



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 06:30 PM EST

PDB ID : 3JAQ
EMDB ID : EMD-3049
Title : Structure of a partial yeast 48S preinitiation complex in open conformation
Authors : Llacer, J.L.; Hussain, T.; Ramakrishnan, V.
Deposited on : 2015-06-18
Resolution : 6.00 Å (reported)
Based on initial models : 3CW2, 1YFG, 3J81, 4U1E, 2D74

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:

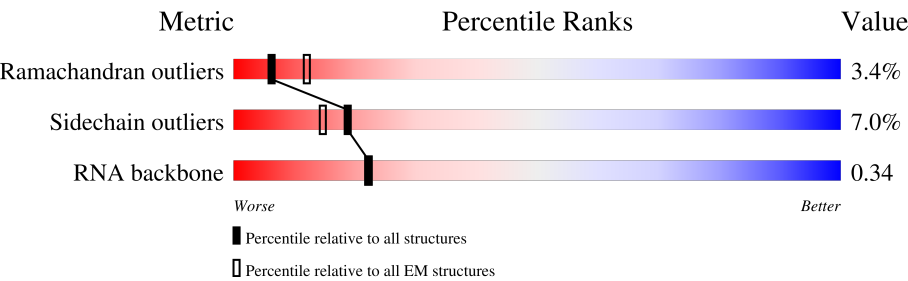
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 6.00 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	1	75	<div><div>45%</div><div>41%</div><div>13%</div></div>
2	2	1781	<div><div>53%</div><div>47%</div></div>
3	3	25	<div><div>8%</div><div>92%</div></div>
4	A	254	<div><div>73%</div><div>9%</div><div>18%</div></div>
5	B	255	<div><div>78%</div><div>9%</div><div>13%</div></div>
6	C	259	<div><div>6%</div><div>76%</div><div>7%</div><div>16%</div></div>
7	D	237	<div><div>9%</div><div>86%</div><div>8%</div><div>6%</div></div>
8	E	261	<div><div>5%</div><div>90%</div><div>9%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	F	227	
10	G	236	
11	H	190	
12	I	201	
13	J	188	
14	K	106	
15	L	156	
16	M	134	
17	N	151	
18	O	137	
19	P	142	
20	Q	143	
21	R	136	
22	S	146	
23	T	144	
24	U	117	
25	V	87	
26	W	130	
27	X	145	
28	Y	135	
29	Z	108	
30	a	119	
31	b	82	
32	c	67	
33	d	56	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	e	63	
35	f	150	
36	g	326	
37	h	25	
38	i	153	
39	j	304	
40	k	527	
41	l	285	
42	m	108	
43	o	92	
44	p	88	
45	q	347	
46	r	34	
47	s	52	

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 89768 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called Met-tRNAi.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	75	Total	C	N	O	P	0	0
			1639	734	298	531	76		

- Molecule 2 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1780	Total	C	N	O	P	0	0
			37797	16892	6658	12467	1780		

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	2	Total	C	N	O	P	0	0
			42	19	7	14	2		

- Molecule 4 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	208	Total	C	N	O	S	0	0
			1626	1040	286	298	2		

- Molecule 5 is a protein called eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	222	Total	C	N	O	S	0	0
			1769	1117	324	325	3		

- Molecule 6 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	217	Total	C	N	O	S	0	0
			1629	1041	287	297	4		

- Molecule 7 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	223	Total	C	N	O	S	0	0
			1744	1108	313	318	5		

- Molecule 8 is a protein called eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 9 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 10 is a protein called eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	226	Total	C	N	O	S	0	0
			1812	1134	348	326	4		

- Molecule 11 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	184	Total	C	N	O	S	0	0
			1483	950	270	263			

- Molecule 12 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	188	Total	C	N	O	S	0	0
			1489	923	300	265	1		

- Molecule 13 is a protein called uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 14 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 15 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 16 is a protein called eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	117	Total	C	N	O	S	0	0
			885	553	161	171			

- Molecule 17 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	150	Total	C	N	O	S	0	0
			1187	756	223	206	2		

- Molecule 18 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	127	Total	C	N	O	S	0	0
			942	578	188	173	3		

- Molecule 19 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	119	Total	C	N	O	S	0	0
			943	604	171	163	5		

- Molecule 20 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	141	Total	C	N	O	S	0	0
			1105	709	204	192			

- Molecule 21 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	111	Total	C	N	O	S	0	0
			892	554	165	170	3		

- Molecule 22 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	145	Total	C	N	O	S	0	0
			1193	741	240	210	2		

- Molecule 23 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	143	Total	C	N	O	S	0	0
			1110	693	210	207			

- Molecule 24 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 25 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 26 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 27 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	144	Total	C	N	O	S	0	0
			1119	708	218	191	2		

- Molecule 28 is a protein called eS24.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	Y	134	Total	C	N	O		
			1061	665	207	189	0	0

- Molecule 29 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	70	Total	C	N	O	S		
			558	355	104	98	1	0	0

- Molecule 30 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	98	Total	C	N	O	S		
			779	480	165	129	5	0	0

- Molecule 31 is a protein called eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	81	Total	C	N	O	S		
			609	379	112	113	5	0	0

- Molecule 32 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	62	Total	C	N	O	S		
			487	301	97	88	1	0	0

- Molecule 33 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	53	Total	C	N	O	S		
			446	280	89	76	1	0	0

- Molecule 34 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	54	Total	C	N	O	S		
			433	271	88	73	1	0	0

- Molecule 35 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	69	Total	C	N	O	S	0	0
			549	352	102	91	4		

- Molecule 36 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	318	Total	C	N	O	S	0	0
			2466	1561	430	470	5		

- Molecule 37 is a protein called eL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 38 is a protein called eIF1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	95	Total	C	N	O	S	0	0
			765	475	142	143	5		

- Molecule 39 is a protein called eIF2 alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	249	Total	C	N	O	S	0	0
			2006	1283	333	382	8		

- Molecule 40 is a protein called eIF2 gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	396	Total	C	N	O	S	0	0
			3034	1932	542	544	16		

- Molecule 41 is a protein called eIF2 beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	128	Total	C	N	O	S	0	0
			1036	661	186	182	7		

- Molecule 42 is a protein called eIF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	86	Total	C	N	O	S	0	0
			695	439	128	124	4		

- Molecule 43 is a protein called eIF3a.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	o	92	Total	C	N	O	0	0
			460	276	92	92		

- Molecule 44 is a protein called eIF3c.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	p	88	Total	C	N	O	0	0
			440	264	88	88		

- Molecule 45 is a protein called eIF3i.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	342	Total	C	N	O	S	0	0
			2693	1711	443	530	9		

- Molecule 46 is a protein called eIF3b.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	34	Total	C	N	O	S	0	0
			300	192	52	54	2		

- Molecule 47 is a protein called eIF3g.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	s	52	Total	C	N	O	0	0
			418	257	82	79		

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	2	79	Total	Mg	0
			79	79	
48	C	1	Total	Mg	0
			1	1	
48	Q	1	Total	Mg	0
			1	1	

Continued on next page...

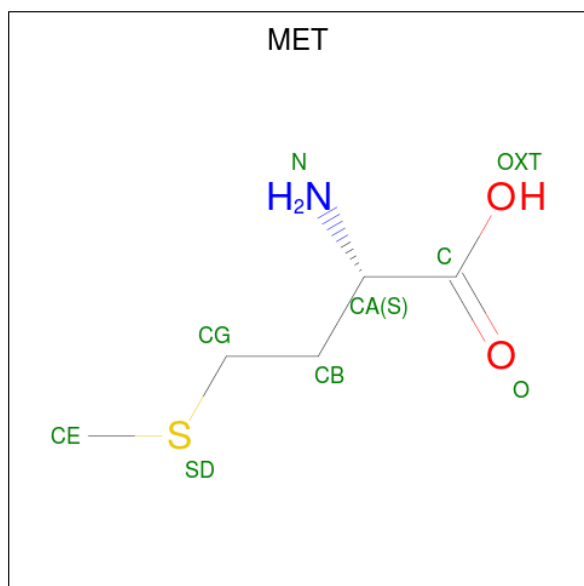
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
48	k	1	Total	Mg	0
			1	1	

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
49	a	1	Total	Zn	0
			1	1	
49	b	1	Total	Zn	0
			1	1	
49	f	1	Total	Zn	0
			1	1	
49	l	1	Total	Zn	0
			1	1	

- Molecule 50 is METHIONINE (three-letter code: MET) (formula: C₅H₁₁NO₂S).



Mol	Chain	Residues	Atoms					AltConf
50	k	1	Total	C	N	O	S	0
			8	5	1	1	1	

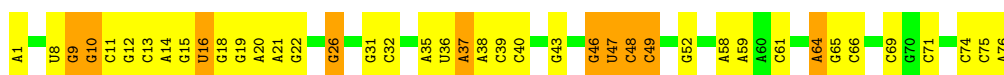
- Molecule 51 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).

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.

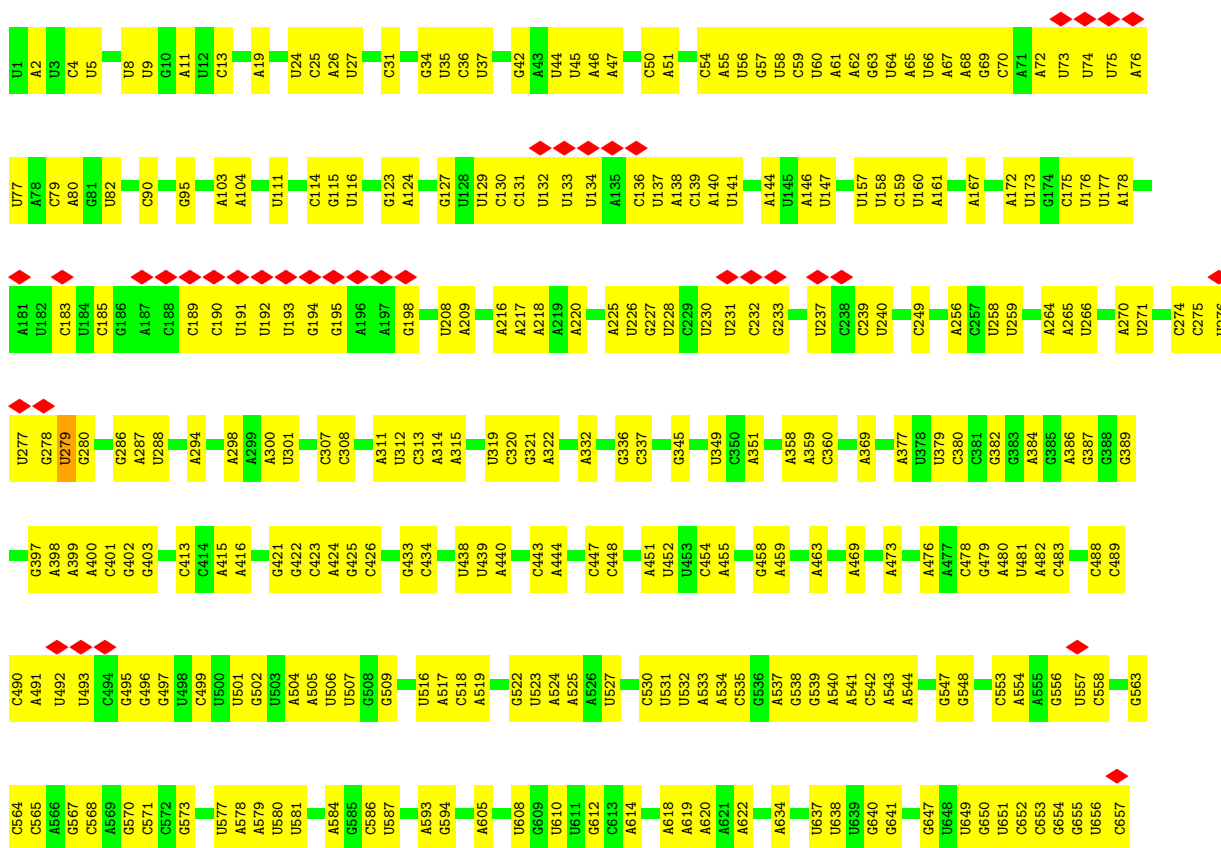
• Molecule 1: Met-tRNAi

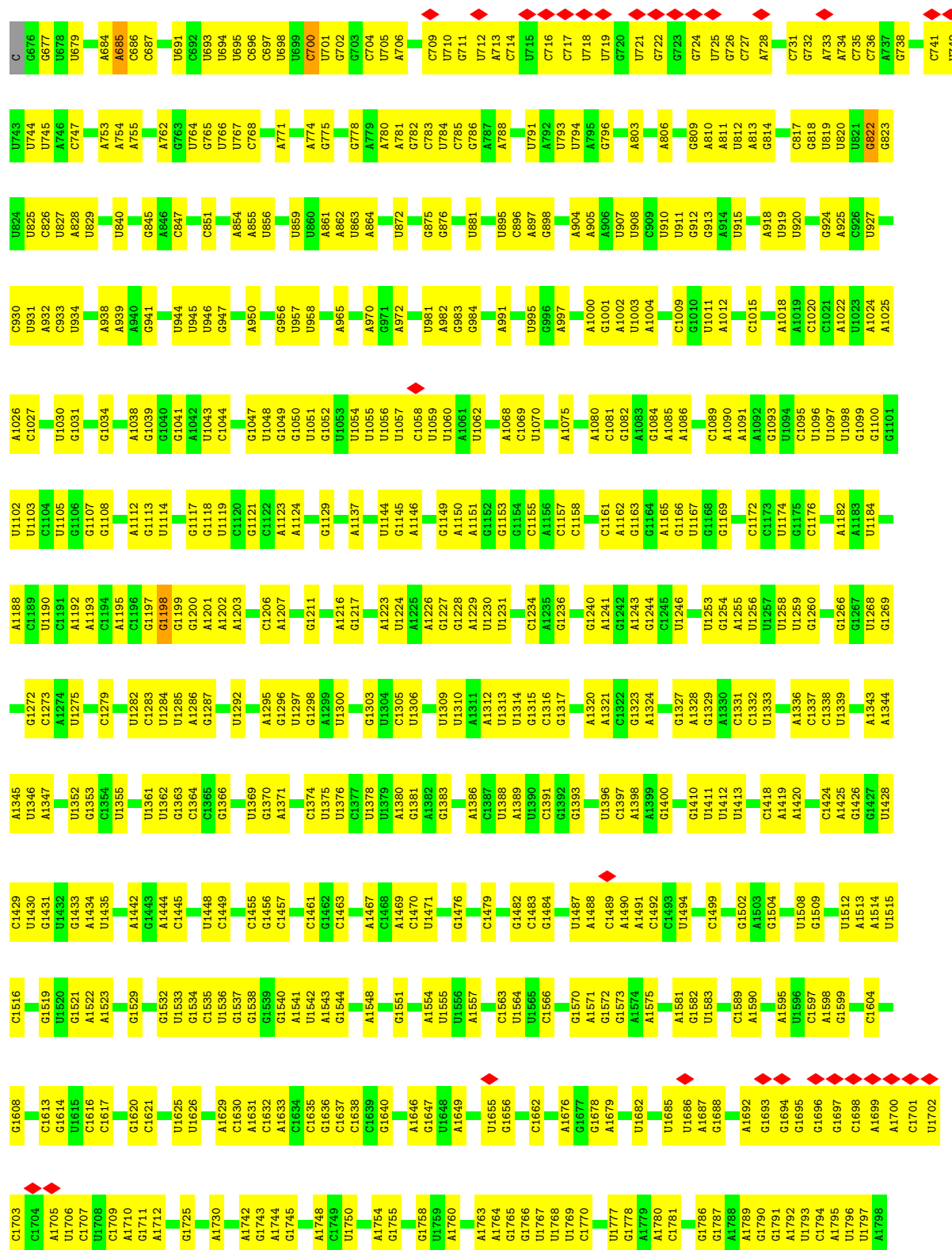
Chain 1: 



• Molecule 2: 18S rRNA

Chain 2: 



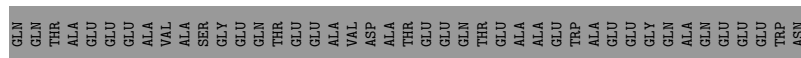


• Molecule 3: mRNA

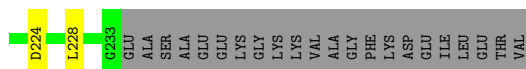
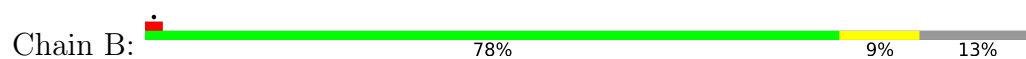




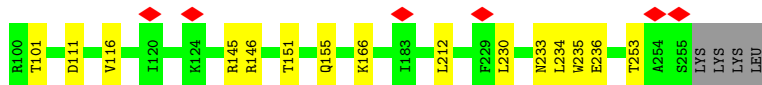
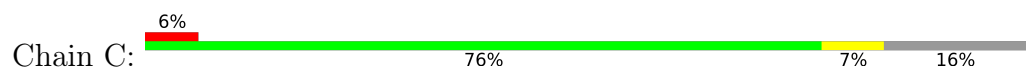
• Molecule 4: uS2



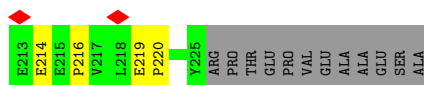
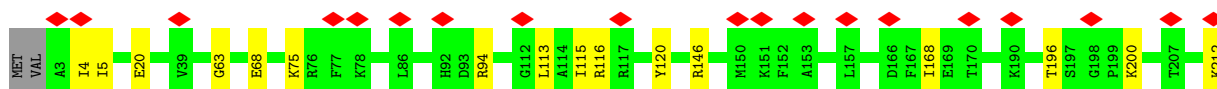
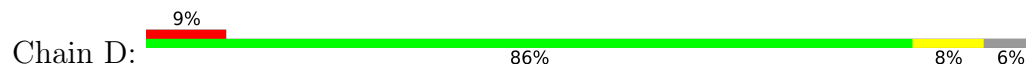
• Molecule 5: eS1



• Molecule 6: uS5

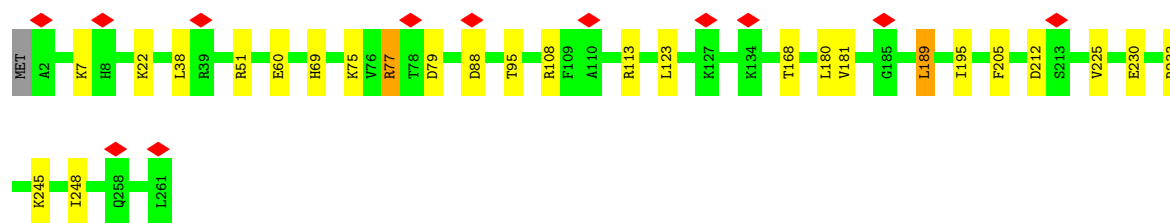


• Molecule 7: uS3

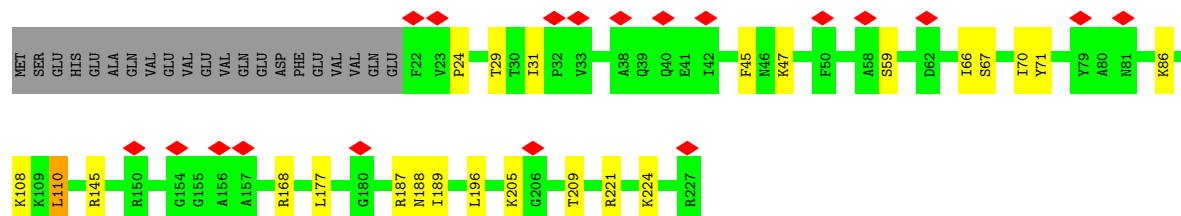
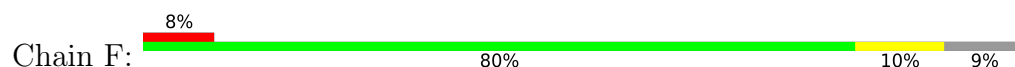


• Molecule 8: eS4

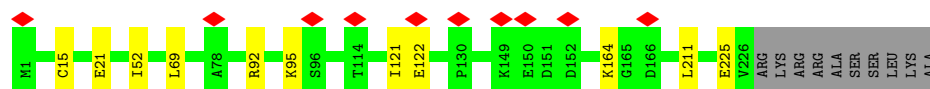




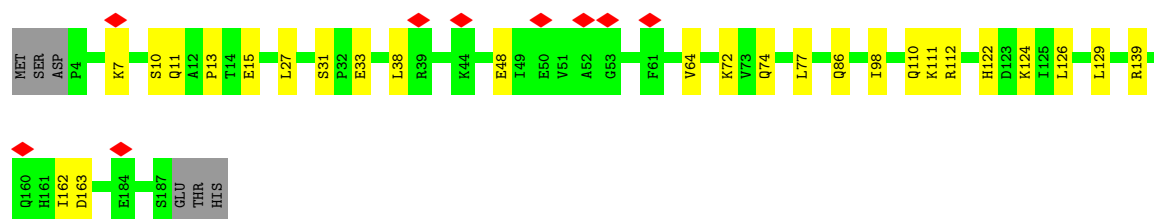
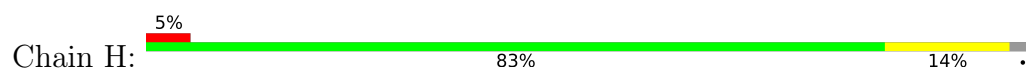
• Molecule 9: uS7



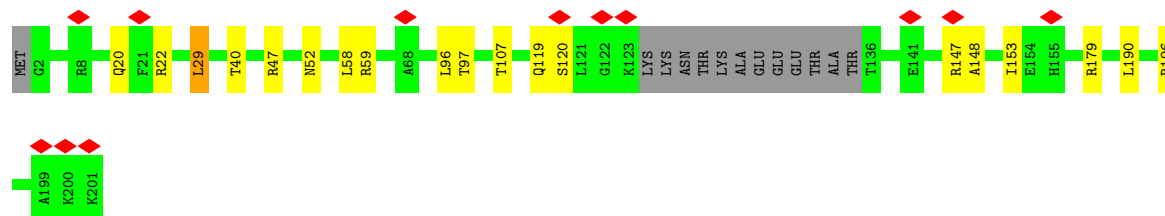
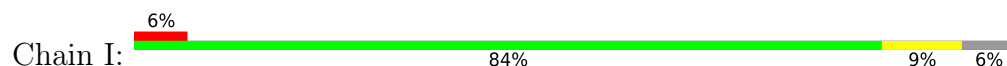
• Molecule 10: eS6




• Molecule 11: eS7



• Molecule 12: eS8




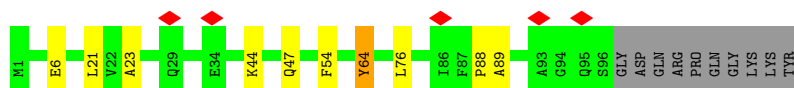
• Molecule 13: uS4

Chain J:  87% 10%



- Molecule 14: eS10

Chain K:  5% 81% 8% 9%




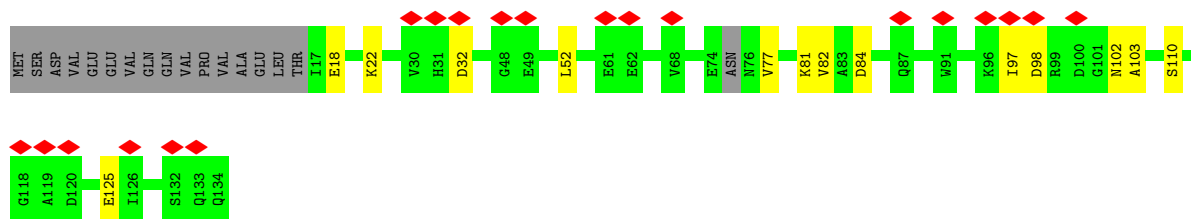
- Molecule 15: uS17

Chain L:  10% 94%



- Molecule 16: eS12

Chain M:  15% 77% 10% 13%




- Molecule 17: uS15

Chain N:  93% 5%



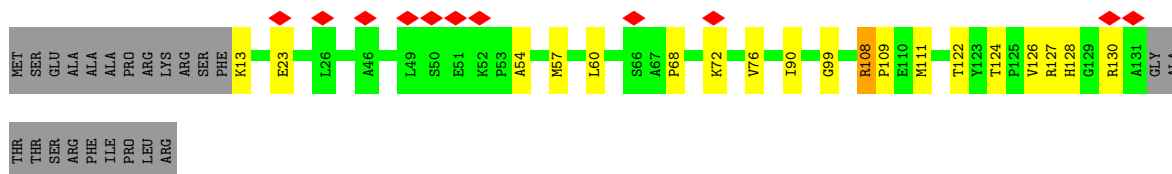
- Molecule 18: uS11

Chain O:  83% 9% 7%

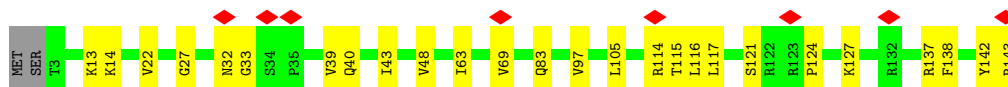
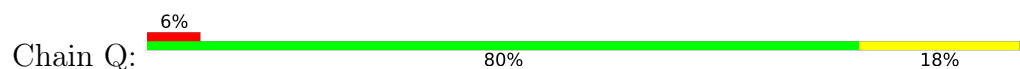


- Molecule 19: uS19

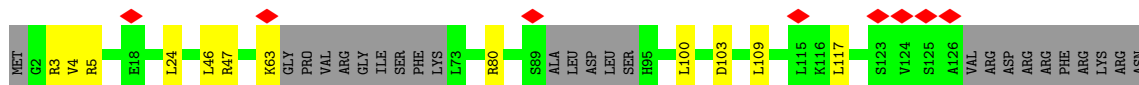
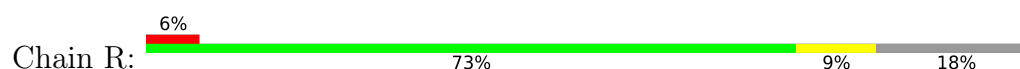
Chain P:  8% 70% 13% 16%



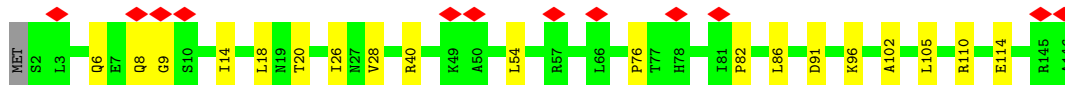
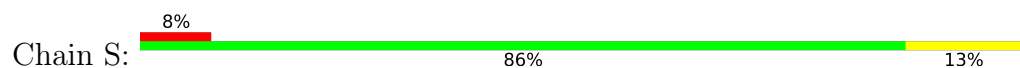
• Molecule 20: uS9



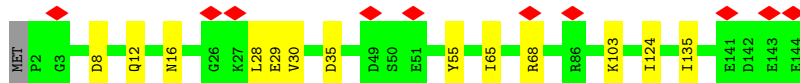
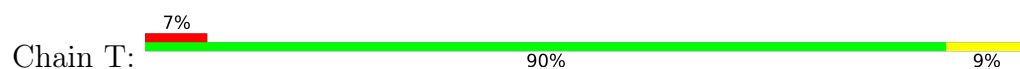
• Molecule 21: eS17



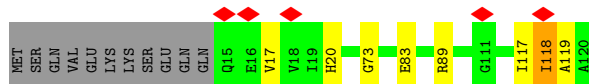
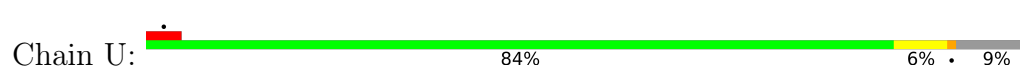
• Molecule 22: uS13



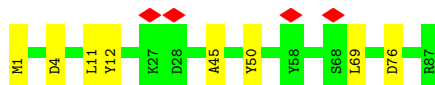
• Molecule 23: eS19



• Molecule 24: uS10



• Molecule 25: eS21




- Molecule 26: uS8

Chain W:  92% 7%




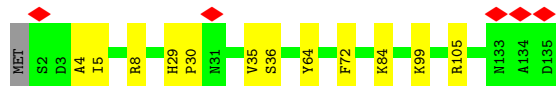
- Molecule 27: uS12

Chain X:  6% 86% 13%



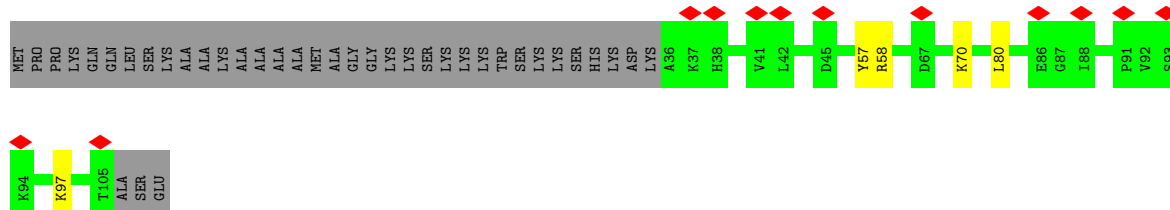
- Molecule 28: eS24

Chain Y:  90% 9%



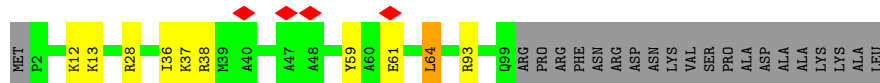
- Molecule 29: eS25

Chain Z:  11% 60% 5% 35%



- Molecule 30: eS26

Chain a:  74% 8% 18%




- Molecule 31: eS27

Chain b:  93% 6%




- Molecule 32: eS28

Chain c: 




• Molecule 33: uS14

Chain d: 




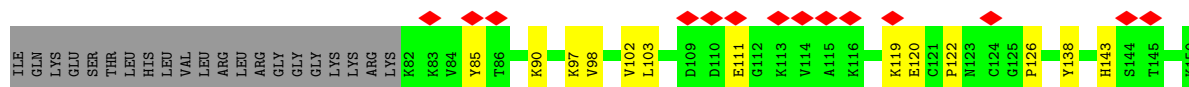
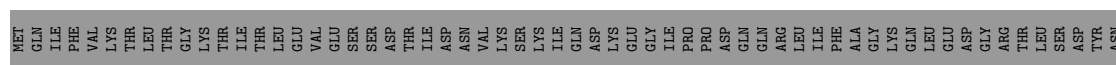
• Molecule 34: eS30

Chain e: 

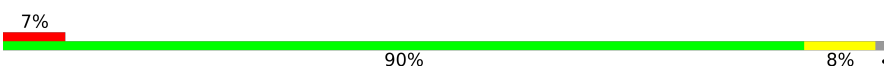


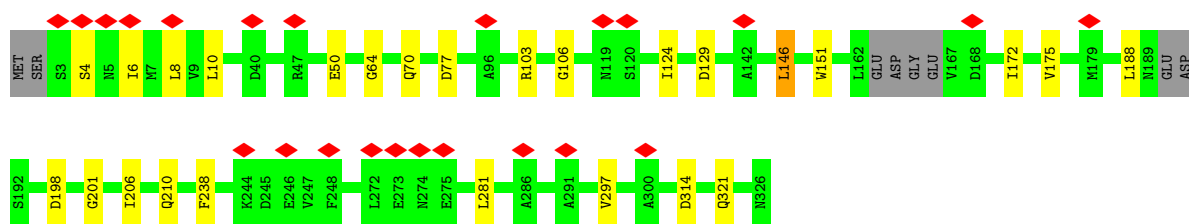
• Molecule 35: eS31

Chain f: 



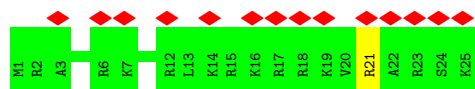
• Molecule 36: RACK1

Chain g: 



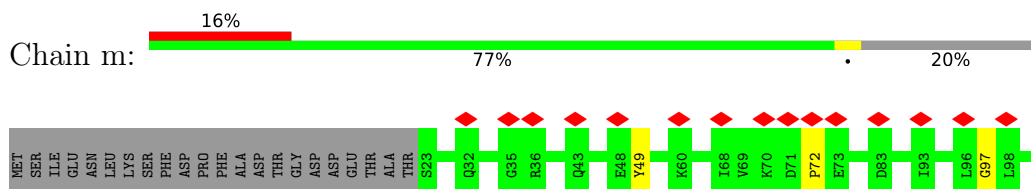
• Molecule 37: eL41

Chain h: 

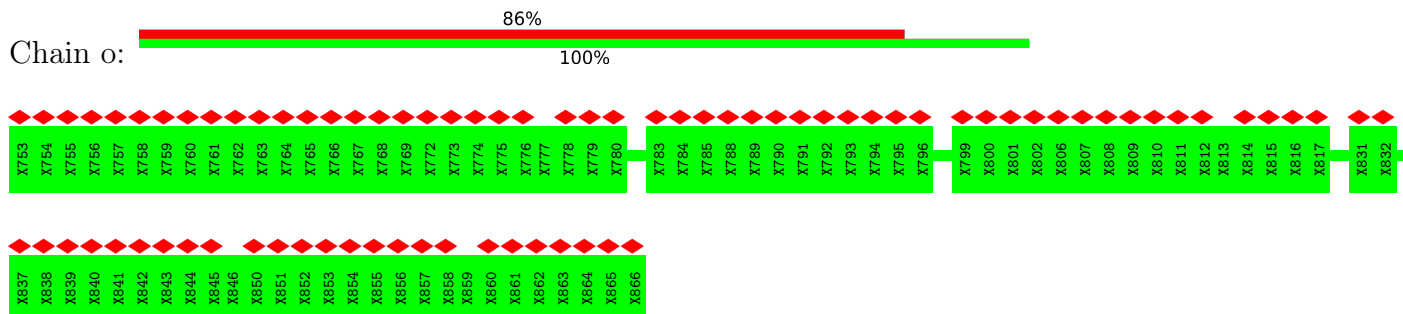


• Molecule 38: eIF1A

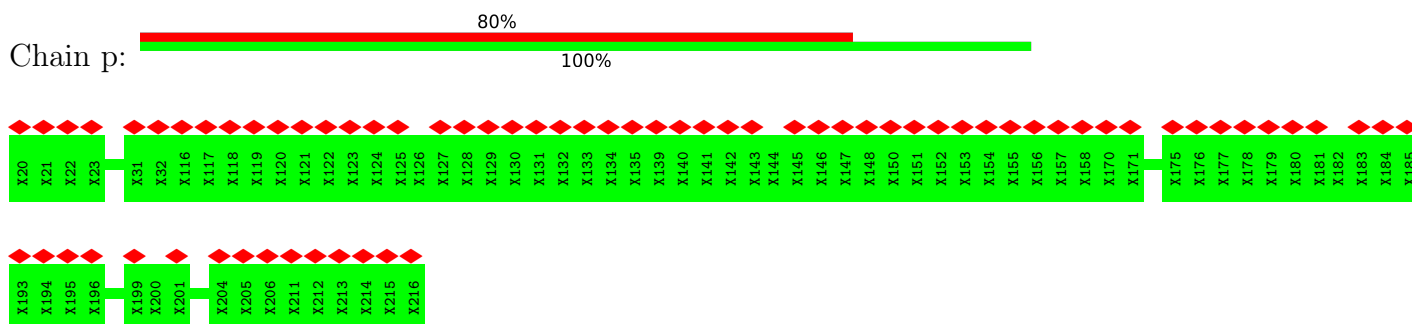
- Molecule 42: eIF1



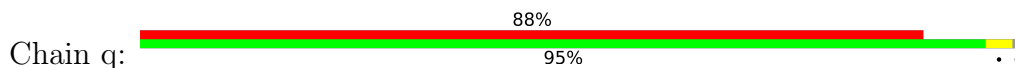
- Molecule 43: eIF3a

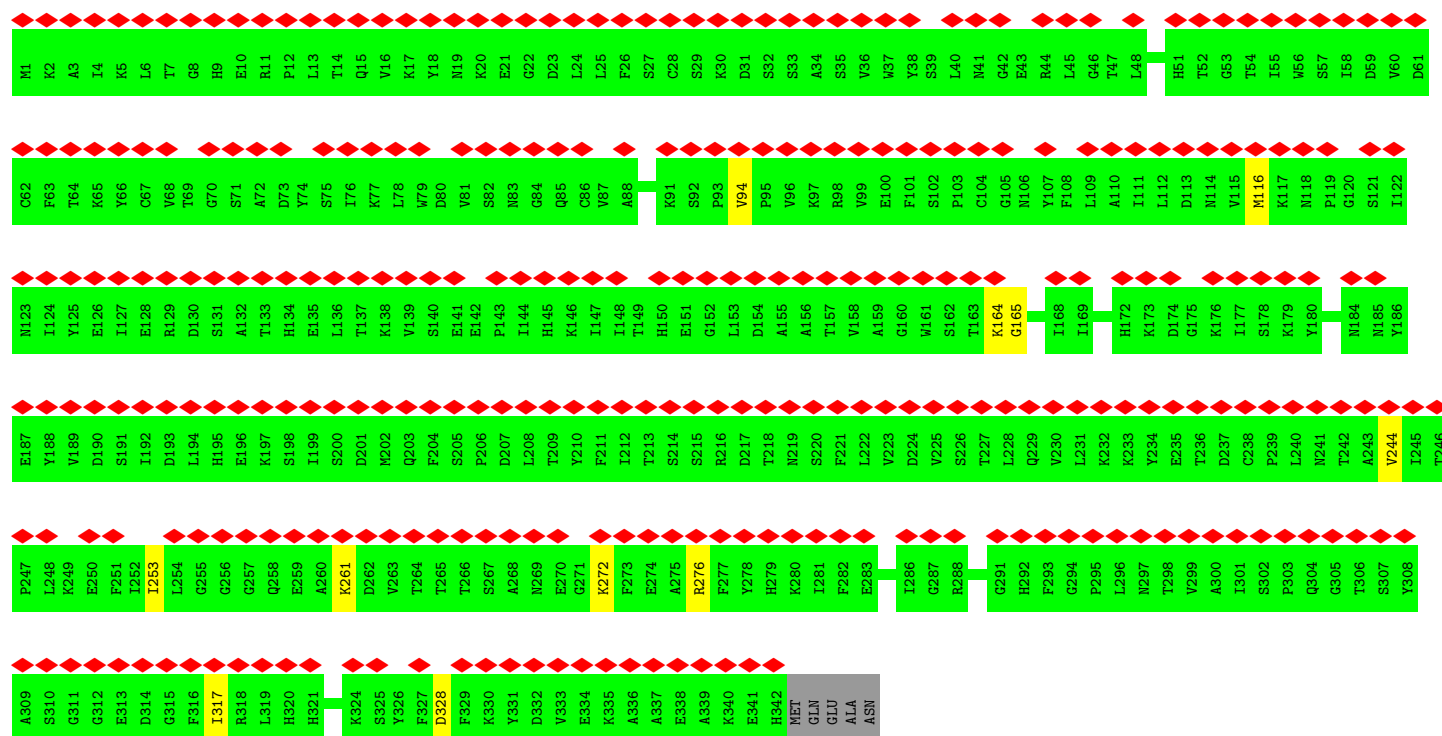


- Molecule 44: eIF3c



- Molecule 45: eIF3i





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	4547	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27	Depositor
Minimum defocus (nm)	4000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.207	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.04	Depositor
Map size (\AA)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 7MG, H2U, MG, T6A, 5MC, RIA, 1MA, 2MG, 1MG, ZN, GCP, M2G

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	0.45	2/1530 (0.1%)	0.76	4/2380 (0.2%)
2	2	0.24	0/42269	0.65	5/65862 (0.0%)
3	3	0.22	0/46	0.64	0/69
4	A	0.42	0/1666	0.63	1/2279 (0.0%)
5	B	0.40	0/1793	0.61	0/2414
6	C	0.40	0/1659	0.59	0/2252
7	D	0.41	0/1769	0.61	0/2378
8	E	0.40	0/2122	0.62	1/2861 (0.0%)
9	F	0.40	0/1628	0.63	1/2198 (0.0%)
10	G	0.38	0/1835	0.60	0/2451
11	H	0.41	0/1507	0.62	0/2028
12	I	0.41	0/1515	0.63	2/2029 (0.1%)
13	J	0.40	0/1495	0.67	2/2001 (0.1%)
14	K	0.46	0/831	0.61	0/1123
15	L	0.42	0/1276	0.58	0/1718
16	M	0.40	0/891	0.65	0/1201
17	N	0.39	0/1210	0.60	0/1628
18	O	0.39	0/953	0.61	0/1279
19	P	0.41	0/962	0.62	0/1294
20	Q	0.41	0/1125	0.62	0/1510
21	R	0.39	0/899	0.60	0/1204
22	S	0.40	0/1212	0.66	0/1629
23	T	0.40	0/1129	0.58	0/1520
24	U	0.39	0/857	0.61	0/1158
25	V	0.38	0/696	0.61	0/938
26	W	0.40	0/1039	0.64	1/1399 (0.1%)
27	X	0.42	0/1137	0.66	2/1516 (0.1%)
28	Y	0.40	0/1075	0.59	0/1433
29	Z	0.41	0/567	0.60	0/762
30	a	0.38	0/791	0.64	0/1059
31	b	0.39	0/619	0.62	0/837
32	c	0.37	0/489	0.65	0/655

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.43	0/457	0.58	0/607
34	e	0.40	0/440	0.61	0/586
35	f	0.45	0/562	0.72	1/751 (0.1%)
36	g	0.41	0/2521	0.58	0/3431
37	h	0.35	0/234	0.61	0/300
38	i	0.38	0/775	0.60	0/1034
39	j	0.41	0/2034	0.63	0/2737
40	k	0.39	0/3079	0.60	0/4157
41	l	0.41	0/1051	0.57	0/1402
42	m	0.39	0/703	0.58	0/938
45	q	0.42	0/2757	0.57	0/3733
46	r	0.42	0/306	0.52	0/407
47	s	0.39	0/426	0.54	0/571
All	All	0.34	2/93937 (0.0%)	0.64	20/135719 (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
27	X	0	1
28	Y	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1	A	OP3-P	-9.98	1.49	1.61
1	1	65	G	P-O5'	-6.66	1.53	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	f	126	PRO	CA-N-CD	-8.85	99.11	111.50
1	1	65	G	OP1-P-OP2	-8.39	107.01	119.60
2	2	685	A	C2'-C3'-O3'	6.95	124.81	113.70
12	I	29	LEU	CA-CB-CG	6.73	130.78	115.30
1	1	65	G	O5'-P-OP2	6.33	118.29	110.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	X	63	GLN	Peptide
28	Y	29	HIS	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	206/254 (81%)	177 (86%)	23 (11%)	6 (3%)	4	29
5	B	218/255 (86%)	191 (88%)	18 (8%)	9 (4%)	3	22
6	C	215/259 (83%)	193 (90%)	17 (8%)	5 (2%)	6	34
7	D	221/237 (93%)	198 (90%)	17 (8%)	6 (3%)	5	31
8	E	258/261 (99%)	230 (89%)	23 (9%)	5 (2%)	8	38
9	F	204/227 (90%)	170 (83%)	28 (14%)	6 (3%)	4	29
10	G	224/236 (95%)	204 (91%)	17 (8%)	3 (1%)	12	48
11	H	182/190 (96%)	166 (91%)	8 (4%)	8 (4%)	2	22
12	I	184/201 (92%)	163 (89%)	12 (6%)	9 (5%)	2	20
13	J	180/188 (96%)	153 (85%)	19 (11%)	8 (4%)	2	22
14	K	94/106 (89%)	80 (85%)	9 (10%)	5 (5%)	2	19
15	L	153/156 (98%)	133 (87%)	16 (10%)	4 (3%)	5	31
16	M	113/134 (84%)	86 (76%)	16 (14%)	11 (10%)	0	9
17	N	148/151 (98%)	141 (95%)	5 (3%)	2 (1%)	11	46
18	O	125/137 (91%)	101 (81%)	16 (13%)	8 (6%)	1	16
19	P	117/142 (82%)	91 (78%)	18 (15%)	8 (7%)	1	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	Q	139/143 (97%)	114 (82%)	13 (9%)	12 (9%)	1	11
21	R	105/136 (77%)	92 (88%)	10 (10%)	3 (3%)	4	29
22	S	143/146 (98%)	115 (80%)	20 (14%)	8 (6%)	2	18
23	T	141/144 (98%)	128 (91%)	13 (9%)	0	100	100
24	U	104/117 (89%)	88 (85%)	11 (11%)	5 (5%)	2	20
25	V	85/87 (98%)	79 (93%)	4 (5%)	2 (2%)	6	33
26	W	127/130 (98%)	114 (90%)	9 (7%)	4 (3%)	4	27
27	X	142/145 (98%)	121 (85%)	13 (9%)	8 (6%)	2	18
28	Y	132/135 (98%)	120 (91%)	8 (6%)	4 (3%)	4	28
29	Z	68/108 (63%)	55 (81%)	12 (18%)	1 (2%)	10	45
30	a	96/119 (81%)	83 (86%)	8 (8%)	5 (5%)	2	19
31	b	79/82 (96%)	69 (87%)	8 (10%)	2 (2%)	5	32
32	c	60/67 (90%)	56 (93%)	3 (5%)	1 (2%)	9	42
33	d	51/56 (91%)	37 (72%)	12 (24%)	2 (4%)	3	23
34	e	52/63 (82%)	41 (79%)	9 (17%)	2 (4%)	3	24
35	f	67/150 (45%)	50 (75%)	12 (18%)	5 (8%)	1	13
36	g	312/326 (96%)	267 (86%)	39 (12%)	6 (2%)	8	38
37	h	23/25 (92%)	23 (100%)	0	0	100	100
38	i	93/153 (61%)	82 (88%)	8 (9%)	3 (3%)	4	26
39	j	243/304 (80%)	212 (87%)	24 (10%)	7 (3%)	4	29
40	k	388/527 (74%)	335 (86%)	39 (10%)	14 (4%)	3	25
41	l	120/285 (42%)	106 (88%)	13 (11%)	1 (1%)	19	60
42	m	84/108 (78%)	74 (88%)	8 (10%)	2 (2%)	6	33
45	q	340/347 (98%)	307 (90%)	29 (8%)	4 (1%)	13	50
46	r	32/34 (94%)	30 (94%)	2 (6%)	0	100	100
47	s	50/52 (96%)	44 (88%)	5 (10%)	1 (2%)	7	38
All	All	6118/7123 (86%)	5319 (87%)	594 (10%)	205 (3%)	6	26

5 of 205 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	H	31	SER
11	H	64	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	H	74	GLN
14	K	88	PRO
19	P	126	VAL

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	
4	A	174/211 (82%)	159 (91%)	15 (9%)	10	33
5	B	198/228 (87%)	182 (92%)	16 (8%)	11	35
6	C	176/203 (87%)	161 (92%)	15 (8%)	10	33
7	D	185/196 (94%)	171 (92%)	14 (8%)	13	37
8	E	223/224 (100%)	201 (90%)	22 (10%)	8	26
9	F	174/194 (90%)	156 (90%)	18 (10%)	7	25
10	G	192/200 (96%)	184 (96%)	8 (4%)	30	54
11	H	164/170 (96%)	146 (89%)	18 (11%)	6	23
12	I	147/159 (92%)	138 (94%)	9 (6%)	18	44
13	J	153/158 (97%)	144 (94%)	9 (6%)	19	45
14	K	88/96 (92%)	82 (93%)	6 (7%)	16	41
15	L	136/137 (99%)	131 (96%)	5 (4%)	34	58
16	M	93/109 (85%)	90 (97%)	3 (3%)	39	62
17	N	127/128 (99%)	119 (94%)	8 (6%)	18	43
18	O	96/104 (92%)	90 (94%)	6 (6%)	18	43
19	P	101/119 (85%)	89 (88%)	12 (12%)	5	20
20	Q	117/119 (98%)	103 (88%)	14 (12%)	5	20
21	R	102/124 (82%)	93 (91%)	9 (9%)	10	31
22	S	128/129 (99%)	117 (91%)	11 (9%)	10	33
23	T	117/118 (99%)	104 (89%)	13 (11%)	6	22
24	U	96/107 (90%)	92 (96%)	4 (4%)	30	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	V	73/73 (100%)	67 (92%)	6 (8%)	11	34
26	W	110/111 (99%)	106 (96%)	4 (4%)	35	59
27	X	119/120 (99%)	109 (92%)	10 (8%)	11	34
28	Y	108/109 (99%)	101 (94%)	7 (6%)	17	42
29	Z	60/88 (68%)	56 (93%)	4 (7%)	16	41
30	a	83/100 (83%)	77 (93%)	6 (7%)	14	39
31	b	71/72 (99%)	68 (96%)	3 (4%)	30	54
32	c	54/59 (92%)	51 (94%)	3 (6%)	21	46
33	d	46/48 (96%)	43 (94%)	3 (6%)	17	42
34	e	47/55 (86%)	42 (89%)	5 (11%)	6	24
35	f	58/133 (44%)	51 (88%)	7 (12%)	5	20
36	g	265/272 (97%)	244 (92%)	21 (8%)	12	36
37	h	23/23 (100%)	22 (96%)	1 (4%)	29	54
38	i	81/130 (62%)	75 (93%)	6 (7%)	13	38
39	j	224/274 (82%)	193 (86%)	31 (14%)	3	17
40	k	332/449 (74%)	324 (98%)	8 (2%)	49	69
41	l	119/246 (48%)	114 (96%)	5 (4%)	30	54
42	m	77/96 (80%)	76 (99%)	1 (1%)	69	82
45	q	297/301 (99%)	290 (98%)	7 (2%)	49	69
46	r	33/33 (100%)	33 (100%)	0	100	100
47	s	43/43 (100%)	43 (100%)	0	100	100
All	All	5310/6068 (88%)	4937 (93%)	373 (7%)	19	40

5 of 373 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	U	20	HIS
35	f	97	LYS
25	V	50	TYR
28	Y	99	LYS
36	g	124	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
21	R	29	GLN
42	m	79	GLN
25	V	33	GLN
42	m	67	ASN
40	k	248	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	73/75 (97%)	38 (52%)	12 (16%)
2	2	1778/1781 (99%)	814 (45%)	118 (6%)
3	3	1/25 (4%)	0	0
All	All	1852/1881 (98%)	852 (46%)	130 (7%)

5 of 852 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	8	U
1	1	9	1MG
1	1	10	2MG
1	1	11	C
1	1	12	G

5 of 130 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	1488	A
2	2	1537	G
2	2	454	C
2	2	451	A
2	2	1613	C

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

11 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
1	5MC	1	48	1	18,22,23	1.09	1 (5%)	26,32,35	1.45	4 (15%)
1	H2U	1	16	1	18,21,22	0.86	1 (5%)	21,30,33	1.23	2 (9%)
1	1MA	1	58	1	16,25,26	1.80	4 (25%)	18,37,40	1.25	3 (16%)
1	H2U	1	47	1	18,21,22	0.78	1 (5%)	21,30,33	1.36	3 (14%)
1	1MG	1	9	1	18,26,27	1.05	1 (5%)	19,39,42	1.58	4 (21%)
1	2MG	1	10	1	18,26,27	0.98	0	16,38,41	1.48	3 (18%)
1	5MC	1	49	1	18,22,23	1.08	1 (5%)	26,32,35	1.38	5 (19%)
1	RIA	1	64	1	31,38,39	1.21	3 (9%)	39,57,60	2.50	11 (28%)
1	M2G	1	26	1	20,27,28	1.69	2 (10%)	22,40,43	1.27	5 (22%)
1	7MG	1	46	1	22,26,27	1.49	4 (18%)	29,39,42	2.52	6 (20%)
1	T6A	1	37	1	27,34,35	1.10	2 (7%)	29,49,52	2.41	9 (31%)

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
1	5MC	1	48	1	-	1/7/25/26	0/2/2/2
1	H2U	1	16	1	-	3/7/38/39	0/2/2/2
1	1MA	1	58	1	-	1/3/25/26	0/3/3/3
1	H2U	1	47	1	-	5/7/38/39	0/2/2/2
1	1MG	1	9	1	-	0/3/25/26	0/3/3/3
1	2MG	1	10	1	-	2/5/27/28	0/3/3/3
1	5MC	1	49	1	-	3/7/25/26	0/2/2/2
1	RIA	1	64	1	-	4/13/51/52	0/4/4/4
1	M2G	1	26	1	-	6/7/29/30	0/3/3/3
1	7MG	1	46	1	-	0/7/37/38	0/3/3/3
1	T6A	1	37	1	-	13/19/41/42	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)
1	1	58	1MA	C2-N3	5.47	1.35	1.29
1	1	26	M2G	C2-N3	5.41	1.37	1.30
1	1	64	RIA	P'-O3X	-3.69	1.40	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	26	M2G	C2-N2	3.66	1.42	1.35
1	1	58	1MA	C6-N6	3.41	1.36	1.27

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	64	RIA	O2A-C1'-O1'	-8.59	102.13	111.43
1	1	46	7MG	N9-C4-N3	8.43	138.07	125.47
1	1	37	T6A	C2-N1-C6	7.40	122.94	116.59
1	1	64	RIA	O2A-C1'-C2'	-6.66	94.14	107.96
1	1	37	T6A	N6-C10-N11	5.98	122.12	113.76

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	16	H2U	C3'-C4'-C5'-O5'
1	1	26	M2G	C3'-C4'-C5'-O5'
1	1	26	M2G	N1-C2-N2-CM1
1	1	26	M2G	N3-C2-N2-CM1
1	1	37	T6A	C5-C6-N6-C10

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 88 ligands modelled in this entry, 86 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
51	GCP	k	603	48	27,34,34	1.91	7 (25%)	34,54,54	1.97	8 (23%)
50	MET	k	601	-	6,7,8	0.45	0	2,7,9	0.38	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
51	GCP	k	603	48	-	0/15/38/38	0/3/3/3
50	MET	k	601	-	-	0/5/6/8	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	k	603	GCP	PG-O1G	5.35	1.61	1.50
51	k	603	GCP	C5-C6	4.78	1.49	1.41
51	k	603	GCP	PG-O3G	-2.83	1.48	1.54
51	k	603	GCP	PB-O3A	2.77	1.61	1.58
51	k	603	GCP	PG-O2G	2.76	1.61	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	k	603	GCP	C2-N3-C4	5.27	121.38	115.36
51	k	603	GCP	C2-N1-C6	4.02	122.31	115.93
51	k	603	GCP	C4-C5-C6	-3.99	116.99	120.80
51	k	603	GCP	C5-C6-N1	-3.75	118.31	123.43
51	k	603	GCP	N3-C2-N1	-3.54	122.51	127.22

There are no chirality outliers.

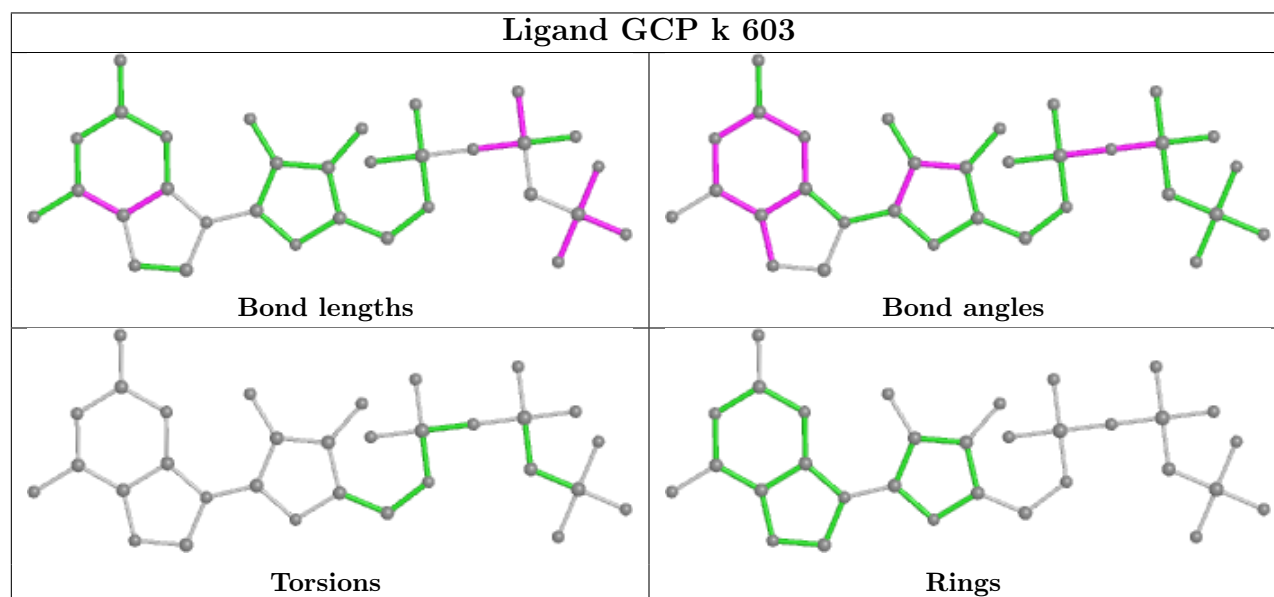
There are no torsion outliers.

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
44	p	6
43	o	6

The worst 5 of 12 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	p	32:UNK	C	116:UNK	N	41.18
1	p	158:UNK	C	170:UNK	N	14.29
1	p	185:UNK	C	193:UNK	N	9.56
1	o	846:UNK	C	850:UNK	N	7.84
1	o	818:UNK	C	829:UNK	N	7.14

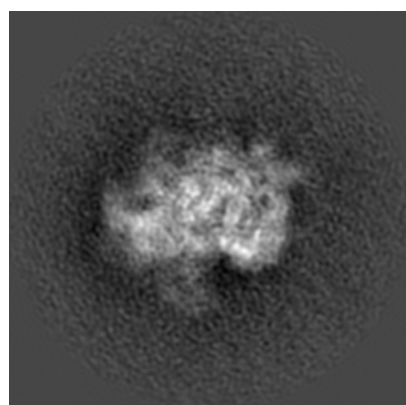
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3049. These allow visual inspection of the internal detail of the map and identification of artifacts.

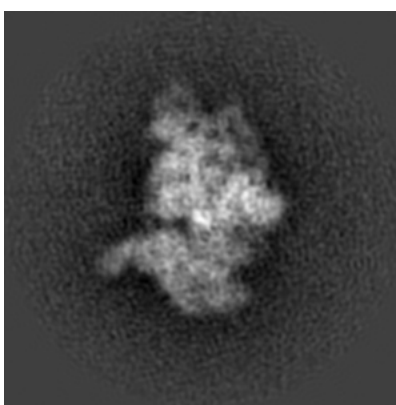
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

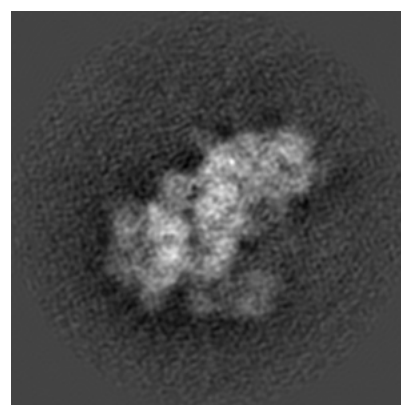
6.1.1 Primary map



X



Y

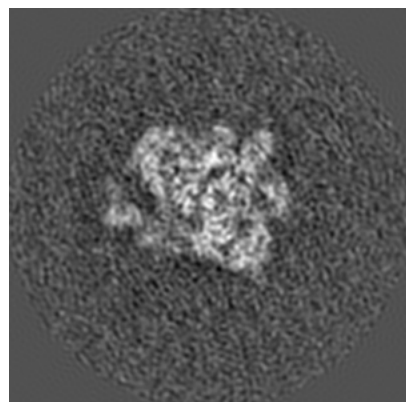


Z

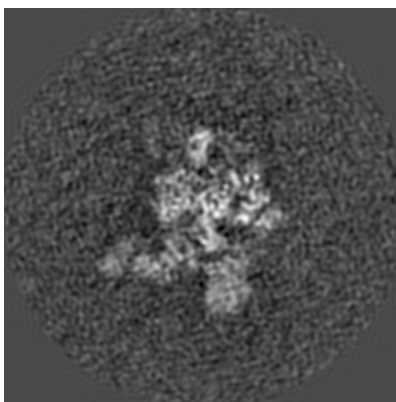
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

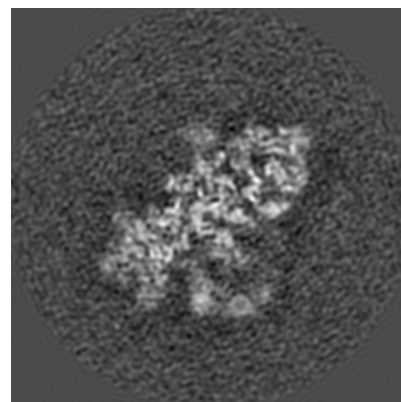
6.2.1 Primary map



X Index: 150



Y Index: 150

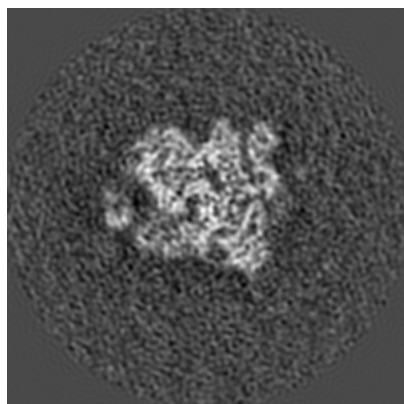


Z Index: 150

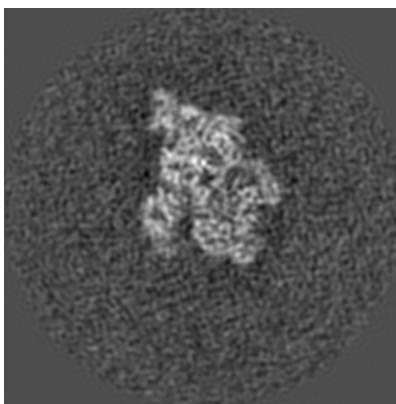
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

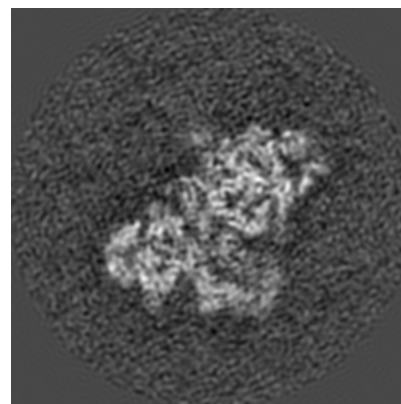
6.3.1 Primary map



X Index: 155



Y Index: 171



Z Index: 143

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

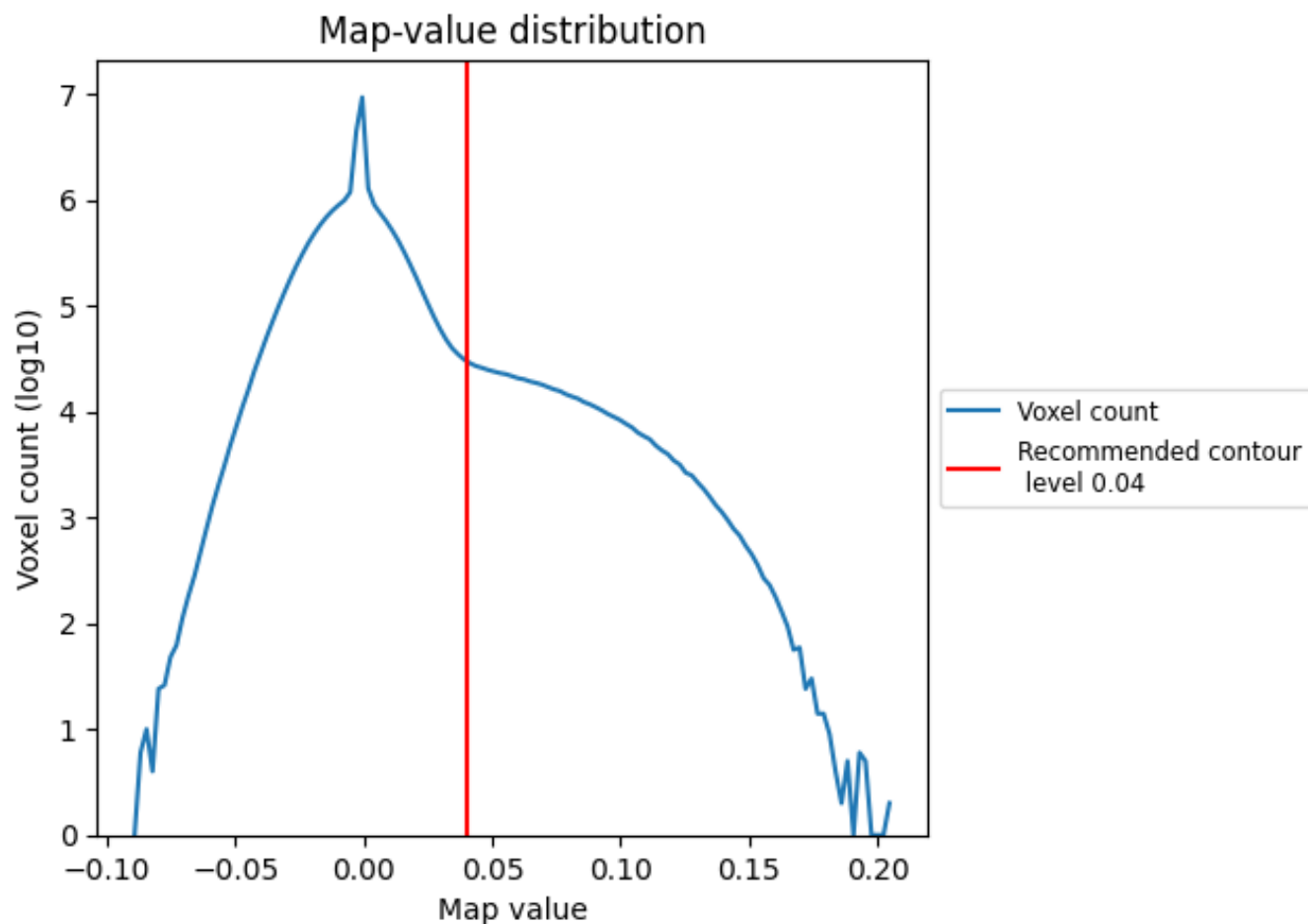
6.5 Mask visualisation

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

7 Map analysis [i](#)

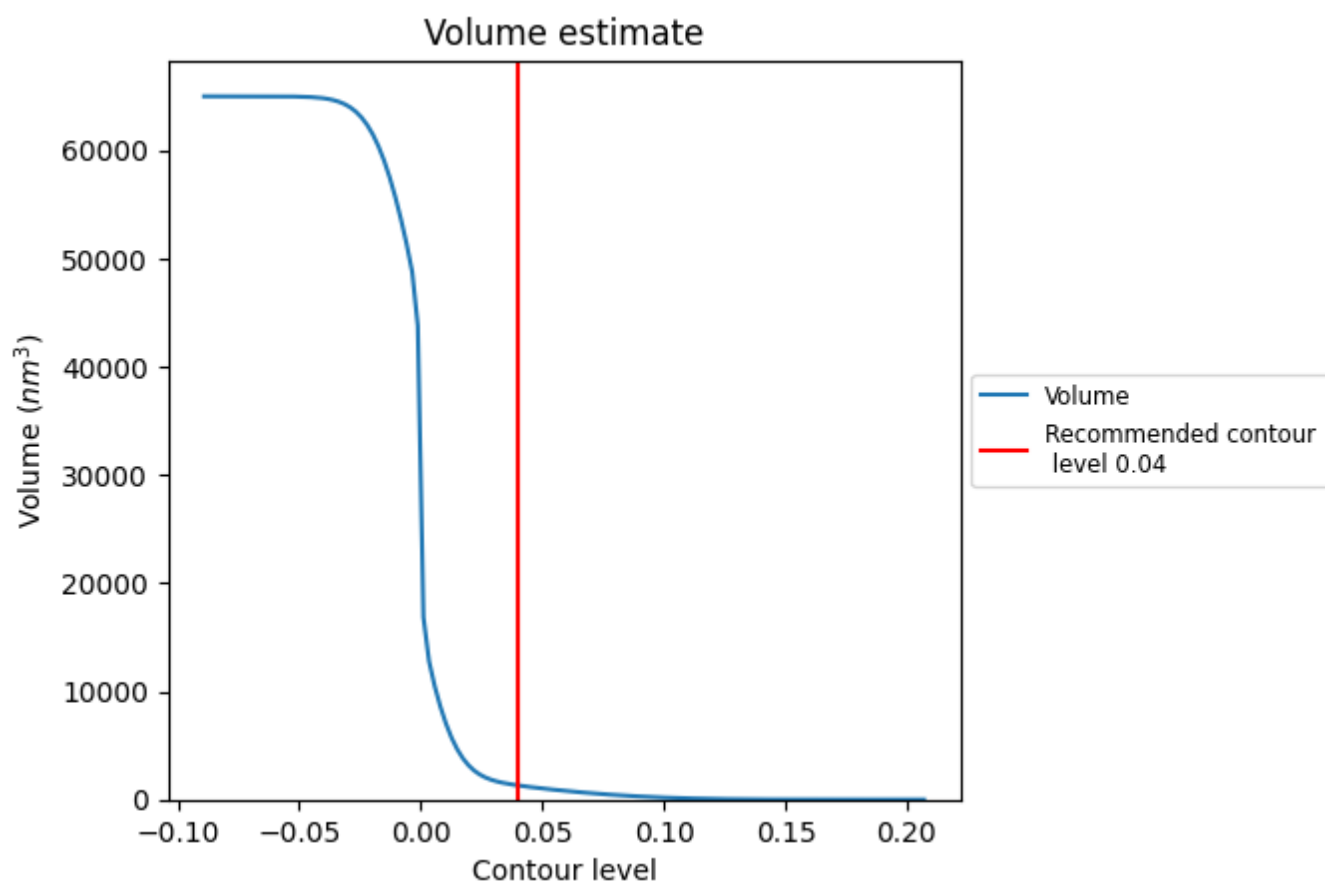
This section contains the results of statistical analysis of the map.

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.

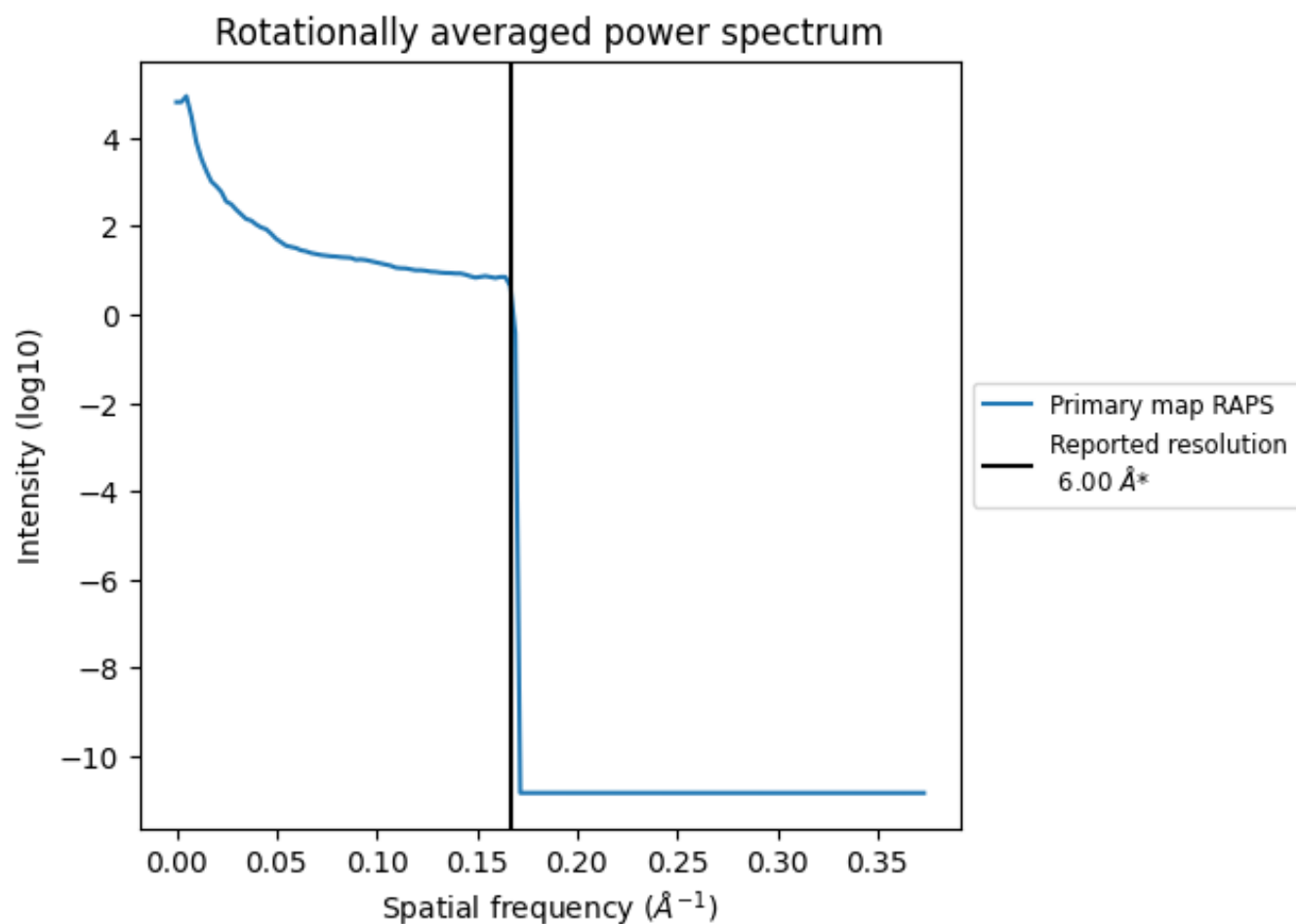
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1309 nm^3 ; this corresponds to an approximate mass of 1182 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 ⓘ

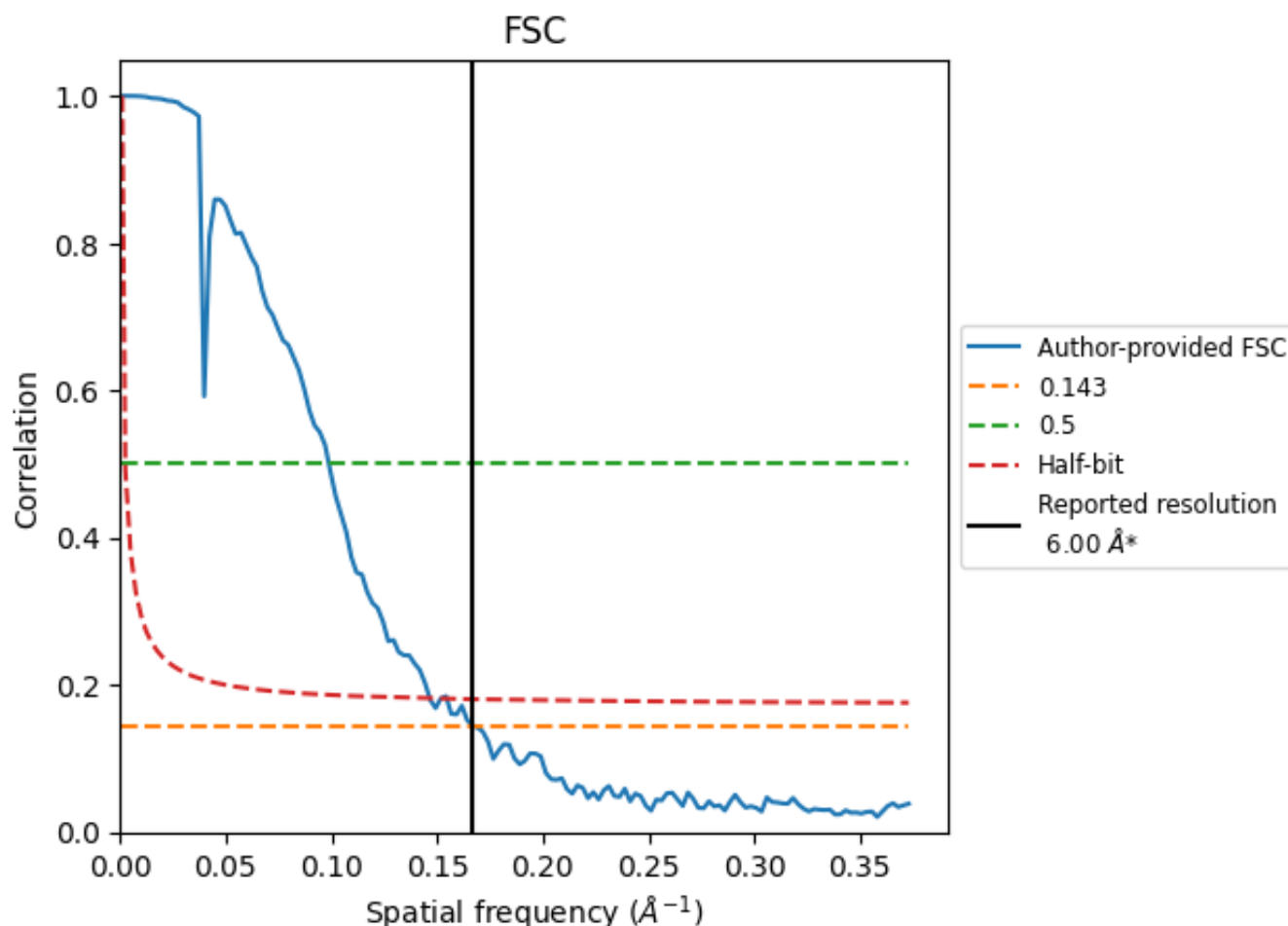


*Reported resolution corresponds to spatial frequency of 0.167 Å⁻¹

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 0.167 Å⁻¹

8.2 Resolution estimates [i](#)

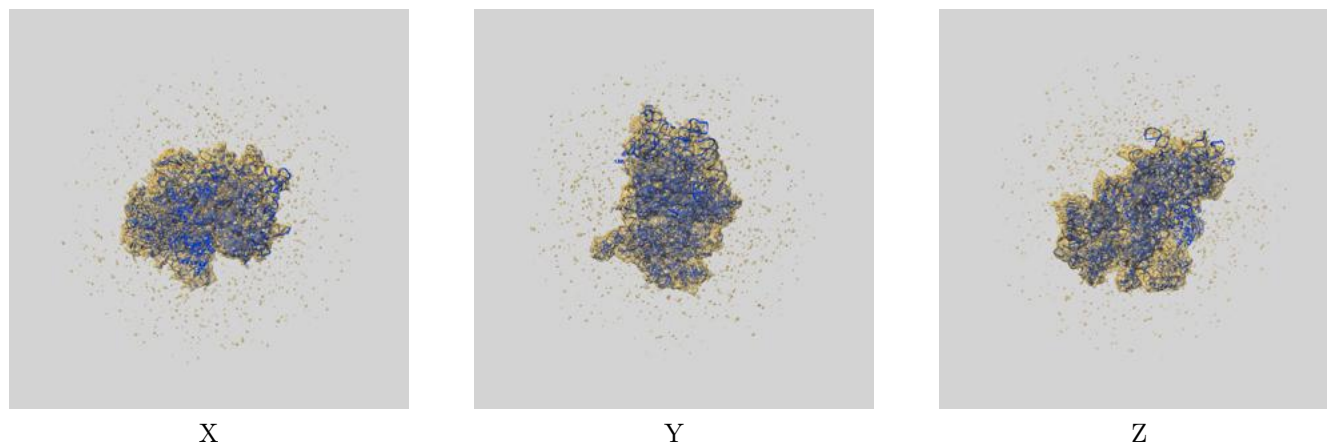
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.00	-	-
Author-provided FSC curve	5.95	10.12	6.83
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

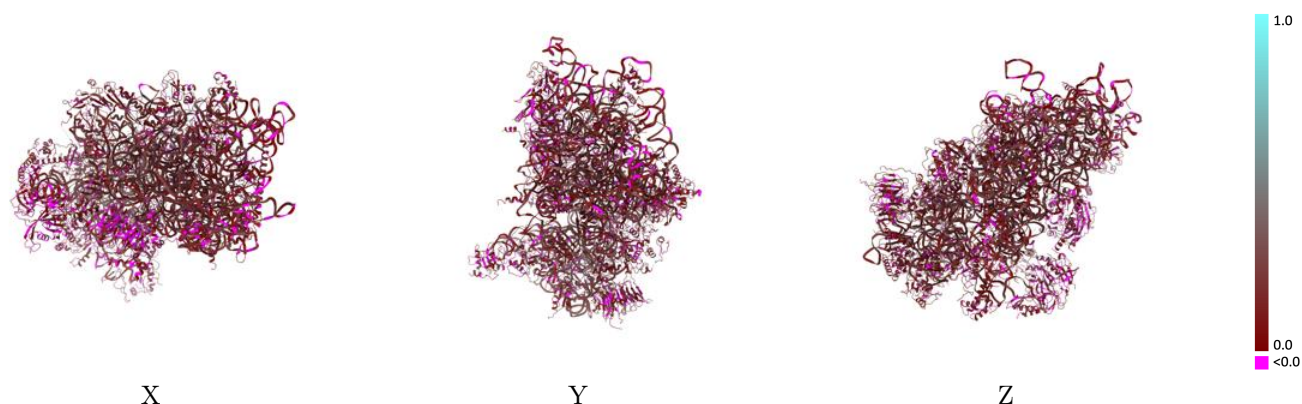
This section contains information regarding the fit between EMDB map EMD-3049 and PDB model 3JAQ. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



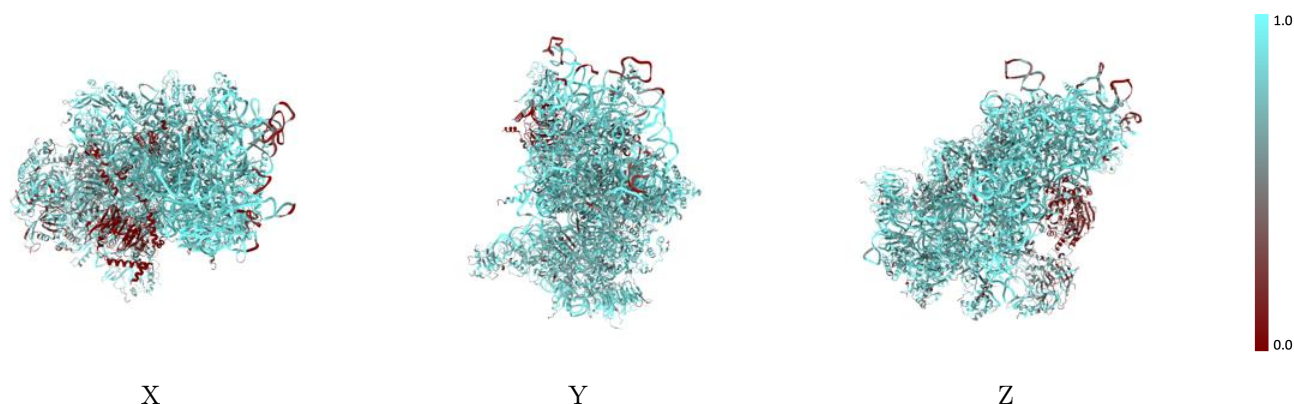
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



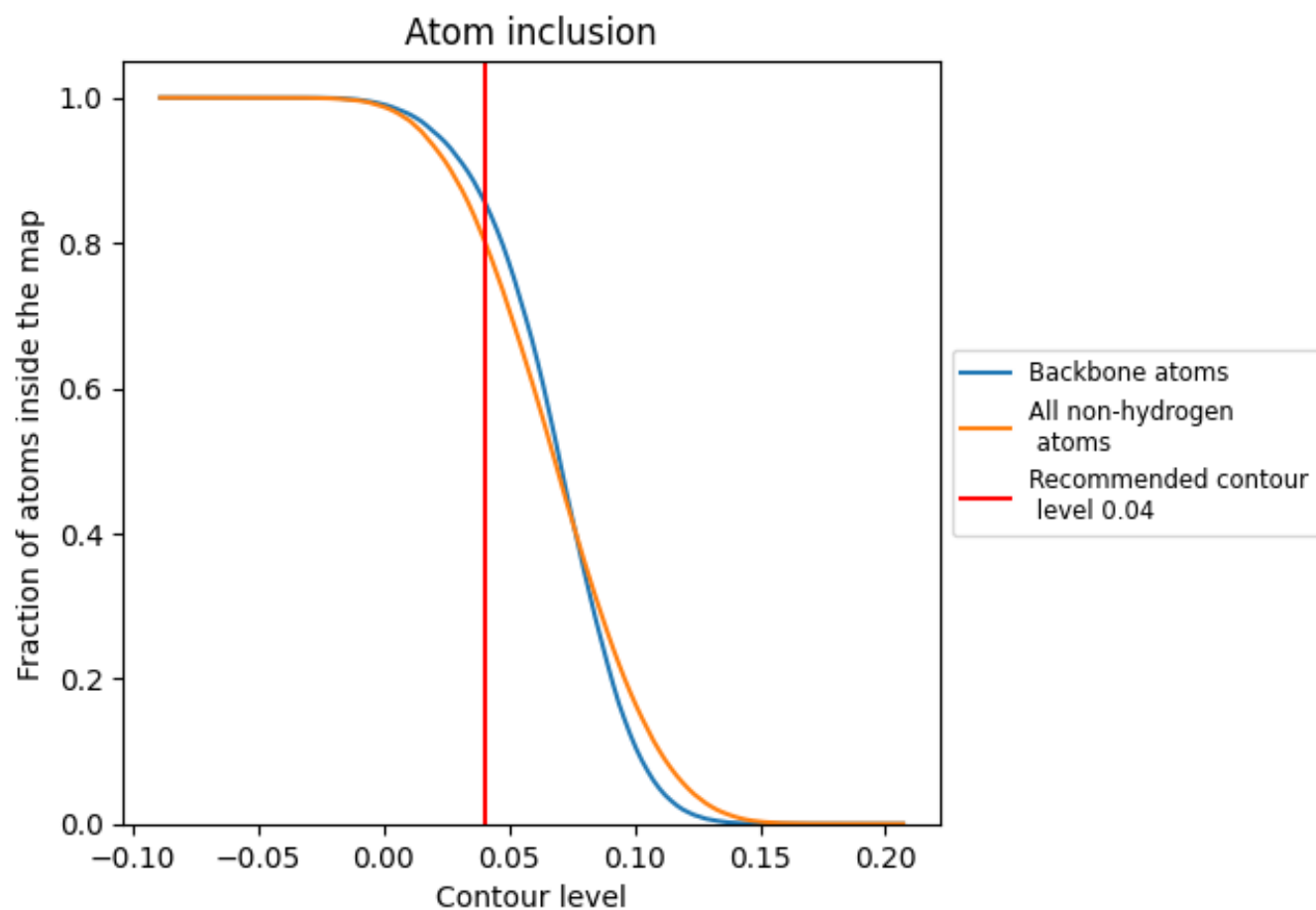
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 80% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8038	 0.1620
1	 0.9231	 0.1750
2	 0.9241	 0.1950
3	 0.3810	 0.2400
A	 0.8200	 0.1520
B	 0.8362	 0.1370
C	 0.7478	 0.1680
D	 0.7354	 0.1560
E	 0.7917	 0.1540
F	 0.7583	 0.1520
G	 0.8215	 0.1310
H	 0.8109	 0.1520
I	 0.8236	 0.1460
J	 0.7924	 0.1490
K	 0.7940	 0.1450
L	 0.7259	 0.1560
M	 0.7296	 0.1240
N	 0.8283	 0.1650
O	 0.8386	 0.1190
P	 0.7963	 0.1290
Q	 0.8030	 0.1390
R	 0.7793	 0.1580
S	 0.7849	 0.1280
T	 0.8296	 0.1290
U	 0.7892	 0.1510
V	 0.7751	 0.1670
W	 0.7600	 0.1480
X	 0.7619	 0.1660
Y	 0.8074	 0.1440
Z	 0.6796	 0.1480
a	 0.7761	 0.1550
b	 0.8505	 0.1700
c	 0.7966	 0.1710
d	 0.8150	 0.1530
e	 0.7542	 0.1830



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	 0.6981	 0.1200
g	 0.8362	 0.1270
h	 0.4009	 0.0700
i	 0.6506	 0.1460
j	 0.6843	 0.1390
k	 0.5691	 0.0870
l	 0.6894	 0.1340
m	 0.6061	 0.1630
o	 0.2043	 0.1540
p	 0.2477	 0.1960
q	 0.1280	 0.0570
r	 0.0000	 0.0860
s	 0.0321	 0.1180