Full wwPDB EM Validation Report

Oct 6, 2024 – 03:22 am BST

PDB ID	:	8P4K
EMDB ID	:	EMD-17410
Title	:	Vaccinia Virus palisade layer A10 trimer
Authors	:	Datler, J.; Hansen, J.M.; Thader, A.; Schloegl, A.; Hodirnau, V.V.; Schur, F.K.M.
Deposited on	:	2023-05-22
Resolution	:	3.80 Å(reported)
Based on initial model	:	.

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 (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:

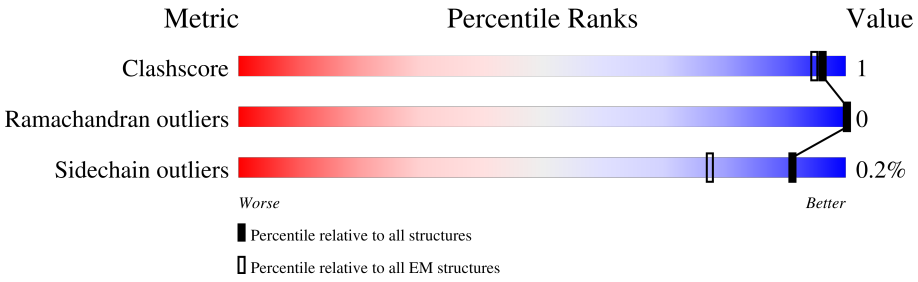
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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 <=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	599	33% 90% 9%
1	B	599	33% 90% 10%
1	C	599	33% 91% 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 29211 atoms, of which 14643 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 Core protein OPG136.

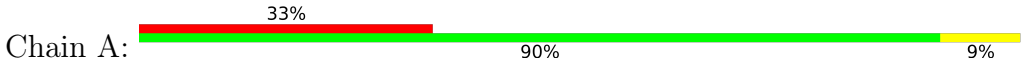
Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	599	Total	C	H	N	O	S	0	0
			9737	3123	4881	803	904	26		
1	B	599	Total	C	H	N	O	S	0	0
			9737	3123	4881	803	904	26		
1	C	599	Total	C	H	N	O	S	0	0
			9737	3123	4881	803	904	26		

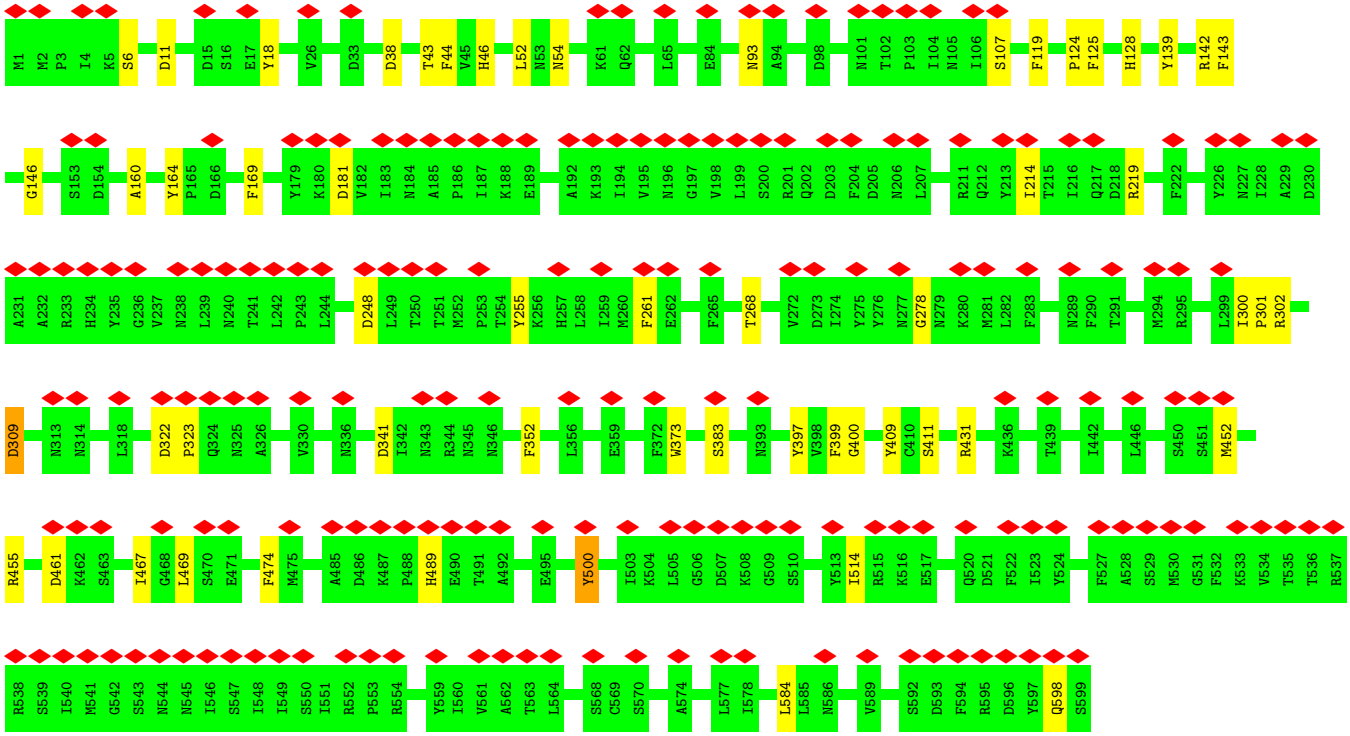
3 Residue-property plots (i)

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: Core protein OPG136

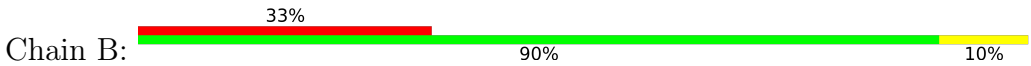
Chain A:

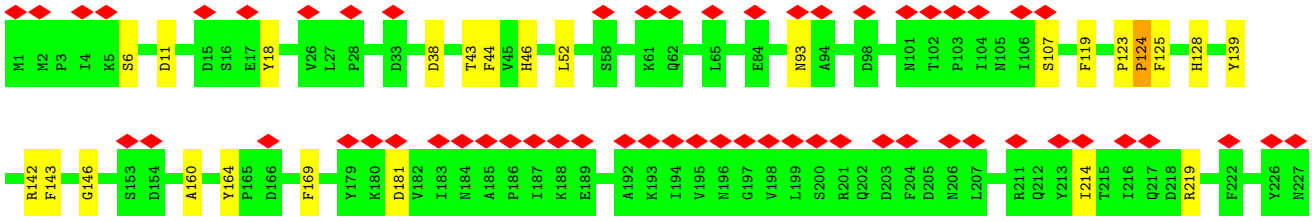


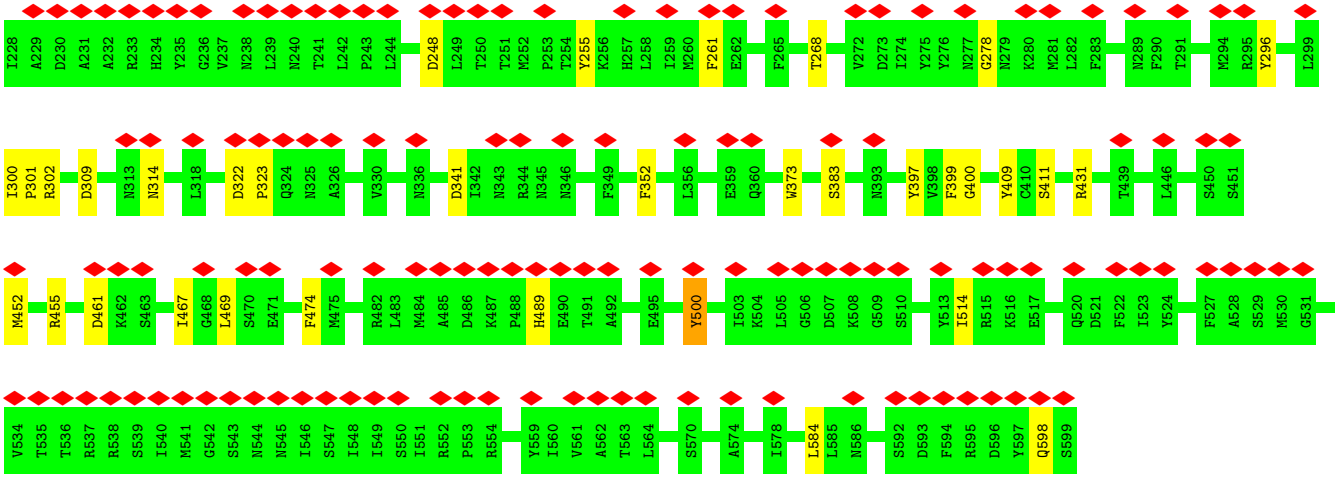


• Molecule 1: Core protein OPG136

Chain B:

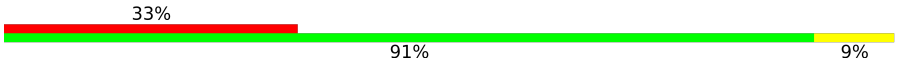


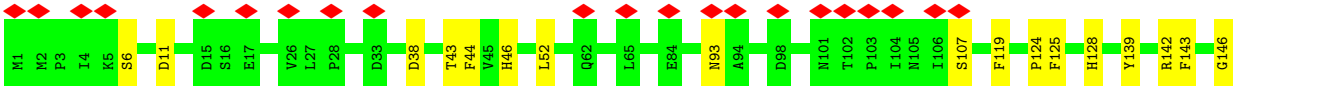


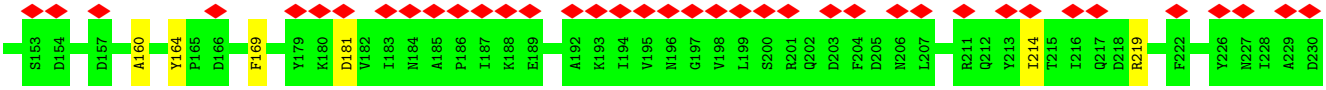


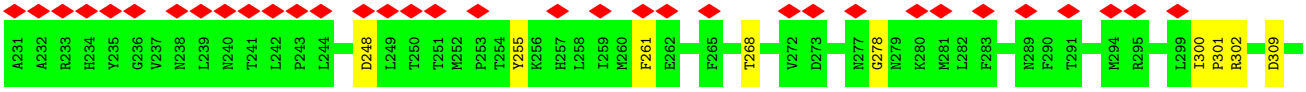
- Molecule 1: Core protein OPG136

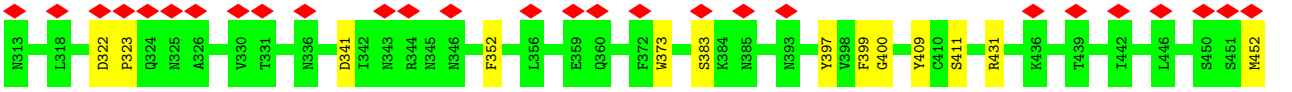
Chain C:

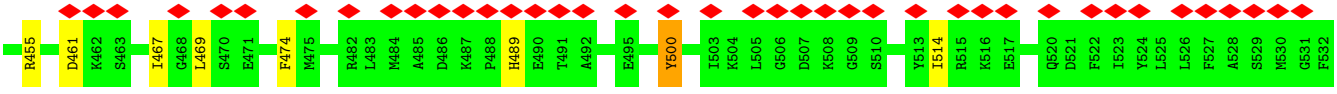


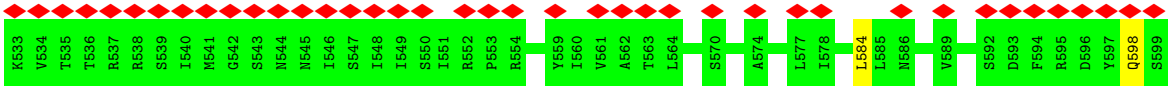












4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	24943	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	53.04	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	17.903	Depositor
Minimum map value	-12.965	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.205	Depositor
Recommended contour level	0.9	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	A	1.03	14/4959 (0.3%)	1.25	41/6722 (0.6%)
1	B	1.03	14/4959 (0.3%)	1.25	42/6722 (0.6%)
1	C	1.03	14/4959 (0.3%)	1.25	41/6722 (0.6%)
All	All	1.03	42/14877 (0.3%)	1.25	124/20166 (0.6%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	352	PHE	CB-CG	-10.78	1.33	1.51
1	A	352	PHE	CB-CG	-10.76	1.33	1.51
1	B	352	PHE	CB-CG	-10.76	1.33	1.51
1	B	169	PHE	CB-CG	-10.13	1.34	1.51
1	A	169	PHE	CB-CG	-10.13	1.34	1.51
1	C	169	PHE	CB-CG	-10.07	1.34	1.51
1	C	373	TRP	CB-CG	-8.61	1.34	1.50
1	A	373	TRP	CB-CG	-8.60	1.34	1.50
1	B	373	TRP	CB-CG	-8.57	1.34	1.50
1	B	143	PHE	CB-CG	-7.48	1.38	1.51
1	C	143	PHE	CB-CG	-7.48	1.38	1.51
1	A	143	PHE	CB-CG	-7.47	1.38	1.51
1	A	399	PHE	CB-CG	-7.42	1.38	1.51
1	C	399	PHE	CB-CG	-7.39	1.38	1.51
1	B	399	PHE	CB-CG	-7.37	1.38	1.51
1	C	128	HIS	CB-CG	-6.93	1.37	1.50
1	A	128	HIS	CB-CG	-6.92	1.37	1.50
1	B	128	HIS	CB-CG	-6.89	1.37	1.50
1	B	125	PHE	CB-CG	-5.90	1.41	1.51
1	A	125	PHE	CB-CG	-5.88	1.41	1.51
1	B	474	PHE	CB-CG	-5.88	1.41	1.51
1	A	474	PHE	CB-CG	-5.88	1.41	1.51
1	C	125	PHE	CB-CG	-5.87	1.41	1.51
1	C	474	PHE	CB-CG	-5.84	1.41	1.51
1	A	119	PHE	CB-CG	-5.75	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	119	PHE	CB-CG	-5.73	1.41	1.51
1	C	119	PHE	CB-CG	-5.72	1.41	1.51
1	B	46	HIS	CB-CG	-5.54	1.40	1.50
1	C	46	HIS	CB-CG	-5.53	1.40	1.50
1	A	46	HIS	CB-CG	-5.52	1.40	1.50
1	C	373	TRP	CD2-CE2	-5.51	1.34	1.41
1	A	373	TRP	CD2-CE2	-5.51	1.34	1.41
1	C	409	TYR	CB-CG	-5.50	1.43	1.51
1	A	409	TYR	CB-CG	-5.49	1.43	1.51
1	B	409	TYR	CB-CG	-5.48	1.43	1.51
1	B	373	TRP	CD2-CE2	-5.44	1.34	1.41
1	A	411	SER	CB-OG	-5.25	1.35	1.42
1	A	139	TYR	CB-CG	-5.22	1.43	1.51
1	B	139	TYR	CB-CG	-5.21	1.43	1.51
1	B	411	SER	CB-OG	-5.21	1.35	1.42
1	C	139	TYR	CB-CG	-5.21	1.43	1.51
1	C	411	SER	CB-OG	-5.18	1.35	1.42

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	467	ILE	C-N-CA	14.89	153.57	122.30
1	A	467	ILE	C-N-CA	14.87	153.53	122.30
1	C	467	ILE	C-N-CA	14.85	153.48	122.30
1	B	6	SER	C-N-CA	14.29	157.42	121.70
1	C	6	SER	C-N-CA	14.29	157.41	121.70
1	A	6	SER	C-N-CA	14.28	157.40	121.70
1	B	598	GLN	C-N-CA	14.16	157.10	121.70
1	A	598	GLN	C-N-CA	14.16	157.09	121.70
1	C	598	GLN	C-N-CA	14.15	157.07	121.70
1	A	341	ASP	C-N-CA	13.64	155.80	121.70
1	B	341	ASP	C-N-CA	13.63	155.78	121.70
1	C	341	ASP	C-N-CA	13.63	155.77	121.70
1	A	452	MET	C-N-CA	12.91	153.99	121.70
1	B	452	MET	C-N-CA	12.91	153.98	121.70
1	C	452	MET	C-N-CA	12.91	153.97	121.70
1	C	455	ARG	C-N-CA	12.79	153.66	121.70
1	B	455	ARG	C-N-CA	12.78	153.65	121.70
1	A	455	ARG	C-N-CA	12.76	153.60	121.70
1	B	461	ASP	C-N-CA	12.70	153.45	121.70
1	C	461	ASP	C-N-CA	12.70	153.44	121.70
1	A	461	ASP	C-N-CA	12.69	153.44	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	107	SER	C-N-CA	12.68	153.40	121.70
1	B	107	SER	C-N-CA	12.68	153.39	121.70
1	C	107	SER	C-N-CA	12.68	153.39	121.70
1	C	93	ASN	C-N-CA	12.53	153.02	121.70
1	B	93	ASN	C-N-CA	12.53	153.01	121.70
1	A	514	ILE	C-N-CA	12.52	153.00	121.70
1	A	93	ASN	C-N-CA	12.52	153.00	121.70
1	C	514	ILE	C-N-CA	12.52	153.00	121.70
1	B	514	ILE	C-N-CA	12.51	152.97	121.70
1	B	400	GLY	C-N-CA	12.12	152.00	121.70
1	A	400	GLY	C-N-CA	12.12	152.00	121.70
1	C	400	GLY	C-N-CA	12.12	151.99	121.70
1	A	248	ASP	C-N-CA	12.05	151.83	121.70
1	C	248	ASP	C-N-CA	12.04	151.80	121.70
1	B	248	ASP	C-N-CA	12.02	151.75	121.70
1	B	52	LEU	C-N-CA	11.81	151.22	121.70
1	C	52	LEU	C-N-CA	11.81	151.22	121.70
1	A	52	LEU	C-N-CA	11.80	151.21	121.70
1	C	160	ALA	C-N-CA	11.72	151.00	121.70
1	B	160	ALA	C-N-CA	11.71	150.98	121.70
1	A	160	ALA	C-N-CA	11.70	150.96	121.70
1	A	278	GLY	C-N-CA	11.63	150.78	121.70
1	B	278	GLY	C-N-CA	11.63	150.78	121.70
1	C	278	GLY	C-N-CA	11.63	150.77	121.70
1	B	469	LEU	C-N-CA	11.53	150.51	121.70
1	A	469	LEU	C-N-CA	11.51	150.48	121.70
1	C	469	LEU	C-N-CA	11.50	150.45	121.70
1	A	214	ILE	C-N-CA	11.45	150.33	121.70
1	B	214	ILE	C-N-CA	11.45	150.33	121.70
1	C	214	ILE	C-N-CA	11.45	150.32	121.70
1	A	383	SER	C-N-CA	11.43	150.27	121.70
1	B	383	SER	C-N-CA	11.43	150.27	121.70
1	C	383	SER	C-N-CA	11.41	150.22	121.70
1	B	119	PHE	C-N-CA	11.26	149.85	121.70
1	A	119	PHE	C-N-CA	11.24	149.81	121.70
1	C	119	PHE	C-N-CA	11.23	149.79	121.70
1	B	181	ASP	C-N-CA	11.18	149.66	121.70
1	A	181	ASP	C-N-CA	11.17	149.63	121.70
1	C	181	ASP	C-N-CA	11.17	149.62	121.70
1	A	489	HIS	C-N-CA	11.15	149.59	121.70
1	B	489	HIS	C-N-CA	11.14	149.55	121.70
1	C	489	HIS	C-N-CA	11.13	149.53	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	268	THR	C-N-CA	11.01	149.21	121.70
1	C	268	THR	C-N-CA	11.01	149.22	121.70
1	A	268	THR	C-N-CA	11.00	149.20	121.70
1	C	474	PHE	C-N-CA	10.94	149.05	121.70
1	B	474	PHE	C-N-CA	10.93	149.03	121.70
1	A	474	PHE	C-N-CA	10.92	149.01	121.70
1	C	431	ARG	NE-CZ-NH2	-10.59	115.00	120.30
1	B	431	ARG	NE-CZ-NH2	-10.58	115.01	120.30
1	A	431	ARG	NE-CZ-NH2	-10.48	115.06	120.30
1	C	261	PHE	C-N-CA	10.29	147.43	121.70
1	A	261	PHE	C-N-CA	10.27	147.38	121.70
1	B	261	PHE	C-N-CA	10.27	147.38	121.70
1	B	309	ASP	C-N-CA	10.18	147.14	121.70
1	A	309	ASP	C-N-CA	10.17	147.14	121.70
1	C	309	ASP	C-N-CA	10.17	147.12	121.70
1	A	146	GLY	C-N-CA	10.10	146.96	121.70
1	B	146	GLY	C-N-CA	10.10	146.96	121.70
1	C	146	GLY	C-N-CA	10.08	146.89	121.70
1	A	124	PRO	C-N-CA	9.98	146.66	121.70
1	B	124	PRO	C-N-CA	9.97	146.63	121.70
1	C	124	PRO	C-N-CA	9.95	146.57	121.70
1	B	255	TYR	C-N-CA	9.65	145.82	121.70
1	A	255	TYR	C-N-CA	9.63	145.79	121.70
1	C	255	TYR	C-N-CA	9.63	145.78	121.70
1	A	139	TYR	C-N-CA	8.66	143.35	121.70
1	C	139	TYR	C-N-CA	8.66	143.34	121.70
1	B	139	TYR	C-N-CA	8.64	143.30	121.70
1	A	219	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	B	219	ARG	NE-CZ-NH2	-8.31	116.15	120.30
1	C	219	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	C	142	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	C	142	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	A	142	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	B	142	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	A	142	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	B	142	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	A	164	TYR	CB-CG-CD1	-6.97	116.82	121.00
1	C	164	TYR	CB-CG-CD1	-6.95	116.83	121.00
1	B	302	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	A	302	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	B	164	TYR	CB-CG-CD1	-6.90	116.86	121.00
1	C	302	ARG	NE-CZ-NH2	-6.84	116.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	474	PHE	CB-CG-CD2	-6.61	116.18	120.80
1	B	474	PHE	CB-CG-CD2	-6.57	116.20	120.80
1	A	474	PHE	CB-CG-CD2	-6.56	116.21	120.80
1	C	397	TYR	CB-CG-CD2	-5.89	117.47	121.00
1	A	397	TYR	CB-CG-CD2	-5.84	117.50	121.00
1	B	397	TYR	CB-CG-CD2	-5.76	117.55	121.00
1	B	248	ASP	CB-CG-OD1	5.53	123.28	118.30
1	C	248	ASP	CB-CG-OD1	5.52	123.26	118.30
1	A	248	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	474	PHE	CB-CG-CD1	5.37	124.56	120.80
1	A	474	PHE	CB-CG-CD1	5.36	124.55	120.80
1	C	474	PHE	CB-CG-CD1	5.33	124.53	120.80
1	A	431	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	C	431	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	431	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	296	TYR	CB-CG-CD1	-5.04	117.98	121.00
1	B	18	TYR	CB-CG-CD1	-5.02	117.99	121.00
1	C	474	PHE	CB-CA-C	-5.01	100.38	110.40
1	A	18	TYR	CB-CG-CD1	-5.01	118.00	121.00

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	4856	4881	4857	8	0
1	B	4856	4881	4857	8	0
1	C	4856	4881	4857	6	0
All	All	14568	14643	14571	22	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 1.

All (22) 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:B:11:ASP:OD1	1:B:11:ASP:N	2.36	0.59
1:B:38:ASP:N	1:B:38:ASP:OD1	2.35	0.57
1:C:11:ASP:OD1	1:C:11:ASP:N	2.36	0.57
1:C:38:ASP:N	1:C:38:ASP:OD1	2.35	0.57
1:A:38:ASP:OD1	1:A:38:ASP:N	2.35	0.57
1:A:11:ASP:N	1:A:11:ASP:OD1	2.36	0.55
1:C:43:THR:OG1	1:C:44:PHE:N	2.44	0.51
1:A:43:THR:OG1	1:A:44:PHE:N	2.44	0.50
1:B:43:THR:OG1	1:B:44:PHE:N	2.44	0.50
1:A:300:ILE:N	1:A:301:PRO:CD	2.79	0.46
1:B:300:ILE:N	1:B:301:PRO:CD	2.79	0.46
1:C:500:TYR:HB3	1:C:584:LEU:HD13	1.99	0.45
1:C:300:ILE:N	1:C:301:PRO:CD	2.79	0.45
1:B:500:TYR:HB3	1:B:584:LEU:HD13	1.99	0.45
1:C:322:ASP:HB2	1:C:323:PRO:CD	2.47	0.44
1:A:500:TYR:HB3	1:A:584:LEU:HD13	1.99	0.44
1:A:309:ASP:OD1	1:A:309:ASP:N	2.49	0.44
1:A:322:ASP:HB2	1:A:323:PRO:CD	2.47	0.44
1:B:322:ASP:HB2	1:B:323:PRO:CD	2.47	0.44
1:B:314:ASN:OD1	1:B:314:ASN:N	2.49	0.42
1:A:54:ASN:OD1	1:A:54:ASN:N	2.52	0.42
1:B:123:PRO:HA	1:B:124:PRO:HD3	1.94	0.40

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	597/599 (100%)	591 (99%)	6 (1%)	0	100	100
1	B	597/599 (100%)	591 (99%)	6 (1%)	0	100	100
1	C	597/599 (100%)	591 (99%)	6 (1%)	0	100	100
All	All	1791/1797 (100%)	1773 (99%)	18 (1%)	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	A	554/554 (100%)	553 (100%)	1 (0%)	92	94
1	B	554/554 (100%)	553 (100%)	1 (0%)	92	94
1	C	554/554 (100%)	553 (100%)	1 (0%)	92	94
All	All	1662/1662 (100%)	1659 (100%)	3 (0%)	91	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	500	TYR
1	B	500	TYR
1	C	500	TYR

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

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

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.

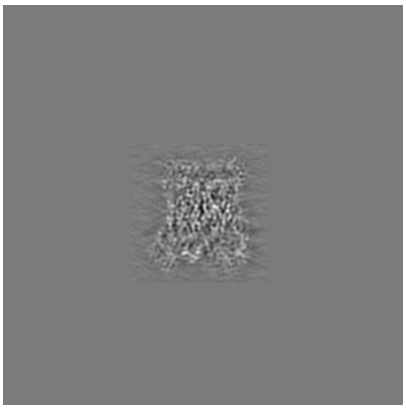
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17410. These allow visual inspection of the internal detail of the map and identification of artifacts.

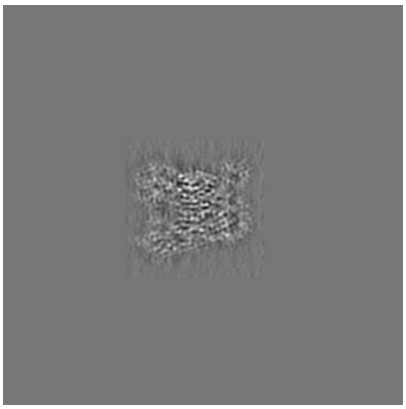
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

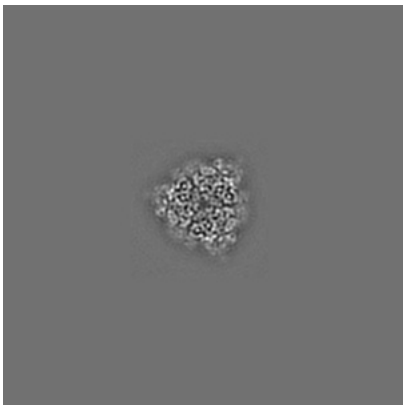
6.1.1 Primary map



X

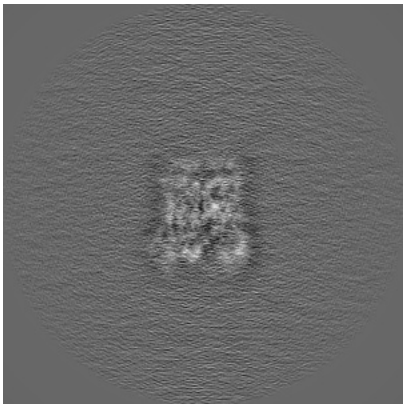


Y

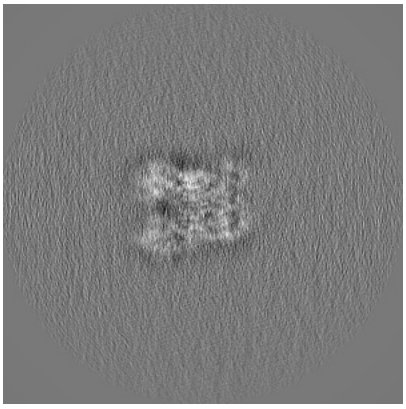


Z

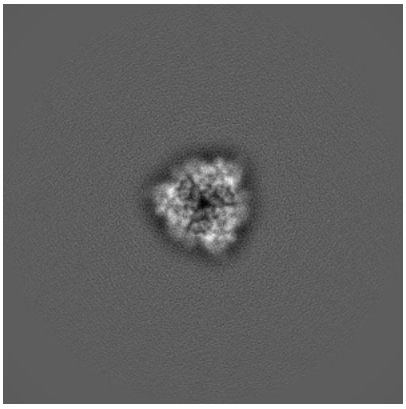
6.1.2 Raw map



X



Y



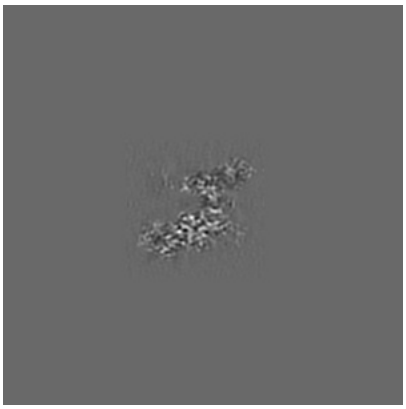
Z

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

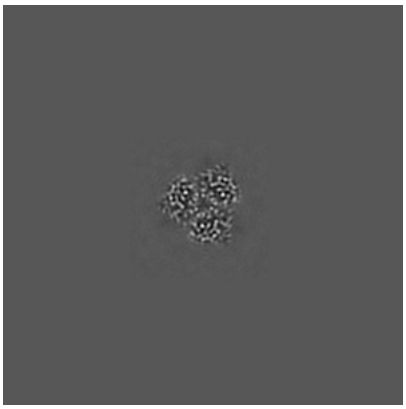
6.2 Central slices (i)

6.2.1 Primary map

X Index: 160

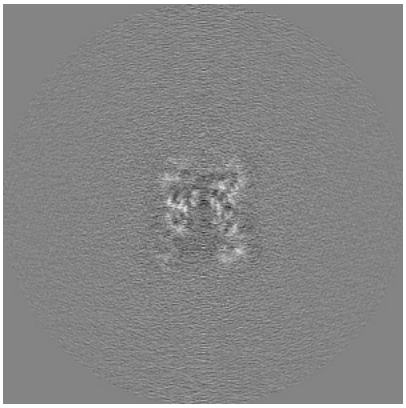


Y Index: 160

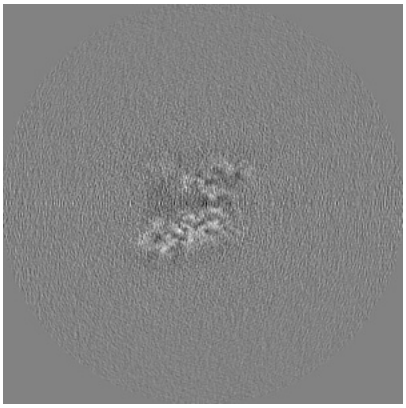


Z Index: 160

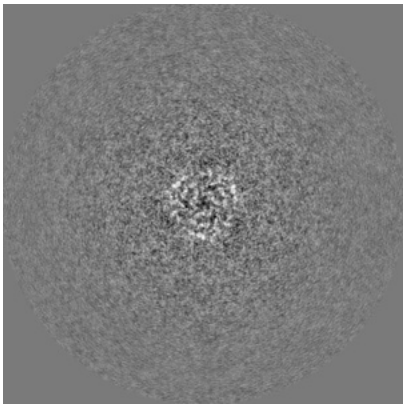
6.2.2 Raw map



X Index: 160



Y Index: 160



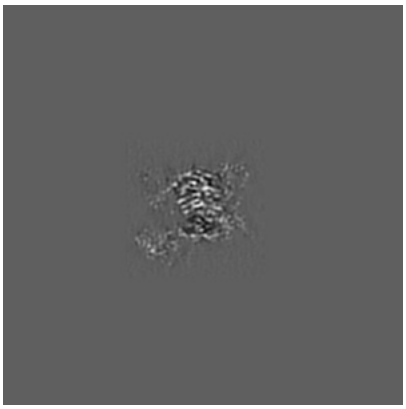
Z Index: 160

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

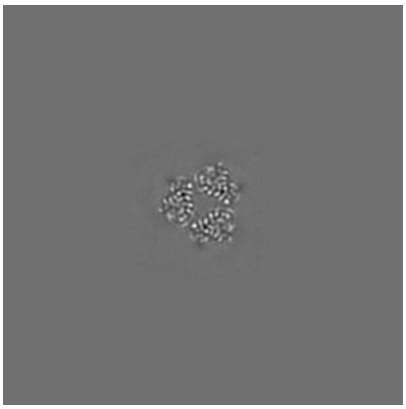
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 173

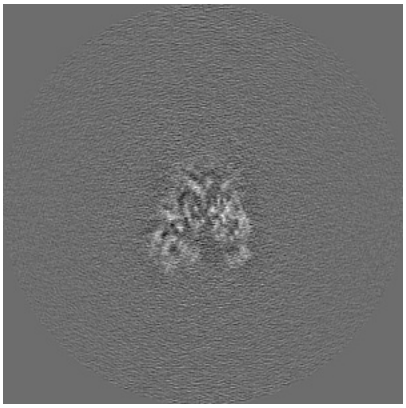


Y Index: 172

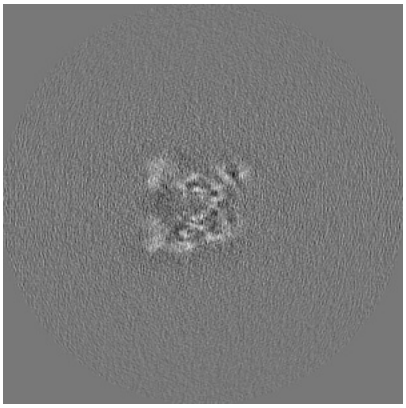


Z Index: 151

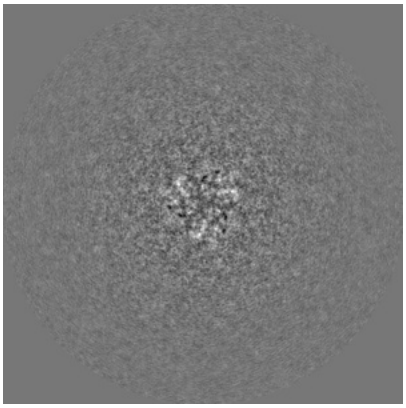
6.3.2 Raw map



X Index: 173



Y Index: 155

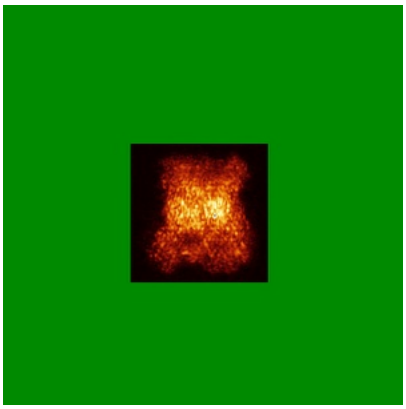


Z Index: 157

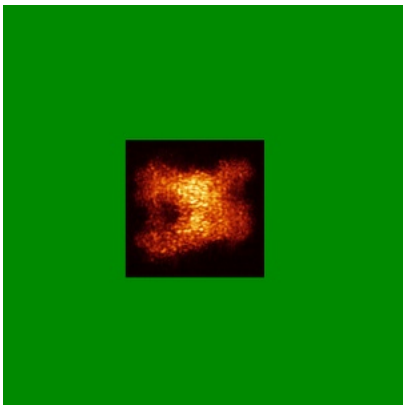
The images above show the largest variance slices of the map in three orthogonal directions.

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

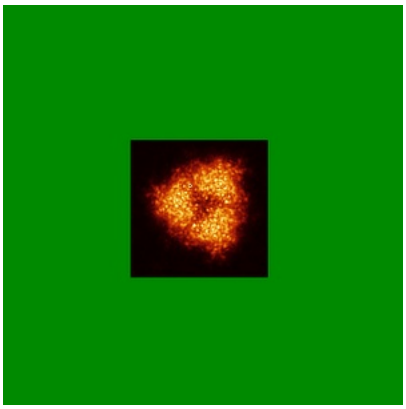
6.4.1 Primary map



X

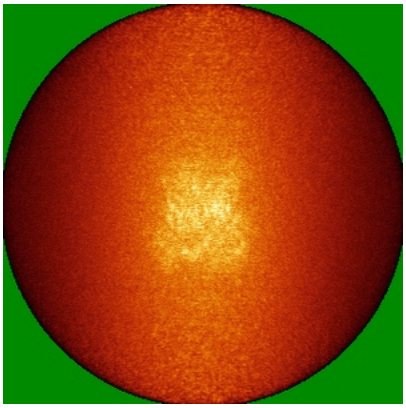


Y

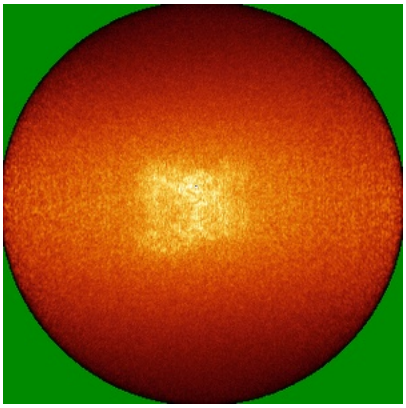


Z

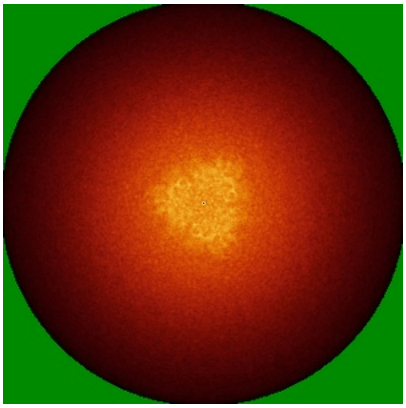
6.4.2 Raw map



X



Y

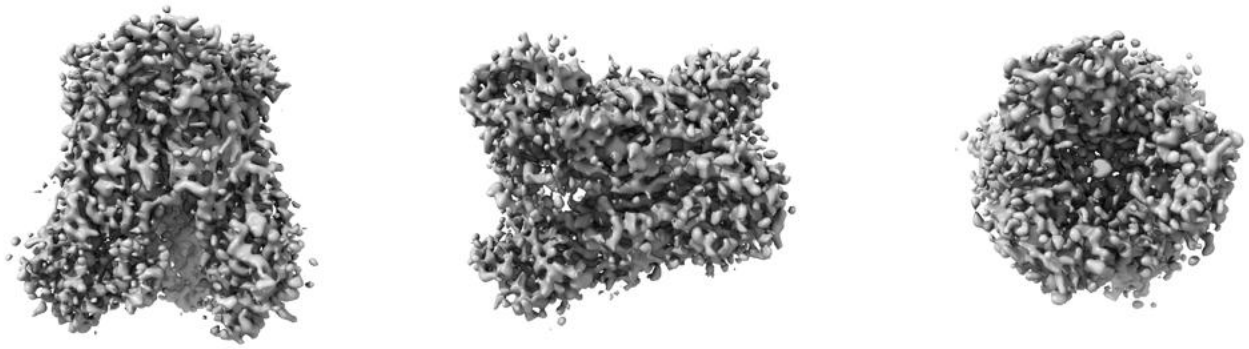


Z

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)

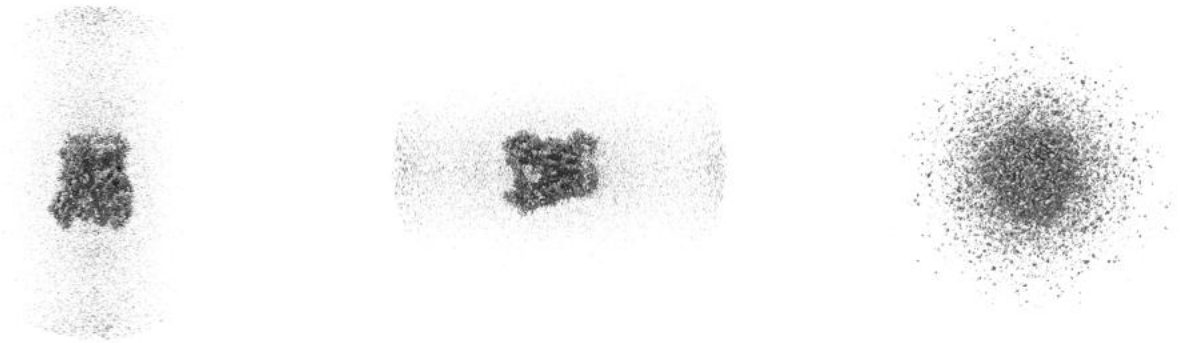
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.9. 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.

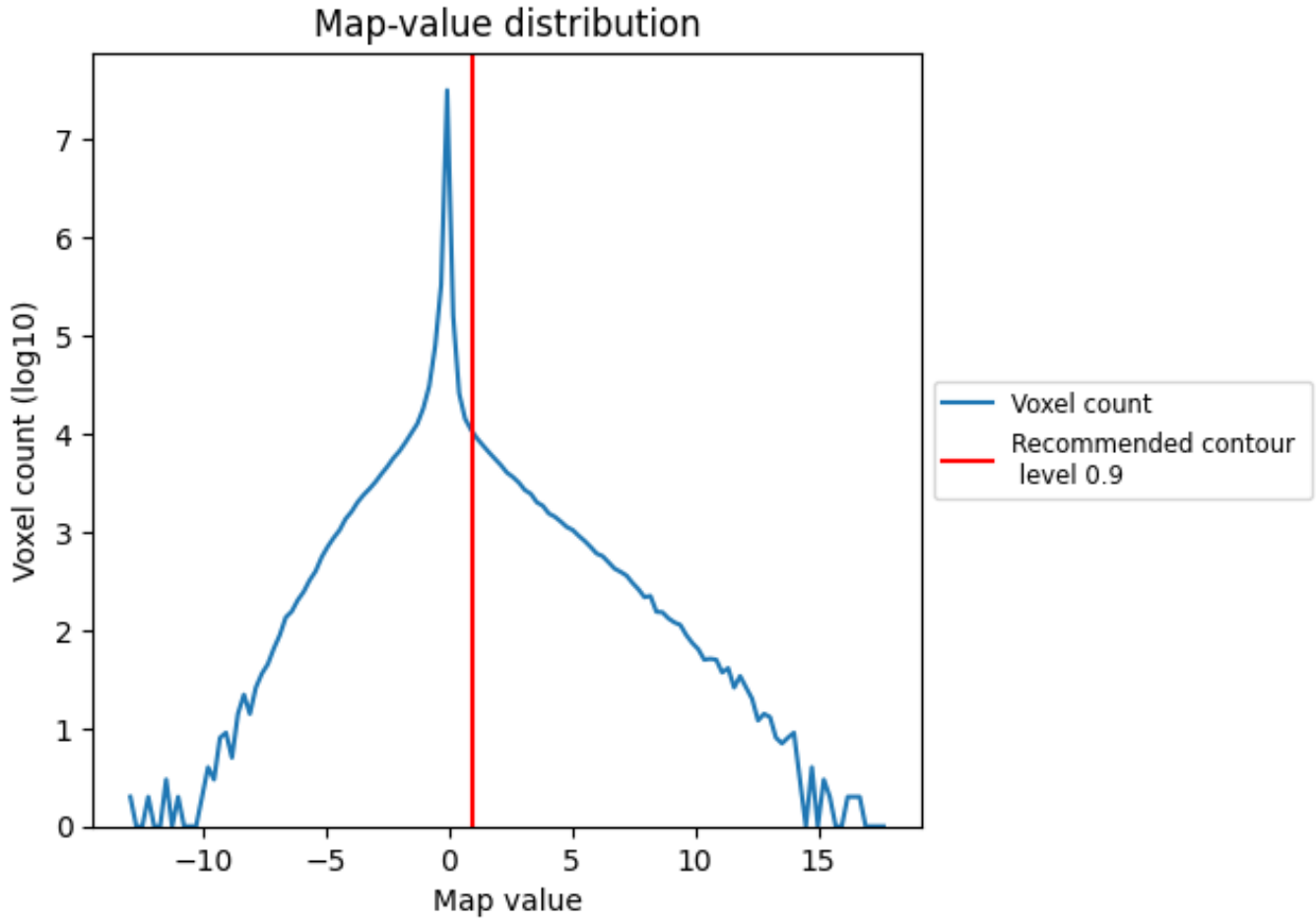
6.6 Mask visualisation (i)

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

7 Map analysis

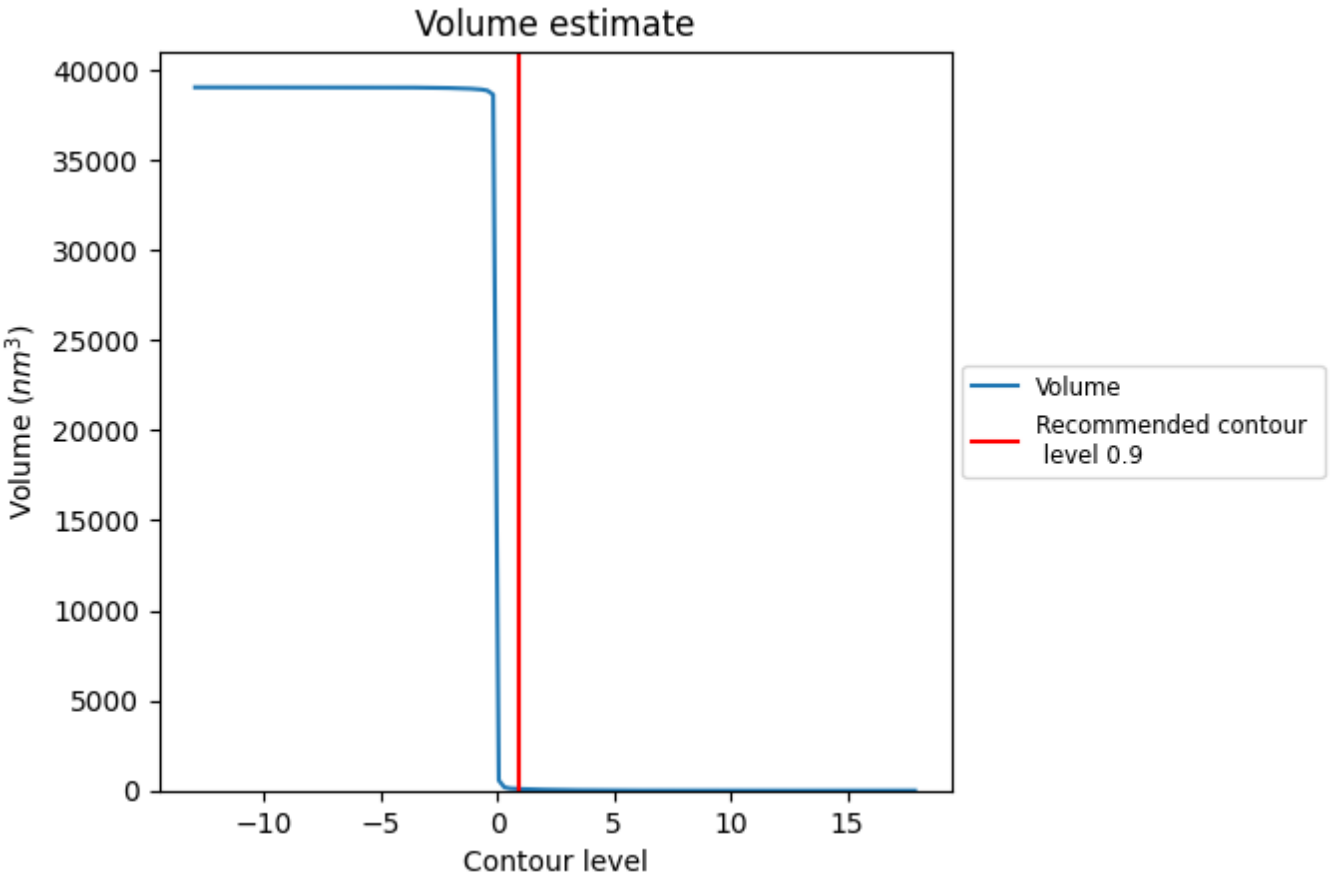
This section contains the results of statistical analysis of the map.

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.

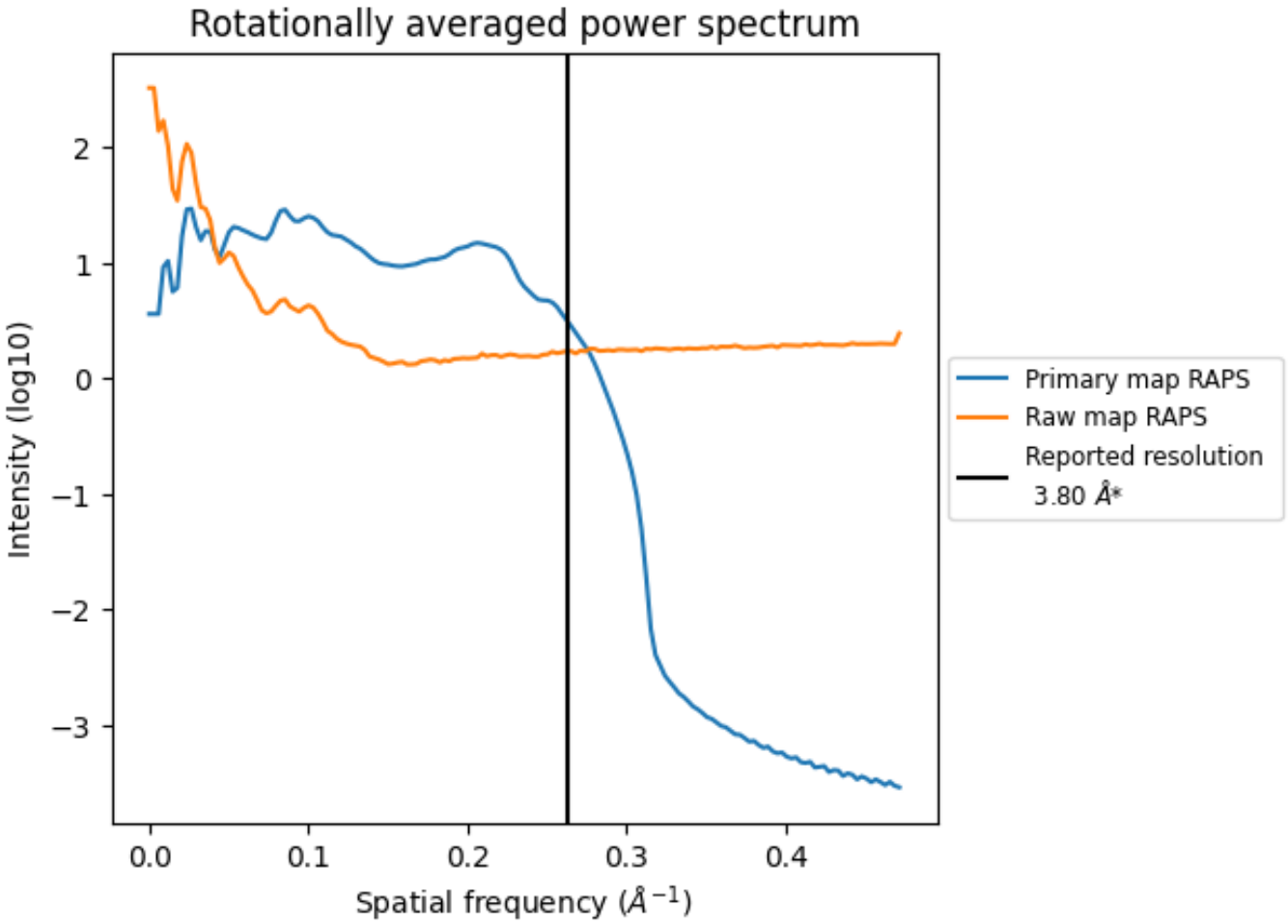
7.2 Volume estimate



The volume at the recommended contour level is 93 nm^3; this corresponds to an approximate mass of 84 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)

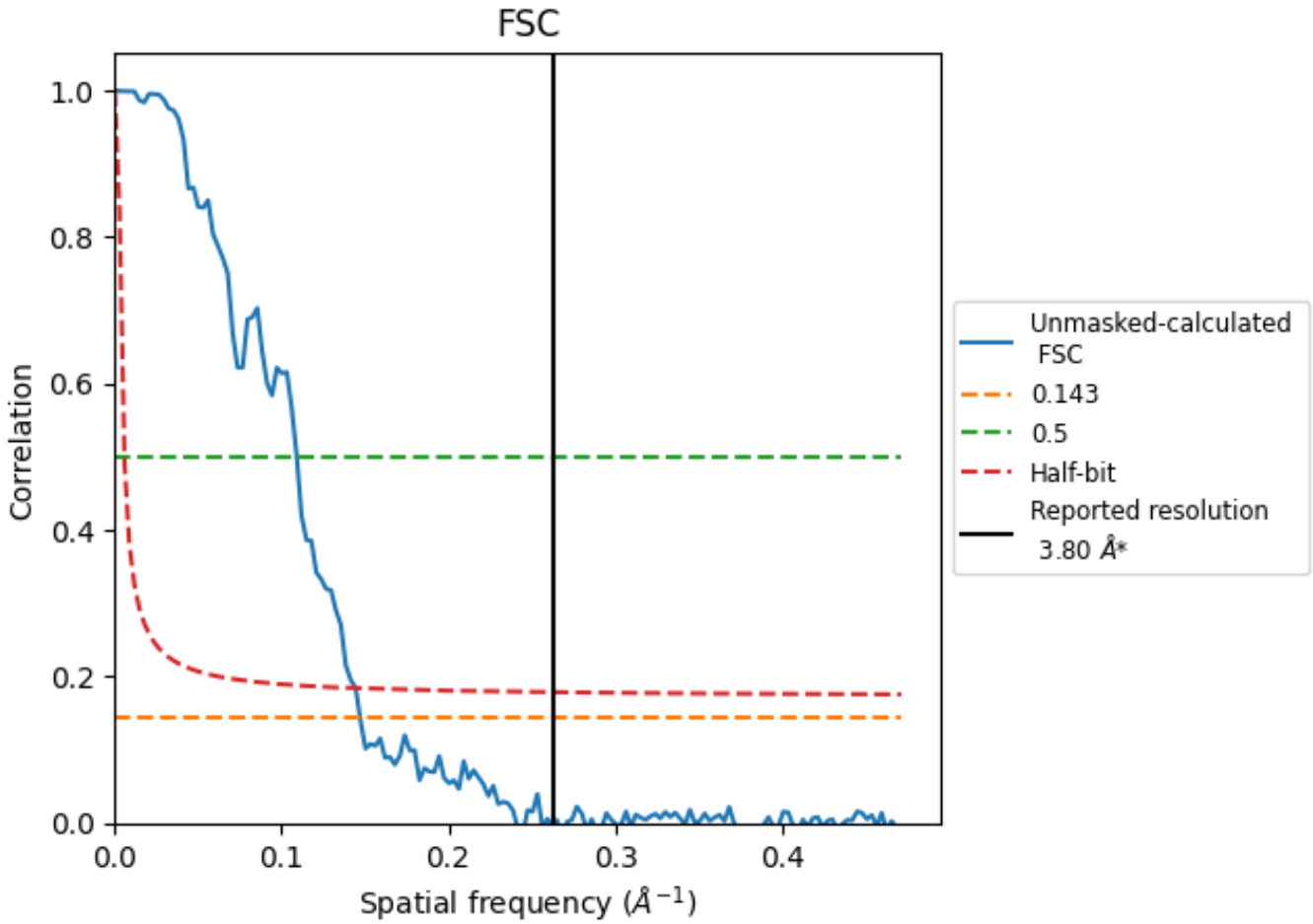


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

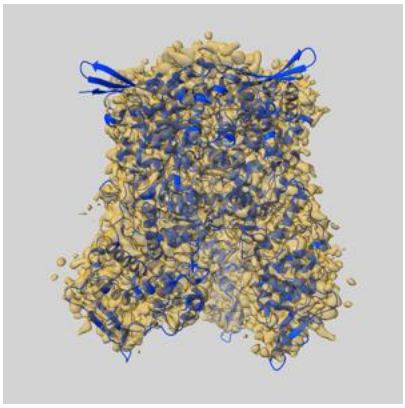
Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
	0.143	0.5	Half-bit	Other
Reported by author	-	-	-	3.80
Author-provided FSC curve	-	-	-	-
Unmasked-calculated*	6.79	9.17	6.92	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

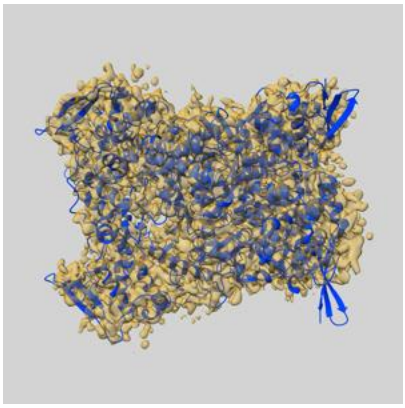
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17410 and PDB model 8P4K. Per-residue inclusion information can be found in section 3 on page 4.

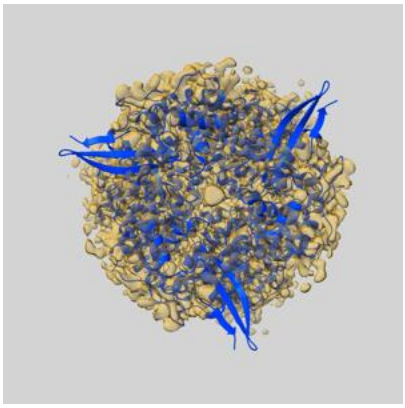
9.1 Map-model overlay



X



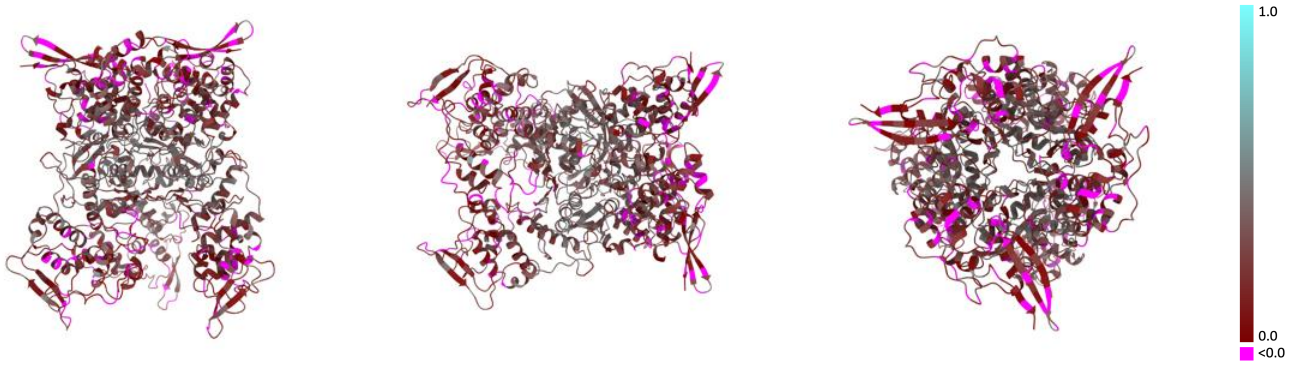
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9 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.

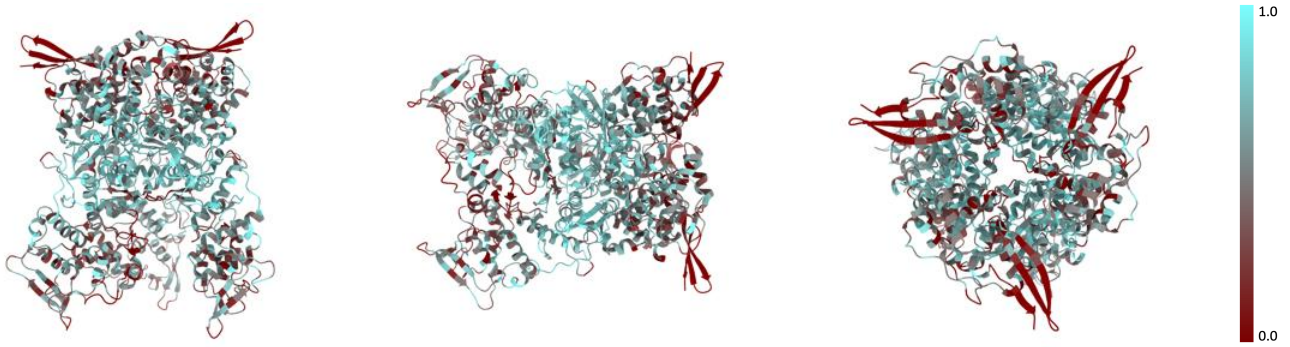
9.2 Q-score mapped to coordinate model



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.

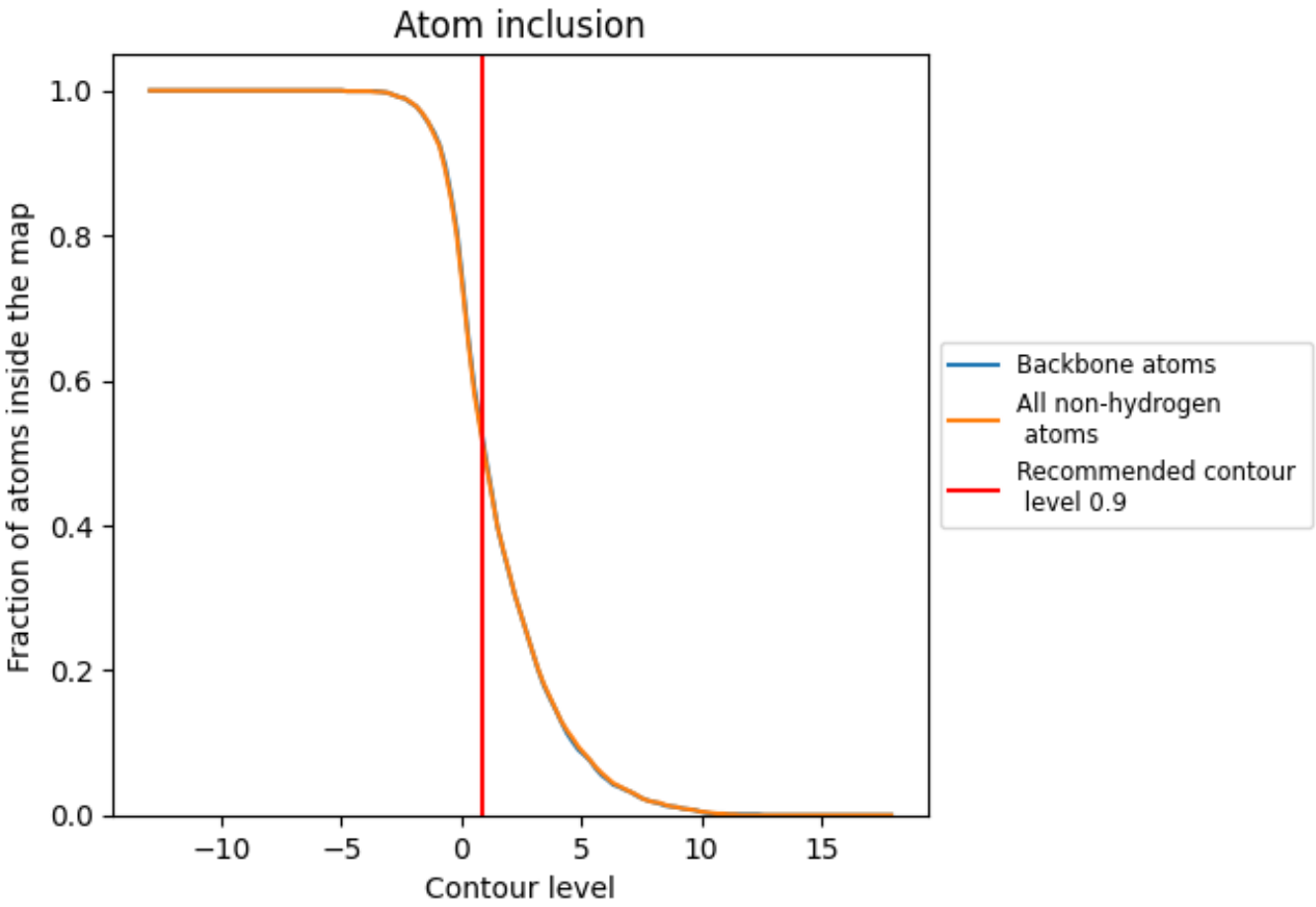
9.3 Atom inclusion mapped to coordinate model



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 (0.9).

9.4 Atom inclusion (i)



At the recommended contour level, 52% of all backbone atoms, 51% 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 (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5110	0.2150
A	0.5210	0.2150
B	0.5190	0.2150
C	0.5220	0.2140