



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 04:31 PM UTC

PDB ID : 9NJF / pdb_00009njf
EMDB ID : EMD-40923
Title : E. coli pre-elongation complex without an A-site tRNA with EQ2-YbiT in Non-hydrolytic 1/PtIM(a) conformation
Authors : Singh, S.; Hunt, J.F.
Deposited on : 2025-02-27
Resolution : 3.40 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

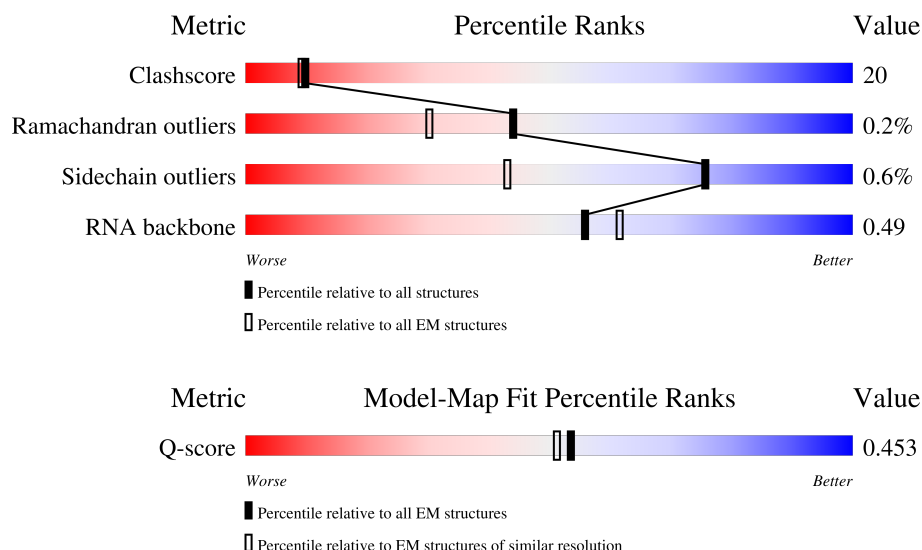
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.



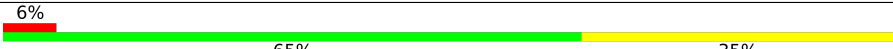
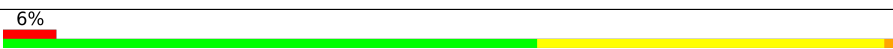
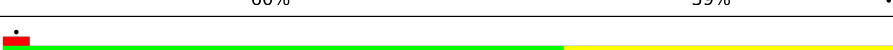
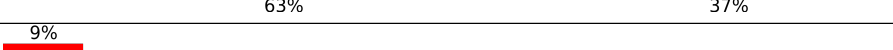
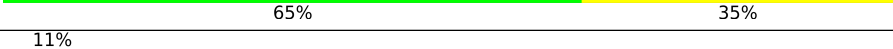
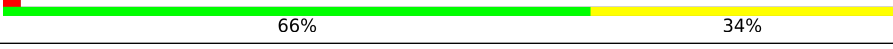
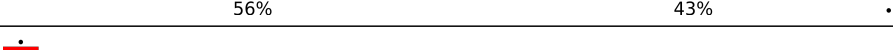
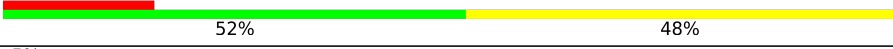
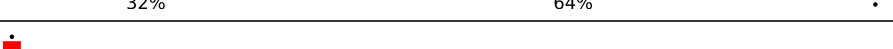
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	220	54% 69% 30%
2	10	131	89% 44% 53% .
3	11	141	86% 33% 57% 10% .

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Mol	Chain	Length	Quality of chain
4	13	142	
5	14	123	
6	15	143	
7	16	136	
8	17	120	
9	18	116	
10	19	114	
11	2	271	
12	20	117	
13	21	103	
14	22	110	
15	23	93	
16	24	102	
17	25	94	
18	27	75	
19	28	77	
20	29	63	
21	3	209	
22	30	58	
23	31	66	
24	32	56	
25	33	50	
26	34	46	
27	35	64	
28	36	38	

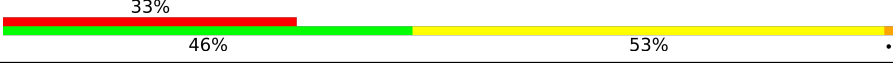
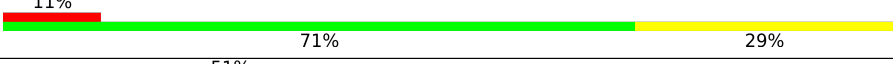
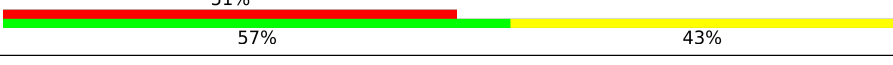
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Mol	Chain	Length	Quality of chain
29	4	201	
30	5	177	
31	6	176	
32	9	149	
33	M	6	
34	R1	2903	
35	R2	119	
36	R3	1538	
37	T	76	
38	Y	530	
39	sb	218	
40	sc	206	
41	sd	205	
42	se	157	
43	sf	100	
44	sg	151	
45	sh	129	
46	si	127	
47	sj	98	
48	sk	116	
49	sl	123	
50	sm	114	
51	sn	100	
52	so	88	
53	sp	82	

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Mol	Chain	Length	Quality of chain
54	sq	80	
55	sr	65	
56	ss	79	
57	st	85	
58	su	65	

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 151792 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 uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	220	Total	C	N	O	S	0	0
			1353	804	270	277	2		

- Molecule 2 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	10	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 3 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	11	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 4 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	13	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 5 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	14	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 6 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	15	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 7 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	16	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 8 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	17	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 9 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	18	116	Total	C	N	O	S	0	0
			892	552	178	162			

- Molecule 10 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	19	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	2	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 12 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	20	117	Total	C	N	O	S	0	0
			947	604	192	151			

- Molecule 13 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	21	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 14 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	22	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 15 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	23	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 16 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	24	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 17 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	25	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 18 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	27	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 19 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	28	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 20 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	29	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 21 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	3	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 22 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	30	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 23 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	31	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 24 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	32	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 25 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	33	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	34	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 27 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	35	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 28 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	36	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 29 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 31 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	6	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 32 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	9	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 33 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	M	6	Total	C	N	O	P	0	0
			123	58	24	35	6		

- Molecule 34 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	R1	2903	Total	C	N	O	P	0	0
			62318	27801	11467	20148	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R1	1847	G	A	conflict	GB 2019144442

- Molecule 35 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	R2	119	Total	C	N	O	P	0	0
			2546	1135	466	827	118		

- Molecule 36 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	R3	1538	Total	C	N	O	P	0	0
			32992	14716	6049	10690	1537		

- Molecule 37 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	T	76	Total	C	N	O	P	0	0
			1621	724	295	527	75		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	34	A	U	conflict	GB 1845258627

- Molecule 38 is a protein called Probable ATP-binding protein YbiT.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Y	530	Total	C	N	O	S	0	0
			4210	2659	718	814	19		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	181	GLN	GLU	conflict	UNP P0A9U3
Y	464	GLN	GLU	conflict	UNP P0A9U3

- Molecule 39 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	sb	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 40 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	sc	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 41 is a protein called 30S ribosomal protein S4.

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

- Molecule 42 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	se	157	Total	C	N	O	S	0	0
			1156	719	218	213	6		

- Molecule 43 is a protein called 30S ribosomal protein S6, non-modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	sf	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 44 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	sg	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 45 is a protein called 30S ribosomal protein S8.

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

- Molecule 46 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 47 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	sj	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 48 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	sk	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 49 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 50 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	sm	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 51 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 52 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 53 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 54 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	sq	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 55 is a protein called 30S ribosomal protein S18.

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

- Molecule 56 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	ss	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 57 is a protein called 30S ribosomal protein S20.

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

- Molecule 58 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	su	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

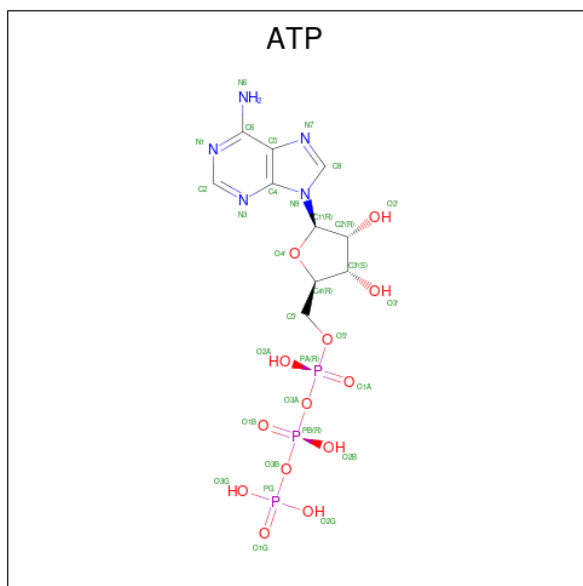
- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	18	1	Total	Mg	0
			1	1	
59	32	1	Total	Mg	0
			1	1	
59	33	1	Total	Mg	0
			1	1	
59	R1	92	Total	Mg	0
			92	92	
59	R2	2	Total	Mg	0
			2	2	
59	R3	27	Total	Mg	0
			27	27	

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
60	36	1	Total	Zn	0
			1	1	

- Molecule 61 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

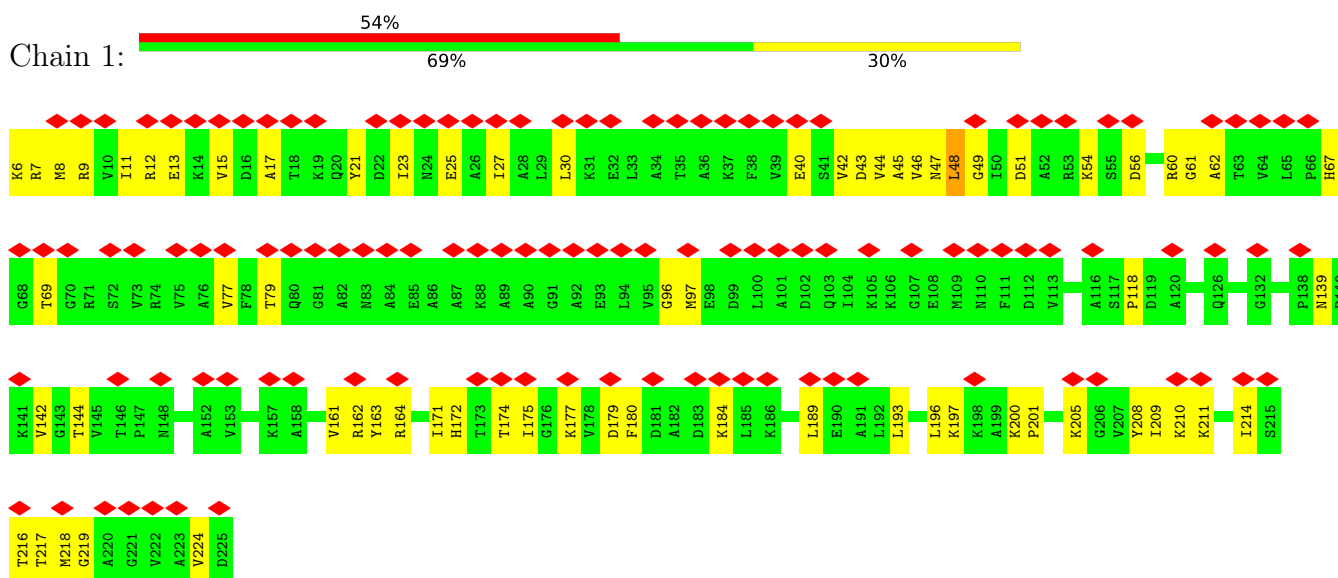
- Molecule 62 is SODIUM ION (CCD ID: NA) (formula: Na).

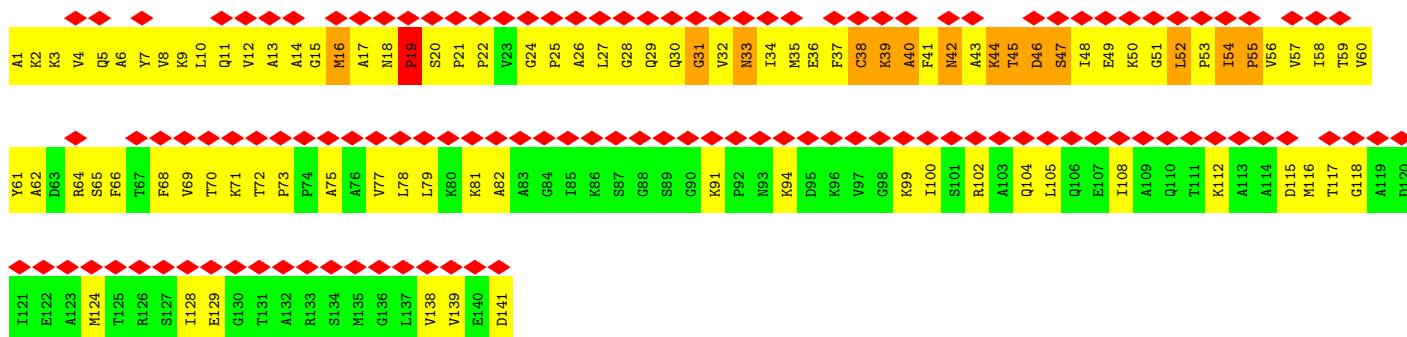
Mol	Chain	Residues	Atoms		AltConf
62	Y	2	Total	Na	0
			2	2	

3 Residue-property plots

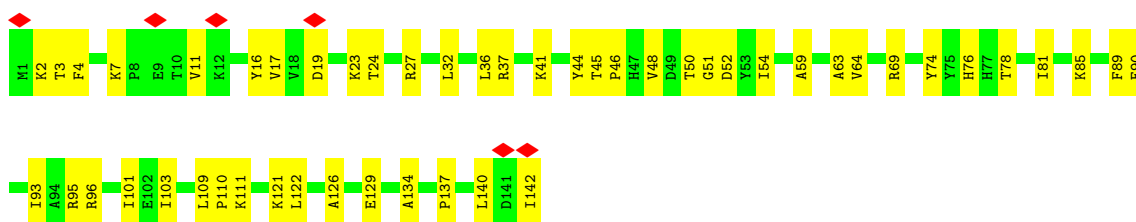
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Large ribosomal subunit protein uL1

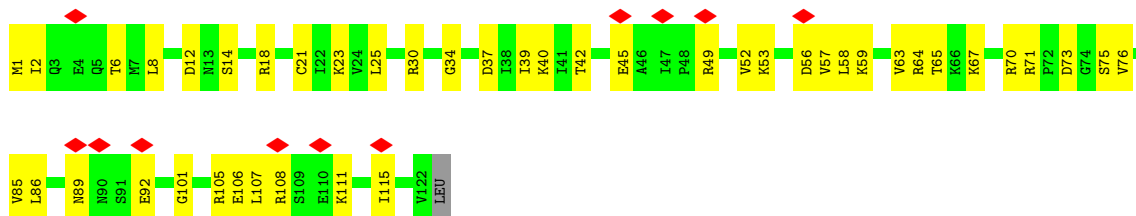




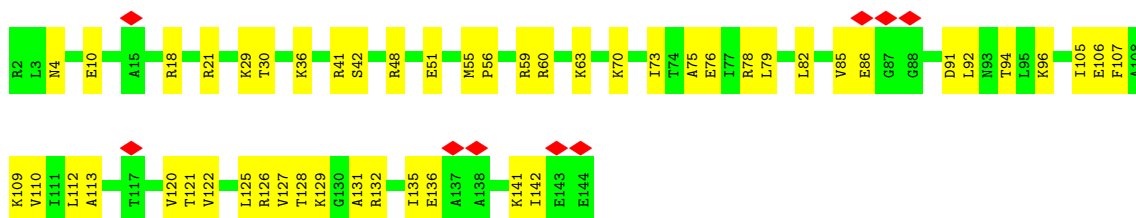
• Molecule 4: Large ribosomal subunit protein uL13



• Molecule 5: Large ribosomal subunit protein uL14

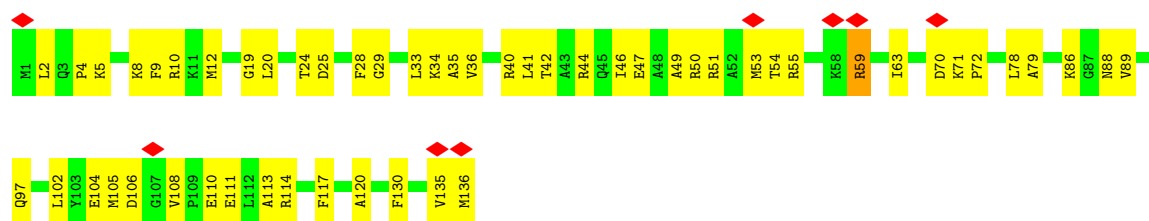


• Molecule 6: 50S ribosomal protein L15

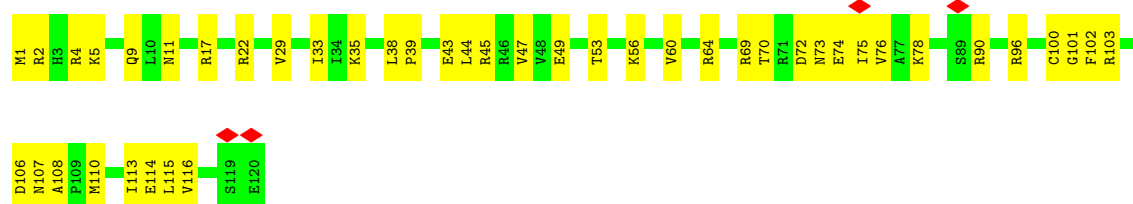


• Molecule 7: 50S ribosomal protein L16

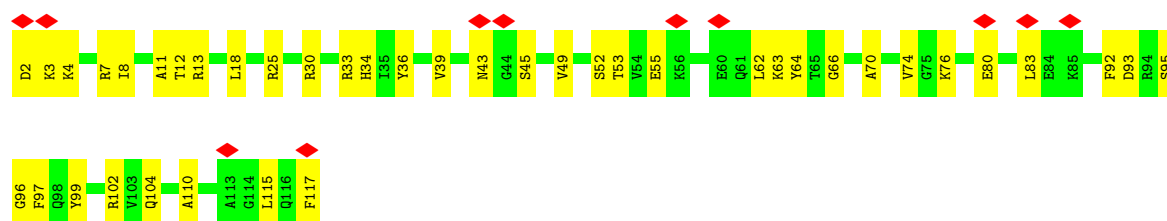




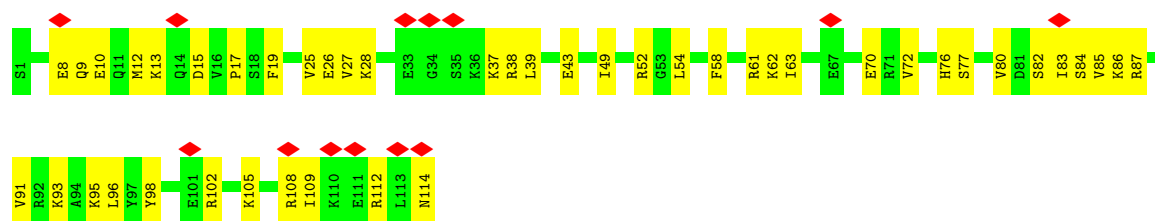
- Molecule 8: Large ribosomal subunit protein bL17



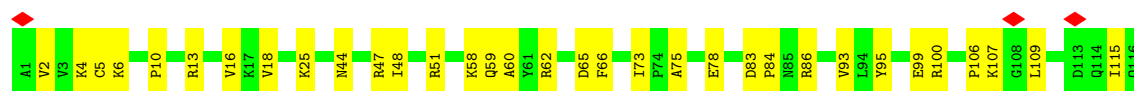
- Molecule 9: Large ribosomal subunit protein uL18

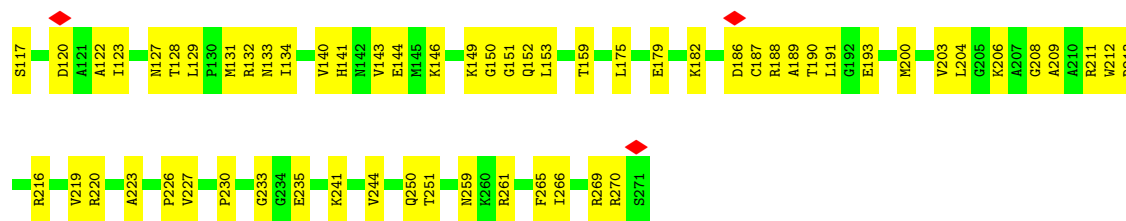


- Molecule 10: 50S ribosomal protein L19



- Molecule 11: 50S ribosomal protein L2

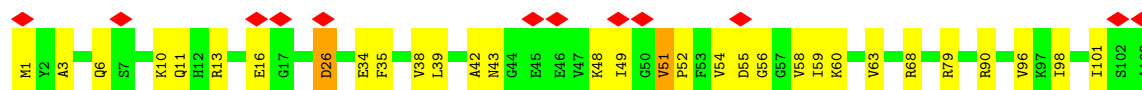




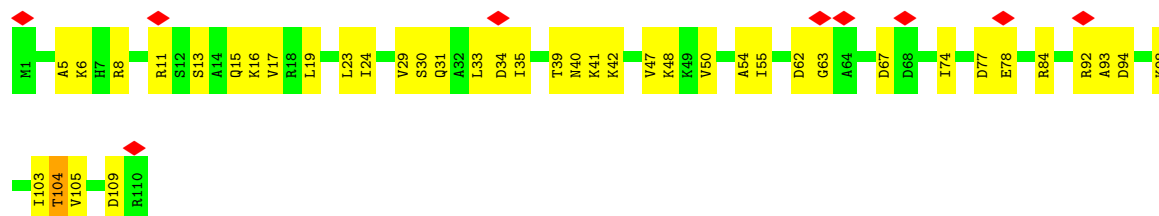
- Molecule 12: Large ribosomal subunit protein bL20



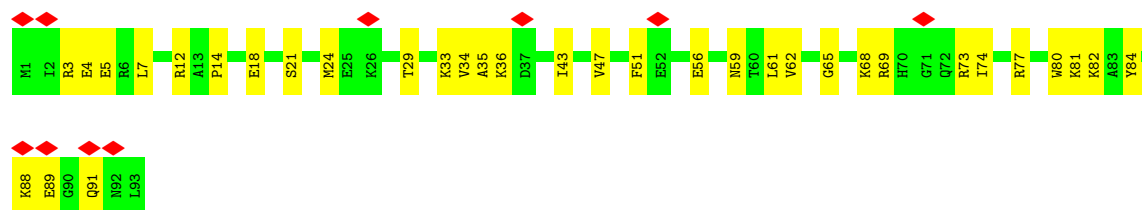
- Molecule 13: Large ribosomal subunit protein bL21



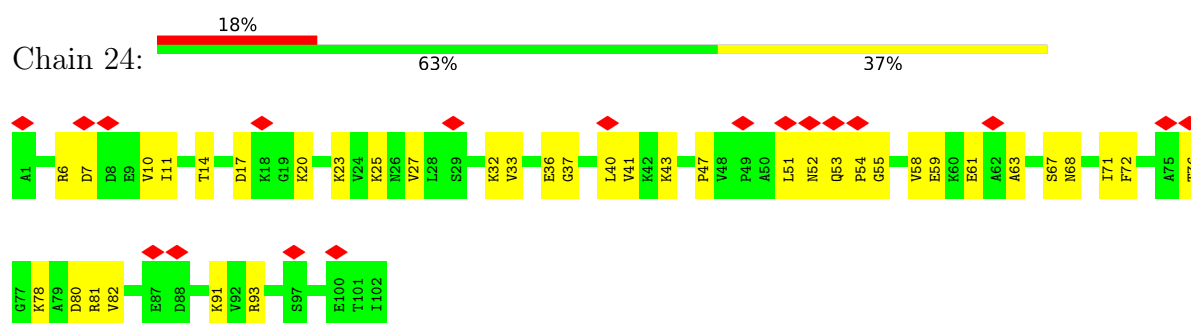
- Molecule 14: Large ribosomal subunit protein uL22



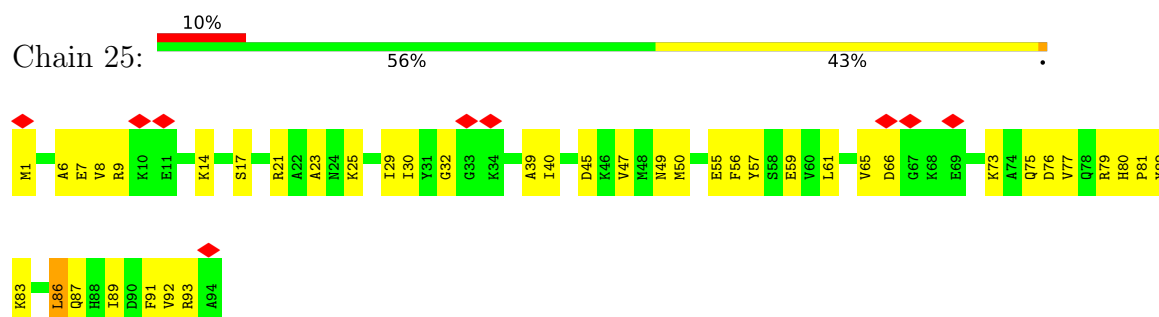
- Molecule 15: Large ribosomal subunit protein uL23



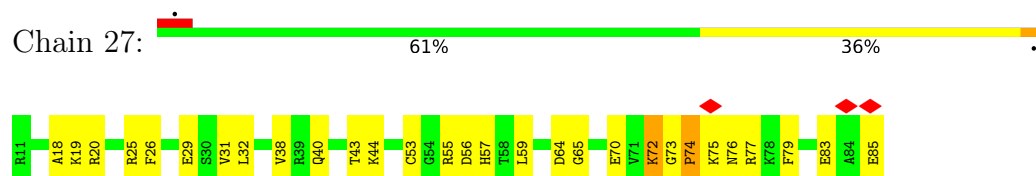
- Molecule 16: Large ribosomal subunit protein uL24



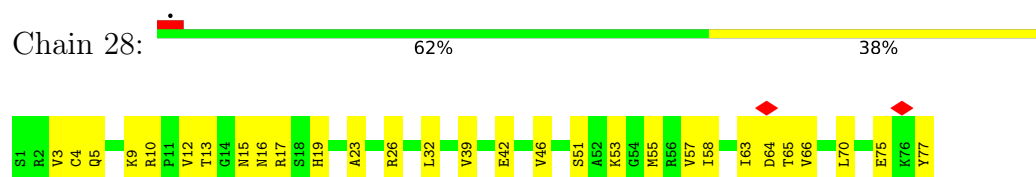
- Molecule 17: Large ribosomal subunit protein bL25



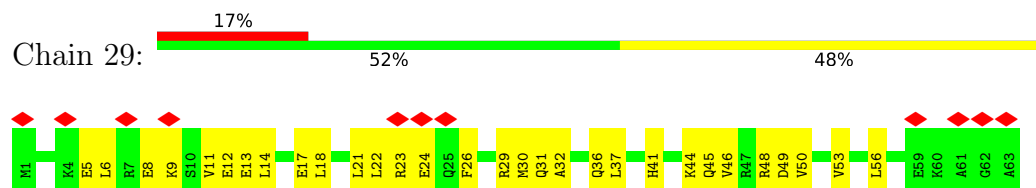
- Molecule 18: 50S ribosomal protein L27



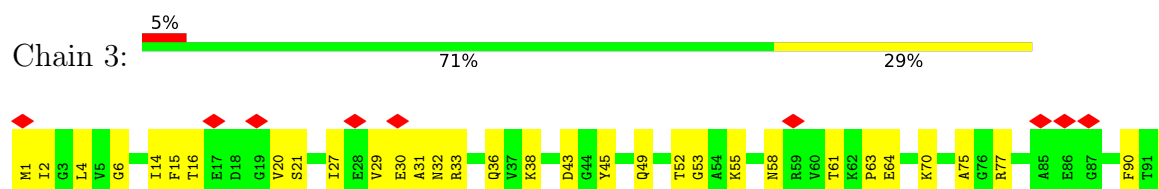
- Molecule 19: 50S ribosomal protein L28

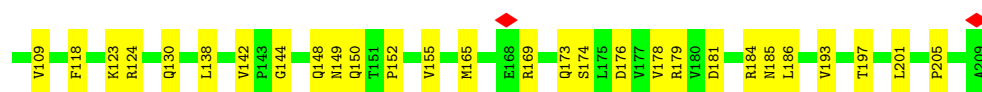


- Molecule 20: Large ribosomal subunit protein uL29



- Molecule 21: 50S ribosomal protein L3

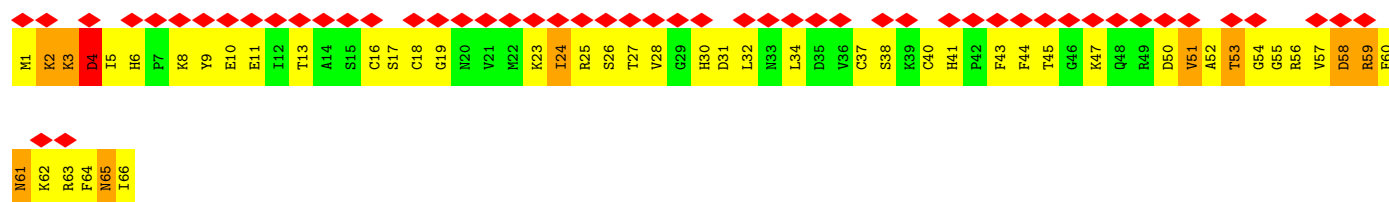
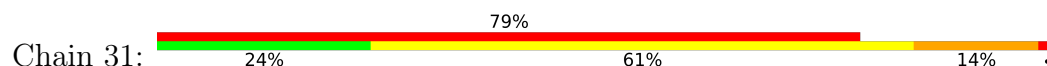




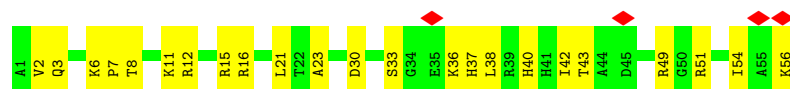
- Molecule 22: 50S ribosomal protein L30



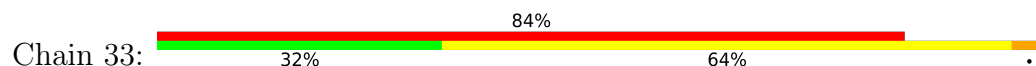
- Molecule 23: Large ribosomal subunit protein bL31



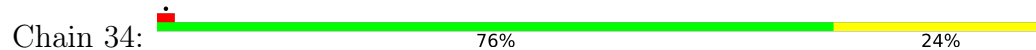
- Molecule 24: 50S ribosomal protein L32



- Molecule 25: Large ribosomal subunit protein bL33



- Molecule 26: 50S ribosomal protein L34

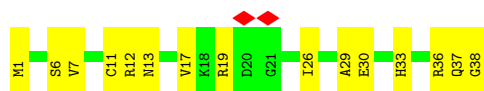


- Molecule 27: Large ribosomal subunit protein bL35

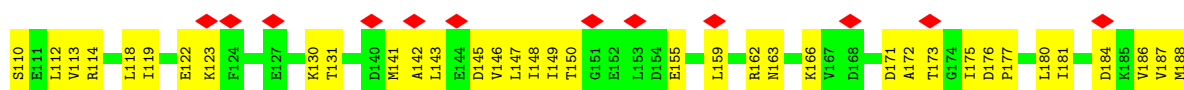




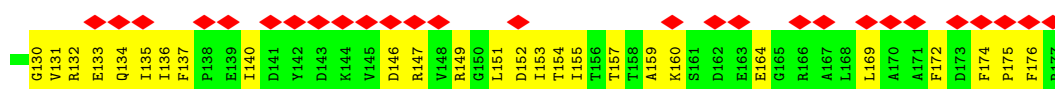
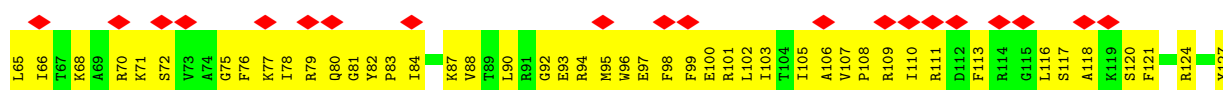
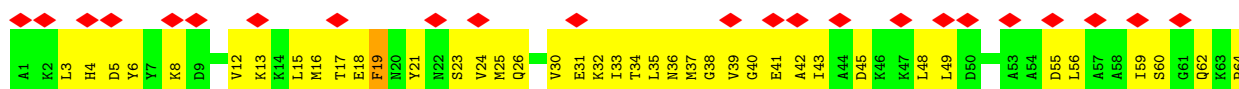
- Molecule 28: 50S ribosomal protein L36



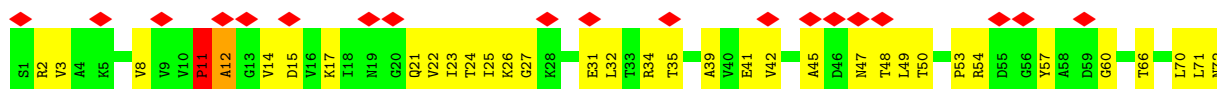
- Molecule 29: Large ribosomal subunit protein uL4

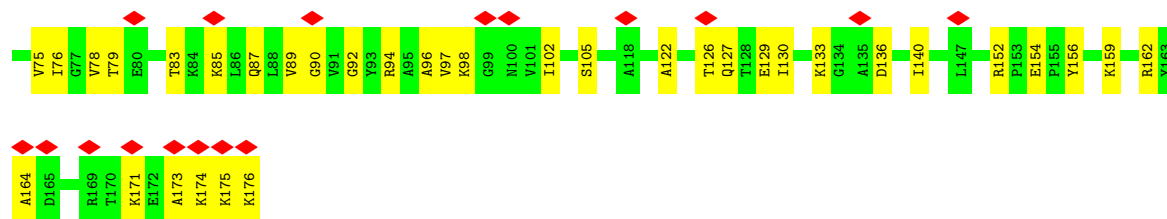


- Molecule 30: 50S ribosomal protein L5

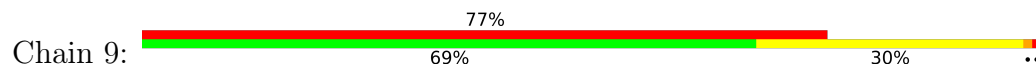


- Molecule 31: Large ribosomal subunit protein uL6

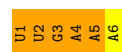




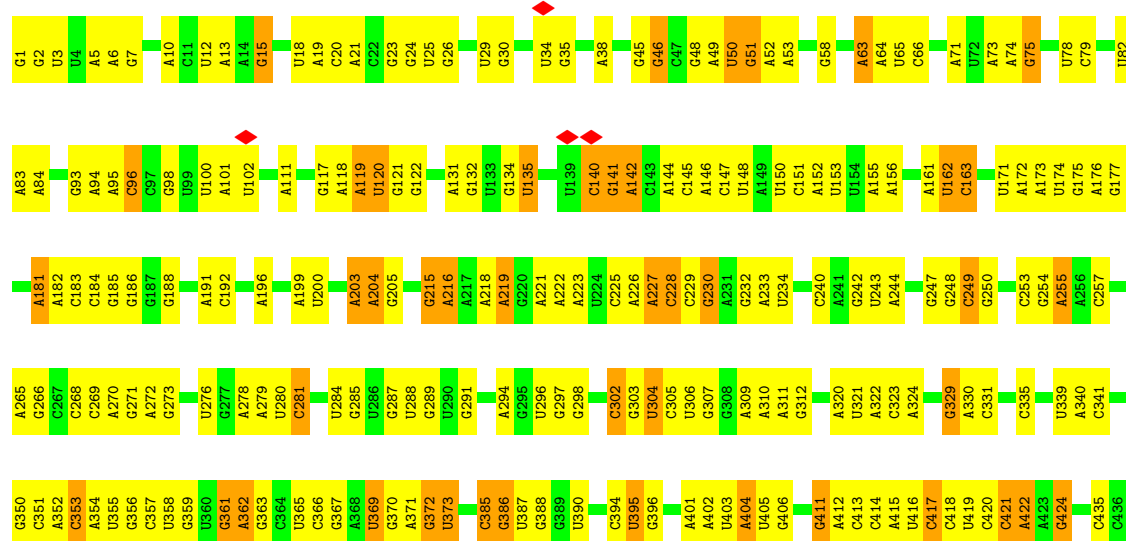
• Molecule 32: Large ribosomal subunit protein bL9



• Molecule 33: mRNA

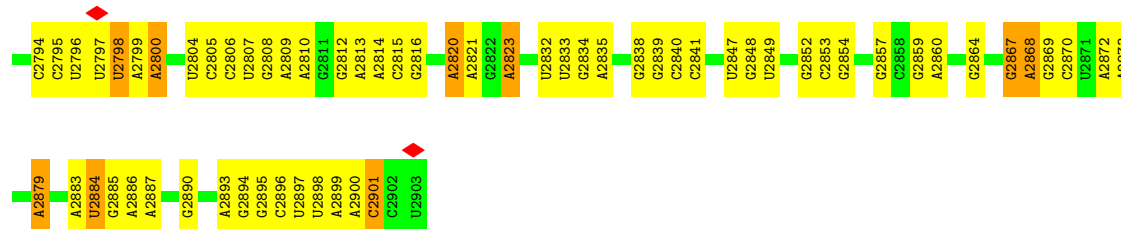


• Molecule 34: 23S ribosomal RNA

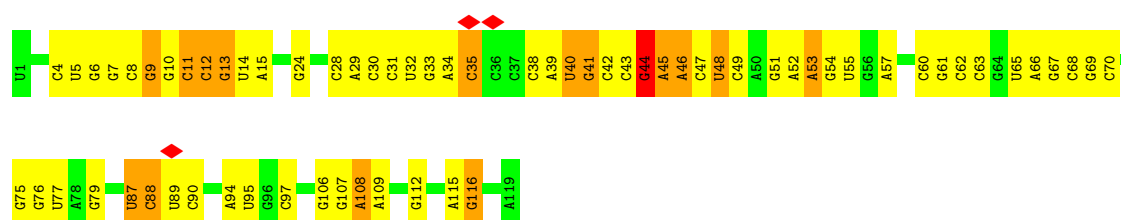




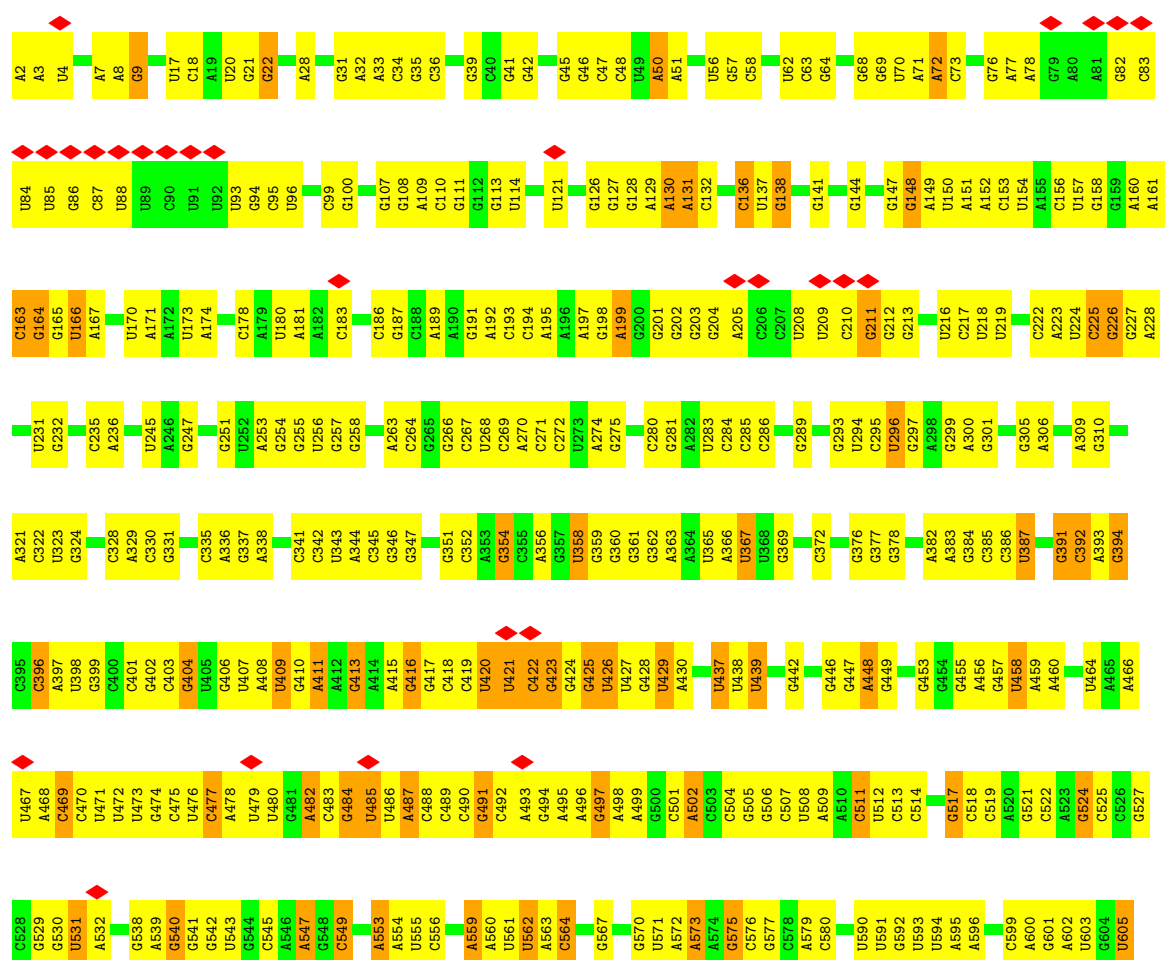
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• Molecule 35: 5S ribosomal RNA



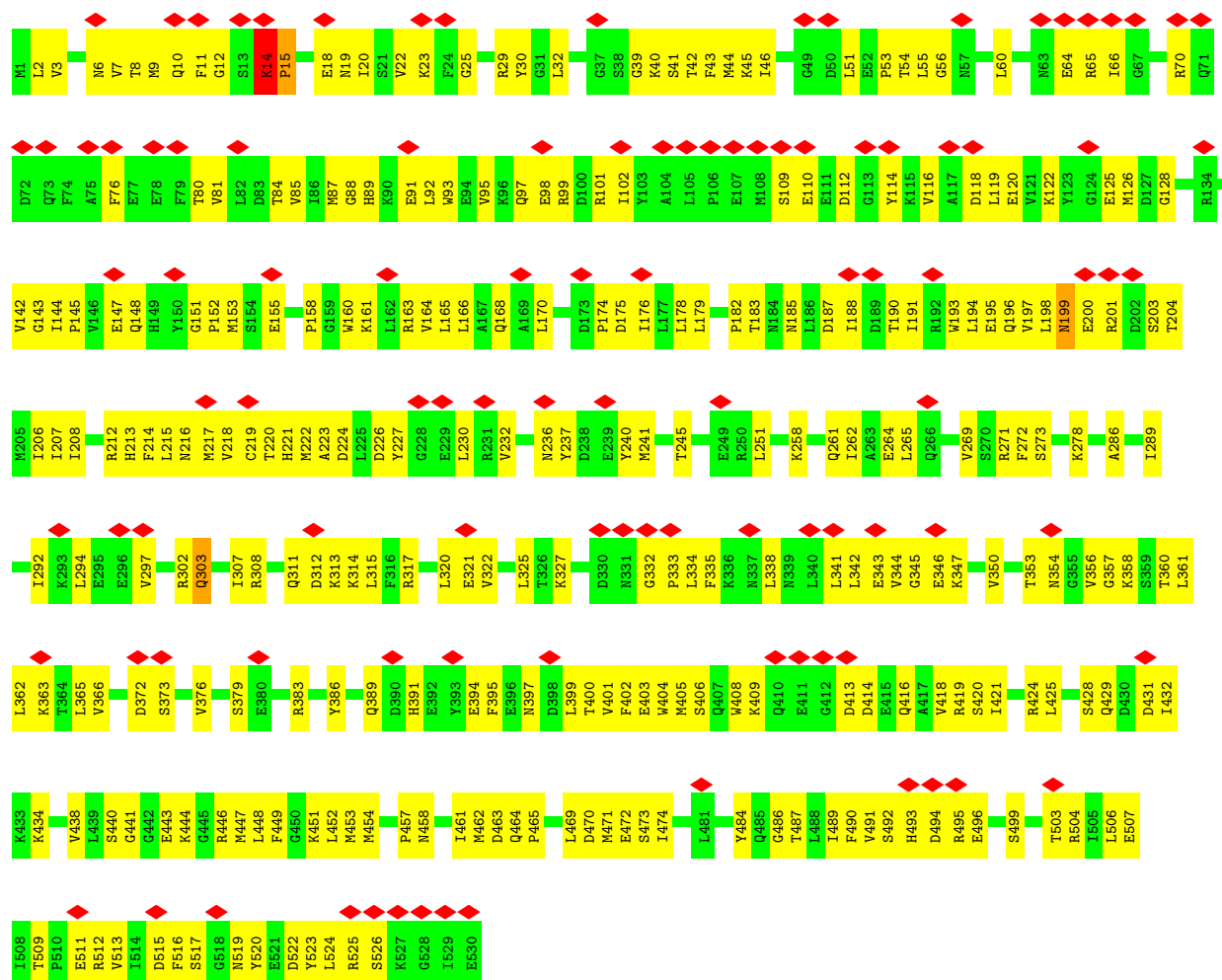
• Molecule 36: 16S ribosomal RNA



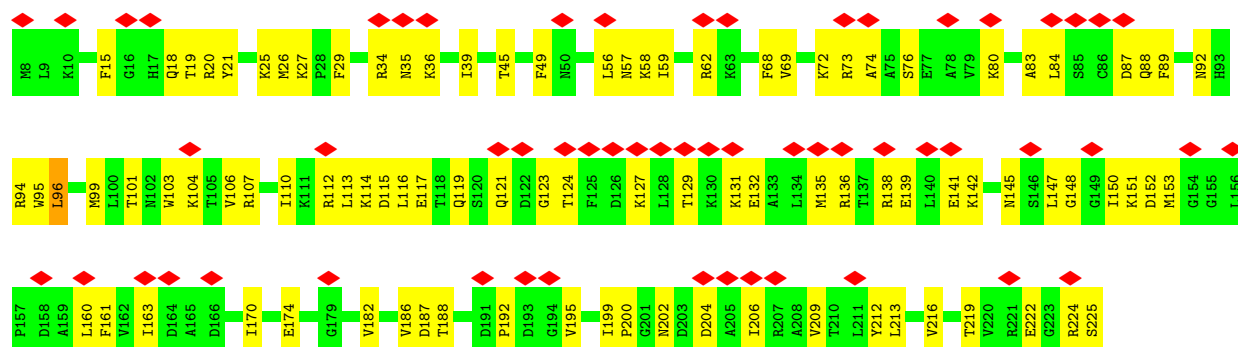




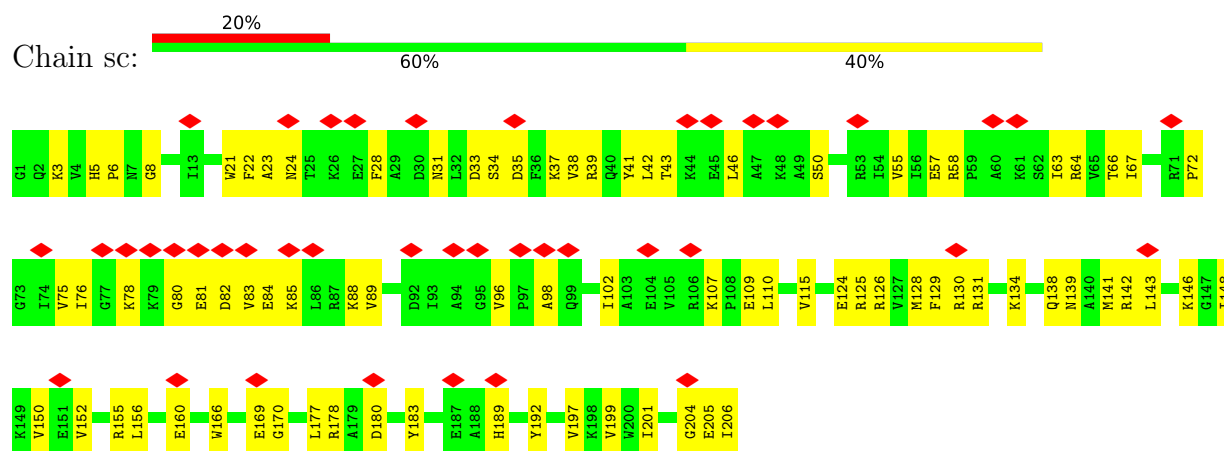
• Molecule 38: Probable ATP-binding protein YbiT



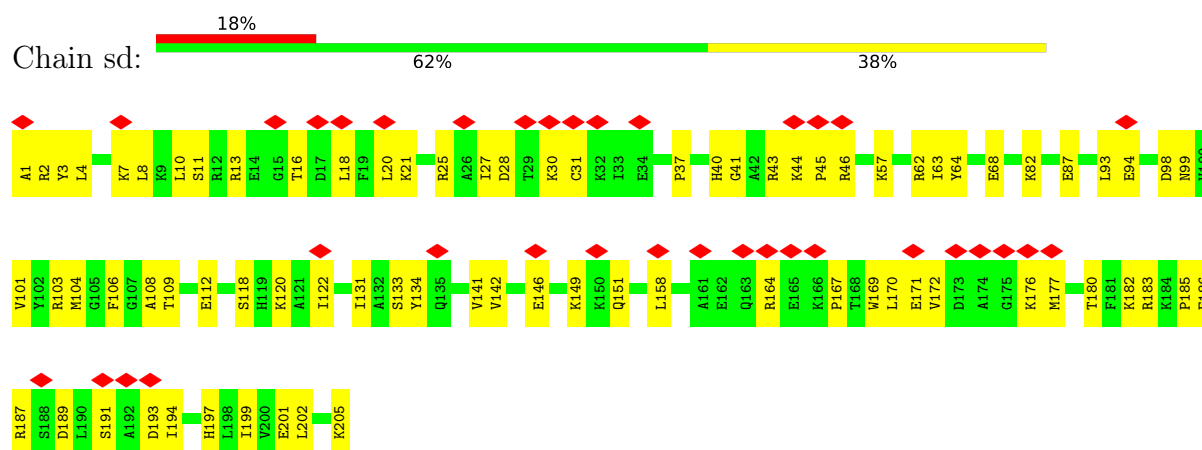
• Molecule 39: Small ribosomal subunit protein uS2



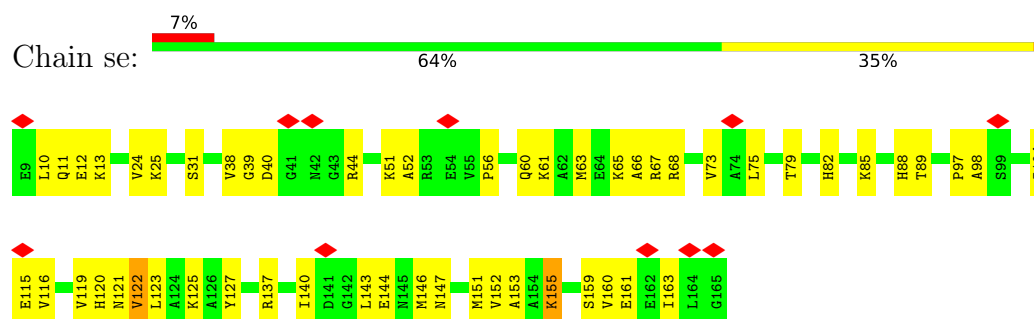
- Molecule 40: Small ribosomal subunit protein uS3



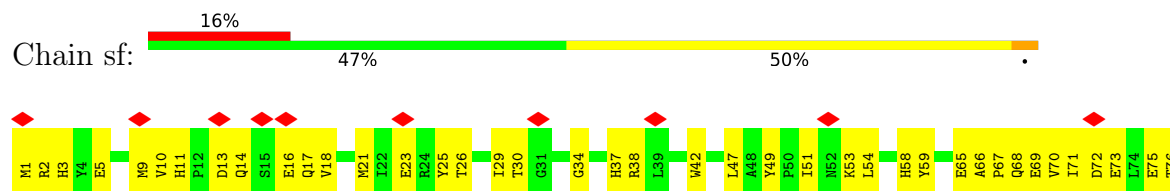
- Molecule 41: 30S ribosomal protein S4

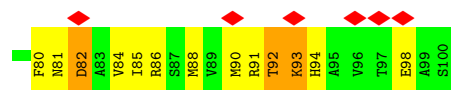


- Molecule 42: Small ribosomal subunit protein uS5

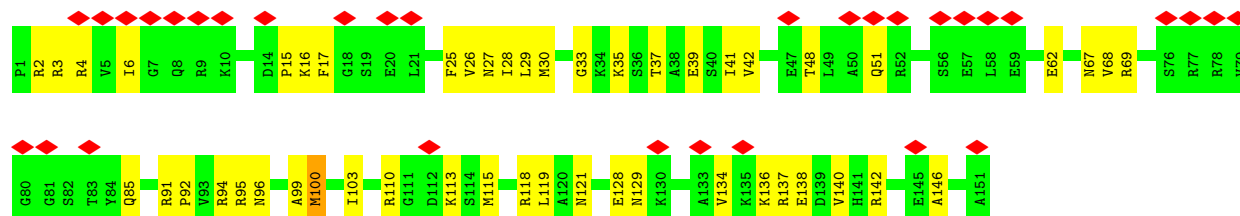


- Molecule 43: 30S ribosomal protein S6, non-modified isoform

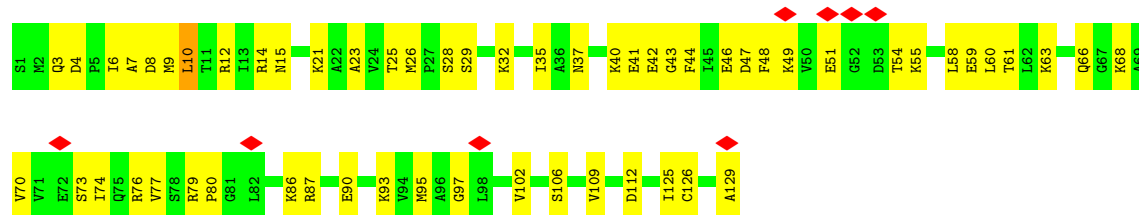




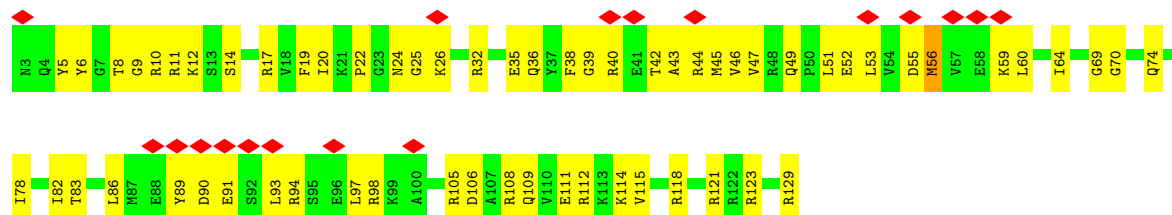
- Molecule 44: 30S ribosomal protein S7



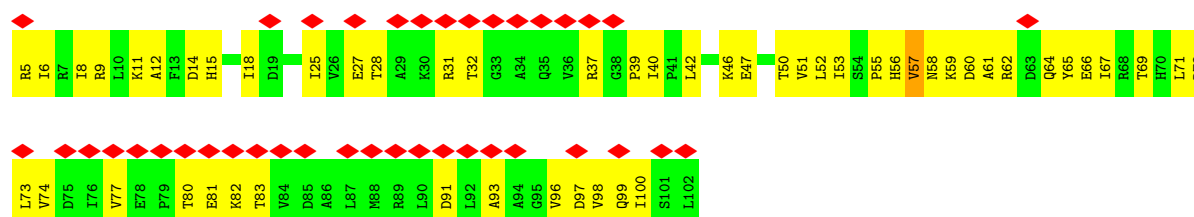
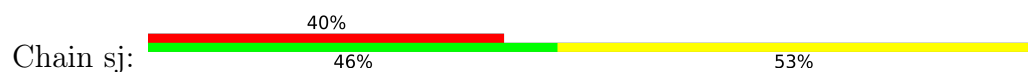
- Molecule 45: 30S ribosomal protein S8



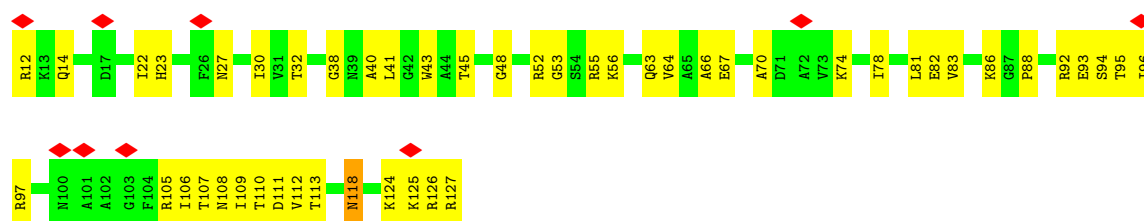
- Molecule 46: Small ribosomal subunit protein uS9



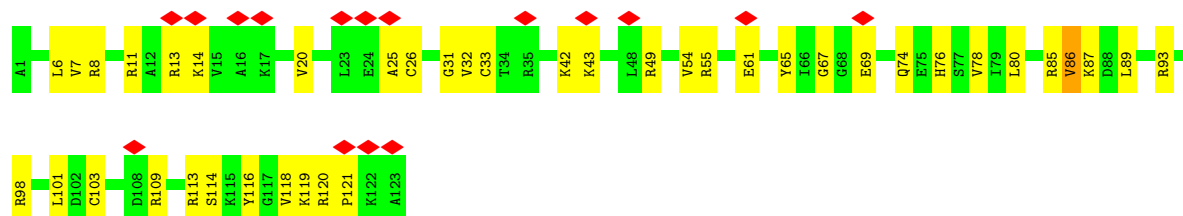
- Molecule 47: 30S ribosomal protein S10



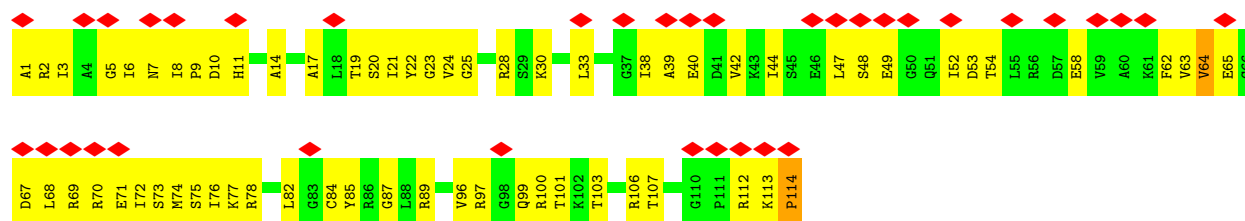
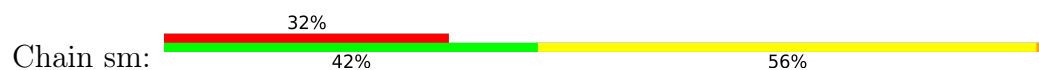
- Molecule 48: Small ribosomal subunit protein uS11



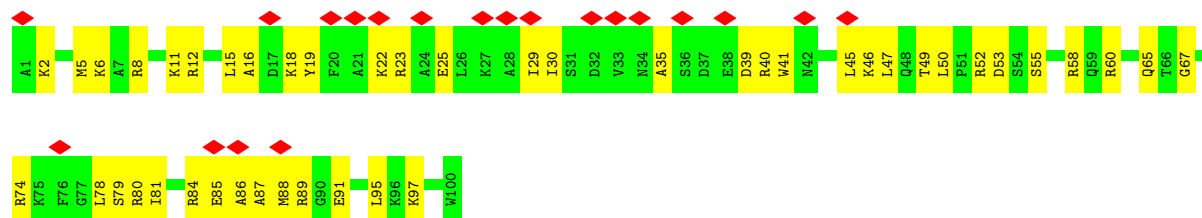
• Molecule 49: Small ribosomal subunit protein uS12



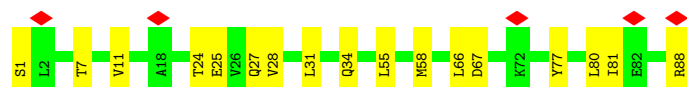
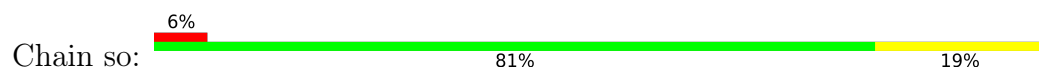
• Molecule 50: 30S ribosomal protein S13



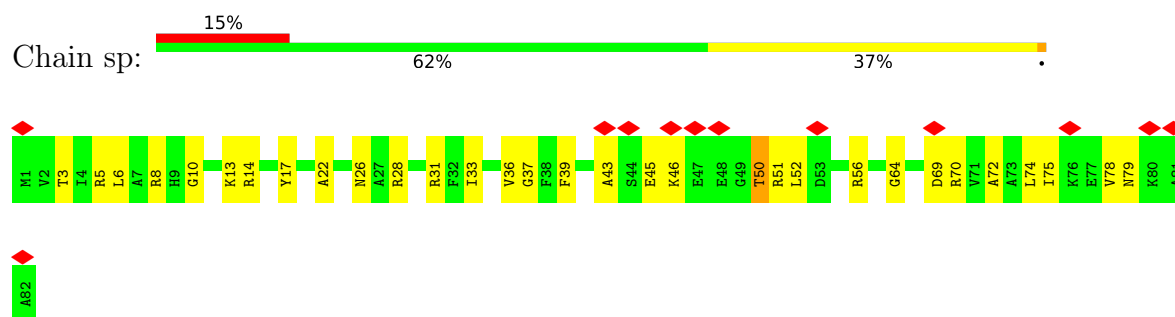
• Molecule 51: Small ribosomal subunit protein uS14



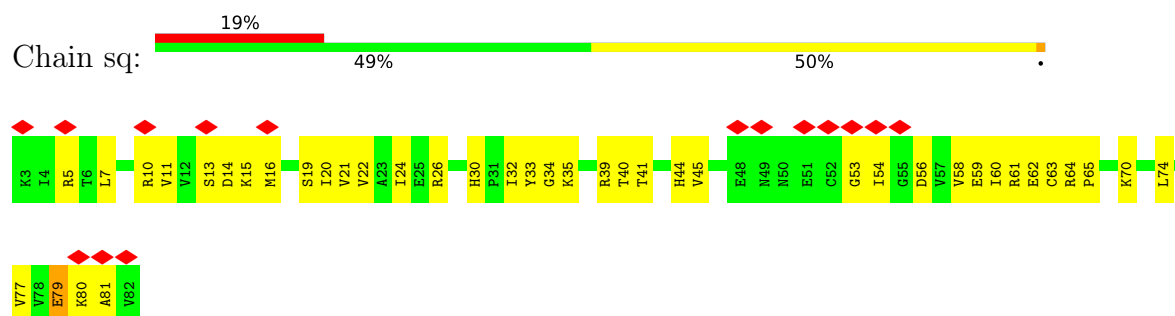
• Molecule 52: Small ribosomal subunit protein uS15



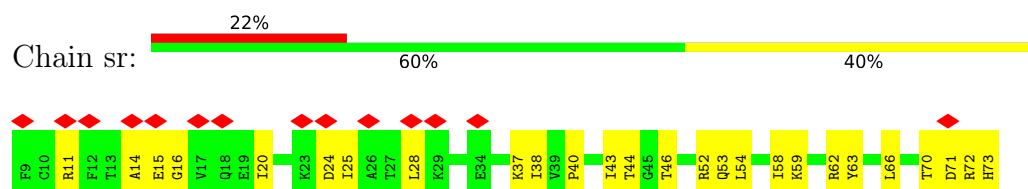
- Molecule 53: Small ribosomal subunit protein bS16



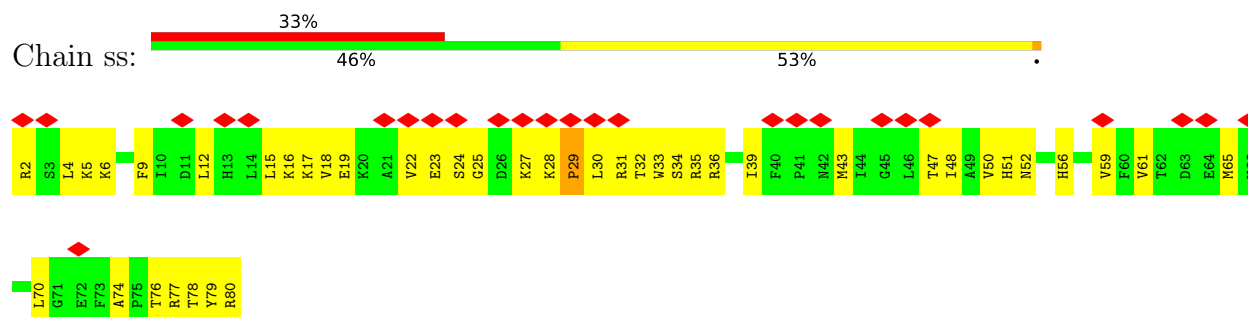
- Molecule 54: Small ribosomal subunit protein uS17



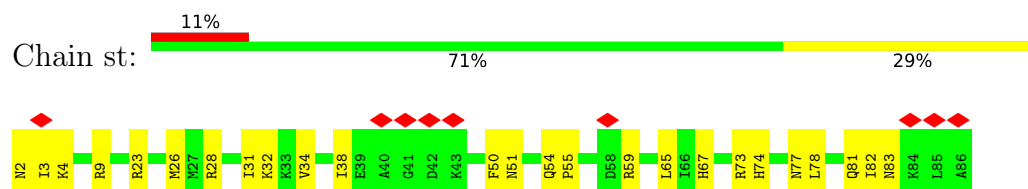
- Molecule 55: 30S ribosomal protein S18



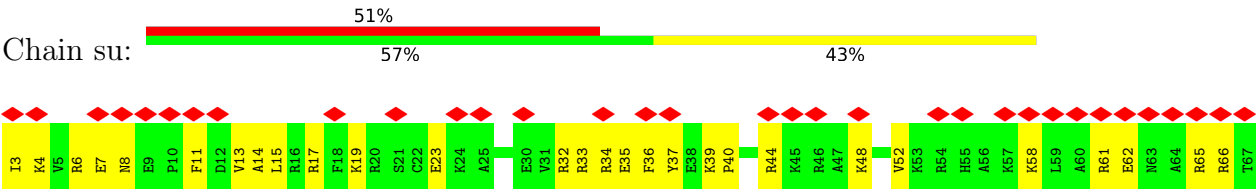
- Molecule 56: 30S ribosomal protein S19



- Molecule 57: 30S ribosomal protein S20



- Molecule 58: Small ribosomal subunit protein bS21



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23587	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.483	Depositor
Minimum map value	-0.984	Depositor
Average map value	0.035	Depositor
Map value standard deviation	0.163	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	335.04, 335.04, 335.04	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.047, 1.047, 1.047	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.15	0/1361	0.39	0/1796
2	10	0.37	1/1001 (0.1%)	0.72	0/1350
3	11	0.94	8/1046 (0.8%)	1.65	22/1410 (1.6%)
4	13	0.24	0/1152	0.34	0/1551
5	14	0.22	0/947	0.40	0/1268
6	15	0.23	0/1054	0.40	0/1403
7	16	0.27	0/1093	0.45	0/1460
8	17	0.28	0/973	0.49	0/1301
9	18	0.21	0/901	0.40	0/1206
10	19	0.21	0/929	0.40	0/1242
11	2	0.24	0/2121	0.40	0/2852
12	20	0.31	0/960	0.42	0/1278
13	21	0.27	0/829	0.54	1/1107 (0.1%)
14	22	0.22	0/864	0.47	0/1156
15	23	0.23	0/744	0.45	0/994
16	24	0.22	0/787	0.39	0/1051
17	25	0.22	0/766	0.41	0/1025
18	27	0.26	0/582	0.39	0/769
19	28	0.23	0/635	0.36	0/848
20	29	0.24	0/510	0.47	0/677
21	3	0.22	0/1586	0.39	0/2134
22	30	0.31	0/453	0.52	0/605
23	31	3.36	8/531 (1.5%)	1.96	14/709 (2.0%)
24	32	0.20	0/450	0.36	0/599
25	33	3.03	6/416 (1.4%)	0.87	1/554 (0.2%)
26	34	0.21	0/380	0.40	0/498
27	35	0.21	0/513	0.42	0/676
28	36	0.24	0/303	0.35	0/397
29	4	0.21	0/1571	0.40	0/2113
30	5	0.35	0/1434	0.58	0/1926
31	6	0.40	2/1343 (0.1%)	0.69	3/1816 (0.2%)
32	9	0.18	0/1122	0.53	1/1515 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	M	0.22	0/138	0.46	0/211
34	R1	0.27	7/69797 (0.0%)	0.35	18/108890 (0.0%)
35	R2	1.11	6/2847 (0.2%)	0.35	0/4440
36	R3	0.54	18/36940 (0.0%)	0.31	1/57624 (0.0%)
37	T	0.19	0/1812	0.34	0/2824
38	Y	0.23	0/4285	0.48	0/5774
39	sb	0.18	0/1735	0.47	0/2338
40	sc	0.22	0/1651	0.40	0/2225
41	sd	0.21	0/1665	0.43	0/2227
42	se	0.36	1/1169 (0.1%)	0.58	1/1573 (0.1%)
43	sf	0.32	0/835	0.66	0/1128
44	sg	0.27	1/1195 (0.1%)	0.42	0/1602
45	sh	0.26	0/989	0.49	0/1326
46	si	0.20	0/1034	0.47	0/1375
47	sj	0.21	0/796	0.44	0/1077
48	sk	0.30	1/885 (0.1%)	0.46	0/1195
49	sl	0.24	0/969	0.51	0/1300
50	sm	0.51	2/892 (0.2%)	1.00	4/1193 (0.3%)
51	sn	0.19	0/817	0.46	0/1088
52	so	0.18	0/722	0.38	0/964
53	sp	0.18	0/659	0.41	0/884
54	sq	0.26	0/657	0.38	0/881
55	sr	0.19	0/544	0.34	0/731
56	ss	0.87	3/652 (0.5%)	1.01	4/877 (0.5%)
57	st	0.25	0/671	0.41	0/888
58	su	0.21	0/550	0.61	0/728
All	All	0.45	64/164263 (0.0%)	0.42	70/244649 (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
2	10	0	4
3	11	0	5
7	16	0	1
23	31	0	3
25	33	0	1
31	6	0	1
32	9	0	1
38	Y	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
43	sf	0	2
46	si	0	1
49	sl	0	1
51	sn	0	1
58	su	0	2
All	All	0	24

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	31	61	ASN	CA-CB	42.20	2.28	1.53
23	31	65	ASN	CA-CB	40.42	2.18	1.53
23	31	3	LYS	CA-C	32.79	1.96	1.52
25	33	38	PHE	CE2-CZ	30.47	2.30	1.38
36	R3	1268	G	C2-N3	28.51	1.89	1.32

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	11	55	PRO	CB-CG-CD	23.08	179.94	106.10
34	R1	2290	G	C8-N9-C4	-22.40	39.20	106.40
23	31	58	ASP	CA-C-N	21.83	163.64	122.60
23	31	58	ASP	C-N-CA	21.83	163.64	122.60
3	11	55	PRO	CA-CB-CG	-20.87	64.85	104.50

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	10	106	PHE	Peptide
2	10	118	ILE	Peptide
2	10	12	VAL	Peptide
2	10	64	VAL	Peptide
3	11	16	MET	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	1353	0	1159	67	0
2	10	988	0	1025	162	0
3	11	1032	0	1088	264	0
4	13	1129	0	1162	46	0
5	14	938	0	1012	35	0
6	15	1045	0	1117	48	0
7	16	1074	0	1157	48	0
8	17	960	0	1000	43	0
9	18	892	0	922	41	0
10	19	917	0	965	35	0
11	2	2082	0	2157	84	0
12	20	947	0	1022	65	0
13	21	816	0	839	33	0
14	22	857	0	922	38	0
15	23	738	0	807	40	0
16	24	779	0	834	35	0
17	25	753	0	780	37	0
18	27	575	0	592	26	0
19	28	625	0	655	21	0
20	29	509	0	543	27	0
21	3	1565	0	1616	55	0
22	30	449	0	491	33	0
23	31	522	0	524	299	0
24	32	444	0	461	25	0
25	33	409	0	440	172	0
26	34	377	0	418	12	0
27	35	504	0	574	23	0
28	36	302	0	340	17	0
29	4	1552	0	1619	61	0
30	5	1410	0	1447	172	0
31	6	1323	0	1374	62	0
32	9	1111	0	1148	40	0
33	M	123	0	65	7	0
34	R1	62318	0	31344	1596	0
35	R2	2546	0	1292	128	0
36	R3	32992	0	16608	939	0
37	T	1621	0	825	53	0
38	Y	4210	0	4172	243	0
39	sb	1704	0	1732	79	0
40	sc	1624	0	1699	67	0
41	sd	1643	0	1710	84	0
42	se	1156	0	1199	51	0
43	sf	817	0	808	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	sg	1181	0	1240	51	0
45	sh	979	0	1034	67	0
46	si	1022	0	1070	60	0
47	sj	786	0	828	51	0
48	sk	869	0	878	52	0
49	sl	955	0	1019	51	0
50	sm	883	0	944	93	0
51	sn	805	0	847	47	0
52	so	714	0	737	13	0
53	sp	649	0	666	29	0
54	sq	648	0	691	47	0
55	sr	535	0	552	25	0
56	ss	637	0	665	37	0
57	st	665	0	714	30	0
58	su	544	0	579	36	0
59	18	1	0	0	0	0
59	32	1	0	0	0	0
59	33	1	0	0	0	0
59	R1	92	0	0	0	0
59	R2	2	0	0	0	0
59	R3	27	0	0	0	0
60	36	1	0	0	0	0
61	Y	62	0	22	5	0
62	Y	2	0	0	0	0
All	All	151792	0	104150	4944	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 20.

The worst 5 of 4944 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)
25:33:38:PHE:CD2	25:33:38:PHE:CG	1.78	1.69
35:R2:44:G:C5	35:R2:44:G:C6	1.80	1.68
25:33:38:PHE:CG	25:33:38:PHE:CD1	1.77	1.66
36:R3:1310:G:C5	36:R3:1310:G:C6	1.80	1.61
36:R3:1311:A:C5	36:R3:1311:A:C6	1.86	1.60

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1	218/220 (99%)	203 (93%)	14 (6%)	1 (0%)	24	54
2	10	129/131 (98%)	89 (69%)	40 (31%)	0	100	100
3	11	139/141 (99%)	103 (74%)	34 (24%)	2 (1%)	9	31
4	13	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
5	14	120/123 (98%)	104 (87%)	16 (13%)	0	100	100
6	15	141/143 (99%)	126 (89%)	15 (11%)	0	100	100
7	16	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
8	17	118/120 (98%)	105 (89%)	13 (11%)	0	100	100
9	18	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
10	19	112/114 (98%)	101 (90%)	11 (10%)	0	100	100
11	2	269/271 (99%)	245 (91%)	24 (9%)	0	100	100
12	20	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
13	21	101/103 (98%)	89 (88%)	12 (12%)	0	100	100
14	22	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
15	23	91/93 (98%)	78 (86%)	13 (14%)	0	100	100
16	24	100/102 (98%)	84 (84%)	16 (16%)	0	100	100
17	25	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
18	27	73/75 (97%)	63 (86%)	9 (12%)	1 (1%)	9	31
19	28	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
20	29	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
21	3	207/209 (99%)	193 (93%)	14 (7%)	0	100	100
22	30	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
23	31	64/66 (97%)	46 (72%)	17 (27%)	1 (2%)	7	29
24	32	54/56 (96%)	49 (91%)	5 (9%)	0	100	100
25	33	48/50 (96%)	34 (71%)	14 (29%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	34	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
27	35	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
28	36	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
29	4	199/201 (99%)	185 (93%)	14 (7%)	0	100	100
30	5	175/177 (99%)	153 (87%)	22 (13%)	0	100	100
31	6	174/176 (99%)	158 (91%)	15 (9%)	1 (1%)	21	50
32	9	147/149 (99%)	133 (90%)	13 (9%)	1 (1%)	18	47
38	Y	528/530 (100%)	482 (91%)	42 (8%)	4 (1%)	16	44
39	sb	216/218 (99%)	200 (93%)	16 (7%)	0	100	100
40	sc	204/206 (99%)	194 (95%)	10 (5%)	0	100	100
41	sd	203/205 (99%)	181 (89%)	22 (11%)	0	100	100
42	se	155/157 (99%)	131 (84%)	23 (15%)	1 (1%)	21	50
43	sf	98/100 (98%)	79 (81%)	19 (19%)	0	100	100
44	sg	149/151 (99%)	137 (92%)	12 (8%)	0	100	100
45	sh	127/129 (98%)	114 (90%)	13 (10%)	0	100	100
46	si	125/127 (98%)	102 (82%)	22 (18%)	1 (1%)	16	44
47	sj	96/98 (98%)	88 (92%)	7 (7%)	1 (1%)	12	40
48	sk	114/116 (98%)	102 (90%)	12 (10%)	0	100	100
49	sl	121/123 (98%)	91 (75%)	30 (25%)	0	100	100
50	sm	112/114 (98%)	95 (85%)	17 (15%)	0	100	100
51	sn	98/100 (98%)	77 (79%)	21 (21%)	0	100	100
52	so	86/88 (98%)	81 (94%)	5 (6%)	0	100	100
53	sp	80/82 (98%)	67 (84%)	13 (16%)	0	100	100
54	sq	78/80 (98%)	67 (86%)	11 (14%)	0	100	100
55	sr	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
56	ss	77/79 (98%)	68 (88%)	9 (12%)	0	100	100
57	st	83/85 (98%)	81 (98%)	2 (2%)	0	100	100
58	su	63/65 (97%)	42 (67%)	20 (32%)	1 (2%)	7	29
All	All	6591/6699 (98%)	5858 (89%)	718 (11%)	15 (0%)	44	71

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	118	PRO
3	11	19	PRO
3	11	52	LEU
38	Y	15	PRO
46	si	90	ASP

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	1	106/171 (62%)	105 (99%)	1 (1%)	70	76
2	10	100/100 (100%)	100 (100%)	0	100	100
3	11	109/109 (100%)	109 (100%)	0	100	100
4	13	116/116 (100%)	115 (99%)	1 (1%)	70	76
5	14	103/104 (99%)	102 (99%)	1 (1%)	68	75
6	15	102/102 (100%)	102 (100%)	0	100	100
7	16	109/109 (100%)	109 (100%)	0	100	100
8	17	100/100 (100%)	99 (99%)	1 (1%)	68	75
9	18	86/86 (100%)	86 (100%)	0	100	100
10	19	99/99 (100%)	99 (100%)	0	100	100
11	2	216/216 (100%)	216 (100%)	0	100	100
12	20	89/89 (100%)	87 (98%)	2 (2%)	45	63
13	21	84/84 (100%)	83 (99%)	1 (1%)	63	72
14	22	93/93 (100%)	92 (99%)	1 (1%)	65	74
15	23	80/80 (100%)	80 (100%)	0	100	100
16	24	83/83 (100%)	83 (100%)	0	100	100
17	25	78/78 (100%)	77 (99%)	1 (1%)	61	71
18	27	57/57 (100%)	56 (98%)	1 (2%)	51	67
19	28	67/67 (100%)	65 (97%)	2 (3%)	36	59
20	29	55/55 (100%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	3	164/164 (100%)	162 (99%)	2 (1%)	63	72
22	30	48/48 (100%)	48 (100%)	0	100	100
23	31	59/59 (100%)	59 (100%)	0	100	100
24	32	47/47 (100%)	47 (100%)	0	100	100
25	33	45/45 (100%)	45 (100%)	0	100	100
26	34	38/38 (100%)	38 (100%)	0	100	100
27	35	51/51 (100%)	51 (100%)	0	100	100
28	36	34/34 (100%)	34 (100%)	0	100	100
29	4	165/165 (100%)	164 (99%)	1 (1%)	78	80
30	5	148/148 (100%)	147 (99%)	1 (1%)	76	78
31	6	137/137 (100%)	135 (98%)	2 (2%)	57	69
32	9	114/114 (100%)	114 (100%)	0	100	100
38	Y	456/456 (100%)	453 (99%)	3 (1%)	76	78
39	sb	180/180 (100%)	178 (99%)	2 (1%)	65	74
40	sc	170/170 (100%)	170 (100%)	0	100	100
41	sd	172/172 (100%)	172 (100%)	0	100	100
42	se	119/119 (100%)	119 (100%)	0	100	100
43	sf	87/87 (100%)	86 (99%)	1 (1%)	65	74
44	sg	124/124 (100%)	124 (100%)	0	100	100
45	sh	104/104 (100%)	103 (99%)	1 (1%)	68	75
46	si	105/105 (100%)	103 (98%)	2 (2%)	50	66
47	sj	86/86 (100%)	86 (100%)	0	100	100
48	sk	89/89 (100%)	89 (100%)	0	100	100
49	sl	103/103 (100%)	103 (100%)	0	100	100
50	sm	92/92 (100%)	90 (98%)	2 (2%)	45	63
51	sn	83/83 (100%)	82 (99%)	1 (1%)	63	72
52	so	76/76 (100%)	76 (100%)	0	100	100
53	sp	65/65 (100%)	63 (97%)	2 (3%)	35	59
54	sq	74/74 (100%)	73 (99%)	1 (1%)	59	70
55	sr	56/56 (100%)	56 (100%)	0	100	100
56	ss	70/70 (100%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	st	65/65 (100%)	65 (100%)	0	100	100
58	su	55/55 (100%)	55 (100%)	0	100	100
All	All	5413/5479 (99%)	5380 (99%)	33 (1%)	76	80

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	sm	103	THR
51	sn	39	ASP
54	sq	79	GLU
21	3	70	LYS
19	28	19	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
24	32	5	ASN
46	si	74	GLN
32	9	11	ASN
44	sg	147	ASN
57	st	54	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
33	M	6/6 (100%)	4 (66%)	1 (16%)
34	R1	2902/2903 (99%)	542 (18%)	11 (0%)
35	R2	118/119 (99%)	20 (16%)	2 (1%)
36	R3	1536/1538 (99%)	320 (20%)	3 (0%)
37	T	75/76 (98%)	27 (36%)	1 (1%)
All	All	4637/4642 (99%)	913 (19%)	18 (0%)

5 of 913 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
33	M	2	U
33	M	3	G
33	M	4	A
33	M	5	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	R1	10	A

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	R3	391	G
37	T	21	A
36	R3	1297	G
34	R1	1130	U
35	R2	87	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 129 ligands modelled in this entry, 127 are monoatomic - leaving 2 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	$\# Z > 2$
61	ATP	Y	602	62	32,33,33	0.41	0	48,52,52	0.35	0
61	ATP	Y	601	62	32,33,33	0.43	0	48,52,52	0.42	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
61	ATP	Y	602	62	-	8/22/38/38	0/3/3/3
61	ATP	Y	601	62	-	7/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

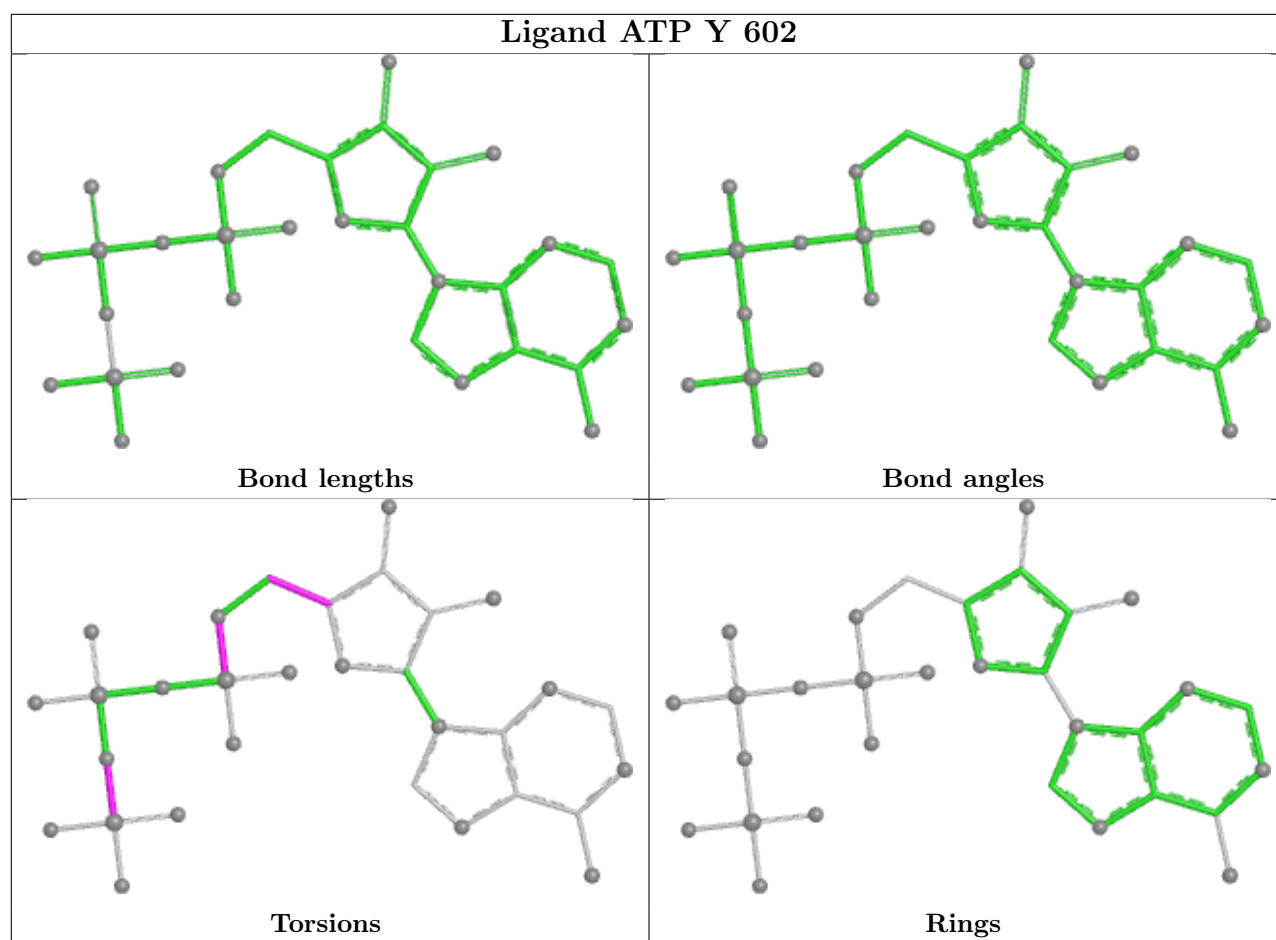
Mol	Chain	Res	Type	Atoms
61	Y	602	ATP	PB-O3B-PG-O2G
61	Y	602	ATP	C5'-O5'-PA-O1A
61	Y	602	ATP	C5'-O5'-PA-O2A
61	Y	602	ATP	C5'-O5'-PA-O3A
61	Y	602	ATP	O4'-C4'-C5'-O5'

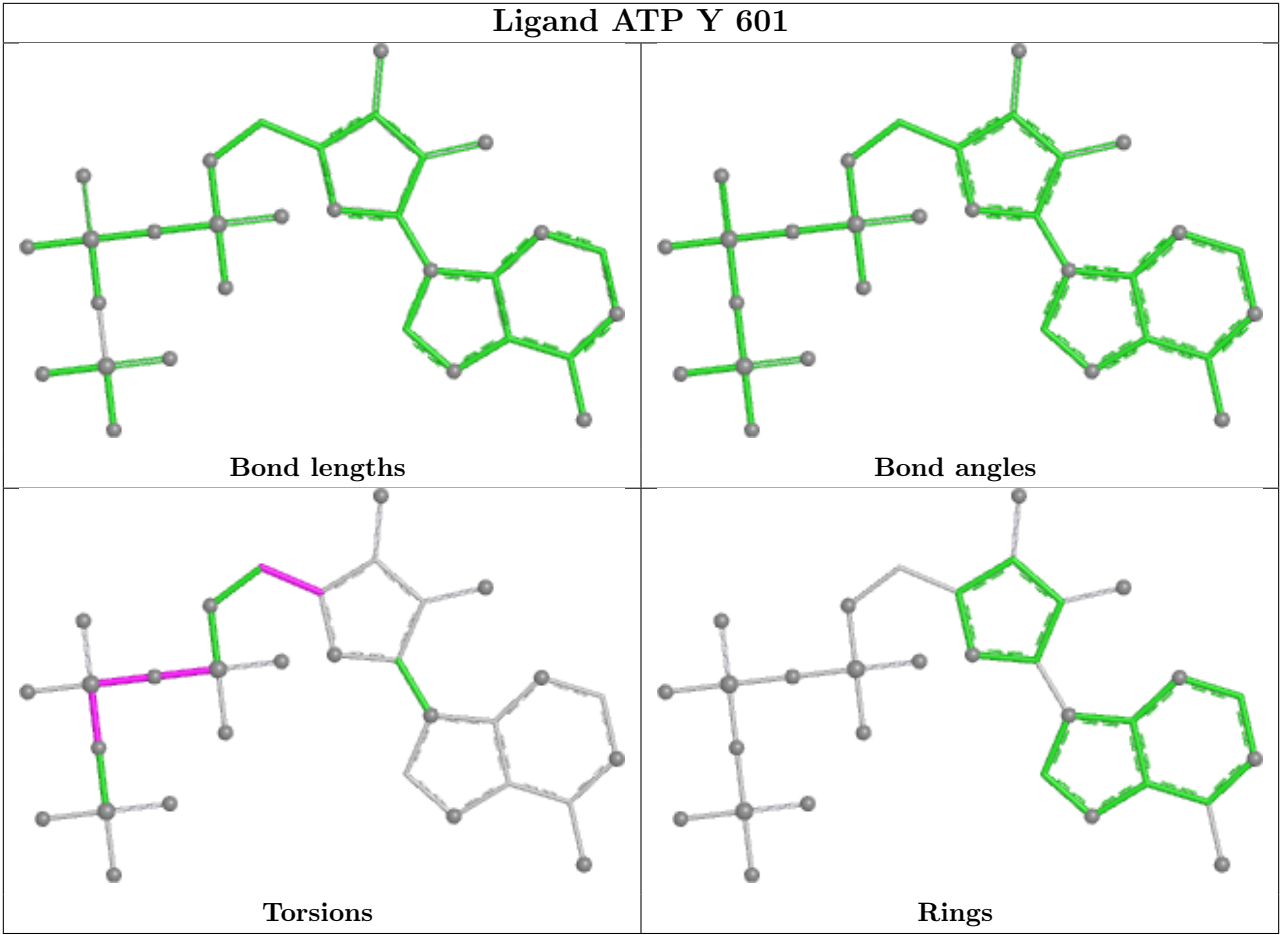
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	Y	602	ATP	2	0
61	Y	601	ATP	3	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
36	R3	1
9	18	1
23	31	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R3	1301:U	O3'	1303:C	P	5.76
1	18	2:ASP	C	3:LYS	N	3.13
1	31	58:ASP	C	59:ARG	N	1.67

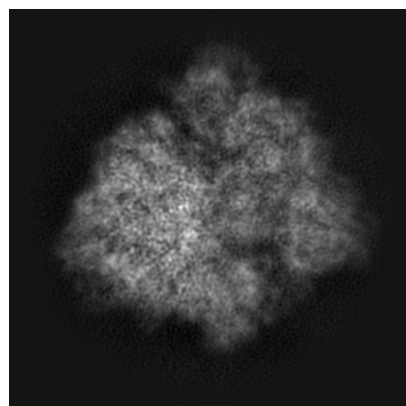
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40923. These allow visual inspection of the internal detail of the map and identification of artifacts.

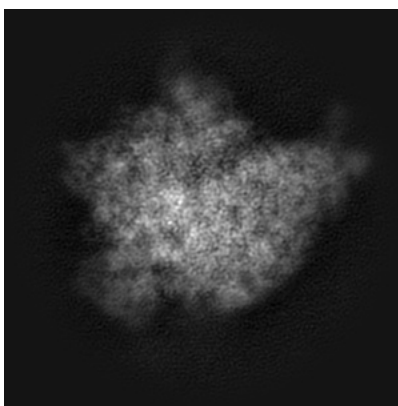
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

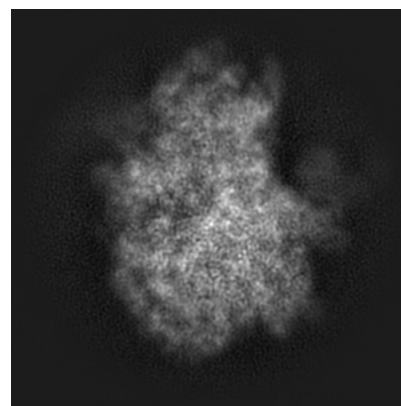
6.1.1 Primary map



X

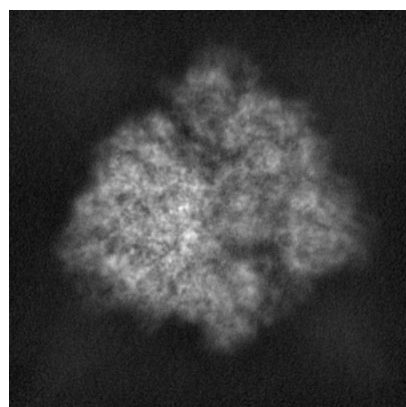


Y

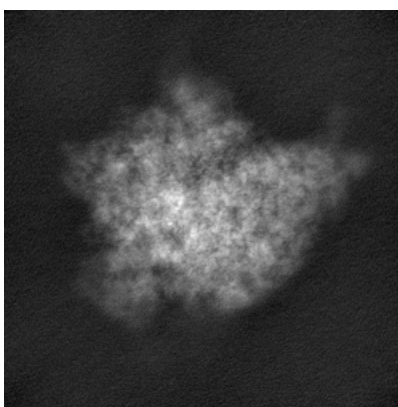


Z

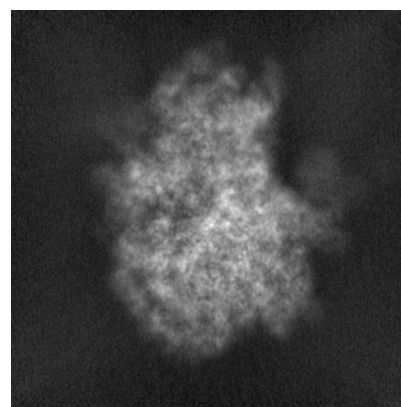
6.1.2 Raw map



X



Y

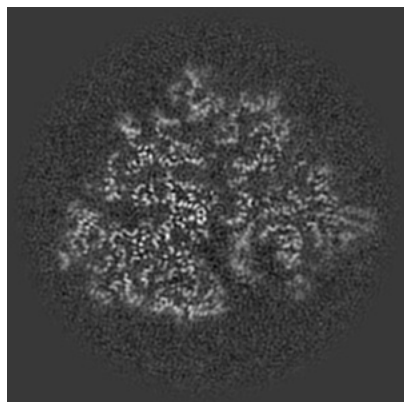


Z

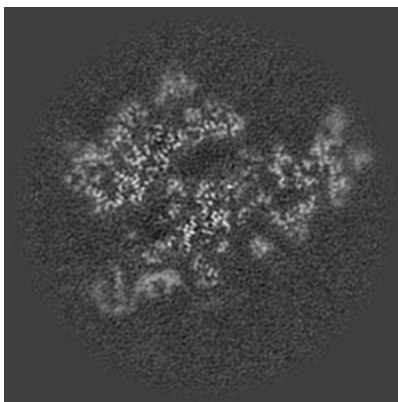
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

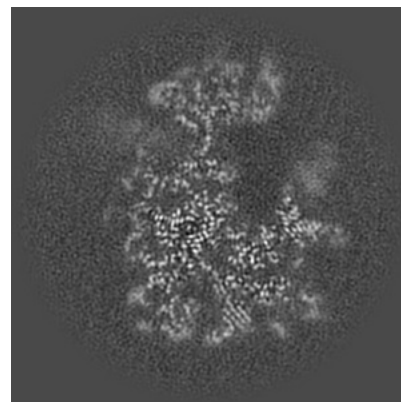
6.2.1 Primary map



X Index: 160

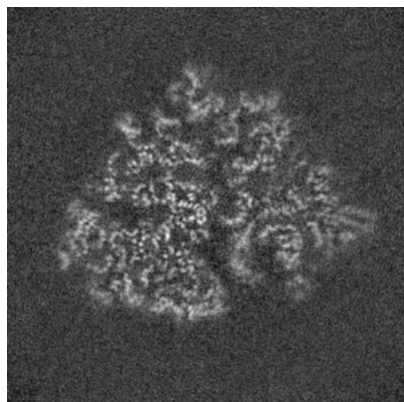


Y Index: 160

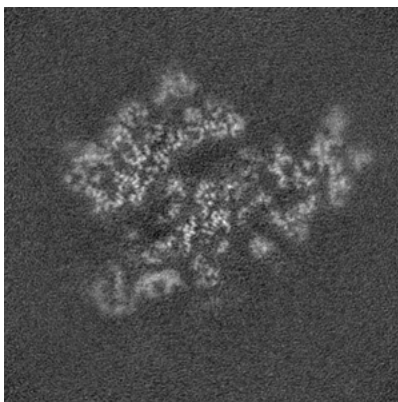


Z Index: 160

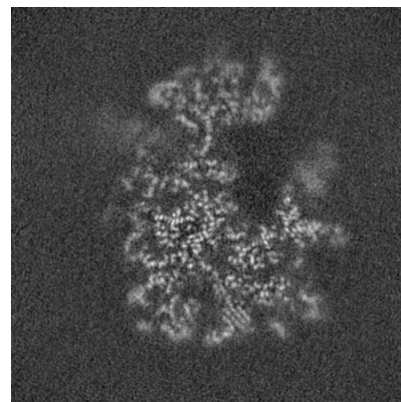
6.2.2 Raw map



X Index: 160



Y Index: 160

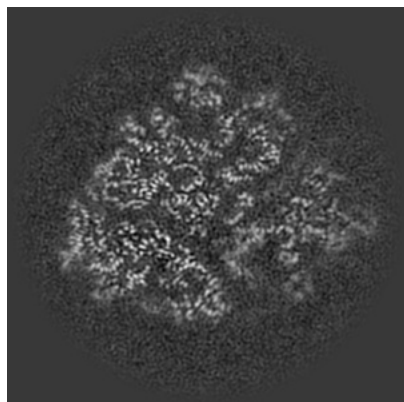


Z Index: 160

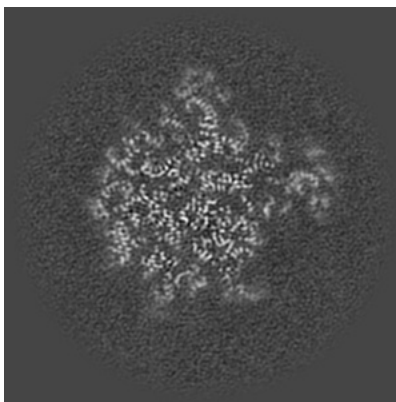
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

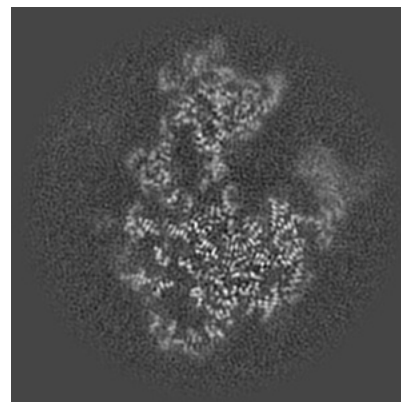
6.3.1 Primary map



X Index: 164

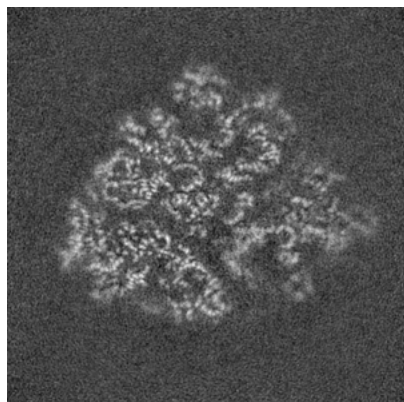


Y Index: 137

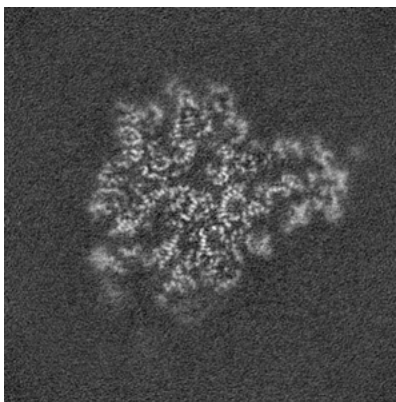


Z Index: 140

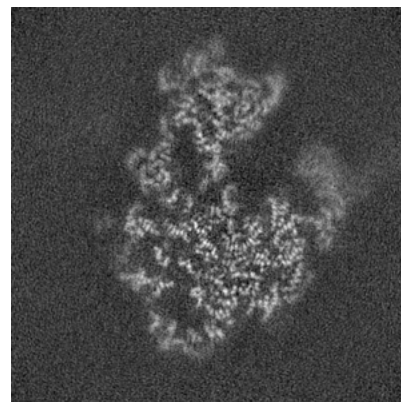
6.3.2 Raw map



X Index: 164



Y Index: 148

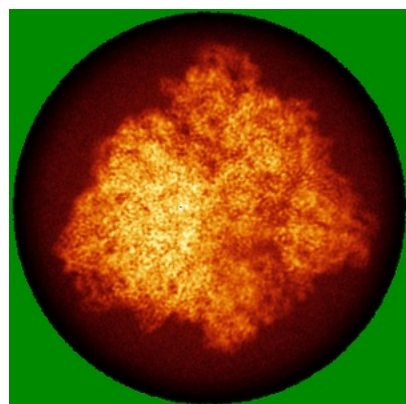


Z Index: 140

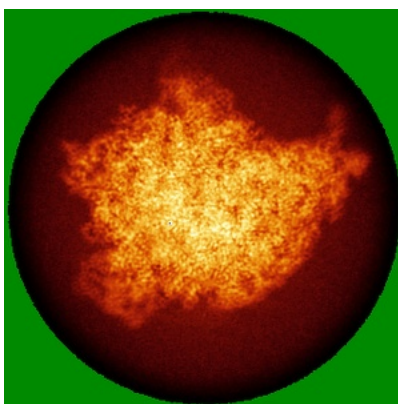
The images above show the largest variance slices of the map in three orthogonal directions.

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

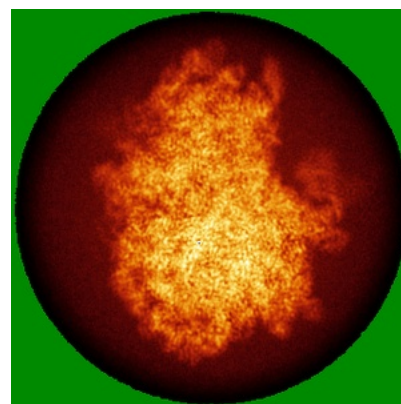
6.4.1 Primary map



X

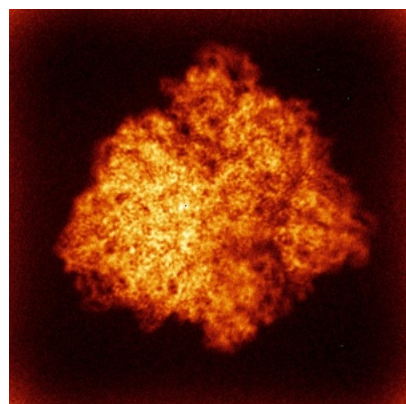


Y

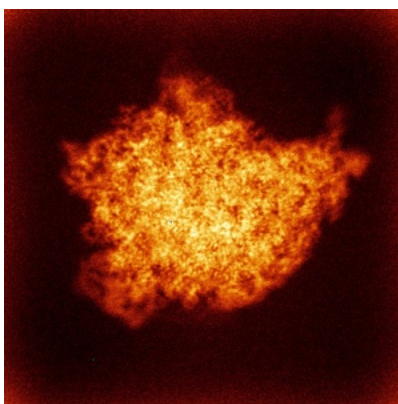


Z

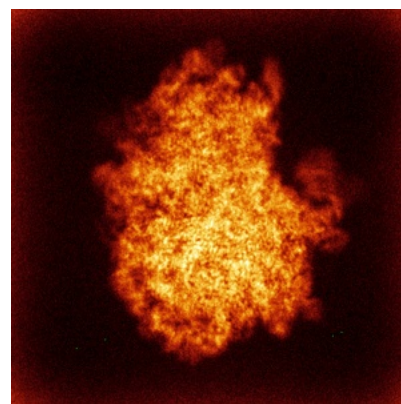
6.4.2 Raw map



X



Y

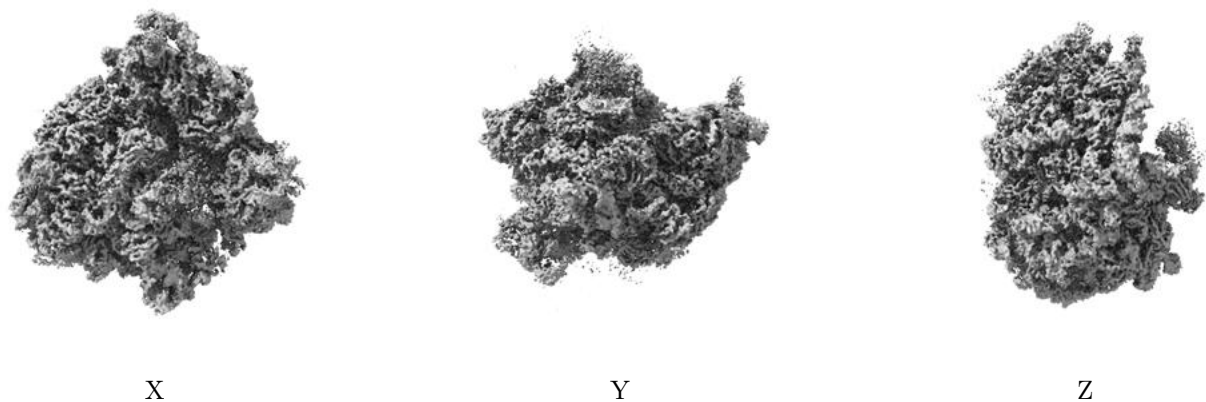


Z

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.

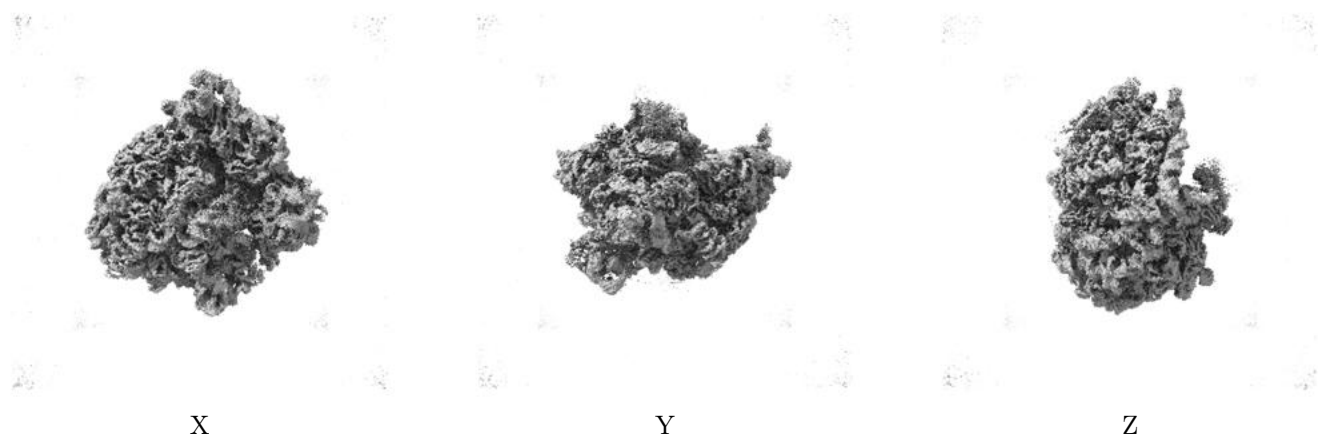
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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



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.

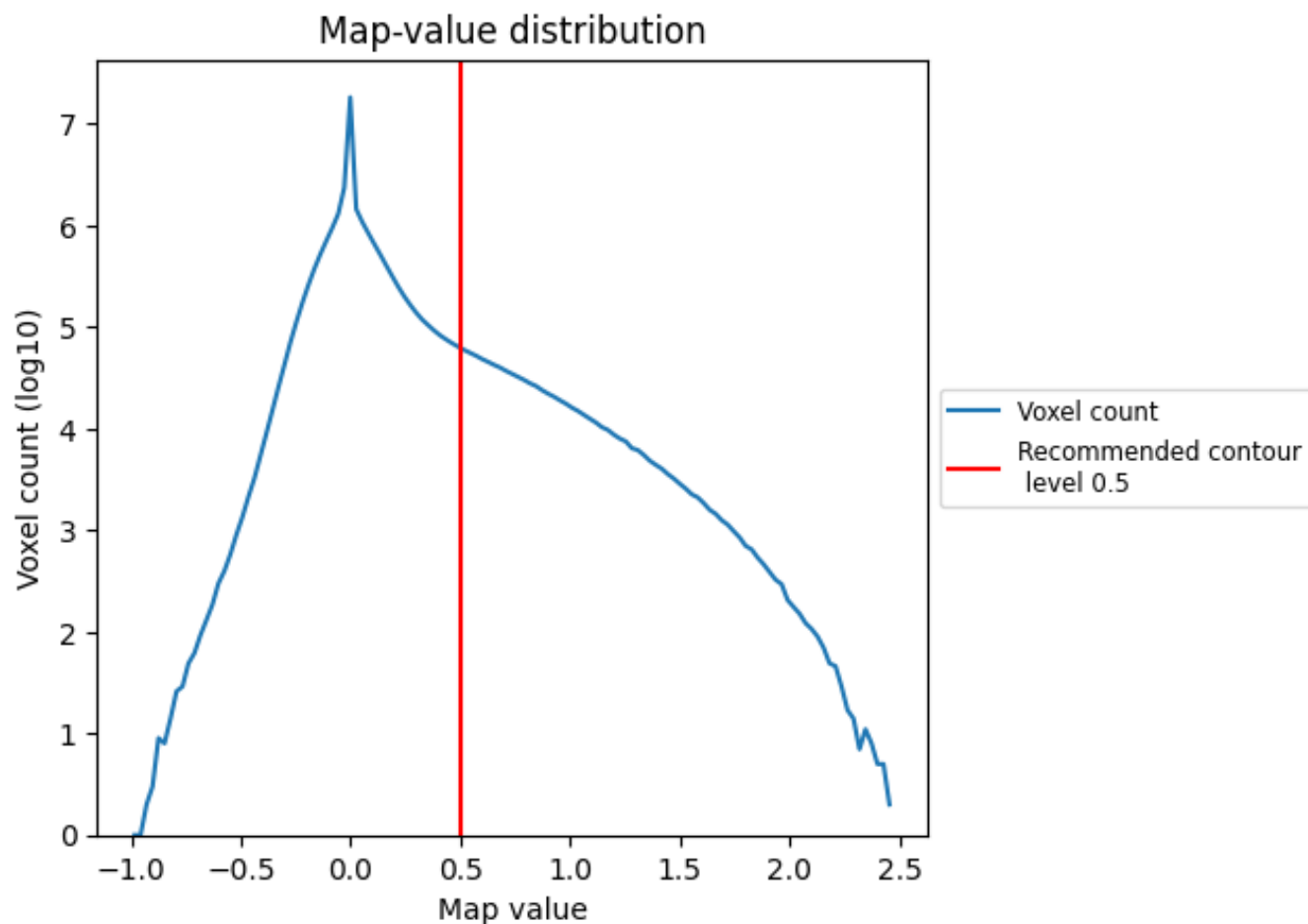
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

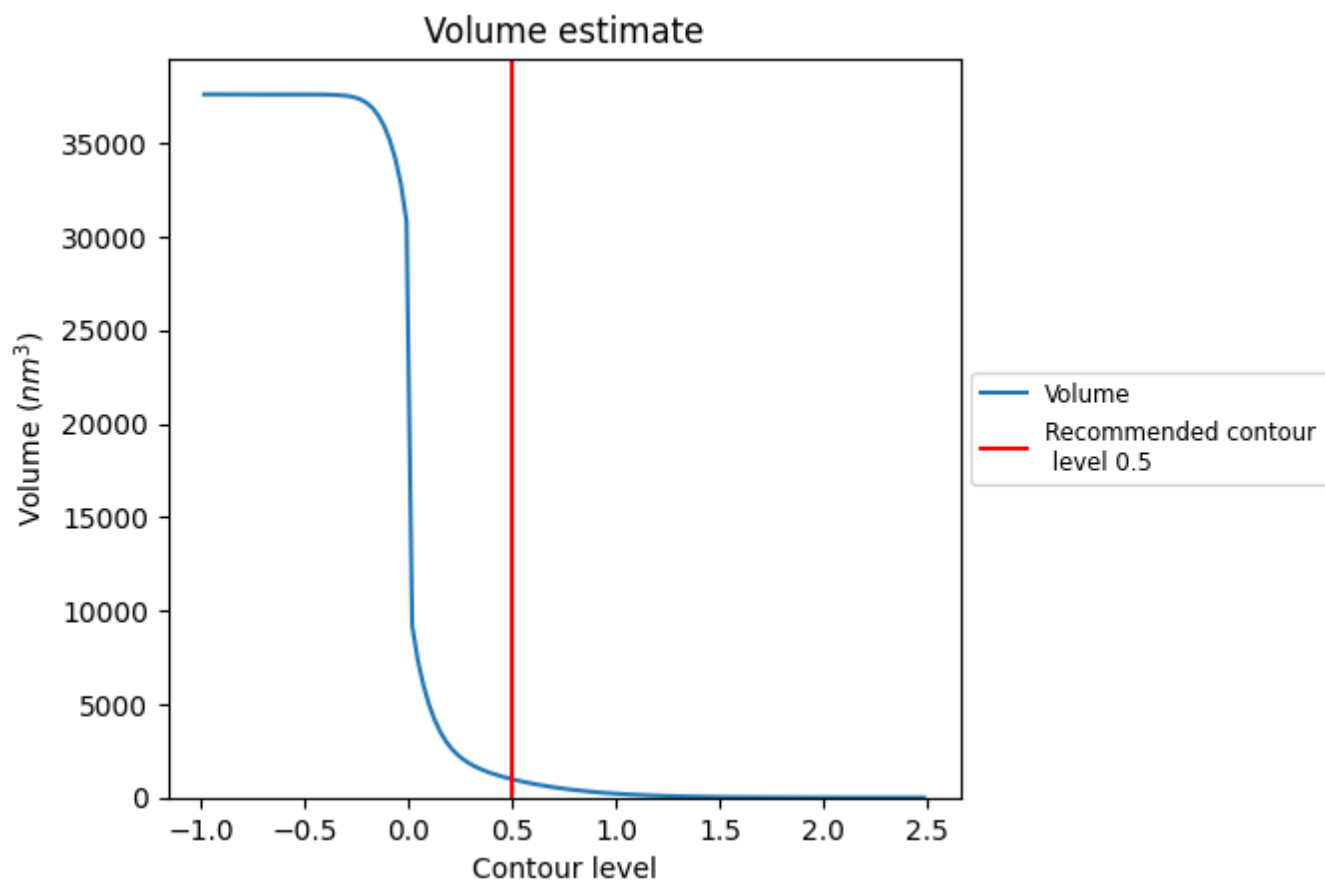
This section contains the results of statistical analysis of the map.

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.

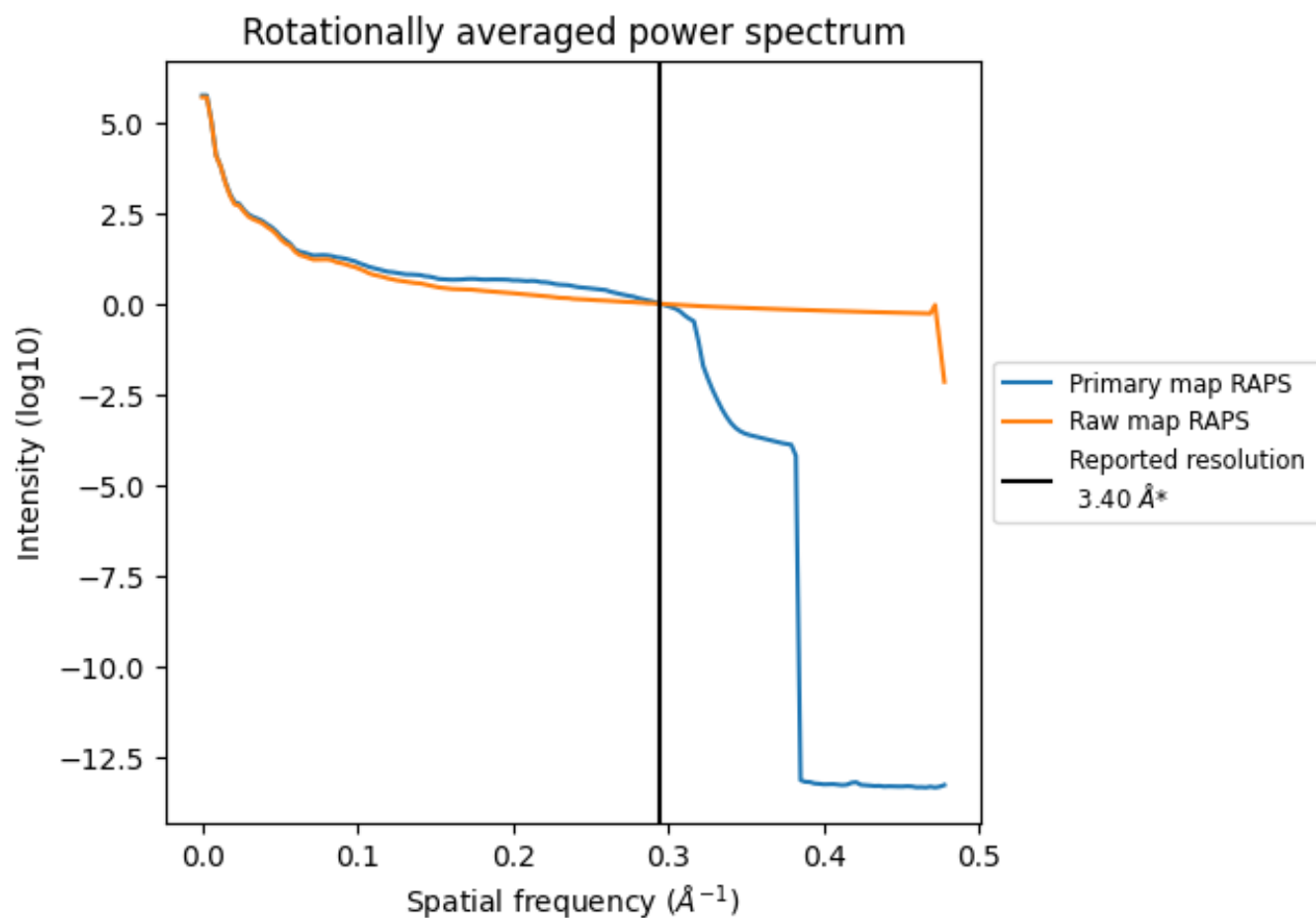
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 979 nm³; this corresponds to an approximate mass of 885 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 ⓘ

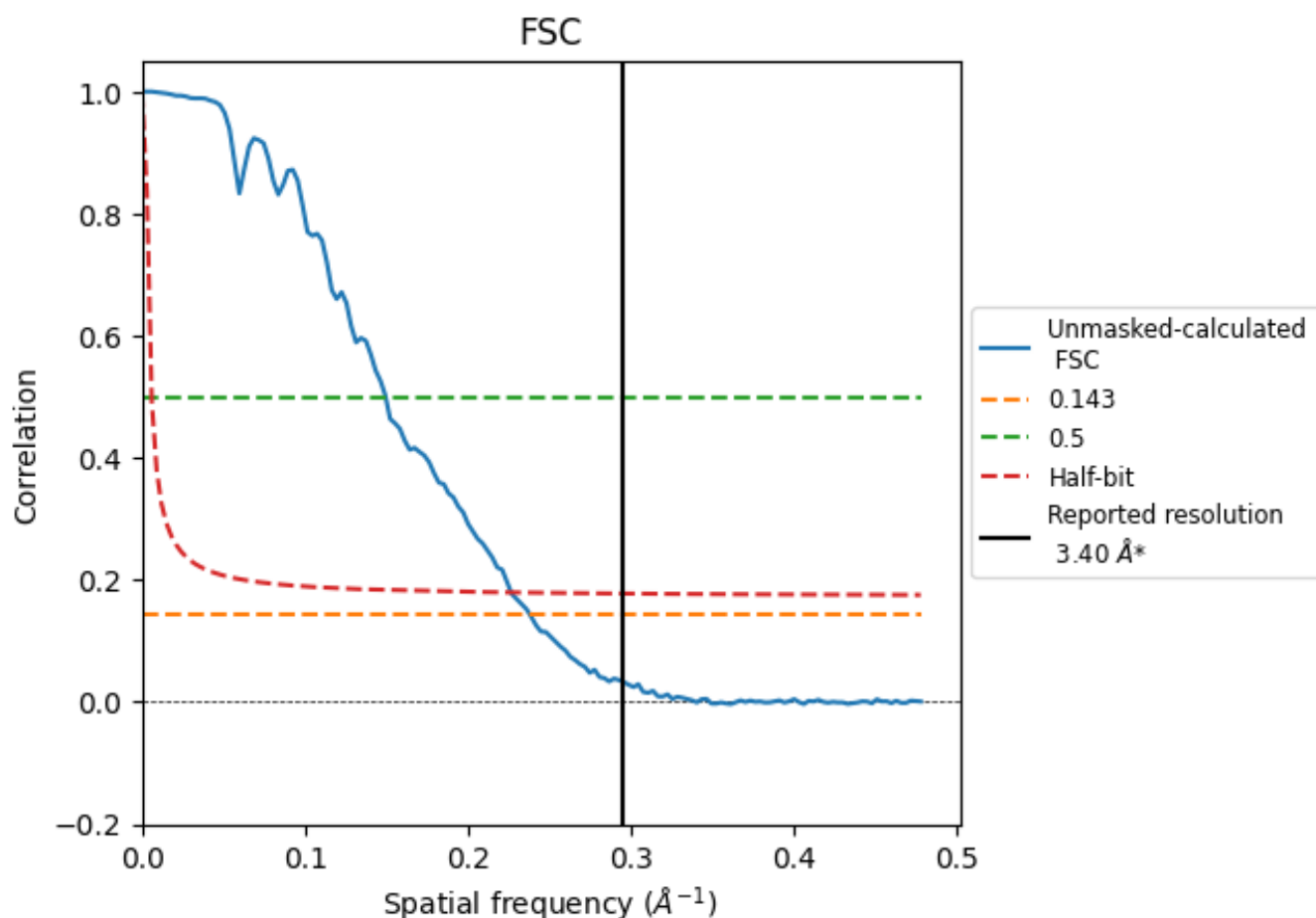


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

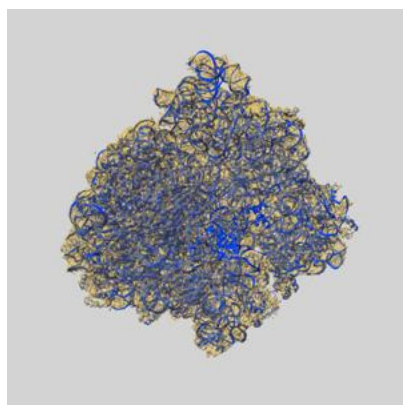
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.20	6.69	4.42

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.20 differs from the reported value 3.4 by more than 10 %

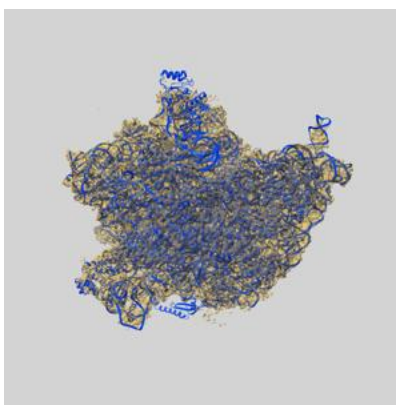
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40923 and PDB model 9NJF. Per-residue inclusion information can be found in section [3](#) on page [16](#).

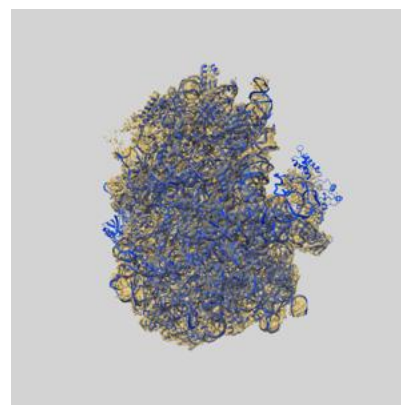
9.1 Map-model overlay [i](#)



X



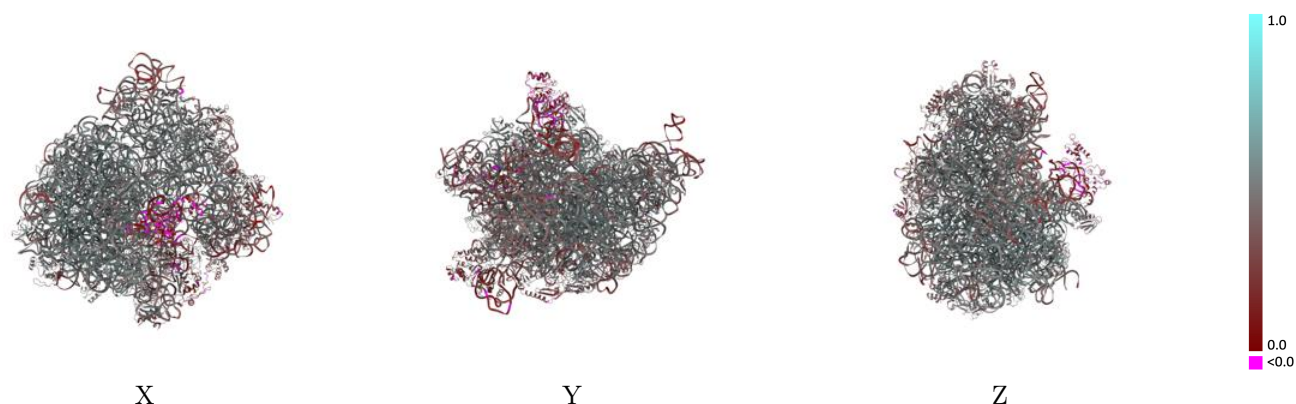
Y



Z

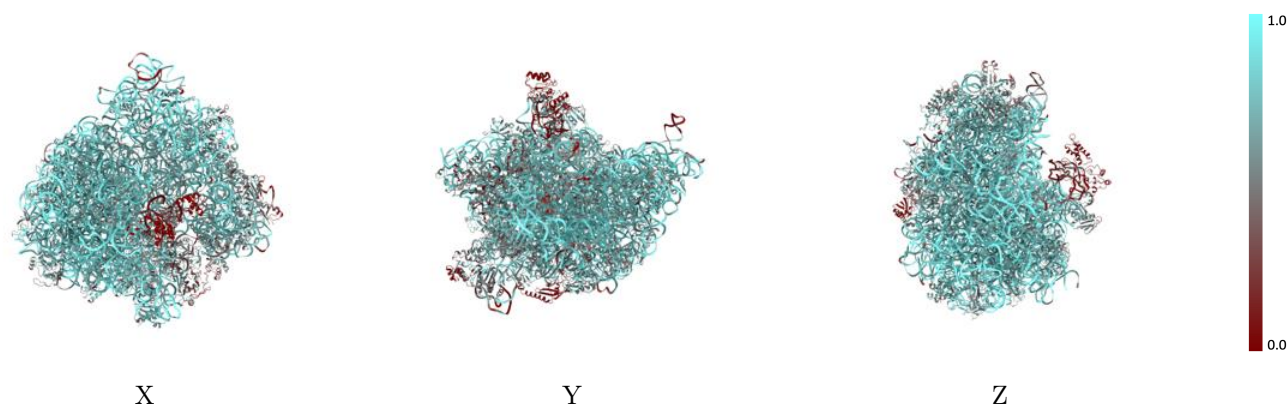
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



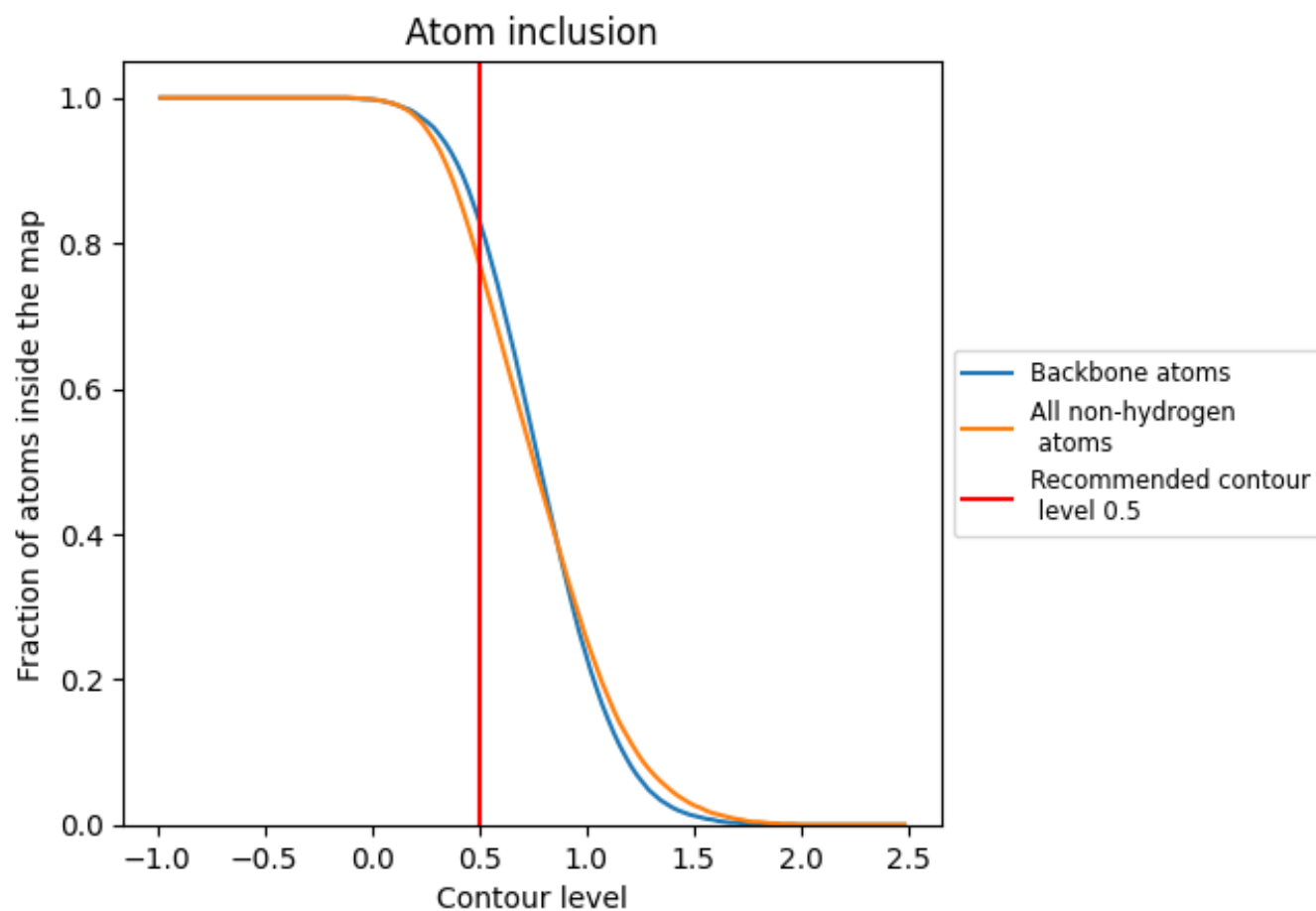
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 77% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7740	 0.4530
1	 0.4030	 0.3290
10	 0.1120	 0.1550
11	 0.1420	 0.1250
13	 0.7410	 0.5170
14	 0.6580	 0.5130
15	 0.7280	 0.5040
16	 0.7240	 0.5100
17	 0.7480	 0.5070
18	 0.6610	 0.4530
19	 0.6780	 0.5060
2	 0.7620	 0.5370
20	 0.7740	 0.5090
21	 0.6880	 0.4780
22	 0.6900	 0.5100
23	 0.6560	 0.4850
24	 0.5930	 0.4500
25	 0.6860	 0.4830
27	 0.7510	 0.5360
28	 0.7650	 0.5270
29	 0.6380	 0.4240
3	 0.7260	 0.5110
30	 0.6910	 0.4800
31	 0.2170	 0.1040
32	 0.7580	 0.5150
33	 0.1620	 0.0880
34	 0.7910	 0.5400
35	 0.7290	 0.5330
36	 0.7170	 0.5370
4	 0.6440	 0.4700
5	 0.4700	 0.3290
6	 0.5730	 0.4290
9	 0.2010	 0.3180
M	 0.6420	 0.3860
R1	 0.8690	 0.4730



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Chain	Atom inclusion	Q-score
R2	 0.8620	 0.4220
R3	 0.8560	 0.4520
T	 0.7920	 0.3840
Y	 0.5900	 0.4100
sb	 0.5410	 0.3920
sc	 0.5780	 0.4470
sd	 0.5930	 0.4240
se	 0.6920	 0.4800
sf	 0.6120	 0.4330
sg	 0.5790	 0.4040
sh	 0.6710	 0.4690
si	 0.5880	 0.4100
sj	 0.4460	 0.3840
sk	 0.6530	 0.4570
sl	 0.6660	 0.4930
sm	 0.5110	 0.3820
sn	 0.6000	 0.4000
so	 0.7010	 0.4700
sp	 0.6600	 0.4670
sq	 0.6140	 0.4700
sr	 0.6460	 0.4690
ss	 0.5230	 0.4020
st	 0.6780	 0.4400
su	 0.4330	 0.3510