



Full wwPDB EM Validation Report ⓘ

Apr 2, 2025 – 02:51 am BST

PDB ID : 7A6A / pdb_00007a6a
EMDB ID : EMD-11668
Title : 1.15 Å structure of human apoferritin obtained from Titan Mono- BCOR microscope
Authors : Yip, K.M.; Fischer, N.; Chari, A.; Stark, H.
Deposited on : 2020-08-25
Resolution : 1.15 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

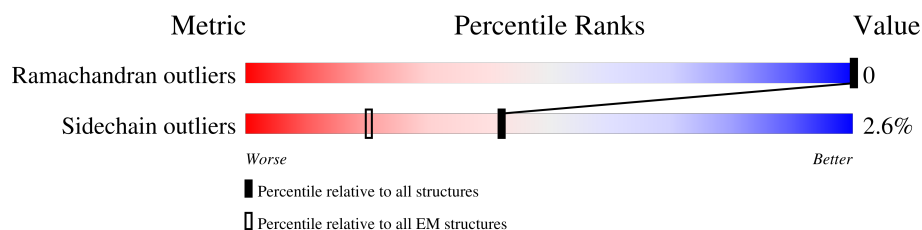
EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **NOT EXECUTED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

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 1.15 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	183	91% • 5%
1	2	183	91% • 5%
1	4	183	91% • 5%
1	6	183	91% • 5%
1	A	183	91% • 5%
1	B	183	91% • 5%
1	E	183	91% • 5%
1	F	183	91% • 5%
1	G	183	91% • 5%

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Mol	Chain	Length	Quality of chain
1	H	183	 91% • 5%
1	I	183	 91% • 5%
1	K	183	 91% • 5%
1	M	183	 91% • 5%
1	O	183	 91% • 5%
1	P	183	 91% • 5%
1	Q	183	 91% • 5%
1	S	183	 91% • 5%
1	U	183	 91% • 5%
1	W	183	 91% • 5%
1	X	183	 91% • 5%
1	Y	183	 91% • 5%
1	a	183	 91% • 5%
1	e	183	 91% • 5%
1	r	183	 91% • 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 41613 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 Ferritin heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	1	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	K	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	a	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	B	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	E	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	e	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	r	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	G	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	I	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	M	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	O	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	Q	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	S	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	U	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	W	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	Y	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	4	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	F	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	H	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	P	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	X	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		
1	6	173	Total	C	N	O	S	14	0
			1540	963	273	299	5		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	GLN	LYS	conflict	UNP P02794
1	86	GLN	LYS	conflict	UNP P02794
K	86	GLN	LYS	conflict	UNP P02794
a	86	GLN	LYS	conflict	UNP P02794
B	86	GLN	LYS	conflict	UNP P02794
E	86	GLN	LYS	conflict	UNP P02794
e	86	GLN	LYS	conflict	UNP P02794
r	86	GLN	LYS	conflict	UNP P02794
G	86	GLN	LYS	conflict	UNP P02794
I	86	GLN	LYS	conflict	UNP P02794
M	86	GLN	LYS	conflict	UNP P02794
O	86	GLN	LYS	conflict	UNP P02794
Q	86	GLN	LYS	conflict	UNP P02794
S	86	GLN	LYS	conflict	UNP P02794
U	86	GLN	LYS	conflict	UNP P02794
W	86	GLN	LYS	conflict	UNP P02794
Y	86	GLN	LYS	conflict	UNP P02794
2	86	GLN	LYS	conflict	UNP P02794
4	86	GLN	LYS	conflict	UNP P02794
F	86	GLN	LYS	conflict	UNP P02794
H	86	GLN	LYS	conflict	UNP P02794
P	86	GLN	LYS	conflict	UNP P02794
X	86	GLN	LYS	conflict	UNP P02794
6	86	GLN	LYS	conflict	UNP P02794

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
2	A	2	Total 2	Na 2	0
2	1	2	Total 2	Na 2	0
2	K	1	Total 1	Na 1	0
2	a	1	Total 1	Na 1	0
2	B	2	Total 2	Na 2	0
2	E	1	Total 1	Na 1	0
2	e	1	Total 1	Na 1	0
2	r	1	Total 1	Na 1	0
2	G	1	Total 1	Na 1	0
2	I	1	Total 1	Na 1	0
2	M	2	Total 2	Na 2	0
2	O	1	Total 1	Na 1	0
2	Q	1	Total 1	Na 1	0
2	S	1	Total 1	Na 1	0
2	U	1	Total 1	Na 1	0
2	W	1	Total 1	Na 1	0
2	Y	1	Total 1	Na 1	0
2	2	2	Total 2	Na 2	0
2	4	2	Total 2	Na 2	0
2	F	1	Total 1	Na 1	0
2	H	2	Total 2	Na 2	0

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Mol	Chain	Residues	Atoms		AltConf
2	P	1	Total 1	Na 1	0
2	X	1	Total 1	Na 1	0
2	6	2	Total 2	Na 2	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	194	Total 194	O 194	0
3	1	194	Total 194	O 194	0
3	K	193	Total 193	O 193	0
3	a	192	Total 192	O 192	0
3	B	193	Total 193	O 193	0
3	E	192	Total 192	O 192	0
3	e	194	Total 194	O 194	0
3	r	192	Total 192	O 192	0
3	G	194	Total 194	O 194	0
3	I	191	Total 191	O 191	0
3	M	192	Total 192	O 192	0
3	O	193	Total 193	O 193	0
3	Q	194	Total 194	O 194	0
3	S	193	Total 193	O 193	0
3	U	191	Total 191	O 191	0
3	W	193	Total 193	O 193	0

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Mol	Chain	Residues	Atoms		AltConf
3	Y	192	Total 192	O 192	0
3	2	192	Total 192	O 192	0
3	4	192	Total 192	O 192	0
3	F	191	Total 191	O 191	0
3	H	193	Total 193	O 193	0
3	P	192	Total 192	O 192	0
3	X	192	Total 192	O 192	0
3	6	192	Total 192	O 192	0

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ferritin heavy chain

Chain A:  91% 5%

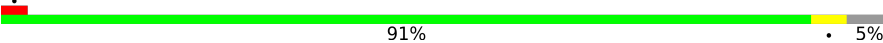


- Molecule 1: Ferritin heavy chain

Chain 1:  91% 5%



- Molecule 1: Ferritin heavy chain

Chain K:  91% 5%




- Molecule 1: Ferritin heavy chain

Chain a:  91% 5%

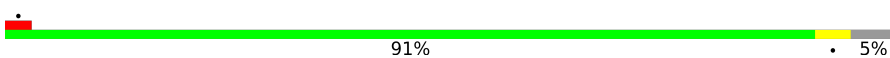


- Molecule 1: Ferritin heavy chain

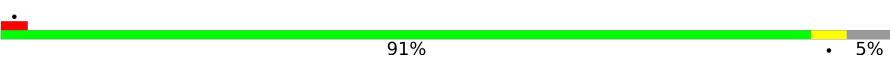
Chain B:  91% 5%



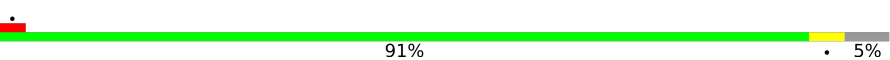
● Molecule 1: Ferritin heavy chain

Chain E:  91% 5%

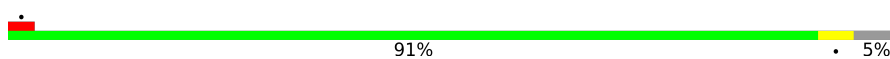
● Molecule 1: Ferritin heavy chain

Chain e:  91% 5%


● Molecule 1: Ferritin heavy chain

Chain r:  91% 5%

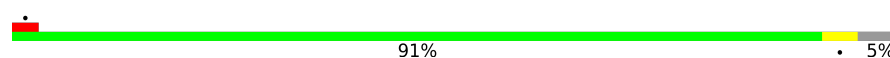
● Molecule 1: Ferritin heavy chain

Chain G:  91% 5%

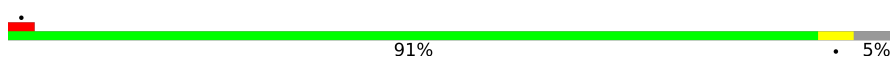
● Molecule 1: Ferritin heavy chain

Chain I:  91% 5%

● Molecule 1: Ferritin heavy chain

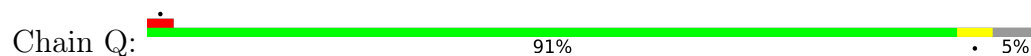
Chain M:  91% 5%

● Molecule 1: Ferritin heavy chain

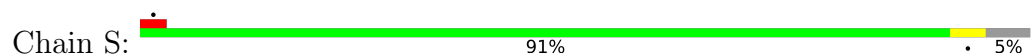
Chain O:  91% 5%



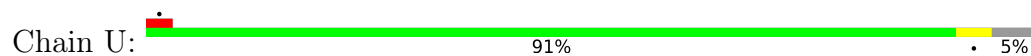
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



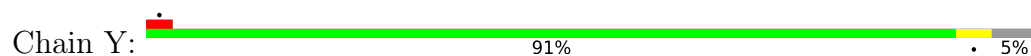
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain



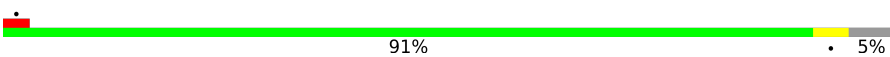
- Molecule 1: Ferritin heavy chain



- Molecule 1: Ferritin heavy chain

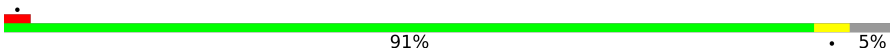


- Molecule 1: Ferritin heavy chain

Chain 4:  91% 5%

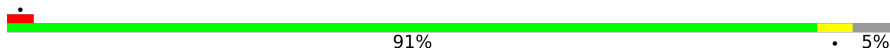


• Molecule 1: Ferritin heavy chain

Chain F:  91% 5%

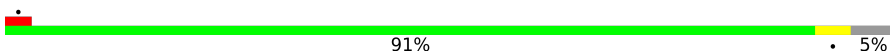


• Molecule 1: Ferritin heavy chain

Chain H:  91% 5%

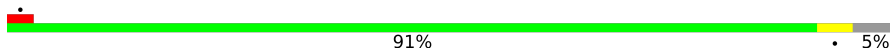


• Molecule 1: Ferritin heavy chain

Chain P:  91% 5%

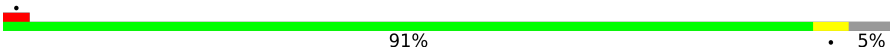


• Molecule 1: Ferritin heavy chain

Chain X:  91% 5%



• Molecule 1: Ferritin heavy chain

Chain 6:  91% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, O	Depositor
Number of particles used	797000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.056	Depositor
Minimum map value	-0.323	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.15	Depositor
Map size (\AA)	236.16, 236.16, 236.16	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.492, 0.492, 0.492	Depositor

5 Model quality

5.1 Standard geometry

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

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	1	0.87	0/1561	0.88	1/2096 (0.0%)
1	2	0.87	0/1561	0.89	1/2096 (0.0%)
1	4	0.87	0/1561	0.89	1/2096 (0.0%)
1	6	0.87	0/1561	0.89	1/2096 (0.0%)
1	A	0.87	0/1561	0.88	1/2096 (0.0%)
1	B	0.87	0/1561	0.88	1/2096 (0.0%)
1	E	0.87	0/1561	0.88	1/2096 (0.0%)
1	F	0.87	0/1561	0.89	1/2096 (0.0%)
1	G	0.87	0/1561	0.88	1/2096 (0.0%)
1	H	0.87	0/1561	0.89	1/2096 (0.0%)
1	I	0.87	0/1561	0.88	1/2096 (0.0%)
1	K	0.87	0/1561	0.88	1/2096 (0.0%)
1	M	0.87	0/1561	0.88	1/2096 (0.0%)
1	O	0.87	0/1561	0.88	1/2096 (0.0%)
1	P	0.87	0/1561	0.88	1/2096 (0.0%)
1	Q	0.87	0/1561	0.88	1/2096 (0.0%)
1	S	0.87	0/1561	0.88	1/2096 (0.0%)
1	U	0.87	0/1561	0.89	1/2096 (0.0%)
1	W	0.87	0/1561	0.88	1/2096 (0.0%)
1	X	0.87	0/1561	0.88	1/2096 (0.0%)
1	Y	0.87	0/1561	0.88	1/2096 (0.0%)
1	a	0.87	0/1561	0.88	1/2096 (0.0%)
1	e	0.87	0/1561	0.88	1/2096 (0.0%)
1	r	0.87	0/1561	0.88	1/2096 (0.0%)
All	All	0.87	0/37464	0.88	24/50304 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	1
1	2	0	1
1	4	0	1
1	6	0	1
1	A	0	1
1	B	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	K	0	1
1	M	0	1
1	O	0	1
1	P	0	1
1	Q	0	1
1	S	0	1
1	U	0	1
1	W	0	1
1	X	0	1
1	Y	0	1
1	a	0	1
1	e	0	1
1	r	0	1
All	All	0	24

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	9	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	e	9	ARG	NE-CZ-NH2	5.71	123.16	120.30
1	G	9	ARG	NE-CZ-NH2	5.71	123.16	120.30
1	Y	9	ARG	NE-CZ-NH2	5.71	123.16	120.30
1	4	9	ARG	NE-CZ-NH2	5.71	123.16	120.30
1	a	9	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	r	9	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	I	9	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	U	9	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	2	9	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	6	9	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	1	9	ARG	NE-CZ-NH2	5.69	123.14	120.30
1	B	9	ARG	NE-CZ-NH2	5.69	123.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	9	ARG	NE-CZ-NH2	5.69	123.14	120.30
1	M	9	ARG	NE-CZ-NH2	5.69	123.14	120.30
1	Q	9	ARG	NE-CZ-NH2	5.69	123.14	120.30
1	W	9	ARG	NE-CZ-NH2	5.69	123.14	120.30
1	H	9	ARG	NE-CZ-NH2	5.69	123.14	120.30
1	P	9	ARG	NE-CZ-NH2	5.69	123.14	120.30
1	X	9	ARG	NE-CZ-NH2	5.69	123.14	120.30
1	F	9	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	O	9	ARG	NE-CZ-NH2	5.67	123.13	120.30
1	A	9	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	K	9	ARG	NE-CZ-NH2	5.64	123.12	120.30

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	137	TYR	Sidechain
1	2	137	TYR	Sidechain
1	4	137	TYR	Sidechain
1	6	137	TYR	Sidechain
1	A	137	TYR	Sidechain
1	B	137	TYR	Sidechain
1	E	137	TYR	Sidechain
1	F	137	TYR	Sidechain
1	G	137	TYR	Sidechain
1	H	137	TYR	Sidechain
1	I	137	TYR	Sidechain
1	K	137	TYR	Sidechain
1	M	137	TYR	Sidechain
1	O	137	TYR	Sidechain
1	P	137	TYR	Sidechain
1	Q	137	TYR	Sidechain
1	S	137	TYR	Sidechain
1	U	137	TYR	Sidechain
1	W	137	TYR	Sidechain
1	X	137	TYR	Sidechain
1	Y	137	TYR	Sidechain
1	a	137	TYR	Sidechain
1	e	137	TYR	Sidechain
1	r	137	TYR	Sidechain

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	1	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	2	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	4	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	6	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	A	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	B	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	E	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	F	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	G	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	H	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	I	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	K	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	M	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	O	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	P	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	Q	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	S	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	U	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	W	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	X	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	Y	184/183 (100%)	181 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	e	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
1	r	184/183 (100%)	181 (98%)	3 (2%)	0	100	100
All	All	4416/4392 (100%)	4344 (98%)	72 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	165/162 (102%)	159 (96%)	6 (4%)	30	2
1	2	165/162 (102%)	159 (96%)	6 (4%)	30	2
1	4	165/162 (102%)	159 (96%)	6 (4%)	30	2
1	6	165/162 (102%)	159 (96%)	6 (4%)	30	2
1	A	165/162 (102%)	159 (96%)	6 (4%)	30	2
1	B	165/162 (102%)	159 (96%)	6 (4%)	30	2
1	E	165/162 (102%)	159 (96%)	6 (4%)	30	2
1	F	165/162 (102%)	159 (96%)	6 (4%)	30	2
1	G	165/162 (102%)	159 (96%)	6 (4%)	30	2
1	H	165/162 (102%)	159 (96%)	6 (4%)	30	2
1	I	165/162 (102%)	159 (96%)	6 (4%)	30	2
1	K	165/162 (102%)	159 (96%)	6 (4%)	30	2
1	M	165/162 (102%)	159 (96%)	6 (4%)	30	2
1	O	165/162 (102%)	159 (96%)	6 (4%)	30	2
1	P	165/162 (102%)	159 (96%)	6 (4%)	30	2
1	Q	165/162 (102%)	159 (96%)	6 (4%)	30	2
1	S	165/162 (102%)	159 (96%)	6 (4%)	30	2
1	U	165/162 (102%)	159 (96%)	6 (4%)	30	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	W	165/162 (102%)	159 (96%)	6 (4%)	30 2
1	X	165/162 (102%)	159 (96%)	6 (4%)	30 2
1	Y	165/162 (102%)	159 (96%)	6 (4%)	30 2
1	a	165/162 (102%)	159 (96%)	6 (4%)	30 2
1	e	165/162 (102%)	159 (96%)	6 (4%)	30 2
1	r	165/162 (102%)	159 (96%)	6 (4%)	30 2
All	All	3960/3888 (102%)	3816 (96%)	144 (4%)	42 2

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53[A]	LYS
1	A	53[B]	LYS
1	A	117	LEU
1	A	157	LYS
1	A	162[A]	GLU
1	A	162[B]	GLU
1	1	53[A]	LYS
1	1	53[B]	LYS
1	1	117	LEU
1	1	157	LYS
1	1	162[A]	GLU
1	1	162[B]	GLU
1	K	53[A]	LYS
1	K	53[B]	LYS
1	K	117	LEU
1	K	157	LYS
1	K	162[A]	GLU
1	K	162[B]	GLU
1	a	53[A]	LYS
1	a	53[B]	LYS
1	a	117	LEU
1	a	157	LYS
1	a	162[A]	GLU
1	a	162[B]	GLU
1	B	53[A]	LYS
1	B	53[B]	LYS
1	B	117	LEU
1	B	157	LYS
1	B	162[A]	GLU

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Mol	Chain	Res	Type
1	B	162[B]	GLU
1	E	53[A]	LYS
1	E	53[B]	LYS
1	E	117	LEU
1	E	157	LYS
1	E	162[A]	GLU
1	E	162[B]	GLU
1	e	53[A]	LYS
1	e	53[B]	LYS
1	e	117	LEU
1	e	157	LYS
1	e	162[A]	GLU
1	e	162[B]	GLU
1	r	53[A]	LYS
1	r	53[B]	LYS
1	r	117	LEU
1	r	157	LYS
1	r	162[A]	GLU
1	r	162[B]	GLU
1	G	53[A]	LYS
1	G	53[B]	LYS
1	G	117	LEU
1	G	157	LYS
1	G	162[A]	GLU
1	G	162[B]	GLU
1	I	53[A]	LYS
1	I	53[B]	LYS
1	I	117	LEU
1	I	157	LYS
1	I	162[A]	GLU
1	I	162[B]	GLU
1	M	53[A]	LYS
1	M	53[B]	LYS
1	M	117	LEU
1	M	157	LYS
1	M	162[A]	GLU
1	M	162[B]	GLU
1	O	53[A]	LYS
1	O	53[B]	LYS
1	O	117	LEU
1	O	157	LYS
1	O	162[A]	GLU

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Mol	Chain	Res	Type
1	O	162[B]	GLU
1	Q	53[A]	LYS
1	Q	53[B]	LYS
1	Q	117	LEU
1	Q	157	LYS
1	Q	162[A]	GLU
1	Q	162[B]	GLU
1	S	53[A]	LYS
1	S	53[B]	LYS
1	S	117	LEU
1	S	157	LYS
1	S	162[A]	GLU
1	S	162[B]	GLU
1	U	53[A]	LYS
1	U	53[B]	LYS
1	U	117	LEU
1	U	157	LYS
1	U	162[A]	GLU
1	U	162[B]	GLU
1	W	53[A]	LYS
1	W	53[B]	LYS
1	W	117	LEU
1	W	157	LYS
1	W	162[A]	GLU
1	W	162[B]	GLU
1	Y	53[A]	LYS
1	Y	53[B]	LYS
1	Y	117	LEU
1	Y	157	LYS
1	Y	162[A]	GLU
1	Y	162[B]	GLU
1	2	53[A]	LYS
1	2	53[B]	LYS
1	2	117	LEU
1	2	157	LYS
1	2	162[A]	GLU
1	2	162[B]	GLU
1	4	53[A]	LYS
1	4	53[B]	LYS
1	4	117	LEU
1	4	157	LYS
1	4	162[A]	GLU

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Mol	Chain	Res	Type
1	4	162[B]	GLU
1	F	53[A]	LYS
1	F	53[B]	LYS
1	F	117	LEU
1	F	157	LYS
1	F	162[A]	GLU
1	F	162[B]	GLU
1	H	53[A]	LYS
1	H	53[B]	LYS
1	H	117	LEU
1	H	157	LYS
1	H	162[A]	GLU
1	H	162[B]	GLU
1	P	53[A]	LYS
1	P	53[B]	LYS
1	P	117	LEU
1	P	157	LYS
1	P	162[A]	GLU
1	P	162[B]	GLU
1	X	53[A]	LYS
1	X	53[B]	LYS
1	X	117	LEU
1	X	157	LYS
1	X	162[A]	GLU
1	X	162[B]	GLU
1	6	53[A]	LYS
1	6	53[B]	LYS
1	6	117	LEU
1	6	157	LYS
1	6	162[A]	GLU
1	6	162[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	98	ASN
1	A	105	HIS
1	A	136	HIS
1	1	14	GLN
1	1	98	ASN
1	1	105	HIS

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Mol	Chain	Res	Type
1	1	136	HIS
1	K	14	GLN
1	K	98	ASN
1	K	105	HIS
1	K	136	HIS
1	a	14	GLN
1	a	98	ASN
1	a	105	HIS
1	a	136	HIS
1	B	14	GLN
1	B	98	ASN
1	B	105	HIS
1	B	136	HIS
1	E	14	GLN
1	E	98	ASN
1	E	105	HIS
1	E	136	HIS
1	e	14	GLN
1	e	98	ASN
1	e	105	HIS
1	e	136	HIS
1	r	14	GLN
1	r	98	ASN
1	r	105	HIS
1	r	136	HIS
1	G	14	GLN
1	G	98	ASN
1	G	105	HIS
1	G	136	HIS
1	I	14	GLN
1	I	98	ASN
1	I	105	HIS
1	I	136	HIS
1	M	14	GLN
1	M	98	ASN
1	M	105	HIS
1	M	136	HIS
1	O	14	GLN
1	O	98	ASN
1	O	105	HIS
1	O	136	HIS
1	Q	14	GLN

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Mol	Chain	Res	Type
1	Q	98	ASN
1	Q	105	HIS
1	Q	136	HIS
1	S	14	GLN
1	S	98	ASN
1	S	105	HIS
1	S	136	HIS
1	U	14	GLN
1	U	98	ASN
1	U	105	HIS
1	U	136	HIS
1	W	14	GLN
1	W	98	ASN
1	W	105	HIS
1	W	136	HIS
1	Y	14	GLN
1	Y	98	ASN
1	Y	105	HIS
1	Y	136	HIS
1	2	14	GLN
1	2	98	ASN
1	2	105	HIS
1	2	136	HIS
1	4	14	GLN
1	4	98	ASN
1	4	105	HIS
1	4	136	HIS
1	F	14	GLN
1	F	98	ASN
1	F	105	HIS
1	F	136	HIS
1	H	14	GLN
1	H	98	ASN
1	H	105	HIS
1	H	136	HIS
1	P	14	GLN
1	P	98	ASN
1	P	105	HIS
1	P	136	HIS
1	X	14	GLN
1	X	98	ASN
1	X	105	HIS

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Mol	Chain	Res	Type
1	X	136	HIS
1	6	14	GLN
1	6	98	ASN
1	6	105	HIS
1	6	136	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

24 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	CSX	r	90	1	3,6,7	0.78	0	1,6,8	2.06	1 (100%)
1	CSX	P	90	1	3,6,7	0.77	0	1,6,8	2.04	1 (100%)
1	CSX	M	90	1	3,6,7	0.76	0	1,6,8	2.04	1 (100%)
1	CSX	U	90	1	3,6,7	0.78	0	1,6,8	2.06	1 (100%)
1	CSX	Y	90	1	3,6,7	0.78	0	1,6,8	2.06	1 (100%)
1	CSX	A	90	1	3,6,7	0.77	0	1,6,8	2.03	1 (100%)
1	CSX	2	90	1	3,6,7	0.77	0	1,6,8	2.05	1 (100%)
1	CSX	4	90	1	3,6,7	0.78	0	1,6,8	2.05	1 (100%)
1	CSX	e	90	1	3,6,7	0.78	0	1,6,8	2.05	1 (100%)
1	CSX	I	90	1	3,6,7	0.78	0	1,6,8	2.05	1 (100%)
1	CSX	H	90	1	3,6,7	0.77	0	1,6,8	2.05	1 (100%)
1	CSX	S	90	1	3,6,7	0.77	0	1,6,8	2.04	1 (100%)
1	CSX	K	90	1	3,6,7	0.78	0	1,6,8	2.06	1 (100%)
1	CSX	B	90	1	3,6,7	0.77	0	1,6,8	2.05	1 (100%)
1	CSX	G	90	1	3,6,7	0.76	0	1,6,8	2.04	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSX	W	90	1	3,6,7	0.76	0	1,6,8	2.04	1 (100%)
1	CSX	E	90	1	3,6,7	0.78	0	1,6,8	2.05	1 (100%)
1	CSX	Q	90	1	3,6,7	0.78	0	1,6,8	2.05	1 (100%)
1	CSX	a	90	1	3,6,7	0.79	0	1,6,8	2.06	1 (100%)
1	CSX	X	90	1	3,6,7	0.78	0	1,6,8	2.05	1 (100%)
1	CSX	O	90	1	3,6,7	0.78	0	1,6,8	2.06	1 (100%)
1	CSX	F	90	1	3,6,7	0.77	0	1,6,8	2.04	1 (100%)
1	CSX	6	90	1	3,6,7	0.77	0	1,6,8	2.04	1 (100%)
1	CSX	1	90	1	3,6,7	0.78	0	1,6,8	2.05	1 (100%)

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	CSX	r	90	1	-	0/1/5/7	-
1	CSX	P	90	1	-	0/1/5/7	-
1	CSX	M	90	1	-	0/1/5/7	-
1	CSX	U	90	1	-	0/1/5/7	-
1	CSX	Y	90	1	-	0/1/5/7	-
1	CSX	A	90	1	-	0/1/5/7	-
1	CSX	2	90	1	-	0/1/5/7	-
1	CSX	4	90	1	-	0/1/5/7	-
1	CSX	e	90	1	-	0/1/5/7	-
1	CSX	I	90	1	-	0/1/5/7	-
1	CSX	H	90	1	-	0/1/5/7	-
1	CSX	S	90	1	-	0/1/5/7	-
1	CSX	K	90	1	-	0/1/5/7	-
1	CSX	B	90	1	-	0/1/5/7	-
1	CSX	G	90	1	-	0/1/5/7	-
1	CSX	W	90	1	-	0/1/5/7	-
1	CSX	E	90	1	-	0/1/5/7	-
1	CSX	Q	90	1	-	0/1/5/7	-
1	CSX	a	90	1	-	0/1/5/7	-
1	CSX	X	90	1	-	0/1/5/7	-
1	CSX	O	90	1	-	0/1/5/7	-
1	CSX	F	90	1	-	0/1/5/7	-
1	CSX	6	90	1	-	0/1/5/7	-
1	CSX	1	90	1	-	0/1/5/7	-

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	90	CSX	CA-CB-SG	-2.06	108.85	113.36
1	O	90	CSX	CA-CB-SG	-2.06	108.85	113.36
1	U	90	CSX	CA-CB-SG	-2.06	108.85	113.36
1	K	90	CSX	CA-CB-SG	-2.06	108.85	113.36
1	r	90	CSX	CA-CB-SG	-2.06	108.85	113.36
1	Y	90	CSX	CA-CB-SG	-2.06	108.85	113.36
1	B	90	CSX	CA-CB-SG	-2.05	108.87	113.36
1	2	90	CSX	CA-CB-SG	-2.05	108.87	113.36
1	H	90	CSX	CA-CB-SG	-2.05	108.87	113.36
1	1	90	CSX	CA-CB-SG	-2.05	108.88	113.36
1	4	90	CSX	CA-CB-SG	-2.05	108.88	113.36
1	E	90	CSX	CA-CB-SG	-2.05	108.88	113.36
1	e	90	CSX	CA-CB-SG	-2.05	108.88	113.36
1	I	90	CSX	CA-CB-SG	-2.05	108.88	113.36
1	X	90	CSX	CA-CB-SG	-2.05	108.88	113.36
1	Q	90	CSX	CA-CB-SG	-2.05	108.88	113.36
1	G	90	CSX	CA-CB-SG	-2.04	108.91	113.36
1	M	90	CSX	CA-CB-SG	-2.04	108.91	113.36
1	S	90	CSX	CA-CB-SG	-2.04	108.91	113.36
1	W	90	CSX	CA-CB-SG	-2.04	108.91	113.36
1	F	90	CSX	CA-CB-SG	-2.04	108.91	113.36
1	P	90	CSX	CA-CB-SG	-2.04	108.91	113.36
1	6	90	CSX	CA-CB-SG	-2.04	108.91	113.36
1	A	90	CSX	CA-CB-SG	-2.03	108.92	113.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 32 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 [i](#)

There are no chain breaks in this entry.

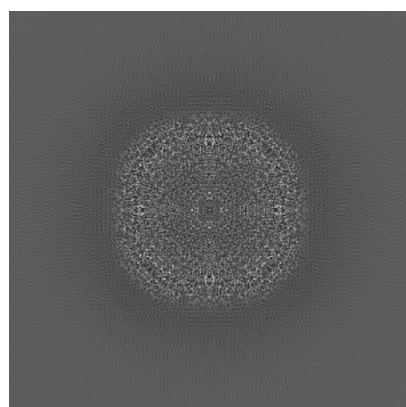
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11668. These allow visual inspection of the internal detail of the map and identification of artifacts.

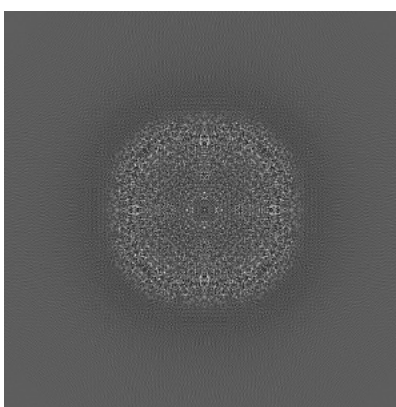
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

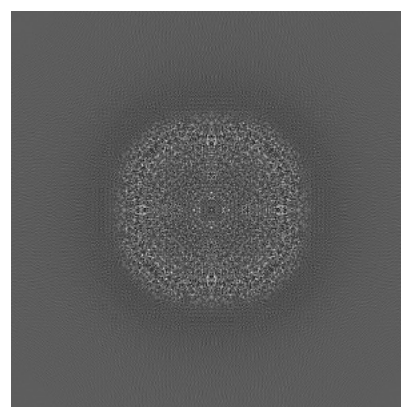
6.1.1 Primary map



X



Y

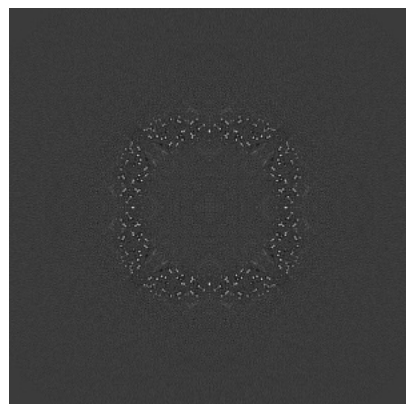


Z

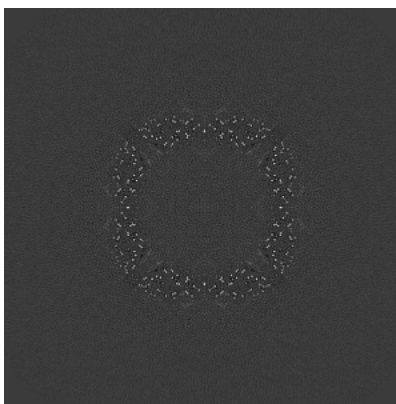
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

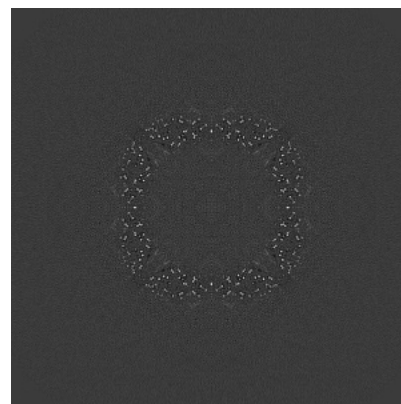
6.2.1 Primary map



X Index: 240



Y Index: 240

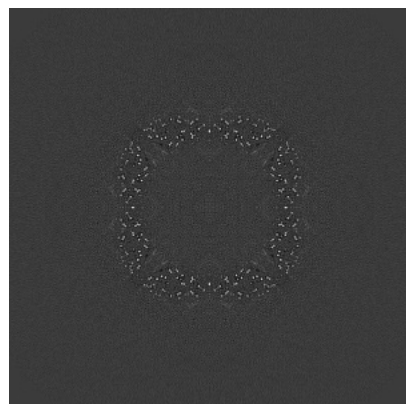


Z Index: 240

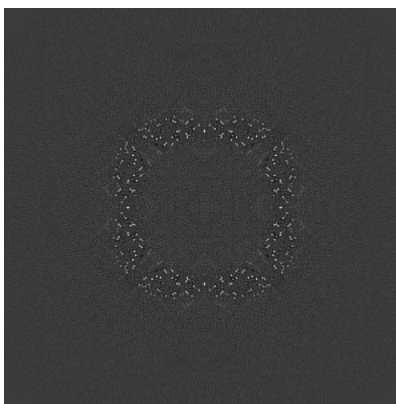
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

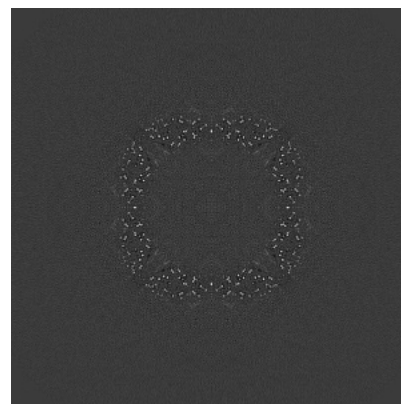
6.3.1 Primary map



X Index: 240



Y Index: 240

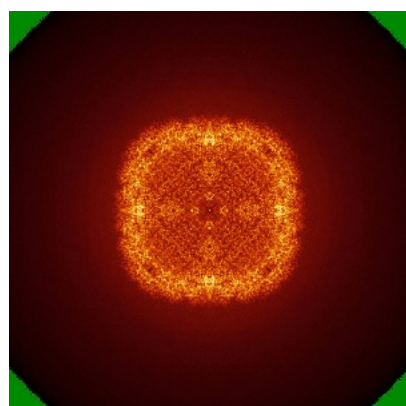


Z Index: 240

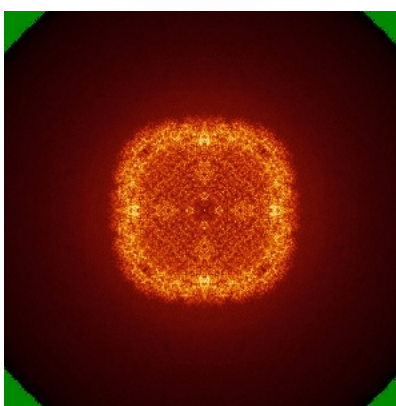
The images above show the largest variance slices of the map in three orthogonal directions.

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

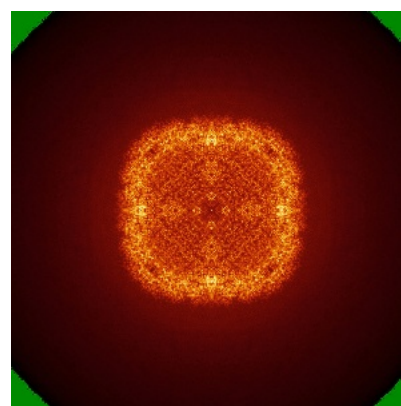
6.4.1 Primary map



X



Y

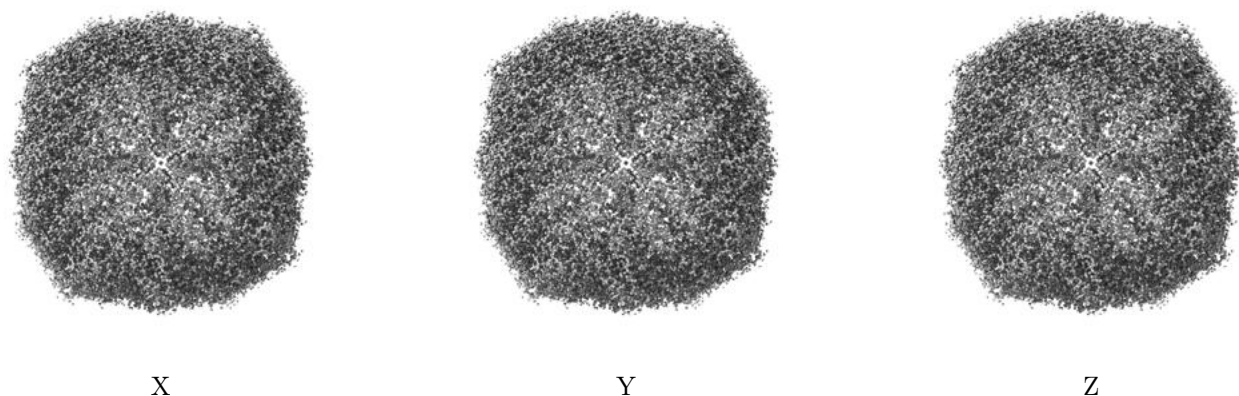


Z

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 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

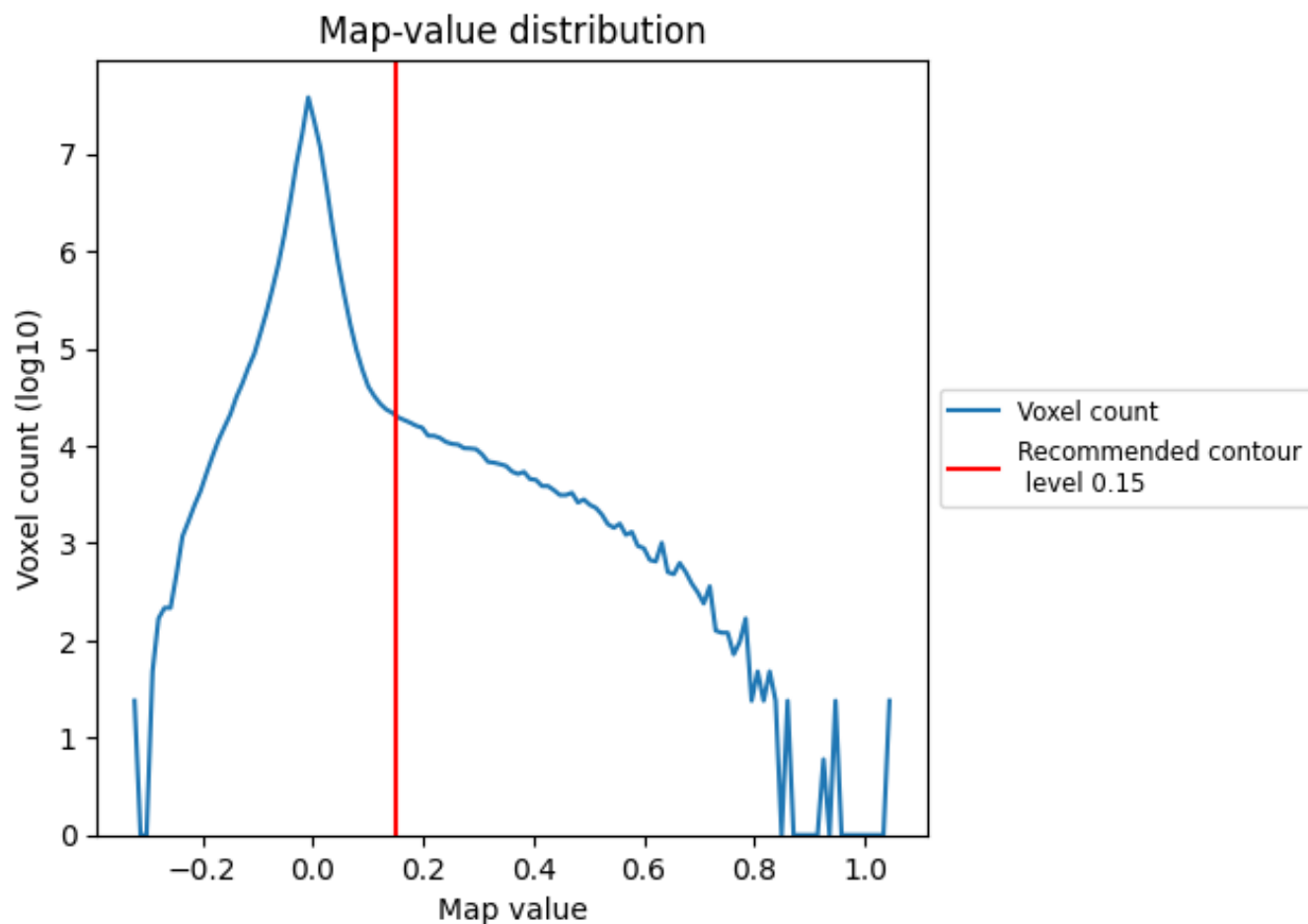
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

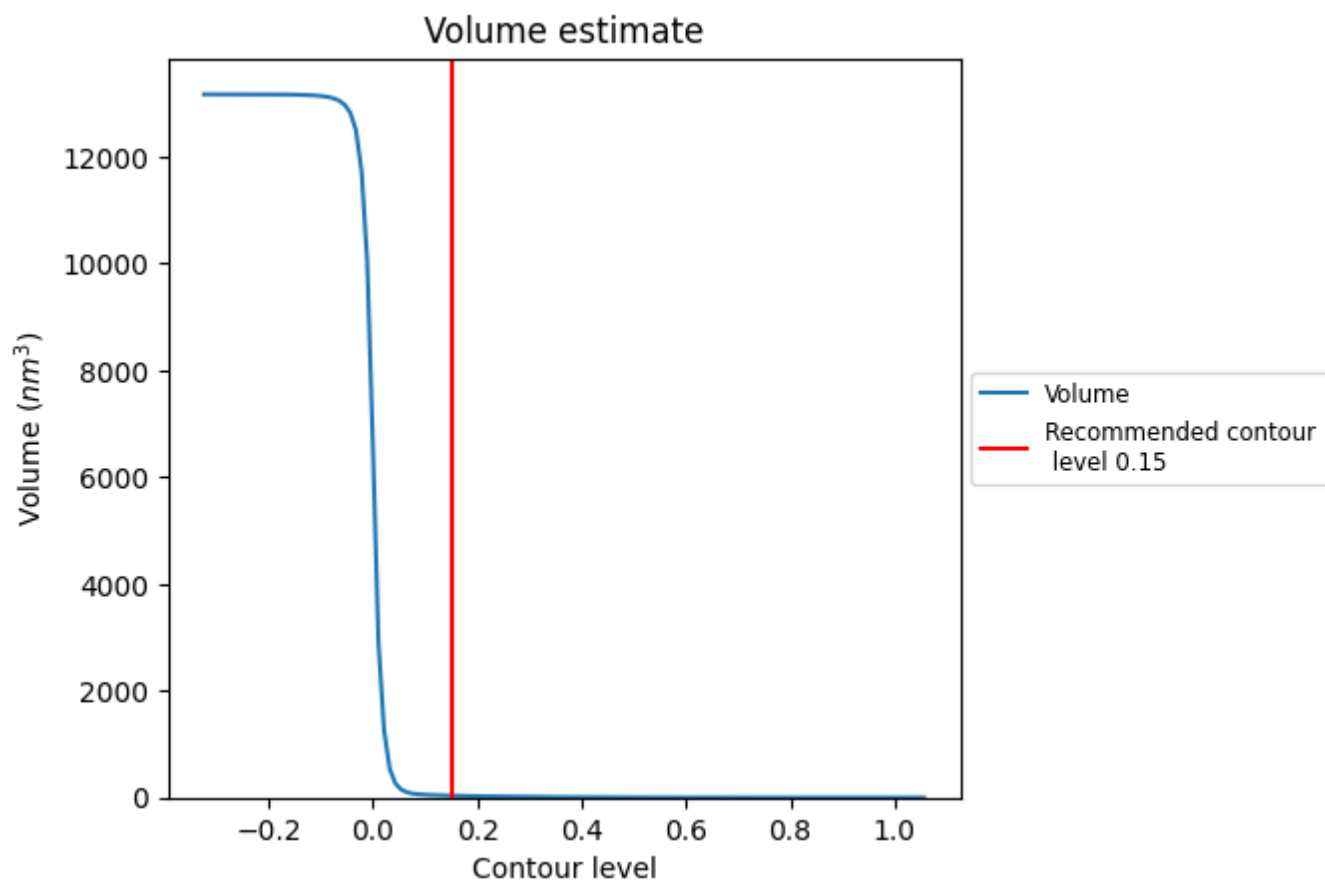
This section contains the results of statistical analysis of the map.

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.

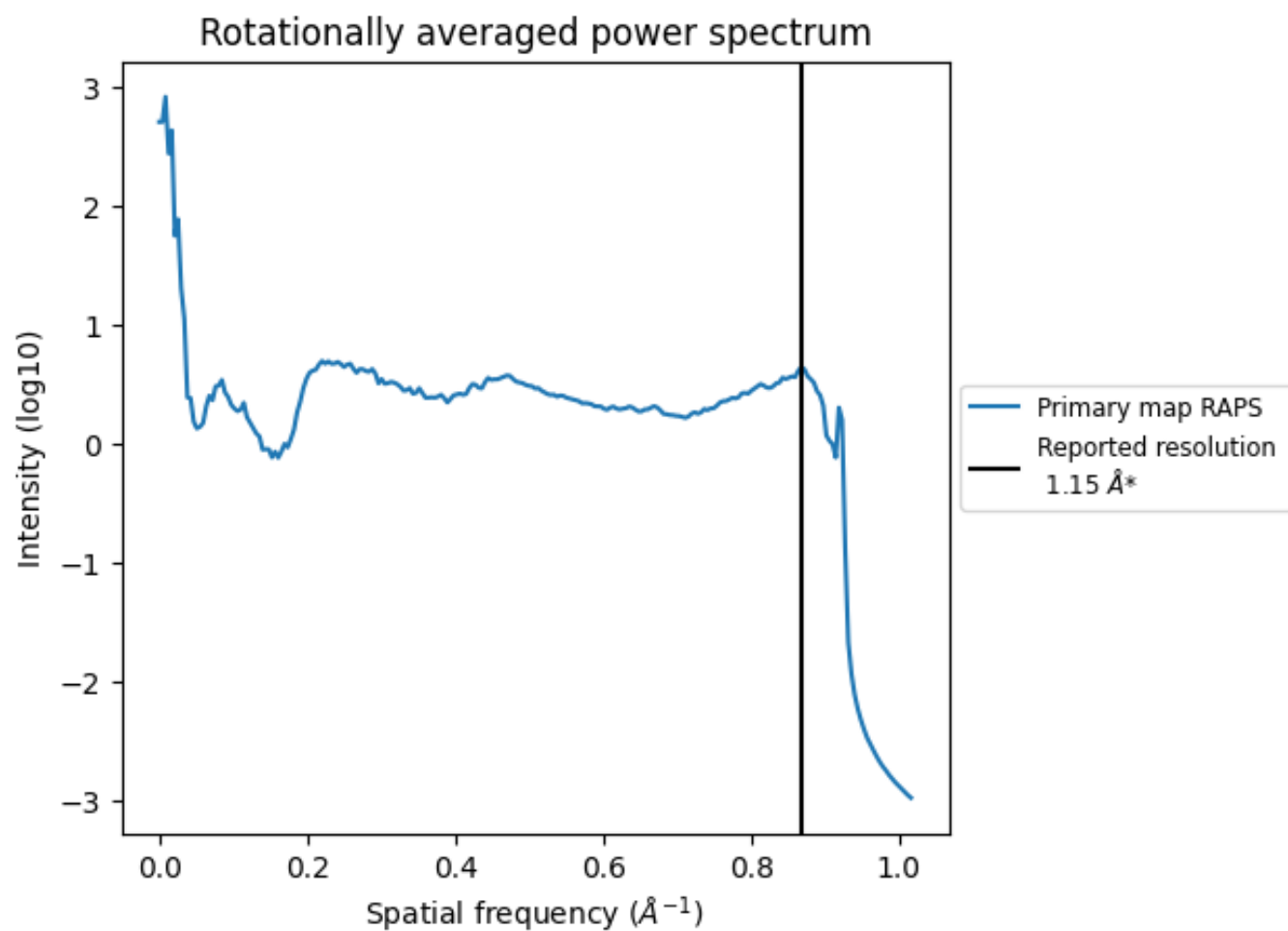
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 36 nm^3 ; this corresponds to an approximate mass of 32 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 0.870 Å⁻¹

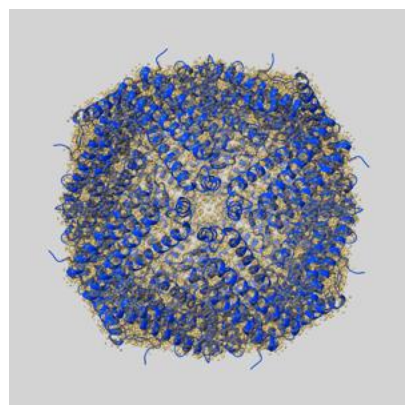
8 Fourier-Shell correlation ⓘ

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

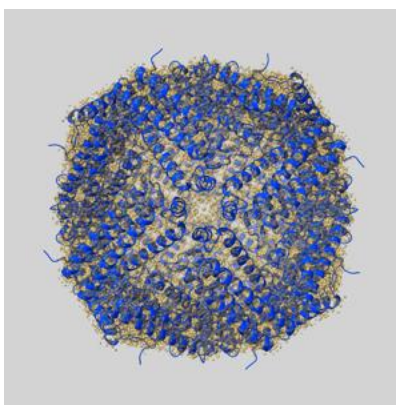
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11668 and PDB model 7A6A. Per-residue inclusion information can be found in section [3](#) on page [9](#).

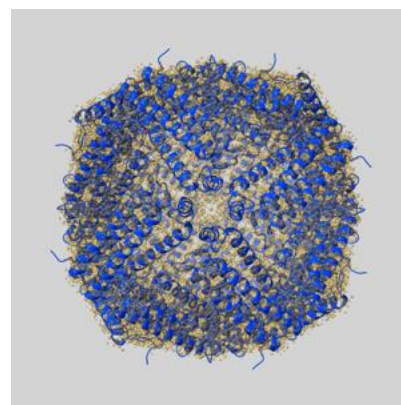
9.1 Map-model overlay [i](#)



X



Y



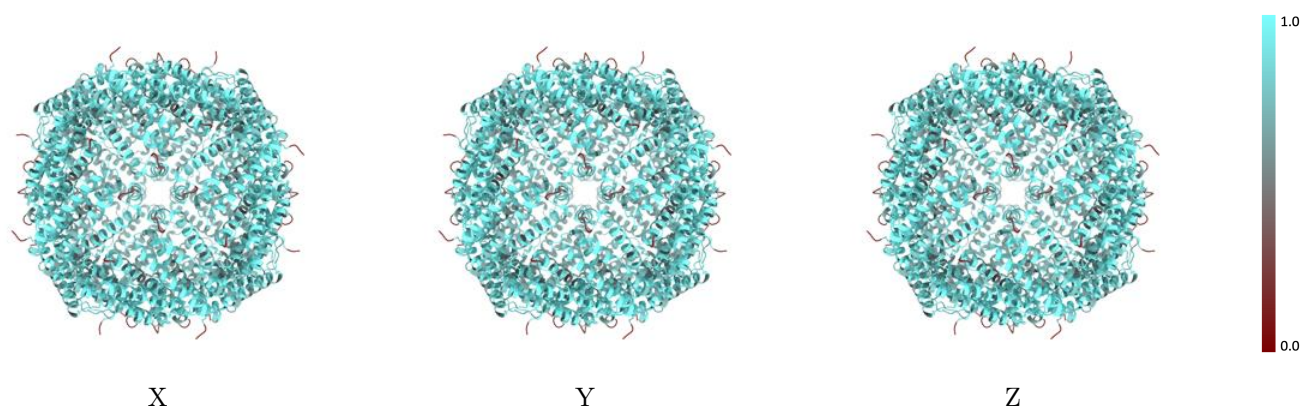
Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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

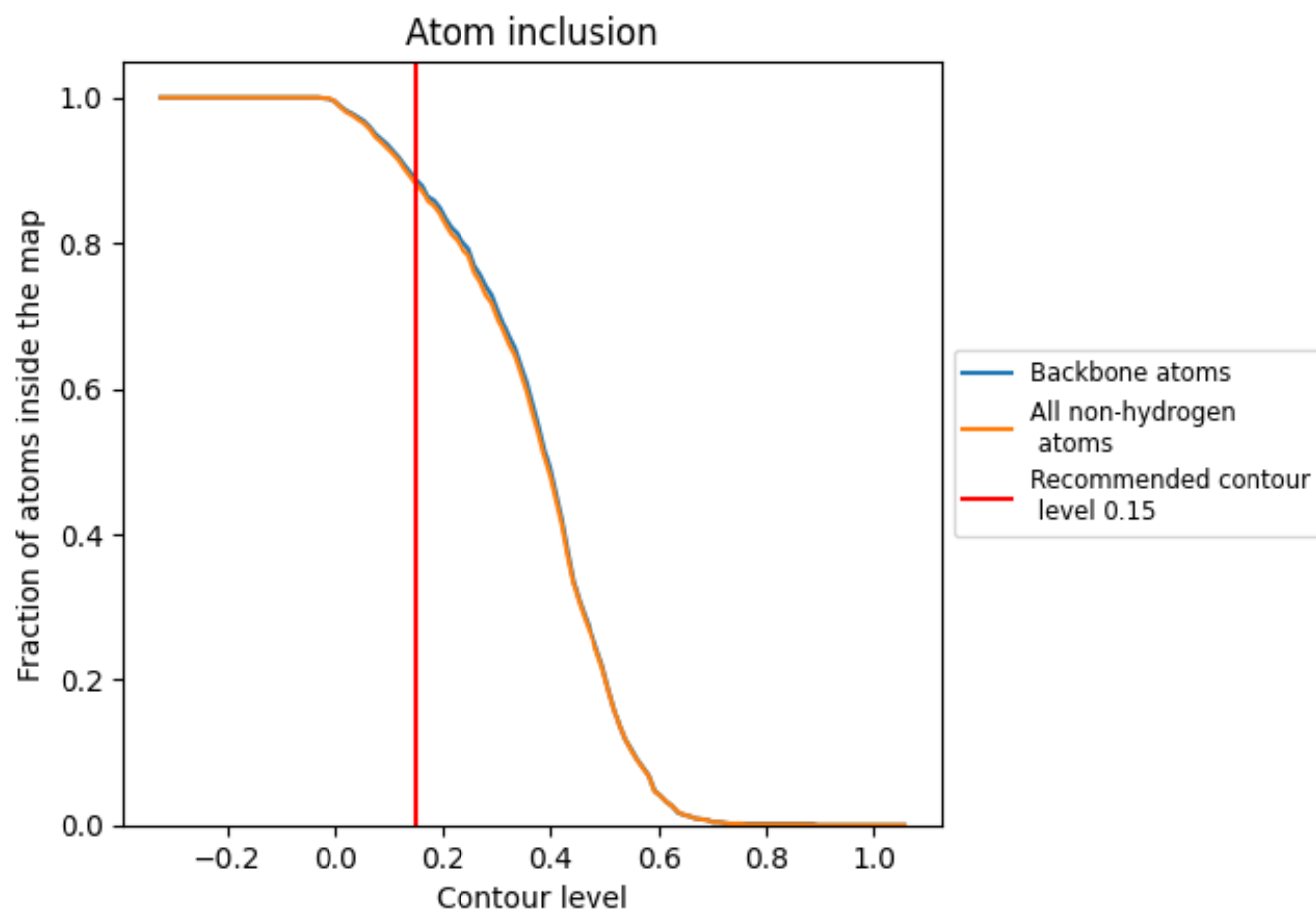
Q-score is only calculated for structures below 1.25 Å in resolution. The reported resolution for this entry is above 1.25 Å and so Q-score has not been calculated.

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 (0.15).

9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	<div></div> 0.8820
1	<div></div> 0.8830
2	<div></div> 0.8830
4	<div></div> 0.8830
6	<div></div> 0.8830
A	<div></div> 0.8830
B	<div></div> 0.8830
E	<div></div> 0.8830
F	<div></div> 0.8830
G	<div></div> 0.8830
H	<div></div> 0.8830
I	<div></div> 0.8830
K	<div></div> 0.8830
M	<div></div> 0.8830
O	<div></div> 0.8830
P	<div></div> 0.8830
Q	<div></div> 0.8830
S	<div></div> 0.8830
U	<div></div> 0.8830
W	<div></div> 0.8830
X	<div></div> 0.8830
Y	<div></div> 0.8830
a	<div></div> 0.8830
e	<div></div> 0.8830
r	<div></div> 0.8830

