



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 10:04 PM UTC

PDB ID : 7ST7 / pdb_00007st7
EMDB ID : EMD-25421
Title : Pre translocation intermediate stalled with viomycin and bound with EF-G in a GDP and Pi state (Structure III-vio)
Authors : Carbone, C.E.; Korostelev, A.A.
Deposited on : 2021-11-12
Resolution : 3.20 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

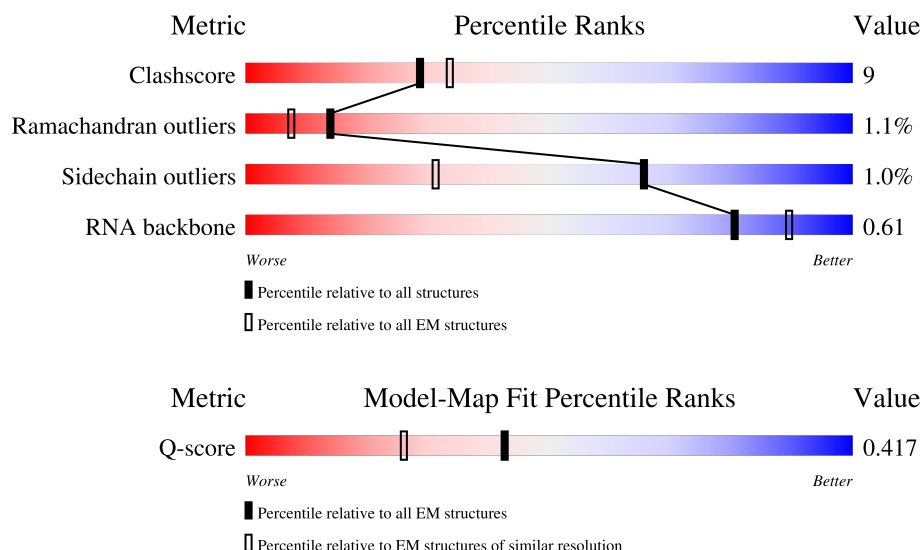
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.



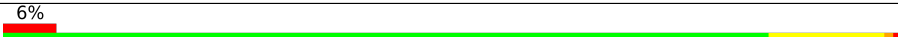
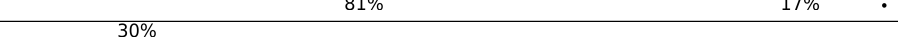
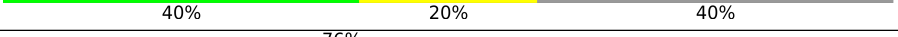
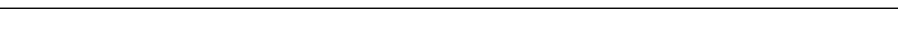
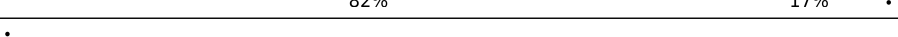
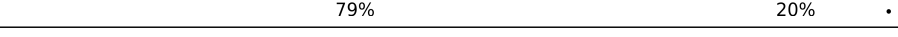
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	1	2903	
2	2	120	
3	b	271	

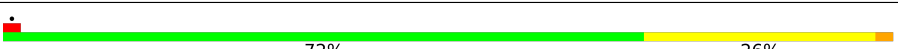
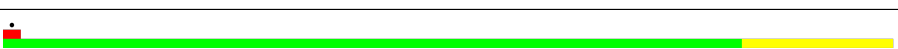
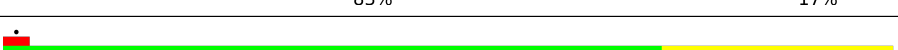
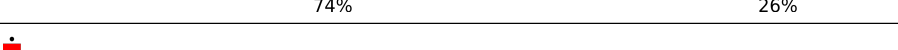
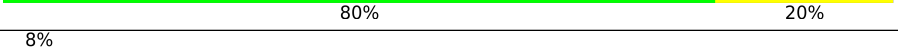
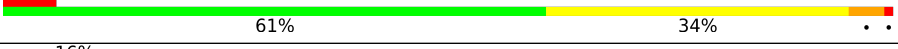
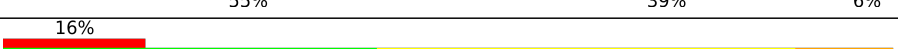
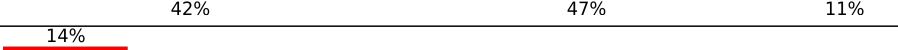
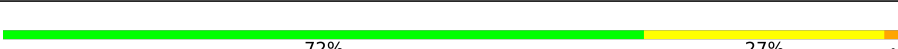
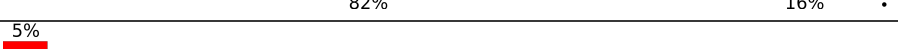
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Mol	Chain	Length	Quality of chain
4	c	209	 77% 22% .
5	d	201	 82% 17% .
6	e	177	 5% 76% 23% .
7	f	176	 6% 86% 13% ..
8	g	149	 87% 81% 17% .
9	a	223	 30% 40% 20% 40%
10	i	141	 76% 59% 37% . .
11	j	142	 82% 17% .
12	k	122	 78% 20% .
13	l	143	 72% 27% .
14	m	136	 82% 17% .
15	n	120	 79% 20% .
16	o	116	 76% 22% .
17	p	114	 79% 21% .
18	q	117	 82% 16% .
19	r	103	 80% 19% .
20	s	110	 80% 20% .
21	t	93	 76% 24% .
22	u	102	 86% 13% .
23	v	94	 77% 23% .
24	w	75	 80% 20% .
25	x	77	 81% 17% .
26	y	63	 6% 81% 17% .
27	z	58	 83% 12% . .
28	A	66	 38% 71% 27% .

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Mol	Chain	Length	Quality of chain
29	B	56	
30	C	50	
31	D	46	
32	E	64	
33	F	38	
34	H	206	
35	L	151	
36	N	127	
37	O	98	
38	R	114	
39	S	100	
40	X	79	
41	3	1539	
42	4	19	
43	G	218	
44	I	205	
45	J	157	
46	K	100	
47	M	129	
48	P	116	
49	Q	123	
50	T	88	
51	U	82	
52	V	80	
53	W	65	

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Mol	Chain	Length	Quality of chain
54	Y	85	5% 71% 29%
55	Z	65	17% 69% 26%
56	8	697	19% 74% 24%
57	6	77	58% 30% 12%
58	5	76	24% 50% 24%
59	h	6	17% 17% 67%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 153555 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 802133627

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	120	A	-	insertion	GB 1266961702

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	b	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	c	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	e	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	g	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 9 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	134	Total	C	N	O	S	0	0
			1027	645	186	194	2		

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	i	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	j	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	k	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	l	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	m	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	n	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
16	o	116	Total	C	N	O	0	0
			892	552	178	162		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	p	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	q	117	Total	C	N	O	0	0
			947	604	192	151		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	r	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	s	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	t	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	u	102	Total	C	N	O		0	0
			780	492	146	142			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	v	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	w	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	x	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	B	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	C	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	D	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	E	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 33 is a protein called 50S ribosomal protein L36.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	H	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 35 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 36 is a protein called 30S ribosomal protein S9.

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

- Molecule 37 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	O	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 38 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	R	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 39 is a protein called 30S ribosomal protein S14.

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

- Molecule 40 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	X	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 41 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	3	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 42 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	4	19	Total	C	N	O	P	0	0
			413	186	85	124	18		

- Molecule 43 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	G	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 44 is a protein called 30S ribosomal protein S4.

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

- Molecule 45 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	J	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

- Molecule 46 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	K	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 47 is a protein called 30S ribosomal protein S8.

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

- Molecule 48 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	P	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 49 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Q	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 50 is a protein called 30S ribosomal protein S15.

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

- Molecule 51 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	U	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 52 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	V	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 53 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	W	65	Total	C	N	O	S	0	0
			536	339	100	96	1		

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Y	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 55 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Z	65	Total	C	N	O	S	0	0
			545	335	117	92	1		

- Molecule 56 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	8	697	Total	C	N	O	S	0	0
			5400	3403	929	1043	25		

- Molecule 57 is a RNA chain called tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	6	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

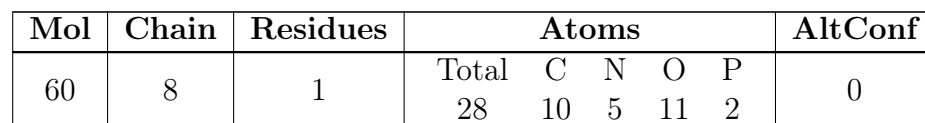
- Molecule 58 is a RNA chain called tRNA Pro.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	5	76	Total	C	N	O	P	0	0
			1625	723	290	536	76		

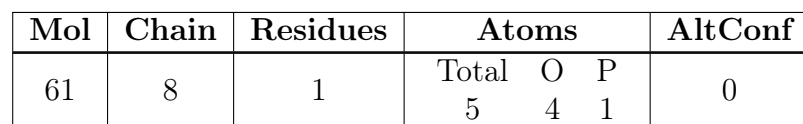
- Molecule 59 is a protein called Viomycin.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	h	6	Total	C	N	O	0	0
			48	25	13	10		

- Molecule 60 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).



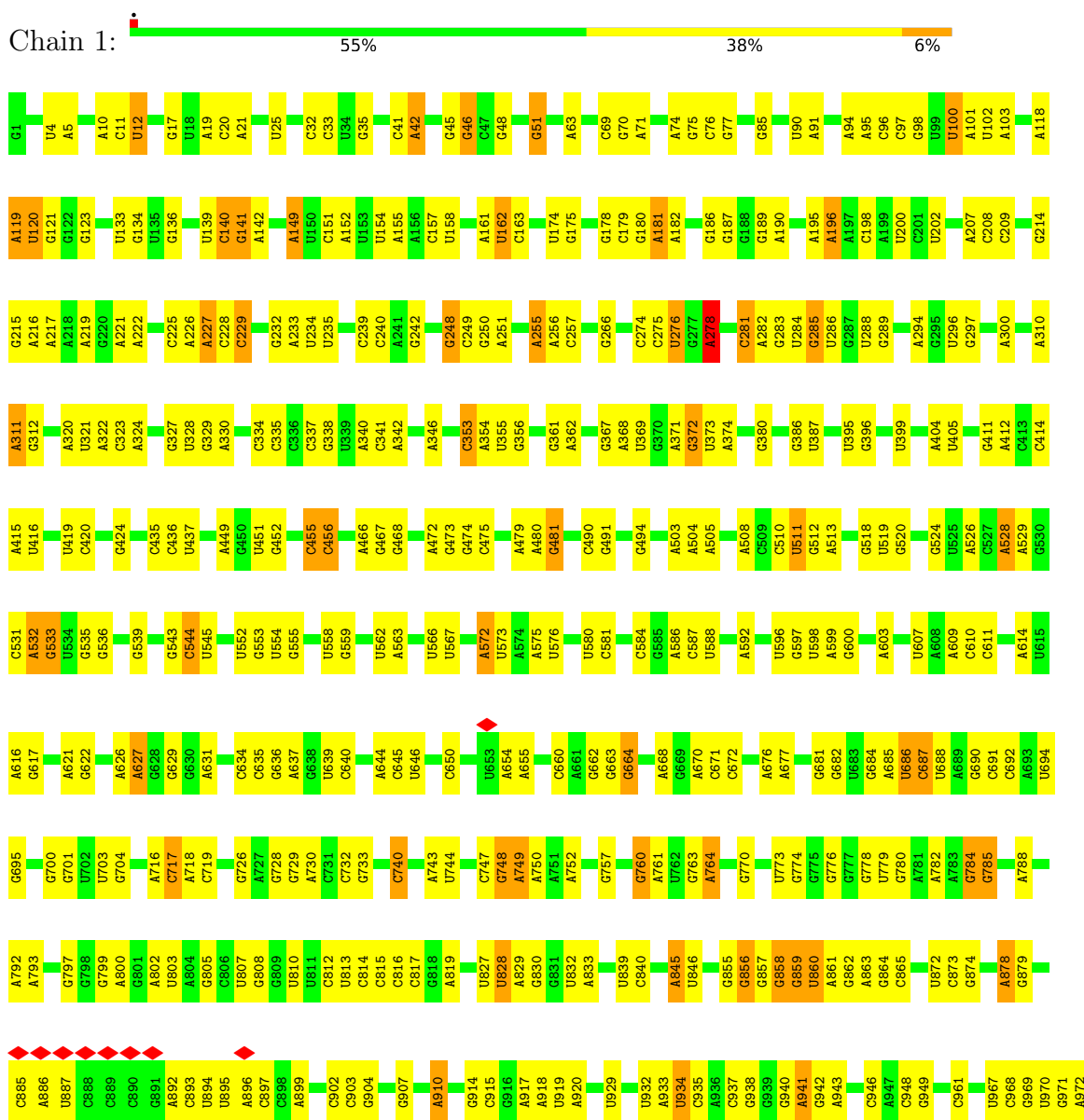
- Molecule 61 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



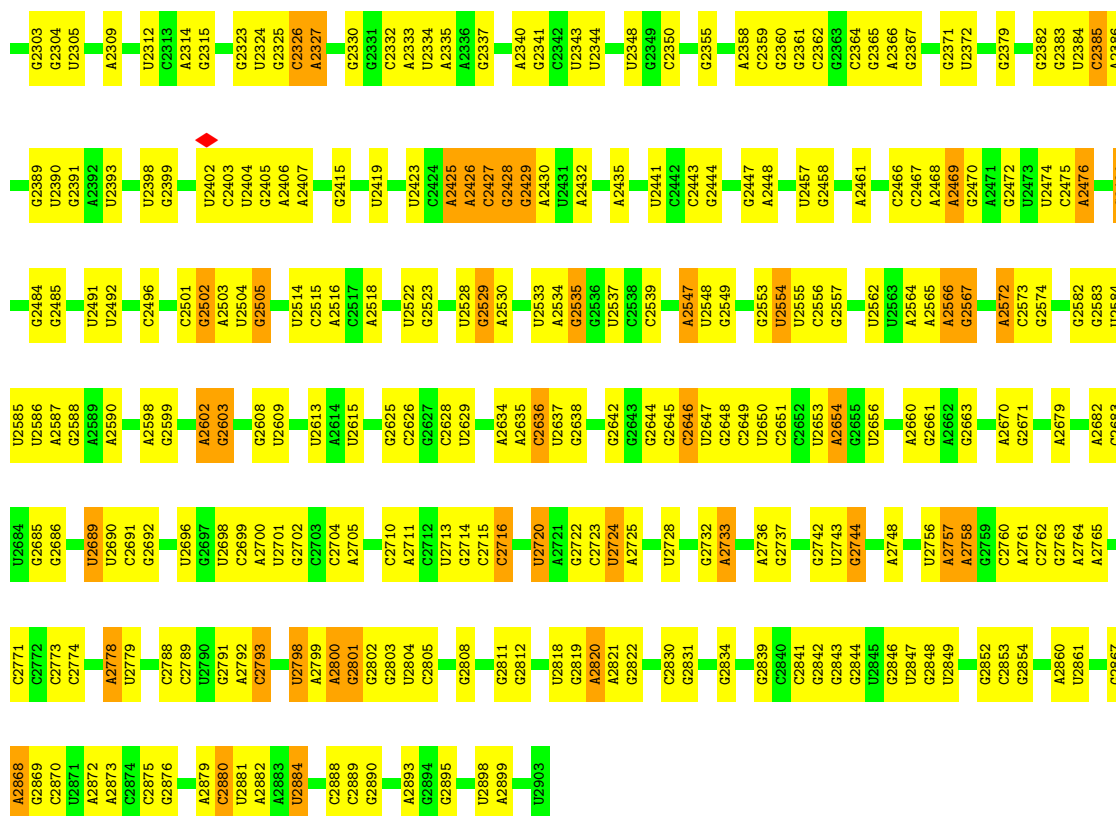
3 Residue-property plots

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

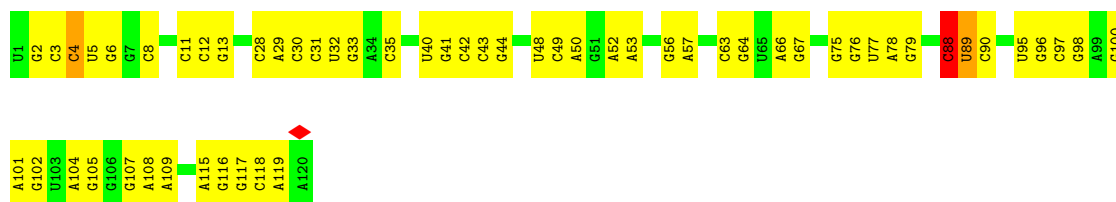
• Molecule 1: 23S rRNA



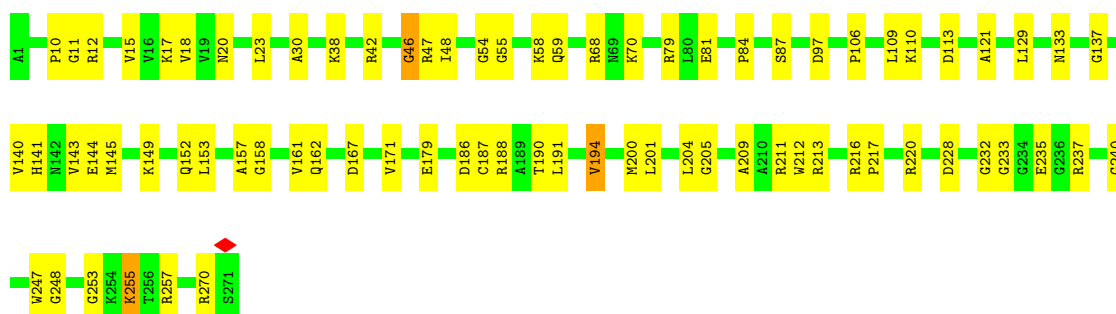




• Molecule 2: 5S rRNA

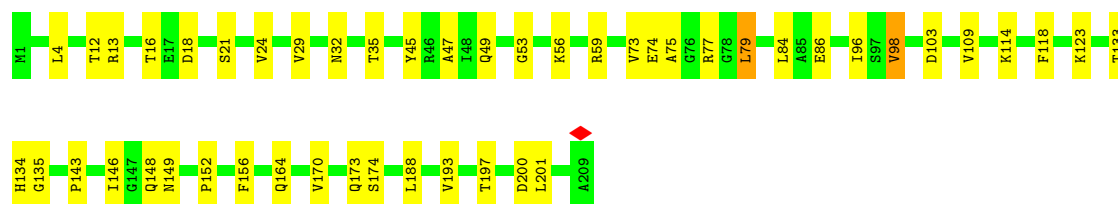


• Molecule 3: 50S ribosomal protein L2



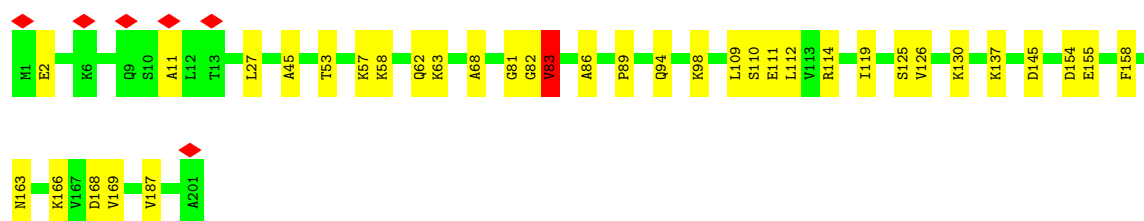
• Molecule 4: 50S ribosomal protein L3

Chain c:  77% 22% .



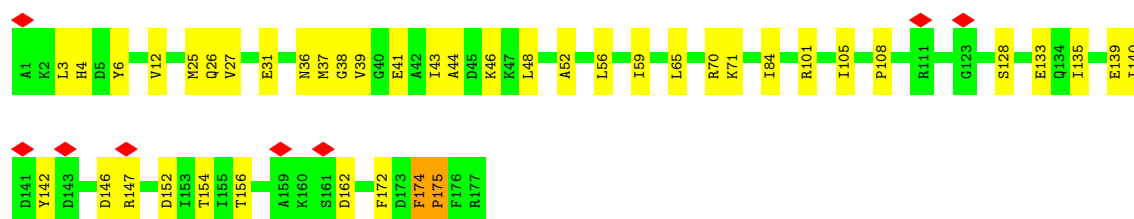
- Molecule 5: 50S ribosomal protein L4

Chain d:  82% 17% .



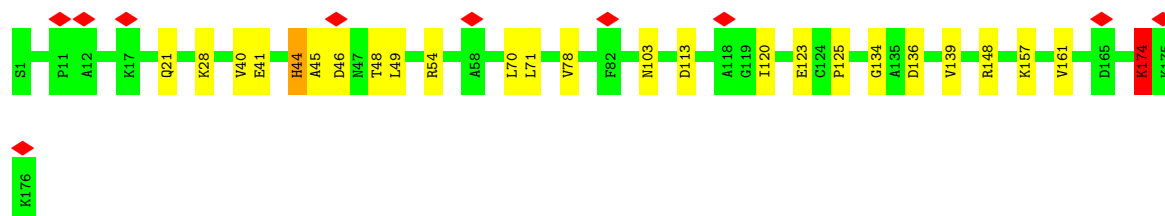
- Molecule 6: 50S ribosomal protein L5

Chain e:  5% 76% 23% .



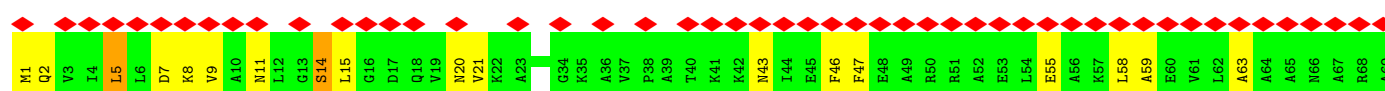
- Molecule 7: 50S ribosomal protein L6

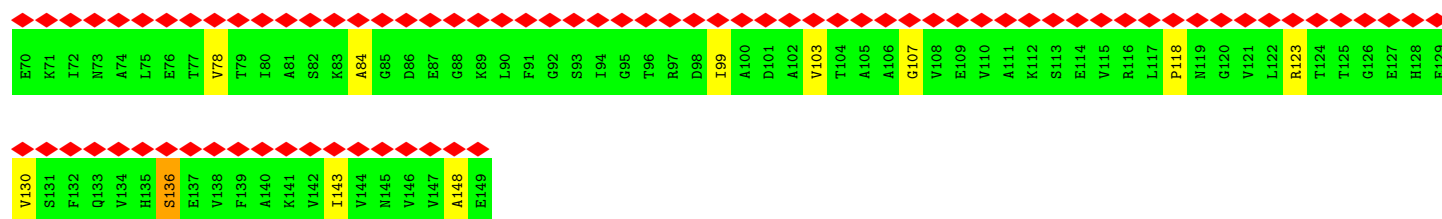
Chain f:  6% 86% 13% ..



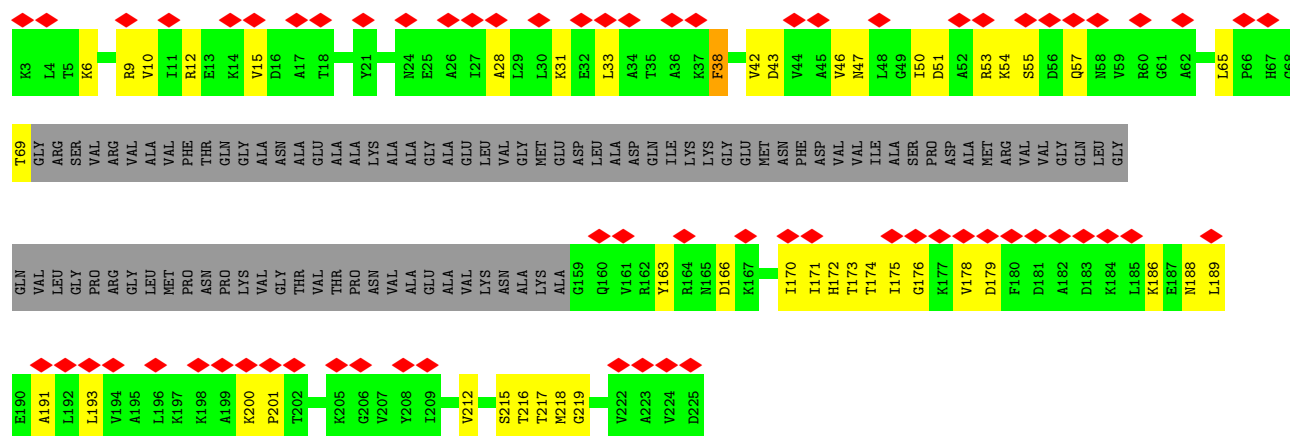
- Molecule 8: 50S ribosomal protein L9

Chain g:  87% 81% 17% .

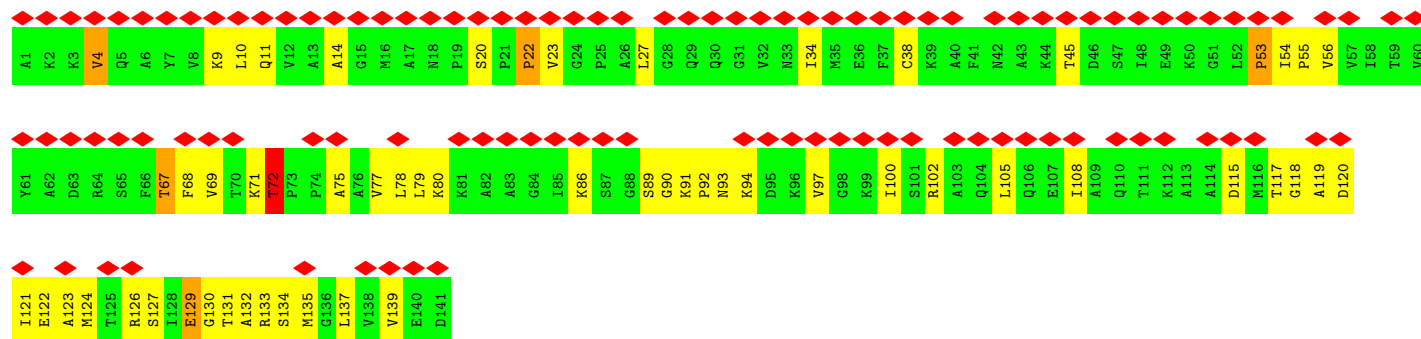
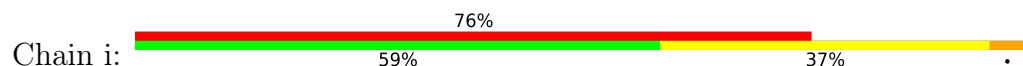




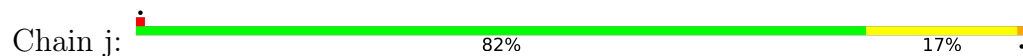
• Molecule 9: 50S ribosomal protein L1



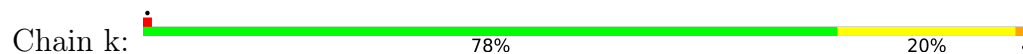
• Molecule 10: 50S ribosomal protein L11

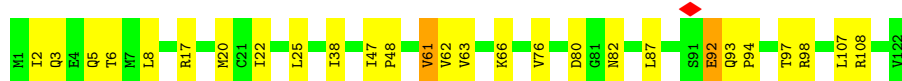


• Molecule 11: 50S ribosomal protein L13

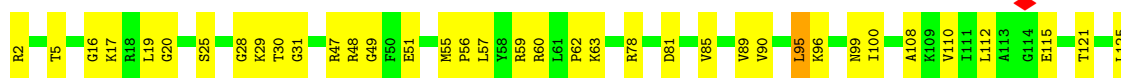


• Molecule 12: 50S ribosomal protein L14

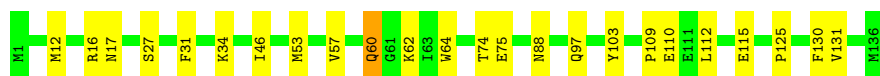
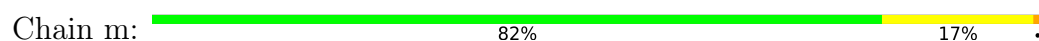




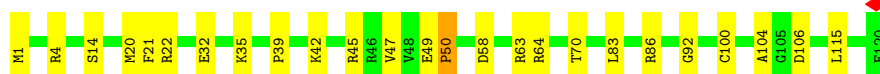
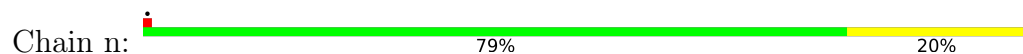
- Molecule 13: 50S ribosomal protein L15



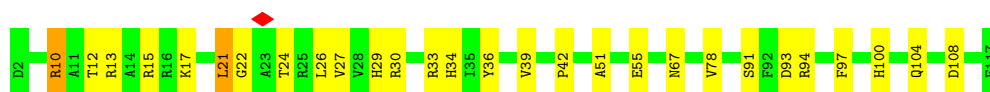
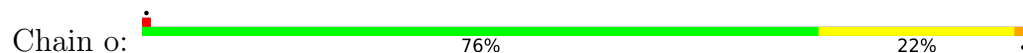
- Molecule 14: 50S ribosomal protein L16



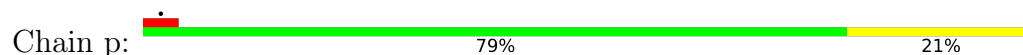
- Molecule 15: 50S ribosomal protein L17



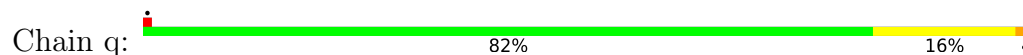
- Molecule 16: 50S ribosomal protein L18

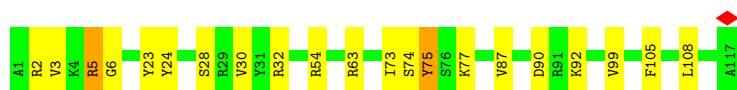


- Molecule 17: 50S ribosomal protein L19

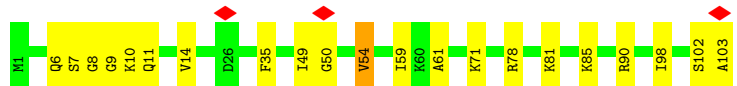
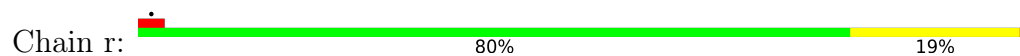


- Molecule 18: 50S ribosomal protein L20

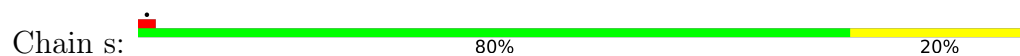




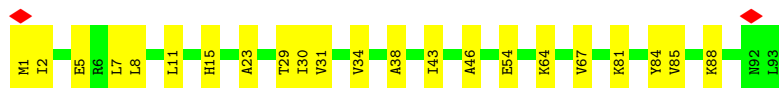
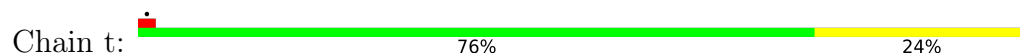
- Molecule 19: 50S ribosomal protein L21



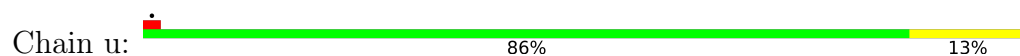
- Molecule 20: 50S ribosomal protein L22



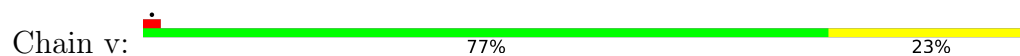
- Molecule 21: 50S ribosomal protein L23



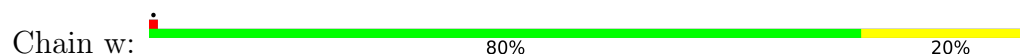
- Molecule 22: 50S ribosomal protein L24



- Molecule 23: 50S ribosomal protein L25

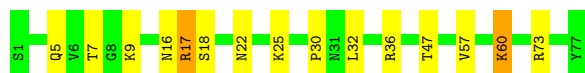


- Molecule 24: 50S ribosomal protein L27



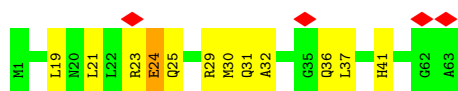
- Molecule 25: 50S ribosomal protein L28

Chain x:  81% 17%



- Molecule 26: 50S ribosomal protein L29

Chain y:  6% 81% 17%



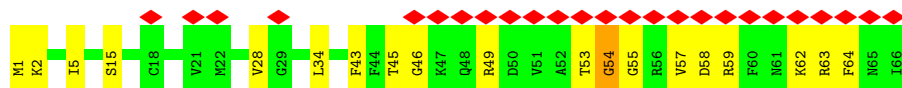
- Molecule 27: 50S ribosomal protein L30

Chain z:  83% 12%



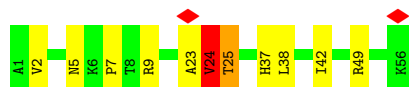
- Molecule 28: 50S ribosomal protein L31

Chain A:  38% 71% 27%



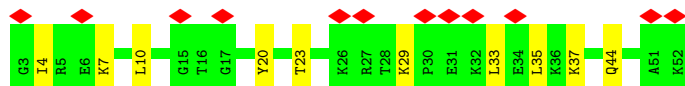
- Molecule 29: 50S ribosomal protein L32

Chain B:  80% 16%



- Molecule 30: 50S ribosomal protein L33

Chain C:  24% 80% 20%



- Molecule 31: 50S ribosomal protein L34

Chain D:  72% 26%



- Molecule 32: 50S ribosomal protein L35

Chain E:  83% 17%



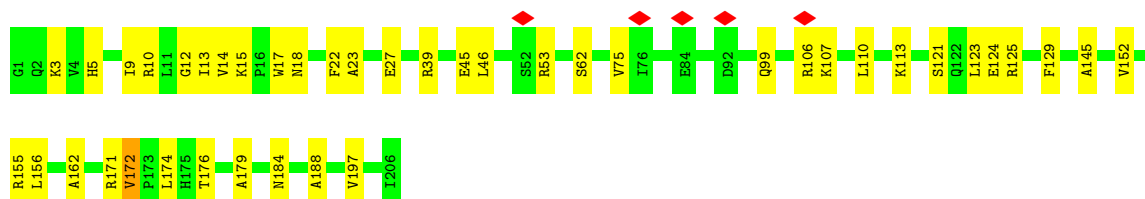
- Molecule 33: 50S ribosomal protein L36

Chain F:  74% 26%



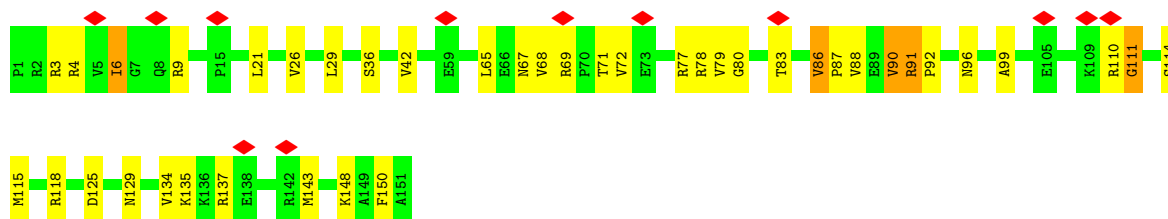
- Molecule 34: 30S ribosomal protein S3

Chain H:  80% 20%



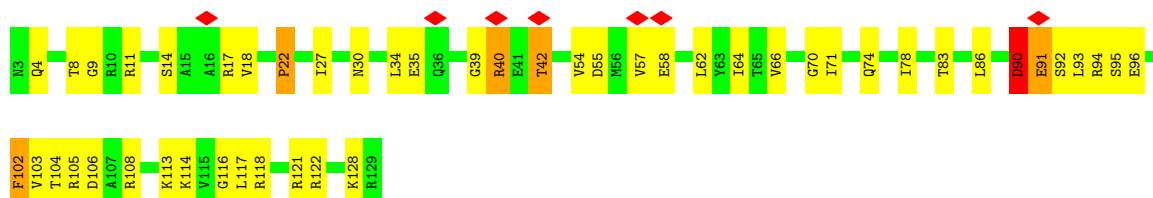
- Molecule 35: 30S ribosomal protein S7

Chain L:  8% 73% 24%

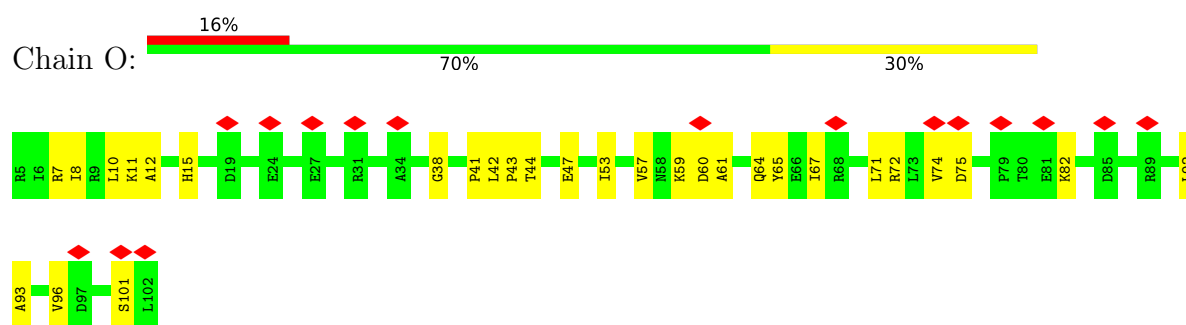


- Molecule 36: 30S ribosomal protein S9

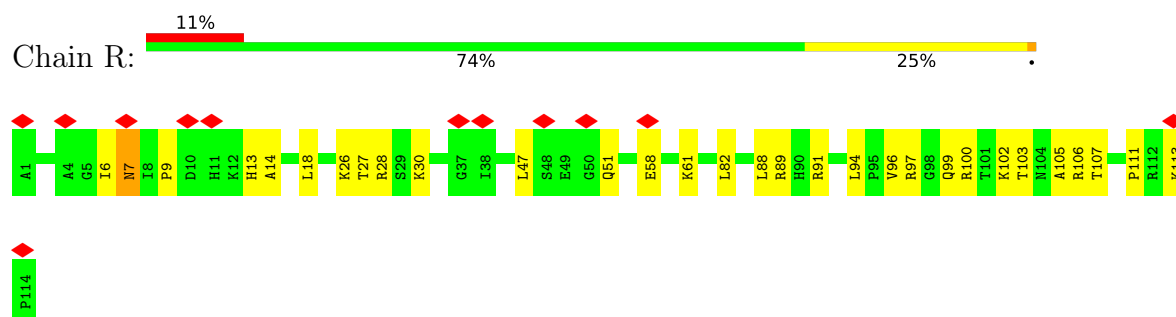
Chain N:  6% 61% 34%



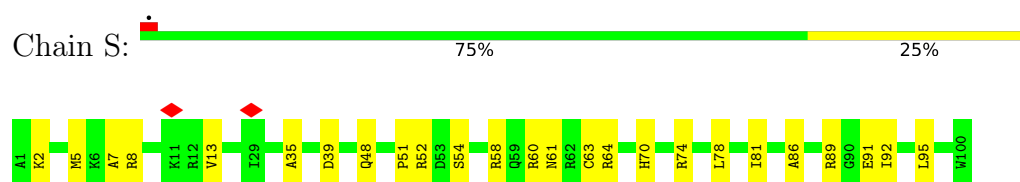
- Molecule 37: 30S ribosomal protein S10



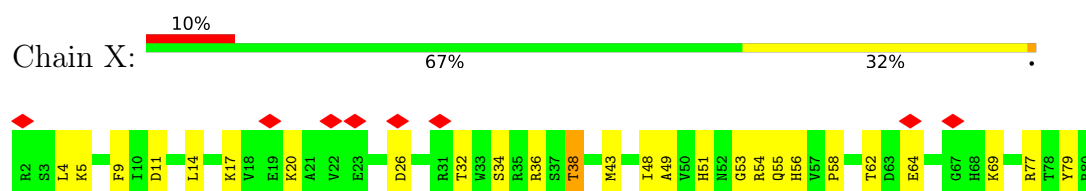
- Molecule 38: 30S ribosomal protein S13



- Molecule 39: 30S ribosomal protein S14

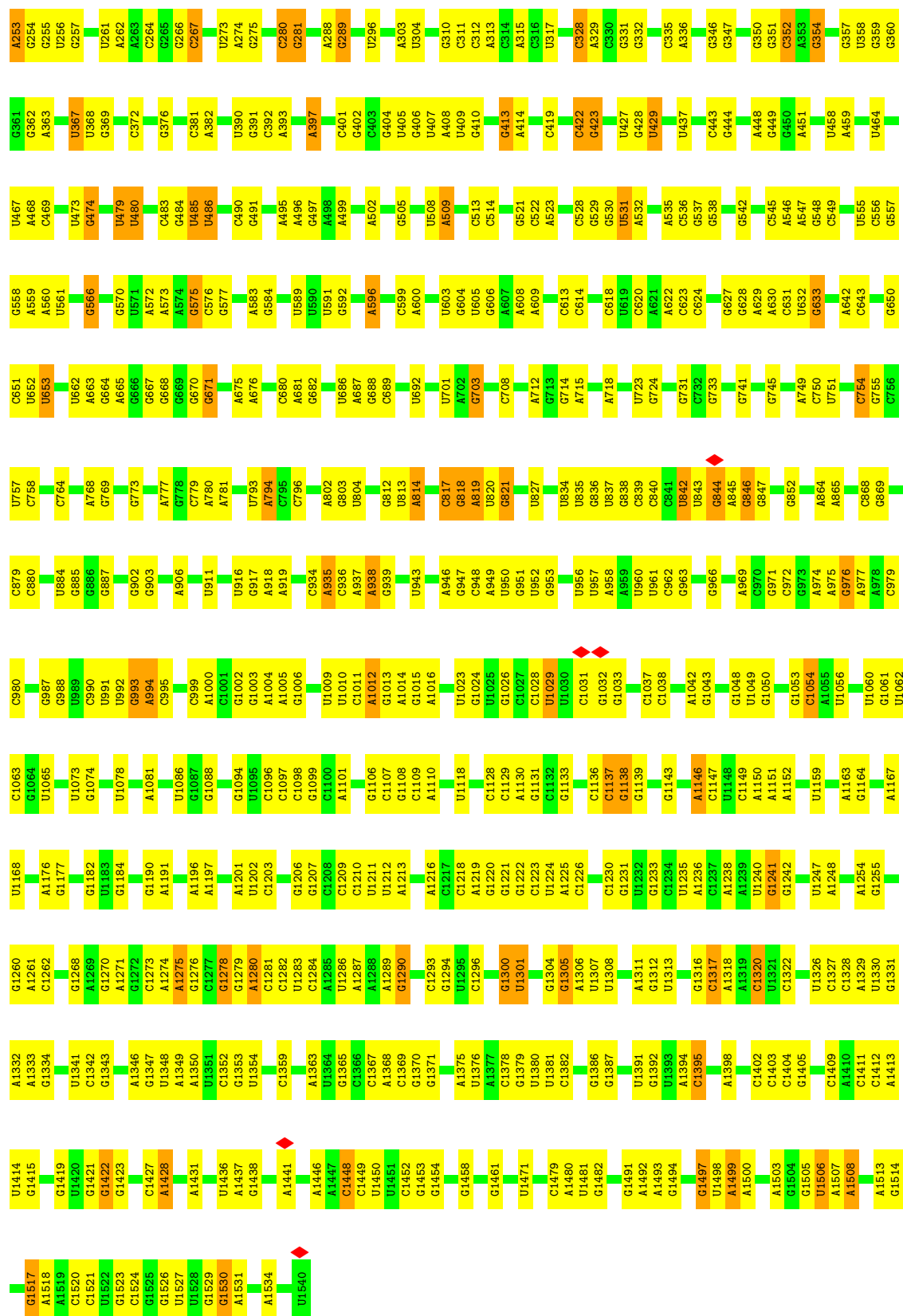


- Molecule 40: 30S ribosomal protein S19

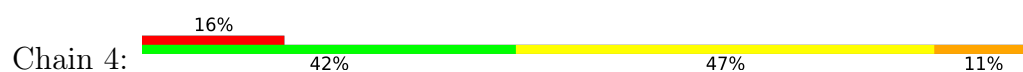


- Molecule 41: 16S rRNA

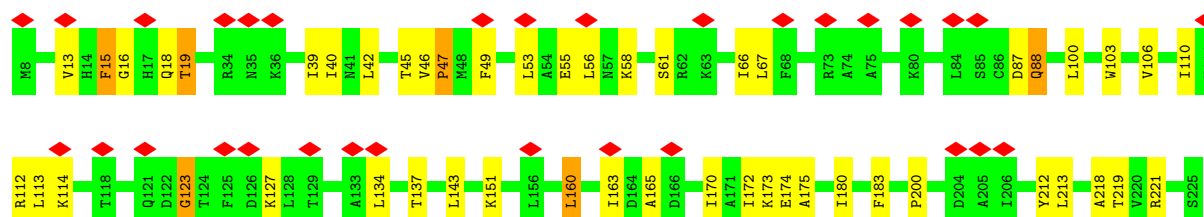
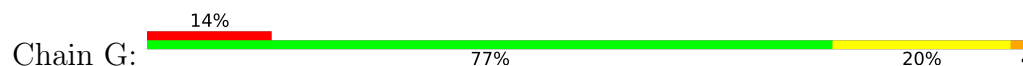




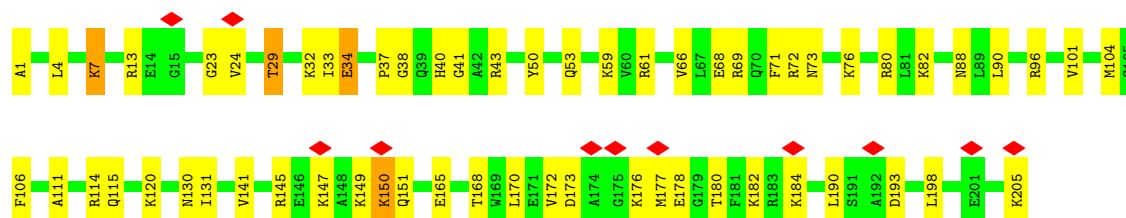
• Molecule 42: mRNA



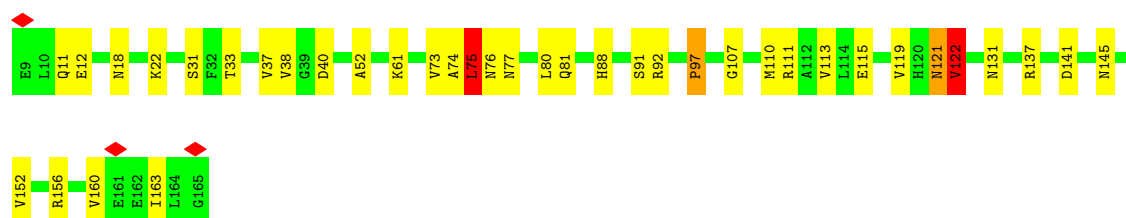
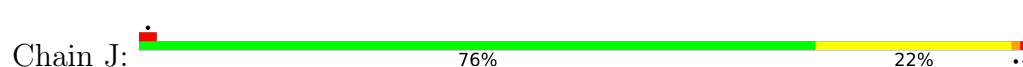
• Molecule 43: 30S ribosomal protein S2



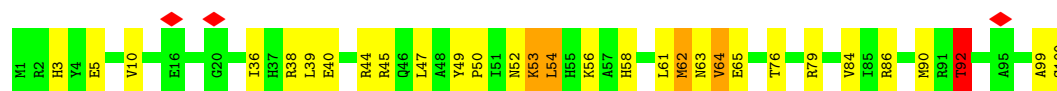
• Molecule 44: 30S ribosomal protein S4



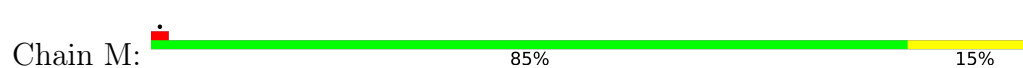
• Molecule 45: 30S ribosomal protein S5

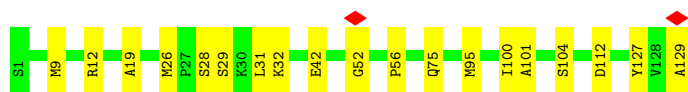


• Molecule 46: 30S ribosomal protein S6



• Molecule 47: 30S ribosomal protein S8

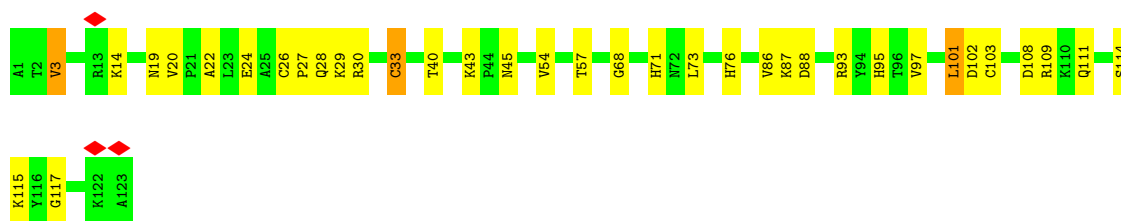




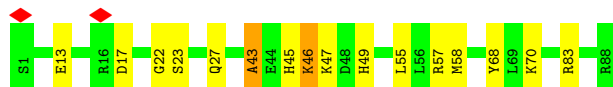
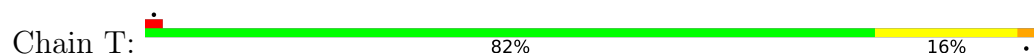
- Molecule 48: 30S ribosomal protein S11



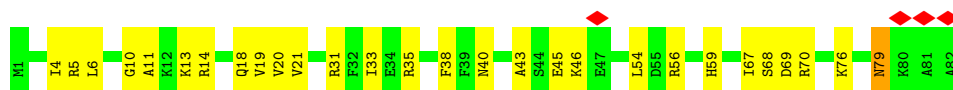
- Molecule 49: 30S ribosomal protein S12



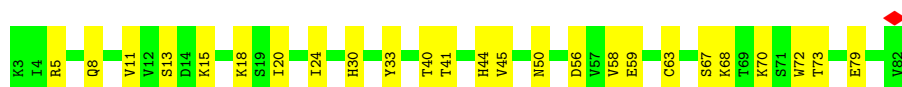
- Molecule 50: 30S ribosomal protein S15



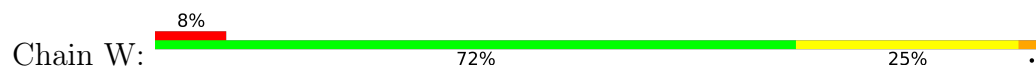
- Molecule 51: 30S ribosomal protein S16

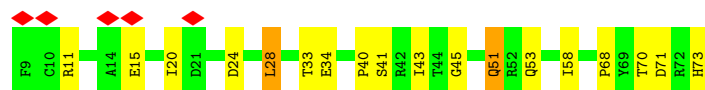


- Molecule 52: 30S ribosomal protein S17



- Molecule 53: 30S ribosomal protein S18

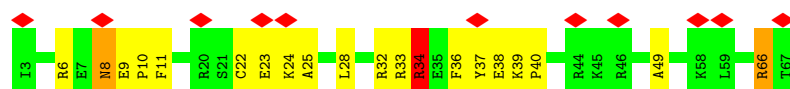




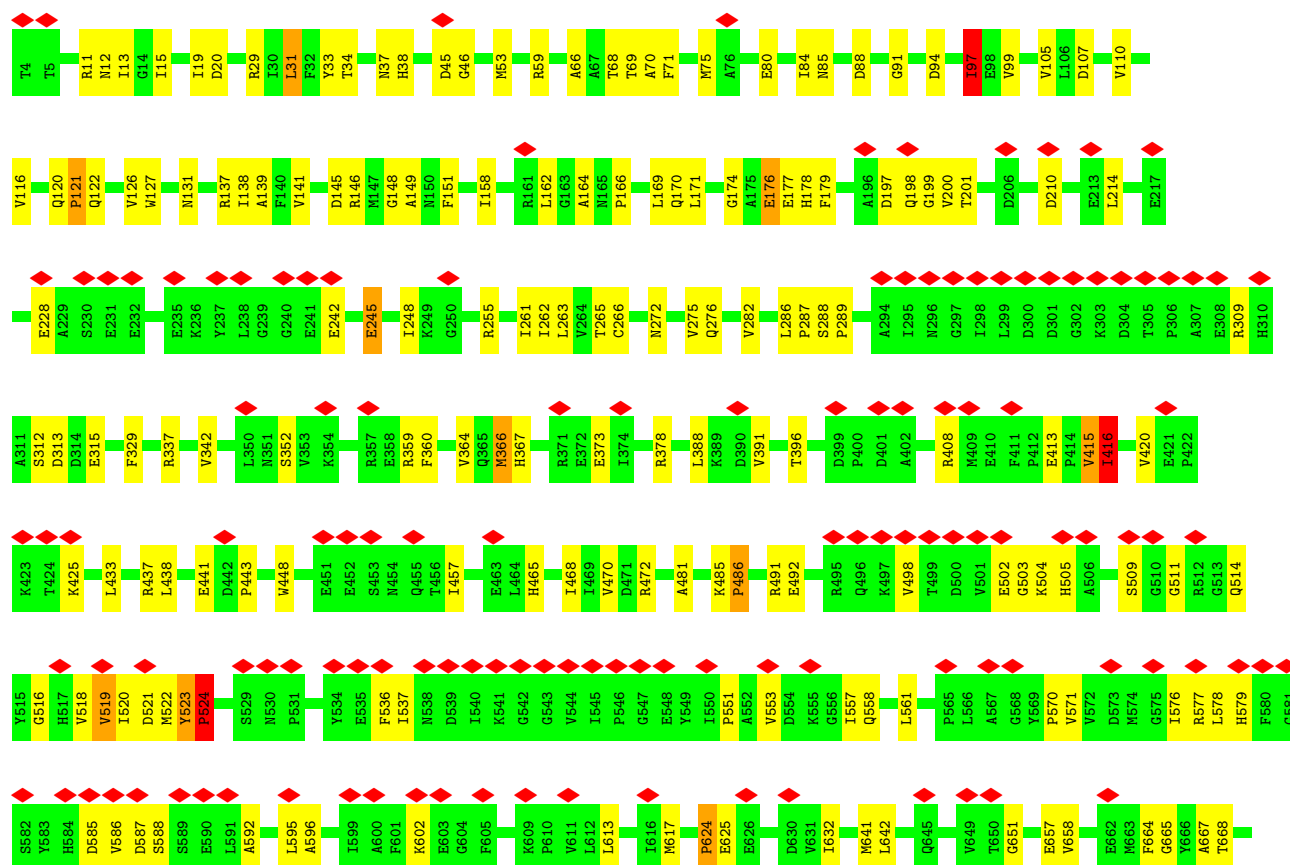
- Molecule 54: 30S ribosomal protein S20

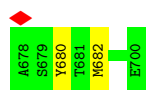


- Molecule 55: 30S ribosomal protein S21

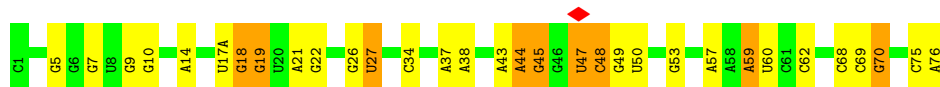


- Molecule 56: Elongation factor G

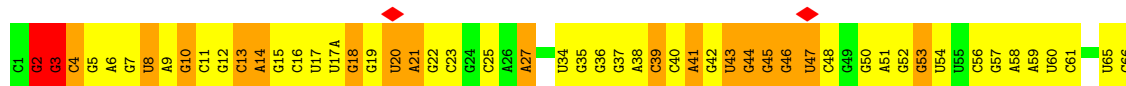




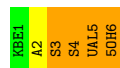
- Molecule 57: tRNA fMet



- Molecule 58: tRNA Pro



- Molecule 59: Viomycin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20167	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.5	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	20.132	Depositor
Minimum map value	-8.010	Depositor
Average map value	0.009	Depositor
Map value standard deviation	1.134	Depositor
Recommended contour level	2.65	Depositor
Map size ($\text{\AA}$)	389.76, 389.76, 389.76	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.87, 0.87, 0.87	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, DPP, 5OH, KBE, UAL, GDP

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	1	0.44	3/69796 (0.0%)	0.54	12/108888 (0.0%)
2	2	0.45	0/2872	0.53	1/4479 (0.0%)
3	b	0.43	0/2122	0.93	7/2852 (0.2%)
4	c	0.38	0/1586	0.84	4/2134 (0.2%)
5	d	0.39	0/1571	0.82	3/2113 (0.1%)
6	e	0.44	1/1435 (0.1%)	0.92	5/1926 (0.3%)
7	f	0.41	0/1343	0.82	2/1816 (0.1%)
8	g	0.47	0/1122	0.93	3/1515 (0.2%)
9	a	0.46	0/1034	0.98	5/1387 (0.4%)
10	i	0.55	0/1046	1.08	6/1410 (0.4%)
11	j	0.39	0/1152	0.86	4/1551 (0.3%)
12	k	0.44	0/948	0.95	2/1268 (0.2%)
13	l	0.40	0/1054	0.95	5/1403 (0.4%)
14	m	0.39	0/1093	0.85	3/1460 (0.2%)
15	n	0.38	0/974	0.92	3/1301 (0.2%)
16	o	0.39	0/902	0.92	3/1209 (0.2%)
17	p	0.39	0/929	0.85	1/1242 (0.1%)
18	q	0.37	0/960	0.85	3/1278 (0.2%)
19	r	0.40	0/829	0.92	2/1107 (0.2%)
20	s	0.38	0/864	0.84	2/1156 (0.2%)
21	t	0.39	0/745	0.78	0/994
22	u	0.41	0/788	0.93	3/1051 (0.3%)
23	v	0.39	0/766	0.78	0/1025
24	w	0.33	0/582	0.72	0/769
25	x	0.36	0/635	0.85	2/848 (0.2%)
26	y	0.34	0/510	0.87	1/677 (0.1%)
27	z	0.48	0/453	1.04	3/605 (0.5%)
28	A	0.43	0/532	0.96	4/709 (0.6%)
29	B	0.45	1/450 (0.2%)	0.91	2/599 (0.3%)
30	C	0.35	0/417	0.73	0/554
31	D	0.40	0/380	0.89	1/498 (0.2%)
32	E	0.40	0/513	0.86	0/676

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	F	0.35	0/303	0.77	0/397
34	H	0.40	0/1652	0.87	3/2225 (0.1%)
35	L	0.44	0/1196	1.02	8/1602 (0.5%)
36	N	0.46	0/1034	1.07	7/1375 (0.5%)
37	O	0.42	0/797	0.95	3/1077 (0.3%)
38	R	0.39	0/893	0.86	1/1193 (0.1%)
39	S	0.39	0/817	0.90	2/1088 (0.2%)
40	X	0.40	0/653	0.95	1/877 (0.1%)
41	3	0.45	0/36963	0.52	4/57662 (0.0%)
42	4	0.52	0/465	0.54	0/725
43	G	0.46	0/1736	1.01	13/2338 (0.6%)
44	I	0.44	1/1665 (0.1%)	0.99	10/2227 (0.4%)
45	J	0.42	0/1170	0.98	10/1573 (0.6%)
46	K	0.52	0/836	1.09	9/1128 (0.8%)
47	M	0.38	0/989	0.80	0/1326
48	P	0.41	0/886	0.98	6/1195 (0.5%)
49	Q	0.46	0/969	1.08	6/1300 (0.5%)
50	T	0.34	0/722	0.85	1/964 (0.1%)
51	U	0.40	0/659	0.91	3/884 (0.3%)
52	V	0.41	0/658	0.86	2/881 (0.2%)
53	W	0.38	0/545	0.98	3/731 (0.4%)
54	Y	0.38	0/671	0.90	2/888 (0.2%)
55	Z	0.56	0/551	1.29	5/728 (0.7%)
56	8	0.44	0/5502	0.95	24/7446 (0.3%)
57	6	0.43	0/1832	0.56	0/2855
58	5	0.46	0/1815	0.71	5/2829 (0.2%)
59	h	3.16	2/11 (18.2%)	0.75	0/13
All	All	0.44	8/166393 (0.0%)	0.67	220/248027 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	3
46	K	0	1
All	All	0	4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1082	U	O3'-P	7.06	1.71	1.61
59	h	3	SER	CA-C	-6.69	1.38	1.52
1	1	1104	C	C3'-O3'	6.53	1.51	1.42
59	h	4	SER	CA-C	-6.14	1.40	1.52
1	1	1104	C	O3'-P	6.13	1.70	1.61

The worst 5 of 220 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1082	U	C2'-C3'-O3'	13.65	134.17	113.70
27	z	13	ILE	N-CA-C	12.38	122.31	110.30
43	G	18	GLN	N-CA-CB	-11.48	101.08	114.17
56	8	174	GLY	N-CA-C	10.07	123.44	111.35
49	Q	43	LYS	N-CA-C	9.98	127.33	113.16

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	202	U	Sidechain
1	1	25	U	Sidechain
1	1	511	U	Sidechain
46	K	53	LYS	Peptide

5.2 Too-close contacts [i](#)

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	1	62317	0	31346	1043	0
2	2	2568	0	1303	59	0
3	b	2083	0	2157	54	0
4	c	1565	0	1616	37	0
5	d	1552	0	1619	26	0
6	e	1411	0	1447	27	0
7	f	1323	0	1374	17	0
8	g	1111	0	1148	17	0
9	a	1027	0	1092	31	0
10	i	1032	0	1088	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	j	1129	0	1162	22	0
12	k	939	0	1012	19	0
13	l	1045	0	1117	30	0
14	m	1074	0	1157	16	0
15	n	961	0	1000	20	0
16	o	892	0	923	21	0
17	p	917	0	965	22	0
18	q	947	0	1022	20	0
19	r	816	0	839	15	0
20	s	857	0	922	15	0
21	t	739	0	807	13	0
22	u	780	0	834	7	0
23	v	753	0	780	16	0
24	w	575	0	592	15	0
25	x	625	0	655	13	0
26	y	509	0	543	8	0
27	z	449	0	491	9	0
28	A	523	0	524	20	0
29	B	444	0	461	9	0
30	C	410	0	440	8	0
31	D	377	0	418	12	0
32	E	504	0	574	9	0
33	F	302	0	341	8	0
34	H	1625	0	1699	25	0
35	L	1182	0	1240	28	0
36	N	1022	0	1070	39	0
37	O	787	0	828	22	0
38	R	884	0	944	24	0
39	S	805	0	847	18	0
40	X	638	0	665	24	0
41	3	33012	0	16618	576	0
42	4	413	0	209	8	0
43	G	1705	0	1732	24	0
44	I	1643	0	1710	46	0
45	J	1157	0	1199	23	0
46	K	818	0	808	15	0
47	M	979	0	1034	12	0
48	P	870	0	878	22	0
49	Q	955	0	1019	24	0
50	T	714	0	737	11	0
51	U	649	0	666	24	0
52	V	649	0	691	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	W	536	0	552	11	0
54	Y	665	0	714	22	0
55	Z	545	0	579	11	0
56	8	5400	0	5363	104	0
57	6	1640	0	837	19	0
58	5	1625	0	821	45	0
59	h	48	0	40	7	0
60	8	28	0	12	2	0
61	8	5	0	0	1	0
All	All	153555	0	105281	2425	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 9.

The worst 5 of 2425 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)
1:1:1071:G:N2	1:1:1090:A:H62	1.26	1.27
1:1:1056:G:N2	1:1:1102:C:H5	1.33	1.24
1:1:1071:G:H22	1:1:1090:A:N6	1.39	1.18
12:k:48:PRO:HB3	41:3:1423:G:H5 ⁷	1.23	1.17
1:1:1056:G:N2	1:1:1102:C:C5	2.13	1.15

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	
3	b	269/271 (99%)	231 (86%)	33 (12%)	5 (2%)	6	33
4	c	207/209 (99%)	181 (87%)	25 (12%)	1 (0%)	24	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	d	199/201 (99%)	188 (94%)	10 (5%)	1 (0%)	24	59
6	e	175/177 (99%)	155 (89%)	18 (10%)	2 (1%)	11	43
7	f	174/176 (99%)	152 (87%)	19 (11%)	3 (2%)	7	35
8	g	147/149 (99%)	133 (90%)	13 (9%)	1 (1%)	18	52
9	a	130/223 (58%)	112 (86%)	18 (14%)	0	100	100
10	i	139/141 (99%)	117 (84%)	20 (14%)	2 (1%)	9	39
11	j	140/142 (99%)	128 (91%)	11 (8%)	1 (1%)	18	52
12	k	120/122 (98%)	99 (82%)	19 (16%)	2 (2%)	7	35
13	l	141/143 (99%)	121 (86%)	20 (14%)	0	100	100
14	m	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
15	n	118/120 (98%)	101 (86%)	17 (14%)	0	100	100
16	o	114/116 (98%)	103 (90%)	10 (9%)	1 (1%)	14	47
17	p	112/114 (98%)	102 (91%)	10 (9%)	0	100	100
18	q	115/117 (98%)	110 (96%)	4 (4%)	1 (1%)	14	47
19	r	101/103 (98%)	85 (84%)	15 (15%)	1 (1%)	12	45
20	s	108/110 (98%)	99 (92%)	9 (8%)	0	100	100
21	t	91/93 (98%)	78 (86%)	13 (14%)	0	100	100
22	u	100/102 (98%)	81 (81%)	18 (18%)	1 (1%)	12	45
23	v	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
24	w	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
25	x	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
26	y	61/63 (97%)	57 (93%)	3 (5%)	1 (2%)	7	36
27	z	56/58 (97%)	51 (91%)	4 (7%)	1 (2%)	6	34
28	A	64/66 (97%)	57 (89%)	7 (11%)	0	100	100
29	B	54/56 (96%)	48 (89%)	5 (9%)	1 (2%)	6	33
30	C	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
31	D	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
32	E	62/64 (97%)	56 (90%)	5 (8%)	1 (2%)	7	36
33	F	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
34	H	204/206 (99%)	184 (90%)	19 (9%)	1 (0%)	24	59
35	L	149/151 (99%)	129 (87%)	18 (12%)	2 (1%)	9	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	N	125/127 (98%)	94 (75%)	26 (21%)	5 (4%)	2	17
37	O	96/98 (98%)	78 (81%)	17 (18%)	1 (1%)	12	45
38	R	112/114 (98%)	99 (88%)	12 (11%)	1 (1%)	14	47
39	S	98/100 (98%)	80 (82%)	15 (15%)	3 (3%)	3	22
40	X	77/79 (98%)	69 (90%)	8 (10%)	0	100	100
43	G	216/218 (99%)	187 (87%)	28 (13%)	1 (0%)	24	59
44	I	203/205 (99%)	177 (87%)	24 (12%)	2 (1%)	12	45
45	J	155/157 (99%)	131 (84%)	20 (13%)	4 (3%)	4	26
46	K	98/100 (98%)	82 (84%)	13 (13%)	3 (3%)	3	22
47	M	127/129 (98%)	119 (94%)	8 (6%)	0	100	100
48	P	114/116 (98%)	90 (79%)	22 (19%)	2 (2%)	6	34
49	Q	121/123 (98%)	98 (81%)	17 (14%)	6 (5%)	1	13
50	T	86/88 (98%)	77 (90%)	8 (9%)	1 (1%)	10	42
51	U	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	9	40
52	V	78/80 (98%)	67 (86%)	10 (13%)	1 (1%)	9	40
53	W	63/65 (97%)	57 (90%)	6 (10%)	0	100	100
54	Y	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
55	Z	63/65 (97%)	43 (68%)	15 (24%)	5 (8%)	1	5
56	8	695/697 (100%)	622 (90%)	65 (9%)	8 (1%)	10	42
59	h	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	6544/6743 (97%)	5750 (88%)	721 (11%)	73 (1%)	14	43

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	d	83	VAL
6	e	175	PRO
7	f	45	ALA
8	g	136	SER
12	k	92	GLU

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	
3	b	216/216 (100%)	213 (99%)	3 (1%)	59	77
4	c	164/164 (100%)	162 (99%)	2 (1%)	63	79
5	d	165/165 (100%)	164 (99%)	1 (1%)	78	84
6	e	148/148 (100%)	147 (99%)	1 (1%)	76	83
7	f	137/137 (100%)	137 (100%)	0	100	100
8	g	114/114 (100%)	112 (98%)	2 (2%)	51	74
9	a	110/174 (63%)	110 (100%)	0	100	100
10	i	109/109 (100%)	105 (96%)	4 (4%)	30	63
11	j	116/116 (100%)	115 (99%)	1 (1%)	70	81
12	k	103/103 (100%)	102 (99%)	1 (1%)	68	80
13	l	102/102 (100%)	100 (98%)	2 (2%)	48	72
14	m	109/109 (100%)	109 (100%)	0	100	100
15	n	100/100 (100%)	99 (99%)	1 (1%)	68	80
16	o	86/86 (100%)	86 (100%)	0	100	100
17	p	99/99 (100%)	98 (99%)	1 (1%)	68	80
18	q	89/89 (100%)	89 (100%)	0	100	100
19	r	84/84 (100%)	84 (100%)	0	100	100
20	s	93/93 (100%)	93 (100%)	0	100	100
21	t	80/80 (100%)	79 (99%)	1 (1%)	61	78
22	u	83/83 (100%)	82 (99%)	1 (1%)	63	79
23	v	78/78 (100%)	77 (99%)	1 (1%)	61	78
24	w	57/57 (100%)	56 (98%)	1 (2%)	51	74
25	x	67/67 (100%)	67 (100%)	0	100	100
26	y	55/55 (100%)	55 (100%)	0	100	100
27	z	48/48 (100%)	48 (100%)	0	100	100
28	A	59/59 (100%)	58 (98%)	1 (2%)	53	75
29	B	47/47 (100%)	44 (94%)	3 (6%)	16	48
30	C	45/45 (100%)	45 (100%)	0	100	100
31	D	38/38 (100%)	37 (97%)	1 (3%)	40	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	E	51/51 (100%)	51 (100%)	0	100	100
33	F	34/34 (100%)	34 (100%)	0	100	100
34	H	170/170 (100%)	168 (99%)	2 (1%)	63	79
35	L	124/124 (100%)	122 (98%)	2 (2%)	55	75
36	N	105/105 (100%)	105 (100%)	0	100	100
37	O	86/86 (100%)	86 (100%)	0	100	100
38	R	92/92 (100%)	91 (99%)	1 (1%)	65	79
39	S	83/83 (100%)	82 (99%)	1 (1%)	63	79
40	X	70/70 (100%)	69 (99%)	1 (1%)	59	77
43	G	180/180 (100%)	178 (99%)	2 (1%)	65	79
44	I	172/172 (100%)	171 (99%)	1 (1%)	78	84
45	J	119/119 (100%)	119 (100%)	0	100	100
46	K	87/87 (100%)	85 (98%)	2 (2%)	44	70
47	M	104/104 (100%)	104 (100%)	0	100	100
48	P	89/89 (100%)	88 (99%)	1 (1%)	65	79
49	Q	103/103 (100%)	101 (98%)	2 (2%)	50	73
50	T	76/76 (100%)	75 (99%)	1 (1%)	61	78
51	U	65/65 (100%)	64 (98%)	1 (2%)	57	76
52	V	74/74 (100%)	73 (99%)	1 (1%)	59	77
53	W	56/56 (100%)	55 (98%)	1 (2%)	51	74
54	Y	65/65 (100%)	65 (100%)	0	100	100
55	Z	55/55 (100%)	54 (98%)	1 (2%)	51	74
56	8	574/574 (100%)	567 (99%)	7 (1%)	63	79
59	h	2/2 (100%)	2 (100%)	0	100	100
All	All	5437/5501 (99%)	5382 (99%)	55 (1%)	65	80

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	H	156	LEU
43	G	47	PRO
56	8	551	PRO
56	8	97	ILE
34	H	172	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 118 such sidechains are listed below:

Mol	Chain	Res	Type
26	y	20	ASN
56	8	157	GLN
36	N	4	GLN
56	8	85	ASN
50	T	27	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2902/2903 (99%)	413 (14%)	11 (0%)
2	2	119/120 (99%)	12 (10%)	1 (0%)
41	3	1538/1539 (99%)	175 (11%)	3 (0%)
42	4	18/19 (94%)	5 (27%)	0
57	6	76/77 (98%)	18 (23%)	0
58	5	75/76 (98%)	22 (29%)	4 (5%)
All	All	4728/4734 (99%)	645 (13%)	19 (0%)

5 of 645 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	12	U
1	1	35	G
1	1	42	A
1	1	46	G

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
41	3	1012	A
58	5	41	A
58	5	45	G
58	5	3	G
1	1	2326	C

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

4 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$
59	5OH	h	6	59	7,12,13	0.71	0	4,16,18	1.34	1 (25%)
59	DPP	h	2	59	4,5,6	0.49	0	1,5,7	0.07	0
59	KBE	h	1	59	8,8,9	0.57	0	6,8,10	1.18	0
59	UAL	h	5	59	6,8,9	2.38	2 (33%)	4,9,11	1.87	1 (25%)

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
59	5OH	h	6	59	-	0/2/18/20	0/1/1/1
59	DPP	h	2	59	-	0/2/4/6	-
59	KBE	h	1	59	-	0/7/7/8	-
59	UAL	h	5	59	-	0/3/7/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	h	5	UAL	C1-N1	-4.98	1.32	1.40
59	h	5	UAL	C-CA	-2.84	1.40	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	h	5	UAL	O-C-CA	-3.27	121.29	125.39
59	h	6	5OH	CR-CB-CA	-2.41	110.06	112.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	h	6	5OH	4	0
59	h	2	DPP	1	0
59	h	5	UAL	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
60	GDP	8	801	-	29,30,30	1.13	4 (13%)	45,47,47	1.75	6 (13%)
61	PO4	8	802	-	4,4,4	1.16	0	6,6,6	0.72	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
60	GDP	8	801	-	-	0/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	8	801	GDP	C5-C4	2.83	1.46	1.38
60	8	801	GDP	C6-N1	-2.43	1.34	1.38
60	8	801	GDP	C5-N7	-2.22	1.34	1.39
60	8	801	GDP	C4-N9	-2.20	1.32	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	8	801	GDP	C5-C4-N3	-5.60	119.48	128.39
60	8	801	GDP	C2-N3-C4	4.86	120.67	112.30
60	8	801	GDP	N9-C4-N3	3.91	133.76	125.95
60	8	801	GDP	C6-C5-N7	3.50	136.66	130.29
60	8	801	GDP	C4-C5-N7	-2.58	106.58	110.67

There are no chirality outliers.

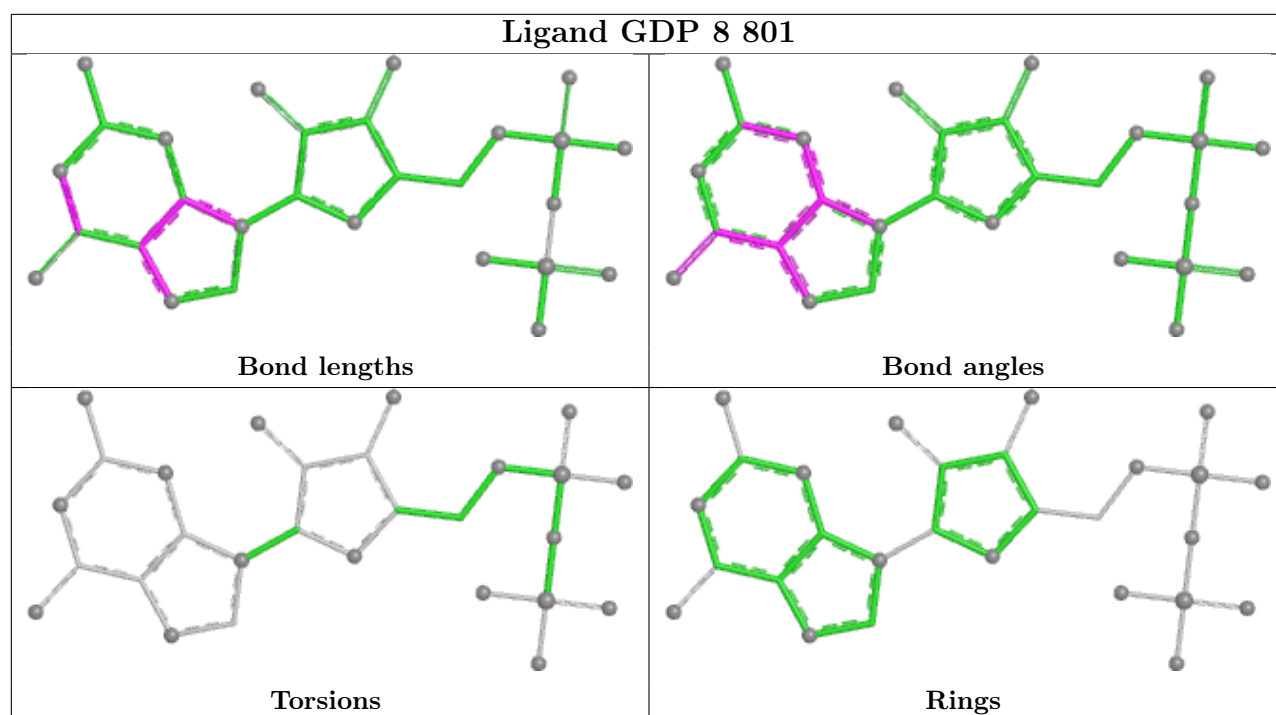
There are no torsion outliers.

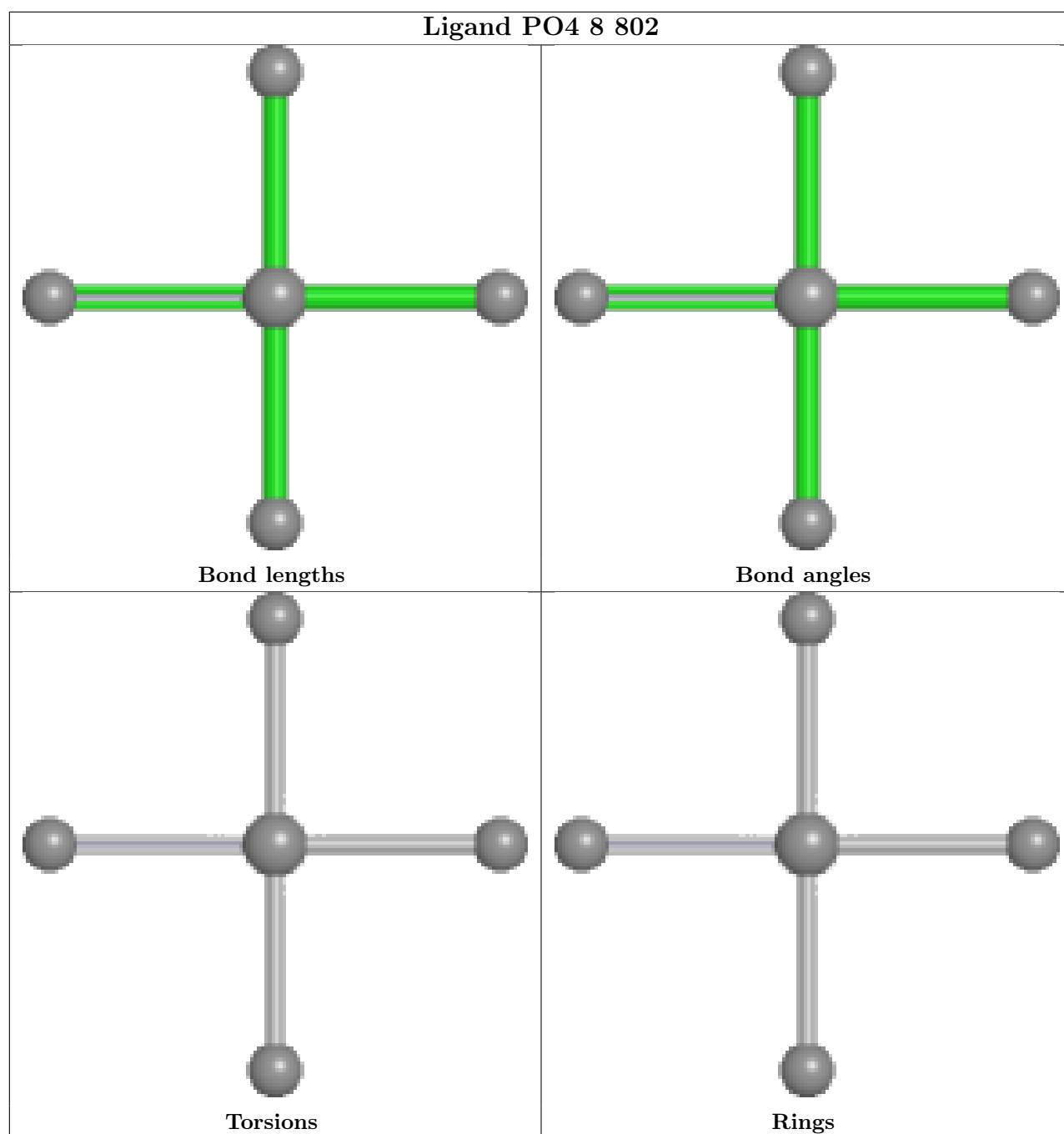
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	8	801	GDP	2	0
61	8	802	PO4	1	0

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](#)

There are no chain breaks in this entry.

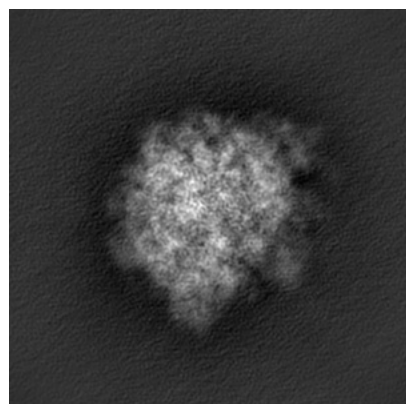
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25421. These allow visual inspection of the internal detail of the map and identification of artifacts.

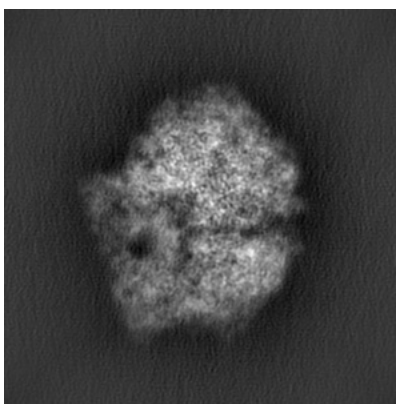
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

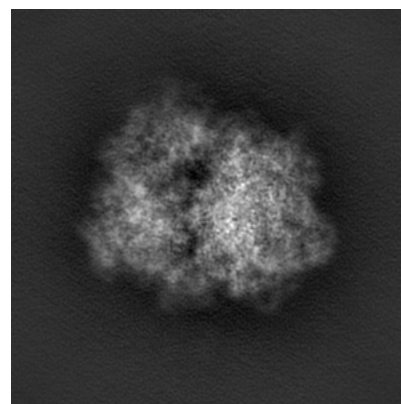
6.1.1 Primary map



X

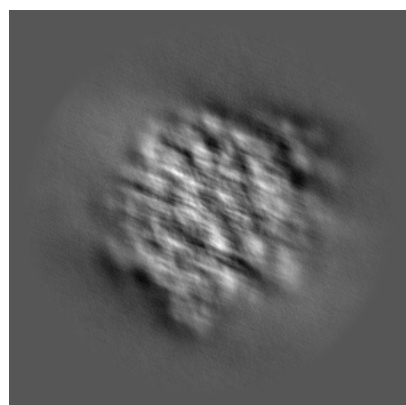


Y

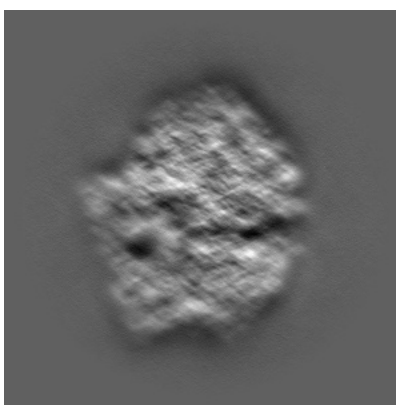


Z

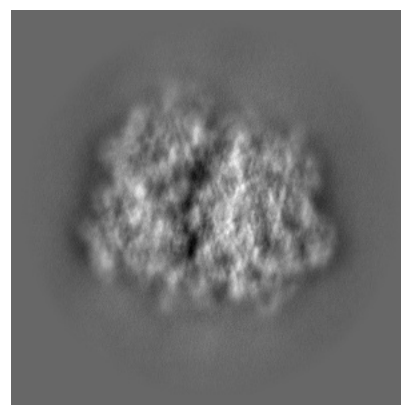
6.1.2 Raw map



X



Y

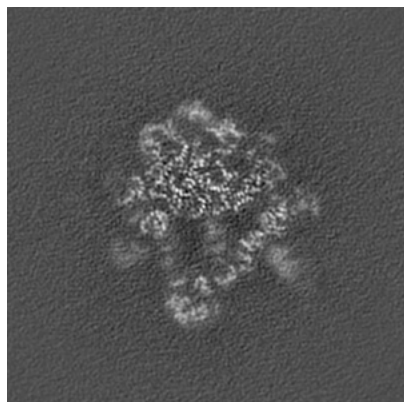


Z

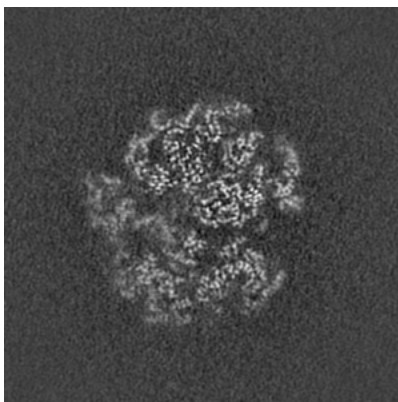
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

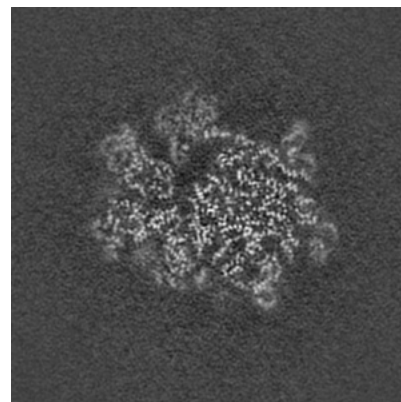
6.2.1 Primary map



X Index: 224

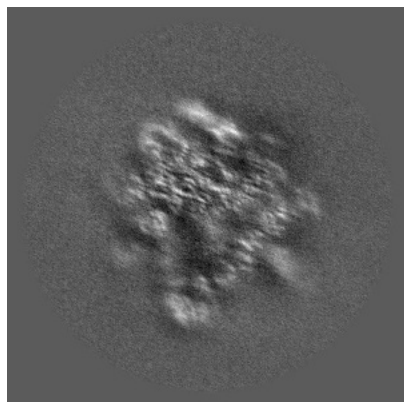


Y Index: 224

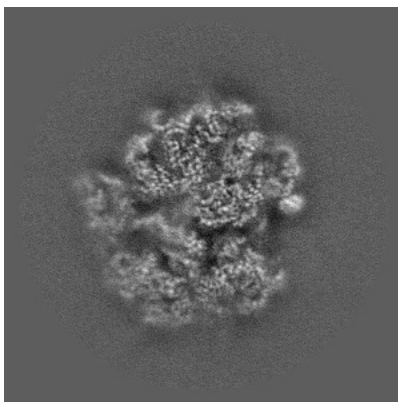


Z Index: 224

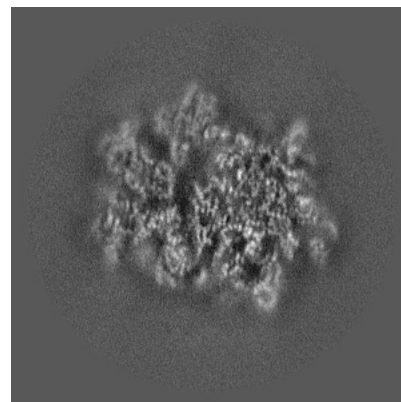
6.2.2 Raw map



X Index: 224



Y Index: 224

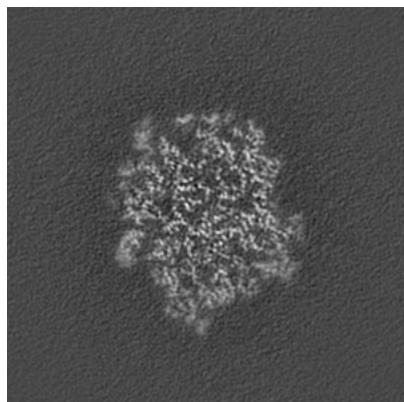


Z Index: 224

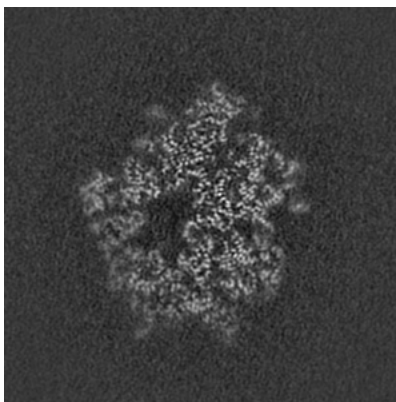
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

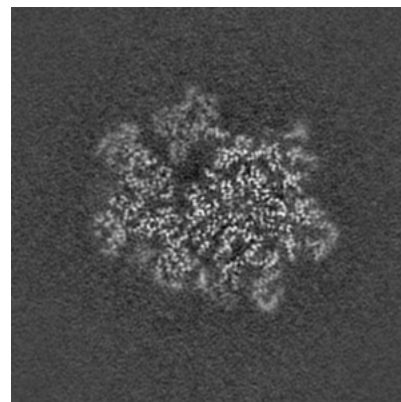
6.3.1 Primary map



X Index: 251

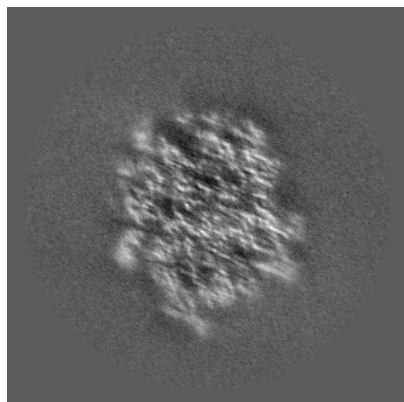


Y Index: 209

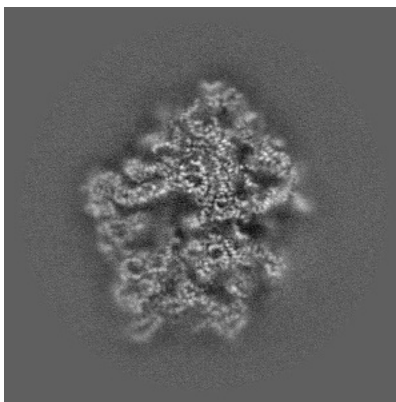


Z Index: 227

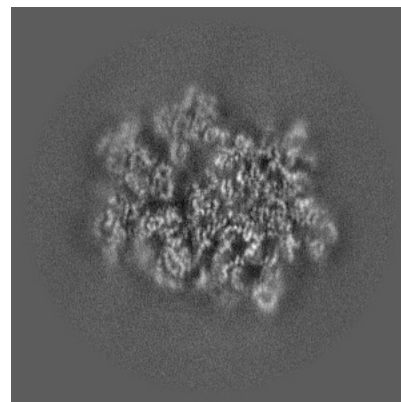
6.3.2 Raw map



X Index: 251



Y Index: 200

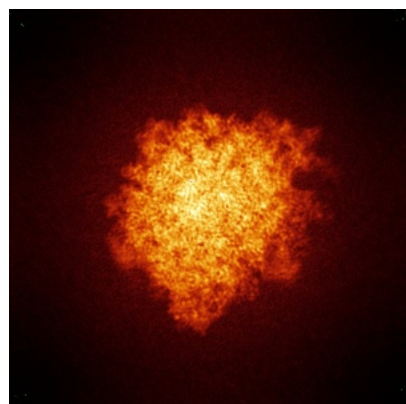


Z Index: 226

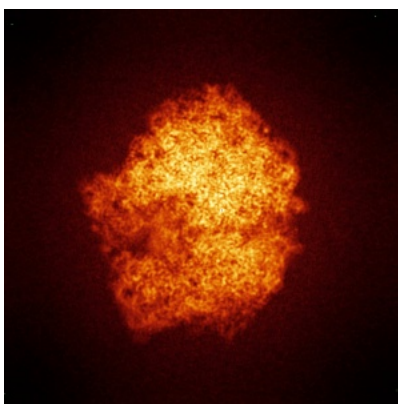
The images above show the largest variance slices of the map in three orthogonal directions.

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

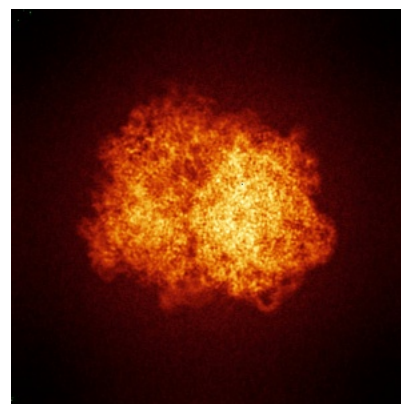
6.4.1 Primary map



X

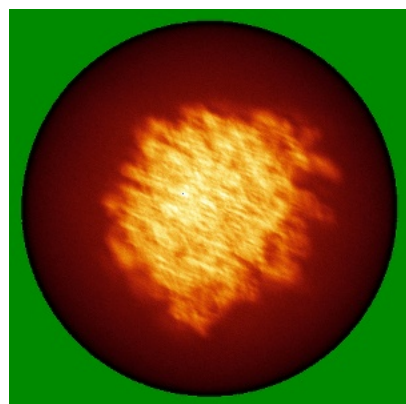


Y

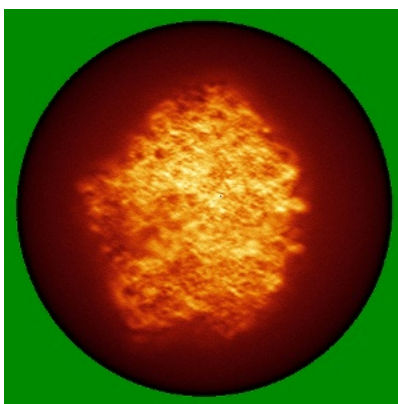


Z

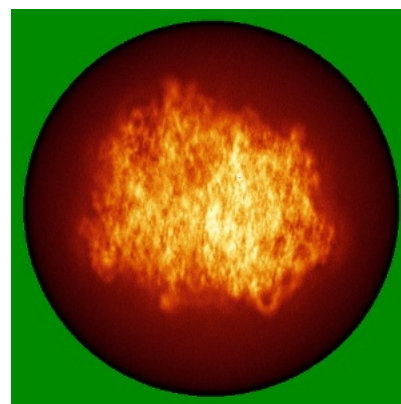
6.4.2 Raw map



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 2.65. 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.

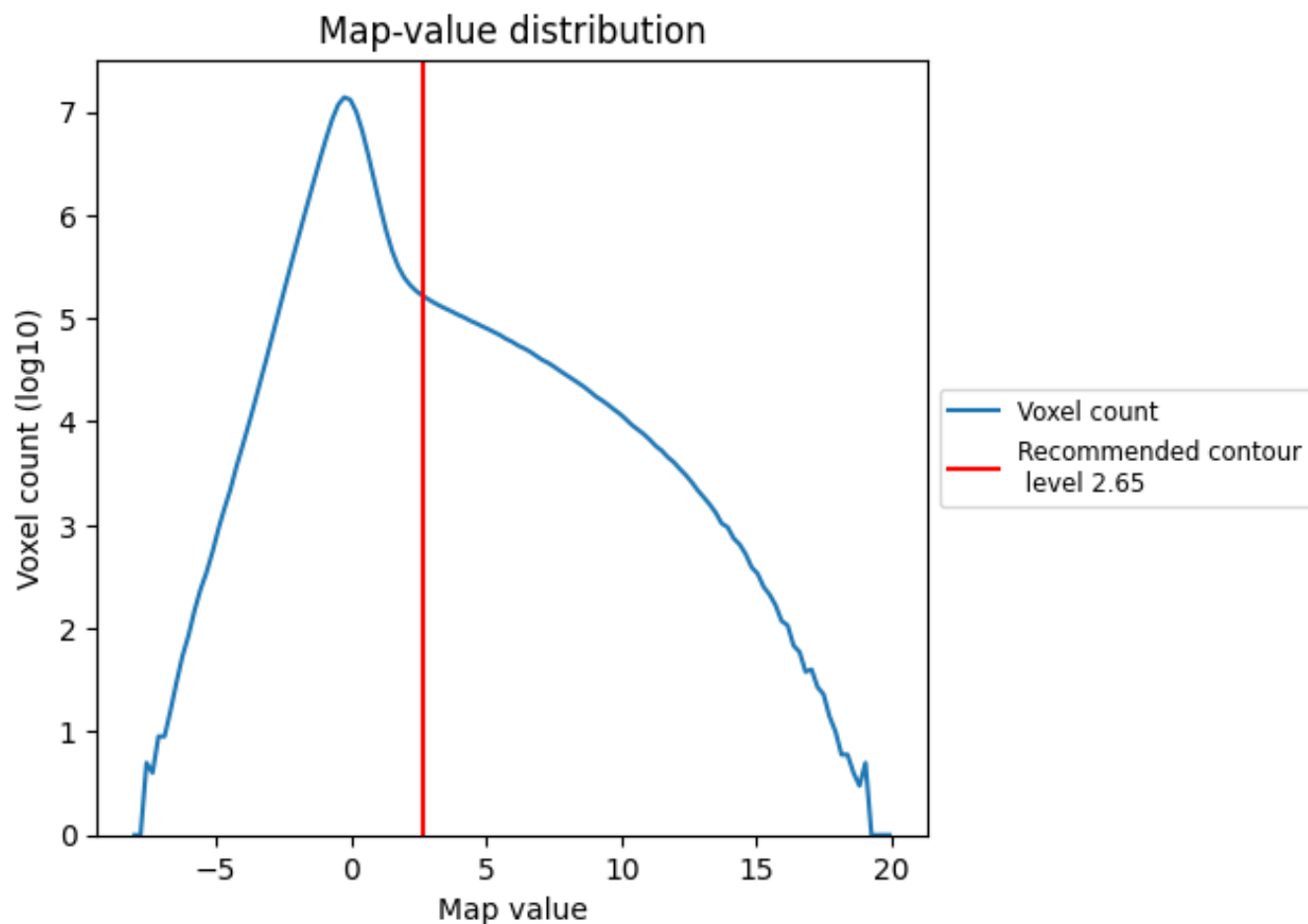
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

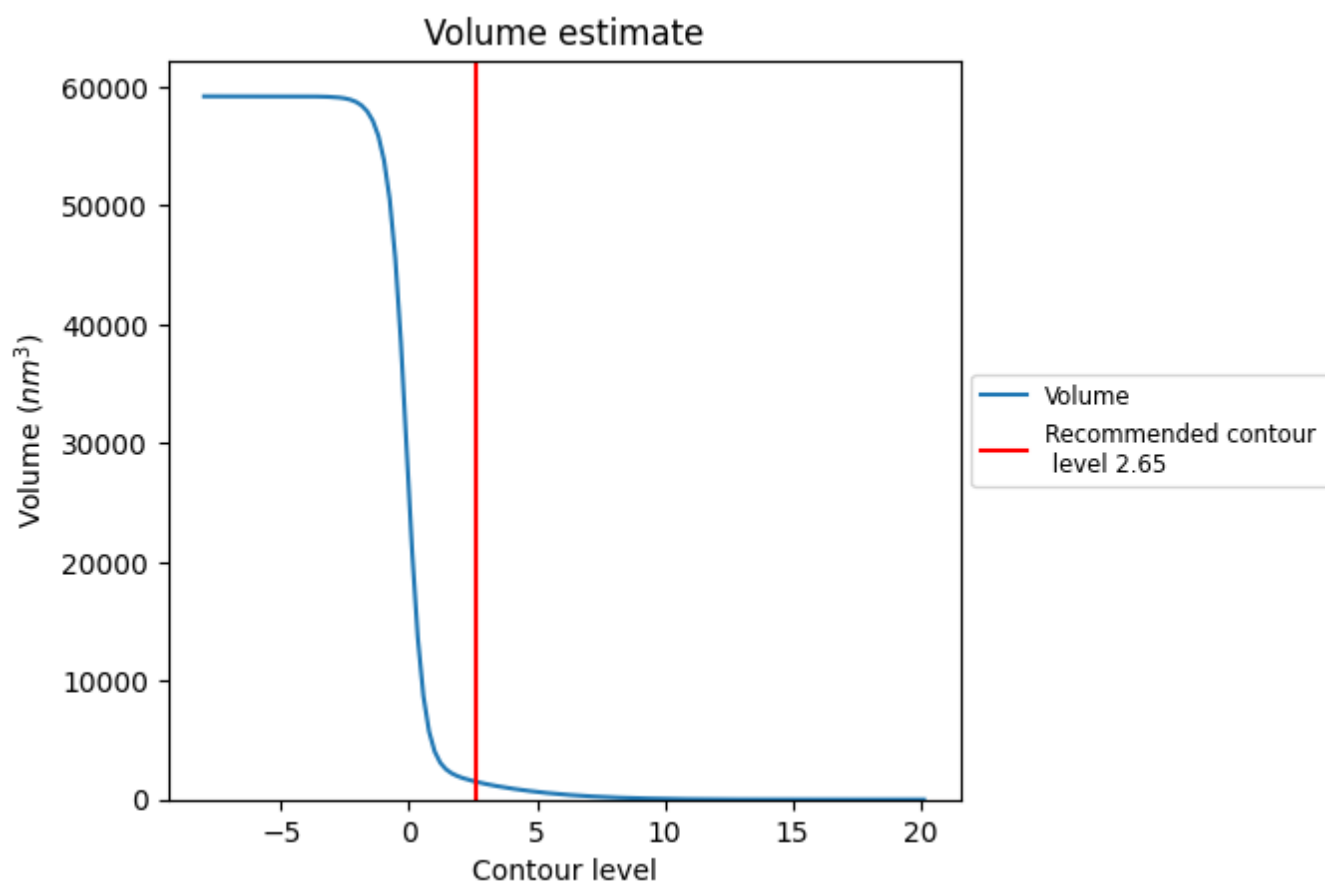
This section contains the results of statistical analysis of the map.

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.

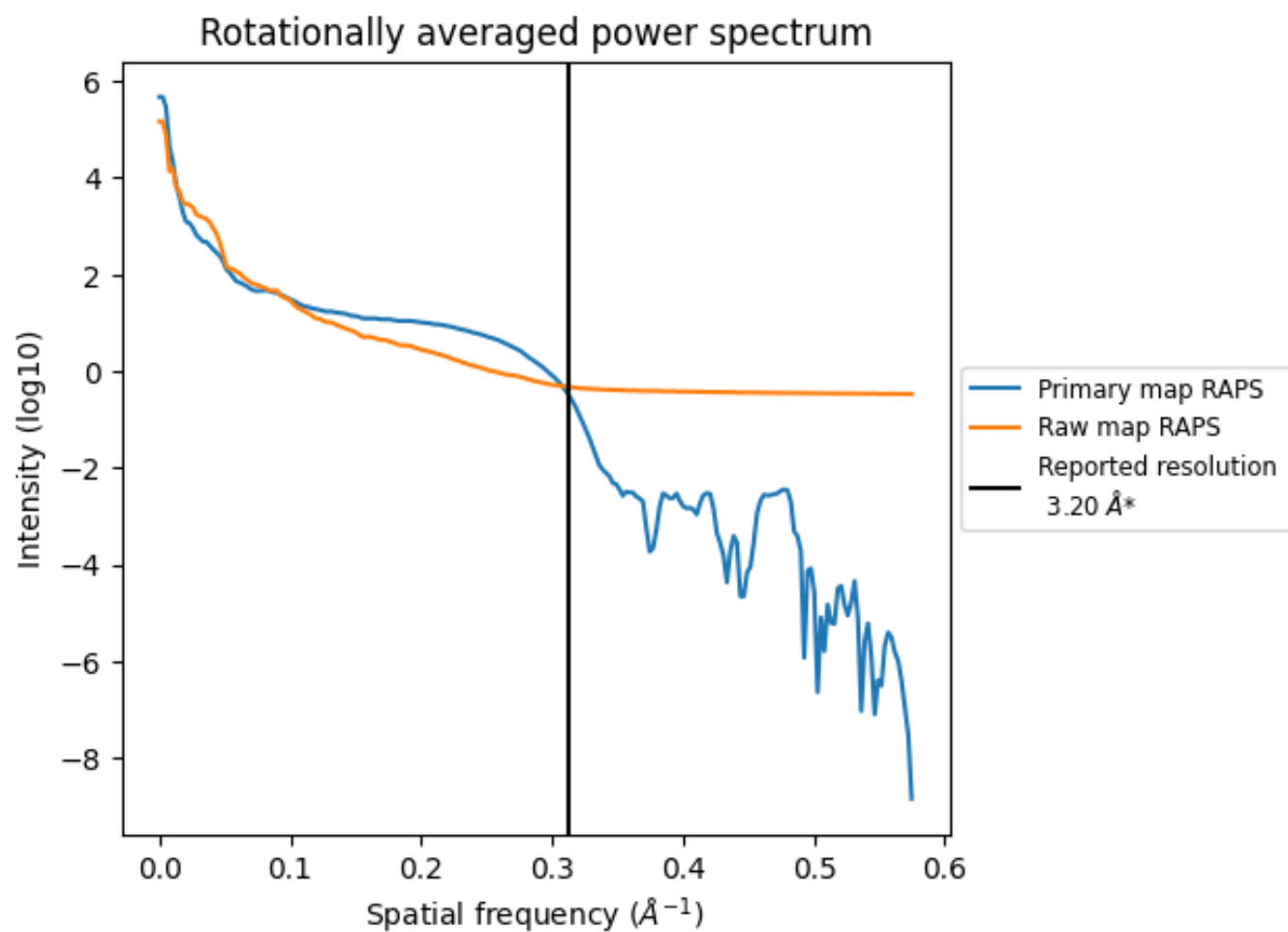
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1485 nm³; this corresponds to an approximate mass of 1341 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 ⓘ

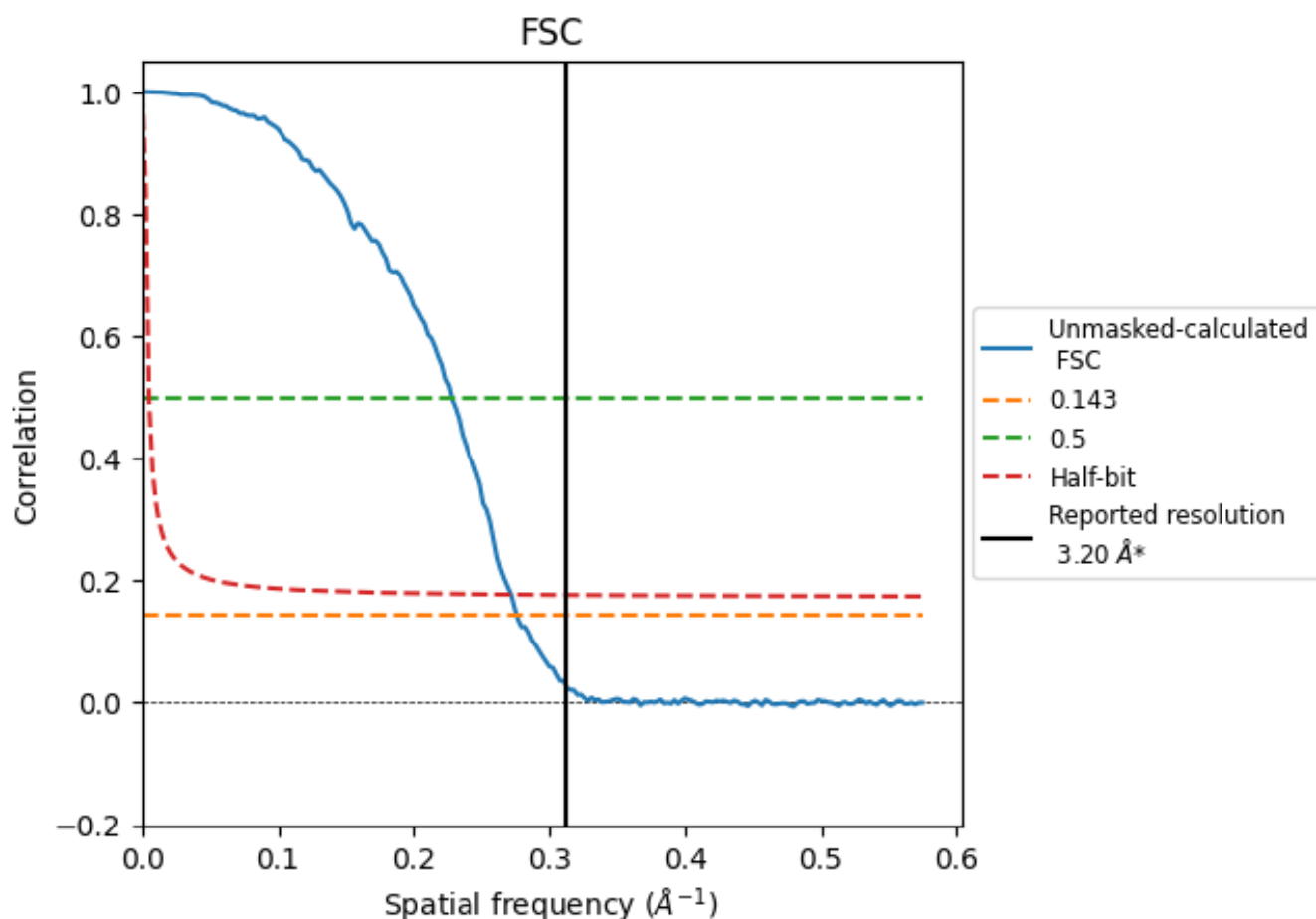


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

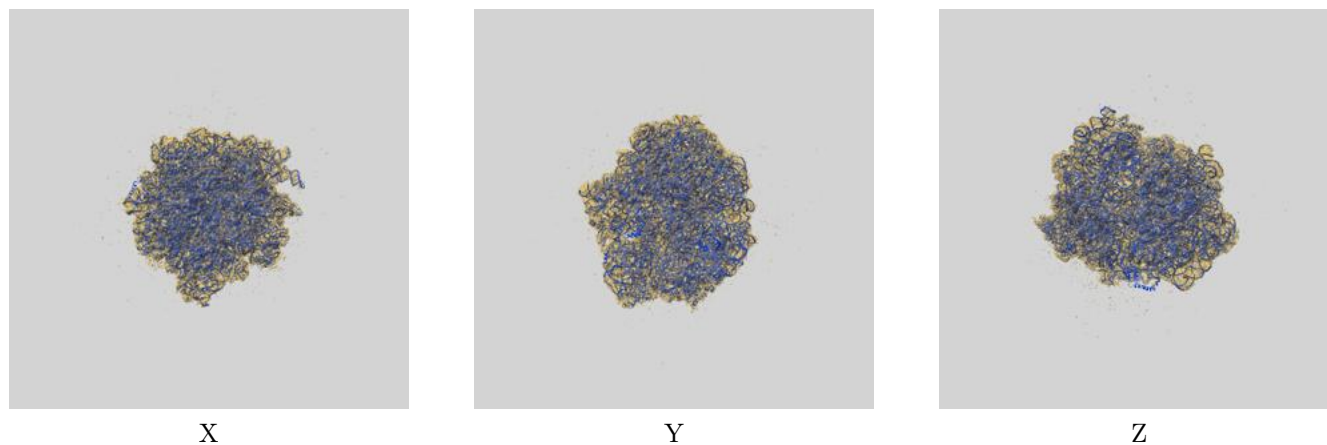
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.62	4.39	3.68

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.62 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

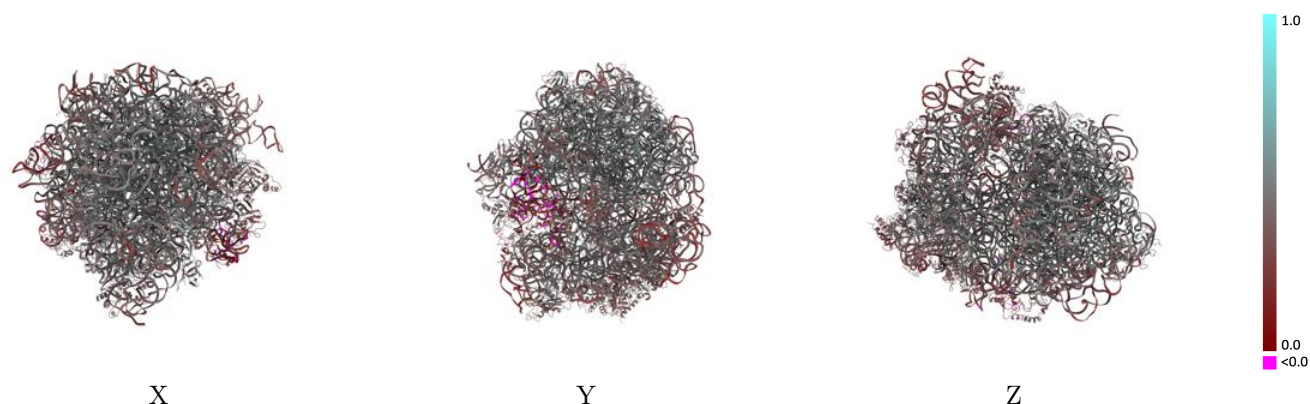
This section contains information regarding the fit between EMDB map EMD-25421 and PDB model 7ST7. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



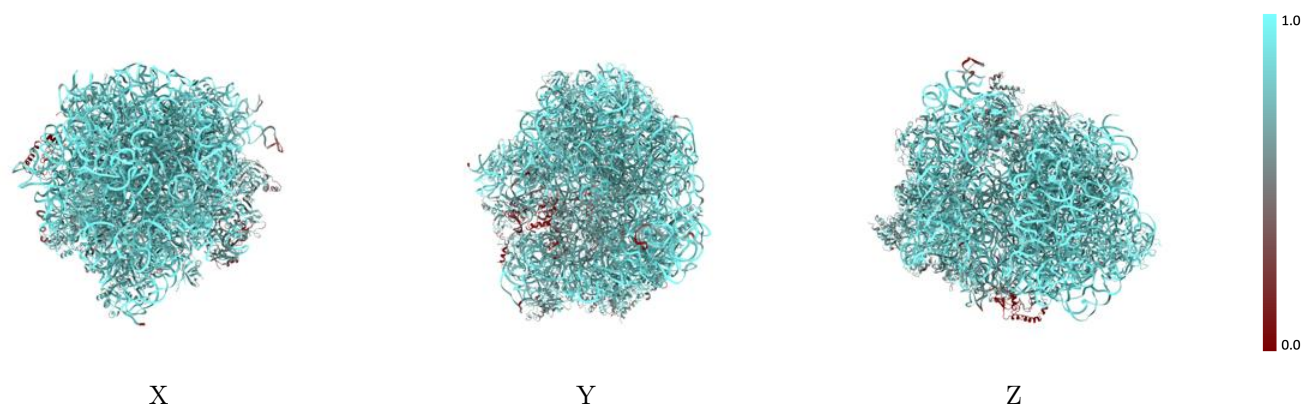
The images above show the 3D surface view of the map at the recommended contour level 2.65 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



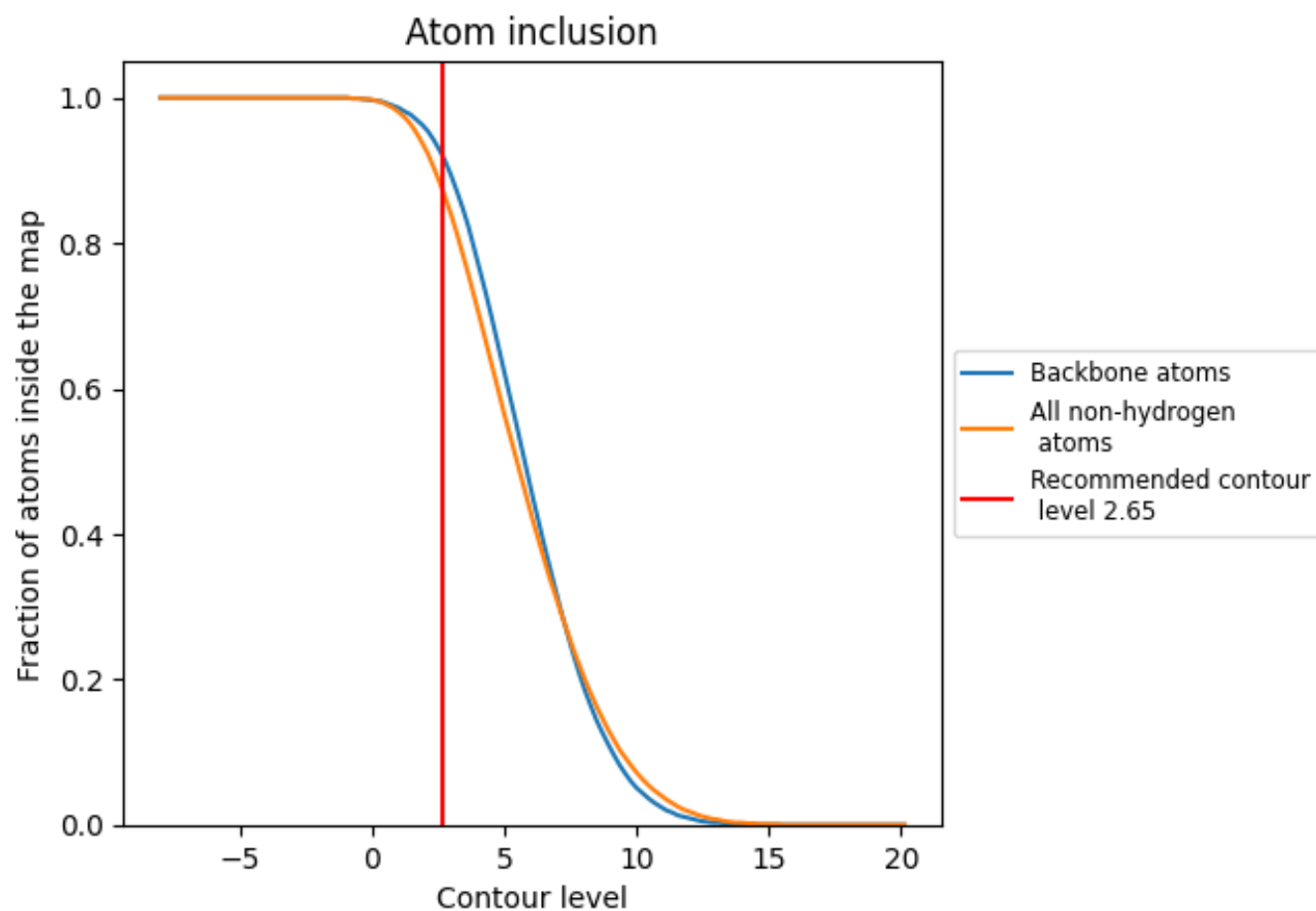
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.65).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 87% 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 (2.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8740	 0.4170
1	 0.9470	 0.4330
2	 0.9500	 0.3950
3	 0.9320	 0.4040
4	 0.7120	 0.3500
5	 0.8200	 0.2800
6	 0.8870	 0.3560
8	 0.6140	 0.3610
A	 0.5490	 0.2820
B	 0.8510	 0.4670
C	 0.6020	 0.4440
D	 0.8900	 0.4930
E	 0.8840	 0.4980
F	 0.7880	 0.4840
G	 0.6360	 0.3710
H	 0.7460	 0.4200
I	 0.7600	 0.3730
J	 0.8170	 0.4460
K	 0.7790	 0.3680
L	 0.6790	 0.3660
M	 0.8170	 0.4440
N	 0.7570	 0.3710
O	 0.6780	 0.3770
P	 0.8380	 0.4440
Q	 0.8060	 0.4730
R	 0.7310	 0.3740
S	 0.7920	 0.3860
T	 0.8390	 0.4310
U	 0.7800	 0.4250
V	 0.8400	 0.4260
W	 0.8000	 0.4220
X	 0.7510	 0.3750
Y	 0.7770	 0.3740
Z	 0.6450	 0.3370
a	 0.4430	 0.2350



Continued on next page...

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Chain	Atom inclusion	Q-score
b	 0.8730	 0.4980
c	 0.8630	 0.4830
d	 0.8140	 0.4510
e	 0.7580	 0.3800
f	 0.7600	 0.3920
g	 0.1300	 0.3110
h	 0.8330	 0.4660
i	 0.2450	 0.2020
j	 0.8710	 0.4710
k	 0.8330	 0.4900
l	 0.8470	 0.4590
m	 0.8450	 0.4790
n	 0.8960	 0.4760
o	 0.8390	 0.4110
p	 0.8140	 0.4730
q	 0.8820	 0.4760
r	 0.8430	 0.4640
s	 0.8410	 0.4770
t	 0.8080	 0.4470
u	 0.8260	 0.4340
v	 0.8240	 0.4420
w	 0.8750	 0.4880
x	 0.8450	 0.4780
y	 0.8030	 0.4010
z	 0.8440	 0.4650