



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 03:13 PM EDT

PDB ID : 6D1W
EMDB ID : EMD-7786
Title : human PKD2 F604P mutant
Authors : Zheng, W.; Yang, X.; Bulkley, D.; Chen, X.Z.; Cao, E.
Deposited on : 2018-04-12
Resolution : 3.54 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
Mogul : 2022.3.0, CSD as543be (2022)
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

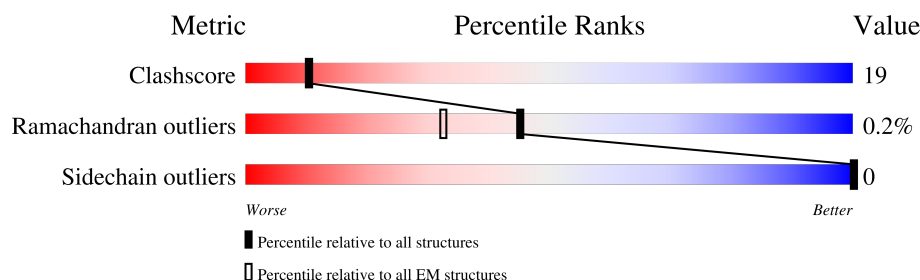
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.54 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	A	740	<div> <div>5%</div> <div>37%</div> <div>24%</div> <div>39%</div> </div>
1	B	740	<div> <div>5%</div> <div>36%</div> <div>24%</div> <div>39%</div> </div>
1	C	740	<div> <div>5%</div> <div>36%</div> <div>24%</div> <div>39%</div> </div>
1	D	740	<div> <div>5%</div> <div>36%</div> <div>24%</div> <div>39%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14492 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 Polycystin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	451	Total	C	N	O	S	0	0
			3581	2381	575	607	18		
1	B	451	Total	C	N	O	S	0	0
			3581	2381	575	607	18		
1	C	451	Total	C	N	O	S	0	0
			3581	2381	575	607	18		
1	D	451	Total	C	N	O	S	0	0
			3581	2381	575	607	18		

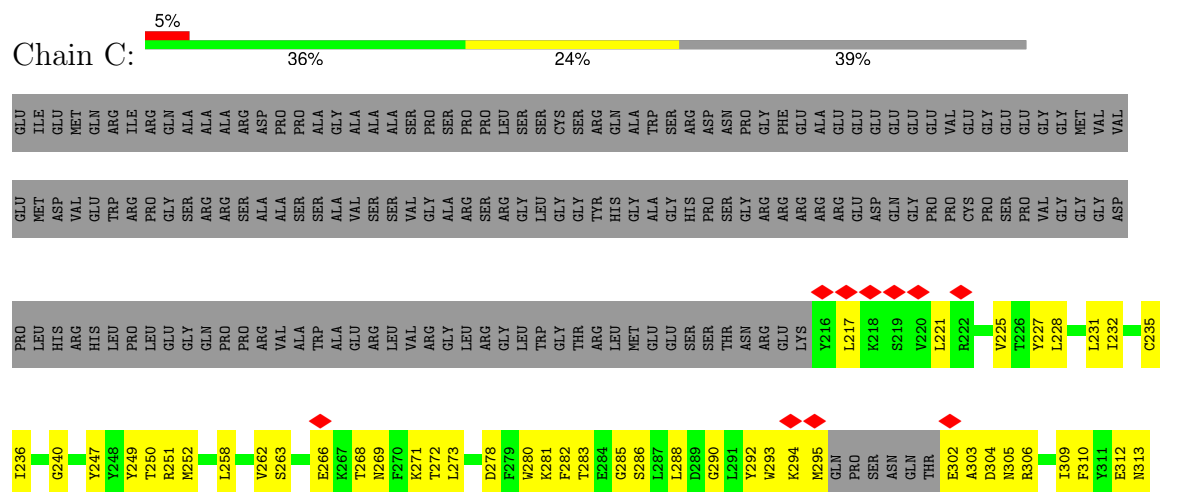
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	604	PRO	PHE	engineered mutation	UNP Q13563
B	604	PRO	PHE	engineered mutation	UNP Q13563
C	604	PRO	PHE	engineered mutation	UNP Q13563
D	604	PRO	PHE	engineered mutation	UNP Q13563

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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



L314	P319	R320	I321	R322	Q323	L324	R325	V326	R327	E340	I341	Y345	Y348	S349	S352	E353	D354	R355	A356	P357	F358	G359	P360	R361	W366	E371	S377	S378	H379	W380	G381	I382	I383	A384	T385	G388	A389	G390	Y391	Y392	L393	D394	L395	S396	R399	T402	L409					
K410	L415	D416	R417		R420	L421	T422	F423	I424	V428	Y429	W430	A431	N432	I433	N434	L435	F436	C437		R440	L441	L442	F445	F446	A447	T448	G450	G450		S454	W455	Q456	L460	K461	L462	I463	R464	Y465	V466	T467	T468	F469	D470	F471		C476	F480	I484	F485	V488	
L493	GLU	ILE	ARG	ILE	HIS	LYS	LEU	HIS	PHE	R504	S505	F506	W507	N508	I526	Y527	S530	N531	V532	L535	L536	Q537	F538	L539	P546	N547	F548	E549	H550	A562	T565	V566	F567	F568	V569	W570	K572	K575	F576	I577	N578	F579	N580	R581	T582	M583	S584	Q585	L586	S587		
T588	T589	M590	S591	R592	C593	A594	K595	D596	L597	F598	G599	F600	A601	I602	A612	Q613	L614	G620	V623	D624	D625	F626	F634	T635	Q636	F637	R638	D643	R654	P658	F664	F667	M668	F669	I671	N674	M675	F676	L677	A678	I679	I680	N681	D682	THR	TYR	SER	GLU				
VAL	LYS	SER	ASP	LEU	ALA	GLN	LYS	ALA	GLU	GLU	MET	GLU	PHE	THR	LYS	ASP	LEU	HIS	ARG	GLY	GLY	TYR	HIS	LYS	LEU	GLN	LEU	VAL	ASP	ILE	SER	GLU	SER	LEU	ARG	GLN	GLY	GLY	LYS	LEU	ASN	PHE	ASP	GLU	LEU	ARG	GLN	ASP	LEU	VAL	LYS	
GLY	LYS	GLY	HIS	THR	ASP	ALA	GLU	GLU	ALA	ILE	THR	LYS	TYR	ASP	GLN	ASP	ASP	GLN	THR	GLU	HIS	GLU	THR	GLU	HIS	GLU	MET	ARG	ASP	ASP	GLY	GLU	ARG	ASP	LEU	ASP	LEU	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY		

• Molecule 1: Polycystin-2



GLU	ILE	GLU	MET	GLN	ARG	ILE	ARG	GLN	ILE	ALA	ALA	ASP	PRO	ALA	ALA	GLY	VAL	ALA	ALA	VAL	SER	VAL	GLY	GLY	PRO	PRO	PRO	GLU	ASP	ASP	ASN	PRO	GLY	GLY	PHE	GLU	ALA	GLU	GLU	GLY	GLY	VAL	GLU	GLY	GLY	GLY	GLY	GLY	VAL																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
PRO	LEU	HIS	ARG	HIS	LEU	PRO	LEU	GLY	GLN	GLY	SER	ALA	ALA	TRP	ALA	VAL	VAL	VAL	VAL	VAL	VAL	VAL	GLY	GLY	ARG	ARG	ARG	ARG	ARG	GLU	GLU	GLU	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GL

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	387454	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.219	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	233.3952, 233.3952, 233.3952	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2156, 1.2156, 1.2156	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	1/3677 (0.0%)	0.47	0/5008
1	B	0.44	1/3677 (0.0%)	0.47	0/5008
1	C	0.44	1/3677 (0.0%)	0.47	0/5008
1	D	0.44	1/3677 (0.0%)	0.47	0/5008
All	All	0.44	4/14708 (0.0%)	0.47	0/20032

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	356	ALA	C-N	-10.18	1.15	1.34
1	A	356	ALA	C-N	-10.14	1.15	1.34
1	D	356	ALA	C-N	-10.14	1.15	1.34
1	B	356	ALA	C-N	-10.13	1.15	1.34

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	A	3581	0	3473	147	0
1	B	3581	0	3473	146	0
1	C	3581	0	3473	147	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3581	0	3473	147	0
2	A	42	0	39	0	0
2	B	42	0	39	0	0
2	C	42	0	39	0	0
2	D	42	0	39	0	0
All	All	14492	0	14048	531	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 19.

The worst 5 of 531 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:D:319:PRO:HB2	1:D:395:LEU:HD12	1.60	0.83
1:B:319:PRO:HB2	1:B:395:LEU:HD12	1.61	0.83
1:A:319:PRO:HB2	1:A:395:LEU:HD12	1.61	0.82
1:C:319:PRO:HB2	1:C:395:LEU:HD12	1.60	0.82
1:B:505:SER:H	1:B:508:ASN:HB2	1.57	0.70

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	445/740 (60%)	415 (93%)	29 (6%)	1 (0%)	44	74
1	B	445/740 (60%)	415 (93%)	29 (6%)	1 (0%)	44	74
1	C	445/740 (60%)	415 (93%)	29 (6%)	1 (0%)	44	74
1	D	445/740 (60%)	415 (93%)	29 (6%)	1 (0%)	44	74
All	All	1780/2960 (60%)	1660 (93%)	116 (6%)	4 (0%)	45	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	532	VAL
1	B	532	VAL
1	C	532	VAL
1	D	532	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/647 (57%)	368 (100%)	0	100	100
1	B	368/647 (57%)	368 (100%)	0	100	100
1	C	368/647 (57%)	368 (100%)	0	100	100
1	D	368/647 (57%)	368 (100%)	0	100	100
All	All	1472/2588 (57%)	1472 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	636	GLN
1	D	543	ASN
1	D	636	GLN
1	D	560	ASN
1	B	458	GLN

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](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	802	1	14,14,15	0.39	0	17,19,21	0.68	1 (5%)
2	NAG	A	801	1	14,14,15	0.19	0	17,19,21	0.45	0
2	NAG	D	801	1	14,14,15	0.18	0	17,19,21	0.45	0
2	NAG	D	802	1	14,14,15	0.40	0	17,19,21	0.68	1 (5%)
2	NAG	B	801	1	14,14,15	0.19	0	17,19,21	0.45	0
2	NAG	D	803	1	14,14,15	0.20	0	17,19,21	0.35	0
2	NAG	C	801	1	14,14,15	0.20	0	17,19,21	0.45	0
2	NAG	A	803	1	14,14,15	0.19	0	17,19,21	0.35	0
2	NAG	C	802	1	14,14,15	0.38	0	17,19,21	0.68	1 (5%)
2	NAG	B	803	1	14,14,15	0.20	0	17,19,21	0.35	0
2	NAG	A	802	1	14,14,15	0.40	0	17,19,21	0.67	1 (5%)
2	NAG	C	803	1	14,14,15	0.19	0	17,19,21	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	802	1	-	2/6/23/26	0/1/1/1
2	NAG	A	801	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	801	1	-	2/6/23/26	0/1/1/1
2	NAG	D	802	1	-	2/6/23/26	0/1/1/1
2	NAG	B	801	1	-	2/6/23/26	0/1/1/1
2	NAG	D	803	1	-	4/6/23/26	0/1/1/1
2	NAG	C	801	1	-	2/6/23/26	0/1/1/1
2	NAG	A	803	1	-	4/6/23/26	0/1/1/1
2	NAG	C	802	1	-	2/6/23/26	0/1/1/1
2	NAG	B	803	1	-	4/6/23/26	0/1/1/1
2	NAG	A	802	1	-	2/6/23/26	0/1/1/1
2	NAG	C	803	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	802	NAG	C1-O5-C5	2.40	115.40	112.19
2	C	802	NAG	C1-O5-C5	2.36	115.35	112.19
2	D	802	NAG	C1-O5-C5	2.36	115.35	112.19
2	A	802	NAG	C1-O5-C5	2.33	115.31	112.19

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NAG	C4-C5-C6-O6
2	B	801	NAG	C4-C5-C6-O6
2	C	801	NAG	C4-C5-C6-O6
2	D	801	NAG	C4-C5-C6-O6
2	A	802	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1
1	D	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	356:ALA	C	357:PRO	N	1.15
1	B	356:ALA	C	357:PRO	N	1.15
1	D	356:ALA	C	357:PRO	N	1.15
1	C	356:ALA	C	357:PRO	N	1.14

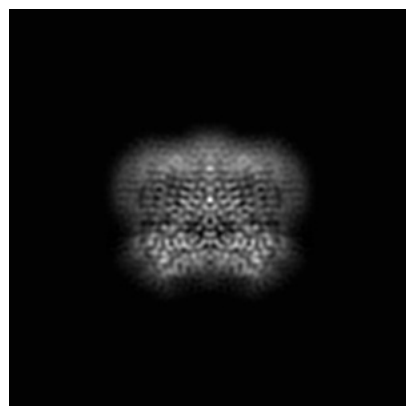
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7786. These allow visual inspection of the internal detail of the map and identification of artifacts.

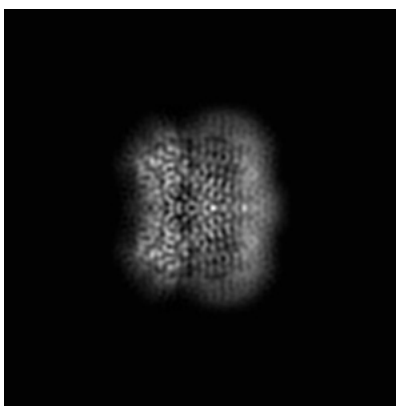
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

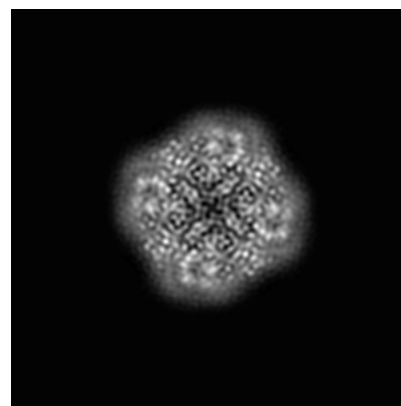
6.1.1 Primary map



X

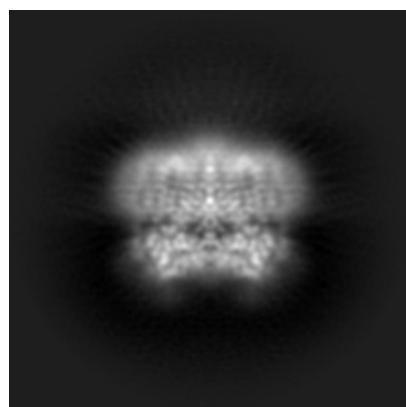


Y

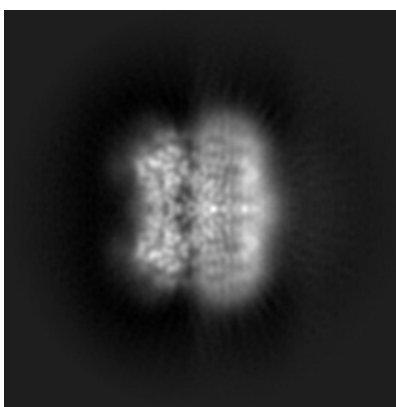


Z

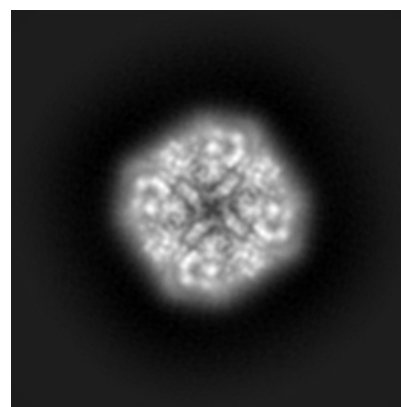
6.1.2 Raw map



X



Y



Z

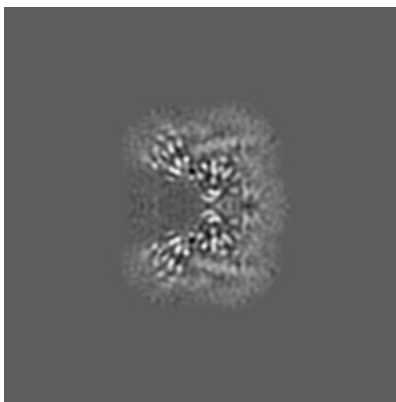
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

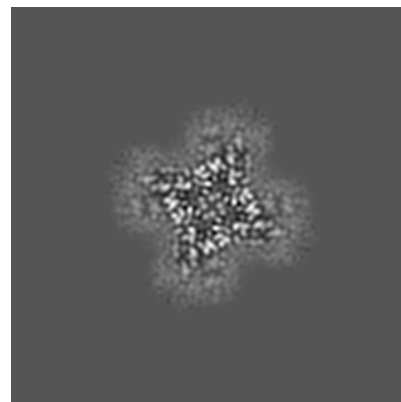
6.2.1 Primary map



X Index: 96

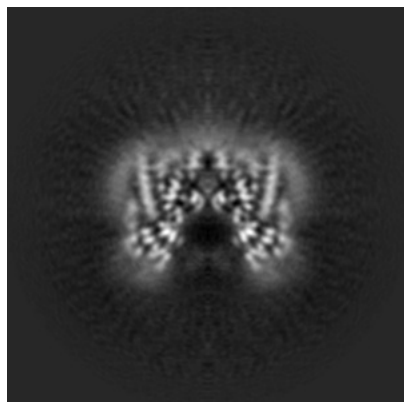


Y Index: 96

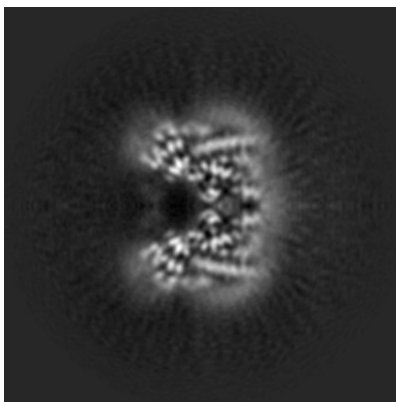


Z Index: 96

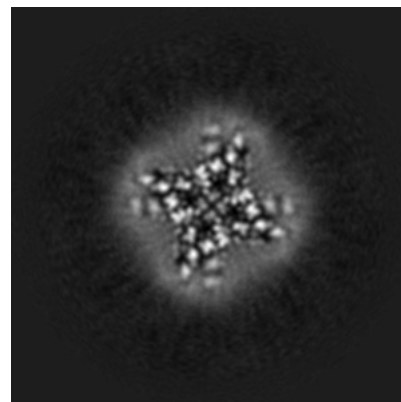
6.2.2 Raw map



X Index: 96



Y Index: 96

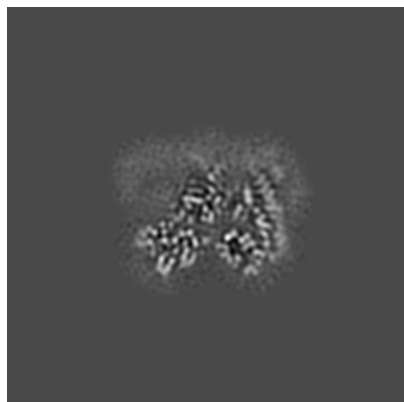


Z Index: 96

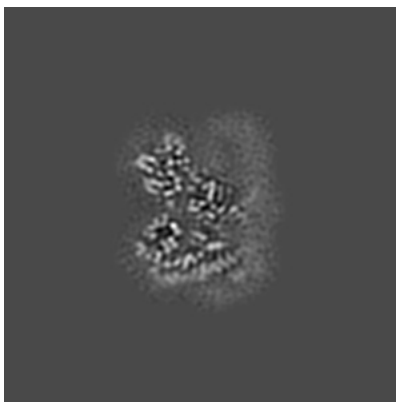
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

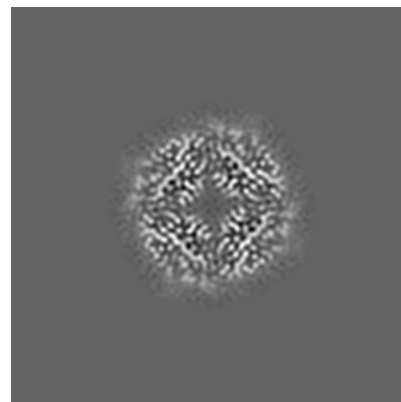
6.3.1 Primary map



X Index: 109

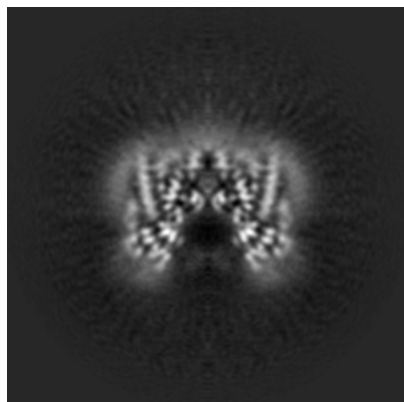


Y Index: 109

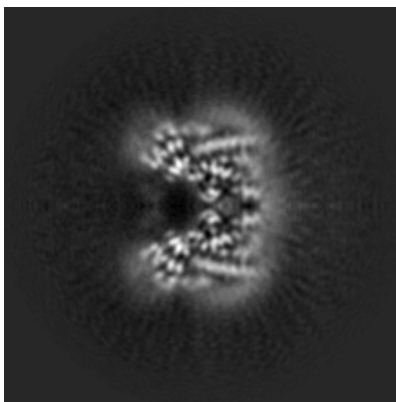


Z Index: 78

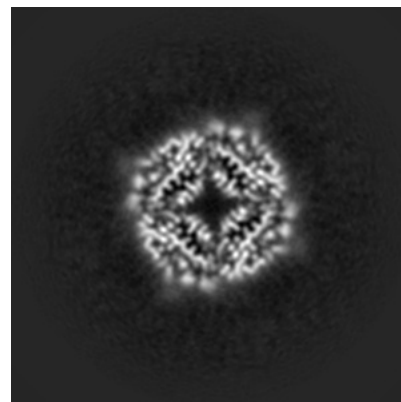
6.3.2 Raw map



X Index: 96



Y Index: 96

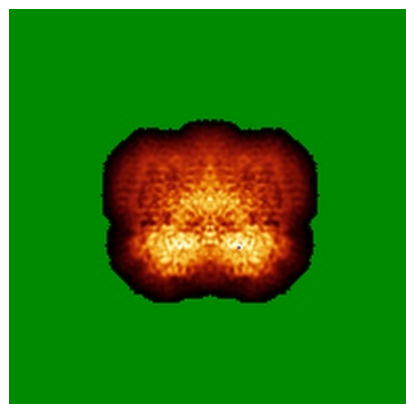


Z Index: 78

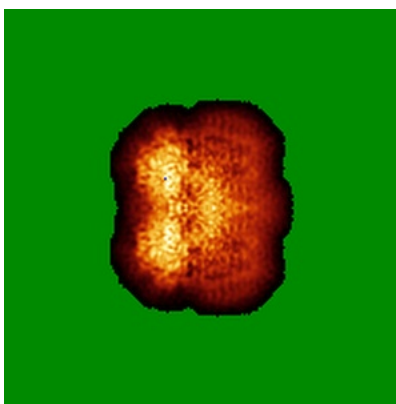
The images above show the largest variance slices of the map in three orthogonal directions.

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

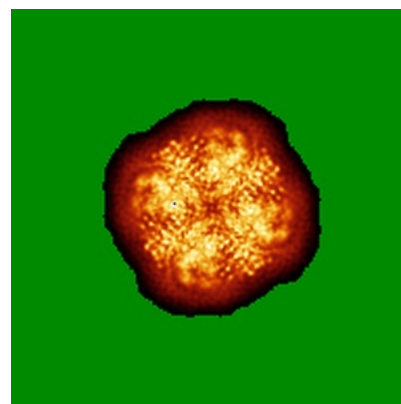
6.4.1 Primary map



X

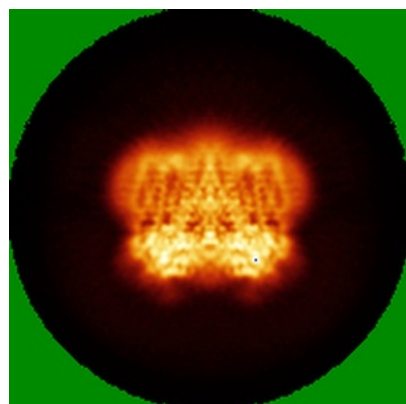


Y

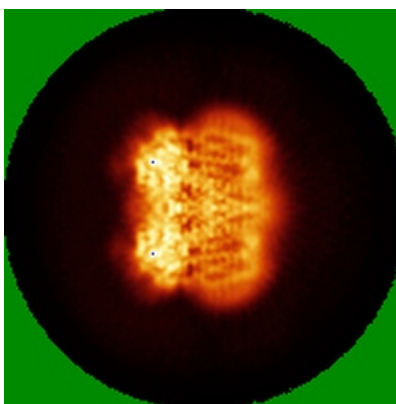


Z

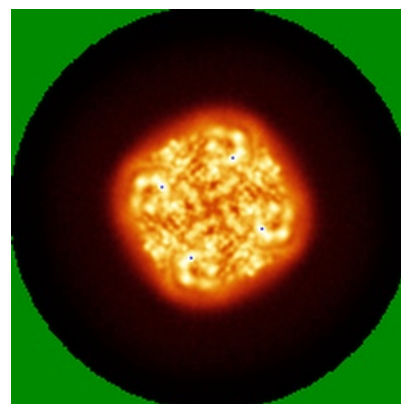
6.4.2 Raw map



X



Y

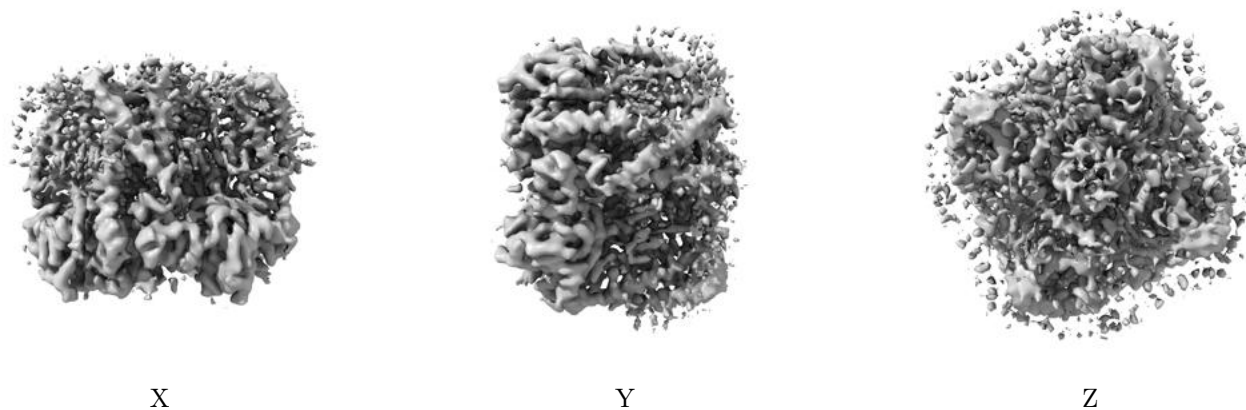


Z

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.

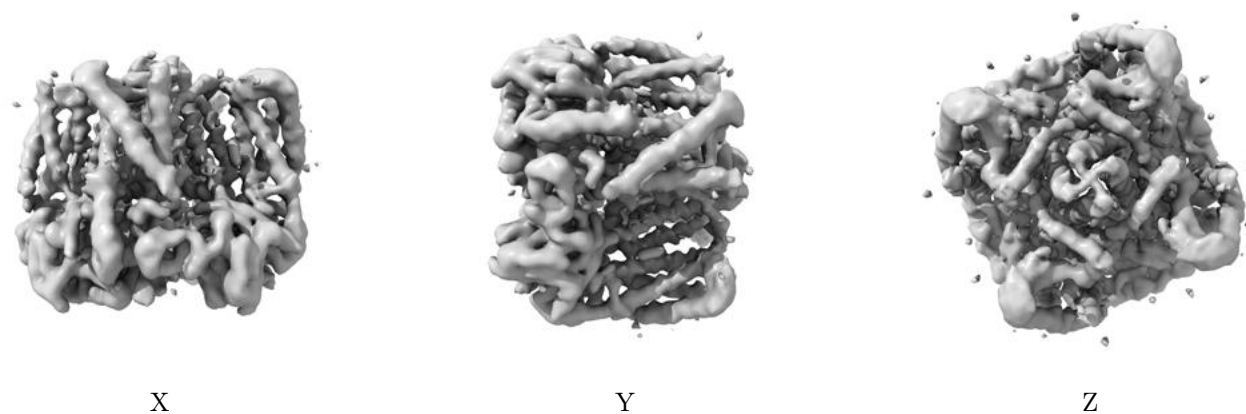
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

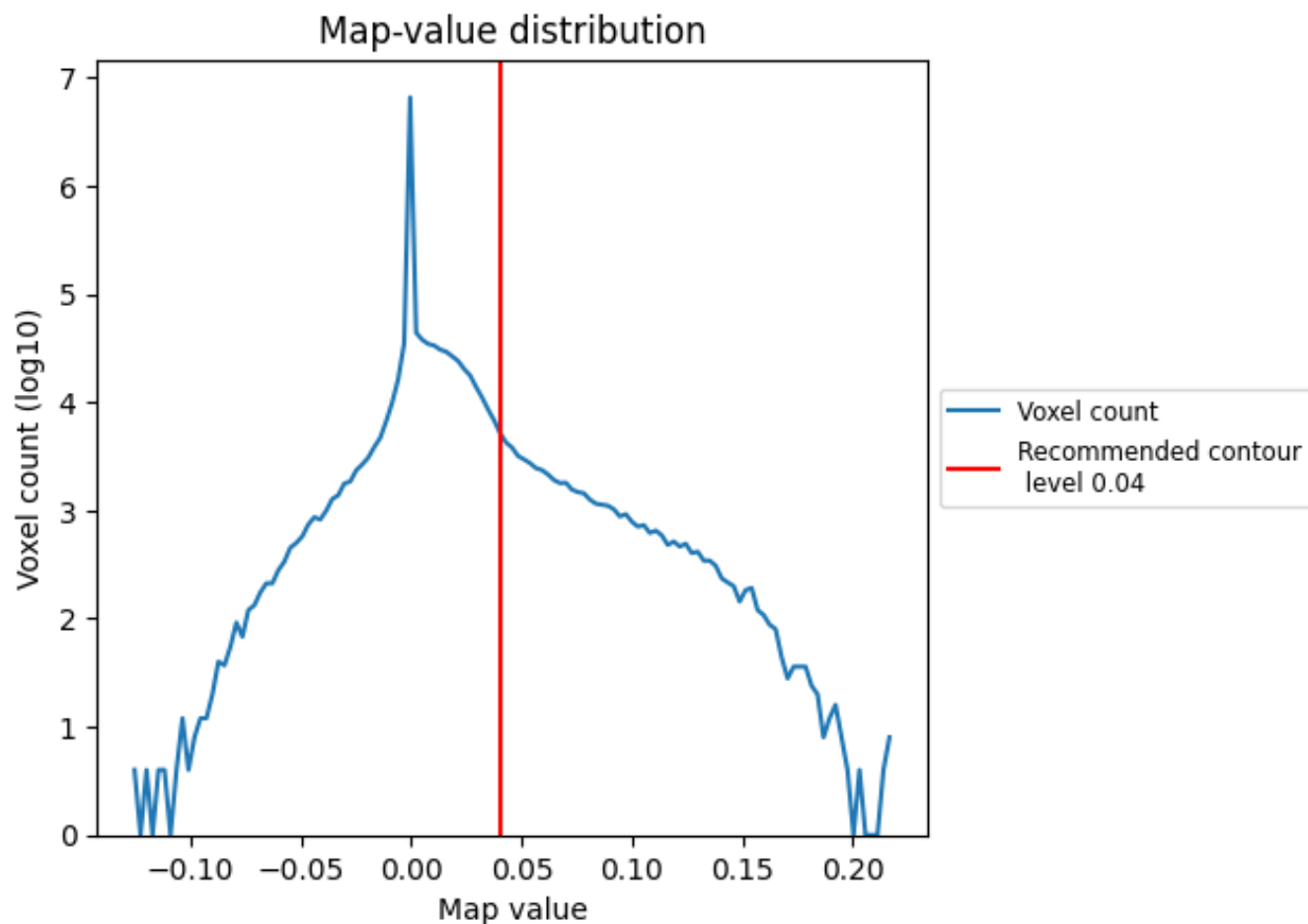
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

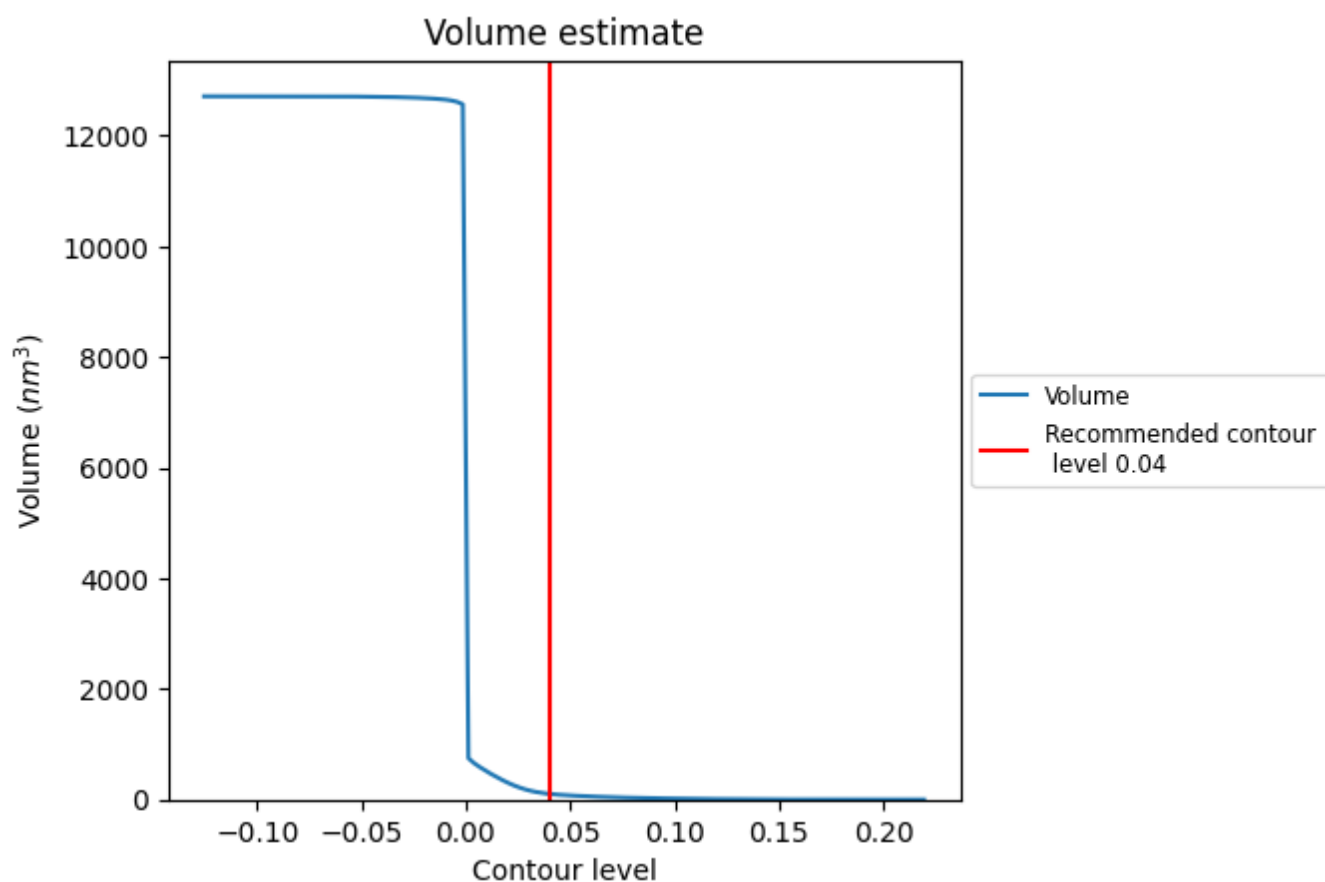
This section contains the results of statistical analysis of the map.

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.

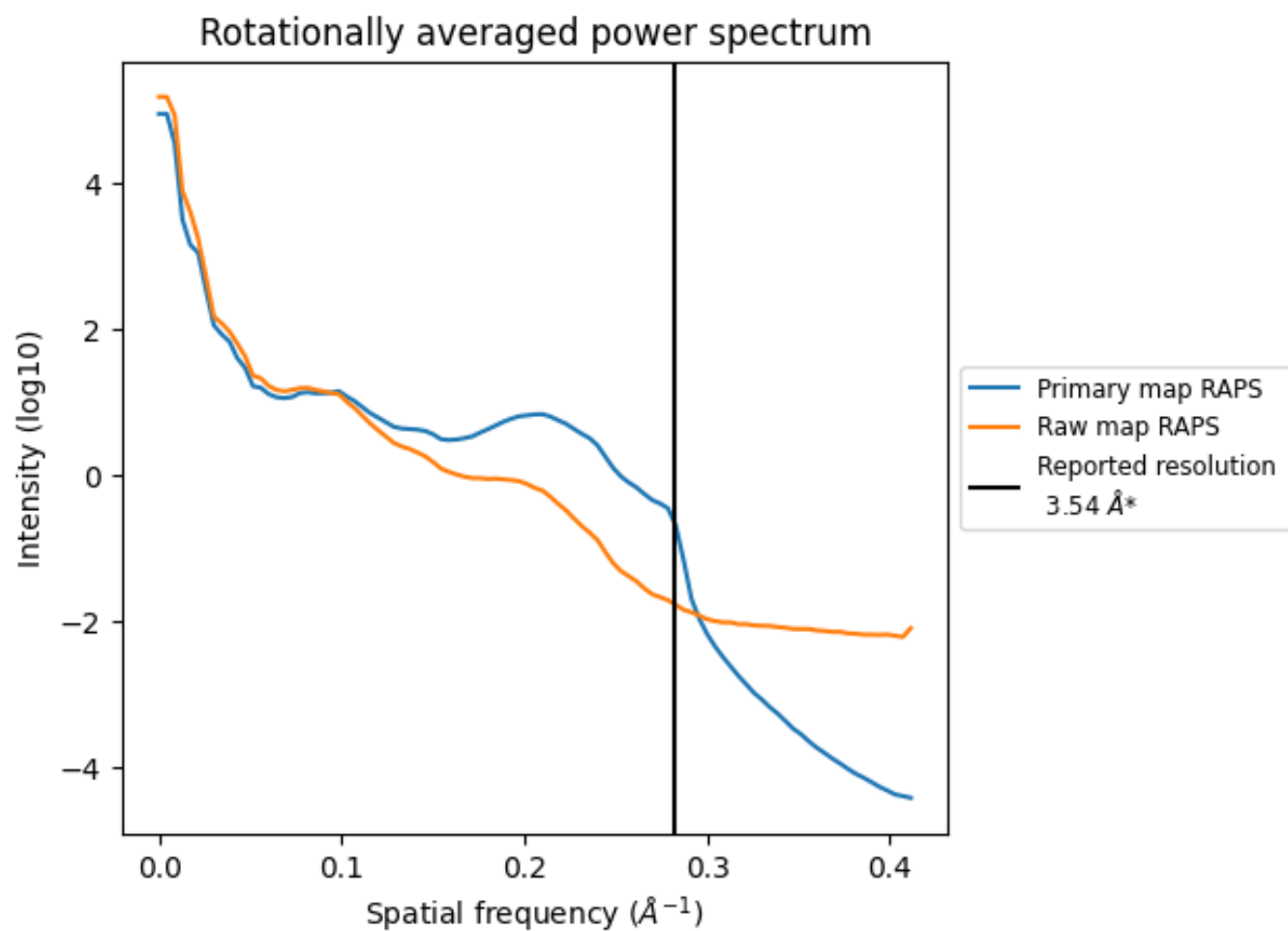
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 nm^3 ; this corresponds to an approximate mass of 93 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 ⓘ

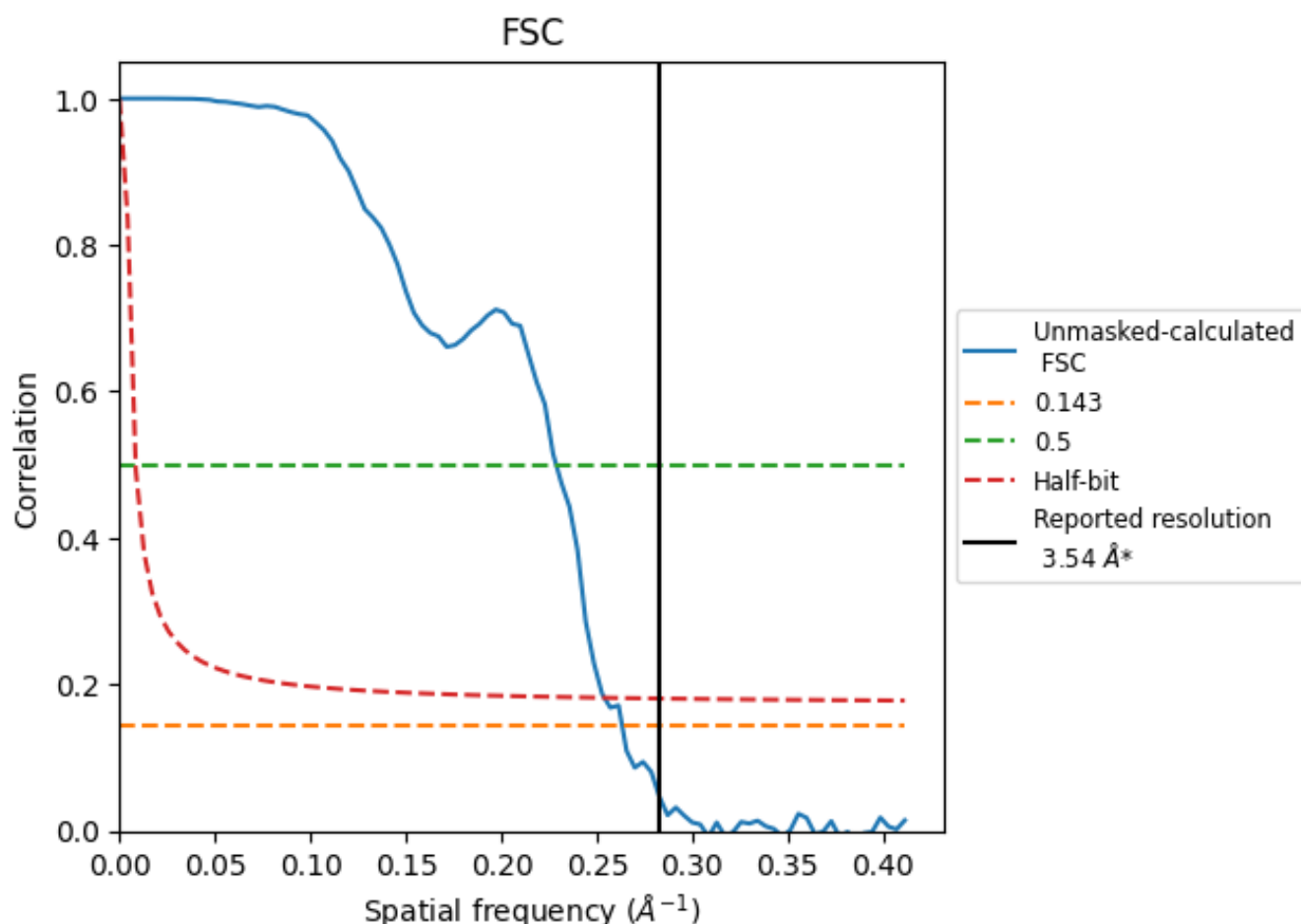


*Reported resolution corresponds to spatial frequency of 0.282 Å⁻¹

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 0.282 Å⁻¹

8.2 Resolution estimates [i](#)

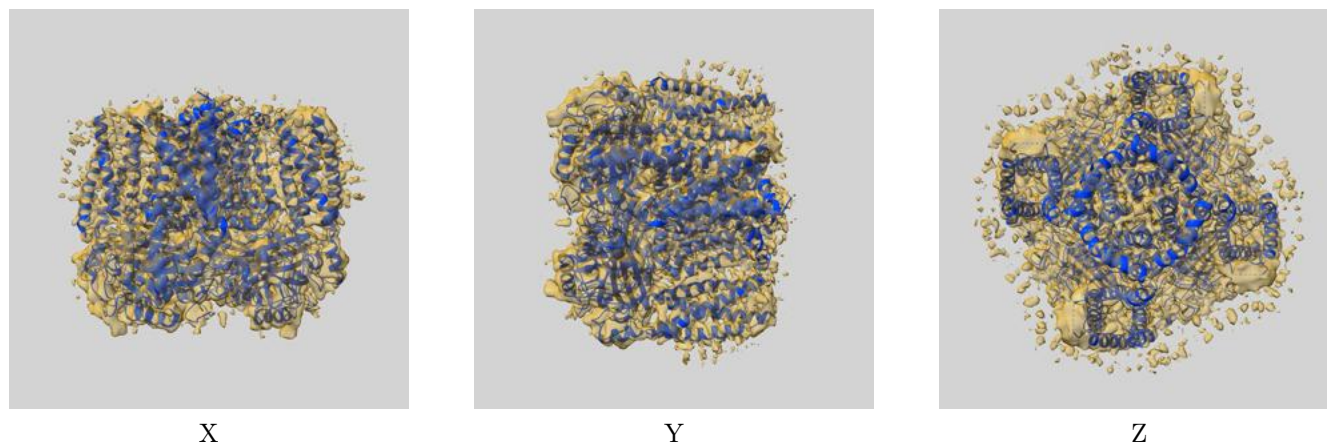
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.54	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	4.37	3.94

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

9 Map-model fit [i](#)

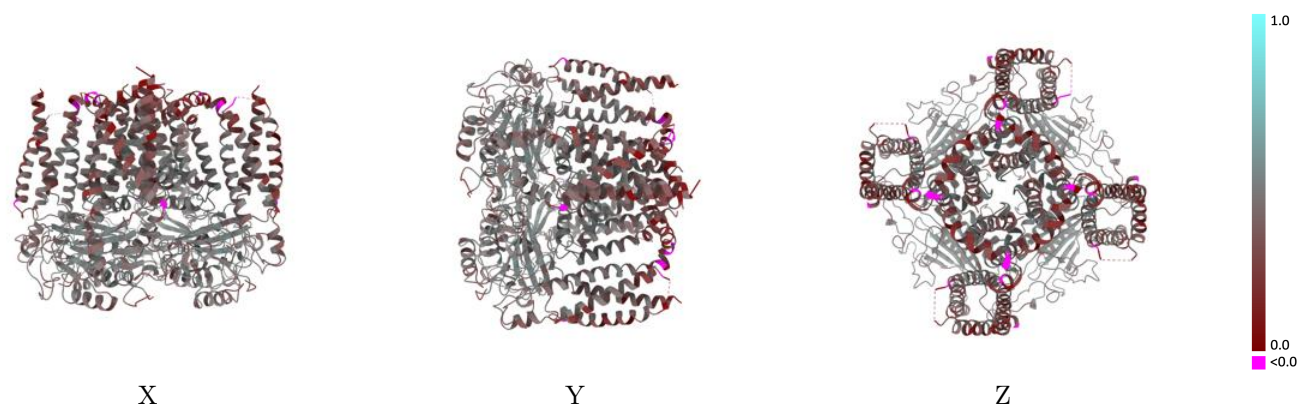
This section contains information regarding the fit between EMDB map EMD-7786 and PDB model 6D1W. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



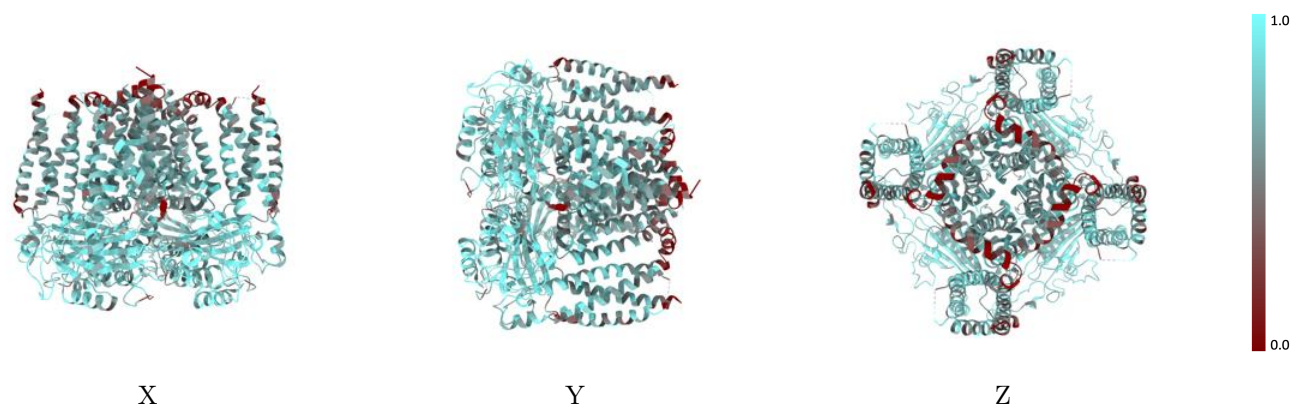
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



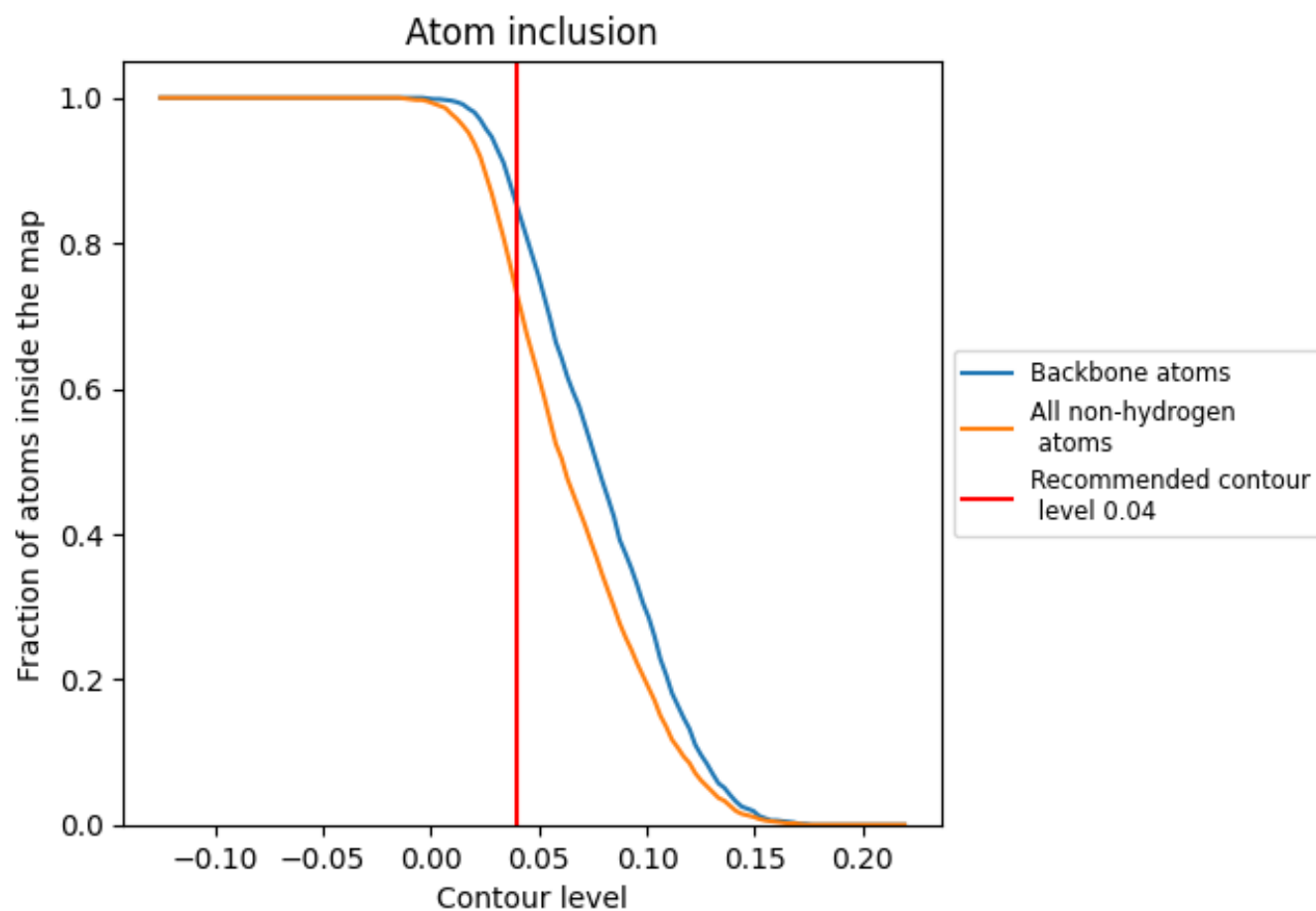
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 73% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7270	<div></div> 0.4050
A	<div></div> 0.7270	<div></div> 0.4050
B	<div></div> 0.7260	<div></div> 0.4040
C	<div></div> 0.7280	<div></div> 0.4050
D	<div></div> 0.7270	<div></div> 0.4040

