



## Full wwPDB EM Validation Report ⓘ

May 18, 2024 – 10:42 AM EDT

PDB ID : 7JSE  
EMDB ID : EMD-22451  
Title : Adeno-Associated Virus Origin Binding Domain in complex with ssDNA  
Authors : Escalante, C.R.  
Deposited on : 2020-08-14  
Resolution : 4.60 Å (reported)  
Based on initial model : 5BYG

This is a Full wwPDB EM Validation 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.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

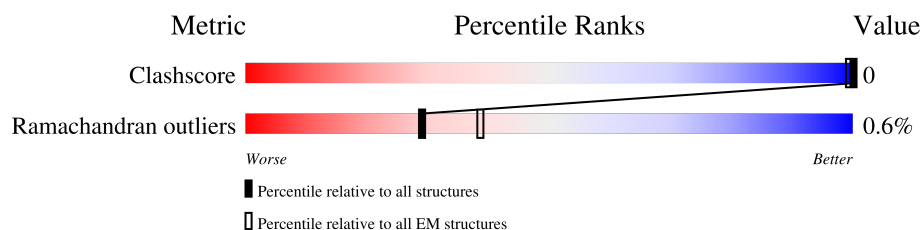
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*








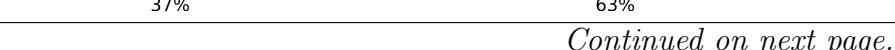

The reported resolution of this entry is 4.60 Å.

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	158937	4297
Ramachandran outliers	154571	4023

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	A	537	 37% 63%
1	B	537	 36% 63%
1	C	537	 37% 63%
1	D	537	 37% 63%
1	E	537	 37% 63%
1	F	537	 37% 63%
1	G	537	 37% 63%
1	H	537	 37% 63%
1	I	537	 37% 63%

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Mol	Chain	Length	Quality of chain
1	J	537	
1	K	537	
1	L	537	
1	M	537	
1	N	537	
1	O	537	
1	P	537	
2	Q	4	
2	R	4	
2	S	4	
2	T	4	
2	U	4	
2	V	4	
2	W	4	
2	X	4	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13288 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 Protein Rep68.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	198	Total 792	C 396	N 198	O 198	0	0
1	B	198	Total 792	C 396	N 198	O 198	0	0
1	C	198	Total 792	C 396	N 198	O 198	0	0
1	D	198	Total 792	C 396	N 198	O 198	0	0
1	E	198	Total 792	C 396	N 198	O 198	0	0
1	F	198	Total 792	C 396	N 198	O 198	0	0
1	G	198	Total 792	C 396	N 198	O 198	0	0
1	H	198	Total 792	C 396	N 198	O 198	0	0
1	I	198	Total 792	C 396	N 198	O 198	0	0
1	J	198	Total 792	C 396	N 198	O 198	0	0
1	K	198	Total 792	C 396	N 198	O 198	0	0
1	L	198	Total 792	C 396	N 198	O 198	0	0
1	M	198	Total 792	C 396	N 198	O 198	0	0
1	N	198	Total 792	C 396	N 198	O 198	0	0
1	O	198	Total 792	C 396	N 198	O 198	0	0
1	P	198	Total 792	C 396	N 198	O 198	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P03132
A	17	GLU	GLY	conflict	UNP P03132
A	151	SER	CYS	engineered mutation	UNP P03132
B	0	GLY	-	expression tag	UNP P03132
B	17	GLU	GLY	conflict	UNP P03132
B	151	SER	CYS	engineered mutation	UNP P03132
C	0	GLY	-	expression tag	UNP P03132
C	17	GLU	GLY	conflict	UNP P03132
C	151	SER	CYS	engineered mutation	UNP P03132
D	0	GLY	-	expression tag	UNP P03132
D	17	GLU	GLY	conflict	UNP P03132
D	151	SER	CYS	engineered mutation	UNP P03132
E	0	GLY	-	expression tag	UNP P03132
E	17	GLU	GLY	conflict	UNP P03132
E	151	SER	CYS	engineered mutation	UNP P03132
F	0	GLY	-	expression tag	UNP P03132
F	17	GLU	GLY	conflict	UNP P03132
F	151	SER	CYS	engineered mutation	UNP P03132
G	0	GLY	-	expression tag	UNP P03132
G	17	GLU	GLY	conflict	UNP P03132
G	151	SER	CYS	engineered mutation	UNP P03132
H	0	GLY	-	expression tag	UNP P03132
H	17	GLU	GLY	conflict	UNP P03132
H	151	SER	CYS	engineered mutation	UNP P03132
I	0	GLY	-	expression tag	UNP P03132
I	17	GLU	GLY	conflict	UNP P03132
I	151	SER	CYS	engineered mutation	UNP P03132
J	0	GLY	-	expression tag	UNP P03132
J	17	GLU	GLY	conflict	UNP P03132
J	151	SER	CYS	engineered mutation	UNP P03132
K	0	GLY	-	expression tag	UNP P03132
K	17	GLU	GLY	conflict	UNP P03132
K	151	SER	CYS	engineered mutation	UNP P03132
L	0	GLY	-	expression tag	UNP P03132
L	17	GLU	GLY	conflict	UNP P03132
L	151	SER	CYS	engineered mutation	UNP P03132
M	0	GLY	-	expression tag	UNP P03132
M	17	GLU	GLY	conflict	UNP P03132
M	151	SER	CYS	engineered mutation	UNP P03132
N	0	GLY	-	expression tag	UNP P03132
N	17	GLU	GLY	conflict	UNP P03132
N	151	SER	CYS	engineered mutation	UNP P03132
O	0	GLY	-	expression tag	UNP P03132

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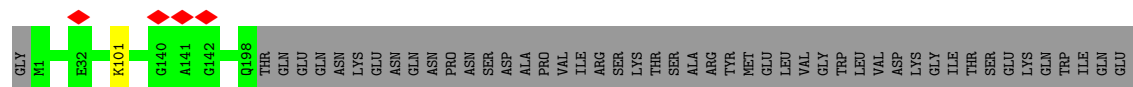
Chain	Residue	Modelled	Actual	Comment	Reference
O	17	GLU	GLY	conflict	UNP P03132
O	151	SER	CYS	engineered mutation	UNP P03132
P	0	GLY	-	expression tag	UNP P03132
P	17	GLU	GLY	conflict	UNP P03132
P	151	SER	CYS	engineered mutation	UNP P03132

- Molecule 2 is a DNA chain called DNA (5'-D(\*TP\*TP\*TP\*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Q	4	Total	C	N	O	P	0	0
			77	40	8	26	3		
2	R	4	Total	C	N	O	P	0	0
			77	40	8	26	3		
2	S	4	Total	C	N	O	P	0	0
			77	40	8	26	3		
2	T	4	Total	C	N	O	P	0	0
			77	40	8	26	3		
2	U	4	Total	C	N	O	P	0	0
			77	40	8	26	3		
2	V	4	Total	C	N	O	P	0	0
			77	40	8	26	3		
2	W	4	Total	C	N	O	P	0	0
			77	40	8	26	3		
2	X	4	Total	C	N	O	P	0	0
			77	40	8	26	3		



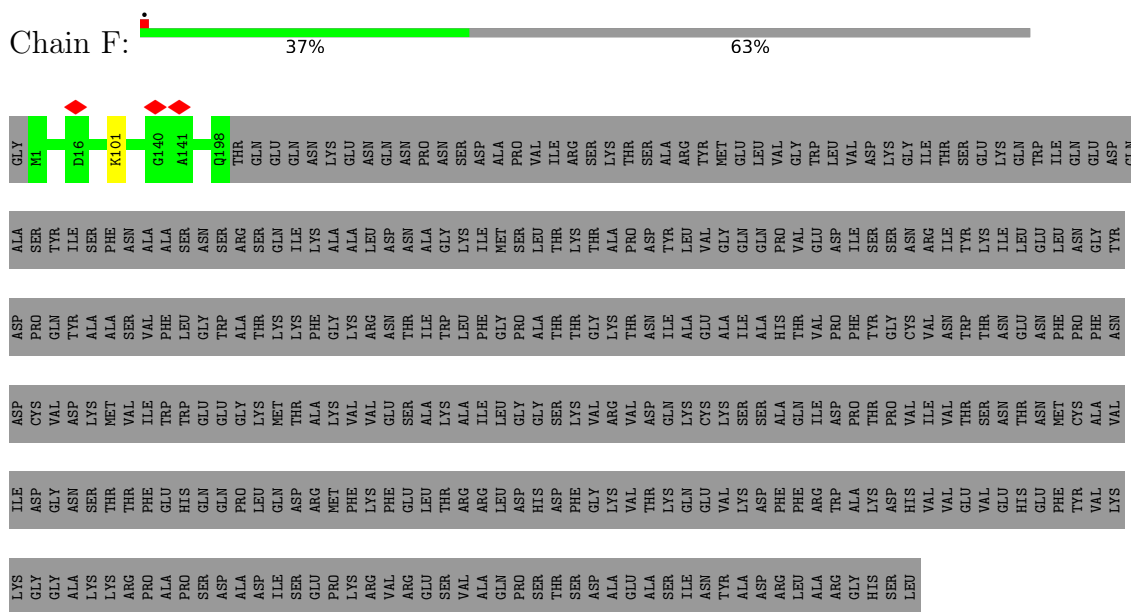
Chain C:  37% 63%



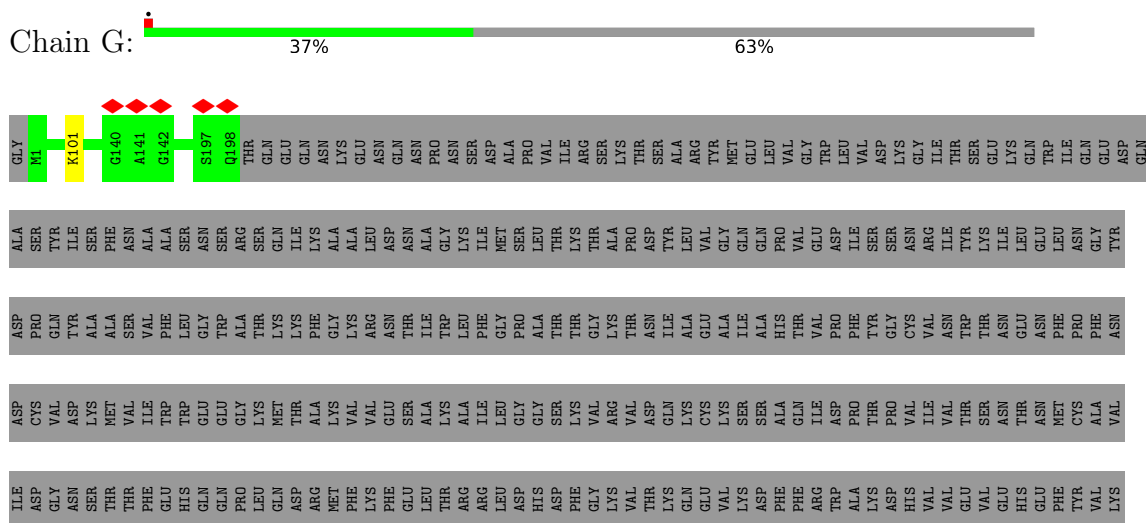


LYS	VAL	ASN	TTR	GLN
GLY	ILE	ASP	ASP	ALA
GLY	ASP	CYS	PRO	SER
ALA	GLY	VAL	GLN	TYR
LYS	ASN	ASP	TYR	ILE
LYS	SER	MET	ALA	SER
ARG	THR	VAL	ALA	PHE
PRO	THR	ILE	SER	ASN
ALA	GLU	TRP	VAL	ALA
PRO	HIS	TRP	LEU	SER
SER	GLN	GLU	GLY	ASN
ASP	GLN	GLU	TRP	SER
ALA	PRO	GLY	ALA	ARG
ASP	LEU	LYS	THR	SER
ILE	GLN	MET	LYS	GLN
SER	ASP	THR	LYS	ILE
GLU	ARG	ALA	PHE	LYS
PRO	MET	LYS	GLY	ALA
LYS	PHE	VAL	LYS	ALA
ARG	LYS	VAL	ARG	LEU
VAL	PHE	GLU	ASN	ASP
ARG	GLU	SER	THR	ASN
GLU	LEU	ALA	ILE	ALA
SER	THR	LYS	TRP	GLY
VAL	ARG	ALA	LEU	LYS
GLN	ARG	ILE	PHE	ILE
PRO	LEU	LEU	GLY	MET
SER	ASP	GLY	PRO	SER
THR	HIS	GLY	ALA	LEU
ASP	ASP	SER	ALA	THR
SER	PHE	LYS	THR	LYS
ASP	GLY	VAL	GLY	THR
ALA	LYS	ARG	LYS	ALA
GLU	VAL	VAL	THR	PRO
ALA	THR	ASP	ASN	ASP
SER	LYS	GLN	ILE	TYR
ARG	PHE	GLN	ALA	GLN
LEU	PHE	GLN	HIS	PRO
ALA	ARG	ILE	THR	VAL
ALA	TRP	ASP	VAL	GLU
ARG	ALA	PRO	ILE	ASP
GLY	ALA	THR	PHE	ILE
HIS	LYS	THR	TYR	SER
SER	ASP	PRO	GLY	SER
LEU	HIS	VAL	CYS	ASN
	VAL	VAL	ASN	ILE
	GLU	THR	TRP	TYR
	VAL	SER	THR	LYS
	GLU	ASN	THR	ILE
	HIS	THR	GLU	LEU
	GLU	ASN	ASN	GLU
	PHE	MET	PHE	LEU
	TYR	CYS	PRO	ASN
	VAL	ALA	PHE	GLY

- Molecule 1: Protein Rep68



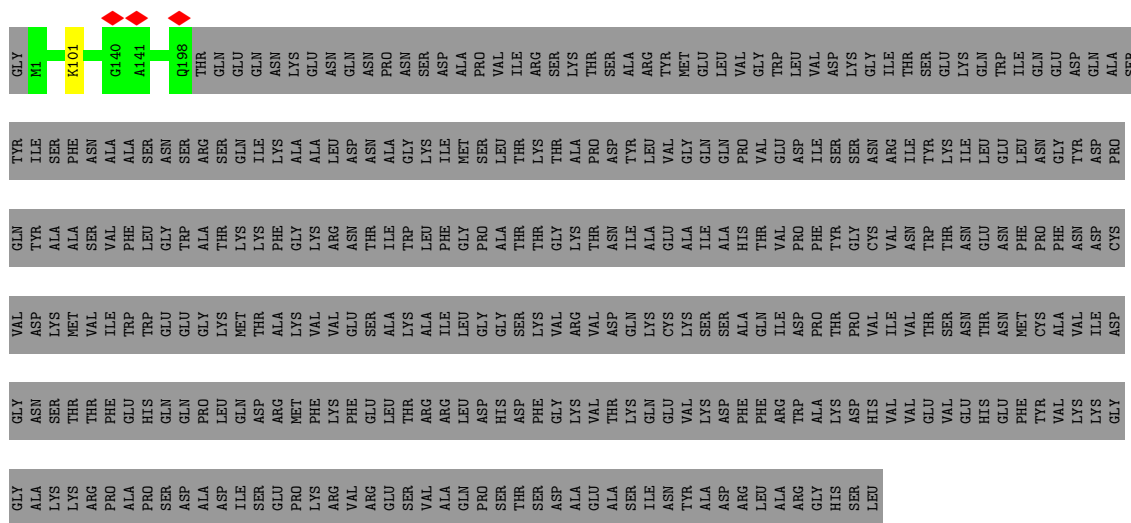
- Molecule 1: Protein Rep68



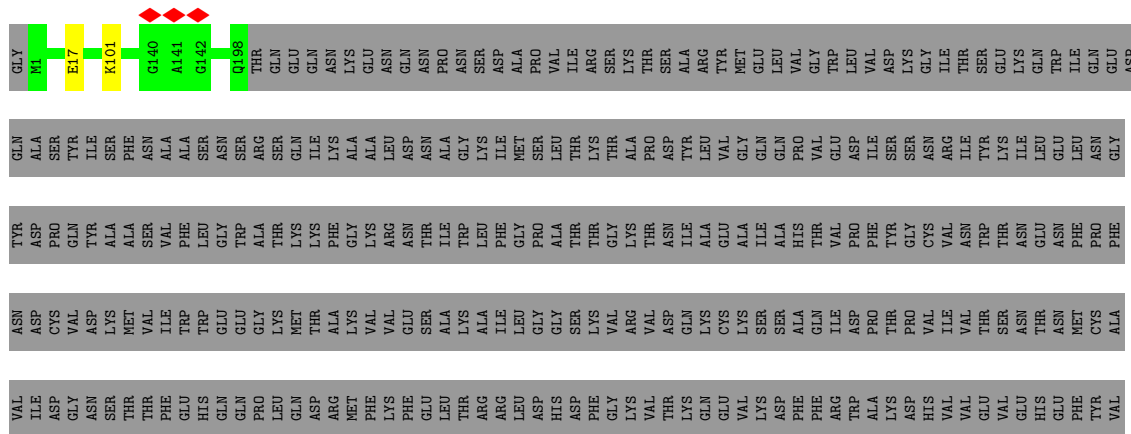


[illegible]

- Molecule 1: Protein Rep68



- Molecule 1: Protein Rep68







- Molecule 2: DNA (5'-D(\*TP\*TP\*TP\*T)-3')

Chain T:  25% 100%



- Molecule 2: DNA (5'-D(\*TP\*TP\*TP\*T)-3')

Chain U:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(\*TP\*TP\*TP\*T)-3')

Chain V:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(\*TP\*TP\*TP\*T)-3')

Chain W:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: DNA (5'-D(\*TP\*TP\*TP\*T)-3')

Chain X:  25% 100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	46031	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 ( $e^-/\text{\AA}^2$ )	92.03	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.872	Depositor
Minimum map value	-0.228	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.23	Depositor
Map size (Å)	329.92004, 329.92004, 329.92004	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82480013, 0.82480013, 0.82480013	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	A	0.23	0/791	0.46	0/987
1	B	0.23	0/791	0.46	0/987
1	C	0.23	0/791	0.45	0/987
1	D	0.23	0/791	0.46	0/987
1	E	0.24	0/791	0.46	0/987
1	F	0.24	0/791	0.46	0/987
1	G	0.23	0/791	0.46	0/987
1	H	0.24	0/791	0.46	0/987
1	I	0.23	0/791	0.46	0/987
1	J	0.23	0/791	0.46	0/987
1	K	0.23	0/791	0.46	0/987
1	L	0.23	0/791	0.46	0/987
1	M	0.24	0/791	0.46	0/987
1	N	0.23	0/791	0.46	0/987
1	O	0.23	0/791	0.44	0/987
1	P	0.23	0/791	0.46	0/987
2	Q	0.49	0/84	1.27	0/128
2	R	0.43	0/84	1.26	0/128
2	S	0.41	0/84	1.26	0/128
2	T	0.41	0/84	1.25	0/128
2	U	0.44	0/84	1.26	0/128
2	V	0.42	0/84	1.25	0/128
2	W	0.45	0/84	1.25	0/128
2	X	0.43	0/84	1.26	0/128
All	All	0.25	0/13328	0.54	0/16816

There are no bond length outliers.

There are no bond angle outliers.

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	A	792	0	208	0	0
1	B	792	0	208	0	0
1	C	792	0	208	0	0
1	D	792	0	208	0	0
1	E	792	0	208	0	0
1	F	792	0	208	0	0
1	G	792	0	208	0	0
1	H	792	0	208	0	0
1	I	792	0	208	0	0
1	J	792	0	208	0	0
1	K	792	0	208	0	0
1	L	792	0	208	0	0
1	M	792	0	208	0	0
1	N	792	0	208	0	0
1	O	792	0	208	0	0
1	P	792	0	208	0	0
2	Q	77	0	50	0	0
2	R	77	0	50	0	0
2	S	77	0	50	0	0
2	T	77	0	50	0	0
2	U	77	0	50	0	0
2	V	77	0	50	0	0
2	W	77	0	50	0	0
2	X	77	0	50	0	0
All	All	13288	0	3728	0	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 0.

There are no clashes within the asymmetric unit.

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	A	196/537 (36%)	171 (87%)	24 (12%)	1 (0%)	29	68
1	B	196/537 (36%)	171 (87%)	23 (12%)	2 (1%)	15	54
1	C	196/537 (36%)	172 (88%)	23 (12%)	1 (0%)	29	68
1	D	196/537 (36%)	173 (88%)	22 (11%)	1 (0%)	29	68
1	E	196/537 (36%)	173 (88%)	22 (11%)	1 (0%)	29	68
1	F	196/537 (36%)	174 (89%)	21 (11%)	1 (0%)	29	68
1	G	196/537 (36%)	171 (87%)	24 (12%)	1 (0%)	29	68
1	H	196/537 (36%)	173 (88%)	22 (11%)	1 (0%)	29	68
1	I	196/537 (36%)	174 (89%)	21 (11%)	1 (0%)	29	68
1	J	196/537 (36%)	173 (88%)	22 (11%)	1 (0%)	29	68
1	K	196/537 (36%)	173 (88%)	22 (11%)	1 (0%)	29	68
1	L	196/537 (36%)	172 (88%)	22 (11%)	2 (1%)	15	54
1	M	196/537 (36%)	173 (88%)	22 (11%)	1 (0%)	29	68
1	N	196/537 (36%)	173 (88%)	22 (11%)	1 (0%)	29	68
1	O	196/537 (36%)	172 (88%)	22 (11%)	2 (1%)	15	54
1	P	196/537 (36%)	172 (88%)	22 (11%)	2 (1%)	15	54
All	All	3136/8592 (36%)	2760 (88%)	356 (11%)	20 (1%)	29	65

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	LYS
1	B	101	LYS
1	C	101	LYS
1	D	101	LYS
1	E	101	LYS
1	F	101	LYS

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Mol	Chain	Res	Type
1	G	101	LYS
1	H	101	LYS
1	I	101	LYS
1	J	101	LYS
1	K	101	LYS
1	L	101	LYS
1	M	101	LYS
1	N	101	LYS
1	O	101	LYS
1	P	101	LYS
1	B	17	GLU
1	O	17	GLU
1	L	17	GLU
1	P	17	GLU

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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](#)

There are no ligands in this entry.

## 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.

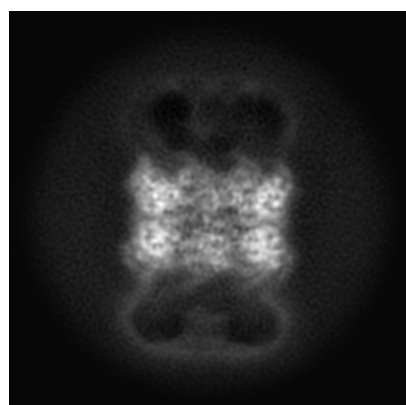
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22451. These allow visual inspection of the internal detail of the map and identification of artifacts.

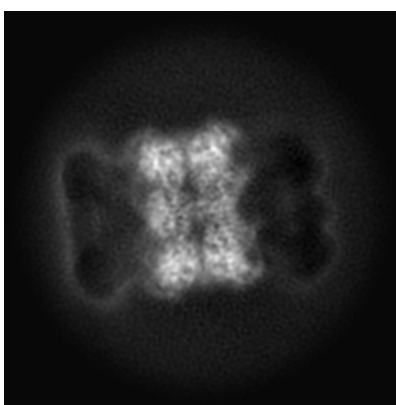
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

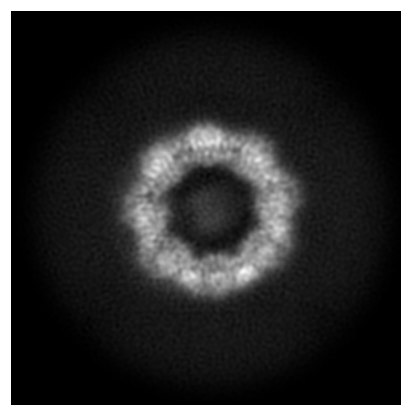
#### 6.1.1 Primary map



X



Y

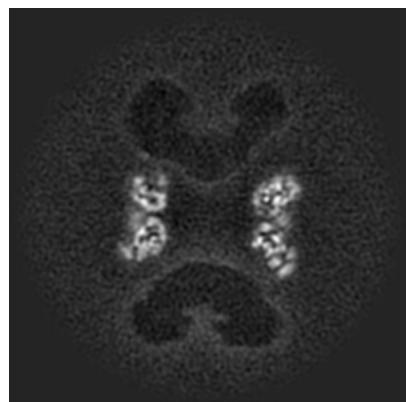


Z

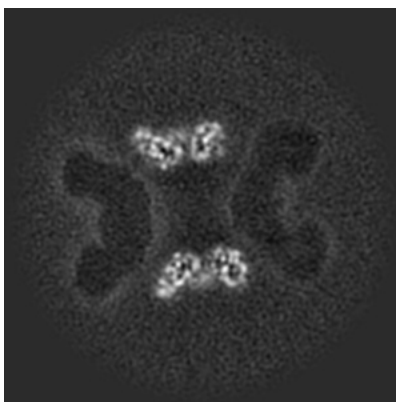
The images above show the map projected in three orthogonal directions.

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

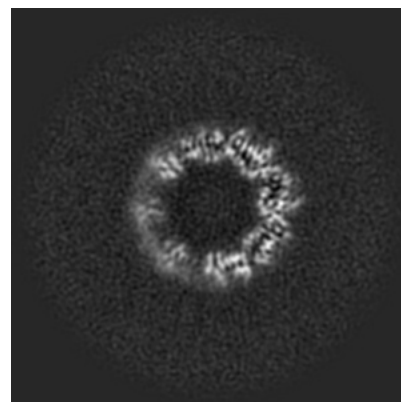
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

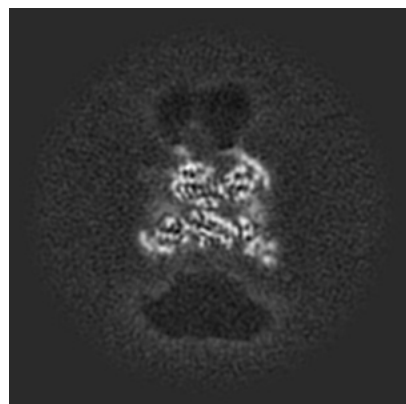


Z Index: 200

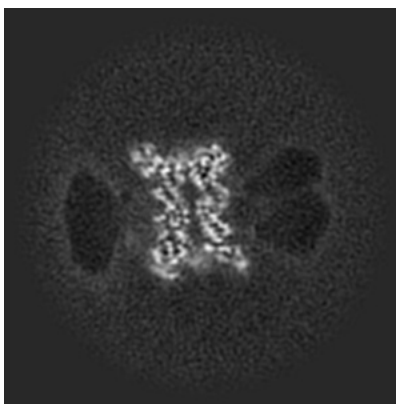
The images above show central slices of the map in three orthogonal directions.

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

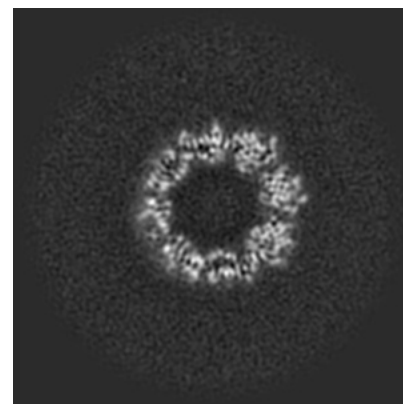
### 6.3.1 Primary map



X Index: 143



Y Index: 251

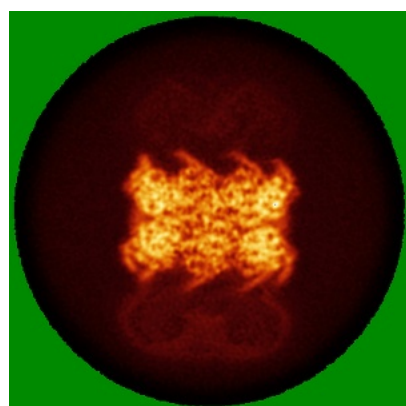


Z Index: 208

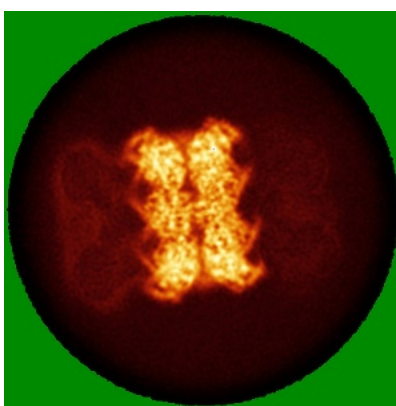
The images above show the largest variance slices of the map in three orthogonal directions.

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

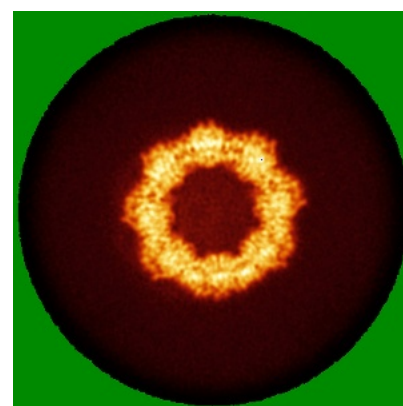
### 6.4.1 Primary map



X



Y

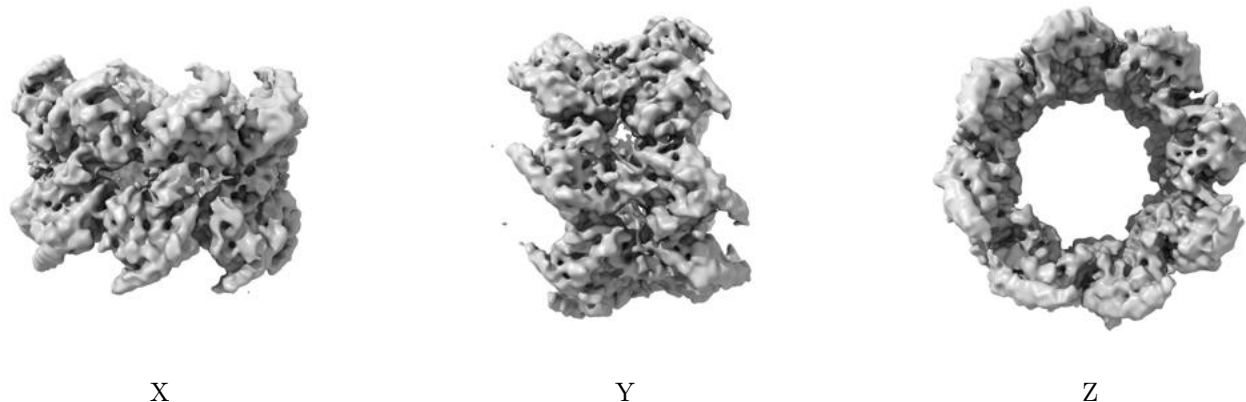


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.23. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

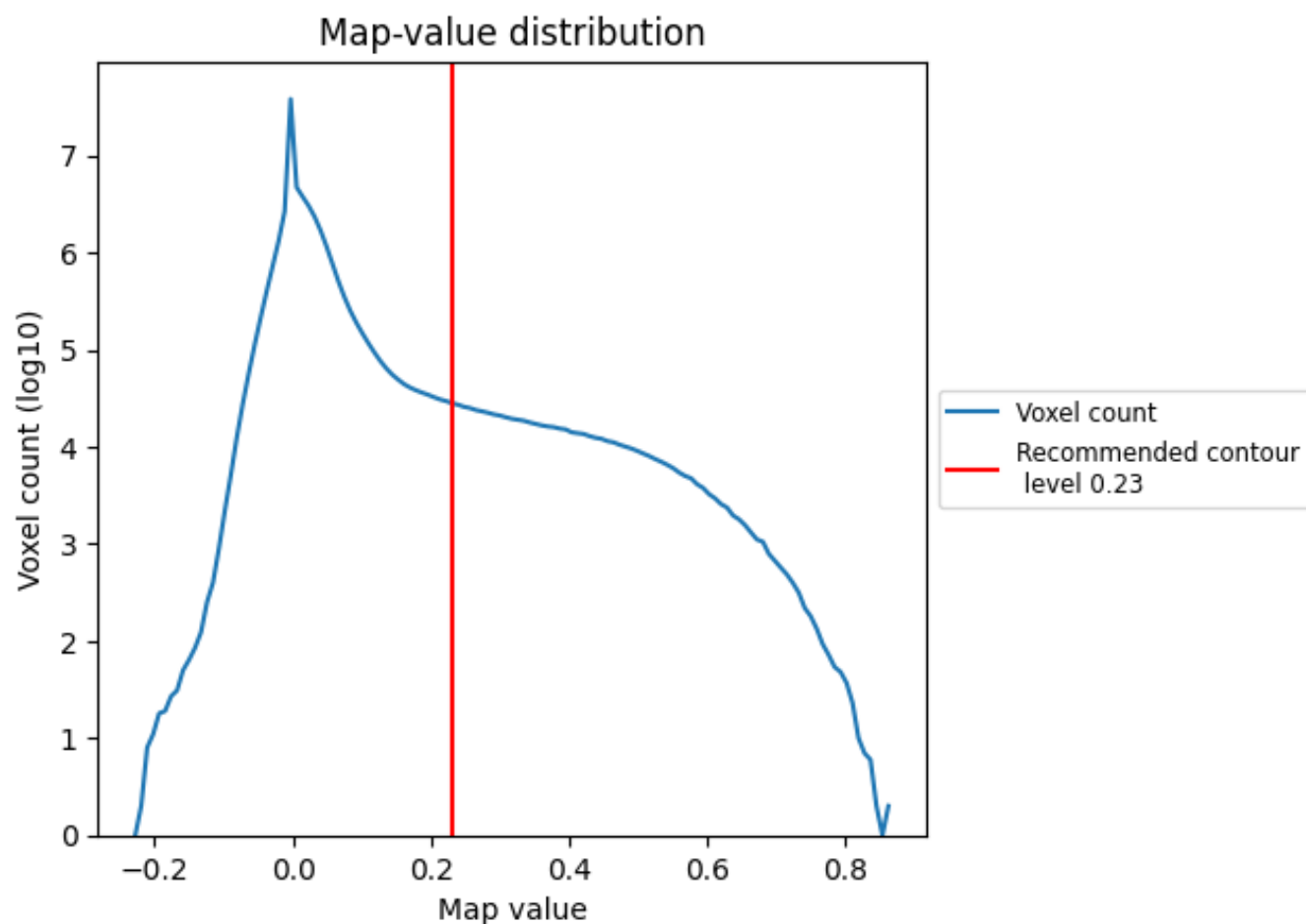
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

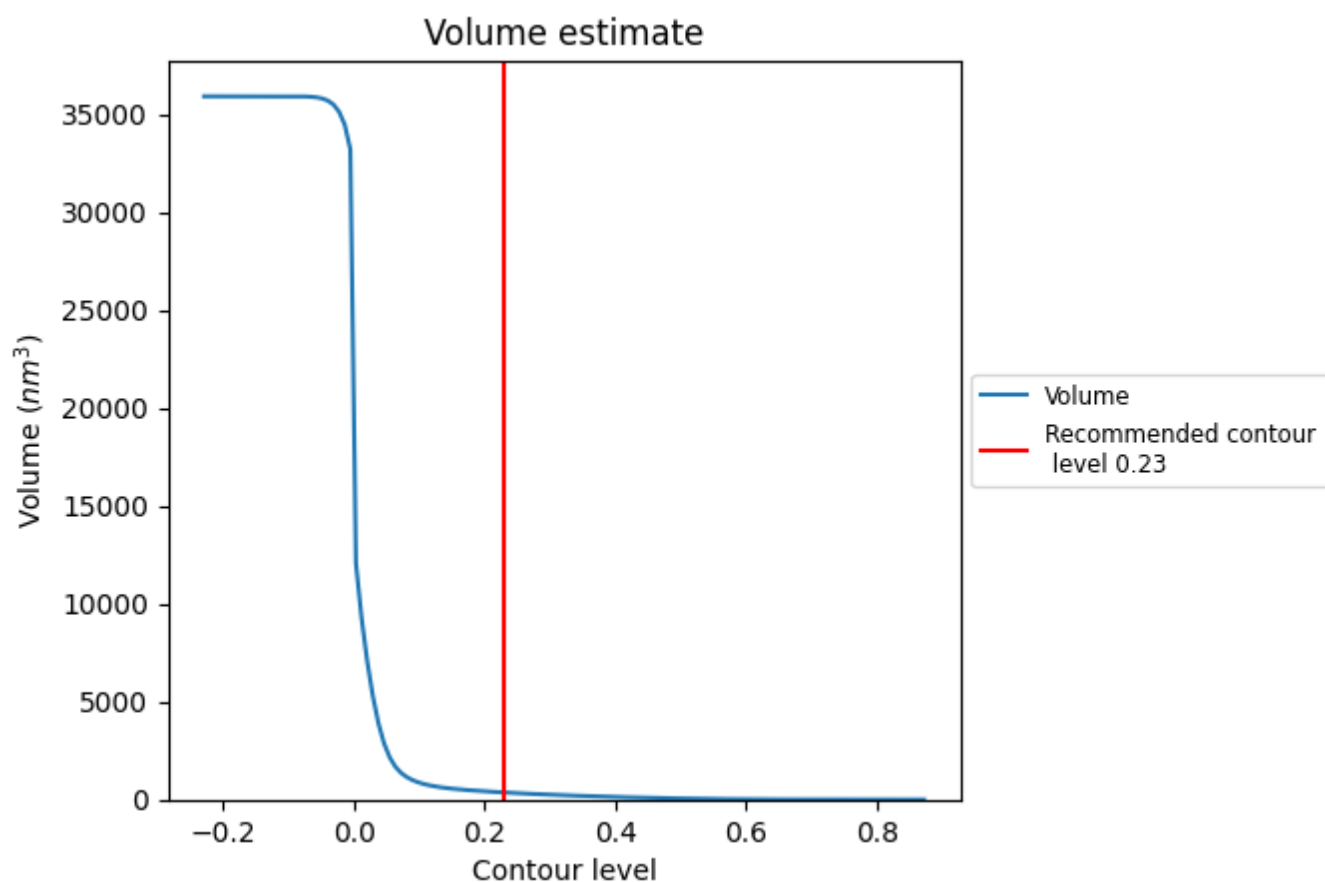
### 7.1 Map-value distribution [i](#)



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



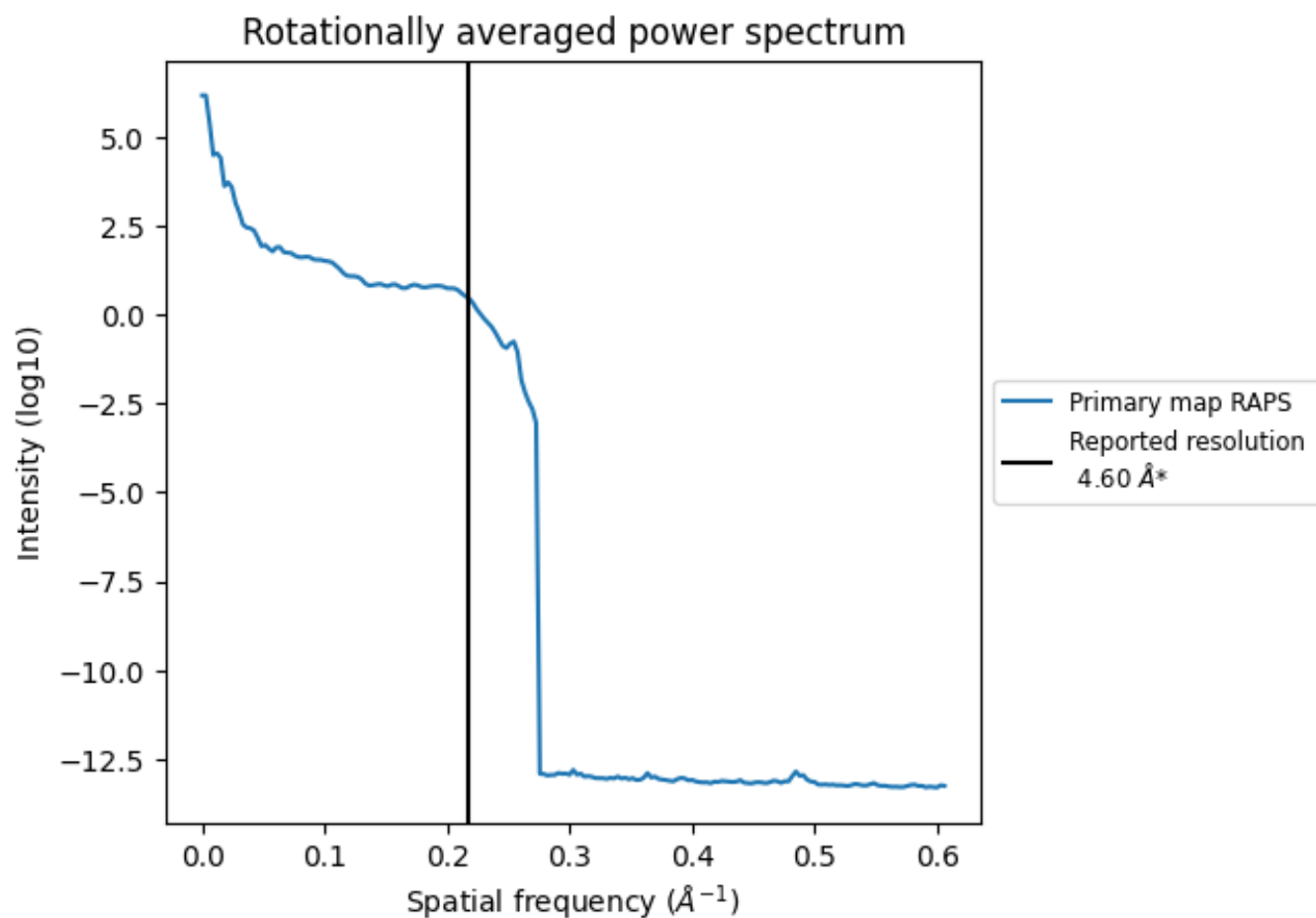
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 361 nm<sup>3</sup>; this corresponds to an approximate mass of 326 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 0.217 Å<sup>-1</sup>

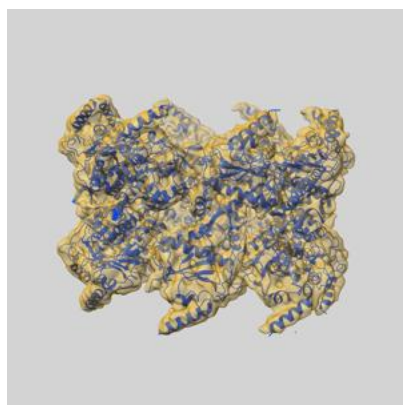
## 8 Fourier-Shell correlation

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

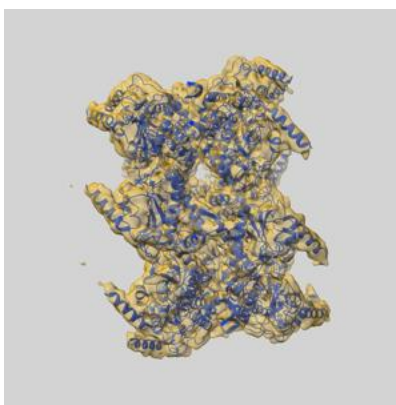
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22451 and PDB model 7JSE. Per-residue inclusion information can be found in section [3](#) on page [7](#).

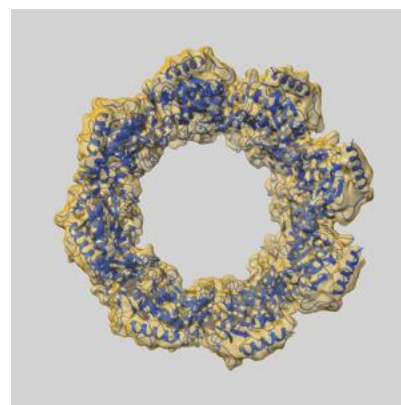
### 9.1 Map-model overlay [i](#)



X



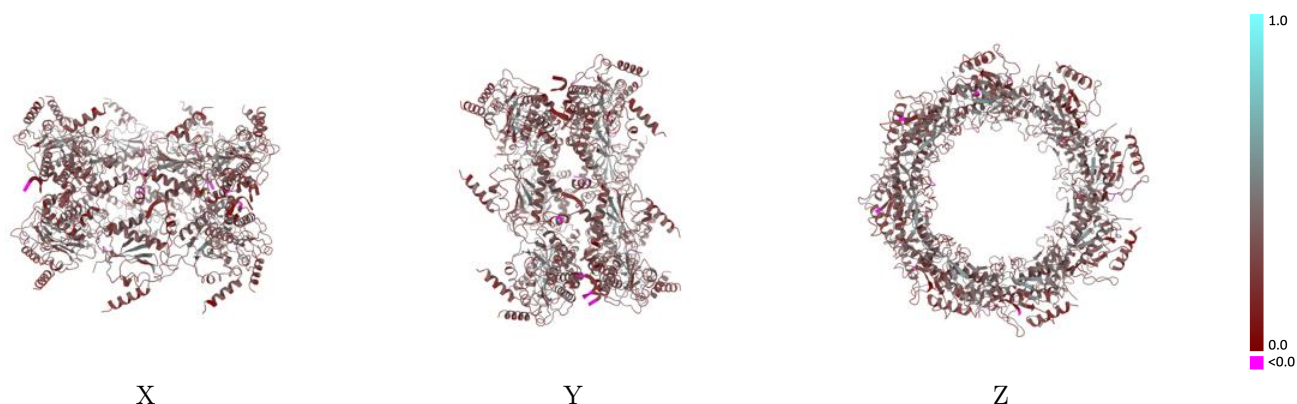
Y



Z

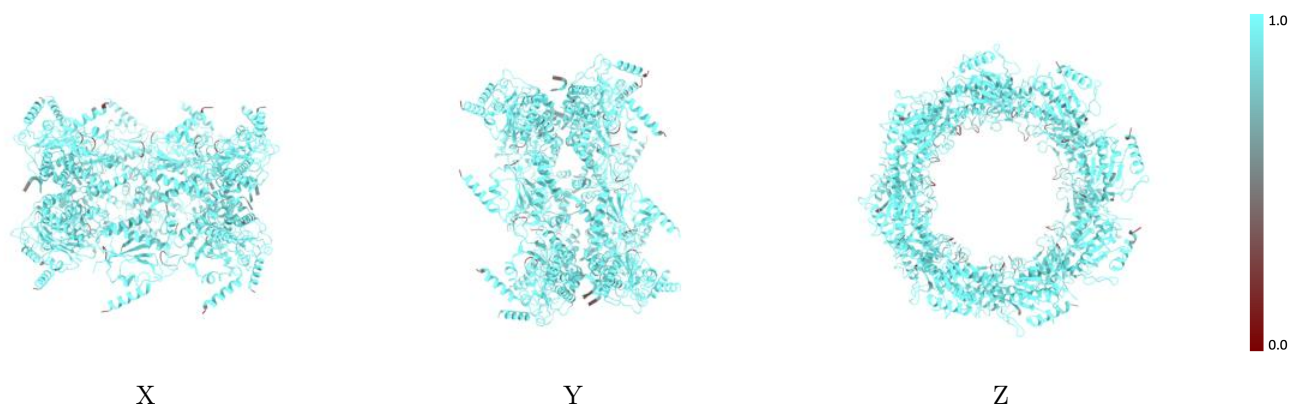
The images above show the 3D surface view of the map at the recommended contour level 0.23 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



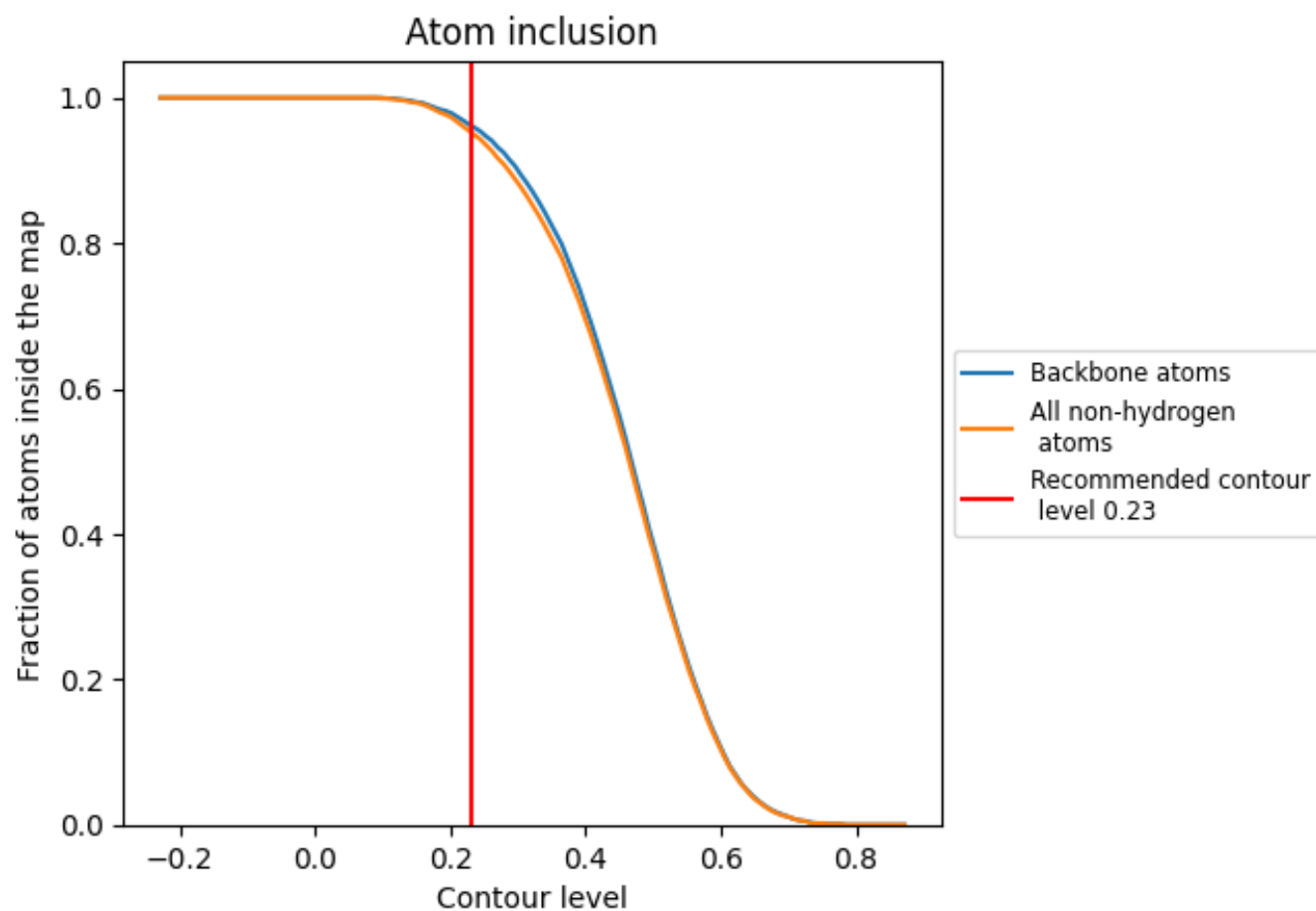
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.23).



















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.23) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9530	 0.3240
A	 0.9630	 0.3260
B	 0.9660	 0.3360
C	 0.9700	 0.3360
D	 0.9670	 0.3340
E	 0.9670	 0.3300
F	 0.9660	 0.3350
G	 0.9630	 0.3360
H	 0.9610	 0.3260
I	 0.9650	 0.3350
J	 0.9650	 0.3230
K	 0.9630	 0.3340
L	 0.9620	 0.3450
M	 0.9580	 0.3330
N	 0.9580	 0.3350
O	 0.9630	 0.3250
P	 0.9630	 0.3340
Q	 0.7530	 0.1350
R	 0.7790	 0.2000
S	 0.6750	 0.0930
T	 0.6620	 0.1220
U	 0.7790	 0.1510
V	 0.6880	 0.0860
W	 0.8440	 0.2270
X	 0.6750	 0.1570

