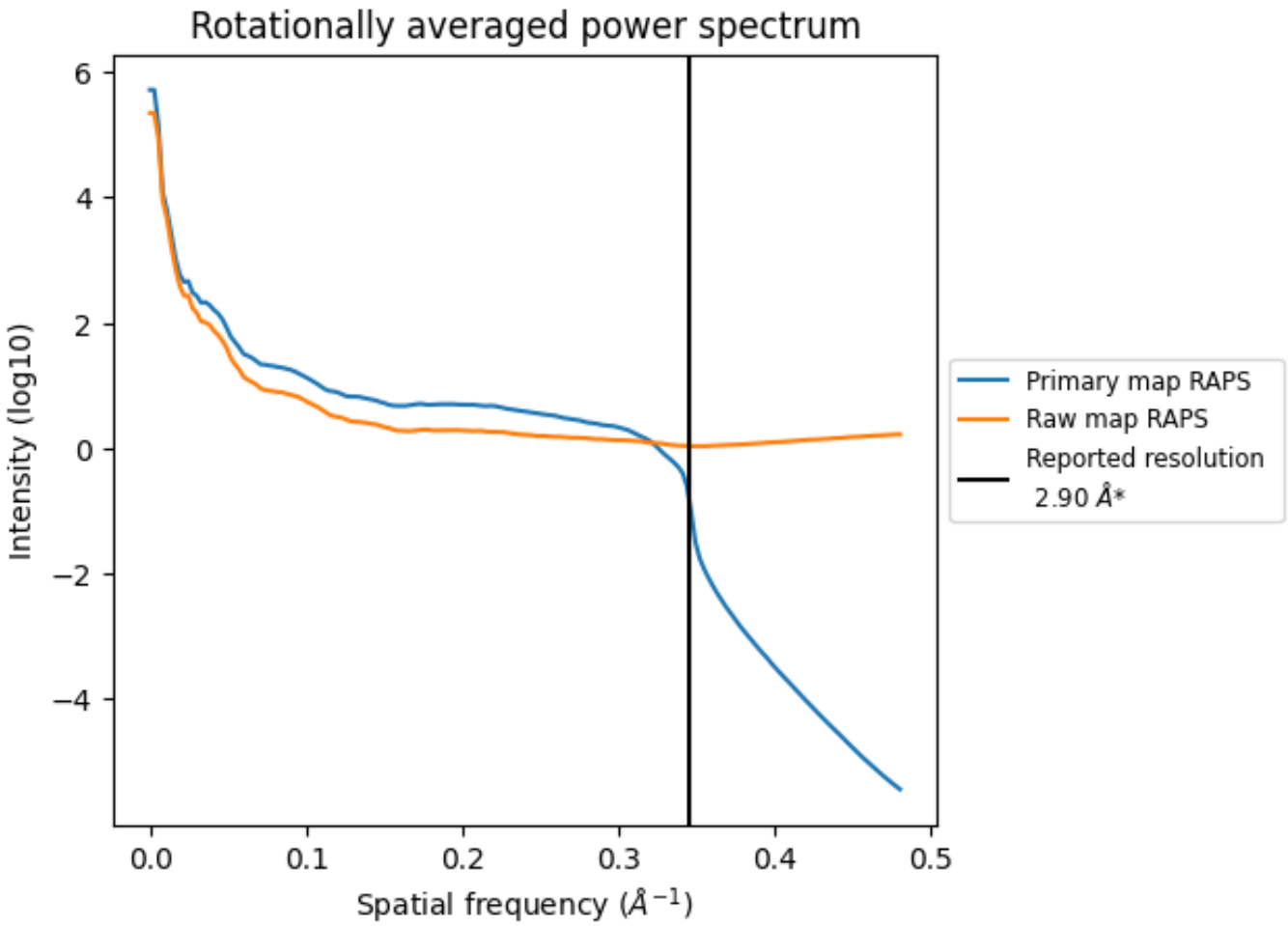
7.2 Volume estimate (i)



The volume at the recommended contour level is 560 nm^3; this corresponds to an approximate mass of 505 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)

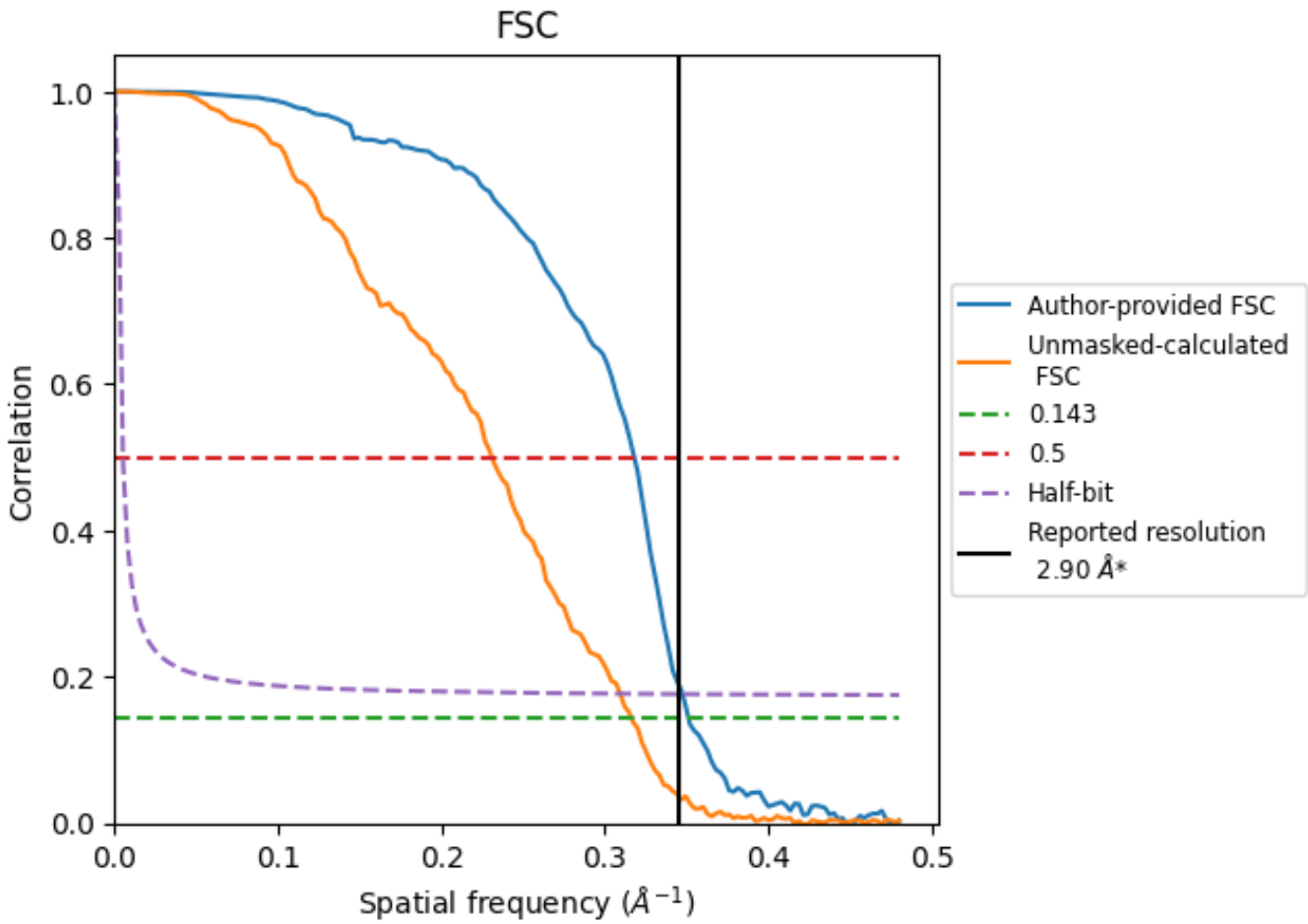


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



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

8.2 Resolution estimates (i)

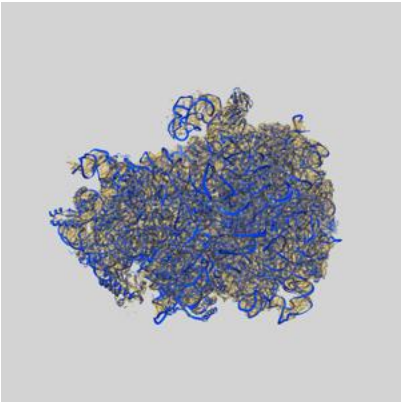
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.85	3.14	2.88
Unmasked-calculated*	3.16	4.33	3.23

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

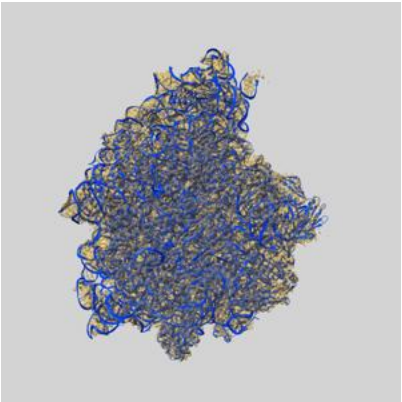
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12331 and PDB model 7NHK. Per-residue inclusion information can be found in section 3 on page 16.

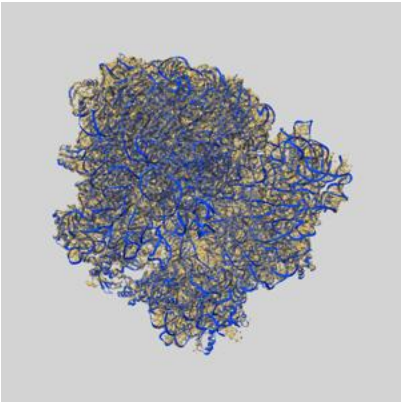
9.1 Map-model overlay (i)



X



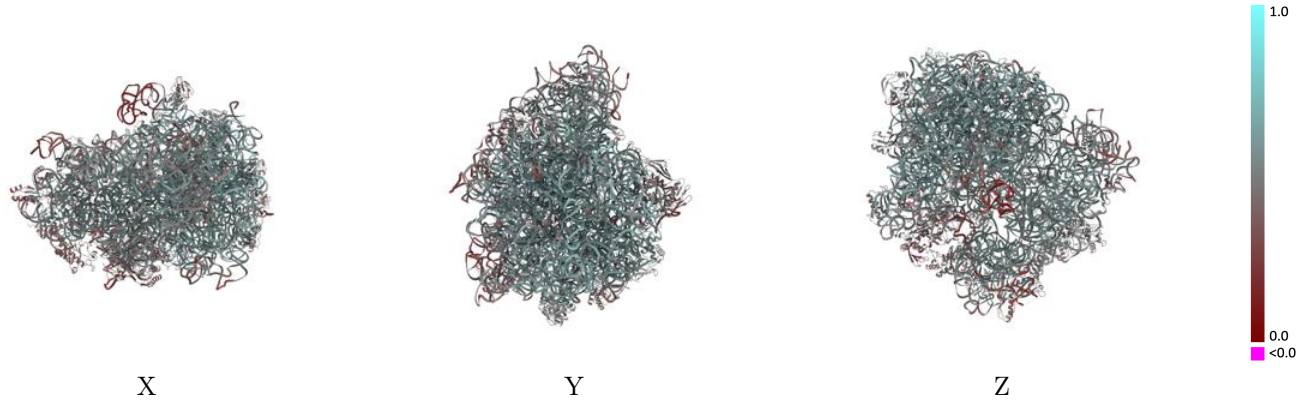
Y



Z

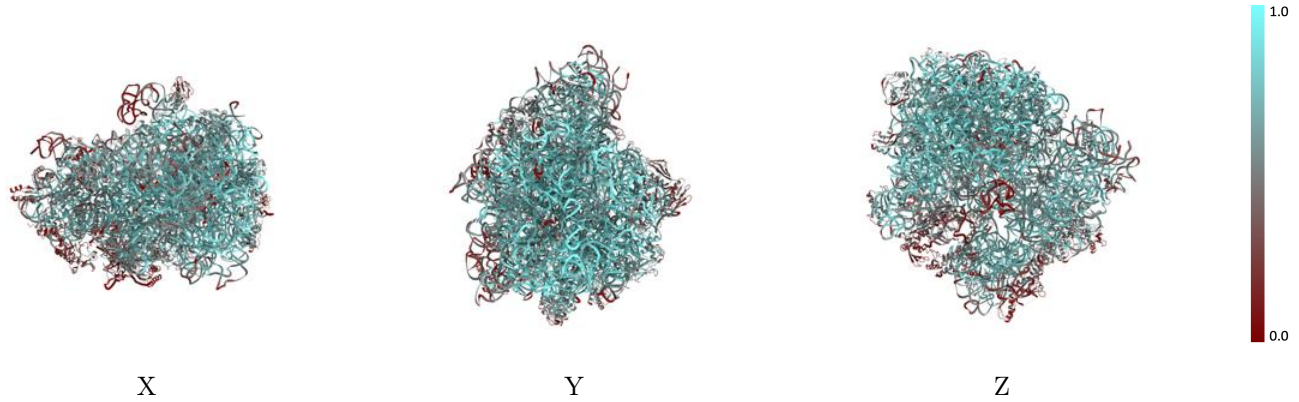
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



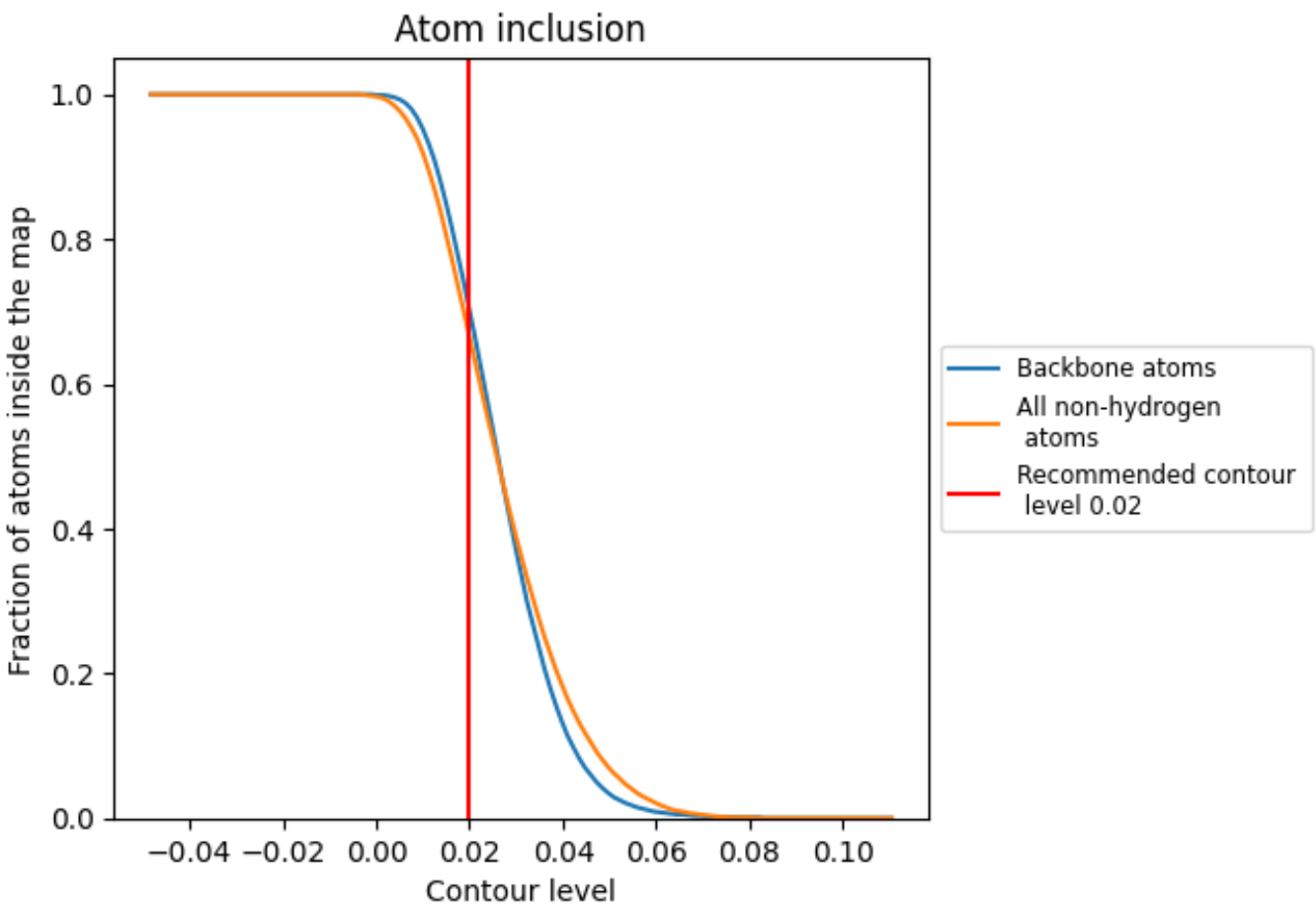
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



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

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6650	0.5190
0	0.4790	0.4870
1	0.4820	0.4540
2	0.5660	0.5120
3	0.1780	0.3520
4	0.7230	0.5470
5	0.6190	0.4940
6	0.6790	0.5650
7	0.7000	0.5540
8	0.6760	0.5430
A	0.7760	0.5490
B	0.6660	0.5180
D	0.6170	0.5310
F	0.0090	0.2090
G	0.6600	0.5440
H	0.6510	0.5380
I	0.5920	0.5100
J	0.2410	0.3860
K	0.3870	0.4400
M	0.6330	0.5320
N	0.5690	0.5210
O	0.5820	0.5230
P	0.6500	0.5200
Q	0.6300	0.5130
R	0.5130	0.4800
S	0.5960	0.5210
T	0.6870	0.5450
U	0.6010	0.5280
V	0.6530	0.5410
W	0.5560	0.4980
X	0.4440	0.4770
Y	0.6830	0.5470
Z	0.5450	0.5270
a	0.7060	0.5240
b	0.4770	0.4650

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Chain	Atom inclusion	Q-score
c	0.2960	0.4040
d	0.4690	0.4680
e	0.3860	0.4400
f	0.4550	0.4680
g	0.1820	0.3860
h	0.4010	0.4450
i	0.4260	0.4650
j	0.4590	0.4730
k	0.3980	0.4400
l	0.3290	0.4180
m	0.5530	0.5240
n	0.3880	0.4430
o	0.6110	0.5130
p	0.4130	0.4270
q	0.4640	0.4640
r	0.4250	0.4640
s	0.2610	0.4180
t	0.4150	0.4400
u	0.4680	0.4530