wwPDB EM Validation Summary Report (i)

May 16, 2024 – 11:36 AM EDT

PDB ID	:	8V5K
EMDB ID	:	EMD-42983
Title	:	Structure of the Human Respirovirus 3 Fusion Protein Bound to Camelid Nanobodies 4C03 and 4C06
Authors	:	Johnson, N.V.; Ramamohan, A.R.; McLellan, J.S.
Deposited on	:	2023-11-30
Resolution	:	2.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

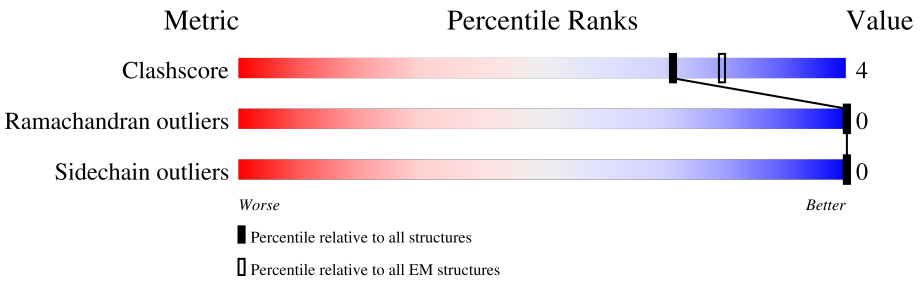
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=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	498	77% 7% 16%
1	B	498	77% 8% 16%
1	C	498	77% 7% 16%
2	D	124	5% 96%
2	E	124	93% 7%
2	F	124	6% 94% 6%
3	G	117	21% 84% 16%
3	H	117	21% 85% 15%

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Mol	Chain	Length	Quality of chain
3	I	117	24% 86% 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15336 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	419	3256	2061	557	622	16	0	0
1	B	419	3256	2061	557	622	16	0	0
1	C	419	3256	2061	557	622	16	0	0

There are 117 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	PRO	ILE	conflict	UNP T1UCV5
A	186	CYS	SER	conflict	UNP T1UCV5
A	195	CYS	ALA	conflict	UNP T1UCV5
A	198	LEU	GLN	conflict	UNP T1UCV5
A	201	LEU	ILE	conflict	UNP T1UCV5
A	204	ASP	THR	conflict	UNP T1UCV5
A	452	ASN	ASP	conflict	UNP T1UCV5
A	485	GLU	-	expression tag	UNP T1UCV5
A	486	ASP	-	expression tag	UNP T1UCV5
A	487	LYS	-	expression tag	UNP T1UCV5
A	488	ILE	-	expression tag	UNP T1UCV5
A	489	GLU	-	expression tag	UNP T1UCV5
A	490	GLU	-	expression tag	UNP T1UCV5
A	491	ILE	-	expression tag	UNP T1UCV5
A	492	LEU	-	expression tag	UNP T1UCV5
A	493	SER	-	expression tag	UNP T1UCV5
A	494	LYS	-	expression tag	UNP T1UCV5
A	495	ILE	-	expression tag	UNP T1UCV5
A	496	TYR	-	expression tag	UNP T1UCV5
A	497	HIS	-	expression tag	UNP T1UCV5
A	498	ILE	-	expression tag	UNP T1UCV5
A	499	GLU	-	expression tag	UNP T1UCV5
A	500	ASN	-	expression tag	UNP T1UCV5
A	501	GLU	-	expression tag	UNP T1UCV5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	502	ILE	-	expression tag	UNP T1UCV5
A	503	ALA	-	expression tag	UNP T1UCV5
A	504	ARG	-	expression tag	UNP T1UCV5
A	505	ILE	-	expression tag	UNP T1UCV5
A	506	LYS	-	expression tag	UNP T1UCV5
A	507	LYS	-	expression tag	UNP T1UCV5
A	508	LEU	-	expression tag	UNP T1UCV5
A	509	ILE	-	expression tag	UNP T1UCV5
A	510	GLY	-	expression tag	UNP T1UCV5
A	511	GLU	-	expression tag	UNP T1UCV5
A	512	ALA	-	expression tag	UNP T1UCV5
A	513	GLU	-	expression tag	UNP T1UCV5
A	514	PRO	-	expression tag	UNP T1UCV5
A	515	GLU	-	expression tag	UNP T1UCV5
A	516	ALA	-	expression tag	UNP T1UCV5
B	165	PRO	ILE	conflict	UNP T1UCV5
B	186	CYS	SER	conflict	UNP T1UCV5
B	195	CYS	ALA	conflict	UNP T1UCV5
B	198	LEU	GLN	conflict	UNP T1UCV5
B	201	LEU	ILE	conflict	UNP T1UCV5
B	204	ASP	THR	conflict	UNP T1UCV5
B	452	ASN	ASP	conflict	UNP T1UCV5
B	485	GLU	-	expression tag	UNP T1UCV5
B	486	ASP	-	expression tag	UNP T1UCV5
B	487	LYS	-	expression tag	UNP T1UCV5
B	488	ILE	-	expression tag	UNP T1UCV5
B	489	GLU	-	expression tag	UNP T1UCV5
B	490	GLU	-	expression tag	UNP T1UCV5
B	491	ILE	-	expression tag	UNP T1UCV5
B	492	LEU	-	expression tag	UNP T1UCV5
B	493	SER	-	expression tag	UNP T1UCV5
B	494	LYS	-	expression tag	UNP T1UCV5
B	495	ILE	-	expression tag	UNP T1UCV5
B	496	TYR	-	expression tag	UNP T1UCV5
B	497	HIS	-	expression tag	UNP T1UCV5
B	498	ILE	-	expression tag	UNP T1UCV5
B	499	GLU	-	expression tag	UNP T1UCV5
B	500	ASN	-	expression tag	UNP T1UCV5
B	501	GLU	-	expression tag	UNP T1UCV5
B	502	ILE	-	expression tag	UNP T1UCV5
B	503	ALA	-	expression tag	UNP T1UCV5
B	504	ARG	-	expression tag	UNP T1UCV5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	505	ILE	-	expression tag	UNP T1UCV5
B	506	LYS	-	expression tag	UNP T1UCV5
B	507	LYS	-	expression tag	UNP T1UCV5
B	508	LEU	-	expression tag	UNP T1UCV5
B	509	ILE	-	expression tag	UNP T1UCV5
B	510	GLY	-	expression tag	UNP T1UCV5
B	511	GLU	-	expression tag	UNP T1UCV5
B	512	ALA	-	expression tag	UNP T1UCV5
B	513	GLU	-	expression tag	UNP T1UCV5
B	514	PRO	-	expression tag	UNP T1UCV5
B	515	GLU	-	expression tag	UNP T1UCV5
B	516	ALA	-	expression tag	UNP T1UCV5
C	165	PRO	ILE	conflict	UNP T1UCV5
C	186	CYS	SER	conflict	UNP T1UCV5
C	195	CYS	ALA	conflict	UNP T1UCV5
C	198	LEU	GLN	conflict	UNP T1UCV5
C	201	LEU	ILE	conflict	UNP T1UCV5
C	204	ASP	THR	conflict	UNP T1UCV5
C	452	ASN	ASP	conflict	UNP T1UCV5
C	485	GLU	-	expression tag	UNP T1UCV5
C	486	ASP	-	expression tag	UNP T1UCV5
C	487	LYS	-	expression tag	UNP T1UCV5
C	488	ILE	-	expression tag	UNP T1UCV5
C	489	GLU	-	expression tag	UNP T1UCV5
C	490	GLU	-	expression tag	UNP T1UCV5
C	491	ILE	-	expression tag	UNP T1UCV5
C	492	LEU	-	expression tag	UNP T1UCV5
C	493	SER	-	expression tag	UNP T1UCV5
C	494	LYS	-	expression tag	UNP T1UCV5
C	495	ILE	-	expression tag	UNP T1UCV5
C	496	TYR	-	expression tag	UNP T1UCV5
C	497	HIS	-	expression tag	UNP T1UCV5
C	498	ILE	-	expression tag	UNP T1UCV5
C	499	GLU	-	expression tag	UNP T1UCV5
C	500	ASN	-	expression tag	UNP T1UCV5
C	501	GLU	-	expression tag	UNP T1UCV5
C	502	ILE	-	expression tag	UNP T1UCV5
C	503	ALA	-	expression tag	UNP T1UCV5
C	504	ARG	-	expression tag	UNP T1UCV5
C	505	ILE	-	expression tag	UNP T1UCV5
C	506	LYS	-	expression tag	UNP T1UCV5
C	507	LYS	-	expression tag	UNP T1UCV5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	508	LEU	-	expression tag	UNP T1UCV5
C	509	ILE	-	expression tag	UNP T1UCV5
C	510	GLY	-	expression tag	UNP T1UCV5
C	511	GLU	-	expression tag	UNP T1UCV5
C	512	ALA	-	expression tag	UNP T1UCV5
C	513	GLU	-	expression tag	UNP T1UCV5
C	514	PRO	-	expression tag	UNP T1UCV5
C	515	GLU	-	expression tag	UNP T1UCV5
C	516	ALA	-	expression tag	UNP T1UCV5

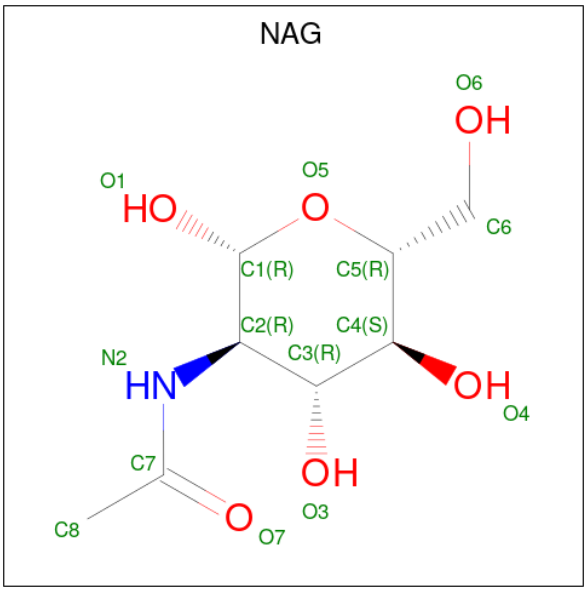
- Molecule 2 is a protein called Camelid Nanobody 4C03.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	124	966	607	174	181	4	0	0
2	E	124	966	607	174	181	4	0	0
2	F	124	966	607	174	181	4	0	0

- Molecule 3 is a protein called Camelid Nanobody 4C06.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	117	876	542	153	178	3	0	0
3	H	117	876	542	153	178	3	0	0
3	I	117	876	542	153	178	3	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



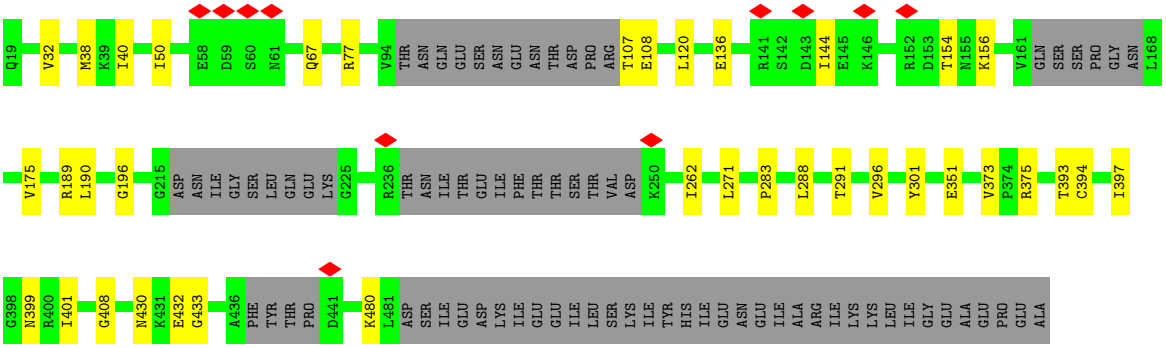
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	14	8	1	5	0
4	B	1	14	8	1	5	0
4	C	1	14	8	1	5	0

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.

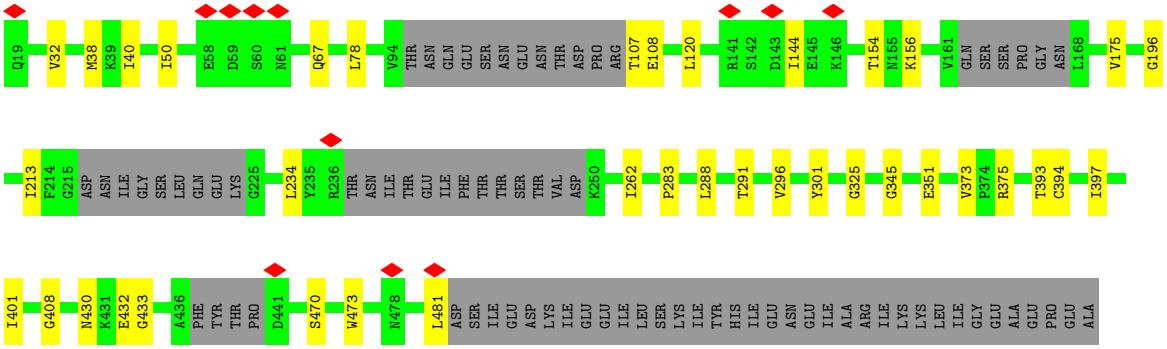
- Molecule 1: Fusion glycoprotein F0

Chain A:



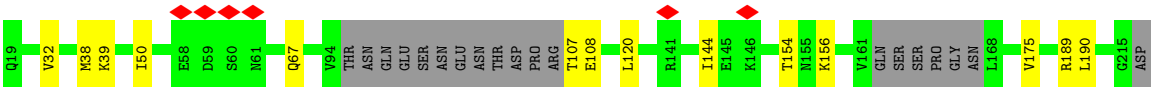
- Molecule 1: Fusion glycoprotein F0

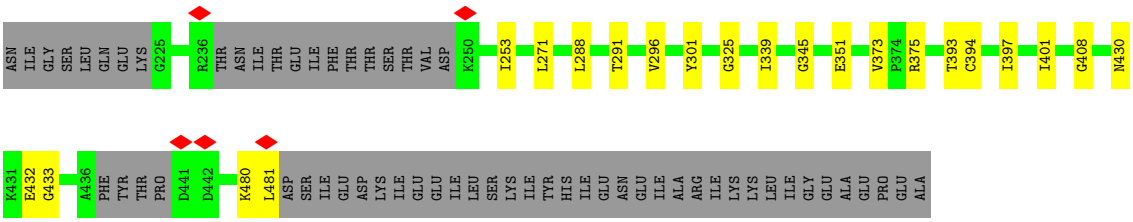
Chain B:



- Molecule 1: Fusion glycoprotein F0

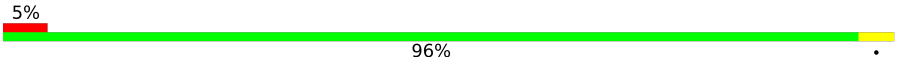
Chain C:

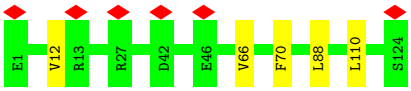




• Molecule 2: Camelid Nanobody 4C03

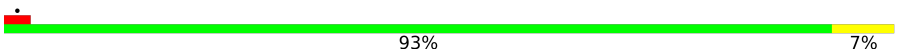
Chain D:

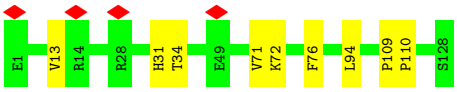




• Molecule 2: Camelid Nanobody 4C03

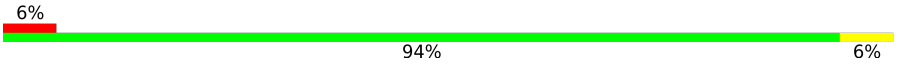
Chain E:

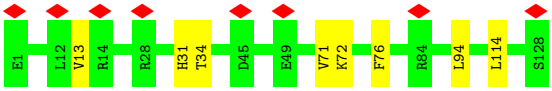




• Molecule 2: Camelid Nanobody 4C03

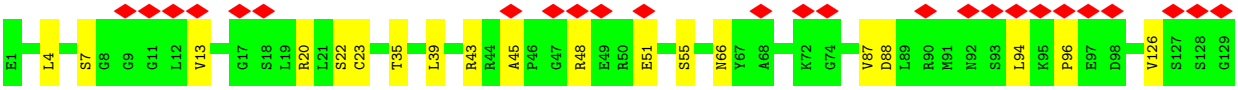
Chain F:





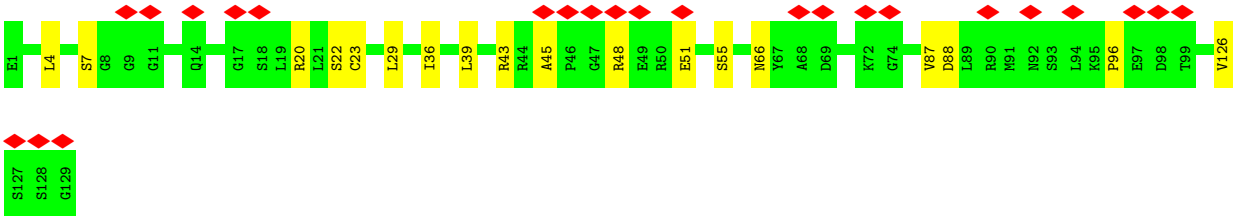
• Molecule 3: Camelid Nanobody 4C06

Chain G:



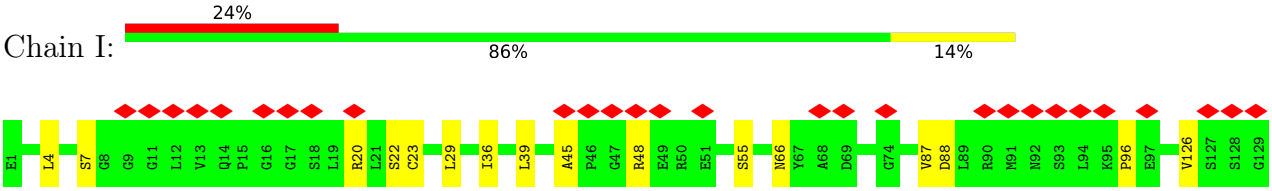
• Molecule 3: Camelid Nanobody 4C06

Chain H:



• Molecule 3: Camelid Nanobody 4C06

Chain I:


24%
86%
14%
E1
L4
S7
G8
G9
G11
L12
V13
Q14
P15
G16
G17
S18
L19
R20
L21
S22
C23
L29
I36
L39
A45
P46
G47
R48
E49
R50
E51
S55
N66
Y67
A68
D69
G74
V87
D88
L89
R90
M91
N92
S93
L94
K95
P96
E97
V126
S127
S128
G129

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	336418	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.525	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	300.8, 300.8, 300.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93999994, 0.93999994, 0.93999994	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.38	0/3297	0.51	0/4460
1	B	0.37	0/3297	0.51	1/4460 (0.0%)
1	C	0.37	0/3297	0.50	0/4460
2	D	0.37	0/989	0.50	0/1343
2	E	0.38	0/989	0.51	0/1343
2	F	0.37	0/989	0.50	0/1343
3	G	0.35	0/890	0.51	0/1206
3	H	0.34	0/890	0.51	0/1206
3	I	0.32	0/890	0.50	0/1206
All	All	0.37	0/15528	0.51	1/21027 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	78	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3256	0	3329	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3256	0	3329	26	0
1	C	3256	0	3329	26	0
2	D	966	0	937	3	0
2	E	966	0	937	5	0
2	F	966	0	937	5	0
3	G	876	0	855	10	0
3	H	876	0	855	9	0
3	I	876	0	855	8	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
All	All	15336	0	15402	108	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 4.

The worst 5 of 108 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)
1:A:154:THR:HG22	1:A:156:LYS:H	1.48	0.79
1:B:154:THR:HG22	1:B:156:LYS:H	1.48	0.77
1:C:154:THR:HG22	1:C:156:LYS:H	1.49	0.76
1:A:38:MET:HE2	1:A:291:THR:HG21	1.78	0.66
1:C:393:THR:HG21	1:C:397:ILE:HA	1.81	0.63

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	407/498 (82%)	402 (99%)	5 (1%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	407/498 (82%)	401 (98%)	6 (2%)	0	100	100
1	C	407/498 (82%)	403 (99%)	4 (1%)	0	100	100
2	D	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
2	E	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
2	F	122/124 (98%)	121 (99%)	1 (1%)	0	100	100
3	G	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
3	H	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
3	I	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
All	All	1932/2217 (87%)	1908 (99%)	24 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	A	369/442 (84%)	369 (100%)	0	100	100
1	B	369/442 (84%)	369 (100%)	0	100	100
1	C	369/442 (84%)	369 (100%)	0	100	100
2	D	100/100 (100%)	100 (100%)	0	100	100
2	E	100/100 (100%)	100 (100%)	0	100	100
2	F	100/100 (100%)	100 (100%)	0	100	100
3	G	94/94 (100%)	94 (100%)	0	100	100
3	H	94/94 (100%)	94 (100%)	0	100	100
3	I	94/94 (100%)	94 (100%)	0	100	100
All	All	1689/1908 (88%)	1689 (100%)	0	100	100

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

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

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)

3 ligands 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	$\#\|Z\| > 2$
4	NAG	A	601	1	14,14,15	0.17	0	17,19,21	0.72	1 (5%)
4	NAG	B	601	1	14,14,15	0.34	0	17,19,21	0.88	1 (5%)
4	NAG	C	601	1	14,14,15	0.25	0	17,19,21	0.82	1 (5%)

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
4	NAG	A	601	1	-	2/6/23/26	0/1/1/1
4	NAG	B	601	1	-	2/6/23/26	0/1/1/1
4	NAG	C	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	601	NAG	C1-O5-C5	3.31	116.68	112.19
4	C	601	NAG	C1-O5-C5	3.01	116.27	112.19
4	A	601	NAG	C1-O5-C5	2.63	115.76	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	O5-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6
4	C	601	NAG	C4-C5-C6-O6
4	B	601	NAG	C4-C5-C6-O6
4	C	601	NAG	O5-C5-C6-O6

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.

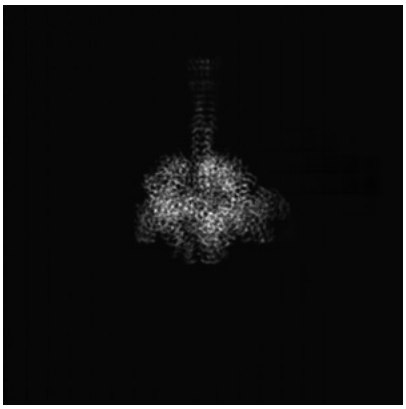
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-42983. These allow visual inspection of the internal detail of the map and identification of artifacts.

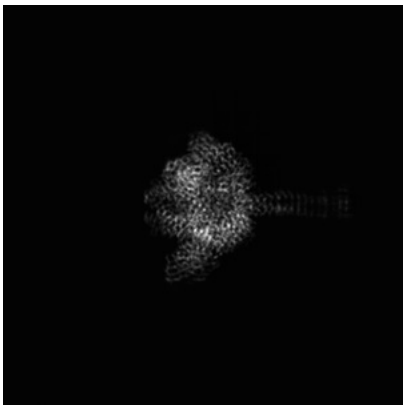
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

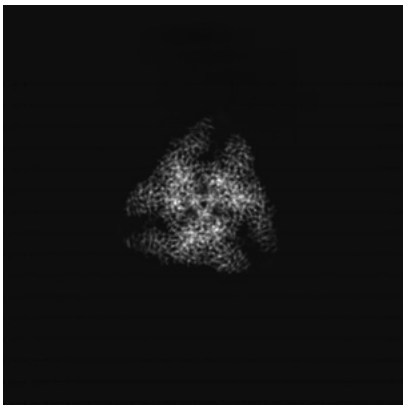
6.1.1 Primary map



X

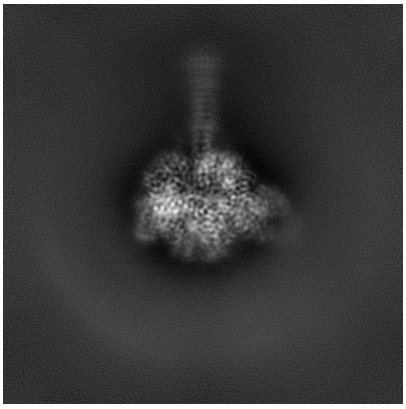


Y

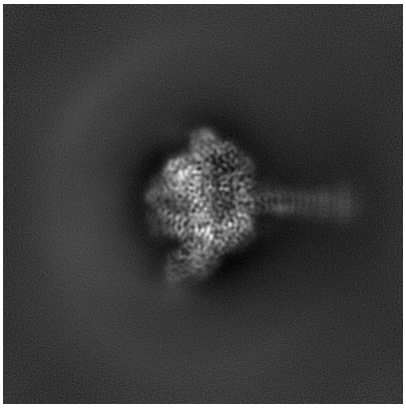


Z

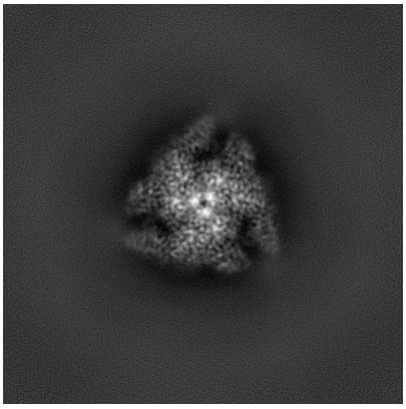
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

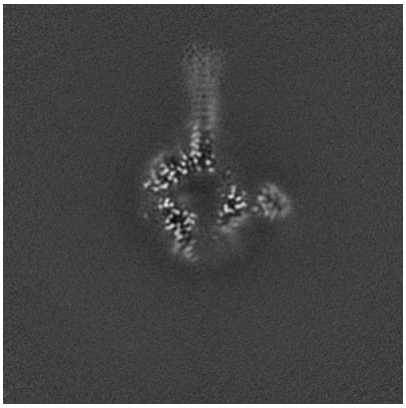
6.2.1 Primary map

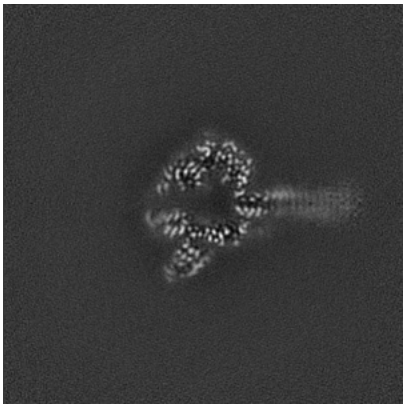
X Index: 160

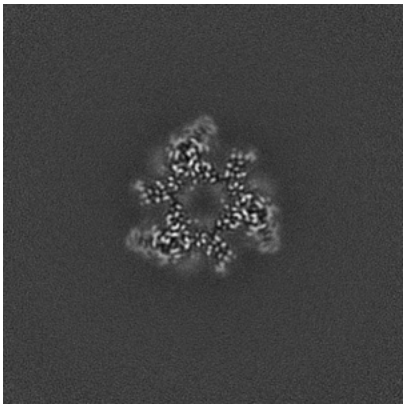
Y Index: 160

Z Index: 160

6.2.2 Raw map


X Index: 160


Y Index: 160


Z Index: 160

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

6.3 Largest variance slices (i)

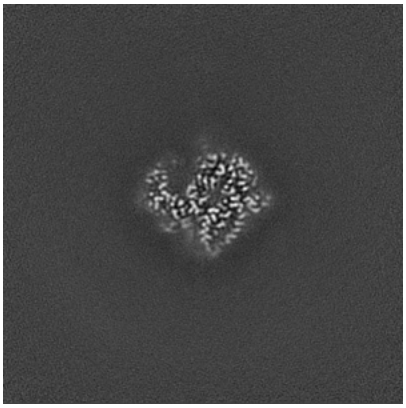
6.3.1 Primary map

X Index: 140

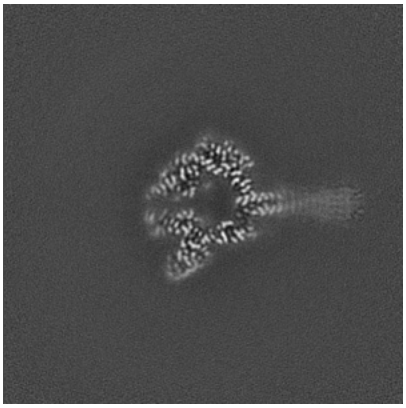
Y Index: 164

Z Index: 153

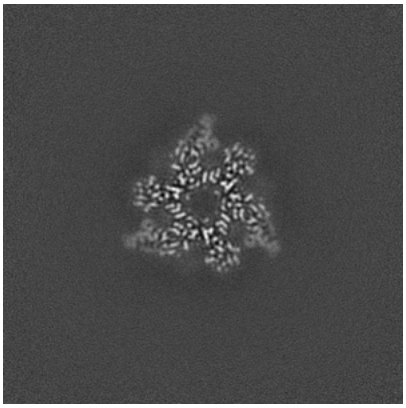
6.3.2 Raw map



X Index: 139



Y Index: 164

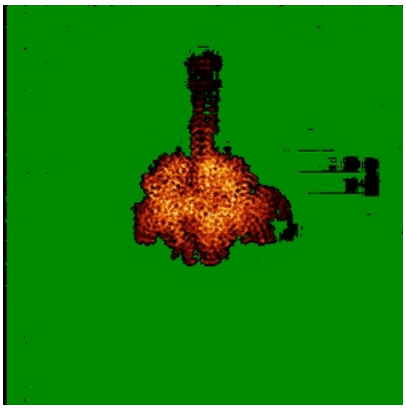


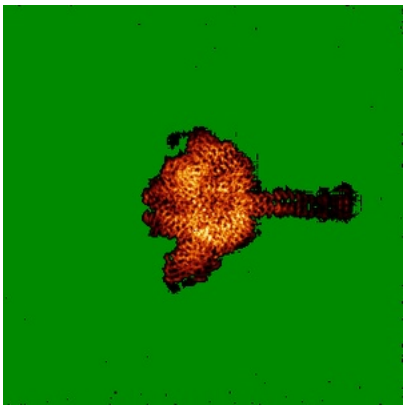
Z Index: 154

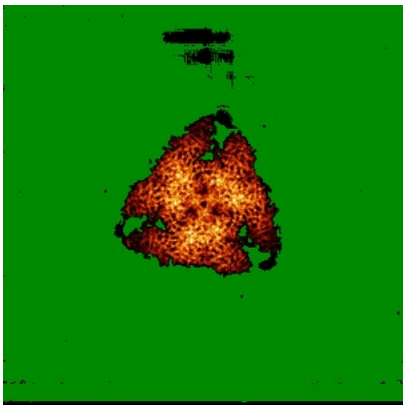
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

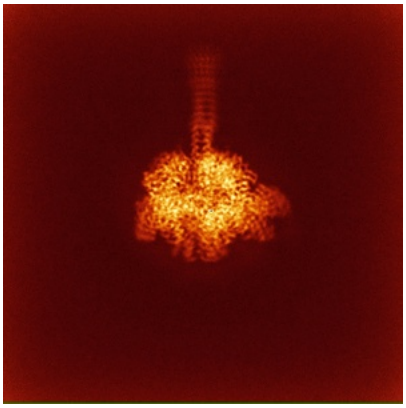
6.4.1 Primary map

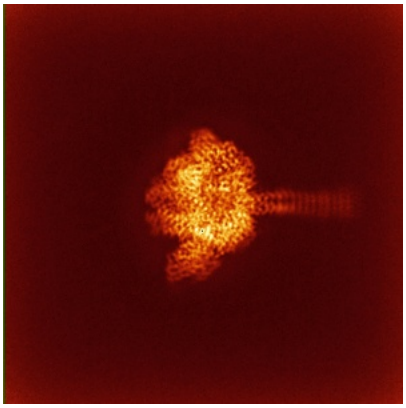

X

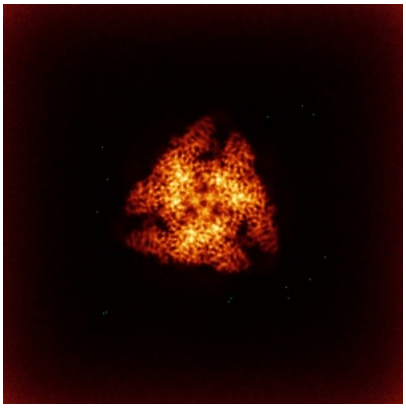

Y


Z

6.4.2 Raw map


X


Y


Z

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

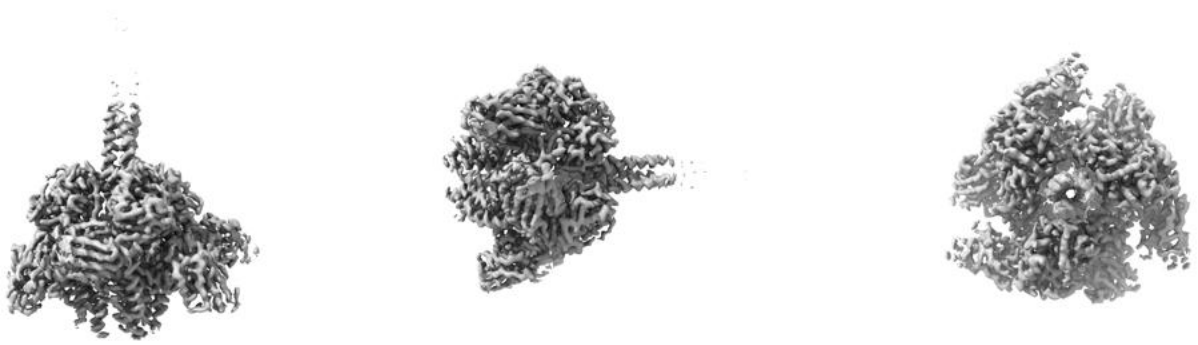
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

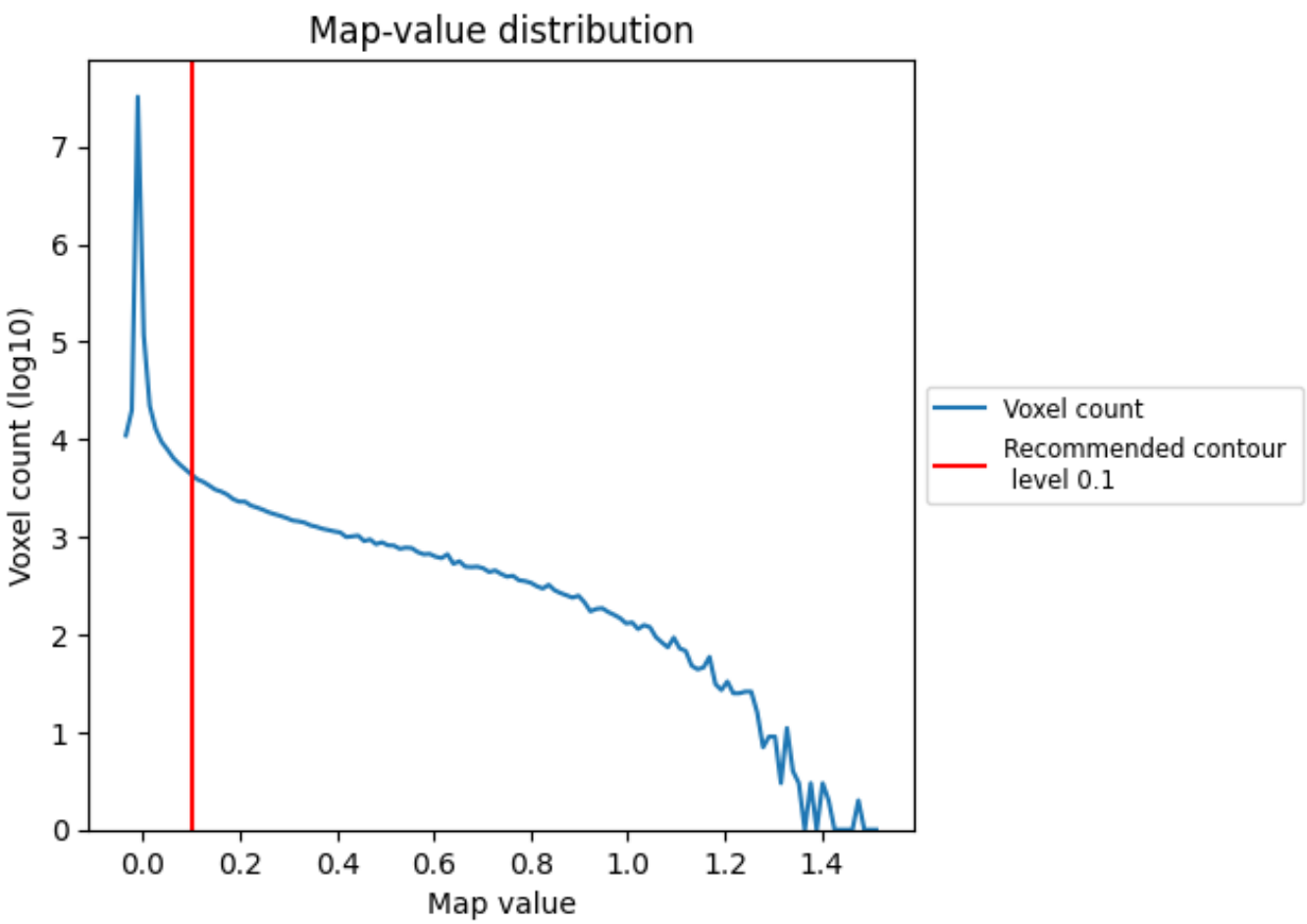
6.6 Mask visualisation (i)

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

7 Map analysis (i)

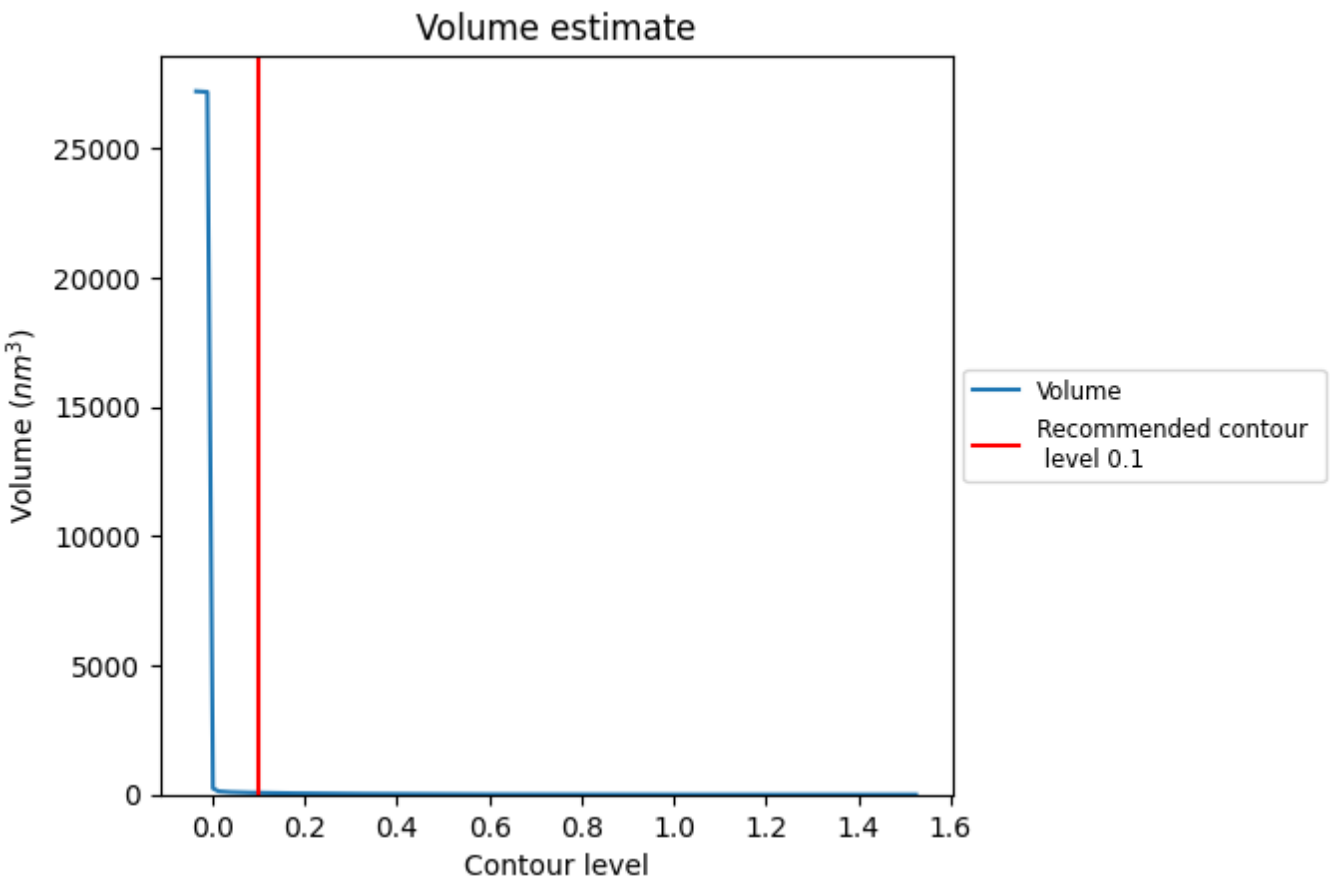
This section contains the results of statistical analysis of the map.

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.

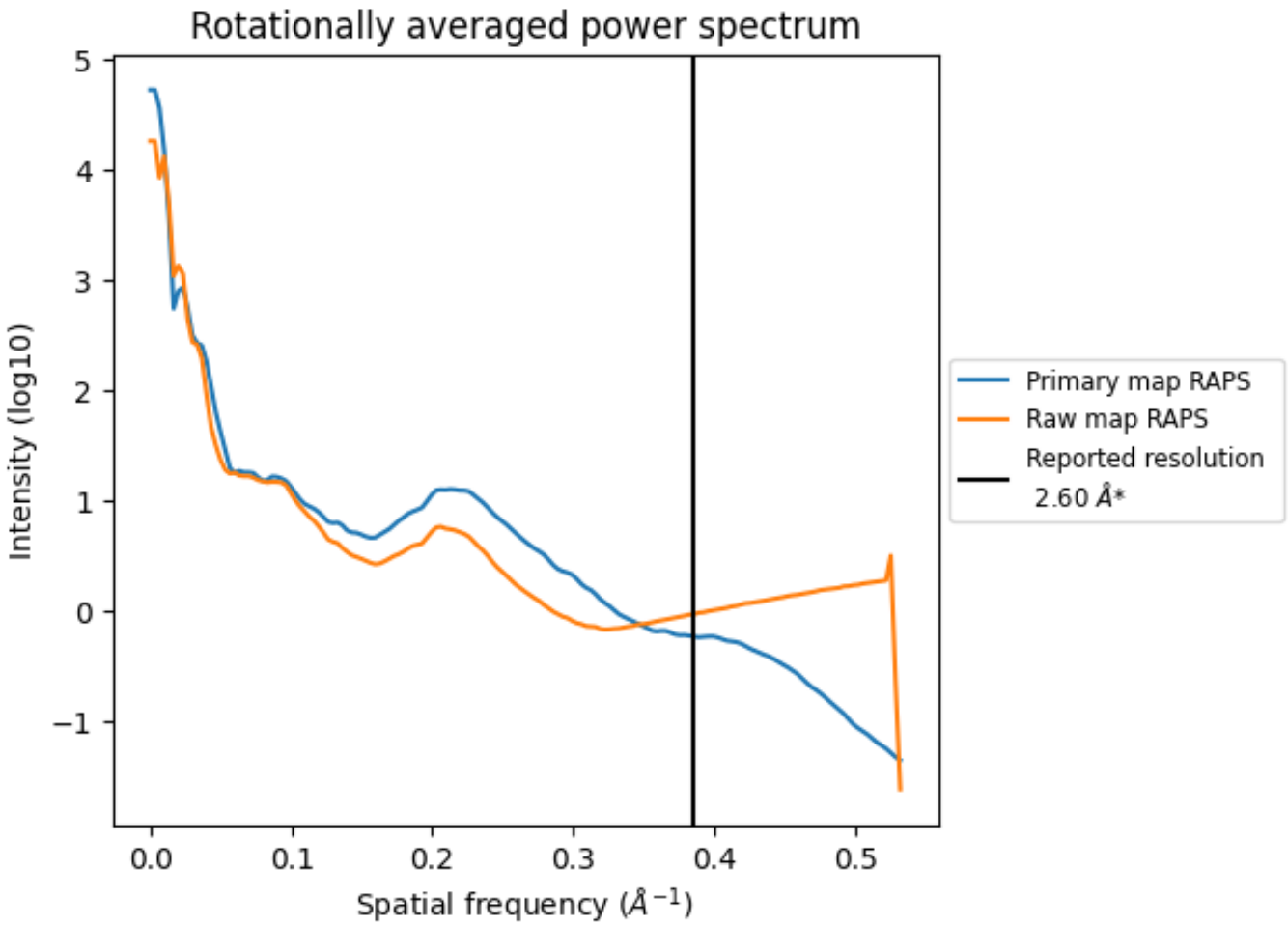
7.2 Volume estimate (i)



The volume at the recommended contour level is 67 nm^3; this corresponds to an approximate mass of 61 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 (i)

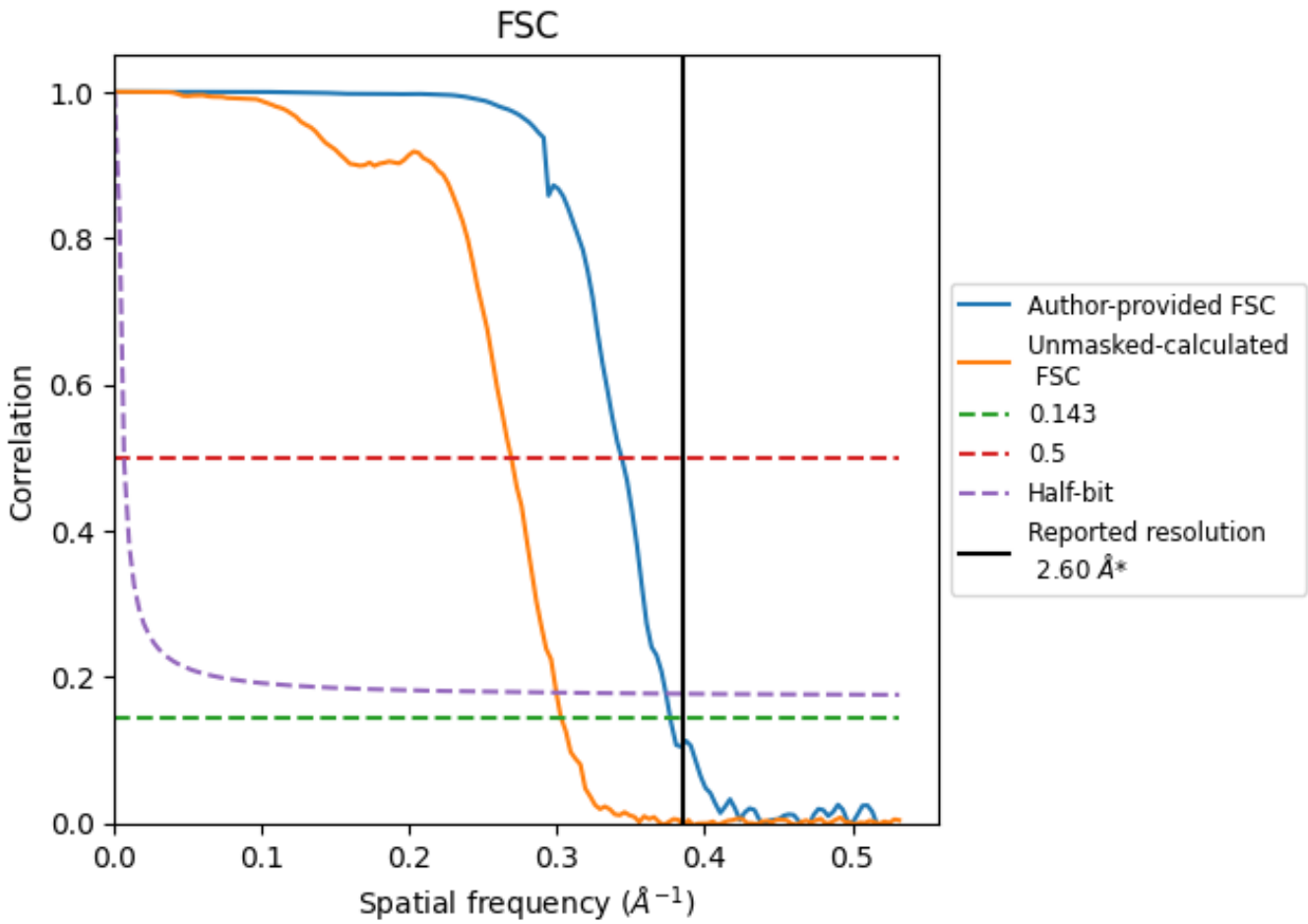


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8.2 Resolution estimates (i)

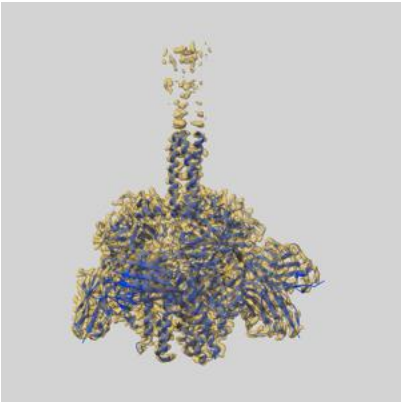
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.65	2.91	2.68
Unmasked-calculated*	3.30	3.72	3.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.30 differs from the reported value 2.6 by more than 10 %

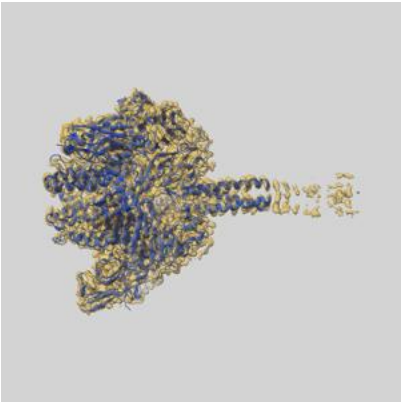
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-42983 and PDB model 8V5K. Per-residue inclusion information can be found in section 3 on page 9.

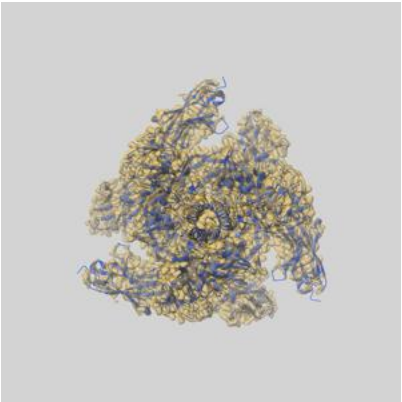
9.1 Map-model overlay (i)



X



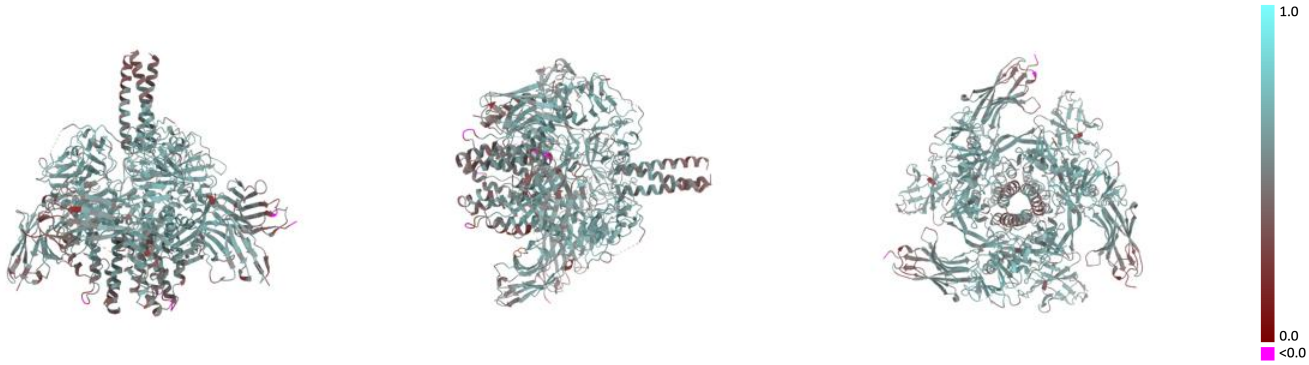
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

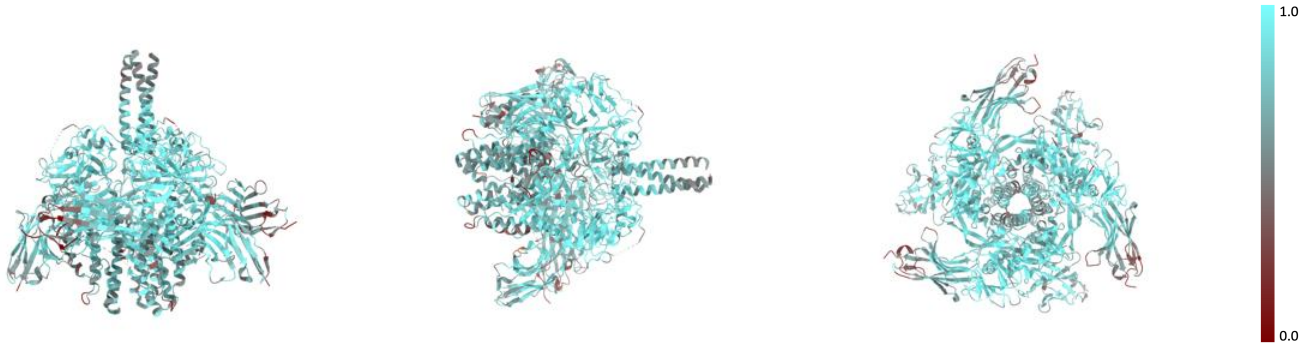
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

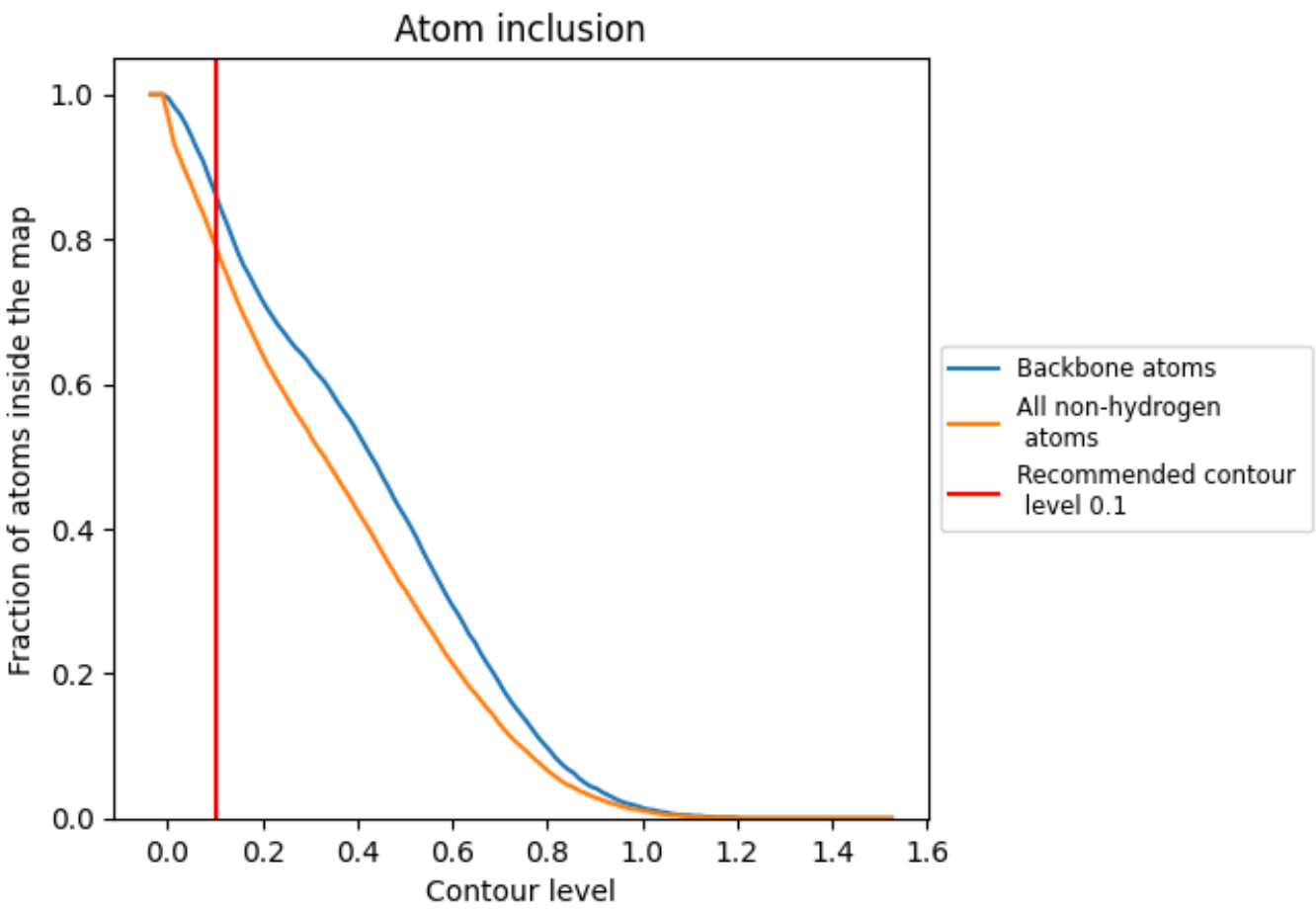
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7920	0.5520
A	0.8290	0.5680
B	0.8260	0.5690
C	0.8340	0.5750
D	0.7830	0.5490
E	0.7940	0.5450
F	0.7690	0.5470
G	0.6770	0.4920
H	0.6570	0.4870
I	0.6530	0.4870