



wwPDB EM Validation Summary Report ⓘ

Apr 17, 2024 – 05:57 pm BST

PDB ID : 8PEG
EMDB ID : EMD-17631
Title : Escherichia coli paused disome complex (queueing 70S non-rotated closed PRE state)
Authors : Fluegel, T.; Schacherl, M.
Deposited on : 2023-06-13
Resolution : 3.30 Å(reported)
Based on initial model : 7N1P

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:

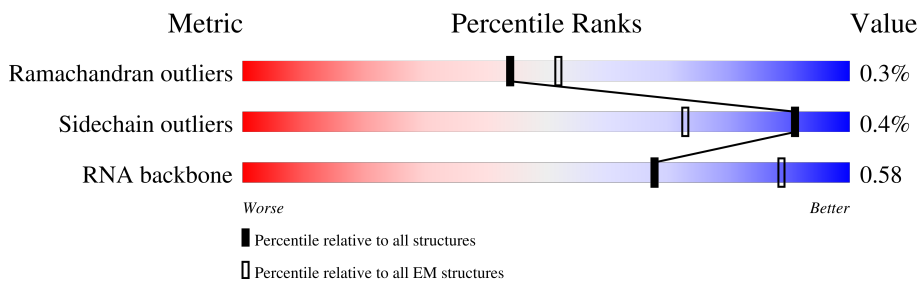
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 Å.

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





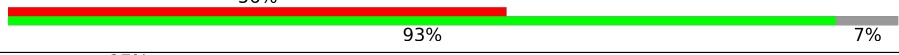
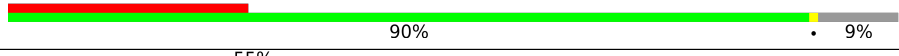
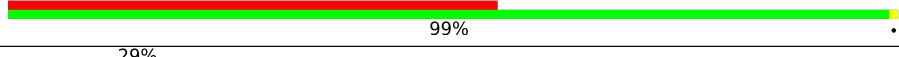
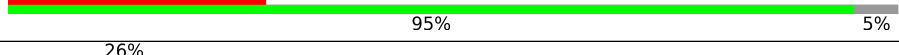


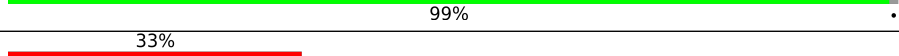
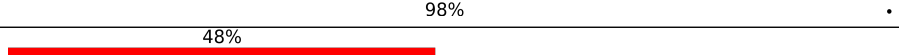
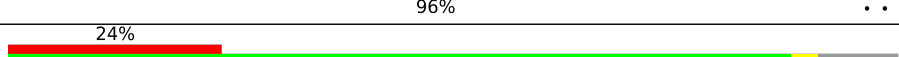
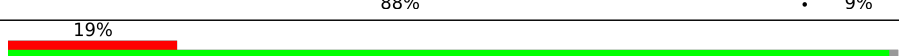
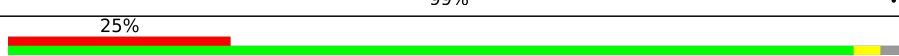
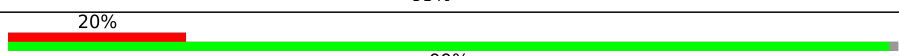
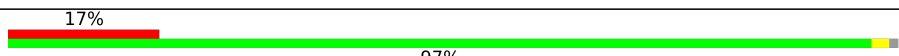
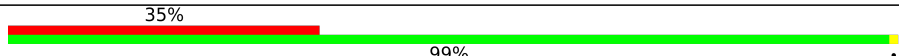
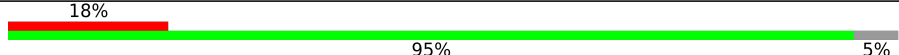
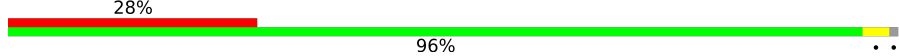
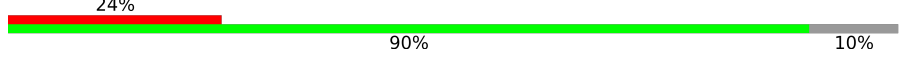
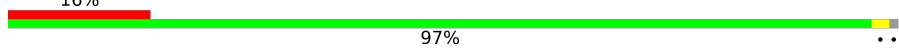
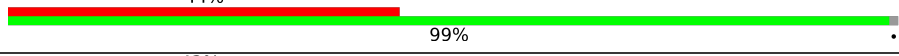


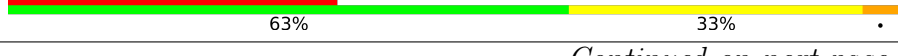

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	0	38	100%
2	1	78	96%
3	2	63	16% 98%
4	3	59	10% 93% 5%
5	4	70	53% 94%
6	5	57	5% 98%
7	6	65	98%
8	7	2903	81% 19%

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Mol	Chain	Length	Quality of chain
9	8	120	
10	A	1542	
11	B	241	
12	C	233	
13	D	206	
14	E	167	
15	F	135	
16	G	179	
17	H	130	
18	I	130	
19	J	103	
20	K	129	
21	L	124	
22	M	118	
23	N	101	
24	O	89	
25	P	82	
26	Q	84	
27	R	75	
28	S	92	
29	T	87	
30	U	71	
31	V	30	
32	W	76	
33	X	78	

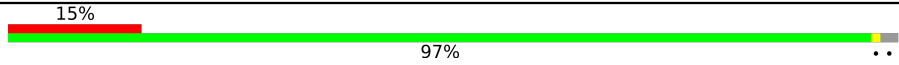
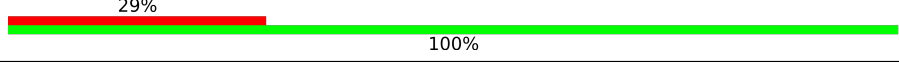
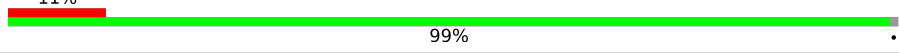
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Mol	Chain	Length	Quality of chain
34	Y	76	
35	Z	557	
36	a	234	
37	b	273	
38	c	209	
39	d	201	
40	e	179	
41	f	177	
42	g	55	
43	h	136	
44	i	149	
45	j	165	
46	k	142	
47	l	46	
48	m	142	
49	n	123	
50	o	144	
51	p	18	
52	q	127	
53	r	117	
54	s	115	
55	t	118	
56	u	103	
57	v	110	
58	w	100	

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Mol	Chain	Length	Quality of chain
59	x	104	 15% 97% ..
60	y	94	 29% 100%
61	z	85	 11% 99% .

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 153284 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 50S ribosomal protein L36.

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

- Molecule 2 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	77	625	388	129	106	2	0	0

- Molecule 3 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	63	509	313	99	95	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	58	449	281	87	79	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	67	529	328	100	95	6	0	0

- Molecule 6 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	56	444	269	94	80	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	64	504	323	105	74	2	0	0

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	7	2903	62335	27815	11467	20150	2903	0	0

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	8	120	2569	1144	468	837	120	0	0

- Molecule 10 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	A	1542	33092	14767	6064	10719	1542	0	0

- Molecule 11 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	B	224	1751	1108	314	321	8	0	0

- Molecule 12 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	C	212	1658	1049	311	294	4	0	0

- Molecule 13 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	E	158	1166	725	220	215	6	0	0

- Molecule 15 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	F	106	862	545	156	154	7	0	0

- Molecule 16 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	G	155	1228	767	237	220	4	0	0

- Molecule 17 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 19 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	J	100	803	502	154	146	1	0	0

- Molecule 20 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	K	118	884	545	175	161	3	0	0

- Molecule 21 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 22 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 23 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 24 is a protein called 30S ribosomal protein S15.

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

- Molecule 25 is a protein called 30S ribosomal protein S16.

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

- Molecule 26 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 27 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	R	74	624	395	122	105	2	0	0

- Molecule 28 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 29 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	U	70	Total	C	N	O	S	0	0
			584	363	122	98	1		

- Molecule 31 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	V	30	Total	C	N	O	P	0	0
			648	290	124	204	30		

- Molecule 32 is a RNA chain called tRNA-Phe (P-site).

Mol	Chain	Residues	Atoms					AltConf	Trace	
32	W	76	Total	C	N	O	P	S	0	0
			1632	731	289	534	76	2		

- Molecule 33 is a RNA chain called tRNA-Ser (E-site).

Mol	Chain	Residues	Atoms					AltConf	Trace	
33	X	78	Total	C	N	O	P	S	0	0
			1683	750	304	548	78	3		

- Molecule 34 is a RNA chain called tRNA-Val (A-site).

Mol	Chain	Residues	Atoms					AltConf	Trace	
34	Y	76	Total	C	N	O	P	S	0	0
			1631	728	292	534	76	1		

- Molecule 35 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	Z	170	Total	C	N	O	0	0
			1319	830	228	261		

- Molecule 36 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	a	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 37 is a protein called 50S ribosomal protein L2.

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

- Molecule 38 is a protein called 50S ribosomal protein L3.

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

- Molecule 39 is a protein called 50S ribosomal protein L4.

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

- Molecule 40 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	e	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 41 is a protein called 50S ribosomal protein L6.

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

- Molecule 42 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	g	52	Total	C	N	O	0	0
			427	275	78	74		

- Molecule 43 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	h	136	Total	C	N	O	S	1	0
			1085	692	209	178	6		

- Molecule 44 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	i	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 45 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	j	135	Total	C	N	O	S	0	0
			1023	648	179	192	4		

- Molecule 46 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	k	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 47 is a protein called 50S ribosomal protein L34.

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

- Molecule 48 is a protein called 50S ribosomal protein L13.

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

- Molecule 49 is a protein called 50S ribosomal protein L14.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	o	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 51 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	p	18	Total	C	N	O	0	0
			101	63	18	20		

- Molecule 52 is a protein called 50S ribosomal protein L17.

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

- Molecule 53 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	r	116	Total	C	N	O	0	0
			891	552	178	161		

- Molecule 54 is a protein called 50S ribosomal protein L19.

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

- Molecule 55 is a protein called 50S ribosomal protein L20.

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

- Molecule 56 is a protein called 50S ribosomal protein L21.

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

- Molecule 57 is a protein called 50S ribosomal protein L22.

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

- Molecule 58 is a protein called 50S ribosomal protein L23.

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

- Molecule 59 is a protein called 50S ribosomal protein L24.

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

- Molecule 60 is a protein called 50S ribosomal protein L25.

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

- Molecule 61 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	z	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

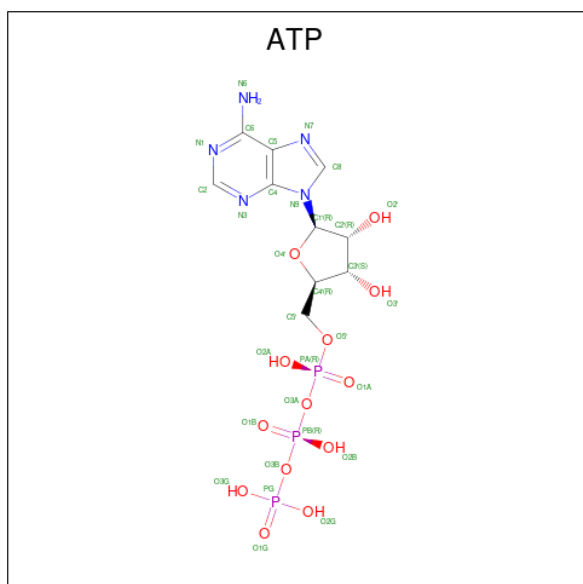
- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
62	0	1	Total	Zn	0
			1	1	
62	4	1	Total	Zn	0
			1	1	

- Molecule 63 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
63	7	193	Total Mg 193 193	0
63	A	63	Total Mg 63 63	0
63	X	1	Total Mg 1 1	0
63	Y	1	Total Mg 1 1	0
63	b	1	Total Mg 1 1	0
63	o	1	Total Mg 1 1	0

- Molecule 64 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



3 Residue-property plots [i](#)

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

- Molecule 1: 50S ribosomal protein L36

Chain 0:  100%



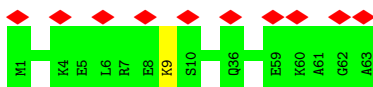
- Molecule 2: 50S ribosomal protein L28

Chain 1:  96%




- Molecule 3: 50S ribosomal protein L29

Chain 2:  16% 98%




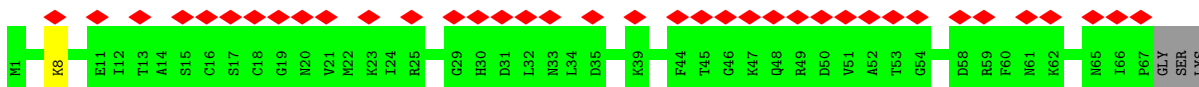
- Molecule 4: 50S ribosomal protein L30

Chain 3:  10% 93% 5%

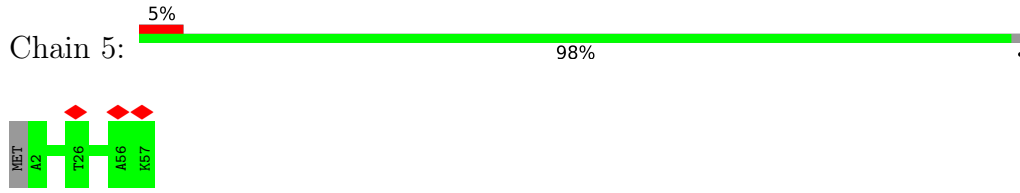


- Molecule 5: Large ribosomal subunit protein bL31A

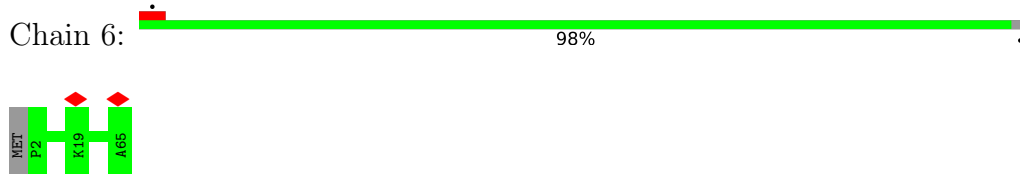
Chain 4:  53% 94%



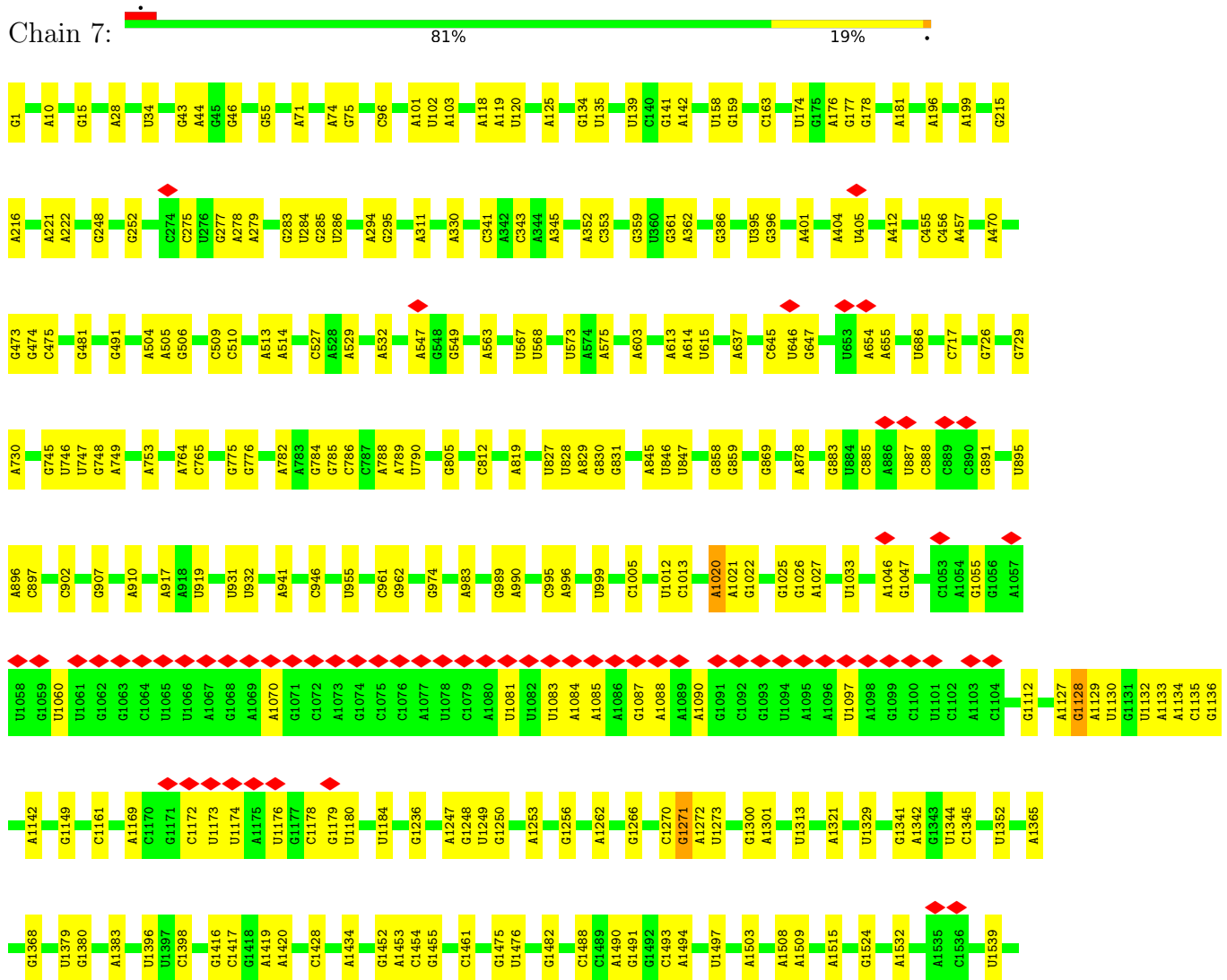
• Molecule 6: 50S ribosomal protein L32

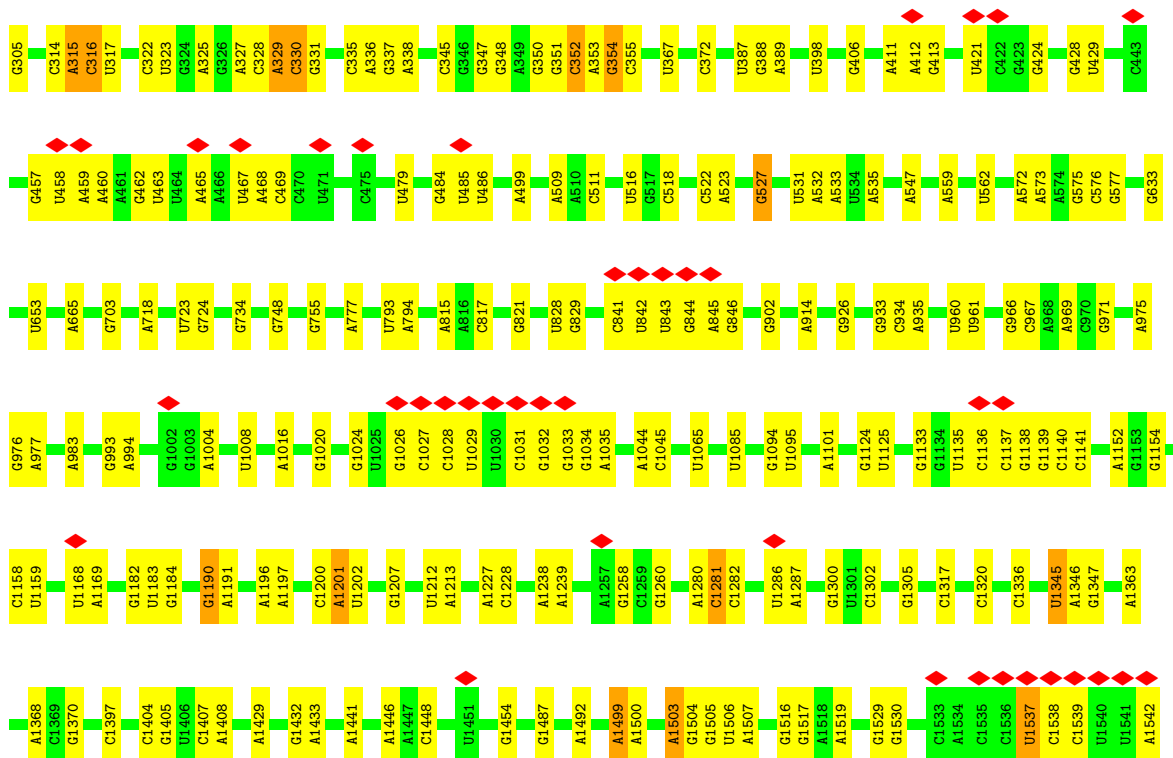


• Molecule 7: 50S ribosomal protein L35

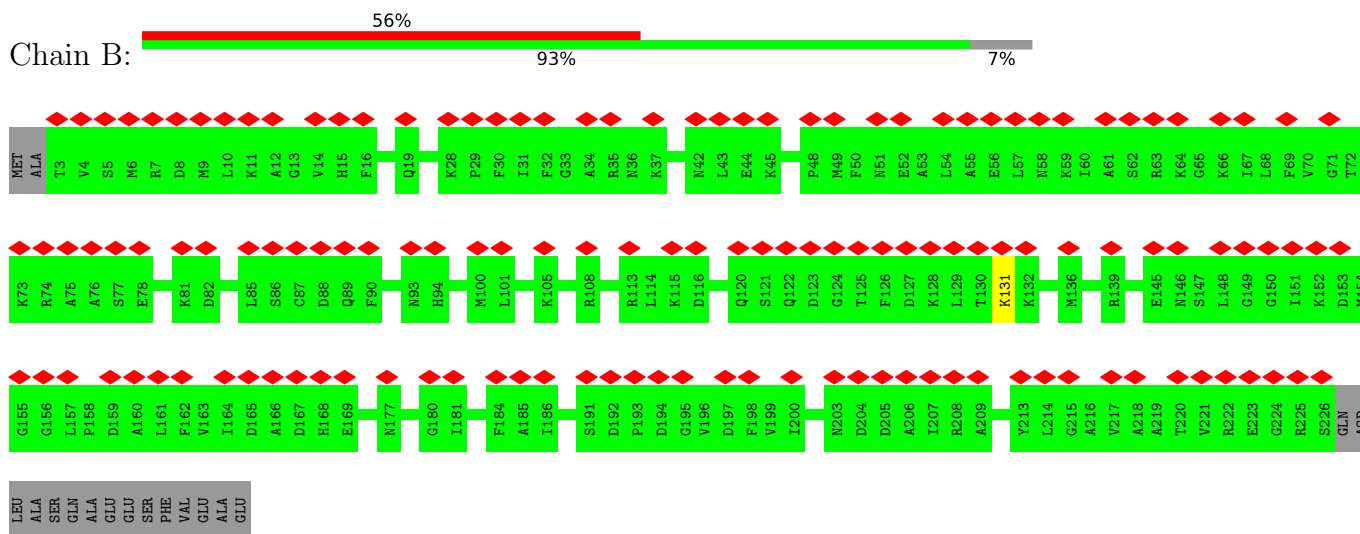


• Molecule 8: 23S ribosomal RNA

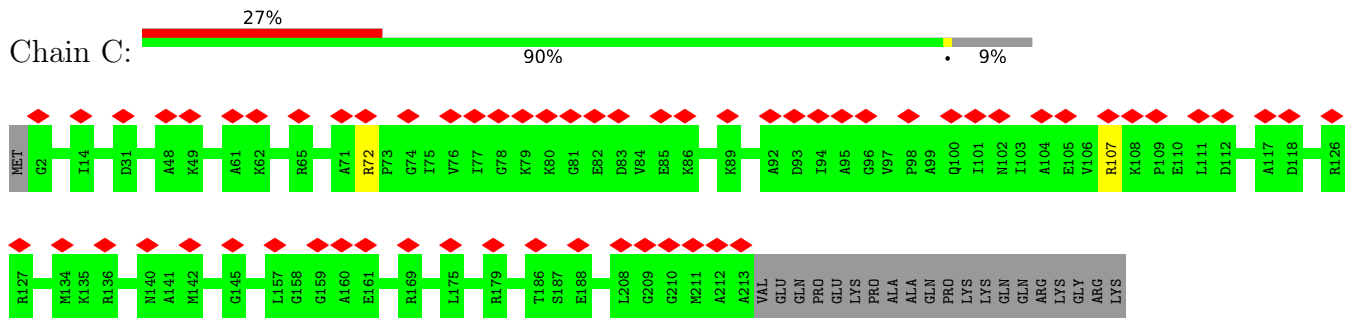




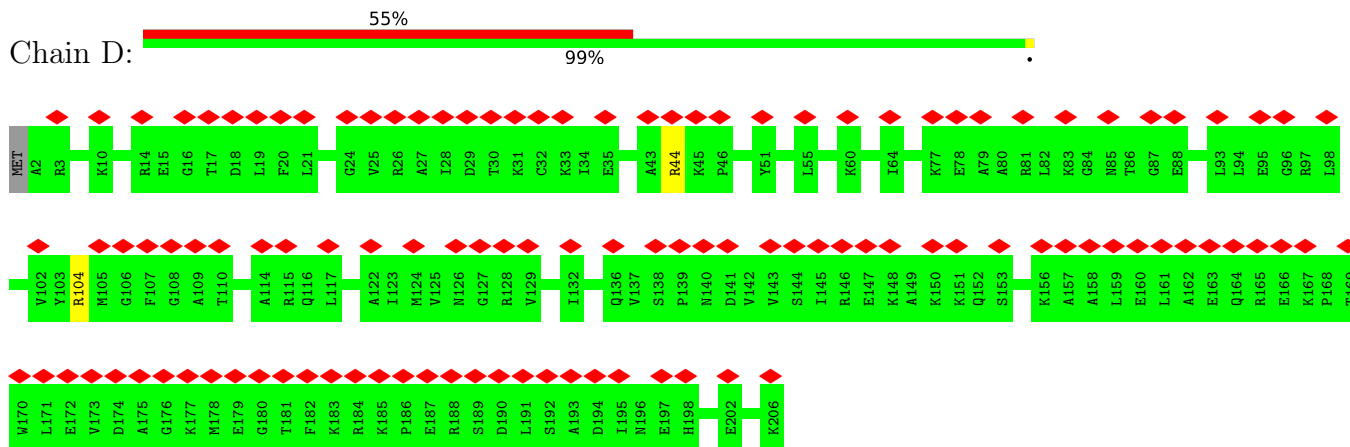
• Molecule 11: Small ribosomal subunit protein uS2



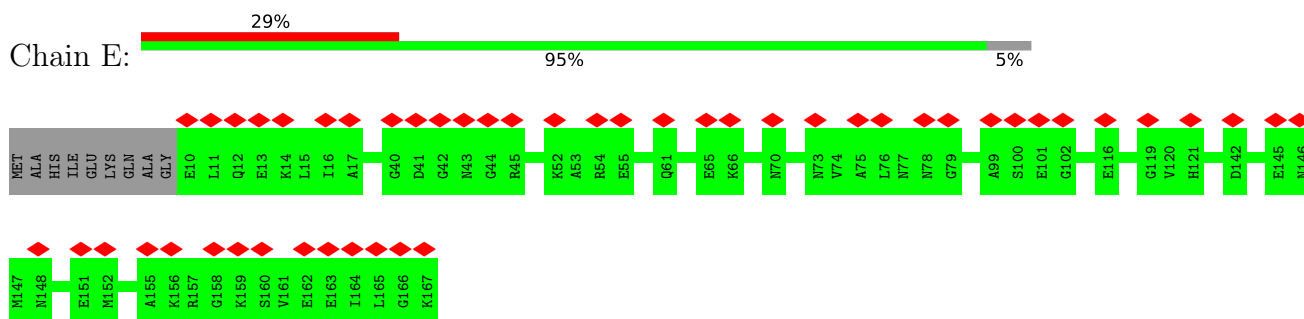
• Molecule 12: Small ribosomal subunit protein uS3



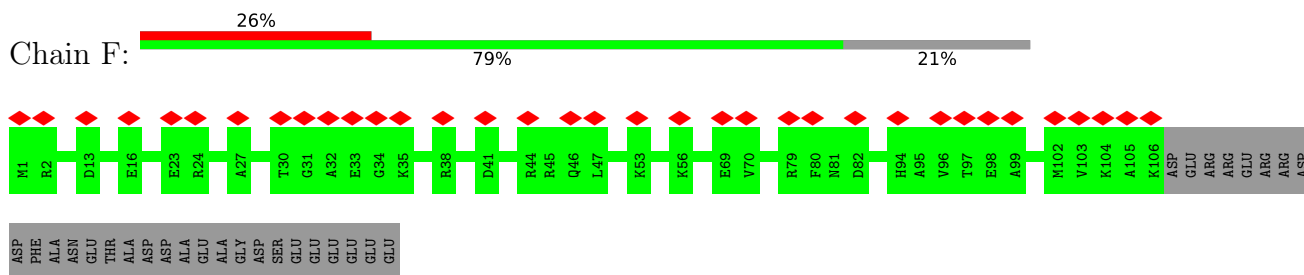
• Molecule 13: Small ribosomal subunit protein uS4



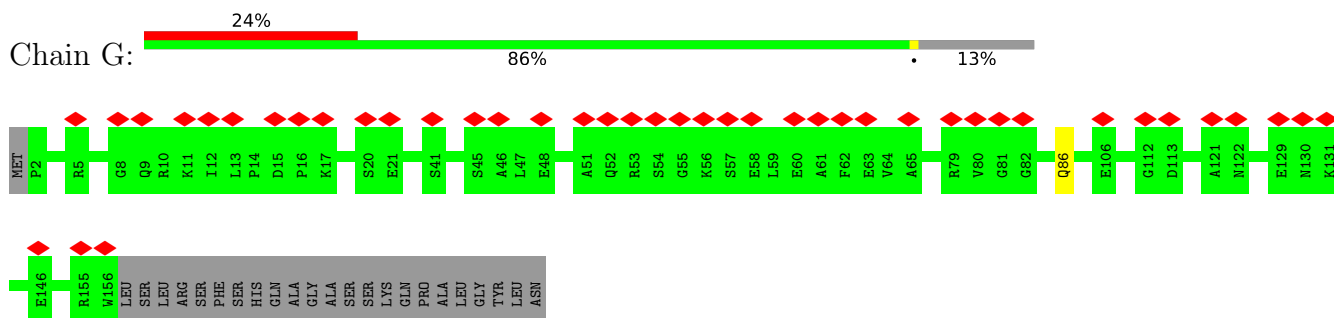
• Molecule 14: Small ribosomal subunit protein uS5



• Molecule 15: 30S ribosomal protein S6

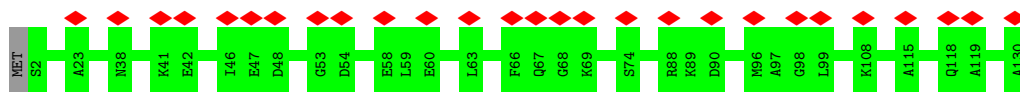


• Molecule 16: 30S ribosomal protein S7

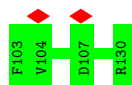
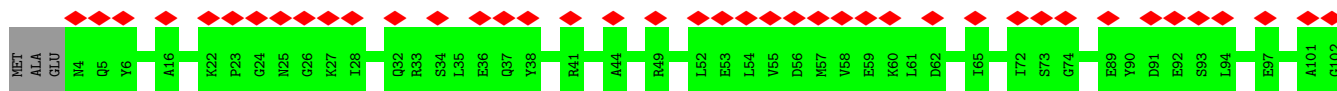


• Molecule 17: Small ribosomal subunit protein uS8

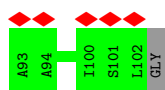
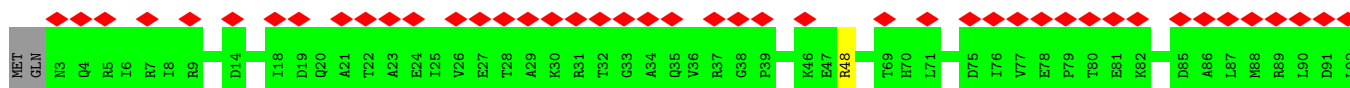




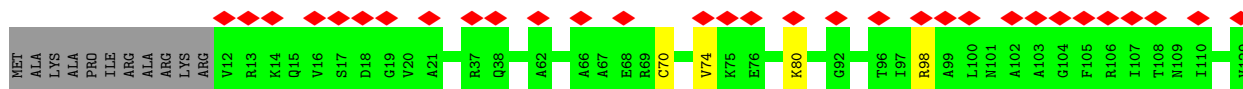
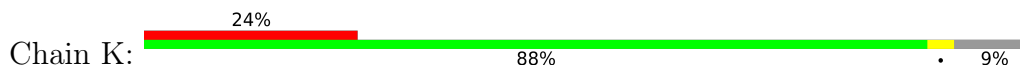
- Molecule 18: Small ribosomal subunit protein uS9



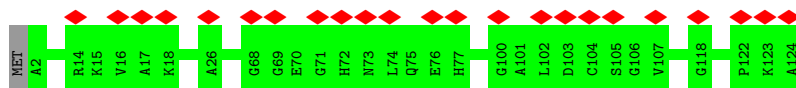
- Molecule 19: 30S ribosomal protein S10



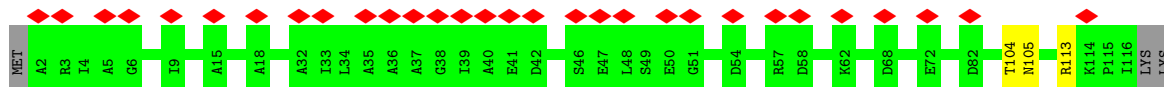
- Molecule 20: Small ribosomal subunit protein uS11



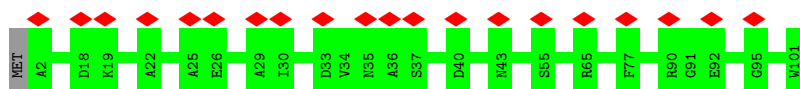
- Molecule 21: Small ribosomal subunit protein uS12



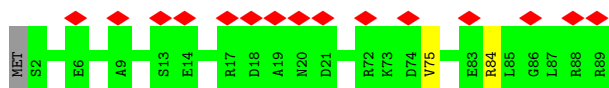
- Molecule 22: Small ribosomal subunit protein uS13



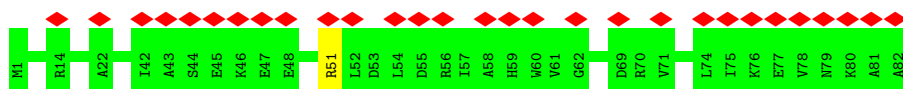
- Molecule 23: Small ribosomal subunit protein uS14



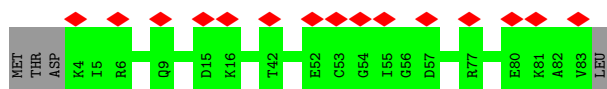
- Molecule 24: 30S ribosomal protein S15



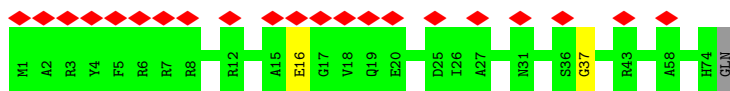
- Molecule 25: 30S ribosomal protein S16



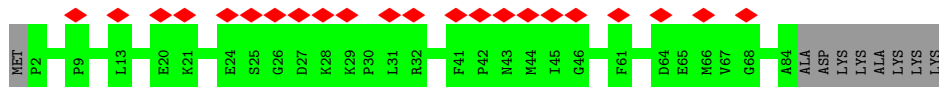
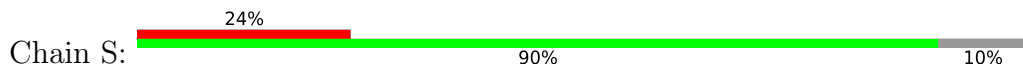
- Molecule 26: Small ribosomal subunit protein uS17



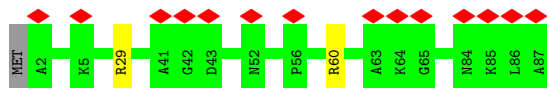
- Molecule 27: Small ribosomal subunit protein bS18



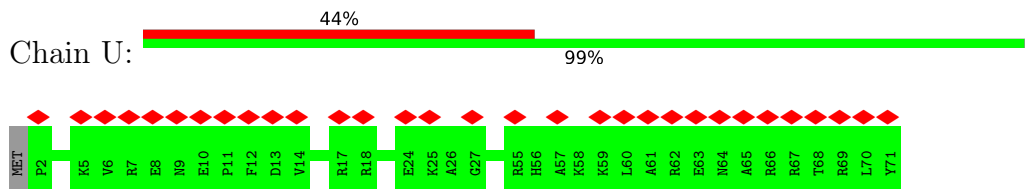
- Molecule 28: Small ribosomal subunit protein uS19



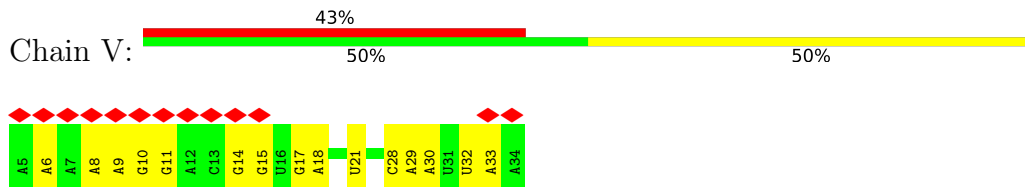
- Molecule 29: Small ribosomal subunit protein bS20



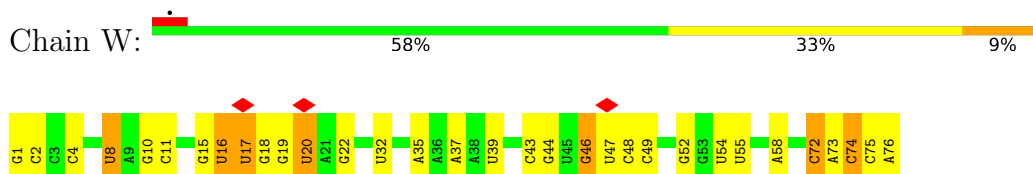
• Molecule 30: 30S ribosomal protein S21



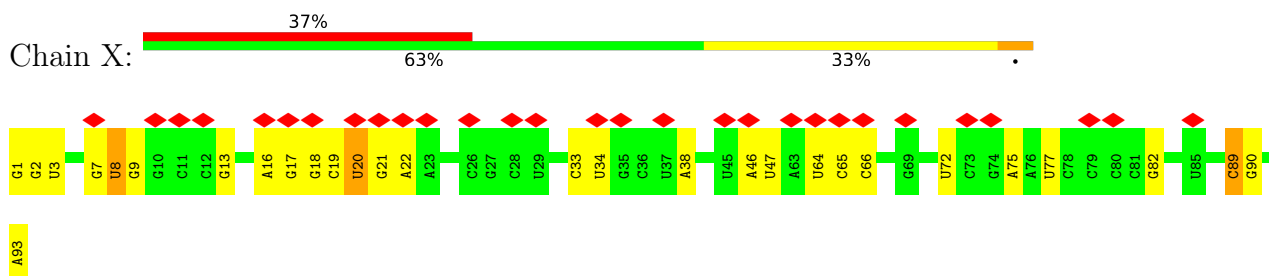
• Molecule 31: mRNA



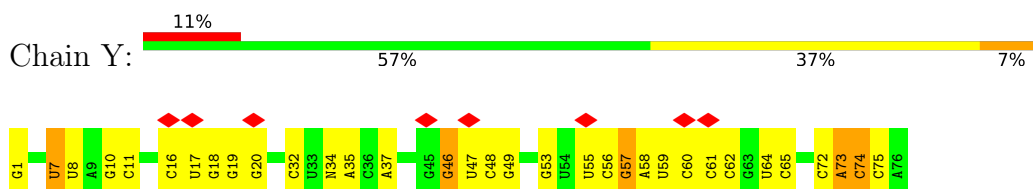
• Molecule 32: tRNA-Phe (P-site)



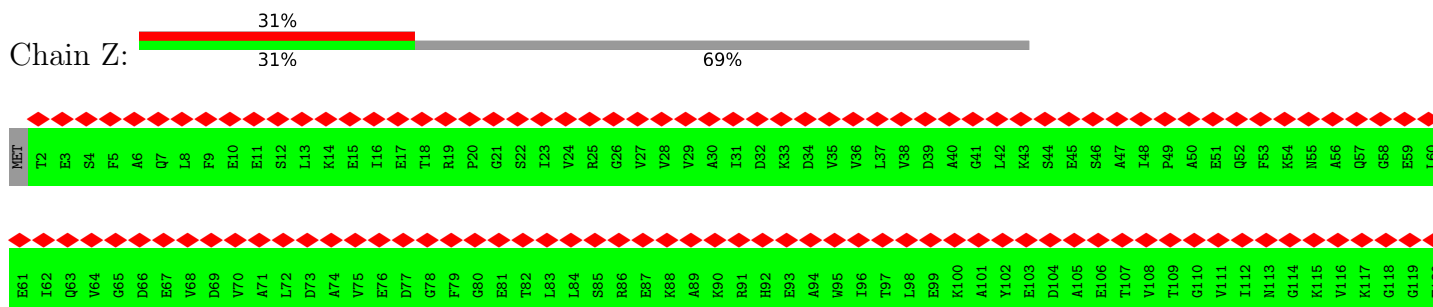
• Molecule 33: tRNA-Ser (E-site)

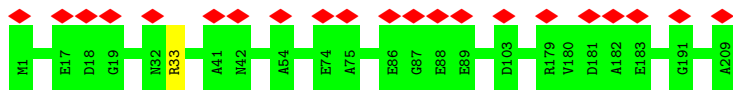


• Molecule 34: tRNA-Val (A-site)

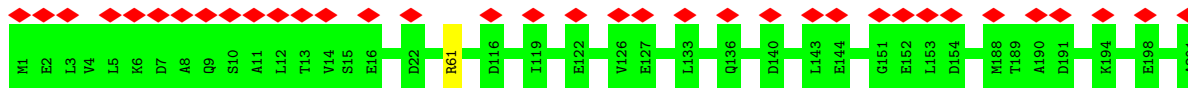


• Molecule 35: 30S ribosomal protein S1

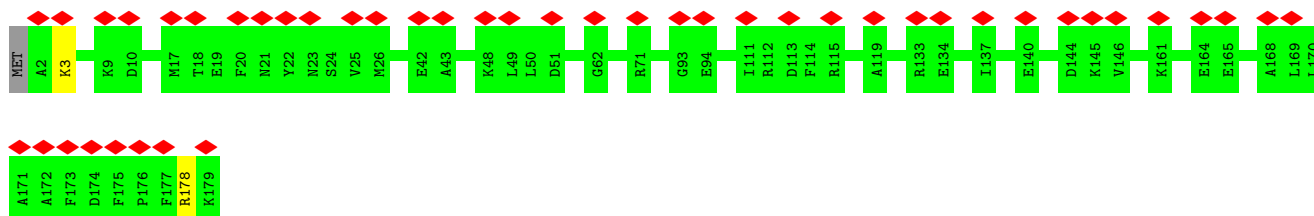




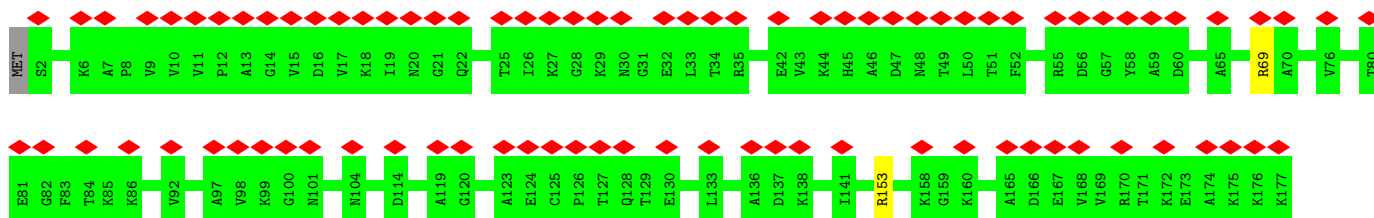
- Molecule 39: 50S ribosomal protein L4



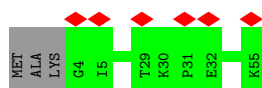
- Molecule 40: 50S ribosomal protein L5



- Molecule 41: 50S ribosomal protein L6



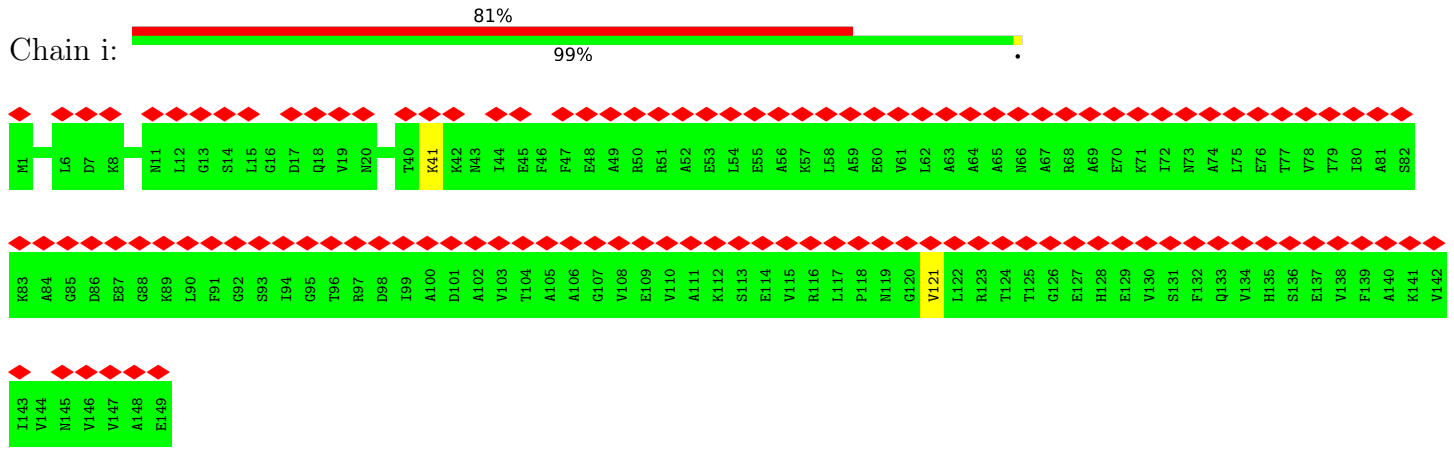
- Molecule 42: 50S ribosomal protein L33



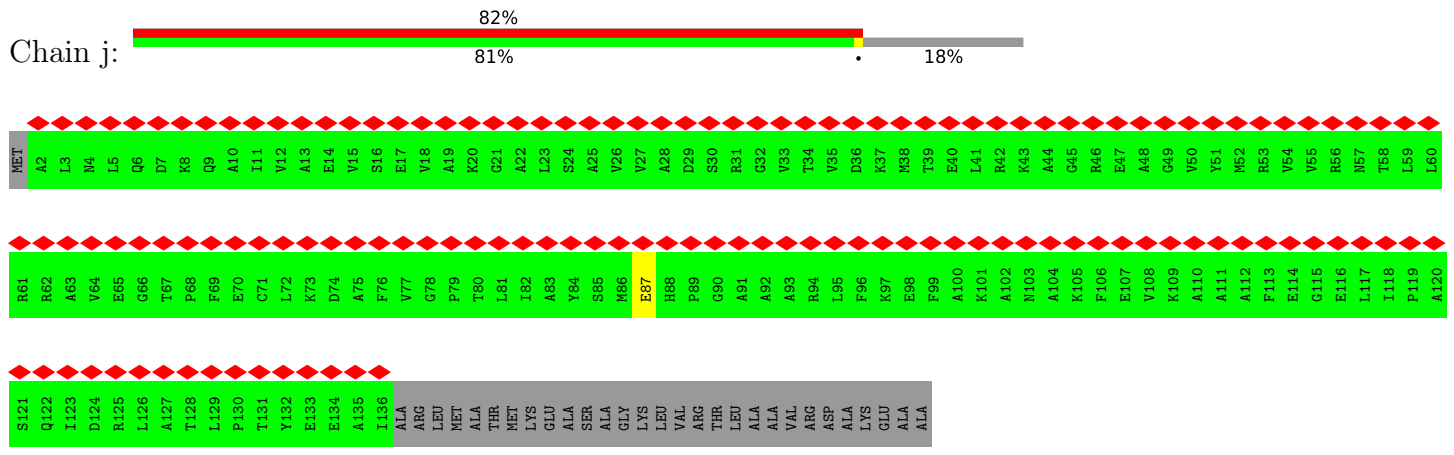
- Molecule 43: 50S ribosomal protein L16



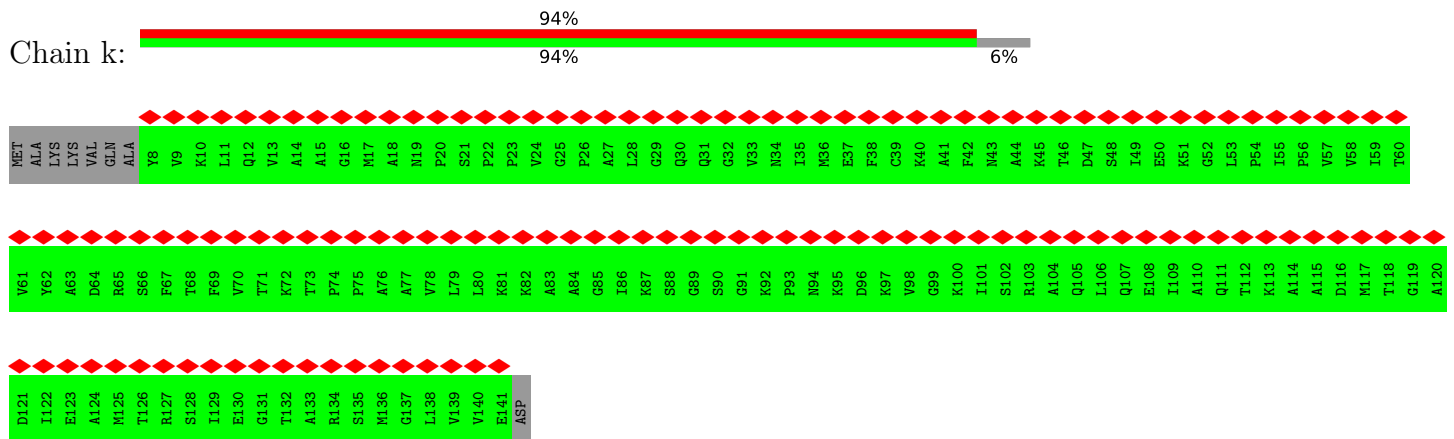
- Molecule 44: 50S ribosomal protein L9



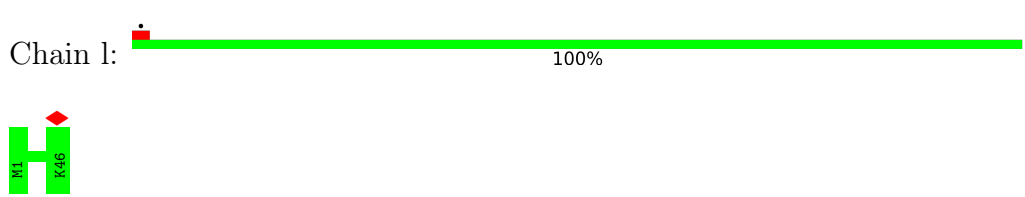
• Molecule 45: Large ribosomal subunit protein uL10



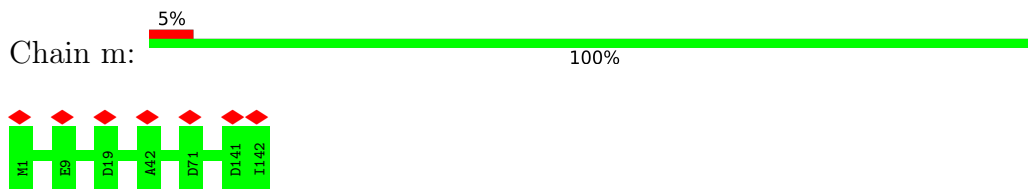
• Molecule 46: 50S ribosomal protein L11



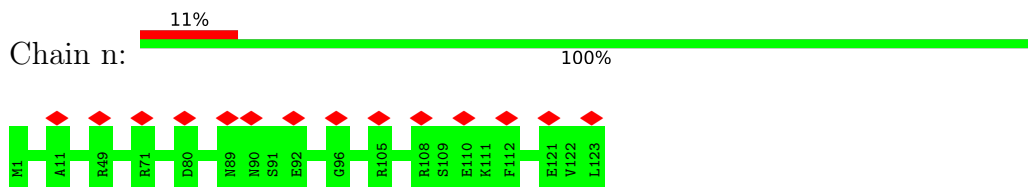
• Molecule 47: 50S ribosomal protein L34



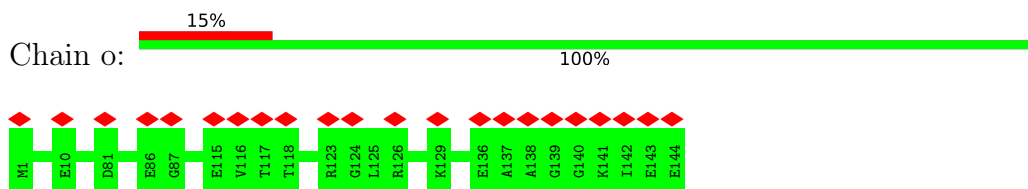
- Molecule 48: 50S ribosomal protein L13



- Molecule 49: 50S ribosomal protein L14



- Molecule 50: 50S ribosomal protein L15

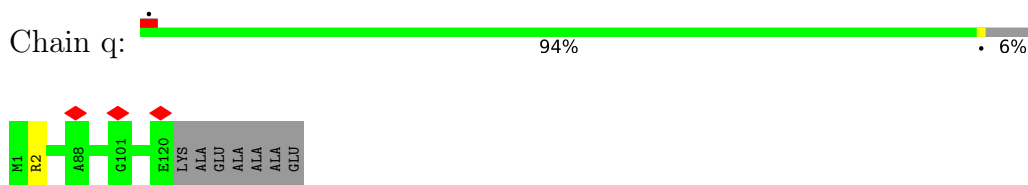


- Molecule 51: Nascent chain

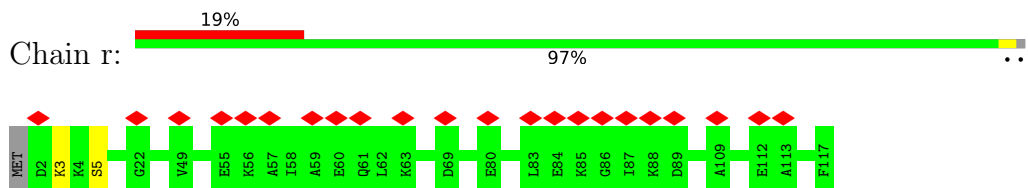


There are no outlier residues recorded for this chain.

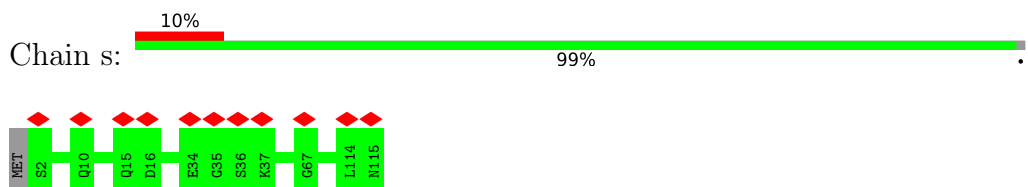
- Molecule 52: 50S ribosomal protein L17



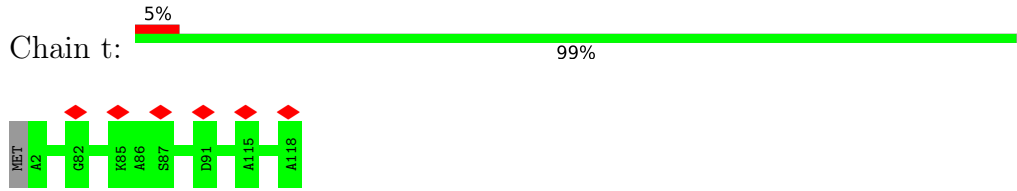
- Molecule 53: 50S ribosomal protein L18



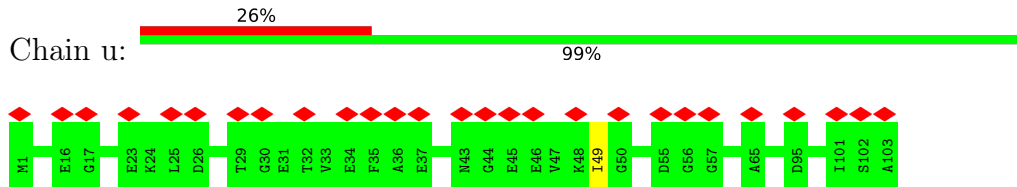
- Molecule 54: 50S ribosomal protein L19



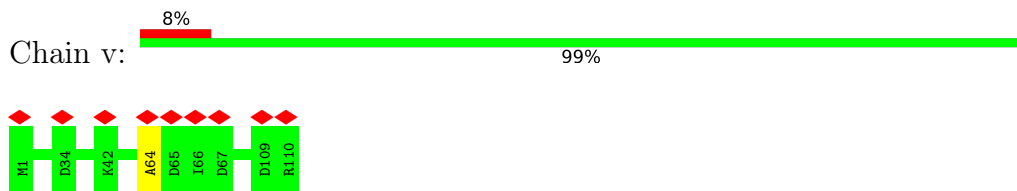
- Molecule 55: 50S ribosomal protein L20



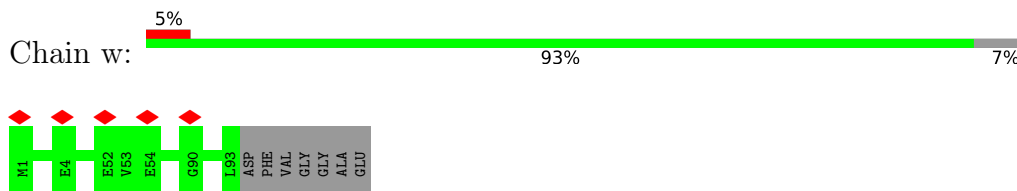
- Molecule 56: 50S ribosomal protein L21



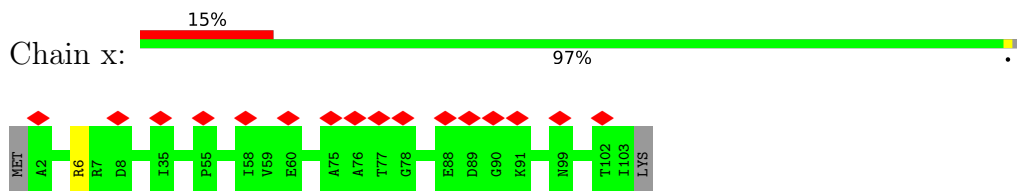
- Molecule 57: 50S ribosomal protein L22



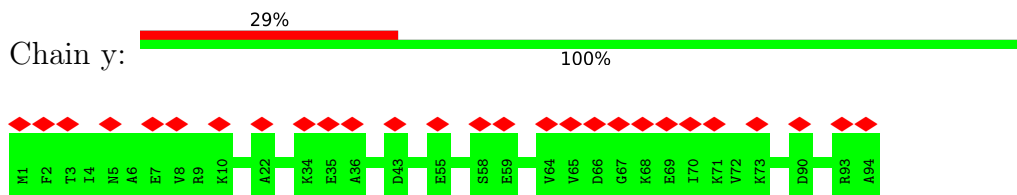
- Molecule 58: 50S ribosomal protein L23



- Molecule 59: 50S ribosomal protein L24

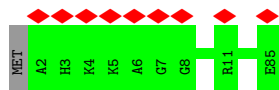


- Molecule 60: 50S ribosomal protein L25



- Molecule 61: 50S ribosomal protein L27





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	32334	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	24.520	Depositor
Minimum map value	-6.989	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.5	Depositor
Map size (Å)	744.11993, 744.11993, 744.11993	wwPDB
Map dimensions	702, 702, 702	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, 4OC, PSU, MIA, G7M, 5MC, OMU, OMG, 7MG, 6MZ, OMC, UR3, MG, MA6, 2MG, H2U, CM0, 1MG, 3TD, 12A, 5MU, RSP, ZN, ATP, 2MA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.23	0/303	0.60	0/397
2	1	0.25	0/635	0.63	0/848
3	2	0.25	0/510	0.54	0/677
4	3	0.24	0/453	0.61	0/605
5	4	0.27	0/539	0.58	0/721
6	5	0.25	0/450	0.58	0/599
7	6	0.24	0/513	0.56	0/676
8	7	0.23	1/69284 (0.0%)	0.75	60/108082 (0.1%)
9	8	0.23	0/2872	0.76	6/4478 (0.1%)
10	A	0.23	0/36772	0.75	47/57358 (0.1%)
11	B	0.26	0/1782	0.53	0/2401
12	C	0.26	0/1685	0.57	0/2270
13	D	0.25	0/1665	0.56	0/2227
14	E	0.27	0/1179	0.55	0/1584
15	F	0.25	0/881	0.54	0/1189
16	G	0.27	0/1246	0.55	0/1672
17	H	0.26	0/989	0.57	0/1326
18	I	0.26	0/1034	0.60	0/1375
19	J	0.28	0/813	0.67	0/1100
20	K	0.26	0/900	0.59	0/1215
21	L	0.27	0/969	0.64	0/1300
22	M	0.31	0/900	0.64	0/1204
23	N	0.26	0/817	0.62	0/1088
24	O	0.24	0/722	0.63	0/964
25	P	0.26	0/659	0.62	0/884
26	Q	0.27	0/657	0.61	0/881
27	R	0.30	0/635	0.65	0/849
28	S	0.26	0/680	0.54	0/915
29	T	0.25	0/676	0.55	0/895
30	U	0.30	0/592	0.64	0/785
31	V	0.26	0/727	0.80	0/1132

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	W	0.34	1/1585 (0.1%)	0.86	4/2467 (0.2%)
33	X	0.35	1/1728 (0.1%)	0.91	1/2686 (0.0%)
34	Y	0.43	1/1672 (0.1%)	0.97	7/2599 (0.3%)
35	Z	0.25	0/1334	0.52	0/1799
36	a	0.24	0/1033	0.50	0/1387
37	b	0.26	0/2121	0.63	1/2852 (0.0%)
38	c	0.26	0/1586	0.56	0/2134
39	d	0.25	0/1571	0.53	0/2113
40	e	0.25	0/1444	0.55	0/1937
41	f	0.25	0/1343	0.55	0/1816
42	g	0.25	0/434	0.54	0/576
43	h	0.27	0/1104	0.60	0/1474
44	i	0.25	0/1121	0.54	0/1515
45	j	0.27	0/1037	0.55	0/1400
46	k	0.27	0/993	0.56	0/1341
47	l	0.29	0/380	0.65	0/498
48	m	0.25	0/1152	0.55	0/1551
49	n	0.27	0/955	0.63	0/1279
50	o	0.27	0/1062	0.62	0/1413
51	p	0.82	0/36	1.05	0/48
52	q	0.26	0/973	0.61	0/1301
53	r	0.25	0/901	0.61	0/1209
54	s	0.26	0/929	0.56	0/1242
55	t	0.25	0/960	0.53	0/1278
56	u	0.26	0/829	0.59	0/1107
57	v	0.24	0/864	0.57	0/1156
58	w	0.25	0/744	0.54	0/994
59	x	0.26	0/787	0.54	0/1051
60	y	0.26	0/766	0.54	0/1025
61	z	0.25	0/642	0.56	0/848
All	All	0.25	4/164625 (0.0%)	0.71	126/245793 (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
13	D	0	1
19	J	0	1
20	K	0	1
24	O	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
25	P	0	1
29	T	0	2
39	d	0	1
41	f	0	1
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	Y	1	G	OP3-P	-7.60	1.52	1.61
8	7	1	G	OP3-P	-7.55	1.52	1.61
32	W	1	G	OP3-P	-7.52	1.52	1.61
33	X	1	G	OP3-P	-7.50	1.52	1.61

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	7	1129	A	P-O3'-C3'	-12.54	104.65	119.70
8	7	2605	PSU	P-O3'-C3'	-11.15	106.32	119.70
10	A	1407	5MC	P-O3'-C3'	-10.99	106.51	119.70
8	7	2453	A	P-O3'-C3'	-10.77	106.78	119.70
10	A	1408	A	P-O3'-C3'	-10.70	106.86	119.70

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	D	104	ARG	Sidechain
19	J	48	ARG	Sidechain
20	K	98	ARG	Sidechain
24	O	84	ARG	Sidechain
25	P	51	ARG	Sidechain

5.2 Too-close contacts

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

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	0	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
2	1	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
3	2	61/63 (97%)	60 (98%)	0	1 (2%)	9	36
4	3	56/59 (95%)	49 (88%)	5 (9%)	2 (4%)	3	20
5	4	65/70 (93%)	49 (75%)	16 (25%)	0	100	100
6	5	54/57 (95%)	54 (100%)	0	0	100	100
7	6	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
11	B	222/241 (92%)	209 (94%)	12 (5%)	1 (0%)	29	61
12	C	210/233 (90%)	208 (99%)	2 (1%)	0	100	100
13	D	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
14	E	156/167 (93%)	151 (97%)	5 (3%)	0	100	100
15	F	104/135 (77%)	103 (99%)	1 (1%)	0	100	100
16	G	153/179 (86%)	149 (97%)	4 (3%)	0	100	100
17	H	127/130 (98%)	127 (100%)	0	0	100	100
18	I	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
19	J	98/103 (95%)	93 (95%)	5 (5%)	0	100	100
20	K	116/129 (90%)	102 (88%)	11 (10%)	3 (3%)	5	27
21	L	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
22	M	113/118 (96%)	106 (94%)	7 (6%)	0	100	100
23	N	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
24	O	86/89 (97%)	83 (96%)	2 (2%)	1 (1%)	13	42
25	P	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
26	Q	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
27	R	72/75 (96%)	63 (88%)	7 (10%)	2 (3%)	5	25
28	S	81/92 (88%)	80 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	T	84/87 (97%)	84 (100%)	0	0	100	100
30	U	68/71 (96%)	61 (90%)	7 (10%)	0	100	100
35	Z	168/557 (30%)	161 (96%)	7 (4%)	0	100	100
36	a	130/234 (56%)	126 (97%)	4 (3%)	0	100	100
37	b	269/273 (98%)	262 (97%)	6 (2%)	1 (0%)	34	66
38	c	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
39	d	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
40	e	176/179 (98%)	171 (97%)	5 (3%)	0	100	100
41	f	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
42	g	50/55 (91%)	50 (100%)	0	0	100	100
43	h	135/136 (99%)	134 (99%)	1 (1%)	0	100	100
44	i	147/149 (99%)	132 (90%)	14 (10%)	1 (1%)	22	54
45	j	133/165 (81%)	122 (92%)	11 (8%)	0	100	100
46	k	132/142 (93%)	124 (94%)	8 (6%)	0	100	100
47	l	44/46 (96%)	44 (100%)	0	0	100	100
48	m	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
49	n	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
50	o	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
51	p	4/18 (22%)	3 (75%)	1 (25%)	0	100	100
52	q	118/127 (93%)	113 (96%)	5 (4%)	0	100	100
53	r	114/117 (97%)	105 (92%)	7 (6%)	2 (2%)	8	35
54	s	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
55	t	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
56	u	101/103 (98%)	93 (92%)	7 (7%)	1 (1%)	15	46
57	v	108/110 (98%)	96 (89%)	11 (10%)	1 (1%)	17	48
58	w	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
59	x	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
60	y	92/94 (98%)	92 (100%)	0	0	100	100
61	z	82/85 (96%)	77 (94%)	5 (6%)	0	100	100
All	All	6208/7029 (88%)	5944 (96%)	248 (4%)	16 (0%)	44	71

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
57	v	64	ALA
4	3	21	LYS
20	K	70	CYS
20	K	80	LYS
53	r	5	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	34/34 (100%)	34 (100%)	0	100	100
2	1	67/68 (98%)	65 (97%)	2 (3%)	41	68
3	2	55/55 (100%)	55 (100%)	0	100	100
4	3	48/49 (98%)	47 (98%)	1 (2%)	53	75
5	4	60/62 (97%)	59 (98%)	1 (2%)	60	78
6	5	47/48 (98%)	47 (100%)	0	100	100
7	6	51/52 (98%)	51 (100%)	0	100	100
11	B	186/199 (94%)	186 (100%)	0	100	100
12	C	172/190 (90%)	170 (99%)	2 (1%)	71	83
13	D	172/173 (99%)	171 (99%)	1 (1%)	86	91
14	E	120/126 (95%)	120 (100%)	0	100	100
15	F	92/116 (79%)	92 (100%)	0	100	100
16	G	128/147 (87%)	127 (99%)	1 (1%)	81	89
17	H	104/105 (99%)	104 (100%)	0	100	100
18	I	105/107 (98%)	105 (100%)	0	100	100
19	J	88/90 (98%)	88 (100%)	0	100	100
20	K	91/99 (92%)	91 (100%)	0	100	100
21	L	103/104 (99%)	103 (100%)	0	100	100
22	M	93/96 (97%)	90 (97%)	3 (3%)	39	67
23	N	83/84 (99%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	O	76/77 (99%)	76 (100%)	0	100	100
25	P	65/65 (100%)	65 (100%)	0	100	100
26	Q	74/78 (95%)	74 (100%)	0	100	100
27	R	64/65 (98%)	64 (100%)	0	100	100
28	S	72/79 (91%)	72 (100%)	0	100	100
29	T	65/66 (98%)	65 (100%)	0	100	100
30	U	59/61 (97%)	59 (100%)	0	100	100
35	Z	143/461 (31%)	143 (100%)	0	100	100
36	a	110/181 (61%)	110 (100%)	0	100	100
37	b	216/218 (99%)	216 (100%)	0	100	100
38	c	164/164 (100%)	163 (99%)	1 (1%)	86	91
39	d	165/165 (100%)	165 (100%)	0	100	100
40	e	149/150 (99%)	147 (99%)	2 (1%)	69	82
41	f	137/138 (99%)	136 (99%)	1 (1%)	84	90
42	g	47/49 (96%)	47 (100%)	0	100	100
43	h	110/109 (101%)	109 (99%)	1 (1%)	78	87
44	i	114/114 (100%)	113 (99%)	1 (1%)	78	87
45	j	103/123 (84%)	102 (99%)	1 (1%)	76	86
46	k	104/110 (94%)	104 (100%)	0	100	100
47	l	38/38 (100%)	38 (100%)	0	100	100
48	m	116/116 (100%)	116 (100%)	0	100	100
49	n	104/104 (100%)	104 (100%)	0	100	100
50	o	103/103 (100%)	103 (100%)	0	100	100
51	p	4/4 (100%)	4 (100%)	0	100	100
52	q	100/103 (97%)	99 (99%)	1 (1%)	76	86
53	r	86/87 (99%)	86 (100%)	0	100	100
54	s	99/100 (99%)	99 (100%)	0	100	100
55	t	89/90 (99%)	89 (100%)	0	100	100
56	u	84/84 (100%)	84 (100%)	0	100	100
57	v	93/93 (100%)	93 (100%)	0	100	100
58	w	80/84 (95%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
59	x	83/85 (98%)	82 (99%)	1 (1%)	71	83
60	y	78/78 (100%)	78 (100%)	0	100	100
61	z	62/63 (98%)	62 (100%)	0	100	100
All	All	5155/5709 (90%)	5135 (100%)	20 (0%)	91	95

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	f	69	ARG
45	j	87	GLU
59	x	6	ARG
52	q	2	ARG
13	D	44	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
41	f	101	ASN
46	k	105	GLN
57	v	61	ASN
54	s	10	GLN
20	K	119	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	1538/1542 (99%)	248 (16%)	20 (1%)
31	V	29/30 (96%)	14 (48%)	3 (10%)
32	W	74/76 (97%)	23 (31%)	2 (2%)
33	X	74/78 (94%)	25 (33%)	4 (5%)
34	Y	73/76 (96%)	25 (34%)	7 (9%)
8	7	2898/2903 (99%)	485 (16%)	55 (1%)
9	8	119/120 (99%)	14 (11%)	1 (0%)
All	All	4805/4825 (99%)	834 (17%)	92 (1%)

5 of 834 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	10	A

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Mol	Chain	Res	Type
8	7	15	G
8	7	28	A
8	7	34	U
8	7	44	A

5 of 92 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	84	U
10	A	1201	A
10	A	181	A
10	A	522	C
10	A	1432	G

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

55 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
10	5MC	A	1407	10	18,22,23	0.33	0	26,32,35	0.58	0
8	PSU	7	2605	8	18,21,22	0.86	1 (5%)	22,30,33	0.54	0
34	4SU	Y	7	34	18,21,22	0.37	0	26,30,33	1.35	3 (11%)
10	G7M	A	527	10	20,26,27	1.13	3 (15%)	17,39,42	0.39	0
8	PSU	7	2504	8	18,21,22	0.87	1 (5%)	22,30,33	0.61	0
32	G7M	W	46	32	20,26,27	2.81	7 (35%)	17,39,42	1.13	1 (5%)
32	H2U	W	16	32	18,21,22	3.08	5 (27%)	21,30,33	2.03	5 (23%)
8	OMU	7	2552	8	19,22,23	0.21	0	26,31,34	0.50	0
10	MA6	A	1519	10	18,26,27	0.75	1 (5%)	19,38,41	0.42	0
8	5MU	7	747	8	19,22,23	0.23	0	28,32,35	0.33	0
10	2MG	A	1516	10	18,26,27	1.04	2 (11%)	16,38,41	0.73	0
10	UR3	A	1498	10	19,22,23	0.30	0	26,32,35	0.67	0
8	2MG	7	2445	8	18,26,27	1.02	2 (11%)	16,38,41	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	5MU	X	71	33	19,22,23	0.25	0	28,32,35	0.27	0
32	5MU	W	54	32	19,22,23	0.25	0	28,32,35	0.37	0
33	PSU	X	72	33	18,21,22	0.87	1 (5%)	22,30,33	0.61	0
10	4OC	A	1402	10	20,23,24	0.38	0	26,32,35	0.41	0
32	PSU	W	39	32	18,21,22	4.65	8 (44%)	22,30,33	1.89	5 (22%)
8	2MA	7	2503	8	17,25,26	0.94	2 (11%)	17,37,40	0.95	1 (5%)
8	PSU	7	2580	8	18,21,22	0.85	1 (5%)	22,30,33	0.97	1 (4%)
8	3TD	7	1915	8	19,22,23	0.83	1 (5%)	21,32,35	0.59	0
33	RSP	X	33	33	17,21,22	4.18	7 (41%)	22,30,33	0.72	0
8	PSU	7	2604	8	18,21,22	0.87	1 (5%)	22,30,33	0.67	0
32	H2U	W	17	32	18,21,22	3.07	5 (27%)	21,30,33	2.01	5 (23%)
33	H2U	X	20	33	18,21,22	3.07	5 (27%)	21,30,33	2.05	4 (19%)
8	2MG	7	1835	8	18,26,27	1.03	2 (11%)	16,38,41	0.79	0
8	PSU	7	746	8,63	18,21,22	0.88	1 (5%)	22,30,33	0.62	0
8	H2U	7	2449	8	18,21,22	4.41	14 (77%)	21,30,33	2.21	5 (23%)
10	5MC	A	967	10	18,22,23	4.04	7 (38%)	26,32,35	1.01	2 (7%)
8	1MG	7	745	8	18,26,27	0.97	1 (5%)	19,39,42	0.71	0
34	6MZ	Y	37	34	18,25,26	0.66	0	16,36,39	0.58	1 (6%)
10	PSU	A	516	10,63	18,21,22	0.89	1 (5%)	22,30,33	1.14	3 (13%)
8	G7M	7	2069	8	20,26,27	1.12	3 (15%)	17,39,42	0.53	0
32	PSU	W	32	32	18,21,22	4.66	8 (44%)	22,30,33	1.82	5 (22%)
33	12A	X	38	10,33	29,36,37	4.79	16 (55%)	34,52,55	3.02	9 (26%)
34	5MU	Y	54	34	19,22,23	0.24	0	28,32,35	0.21	0
34	PSU	Y	55	34	18,21,22	0.88	1 (5%)	22,30,33	0.58	0
32	PSU	W	55	32	18,21,22	0.90	1 (5%)	22,30,33	0.70	0
8	5MC	7	1962	8	18,22,23	0.33	0	26,32,35	0.52	0
32	H2U	W	20	32	18,21,22	3.07	5 (27%)	21,30,33	2.01	5 (23%)
34	CM0	Y	34	34	23,26,27	1.11	1 (4%)	27,37,40	0.56	0
32	MIA	W	37	32	24,31,32	2.36	3 (12%)	26,44,47	2.55	7 (26%)
10	2MG	A	966	10	18,26,27	2.83	7 (38%)	16,38,41	1.43	4 (25%)
10	2MG	A	1207	10	18,26,27	1.01	3 (16%)	16,38,41	0.88	1 (6%)
8	6MZ	7	2030	8	18,25,26	0.73	0	16,36,39	1.02	2 (12%)
8	OMG	7	2251	8,32	18,26,27	1.02	2 (11%)	19,38,41	0.69	0
8	PSU	7	2457	8	18,21,22	0.85	1 (5%)	22,30,33	0.78	1 (4%)
8	OMC	7	2498	8,63	19,22,23	0.30	0	26,31,34	0.34	0
32	4SU	W	8	32	18,21,22	3.79	7 (38%)	26,30,33	2.23	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PSU	7	955	8	18,21,22	0.86	1 (5%)	22,30,33	0.59	0
8	5MU	7	1939	8,63	19,22,23	0.27	0	28,32,35	0.40	0
10	MA6	A	1518	10	18,26,27	0.73	0	19,38,41	0.54	0
33	4SU	X	8	33	18,21,22	3.81	7 (38%)	26,30,33	2.26	4 (15%)
34	7MG	Y	46	34	22,26,27	3.88	10 (45%)	29,39,42	2.08	9 (31%)
8	6MZ	7	1618	8	18,25,26	0.68	0	16,36,39	0.83	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
10	5MC	A	1407	10	-	0/7/25/26	0/2/2/2
8	PSU	7	2605	8	-	0/7/25/26	0/2/2/2
34	4SU	Y	7	34	-	0/7/25/26	0/2/2/2
10	G7M	A	527	10	-	2/3/25/26	0/3/3/3
8	PSU	7	2504	8	-	0/7/25/26	0/2/2/2
32	G7M	W	46	32	-	3/3/25/26	0/3/3/3
32	H2U	W	16	32	-	1/7/38/39	0/2/2/2
8	OMU	7	2552	8	-	0/9/27/28	0/2/2/2
10	MA6	A	1519	10	-	4/7/29/30	0/3/3/3
8	5MU	7	747	8	-	0/7/25/26	0/2/2/2
10	2MG	A	1516	10	-	1/5/27/28	0/3/3/3
10	UR3	A	1498	10	-	2/7/25/26	0/2/2/2
8	2MG	7	2445	8	-	2/5/27/28	0/3/3/3
33	5MU	X	71	33	-	0/7/25/26	0/2/2/2
32	5MU	W	54	32	-	4/7/25/26	0/2/2/2
33	PSU	X	72	33	-	0/7/25/26	0/2/2/2
10	4OC	A	1402	10	-	0/9/29/30	0/2/2/2
32	PSU	W	39	32	-	0/7/25/26	0/2/2/2
8	2MA	7	2503	8	-	0/3/25/26	0/3/3/3
8	PSU	7	2580	8	-	0/7/25/26	0/2/2/2
8	3TD	7	1915	8	-	0/7/25/26	0/2/2/2
33	RSP	X	33	33	-	1/7/25/26	0/2/2/2
8	PSU	7	2604	8	-	0/7/25/26	0/2/2/2
32	H2U	W	17	32	-	6/7/38/39	0/2/2/2
33	H2U	X	20	33	-	5/7/38/39	0/2/2/2
8	2MG	7	1835	8	-	1/5/27/28	0/3/3/3
8	PSU	7	746	8,63	-	6/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	H2U	7	2449	8	-	0/7/38/39	0/2/2/2
10	5MC	A	967	10	-	0/7/25/26	0/2/2/2
8	1MG	7	745	8	-	0/3/25/26	0/3/3/3
34	6MZ	Y	37	34	-	0/5/27/28	0/3/3/3
10	PSU	A	516	10,63	-	0/7/25/26	0/2/2/2
8	G7M	7	2069	8	-	1/3/25/26	0/3/3/3
32	PSU	W	32	32	-	0/7/25/26	0/2/2/2
33	12A	X	38	10,33	-	10/21/43/44	0/3/3/3
34	5MU	Y	54	34	-	0/7/25/26	0/2/2/2
34	PSU	Y	55	34	-	4/7/25/26	0/2/2/2
32	PSU	W	55	32	-	0/7/25/26	0/2/2/2
8	5MC	7	1962	8	-	4/7/25/26	0/2/2/2
32	H2U	W	20	32	-	3/7/38/39	0/2/2/2
34	CM0	Y	34	34	-	2/12/30/31	0/2/2/2
32	MIA	W	37	32	-	4/11/33/34	0/3/3/3
10	2MG	A	966	10	-	0/5/27/28	0/3/3/3
10	2MG	A	1207	10	-	0/5/27/28	0/3/3/3
8	6MZ	7	2030	8	-	1/5/27/28	0/3/3/3
8	OMG	7	2251	8,32	-	3/5/27/28	0/3/3/3
8	PSU	7	2457	8	-	0/7/25/26	0/2/2/2
8	OMC	7	2498	8,63	-	2/9/27/28	0/2/2/2
32	4SU	W	8	32	-	2/7/25/26	0/2/2/2
8	PSU	7	955	8	-	0/7/25/26	0/2/2/2
8	5MU	7	1939	8,63	-	0/7/25/26	0/2/2/2
10	MA6	A	1518	10	-	0/7/29/30	0/3/3/3
33	4SU	X	8	33	-	2/7/25/26	0/2/2/2
34	7MG	Y	46	34	-	1/7/37/38	0/3/3/3
8	6MZ	7	1618	8	-	2/5/27/28	0/3/3/3

The worst 5 of 155 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	X	38	12A	C2-S2	14.59	1.88	1.75
32	W	32	PSU	C6-C5	12.17	1.49	1.35
32	W	39	PSU	C6-C5	12.14	1.49	1.35
33	X	33	RSP	C2-N3	11.88	1.49	1.36
33	X	38	12A	C2'-C3'	-10.51	1.24	1.53

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	X	38	12A	N6-C6-N1	-11.23	98.72	118.84
32	W	37	MIA	C11-S10-C2	9.96	109.70	102.27
33	X	38	12A	C2M-S2-C2	9.30	109.21	102.27
33	X	8	4SU	C4-N3-C2	-7.94	119.63	127.34
32	W	8	4SU	C4-N3-C2	-7.83	119.74	127.34

There are no chirality outliers.

5 of 79 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	527	G7M	O4'-C4'-C5'-O5'
10	A	527	G7M	C3'-C4'-C5'-O5'
10	A	1516	2MG	N3-C2-N2-CM2
10	A	1519	MA6	C5-C6-N6-C10
8	7	746	PSU	C2'-C1'-C5-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 264 ligands modelled in this entry, 262 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
64	ATP	7	3193	-	26,33,33	3.48	10 (38%)	31,52,52	2.24	7 (22%)
64	ATP	7	3194	-	26,33,33	3.46	10 (38%)	31,52,52	2.19	7 (22%)

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
64	ATP	7	3193	-	-	6/18/38/38	0/3/3/3
64	ATP	7	3194	-	-	4/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	7	3194	ATP	C2'-C3'	-10.66	1.24	1.53
64	7	3193	ATP	C2'-C3'	-10.60	1.24	1.53
64	7	3194	ATP	O4'-C1'	7.46	1.51	1.41
64	7	3193	ATP	O4'-C1'	7.46	1.51	1.41
64	7	3193	ATP	O4'-C4'	-6.45	1.30	1.45

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	7	3193	ATP	C5-C6-N6	6.65	130.46	120.35
64	7	3194	ATP	C5-C6-N6	6.60	130.39	120.35
64	7	3194	ATP	N3-C2-N1	-5.50	120.08	128.68
64	7	3193	ATP	N3-C2-N1	-5.46	120.14	128.68
64	7	3193	ATP	C1'-N9-C4	4.93	135.31	126.64

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

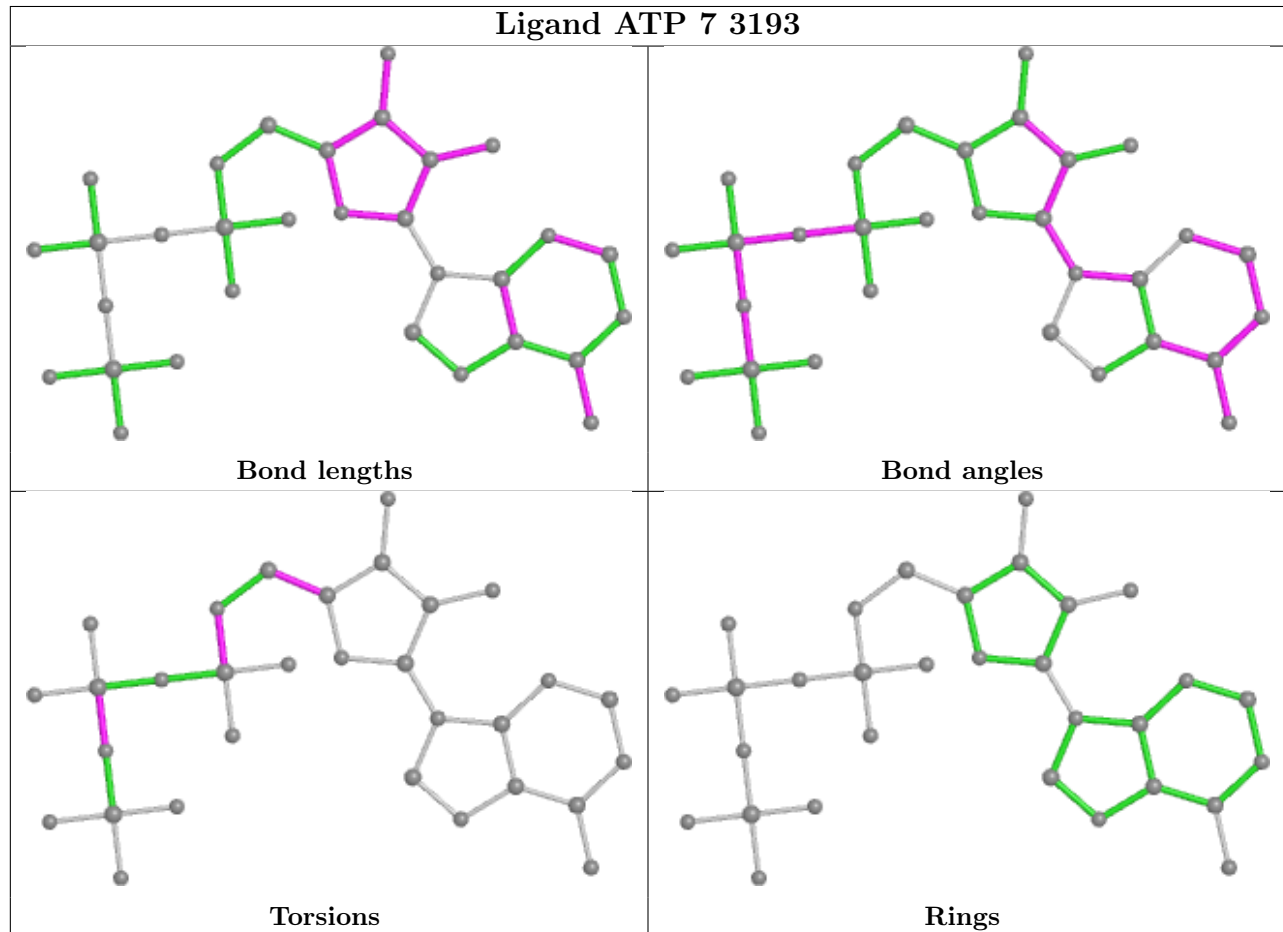
Mol	Chain	Res	Type	Atoms
64	7	3193	ATP	C5'-O5'-PA-O1A
64	7	3194	ATP	C5'-O5'-PA-O3A
64	7	3193	ATP	C3'-C4'-C5'-O5'
64	7	3193	ATP	C5'-O5'-PA-O3A
64	7	3193	ATP	C5'-O5'-PA-O2A

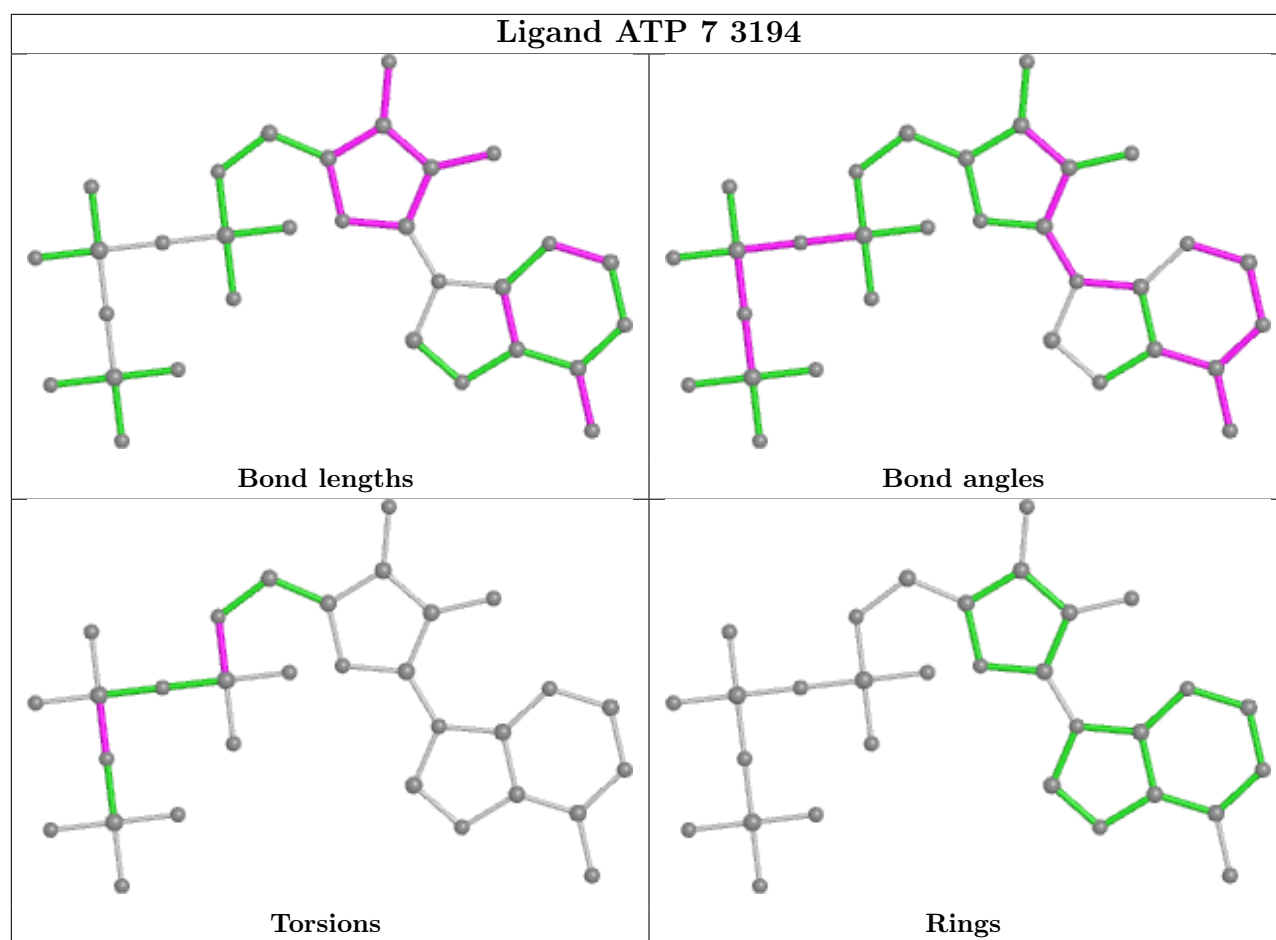
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
33	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	47:U	O3'	63:A	P	17.15

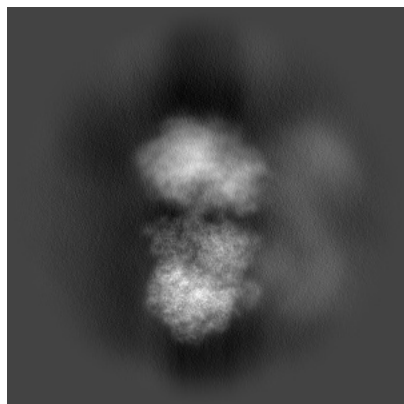
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17631. These allow visual inspection of the internal detail of the map and identification of artifacts.

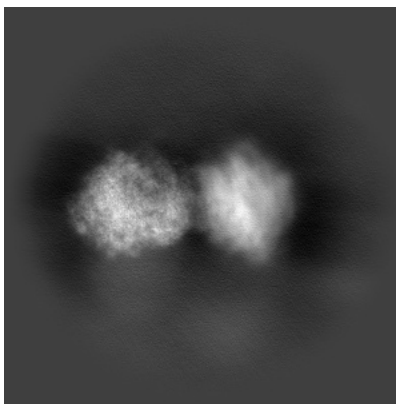
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

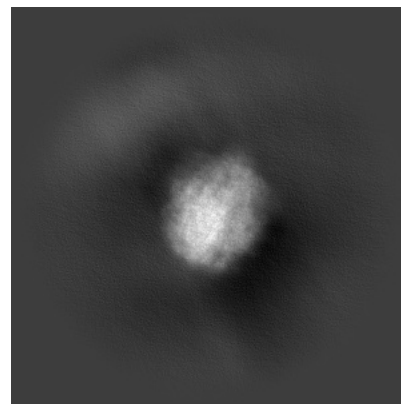
6.1.1 Primary map



X

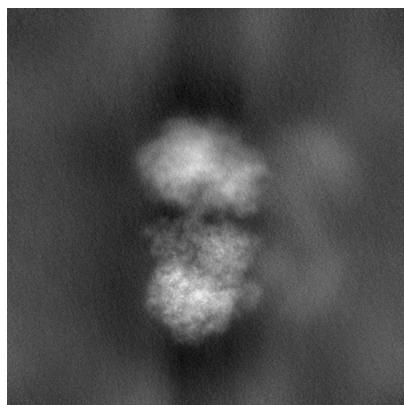


Y

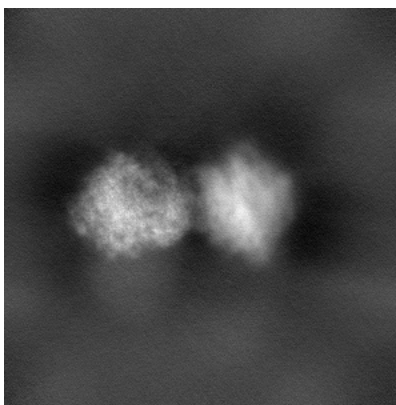


Z

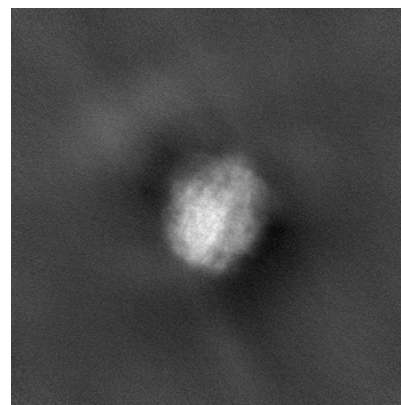
6.1.2 Raw map



X



Y

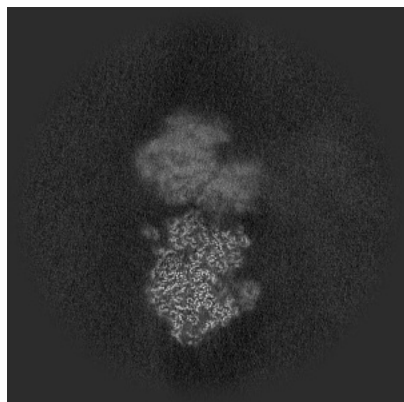


Z

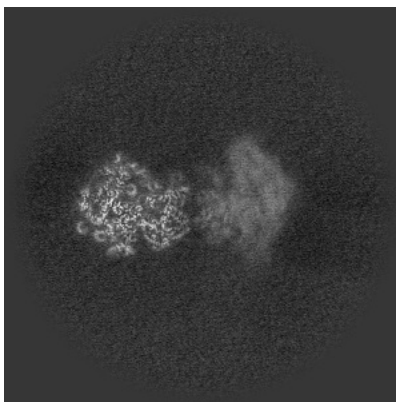
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

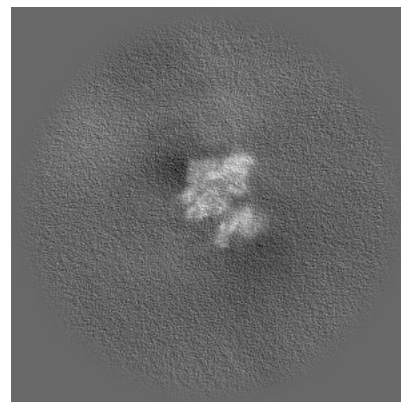
6.2.1 Primary map



X Index: 351

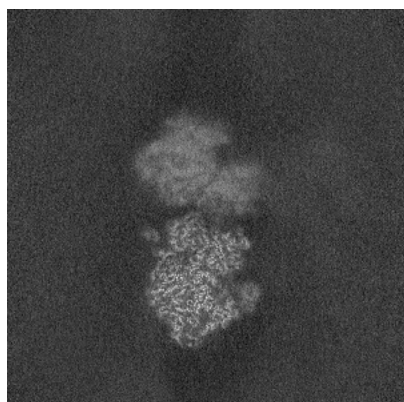


Y Index: 351

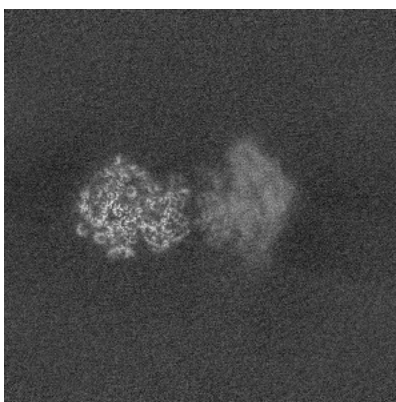


Z Index: 351

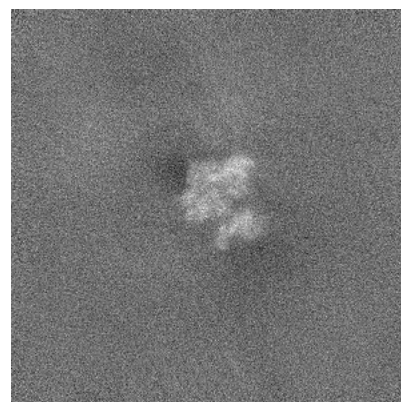
6.2.2 Raw map



X Index: 351



Y Index: 351

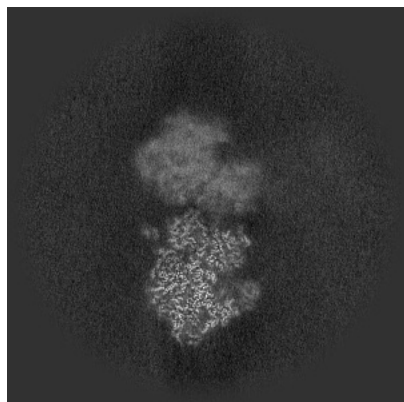


Z Index: 351

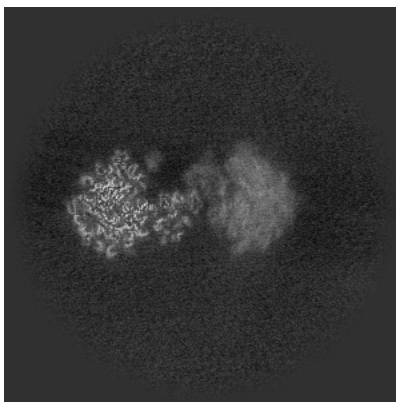
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

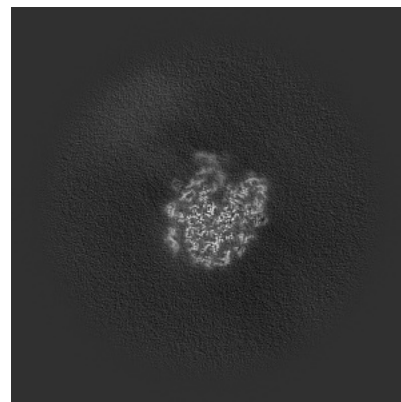
6.3.1 Primary map



X Index: 352

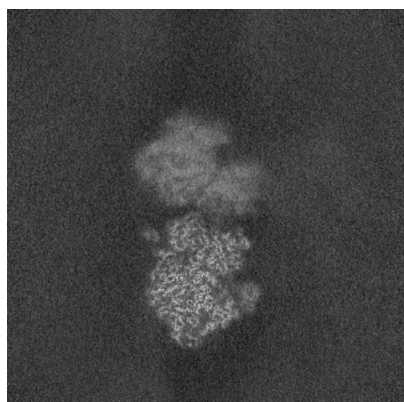


Y Index: 324

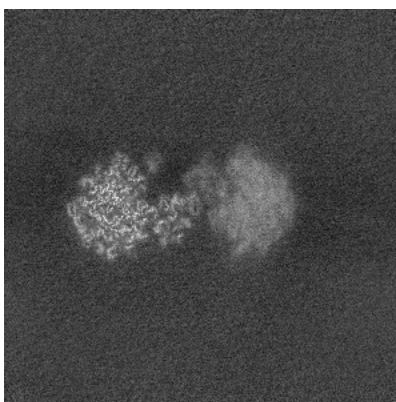


Z Index: 202

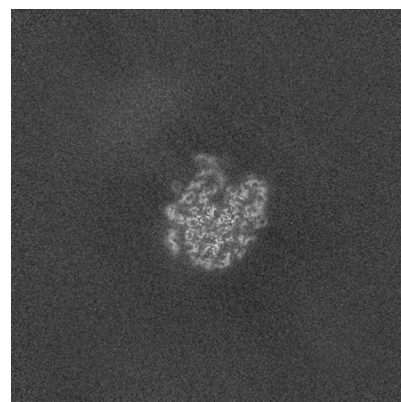
6.3.2 Raw map



X Index: 351



Y Index: 323

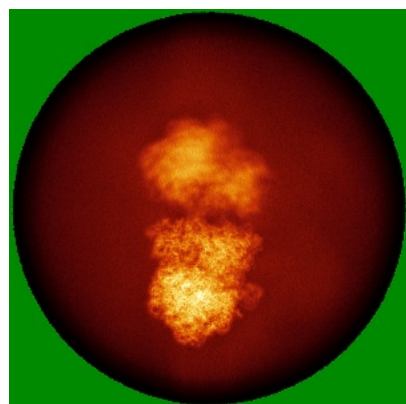


Z Index: 202

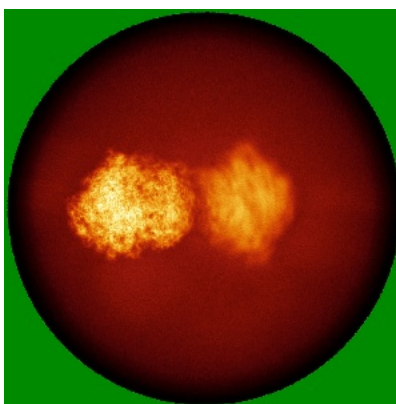
The images above show the largest variance slices of the map in three orthogonal directions.

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

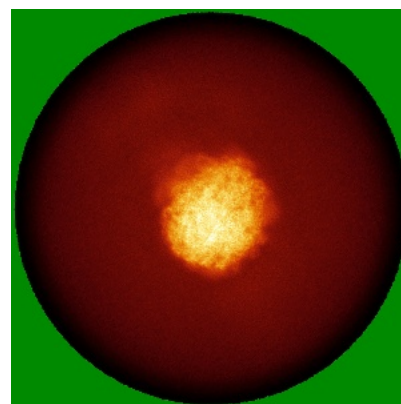
6.4.1 Primary map



X

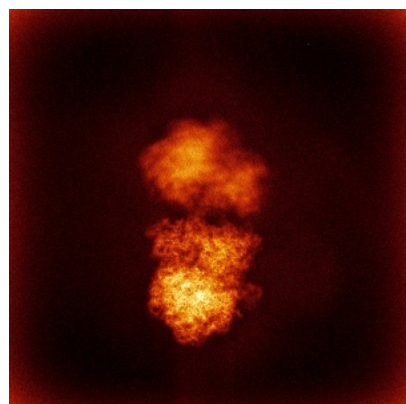


Y

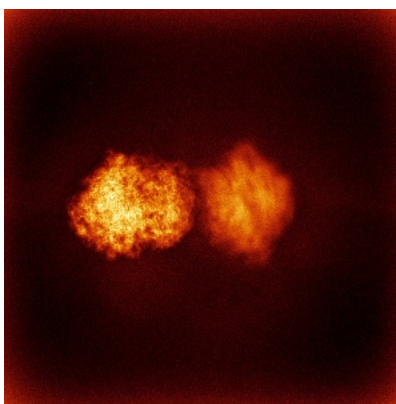


Z

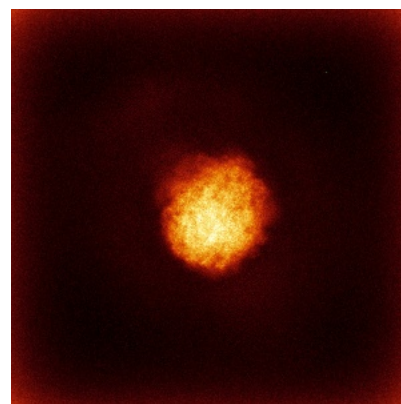
6.4.2 Raw map



X



Y

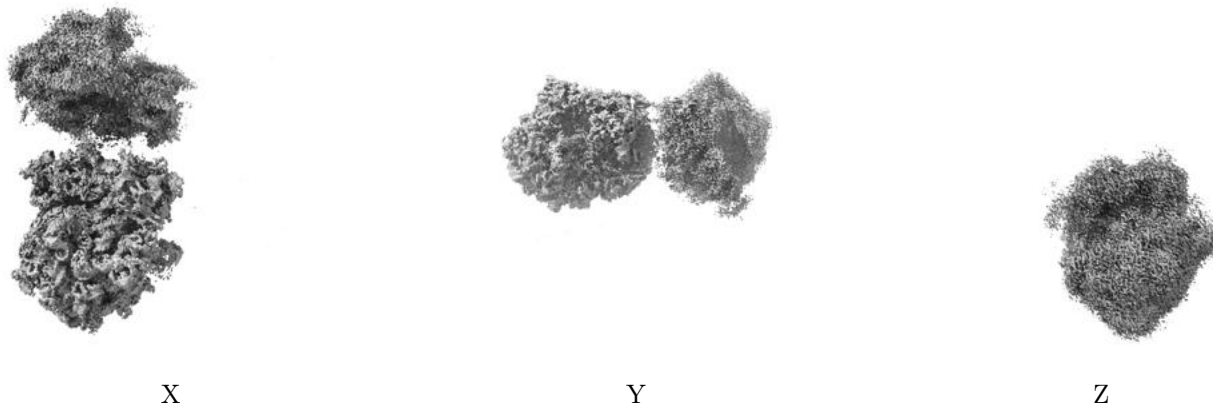


Z

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.

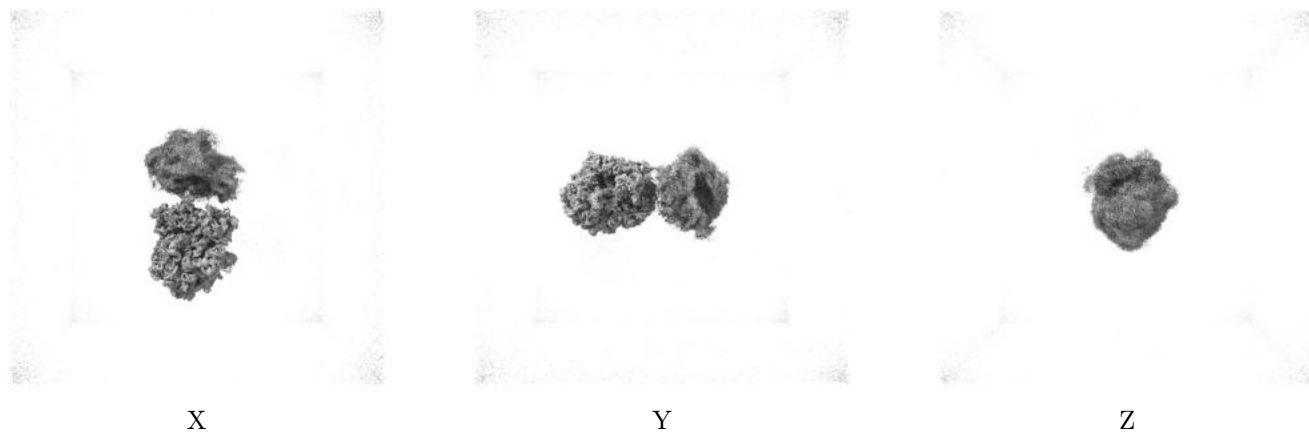
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.5. 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.

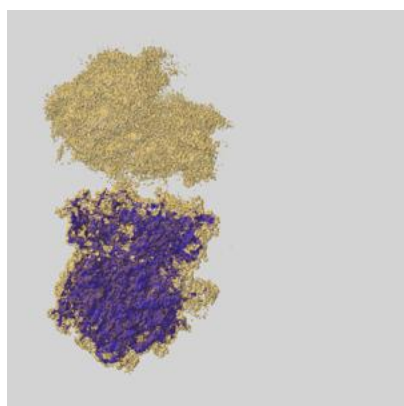
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

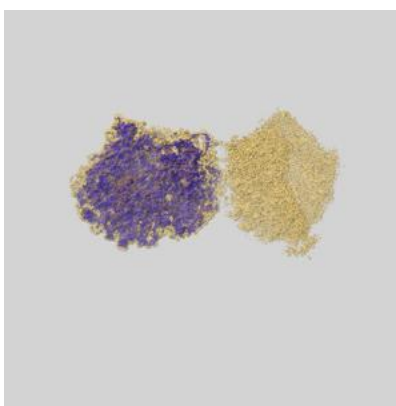
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

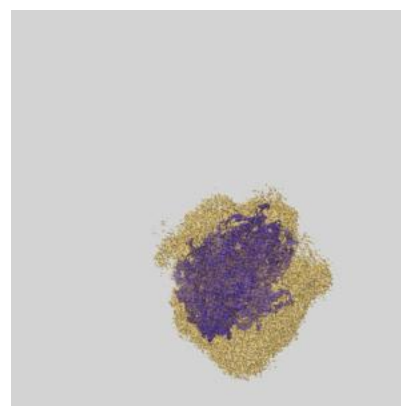
6.6.1 emd_17631_msk_1.map [i](#)



X



Y

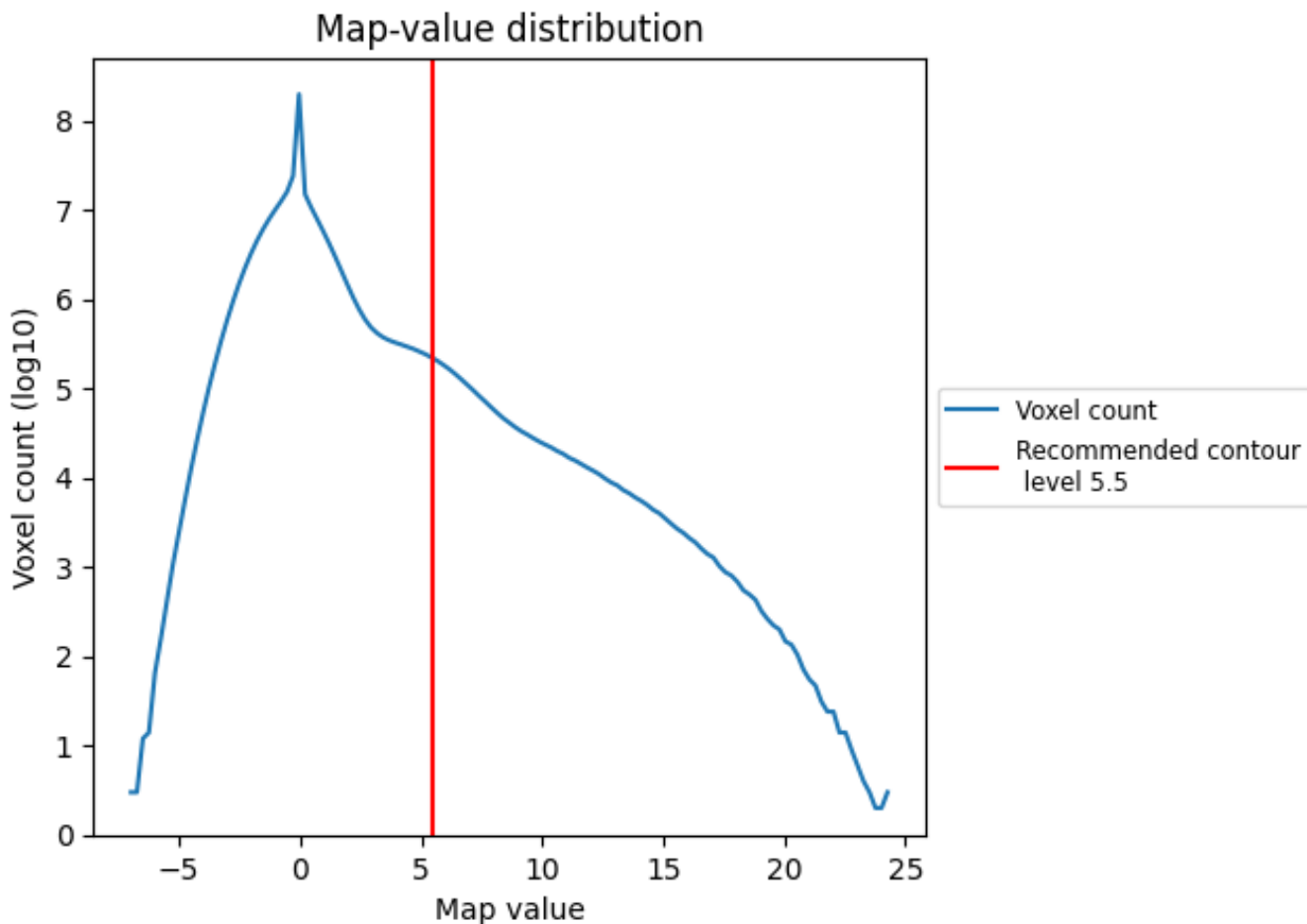


Z

7 Map analysis [i](#)

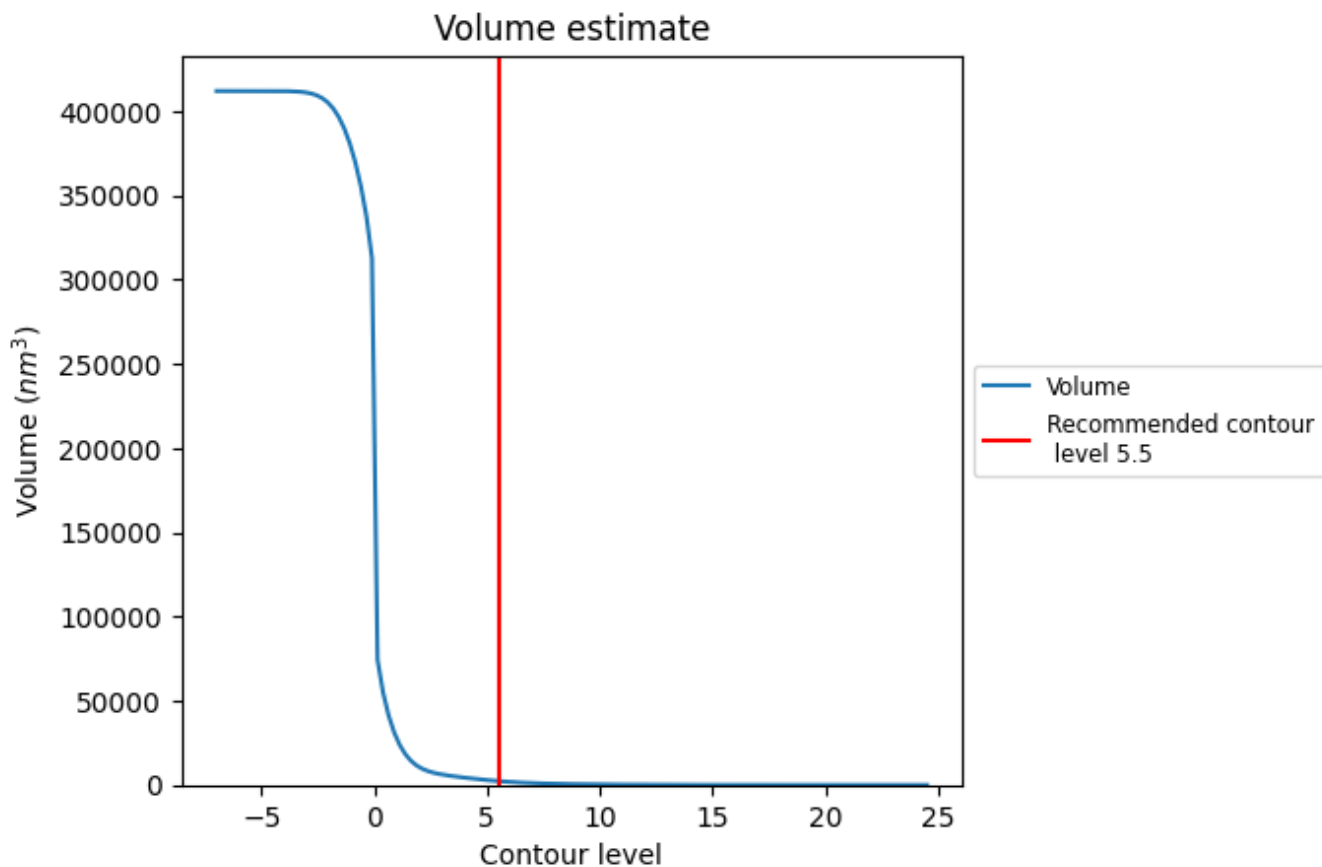
This section contains the results of statistical analysis of the map.

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.

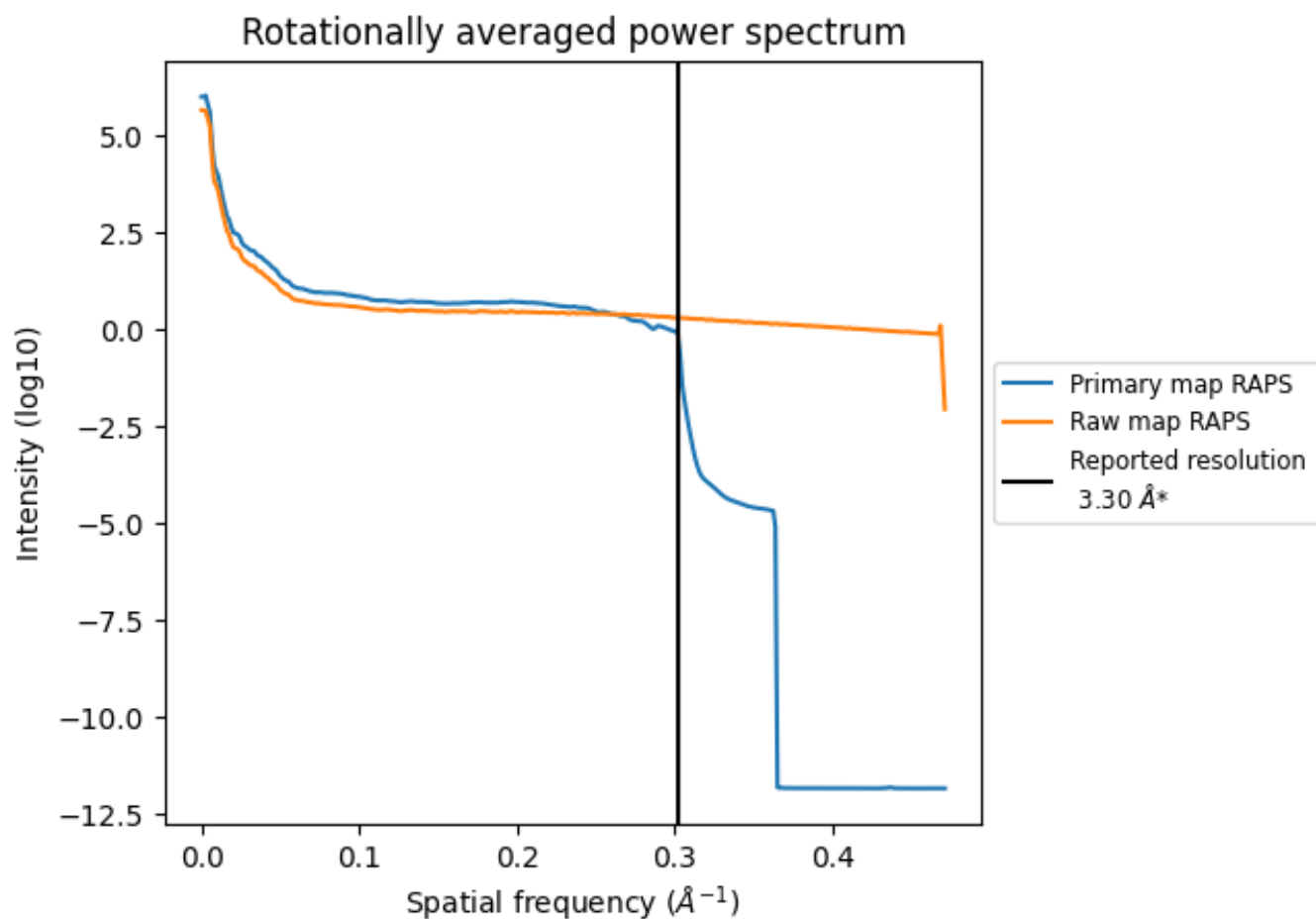
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 2321 nm³; this corresponds to an approximate mass of 2097 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

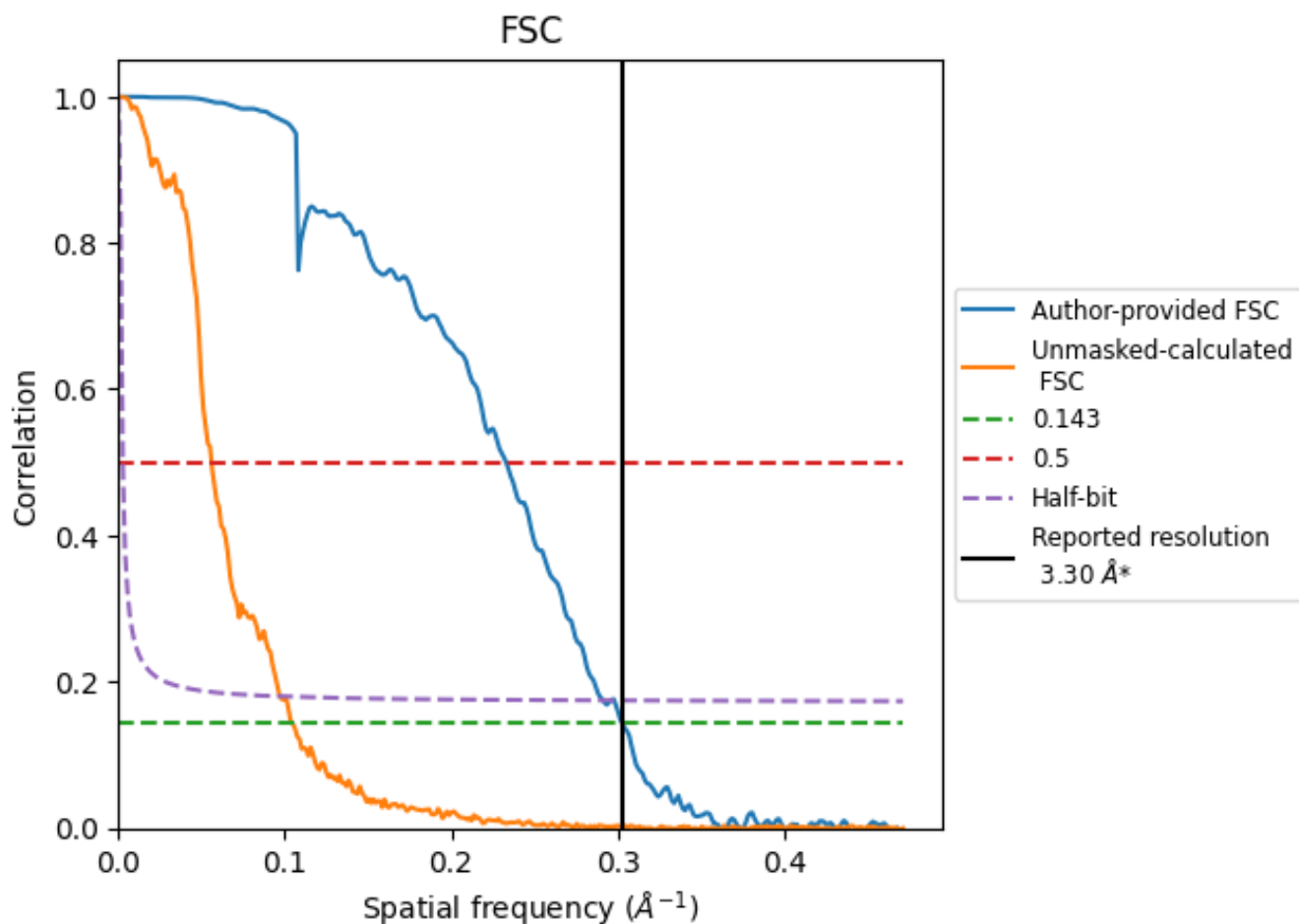


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

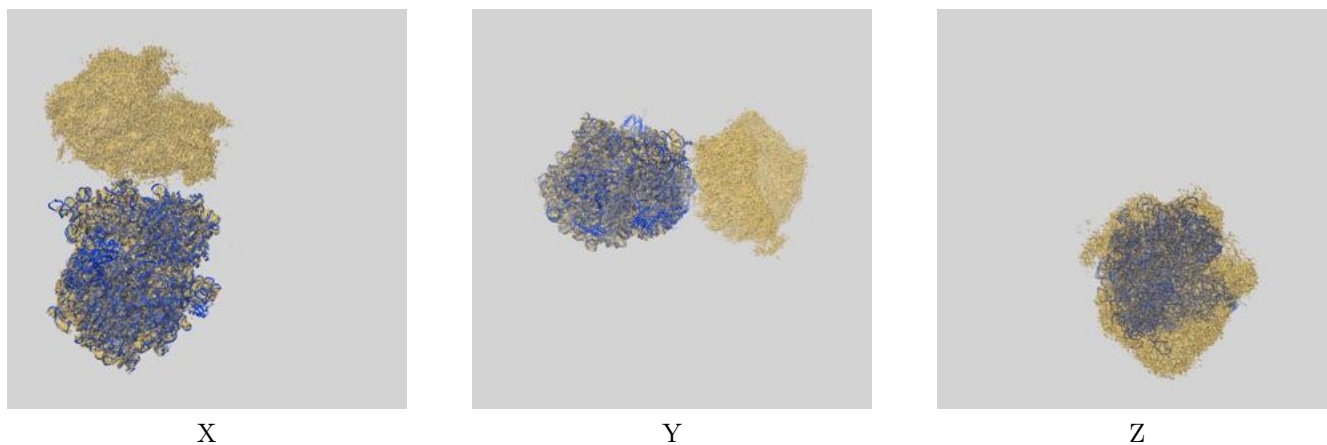
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	4.29	3.43
Unmasked-calculated*	9.55	17.86	10.29

*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 9.55 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

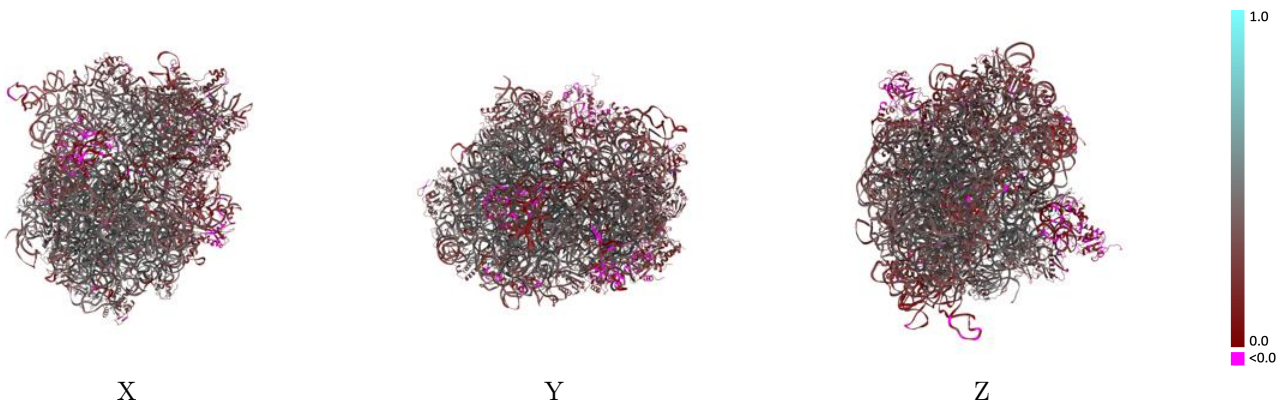
This section contains information regarding the fit between EMDB map EMD-17631 and PDB model 8PEG. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



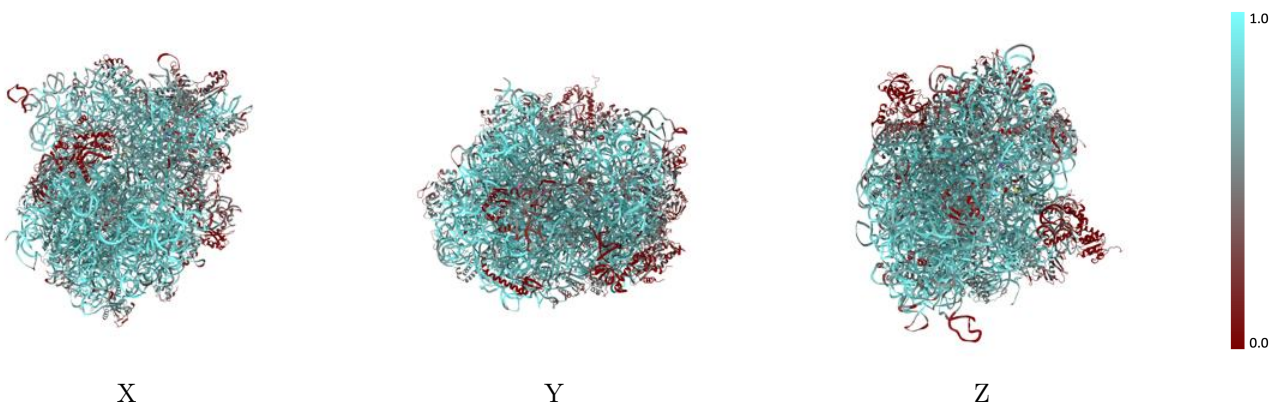
The images above show the 3D surface view of the map at the recommended contour level 5.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



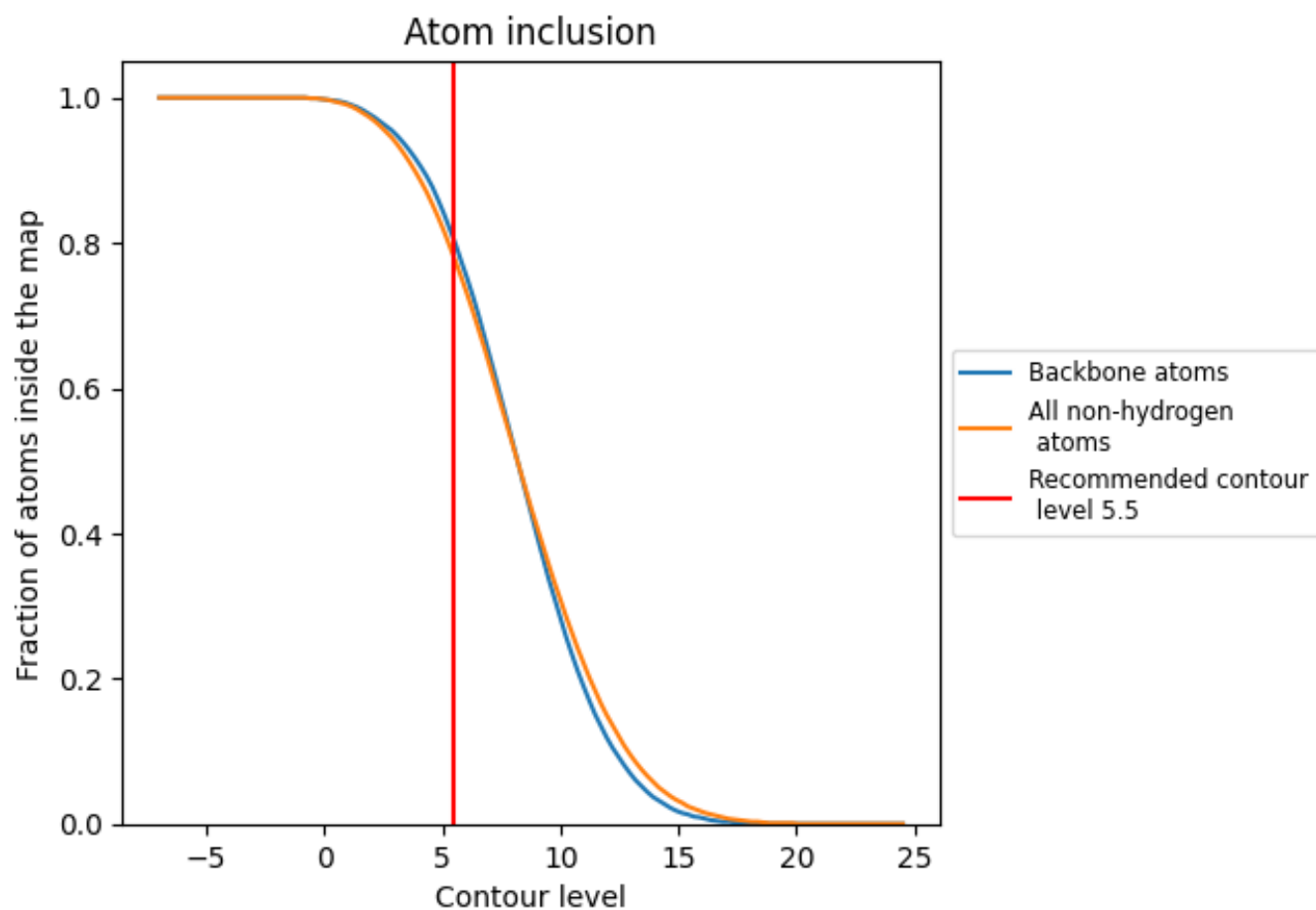
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 78% 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 (5.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7800	 0.3630
0	 0.7610	 0.4130
1	 0.8090	 0.4020
2	 0.6320	 0.3090
3	 0.7210	 0.3630
4	 0.3780	 0.2010
5	 0.7900	 0.3470
6	 0.8290	 0.4340
7	 0.9180	 0.4110
8	 0.8780	 0.3560
A	 0.8640	 0.3640
B	 0.3460	 0.2990
C	 0.5230	 0.3260
D	 0.3700	 0.2740
E	 0.5380	 0.3610
F	 0.4930	 0.3070
G	 0.5300	 0.2790
H	 0.5780	 0.3240
I	 0.5290	 0.2840
J	 0.4160	 0.2480
K	 0.5900	 0.3500
L	 0.6450	 0.3460
M	 0.5820	 0.2860
N	 0.5870	 0.2680
O	 0.6460	 0.3180
P	 0.4820	 0.2940
Q	 0.6110	 0.3030
R	 0.5390	 0.3110
S	 0.5630	 0.3100
T	 0.6430	 0.2560
U	 0.4550	 0.2610
V	 0.4770	 0.1880
W	 0.8510	 0.3100
X	 0.4590	 0.1490
Y	 0.7860	 0.3090



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Z	 0.0000	 0.0600
a	 0.0440	 0.0890
b	 0.8440	 0.4280
c	 0.6940	 0.4050
d	 0.6410	 0.3650
e	 0.5680	 0.2820
f	 0.4000	 0.2980
g	 0.6710	 0.3550
h	 0.6920	 0.3990
i	 0.1790	 0.2430
j	 0.0010	 0.0690
k	 0.0000	 0.0560
l	 0.9240	 0.4250
m	 0.7660	 0.3850
n	 0.6460	 0.4050
o	 0.6890	 0.3830
p	 0.8810	 0.3740
q	 0.8200	 0.3690
r	 0.6260	 0.3100
s	 0.6730	 0.3780
t	 0.7740	 0.4070
u	 0.5970	 0.3880
v	 0.7640	 0.4130
w	 0.7300	 0.3440
x	 0.6170	 0.3450
y	 0.5380	 0.3360
z	 0.8090	 0.3960