



## wwPDB EM Validation Summary Report ⓘ

Nov 5, 2024 – 08:40 pm GMT

PDB ID : 7ZAI  
EMDB ID : EMD-14581  
Title : Cryo-EM structure of a *Pyrococcus abyssi* 30S bound to Met-initiator tRNA, mRNA and aIF1A.  
Authors : Coureux, P.D.; Bourgeois, G.; Mechulam, Y.; Schmitt, E.; Kazan, R.  
Deposited on : 2022-03-22  
Resolution : 2.60 Å(reported)  
Based on initial model : 7ZHG

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

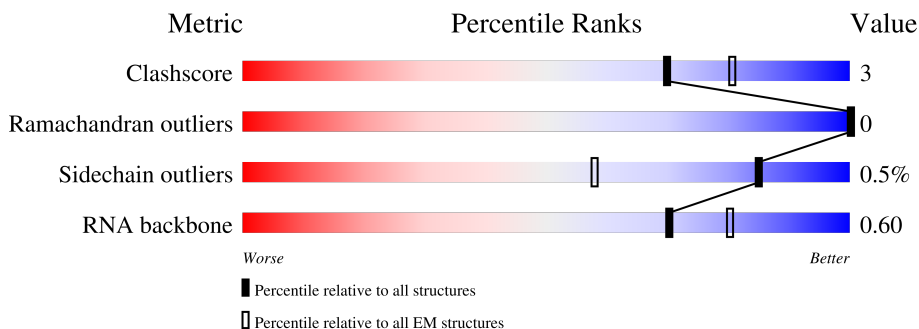
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.60 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.







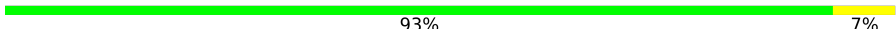






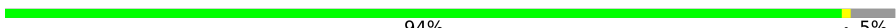


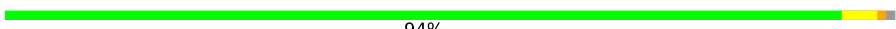

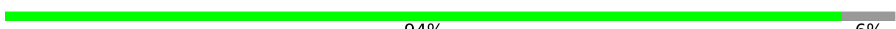



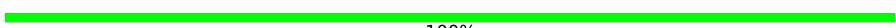




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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  $\geq 3$ , 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	2	1497	
2	A	199	
3	B	202	
4	C	63	
5	D	180	
6	E	243	
7	F	236	

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Mol	Chain	Length	Quality of chain
8	G	125	 90% 9% .
9	H	215	 89% 10%
10	I	130	 93% 6% .
11	J	127	 87% 11% .
12	K	135	 93% 7%
13	L	102	 88% 10% .
14	M	137	 88% 5% 7%
15	N	147	 93% 6% .
16	O	148	 93% . 5%
17	P	56	 91% 7% .
18	Q	158	 90% 6% .
19	R	113	 94% . 5%
20	S	67	 88% 7% .
21	T	132	 89% 5% 6%
22	U	150	 94% . ..
23	V	99	 88% 9% .
24	W	65	 94% 6%
25	X	71	 83% 8% 8%
26	Y	51	 49% 47% .
27	Z	210	 86% 7% 7%
28	0	36	 100%
29	3	123	 70% 28% ..
30	5	25	 72% 16% 12%
31	4	77	 39% 40% 17% .
32	6	134	 55% 13% 31%

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 64649 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1497	Total	C	N	O	P	0	0
			32312	14418	5959	10438	1497		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	17	4AC	C	modified residue	GB 5457433
2	53	4AC	C	modified residue	GB 5457433
2	286	4AC	C	modified residue	GB 5457433
2	303	4AC	C	modified residue	GB 5457433
2	319	4AC	C	modified residue	GB 5457433
2	379	4AC	C	modified residue	GB 5457433
2	394	4AC	C	modified residue	GB 5457433
2	479	4AC	C	modified residue	GB 5457433
2	511	4AC	C	modified residue	GB 5457433
2	546	4AC	C	modified residue	GB 5457433
2	590	4AC	C	modified residue	GB 5457433
2	626	4AC	C	modified residue	GB 5457433
2	636	4AC	C	modified residue	GB 5457433
2	703	4AC	C	modified residue	GB 5457433
2	718	4AC	C	modified residue	GB 5457433
2	731	4AC	C	modified residue	GB 5457433
2	751	4AC	C	modified residue	GB 5457433
2	828	4AC	C	modified residue	GB 5457433
2	839	4AC	C	modified residue	GB 5457433
2	848	4AC	C	modified residue	GB 5457433
2	851	4AC	C	modified residue	GB 5457433
2	868	4AC	C	modified residue	GB 5457433
2	957	4AC	C	modified residue	GB 5457433
2	1028	4AC	C	modified residue	GB 5457433
2	1147	4AC	C	modified residue	GB 5457433
2	1184	4AC	C	modified residue	GB 5457433
2	1233	4AC	C	modified residue	GB 5457433
2	1239	4AC	C	modified residue	GB 5457433

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Chain	Residue	Modelled	Actual	Comment	Reference
2	1479	4AC	C	modified residue	GB 5457433

- Molecule 2 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	188	Total	C	N	O	S	0	0
			1531	993	268	266	4		

- Molecule 3 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	196	Total	C	N	O	S	0	0
			1571	1017	269	281	4		

- Molecule 4 is a protein called Zn-ribbon RNA-binding protein involved in translation.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	57	Total	C	N	O	S	0	0
			449	285	80	76	8		

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	173	Total	C	N	O	S	0	0
			1452	913	280	255	4		

- Molecule 6 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	242	Total	C	N	O	S	0	0
			1983	1281	358	339	5		

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	229	Total	C	N	O	S	0	0
			1808	1147	334	320	7		

- Molecule 8 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	124	Total	C	N	O	S	0	0
			977	621	178	176	2		

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	214	Total	C	N	O	S	0	0
			1725	1095	323	300	7		

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	129	Total	C	N	O	S	0	0
			1034	668	184	180	2		

- Molecule 11 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	125	Total	C	N	O		0	0
			986	612	205	169			

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	135	Total	C	N	O	S	0	0
			1073	673	207	189	4		

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	100	Total	C	N	O	S	0	0
			809	502	157	147	3		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	127	Total	C	N	O	S	0	0
			955	591	190	172	2		

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	146	Total	C	N	O	S	0	0
			1148	727	224	194	3		

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	141	Total	C	N	O	S	0	0
			1134	712	224	193	5		

- Molecule 17 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	55	Total	C	N	O	S	0	0
			455	288	95	67	5		

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	151	Total	C	N	O	S	0	0
			1257	801	239	213	4		

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	107	Total	C	N	O	S	0	0
			884	562	172	147	3		

- Molecule 20 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	64	Total	C	N	O	S	0	0
			541	343	104	93	1		

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	124	Total	C	N	O	S	0	0
			1007	641	191	168	7		

- Molecule 22 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	U	149	Total	C	N	O	0	0
			1223	790	221	212		

- Molecule 23 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	V	96	Total	C	N	O	S	0
			808	528	129	148	3	0

- Molecule 24 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	W	61	Total	C	N	O	S	0
			470	294	91	80	5	0

- Molecule 25 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	X	65	Total	C	N	O		0
			516	316	103	97		0

- Molecule 26 is a protein called 30S ribosomal protein S27ae.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Y	49	Total	C	N	O	S	0
			400	257	76	62	5	0

- Molecule 27 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	Z	196	Total	C	N	O	S	0
			1541	983	284	270	4	0

- Molecule 28 is a protein called 50S ribosomal protein L41e.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	0	36	Total	C	N	O	S	0
			343	218	84	39	2	0

- Molecule 29 is a protein called 50S ribosomal protein L7Ae.



Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	122	Total	C	N	O	S	0	0
			933	594	156	180	3		

- Molecule 30 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	22	Total	C	N	O	P	0	0
			474	212	88	152	22		

- Molecule 31 is a RNA chain called tRNA-MET.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	4	77	Total	C	N	O	P	S	0	0
			1644	734	296	536	77	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	A	-	engineered mutation	GB 1334604293
4	72	U	A	engineered mutation	GB 1334604293

- Molecule 32 is a protein called Translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	6	92	Total	C	N	O	S	0	0
			751	479	142	127	3		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	-20	MET	-	initiating methionine	UNP Q9V138
6	-19	GLY	-	expression tag	UNP Q9V138
6	-18	SER	-	expression tag	UNP Q9V138
6	-17	SER	-	expression tag	UNP Q9V138
6	-16	SER	-	expression tag	UNP Q9V138
6	-15	HIS	-	expression tag	UNP Q9V138
6	-14	HIS	-	expression tag	UNP Q9V138
6	-13	HIS	-	expression tag	UNP Q9V138
6	-12	HIS	-	expression tag	UNP Q9V138
6	-11	HIS	-	expression tag	UNP Q9V138
6	-10	HIS	-	expression tag	UNP Q9V138
6	-9	SER	-	expression tag	UNP Q9V138
6	-8	SER	-	expression tag	UNP Q9V138

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Chain	Residue	Modelled	Actual	Comment	Reference
6	-7	GLY	-	expression tag	UNP Q9V138
6	-6	LEU	-	expression tag	UNP Q9V138
6	-5	VAL	-	expression tag	UNP Q9V138
6	-4	PRO	-	expression tag	UNP Q9V138
6	-3	ARG	-	expression tag	UNP Q9V138
6	-2	GLY	-	expression tag	UNP Q9V138
6	-1	SER	-	expression tag	UNP Q9V138
6	0	HIS	-	expression tag	UNP Q9V138

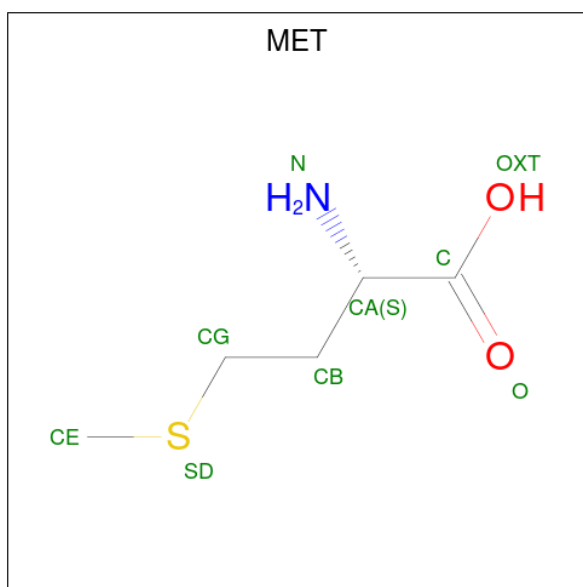
- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	2	59	Total 59	Mg 59	0
33	F	1	Total 1	Mg 1	0
33	5	1	Total 1	Mg 1	0
33	4	1	Total 1	Mg 1	0

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
34	C	2	Total 2	Zn 2	0
34	F	1	Total 1	Zn 1	0
34	P	1	Total 1	Zn 1	0
34	R	1	Total 1	Zn 1	0
34	W	1	Total 1	Zn 1	0

- Molecule 35 is METHIONINE (three-letter code: MET) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>S).



Mol	Chain	Residues	Atoms					AltConf
35	4	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
36	2	342	Total	O	0
			342	342	
36	D	1	Total	O	0
			1	1	
36	F	2	Total	O	0
			2	2	
36	H	2	Total	O	0
			2	2	
36	K	4	Total	O	0
			4	4	
36	L	1	Total	O	0
			1	1	
36	M	7	Total	O	0
			7	7	
36	N	1	Total	O	0
			1	1	
36	Q	3	Total	O	0
			3	3	
36	S	1	Total	O	0
			1	1	
36	U	3	Total	O	0
			3	3	

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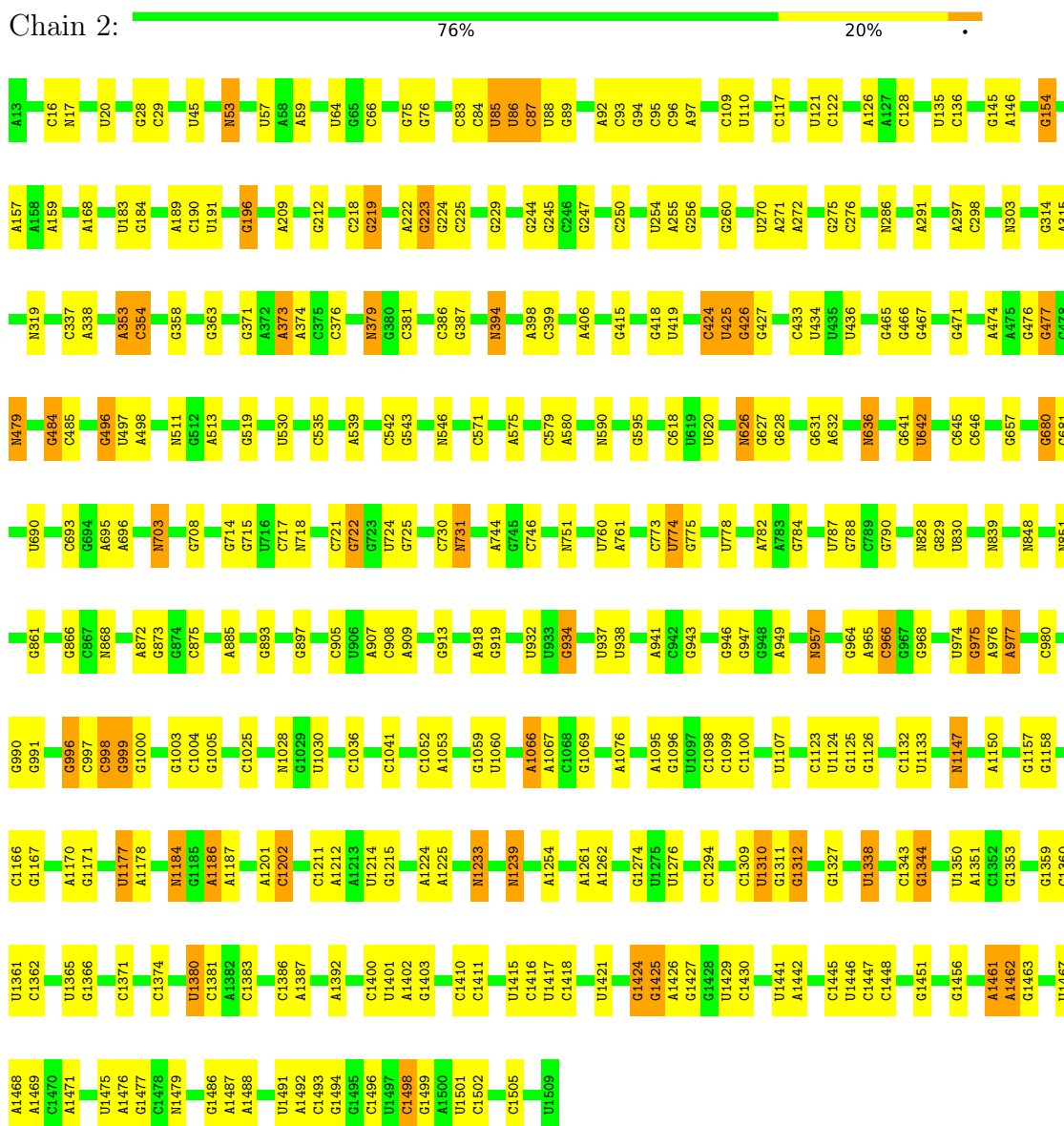
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Mol	Chain	Residues	Atoms		AltConf
36	0	3	Total 3	O 3	0
36	5	4	Total 4	O 4	0
36	4	5	Total 5	O 5	0

### 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: 16S rRNA



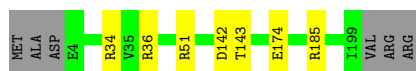
#### • Molecule 2: 30S ribosomal protein S3Ae

Chain A:  92% • 6%




- Molecule 3: 30S ribosomal protein S2

Chain B:  94% • •




- Molecule 4: Zn-ribbon RNA-binding protein involved in translation

Chain C:  84% 6% 10%



- Molecule 5: 30S ribosomal protein S4

Chain D:  91% 5% • •



- Molecule 6: 30S ribosomal protein S4e

Chain E:  91% 9%




- Molecule 7: 30S ribosomal protein S5

Chain F:  92% 6% •




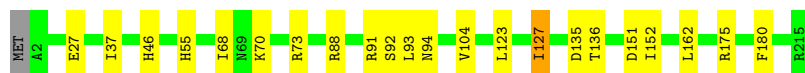
- Molecule 8: 30S ribosomal protein S6e

Chain G:  90% 9% •



- Molecule 9: 30S ribosomal protein S7

Chain H:  89% 10%




- Molecule 10: 30S ribosomal protein S8

Chain I:  93% 6%



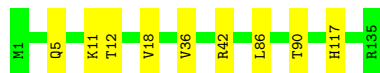
- Molecule 11: 30S ribosomal protein S8e

Chain J:  87% 11%




- Molecule 12: 30S ribosomal protein S9

Chain K:  93% 7%




- Molecule 13: 30S ribosomal protein S10

Chain L:  88% 10%



- Molecule 14: 30S ribosomal protein S11

Chain M:  88% 5% 7%




- Molecule 15: 30S ribosomal protein S12

Chain N:  93% 6%



- Molecule 16: 30S ribosomal protein S13

Chain O:  93% • 5%




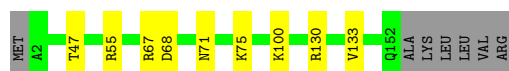
- Molecule 17: 30S ribosomal protein S14 type Z

Chain P:  91% 7% •



- Molecule 18: 30S ribosomal protein S15

Chain Q:  90% 6% •




- Molecule 19: 30S ribosomal protein S17

Chain R:  94% • 5%




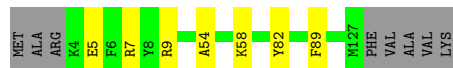
- Molecule 20: 30S ribosomal protein S17e

Chain S:  88% 7% •



- Molecule 21: 30S ribosomal protein S19

Chain T:  89% 5% 6%




- Molecule 22: 30S ribosomal protein S19e

Chain U:  94% • •



- Molecule 23: 30S ribosomal protein S24e



Chain V:  88% 9% .




- Molecule 24: 30S ribosomal protein S27e

Chain W:  94% 6%



- Molecule 25: 30S ribosomal protein S28e

Chain X:  83% 8% 8%




- Molecule 26: 30S ribosomal protein S27ae

Chain Y:  49% 47% .



- Molecule 27: 30S ribosomal protein S3

Chain Z:  86% 7% 7%



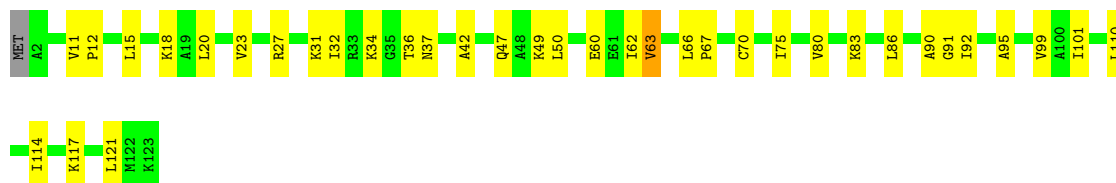
- Molecule 28: 50S ribosomal protein L41e

Chain 0:  100%

There are no outlier residues recorded for this chain.

- Molecule 29: 50S ribosomal protein L7Ae

Chain 3:  70% 28% ..



- Molecule 30: mRNA

Chain 5:  72% 16% 12%



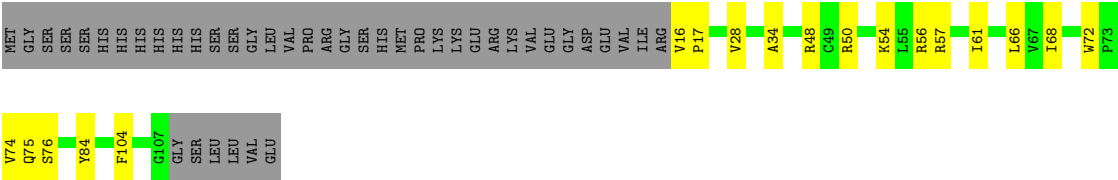
● Molecule 31: tRNA-MET

Chain 4:  39% 40% 17% .



● Molecule 32: Translation initiation factor 1A

Chain 6:  55% 13% 31%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	382130	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	39	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.074	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0016	Depositor
Map size ( $\text{\AA}$ )	371.52002, 371.52002, 371.52002	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.8600001, 0.8600001, 0.8600001	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A2M, MA6, 6MZ, H2U, B8H, OMC, OMG, OMU, 4SU, 5MC, PSU, MG, UR3, 5MU, ZN, LHH, 4AC

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	2	0.42	0/34435	0.79	2/53681 (0.0%)
2	A	0.28	0/1557	0.48	0/2087
3	B	0.27	0/1602	0.48	0/2165
4	C	0.28	0/463	0.50	0/628
5	D	0.27	0/1476	0.52	0/1980
6	E	0.28	0/2032	0.53	0/2742
7	F	0.27	0/1838	0.54	0/2478
8	G	0.26	0/993	0.53	0/1329
9	H	0.27	0/1762	0.50	0/2366
10	I	0.29	0/1055	0.54	0/1415
11	J	0.27	0/995	0.58	0/1327
12	K	0.26	0/1089	0.55	0/1459
13	L	0.24	0/817	0.54	0/1097
14	M	0.26	0/973	0.56	0/1311
15	N	0.28	0/1165	0.54	0/1547
16	O	0.26	0/1153	0.54	0/1551
17	P	0.29	0/465	0.58	0/613
18	Q	0.27	0/1285	0.51	0/1727
19	R	0.29	0/907	0.53	0/1225
20	S	0.27	0/548	0.50	0/725
21	T	0.26	0/1026	0.51	0/1371
22	U	0.28	0/1253	0.51	0/1689
23	V	0.29	0/826	0.46	0/1108
24	W	0.26	0/476	0.52	0/641
25	X	0.26	0/518	0.60	0/694
26	Y	0.24	0/412	0.51	0/549
27	Z	0.27	0/1563	0.52	0/2099
28	0	0.28	0/349	0.63	0/451
29	3	0.24	0/945	0.47	0/1274
30	5	0.32	0/531	0.73	0/826
31	4	0.69	8/1724 (0.5%)	1.23	11/2687 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	6	0.23	0/767	0.54	0/1037
All	All	0.37	8/67000 (0.0%)	0.71	13/97879 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	76	A	N3-C4	15.91	1.44	1.34
31	4	76	A	C8-N7	11.15	1.39	1.31
31	4	76	A	C6-N1	9.62	1.42	1.35
31	4	76	A	C5-C4	7.89	1.44	1.38
31	4	76	A	C6-N6	7.10	1.39	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	4	75	C	OP1-P-O3'	-27.71	44.24	105.20
31	4	76	A	C2-N3-C4	19.58	120.39	110.60
31	4	75	C	OP2-P-O3'	18.10	145.03	105.20
31	4	76	A	N1-C2-N3	-15.53	121.54	129.30
31	4	76	A	N7-C8-N9	-11.57	108.02	113.80

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	2	32312	0	16354	161	0
2	A	1531	0	1623	3	0
3	B	1571	0	1630	4	0
4	C	449	0	435	2	0
5	D	1452	0	1521	7	0
6	E	1983	0	2060	14	0
7	F	1808	0	1879	8	0
8	G	977	0	1037	9	0
9	H	1725	0	1780	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	I	1034	0	1069	6	0
11	J	986	0	1070	9	0
12	K	1073	0	1133	5	0
13	L	809	0	859	5	0
14	M	955	0	981	6	0
15	N	1148	0	1248	5	0
16	O	1134	0	1173	2	0
17	P	455	0	476	2	0
18	Q	1257	0	1326	6	0
19	R	884	0	906	1	0
20	S	541	0	573	4	0
21	T	1007	0	1073	4	0
22	U	1223	0	1263	7	0
23	V	808	0	832	6	0
24	W	470	0	496	0	0
25	X	516	0	544	4	0
26	Y	400	0	401	17	0
27	Z	1541	0	1624	10	0
28	0	343	0	407	0	0
29	3	933	0	982	25	0
30	5	474	0	237	0	0
31	4	1644	0	837	50	0
32	6	751	0	773	13	0
33	2	59	0	0	0	0
33	4	1	0	0	0	0
33	5	1	0	0	0	0
33	F	1	0	0	0	0
34	C	2	0	0	0	0
34	F	1	0	0	0	0
34	P	1	0	0	0	0
34	R	1	0	0	0	0
34	W	1	0	0	0	0
35	4	8	0	8	0	0
36	0	3	0	0	0	0
36	2	342	0	0	6	0
36	4	5	0	0	0	0
36	5	4	0	0	0	0
36	D	1	0	0	0	0
36	F	2	0	0	0	0
36	H	2	0	0	0	0
36	K	4	0	0	1	0
36	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	M	7	0	0	0	0
36	N	1	0	0	1	0
36	Q	3	0	0	0	0
36	S	1	0	0	1	0
36	U	3	0	0	1	0
All	All	64649	0	48610	377	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 377 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)
31:4:16:C:H1'	31:4:61:C:OP1	1.17	1.26
31:4:16:C:C1'	31:4:61:C:OP1	1.90	1.19
31:4:16:C:O2'	31:4:61:C:O5'	1.57	1.18
31:4:16:C:O2'	31:4:61:C:C5'	1.92	1.15
26:Y:34:HIS:CD2	26:Y:39:ALA:HB2	1.86	1.10

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	
2	A	186/199 (94%)	183 (98%)	3 (2%)	0	100	100
3	B	194/202 (96%)	190 (98%)	4 (2%)	0	100	100
4	C	55/63 (87%)	55 (100%)	0	0	100	100
5	D	171/180 (95%)	168 (98%)	3 (2%)	0	100	100
6	E	240/243 (99%)	236 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	F	227/236 (96%)	220 (97%)	7 (3%)	0	100	100
8	G	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
9	H	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
10	I	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
11	J	123/127 (97%)	122 (99%)	1 (1%)	0	100	100
12	K	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
13	L	98/102 (96%)	95 (97%)	3 (3%)	0	100	100
14	M	125/137 (91%)	121 (97%)	4 (3%)	0	100	100
15	N	144/147 (98%)	142 (99%)	2 (1%)	0	100	100
16	O	139/148 (94%)	136 (98%)	3 (2%)	0	100	100
17	P	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
18	Q	149/158 (94%)	147 (99%)	2 (1%)	0	100	100
19	R	105/113 (93%)	100 (95%)	5 (5%)	0	100	100
20	S	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
21	T	122/132 (92%)	119 (98%)	3 (2%)	0	100	100
22	U	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
23	V	94/99 (95%)	92 (98%)	2 (2%)	0	100	100
24	W	59/65 (91%)	56 (95%)	3 (5%)	0	100	100
25	X	63/71 (89%)	62 (98%)	1 (2%)	0	100	100
26	Y	47/51 (92%)	41 (87%)	6 (13%)	0	100	100
27	Z	194/210 (92%)	183 (94%)	11 (6%)	0	100	100
28	0	34/36 (94%)	34 (100%)	0	0	100	100
29	3	120/123 (98%)	109 (91%)	11 (9%)	0	100	100
32	6	90/134 (67%)	88 (98%)	2 (2%)	0	100	100
All	All	3635/3854 (94%)	3529 (97%)	106 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	
2	A	160/167 (96%)	160 (100%)	0	100	100
3	B	168/173 (97%)	168 (100%)	0	100	100
4	C	50/55 (91%)	50 (100%)	0	100	100
5	D	156/160 (98%)	155 (99%)	1 (1%)	84	94
6	E	213/214 (100%)	212 (100%)	1 (0%)	86	95
7	F	192/198 (97%)	191 (100%)	1 (0%)	86	95
8	G	107/108 (99%)	107 (100%)	0	100	100
9	H	183/184 (100%)	179 (98%)	4 (2%)	47	72
10	I	106/107 (99%)	106 (100%)	0	100	100
11	J	101/103 (98%)	101 (100%)	0	100	100
12	K	111/111 (100%)	111 (100%)	0	100	100
13	L	89/91 (98%)	88 (99%)	1 (1%)	70	86
14	M	94/104 (90%)	94 (100%)	0	100	100
15	N	120/121 (99%)	119 (99%)	1 (1%)	79	91
16	O	117/123 (95%)	116 (99%)	1 (1%)	75	90
17	P	45/46 (98%)	45 (100%)	0	100	100
18	Q	137/143 (96%)	136 (99%)	1 (1%)	81	93
19	R	96/102 (94%)	96 (100%)	0	100	100
20	S	58/61 (95%)	58 (100%)	0	100	100
21	T	108/114 (95%)	108 (100%)	0	100	100
22	U	126/127 (99%)	124 (98%)	2 (2%)	58	79
23	V	88/90 (98%)	88 (100%)	0	100	100
24	W	53/56 (95%)	53 (100%)	0	100	100
25	X	55/60 (92%)	55 (100%)	0	100	100
26	Y	40/42 (95%)	40 (100%)	0	100	100
27	Z	155/168 (92%)	153 (99%)	2 (1%)	65	84
28	0	34/34 (100%)	34 (100%)	0	100	100
29	3	98/99 (99%)	97 (99%)	1 (1%)	73	88
32	6	80/117 (68%)	80 (100%)	0	100	100
All	All	3140/3278 (96%)	3124 (100%)	16 (0%)	85	95

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	Z	173	LEU
27	Z	168	GLN
15	N	18	LEU
22	U	82	ASN
13	L	32	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1461/1497 (97%)	147 (10%)	1 (0%)
30	5	21/25 (84%)	4 (19%)	0
31	4	76/77 (98%)	20 (26%)	3 (3%)
All	All	1558/1599 (97%)	171 (10%)	4 (0%)

5 of 171 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	16	C
1	2	45	U
1	2	57	U
1	2	59	A
1	2	66	C

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1424	G
31	4	19	G
31	4	60	U
31	4	75	C

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

73 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	2	693	1	18,22,23	0.93	2 (11%)	26,32,35	1.09	3 (11%)
1	OMU	2	787	1	19,22,23	1.26	3 (15%)	26,31,34	1.80	5 (19%)
1	A2M	2	373	1	18,25,26	0.96	1 (5%)	18,36,39	1.25	2 (11%)
1	UR3	2	1467	1	19,22,23	0.92	0	26,32,35	1.42	1 (3%)
1	4AC	2	1184	1	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
1	OMU	2	830	1	19,22,23	1.26	3 (15%)	26,31,34	1.73	4 (15%)
1	4AC	2	703	1	21,24,25	1.02	2 (9%)	29,34,37	1.49	4 (13%)
1	OMG	2	1069	1	18,26,27	0.95	1 (5%)	19,38,41	1.08	2 (10%)
1	OMU	2	774	1	19,22,23	1.24	3 (15%)	26,31,34	1.74	4 (15%)
1	LHH	2	250	1	22,25,26	2.53	8 (36%)	29,35,38	1.26	6 (20%)
1	B8H	2	938	1	19,22,23	0.78	0	22,32,35	1.37	3 (13%)
1	4AC	2	319	1	21,24,25	1.01	2 (9%)	29,34,37	1.39	4 (13%)
1	5MC	2	1025	1	18,22,23	0.94	2 (11%)	26,32,35	1.10	3 (11%)
1	OMG	2	471	1	18,26,27	0.96	1 (5%)	19,38,41	1.06	2 (10%)
1	OMC	2	846	1	19,22,23	0.81	0	26,31,34	0.82	0
1	4AC	2	590	1	21,24,25	1.00	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	2	839	1	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
1	5MC	2	1374	1	18,22,23	0.94	2 (11%)	26,32,35	1.09	2 (7%)
1	4AC	2	53	1	21,24,25	1.00	2 (9%)	29,34,37	1.32	4 (13%)
1	4AC	2	626	1	21,24,25	1.01	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	2	828	1	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
1	4AC	2	1239	1	21,24,25	1.02	2 (9%)	29,34,37	1.32	4 (13%)
1	4AC	2	851	1	21,24,25	1.04	2 (9%)	29,34,37	1.33	5 (17%)
1	5MC	2	535	1	18,22,23	0.95	2 (11%)	26,32,35	1.08	2 (7%)
1	4AC	2	286	1	21,24,25	1.02	2 (9%)	29,34,37	1.32	4 (13%)
1	MA6	2	1487	1	18,26,27	0.89	1 (5%)	19,38,41	1.26	2 (10%)
1	5MC	2	1496	1	18,22,23	0.92	2 (11%)	26,32,35	1.11	2 (7%)
1	4AC	2	394	1	21,24,25	1.00	2 (9%)	29,34,37	1.35	4 (13%)
1	OMC	2	129	1	19,22,23	0.82	0	26,31,34	0.83	0
1	OMC	2	773	1	19,22,23	0.83	0	26,31,34	0.91	1 (3%)
1	6MZ	2	1469	1,33	18,25,26	0.83	1 (5%)	16,36,39	2.14	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	2	1498	1	18,22,23	0.92	2 (11%)	26,32,35	1.24	4 (15%)
1	4AC	2	379	1	21,24,25	1.00	2 (9%)	29,34,37	1.38	4 (13%)
1	OMU	2	64	1	19,22,23	1.24	3 (15%)	26,31,34	1.72	4 (15%)
1	OMG	2	467	1	18,26,27	0.95	1 (5%)	19,38,41	1.11	2 (10%)
1	OMC	2	1036	1	19,22,23	0.82	0	26,31,34	0.83	1 (3%)
1	OMU	2	1177	1	19,22,23	1.23	3 (15%)	26,31,34	1.74	5 (19%)
31	5MU	4	54	31	19,22,23	1.42	6 (31%)	28,32,35	1.86	5 (17%)
1	4AC	2	546	1	21,24,25	1.00	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	2	479	1	21,24,25	1.01	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	2	303	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	2	848	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	2	1147	1	21,24,25	1.02	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	2	511	1	21,24,25	1.03	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	2	1233	1	21,24,25	1.01	2 (9%)	29,34,37	1.39	4 (13%)
1	5MC	2	1202	1	18,22,23	0.94	2 (11%)	26,32,35	1.10	3 (11%)
1	5MC	2	875	1	18,22,23	0.95	2 (11%)	26,32,35	1.11	3 (11%)
1	OMG	2	913	1	18,26,27	0.95	1 (5%)	19,38,41	1.12	2 (10%)
1	4AC	2	1028	1	21,24,25	0.99	2 (9%)	29,34,37	1.32	4 (13%)
1	OMG	2	680	1	18,26,27	0.94	1 (5%)	19,38,41	1.06	2 (10%)
1	LHH	2	1041	1	22,25,26	2.52	8 (36%)	29,35,38	1.24	5 (17%)
31	H2U	4	20	31	18,21,22	1.01	2 (11%)	21,30,33	1.98	1 (4%)
1	4AC	2	718	1	21,24,25	1.00	2 (9%)	29,34,37	1.29	4 (13%)
1	OMU	2	20	1	19,22,23	1.25	3 (15%)	26,31,34	1.81	5 (19%)
1	OMG	2	519	1	18,26,27	0.95	1 (5%)	19,38,41	1.12	2 (10%)
31	OMC	4	32	31	19,22,23	0.85	0	26,31,34	1.05	2 (7%)
1	4AC	2	868	1	21,24,25	1.03	2 (9%)	29,34,37	1.31	5 (17%)
31	4SU	4	8	31	18,21,22	1.72	4 (22%)	26,30,33	2.22	5 (19%)
1	4AC	2	731	1	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
1	MA6	2	1488	1	18,26,27	0.90	1 (5%)	19,38,41	1.28	2 (10%)
1	OMG	2	873	1	18,26,27	0.93	1 (5%)	19,38,41	1.10	2 (10%)
1	4AC	2	751	1	21,24,25	1.02	2 (9%)	29,34,37	1.31	4 (13%)
1	4AC	2	957	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
1	5MC	2	1505	30,1	18,22,23	0.94	2 (11%)	26,32,35	1.12	3 (11%)
1	OMC	2	1376	1	19,22,23	0.82	0	26,31,34	0.81	0
1	OMG	2	934	1	18,26,27	0.95	1 (5%)	19,38,41	1.15	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	4AC	2	636	1	21,24,25	1.02	2 (9%)	29,34,37	1.53	4 (13%)
1	OMG	2	657	1	18,26,27	0.94	1 (5%)	19,38,41	1.06	2 (10%)
1	4AC	2	17	1	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)
31	PSU	4	55	31	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
1	OMC	2	1040	1	19,22,23	0.82	0	26,31,34	0.77	0
1	4AC	2	1479	1	21,24,25	1.00	2 (9%)	29,34,37	1.33	4 (13%)
1	OMU	2	1380	1	19,22,23	1.25	3 (15%)	26,31,34	1.76	5 (19%)

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	2	693	1	-	0/7/25/26	0/2/2/2
1	OMU	2	787	1	-	2/9/27/28	0/2/2/2
1	A2M	2	373	1	-	0/5/27/28	0/3/3/3
1	UR3	2	1467	1	-	0/7/25/26	0/2/2/2
1	4AC	2	1184	1	-	0/11/29/30	0/2/2/2
1	OMU	2	830	1	-	0/9/27/28	0/2/2/2
1	4AC	2	703	1	-	0/11/29/30	0/2/2/2
1	OMG	2	1069	1	-	0/5/27/28	0/3/3/3
1	OMU	2	774	1	-	1/9/27/28	0/2/2/2
1	LHH	2	250	1	-	0/13/31/32	0/2/2/2
1	B8H	2	938	1	-	0/7/25/26	0/2/2/2
1	4AC	2	319	1	-	0/11/29/30	0/2/2/2
1	5MC	2	1025	1	-	1/7/25/26	0/2/2/2
1	OMG	2	471	1	-	0/5/27/28	0/3/3/3
1	OMC	2	846	1	-	0/9/27/28	0/2/2/2
1	4AC	2	590	1	-	0/11/29/30	0/2/2/2
1	4AC	2	839	1	-	0/11/29/30	0/2/2/2
1	5MC	2	1374	1	-	0/7/25/26	0/2/2/2
1	4AC	2	53	1	-	0/11/29/30	0/2/2/2
1	4AC	2	626	1	-	0/11/29/30	0/2/2/2
1	4AC	2	828	1	-	0/11/29/30	0/2/2/2
1	4AC	2	1239	1	-	0/11/29/30	0/2/2/2
1	4AC	2	851	1	-	0/11/29/30	0/2/2/2
1	5MC	2	535	1	-	0/7/25/26	0/2/2/2
1	4AC	2	286	1	-	0/11/29/30	0/2/2/2
1	MA6	2	1487	1	-	0/7/29/30	0/3/3/3
1	5MC	2	1496	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	2	394	1	-	0/11/29/30	0/2/2/2
1	OMC	2	129	1	-	0/9/27/28	0/2/2/2
1	OMC	2	773	1	-	0/9/27/28	0/2/2/2
1	6MZ	2	1469	1,33	-	0/5/27/28	0/3/3/3
1	5MC	2	1498	1	-	4/7/25/26	0/2/2/2
1	4AC	2	379	1	-	0/11/29/30	0/2/2/2
1	OMU	2	64	1	-	2/9/27/28	0/2/2/2
1	OMG	2	467	1	-	1/5/27/28	0/3/3/3
1	OMC	2	1036	1	-	0/9/27/28	0/2/2/2
1	OMU	2	1177	1	-	2/9/27/28	0/2/2/2
31	5MU	4	54	31	-	0/7/25/26	0/2/2/2
1	4AC	2	546	1	-	0/11/29/30	0/2/2/2
1	4AC	2	479	1	-	0/11/29/30	0/2/2/2
1	4AC	2	303	1	-	0/11/29/30	0/2/2/2
1	4AC	2	848	1	-	0/11/29/30	0/2/2/2
1	4AC	2	1147	1	-	0/11/29/30	0/2/2/2
1	4AC	2	511	1	-	1/11/29/30	0/2/2/2
1	4AC	2	1233	1	-	0/11/29/30	0/2/2/2
1	5MC	2	1202	1	-	2/7/25/26	0/2/2/2
1	5MC	2	875	1	-	0/7/25/26	0/2/2/2
1	OMG	2	913	1	-	1/5/27/28	0/3/3/3
1	4AC	2	1028	1	-	0/11/29/30	0/2/2/2
1	OMG	2	680	1	-	0/5/27/28	0/3/3/3
1	LHH	2	1041	1	-	0/13/31/32	0/2/2/2
31	H2U	4	20	31	-	7/7/38/39	0/2/2/2
1	4AC	2	718	1	-	0/11/29/30	0/2/2/2
1	OMU	2	20	1	-	5/9/27/28	0/2/2/2
1	OMG	2	519	1	-	0/5/27/28	0/3/3/3
31	OMC	4	32	31	-	2/9/27/28	0/2/2/2
1	4AC	2	868	1	-	0/11/29/30	0/2/2/2
31	4SU	4	8	31	-	0/7/25/26	0/2/2/2
1	4AC	2	731	1	-	0/11/29/30	0/2/2/2
1	MA6	2	1488	1	-	1/7/29/30	0/3/3/3
1	OMG	2	873	1	-	1/5/27/28	0/3/3/3
1	4AC	2	751	1	-	0/11/29/30	0/2/2/2
1	4AC	2	957	1	-	0/11/29/30	0/2/2/2
1	5MC	2	1505	30,1	-	0/7/25/26	0/2/2/2
1	OMC	2	1376	1	-	2/9/27/28	0/2/2/2
1	OMG	2	934	1	-	2/5/27/28	0/3/3/3
1	4AC	2	636	1	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	2	657	1	-	0/5/27/28	0/3/3/3
1	4AC	2	17	1	-	0/11/29/30	0/2/2/2
31	PSU	4	55	31	-	0/7/25/26	0/2/2/2
1	OMC	2	1040	1	-	0/9/27/28	0/2/2/2
1	4AC	2	1479	1	-	0/11/29/30	0/2/2/2
1	OMU	2	1380	1	-	0/9/27/28	0/2/2/2

The worst 5 of 140 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	250	LHH	C4-N4	6.99	1.49	1.39
1	2	1041	LHH	C4-N4	6.96	1.49	1.39
1	2	250	LHH	C7-N4	6.36	1.49	1.37
1	2	1041	LHH	C7-N4	6.27	1.48	1.37
31	4	8	4SU	C4-S4	-4.49	1.59	1.68

The worst 5 of 235 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	4	20	H2U	C4-N3-C2	-8.41	118.82	125.79
31	4	8	4SU	C4-N3-C2	-7.00	120.54	127.34
1	2	1469	6MZ	C2-N1-C6	6.71	122.34	116.59
31	4	8	4SU	C5-C4-N3	5.97	120.23	114.69
31	4	55	PSU	N1-C2-N3	5.91	121.83	115.13

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	934	OMG	O4'-C4'-C5'-O5'
31	4	20	H2U	C3'-C4'-C5'-O5'
31	4	20	H2U	O4'-C1'-N1-C6
1	2	934	OMG	C3'-C4'-C5'-O5'
1	2	1202	5MC	O4'-C4'-C5'-O5'

There are no ring outliers.

21 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	373	A2M	1	0
1	2	1184	4AC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	703	4AC	3	0
1	2	774	OMU	1	0
1	2	53	4AC	1	0
1	2	626	4AC	1	0
1	2	1239	4AC	1	0
1	2	394	4AC	1	0
1	2	379	4AC	1	0
1	2	1177	OMU	1	0
1	2	479	4AC	1	0
1	2	1147	4AC	1	0
1	2	1233	4AC	1	0
1	2	680	OMG	1	0
31	4	20	H2U	1	0
31	4	32	OMC	1	0
31	4	8	4SU	1	0
1	2	731	4AC	1	0
1	2	957	4AC	1	0
1	2	636	4AC	3	0
1	2	1380	OMU	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 69 ligands modelled in this entry, 68 are monoatomic - leaving 1 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	$\# Z  > 2$
35	MET	4	101	31	6,7,8	1.23	1 (16%)	2,7,9	1.97	1 (50%)

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
35	MET	4	101	31	-	1/5/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	4	101	MET	CB-CA	-2.78	1.49	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	4	101	MET	CE-SD-CG	2.68	109.60	100.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	4	101	MET	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

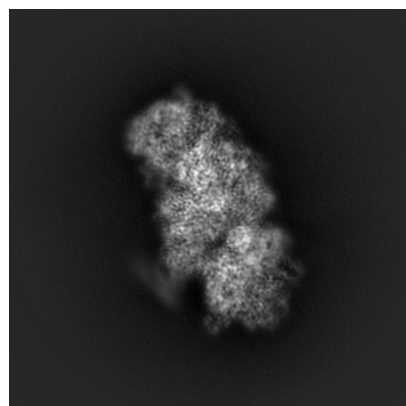
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14581. These allow visual inspection of the internal detail of the map and identification of artifacts.

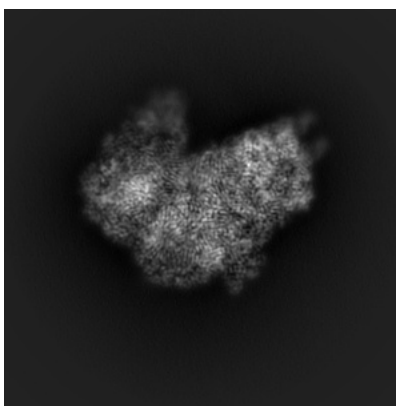
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

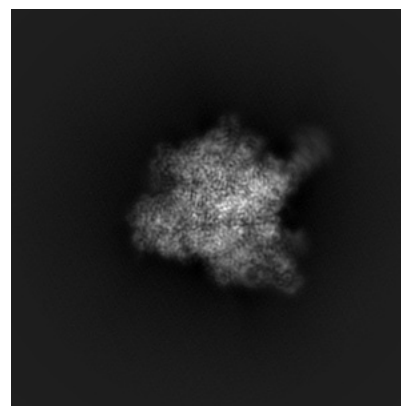
#### 6.1.1 Primary map



X

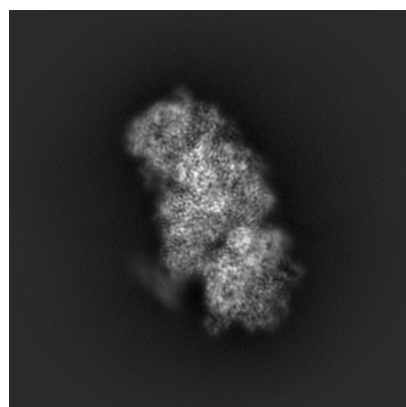


Y

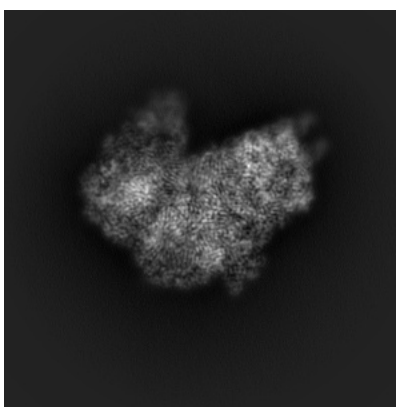


Z

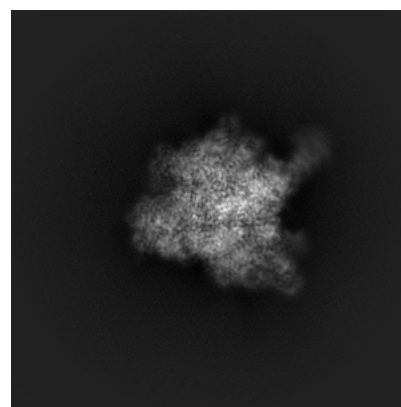
#### 6.1.2 Raw map



X



Y

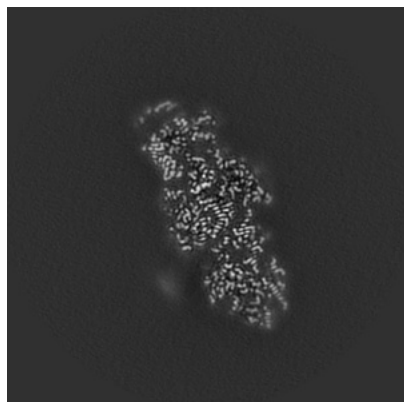


Z

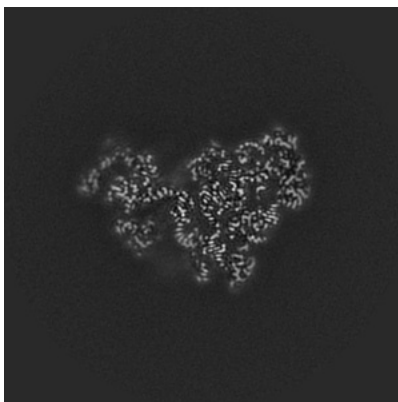
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

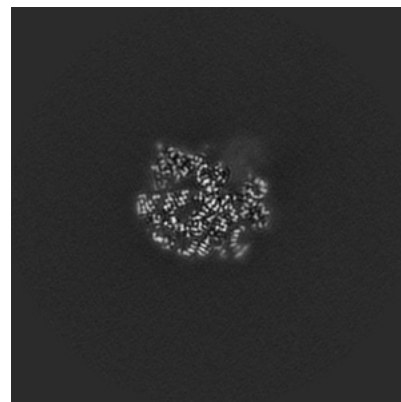
### 6.2.1 Primary map



X Index: 216

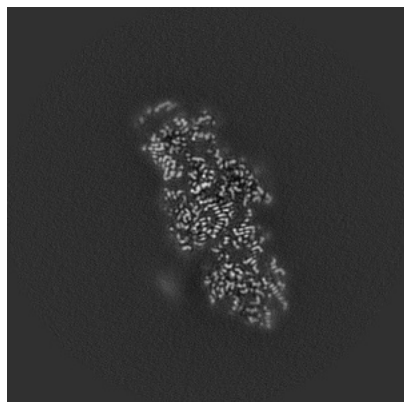


Y Index: 216

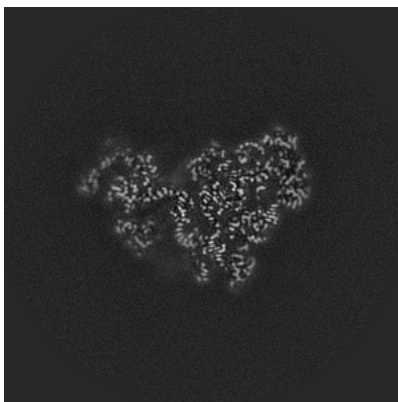


Z Index: 216

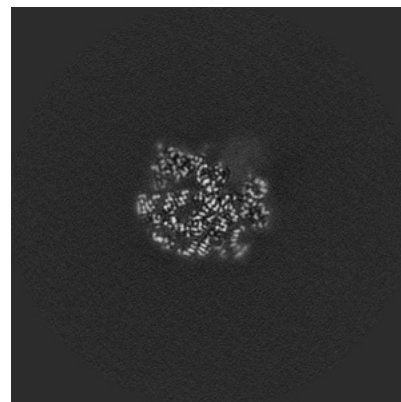
### 6.2.2 Raw map



X Index: 216



Y Index: 216

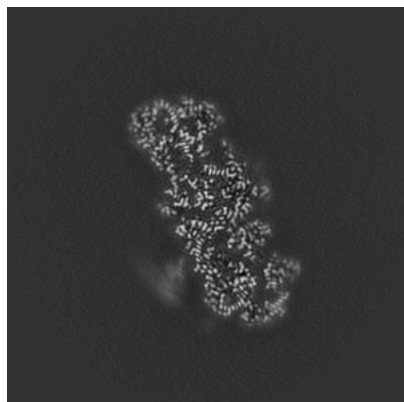


Z Index: 216

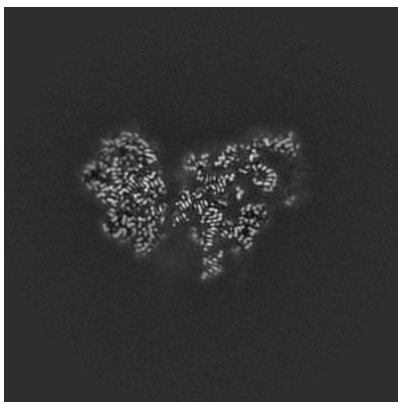
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

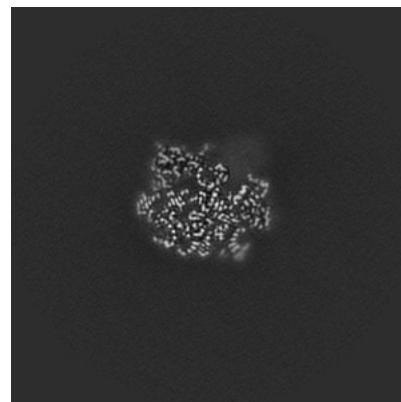
### 6.3.1 Primary map



X Index: 226

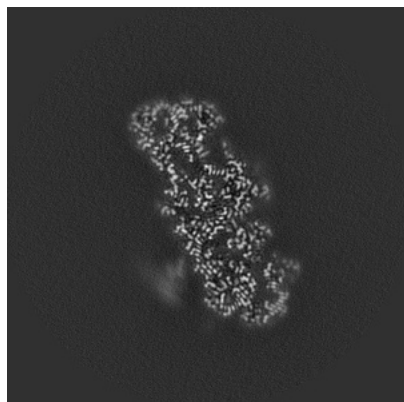


Y Index: 228

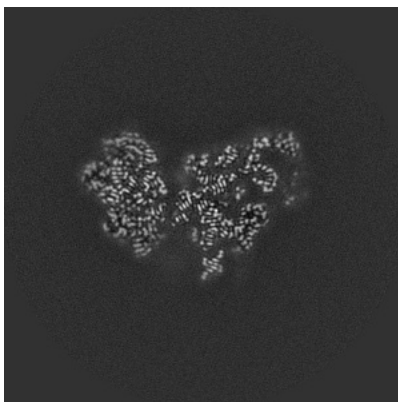


Z Index: 218

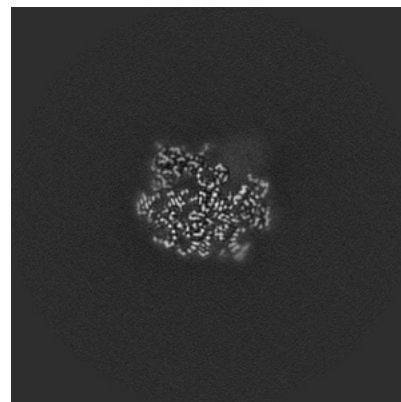
### 6.3.2 Raw map



X Index: 225



Y Index: 227

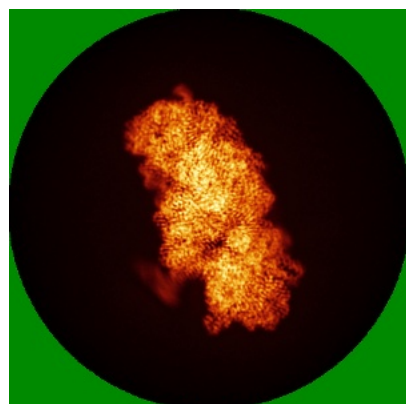


Z Index: 218

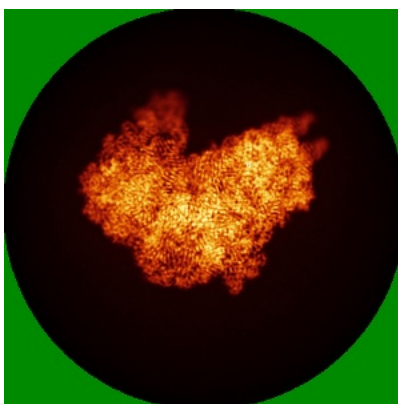
The images above show the largest variance slices of the map in three orthogonal directions.

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

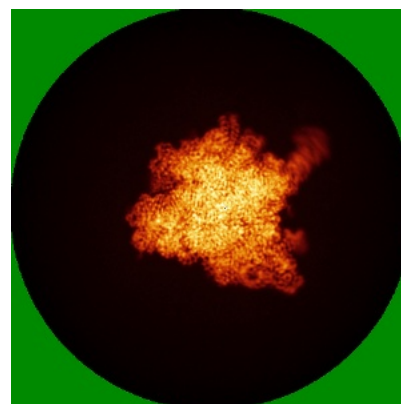
### 6.4.1 Primary map



X

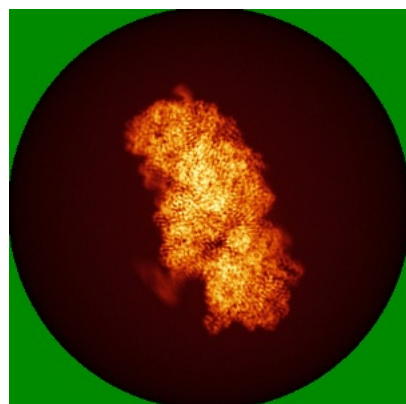


Y

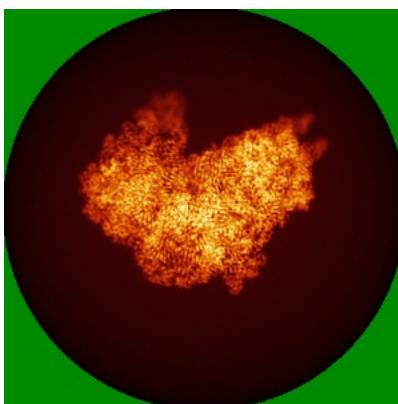


Z

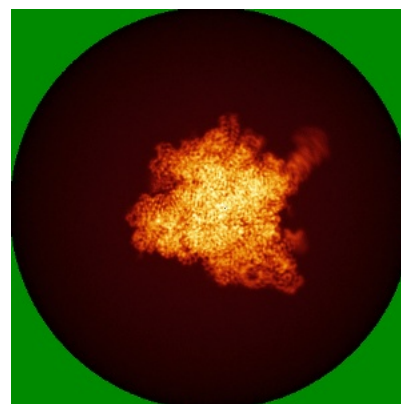
### 6.4.2 Raw map



X



Y



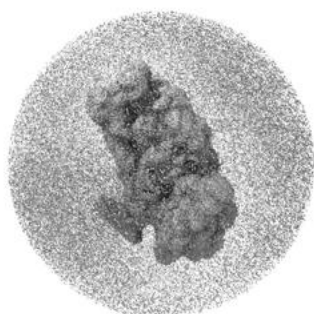
Z

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

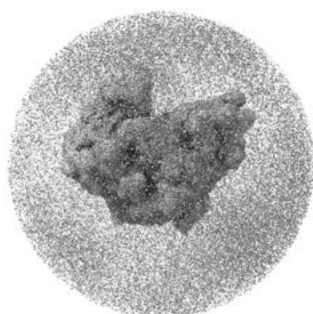


## 6.5 Orthogonal surface views [i](#)

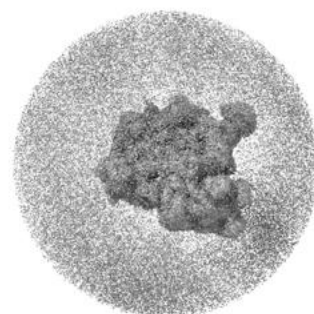
### 6.5.1 Primary map



X



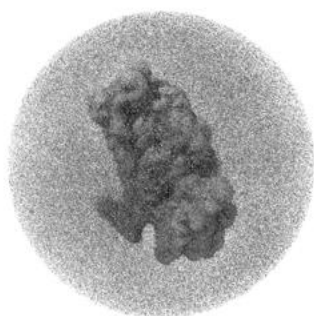
Y



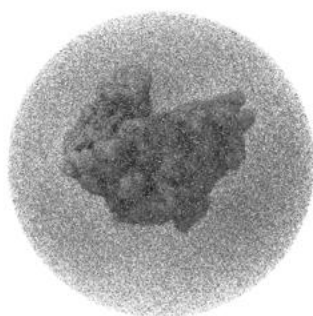
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

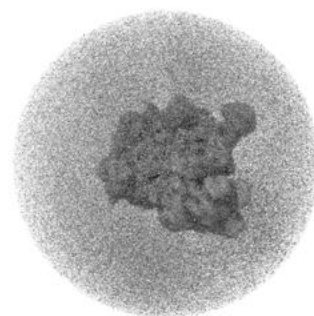
### 6.5.2 Raw map



X



Y



Z

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

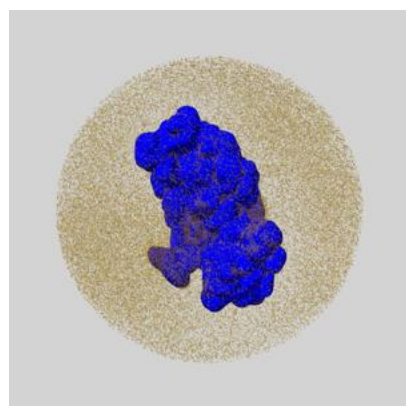
## 6.6 Mask visualisation [i](#)

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

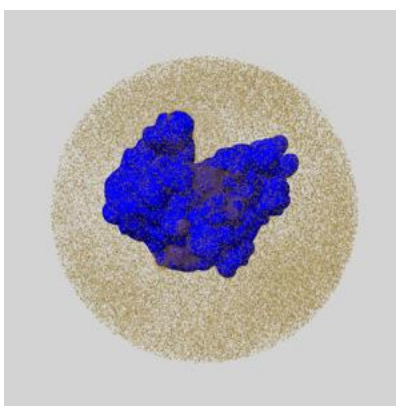
A mask typically either:

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

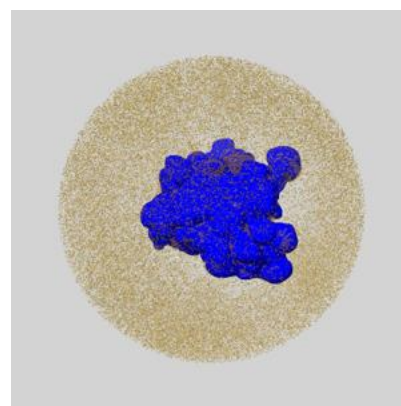
### 6.6.1 emd\_14581\_msk\_1.map [i](#)



X



Y

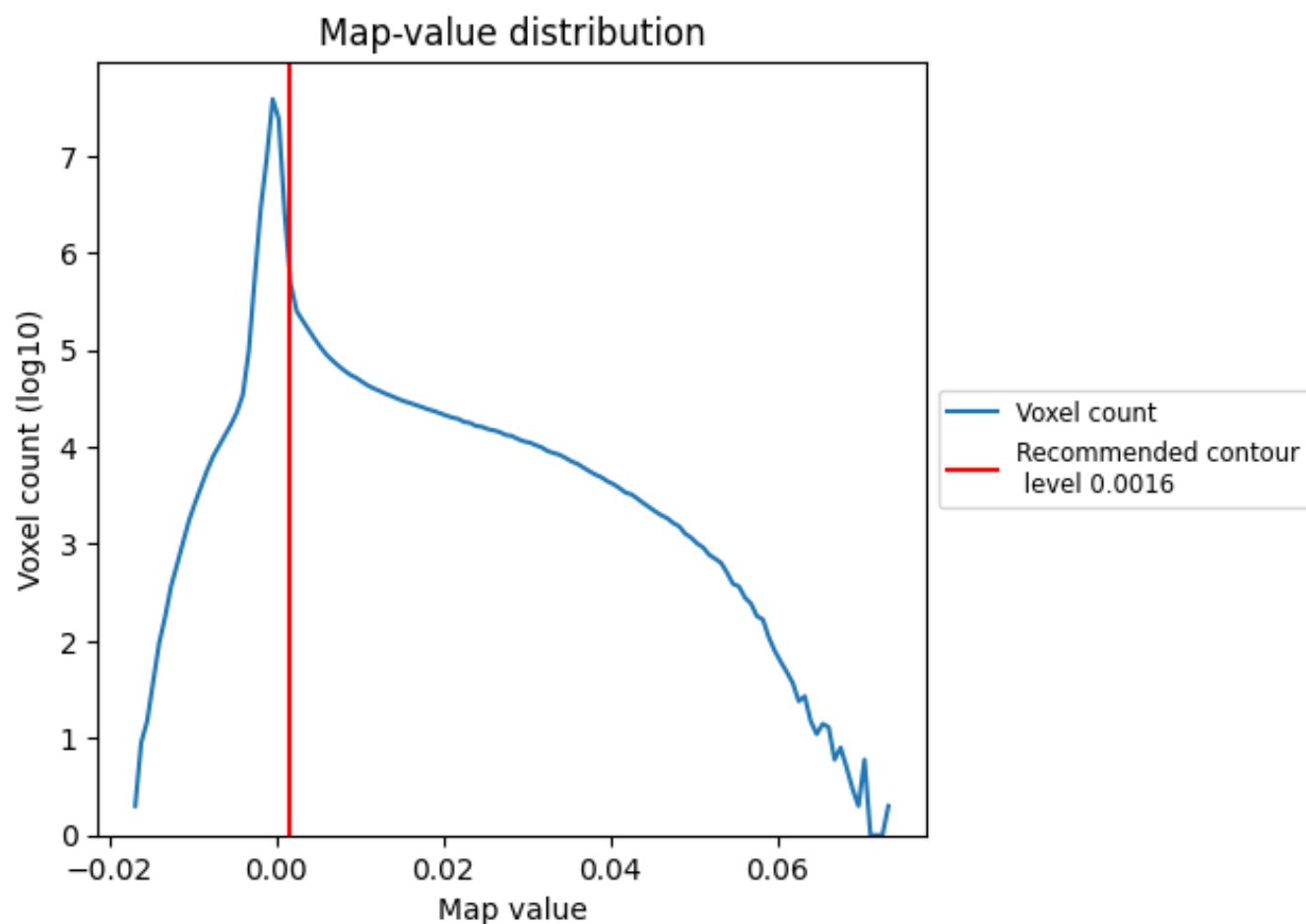


Z

## 7 Map analysis [i](#)

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

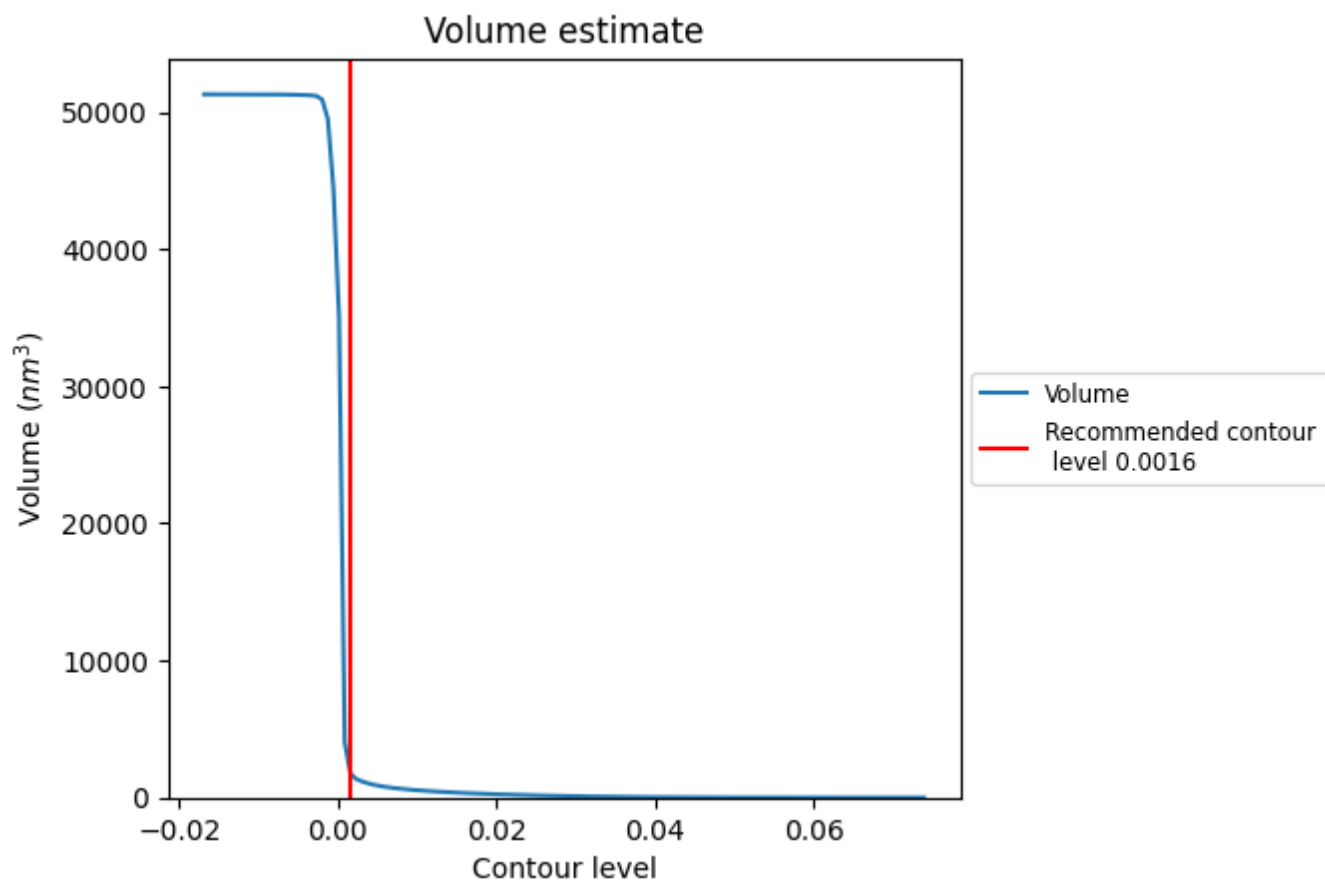
### 7.1 Map-value distribution [i](#)



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



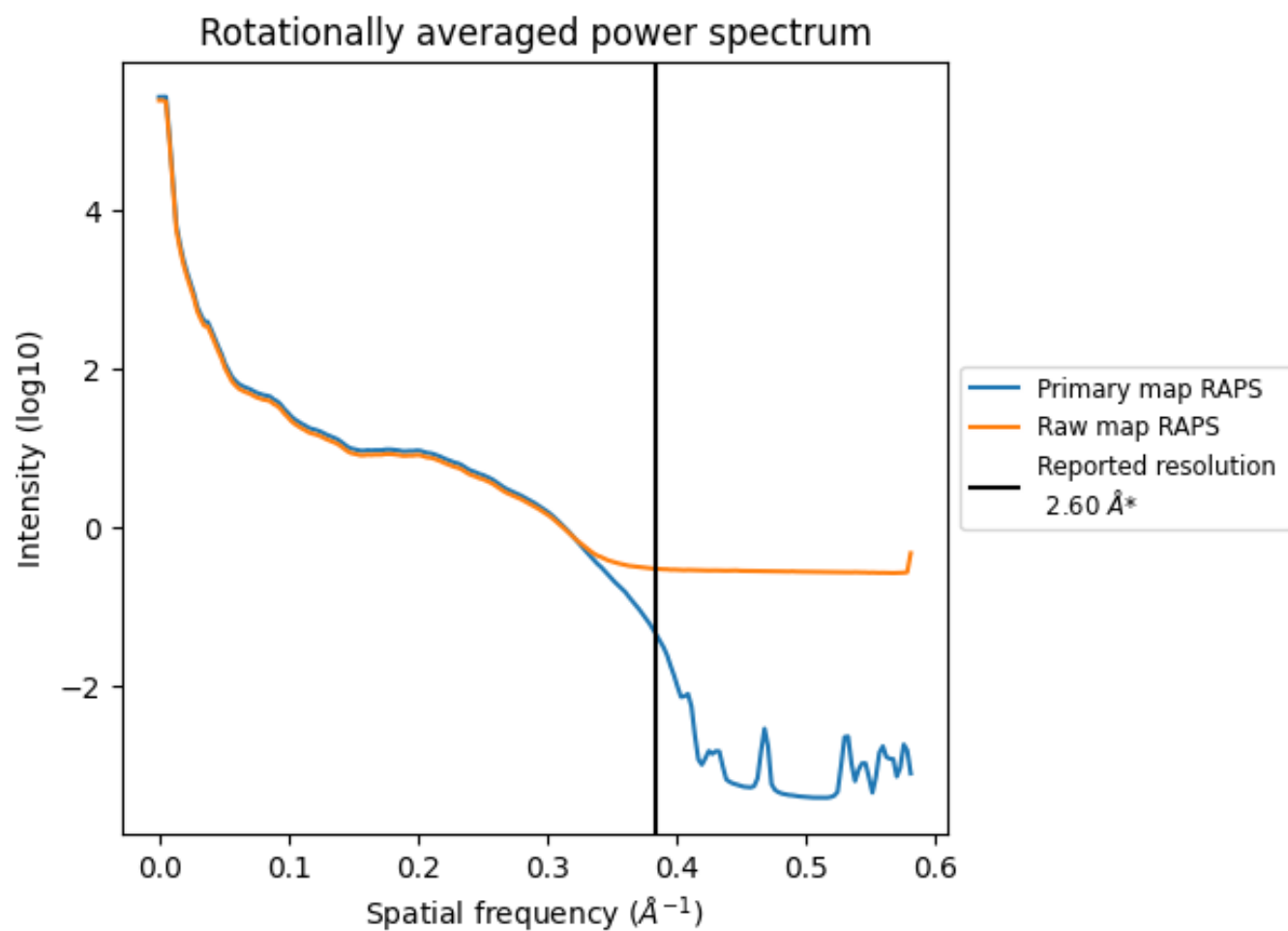
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1745 nm<sup>3</sup>; this corresponds to an approximate mass of 1576 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 ⓘ

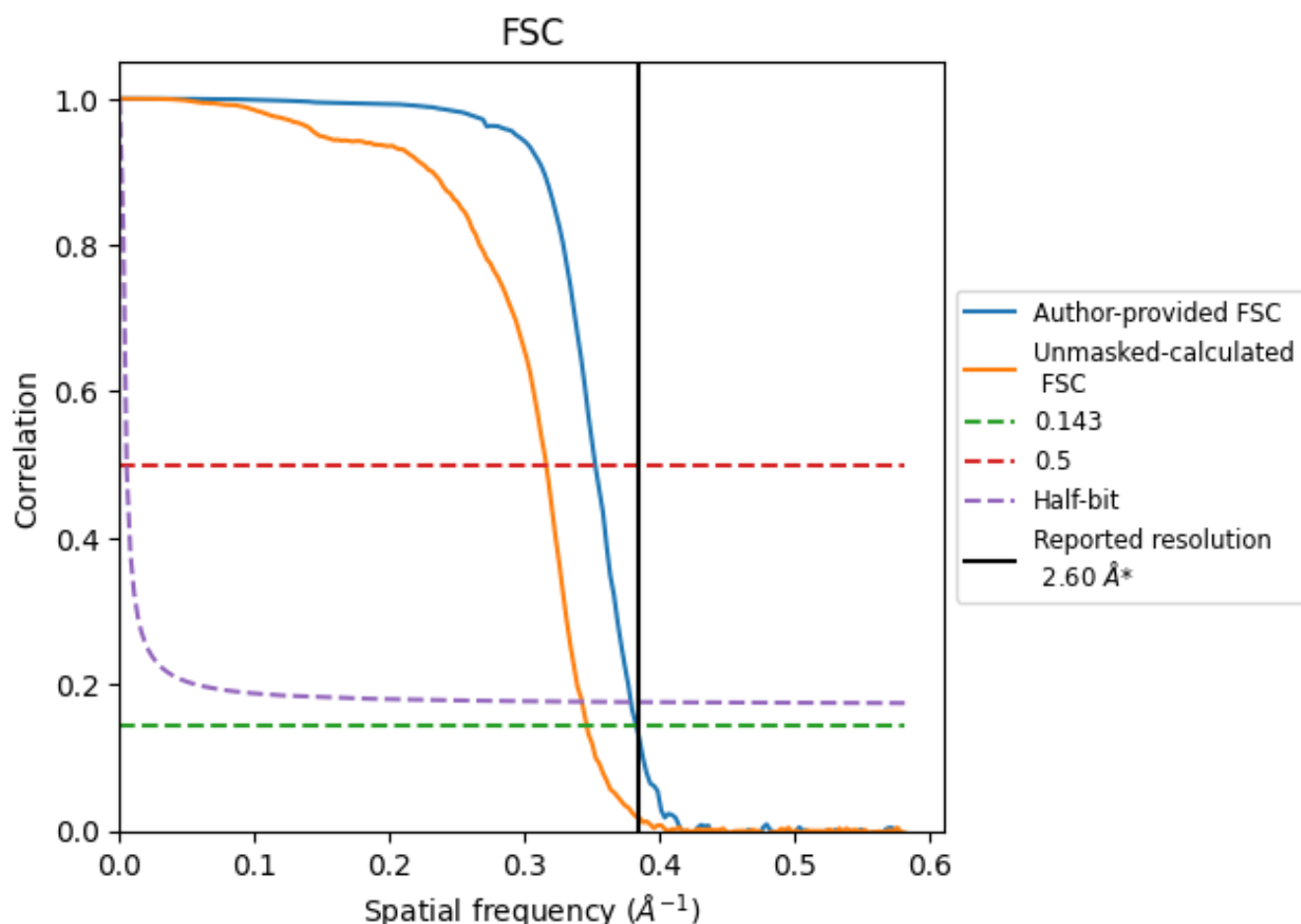


\*Reported resolution corresponds to spatial frequency of 0.385 Å<sup>-1</sup>

## 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  $0.385 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

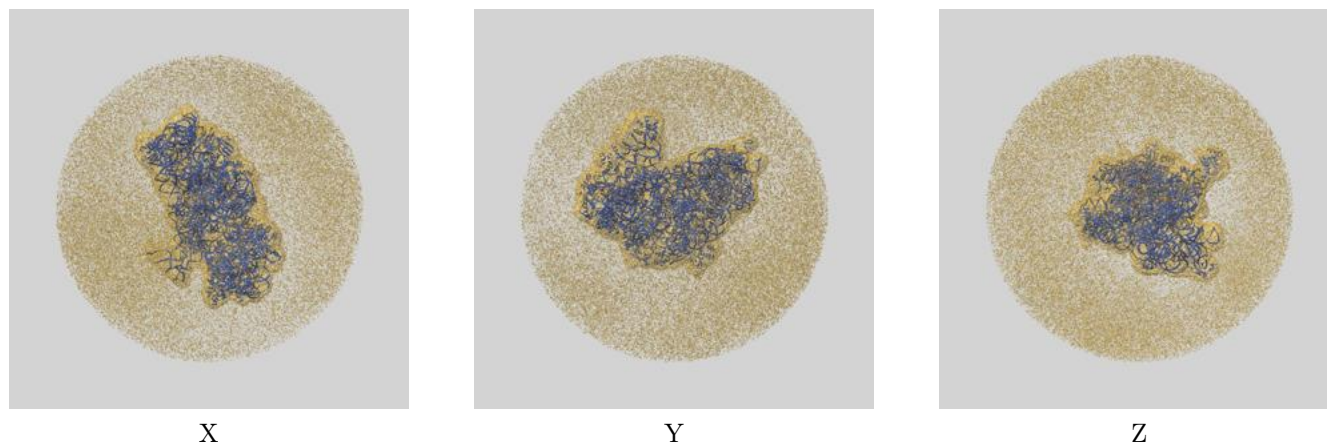
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.61	2.84	2.64
Unmasked-calculated*	2.89	3.17	2.92

\*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 2.89 differs from the reported value 2.6 by more than 10 %

## 9 Map-model fit [i](#)

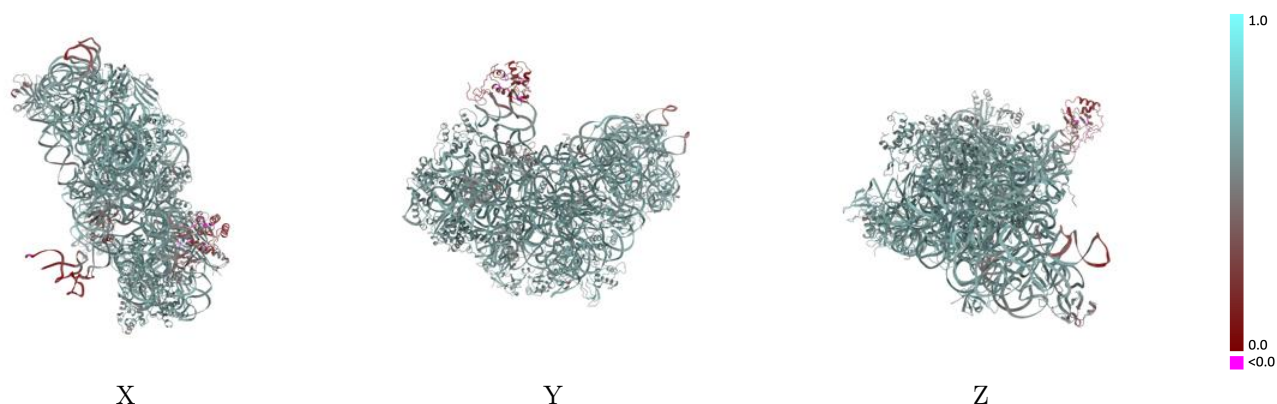
This section contains information regarding the fit between EMDB map EMD-14581 and PDB model 7ZAI. Per-residue inclusion information can be found in section [3](#) on page [13](#).

### 9.1 Map-model overlay [i](#)



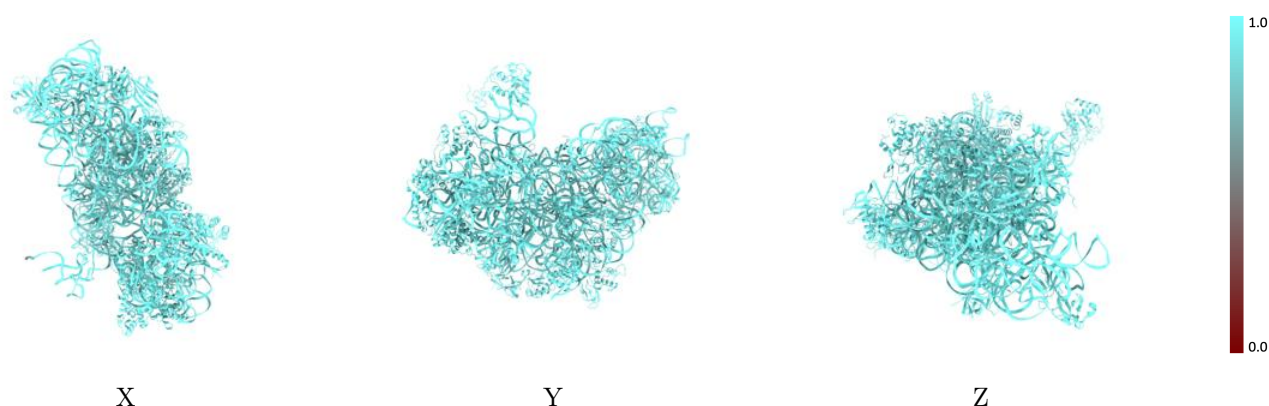
The images above show the 3D surface view of the map at the recommended contour level 0.0016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



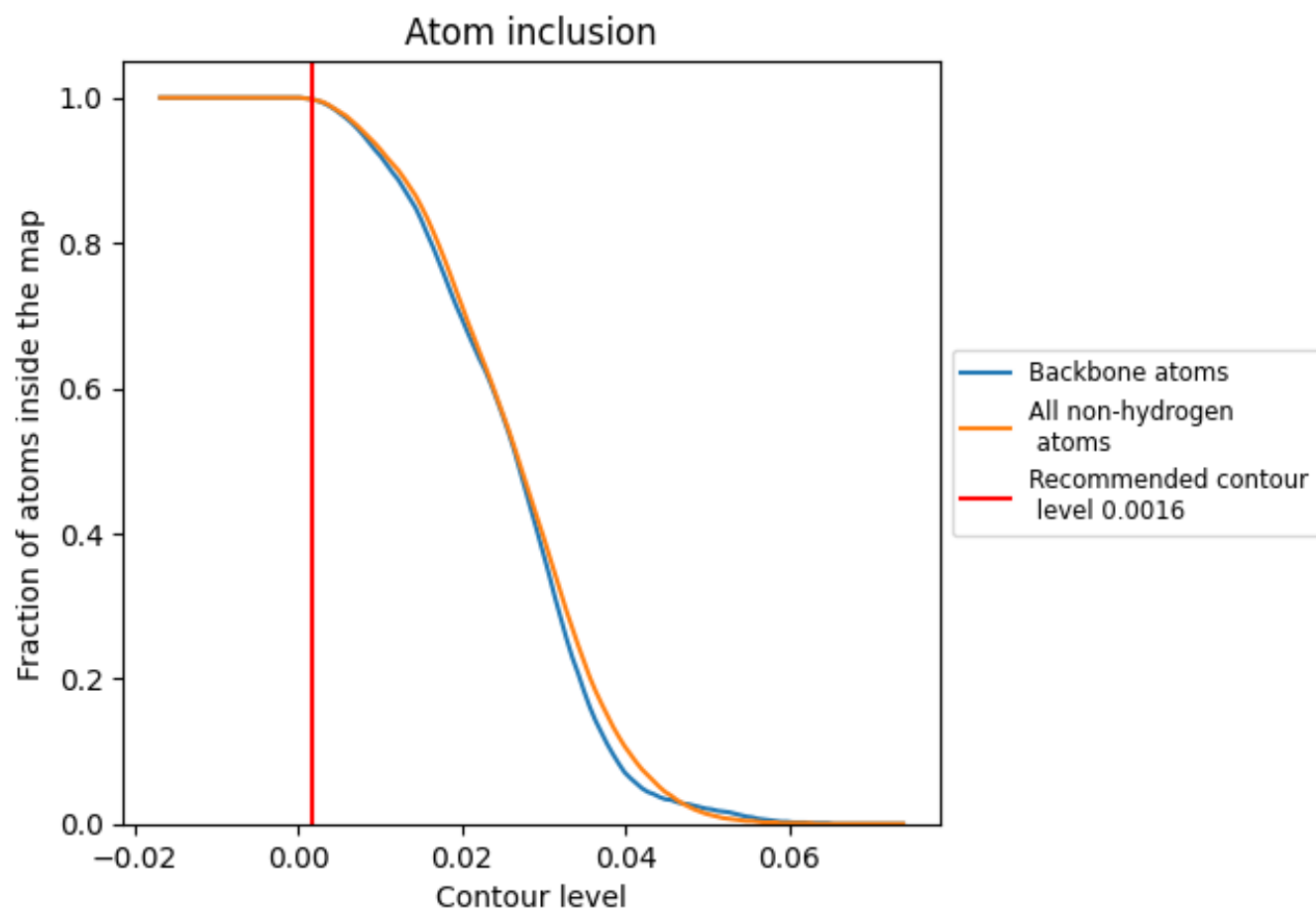
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0016).



































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.0016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9980	 0.5870
0	 1.0000	 0.6320
2	 1.0000	 0.6130
3	 0.9950	 0.2100
4	 0.9860	 0.3190
5	 1.0000	 0.5630
6	 0.9130	 0.4080
A	 1.0000	 0.5920
B	 0.9990	 0.5920
C	 1.0000	 0.6110
D	 1.0000	 0.6190
E	 1.0000	 0.6070
F	 0.9990	 0.6170
G	 1.0000	 0.5310
H	 0.9980	 0.5960
I	 0.9990	 0.6270
J	 1.0000	 0.5980
K	 1.0000	 0.6030
L	 1.0000	 0.5620
M	 0.9990	 0.6110
N	 0.9980	 0.6130
O	 0.9990	 0.5760
P	 0.9980	 0.6010
Q	 1.0000	 0.6020
R	 1.0000	 0.6260
S	 1.0000	 0.5480
T	 1.0000	 0.5750
U	 1.0000	 0.5950
V	 0.9990	 0.5890
W	 1.0000	 0.5890
X	 1.0000	 0.5940
Y	 0.9970	 0.1770
Z	 0.9990	 0.5670

