



## wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 07:44 AM EST

PDB ID : 6C66  
EMDB ID : EMD-7347  
Title : CRISPR RNA-guided surveillance complex, pre-nicking  
Authors : Xiao, Y.; Luo, M.; Liao, M.; Ke, A.  
Deposited on : 2018-01-17  
Resolution : 3.66 Å(reported)

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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  
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) : 2.31.2



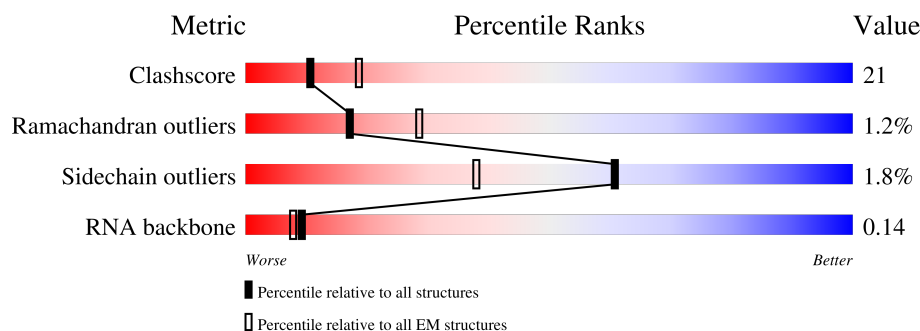
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.66 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


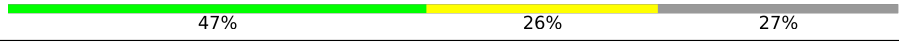
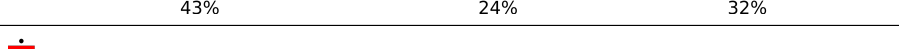
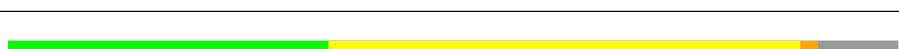

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey 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	G	944	
2	A	549	
3	B	373	
3	C	373	
3	D	373	
3	E	373	
3	F	373	

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Mol	Chain	Length	Quality of chain
3	H	373	
4	I	244	
4	K	244	
5	J	61	
6	L	55	
7	M	254	
8	N	55	
9	O	232	



## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 36255 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CRISPR-associated helicase, Cas3 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	832	Total	C	N	O	S	0	0
			6467	4104	1153	1185	25		

- Molecule 2 is a protein called CRISPR-associated protein, Cse1 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	511	Total	C	N	O	S	0	0
			4053	2573	740	731	9		

- Molecule 3 is a protein called CRISPR-associated protein, Cse4 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	334	Total	C	N	O	S	0	0
			2501	1573	445	478	5		
3	C	367	Total	C	N	O	S	0	0
			2840	1781	509	545	5		
3	D	367	Total	C	N	O	S	0	0
			2835	1779	508	543	5		
3	E	366	Total	C	N	O	S	0	0
			2825	1770	508	542	5		
3	F	366	Total	C	N	O	S	0	0
			2829	1772	508	544	5		
3	H	329	Total	C	N	O	S	0	0
			2553	1603	460	487	3		

- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	177	Total	C	N	O	S	0	0
			1412	887	282	241	2		
4	K	165	Total	C	N	O	S	0	0
			1325	833	264	226	2		



- Molecule 5 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	59	Total	C	N	O	P	0	0
			1267	565	235	409	58		

- Molecule 6 is a DNA chain called Target strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	50	Total	C	N	O	P	0	0
			1012	481	179	302	50		

- Molecule 7 is a protein called CRISPR-associated protein, Cas5e family.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	244	Total	C	N	O	S	0	0
			1916	1215	349	348	4		

- Molecule 8 is a DNA chain called Nontarget strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	38	Total	C	N	O	P	0	0
			766	359	145	224	38		

- Molecule 9 is a protein called CRISPR-associated protein, Cse3 family.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	212	Total	C	N	O	S	0	0
			1652	1028	322	300	2		

- Molecule 10 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
10	G	2	Total	Fe	0
			2	2	



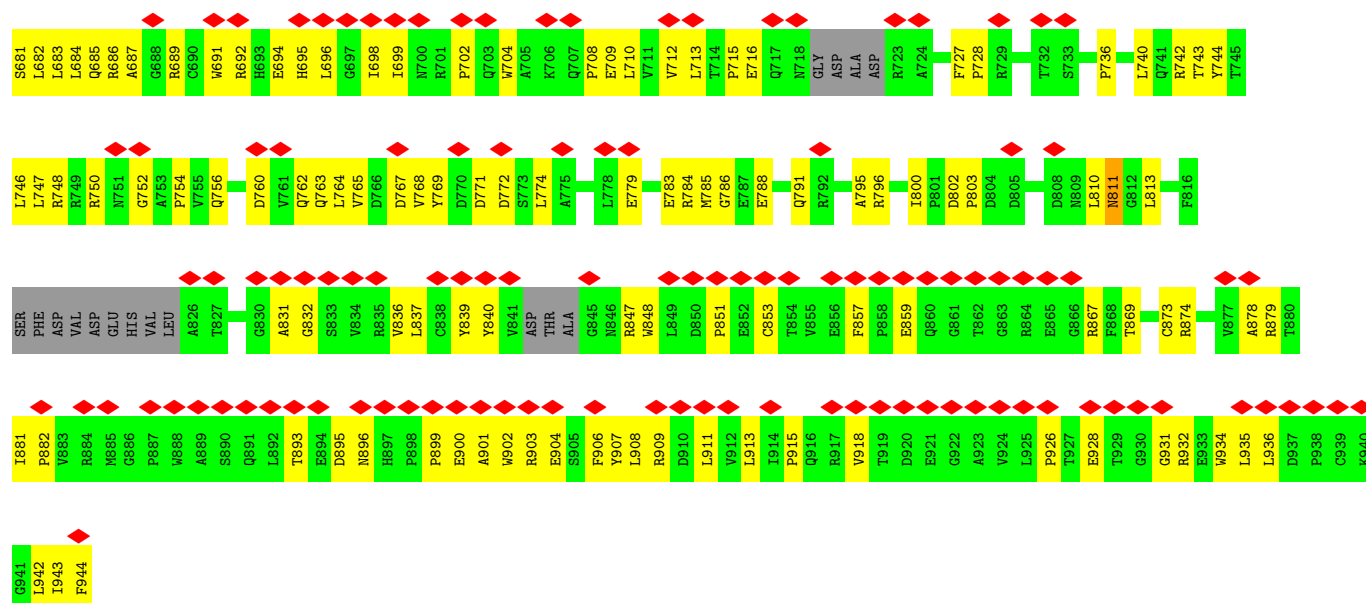
### 3 Residue-property plots

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.

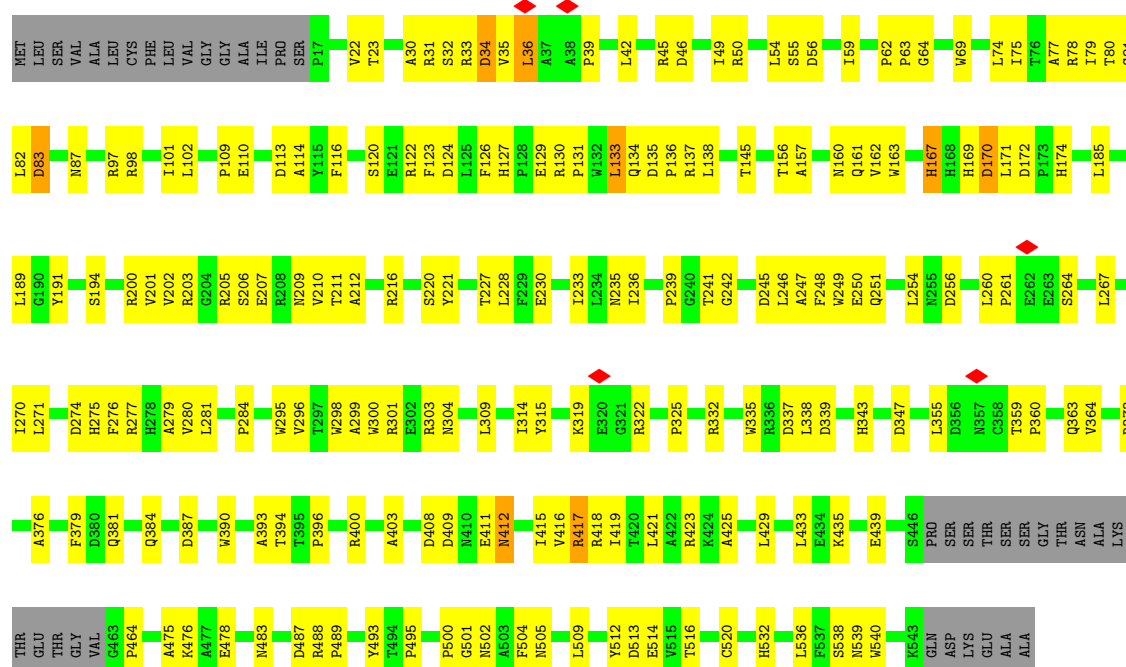
- Molecule 1: CRISPR-associated helicase, Cas3 family



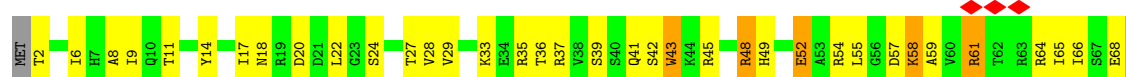
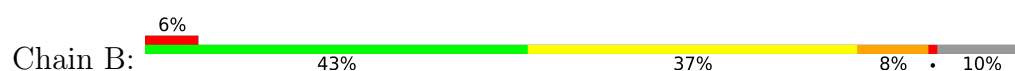




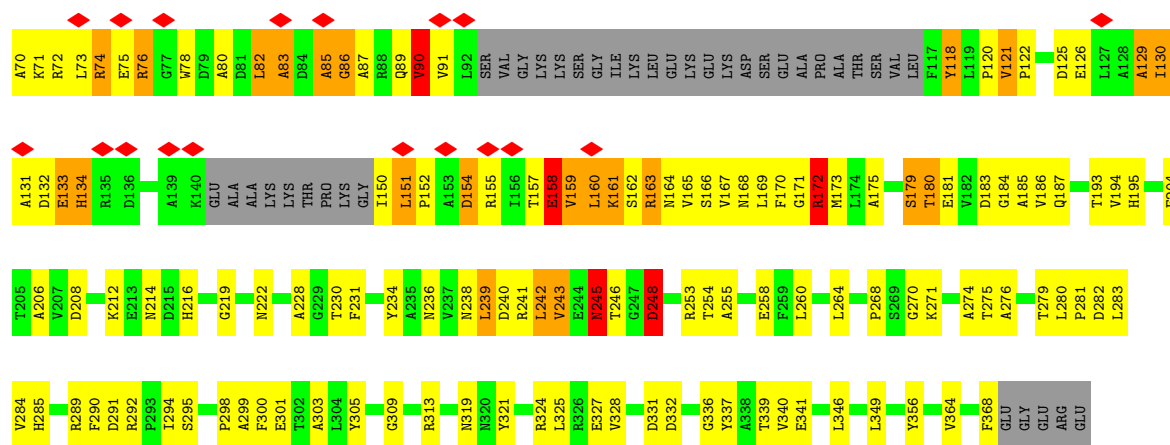
• Molecule 2: CRISPR-associated protein, Cse1 family



• Molecule 3: CRISPR-associated protein, Cse4 family

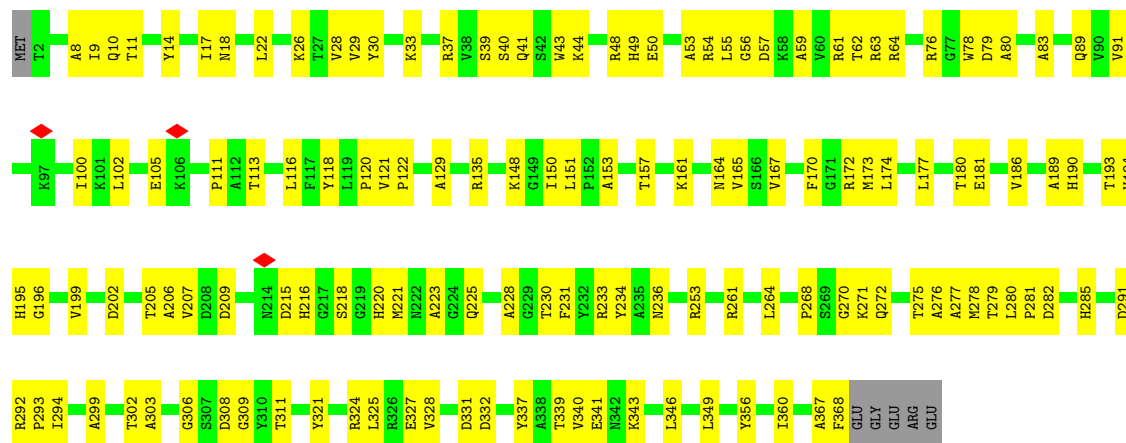






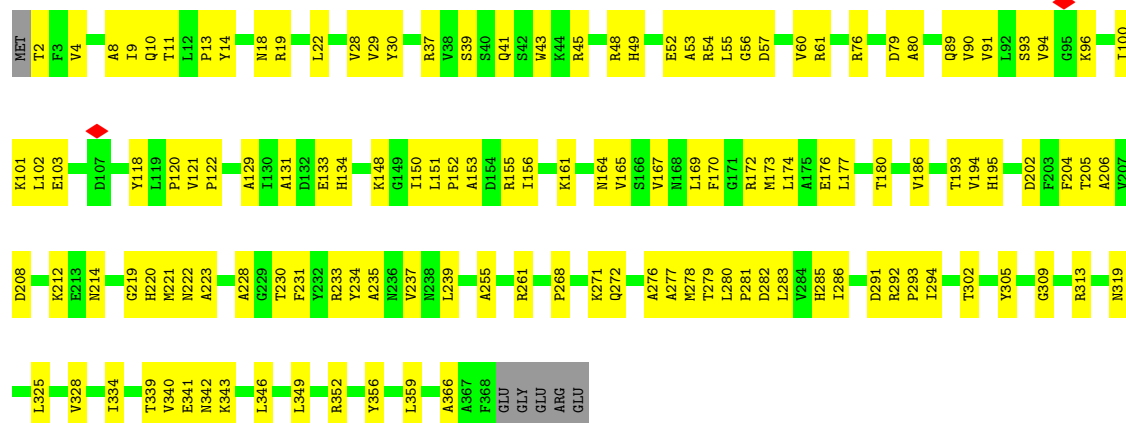
• Molecule 3: CRISPR-associated protein, Cse4 family

Chain C: 61% 37%



• Molecule 3: CRISPR-associated protein, Cse4 family

Chain D: 63% 35%



• Molecule 3: CRISPR-associated protein, Cse4 family



Response	Percentage
Yes, I have used a mobile app to book a flight	65%
No, I have not used a mobile app to book a flight	33%



Response	Percentage
Yes, the U.S. is a threat to my country	60%
No, the U.S. is not a threat to my country	38%



Response	Percentage
Yes	59%
No	29%
Don't know	12%






Chain I:  47%  26%  27%

MET	ASN	ASN	SER	ASP	Y5	I6	L7	A10	V14	A15	A16	V17	S18	K19	L20	I21	V22	R28	R32	L37	A38	P39	E40	D41	F42	R43	M44	R49	V50	V51	Y54	V57	THR	THR	ASP	TYR	ASP	ASP	VAL	ASP	ASP	ARG	ARG	ALA	ALA	SER	LEU	TRP	ASP	V74	V77
F81	Y82	A83	V84	I87	R93	R96	E101	A102	THR	GLU	GLU	GLN	THR	GLY	GLU	PRO	GLN	ASP	SER	GLU	ALA	LEU	THR	GLU	PRO	THR	ALA	GLU	GLU	SER	SER	ALA	THR	LYS	ASP	GLY	LYS	PRO	PRO	R136	R136	L139	A146	M153	S156	Q159	L163				

Chain K:


43% 24% 32%

Position	Amino Acid	Information Content (bits)
1	ALA	0.1
2	GLU	0.1
3	ALA	0.1
4	ALA	0.1
5	VI47	0.1
6	K150	0.1
7	G151	0.1
8	L152	0.1
9	Q159	0.1
10	R160	0.1
11	A165	0.1
12	R166	0.1
13	Q167	0.1
14	R168	0.1
15	L169	0.1
16	V172	0.1
17	H175	0.1
18	L176	0.1
19	L179	0.1
20	Y182	0.1
21	L183	0.1
22	R184	0.1
23	S185	0.1
24	D186	0.1
25	Q187	0.1
26	V188	0.1
27	H189	0.1
28	I190	0.1
29	D191	0.1
30	W192	0.1
31	G193	0.1
32	I194	0.1
33	L195	0.1
34	I196	0.1
35	R197	0.1
36	W202	0.1
37	A210	0.1
38	R211	0.1
39	E212	0.1
40	Q215	0.1
41	D216	0.1
42	E229	0.1
43	GLN	0.1
44	LYS	0.1
45	ASN	0.1
46	LYS	0.1
47	ASN	0.1
48	THR	0.1
49	THR	0.1
50	GLU	0.1
51	GLU	0.1
52	TRP	0.1
53	ASP	0.1
54	ASP	0.1
55	ASP	0.1
56	ASP	0.1
57	ASP	0.1
58	ARG	0.1
59	R136	0.1
60	P137	0.1
61	V141	0.1
62	LEU	0.1
63	TRP	0.1
64	ASP	0.1
65	W74	0.1
66	H75	0.1
67	A76	0.1
68	Y82	0.1
69	A83	0.1
70	H84	0.1
71	A90	0.1
72	R93	0.1
73	R96	0.1
74	P97	0.1
75	Q98	0.1
76	GLU	0.1
77	ALA	0.1
78	GLU	0.1
79	ALA	0.1
80	THR	0.1
81	GLU	0.1
82	GLN	0.1
83	THR	0.1
84	GLY	0.1
85	GLU	0.1
86	PRO	0.1
87	GLN	0.1
88	ASP	0.1
89	SER	0.1
90	GLU	0.1
91	ALA	0.1
92	LEU	0.1
93	THR	0.1
94	GLU	0.1
95	PRO	0.1
96	THR	0.1
97	PRO	0.1
98	ALA	0.1
99	GLU	0.1
100	GLU	0.1

Chain J: 

Label	Color
A1	Green
U2	Yellow
G3	Yellow
G4	Orange
A5	Yellow
C6	Yellow
C7	Orange
G8	Orange
C9	Yellow
C10	Yellow
A11	Yellow
G12	Green
U13	Yellow
G14	Green
A15	Yellow
U16	Green
A17	Yellow
A18	Yellow
G19	Red
U20	Green
G21	Yellow
G22	Yellow
A23	Green
A24	Yellow
U25	Yellow
G26	Yellow
C27	Orange
C28	Yellow
A29	Yellow
U30	Yellow
G31	Yellow
U32	Yellow
G33	Yellow
G34	Green
G35	Yellow
C36	Yellow
U37	Yellow
G38	Yellow
U39	Yellow
G40	Green
G	Grey
U	Grey
G43	Yellow
A44	Yellow
G45	Yellow
C46	Yellow
C47	Yellow
C48	Yellow
C49	Yellow
A50	Yellow
C51	Orange
G52	Yellow
C53	Green
A54	Orange
G55	Red
G56	Yellow
U57	Yellow
G58	Yellow
G59	Yellow
G60	Yellow

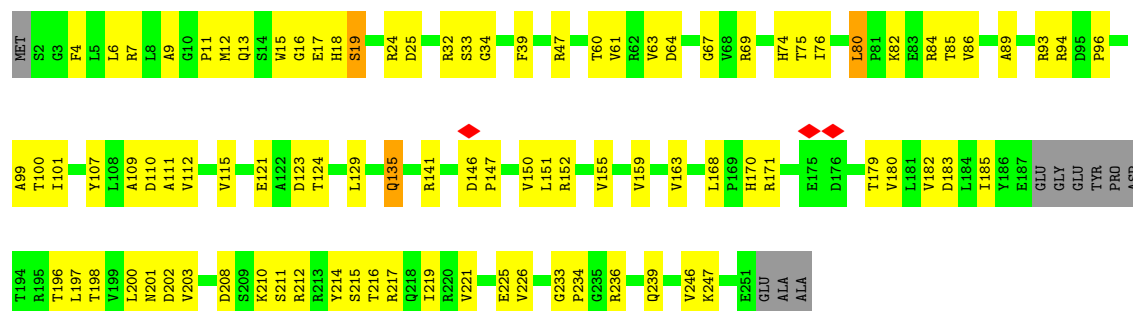
G61

Chain L: 

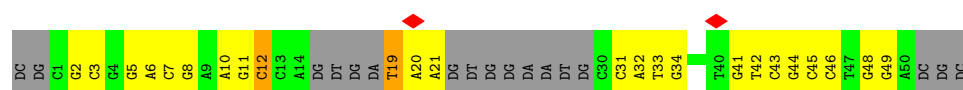
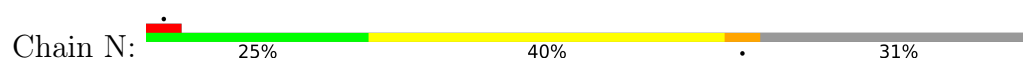
Component	Category
DG	Green
DC	Green
DG	Green
T16	Green
A19	Green
G20	Green
G21	Green
G22	Green
G23	Green
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C25	Green
A26	Green
G27	Green
C30	Green
A31	Green
C32	Green
A33	Green
A38	Green
T39	Yellow
T40	Yellow
C41	Yellow
C44	Yellow
T45	Yellow
T46	Yellow
A50	Yellow
C51	Yellow
G54	Yellow
C55	Yellow
T56	Yellow
T57	Yellow
C58	Yellow
G59	Yellow
T60	Yellow
C61	Yellow
C62	Yellow
G65	Yellow
DC	Grey
DG	Grey

Chain M:  59% 35% ..

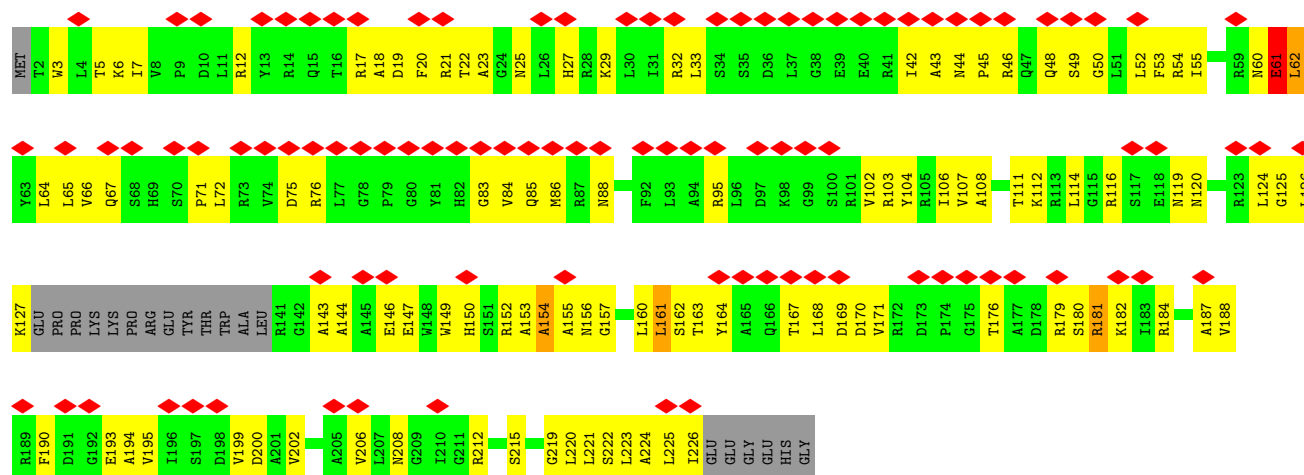
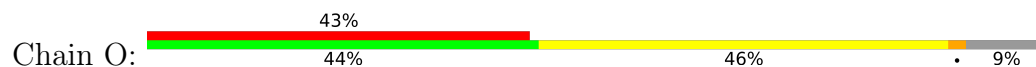




• Molecule 8: Nontarget strand



• Molecule 9: CRISPR-associated protein, Cse3 family





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51889	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.212	Depositor
Minimum map value	-0.102	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	317.44, 317.44, 317.44	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE

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	G	0.30	0/6620	0.57	1/9016 (0.0%)
2	A	0.41	0/4175	0.66	2/5705 (0.0%)
3	B	0.44	0/2551	0.66	1/3476 (0.0%)
3	C	0.44	0/2894	0.60	0/3927
3	D	0.45	0/2889	0.60	0/3920
3	E	0.46	0/2878	0.59	0/3906
3	F	0.45	0/2882	0.59	0/3911
3	H	0.39	0/2598	0.57	0/3524
4	I	0.47	0/1441	0.63	0/1957
4	K	0.40	0/1351	0.60	0/1832
5	J	0.73	0/1417	1.30	15/2208 (0.7%)
6	L	0.91	0/1131	1.00	1/1740 (0.1%)
7	M	0.46	0/1959	0.65	0/2665
8	N	0.70	0/857	0.97	2/1317 (0.2%)
9	O	0.30	0/1680	0.73	1/2270 (0.0%)
All	All	0.46	0/37323	0.69	23/51374 (0.0%)

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	46	C	O4'-C1'-N1	8.73	115.18	108.20
5	J	55	C	N3-C2-O2	-7.97	116.32	121.90
5	J	55	C	C2-N1-C1'	7.58	127.14	118.80
5	J	55	C	N1-C2-O2	7.38	123.33	118.90
5	J	55	C	C6-N1-C2	-7.27	117.39	120.30

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	G	6467	0	6433	318	0
2	A	4053	0	3928	168	0
3	B	2501	0	2352	160	0
3	C	2840	0	2809	123	0
3	D	2835	0	2800	119	0
3	E	2825	0	2796	106	0
3	F	2829	0	2800	117	0
3	H	2553	0	2550	99	0
4	I	1412	0	1427	60	0
4	K	1325	0	1339	46	0
5	J	1267	0	642	87	0
6	L	1012	0	562	39	0
7	M	1916	0	1941	90	0
8	N	766	0	415	24	0
9	O	1652	0	1647	112	0
10	G	2	0	0	0	0
All	All	36255	0	34441	1474	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 21.

The worst 5 of 1474 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)
9:O:167:THR:HB	9:O:168:LEU:HB2	1.46	0.98
5:J:61:G:H2'	9:O:180:SER:HB2	1.45	0.97
5:J:49:C:H2'	5:J:50:A:H8	1.32	0.95
4:K:84:VAL:HG11	4:K:196:ILE:HG12	1.50	0.93
9:O:171:VAL:O	9:O:182:LYS:HA	1.69	0.91

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	
1	G	814/944 (86%)	764 (94%)	43 (5%)	7 (1%)	17	54
2	A	507/549 (92%)	457 (90%)	47 (9%)	3 (1%)	25	62
3	B	328/373 (88%)	243 (74%)	59 (18%)	26 (8%)	1	12
3	C	365/373 (98%)	346 (95%)	18 (5%)	1 (0%)	41	74
3	D	365/373 (98%)	345 (94%)	19 (5%)	1 (0%)	41	74
3	E	364/373 (98%)	337 (93%)	23 (6%)	4 (1%)	14	51
3	F	364/373 (98%)	342 (94%)	21 (6%)	1 (0%)	41	74
3	H	323/373 (87%)	300 (93%)	23 (7%)	0	100	100
4	I	171/244 (70%)	165 (96%)	6 (4%)	0	100	100
4	K	157/244 (64%)	153 (98%)	4 (2%)	0	100	100
7	M	240/254 (94%)	225 (94%)	15 (6%)	0	100	100
9	O	208/232 (90%)	180 (86%)	22 (11%)	6 (3%)	4	32
All	All	4206/4705 (89%)	3857 (92%)	300 (7%)	49 (1%)	17	49

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	221	GLU
1	G	223	PHE
1	G	224	LEU
3	B	70	ALA
3	B	72	ARG

### 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	
1	G	684/779 (88%)	669 (98%)	15 (2%)	52	72
2	A	416/452 (92%)	410 (99%)	6 (1%)	67	82
3	B	241/299 (81%)	212 (88%)	29 (12%)	5	24
3	C	294/299 (98%)	294 (100%)	0	100	100
3	D	292/299 (98%)	292 (100%)	0	100	100
3	E	292/299 (98%)	290 (99%)	2 (1%)	84	91
3	F	293/299 (98%)	292 (100%)	1 (0%)	92	96
3	H	265/299 (89%)	265 (100%)	0	100	100
4	I	142/200 (71%)	141 (99%)	1 (1%)	84	91
4	K	135/200 (68%)	134 (99%)	1 (1%)	84	91
7	M	204/211 (97%)	200 (98%)	4 (2%)	55	74
9	O	168/193 (87%)	166 (99%)	2 (1%)	71	84
All	All	3426/3829 (90%)	3365 (98%)	61 (2%)	61	77

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	65	ILE
7	M	19	SER
3	B	154	ASP
4	K	15	LYS
9	O	61	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	18	ASN
4	K	8	GLN
3	D	134	HIS
4	I	218	HIS
7	M	135	GLN

### 5.3.3 RNA



Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	J	57/61 (93%)	28 (49%)	0

5 of 28 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	J	4	G
5	J	7	C
5	J	8	G
5	J	9	C
5	J	10	C

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



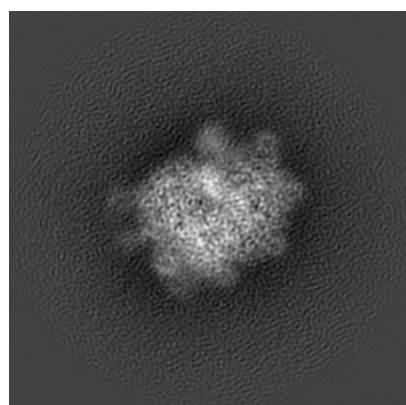
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7347. These allow visual inspection of the internal detail of the map and identification of artifacts.

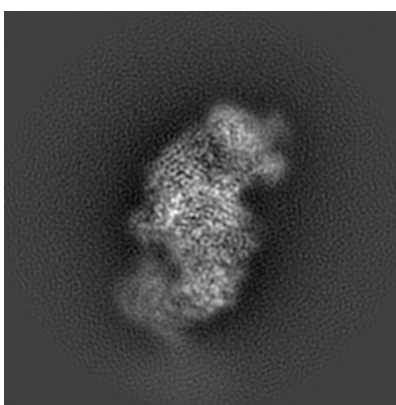
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

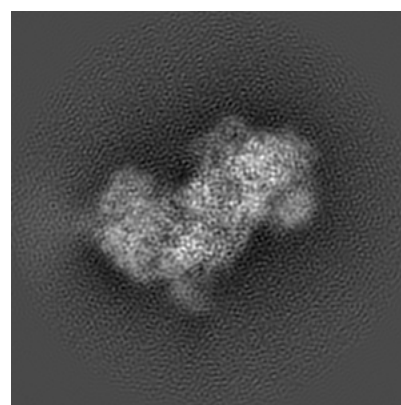
#### 6.1.1 Primary map



X



Y

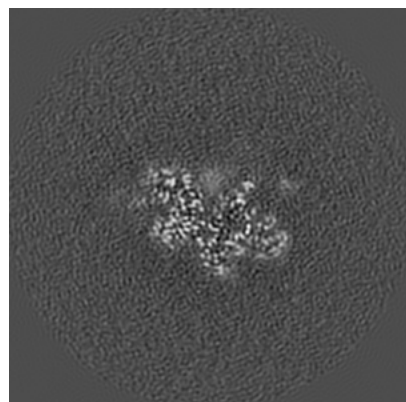


Z

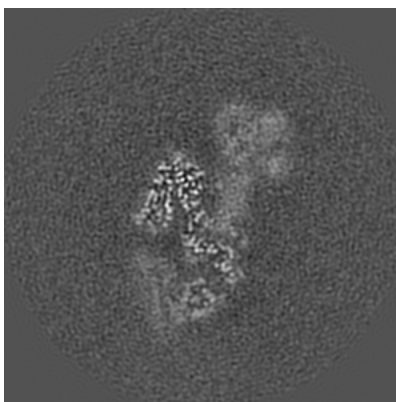
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

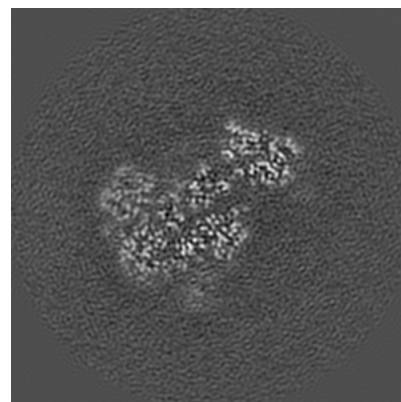
#### 6.2.1 Primary map



X Index: 128



Y Index: 128



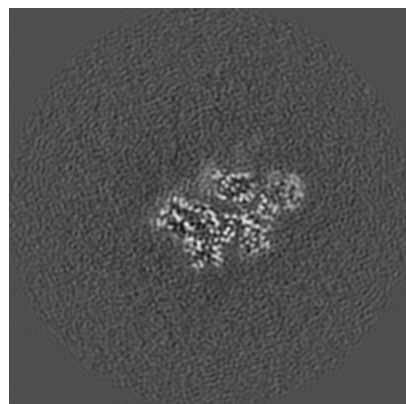
Z Index: 128



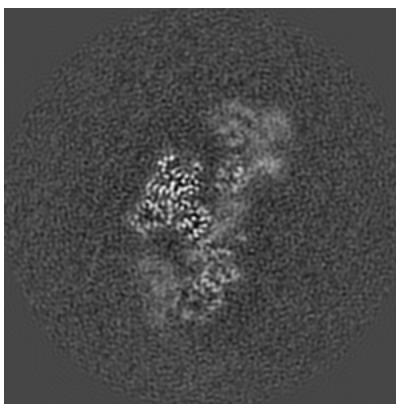
The images above show central slices of the map in three orthogonal directions.

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

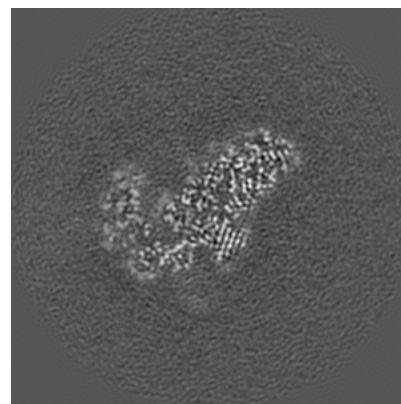
### 6.3.1 Primary map



X Index: 141



Y Index: 132



Z Index: 122

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

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

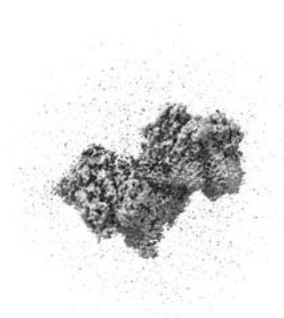
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



## 6.5 Mask visualisation

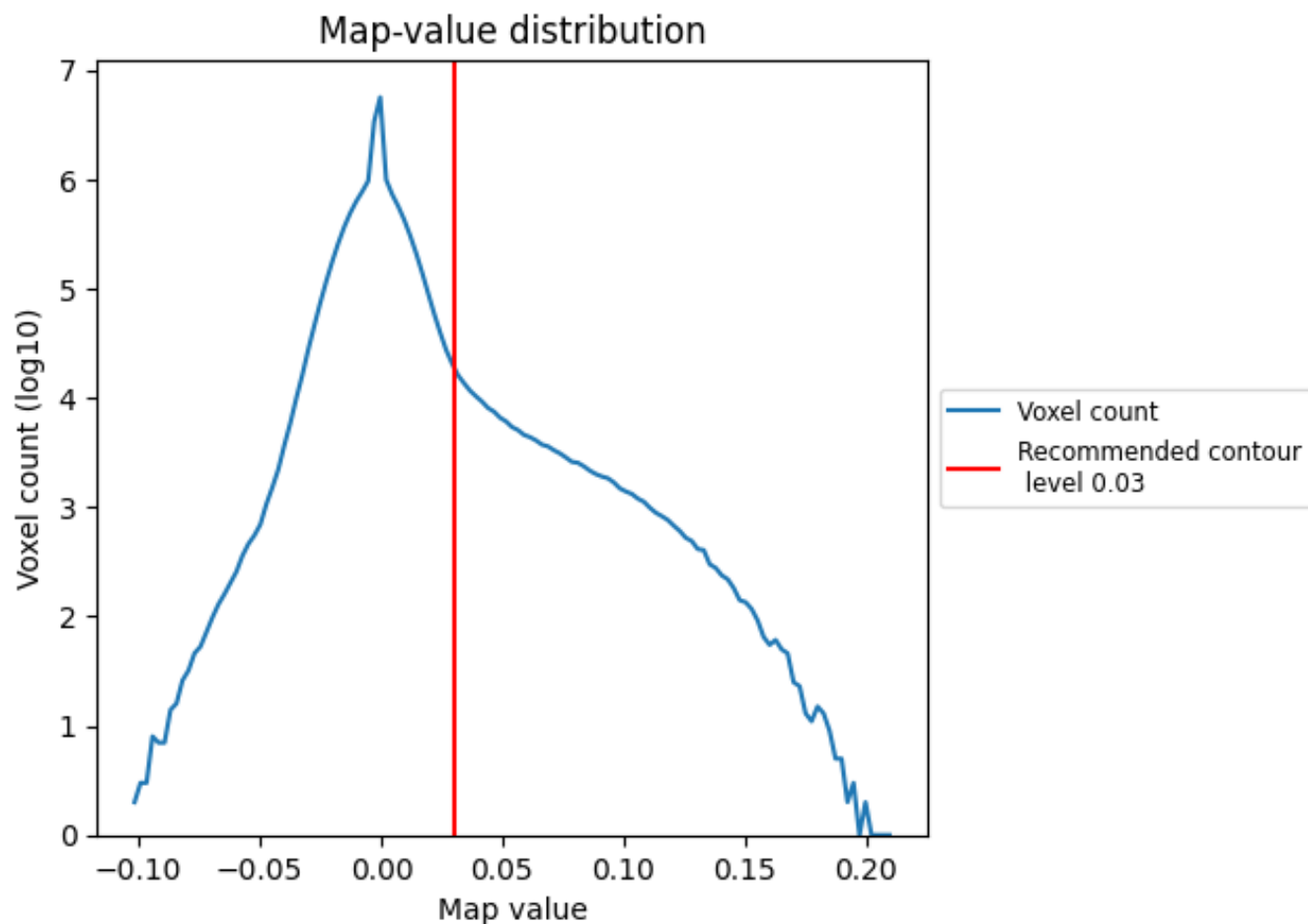
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

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

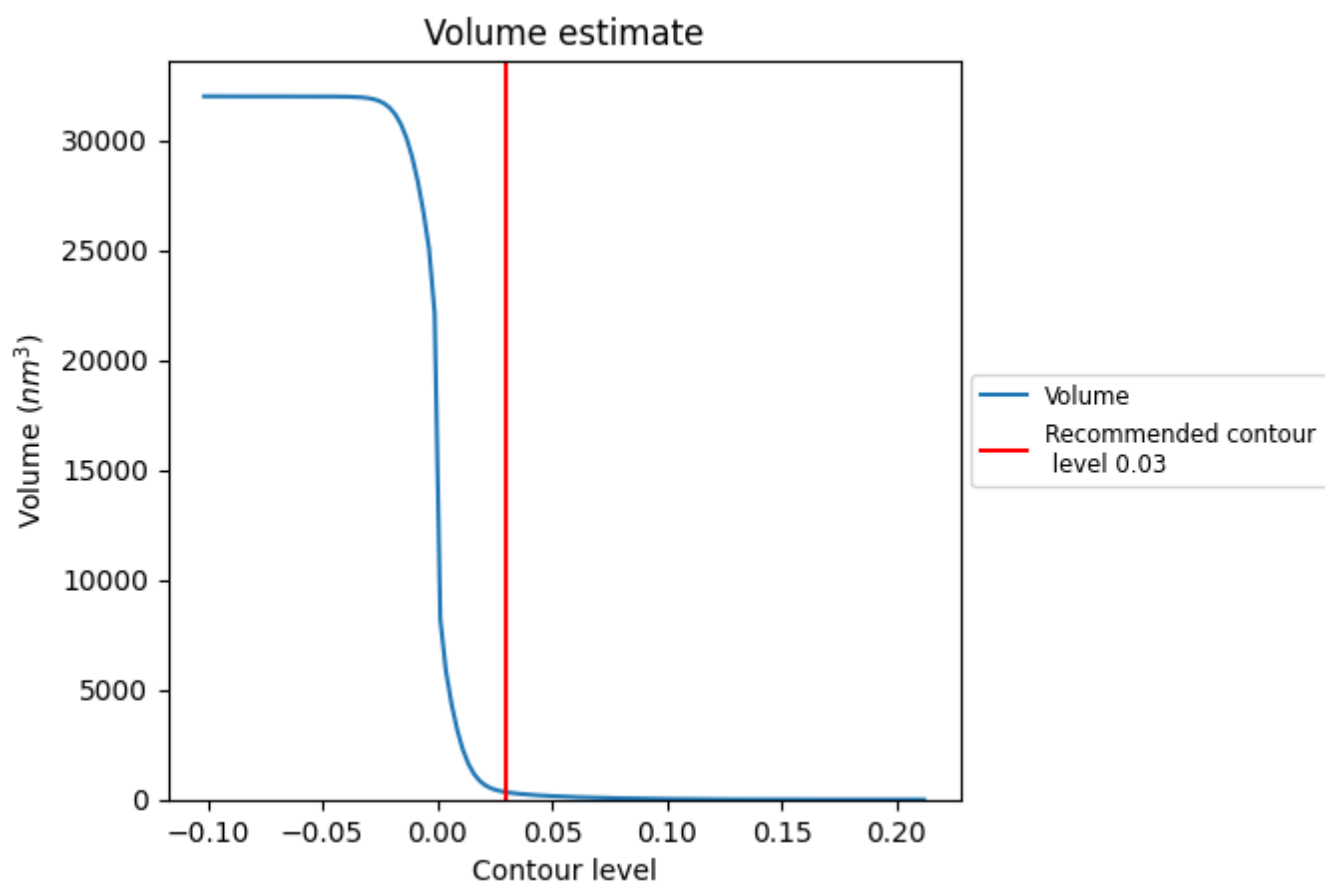
### 7.1 Map-value distribution [i](#)



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



## 7.2 Volume estimate [i](#)

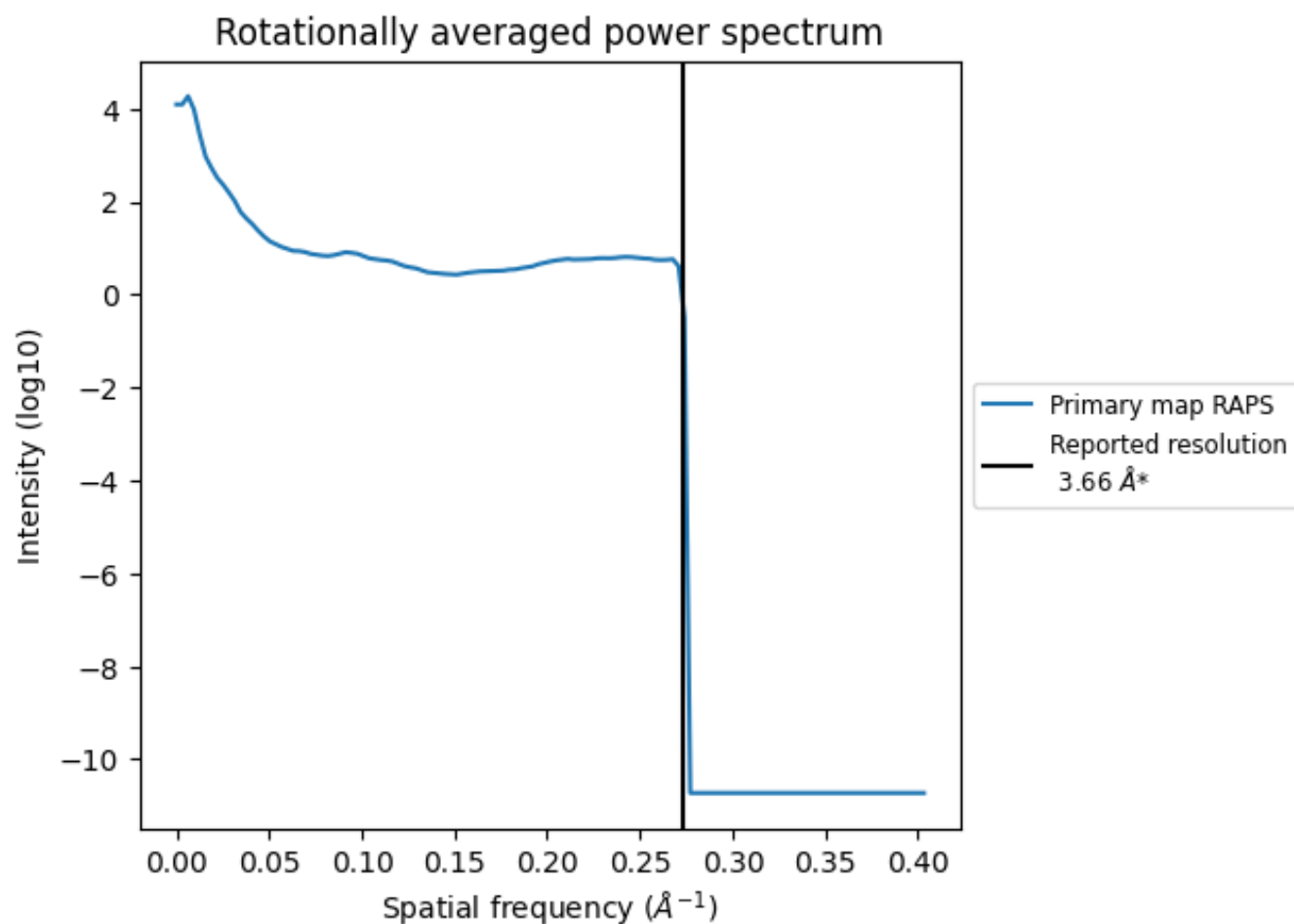


The volume at the recommended contour level is 336 nm<sup>3</sup>; this corresponds to an approximate mass of 304 kDa.

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 0.273  $\text{\AA}^{-1}$



## 8 Fourier-Shell correlation

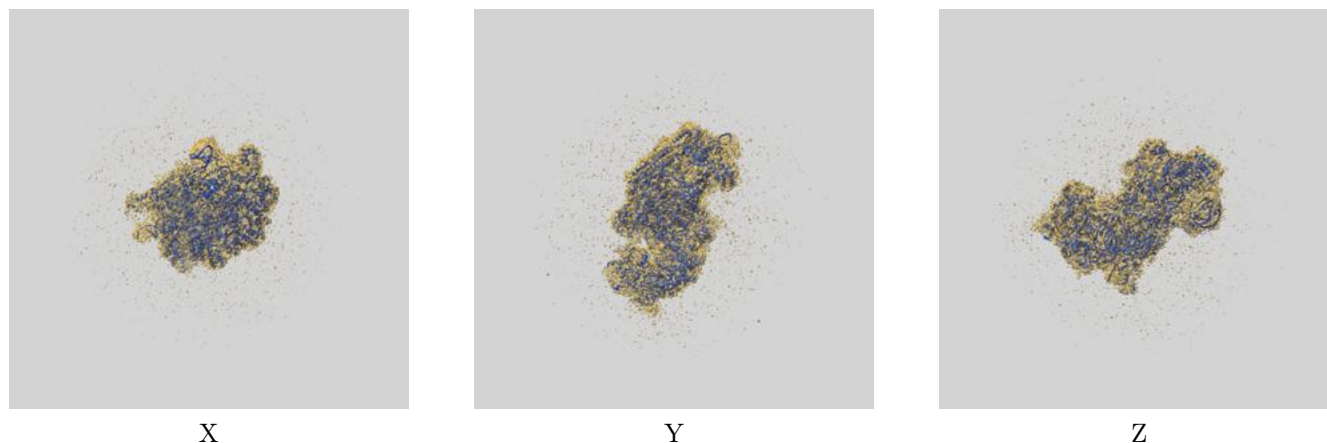
This section was not generated. No FSC curve or half-maps provided.



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

This section contains information regarding the fit between EMDB map EMD-7347 and PDB model 6C66. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

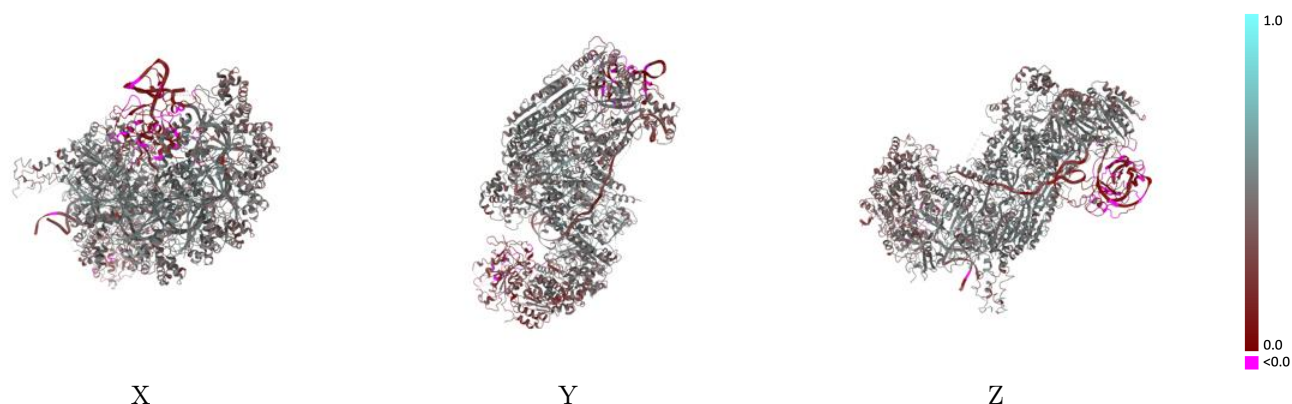
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

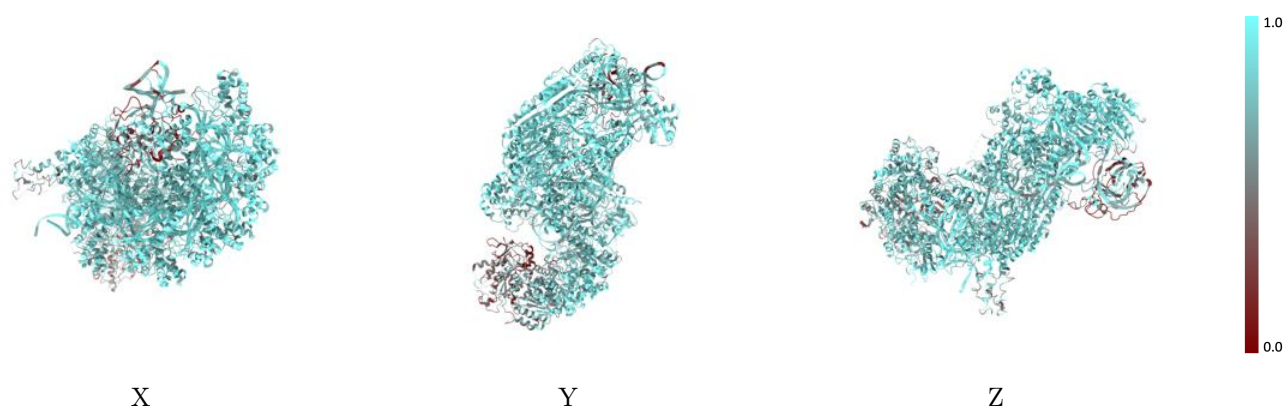


## 9.2 Q-score mapped to coordinate model [i](#)



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.

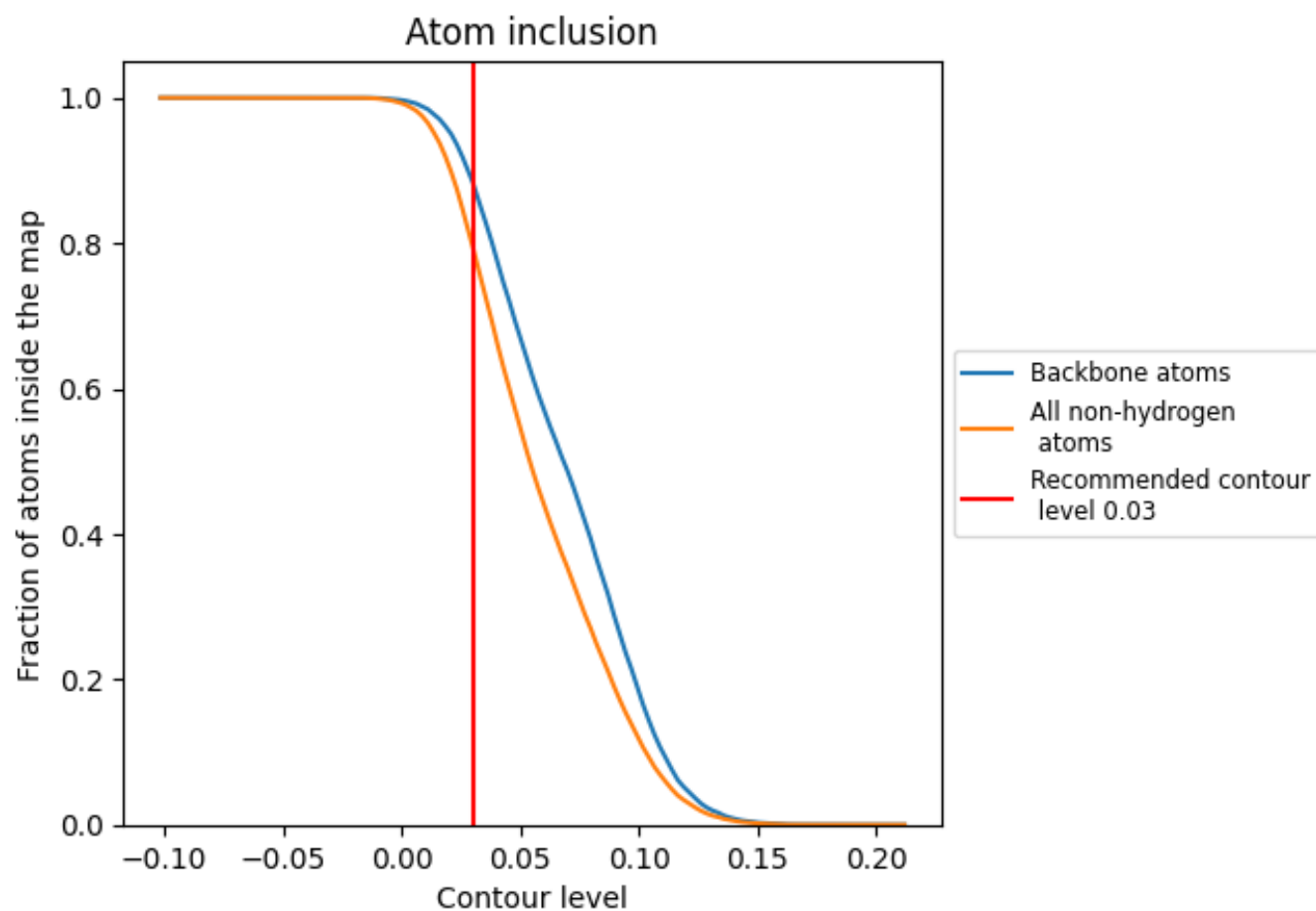
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.03).



## 9.4 Atom inclusion [i](#)



































At the recommended contour level, 88% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7954	 0.4110
A	 0.8523	 0.4530
B	 0.8147	 0.4670
C	 0.8780	 0.4570
D	 0.8731	 0.4690
E	 0.8748	 0.4760
F	 0.8572	 0.4740
G	 0.5967	 0.3130
H	 0.8498	 0.4220
I	 0.8824	 0.4780
J	 0.8532	 0.3670
K	 0.8818	 0.4730
L	 0.9308	 0.4110
M	 0.8709	 0.4740
N	 0.7872	 0.2520
O	 0.4470	 0.1120

