



wwPDB EM Validation Summary Report ⓘ

Oct 5, 2024 – 09:18 am BST

PDB ID : 9FGQ
EMDB ID : EMD-50416
Title : Structure of human APC3loop 375-381 bound to the NCP
Authors : Young, R.V.C.; Muhammad, R.; Alfieri, C.
Deposited on : 2024-05-24
Resolution : 2.50 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 ⓘ 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

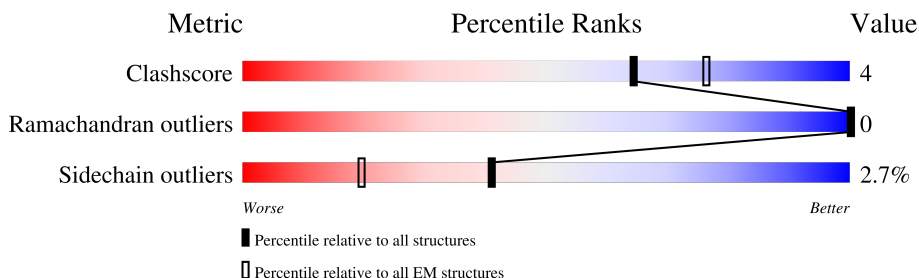
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

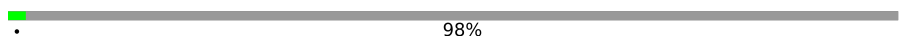
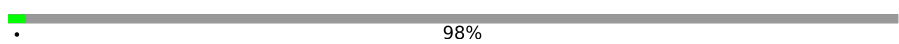






The reported resolution of this entry is 2.50 Å.

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.





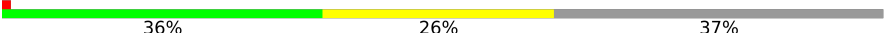
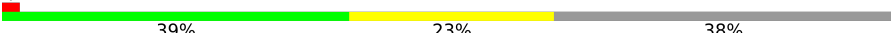
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	K	317	 98%
1	L	317	 98%
2	A	136	 65% 5% 30%
2	E	136	 66% 31%
3	B	103	 74% 22%
3	F	103	 71% 6% 23%
4	C	130	 76% 5% 18%
4	G	130	 80% 18%

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Mol	Chain	Length	Quality of chain
5	D	273	 31% 66%
5	H	273	 32% 66%
6	I	211	 36% 26% 37%
7	J	211	 39% 23% 38%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11519 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 Cell division cycle protein 27 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	K	7	Total	C	N	O	0	0
			60	35	16	9		
1	L	7	Total	C	N	O	0	0
			60	35	16	9		

There are 94 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	172	GLY	-	expression tag	UNP P30260
K	173	GLY	-	expression tag	UNP P30260
K	174	SER	-	expression tag	UNP P30260
K	175	ALA	-	expression tag	UNP P30260
K	446	GLY	-	expression tag	UNP P30260
K	447	SER	-	expression tag	UNP P30260
K	448	ALA	-	expression tag	UNP P30260
K	449	GLY	-	expression tag	UNP P30260
K	450	SER	-	expression tag	UNP P30260
K	451	ALA	-	expression tag	UNP P30260
K	452	GLY	-	expression tag	UNP P30260
K	453	SER	-	expression tag	UNP P30260
K	454	ALA	-	expression tag	UNP P30260
K	455	GLY	-	expression tag	UNP P30260
K	456	SER	-	expression tag	UNP P30260
K	457	ALA	-	expression tag	UNP P30260
K	458	GLY	-	expression tag	UNP P30260
K	459	SER	-	expression tag	UNP P30260
K	460	ALA	-	expression tag	UNP P30260
K	461	GLY	-	expression tag	UNP P30260
K	462	SER	-	expression tag	UNP P30260
K	463	ALA	-	expression tag	UNP P30260
K	464	GLY	-	expression tag	UNP P30260
K	465	SER	-	expression tag	UNP P30260
K	466	ALA	-	expression tag	UNP P30260
K	467	GLY	-	expression tag	UNP P30260

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Chain	Residue	Modelled	Actual	Comment	Reference
K	468	SER	-	expression tag	UNP P30260
K	469	ALA	-	expression tag	UNP P30260
K	470	GLY	-	expression tag	UNP P30260
K	471	SER	-	expression tag	UNP P30260
K	472	ALA	-	expression tag	UNP P30260
K	473	ARG	-	expression tag	UNP P30260
K	474	GLY	-	expression tag	UNP P30260
K	475	VAL	-	expression tag	UNP P30260
K	476	PRO	-	expression tag	UNP P30260
K	477	HIS	-	expression tag	UNP P30260
K	478	ILE	-	expression tag	UNP P30260
K	479	VAL	-	expression tag	UNP P30260
K	480	MET	-	expression tag	UNP P30260
K	481	VAL	-	expression tag	UNP P30260
K	482	ASP	-	expression tag	UNP P30260
K	483	ALA	-	expression tag	UNP P30260
K	484	TYR	-	expression tag	UNP P30260
K	485	LYS	-	expression tag	UNP P30260
K	486	ARG	-	expression tag	UNP P30260
K	487	TYR	-	expression tag	UNP P30260
K	488	LYS	-	expression tag	UNP P30260
L	173	GLY	-	expression tag	UNP P30260
L	174	GLY	-	expression tag	UNP P30260
L	175	SER	-	expression tag	UNP P30260
L	176	ALA	-	expression tag	UNP P30260
L	447	GLY	-	expression tag	UNP P30260
L	448	SER	-	expression tag	UNP P30260
L	449	ALA	-	expression tag	UNP P30260
L	450	GLY	-	expression tag	UNP P30260
L	451	SER	-	expression tag	UNP P30260
L	452	ALA	-	expression tag	UNP P30260
L	453	GLY	-	expression tag	UNP P30260
L	454	SER	-	expression tag	UNP P30260
L	455	ALA	-	expression tag	UNP P30260
L	456	GLY	-	expression tag	UNP P30260
L	457	SER	-	expression tag	UNP P30260
L	458	ALA	-	expression tag	UNP P30260
L	459	GLY	-	expression tag	UNP P30260
L	460	SER	-	expression tag	UNP P30260
L	461	ALA	-	expression tag	UNP P30260
L	462	GLY	-	expression tag	UNP P30260
L	463	SER	-	expression tag	UNP P30260

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Chain	Residue	Modelled	Actual	Comment	Reference
L	464	ALA	-	expression tag	UNP P30260
L	465	GLY	-	expression tag	UNP P30260
L	466	SER	-	expression tag	UNP P30260
L	467	ALA	-	expression tag	UNP P30260
L	468	GLY	-	expression tag	UNP P30260
L	469	SER	-	expression tag	UNP P30260
L	470	ALA	-	expression tag	UNP P30260
L	471	GLY	-	expression tag	UNP P30260
L	472	SER	-	expression tag	UNP P30260
L	473	ALA	-	expression tag	UNP P30260
L	474	ARG	-	expression tag	UNP P30260
L	475	GLY	-	expression tag	UNP P30260
L	476	VAL	-	expression tag	UNP P30260
L	477	PRO	-	expression tag	UNP P30260
L	478	HIS	-	expression tag	UNP P30260
L	479	ILE	-	expression tag	UNP P30260
L	480	VAL	-	expression tag	UNP P30260
L	481	MET	-	expression tag	UNP P30260
L	482	VAL	-	expression tag	UNP P30260
L	483	ASP	-	expression tag	UNP P30260
L	484	ALA	-	expression tag	UNP P30260
L	485	TYR	-	expression tag	UNP P30260
L	486	LYS	-	expression tag	UNP P30260
L	487	ARG	-	expression tag	UNP P30260
L	488	TYR	-	expression tag	UNP P30260
L	489	LYS	-	expression tag	UNP P30260

- Molecule 2 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	95	Total	C	N	O	S	0	0
			783	494	150	135	4		
2	E	94	Total	C	N	O	S	0	0
			773	488	147	134	4		

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	80	Total	C	N	O	S	0	0
			641	405	125	110	1		
3	F	79	Total	C	N	O	S	0	0
			633	399	124	109	1		

- Molecule 4 is a protein called Histone H2A type 2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	107	Total	C	N	O	S	0	0
			822	518	161	142	1		
4	G	107	Total	C	N	O	S	0	0
			822	518	161	142	1		

- Molecule 5 is a protein called Histone H2B type 1-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	93	Total	C	N	O	S	0	0
			729	459	131	137	2		
5	H	93	Total	C	N	O	S	0	0
			729	459	131	137	2		

- Molecule 6 is a DNA chain called DNA (132-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	132	Total	C	N	O	P	0	0
			2688	1277	487	792	132		

- Molecule 7 is a DNA chain called DNA (131-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	131	Total	C	N	O	P	0	0
			2704	1279	509	785	131		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	15	Total	O	0
			15	15	
8	B	12	Total	O	0
			12	12	
8	C	7	Total	O	0
			7	7	
8	D	3	Total	O	0
			3	3	
8	E	9	Total	O	0
			9	9	
8	F	9	Total	O	0
			9	9	

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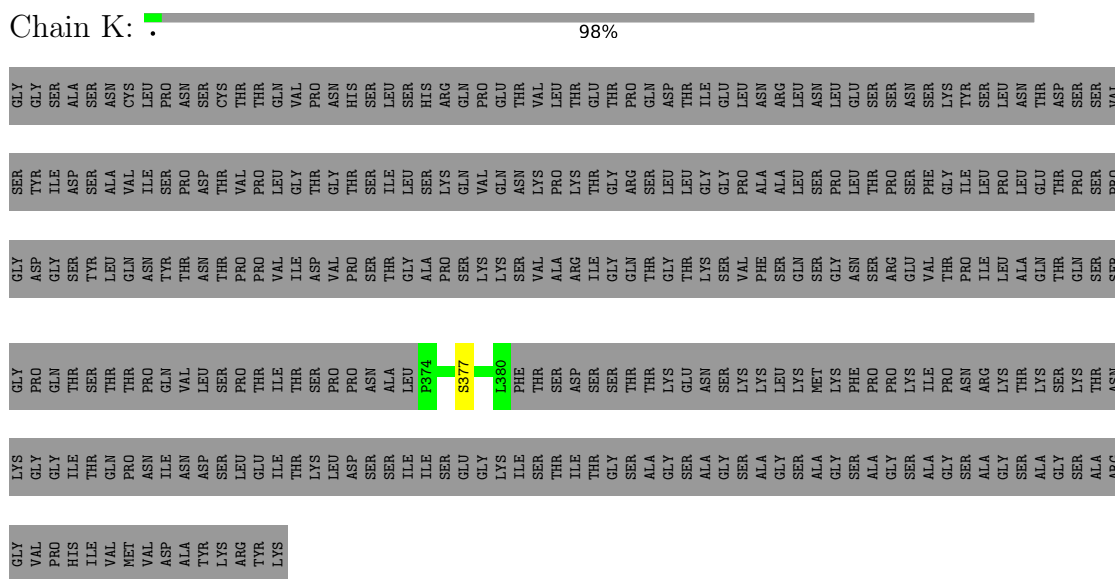
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Mol	Chain	Residues	Atoms		AltConf
8	G	12	Total 12	O 12	0
8	H	5	Total 5	O 5	0
8	I	1	Total 1	O 1	0
8	J	2	Total 2	O 2	0

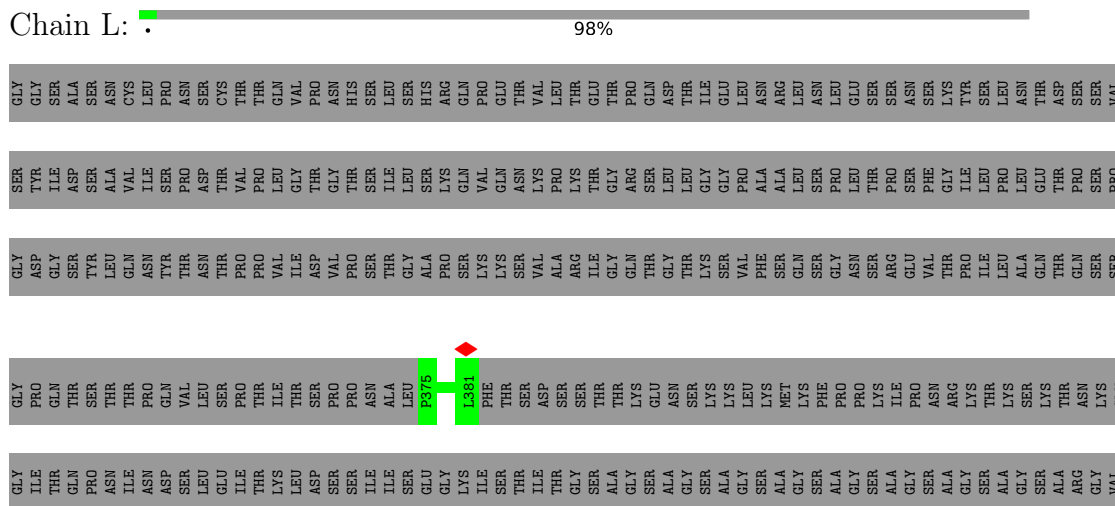
3 Residue-property plots

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

- Molecule 1: Cell division cycle protein 27 homolog



- Molecule 1: Cell division cycle protein 27 homolog



PRO
HIS
ILE
VAL
MET
VAL
ASP
ALA
TYR
LYS
ARG
TYR
LYS

• Molecule 2: Histone H3.1

Chain A:  65% 5% 30%

MET
ALA
ARG
THR
LYS
GLN
THR
ALA
ARG
LYS
SER
THR
GLY
GLY
LYS
ALA
ALA
PRO
ARG
LYS
GLN
LEU
ALA
THR
LYS
ALA
ALA
ARG
LYS
SER
ALA
PRO
ALA
THR
GLY
GLY
VAL
LYS
LYS
PRO
HIS
K39
K56
R69
E73
Q76
S87
R116
R129
E133
ARG
ALA

• Molecule 2: Histone H3.1

Chain E:  66% 0% 31%

MET
ALA
ARG
THR
LYS
GLN
THR
ALA
ARG
LYS
SER
THR
GLY
GLY
LYS
ALA
ALA
PRO
ARG
LYS
GLN
LEU
ALA
THR
LYS
ALA
ALA
ARG
LYS
SER
ALA
PRO
ALA
THR
GLY
GLY
VAL
LYS
LYS
PRO
HIS
R40
Y41
R42
L61
R69
E73
E133
ARG
ALA

• Molecule 3: Histone H4

Chain B:  74% 0% 22%

MET
SER
GLY
ARG
GLY
LYS
GLY
GLY
GLY
LYS
LEU
GLY
LYS
GLY
GLY
ALA
LYS
ARG
HIS
ARG
LYS
VAL
L22
R23
D24
N25
K91
R92
G101
GLY

• Molecule 3: Histone H4

Chain F:  71% 6% 23%


MET
SER
GLY
ARG
GLY
LYS
GLY
GLY
LYS
LEU
GLY
LYS
GLY
GLY
ALA
LYS
ARG
HIS
ARG
LYS
VAL
L22
R23
D24
K31
L37
Y51
H75
A76
K77
G101
GLY

• Molecule 4: Histone H2A type 2-A

Chain C:  76% 5% 18%

MET
SER
GLY
ARG
GLY
LYS
GLN
GLY
LYS
ALA
R11
A12
K13
K36
K74
K75
I79
H82
K95
P117
LYS
LYS
THR
GLU
SER
HIS
HIS
LYS
LYS
ALA
GLY
LYS

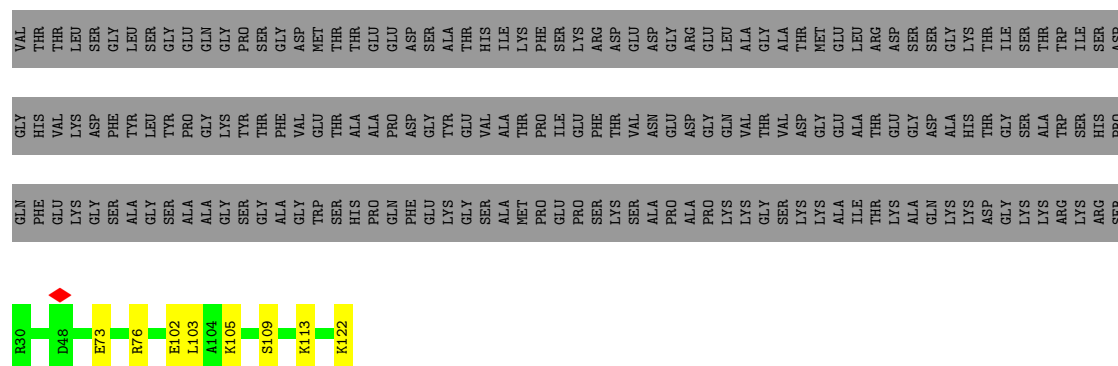
• Molecule 4: Histone H2A type 2-A

Chain G:  80% 0% 18%

MET
SER
GLY
ARG
GLY
LYS
GLN
GLY
LYS
ALA
R11
W73
R88
E92
P117
LYS
LYS
THR
GLU
SER
HIS
HIS
LYS
LYS
ALA
GLY
LYS

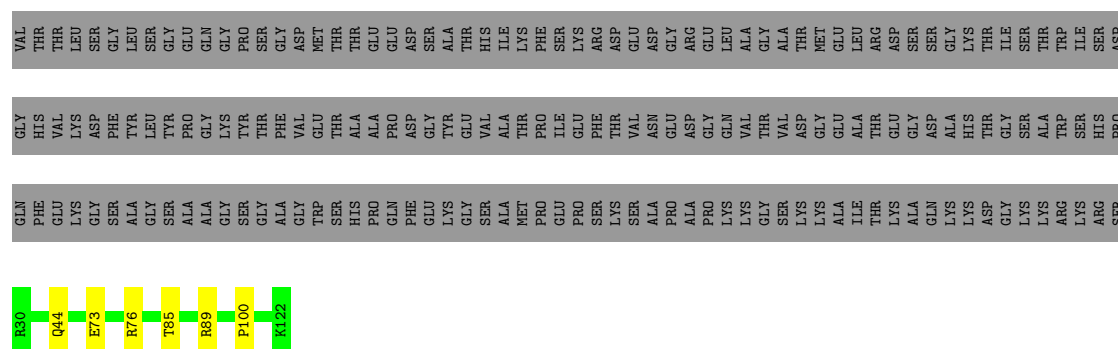
• Molecule 5: Histone H2B type 1-B

Chain D:  31% 0% 66%



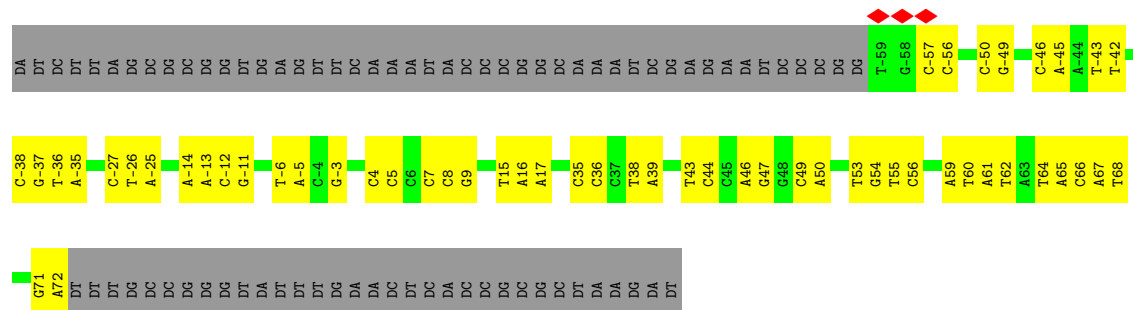
• Molecule 5: Histone H2B type 1-B

Chain H: 32% 66%



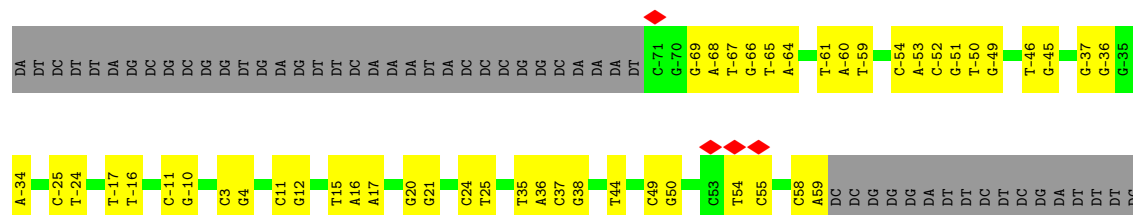
• Molecule 6: DNA (132-MER)

Chain I: 36% 26% 37%



• Molecule 7: DNA (131-MER)

Chain J: 39% 23% 38%



DC	DC	DG	DG	DG	DT	DA	DT	DT	DT	DG	DA	DA	DC	DT	DC	DA	DC	DC	DG	DC	DT	DA	DA	DG	DA	DT
----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----	----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	414277	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	62	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	224.63998, 224.63998, 224.63998	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	K	0.19	0/60	0.74	0/77
1	L	0.20	0/60	0.71	0/77
2	A	0.26	0/794	0.54	0/1065
2	E	0.27	0/783	0.54	0/1050
3	B	0.25	0/648	0.56	0/868
3	F	0.26	0/640	0.57	0/857
4	C	0.26	0/832	0.51	0/1121
4	G	0.25	0/832	0.51	0/1121
5	D	0.25	0/740	0.46	0/994
5	H	0.25	0/740	0.47	0/994
6	I	0.55	0/3011	0.93	0/4640
7	J	0.52	0/3037	0.91	0/4690
All	All	0.42	0/12177	0.76	0/17554

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 [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	K	60	0	67	0	0
1	L	60	0	67	0	0
2	A	783	0	818	6	0
2	E	773	0	811	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	641	0	684	2	0
3	F	633	0	673	4	0
4	C	822	0	880	2	0
4	G	822	0	880	3	0
5	D	729	0	753	4	0
5	H	729	0	753	4	0
6	I	2688	0	1482	35	0
7	J	2704	0	1470	29	0
8	A	15	0	0	0	0
8	B	12	0	0	0	0
8	C	7	0	0	0	0
8	D	3	0	0	0	0
8	E	9	0	0	0	0
8	F	9	0	0	0	0
8	G	12	0	0	0	0
8	H	5	0	0	0	0
8	I	1	0	0	0	0
8	J	2	0	0	0	0
All	All	11519	0	9338	81	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 81 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)
7:J:-65:DT:H2'	7:J:-64:DA:C8	2.28	0.69
6:I:-27:DC:H2''	6:I:-26:DT:H71	1.79	0.65
6:I:55:DT:H2''	6:I:56:DC:C5	2.32	0.65
4:G:92:GLU:HG2	5:H:100:PRO:HB2	1.82	0.62
3:F:75:HIS:O	5:H:89:ARG:NH2	2.34	0.61

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	K	5/317 (2%)	5 (100%)	0	0	100	100
1	L	5/317 (2%)	5 (100%)	0	0	100	100
2	A	93/136 (68%)	93 (100%)	0	0	100	100
2	E	92/136 (68%)	92 (100%)	0	0	100	100
3	B	78/103 (76%)	77 (99%)	1 (1%)	0	100	100
3	F	77/103 (75%)	77 (100%)	0	0	100	100
4	C	105/130 (81%)	102 (97%)	3 (3%)	0	100	100
4	G	105/130 (81%)	103 (98%)	2 (2%)	0	100	100
5	D	91/273 (33%)	90 (99%)	1 (1%)	0	100	100
5	H	91/273 (33%)	87 (96%)	4 (4%)	0	100	100
All	All	742/1918 (39%)	731 (98%)	11 (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	K	7/271 (3%)	6 (86%)	1 (14%)	2	5
1	L	7/271 (3%)	7 (100%)	0	100	100
2	A	83/111 (75%)	81 (98%)	2 (2%)	44	70
2	E	82/111 (74%)	81 (99%)	1 (1%)	67	86
3	B	66/79 (84%)	64 (97%)	2 (3%)	36	63
3	F	65/79 (82%)	64 (98%)	1 (2%)	60	82
4	C	83/99 (84%)	77 (93%)	6 (7%)	12	24
4	G	83/99 (84%)	82 (99%)	1 (1%)	67	86
5	D	80/220 (36%)	78 (98%)	2 (2%)	42	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	H	80/220 (36%)	79 (99%)	1 (1%)	65	85
All	All	636/1560 (41%)	619 (97%)	17 (3%)	41	67

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

Mol	Chain	Res	Type
3	F	77	LYS
5	H	44	GLN
4	C	36	LYS
4	C	74	LYS
4	C	75	LYS

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 oligosaccharides 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 [i](#)

There are no chain breaks in this entry.

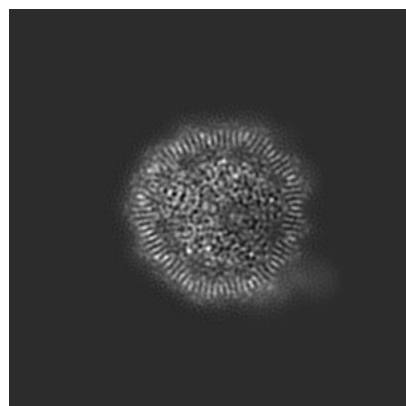
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50416. These allow visual inspection of the internal detail of the map and identification of artifacts.

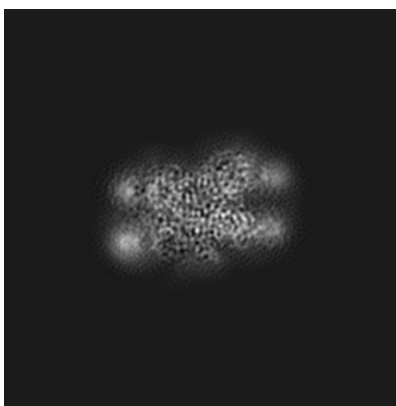
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

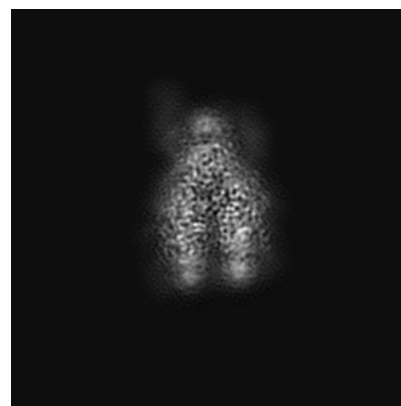
6.1.1 Primary map



X

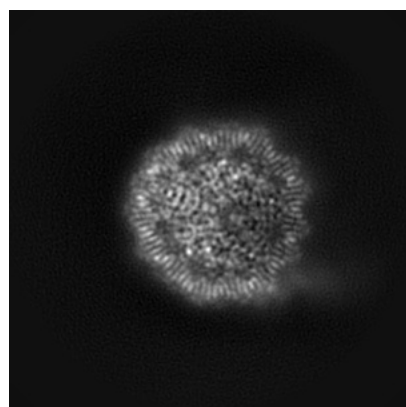


Y

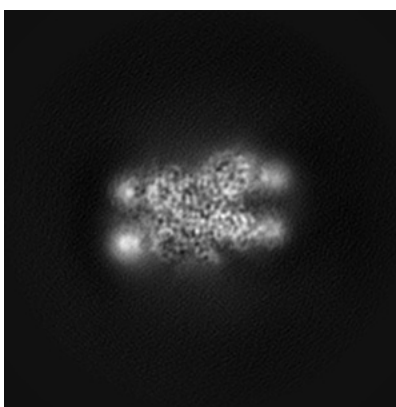


Z

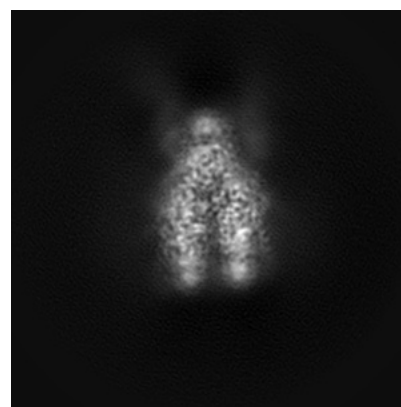
6.1.2 Raw map



X



Y

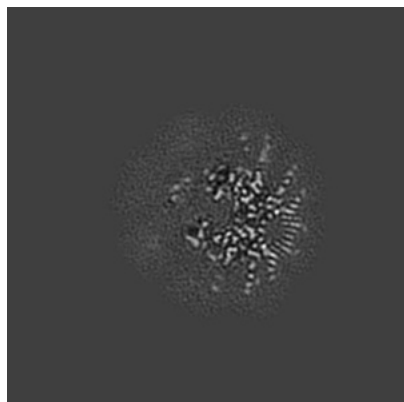


Z

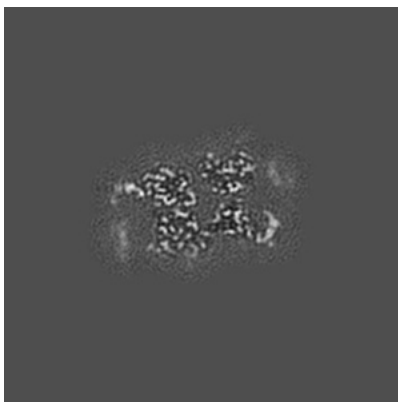
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

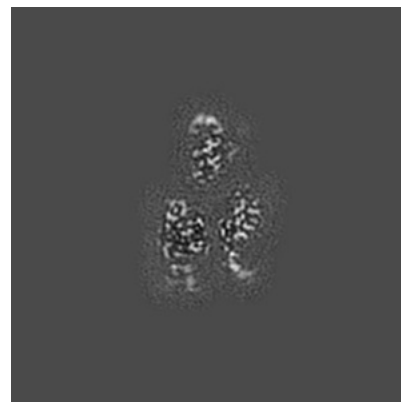
6.2.1 Primary map



X Index: 108

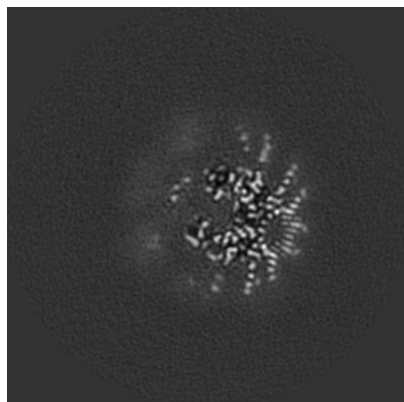


Y Index: 108

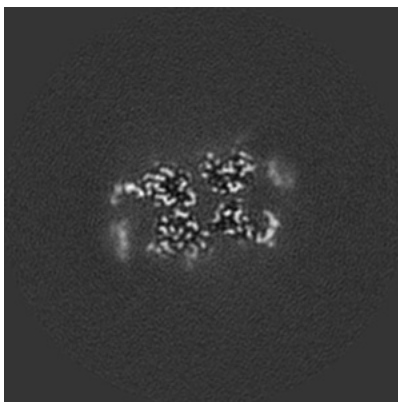


Z Index: 108

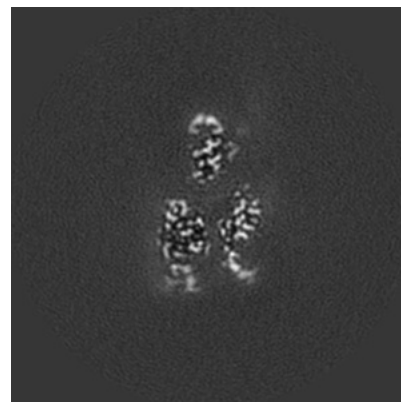
6.2.2 Raw map



X Index: 108



Y Index: 108

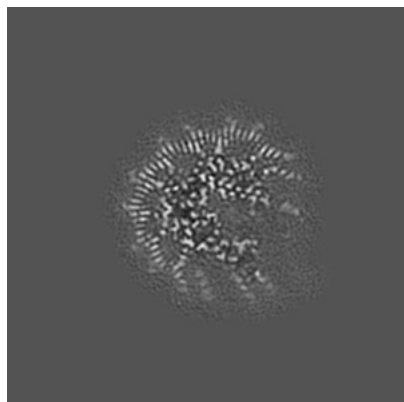


Z Index: 108

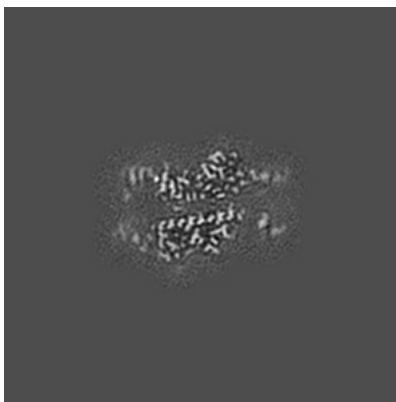
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

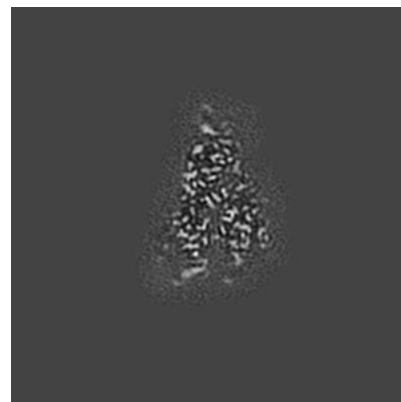
6.3.1 Primary map



X Index: 97

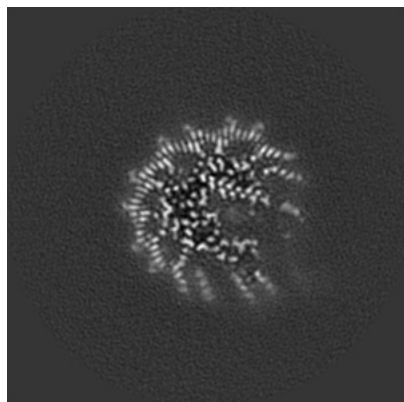


Y Index: 96

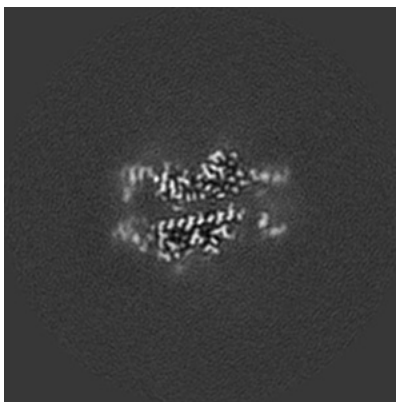


Z Index: 117

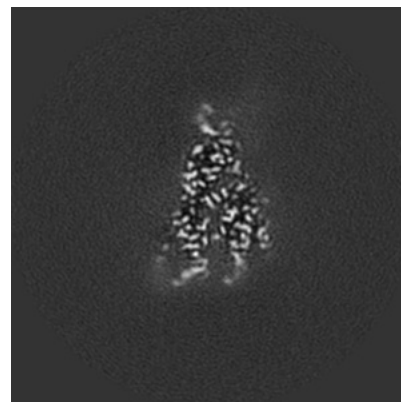
6.3.2 Raw map



X Index: 97



Y Index: 96

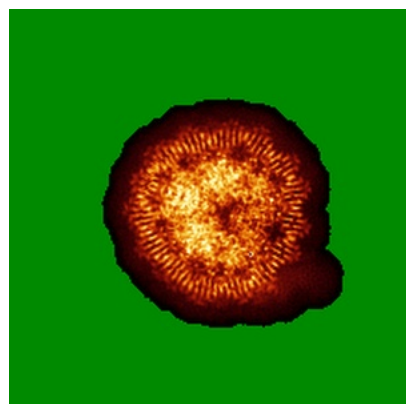


Z Index: 117

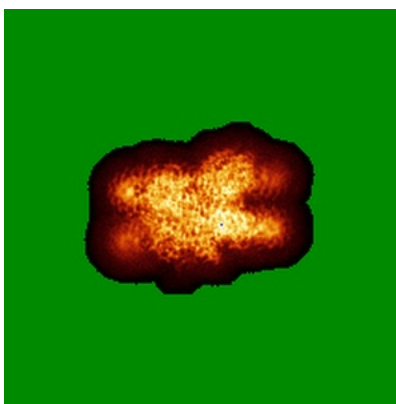
The images above show the largest variance slices of the map in three orthogonal directions.

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

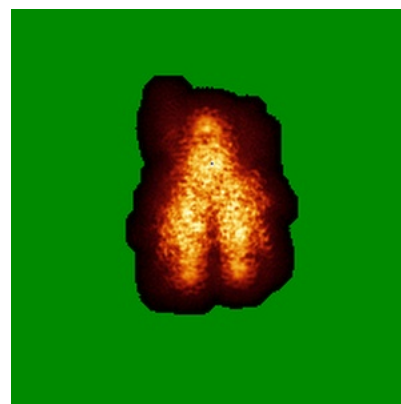
6.4.1 Primary map



X

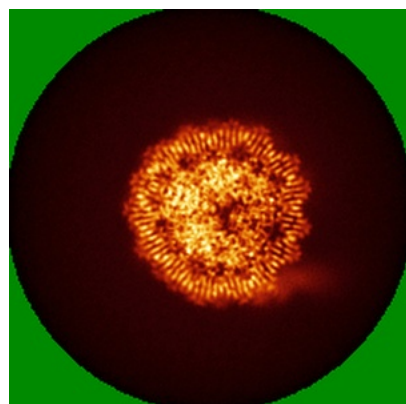


Y

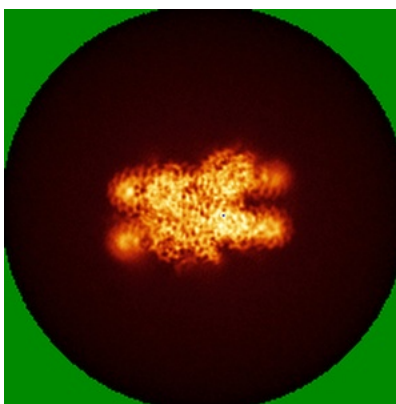


Z

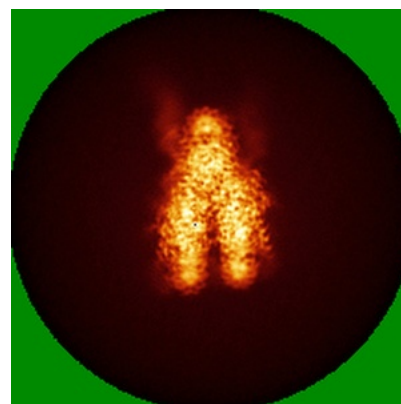
6.4.2 Raw map



X



Y

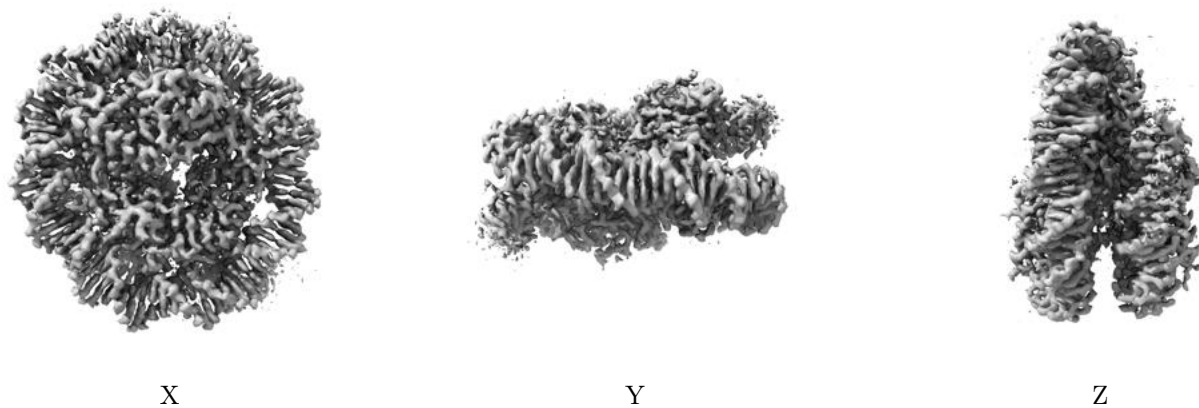


Z

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.

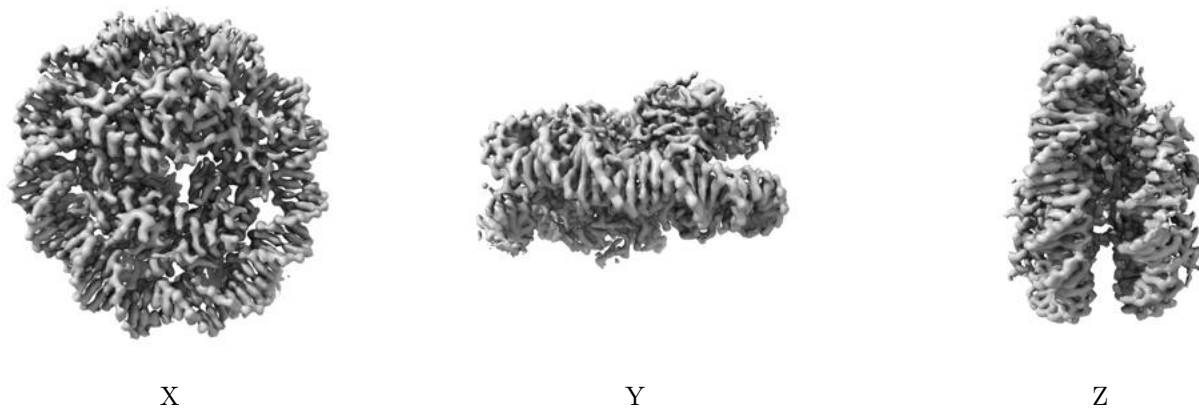
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.017. 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



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.

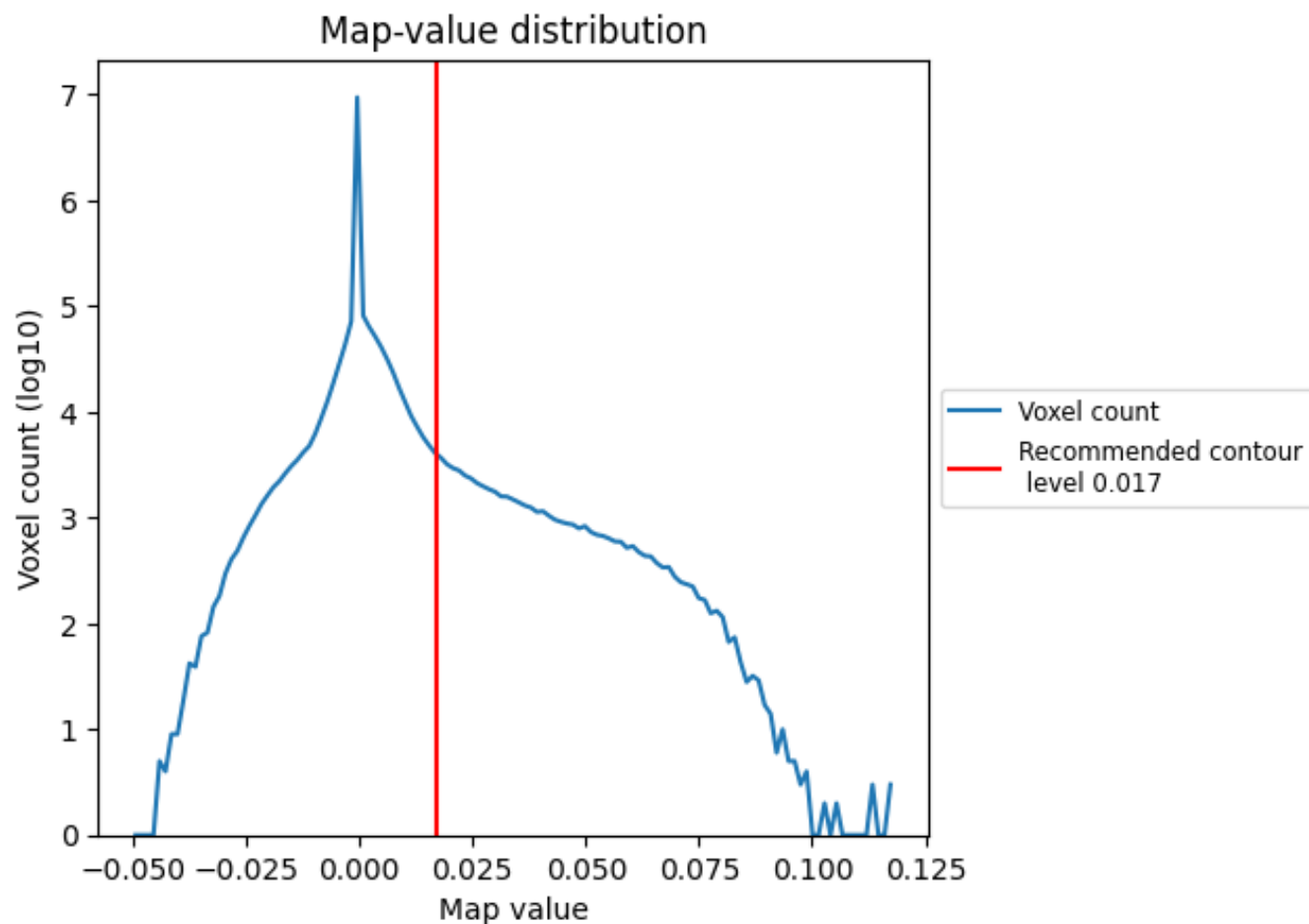
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

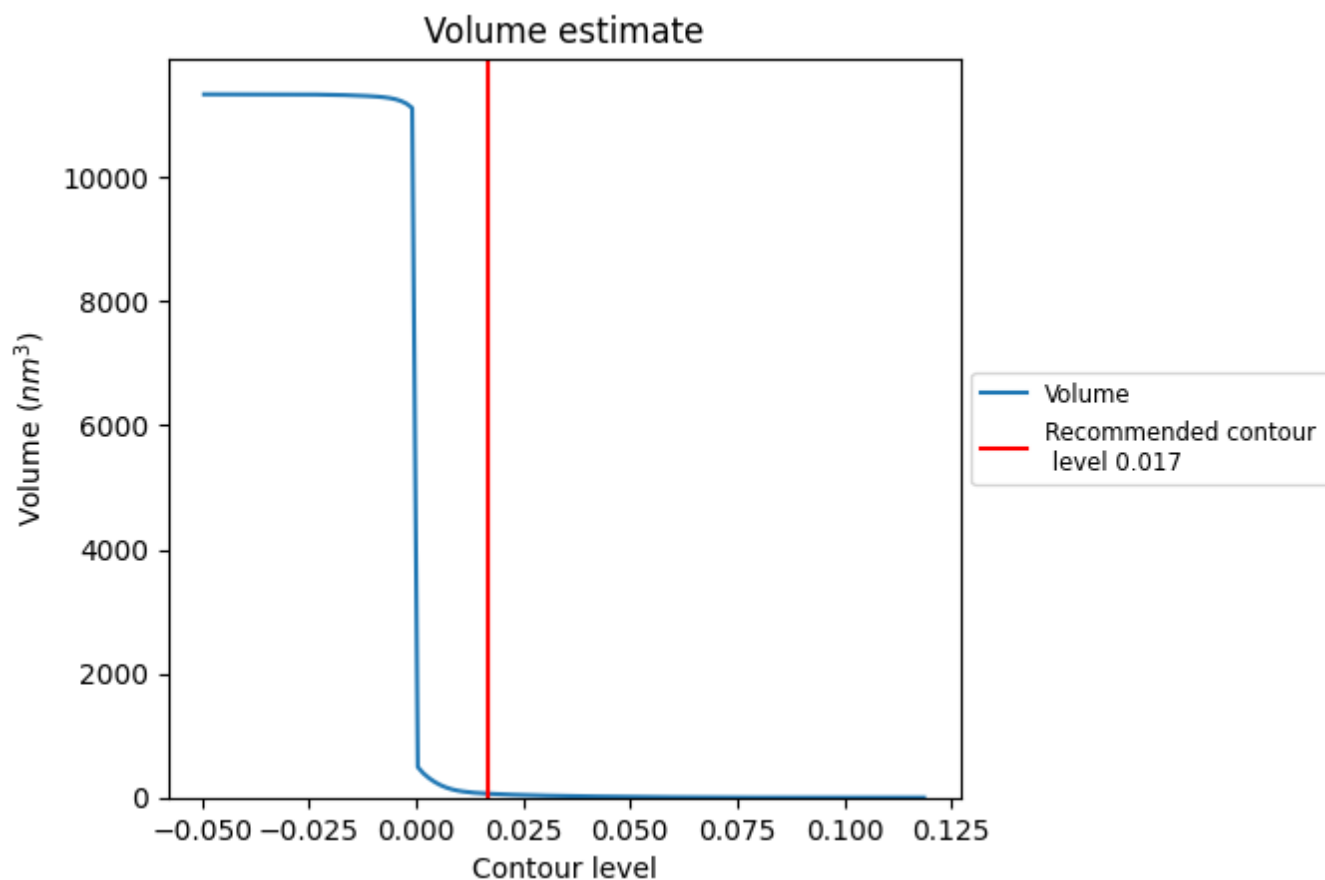
This section contains the results of statistical analysis of the map.

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.

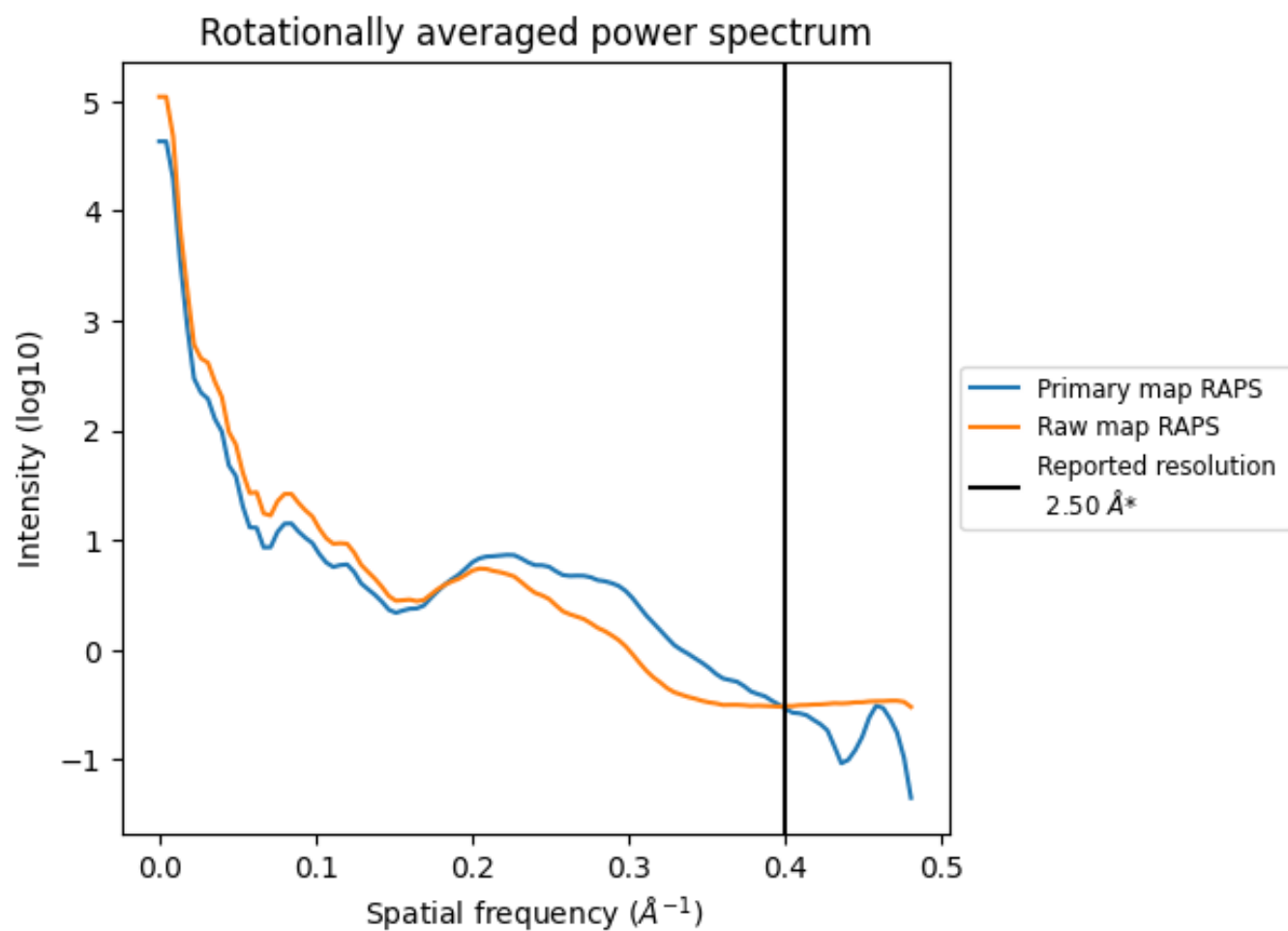
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 62 nm^3 ; this corresponds to an approximate mass of 56 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 ⓘ

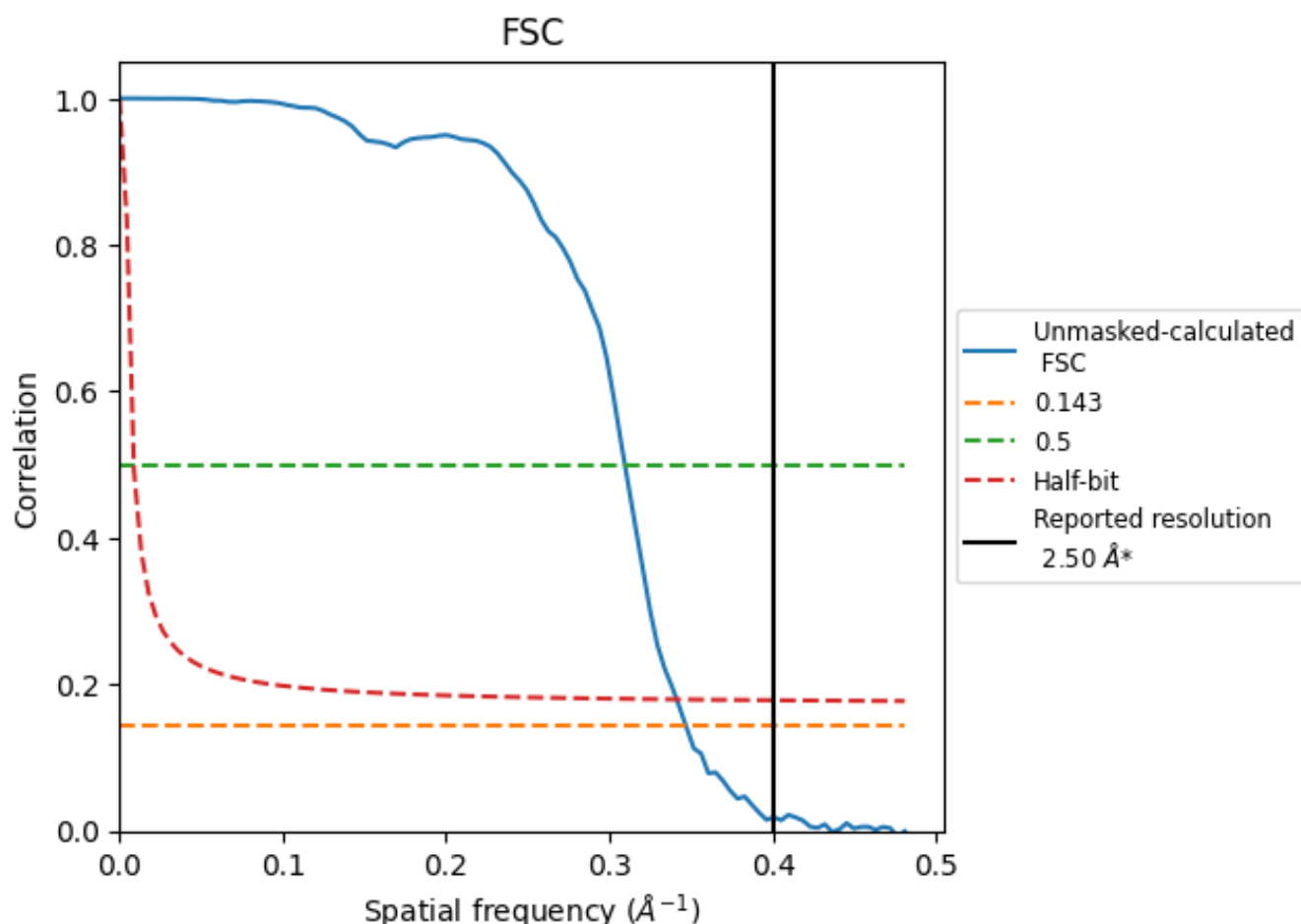


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

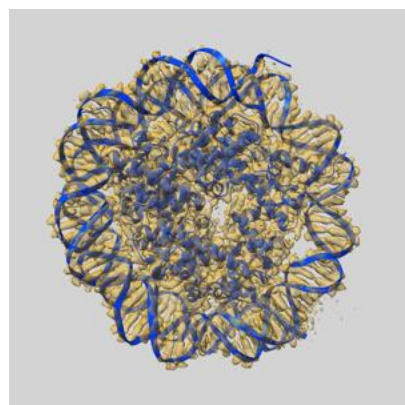
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.88	3.23	2.93

*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 2.88 differs from the reported value 2.5 by more than 10 %

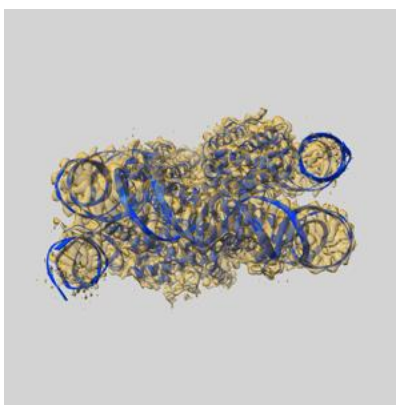
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50416 and PDB model 9FGQ. Per-residue inclusion information can be found in section [3](#) on page [9](#).

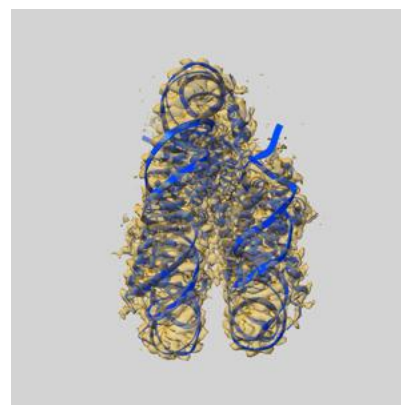
9.1 Map-model overlay [i](#)



X



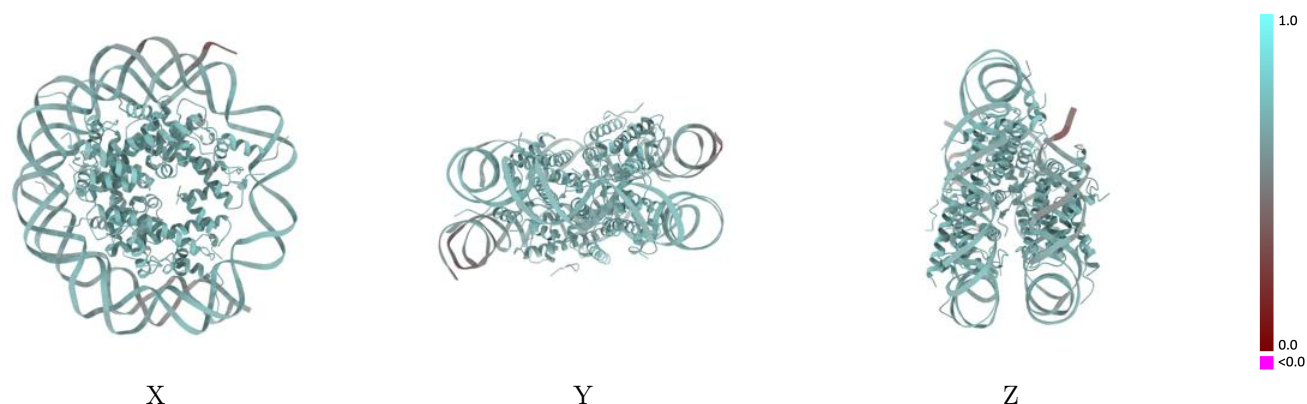
Y



Z

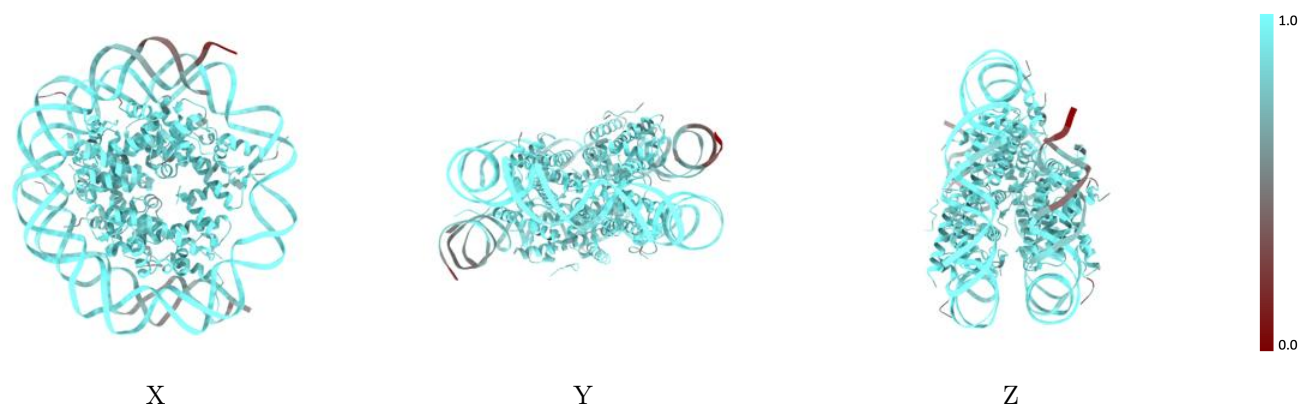
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



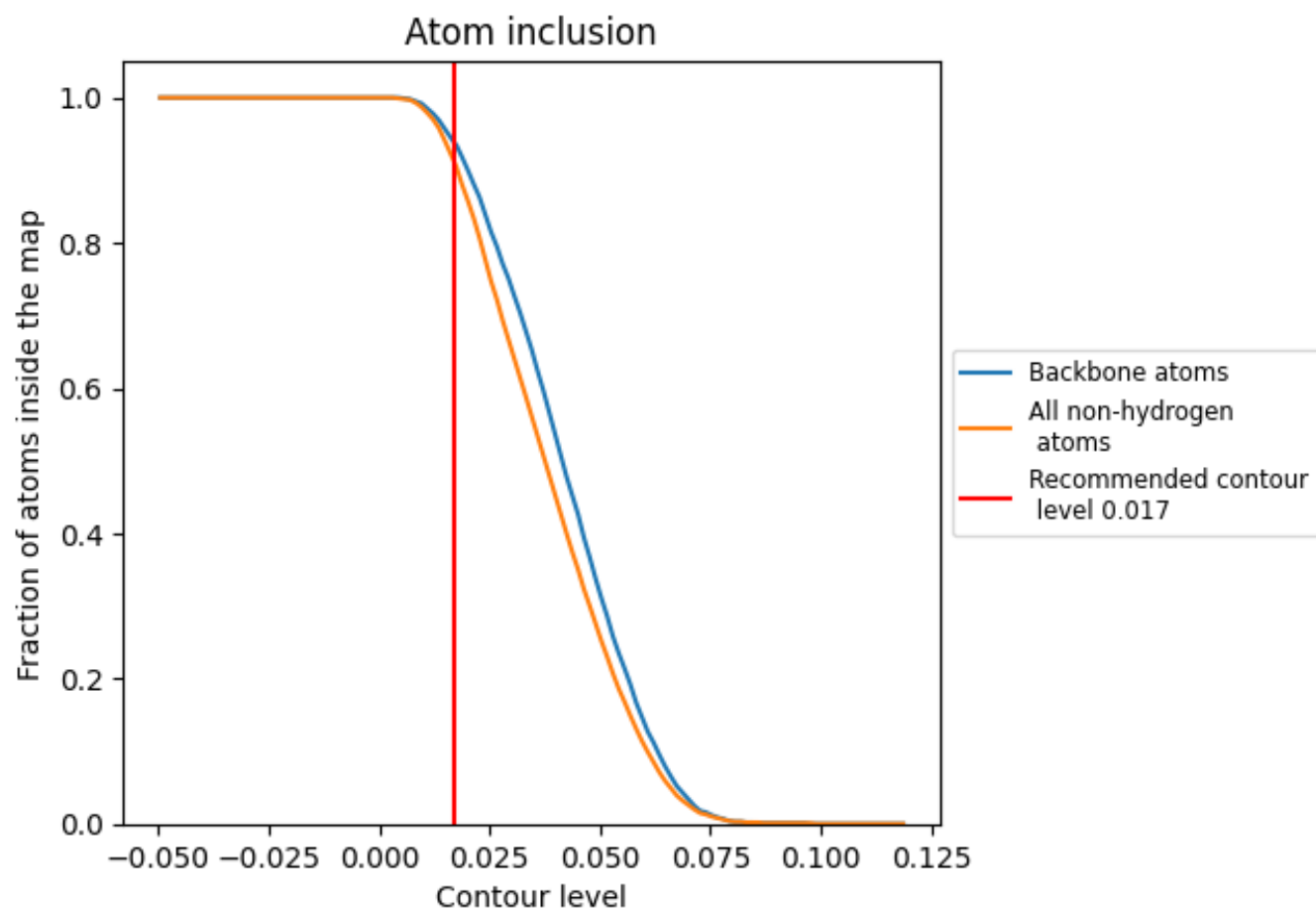
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9120</div>	<div><div></div>0.6510</div>
A	<div><div></div>0.9670</div>	<div><div></div>0.6910</div>
B	<div><div></div>0.9580</div>	<div><div></div>0.6950</div>
C	<div><div></div>0.9200</div>	<div><div></div>0.6720</div>
D	<div><div></div>0.9450</div>	<div><div></div>0.6780</div>
E	<div><div></div>0.9450</div>	<div><div></div>0.6850</div>
F	<div><div></div>0.9620</div>	<div><div></div>0.6920</div>
G	<div><div></div>0.9400</div>	<div><div></div>0.6870</div>
H	<div><div></div>0.9490</div>	<div><div></div>0.6900</div>
I	<div><div></div>0.8780</div>	<div><div></div>0.6110</div>
J	<div><div></div>0.8830</div>	<div><div></div>0.6140</div>
K	<div><div></div>0.8890</div>	<div><div></div>0.6610</div>
L	<div><div></div>0.6850</div>	<div><div></div>0.6450</div>

1.0

0.0

<0.0