Full wwPDB EM Validation Report ⓘ

May 21, 2024 – 10:22 AM JST

PDB ID	:	8XOT
EMDB ID	:	EMD-38540
Title	:	Prohead portal of bacteriophage lambda
Authors	:	Wang, J.W.; Gu, Z.W.
Deposited on	:	2024-01-02
Resolution	:	3.51 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:

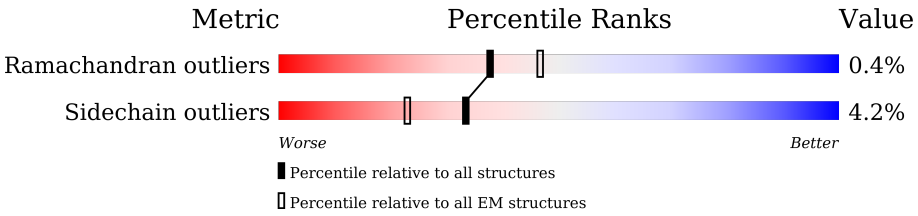
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.51 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	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	B	533	86% · 11%
1	B1	533	86% · 11%
1	B2	533	86% · 11%
1	B3	533	85% · 11%
1	B4	533	84% 5% 11%
1	B5	533	85% · 11%
1	b	533	86% · 11%
1	b1	533	85% · 11%
1	b2	533	86% · 11%

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Mol	Chain	Length	Quality of chain
1	b3	533	
1	b4	533	
1	b5	533	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 44532 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 Portal protein B.

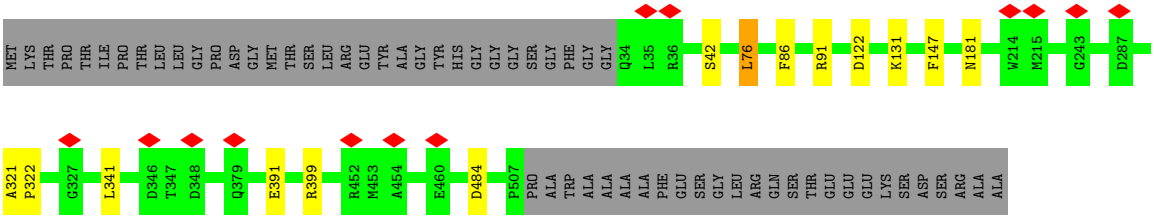
Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	474	Total	C	N	O	S	0	0
			3711	2319	672	697	23		
1	b	474	Total	C	N	O	S	0	0
			3711	2319	672	697	23		
1	B1	474	Total	C	N	O	S	0	0
			3711	2319	672	697	23		
1	b1	474	Total	C	N	O	S	0	0
			3711	2319	672	697	23		
1	B2	474	Total	C	N	O	S	0	0
			3711	2319	672	697	23		
1	b2	474	Total	C	N	O	S	0	0
			3711	2319	672	697	23		
1	B3	474	Total	C	N	O	S	0	0
			3711	2319	672	697	23		
1	b3	474	Total	C	N	O	S	0	0
			3711	2319	672	697	23		
1	B4	474	Total	C	N	O	S	0	0
			3711	2319	672	697	23		
1	b4	474	Total	C	N	O	S	0	0
			3711	2319	672	697	23		
1	B5	474	Total	C	N	O	S	0	0
			3711	2319	672	697	23		
1	b5	474	Total	C	N	O	S	0	0
			3711	2319	672	697	23		

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.

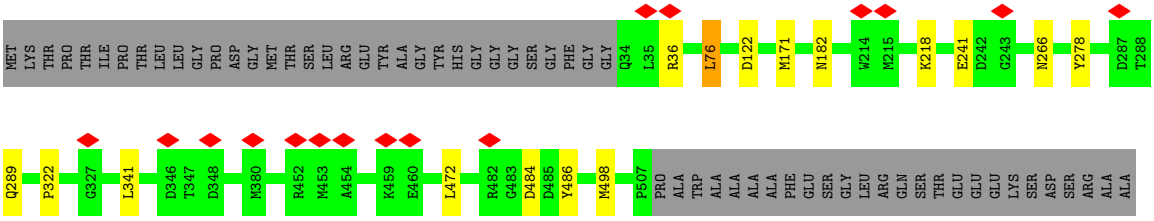
• Molecule 1: Portal protein B

Chain B:



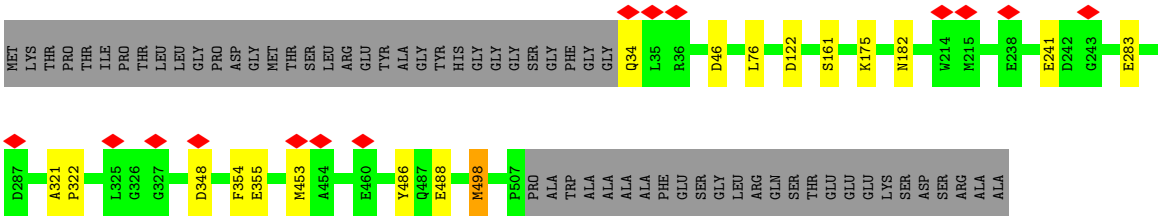
• Molecule 1: Portal protein B

Chain b:



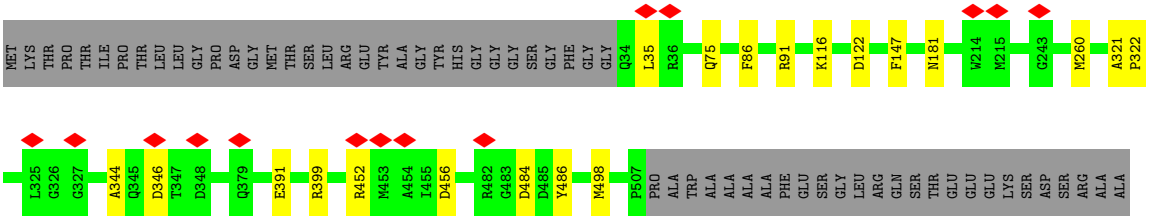
• Molecule 1: Portal protein B

Chain B1:



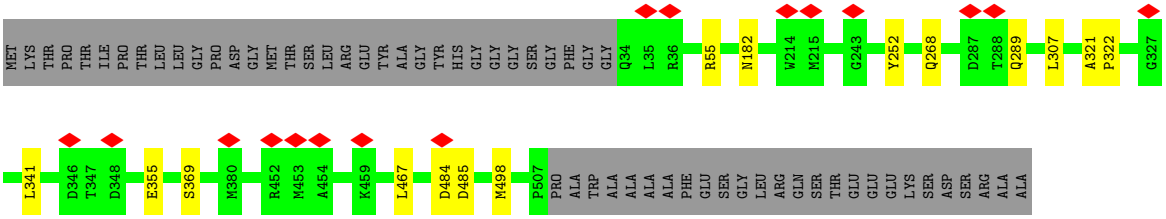
• Molecule 1: Portal protein B

Chain b1:



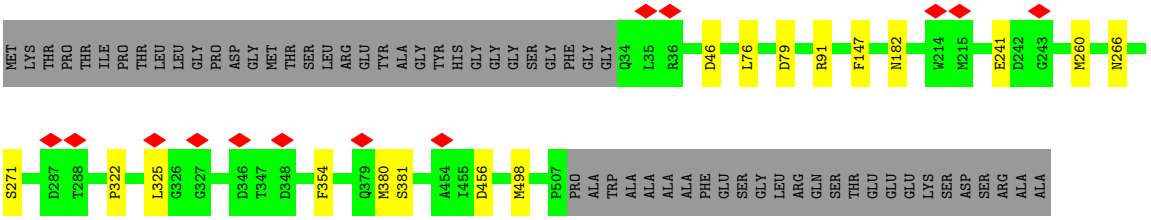
• Molecule 1: Portal protein B

Chain B2:



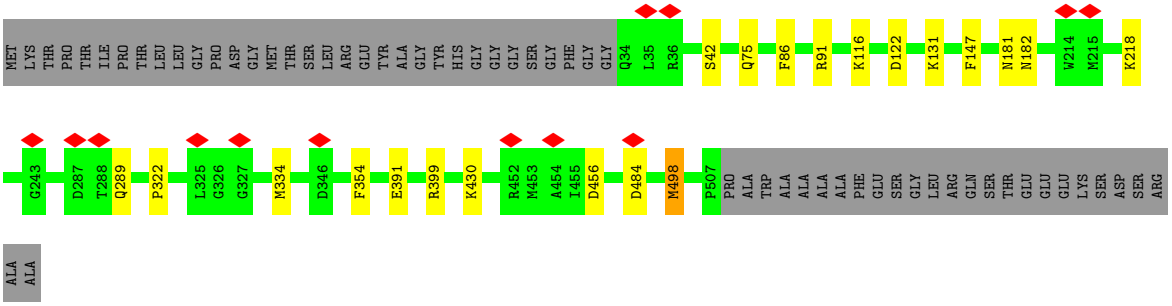
• Molecule 1: Portal protein B

Chain b2:



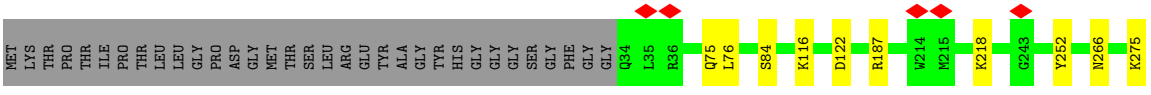
• Molecule 1: Portal protein B

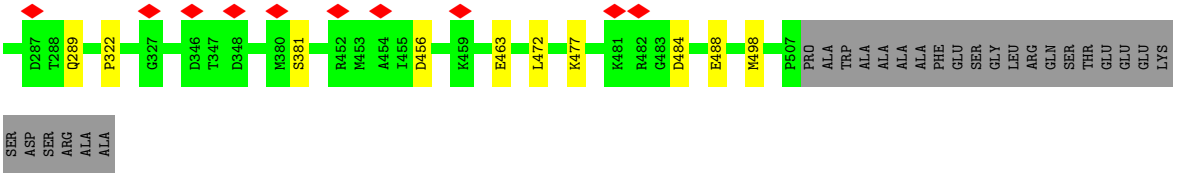
Chain B3:



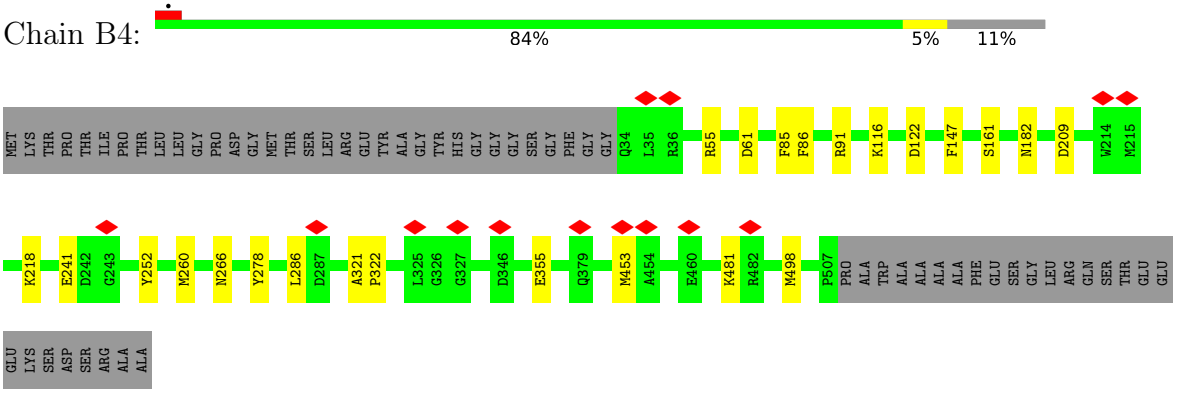
• Molecule 1: Portal protein B

Chain b3:

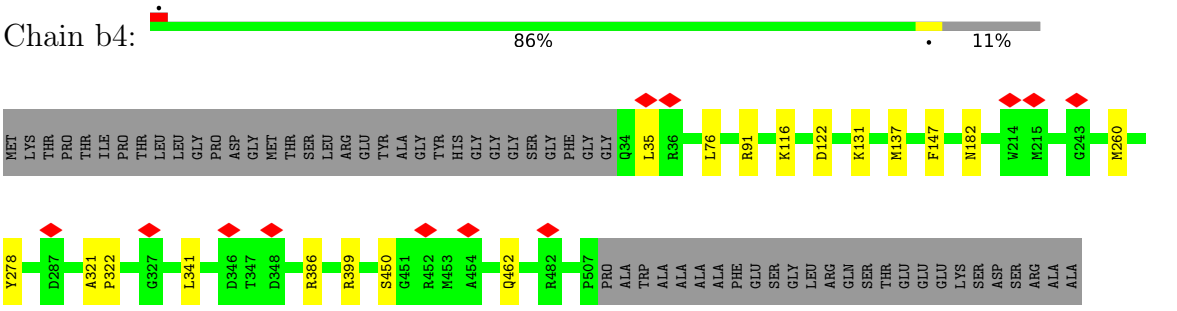




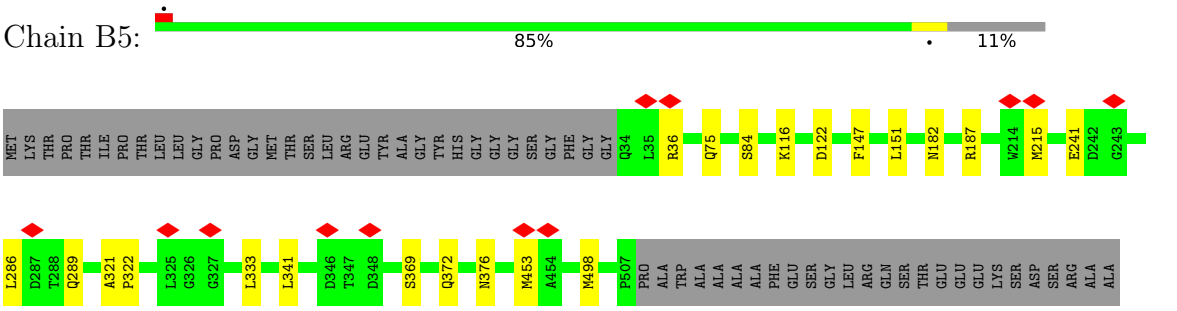
• Molecule 1: Portal protein B



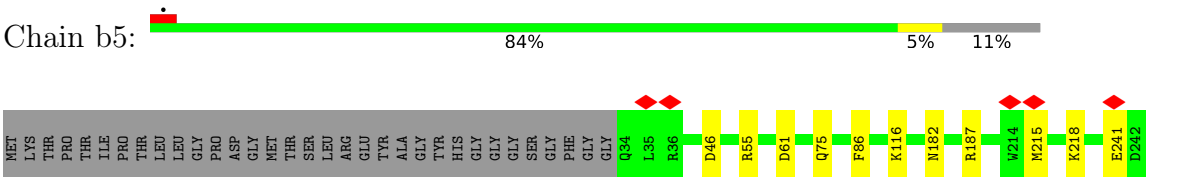
• Molecule 1: Portal protein B

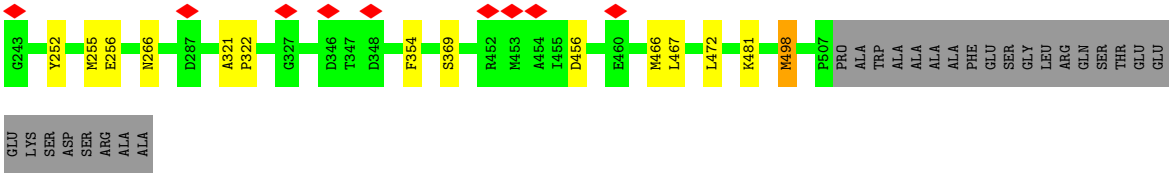


• Molecule 1: Portal protein B



• Molecule 1: Portal protein B




G243
Y252
M255
E256
N266
D287
A321
P322
G327
D346
T347
D348
F354
S369
R452
M453
A454
I455
D456
E460
M466
L467
L472
K481
M498
P507
PRO
ALA
TRP
ALA
ALA
ALA
ALA
PHE
GLU
SER
GLY
LEU
ARG
GLN
SER
THR
GLU
GLU
GLU
LYS
SER
ASP
SER
ARG
ALA
ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50921	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.120	Depositor
Minimum map value	-0.582	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	334.47424, 334.47424, 334.47424	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.30654, 1.30654, 1.30654	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	B	0.31	0/3793	0.57	1/5131 (0.0%)
1	B1	0.31	0/3793	0.59	2/5131 (0.0%)
1	B2	0.31	0/3793	0.59	2/5131 (0.0%)
1	B3	0.32	0/3793	0.59	1/5131 (0.0%)
1	B4	0.32	0/3793	0.60	2/5131 (0.0%)
1	B5	0.32	0/3793	0.60	1/5131 (0.0%)
1	b	0.31	0/3793	0.58	2/5131 (0.0%)
1	b1	0.31	0/3793	0.58	1/5131 (0.0%)
1	b2	0.31	0/3793	0.60	2/5131 (0.0%)
1	b3	0.31	0/3793	0.59	1/5131 (0.0%)
1	b4	0.31	0/3793	0.58	2/5131 (0.0%)
1	b5	0.31	0/3793	0.57	1/5131 (0.0%)
All	All	0.31	0/45516	0.59	18/61572 (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	B	0	1
1	B1	0	1
1	B2	0	1
1	B4	0	1
1	B5	0	1
1	b1	0	1
1	b4	0	1
1	b5	0	1
All	All	0	8

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	b	341	LEU	CA-CB-CG	7.48	132.51	115.30
1	b2	76	LEU	CA-CB-CG	6.85	131.05	115.30
1	b4	76	LEU	CA-CB-CG	6.81	130.97	115.30
1	b	76	LEU	CA-CB-CG	6.76	130.86	115.30
1	B	76	LEU	CA-CB-CG	6.37	129.95	115.30
1	b2	260	MET	CA-CB-CG	6.20	123.84	113.30
1	b4	260	MET	CA-CB-CG	5.66	122.93	113.30
1	B2	341	LEU	CA-CB-CG	5.63	128.24	115.30
1	B2	307	LEU	CA-CB-CG	5.57	128.12	115.30
1	b5	498	MET	CA-CB-CG	5.48	122.62	113.30
1	B1	498	MET	CA-CB-CG	5.48	122.61	113.30
1	B3	498	MET	CA-CB-CG	5.45	122.56	113.30
1	B1	76	LEU	CA-CB-CG	5.45	127.83	115.30
1	B5	341	LEU	CA-CB-CG	5.44	127.82	115.30
1	B4	260	MET	CA-CB-CG	5.43	122.53	113.30
1	b3	76	LEU	CA-CB-CG	5.41	127.73	115.30
1	B4	61	ASP	CB-CG-OD2	5.30	123.07	118.30
1	b1	260	MET	CA-CB-CG	5.23	122.19	113.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	321	ALA	Peptide
1	B1	321	ALA	Peptide
1	B2	321	ALA	Peptide
1	B4	321	ALA	Peptide
1	B5	321	ALA	Peptide
1	b1	321	ALA	Peptide
1	b4	321	ALA	Peptide
1	b5	321	ALA	Peptide

5.2 Too-close contacts (i)

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

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	B	472/533 (89%)	444 (94%)	27 (6%)	1 (0%)	47	80
1	B1	472/533 (89%)	445 (94%)	26 (6%)	1 (0%)	47	80
1	B2	472/533 (89%)	445 (94%)	25 (5%)	2 (0%)	34	71
1	B3	472/533 (89%)	446 (94%)	24 (5%)	2 (0%)	34	71
1	B4	472/533 (89%)	445 (94%)	25 (5%)	2 (0%)	34	71
1	B5	472/533 (89%)	446 (94%)	23 (5%)	3 (1%)	25	64
1	b	472/533 (89%)	442 (94%)	28 (6%)	2 (0%)	34	71
1	b1	472/533 (89%)	446 (94%)	24 (5%)	2 (0%)	34	71
1	b2	472/533 (89%)	448 (95%)	23 (5%)	1 (0%)	47	80
1	b3	472/533 (89%)	448 (95%)	22 (5%)	2 (0%)	34	71
1	b4	472/533 (89%)	446 (94%)	25 (5%)	1 (0%)	47	80
1	b5	472/533 (89%)	451 (96%)	20 (4%)	1 (0%)	47	80
All	All	5664/6396 (89%)	5352 (94%)	292 (5%)	20 (0%)	38	71

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	322	PRO
1	b	322	PRO
1	B1	322	PRO
1	b1	322	PRO
1	b1	344	ALA
1	B2	322	PRO
1	b2	322	PRO
1	B3	322	PRO
1	b3	322	PRO
1	B4	322	PRO
1	b4	322	PRO
1	B5	322	PRO
1	b5	322	PRO
1	B2	289	GLN
1	B3	289	GLN
1	b3	289	GLN
1	b	289	GLN
1	B5	286	LEU

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Mol	Chain	Res	Type
1	B5	289	GLN
1	B4	286	LEU

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	B	373/428 (87%)	361 (97%)	12 (3%)	39	69
1	B1	373/428 (87%)	358 (96%)	15 (4%)	31	64
1	B2	373/428 (87%)	363 (97%)	10 (3%)	44	73
1	B3	373/428 (87%)	354 (95%)	19 (5%)	24	58
1	B4	373/428 (87%)	354 (95%)	19 (5%)	24	58
1	B5	373/428 (87%)	356 (95%)	17 (5%)	27	61
1	b	373/428 (87%)	360 (96%)	13 (4%)	36	67
1	b1	373/428 (87%)	357 (96%)	16 (4%)	29	62
1	b2	373/428 (87%)	359 (96%)	14 (4%)	33	65
1	b3	373/428 (87%)	356 (95%)	17 (5%)	27	61
1	b4	373/428 (87%)	359 (96%)	14 (4%)	33	65
1	b5	373/428 (87%)	350 (94%)	23 (6%)	18	52
All	All	4476/5136 (87%)	4287 (96%)	189 (4%)	33	63

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	42	SER
1	B	76	LEU
1	B	86	PHE
1	B	91	ARG
1	B	122	ASP
1	B	131	LYS
1	B	147	PHE
1	B	181	ASN

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Mol	Chain	Res	Type
1	B	341	LEU
1	B	391	GLU
1	B	399	ARG
1	B	484	ASP
1	b	36	ARG
1	b	76	LEU
1	b	122	ASP
1	b	171	MET
1	b	182	ASN
1	b	218	LYS
1	b	241	GLU
1	b	266	ASN
1	b	278	TYR
1	b	472	LEU
1	b	484	ASP
1	b	486	TYR
1	b	498	MET
1	B1	34	GLN
1	B1	46	ASP
1	B1	122	ASP
1	B1	161	SER
1	B1	175	LYS
1	B1	182	ASN
1	B1	241	GLU
1	B1	283	GLU
1	B1	348	ASP
1	B1	354	PHE
1	B1	355	GLU
1	B1	453	MET
1	B1	486	TYR
1	B1	488	GLU
1	B1	498	MET
1	b1	35	LEU
1	b1	75	GLN
1	b1	86	PHE
1	b1	91	ARG
1	b1	116	LYS
1	b1	122	ASP
1	b1	147	PHE
1	b1	181	ASN
1	b1	346	ASP
1	b1	391	GLU

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Mol	Chain	Res	Type
1	b1	399	ARG
1	b1	452	ARG
1	b1	456	ASP
1	b1	484	ASP
1	b1	486	TYR
1	b1	498	MET
1	B2	55	ARG
1	B2	182	ASN
1	B2	252	TYR
1	B2	268	GLN
1	B2	355	GLU
1	B2	369	SER
1	B2	467	LEU
1	B2	484	ASP
1	B2	485	ASP
1	B2	498	MET
1	b2	46	ASP
1	b2	79	ASP
1	b2	91	ARG
1	b2	147	PHE
1	b2	182	ASN
1	b2	241	GLU
1	b2	266	ASN
1	b2	271	SER
1	b2	325	LEU
1	b2	354	PHE
1	b2	380	MET
1	b2	381	SER
1	b2	456	ASP
1	b2	498	MET
1	B3	42	SER
1	B3	75	GLN
1	B3	86	PHE
1	B3	91	ARG
1	B3	116	LYS
1	B3	122	ASP
1	B3	131	LYS
1	B3	147	PHE
1	B3	181	ASN
1	B3	182	ASN
1	B3	218	LYS
1	B3	334	MET

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Mol	Chain	Res	Type
1	B3	354	PHE
1	B3	391	GLU
1	B3	399	ARG
1	B3	430	LYS
1	B3	456	ASP
1	B3	484	ASP
1	B3	498	MET
1	b3	75	GLN
1	b3	84	SER
1	b3	116	LYS
1	b3	122	ASP
1	b3	187	ARG
1	b3	218	LYS
1	b3	252	TYR
1	b3	266	ASN
1	b3	275	LYS
1	b3	381	SER
1	b3	456	ASP
1	b3	463	GLU
1	b3	472	LEU
1	b3	477	LYS
1	b3	484	ASP
1	b3	488	GLU
1	b3	498	MET
1	B4	55	ARG
1	B4	85	PHE
1	B4	86	PHE
1	B4	91	ARG
1	B4	116	LYS
1	B4	122	ASP
1	B4	147	PHE
1	B4	161	SER
1	B4	182	ASN
1	B4	209	ASP
1	B4	218	LYS
1	B4	241	GLU
1	B4	252	TYR
1	B4	266	ASN
1	B4	278	TYR
1	B4	355	GLU
1	B4	453	MET
1	B4	481	LYS

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Mol	Chain	Res	Type
1	B4	498	MET
1	b4	35	LEU
1	b4	91	ARG
1	b4	116	LYS
1	b4	122	ASP
1	b4	131	LYS
1	b4	137	MET
1	b4	147	PHE
1	b4	182	ASN
1	b4	278	TYR
1	b4	341	LEU
1	b4	386	ARG
1	b4	399	ARG
1	b4	450	SER
1	b4	462	GLN
1	B5	36	ARG
1	B5	75	GLN
1	B5	84	SER
1	B5	116	LYS
1	B5	122	ASP
1	B5	147	PHE
1	B5	151	LEU
1	B5	182	ASN
1	B5	187	ARG
1	B5	215	MET
1	B5	241	GLU
1	B5	333	LEU
1	B5	369	SER
1	B5	372	GLN
1	B5	376	ASN
1	B5	453	MET
1	B5	498	MET
1	b5	46	ASP
1	b5	55	ARG
1	b5	61	ASP
1	b5	75	GLN
1	b5	86	PHE
1	b5	116	LYS
1	b5	182	ASN
1	b5	187	ARG
1	b5	215	MET
1	b5	218	LYS

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Mol	Chain	Res	Type
1	b5	241	GLU
1	b5	252	TYR
1	b5	255	MET
1	b5	256	GLU
1	b5	266	ASN
1	b5	354	PHE
1	b5	369	SER
1	b5	456	ASP
1	b5	466	MET
1	b5	467	LEU
1	b5	472	LEU
1	b5	481	LYS
1	b5	498	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	75	GLN
1	b	268	GLN
1	b	462	GLN
1	B1	268	GLN
1	B1	349	ASN
1	b1	75	GLN
1	b1	356	GLN
1	b1	376	ASN
1	B2	266	ASN
1	B4	266	ASN
1	b4	75	GLN
1	B5	266	ASN
1	b5	356	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

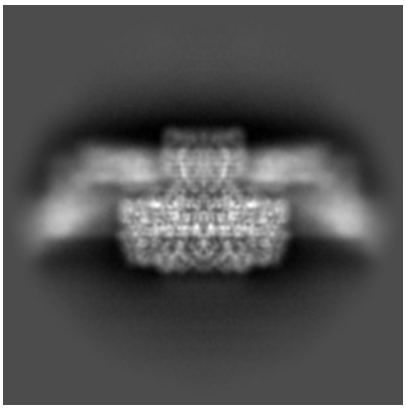
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38540. These allow visual inspection of the internal detail of the map and identification of artifacts.

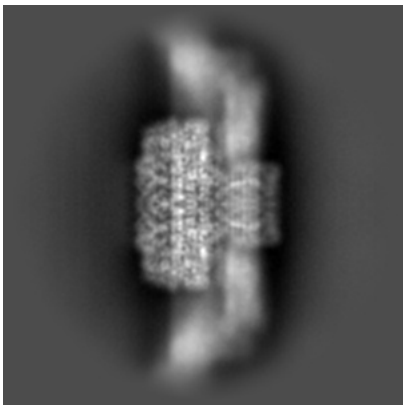
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

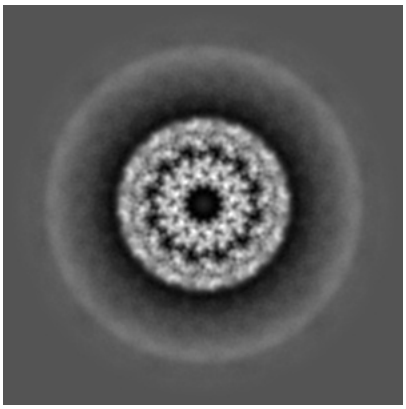
6.1.1 Primary map



X

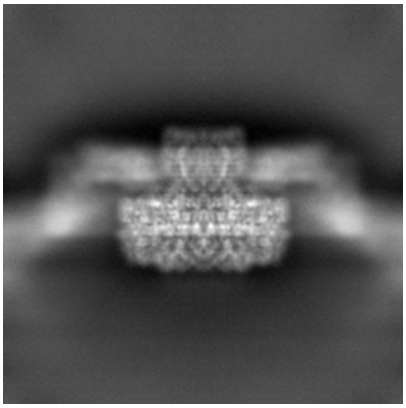


Y

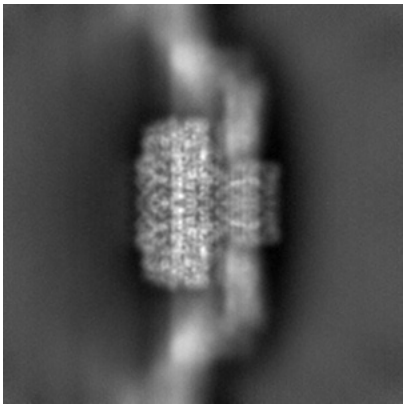


Z

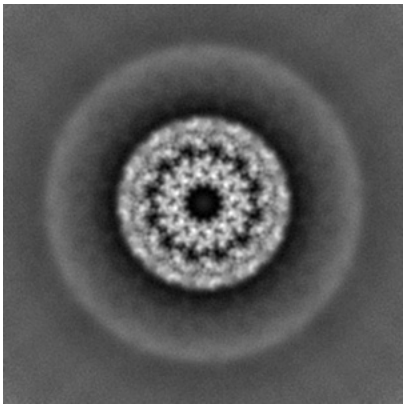
6.1.2 Raw map



X



Y

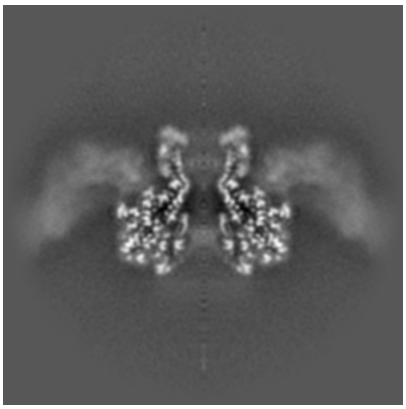


Z

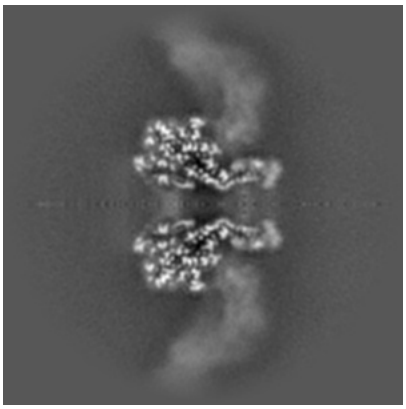
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

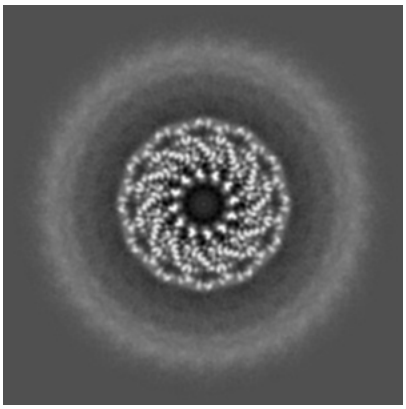
6.2.1 Primary map



X Index: 128

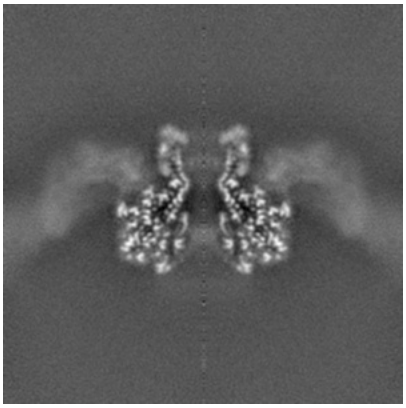


Y Index: 128

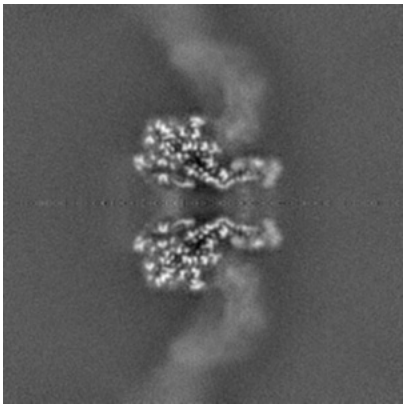


Z Index: 128

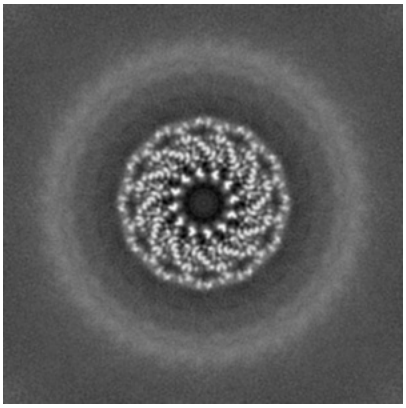
6.2.2 Raw map



X Index: 128



Y Index: 128

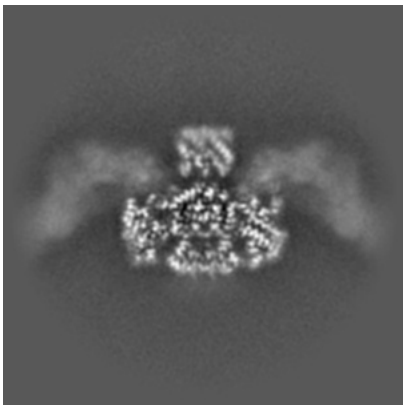


Z Index: 128

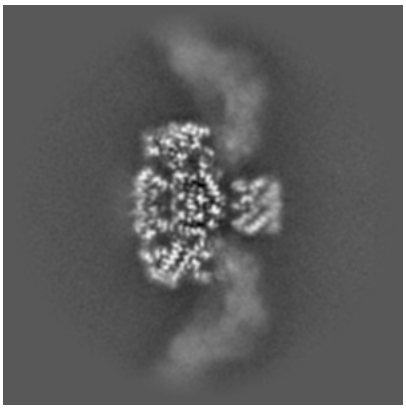
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

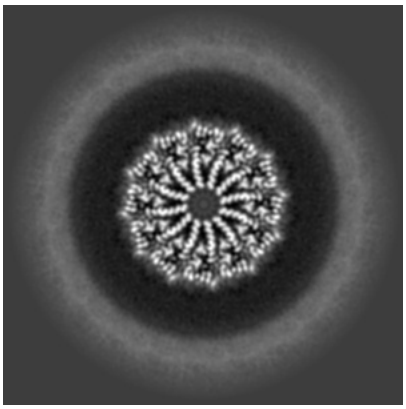
6.3.1 Primary map



X Index: 106

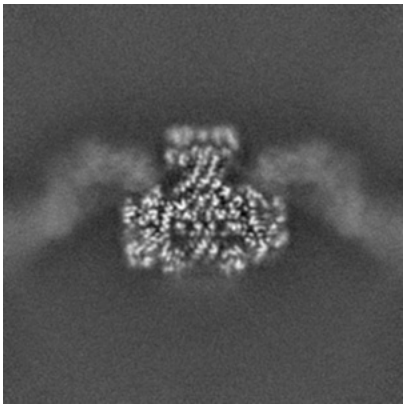


Y Index: 106

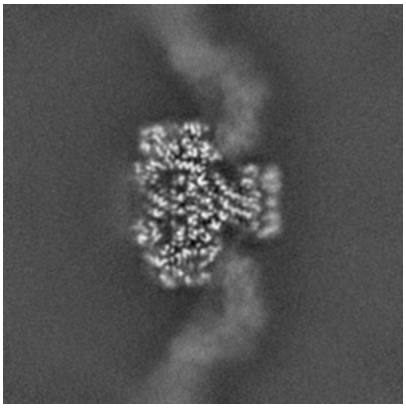


Z Index: 113

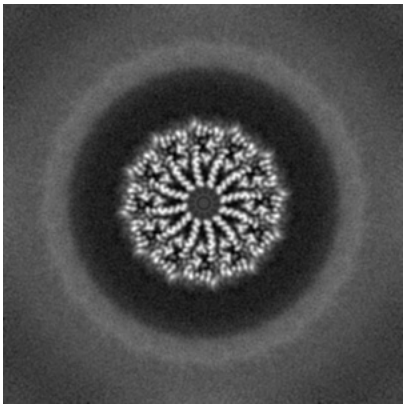
6.3.2 Raw map



X Index: 111



Y Index: 111

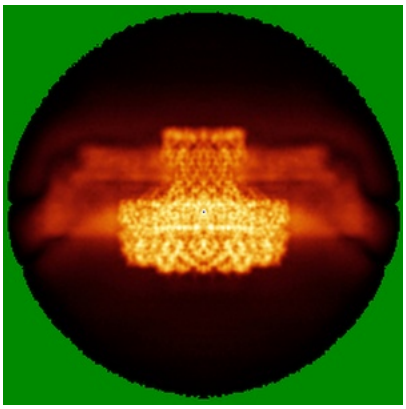


Z Index: 113

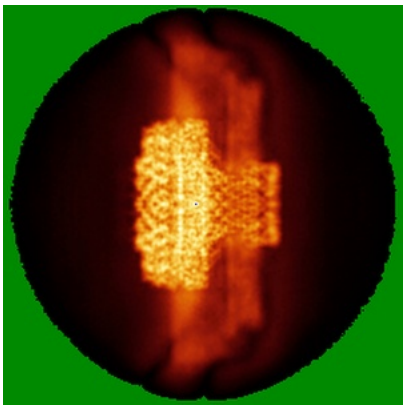
The images above show the largest variance slices of the map in three orthogonal directions.

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

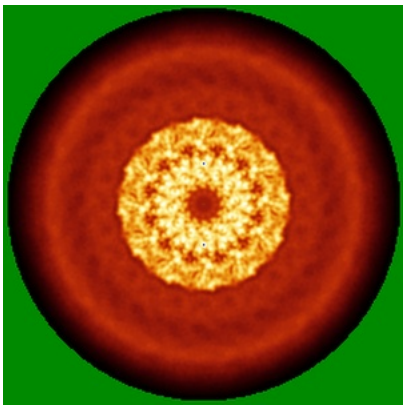
6.4.1 Primary map



X

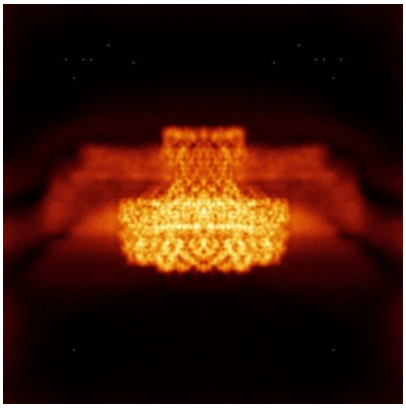


Y

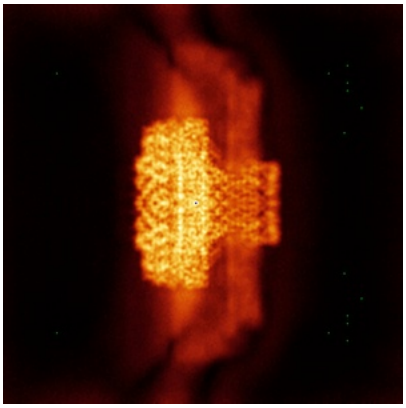


Z

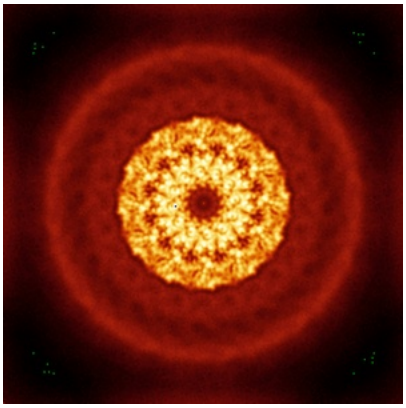
6.4.2 Raw map



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 0.3. 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.

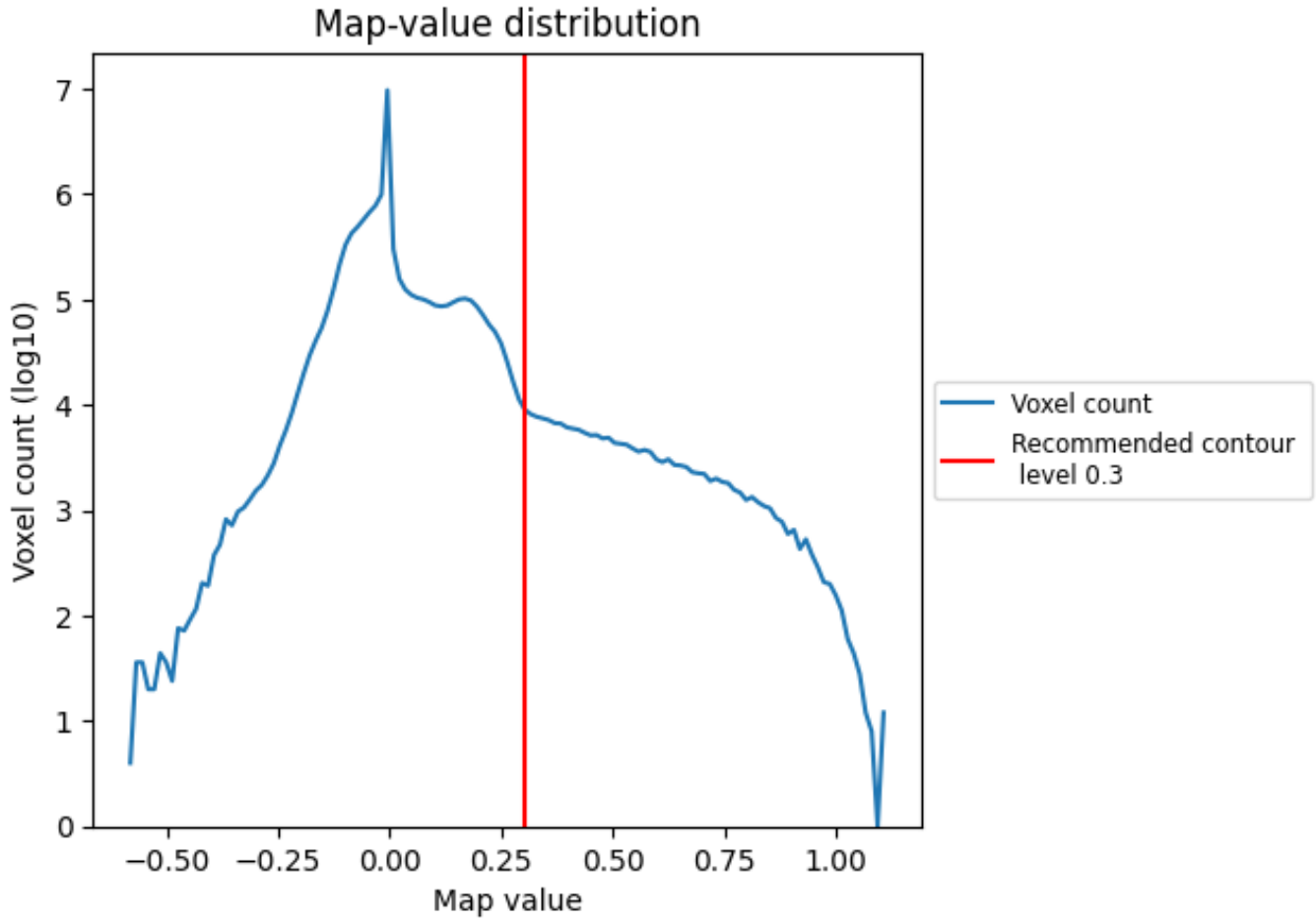
6.6 Mask visualisation (i)

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

7 Map analysis

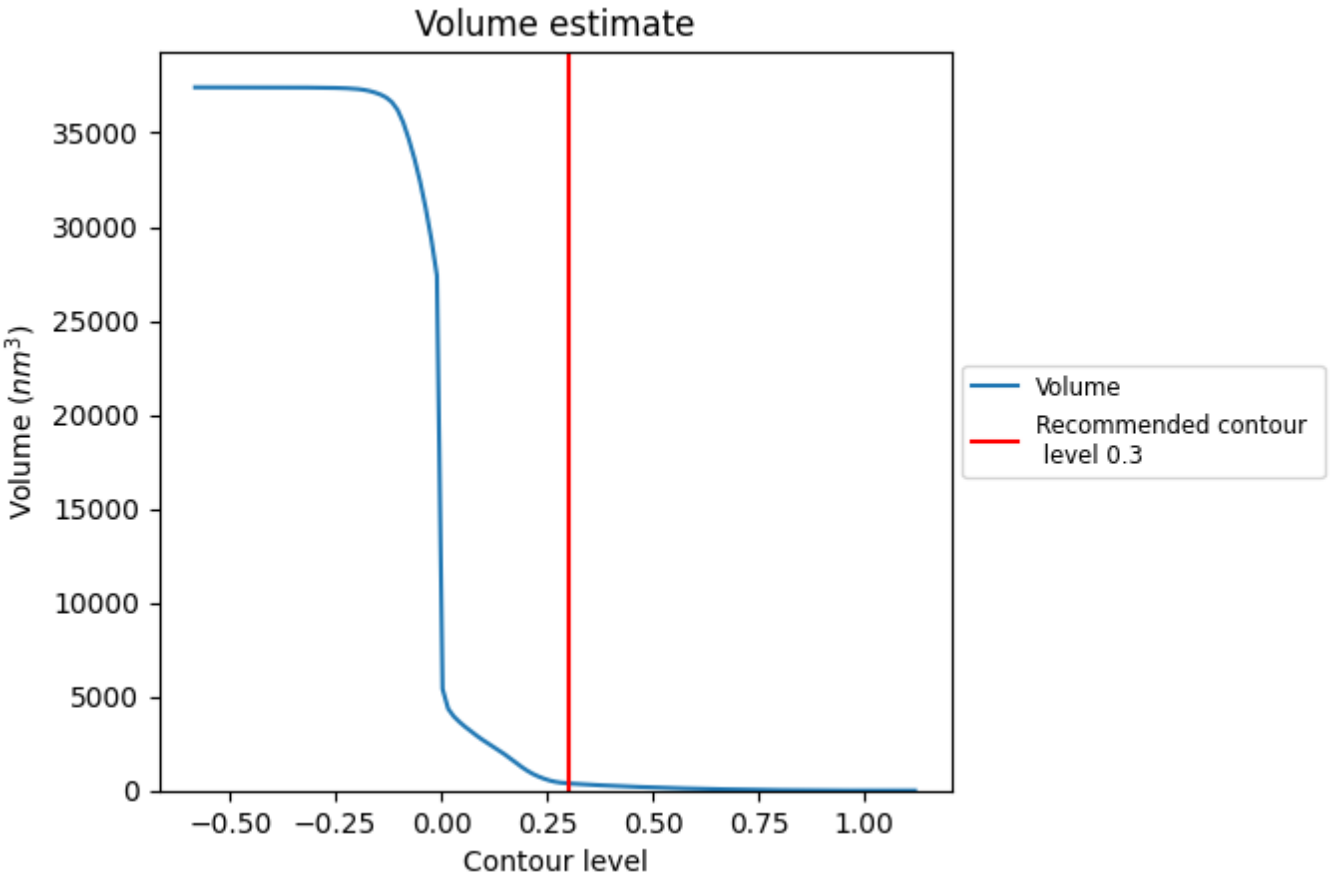
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

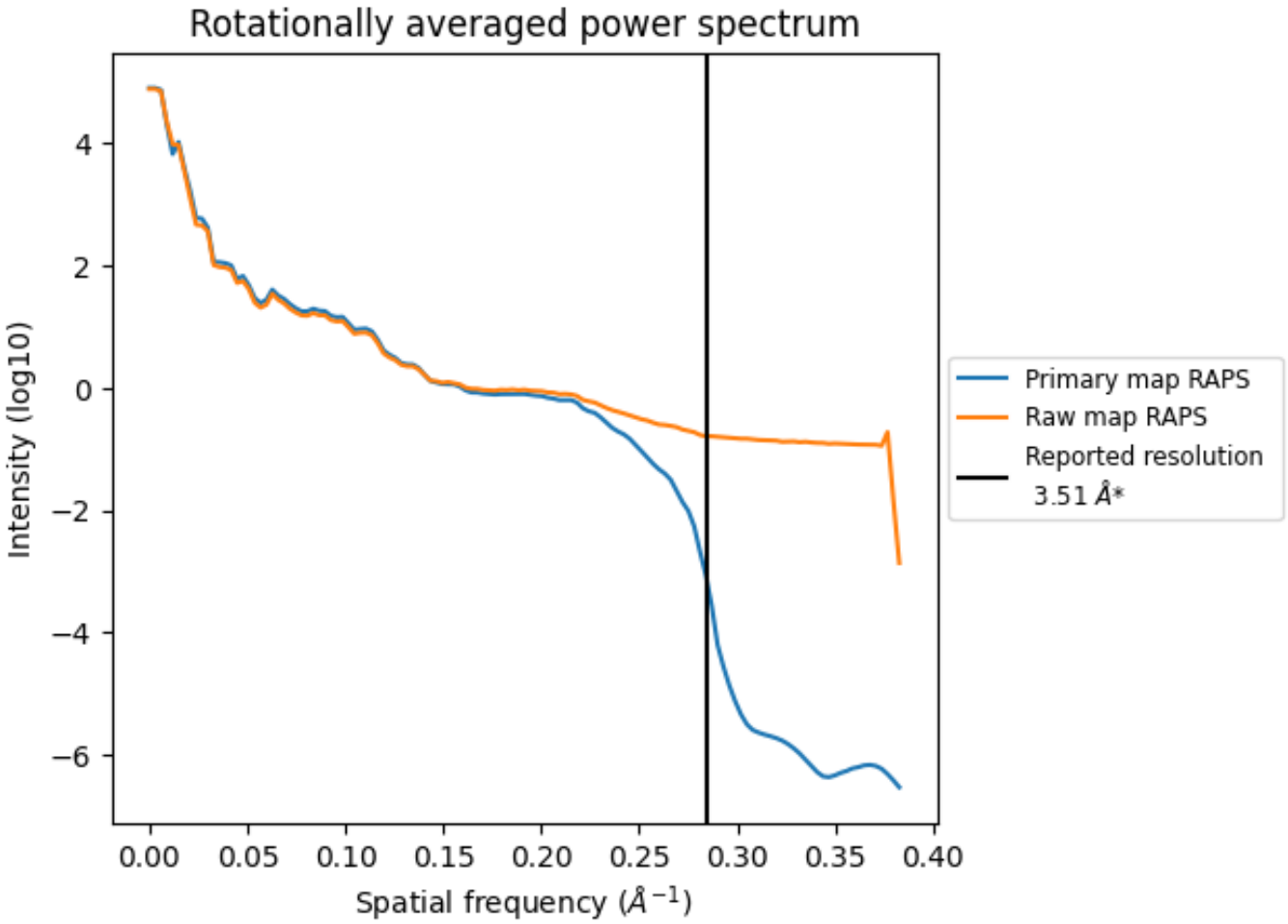
7.2 Volume estimate



The volume at the recommended contour level is 383 nm^3; this corresponds to an approximate mass of 346 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)

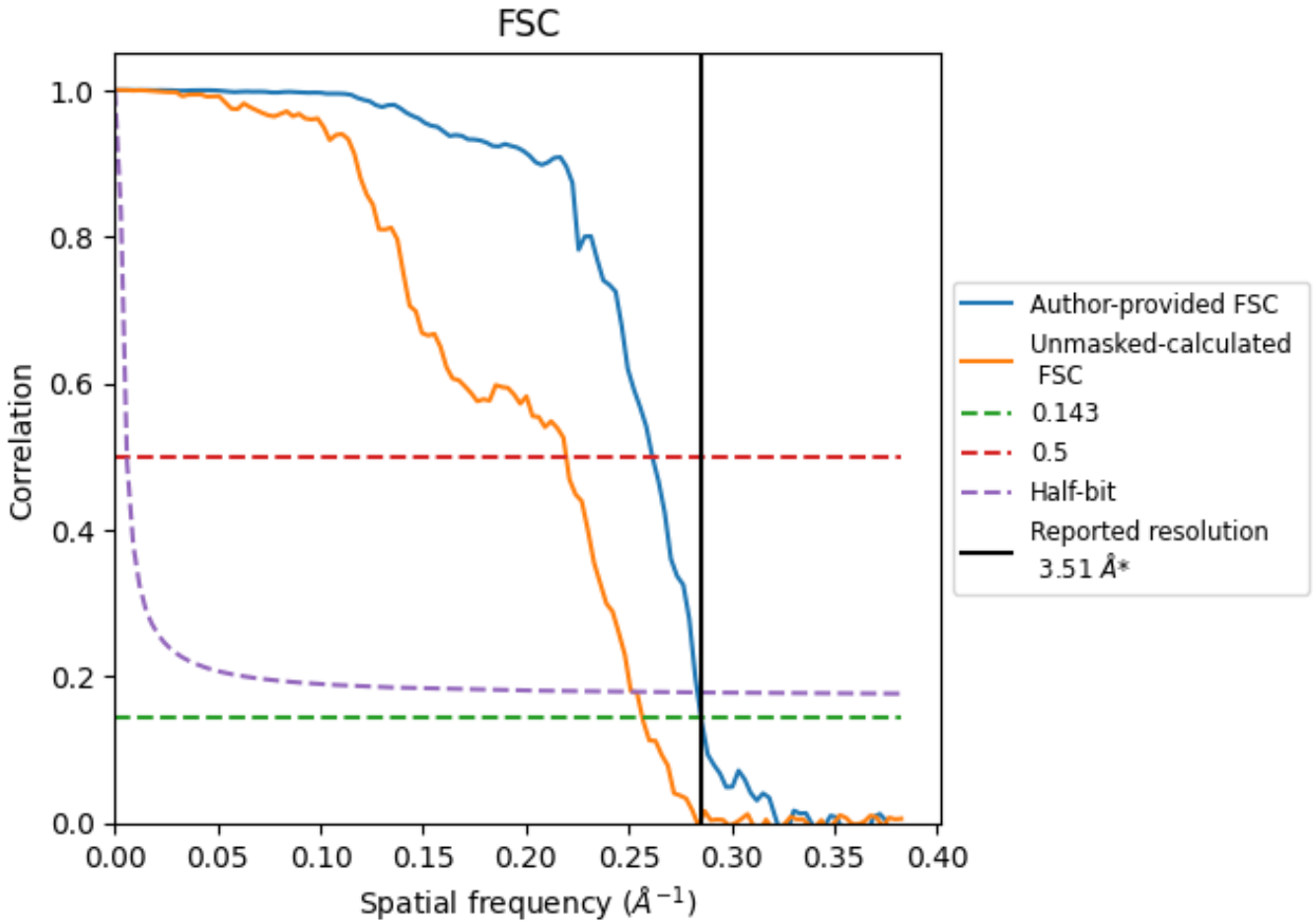


*Reported resolution corresponds to spatial frequency of 0.285 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.285 Å^{-1}

8.2 Resolution estimates (i)

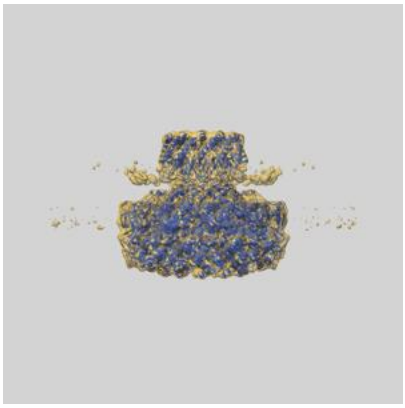
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.51	-	-
Author-provided FSC curve	3.51	3.82	3.53
Unmasked-calculated*	3.89	4.55	3.96

*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 3.89 differs from the reported value 3.51 by more than 10 %

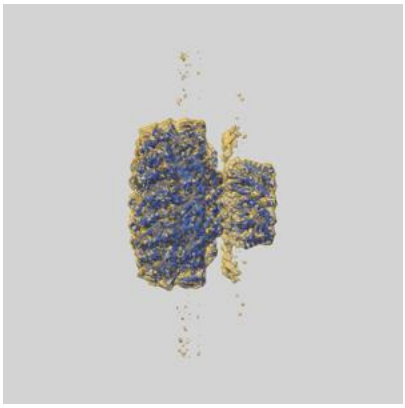
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38540 and PDB model 8XOT. Per-residue inclusion information can be found in section 3 on page 5.

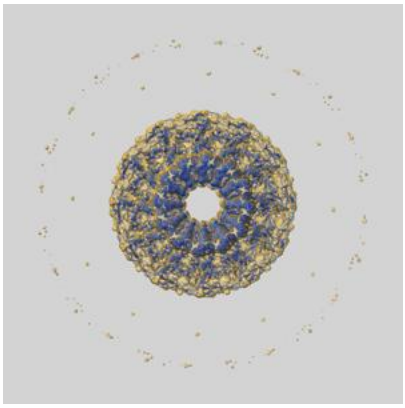
9.1 Map-model overlay



X



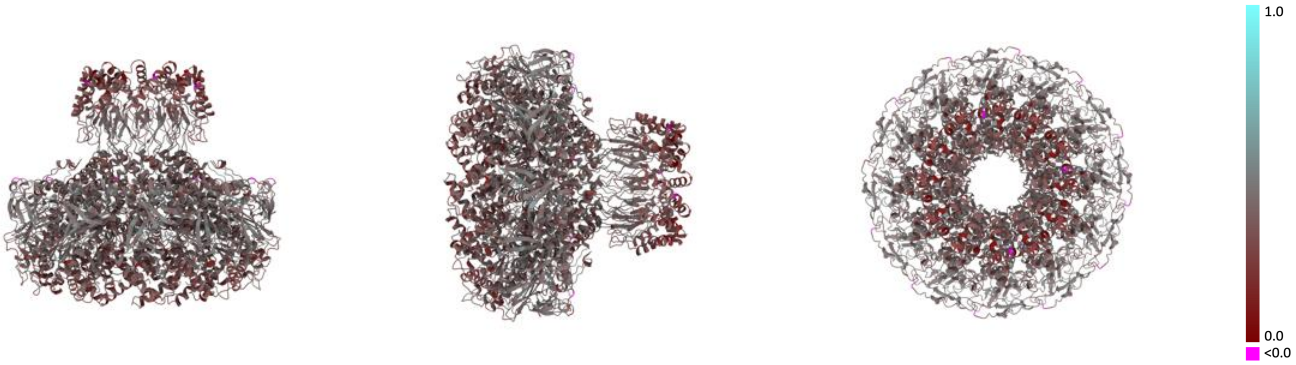
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

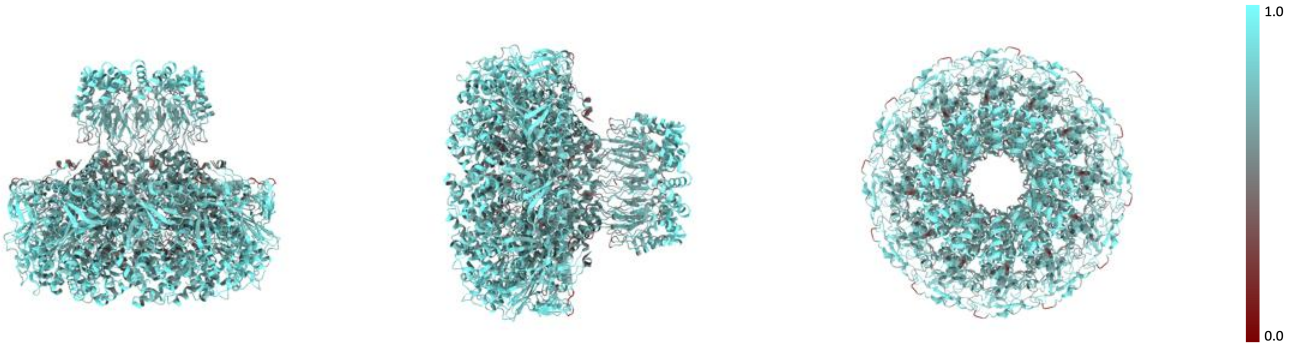
9.2 Q-score mapped to coordinate model (i)



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.

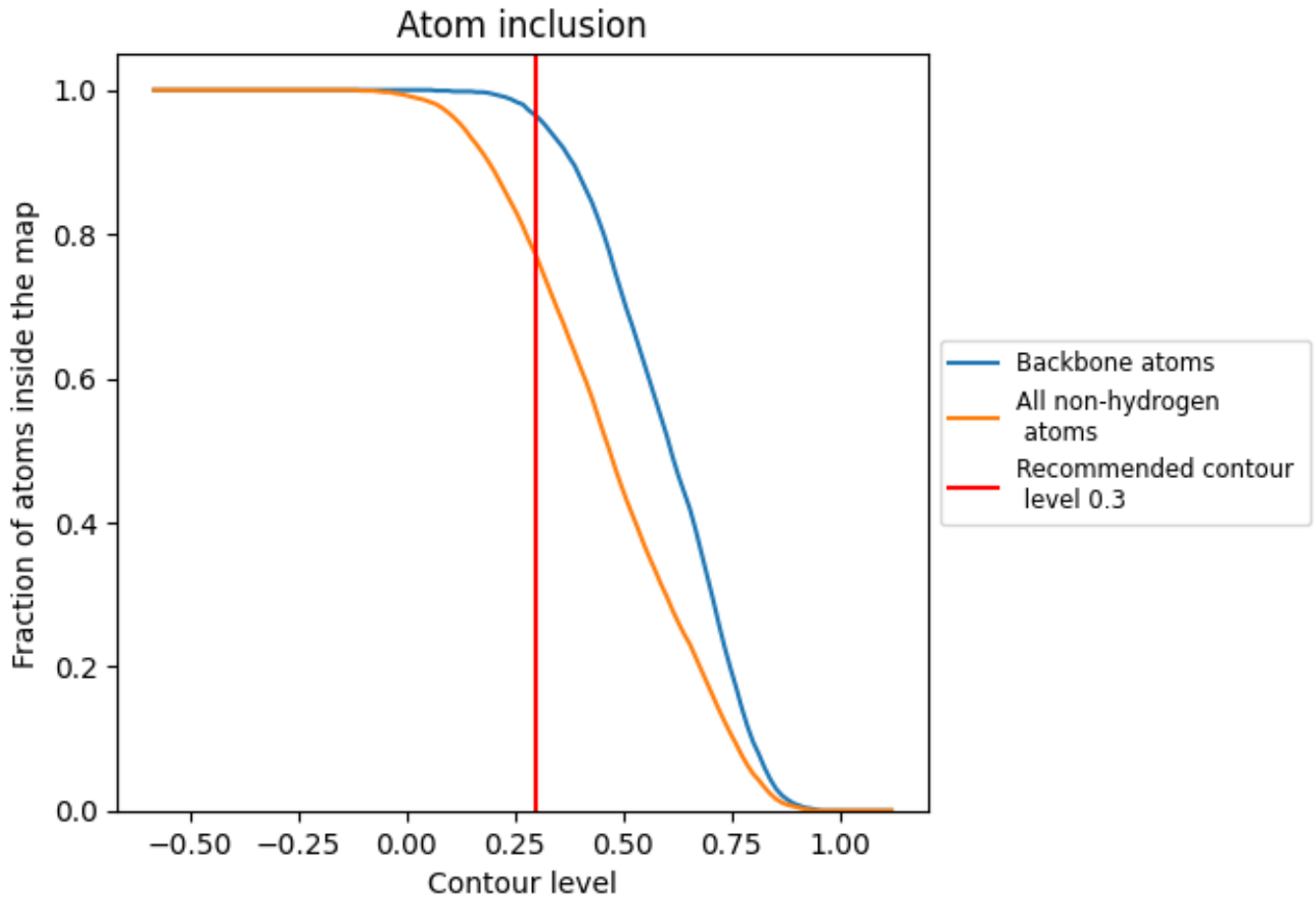
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 77% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7700	0.3770
B	0.7690	0.3760
B1	0.7720	0.3770
B2	0.7670	0.3760
B3	0.7690	0.3780
B4	0.7710	0.3780
B5	0.7700	0.3760
b	0.7670	0.3760
b1	0.7700	0.3750
b2	0.7710	0.3780
b3	0.7670	0.3750
b4	0.7700	0.3780
b5	0.7700	0.3770