



wwPDB EM Validation Summary Report ⓘ

Aug 25, 2026 – 08:51 pm BST

PDB ID : 8CAS / pdb_00008cas
EMDB ID : EMD-16533
Title : Cryo-EM structure of native Otu2-bound ubiquitinated 48S initiation complex (partial)
Authors : Ikeuchi, K.; Buschauer, R.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on : 2023-01-24
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

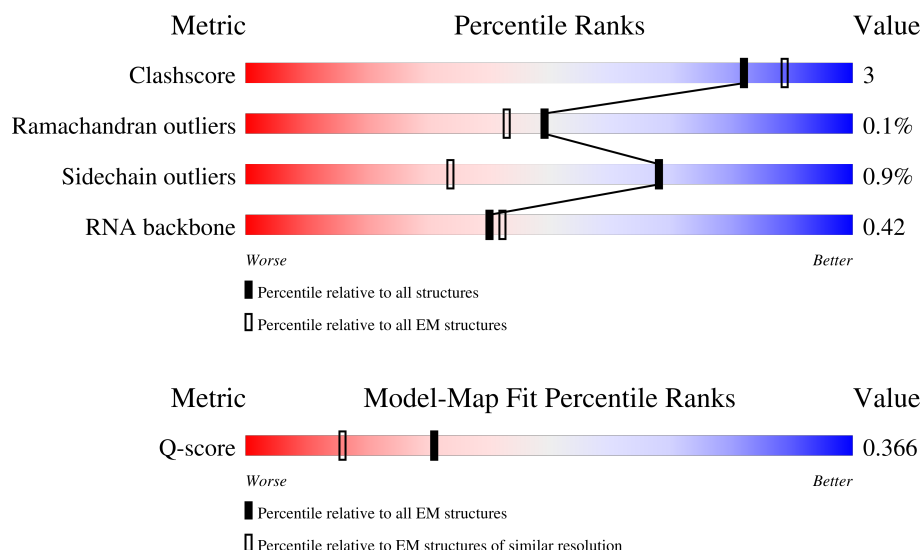
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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.



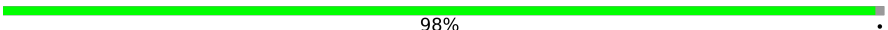
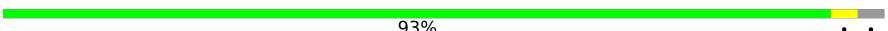
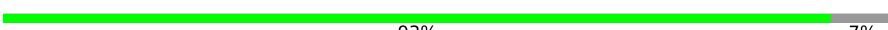
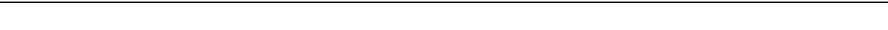
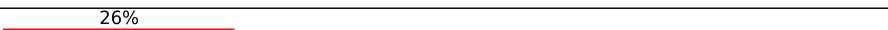
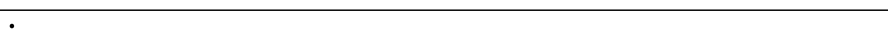
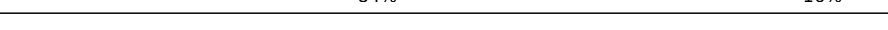
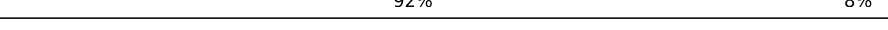
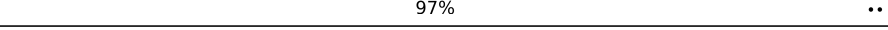
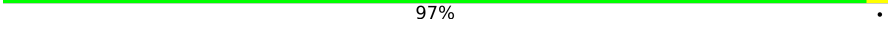
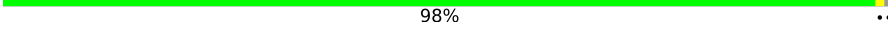
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	P	252	
2	Q	255	
3	R	254	

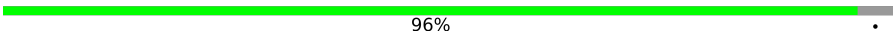
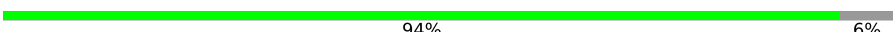
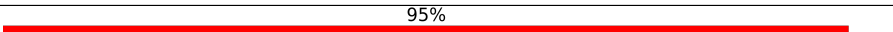
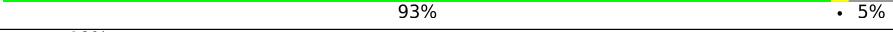
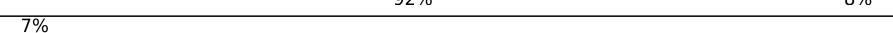
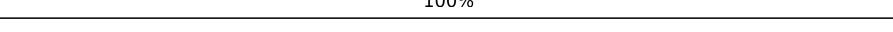
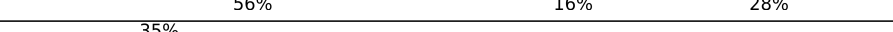
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Mol	Chain	Length	Quality of chain
4	S	261	 98%
5	T	236	 93%
6	V	200	 92% 6%
7	W	197	 93% 7%
8	X	156	 91% 9%
9	Y	151	 99%
10	Z	137	 90% 7%
11	a	87	 100%
12	b	130	 98% ..
13	c	145	 97% ..
14	d	135	 98% ..
15	e	119	 81% 18%
16	f	82	 26% 85% 13%
17	g	63	 84% 16%
18	E	142	 80% 18%
19	B	240	 92% 8%
20	D	105	 84% 12%
21	F	143	 83% 15%
22	H	143	 97% ..
23	I	136	 88% 11%
24	J	146	 97% ..
25	K	144	 98% ..
26	L	121	 83% 17%
27	M	108	 6% 76% 24%
28	N	56	 88% 7% 5%

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Mol	Chain	Length	Quality of chain
29	O	76	 96% .
30	h	319	 88% 10% .
31	i	67	 94% 6%
32	l	347	 95%  93% . 5%
33	r	274	 19% 81%
34	1	75	 48% 39% 8% 5%
35	m	405	 35% 64% 6%
36	o	964	 55% 45% 13%
37	p	763	 39% 83% 15%
38	q	812	 16% 78% 22%
39	3	8	 12% 88% 12%
40	A	153	 61% 5% 34%
41	k	608	 75% 94% 5%
42	2	1800	 61% 33% 5%
43	C	225	 92% 8%
44	y	76	 7% 100%
45	n	25	 56% 16% 28%
46	j	304	 35% 69% 12% 18%
47	G	527	 50% 60% 15% 25%
48	s	285	 36% 38% 7% 55%
49	x	307	 84% 16%
50	U	190	 78% 18% . .

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 86738 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 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	P	206	Total	C	N	O	0	0
			1020	608	206	206		

- Molecule 2 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	Q	226	Total	C	N	O	0	0
			1119	667	226	226		

- Molecule 3 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	R	216	Total	C	N	O	0	0
			1058	626	216	216		

- Molecule 4 is a protein called 40S ribosomal protein S4-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	S	258	Total	C	N	O	0	0
			1267	751	258	258		

- Molecule 5 is a protein called 40S ribosomal protein S6-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	T	228	Total	C	N	O	0	0
			1123	667	228	228		

- Molecule 6 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	V	187	Total	C	N	O	0	0
			919	545	187	187		

- Molecule 7 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	W	184	Total	C	N	O	0	0
			910	542	184	184		

- Molecule 8 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	X	142	Total	C	N	O	0	0
			702	418	142	142		

- Molecule 9 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	Y	150	Total	C	N	O	0	0
			742	442	150	150		

- Molecule 10 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	Z	127	Total	C	N	O	0	0
			620	366	127	127		

- Molecule 11 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	a	87	Total	C	N	O	0	0
			429	255	87	87		

- Molecule 12 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	b	129	Total	C	N	O	0	0
			634	376	129	129		

- Molecule 13 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	c	144	Total	C	N	O	0	0
			704	416	144	144		

- Molecule 14 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	d	134	Total	C	N	O	0	0
			661	393	134	134		

- Molecule 15 is a protein called 40S ribosomal protein S26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	e	97	Total	C	N	O	0	0
			482	288	97	97		

- Molecule 16 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	f	81	Total	C	N	O	0	0
			400	238	81	81		

- Molecule 17 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	g	53	Total	C	N	O	0	0
			261	155	53	53		

- Molecule 18 is a protein called RPS15 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	E	117	Total	C	N	O	0	0
			576	342	117	117		

- Molecule 19 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	B	222	Total	C	N	O	0	0
			1093	649	222	222		

- Molecule 20 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	D	92	Total	C	N	O	0	0
			456	272	92	92		

- Molecule 21 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	F	121	Total	C	N	O	0	0
			595	353	121	121		

- Molecule 22 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	H	141	Total	C	N	O	0	0
			693	411	141	141		

- Molecule 23 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	I	121	Total	C	N	O	0	0
			600	358	121	121		

- Molecule 24 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	J	145	Total	C	N	O	0	0
			715	425	145	145		

- Molecule 25 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	K	143	Total	C	N	O	0	0
			700	414	143	143		

- Molecule 26 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	L	100	Total	C	N	O	0	0
			496	296	100	100		

- Molecule 27 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	M	82	Total	C	N	O	0	0
			407	243	82	82		

- Molecule 28 is a protein called RPS29A isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	N	53	Total	C	N	O	0	0
			260	154	53	53		

- Molecule 29 is a protein called 40S ribosomal protein S31.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	O	73	Total	C	N	O	0	0
			361	215	73	73		

- Molecule 30 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	h	312	Total	C	N	O	0	0
			1538	914	312	312		

- Molecule 31 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	i	63	Total	C	N	O	0	0
			310	184	63	63		

- Molecule 32 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	l	330	Total	C	N	O	0	0
			1624	964	330	330		

- Molecule 33 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	r	53	Total	C	N	O	0	0
			261	155	53	53		

- Molecule 34 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1	75	Total	C	N	O	P	0	0
			1639	734	298	531	76		

- Molecule 35 is a protein called TIF5 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	m	147	Total	C	N	O	0	0
			726	432	147	147		

- Molecule 36 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	o	529	Total	C	N	O	0	0
			2632	1574	529	529		

- Molecule 37 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	p	646	Total	C	N	O	0	0
			3201	1909	646	646		

- Molecule 38 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	q	636	Total	C	N	O	0	0
			3169	1897	636	636		

- Molecule 39 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	3	8	Total	C	N	O	P	0	0
			171	77	32	54	8		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 4C.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	A	101	Total	C	N	O	0	0
			497	295	101	101		

- Molecule 41 is a protein called RLI1 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	k	579	Total	C	N	O	0	0
			2860	1702	579	579		

- Molecule 42 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	2	1763	Total	C	N	O	P	0	0
			37577	16799	6661	12354	1763		

- Molecule 43 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	C	206	Total	C	N	O	0	0
			1020	608	206	206		

- Molecule 44 is a protein called 60S ribosomal protein L40-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	y	76	Total	C	N	O	0	0
			374	222	76	76		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	19	PRO	SER	conflict	UNP P0CH08
y	24	GLU	ASP	conflict	UNP P0CH08
y	28	ALA	SER	conflict	UNP P0CH08

- Molecule 45 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	18	Total	C	N	O	S	0	0
			175	107	48	19	1		

- Molecule 46 is a protein called SUI2 isoform 1.

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

- Molecule 47 is a protein called protein-synthesizing GTPase.

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

- Molecule 48 is a protein called SUI3 isoform 1.

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

- Molecule 49 is a protein called OTU domain-containing protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	259	Total	C	N	O		0	0
			1289	770	259	260			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
x	178	SER	CYS	engineered mutation	UNP P38747

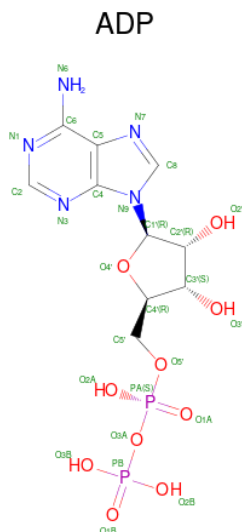
- Molecule 50 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	U	184	Total	C	N	O		0	0
			1473	946	263	264			

- Molecule 51 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
51	N	1	Total	Zn	0
			1	1	
51	O	1	Total	Zn	0
			1	1	
51	m	1	Total	Zn	0
			1	1	
51	s	1	Total	Zn	0
			1	1	

- Molecule 52 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

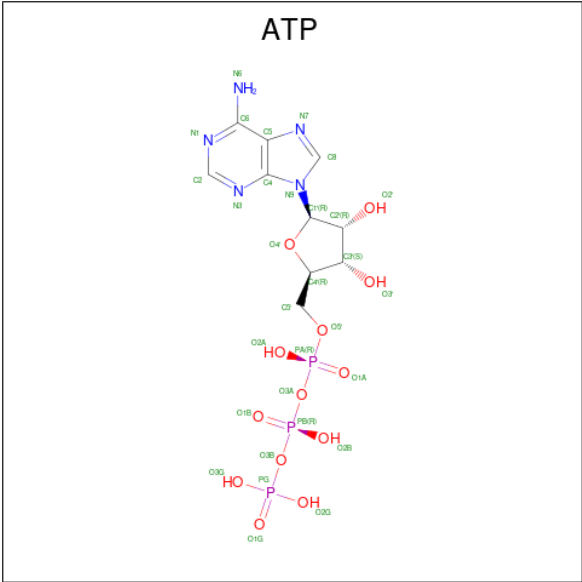


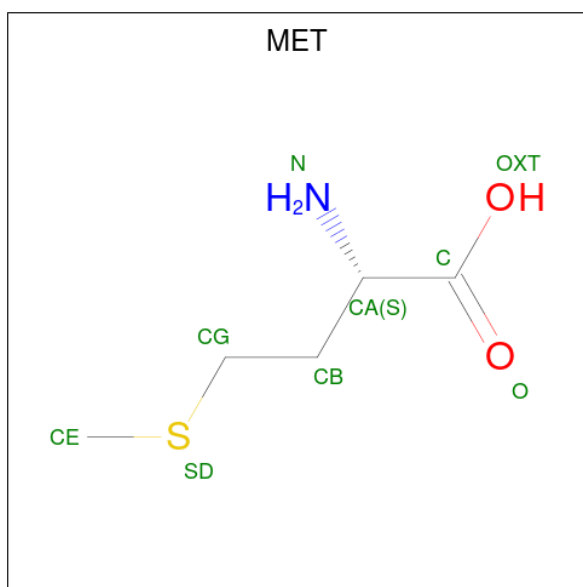
Mol	Chain	Residues	Atoms					AltConf
52	k	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
53	k	2	Total Mg 2 2	0
53	2	2	Total Mg 2 2	0
53	G	1	Total Mg 1 1	0

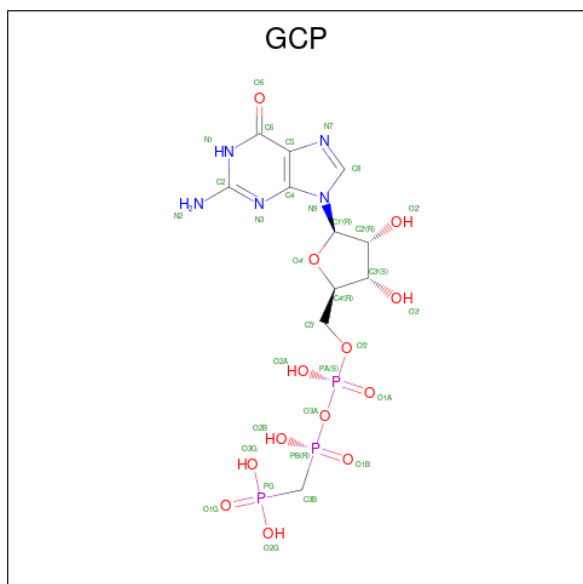
- Molecule 54 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).





Mol	Chain	Residues	Atoms					AltConf
56	G	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 57 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



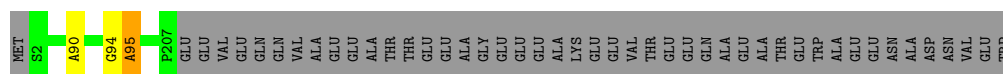
Mol	Chain	Residues	Atoms					AltConf
57	G	1	Total	C	N	O	P	0
			32	11	5	13	3	

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.

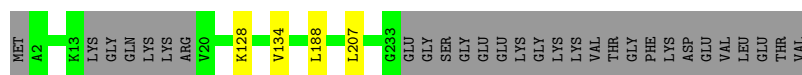
- Molecule 1: 40S ribosomal protein S0-A

Chain P: 



- Molecule 2: 40S ribosomal protein S1-A

Chain Q: 

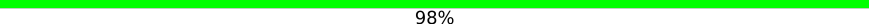


- Molecule 3: 40S ribosomal protein S2

Chain R: 

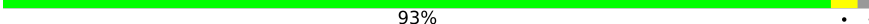


- Molecule 4: 40S ribosomal protein S4-B

Chain S: 



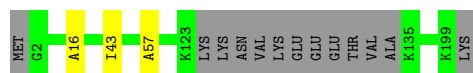
- Molecule 5: 40S ribosomal protein S6-B

Chain T: 

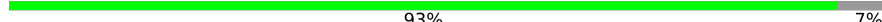


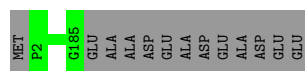
- Molecule 6: 40S ribosomal protein S8-A

Chain V:  92% • 6%



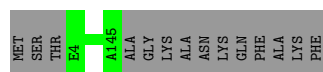
- Molecule 7: 40S ribosomal protein S9-A

Chain W:  93% 7%

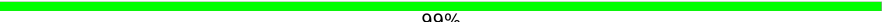


- Molecule 8: 40S ribosomal protein S11-A

Chain X:  91% 9%



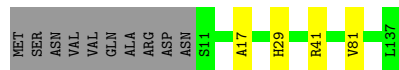
- Molecule 9: 40S ribosomal protein S13

Chain Y:  99% •



- Molecule 10: 40S ribosomal protein S14-A

Chain Z:  90% • 7%

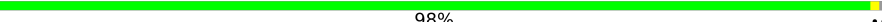


- Molecule 11: 40S ribosomal protein S21-A

Chain a:  100%

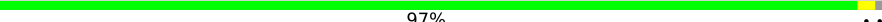
There are no outlier residues recorded for this chain.

- Molecule 12: 40S ribosomal protein S22-A

Chain b:  98% ••

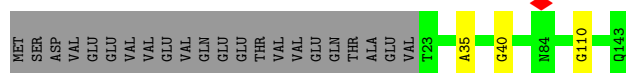
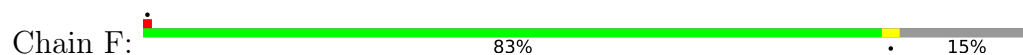


- Molecule 13: 40S ribosomal protein S23-A

Chain c:  97% ••



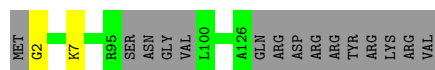
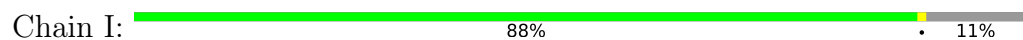
- Molecule 21: 40S ribosomal protein S12



- Molecule 22: 40S ribosomal protein S16-A



- Molecule 23: 40S ribosomal protein S17-A



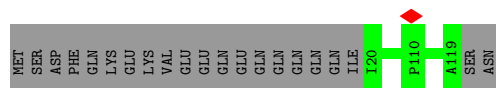
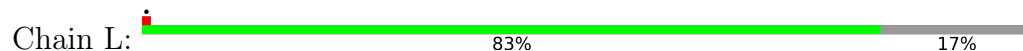
- Molecule 24: 40S ribosomal protein S18-A



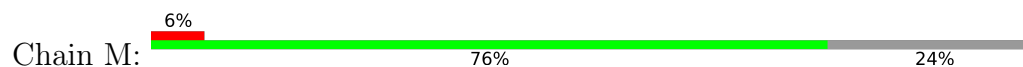
- Molecule 25: 40S ribosomal protein S19-A

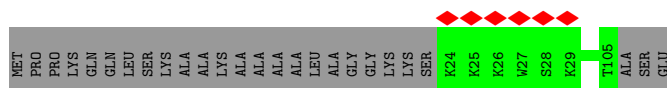


- Molecule 26: 40S ribosomal protein S20



- Molecule 27: 40S ribosomal protein S25-A





- Molecule 28: RPS29A isoform 1

Chain N: 88% 7% 5%



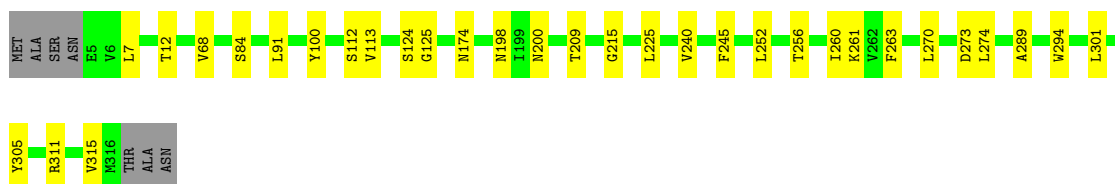
- Molecule 29: 40S ribosomal protein S31

Chain O: 96% .



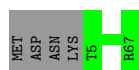
- Molecule 30: Guanine nucleotide-binding protein subunit beta-like protein

Chain h: 88% 10% .



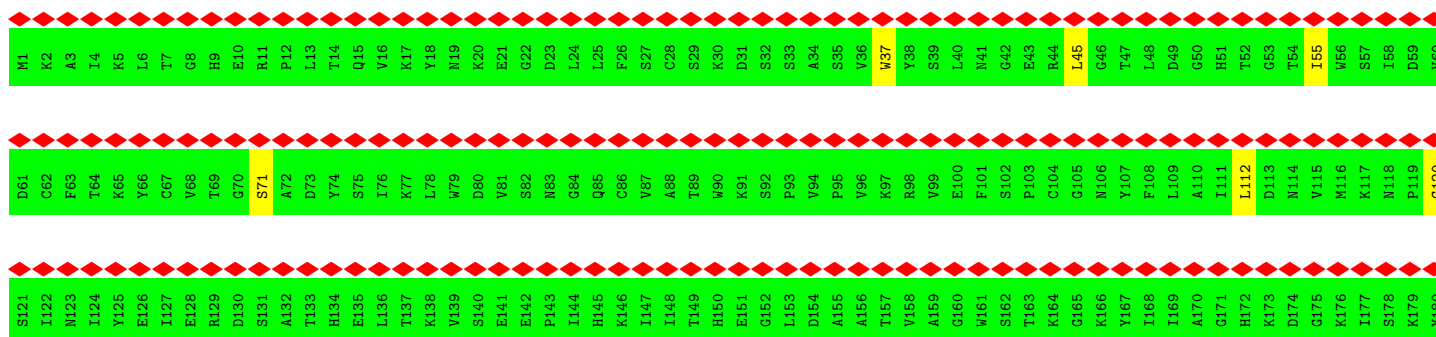
- Molecule 31: 40S ribosomal protein S28-A

Chain i: 94% 6%

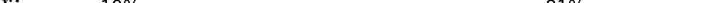


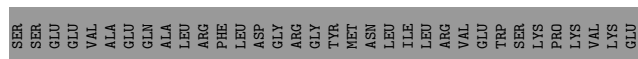
- Molecule 32: Eukaryotic translation initiation factor 3 subunit I

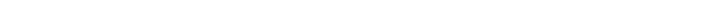
Chain l: 95% 93% . 5%

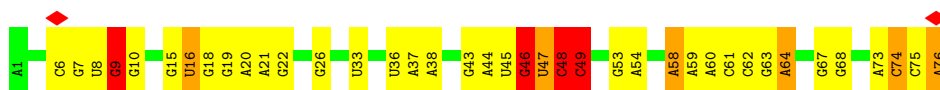




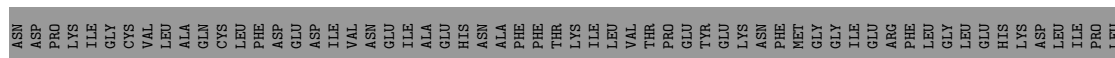
Chain r:  19% 81%



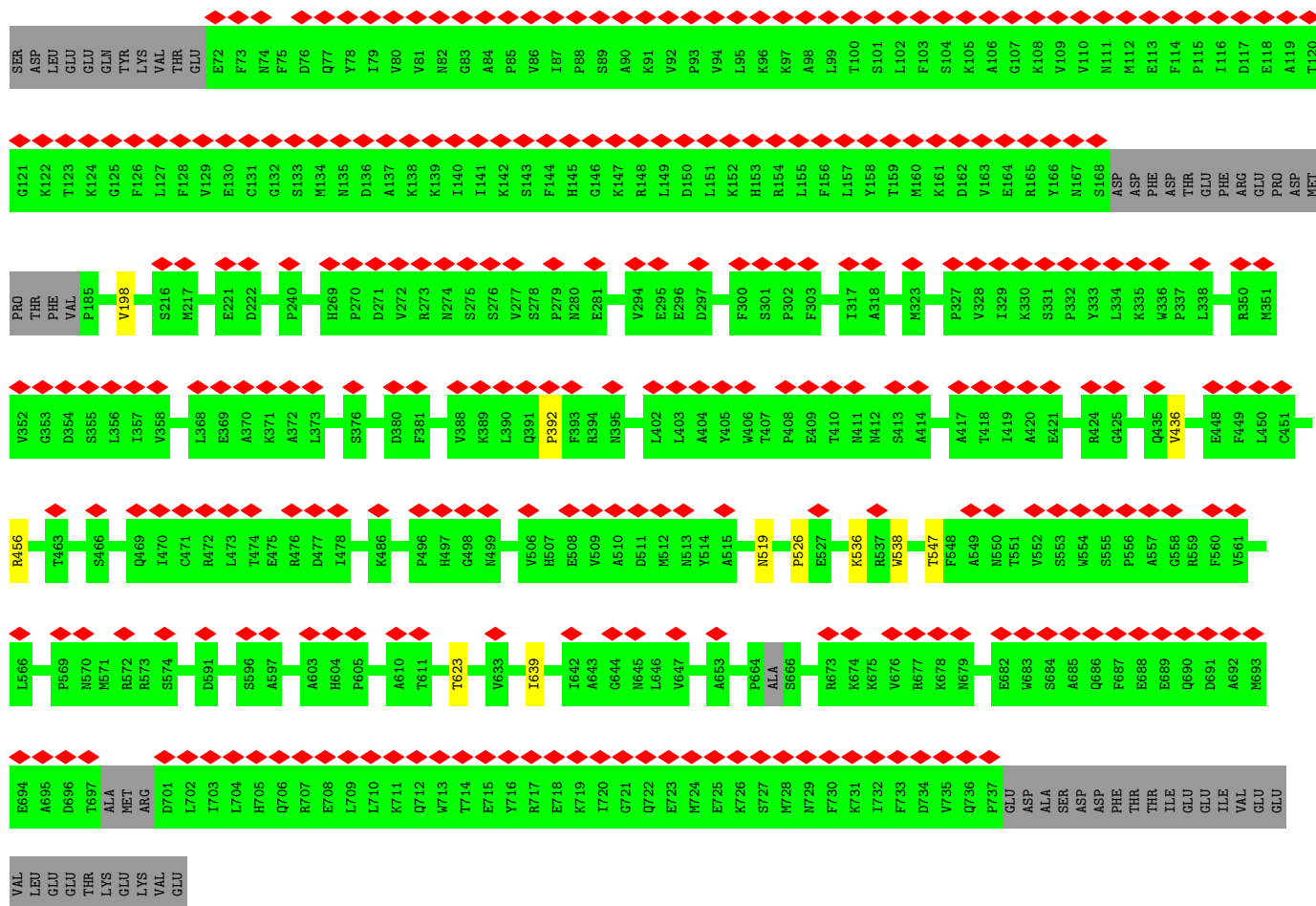
Chain 1:  48% 39% 8% 5%



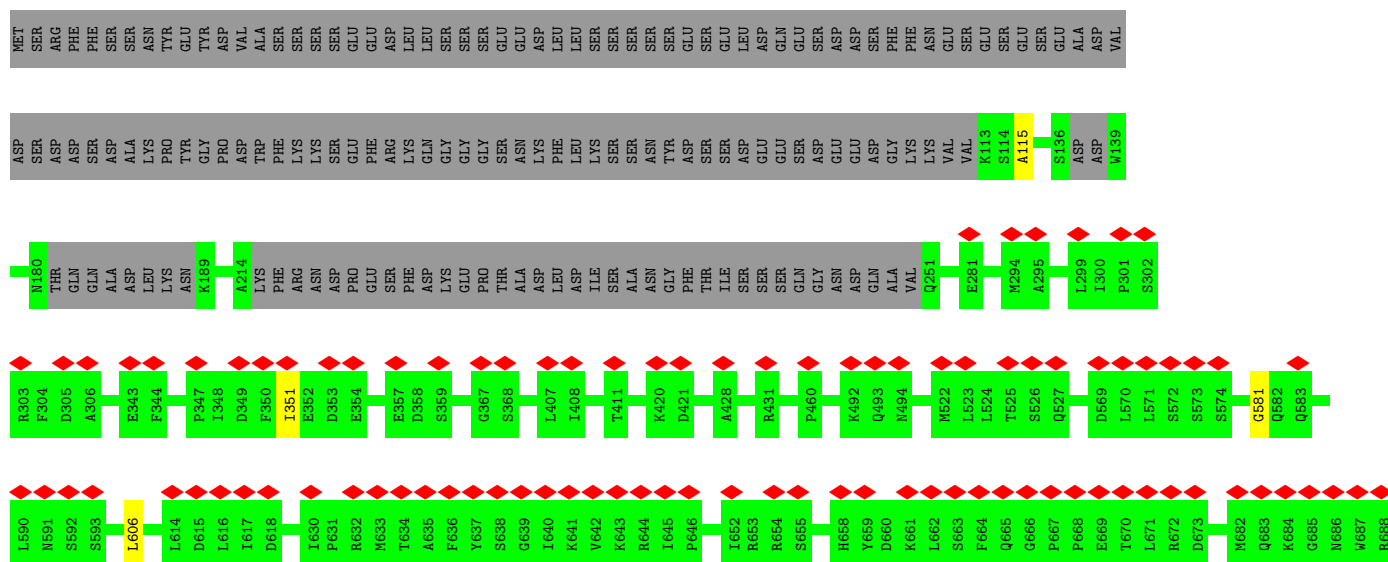
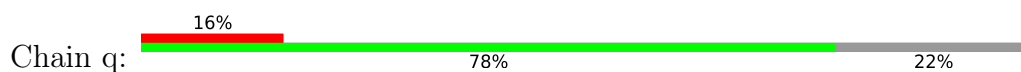
Chain m: 6% 35% 64%

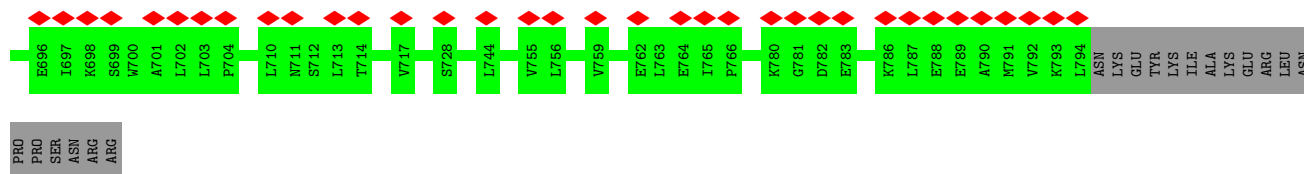


MET	LYS	ASN	PHE	LEU	PRO	ARG	THR	LYS	ASN	ILE	TYR	GLU	TYR	PHE	ASN	ASN	VAL	SER	HIS	SER	ILE	VAL	SER	ARG	ASN	THR	GLN	LEU	LYS	ARG	SER	LYS	ILE	ILE	GLN	MET	THR	THR	GLU	THR	PHE	GLU	ASP	ILE	LYS	LEU	GLU	ASP	PRO	VAL	ASP	ASP	ILE	ASP	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

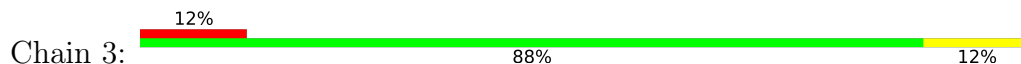


- Molecule 38: Eukaryotic translation initiation factor 3 subunit C

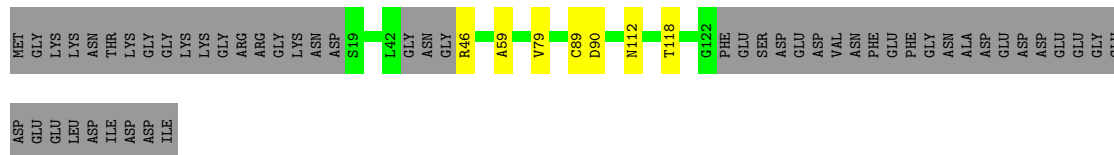




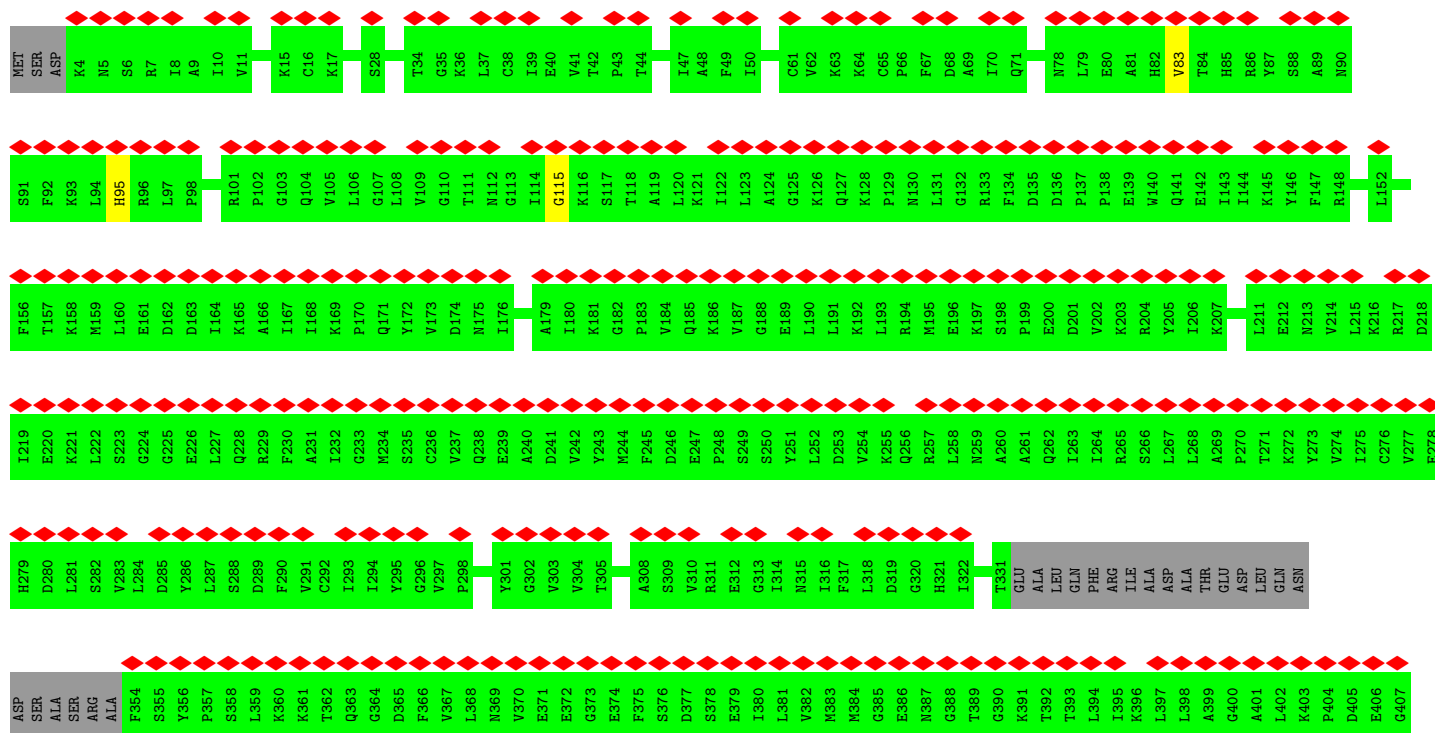
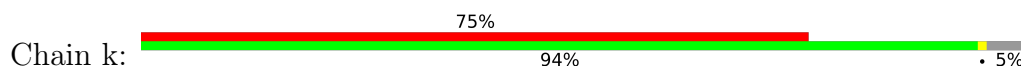
• Molecule 39: mRNA

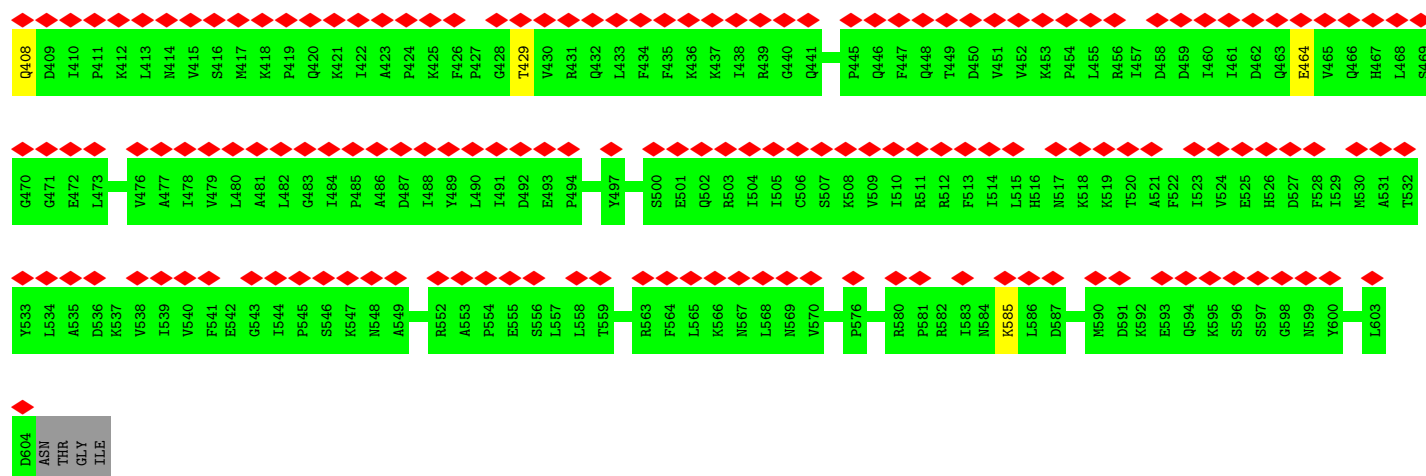


• Molecule 40: Eukaryotic translation initiation factor 4C



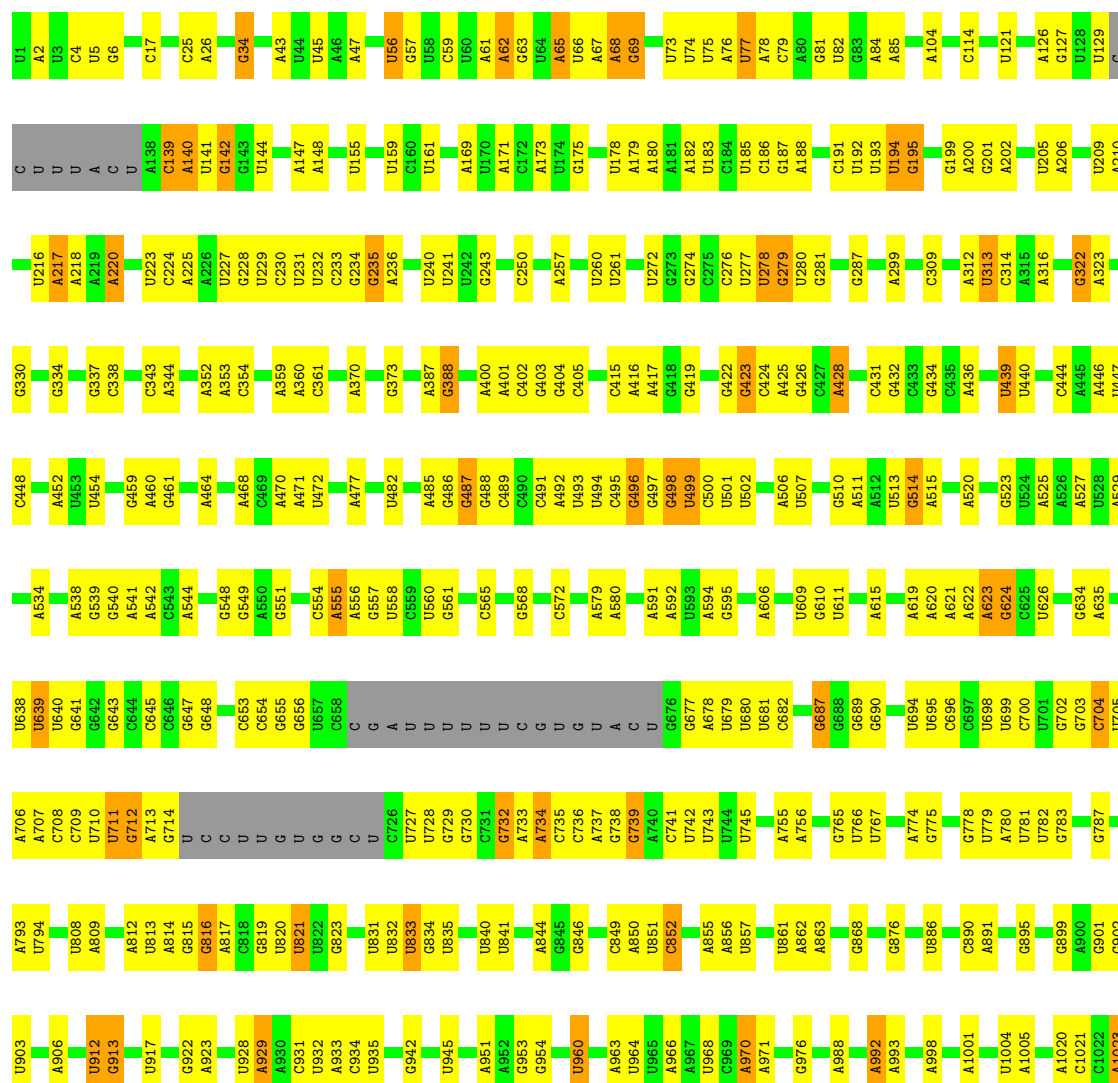
• Molecule 41: RLI1 isoform 1



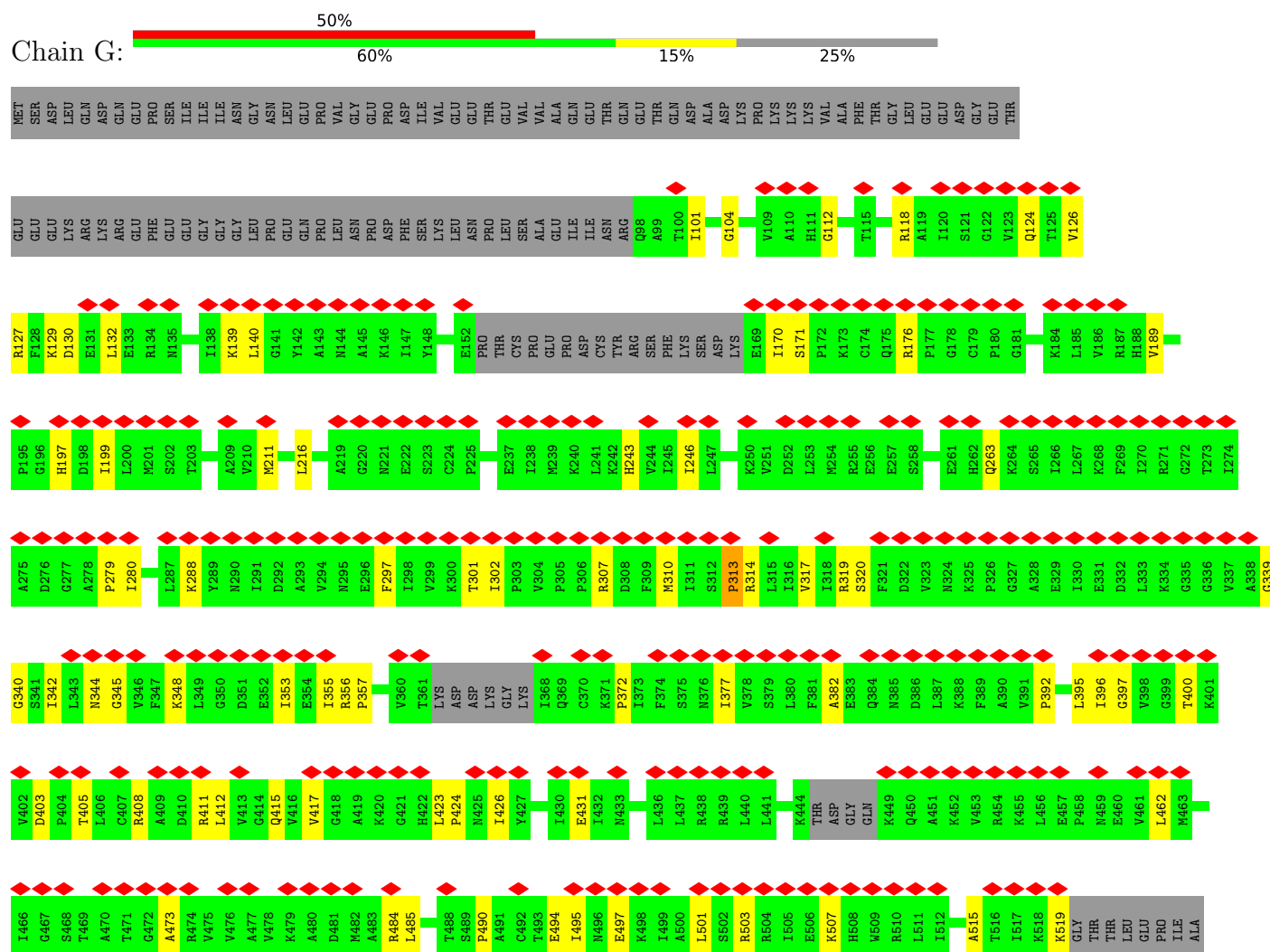


• Molecule 42: 18S ribosomal RNA

Chain 2: 61% 33% 5% •







- Molecule 48: SUI3 isoform 1

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12059	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 ($e^-/\text{\AA}^2$)	46.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.596	Depositor
Minimum map value	-1.857	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	438.9, 438.9, 438.9	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1MA, 1MG, ZN, H2U, ADP, ATP, T6A, 5MC, 2MG, G7M, MG, M2G, GCP, SF4, RIA

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	P	0.30	0/1019	0.59	1/1419 (0.1%)
2	Q	0.27	0/1117	0.68	3/1554 (0.2%)
3	R	0.32	0/1057	0.62	0/1465
4	S	0.33	0/1266	0.72	0/1757
5	T	0.25	0/1122	0.60	0/1559
6	V	0.32	0/917	0.66	0/1271
7	W	0.30	0/909	0.64	0/1265
8	X	0.35	0/701	0.71	0/975
9	Y	0.28	0/741	0.61	0/1031
10	Z	0.28	0/619	0.60	0/856
11	a	0.28	0/428	0.65	0/594
12	b	0.36	0/633	0.60	0/878
13	c	0.35	0/703	0.68	0/973
14	d	0.32	0/660	0.57	0/917
15	e	0.31	0/481	0.71	0/670
16	f	0.35	0/399	0.95	0/554
17	g	0.29	0/260	0.50	0/360
18	E	0.18	0/575	0.50	0/798
19	B	0.23	0/1092	0.53	0/1517
20	D	0.19	0/455	0.59	0/633
21	F	0.21	0/594	0.72	0/824
22	H	0.23	0/692	0.58	1/960 (0.1%)
23	I	0.20	0/598	0.43	0/831
24	J	0.18	0/714	0.50	0/992
25	K	0.19	0/699	0.53	0/968
26	L	0.22	0/495	0.48	0/689
27	M	0.20	0/406	0.53	0/565
28	N	0.28	0/259	0.60	0/358
29	O	0.22	0/360	0.68	0/500
30	h	0.20	0/1537	0.56	0/2137
31	i	0.22	0/309	0.54	0/428
32	l	0.14	0/1622	0.48	0/2252

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	r	0.10	0/260	0.37	0/360
34	l	0.24	0/1529	0.43	0/2376
35	m	0.17	0/725	0.49	0/1008
36	o	0.13	0/2627	0.41	0/3662
37	p	0.17	0/3197	0.49	0/4452
38	q	0.15	0/3163	0.47	1/4412 (0.0%)
39	3	0.25	0/191	0.38	0/295
40	A	0.23	0/495	0.67	0/685
41	k	0.16	0/2858	0.51	0/3977
42	2	0.46	0/42031	0.49	8/65492 (0.0%)
43	C	0.21	0/1019	0.57	0/1419
44	y	0.15	0/373	0.52	0/517
45	n	0.41	0/176	0.72	0/225
46	j	0.27	0/2034	0.73	6/2737 (0.2%)
47	G	0.22	0/3079	0.59	2/4157 (0.0%)
48	s	0.26	1/1051 (0.1%)	0.49	0/1402
49	x	0.15	0/1286	0.43	0/1790
50	U	0.44	0/1498	0.91	2/2019 (0.1%)
All	All	0.36	1/91031 (0.0%)	0.54	24/133535 (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
1	P	0	1
13	c	0	1
16	f	0	2
21	F	0	1
47	G	0	1
50	U	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	s	129	LEU	C-N	6.00	1.38	1.33

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	j	97	LYS	CA-CB-CG	7.08	128.25	114.10
50	U	22	GLN	CA-CB-CG	7.05	128.19	114.10
50	U	157	LYS	CA-CB-CG	7.04	128.18	114.10
46	j	80	LYS	N-CA-C	-6.55	104.89	114.39
22	H	43	ILE	N-CA-C	-6.42	106.73	112.12

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	F	110	GLY	Peptide
1	P	94	GLY	Peptide
13	c	96	VAL	Peptide
16	f	61	THR	Peptide
16	f	80	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	P	1020	0	474	1	0
2	Q	1119	0	501	1	0
3	R	1058	0	497	0	0
4	S	1267	0	571	1	0
5	T	1123	0	514	5	0
6	V	919	0	450	2	0
7	W	910	0	420	0	0
8	X	702	0	304	0	0
9	Y	742	0	345	0	0
10	Z	620	0	311	2	0
11	a	429	0	201	0	0
12	b	634	0	289	1	0
13	c	704	0	324	1	0
14	d	661	0	312	1	0
15	e	482	0	223	1	0
16	f	400	0	180	4	0
17	g	261	0	113	0	0
18	E	576	0	264	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	1093	0	520	0	0
20	D	456	0	196	2	0
21	F	595	0	288	1	0
22	H	693	0	323	1	0
23	I	600	0	259	2	0
24	J	715	0	318	3	0
25	K	700	0	334	2	0
26	L	496	0	207	0	0
27	M	407	0	182	0	0
28	N	260	0	112	3	0
29	O	361	0	162	0	0
30	h	1538	0	736	16	0
31	i	310	0	134	0	0
32	l	1624	0	727	4	0
33	r	261	0	122	0	0
34	1	1639	0	848	13	0
35	m	726	0	316	3	0
36	o	2632	0	1201	0	0
37	p	3201	0	1398	4	0
38	q	3169	0	1370	1	0
39	3	171	0	87	0	0
40	A	497	0	221	4	0
41	k	2860	0	1247	4	0
42	2	37577	0	18905	164	0
43	C	1020	0	482	0	0
44	y	374	0	163	0	0
45	n	175	0	213	3	0
46	j	2006	0	2066	17	0
47	G	3034	0	3195	42	0
48	s	1036	0	1080	11	0
49	x	1289	0	556	1	0
50	U	1473	0	1555	19	0
51	N	1	0	0	0	0
51	O	1	0	0	0	0
51	m	1	0	0	0	0
51	s	1	0	0	0	0
52	k	27	0	12	1	0
53	2	2	0	0	0	0
53	G	1	0	0	0	0
53	k	2	0	0	0	0
54	k	31	0	12	0	0
55	k	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	G	8	0	8	2	0
57	G	32	0	14	1	0
All	All	86738	0	45862	318	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 318 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2:1663:G:H1	42:2:1738:U:H3	1.10	0.95
42:2:699:U:H3	42:2:739:G:H1	0.93	0.91
42:2:1588:G:H1	42:2:1608:U:H3	1.15	0.90
16:f:35:VAL:O	16:f:43:ILE:HA	1.86	0.75
42:2:868:G:H1	42:2:960:U:H3	1.36	0.74

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	204/252 (81%)	179 (88%)	25 (12%)	0	100	100
2	Q	222/255 (87%)	206 (93%)	16 (7%)	0	100	100
3	R	214/254 (84%)	203 (95%)	11 (5%)	0	100	100
4	S	256/261 (98%)	236 (92%)	20 (8%)	0	100	100
5	T	226/236 (96%)	216 (96%)	10 (4%)	0	100	100
6	V	183/200 (92%)	166 (91%)	17 (9%)	0	100	100
7	W	182/197 (92%)	171 (94%)	11 (6%)	0	100	100
8	X	140/156 (90%)	129 (92%)	11 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	Y	148/151 (98%)	136 (92%)	12 (8%)	0	100	100
10	Z	125/137 (91%)	114 (91%)	11 (9%)	0	100	100
11	a	85/87 (98%)	76 (89%)	9 (11%)	0	100	100
12	b	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
13	c	142/145 (98%)	128 (90%)	14 (10%)	0	100	100
14	d	132/135 (98%)	124 (94%)	8 (6%)	0	100	100
15	e	95/119 (80%)	90 (95%)	5 (5%)	0	100	100
16	f	79/82 (96%)	65 (82%)	13 (16%)	1 (1%)	9	35
17	g	51/63 (81%)	44 (86%)	7 (14%)	0	100	100
18	E	115/142 (81%)	105 (91%)	10 (9%)	0	100	100
19	B	220/240 (92%)	211 (96%)	9 (4%)	0	100	100
20	D	90/105 (86%)	81 (90%)	9 (10%)	0	100	100
21	F	119/143 (83%)	98 (82%)	21 (18%)	0	100	100
22	H	139/143 (97%)	125 (90%)	14 (10%)	0	100	100
23	I	117/136 (86%)	113 (97%)	4 (3%)	0	100	100
24	J	143/146 (98%)	133 (93%)	10 (7%)	0	100	100
25	K	141/144 (98%)	135 (96%)	6 (4%)	0	100	100
26	L	98/121 (81%)	93 (95%)	5 (5%)	0	100	100
27	M	80/108 (74%)	77 (96%)	3 (4%)	0	100	100
28	N	51/56 (91%)	51 (100%)	0	0	100	100
29	O	71/76 (93%)	54 (76%)	17 (24%)	0	100	100
30	h	310/319 (97%)	287 (93%)	23 (7%)	0	100	100
31	i	61/67 (91%)	57 (93%)	4 (7%)	0	100	100
32	l	326/347 (94%)	321 (98%)	5 (2%)	0	100	100
33	r	51/274 (19%)	49 (96%)	2 (4%)	0	100	100
35	m	145/405 (36%)	134 (92%)	11 (8%)	0	100	100
36	o	519/964 (54%)	509 (98%)	10 (2%)	0	100	100
37	p	638/763 (84%)	613 (96%)	22 (3%)	3 (0%)	24	55
38	q	624/812 (77%)	597 (96%)	26 (4%)	1 (0%)	43	71
40	A	97/153 (63%)	90 (93%)	6 (6%)	1 (1%)	12	40
41	k	575/608 (95%)	552 (96%)	22 (4%)	1 (0%)	43	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	C	204/225 (91%)	188 (92%)	16 (8%)	0	100	100
44	y	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
45	n	16/25 (64%)	16 (100%)	0	0	100	100
46	j	243/304 (80%)	222 (91%)	20 (8%)	1 (0%)	30	60
47	G	388/527 (74%)	357 (92%)	28 (7%)	3 (1%)	16	45
48	s	120/285 (42%)	117 (98%)	3 (2%)	0	100	100
49	x	253/307 (82%)	251 (99%)	2 (1%)	0	100	100
50	U	182/190 (96%)	173 (95%)	9 (5%)	0	100	100
All	All	8821/11071 (80%)	8283 (94%)	527 (6%)	11 (0%)	49	75

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	f	59	CYS
37	p	392	PRO
37	p	536	LYS
47	G	497	GLU
40	A	118	THR

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	
45	n	17/23 (74%)	17 (100%)	0	100	100
46	j	224/274 (82%)	222 (99%)	2 (1%)	70	78
47	G	332/449 (74%)	329 (99%)	3 (1%)	70	78
48	s	119/246 (48%)	119 (100%)	0	100	100
50	U	163/170 (96%)	160 (98%)	3 (2%)	51	70
All	All	855/1162 (74%)	847 (99%)	8 (1%)	68	78

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	U	34	LEU
50	U	19	GLN
47	G	495	ILE
47	G	423	LEU
50	U	16	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
47	G	384	GLN
47	G	433	ASN
50	U	71	HIS
48	s	176	ASN
50	U	29	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	1	72/75 (96%)	25 (34%)	2 (2%)
39	3	7/8 (87%)	1 (14%)	0
42	2	1759/1800 (97%)	499 (28%)	40 (2%)
All	All	1838/1883 (97%)	525 (28%)	42 (2%)

5 of 525 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	1	8	U
34	1	9	1MG
34	1	10	2MG
34	1	15	G
34	1	16	H2U

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
42	2	1108	G
42	2	1430	U
42	2	1226	A
42	2	1274	C
42	2	1573	A

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	$\# Z > 2$
34	M2G	1	26	34	24,27,28	0.52	0	35,40,43	0.64	0
34	H2U	1	16	34	18,21,22	0.49	0	21,30,33	1.09	1 (4%)
34	5MC	1	49	34	18,22,23	0.55	0	26,32,35	1.15	2 (7%)
34	T6A	1	37	34	31,34,35	1.84	7 (22%)	44,49,52	2.52	15 (34%)
34	1MG	1	9	34	22,26,27	2.87	5 (22%)	33,39,42	2.34	8 (24%)
34	H2U	1	47	34	18,21,22	0.46	0	21,30,33	1.30	2 (9%)
34	5MC	1	48	34	18,22,23	0.53	0	26,32,35	0.79	1 (3%)
34	RIA	1	64	34	35,38,39	4.28	21 (60%)	53,57,60	2.34	13 (24%)
34	2MG	1	10	34	23,26,27	0.48	0	32,38,41	0.66	0
34	1MA	1	58	34	21,25,26	0.45	0	31,37,40	0.86	1 (3%)
34	G7M	1	46	34	23,26,27	2.60	8 (34%)	35,39,42	1.95	9 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	M2G	1	26	34	-	2/11/29/30	0/3/3/3
34	H2U	1	16	34	-	2/7/38/39	0/2/2/2
34	5MC	1	49	34	-	2/7/25/26	0/2/2/2
34	T6A	1	37	34	-	8/23/41/42	0/3/3/3
34	1MG	1	9	34	-	3/7/25/26	0/3/3/3
34	H2U	1	47	34	-	5/7/38/39	0/2/2/2
34	5MC	1	48	34	-	3/7/25/26	0/2/2/2
34	RIA	1	64	34	-	3/17/51/52	0/4/4/4
34	2MG	1	10	34	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	1MA	1	58	34	-	2/7/25/26	0/3/3/3
34	G7M	1	46	34	-	1/7/25/26	0/3/3/3

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	1	64	RIA	C3A-C2A	-12.91	1.24	1.52
34	1	64	RIA	C1'-C2'	11.29	1.67	1.52
34	1	64	RIA	C3'-C2'	-10.44	1.24	1.53
34	1	9	1MG	C2-N3	7.30	1.47	1.34
34	1	9	1MG	C4-N3	6.85	1.50	1.34

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1	9	1MG	C1'-N9-C4	-6.78	106.37	126.50
34	1	64	RIA	C5-C4-N3	-6.64	118.09	126.75
34	1	37	T6A	C12-N11-C10	6.56	132.87	121.94
34	1	9	1MG	C1'-N9-C8	6.21	144.37	126.70
34	1	64	RIA	N3-C2-N1	-6.07	119.11	128.60

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	1	9	1MG	O4'-C4'-C5'-O5'
34	1	9	1MG	C3'-C4'-C5'-O5'
34	1	10	2MG	O4'-C4'-C5'-O5'
34	1	16	H2U	C4'-C5'-O5'-P
34	1	26	M2G	C3'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	1	49	5MC	1	0
34	1	9	1MG	1	0
34	1	48	5MC	1	0
34	1	46	G7M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 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
55	SF4	k	705	-	0,12,12	-	-	-		
52	ADP	k	701	53	27,29,29	1.37	4 (14%)	42,45,45	1.97	10 (23%)
55	SF4	k	706	-	0,12,12	-	-	-		
56	MET	G	601	-	6,7,8	0.50	0	2,7,9	0.33	0
57	GCP	G	603	-	31,34,34	2.04	2 (6%)	47,54,54	0.86	2 (4%)
54	ATP	k	703	53	29,33,33	0.27	0	44,52,52	0.45	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	SF4	k	705	-	-	-	0/6/5/5
52	ADP	k	701	53	-	2/16/32/32	0/3/3/3
57	GCP	G	603	-	-	4/19/38/38	0/3/3/3
56	MET	G	601	-	-	0/5/6/8	-
55	SF4	k	706	-	-	-	0/6/5/5
54	ATP	k	703	53	-	5/22/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	G	603	GCP	PB-O3A	10.40	1.70	1.58
52	k	701	ADP	C5-C4	4.58	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	k	701	ADP	C5-C6	2.75	1.48	1.41
52	k	701	ADP	C8-N7	2.45	1.36	1.31
57	G	603	GCP	PB-O2B	-2.27	1.51	1.56

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	k	701	ADP	C5-C4-N3	-6.27	118.57	126.75
52	k	701	ADP	N3-C4-N9	4.79	134.98	127.08
52	k	701	ADP	C2-N3-C4	3.88	120.92	111.75
52	k	701	ADP	PA-O3A-PB	-3.60	120.49	132.83
52	k	701	ADP	C4-C5-N7	-3.36	106.53	110.62

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	k	701	ADP	O4'-C4'-C5'-O5'
54	k	703	ATP	C5'-O5'-PA-O2A
54	k	703	ATP	C5'-O5'-PA-O3A
57	G	603	GCP	PB-C3B-PG-O1G
57	G	603	GCP	PG-C3B-PB-O2B

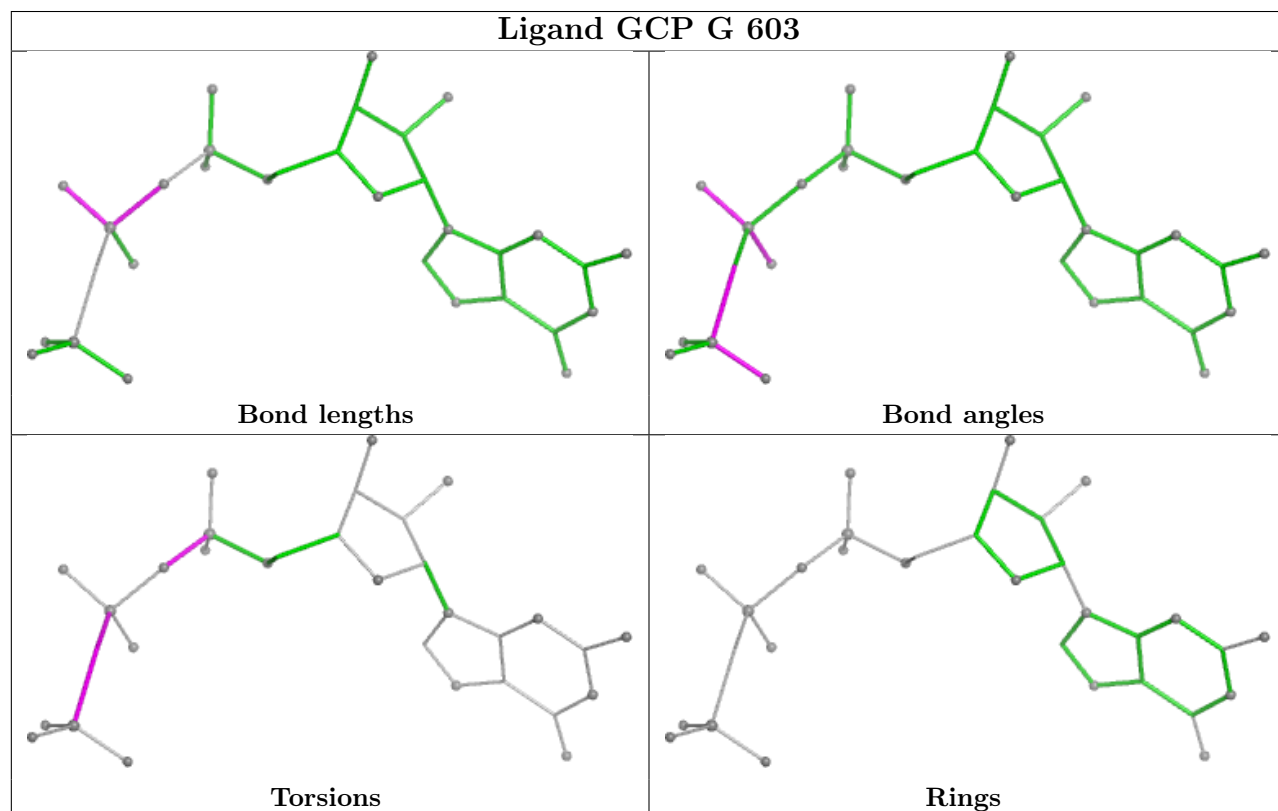
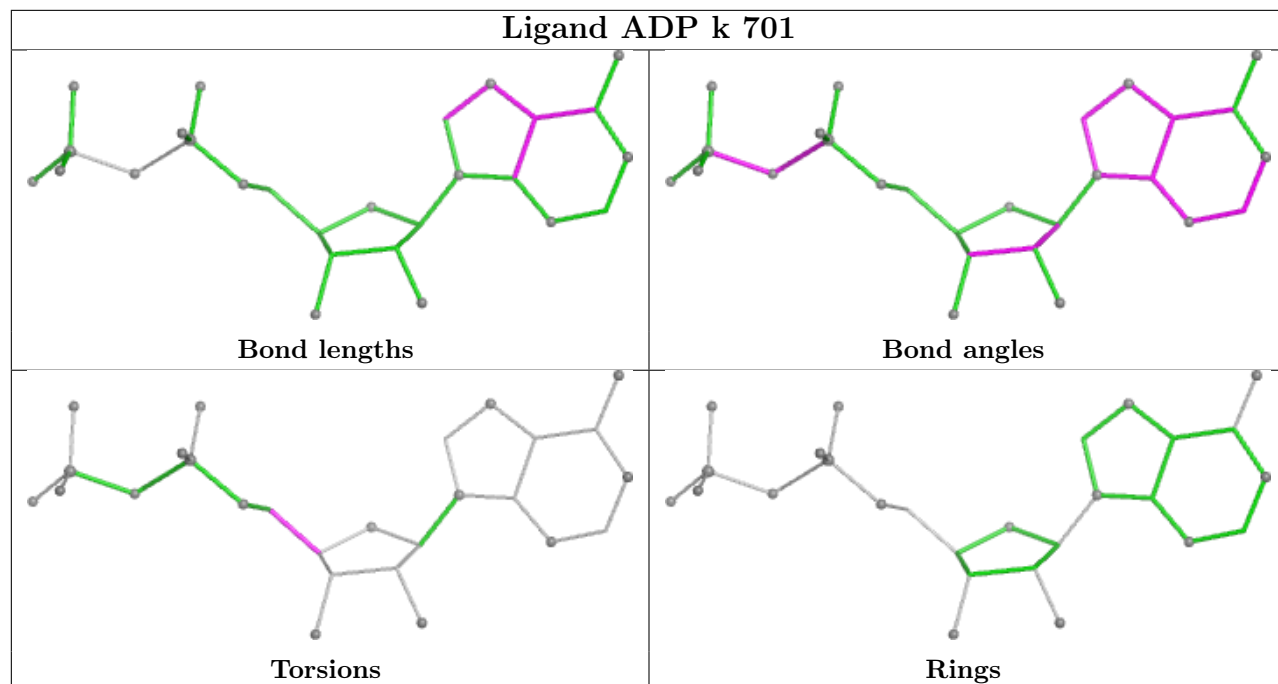
There are no ring outliers.

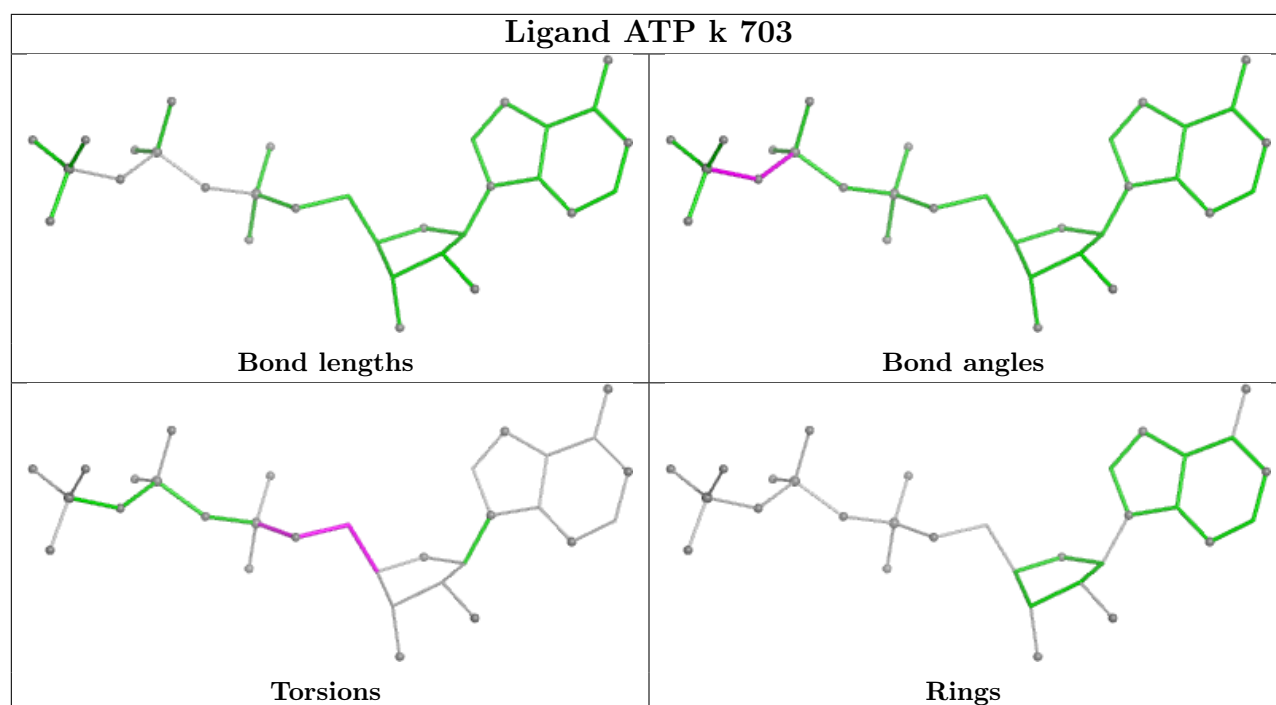
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	k	701	ADP	1	0
56	G	601	MET	2	0
57	G	603	GCP	1	0

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

equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
38	q	2
34	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	q	582:GLN	C	583:GLN	N	4.38
1	q	605:CYS	C	606:LEU	N	4.22
1	1	16:H2U	O3'	18:G	P	4.10

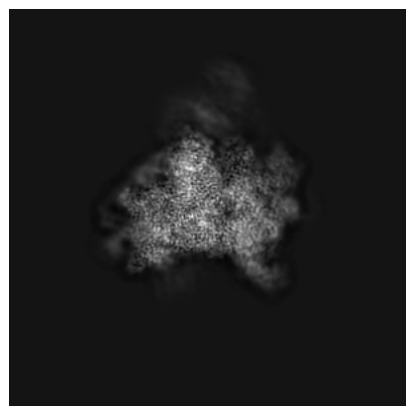
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16533. These allow visual inspection of the internal detail of the map and identification of artifacts.

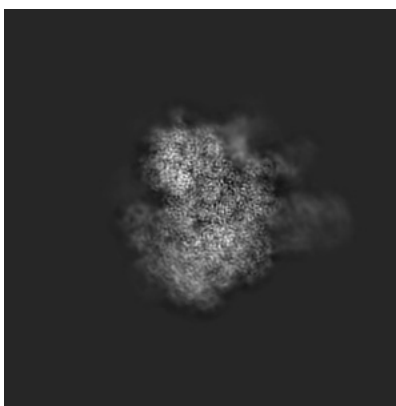
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

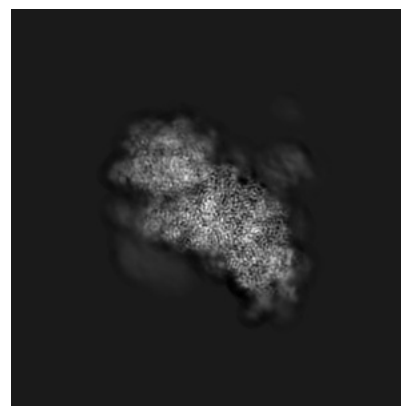
6.1.1 Primary map



X

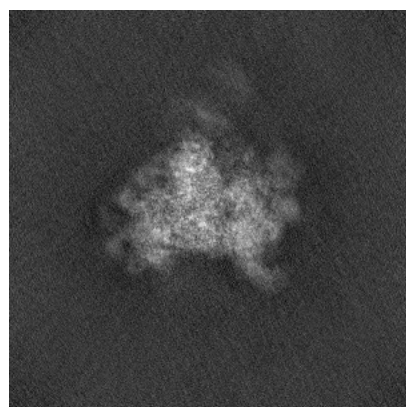


Y

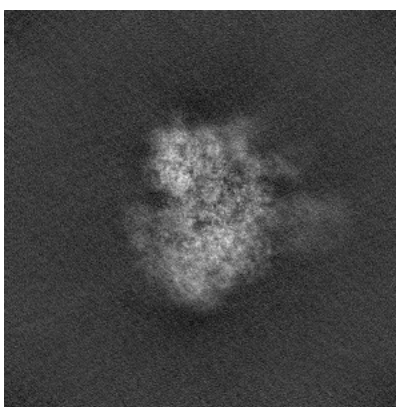


Z

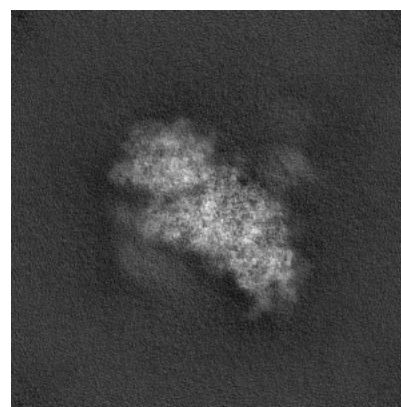
6.1.2 Raw map



X



Y

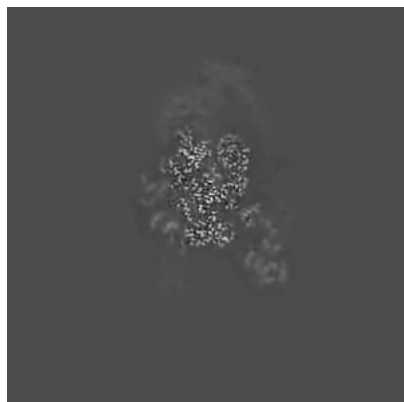


Z

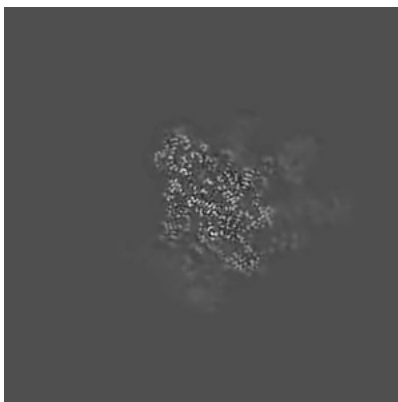
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

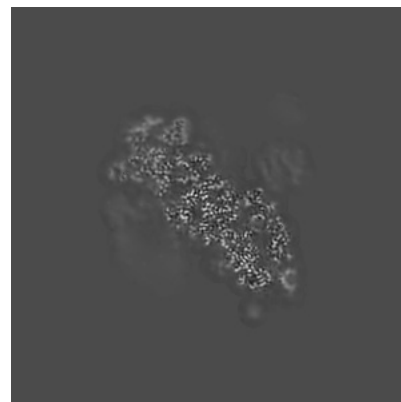
6.2.1 Primary map



X Index: 210

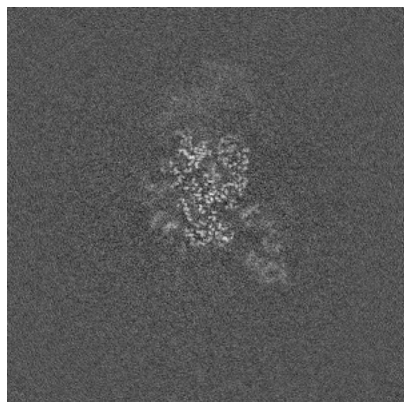


Y Index: 210

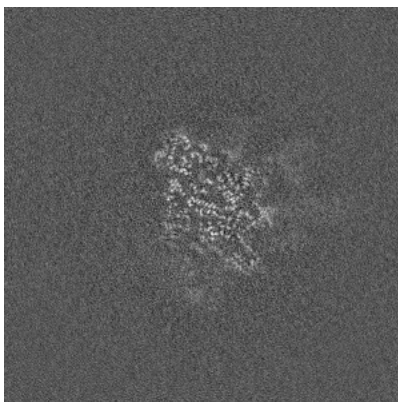


Z Index: 210

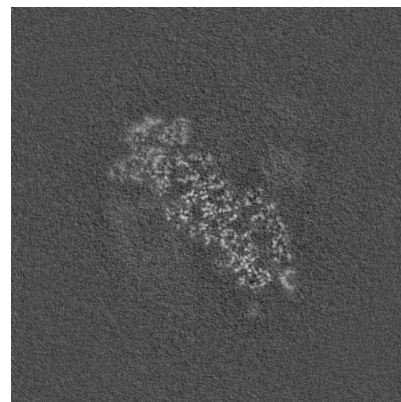
6.2.2 Raw map



X Index: 210



Y Index: 210

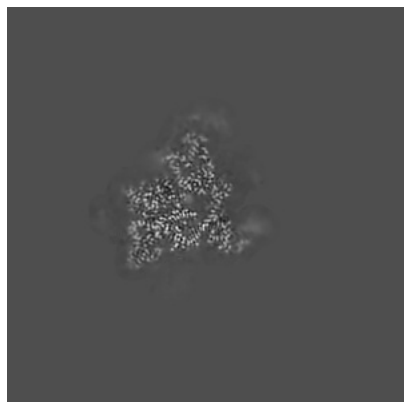


Z Index: 210

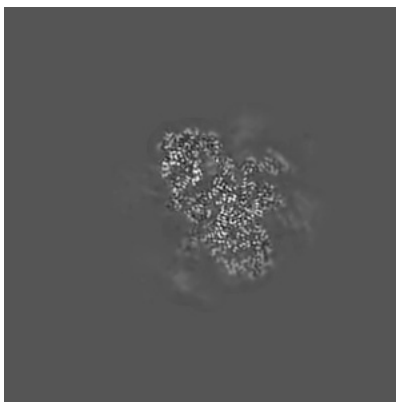
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

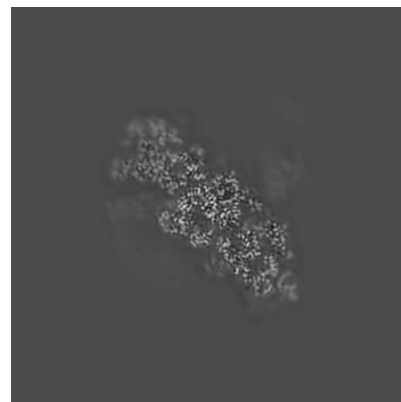
6.3.1 Primary map



X Index: 245

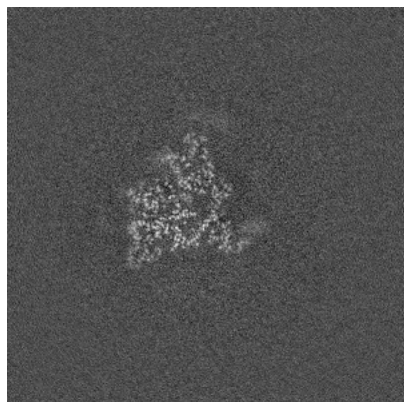


Y Index: 189

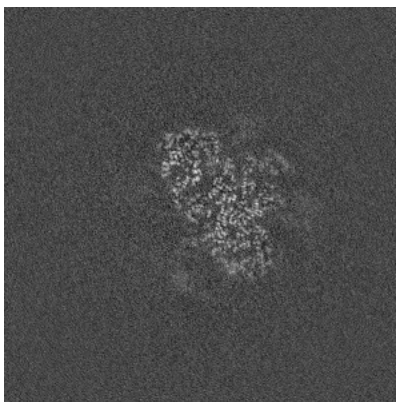


Z Index: 218

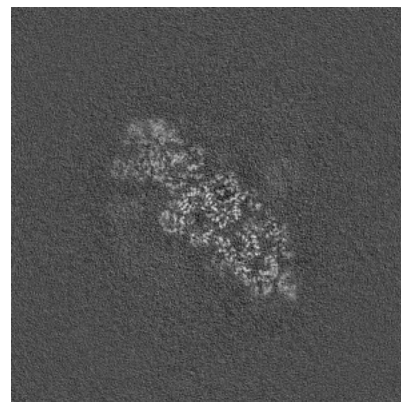
6.3.2 Raw map



X Index: 245



Y Index: 189

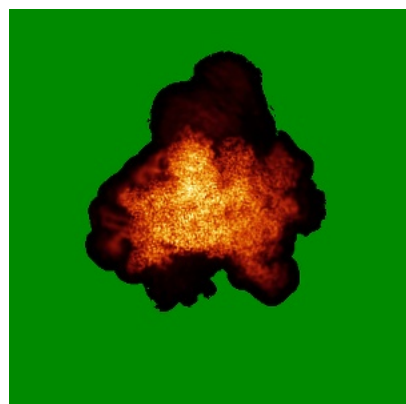


Z Index: 217

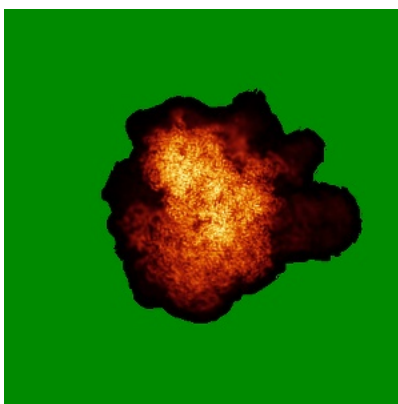
The images above show the largest variance slices of the map in three orthogonal directions.

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

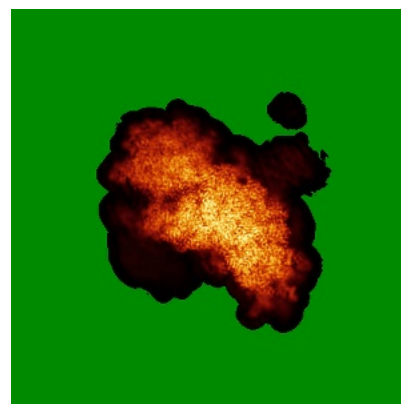
6.4.1 Primary map



X

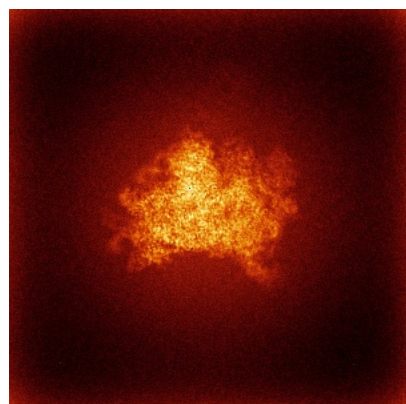


Y

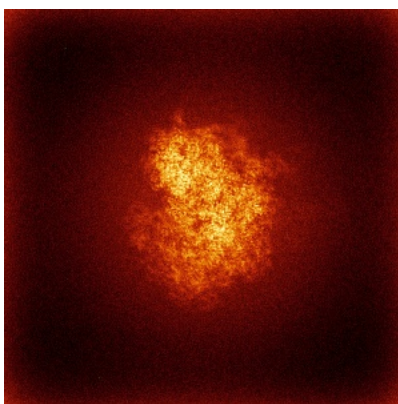


Z

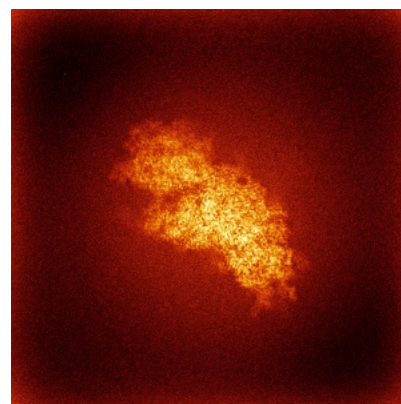
6.4.2 Raw map



X



Y

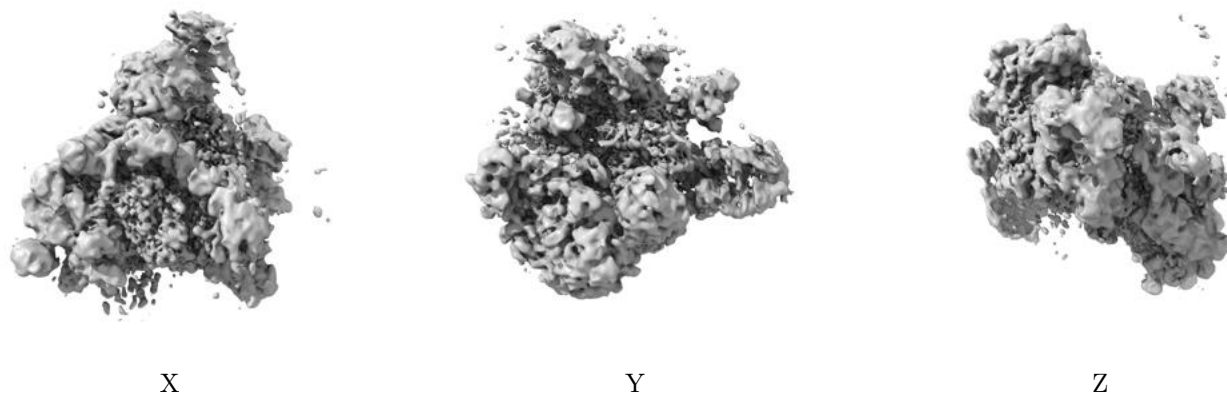


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

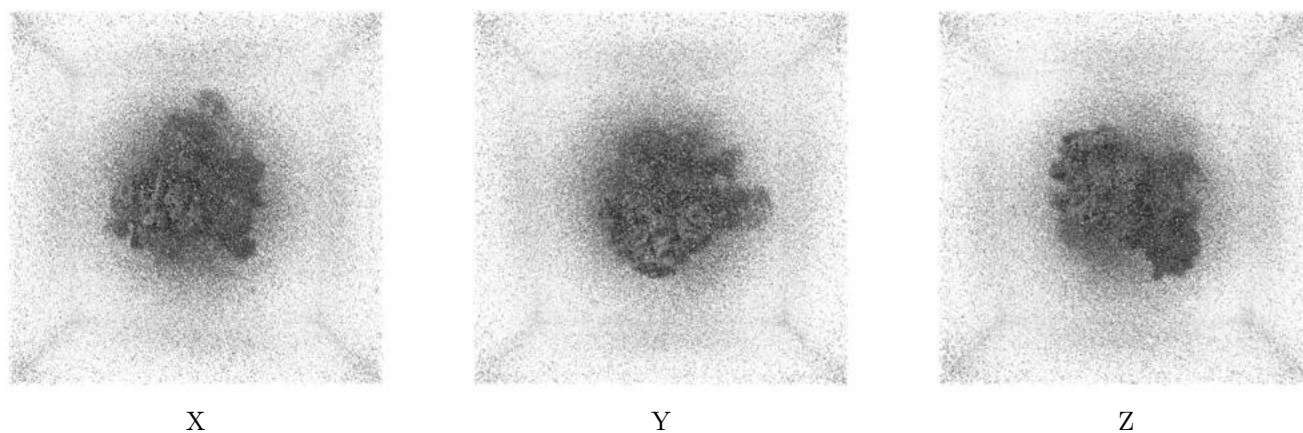
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

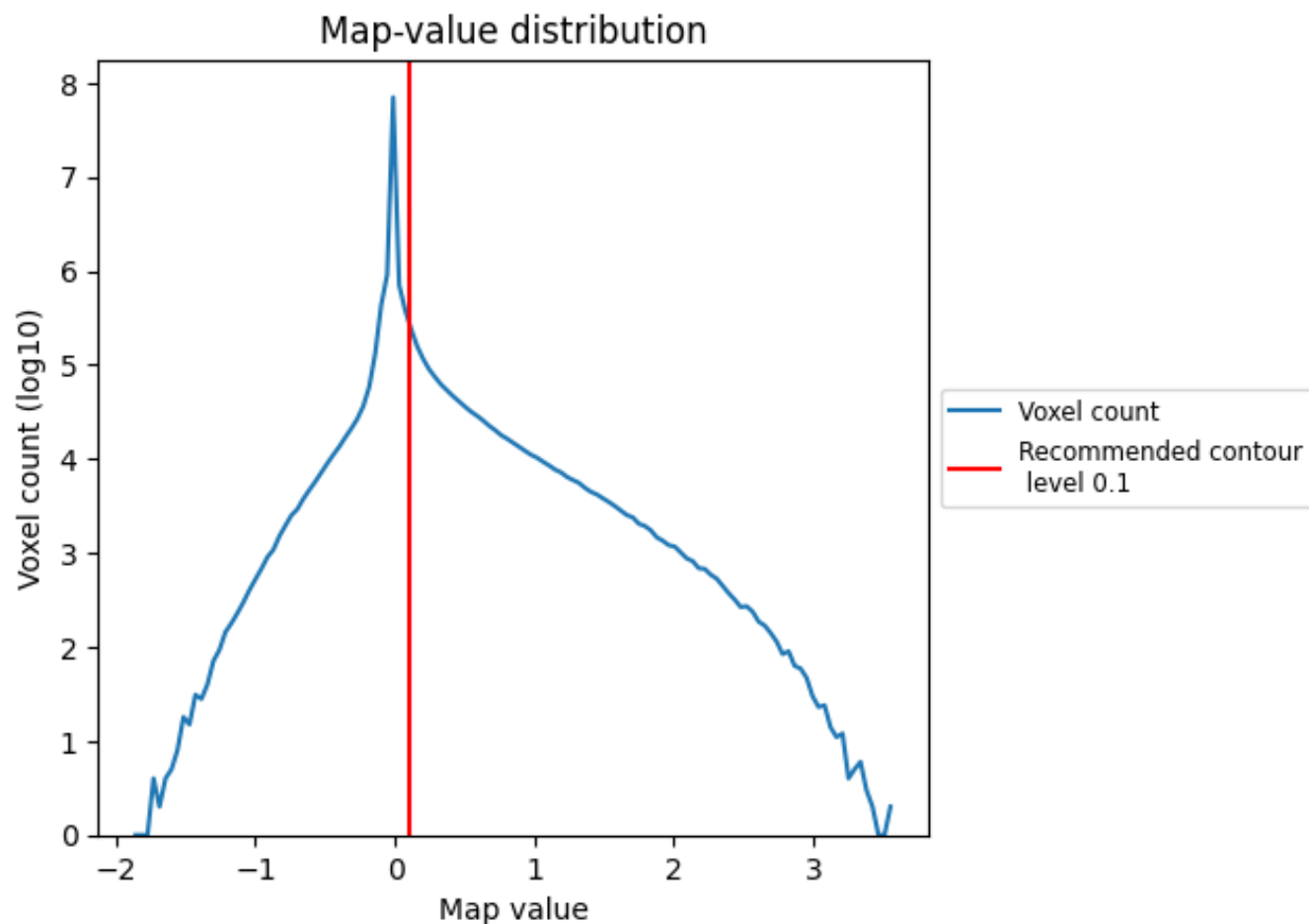
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

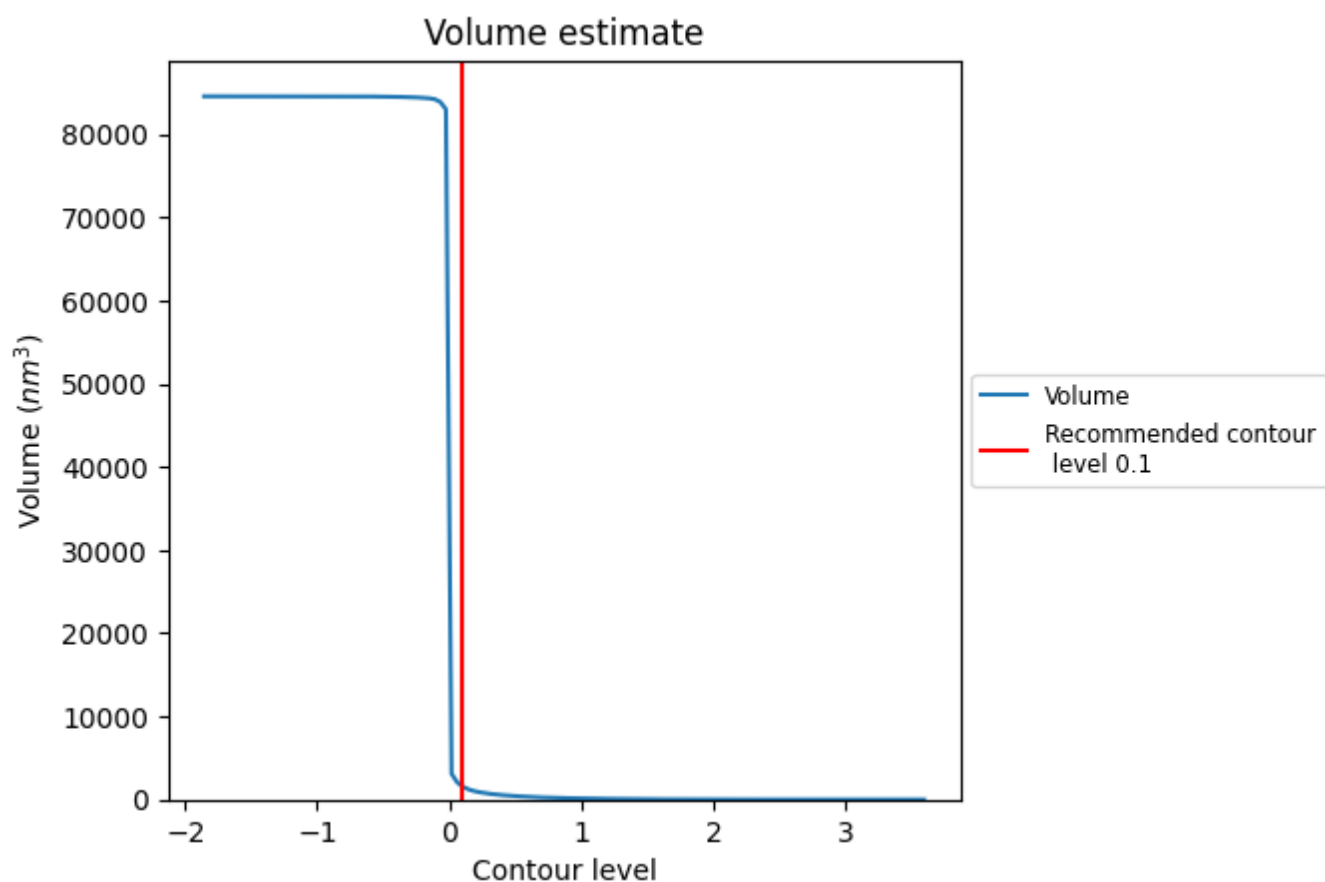
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

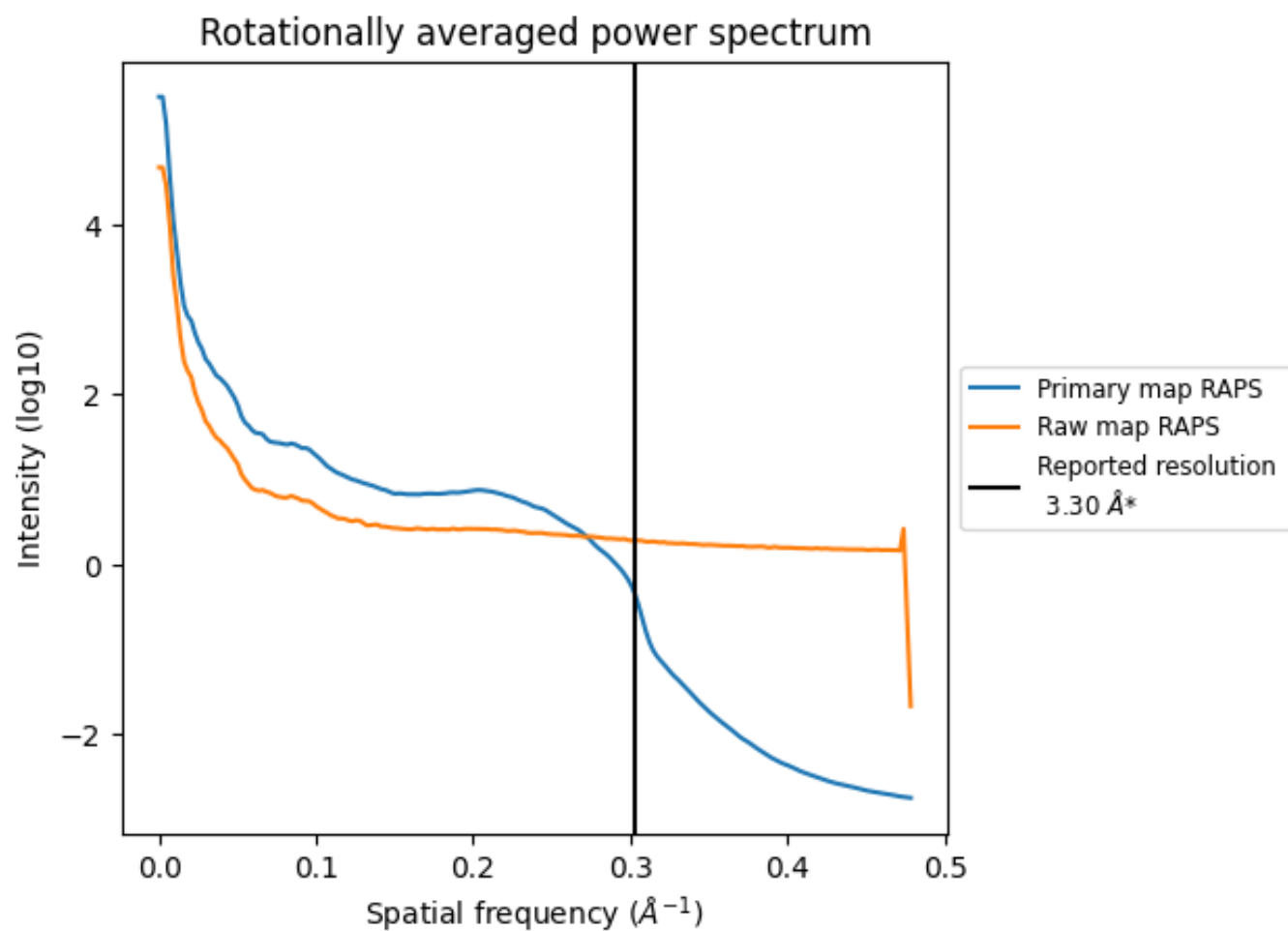
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1582 nm^3 ; this corresponds to an approximate mass of 1429 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 ⓘ

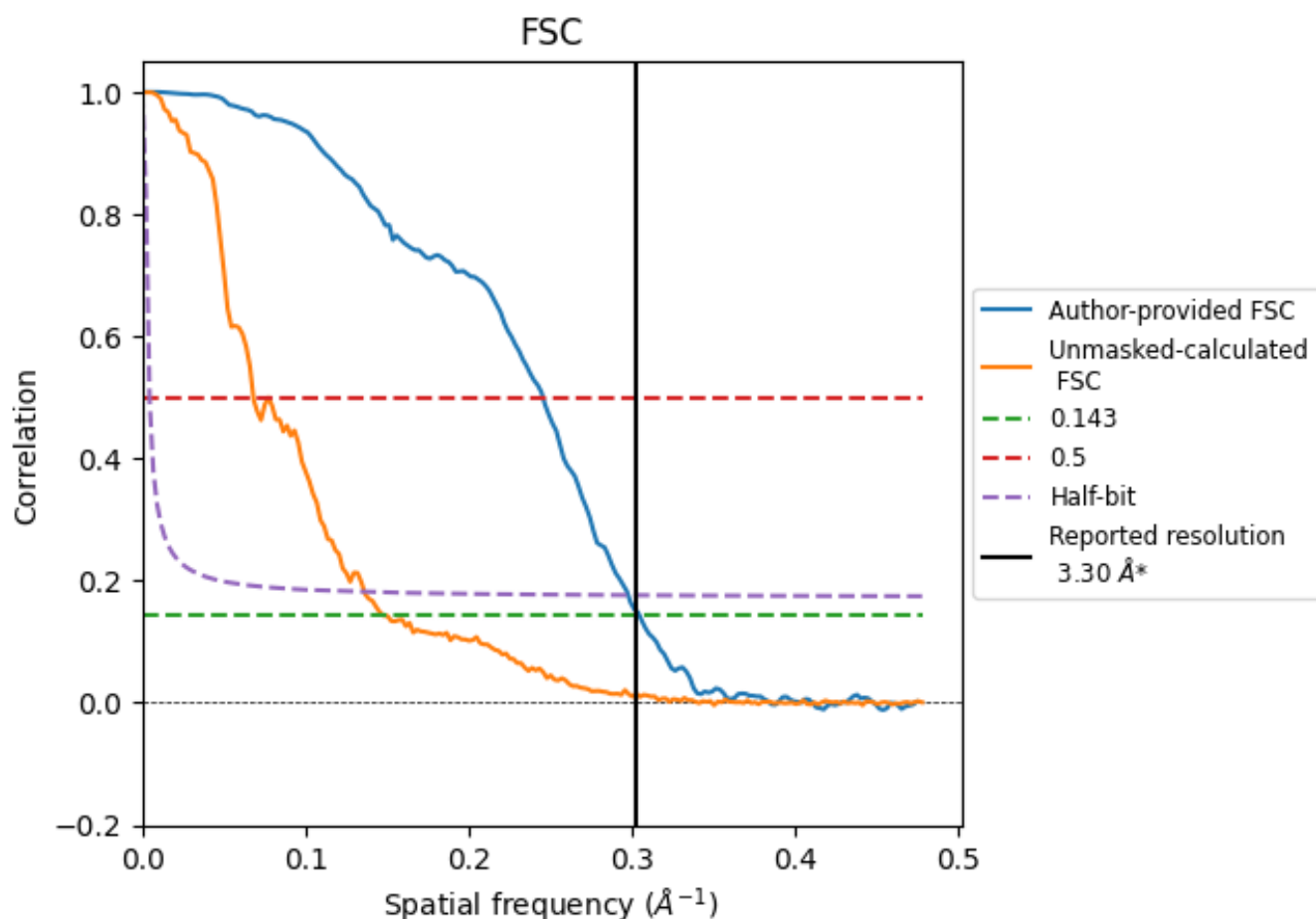


*Reported resolution corresponds to spatial frequency of $0.303 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.303 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

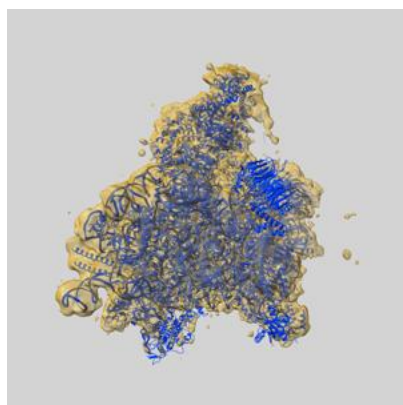
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.28	4.07	3.35
Unmasked-calculated*	6.76	14.66	7.34

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

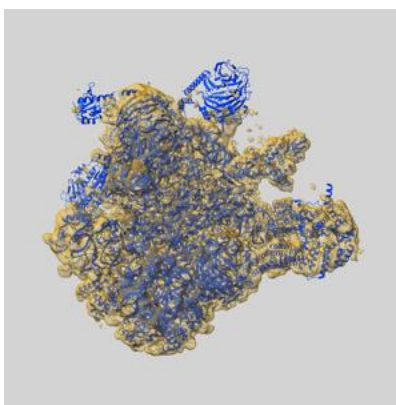
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16533 and PDB model 8CAS. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

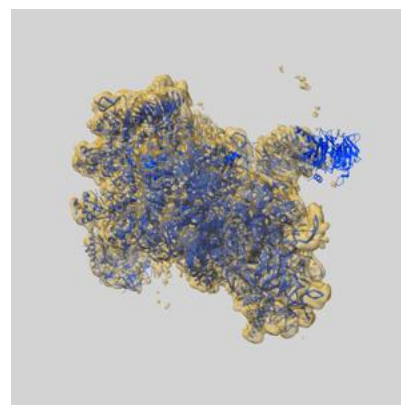
9.1 Map-model overlay [i](#)



X



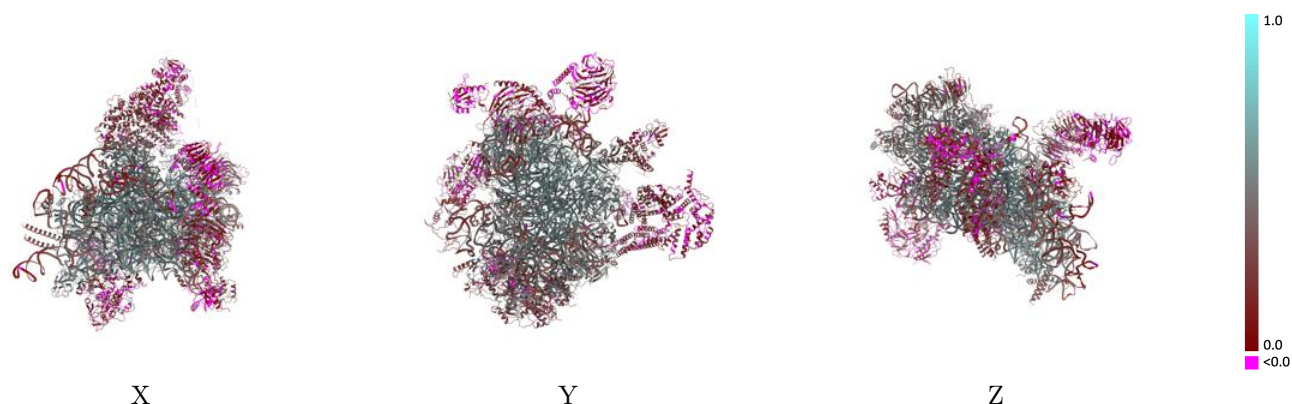
Y



Z

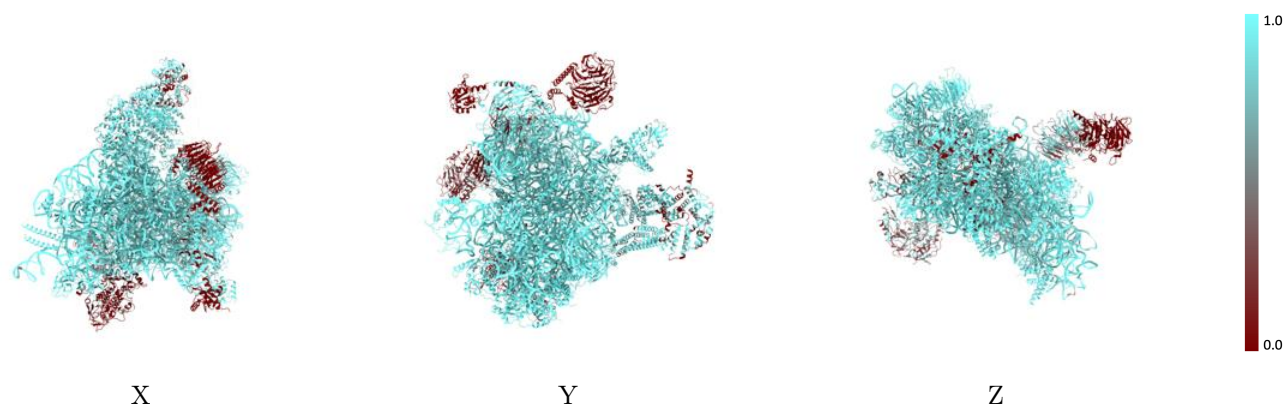
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



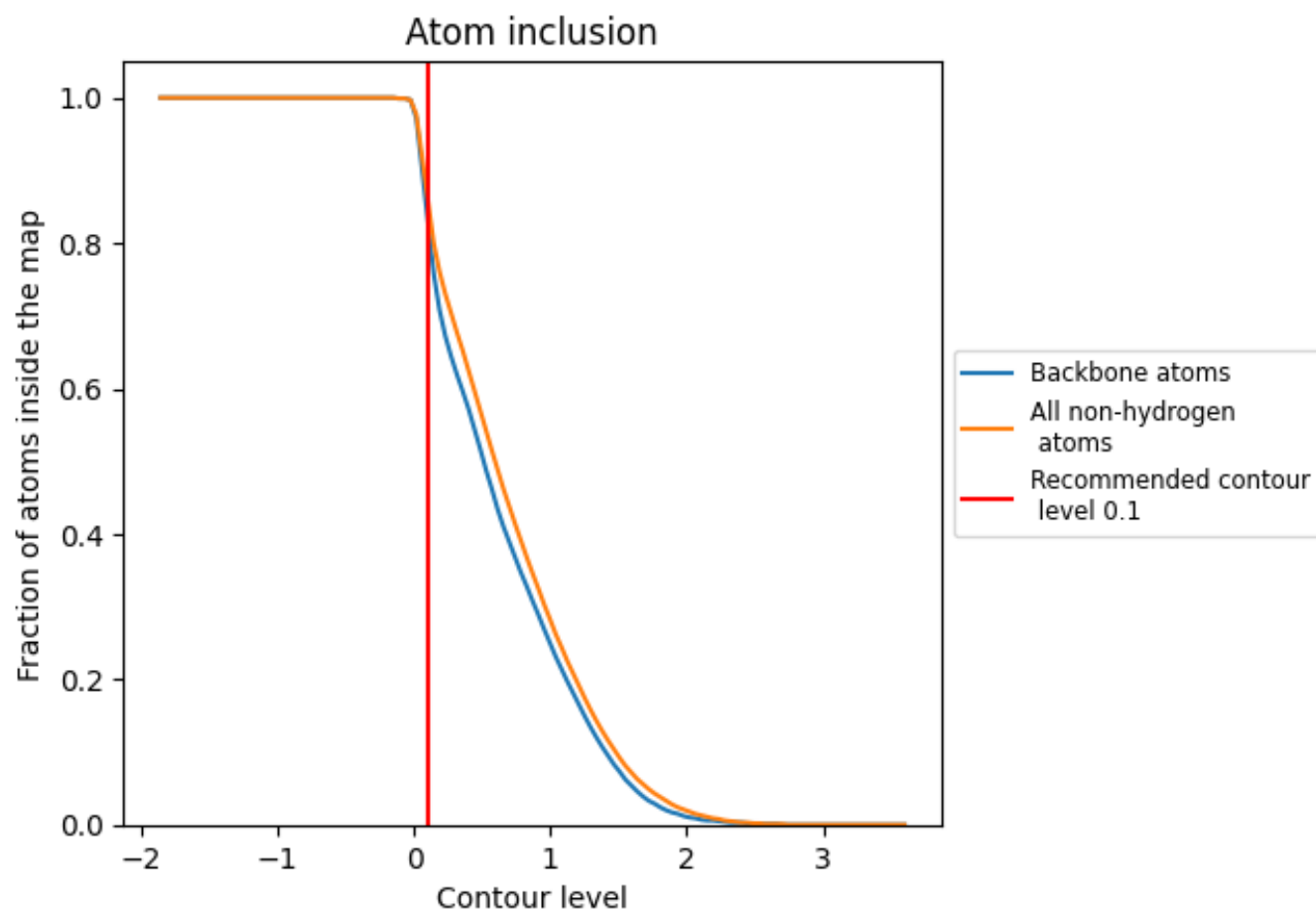
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 86% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8620	 0.3660
1	 0.8970	 0.1700
2	 0.9950	 0.4560
3	 0.8770	 0.3510
A	 0.9840	 0.4580
B	 0.9960	 0.4670
C	 0.9940	 0.4380
D	 1.0000	 0.4090
E	 0.9950	 0.3860
F	 0.9770	 0.2600
G	 0.3010	 0.0530
H	 0.9970	 0.4410
I	 0.9950	 0.4820
J	 0.9870	 0.3810
K	 0.9970	 0.4090
L	 0.9940	 0.4540
M	 0.9160	 0.3250
N	 1.0000	 0.5360
O	 0.9890	 0.2910
P	 0.9950	 0.5290
Q	 0.9970	 0.4820
R	 0.9970	 0.5590
S	 0.9990	 0.5610
T	 0.9990	 0.4860
U	 0.9770	 0.4130
V	 0.9960	 0.5250
W	 0.9980	 0.5270
X	 0.9990	 0.5560
Y	 0.9920	 0.5240
Z	 0.9940	 0.5120
a	 1.0000	 0.5510
b	 0.9970	 0.5750
c	 0.9960	 0.5710
d	 0.9890	 0.5200
e	 0.9980	 0.5470



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Chain	Atom inclusion	Q-score
f	 0.7150	 0.1730
g	 0.9660	 0.4990
h	 0.9990	 0.3600
i	 0.9940	 0.4810
j	 0.4980	 0.0910
k	 0.2220	 0.1230
l	 0.0050	 0.0130
m	 0.7990	 0.2220
n	 0.9870	 0.4940
o	 0.7280	 0.1310
p	 0.5190	 0.1320
q	 0.7760	 0.1620
r	 0.0000	 0.0060
s	 0.1870	 0.0400
x	 0.9830	 0.2410
y	 0.9090	 0.1660