



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 01:21 PM UTC

PDB ID : 8ZKR / pdb_00008zkr
EMDB ID : EMD-60206
Title : Structure of Polycystin-1/Polycystin-2 complex with phosphatidic acid bound
Authors : Chen, M.Y.; Su, Q.; Shi, Y.G.
Deposited on : 2024-05-17
Resolution : 2.80 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

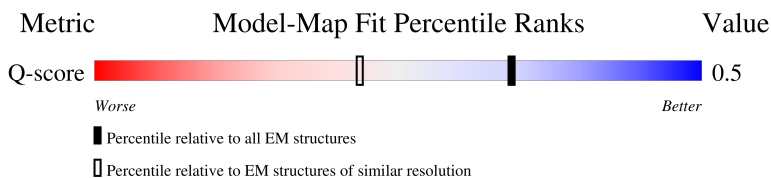
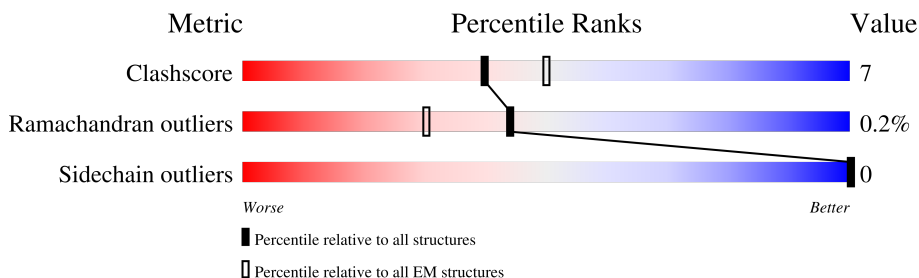
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	1261	
2	B	1007	
2	C	1007	
2	D	1007	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17056 atoms, of which 35 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-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	776	Total	C	N	O	S	0	0
			5278	3375	978	909	16		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3043	MET	-	initiating methionine	UNP P98161
A	3044	ASP	-	expression tag	UNP P98161
A	3045	TYR	-	expression tag	UNP P98161
A	3046	LYS	-	expression tag	UNP P98161
A	3047	ASP	-	expression tag	UNP P98161
A	3048	ASP	-	expression tag	UNP P98161
A	3049	ASP	-	expression tag	UNP P98161
A	3050	ASP	-	expression tag	UNP P98161
A	3051	LYS	-	expression tag	UNP P98161

- Molecule 2 is a protein called Polycystin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	473	Total	C	N	O	S	0	0
			3904	2576	616	691	21		
2	C	472	Total	C	N	O	S	0	0
			3899	2573	615	690	21		
2	D	461	Total	C	N	O	S	0	0
			3798	2507	599	672	20		

There are 117 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-38	MET	-	initiating methionine	UNP Q13563
B	-37	GLY	-	expression tag	UNP Q13563
B	-36	ALA	-	expression tag	UNP Q13563
B	-35	SER	-	expression tag	UNP Q13563

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-34	SER	-	expression tag	UNP Q13563
B	-33	ALA	-	expression tag	UNP Q13563
B	-32	TRP	-	expression tag	UNP Q13563
B	-31	SER	-	expression tag	UNP Q13563
B	-30	HIS	-	expression tag	UNP Q13563
B	-29	PRO	-	expression tag	UNP Q13563
B	-28	GLN	-	expression tag	UNP Q13563
B	-27	PHE	-	expression tag	UNP Q13563
B	-26	GLU	-	expression tag	UNP Q13563
B	-25	LYS	-	expression tag	UNP Q13563
B	-24	GLY	-	expression tag	UNP Q13563
B	-23	GLY	-	expression tag	UNP Q13563
B	-22	GLY	-	expression tag	UNP Q13563
B	-21	SER	-	expression tag	UNP Q13563
B	-20	GLY	-	expression tag	UNP Q13563
B	-19	GLY	-	expression tag	UNP Q13563
B	-18	GLY	-	expression tag	UNP Q13563
B	-17	SER	-	expression tag	UNP Q13563
B	-16	GLY	-	expression tag	UNP Q13563
B	-15	GLY	-	expression tag	UNP Q13563
B	-14	SER	-	expression tag	UNP Q13563
B	-13	ALA	-	expression tag	UNP Q13563
B	-12	TRP	-	expression tag	UNP Q13563
B	-11	SER	-	expression tag	UNP Q13563
B	-10	HIS	-	expression tag	UNP Q13563
B	-9	PRO	-	expression tag	UNP Q13563
B	-8	GLN	-	expression tag	UNP Q13563
B	-7	PHE	-	expression tag	UNP Q13563
B	-6	GLU	-	expression tag	UNP Q13563
B	-5	LYS	-	expression tag	UNP Q13563
B	-4	GLY	-	expression tag	UNP Q13563
B	-3	SER	-	linker	UNP Q13563
B	-2	ALA	-	linker	UNP Q13563
B	-1	ALA	-	linker	UNP Q13563
B	0	ALA	-	linker	UNP Q13563
C	-38	MET	-	initiating methionine	UNP Q13563
C	-37	GLY	-	expression tag	UNP Q13563
C	-36	ALA	-	expression tag	UNP Q13563
C	-35	SER	-	expression tag	UNP Q13563
C	-34	SER	-	expression tag	UNP Q13563
C	-33	ALA	-	expression tag	UNP Q13563
C	-32	TRP	-	expression tag	UNP Q13563

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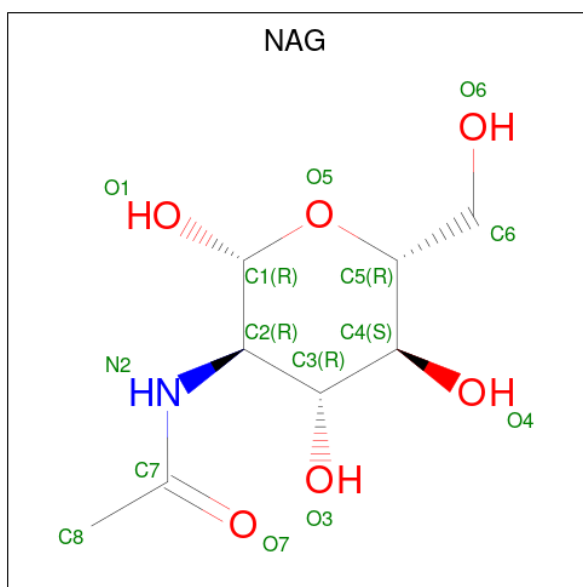
Chain	Residue	Modelled	Actual	Comment	Reference
C	-31	SER	-	expression tag	UNP Q13563
C	-30	HIS	-	expression tag	UNP Q13563
C	-29	PRO	-	expression tag	UNP Q13563
C	-28	GLN	-	expression tag	UNP Q13563
C	-27	PHE	-	expression tag	UNP Q13563
C	-26	GLU	-	expression tag	UNP Q13563
C	-25	LYS	-	expression tag	UNP Q13563
C	-24	GLY	-	expression tag	UNP Q13563
C	-23	GLY	-	expression tag	UNP Q13563
C	-22	GLY	-	expression tag	UNP Q13563
C	-21	SER	-	expression tag	UNP Q13563
C	-20	GLY	-	expression tag	UNP Q13563
C	-19	GLY	-	expression tag	UNP Q13563
C	-18	GLY	-	expression tag	UNP Q13563
C	-17	SER	-	expression tag	UNP Q13563
C	-16	GLY	-	expression tag	UNP Q13563
C	-15	GLY	-	expression tag	UNP Q13563
C	-14	SER	-	expression tag	UNP Q13563
C	-13	ALA	-	expression tag	UNP Q13563
C	-12	TRP	-	expression tag	UNP Q13563
C	-11	SER	-	expression tag	UNP Q13563
C	-10	HIS	-	expression tag	UNP Q13563
C	-9	PRO	-	expression tag	UNP Q13563
C	-8	GLN	-	expression tag	UNP Q13563
C	-7	PHE	-	expression tag	UNP Q13563
C	-6	GLU	-	expression tag	UNP Q13563
C	-5	LYS	-	expression tag	UNP Q13563
C	-4	GLY	-	expression tag	UNP Q13563
C	-3	SER	-	linker	UNP Q13563
C	-2	ALA	-	linker	UNP Q13563
C	-1	ALA	-	linker	UNP Q13563
C	0	ALA	-	linker	UNP Q13563
D	-38	MET	-	initiating methionine	UNP Q13563
D	-37	GLY	-	expression tag	UNP Q13563
D	-36	ALA	-	expression tag	UNP Q13563
D	-35	SER	-	expression tag	UNP Q13563
D	-34	SER	-	expression tag	UNP Q13563
D	-33	ALA	-	expression tag	UNP Q13563
D	-32	TRP	-	expression tag	UNP Q13563
D	-31	SER	-	expression tag	UNP Q13563
D	-30	HIS	-	expression tag	UNP Q13563
D	-29	PRO	-	expression tag	UNP Q13563

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-28	GLN	-	expression tag	UNP Q13563
D	-27	PHE	-	expression tag	UNP Q13563
D	-26	GLU	-	expression tag	UNP Q13563
D	-25	LYS	-	expression tag	UNP Q13563
D	-24	GLY	-	expression tag	UNP Q13563
D	-23	GLY	-	expression tag	UNP Q13563
D	-22	GLY	-	expression tag	UNP Q13563
D	-21	SER	-	expression tag	UNP Q13563
D	-20	GLY	-	expression tag	UNP Q13563
D	-19	GLY	-	expression tag	UNP Q13563
D	-18	GLY	-	expression tag	UNP Q13563
D	-17	SER	-	expression tag	UNP Q13563
D	-16	GLY	-	expression tag	UNP Q13563
D	-15	GLY	-	expression tag	UNP Q13563
D	-14	SER	-	expression tag	UNP Q13563
D	-13	ALA	-	expression tag	UNP Q13563
D	-12	TRP	-	expression tag	UNP Q13563
D	-11	SER	-	expression tag	UNP Q13563
D	-10	HIS	-	expression tag	UNP Q13563
D	-9	PRO	-	expression tag	UNP Q13563
D	-8	GLN	-	expression tag	UNP Q13563
D	-7	PHE	-	expression tag	UNP Q13563
D	-6	GLU	-	expression tag	UNP Q13563
D	-5	LYS	-	expression tag	UNP Q13563
D	-4	GLY	-	expression tag	UNP Q13563
D	-3	SER	-	linker	UNP Q13563
D	-2	ALA	-	linker	UNP Q13563
D	-1	ALA	-	linker	UNP Q13563
D	0	ALA	-	linker	UNP Q13563

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

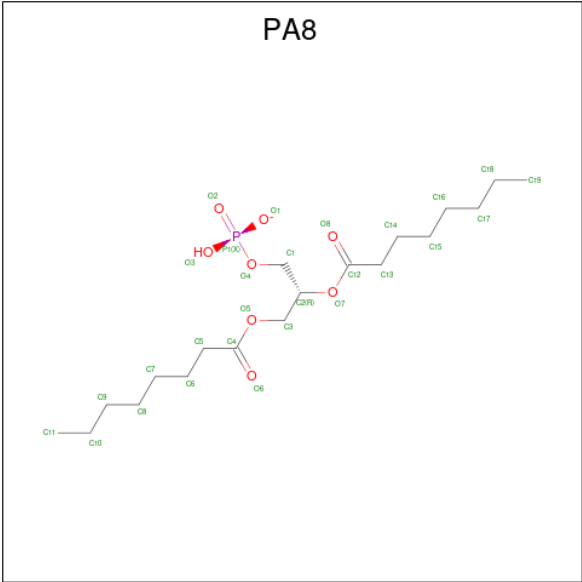


Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	

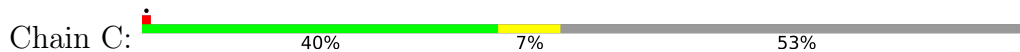
- Molecule 5 is 1,2-DIOCTANOYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PA8) (formula: C₁₉H₃₆O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	D	1	Total	C	H	O	P	0
			63	19	35	8	1	

ALA	ALA	ALA	GLN	ILE	SER	HIS	LEU	GLY	GLY	THR	PRO	VAL	LEU	GLY	ASN	GLY	GLN	PRO	ARG	PRO	ARG	SER	SER	ARG	PRO	SER	SER	SER	GLN	SER	THR	GLU	GLY	GLY	ALA	GLY	GLY	ASN	SER	SER	ASN	VAL	HIS	VAL
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- Molecule 2: Polycystin-2



	ARG	ALA	PRO	PRO	ASP	PRO	GLY	ARG	LEU	ALA	MET	GLY	CYS	ALA	ALA	VAL	GLY	GLY	ALA	SER	LEU	LEU	CYS	GLU	GLN	ARG	GLY	GLY	LEU	GLU	ILE	GLU	GLN	MET	GLN	ARG	ILE	ARG	ASP	PRO	PRO	PRO	ALA	GLY	ALA	ALA	ALA	ALA	ALA	ALA	SER	PRO	SER	PRO	PRO	LEU	SER
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[illegible]

GLY	GLY	TYR	HIS	GLY	ALA	GLY	HIS	PRO	SER	GLY	ARG	ARG	ARG	ARG	GLU	ASP	GLN	GLY	PRO	PRO	VAL	GLY	GLY	GLY	ASP	PRO	PRO	LEU	HIS	LEU	ARG	ALA	TRP	ALA	GLU	ARG	LEU	VAL	VAL	ARG	GLY	GLY	GLY	LEU	LEU	ARG	GLY	LEU	TRP
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GLY
 THR
 ARG
 MET
 MET
 GLU
 GLU
 SER
 SER
 THR
 ASN
 ARG
 GLU
 LYS
 TYR
 LEU
 LYS
 S219
 T238
 M242
 Y247
 Y248
 R251
 M252
 M253
 S254
 L258
 M295
 GLN
 PRO
 SER
 SER
 ASN
 GLN
 THR
 GLU
 ALA
 D304
 M305
 R306
 I309
 N313
 P319
 R322
 E340
 G359
 P360
 R361

L374	A389	L395	S396	R397	E401	F423	N434	L442	V443	V451	W455	L460	I463	I496	R496	I497	H501	Y502	F503	R504	N508	V512	V515	V532	E533	V534	L535	L536	Q537	F538	L539	E540	D541	Q542	A552	V566	W570	I577
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R581	Q585	T589	C593	L597	F604	Q613	V623	D624	D625	T635	I639	I640	L641	I644	E648	E651	I671	L672	L673	N674	M675	F676	L677	N681	D682	T683	Y684	Q694	K695	A696	E697	M698	GLU	LEU	SER	ASP	LEU	ILE	ARG	LYS	GLY	TYR
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ALA LEU VAL LYS LYS LYS LYS ASN THR VAL ASP ASP ASP ILE GLY SER GLU SER LEU ARG GLN GLY GLY LYS LEU ASN PHE ASP ASP GLU LEU ARG GLN ASP ASP LEU LYS GLY GLY LYS THR THR ASP ALA GLU ILE GLU ALA ILE PHE THR LYS TYR ASP GLN ASP GLY ASP GLN GLU LEU

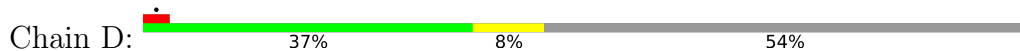
THR	GLU	HIS	GLU	HIS	GLN	MET	ARG	ASP	ASP	LEU	GLU	LYS	GLU	ARG	GLU	ASP	LEU	ASP	LEU	LEU	LEU	PRO	PRO	PRO	MET	SER	SER	SER	PHE	PRO	ARG	ARG	SER	SER	LEU	LEU	ASP	ASP	SER	GLU	GLY	HIS	SER	SER	ARG	ARG	GLY	GLY	SER	SER	LEU
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SER	GLY	VAL	SER	TYR	GLU	GLU	PHE	GLN	VAL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

SER THR GLU GLY MET GLU GLY ALA GLY GLY ASN GLY SER SER ASN VAL HIS VAL

- Molecule 2: Polycystin-2



MET	GLY	ALA	SER	SER	ALA	TRP	SER	SER	HIS	PRO	PRO	PHE	GLN	PHE	GLU	GLY	GLY	GLY	SER	SER	ALA	ALA	HIS	PRO	PRO	GLN	GLN	GLN	GLY	ASP	ALA	ALA	LYS	ARG	PRO	PRO	ALA	PRO	PRO
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	146525	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.537	Depositor
Minimum map value	-2.774	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.140	Depositor
Recommended contour level	0.45	Depositor
Map size ($\text{\AA}$)	260.88, 260.88, 260.88	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	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, PA8, CA

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	0.24	0/5375	0.51	6/7354 (0.1%)
2	B	0.22	1/4007 (0.0%)	0.38	0/5436
2	C	0.37	5/4002 (0.1%)	0.46	2/5429 (0.0%)
2	D	0.15	0/3898	0.36	0/5291
All	All	0.26	6/17282 (0.0%)	0.44	8/23510 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	681	ASN	C-O	-11.14	1.11	1.24
2	B	681	ASN	C-O	-6.62	1.16	1.24
2	C	535	LEU	C-O	-5.79	1.16	1.24
2	C	536	LEU	CA-C	-5.49	1.46	1.52
2	C	537	GLN	CA-C	-5.47	1.46	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	681	ASN	CB-CA-C	-13.70	89.37	110.88
1	A	3063	ARG	N-CA-C	11.70	126.85	112.58
1	A	3306	ALA	N-CA-C	-9.48	98.22	112.54
1	A	3806	TRP	CB-CA-C	-9.30	104.72	115.79
1	A	3806	TRP	N-CA-C	8.75	125.43	109.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	5278	0	4755	93	0
2	B	3904	0	3852	38	0
2	C	3899	0	3847	61	0
2	D	3798	0	3754	60	0
3	B	42	0	39	1	0
3	C	42	0	39	1	0
3	D	28	0	26	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	D	28	35	36	3	0
All	All	17021	35	16348	237	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 7.

The worst 5 of 237 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)
2:C:533:GLU:HA	2:C:536:LEU:CD2	1.90	1.01
1:A:3806:TRP:HA	1:A:3814:TYR:O	1.59	1.01
2:C:533:GLU:HA	2:C:536:LEU:HD23	1.02	0.99
2:C:542:GLN:OE1	2:D:340:GLU:OE2	1.81	0.97
1:A:3580:PHE:CE1	1:A:3584:VAL:HG12	2.03	0.94

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	766/1261 (61%)	673 (88%)	89 (12%)	4 (0%)	24	55
2	B	469/1007 (47%)	427 (91%)	41 (9%)	1 (0%)	43	72
2	C	468/1007 (46%)	434 (93%)	34 (7%)	0	100	100
2	D	457/1007 (45%)	425 (93%)	32 (7%)	0	100	100
All	All	2160/4282 (50%)	1959 (91%)	196 (9%)	5 (0%)	44	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3807	SER
1	A	3065	VAL
1	A	3808	TRP
2	B	306	ARG
1	A	3307	TYR

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	410/1041 (39%)	410 (100%)	0	100	100
2	B	427/860 (50%)	427 (100%)	0	100	100
2	C	427/860 (50%)	427 (100%)	0	100	100
2	D	416/860 (48%)	416 (100%)	0	100	100
All	All	1680/3621 (46%)	1680 (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 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	613	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	681	ASN
2	D	542	GLN
2	D	335	GLN
2	B	430	ASN

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](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 for Mogul analysis.

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	$\# Z > 2$
3	NAG	B	1003	2	14,14,15	0.22	0	17,19,21	0.45	0
5	PA8	D	4201	-	27,27,27	1.14	3 (11%)	30,32,32	1.32	2 (6%)
3	NAG	B	1001	2	14,14,15	0.28	0	17,19,21	0.50	0
3	NAG	D	4203	2	14,14,15	0.24	0	17,19,21	0.39	0
3	NAG	C	1002	2	14,14,15	0.23	0	17,19,21	0.49	0
3	NAG	C	1001	2	14,14,15	0.20	0	17,19,21	0.43	0
3	NAG	D	4202	2	14,14,15	0.88	1 (7%)	17,19,21	1.27	1 (5%)
3	NAG	B	1002	2	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	C	1003	2	14,14,15	0.25	0	17,19,21	0.48	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
3	NAG	B	1003	2	-	1/6/23/26	0/1/1/1
5	PA8	D	4201	-	-	15/29/29/29	-
3	NAG	B	1001	2	-	2/6/23/26	0/1/1/1
3	NAG	D	4203	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1002	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1001	2	-	2/6/23/26	0/1/1/1
3	NAG	D	4202	2	-	4/6/23/26	0/1/1/1
3	NAG	B	1002	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1003	2	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	4202	NAG	O5-C1	3.02	1.48	1.43
5	D	4201	PA8	O7-C2	-2.75	1.40	1.46
5	D	4201	PA8	O5-C4	2.40	1.40	1.33
5	D	4201	PA8	O5-C3	-2.31	1.40	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4202	NAG	C1-O5-C5	4.99	118.88	112.19
5	D	4201	PA8	O7-C12-C13	4.38	120.95	111.48
5	D	4201	PA8	O5-C4-C5	2.78	120.31	111.83

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

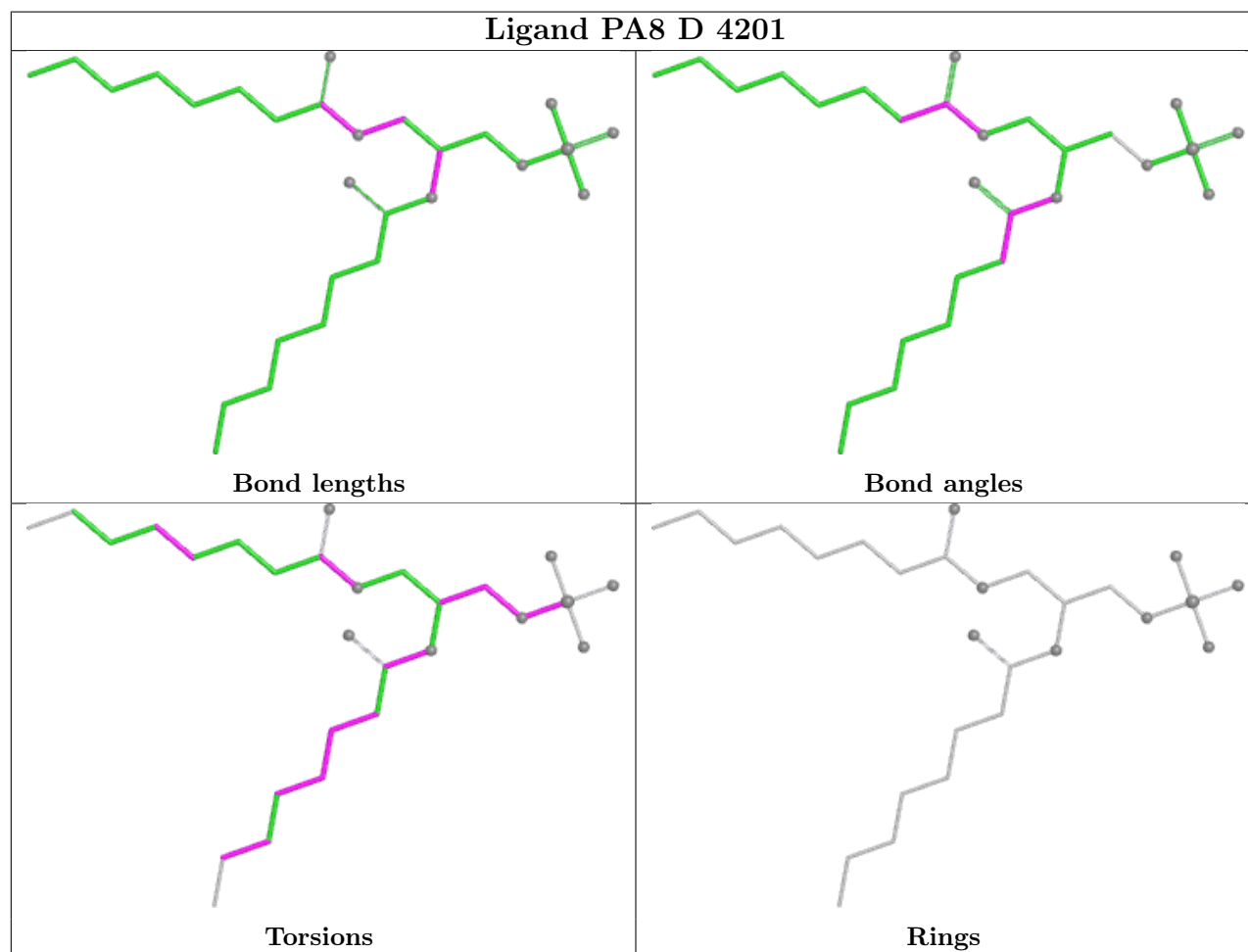
Mol	Chain	Res	Type	Atoms
5	D	4201	PA8	C1-O4-P1-O1
5	D	4201	PA8	C1-O4-P1-O2
5	D	4201	PA8	C1-O4-P1-O3
3	B	1001	NAG	C4-C5-C6-O6
3	D	4203	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	4201	PA8	3	0
3	B	1001	NAG	1	0
3	C	1003	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

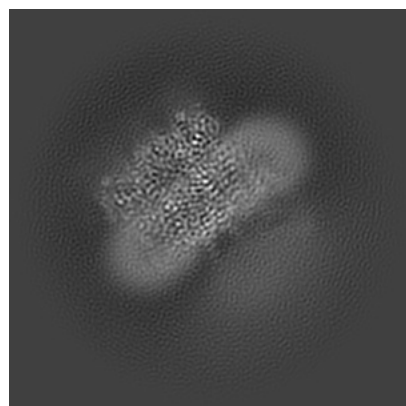
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60206. These allow visual inspection of the internal detail of the map and identification of artifacts.

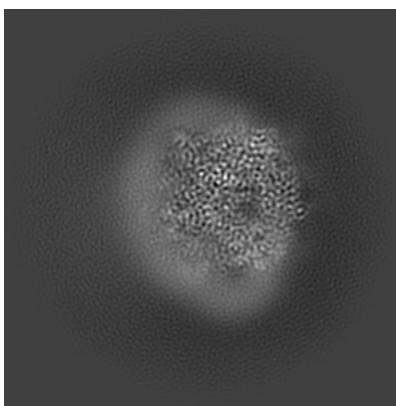
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

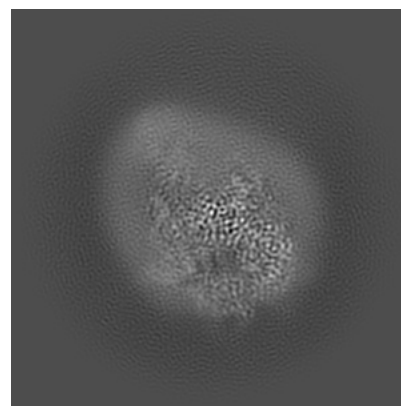
6.1.1 Primary map



X

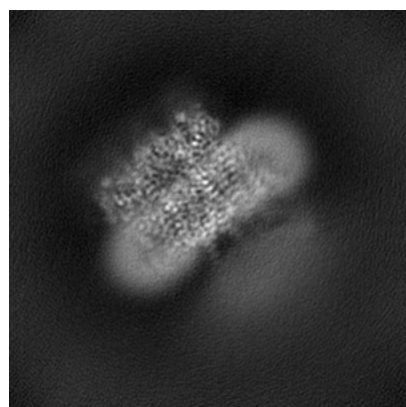


Y

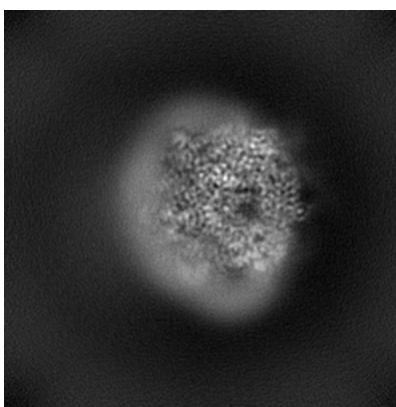


Z

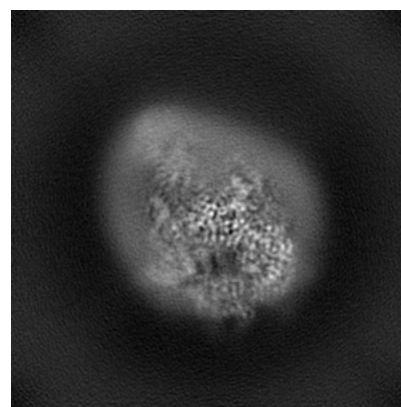
6.1.2 Raw map



X



Y

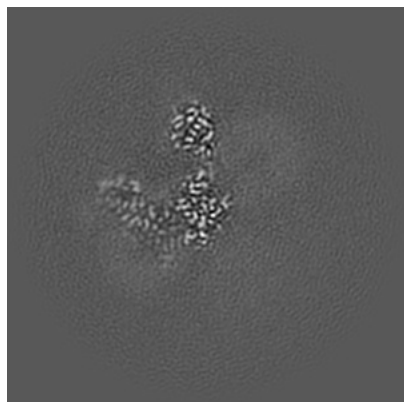


Z

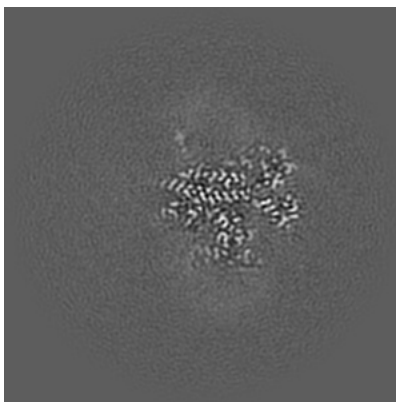
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

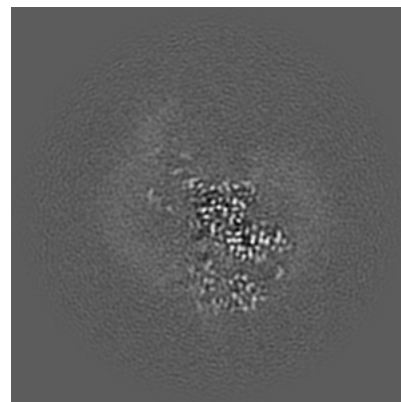
6.2.1 Primary map



X Index: 120

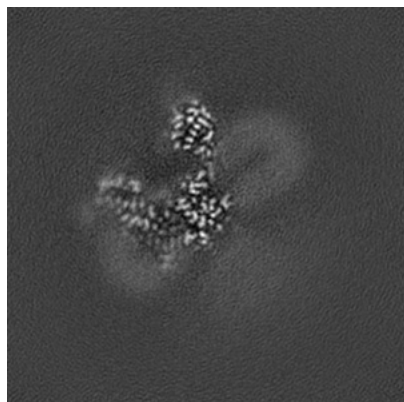


Y Index: 120

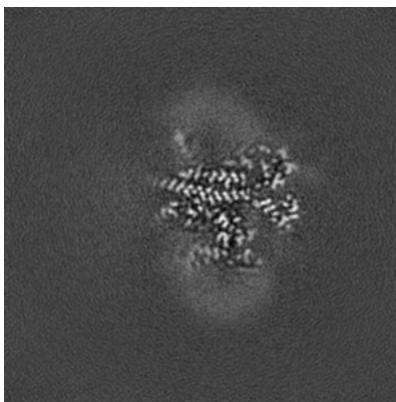


Z Index: 120

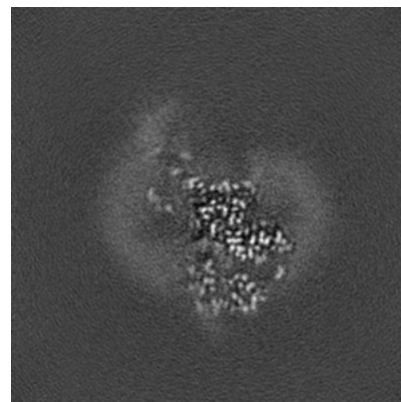
6.2.2 Raw map



X Index: 120



Y Index: 120

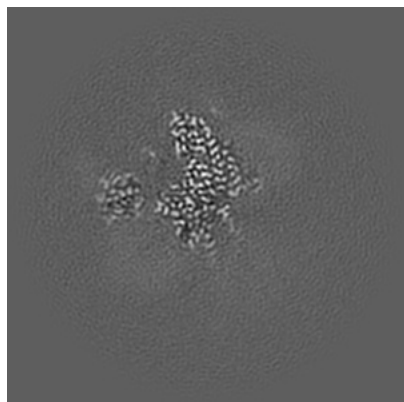


Z Index: 120

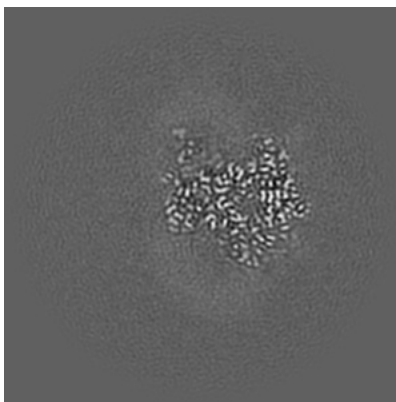
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

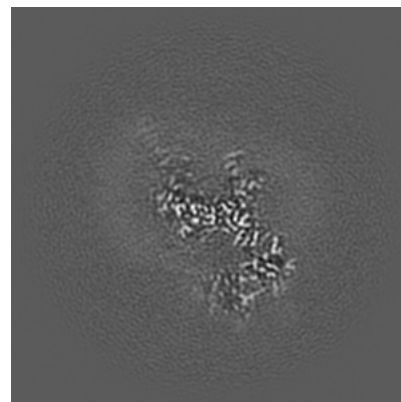
6.3.1 Primary map



X Index: 135

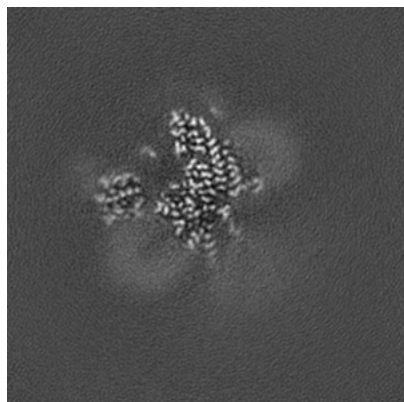


Y Index: 111

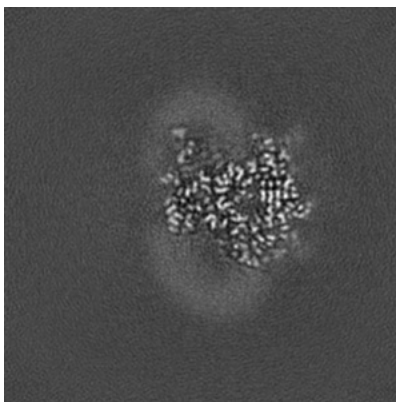


Z Index: 132

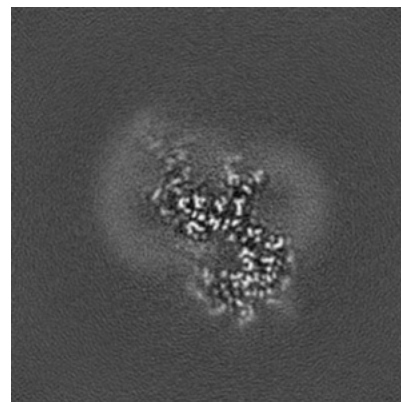
6.3.2 Raw map



X Index: 135



Y Index: 111

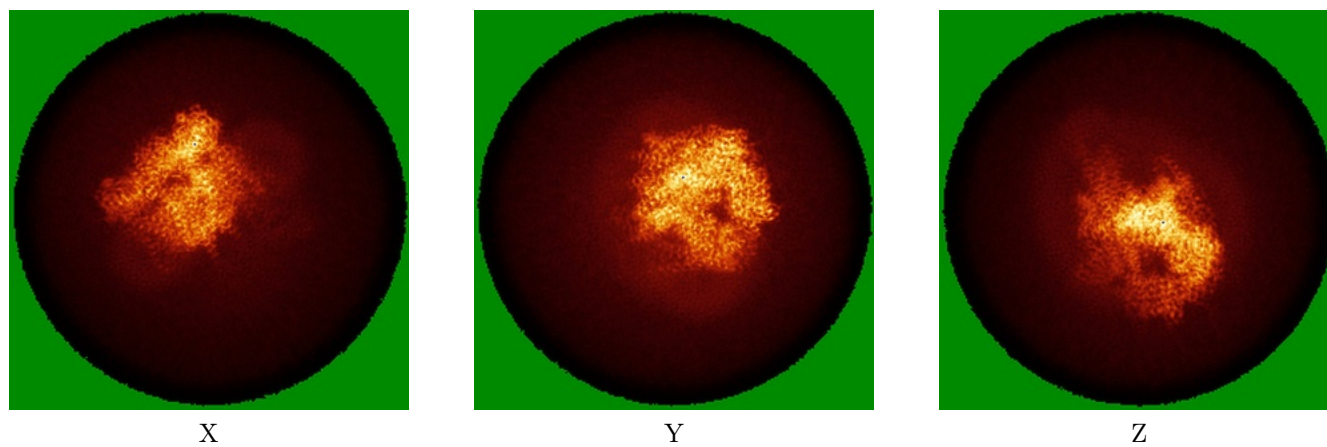


Z Index: 129

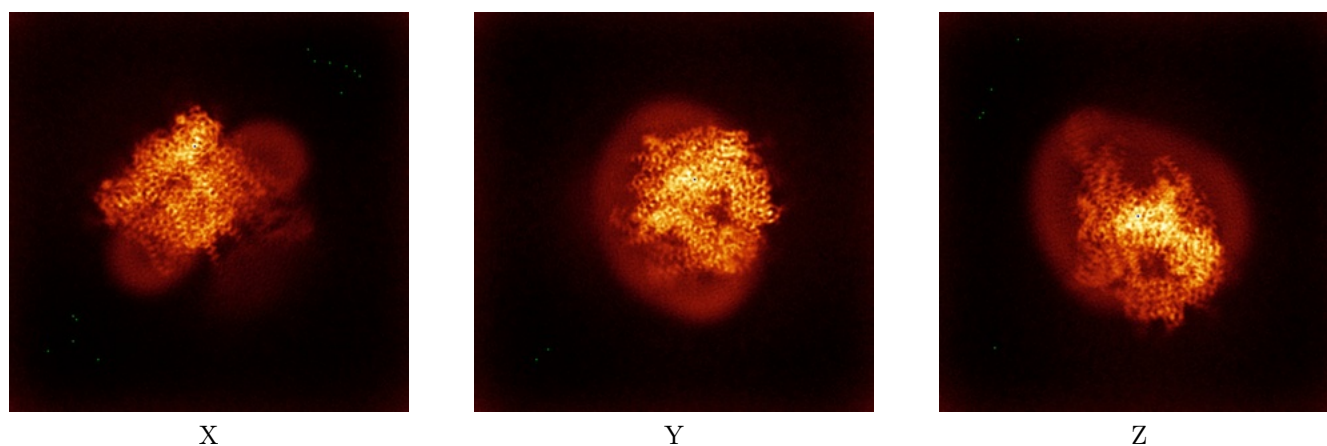
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

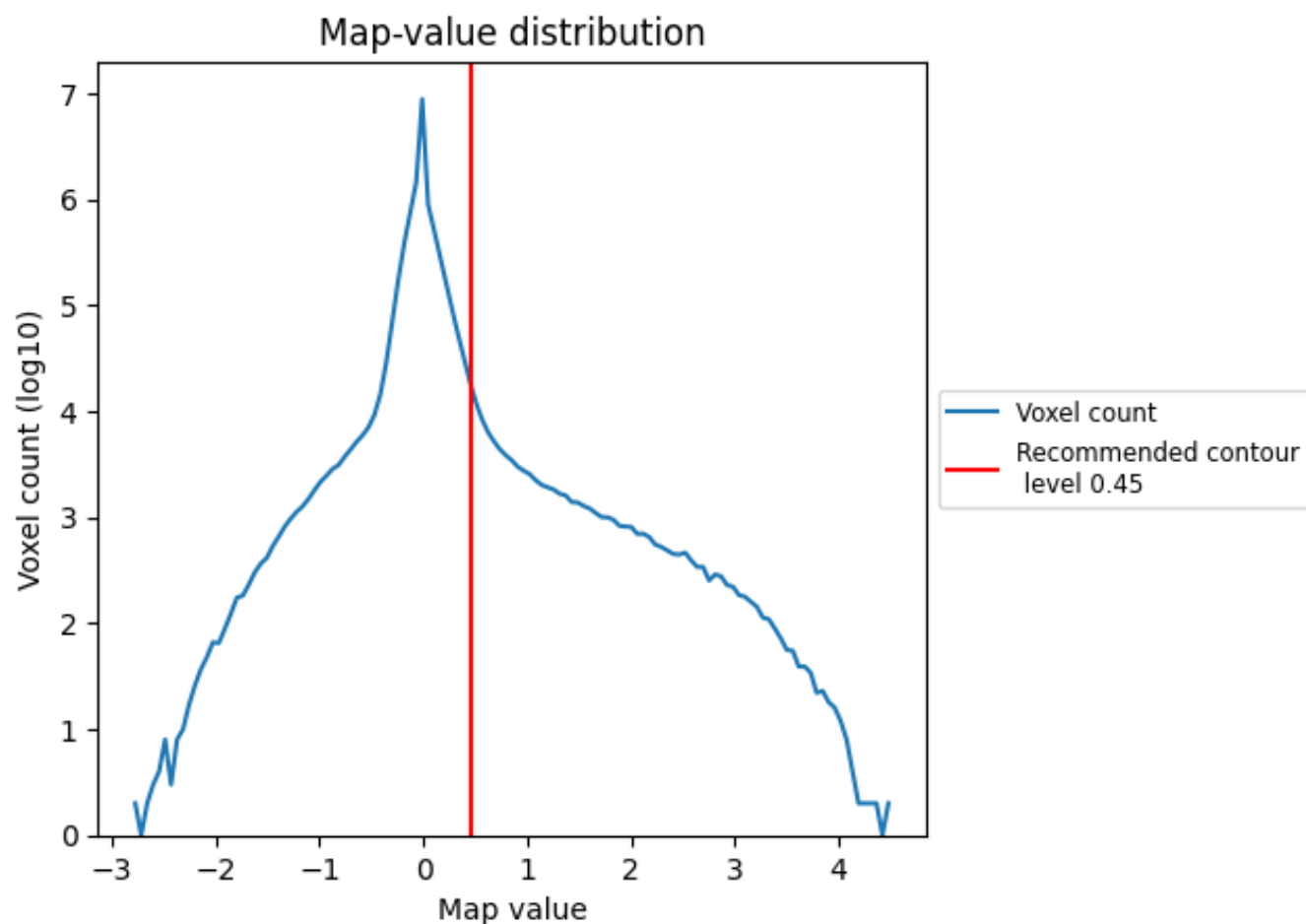
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

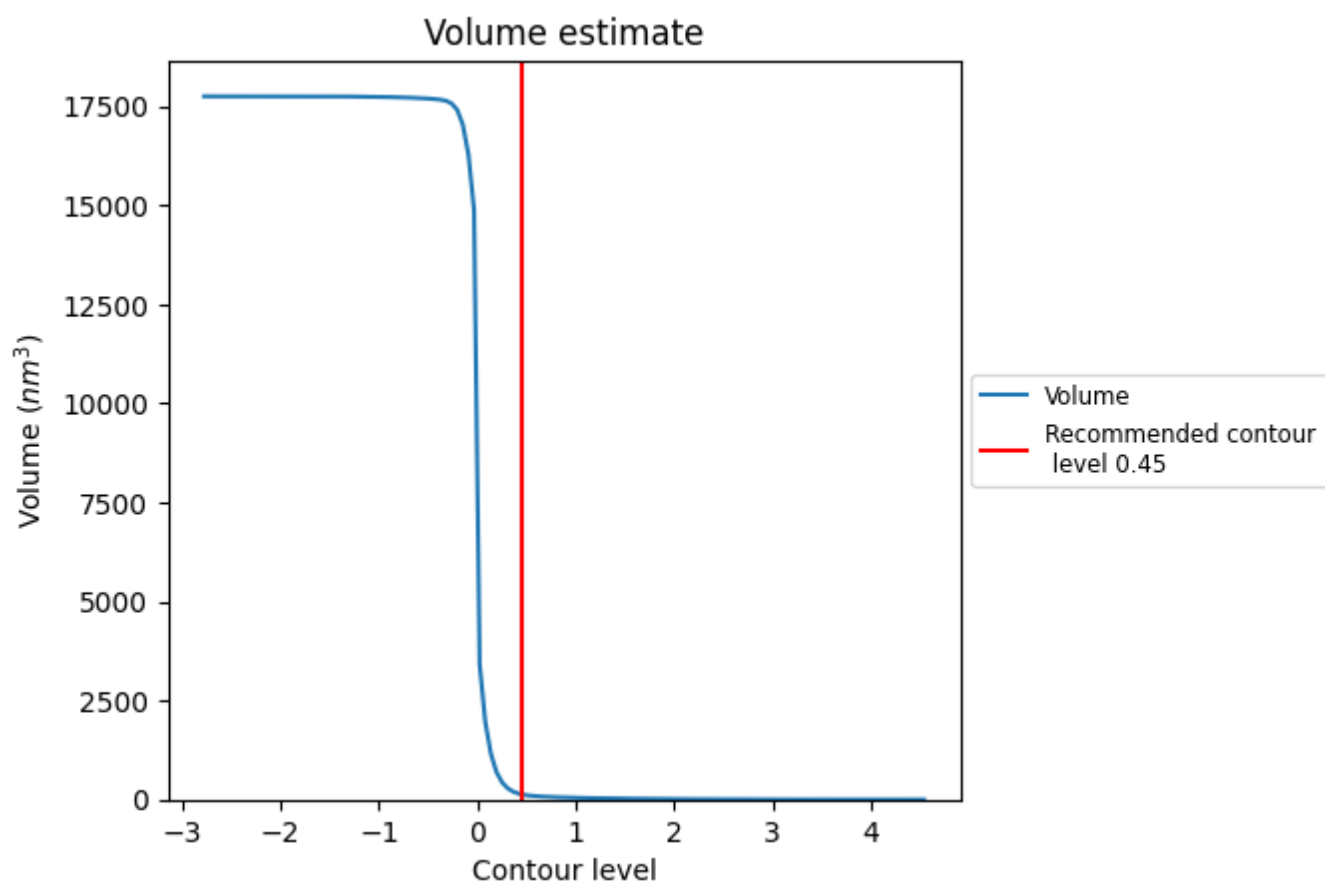
This section contains the results of statistical analysis of the map.

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.

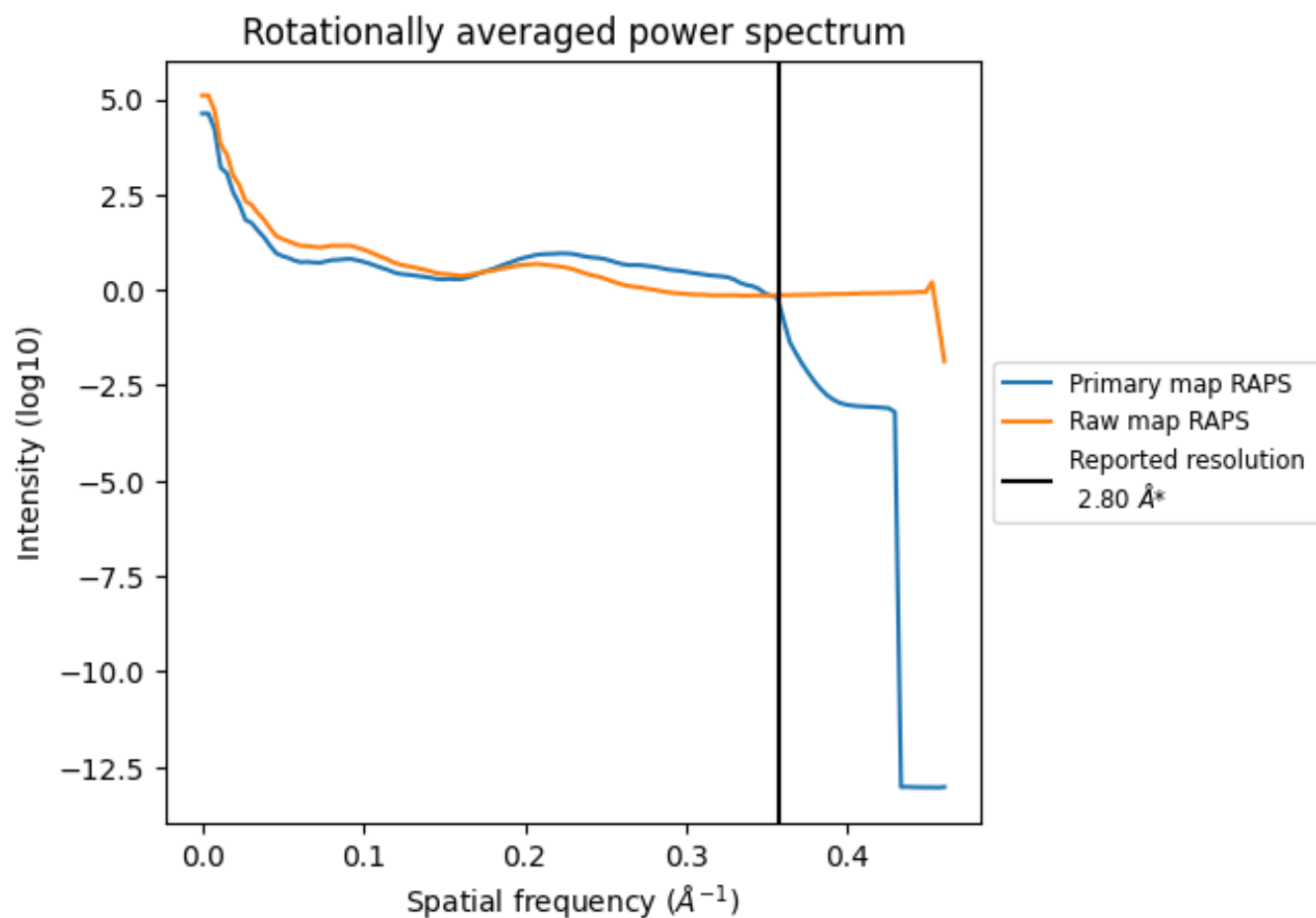
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 133 nm³; this corresponds to an approximate mass of 120 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 ⓘ

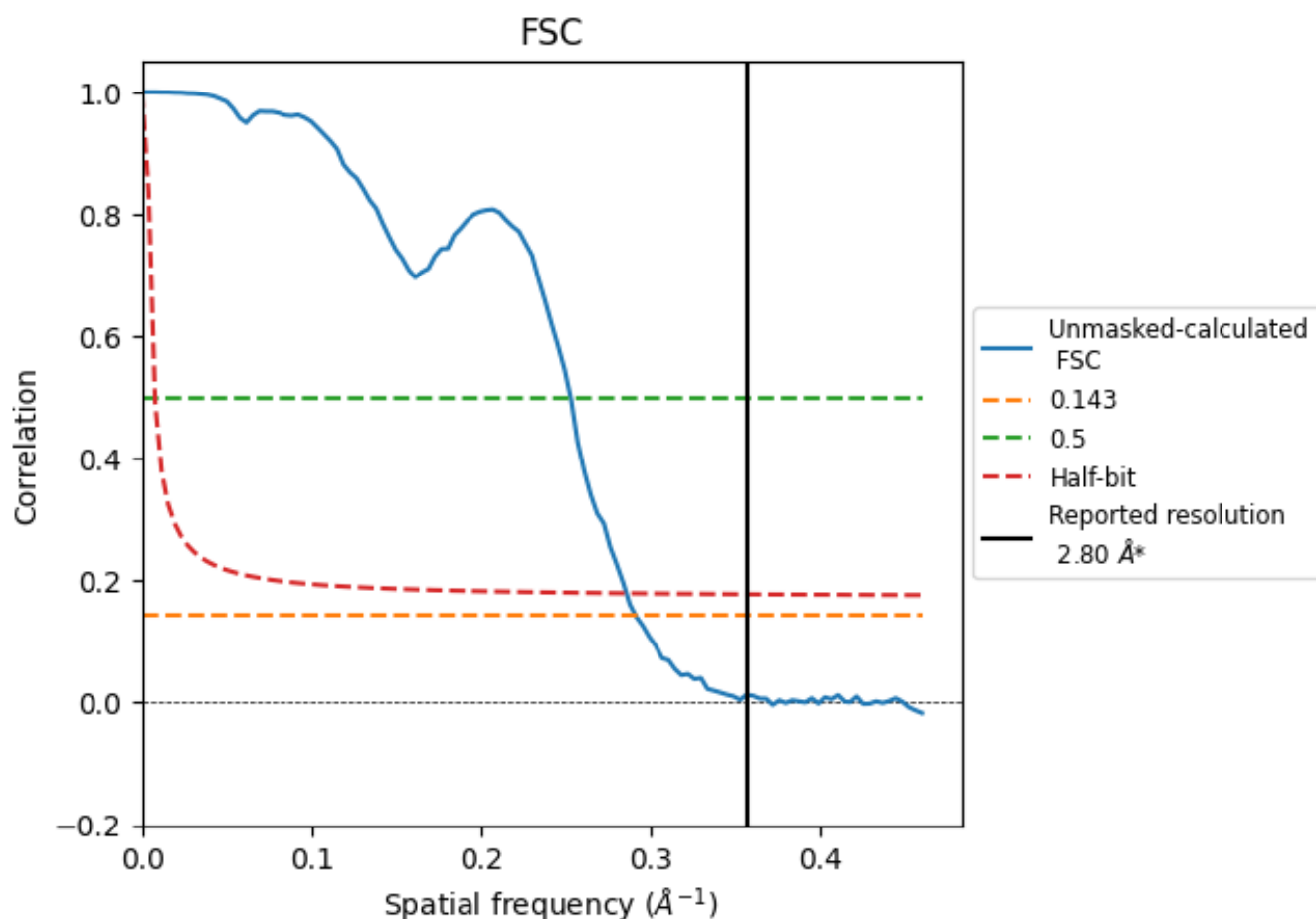


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.44	3.96	3.50

*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 3.44 differs from the reported value 2.8 by more than 10 %

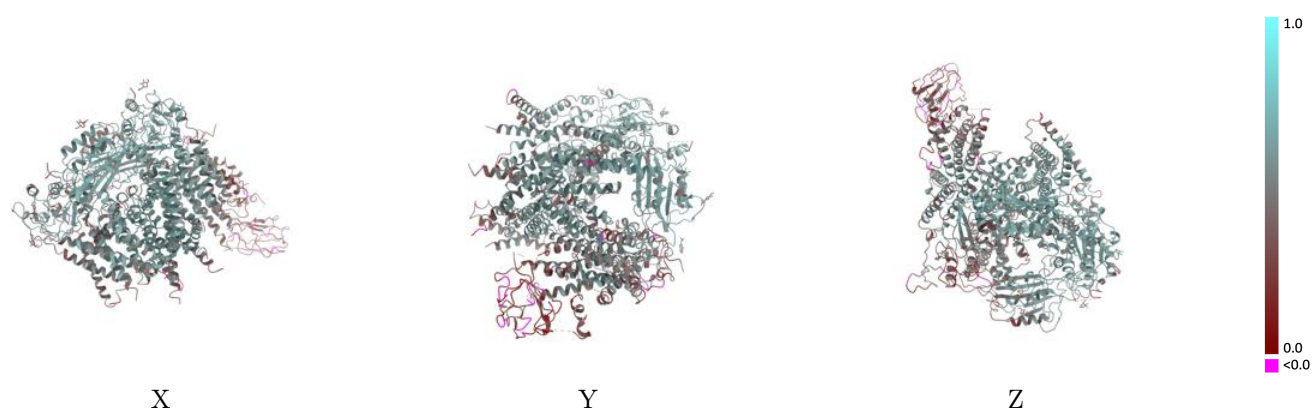
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60206 and PDB model 8ZKR. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

This section was not generated.

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

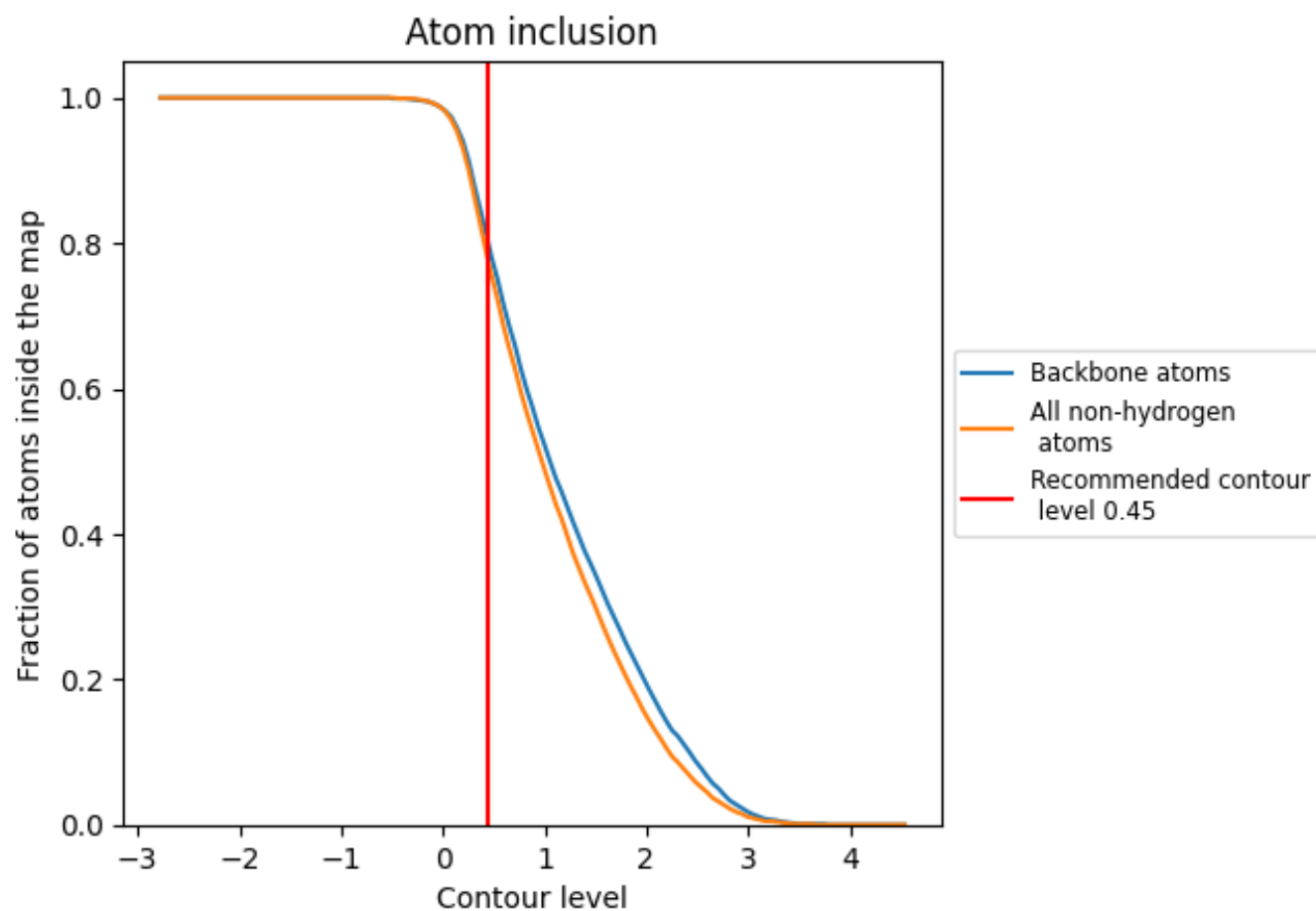


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7720	0.5000
A	0.6110	0.4060
B	0.8720	0.5590
C	0.8820	0.5670
D	0.7780	0.5010

