



## wwPDB EM Validation Summary Report ⓘ

Dec 11, 2022 – 05:09 pm GMT

PDB ID : 6SWD  
EMDB ID : EMD-10323  
Title : IC2 body model of cryo-EM structure of a full archaeal ribosomal translation initiation complex devoid of aIF1 in *P. abyssi*  
Authors : Coureux, P.-D.; Mechulam, Y.; Schmitt, E.  
Deposited on : 2019-09-20  
Resolution : 3.20 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](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.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

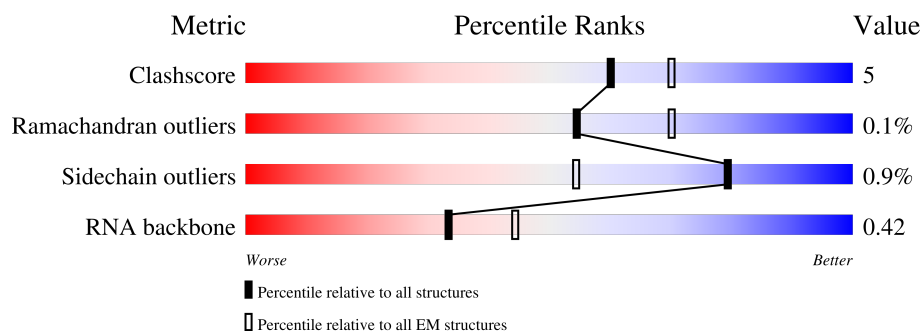
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1044	
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	 80%19%.
9	I	130	 79%19%..
10	J	127	 81%18%.
11	M	137	 81%12%7%.
12	N	147	 88%11%.
13	Q	158	 85%11%.
14	R	113	 84%12%.
15	V	99	 73%22%5%.
16	W	65	 80%17%.
17	0	36	 81%19%
18	5	20	 30%65%25%10%
19	6	113	 55%45%39%16%

## 2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 41548 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1044	Total	C	N	O	P	0	0
			22543	10048	4165	7286	1044		

- 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
			1533	995	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	61	Total	C	N	O	S	0	0
			482	304	85	85	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	175	Total	C	N	O	S	0	0
			1470	924	284	258	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 S8.

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

- Molecule 10 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	126	Total	C	N	O	S	0	0
			996	617	206	173			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	128	Total	C	N	O	S	0	0
			964	597	192	173	2		

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	152	Total	C	N	O	S	0	0
			1262	804	240	214	4		

- Molecule 14 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	109	Total	C	N	O	S	0	0
			900	572	174	151	3		

- Molecule 15 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	94	Total	C	N	O	S	0	0
			790	516	125	146	3		

- Molecule 16 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	63	Total	C	N	O	S	0	0
			481	303	93	80	5		

- Molecule 17 is a protein called 30S ribosomal protein aL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	0	36	Total	C	N	O	S	0	0
			343	218	84	39	2		

- Molecule 18 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	5	20	Total	C	N	O	P	0	0
			430	192	78	140	20		

- Molecule 19 is a protein called Translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	6	95	Total	C	N	O	S	0	0
			777	496	148	130	3		

- Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
20	2	24	Total	Mg	0
			24	24	
20	5	1	Total	Mg	0
			1	1	

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

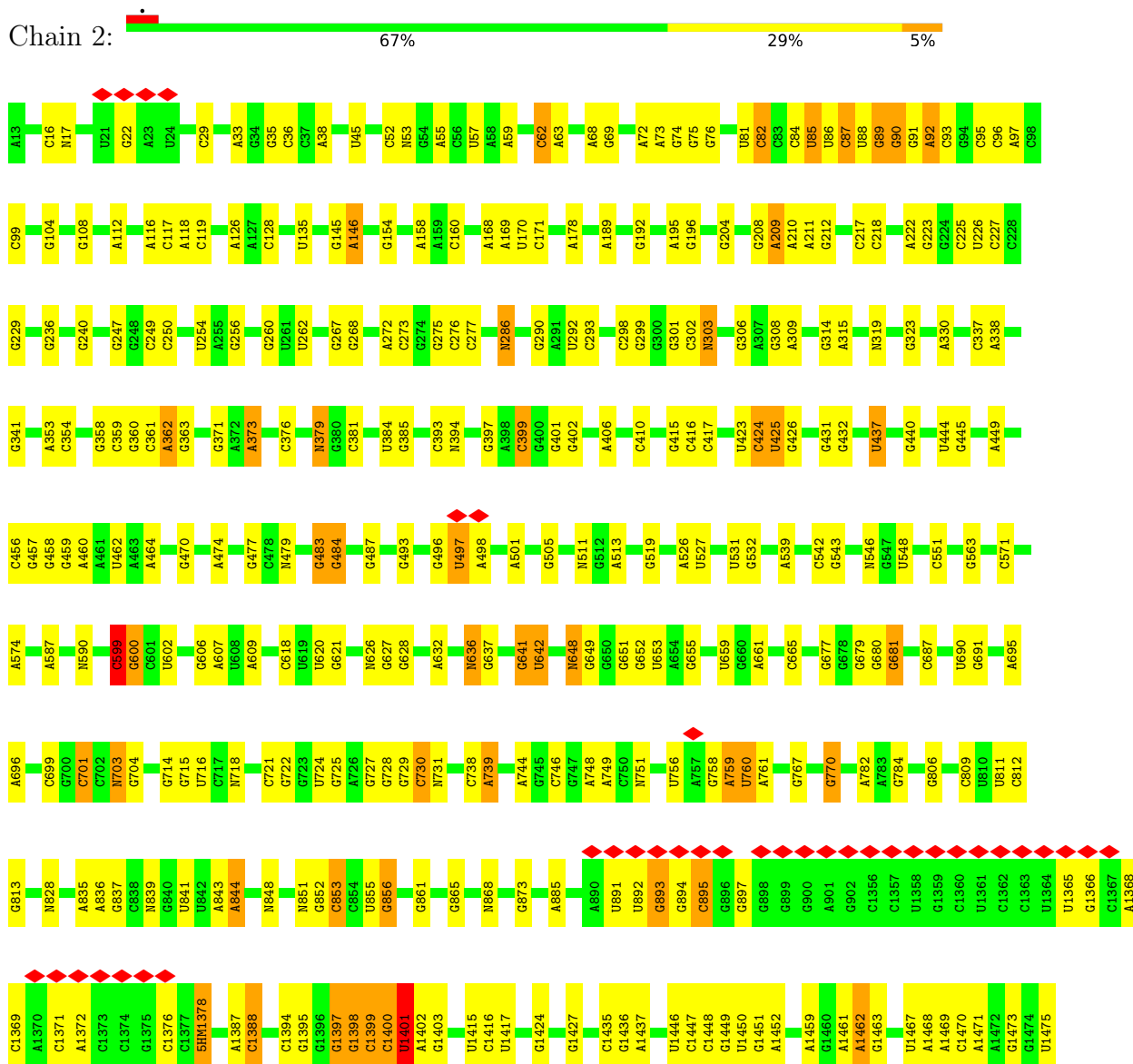
- Molecule 22 is water.

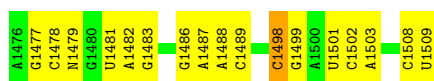
Mol	Chain	Residues	Atoms		AltConf
22	2	24	Total 24	O 24	0
22	F	1	Total 1	O 1	0
22	Q	1	Total 1	O 1	0

### 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.

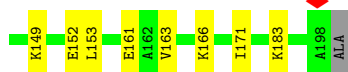
#### • Molecule 1: 16S ribosomal RNA





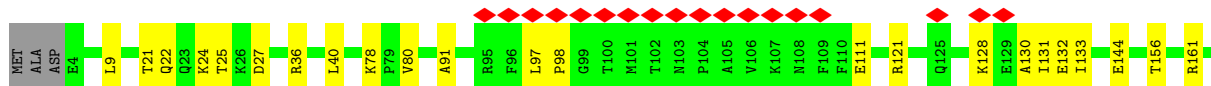
- Molecule 2: 30S ribosomal protein S3Ae

Chain A: 77% 18% 6%



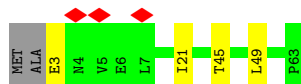
- Molecule 3: 30S ribosomal protein S2

Chain B: 9% 83% 14%



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

Chain C: 5% 90% 6%



- Molecule 5: 30S ribosomal protein S4

Chain D: 83% 14%



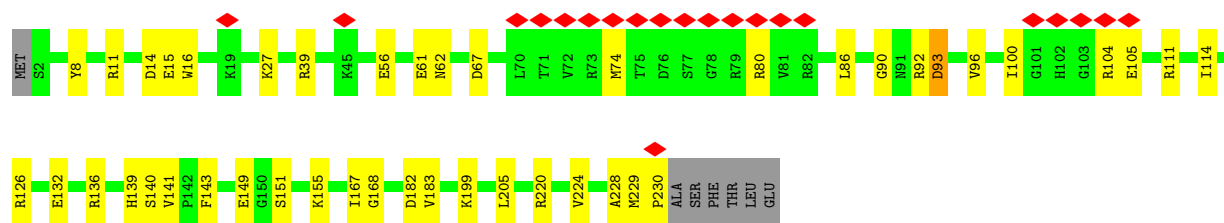
- Molecule 6: 30S ribosomal protein S4e

Chain E: 88% 11%



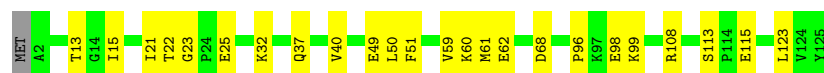
- Molecule 7: 30S ribosomal protein S5

Chain F: 9% 78% 18%



- Molecule 8: 30S ribosomal protein S6e

Chain G: 80% 19% .



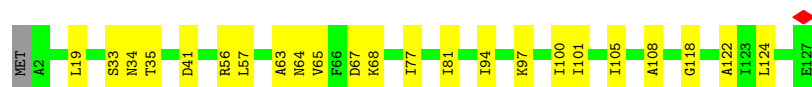
- Molecule 9: 30S ribosomal protein S8

Chain I: 79% 19% ..



- Molecule 10: 30S ribosomal protein S8e

Chain J: 81% 18% .



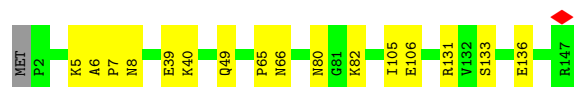
- Molecule 11: 30S ribosomal protein S11

Chain M: 81% 12% 7% .



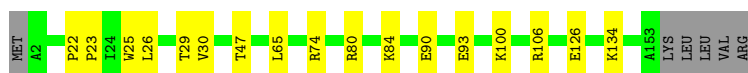
- Molecule 12: 30S ribosomal protein S12

Chain N: 88% 11% .



- Molecule 13: 30S ribosomal protein S15

Chain Q: 85% 11% .



- Molecule 14: 30S ribosomal protein S17

Chain R: 84% 12% .



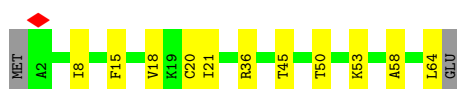
- Molecule 15: 30S ribosomal protein S24e

Chain V: 73% 22% 5%



- Molecule 16: 30S ribosomal protein S27e

Chain W: 80% 17% .



- Molecule 17: 30S ribosomal protein aL41

Chain 0: 81% 19%



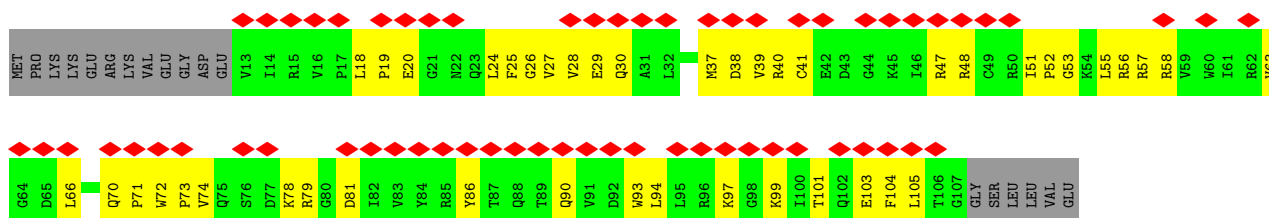
- Molecule 18: mRNA

Chain 5: 30% 65% 25% 10%



- Molecule 19: Translation initiation factor 1A

Chain 6: 55% 45% 39% 16%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	142000	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 ( $e^-/\text{\AA}^2$ )	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.050	Depositor
Minimum map value	-0.019	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	379.32, 379.32, 379.32	wwPDB
Map dimensions	348, 348, 348	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	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, 4AC, 6MZ, UR3, ZN, MA6, LHH, OMC, 5HM, MG

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	1.27	1/24391 (0.0%)	1.10	38/38014 (0.1%)
2	A	0.55	0/1559	0.56	0/2090
3	B	0.53	0/1602	0.55	0/2165
4	C	0.57	0/496	0.60	0/673
5	D	0.62	0/1494	0.58	0/2003
6	E	0.65	0/2032	0.60	0/2742
7	F	0.62	0/1838	0.62	0/2478
8	G	0.42	0/993	0.55	0/1329
9	I	0.71	0/1055	0.61	1/1415 (0.1%)
10	J	0.52	0/1005	0.56	0/1339
11	M	0.51	0/982	0.58	0/1322
12	N	0.62	0/1165	0.59	0/1547
13	Q	0.55	0/1290	0.55	0/1734
14	R	0.68	0/923	0.57	0/1247
15	V	0.66	0/808	0.55	0/1086
16	W	0.43	0/488	0.53	0/659
17	0	0.68	0/349	0.65	0/451
18	5	0.74	0/481	0.93	0/748
19	6	0.31	0/793	0.53	0/1072
All	All	1.02	1/43744 (0.0%)	0.93	39/64114 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
12	N	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	399	C	N1-C6	-5.44	1.33	1.37

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	393	C	C2-N1-C1'	6.82	126.30	118.80
1	2	293	C	C6-N1-C2	-6.49	117.70	120.30
1	2	759	A	O4'-C1'-N9	6.48	113.38	108.20
1	2	1470	C	O5'-P-OP1	-6.15	100.17	105.70
1	2	641	G	N1-C6-O6	-6.01	116.29	119.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	N	5	LYS	Peptide

## 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	22543	0	11390	101	0
2	A	1533	0	1627	25	0
3	B	1571	0	1630	17	0
4	C	482	0	462	4	0
5	D	1470	0	1542	21	0
6	E	1983	0	2060	16	0
7	F	1808	0	1879	30	0
8	G	977	0	1037	13	0
9	I	1034	0	1069	20	0
10	J	996	0	1076	17	0
11	M	964	0	994	10	0
12	N	1148	0	1248	8	0
13	Q	1262	0	1331	13	0
14	R	900	0	921	11	0
15	V	790	0	806	17	0
16	W	481	0	512	9	0
17	0	343	0	407	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	5	430	0	215	3	0
19	6	777	0	806	38	0
20	2	24	0	0	0	0
20	5	1	0	0	0	0
21	C	2	0	0	0	0
21	F	1	0	0	0	0
21	R	1	0	0	0	0
21	W	1	0	0	0	0
22	2	24	0	0	0	0
22	F	1	0	0	0	0
22	Q	1	0	0	0	0
All	All	41548	0	31012	337	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 5.

The worst 5 of 337 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)
6:E:168:VAL:HG23	6:E:169:PRO:HD3	1.51	0.90
2:A:47:ARG:HB3	11:M:34:THR:HG21	1.55	0.88
2:A:47:ARG:NH2	11:M:37:GLU:OE1	2.10	0.84
1:2:303:4AC:O2'	5:D:6:ARG:NH1	2.14	0.80
1:2:651:G:H21	11:M:38:THR:HG21	1.45	0.80

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	186/199 (94%)	170 (91%)	16 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	194/202 (96%)	181 (93%)	13 (7%)	0	100	100
4	C	59/63 (94%)	51 (86%)	8 (14%)	0	100	100
5	D	173/180 (96%)	163 (94%)	10 (6%)	0	100	100
6	E	240/243 (99%)	216 (90%)	23 (10%)	1 (0%)	34	69
7	F	227/236 (96%)	202 (89%)	25 (11%)	0	100	100
8	G	122/125 (98%)	102 (84%)	19 (16%)	1 (1%)	19	58
9	I	127/130 (98%)	117 (92%)	10 (8%)	0	100	100
10	J	124/127 (98%)	113 (91%)	11 (9%)	0	100	100
11	M	126/137 (92%)	110 (87%)	16 (13%)	0	100	100
12	N	144/147 (98%)	124 (86%)	20 (14%)	0	100	100
13	Q	150/158 (95%)	140 (93%)	10 (7%)	0	100	100
14	R	107/113 (95%)	91 (85%)	16 (15%)	0	100	100
15	V	92/99 (93%)	82 (89%)	10 (11%)	0	100	100
16	W	61/65 (94%)	49 (80%)	12 (20%)	0	100	100
17	0	34/36 (94%)	27 (79%)	7 (21%)	0	100	100
19	6	93/113 (82%)	79 (85%)	14 (15%)	0	100	100
All	All	2259/2373 (95%)	2017 (89%)	240 (11%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	E	36	PRO
8	G	96	PRO

### 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	161/167 (96%)	161 (100%)	0	100	100
3	B	168/173 (97%)	167 (99%)	1 (1%)	86	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	54/55 (98%)	52 (96%)	2 (4%)	34	68
5	D	158/160 (99%)	157 (99%)	1 (1%)	86	94
6	E	213/214 (100%)	211 (99%)	2 (1%)	78	91
7	F	192/198 (97%)	185 (96%)	7 (4%)	35	69
8	G	107/108 (99%)	106 (99%)	1 (1%)	78	91
9	I	106/107 (99%)	105 (99%)	1 (1%)	78	91
10	J	102/103 (99%)	102 (100%)	0	100	100
11	M	95/104 (91%)	95 (100%)	0	100	100
12	N	120/121 (99%)	119 (99%)	1 (1%)	81	93
13	Q	137/143 (96%)	137 (100%)	0	100	100
14	R	98/102 (96%)	97 (99%)	1 (1%)	76	90
15	V	86/90 (96%)	86 (100%)	0	100	100
16	W	54/56 (96%)	54 (100%)	0	100	100
17	0	34/34 (100%)	34 (100%)	0	100	100
19	6	83/99 (84%)	83 (100%)	0	100	100
All	All	1968/2034 (97%)	1951 (99%)	17 (1%)	79	91

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	61	TYR
14	R	69	ARG
7	F	80	ARG
7	F	93	ASP
7	F	96	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
8	G	120	ASN
13	Q	85	HIS
9	I	9	ASN
13	Q	112	HIS
12	N	66	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1013/1044 (97%)	211 (20%)	3 (0%)
18	5	19/20 (95%)	7 (36%)	0
All	All	1032/1064 (96%)	218 (21%)	3 (0%)

5 of 218 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	16	C
1	2	29	C
1	2	33	A
1	2	36	C
1	2	38	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	87	C
1	2	599	C
1	2	1387	A

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

32 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	4AC	2	546	1	21,24,25	1.02	2 (9%)	29,34,37	1.21	3 (10%)
1	4AC	2	868	1	21,24,25	1.00	2 (9%)	29,34,37	1.28	3 (10%)
1	OMC	2	1376	1	19,22,23	0.82	0	26,31,34	0.94	1 (3%)
1	4AC	2	394	1	21,24,25	1.03	2 (9%)	29,34,37	1.24	4 (13%)
1	4AC	2	851	1	21,24,25	1.14	2 (9%)	29,34,37	1.40	2 (6%)
1	MA6	2	1487	1	19,26,27	0.91	0	18,38,41	1.21	2 (11%)

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	1.12	2 (9%)	29,34,37	1.48	3 (10%)
1	5HM	2	1378	1	19,23,24	2.89	7 (36%)	25,33,36	0.71	0
1	6MZ	2	1469	20,1	18,25,26	0.84	1 (5%)	16,36,39	2.24	3 (18%)
1	4AC	2	303	1	21,24,25	1.11	3 (14%)	29,34,37	1.30	4 (13%)
1	4AC	2	648	1	21,24,25	1.01	2 (9%)	29,34,37	1.40	4 (13%)
1	4AC	2	828	1	21,24,25	1.01	2 (9%)	29,34,37	1.31	4 (13%)
1	4AC	2	17	1	21,24,25	1.09	2 (9%)	29,34,37	1.28	4 (13%)
1	4AC	2	1479	1	21,24,25	1.13	2 (9%)	29,34,37	1.07	2 (6%)
1	4AC	2	53	1	21,24,25	1.06	2 (9%)	29,34,37	1.24	4 (13%)
1	4AC	2	319	1	21,24,25	1.11	2 (9%)	29,34,37	1.25	3 (10%)
1	A2M	2	373	1	18,25,26	0.97	0	18,36,39	1.36	3 (16%)
1	4AC	2	839	1	21,24,25	1.08	1 (4%)	29,34,37	1.28	3 (10%)
1	4AC	2	718	1	21,24,25	1.06	2 (9%)	29,34,37	1.28	4 (13%)
1	4AC	2	703	1	21,24,25	1.10	1 (4%)	29,34,37	1.78	5 (17%)
1	4AC	2	479	1	21,24,25	1.01	2 (9%)	29,34,37	1.44	4 (13%)
1	LHH	2	250	1	22,25,26	2.55	8 (36%)	29,35,38	1.24	2 (6%)
1	4AC	2	590	1	21,24,25	1.07	2 (9%)	29,34,37	1.43	4 (13%)
1	UR3	2	1467	1	19,22,23	0.91	1 (5%)	26,32,35	1.37	2 (7%)
1	4AC	2	751	1	21,24,25	1.00	2 (9%)	29,34,37	1.16	3 (10%)
1	4AC	2	731	1	21,24,25	1.02	2 (9%)	29,34,37	1.18	3 (10%)
1	4AC	2	848	1	21,24,25	1.10	2 (9%)	29,34,37	1.27	2 (6%)
1	4AC	2	511	1	21,24,25	1.09	1 (4%)	29,34,37	1.31	3 (10%)
1	MA6	2	1488	1	19,26,27	0.89	0	18,38,41	1.21	2 (11%)
1	4AC	2	379	1	21,24,25	1.06	2 (9%)	29,34,37	1.51	4 (13%)
1	4AC	2	286	1	21,24,25	1.09	2 (9%)	29,34,37	1.36	4 (13%)
1	4AC	2	626	1	21,24,25	1.01	2 (9%)	29,34,37	1.26	4 (13%)

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	4AC	2	546	1	-	2/11/29/30	0/2/2/2
1	4AC	2	868	1	-	1/11/29/30	0/2/2/2
1	OMC	2	1376	1	-	2/9/27/28	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	2	394	1	-	2/11/29/30	0/2/2/2
1	4AC	2	851	1	-	0/11/29/30	0/2/2/2
1	MA6	2	1487	1	-	0/7/29/30	0/3/3/3
1	4AC	2	636	1	-	2/11/29/30	0/2/2/2
1	5HM	2	1378	1	-	2/9/27/28	0/2/2/2
1	6MZ	2	1469	20,1	-	0/5/27/28	0/3/3/3
1	4AC	2	303	1	-	0/11/29/30	0/2/2/2
1	4AC	2	648	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	17	1	-	2/11/29/30	0/2/2/2
1	4AC	2	1479	1	-	0/11/29/30	0/2/2/2
1	4AC	2	53	1	-	0/11/29/30	0/2/2/2
1	4AC	2	319	1	-	0/11/29/30	0/2/2/2
1	A2M	2	373	1	-	2/5/27/28	0/3/3/3
1	4AC	2	839	1	-	2/11/29/30	0/2/2/2
1	4AC	2	718	1	-	2/11/29/30	0/2/2/2
1	4AC	2	703	1	-	0/11/29/30	0/2/2/2
1	4AC	2	479	1	-	0/11/29/30	0/2/2/2
1	LHH	2	250	1	-	1/13/31/32	0/2/2/2
1	4AC	2	590	1	-	0/11/29/30	0/2/2/2
1	UR3	2	1467	1	-	1/7/25/26	0/2/2/2
1	4AC	2	751	1	-	0/11/29/30	0/2/2/2
1	4AC	2	731	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	511	1	-	1/11/29/30	0/2/2/2
1	MA6	2	1488	1	-	0/7/29/30	0/3/3/3
1	4AC	2	379	1	-	0/11/29/30	0/2/2/2
1	4AC	2	286	1	-	2/11/29/30	0/2/2/2
1	4AC	2	626	1	-	0/11/29/30	0/2/2/2

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	250	LHH	C4-N4	6.38	1.49	1.39
1	2	1378	5HM	C4-N3	6.16	1.44	1.34
1	2	250	LHH	C7-N4	5.86	1.48	1.37
1	2	1378	5HM	C4-N4	5.29	1.47	1.34
1	2	1378	5HM	C2-N3	5.28	1.47	1.36

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1469	6MZ	C2-N1-C6	6.81	122.43	116.59
1	2	636	4AC	O7-C7-N4	5.50	130.71	121.82
1	2	703	4AC	O7-C7-N4	5.48	130.69	121.82
1	2	1467	UR3	C4-N3-C2	-5.06	119.80	124.56
1	2	851	4AC	O7-C7-N4	4.95	129.83	121.82

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	17	4AC	C3'-C4'-C5'-O5'
1	2	286	4AC	O4'-C4'-C5'-O5'
1	2	286	4AC	C3'-C4'-C5'-O5'
1	2	373	A2M	O4'-C4'-C5'-O5'
1	2	394	4AC	O4'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	636	4AC	3	0
1	2	1378	5HM	1	0
1	2	303	4AC	4	0
1	2	648	4AC	2	0
1	2	703	4AC	5	0
1	2	379	4AC	1	0
1	2	286	4AC	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 30 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	902:G	O3'	1356:C	P	14.11

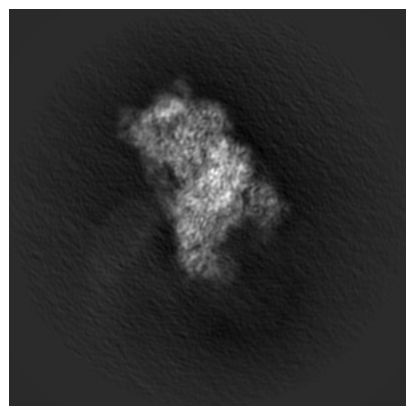
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10323. These allow visual inspection of the internal detail of the map and identification of artifacts.

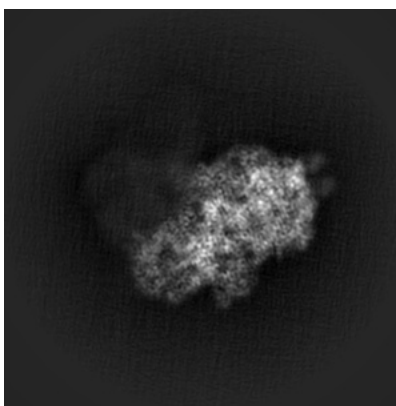
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

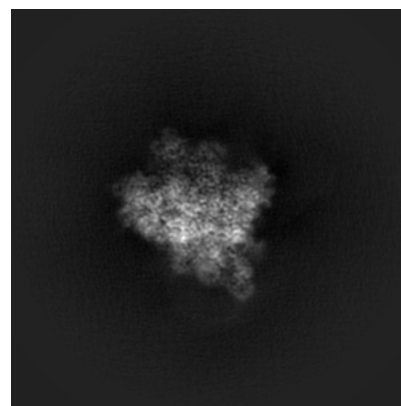
#### 6.1.1 Primary map



X

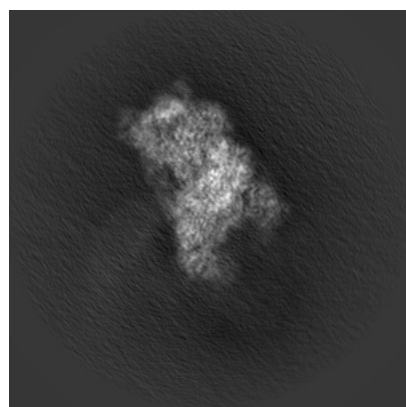


Y

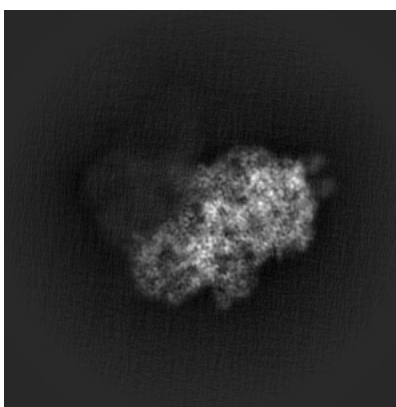


Z

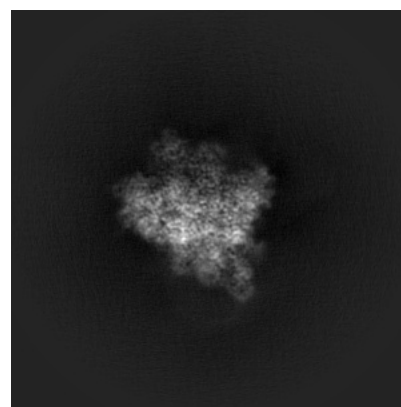
#### 6.1.2 Raw map



X



Y

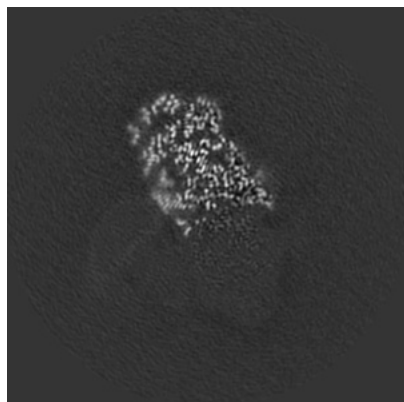


Z

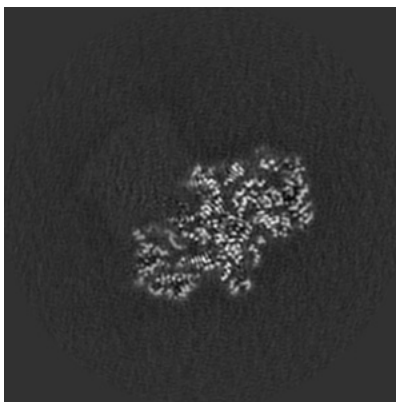
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

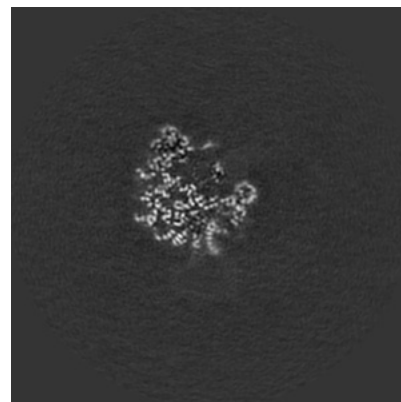
### 6.2.1 Primary map



X Index: 174

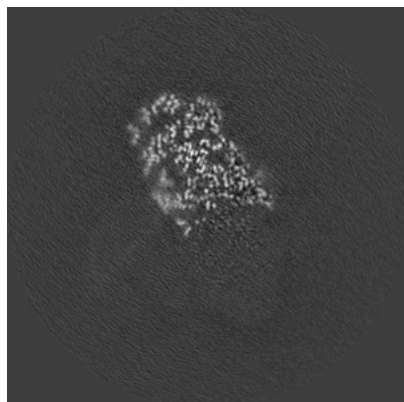


Y Index: 174

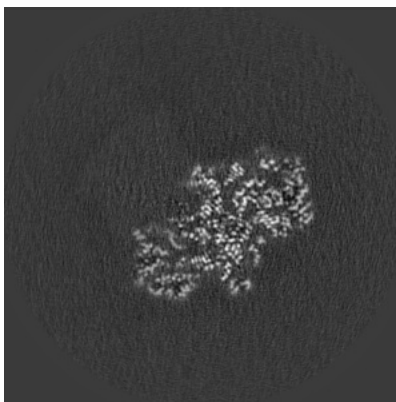


Z Index: 174

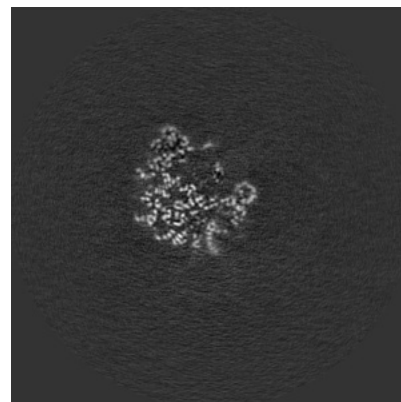
### 6.2.2 Raw map



X Index: 174



Y Index: 174

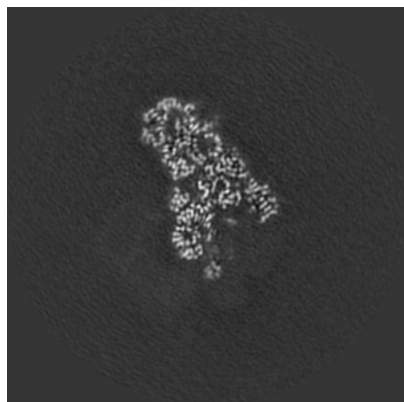


Z Index: 174

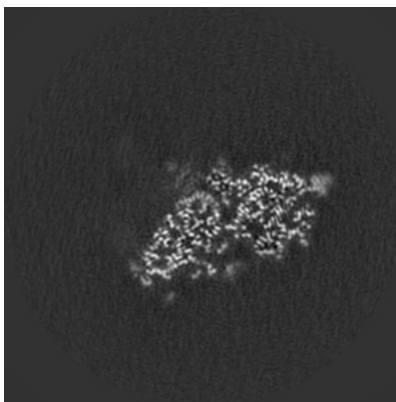
The images above show central slices of the map in three orthogonal directions.

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

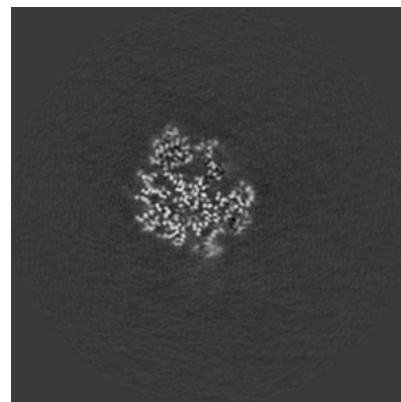
### 6.3.1 Primary map



X Index: 149

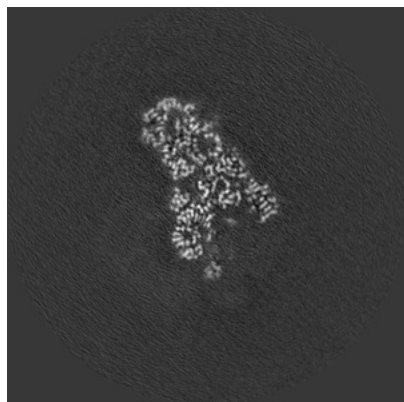


Y Index: 154

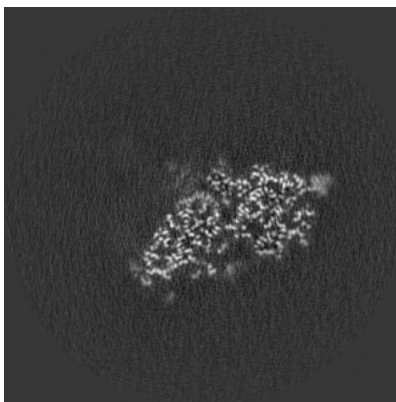


Z Index: 178

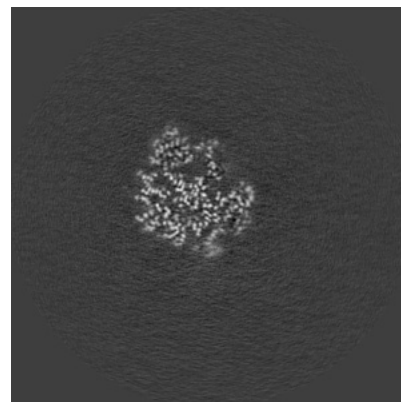
### 6.3.2 Raw map



X Index: 149



Y Index: 154



Z Index: 178

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

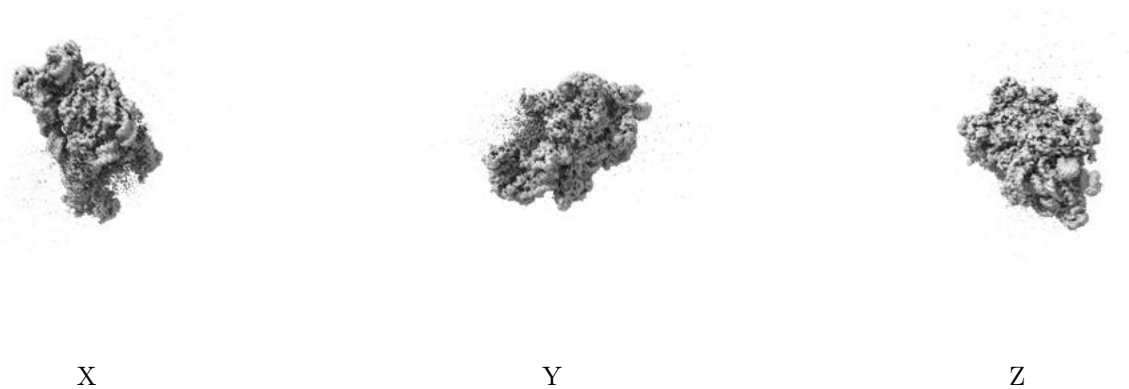
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

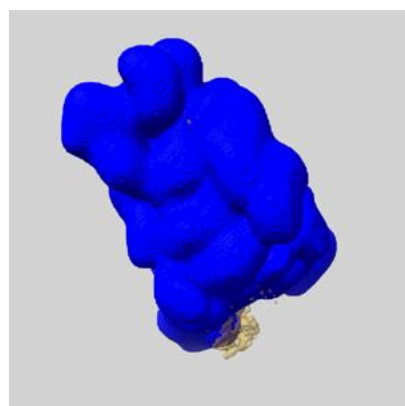
## 6.5 Mask visualisation [i](#)

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

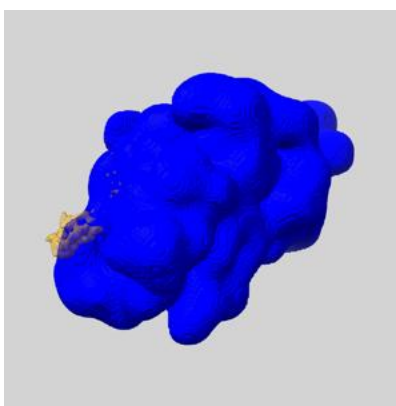
A mask typically either:

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

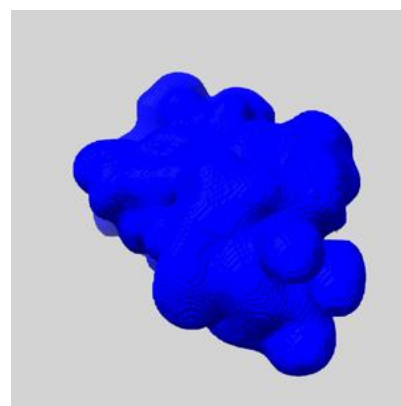
### 6.5.1 emd\_10323\_msk\_1.map [i](#)



X



Y

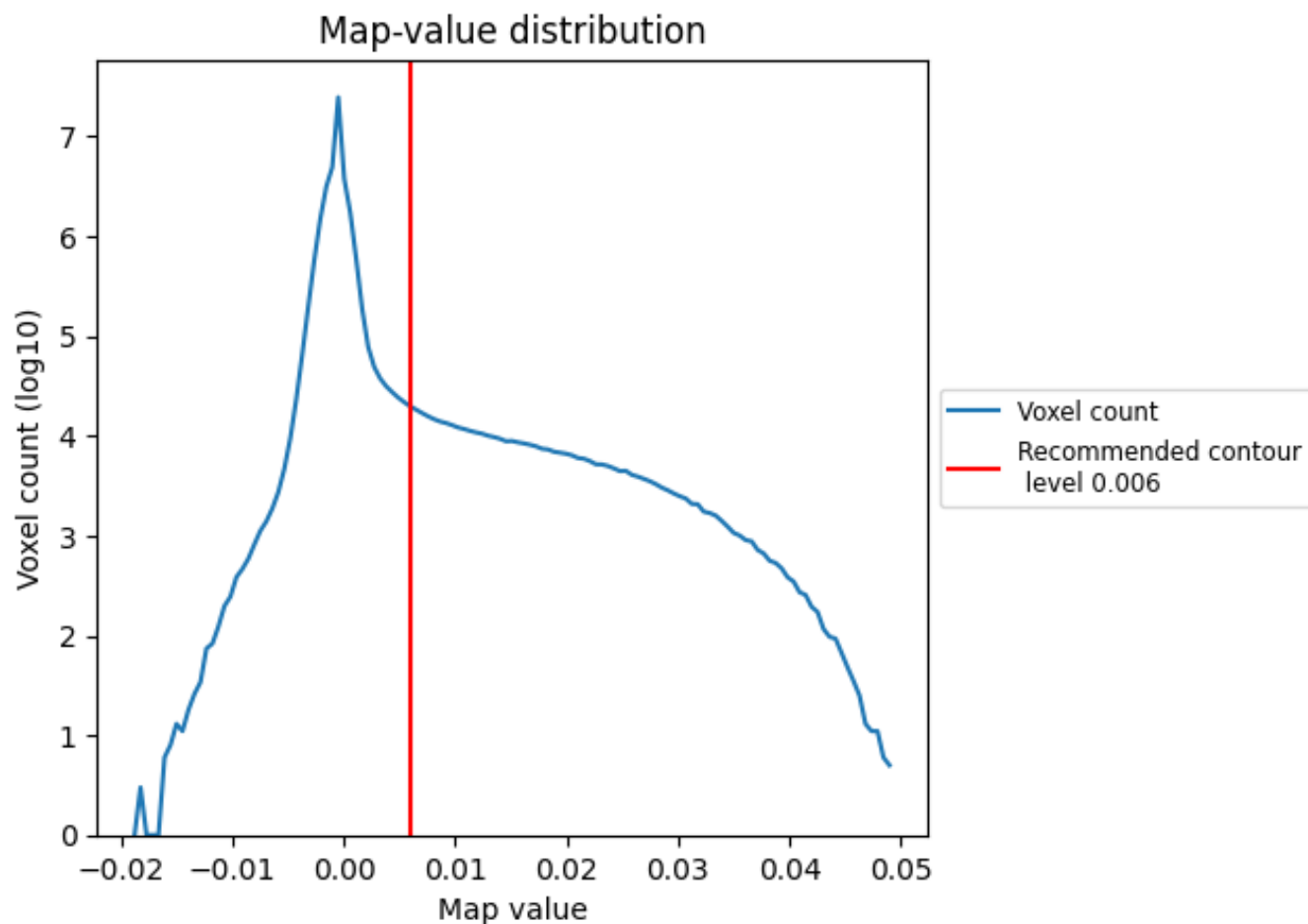


Z

## 7 Map analysis [i](#)

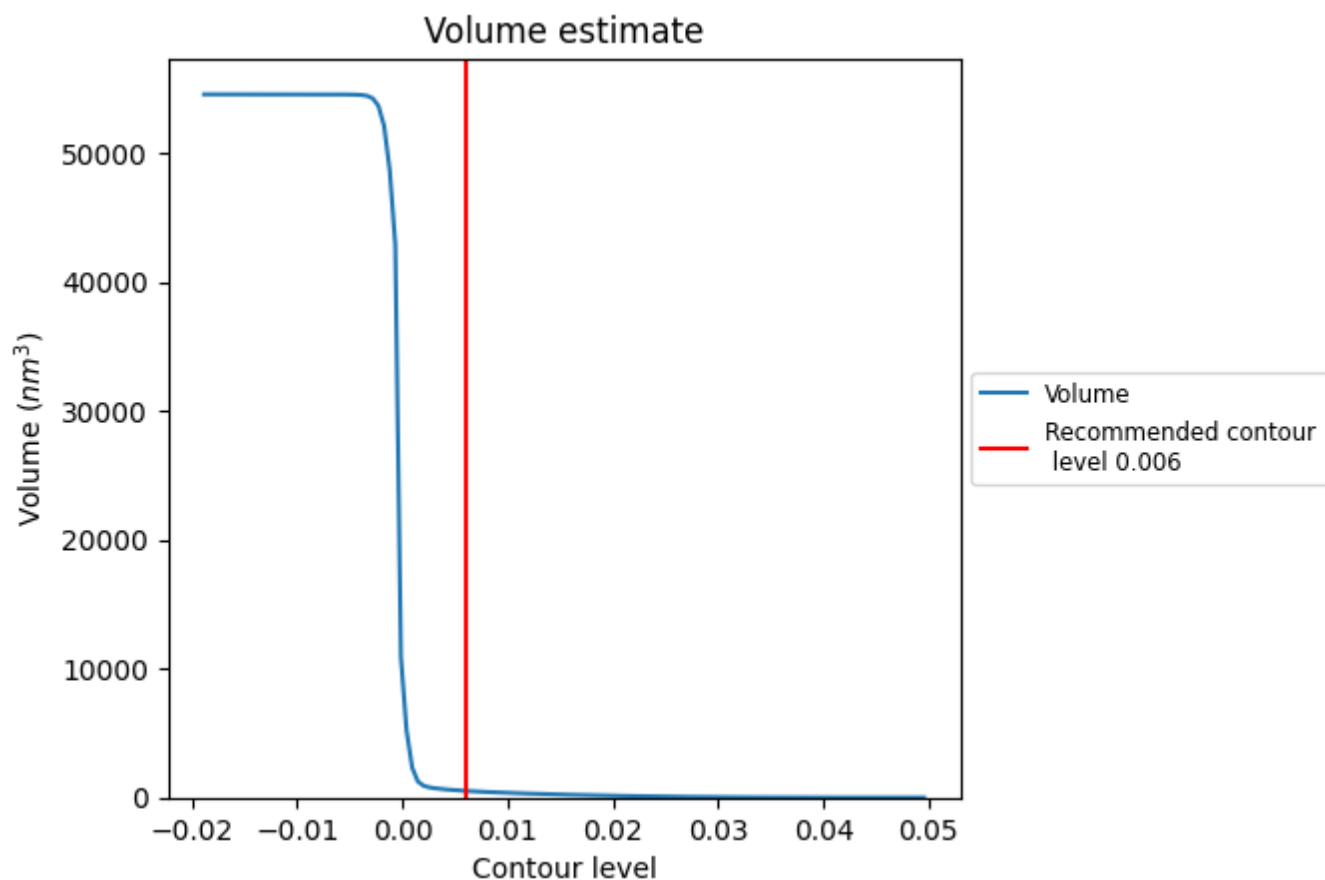
This section contains the results of statistical analysis of the map.

### 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.

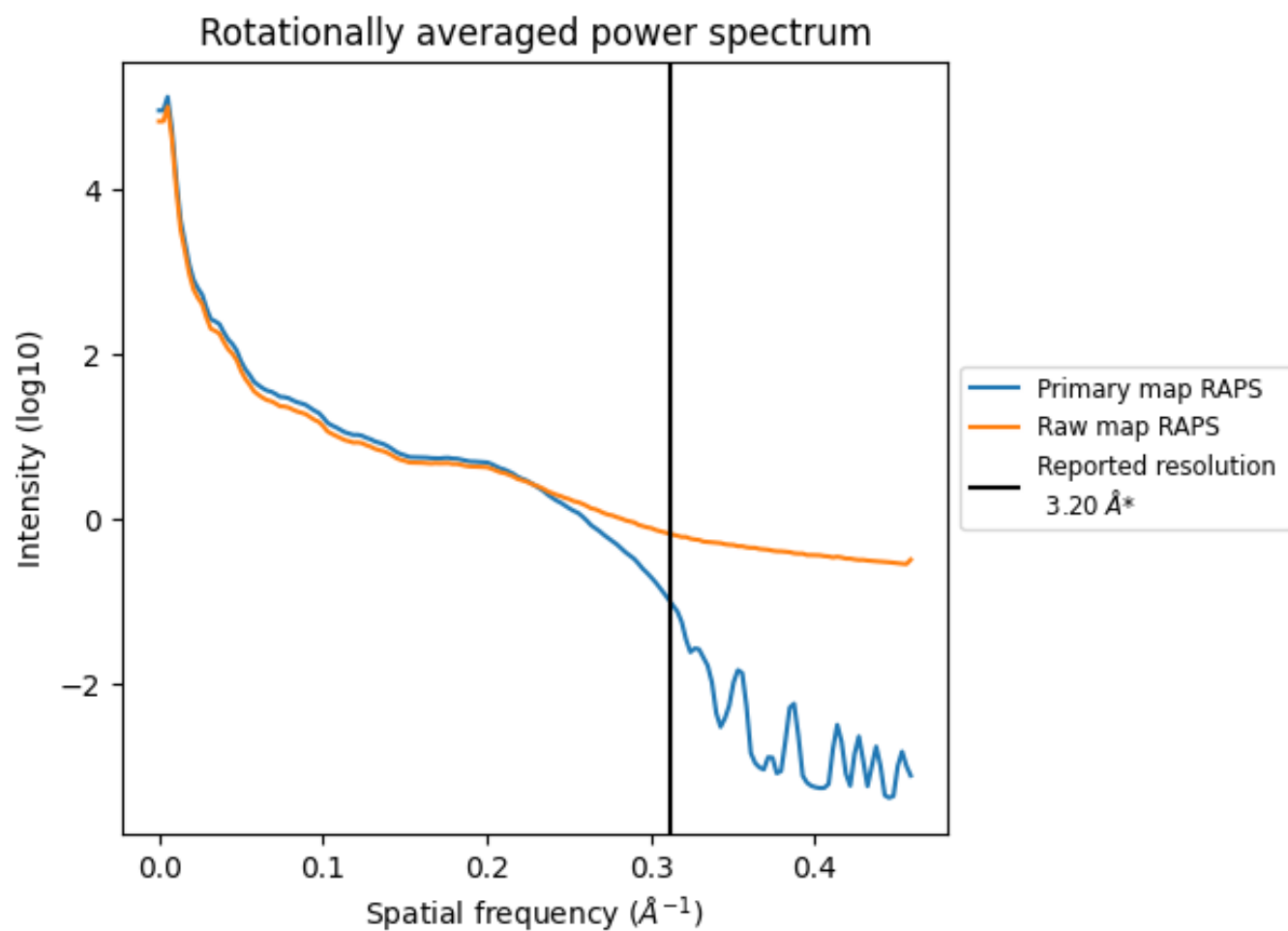
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 519  $\text{nm}^3$ ; this corresponds to an approximate mass of 469 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 ⓘ

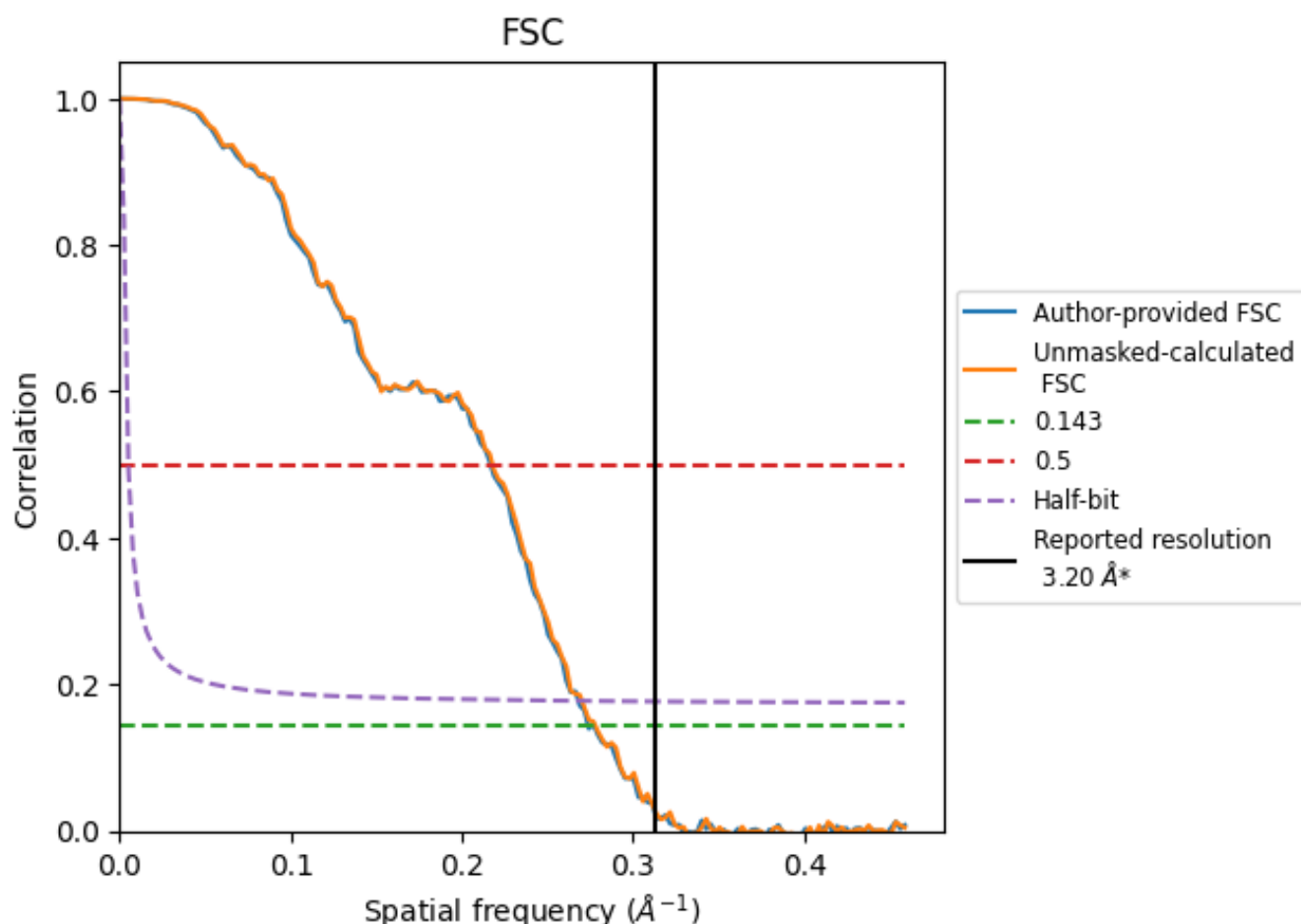


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 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 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.65	4.61	3.73
Unmasked-calculated*	3.60	4.59	3.70

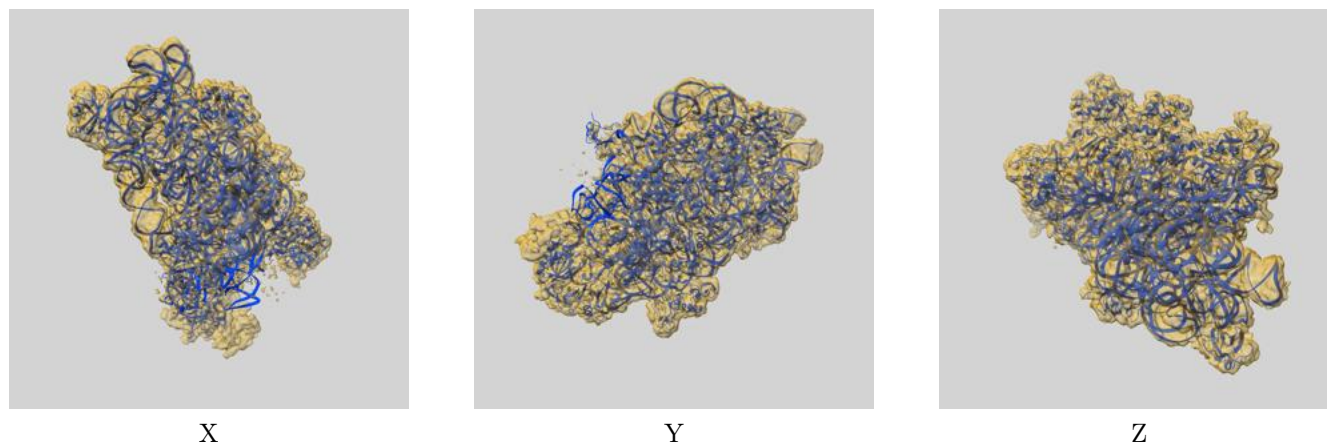
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.65 differs from the reported value 3.2 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.60 differs from the reported value 3.2 by more than 10 %

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

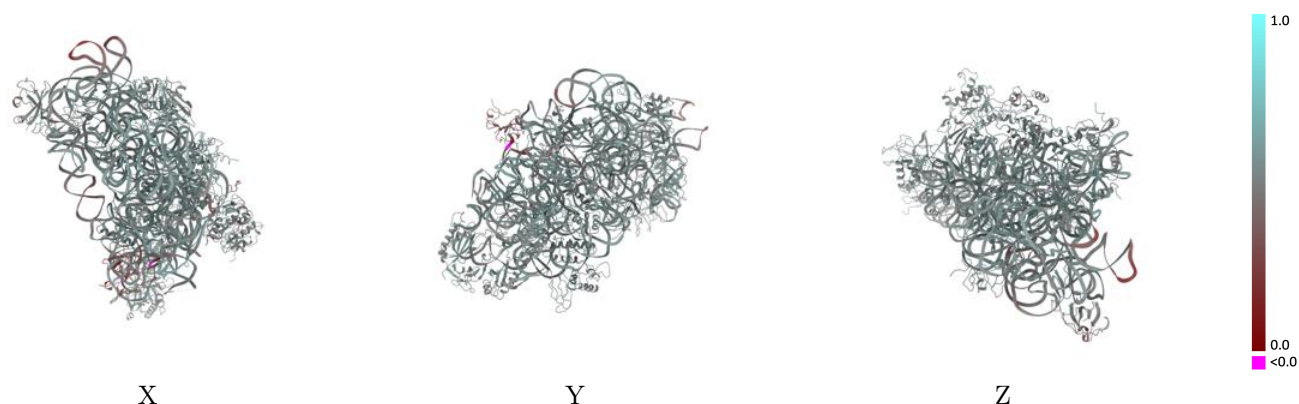
This section contains information regarding the fit between EMDB map EMD-10323 and PDB model 6SWD. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

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



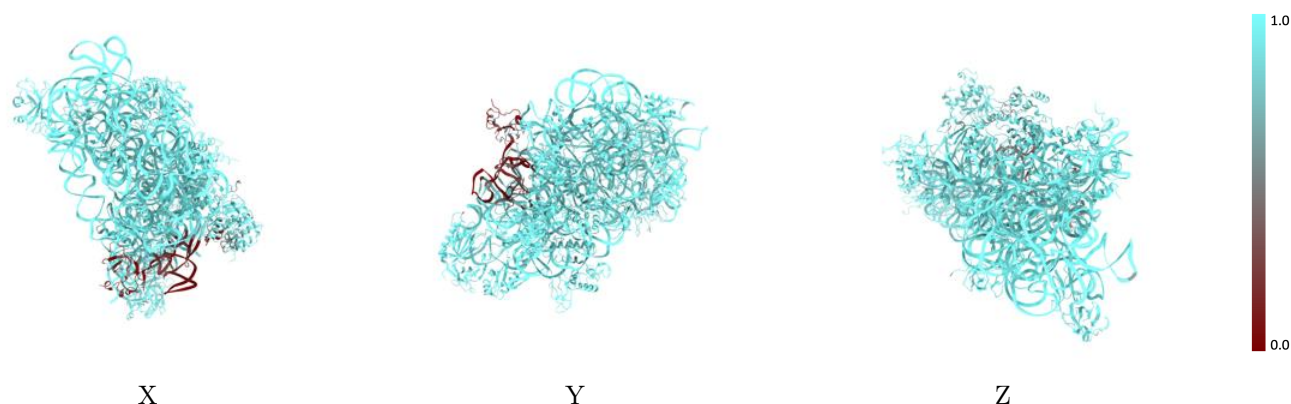
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



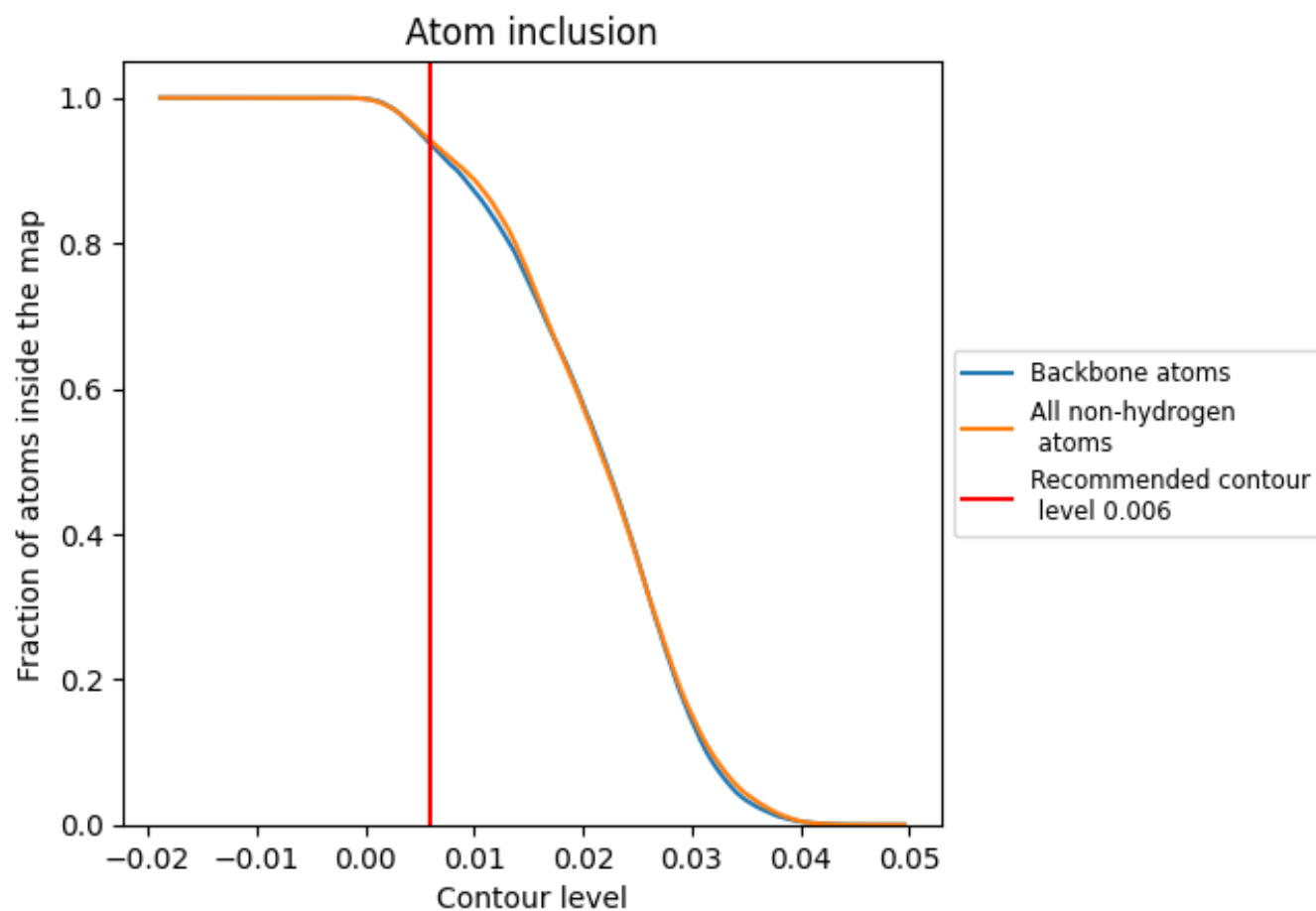
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).









































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9407	 0.5260
0	 0.9465	 0.5410
2	 0.9618	 0.5310
5	 0.6705	 0.4290
6	 0.3066	 0.3220
A	 0.9693	 0.5240
B	 0.8704	 0.5220
C	 0.9175	 0.5140
D	 0.9725	 0.5430
E	 0.9756	 0.5410
F	 0.8799	 0.5310
G	 0.9634	 0.4920
I	 0.9711	 0.5480
J	 0.9697	 0.5350
M	 0.9667	 0.5290
N	 0.9677	 0.5380
Q	 0.9721	 0.5300
R	 0.9713	 0.5460
V	 0.9727	 0.5210
W	 0.9615	 0.5290

