



wwPDB EM Validation Summary Report ⓘ

Apr 9, 2026 – 08:23 PM UTC

PDB ID : 9SRO / pdb_00009sro
EMDB ID : EMD-55145
Title : Cryo-EM structure of SKM-70S ribosomal stalled complex in the rotated state with hybrid tRNAs
Authors : Morici, M.; Corazza, M.; Safdari, H.A.; Wilson, D.N.
Deposited on : 2025-09-24
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

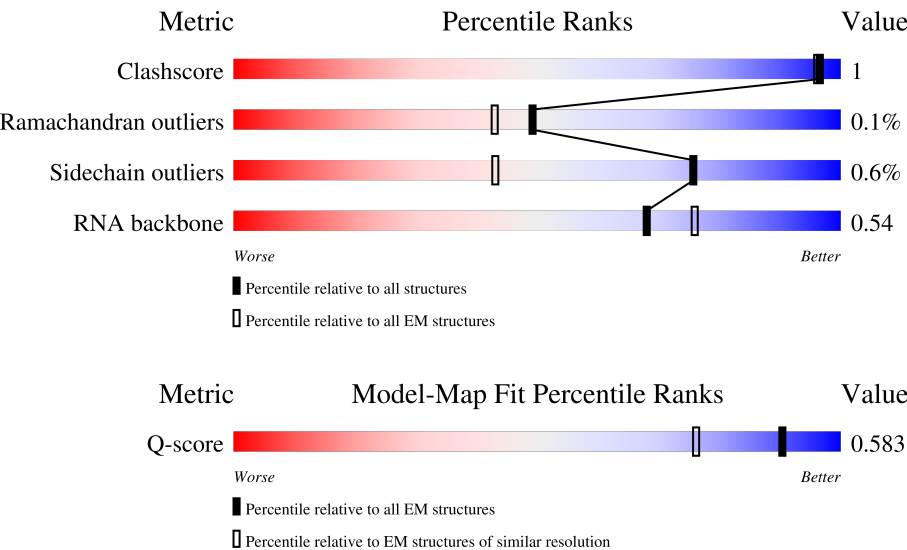
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8728 (2.10 - 3.10)

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

Mol	Chain	Length	Quality of chain
1	3	38	<div><div>71%</div><div>100%</div></div>
2	L	124	<div><div>8%</div><div>94%</div><div>..</div></div>
3	d	209	<div><div>66%</div><div>96%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
4	a	2907	
5	4	70	
6	A	1532	
7	0	55	
8	1	46	
9	2	65	
10	B	241	
11	D	206	
12	E	167	
13	F	135	
14	H	130	
15	I	130	
16	M	118	
17	N	101	
18	O	89	
19	P	82	
20	Q	84	
21	R	75	
22	S	92	
23	T	87	
24	X	136	
25	b	120	
26	c	273	
27	f	179	
28	i	142	

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Mol	Chain	Length	Quality of chain
29	j	123	
30	m	127	
31	n	117	
32	o	115	
33	p	118	
34	q	103	
35	r	110	
36	s	100	
37	v	85	
38	w	78	
39	x	63	
40	y	59	
41	z	57	
42	e	201	
43	g	177	
44	h	149	
45	k	144	
46	u	94	
47	C	233	
48	G	179	
49	J	103	
50	U	71	
51	Y	73	
52	Z	73	
53	l	136	

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Mol	Chain	Length	Quality of chain
54	K	129	<div><div></div><div>25%</div><div></div><div>81%</div><div></div><div>9%</div><div></div><div>9%</div></div>

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 140762 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 Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 2 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	121	Total	C	N	O	S	0	0
			942	582	193	162	5		

- Molecule 3 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	205	Total	C	N	O	S	0	0
			1539	963	283	289	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	2750	Total	C	N	O	P	0	0
			59068	26356	10887	19075	2750		

- Molecule 5 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	58	Total	C	N	O	S	0	0
			464	289	87	82	6		

- Molecule 6 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1501	Total	C	N	O	P	0	0
			32234	14382	5925	10426	1501		

- Molecule 7 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 8 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1	45	Total	C	N	O	S	0	0
			367	222	88	55	2		

- Molecule 9 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2	63	Total	C	N	O	S	0	0
			498	320	104	72	2		

- Molecule 10 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 11 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 12 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 13 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 15 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 16 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 17 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 18 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 19 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	79	Total	C	N	O	S	0	0
			629	394	124	110	1		

- Molecule 20 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 21 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 22 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 23 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	85	Total	C	N	O	S	0	0
			664	411	137	113	3		

- Molecule 24 is a RNA chain called ermBL mRNA transcript.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	10	Total	C	N	O	P	0	0
			215	96	38	71	10		

- Molecule 25 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 26 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	270	Total	C	N	O	S	0	0
			2076	1285	422	362	7		

- Molecule 27 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 28 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	i	140	Total	C	N	O	S	0	0
			1112	703	210	196	3		

- Molecule 29 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 30 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 31 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	n	110	Total	C	N	O		0	0
			845	522	171	152			

- Molecule 32 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	o	113	Total	C	N	O	S	0	0
			908	570	177	160	1		

- Molecule 33 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	p	115	Total	C	N	O		0	0
			933	595	190	148			

- Molecule 34 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	q	97	Total	C	N	O	S	0	0
			773	487	147	138	1		

- Molecule 35 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	r	106	Total	C	N	O	S	0	0
			823	514	159	148	2		

- Molecule 36 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	s	91	Total	C	N	O	S	0	0
			722	455	137	129	1		

- Molecule 37 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	v	71	Total	C	N	O	S	0	0
			540	337	109	93	1		

- Molecule 38 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	w	75	Total	C	N	O	S	0	0
			603	373	126	102	2		

- Molecule 39 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	x	57	Total	C	N	O	S	0	0
			468	288	91	88	1		

- Molecule 40 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	y	52	Total	C	N	O	S	0	0
			401	251	79	69	2		

- Molecule 41 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	z	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 42 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	e	191	Total	C	N	O	S	0	0
			1474	926	272	271	5		

- Molecule 43 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	g	127	Total	C	N	O	S	0	0
			954	599	176	177	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	16	SER	ASP	conflict	UNP A7ZSJ4

- Molecule 44 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	h	28	Total	C	N	O	S	0	0
			212	139	37	35	1		

- Molecule 45 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	130	Total	C	N	O	S	0	0
			955	592	192	169	2		

- Molecule 46 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	u	85	Total	C	N	O	S	0	0
			679	431	126	120	2		

- Molecule 47 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	C	202	Total	C	N	O	S	0	0
			1593	1009	299	282	3		

- Molecule 48 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	G	119	Total	C	N	O	S	0	0
			942	591	181	166	4		

- Molecule 49 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	J	91	Total	C	N	O		0	0
			730	459	140	131			

- Molecule 50 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 51 is a RNA chain called A/P-tRNA-Leu.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Y	73	Total	C	N	O	P	0	0
			1562	697	286	506	73		

- Molecule 52 is a RNA chain called P/E-tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Z	73	Total	C	N	O	P	0	0
			1563	696	286	508	73		

- Molecule 53 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	l	132	Total	C	N	O	S	0	0
			1043	666	200	171	6		

- Molecule 54 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP P0A7R9

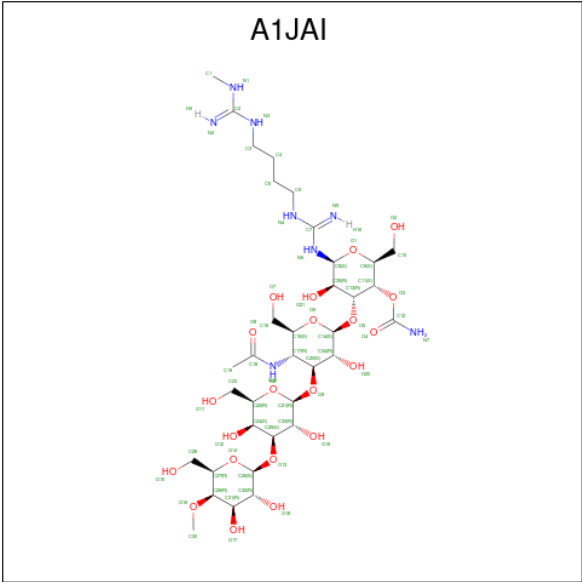
- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	3	1	Total 1	Zn 1	0
55	4	1	Total 1	Zn 1	0

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	d	1	Total 1	Mg 1	0
56	a	191	Total 191	Mg 191	0
56	A	110	Total 110	Mg 110	0
56	B	1	Total 1	Mg 1	0
56	b	5	Total 5	Mg 5	0
56	c	1	Total 1	Mg 1	0

- Molecule 57 is [(2 {S},3 {S},4 {R},5 {R},6 {S})-4-[(2 {S},3 {R},4 {S},5 {R},6 {S})-5-acetamido-6-(hydroxymethyl)-4-[(2 {R},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-4-[(2 {S},3 {R},4 {R},5 {R},6 {R})-6-(hydroxymethyl)-5-methoxy-3,4-bis(oxidanyl)oxan-2-yl]oxy-3,5-bis(oxidanyl)oxan-2-yl]oxy-3-oxidanyl-oxan-2-yl]oxy-2-(hydroxymethyl)-6-[[{N}]-[4-[({N}-methylcarbamimidoyl)amino]butyl]carbamimidoyl]amino]-5-oxidanyl-oxan-3-yl] carbamate (CCD ID: A1JAI) (formula: C₃₅H₆₄N₈O₂₁) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
57	A	1	Total	C	N	O	0
			64	35	8	21	

- Molecule 58 is water.

Mol	Chain	Residues	Atoms		AltConf
58	3	1	Total	O	0
			1	1	
58	L	14	Total	O	0
			14	14	
58	d	7	Total	O	0
			7	7	
58	a	696	Total	O	0
			696	696	
58	4	4	Total	O	0
			4	4	
58	A	767	Total	O	0
			767	767	
58	0	2	Total	O	0
			2	2	
58	1	4	Total	O	0
			4	4	
58	2	2	Total	O	0
			2	2	
58	B	7	Total	O	0
			7	7	
58	D	13	Total	O	0
			13	13	

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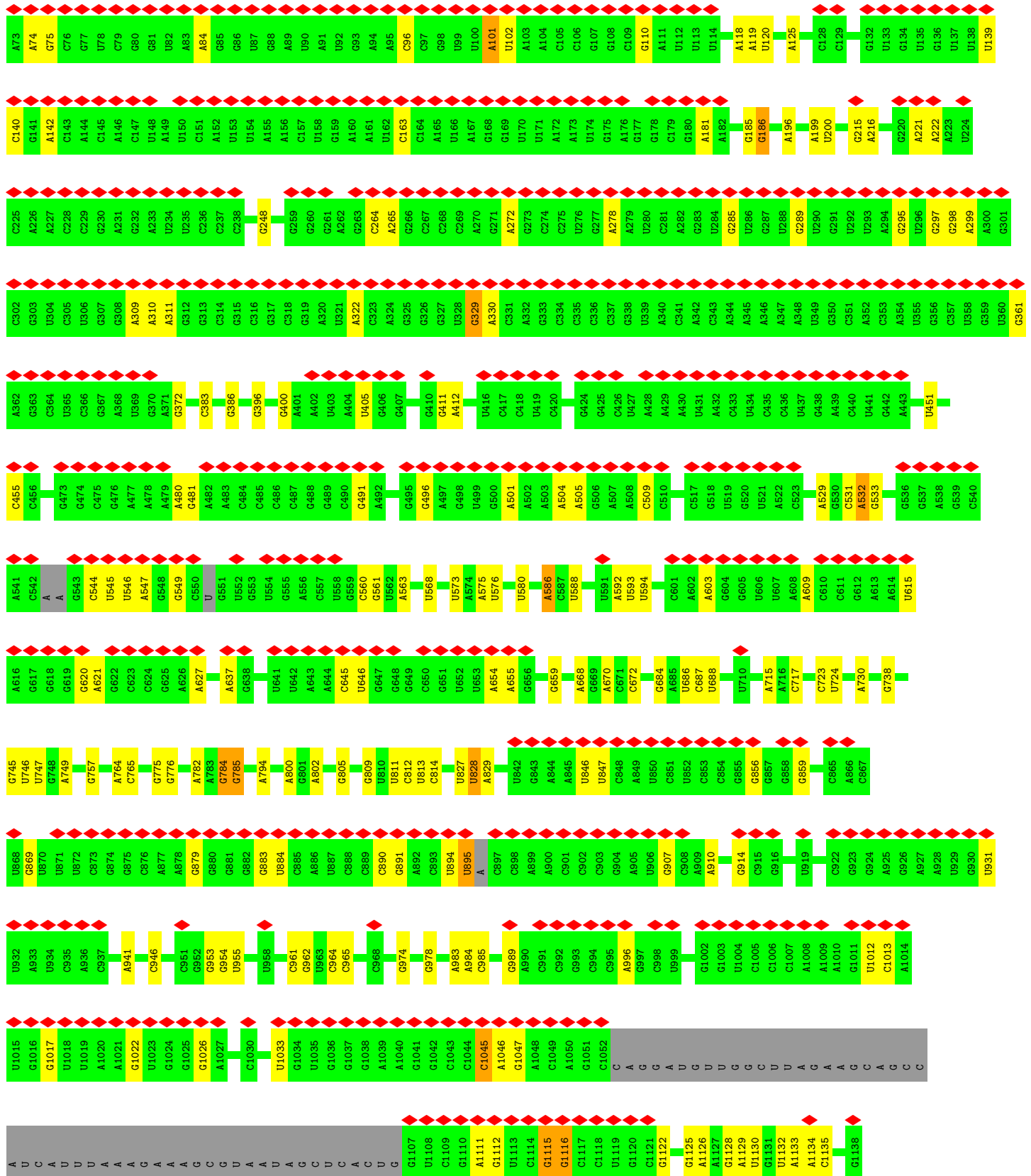
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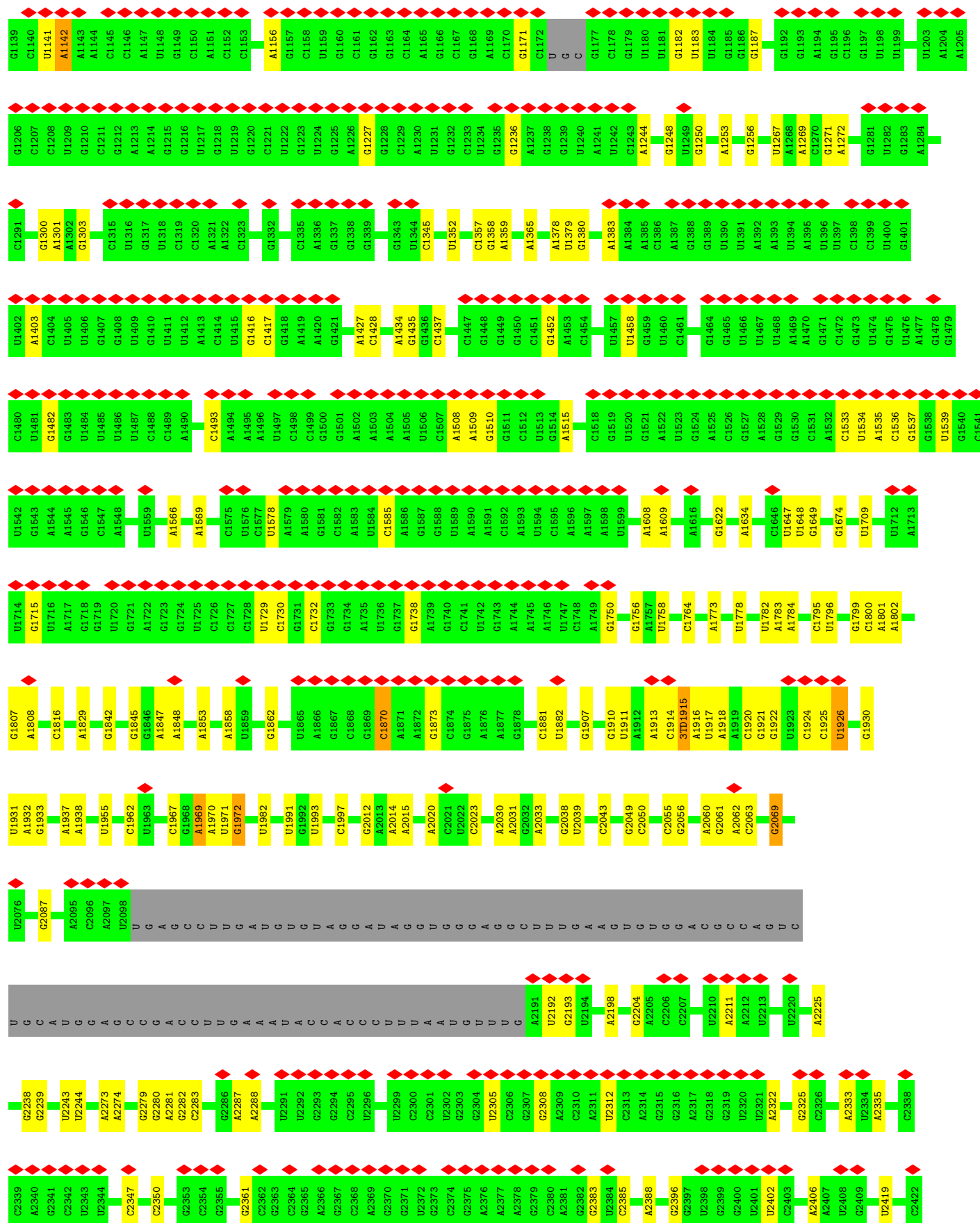
Mol	Chain	Residues	Atoms		AltConf
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58	F	1	Total 1	O 1	0
58	H	15	Total 15	O 15	0
58	I	5	Total 5	O 5	0
58	M	7	Total 7	O 7	0
58	N	17	Total 17	O 17	0
58	O	6	Total 6	O 6	0
58	P	3	Total 3	O 3	0
58	Q	5	Total 5	O 5	0
58	R	8	Total 8	O 8	0
58	S	6	Total 6	O 6	0
58	T	3	Total 3	O 3	0
58	b	2	Total 2	O 2	0
58	c	51	Total 51	O 51	0
58	f	2	Total 2	O 2	0
58	i	6	Total 6	O 6	0
58	j	7	Total 7	O 7	0
58	n	1	Total 1	O 1	0
58	o	6	Total 6	O 6	0
58	p	2	Total 2	O 2	0
58	q	3	Total 3	O 3	0

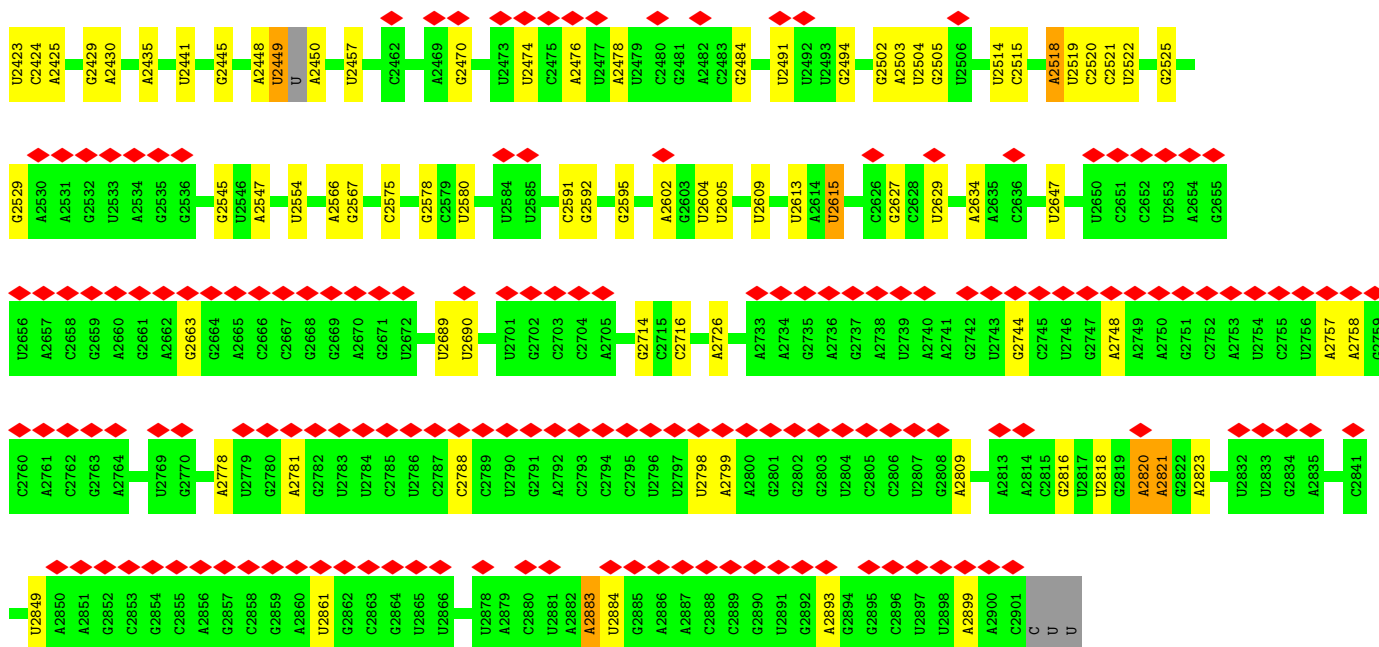
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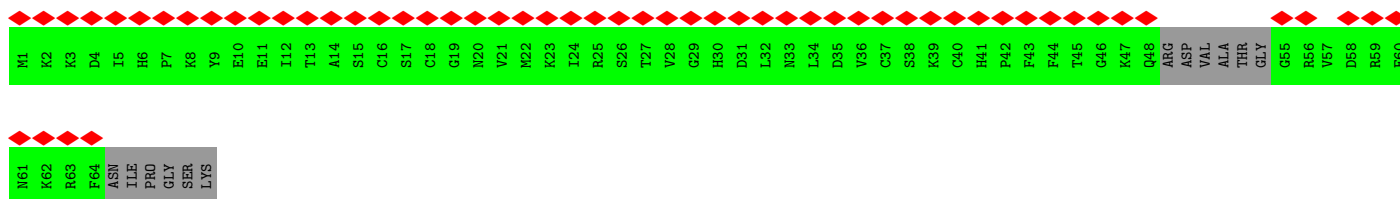
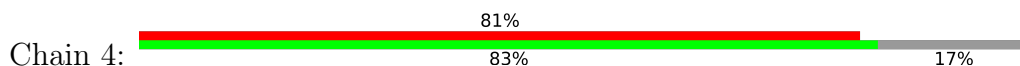
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58	s	1	Total 1	O 1	0
58	v	2	Total 2	O 2	0
58	w	3	Total 3	O 3	0
58	y	1	Total 1	O 1	0
58	z	2	Total 2	O 2	0
58	e	5	Total 5	O 5	0
58	g	1	Total 1	O 1	0
58	h	1	Total 1	O 1	0
58	k	5	Total 5	O 5	0
58	u	2	Total 2	O 2	0
58	C	17	Total 17	O 17	0
58	G	2	Total 2	O 2	0
58	J	10	Total 10	O 10	0
58	U	3	Total 3	O 3	0
58	Y	1	Total 1	O 1	0
58	Z	4	Total 4	O 4	0
58	l	2	Total 2	O 2	0
58	K	6	Total 6	O 6	0

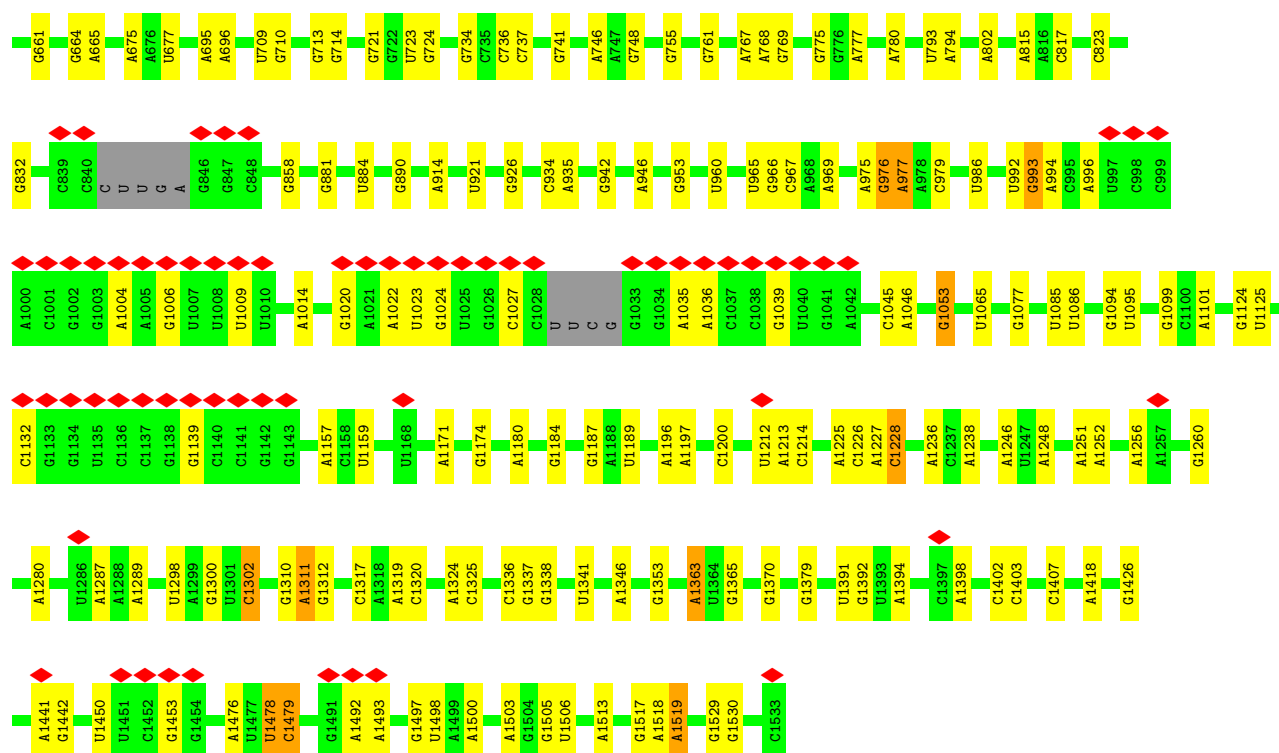




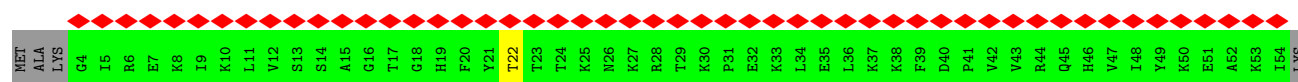


• Molecule 5: Large ribosomal subunit protein bL31A

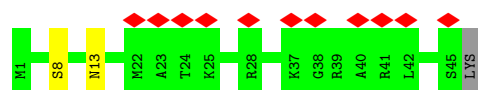




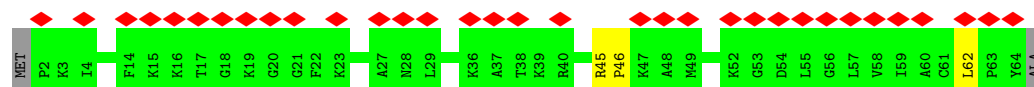
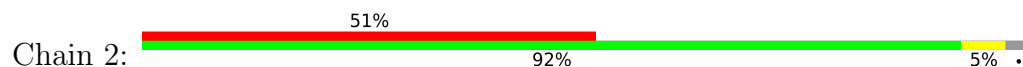
• Molecule 7: Large ribosomal subunit protein bL33



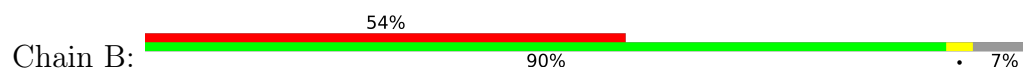
• Molecule 8: Large ribosomal subunit protein bL34

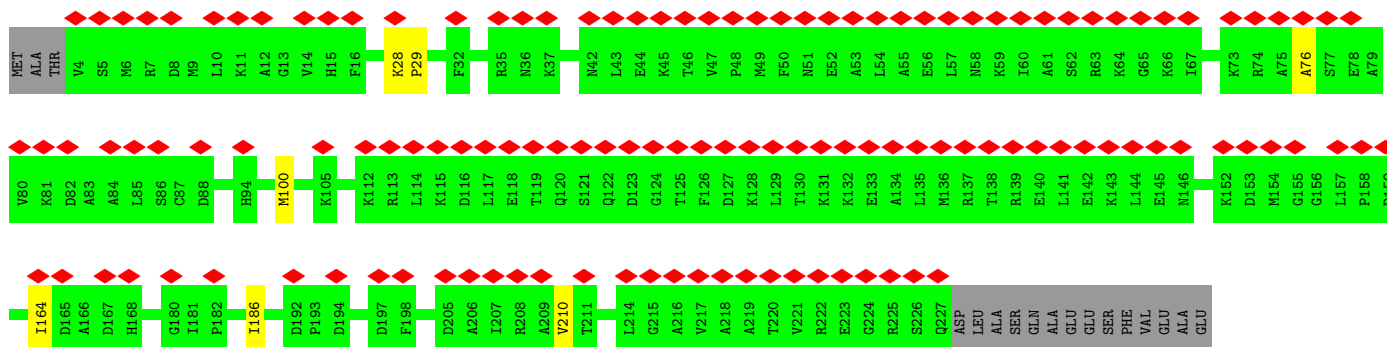


• Molecule 9: Large ribosomal subunit protein bL35

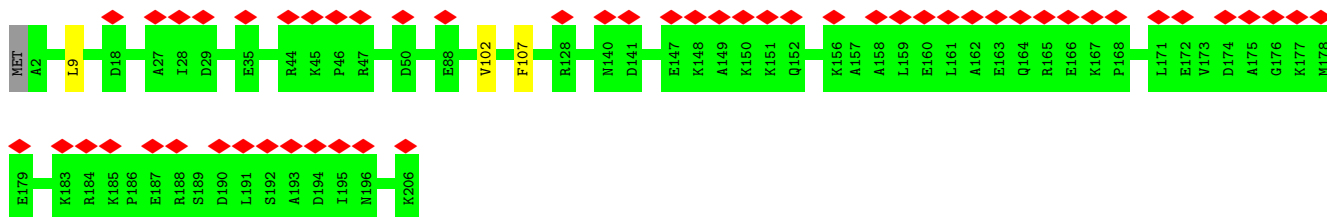


• Molecule 10: Small ribosomal subunit protein uS2

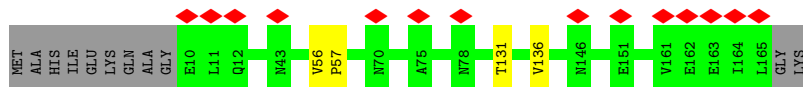
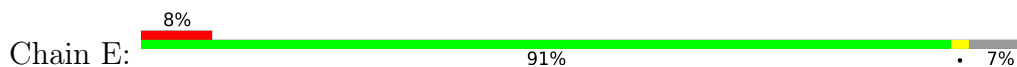




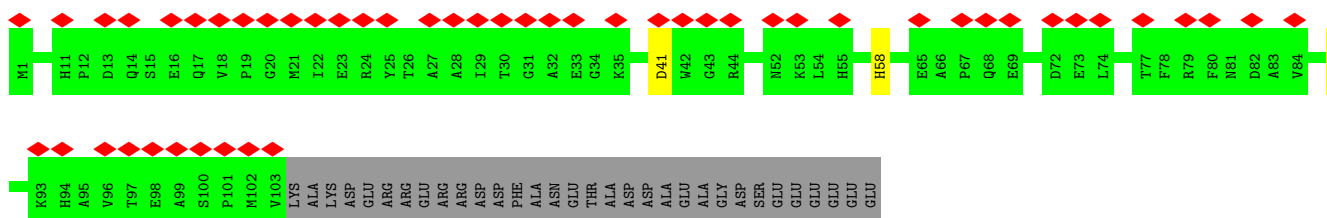
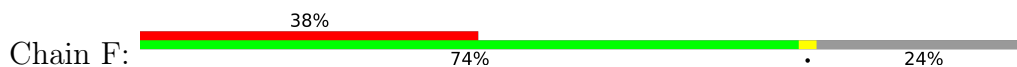
- Molecule 11: Small ribosomal subunit protein uS4



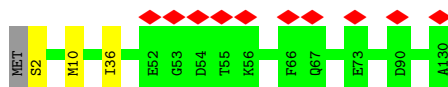
- Molecule 12: Small ribosomal subunit protein uS5



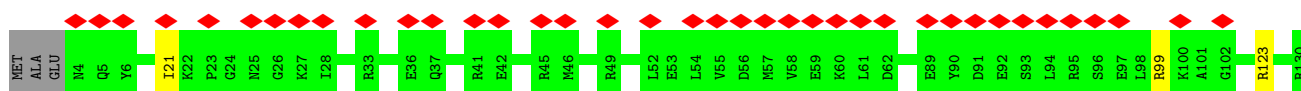
- Molecule 13: Small ribosomal subunit protein bS6, fully modified isoform



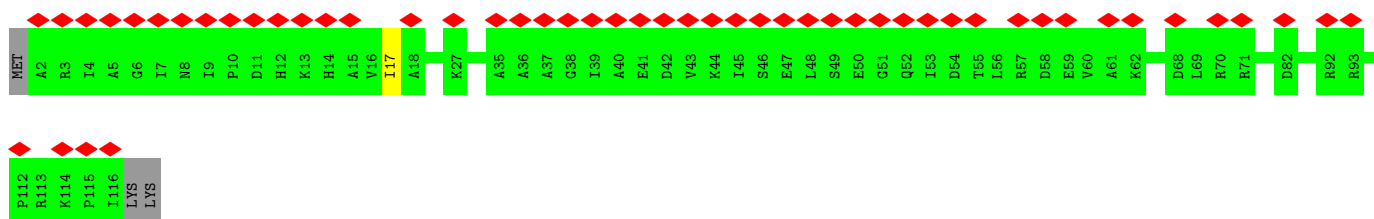
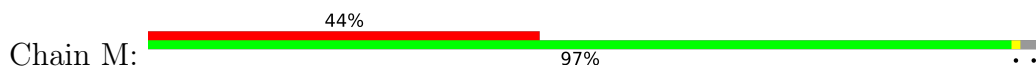
- Molecule 14: Small ribosomal subunit protein uS8



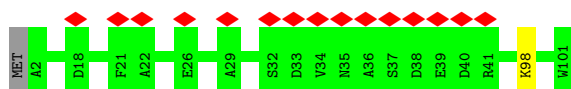
- Molecule 15: Small ribosomal subunit protein uS9



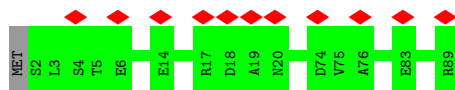
- Molecule 16: Small ribosomal subunit protein uS13



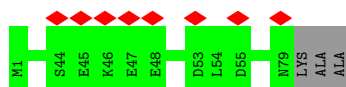
- Molecule 17: Small ribosomal subunit protein uS14



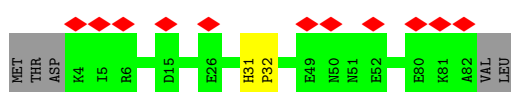
- Molecule 18: Small ribosomal subunit protein uS15



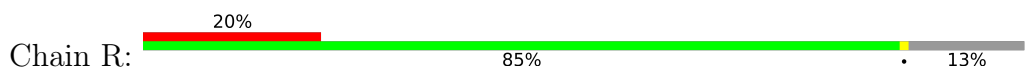
- Molecule 19: Small ribosomal subunit protein bS16

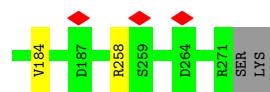


- Molecule 20: Small ribosomal subunit protein uS17

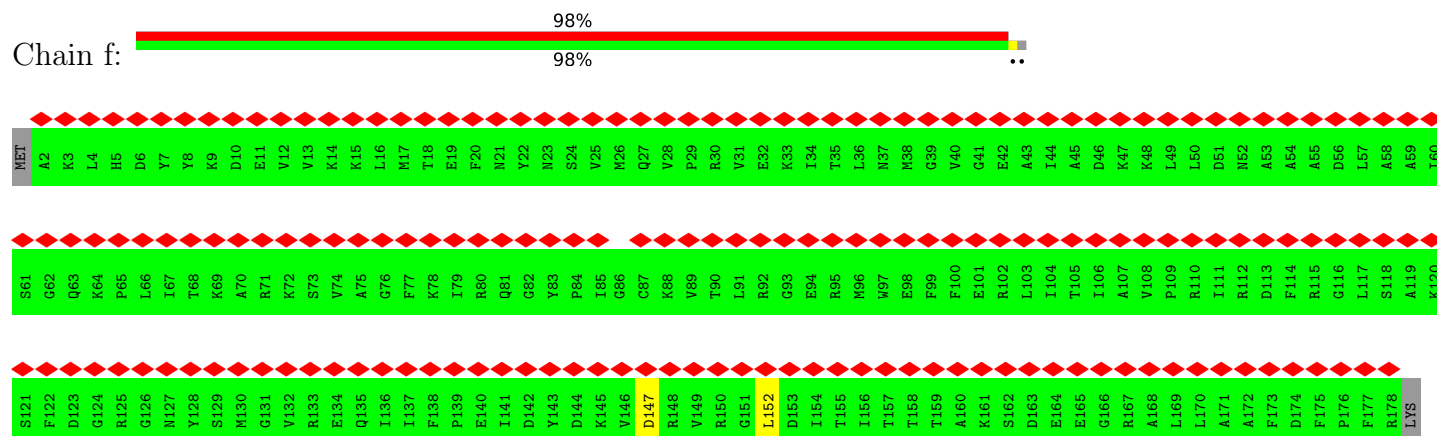


- Molecule 21: Small ribosomal subunit protein bS18

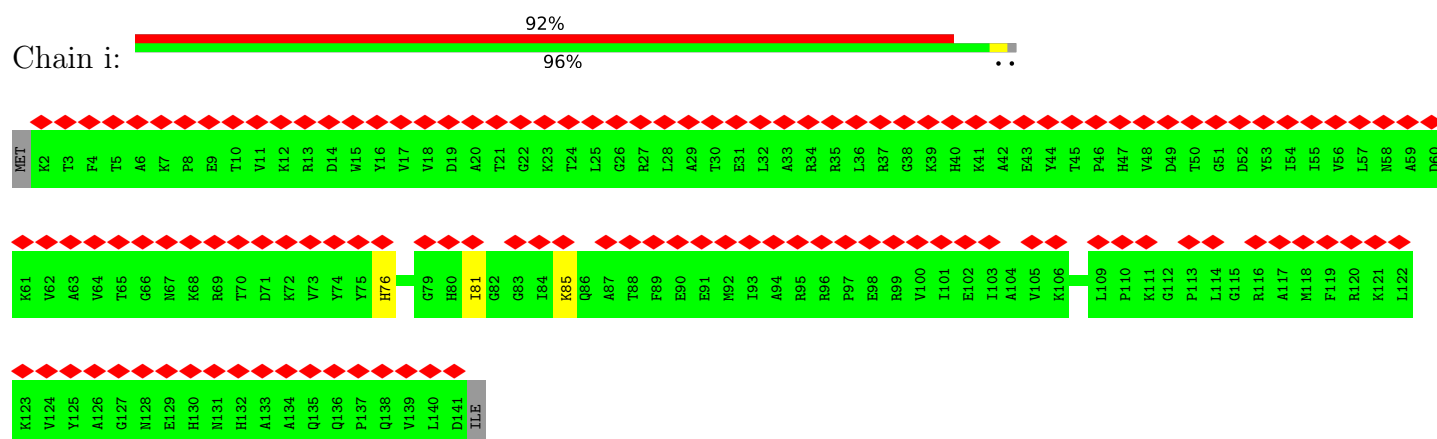




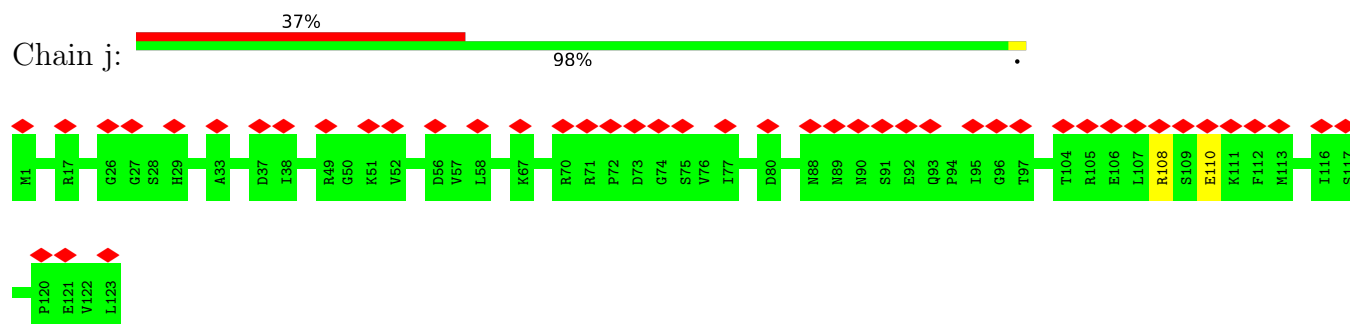
- Molecule 27: Large ribosomal subunit protein uL5



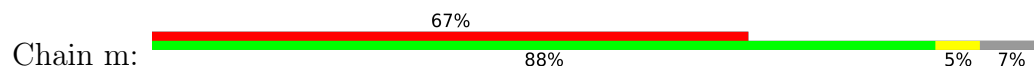
- Molecule 28: Large ribosomal subunit protein uL13

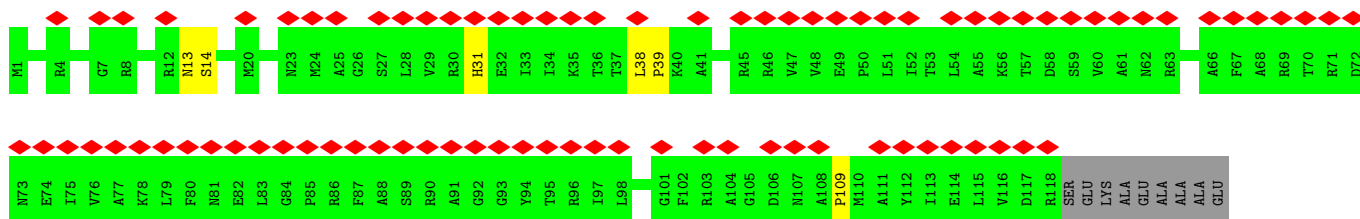


- Molecule 29: Large ribosomal subunit protein uL14

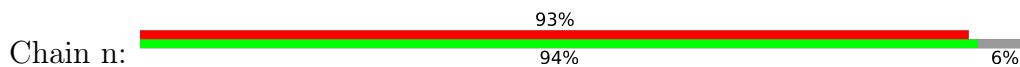


- Molecule 30: Large ribosomal subunit protein bL17

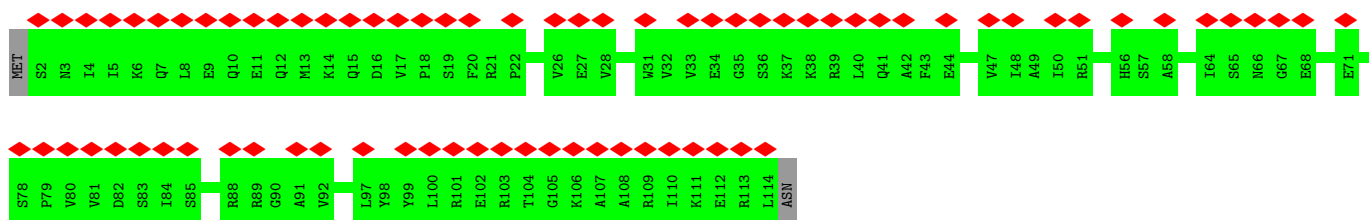




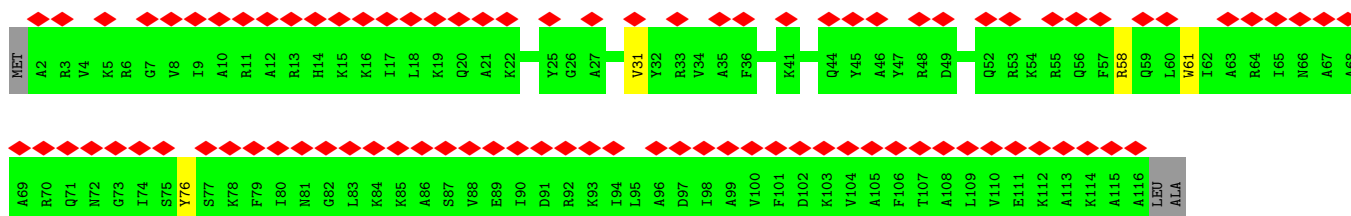
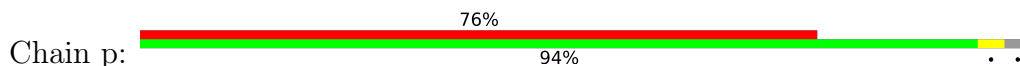
- Molecule 31: Large ribosomal subunit protein uL18



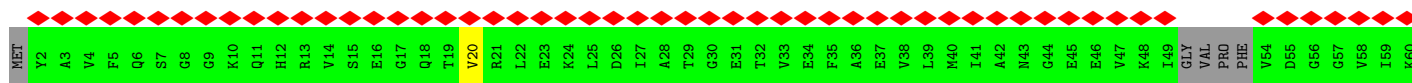
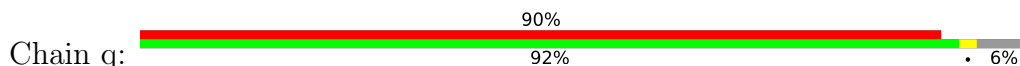
- Molecule 32: Large ribosomal subunit protein bL19

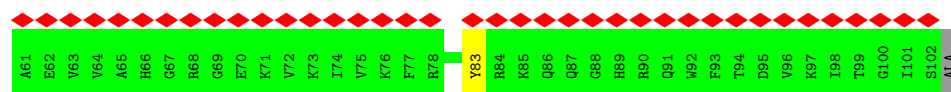


- Molecule 33: Large ribosomal subunit protein bL20



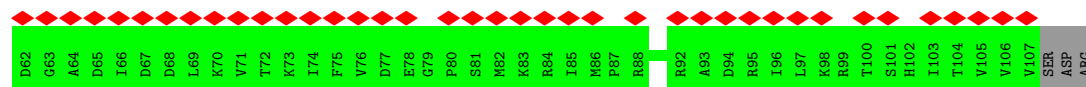
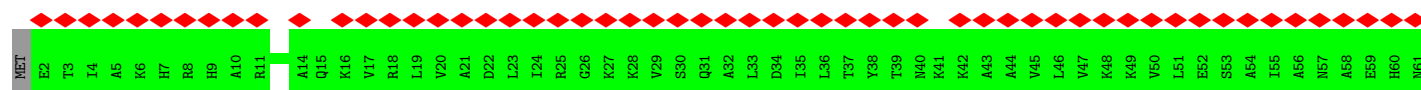
- Molecule 34: Large ribosomal subunit protein bL21





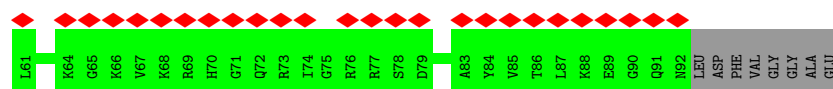
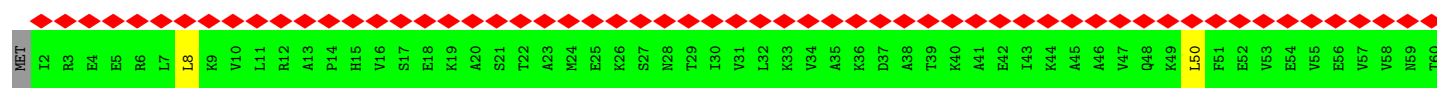
- Molecule 35: Large ribosomal subunit protein uL22

Chain r: 86%
96%



- Molecule 36: Large ribosomal subunit protein uL23

Chain s: 85%
89% 9%



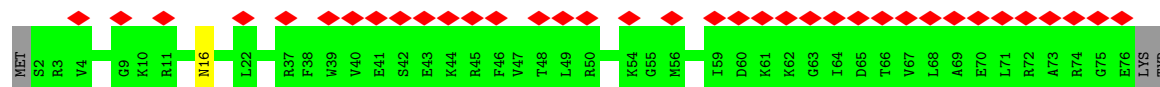
- Molecule 37: Large ribosomal subunit protein bL27

Chain v: 76%
81% 16%



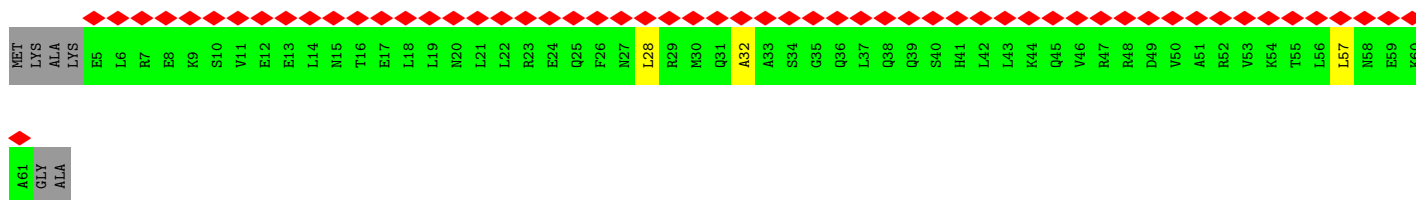
- Molecule 38: Large ribosomal subunit protein bL28

Chain w: 46%
95%

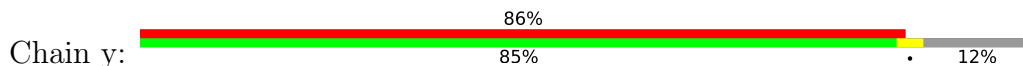


- Molecule 39: Large ribosomal subunit protein uL29

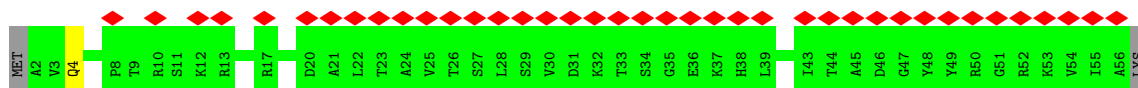
Chain x: 90%
86% 5% 10%



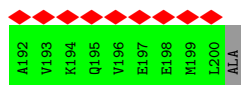
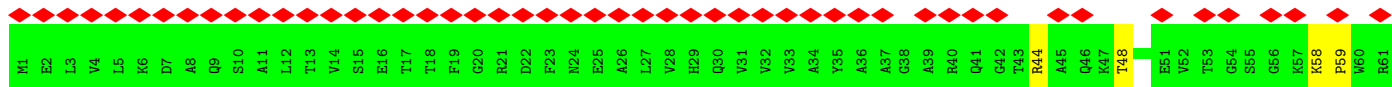
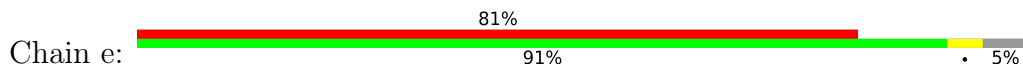
- Molecule 40: Large ribosomal subunit protein uL30



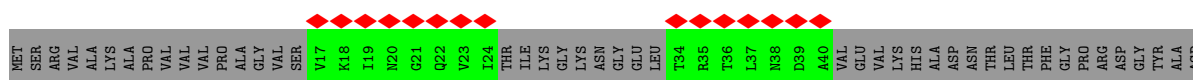
- Molecule 41: Large ribosomal subunit protein bL32

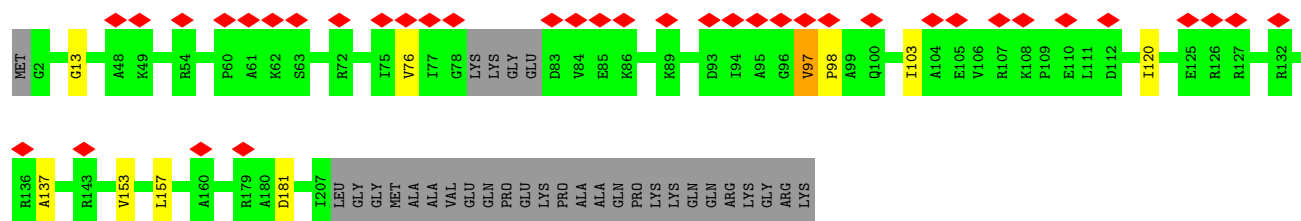


- Molecule 42: Large ribosomal subunit protein uL4

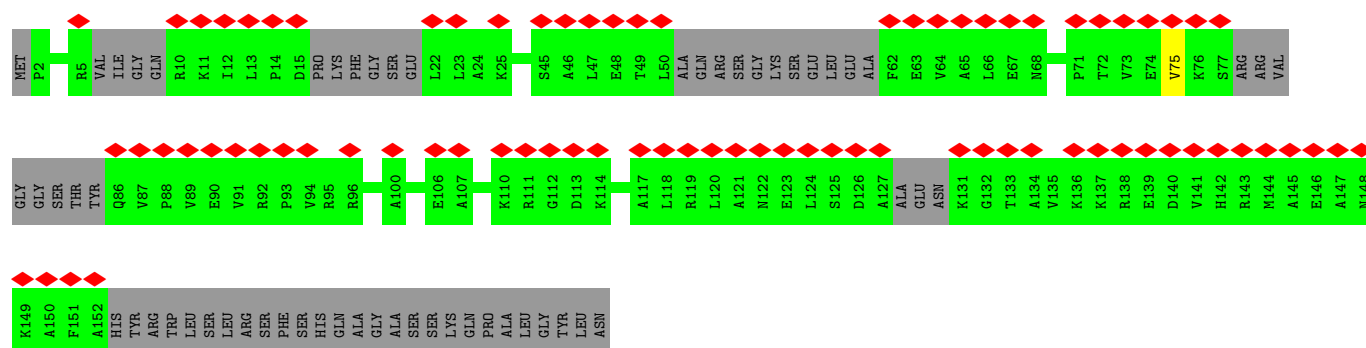
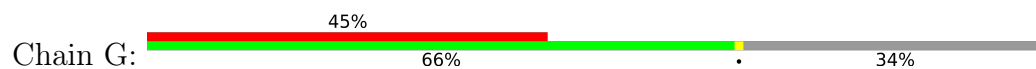


- Molecule 43: Large ribosomal subunit protein uL6

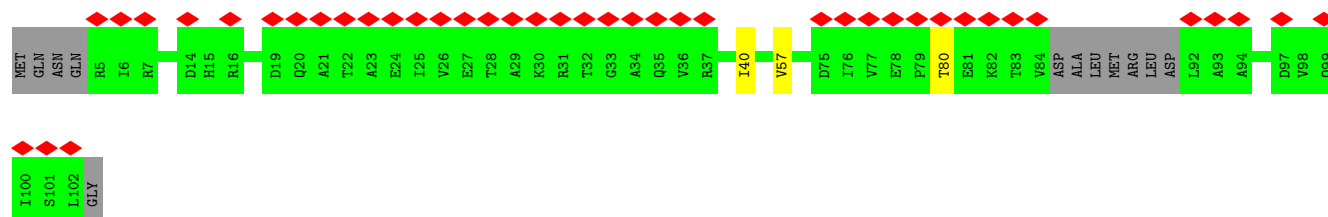
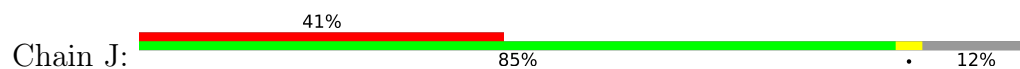




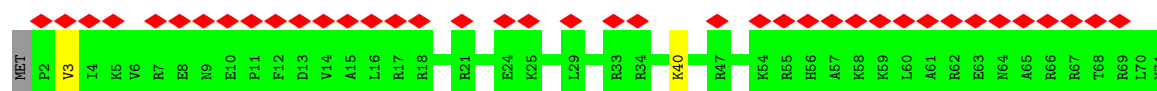
• Molecule 48: Small ribosomal subunit protein uS7



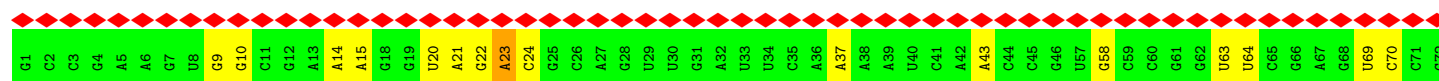
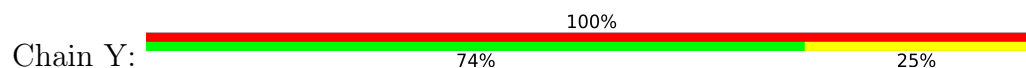
• Molecule 49: Small ribosomal subunit protein uS10



• Molecule 50: Small ribosomal subunit protein bS21

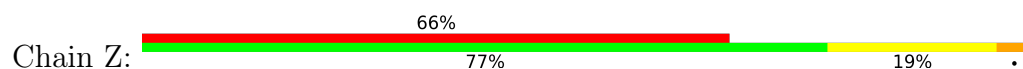


• Molecule 51: A/P-tRNA-Leu

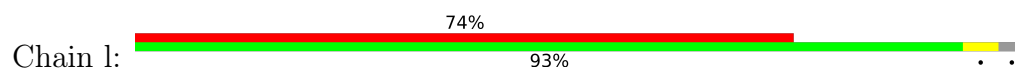




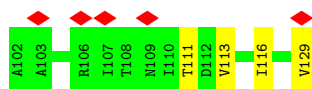
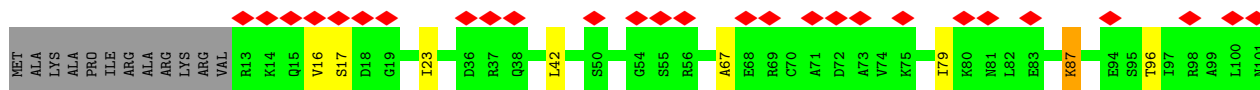
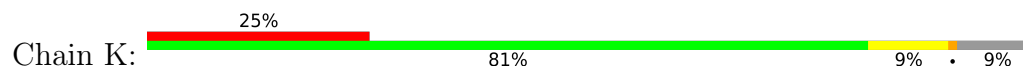
• Molecule 52: P/E-tRNA-fMet



• Molecule 53: Large ribosomal subunit protein uL16



• Molecule 54: Small ribosomal subunit protein uS11



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	121168	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.14	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	359.424, 359.424, 359.424	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, 6MZ, G7M, OMU, PSU, MA6, MEQ, 1MG, MS6, 4OC, 2MA, UR3, 5MU, 2MG, OMG, OMC, D2T, H2U, IAS, ZN, 4D4, A1JAI, 3TD, 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	3	0.59	0/303	0.69	0/397
2	L	0.58	0/945	0.76	0/1268
3	d	0.58	0/1549	0.76	0/2084
4	a	0.57	0/65581	0.78	4/102302 (0.0%)
5	4	0.60	0/472	0.79	0/627
6	A	0.53	0/35839	0.83	8/55896 (0.0%)
7	0	0.57	0/424	0.74	0/565
8	1	0.56	0/370	0.83	0/487
9	2	0.60	0/507	0.84	0/669
10	B	0.57	0/1784	0.86	0/2403
11	D	0.57	0/1665	0.82	0/2227
12	E	0.62	0/1165	0.79	0/1568
13	F	0.57	0/858	0.79	0/1160
14	H	0.61	0/989	0.81	0/1326
15	I	0.60	0/1034	0.81	0/1375
16	M	0.58	0/900	0.85	0/1204
17	N	0.64	0/817	0.84	0/1088
18	O	0.59	0/722	0.88	0/964
19	P	0.60	0/639	0.76	0/859
20	Q	0.57	0/650	0.73	0/871
21	R	0.59	0/544	0.83	0/731
22	S	0.62	0/680	0.79	0/915
23	T	0.59	0/670	0.88	0/888
24	X	0.69	0/240	0.91	2/372 (0.5%)
25	b	0.59	0/2850	0.74	0/4444
26	c	0.62	0/2115	0.76	0/2844
27	f	0.58	0/1434	0.82	0/1926
28	i	0.56	0/1135	0.83	0/1530
29	j	0.57	0/955	0.76	0/1279
30	m	0.58	0/958	0.81	0/1281
31	n	0.59	0/854	0.84	0/1146

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	o	0.56	0/920	0.71	0/1231
33	p	0.53	0/946	0.87	0/1260
34	q	0.58	0/783	0.67	0/1044
35	r	0.57	0/830	0.79	0/1113
36	s	0.56	0/728	0.77	0/973
37	v	0.59	0/547	0.70	0/724
38	w	0.57	0/612	0.77	0/819
39	x	0.53	0/469	0.91	0/626
40	y	0.60	0/405	0.81	0/543
41	z	0.60	0/440	0.82	0/588
42	e	0.56	0/1491	0.83	0/2004
43	g	0.60	0/964	0.80	0/1301
44	h	0.64	0/214	0.83	0/287
45	k	0.59	0/961	0.80	0/1272
46	u	0.59	0/689	0.73	0/922
47	C	0.59	0/1619	0.81	0/2183
48	G	0.59	0/948	0.87	0/1264
49	J	0.62	0/739	0.79	0/999
50	U	0.60	0/597	0.88	0/792
51	Y	0.65	0/1745	0.74	0/2714
52	Z	0.58	0/1746	0.79	1/2719 (0.0%)
53	l	0.57	0/1041	0.77	0/1392
54	K	0.66	0/884	0.79	0/1191
All	All	0.57	0/149966	0.80	15/224657 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	a	0	1
6	A	0	4
9	2	0	1
23	T	0	1
37	v	0	1
38	w	0	1
47	C	0	1
All	All	0	10

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	976	G	O3'-P-O5'	-7.16	93.26	104.00
6	A	1311	A	O3'-P-O5'	-6.03	94.95	104.00
24	X	18	G	C2'-C3'-O3'	5.62	117.93	109.50
6	A	746	A	O3'-P-O5'	-5.50	95.76	104.00
6	A	652	U	O3'-P-O5'	-5.49	95.77	104.00

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	1077	G	Sidechain
6	A	362	G	Sidechain
6	A	575	G	Sidechain
6	A	587	G	Sidechain
4	a	2595	G	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	302	0	340	0	0
2	L	942	0	999	2	0
3	d	1539	0	1586	3	0
4	a	59068	0	29738	70	0
5	4	464	0	462	0	0
6	A	32234	0	16242	44	0
7	0	417	0	451	1	0
8	1	367	0	405	1	0
9	2	498	0	567	1	0
10	B	1753	0	1780	3	0
11	D	1643	0	1707	2	0
12	E	1152	0	1196	2	0
13	F	839	0	833	2	0
14	H	979	0	1031	2	0
15	I	1022	0	1070	1	0
16	M	891	0	952	1	0
17	N	805	0	844	1	0
18	O	714	0	734	0	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	P	629	0	643	0	0
20	Q	641	0	682	1	0
21	R	535	0	552	1	0
22	S	663	0	688	2	0
23	T	664	0	714	1	0
24	X	215	0	107	0	0
25	b	2549	0	1291	0	0
26	c	2076	0	2149	6	0
27	f	1410	0	1444	0	0
28	i	1112	0	1139	2	0
29	j	946	0	1023	0	0
30	m	945	0	989	2	0
31	n	845	0	881	0	0
32	o	908	0	956	0	0
33	p	933	0	1003	3	0
34	q	773	0	793	1	0
35	r	823	0	888	0	0
36	s	722	0	784	1	0
37	v	540	0	562	0	0
38	w	603	0	630	0	0
39	x	468	0	492	1	0
40	y	401	0	433	1	0
41	z	434	0	445	1	0
42	e	1474	0	1550	4	0
43	g	954	0	991	0	0
44	h	212	0	233	1	0
45	k	955	0	1023	1	0
46	u	679	0	707	2	0
47	C	1593	0	1660	4	0
48	G	942	0	1000	0	0
49	J	730	0	770	0	0
50	U	589	0	629	1	0
51	Y	1562	0	793	2	0
52	Z	1563	0	794	5	0
53	l	1043	0	1107	4	0
54	K	877	0	884	7	0
55	3	1	0	0	0	0
55	4	1	0	0	0	0
56	A	110	0	0	0	0
56	B	1	0	0	0	0
56	a	191	0	0	0	0
56	b	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	c	1	0	0	0	0
56	d	1	0	0	0	0
57	A	64	0	0	0	0
58	0	2	0	0	0	0
58	1	4	0	0	0	0
58	2	2	0	0	0	0
58	3	1	0	0	0	0
58	4	4	0	0	0	0
58	A	767	0	0	0	0
58	B	7	0	0	0	0
58	C	17	0	0	0	0
58	D	13	0	0	0	0
58	E	5	0	0	0	0
58	F	1	0	0	0	0
58	G	2	0	0	0	0
58	H	15	0	0	0	0
58	I	5	0	0	0	0
58	J	10	0	0	0	0
58	K	6	0	0	0	0
58	L	14	0	0	0	0
58	M	7	0	0	0	0
58	N	17	0	0	0	0
58	O	6	0	0	0	0
58	P	3	0	0	0	0
58	Q	5	0	0	0	0
58	R	8	0	0	0	0
58	S	6	0	0	0	0
58	T	3	0	0	0	0
58	U	3	0	0	0	0
58	Y	1	0	0	0	0
58	Z	4	0	0	0	0
58	a	696	0	0	0	0
58	b	2	0	0	0	0
58	c	51	0	0	0	0
58	d	7	0	0	0	0
58	e	5	0	0	0	0
58	f	2	0	0	0	0
58	g	1	0	0	0	0
58	h	1	0	0	0	0
58	i	6	0	0	0	0
58	j	7	0	0	0	0
58	k	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	l	2	0	0	0	0
58	n	1	0	0	0	0
58	o	6	0	0	0	0
58	p	2	0	0	0	0
58	q	3	0	0	0	0
58	r	4	0	0	0	0
58	s	1	0	0	0	0
58	u	2	0	0	0	0
58	v	2	0	0	0	0
58	w	3	0	0	0	0
58	y	1	0	0	0	0
58	z	2	0	0	0	0
All	All	140762	0	92366	166	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 166 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:568:U:H1'	4:a:2030:6MZ:H9C1	1.71	0.72
6:A:664:G:H22	6:A:741:G:H1	1.40	0.70
54:K:23:ILE:HG12	54:K:96:THR:HG21	1.74	0.70
6:A:823:C:HO2'	14:H:2:SER:N	1.98	0.61
6:A:677:U:H3	6:A:713:G:H22	1.49	0.60

There are no symmetry-related clashes.

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	3	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
2	L	118/124 (95%)	115 (98%)	3 (2%)	0	100	100
3	d	202/209 (97%)	188 (93%)	14 (7%)	0	100	100
5	4	54/70 (77%)	48 (89%)	6 (11%)	0	100	100
7	0	49/55 (89%)	45 (92%)	4 (8%)	0	100	100
8	1	43/46 (94%)	43 (100%)	0	0	100	100
9	2	61/65 (94%)	57 (93%)	4 (7%)	0	100	100
10	B	222/241 (92%)	213 (96%)	9 (4%)	0	100	100
11	D	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
12	E	154/167 (92%)	150 (97%)	4 (3%)	0	100	100
13	F	101/135 (75%)	98 (97%)	3 (3%)	0	100	100
14	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
15	I	125/130 (96%)	119 (95%)	5 (4%)	1 (1%)	16	34
16	M	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
17	N	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
18	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
19	P	77/82 (94%)	74 (96%)	3 (4%)	0	100	100
20	Q	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
21	R	63/75 (84%)	62 (98%)	1 (2%)	0	100	100
22	S	81/92 (88%)	80 (99%)	1 (1%)	0	100	100
23	T	83/87 (95%)	82 (99%)	1 (1%)	0	100	100
26	c	268/273 (98%)	257 (96%)	11 (4%)	0	100	100
27	f	175/179 (98%)	163 (93%)	12 (7%)	0	100	100
28	i	138/142 (97%)	131 (95%)	7 (5%)	0	100	100
29	j	121/123 (98%)	111 (92%)	9 (7%)	1 (1%)	16	34
30	m	116/127 (91%)	105 (90%)	10 (9%)	1 (1%)	14	30
31	n	108/117 (92%)	99 (92%)	9 (8%)	0	100	100
32	o	111/115 (96%)	105 (95%)	6 (5%)	0	100	100
33	p	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
34	q	93/103 (90%)	85 (91%)	8 (9%)	0	100	100
35	r	104/110 (94%)	96 (92%)	8 (8%)	0	100	100
36	s	89/100 (89%)	75 (84%)	14 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	v	69/85 (81%)	67 (97%)	2 (3%)	0	100	100
38	w	73/78 (94%)	69 (94%)	4 (6%)	0	100	100
39	x	55/63 (87%)	52 (94%)	3 (6%)	0	100	100
40	y	50/59 (85%)	47 (94%)	3 (6%)	0	100	100
41	z	53/57 (93%)	46 (87%)	7 (13%)	0	100	100
42	e	187/201 (93%)	179 (96%)	8 (4%)	0	100	100
43	g	121/177 (68%)	99 (82%)	22 (18%)	0	100	100
44	h	24/149 (16%)	22 (92%)	2 (8%)	0	100	100
45	k	124/144 (86%)	113 (91%)	10 (8%)	1 (1%)	16	34
46	u	81/94 (86%)	73 (90%)	8 (10%)	0	100	100
47	C	198/233 (85%)	191 (96%)	7 (4%)	0	100	100
48	G	107/179 (60%)	103 (96%)	4 (4%)	0	100	100
49	J	87/103 (84%)	80 (92%)	5 (6%)	2 (2%)	5	9
50	U	68/71 (96%)	63 (93%)	5 (7%)	0	100	100
53	l	128/136 (94%)	125 (98%)	3 (2%)	0	100	100
54	K	113/129 (88%)	109 (96%)	4 (4%)	0	100	100
All	All	5147/5809 (89%)	4869 (95%)	272 (5%)	6 (0%)	49	70

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
49	J	57	VAL
49	J	40	ILE
15	I	123	ARG
29	j	108	ARG
30	m	109	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	34/34 (100%)	34 (100%)	0	100	100
2	L	101/103 (98%)	101 (100%)	0	100	100
3	d	161/163 (99%)	160 (99%)	1 (1%)	78	91
5	4	53/62 (86%)	53 (100%)	0	100	100
7	0	46/49 (94%)	46 (100%)	0	100	100
8	1	37/38 (97%)	36 (97%)	1 (3%)	39	67
9	2	51/52 (98%)	51 (100%)	0	100	100
10	B	186/199 (94%)	185 (100%)	1 (0%)	81	92
11	D	172/173 (99%)	172 (100%)	0	100	100
12	E	119/126 (94%)	119 (100%)	0	100	100
13	F	90/116 (78%)	90 (100%)	0	100	100
14	H	104/105 (99%)	104 (100%)	0	100	100
15	I	105/107 (98%)	104 (99%)	1 (1%)	68	86
16	M	93/96 (97%)	93 (100%)	0	100	100
17	N	83/84 (99%)	83 (100%)	0	100	100
18	O	76/77 (99%)	76 (100%)	0	100	100
19	P	64/65 (98%)	64 (100%)	0	100	100
20	Q	73/78 (94%)	73 (100%)	0	100	100
21	R	56/65 (86%)	56 (100%)	0	100	100
22	S	72/79 (91%)	72 (100%)	0	100	100
23	T	65/66 (98%)	65 (100%)	0	100	100
26	c	215/218 (99%)	213 (99%)	2 (1%)	70	87
27	f	148/150 (99%)	146 (99%)	2 (1%)	59	81
28	i	114/116 (98%)	114 (100%)	0	100	100
29	j	104/104 (100%)	103 (99%)	1 (1%)	68	86
30	m	98/103 (95%)	97 (99%)	1 (1%)	68	86
31	n	82/87 (94%)	82 (100%)	0	100	100
32	o	98/100 (98%)	98 (100%)	0	100	100
33	p	88/90 (98%)	88 (100%)	0	100	100
34	q	80/84 (95%)	79 (99%)	1 (1%)	61	82
35	r	89/93 (96%)	89 (100%)	0	100	100
36	s	78/84 (93%)	78 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	v	54/63 (86%)	53 (98%)	1 (2%)	50	75
38	w	65/68 (96%)	65 (100%)	0	100	100
39	x	52/55 (94%)	51 (98%)	1 (2%)	50	75
40	y	43/49 (88%)	42 (98%)	1 (2%)	44	71
41	z	46/48 (96%)	46 (100%)	0	100	100
42	e	157/165 (95%)	155 (99%)	2 (1%)	61	82
43	g	99/138 (72%)	98 (99%)	1 (1%)	68	86
44	h	22/114 (19%)	21 (96%)	1 (4%)	24	50
45	k	92/103 (89%)	92 (100%)	0	100	100
46	u	72/78 (92%)	72 (100%)	0	100	100
47	C	167/190 (88%)	165 (99%)	2 (1%)	63	83
48	G	100/147 (68%)	99 (99%)	1 (1%)	68	86
49	J	80/90 (89%)	79 (99%)	1 (1%)	61	82
50	U	60/61 (98%)	59 (98%)	1 (2%)	53	78
53	l	103/107 (96%)	102 (99%)	1 (1%)	68	86
54	K	89/98 (91%)	86 (97%)	3 (3%)	32	60
All	All	4336/4740 (92%)	4309 (99%)	27 (1%)	76	91

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	e	163	ASN
44	h	37	VAL
54	K	16	VAL
43	g	89	LEU
47	C	97	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
46	u	75	GLN
47	C	102	ASN
17	N	4	GLN
15	I	110	GLN
48	G	68	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	X	9/136 (6%)	4 (44%)	1 (11%)
25	b	118/120 (98%)	17 (14%)	0
4	a	2745/2907 (94%)	354 (12%)	0
51	Y	70/73 (95%)	17 (24%)	3 (4%)
52	Z	71/73 (97%)	12 (16%)	2 (2%)
6	A	1495/1532 (97%)	192 (12%)	22 (1%)
All	All	4508/4841 (93%)	596 (13%)	28 (0%)

5 of 596 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	a	10	A
4	a	15	G
4	a	34	U
4	a	58	G
4	a	62	U

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	1035	A
52	Z	7	G
6	A	1212	U
51	Y	20	U
6	A	1124	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	2MG	A	966	6	23,26,27	0.47	0	33,38,41	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	4OC	A	1402	6	20,23,24	0.43	0	25,32,35	0.52	0
2	D2T	L	89	2	8,9,10	1.05	0	6,11,13	1.72	3 (50%)
4	OMG	a	2251	4,51	23,26,27	0.34	0	32,38,41	0.38	0
6	5MC	A	1407	6	19,22,23	0.74	1 (5%)	26,32,35	0.58	0
54	IAS	K	119	54	6,7,8	0.85	0	3,8,10	0.87	0
4	OMU	a	2552	4	19,22,23	0.27	0	25,31,34	0.37	0
4	3TD	a	1915	4	19,22,23	1.32	3 (15%)	23,32,35	1.03	1 (4%)
6	UR3	A	1498	6	19,22,23	0.42	0	26,32,35	0.73	1 (3%)
6	2MG	A	1516	6	23,26,27	0.39	0	33,38,41	0.53	0
4	G7M	a	2069	4	23,26,27	0.85	1 (4%)	34,39,42	0.66	1 (2%)
4	PSU	a	2580	4,56	18,21,22	1.12	1 (5%)	21,30,33	0.77	0
4	OMC	a	2498	4,56	19,22,23	0.38	0	25,31,34	0.41	0
4	PSU	a	746	4,56	18,21,22	1.09	1 (5%)	21,30,33	0.61	0
4	PSU	a	1917	4	18,21,22	0.96	1 (5%)	21,30,33	0.63	0
53	MS6	l	82	53	5,7,8	0.24	0	2,7,9	0.16	0
3	MEQ	d	150	3	8,9,10	0.43	0	5,10,12	0.27	0
4	5MC	a	1962	4	19,22,23	0.62	1 (5%)	26,32,35	0.49	0
4	PSU	a	955	4	18,21,22	1.05	1 (5%)	21,30,33	0.68	0
4	PSU	a	2504	4	18,21,22	1.06	1 (5%)	21,30,33	0.64	0
6	5MC	A	967	6	19,22,23	0.78	1 (5%)	26,32,35	0.58	0
6	MA6	A	1519	6	23,26,27	0.37	0	33,38,41	0.71	1 (3%)
4	5MU	a	1939	4	19,22,23	0.41	0	27,32,35	0.27	0
4	2MA	a	2503	4,56	22,25,26	0.37	0	32,37,40	0.63	1 (3%)
4	6MZ	a	2030	4	22,25,26	0.49	0	29,36,39	0.55	0
4	PSU	a	2457	4	18,21,22	1.05	1 (5%)	21,30,33	0.63	0
6	MA6	A	1518	6	23,26,27	0.30	0	33,38,41	0.67	1 (3%)
53	4D4	l	81	53	9,11,12	0.52	0	7,13,15	0.59	0
4	2MG	a	1835	4	23,26,27	0.37	0	33,38,41	0.43	0
4	2MG	a	2445	4	23,26,27	0.40	0	33,38,41	0.42	0
4	6MZ	a	1618	4	22,25,26	0.53	0	29,36,39	0.57	0
4	PSU	a	1911	4	18,21,22	1.09	1 (5%)	21,30,33	0.67	0
6	PSU	A	516	6	18,21,22	1.04	2 (11%)	21,30,33	0.69	0
4	PSU	a	2605	4	18,21,22	1.16	1 (5%)	21,30,33	0.73	0
4	PSU	a	2604	4	18,21,22	1.04	1 (5%)	21,30,33	0.71	0
6	G7M	A	527	6	23,26,27	0.69	1 (4%)	34,39,42	0.64	1 (2%)
4	5MU	a	747	4	19,22,23	0.39	0	27,32,35	0.34	0
4	H2U	a	2449	4	18,21,22	0.64	0	19,30,33	0.66	1 (5%)
4	1MG	a	745	4	23,26,27	0.80	1 (4%)	33,39,42	0.48	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
6	2MG	A	966	6	-	0/9/27/28	0/3/3/3
6	4OC	A	1402	6	-	2/9/29/30	0/2/2/2
2	D2T	L	89	2	-	4/7/12/14	-
4	OMG	a	2251	4,51	-	0/9/27/28	0/3/3/3
6	5MC	A	1407	6	-	0/7/25/26	0/2/2/2
54	IAS	K	119	54	-	0/7/7/8	-
4	OMU	a	2552	4	-	0/9/27/28	0/2/2/2
4	3TD	a	1915	4	-	5/7/25/26	0/2/2/2
6	UR3	A	1498	6	-	0/7/25/26	0/2/2/2
6	2MG	A	1516	6	-	0/9/27/28	0/3/3/3
4	G7M	a	2069	4	-	1/7/25/26	0/3/3/3
4	PSU	a	2580	4,56	-	0/7/25/26	0/2/2/2
4	OMC	a	2498	4,56	-	1/9/27/28	0/2/2/2
4	PSU	a	746	4,56	-	2/7/25/26	0/2/2/2
4	PSU	a	1917	4	-	0/7/25/26	0/2/2/2
53	MS6	l	82	53	-	1/4/6/8	-
3	MEQ	d	150	3	-	5/8/9/11	-
4	5MC	a	1962	4	-	0/7/25/26	0/2/2/2
4	PSU	a	955	4	-	0/7/25/26	0/2/2/2
4	PSU	a	2504	4	-	0/7/25/26	0/2/2/2
6	5MC	A	967	6	-	0/7/25/26	0/2/2/2
6	MA6	A	1519	6	-	3/11/29/30	0/3/3/3
4	5MU	a	1939	4	-	0/7/25/26	0/2/2/2
4	2MA	a	2503	4,56	-	1/7/25/26	0/3/3/3
4	6MZ	a	2030	4	-	2/9/27/28	0/3/3/3
4	PSU	a	2457	4	-	0/7/25/26	0/2/2/2
6	MA6	A	1518	6	-	0/11/29/30	0/3/3/3
53	4D4	l	81	53	-	1/11/12/14	-
4	2MG	a	1835	4	-	0/9/27/28	0/3/3/3
4	2MG	a	2445	4	-	0/9/27/28	0/3/3/3
4	6MZ	a	1618	4	-	0/9/27/28	0/3/3/3
4	PSU	a	1911	4	-	0/7/25/26	0/2/2/2
6	PSU	A	516	6	-	0/7/25/26	0/2/2/2
4	PSU	a	2605	4	-	0/7/25/26	0/2/2/2
4	PSU	a	2604	4	-	0/7/25/26	0/2/2/2
6	G7M	A	527	6	-	1/7/25/26	0/3/3/3
4	5MU	a	747	4	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	H2U	a	2449	4	-	0/7/38/39	0/2/2/2
4	1MG	a	745	4	-	0/7/25/26	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	a	1915	3TD	C6-C5	4.31	1.40	1.35
4	a	2580	PSU	C6-C5	4.10	1.39	1.35
4	a	746	PSU	C6-C5	4.09	1.39	1.35
4	a	2504	PSU	C6-C5	4.08	1.39	1.35
4	a	1911	PSU	C6-C5	4.08	1.39	1.35

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	a	1915	3TD	C1'-C5-C4	3.56	123.01	117.61
6	A	1519	MA6	C2-N1-C6	2.79	118.64	111.83
6	A	1518	MA6	C2-N1-C6	2.74	118.53	111.83
4	a	2503	2MA	C5-C4-N3	-2.43	124.62	127.18
2	L	89	D2T	OD1-CG-CB	-2.42	117.38	122.44

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	89	D2T	CA-CB-CG-OD1
2	L	89	D2T	CA-CB-CG-OD2
3	d	150	MEQ	C-CA-CB-CG
6	A	1519	MA6	O4'-C4'-C5'-O5'
4	a	1915	3TD	O4'-C1'-C5-C4

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1402	4OC	2	0
4	a	2030	6MZ	1	0
4	a	2445	2MG	1	0
6	A	527	G7M	1	0
4	a	2449	H2U	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 312 ligands modelled in this entry, 311 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	A1JAI	A	1601	-	63,67,67	0.52	0	89,94,94	0.82	2 (2%)

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
57	A1JAI	A	1601	-	-	7/43/125/125	0/4/4/4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A	1601	A1JAI	O1-C8-N6	3.36	114.28	108.12
57	A	1601	A1JAI	C9-O1-C8	-2.03	109.65	112.47

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	A	1601	A1JAI	O1-C8-N6-C7
57	A	1601	A1JAI	O2-C10-C9-O1
57	A	1601	A1JAI	O2-C10-C9-C11
57	A	1601	A1JAI	O14-C27-C28-O15

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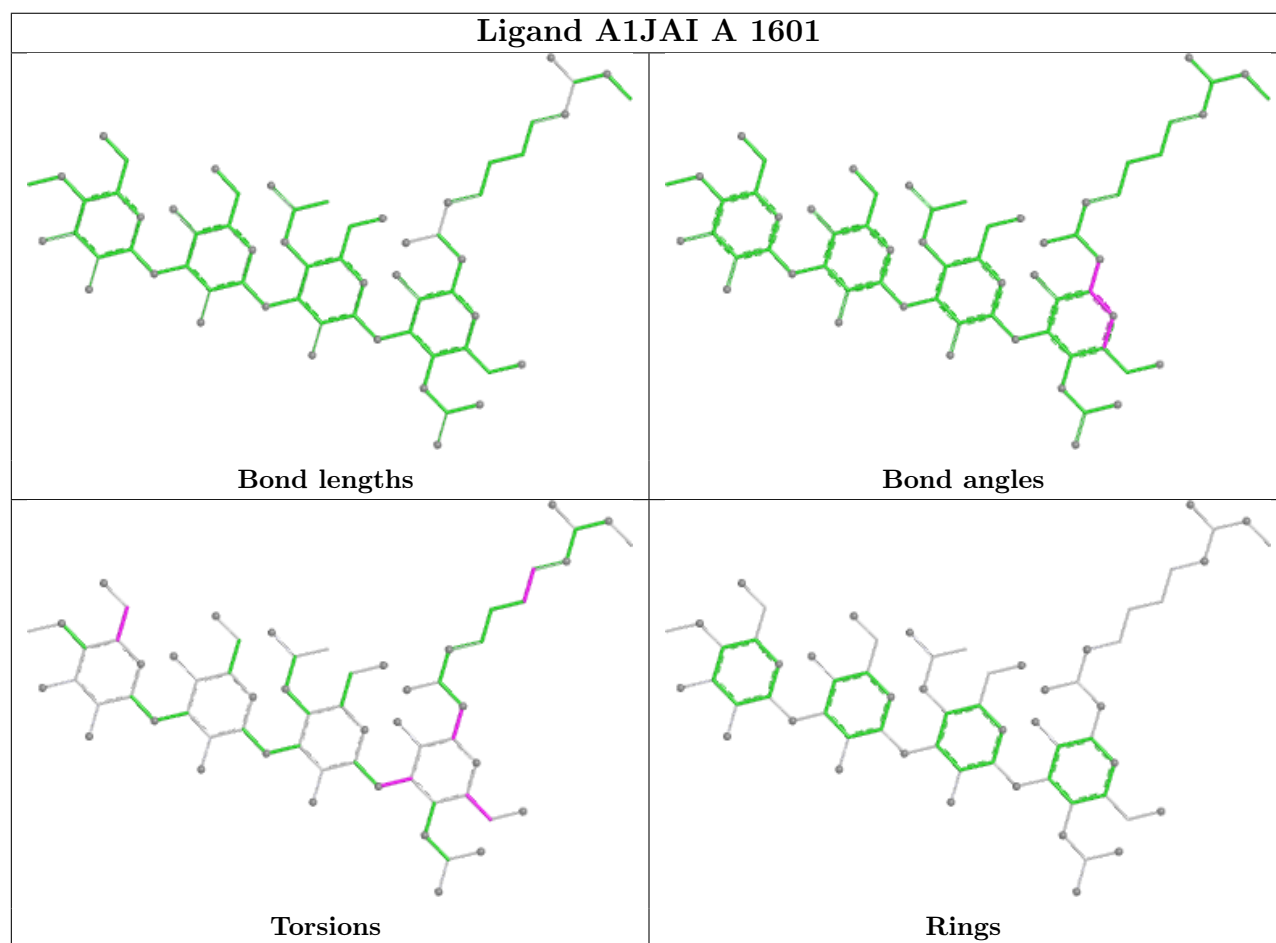
Continued from previous page...

Mol	Chain	Res	Type	Atoms
57	A	1601	A1JAI	C11-C13-O5-C14

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
51	Y	2
52	Z	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	46:G	O3'	57:U	P	9.80
1	Y	15:A	O3'	18:G	P	7.42
1	Z	15:G	O3'	18:G	P	5.11

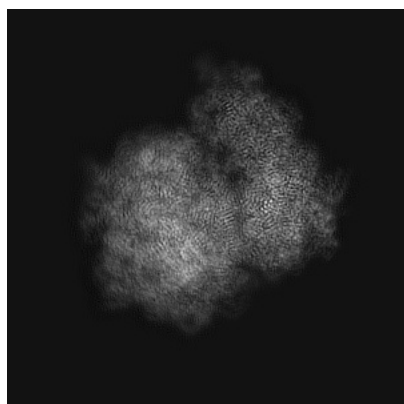
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55145. These allow visual inspection of the internal detail of the map and identification of artifacts.

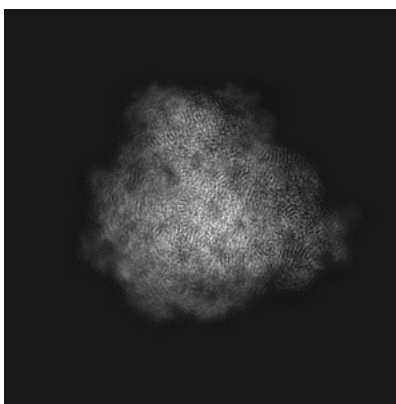
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

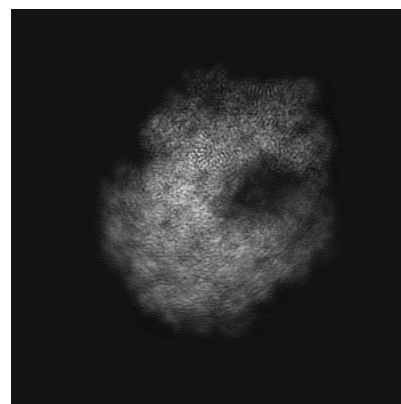
6.1.1 Primary map



X

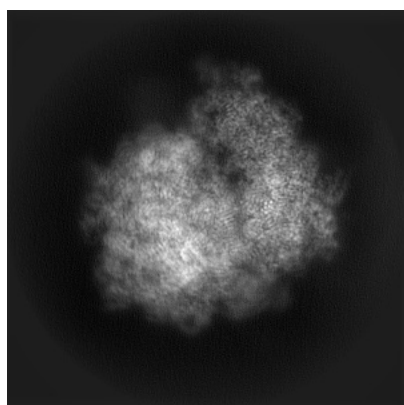


Y

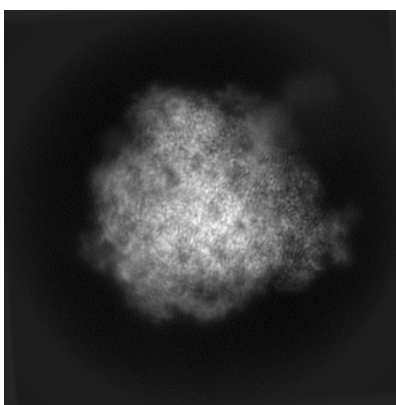


Z

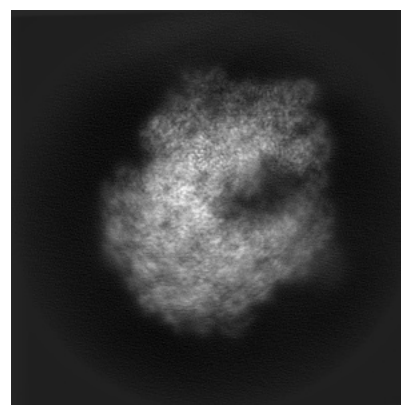
6.1.2 Raw map



X



Y

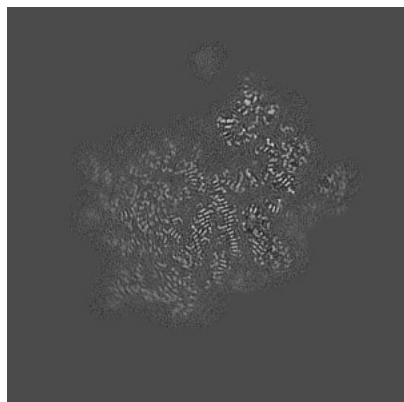


Z

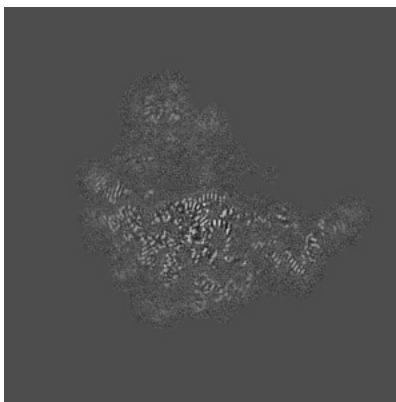
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

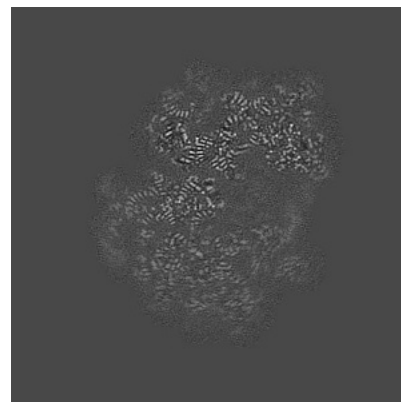
6.2.1 Primary map



X Index: 216

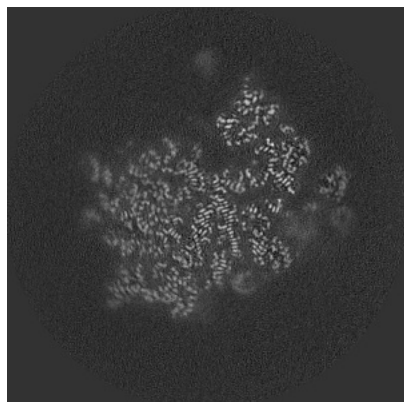


Y Index: 216

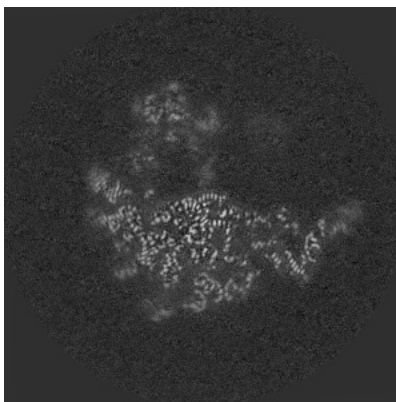


Z Index: 216

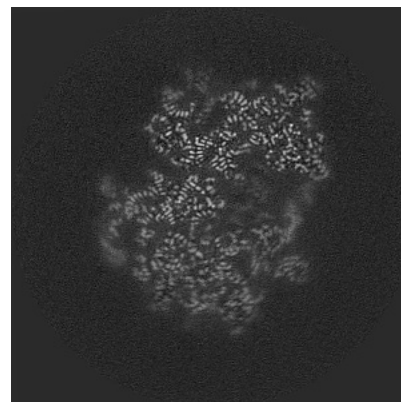
6.2.2 Raw map



X Index: 216



Y Index: 216

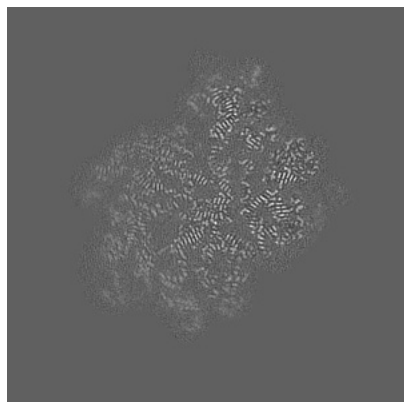


Z Index: 216

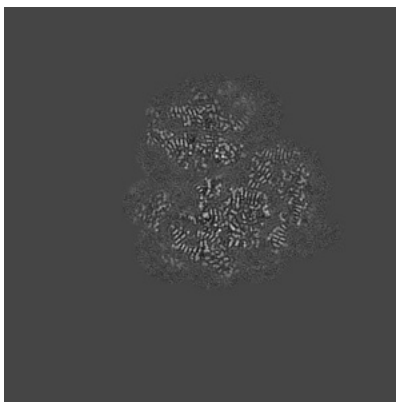
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

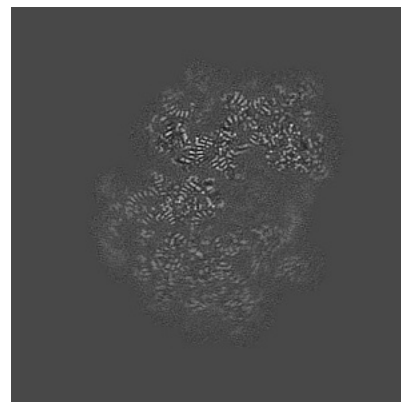
6.3.1 Primary map



X Index: 185

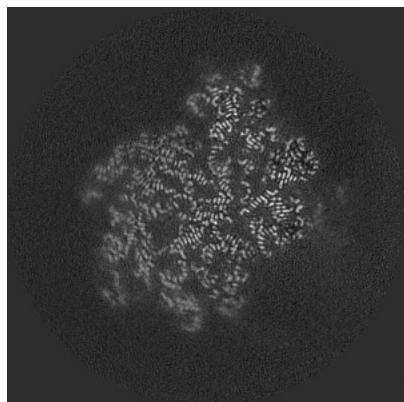


Y Index: 287

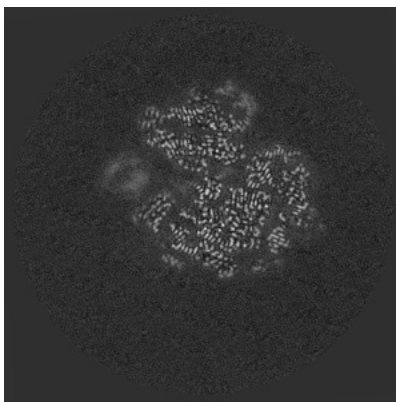


Z Index: 216

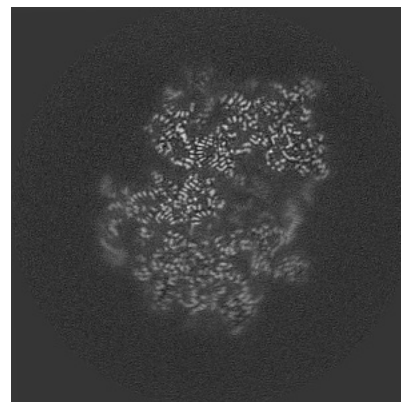
6.3.2 Raw map



X Index: 185



Y Index: 286

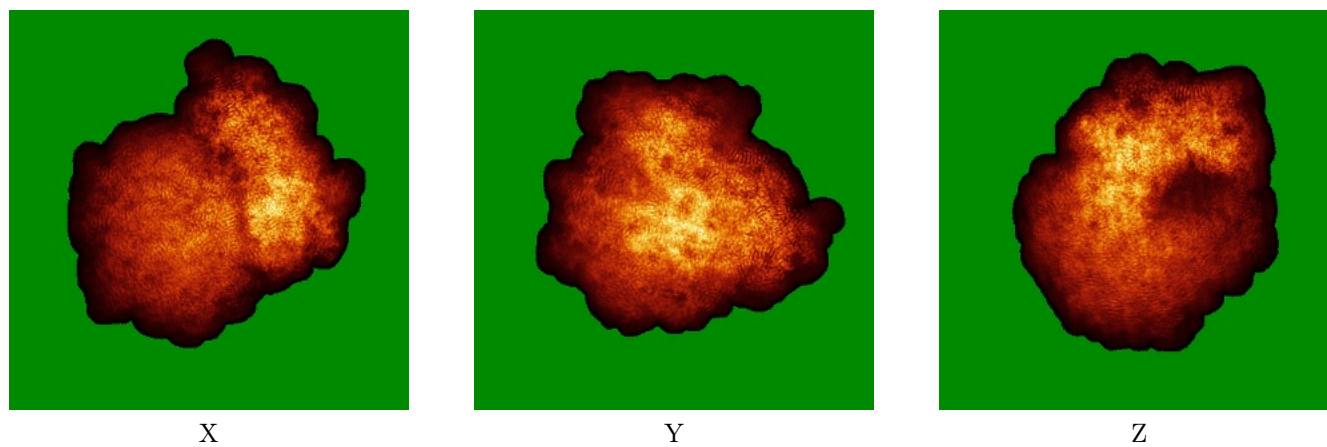


Z Index: 215

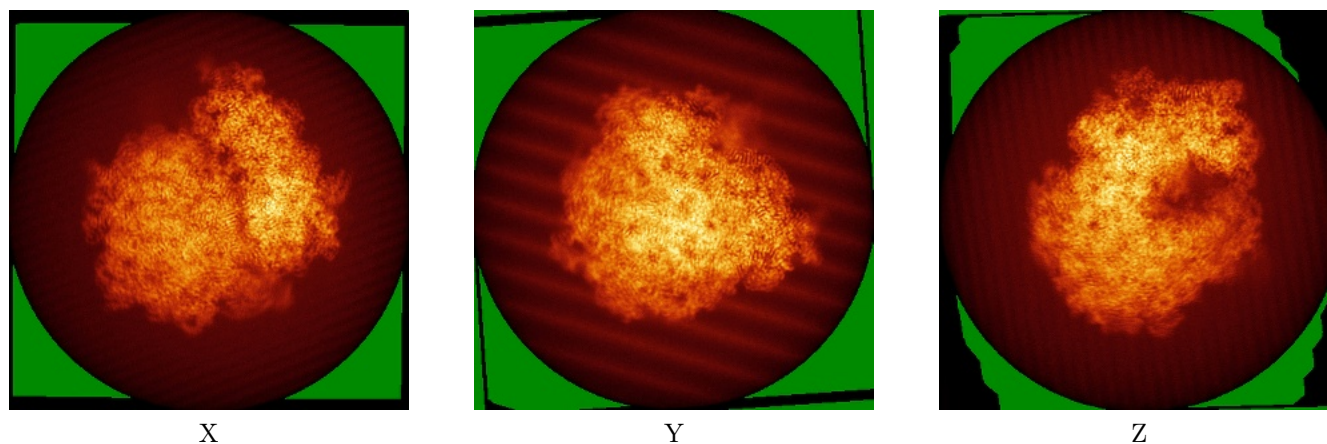
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

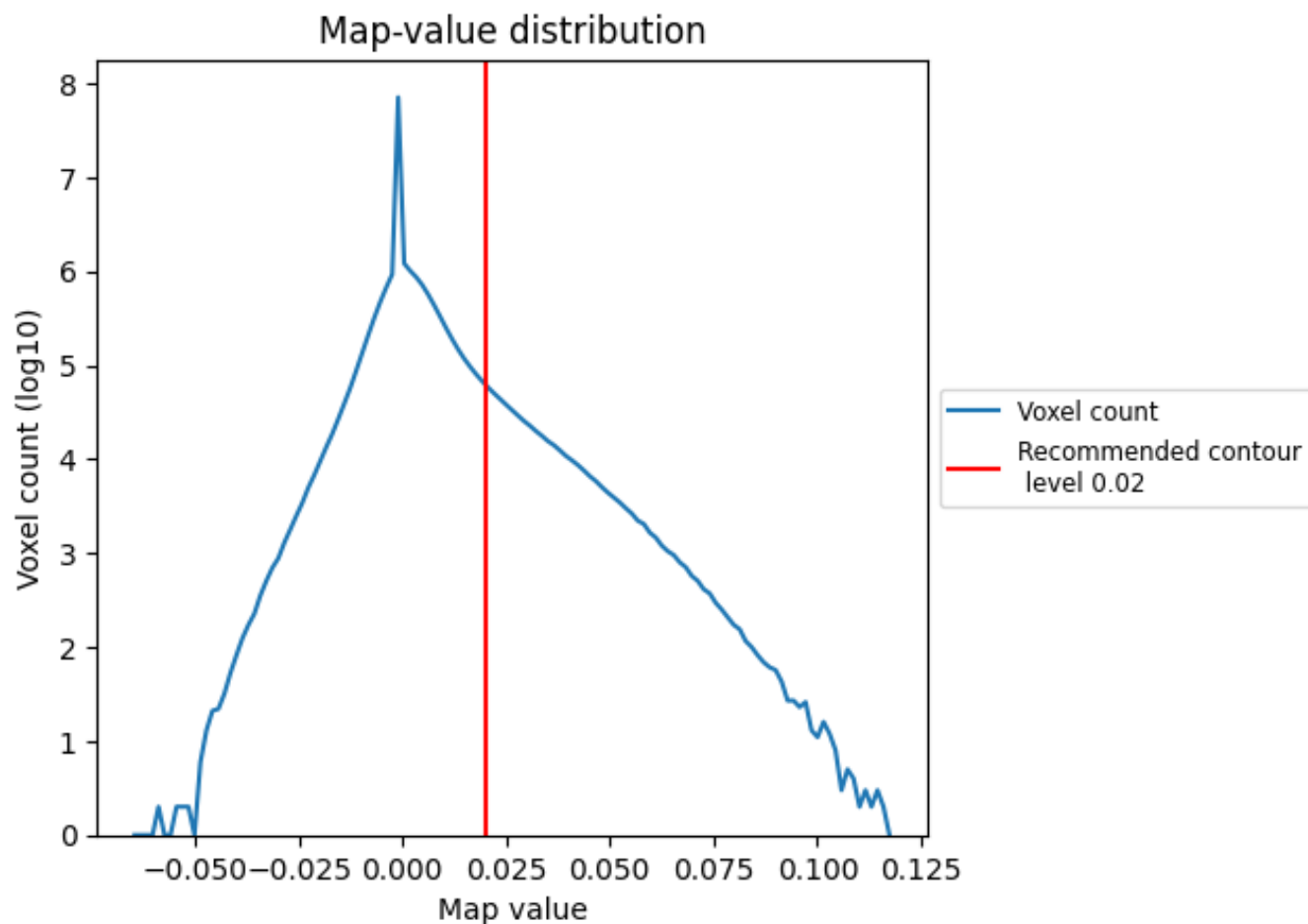
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

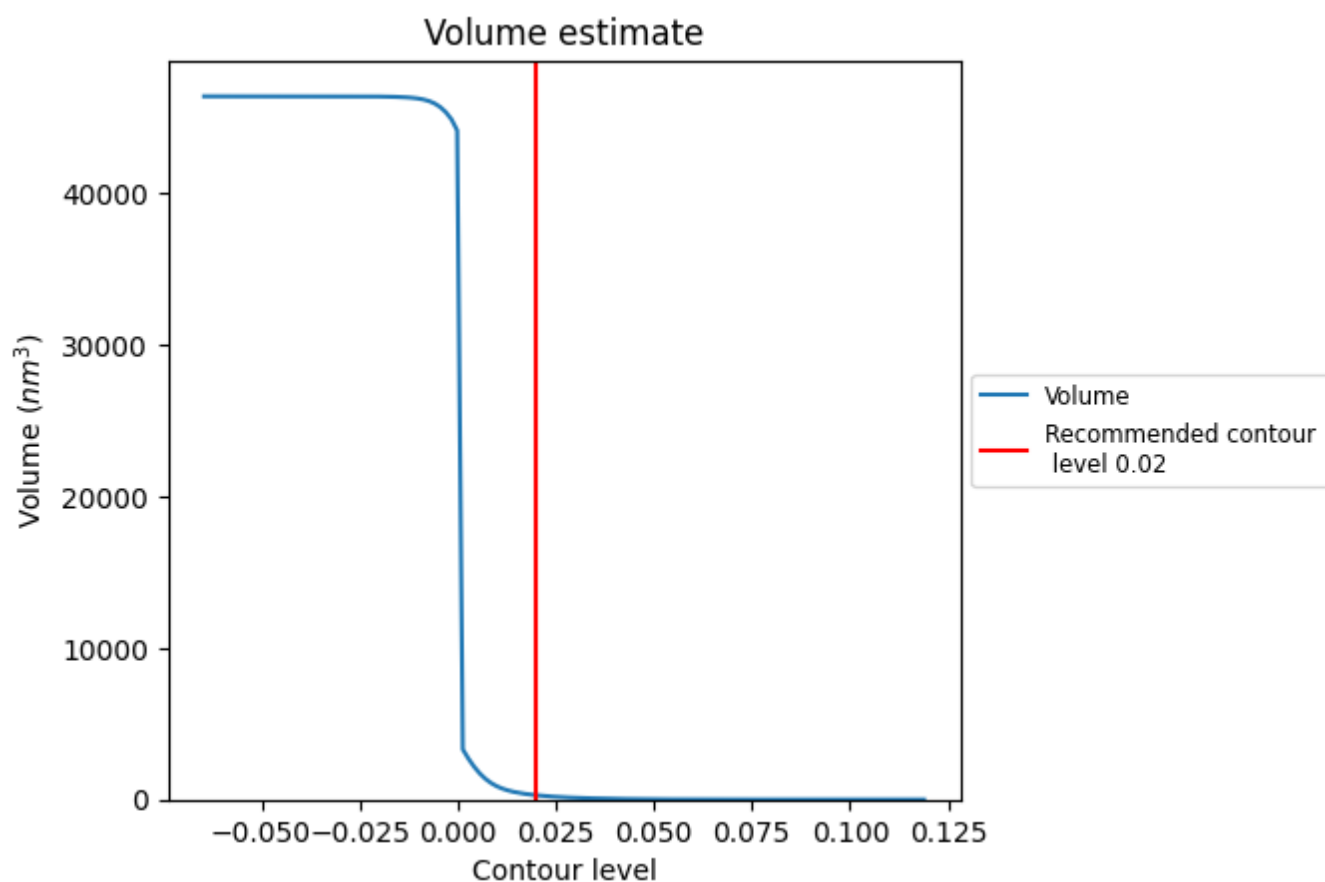
This section contains the results of statistical analysis of the map.

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.

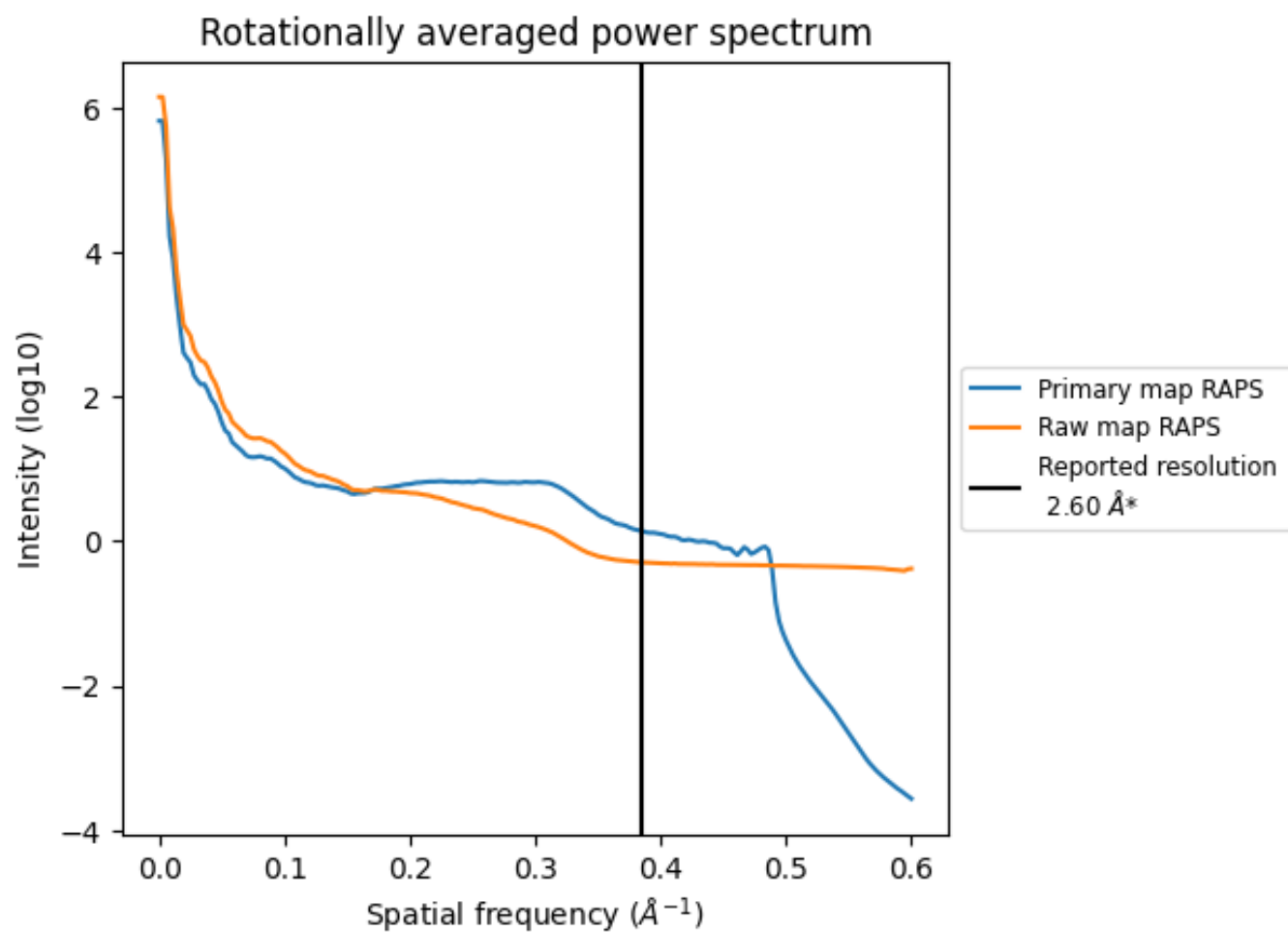
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 286 nm^3 ; this corresponds to an approximate mass of 258 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

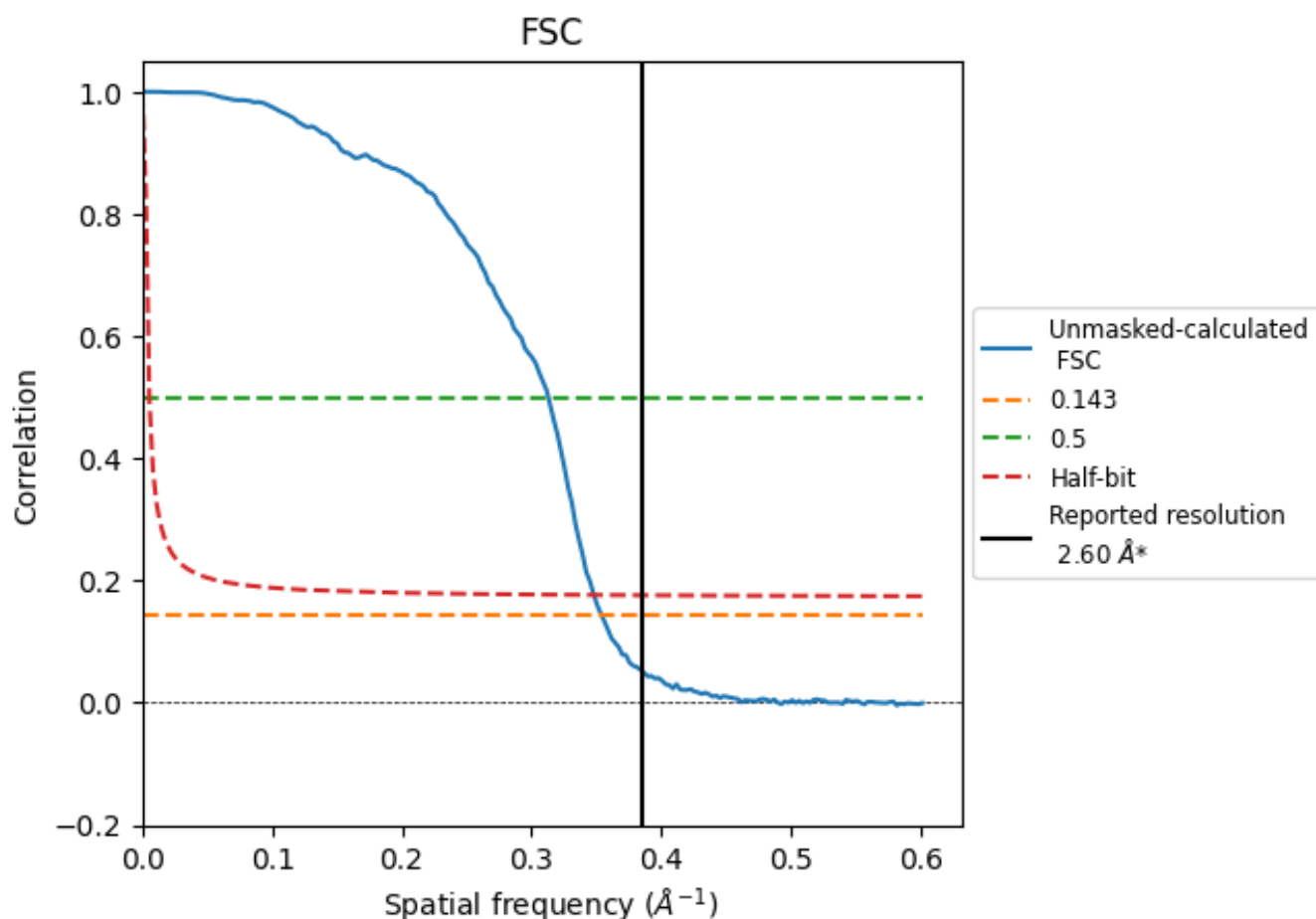


*Reported resolution corresponds to spatial frequency of 0.385 \AA^{-1}

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 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

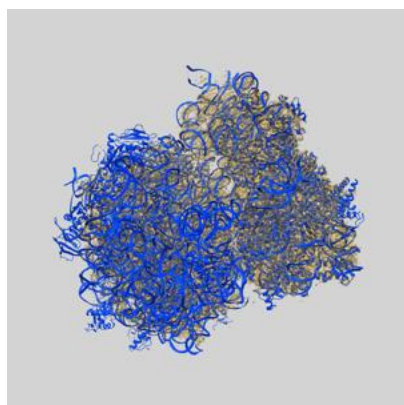
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.82	3.20	2.87

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

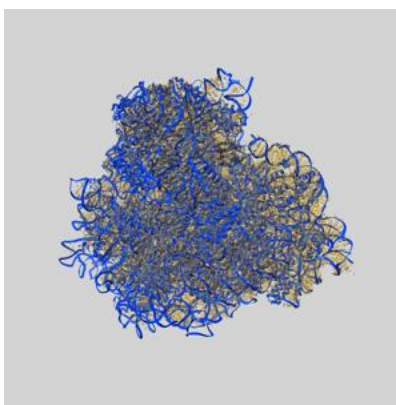
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55145 and PDB model 9SRO. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

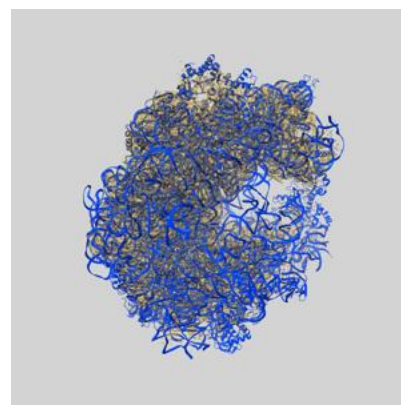
9.1 Map-model overlay [i](#)



X



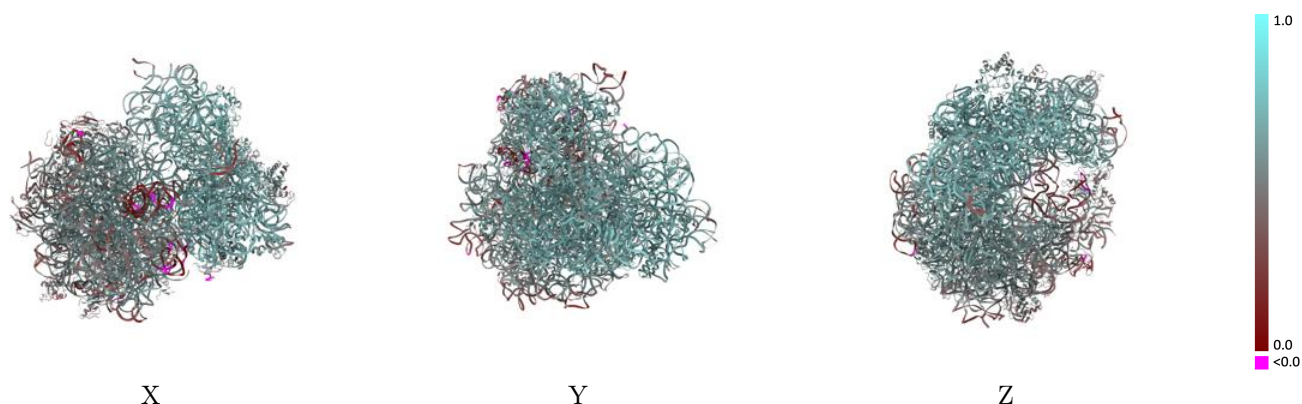
Y



Z

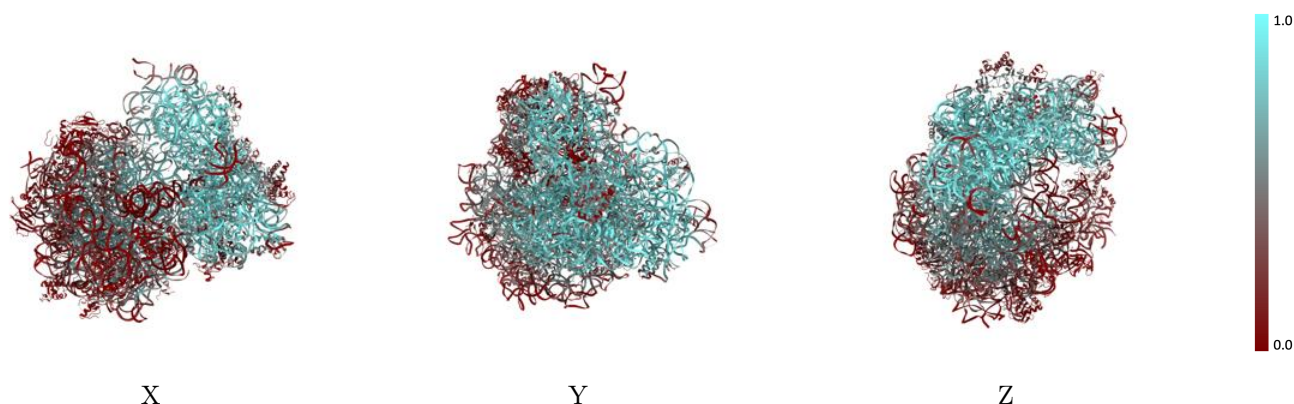
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



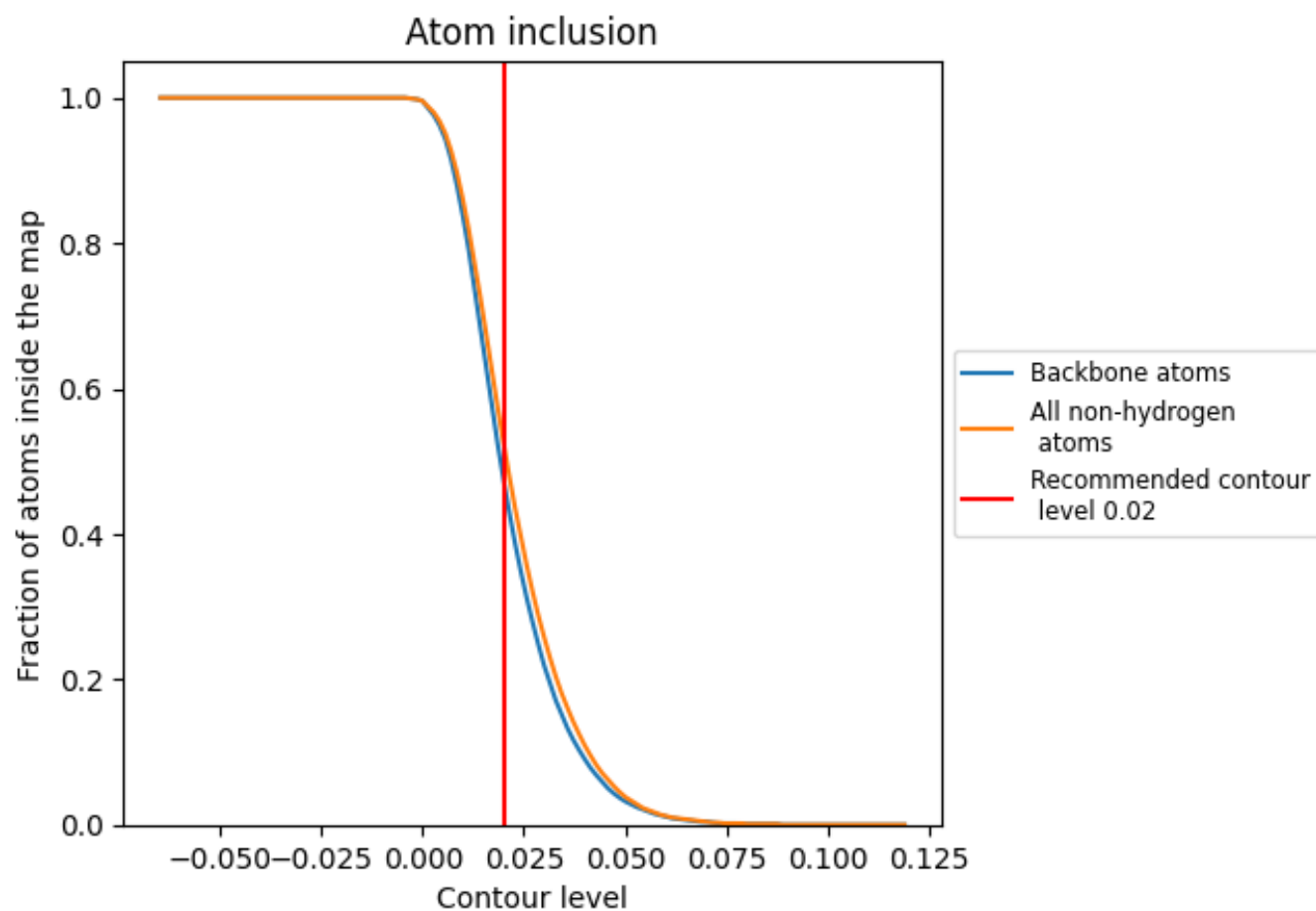
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 47% of all backbone atoms, 52% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5250	 0.5830
0	 0.1300	 0.4970
1	 0.5680	 0.6450
2	 0.3920	 0.6070
3	 0.2800	 0.4870
4	 0.0530	 0.4220
A	 0.8270	 0.6680
B	 0.3620	 0.5630
C	 0.6600	 0.6390
D	 0.6140	 0.6440
E	 0.7550	 0.6740
F	 0.4620	 0.5870
G	 0.3250	 0.5380
H	 0.7560	 0.6820
I	 0.6110	 0.6240
J	 0.5110	 0.5930
K	 0.6210	 0.6190
L	 0.7810	 0.6820
M	 0.4600	 0.5670
N	 0.7290	 0.6710
O	 0.7200	 0.6650
P	 0.7690	 0.6770
Q	 0.6690	 0.6460
R	 0.7000	 0.6430
S	 0.7020	 0.6630
T	 0.6790	 0.6600
U	 0.3950	 0.5620
X	 0.3490	 0.4840
Y	 0.0130	 0.2930
Z	 0.2940	 0.3420
a	 0.4820	 0.5650
b	 0.1210	 0.4440
c	 0.7470	 0.6830
d	 0.2980	 0.5520
e	 0.1410	 0.4590



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Chain	Atom inclusion	Q-score
f	 0.0570	 0.4580
g	 0.0240	 0.4100
h	 0.1480	 0.5010
i	 0.1380	 0.4910
j	 0.4870	 0.6280
k	 0.2260	 0.5310
l	 0.2280	 0.5360
m	 0.2810	 0.5890
n	 0.0440	 0.4340
o	 0.3110	 0.5740
p	 0.2380	 0.5300
q	 0.0740	 0.4670
r	 0.1600	 0.5140
s	 0.1080	 0.4720
u	 0.0270	 0.4050
v	 0.2000	 0.5640
w	 0.4000	 0.5900
x	 0.0220	 0.3610
y	 0.1030	 0.4970
z	 0.2440	 0.5260