



wwPDB EM Validation Summary Report ⓘ

Dec 8, 2025 – 08:00 PM JST

PDB ID : 9LOW / pdb_00009low
EMDB ID : EMD-62726
Title : Structure of gain-of-function polycystin-1/polycystin-2 complex
Authors : Chen, M.Y.; Su, Q.; Shi, Y.G.
Deposited on : 2024-12-13
Resolution : 3.69 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.dev129
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.47

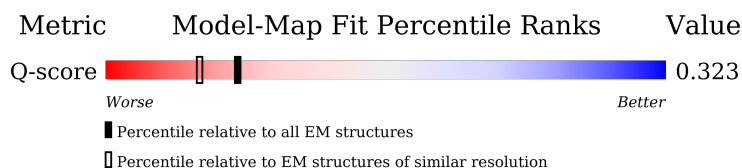
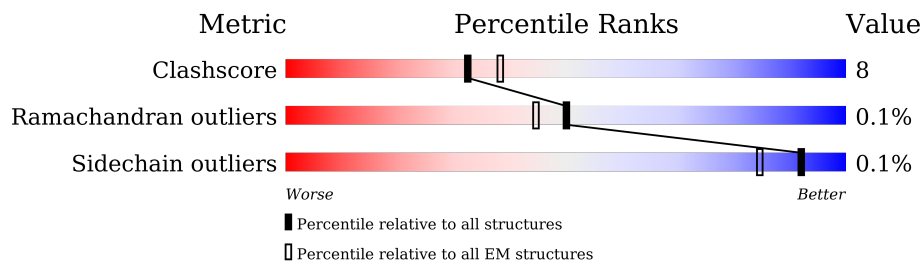
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.69 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	11284 (3.19 - 4.18)

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	1262	
2	B	1005	
2	C	1005	
2	D	1005	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16028 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-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	739	Total	C	N	O	S	0	0
			5474	3528	1001	927	18		

There are 10 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
A	4304	LEU	-	expression tag	UNP P98161

- Molecule 2 is a protein called Polycystin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	476	Total	C	N	O	S	0	0
			3932	2597	621	693	21		
2	C	468	Total	C	N	O	S	0	0
			3860	2550	608	682	20		
2	D	473	Total	C	N	O	S	0	0
			2678	1665	491	517	5		

There are 117 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-36	MET	-	initiating methionine	UNP Q13563
B	-35	GLY	-	expression tag	UNP Q13563
B	-34	ALA	-	expression tag	UNP Q13563

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-33	SER	-	expression tag	UNP Q13563
B	-32	SER	-	expression tag	UNP Q13563
B	-31	ALA	-	expression tag	UNP Q13563
B	-30	TRP	-	expression tag	UNP Q13563
B	-29	SER	-	expression tag	UNP Q13563
B	-28	HIS	-	expression tag	UNP Q13563
B	-27	PRO	-	expression tag	UNP Q13563
B	-26	GLN	-	expression tag	UNP Q13563
B	-25	PHE	-	expression tag	UNP Q13563
B	-24	GLU	-	expression tag	UNP Q13563
B	-23	LYS	-	expression tag	UNP Q13563
B	-22	GLY	-	expression tag	UNP Q13563
B	-21	GLY	-	expression tag	UNP Q13563
B	-20	GLY	-	expression tag	UNP Q13563
B	-19	SER	-	expression tag	UNP Q13563
B	-18	GLY	-	expression tag	UNP Q13563
B	-17	GLY	-	expression tag	UNP Q13563
B	-16	GLY	-	expression tag	UNP Q13563
B	-15	SER	-	expression tag	UNP Q13563
B	-14	GLY	-	expression tag	UNP Q13563
B	-13	GLY	-	expression tag	UNP Q13563
B	-12	SER	-	expression tag	UNP Q13563
B	-11	ALA	-	expression tag	UNP Q13563
B	-10	TRP	-	expression tag	UNP Q13563
B	-9	SER	-	expression tag	UNP Q13563
B	-8	HIS	-	expression tag	UNP Q13563
B	-7	PRO	-	expression tag	UNP Q13563
B	-6	GLN	-	expression tag	UNP Q13563
B	-5	PHE	-	expression tag	UNP Q13563
B	-4	GLU	-	expression tag	UNP Q13563
B	-3	LYS	-	expression tag	UNP Q13563
B	-2	GLY	-	expression tag	UNP Q13563
B	-1	GLY	-	expression tag	UNP Q13563
B	0	SER	-	expression tag	UNP Q13563
B	677	ALA	LEU	engineered mutation	UNP Q13563
B	681	ALA	ASN	engineered mutation	UNP Q13563
C	-36	MET	-	initiating methionine	UNP Q13563
C	-35	GLY	-	expression tag	UNP Q13563
C	-34	ALA	-	expression tag	UNP Q13563
C	-33	SER	-	expression tag	UNP Q13563
C	-32	SER	-	expression tag	UNP Q13563
C	-31	ALA	-	expression tag	UNP Q13563

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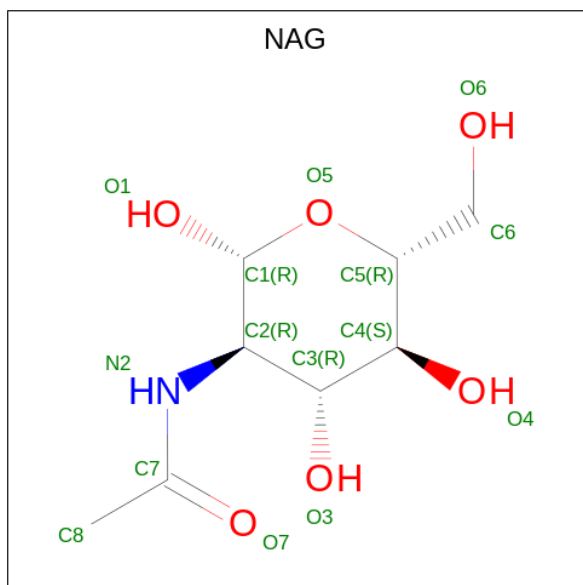
Chain	Residue	Modelled	Actual	Comment	Reference
C	-30	TRP	-	expression tag	UNP Q13563
C	-29	SER	-	expression tag	UNP Q13563
C	-28	HIS	-	expression tag	UNP Q13563
C	-27	PRO	-	expression tag	UNP Q13563
C	-26	GLN	-	expression tag	UNP Q13563
C	-25	PHE	-	expression tag	UNP Q13563
C	-24	GLU	-	expression tag	UNP Q13563
C	-23	LYS	-	expression tag	UNP Q13563
C	-22	GLY	-	expression tag	UNP Q13563
C	-21	GLY	-	expression tag	UNP Q13563
C	-20	GLY	-	expression tag	UNP Q13563
C	-19	SER	-	expression tag	UNP Q13563
C	-18	GLY	-	expression tag	UNP Q13563
C	-17	GLY	-	expression tag	UNP Q13563
C	-16	GLY	-	expression tag	UNP Q13563
C	-15	SER	-	expression tag	UNP Q13563
C	-14	GLY	-	expression tag	UNP Q13563
C	-13	GLY	-	expression tag	UNP Q13563
C	-12	SER	-	expression tag	UNP Q13563
C	-11	ALA	-	expression tag	UNP Q13563
C	-10	TRP	-	expression tag	UNP Q13563
C	-9	SER	-	expression tag	UNP Q13563
C	-8	HIS	-	expression tag	UNP Q13563
C	-7	PRO	-	expression tag	UNP Q13563
C	-6	GLN	-	expression tag	UNP Q13563
C	-5	PHE	-	expression tag	UNP Q13563
C	-4	GLU	-	expression tag	UNP Q13563
C	-3	LYS	-	expression tag	UNP Q13563
C	-2	GLY	-	expression tag	UNP Q13563
C	-1	GLY	-	expression tag	UNP Q13563
C	0	SER	-	expression tag	UNP Q13563
C	677	ALA	LEU	engineered mutation	UNP Q13563
C	681	ALA	ASN	engineered mutation	UNP Q13563
D	-36	MET	-	initiating methionine	UNP Q13563
D	-35	GLY	-	expression tag	UNP Q13563
D	-34	ALA	-	expression tag	UNP Q13563
D	-33	SER	-	expression tag	UNP Q13563
D	-32	SER	-	expression tag	UNP Q13563
D	-31	ALA	-	expression tag	UNP Q13563
D	-30	TRP	-	expression tag	UNP Q13563
D	-29	SER	-	expression tag	UNP Q13563
D	-28	HIS	-	expression tag	UNP Q13563

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-27	PRO	-	expression tag	UNP Q13563
D	-26	GLN	-	expression tag	UNP Q13563
D	-25	PHE	-	expression tag	UNP Q13563
D	-24	GLU	-	expression tag	UNP Q13563
D	-23	LYS	-	expression tag	UNP Q13563
D	-22	GLY	-	expression tag	UNP Q13563
D	-21	GLY	-	expression tag	UNP Q13563
D	-20	GLY	-	expression tag	UNP Q13563
D	-19	SER	-	expression tag	UNP Q13563
D	-18	GLY	-	expression tag	UNP Q13563
D	-17	GLY	-	expression tag	UNP Q13563
D	-16	GLY	-	expression tag	UNP Q13563
D	-15	SER	-	expression tag	UNP Q13563
D	-14	GLY	-	expression tag	UNP Q13563
D	-13	GLY	-	expression tag	UNP Q13563
D	-12	SER	-	expression tag	UNP Q13563
D	-11	ALA	-	expression tag	UNP Q13563
D	-10	TRP	-	expression tag	UNP Q13563
D	-9	SER	-	expression tag	UNP Q13563
D	-8	HIS	-	expression tag	UNP Q13563
D	-7	PRO	-	expression tag	UNP Q13563
D	-6	GLN	-	expression tag	UNP Q13563
D	-5	PHE	-	expression tag	UNP Q13563
D	-4	GLU	-	expression tag	UNP Q13563
D	-3	LYS	-	expression tag	UNP Q13563
D	-2	GLY	-	expression tag	UNP Q13563
D	-1	GLY	-	expression tag	UNP Q13563
D	0	SER	-	expression tag	UNP Q13563
D	677	ALA	LEU	engineered mutation	UNP Q13563
D	681	ALA	ASN	engineered mutation	UNP Q13563

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

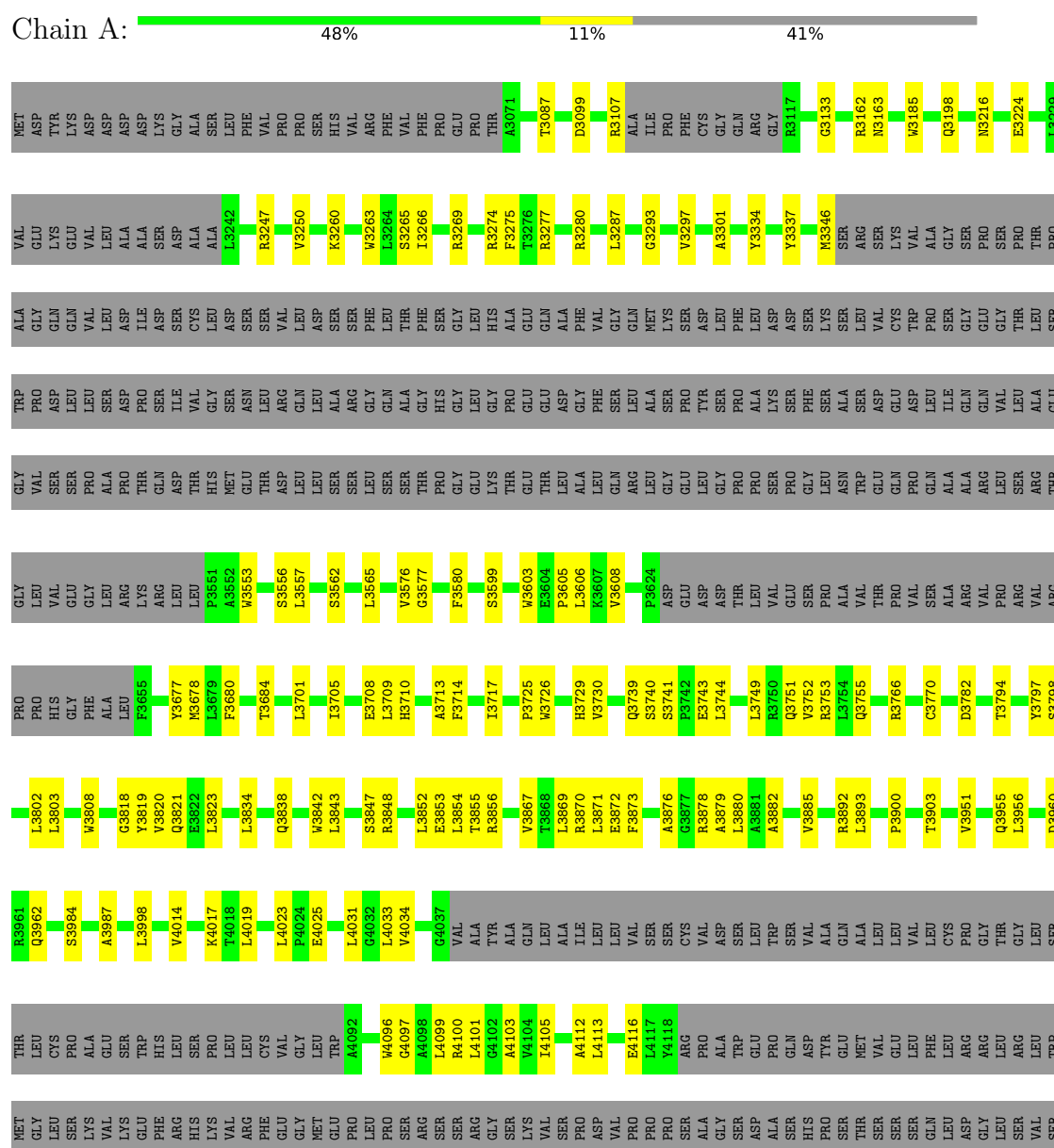


Mol	Chain	Residues	Atoms				AltConf
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

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

• Molecule 1: Polycystin-1



[illegible]

- Molecule 2: Polycystin-2

Chain B: 40% 8% 53%

GLY	ASN	TLE	GLN	ASP	ASN	W570	R355	ARG	TVR	ARG	PRO	MET
GLY	ASN	HIS	VAL	LEU	THR	I571	Y386	LEU	HIS	GLN	ASP	GLY
SER	GLY	ARG	VAL	GLU	ASP	I572	Y387	GLU	GLY	TRP	GLY	ALA
SER	ASN	GLN	ARG	LYS	ASP	I577	G388	GLU	GLY	SER	ALA	SER
VAL	ASN	MET	ARG	GLU	ILE	C593	L395	SER	HIS	ARG	LEU	ALA
VAL	HIS	GLU	ASP	ARG	SER	C593	L395	SER	PRO	ASP	MET	TRP
VAL	HIS	LEU	ASP	ASP	GLU	A610	D416	THR	SER	ASN	ALA	SER
VAL	ASN	VAL	MET	LEU	LEU	A610	R417	ASN	GLY	PRO	GLY	HIS
		VAL	ARG	LEU	GLN	G613	G418	ARG	ARG	GLY	CYS	PRO
		GLU	HIS	LEU	ASN	G613	T419	GLU	ARG	PHE	ALA	GLN
		GLU	SER	ASP	GLY	V618		K215	ARG	GLU	ALA	PHE
		LEU	ILE	HIS	GLY	F619	N432	R222	ARG	ALA	VAL	GLU
		GLU	GLY	SER	GLY	G620	I433	GLU	GLU	GLU	GLY	LYS
		ARG	SER	SER	LYS	T621	N434	V225	ASP	GLU	SER	GLY
		TRP	ILE	LEU	LEU	D622		T226	GLN	GLU	LEU	GLY
		GLU	VAL	PRO	ASN	V623	R440	Y227	GLY	GLU	ALA	SER
		SER	SER	ARG	PHE				PRO	GLU	ALA	GLY
		ASP	LYS	PRO	ASP	C632	E444	Y248	PRO	VAL	PRO	GLY
		ASP	ILE	MET	GLU	T635	I452	M252	CYS	GLU	GLY	GLY
		ALA	ALA	SER	LEU				SER	GLY	LEU	SER
		SER	VAL	ARG	GLN	R654	L460	V262	PRO	GLU	CYS	GLY
		GLN	ILE	SER	ASP	V655		K281	VAL	GLY	GLU	SER
		ILE	VAL	PHE	LEU	L656	I463		GLY	GLY	GLN	ALA
		HIS	LYS	PRO	LYS		V466	Q296	GLY	MET	ARG	TRP
		GLY	LEU	ARG	GLY	V665	T467	PRO	GLY	VAL	GLY	SER
		LEU	ILE	LEU	LYS		L473	SER	ASP	VAL	LEU	HIS
		GLY	MET	ASP	HIS	F669		ASN	PRO	GLU	GLU	PRO
		THR	GLU	ASP	GLY	F670	L473	GLN	LEU	ILE	GLN	PHI
		PRO	ARG	ASP	THR	I671	S518	THR	HIS	ASP	GLU	PHI
		VAL	ALA	GLU	ALA	L672		GLU	ARG	VAL	MET	GLY
		GLY	LYS	GLU	GLU	L673	I522	ALA	HIS	GLU	GLN	LYS
		LEU	LEU	ASP	ILE	N674		ASP	LEU	TRP	ARG	GLY
		ASN	LYS	ASP	GLU	T683	N525	N305	PRO	ARG	ILE	GLY
		GLY	ARG	ASP	ALA		R528	R306	LEU	PRO	ARG	SER
		GLN	ARG	GLU	ILE	W698		GLN	GLY	GLY	GLN	MET
		PRO	GLU	ASP	PHE	GLU	E528	Y309	GLY	SER	ALA	ASN
		ARG	VAL	SER	THR	LEU	E533	ARG	PRO	ARG	ALA	SER
		PRO	LEU	GLY	LYS	SER	L536	E312	PRO	SER	ARG	SER
		ARG	ARG	HIS	TYR	ASP	L536	N313	ARG	ALA	ASP	ARG
		SER	GLY	SER	ASP	LEU	Q537	VAL	VAL	ALA	PRO	ARG
		SER	LEU	SER	GLN	ILE	F538	L316	ALA	SER	PRO	GLN
		ARG	LEU	ARG	ASP	ARG	L539		TRP	SER	ALA	PRO
		PRO	ASP	ARG	GLY	LYS	E540	P319	ALA	ALA	GLY	GLN
		SER	GLY	ARG	ASP	GLY			GLU	VAL	ALA	GLN
		SER	VAL	GLY	GLN	TYR	E549	R325	ARG	SER	ALA	PRO
		SER	ALA	GLY	LEU	HIS			LEU	SER	ALA	GLY
		GLN	GLU	ILE	GLU	LYS	A552	P334	VAL	VAL	SER	ASP
		THR	ASP	SER	THR	ALA	SER	Q335	ARG	GLY	PRO	ALA
		THR	GLU	SER	GLY	LEU	Q555	D336	GLY	ALA	SER	LYS
		GLU	ARG	GLY	HIS	VAL	F558	L337	LEU	ARG	PRO	ARG
		GLY	VAL	VAL	GLU	LYS	F558	R338	ARG	SER	PRO	PRO
		MET	GLY	SER	HIS	LEU	A563	D339	GLY	ARG	PRO	PRO
		GLU	ARG	TYR	GLN	LYS		E343	TRP	GLY	SER	ALA
		GLY	ASP	GLU	GLN	LEU	A563	E343	TRP	LEU	PRO	ALA
		ALA	SER	GLU	MET	LYS	F567		GLY	CYS	ALA	ALA
		GLY	GLU	DUE	ARG	LYS		D364	THR	GLY	SER	ALA

- Molecule 2: Polycystin-2

Chain C: 37% 10% 53%

[illegible]

V406	A407	S408	L409	K410	K411	M412	V413	M414	L415	D416	R417	G418	T419	R420	A421	T422	F423	I424	D425	F426	S427	V428	Y429	M430	A431	M432	I433	M434	L435	F436	C437	V438	V439	R440	L441	L442	V443	Q456	F457	Q458	P459	L460	K461	L462	I463	R464	Y465	V466	T467	T468	F469	D470	F471	F472	L473	A474	A475	C476																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
	F485		V488		V513	I514	V515	V516	L517	S518	V519	V520		L536	Q537	F538		L539		Q542	N543	T544	F545	P546	N547		A552		I561	A562	A563	V564	T565		I571	K572	L573		K595	D596	L597		Y611		L614		V618	F619		V623		F626		I639		I644	N645		E648																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
E651		V655	G657		F664	F676	A677		K688		A692	Q693	Q694	K695	ALA	GLU	MET	LEU	SER	ASP	LEU	ILE	PHE	THR	GLY		THR	LYS	GLU	ALA	HIS	LYS	VAL	LYS	ASN	THR	VAL	ASP	LYS	ASP	ILE	ASP	GLU	SER	LEU	ARG	PHE																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	128014	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.948	Depositor
Minimum map value	-0.397	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.058	Depositor
Recommended contour level	0.15	Depositor
Map size (\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 (\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

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	0.15	0/5602	0.41	0/7636
2	B	0.12	0/4036	0.31	0/5473
2	C	0.13	0/3962	0.36	0/5375
2	D	0.11	0/2699	0.32	0/3726
All	All	0.13	0/16299	0.36	0/22210

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5474	0	5292	124	0
2	B	3932	0	3890	53	0
2	C	3860	0	3821	68	0
2	D	2678	0	1619	19	0
3	B	42	0	39	0	0
3	C	42	0	39	6	0
All	All	16028	0	14700	253	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 8.

The worst 5 of 253 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:375:ASN:HD21	3:C:1001:NAG:C1	1.13	1.57
1:A:3766:ARG:CG	1:A:3878:ARG:HH21	1.44	1.31
1:A:3873:PHE:CE1	1:A:3879:ALA:CB	2.37	1.08
1:A:3766:ARG:HG2	1:A:3878:ARG:HH21	0.98	1.08
2:B:306:ARG:HD3	2:C:340:GLU:OE1	1.58	1.02

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	727/1262 (58%)	650 (89%)	75 (10%)	2 (0%)	37	67
2	B	472/1005 (47%)	450 (95%)	22 (5%)	0	100	100
2	C	464/1005 (46%)	433 (93%)	31 (7%)	0	100	100
2	D	469/1005 (47%)	446 (95%)	23 (5%)	0	100	100
All	All	2132/4277 (50%)	1979 (93%)	151 (7%)	2 (0%)	50	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3876	ALA
1	A	3770	CYS

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	506/1042 (49%)	505 (100%)	1 (0%)	92	96
2	B	429/858 (50%)	429 (100%)	0	100	100
2	C	421/858 (49%)	421 (100%)	0	100	100
2	D	88/858 (10%)	88 (100%)	0	100	100
All	All	1444/3616 (40%)	1443 (100%)	1 (0%)	92	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3802	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	674	ASN
2	C	585	GLN
2	C	379	HIS
2	C	375	ASN
2	C	557	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](#)

6 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	$\# Z > 2$
3	NAG	C	1003	2	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	B	1002	2	14,14,15	0.49	0	17,19,21	0.82	1 (5%)
3	NAG	B	1001	2	14,14,15	0.92	1 (7%)	17,19,21	1.25	1 (5%)
3	NAG	C	1001	2	14,14,15	0.29	0	17,19,21	0.61	0
3	NAG	B	1003	2	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	C	1002	2	14,14,15	0.20	0	17,19,21	0.41	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	C	1003	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1002	2	-	1/6/23/26	0/1/1/1
3	NAG	B	1001	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1001	2	-	5/6/23/26	0/1/1/1
3	NAG	B	1003	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1002	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	NAG	O5-C1	3.28	1.49	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1001	NAG	C1-O5-C5	4.94	118.88	112.19
3	B	1002	NAG	C1-O5-C5	2.64	115.77	112.19

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1001	NAG	C8-C7-N2-C2
3	C	1001	NAG	O7-C7-N2-C2
3	B	1001	NAG	O5-C5-C6-O6
3	C	1002	NAG	C4-C5-C6-O6
3	C	1002	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1001	NAG	6	0

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.

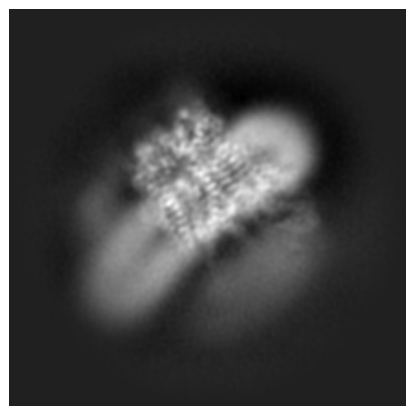
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62726. These allow visual inspection of the internal detail of the map and identification of artifacts.

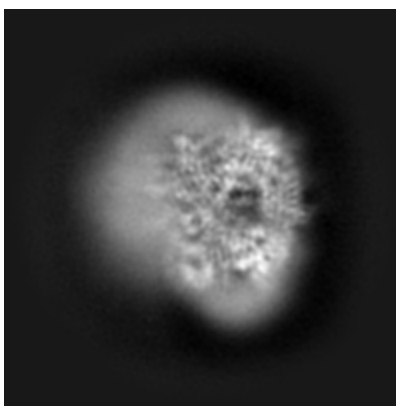
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

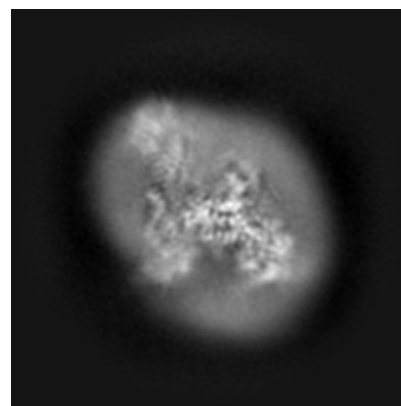
6.1.1 Primary map



X

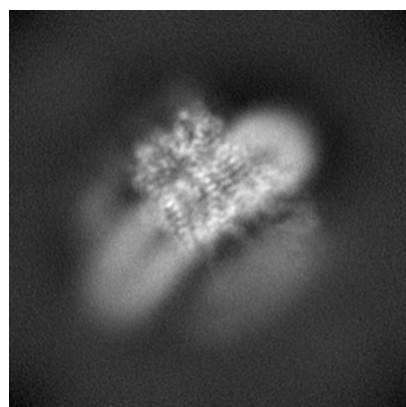


Y

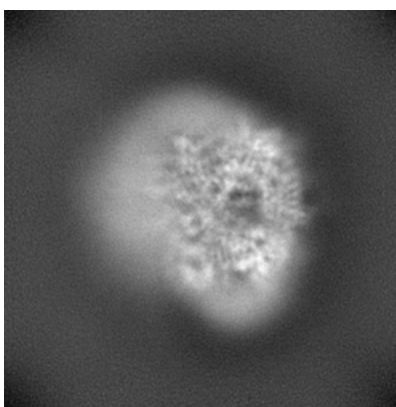


Z

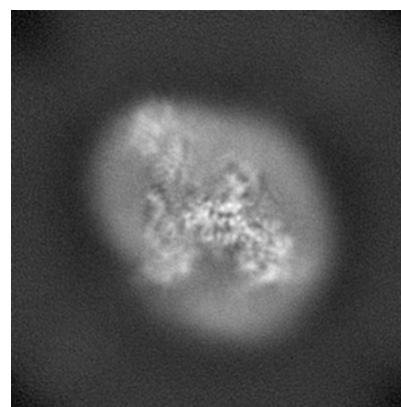
6.1.2 Raw map



X



Y

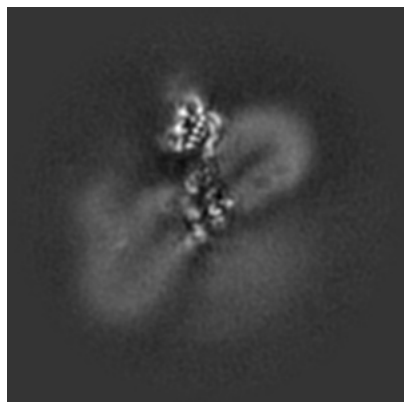


Z

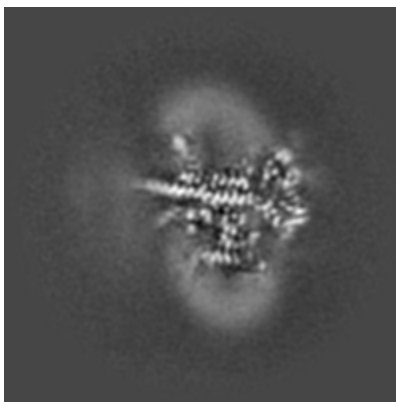
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

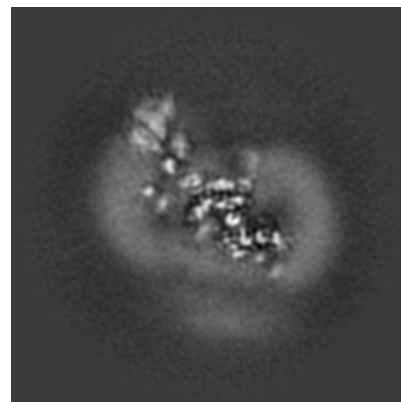
6.2.1 Primary map



X Index: 120

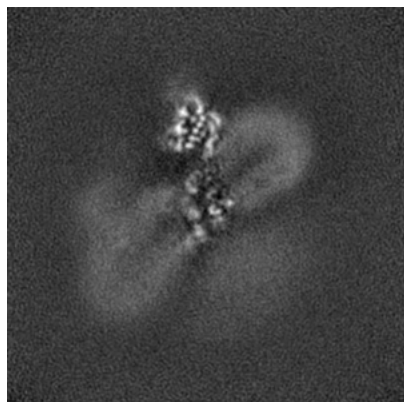


Y Index: 120

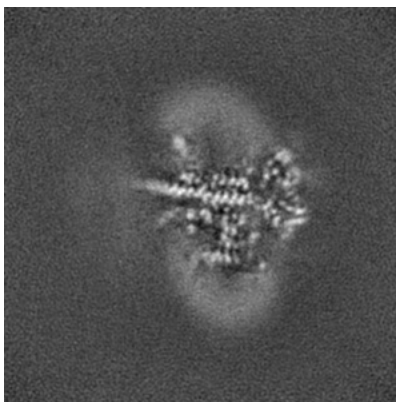


Z Index: 120

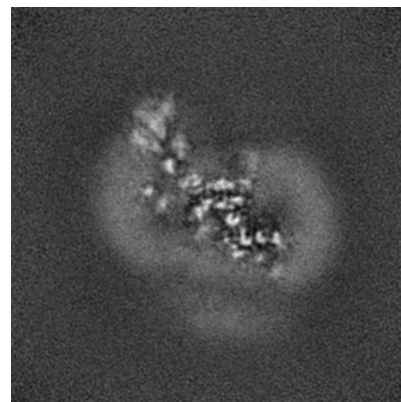
6.2.2 Raw map



X Index: 120



Y Index: 120

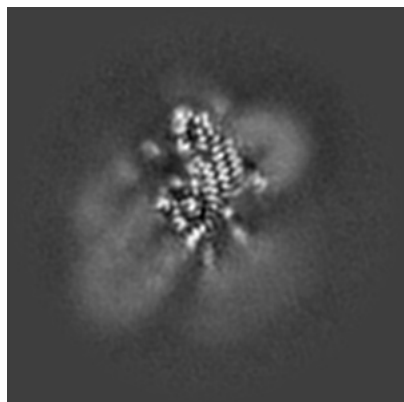


Z Index: 120

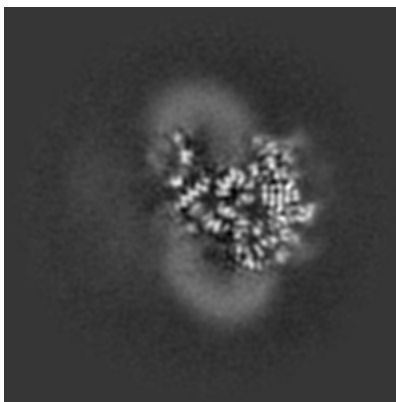
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

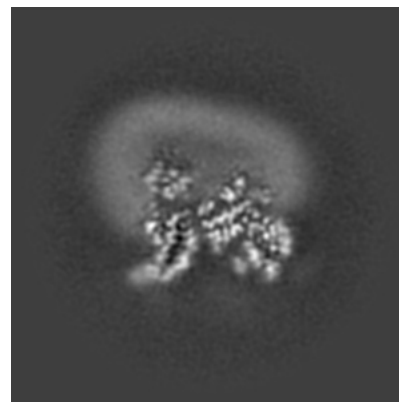
6.3.1 Primary map



X Index: 134

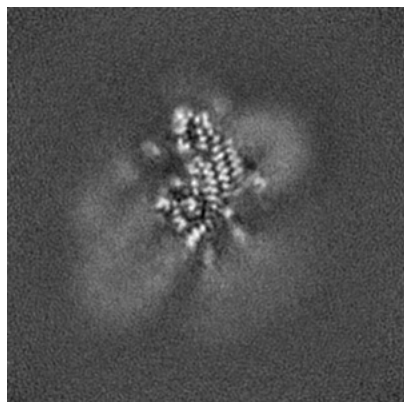


Y Index: 113

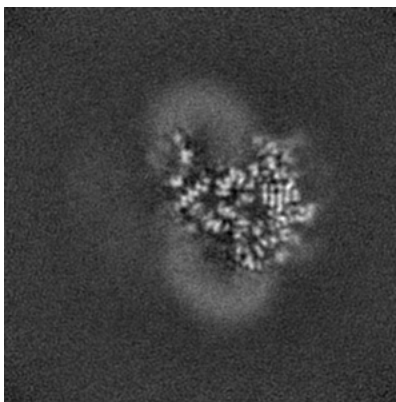


Z Index: 156

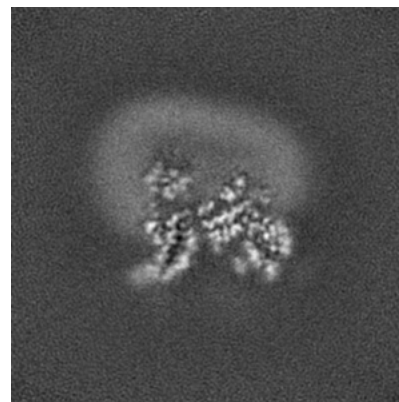
6.3.2 Raw map



X Index: 134



Y Index: 113

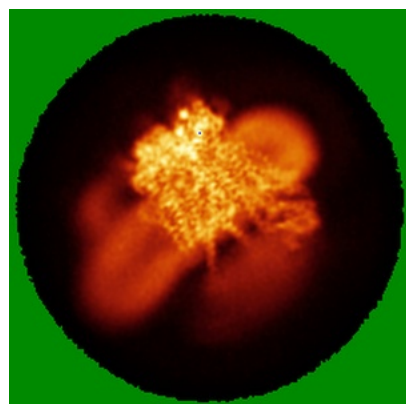


Z Index: 156

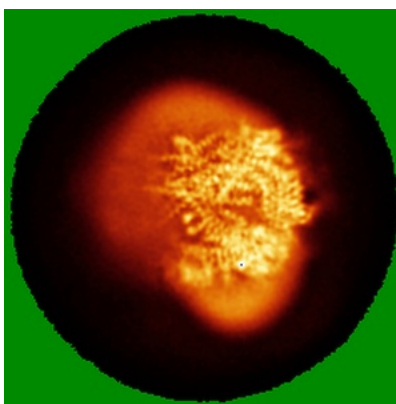
The images above show the largest variance slices of the map in three orthogonal directions.

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

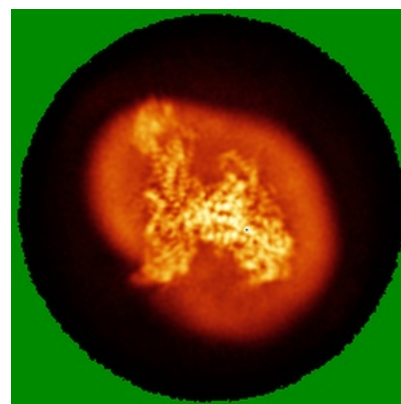
6.4.1 Primary map



X

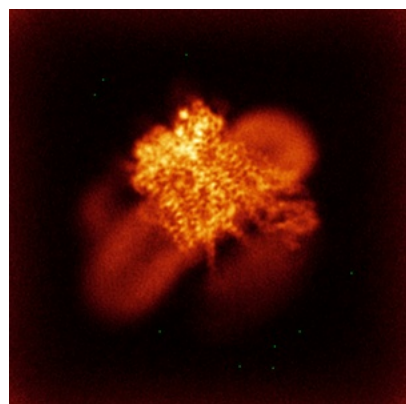


Y

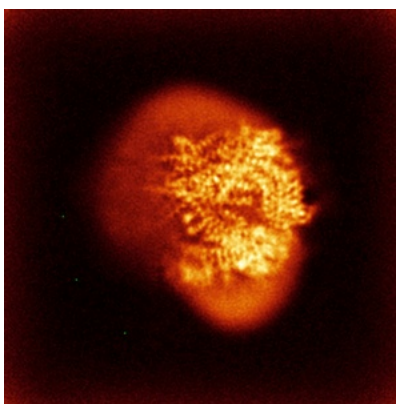


Z

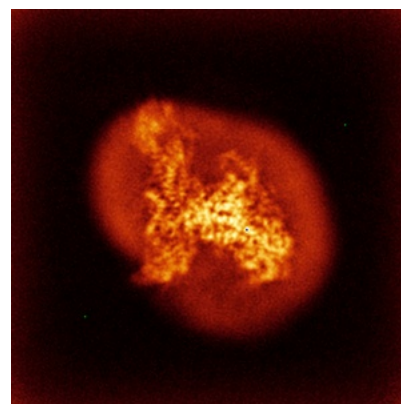
6.4.2 Raw map



X



Y

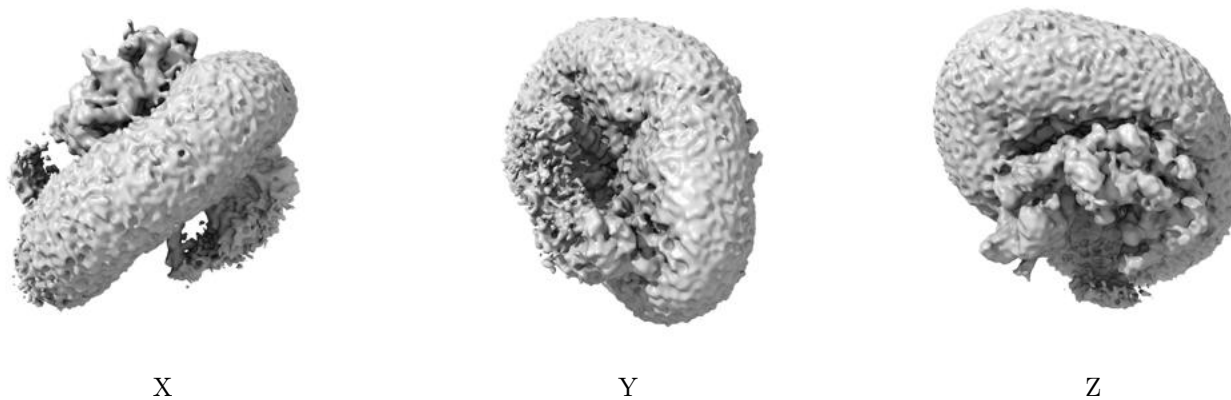


Z

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.

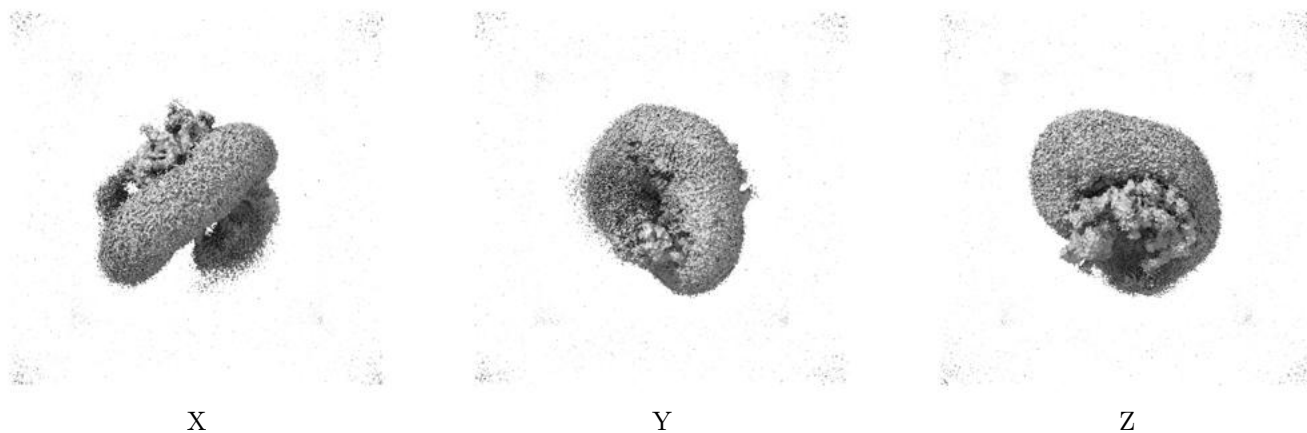
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

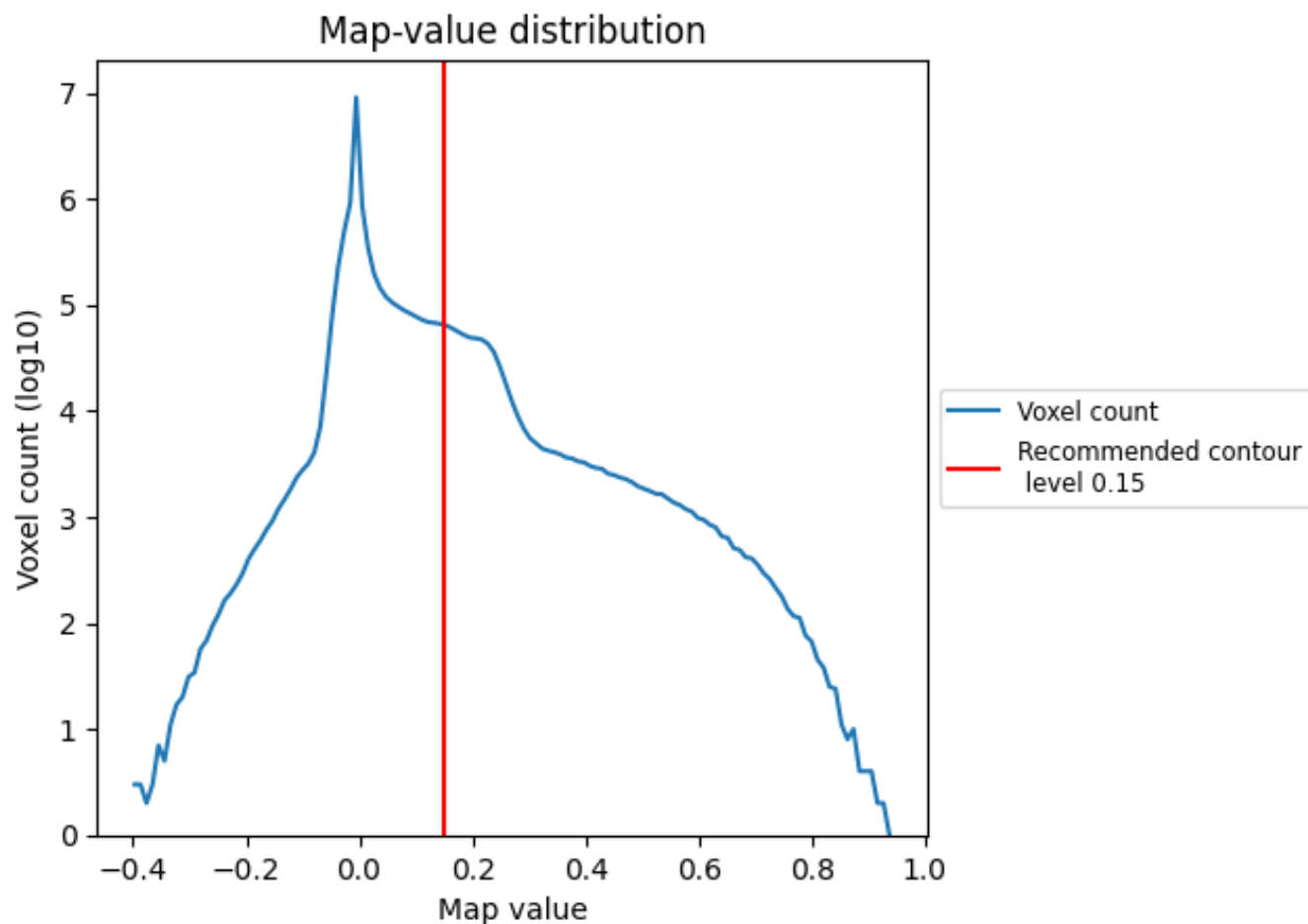
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

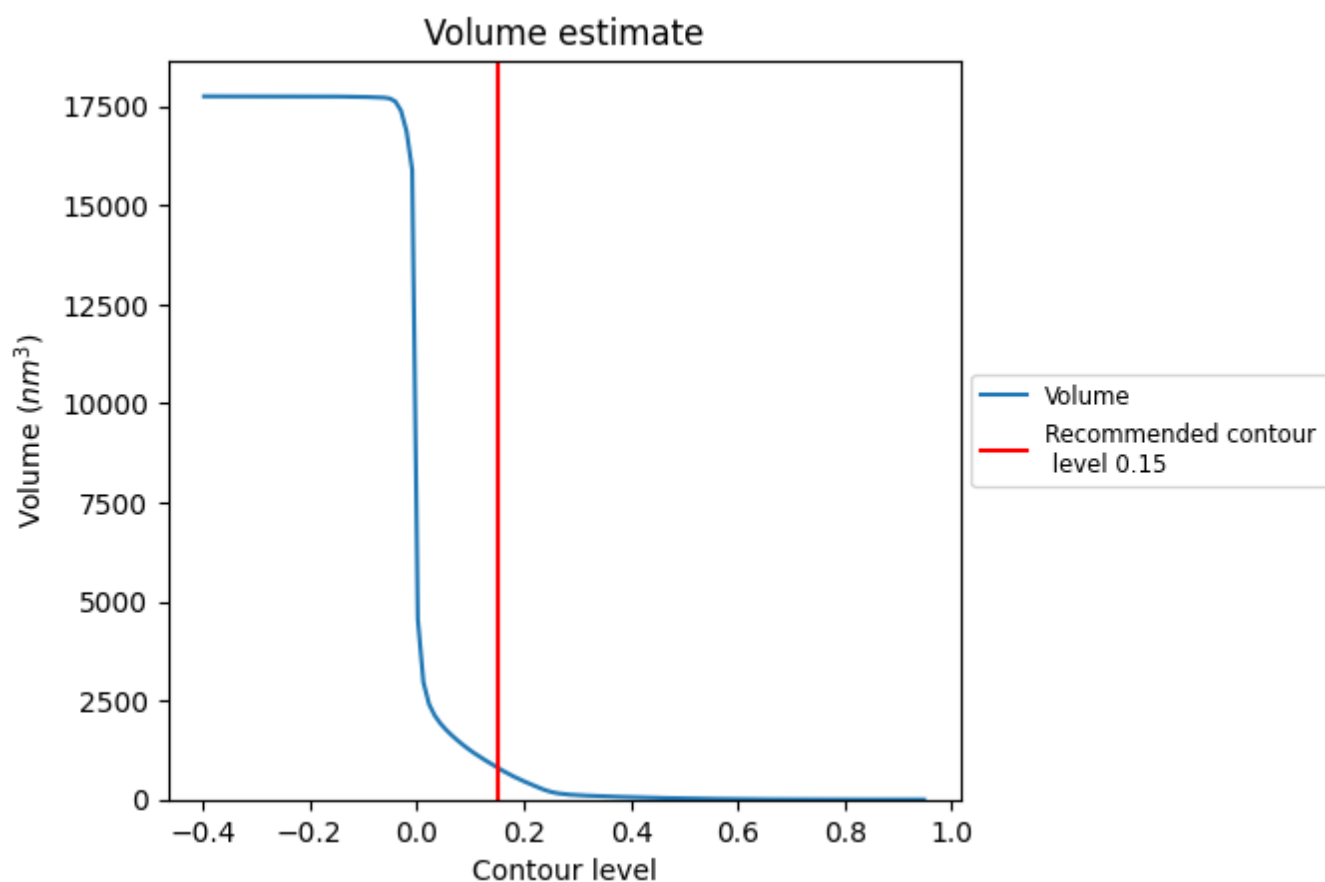
This section contains the results of statistical analysis of the map.

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.

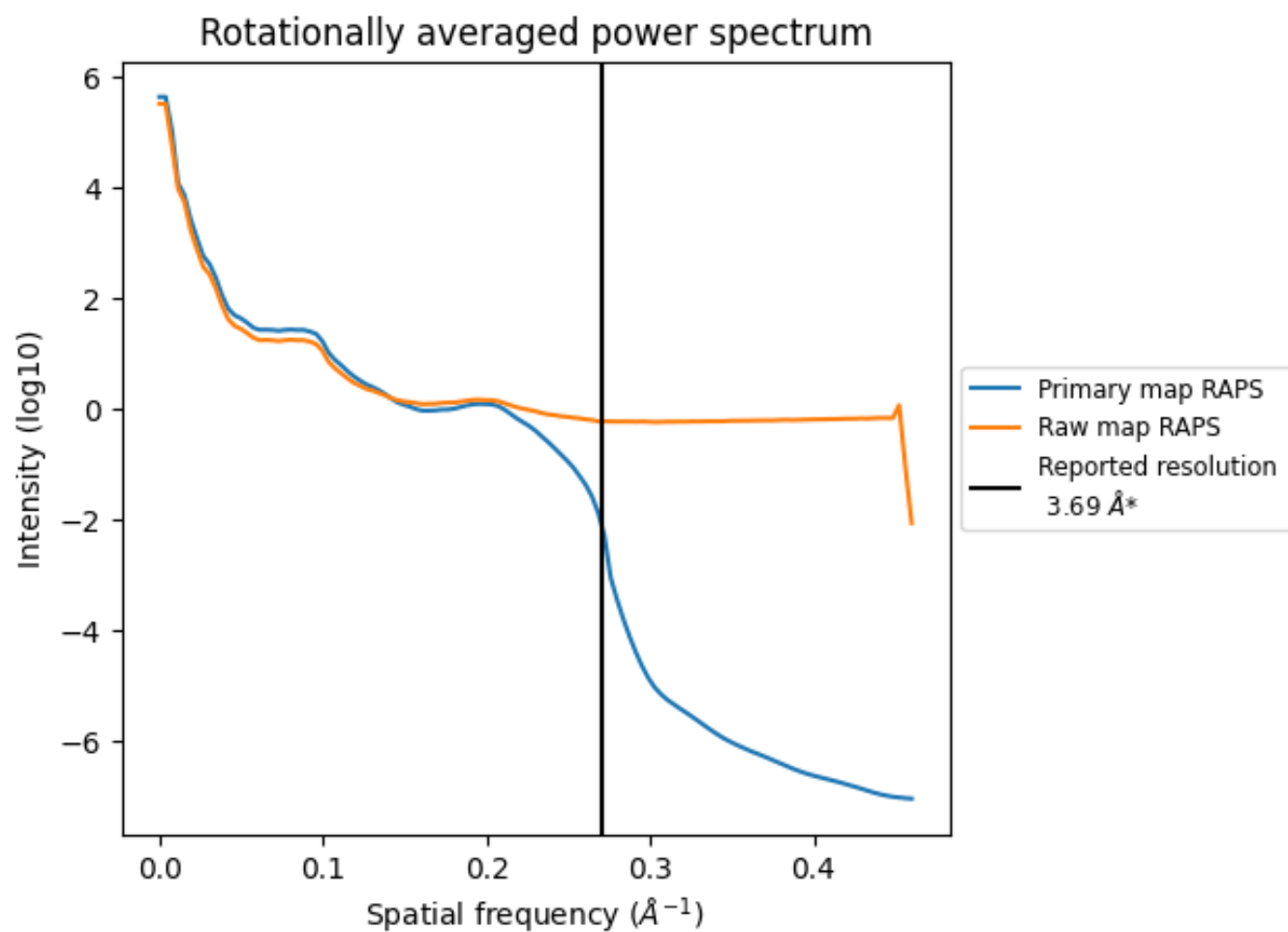
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 814 nm³; this corresponds to an approximate mass of 735 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 ⓘ

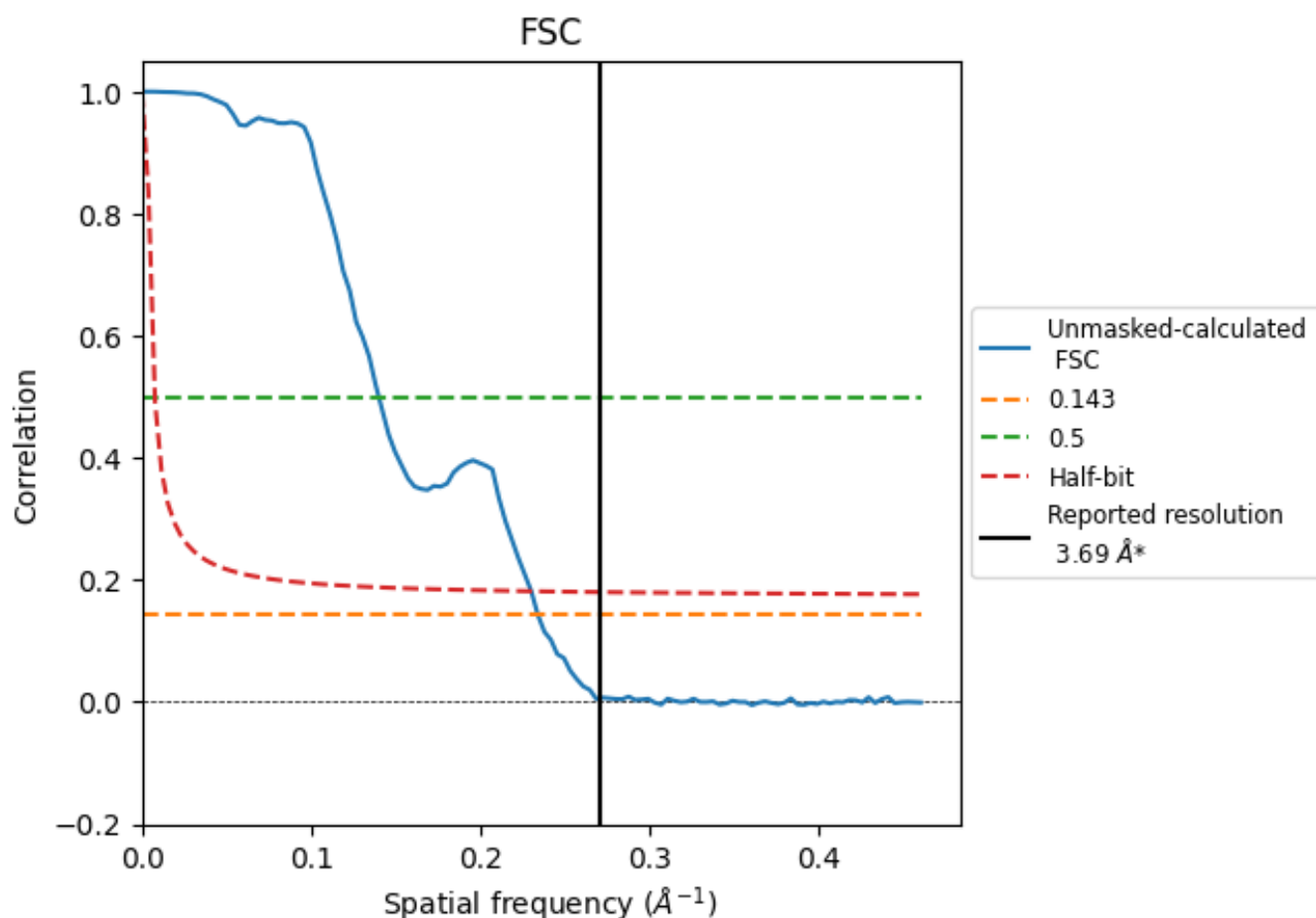


*Reported resolution corresponds to spatial frequency of 0.271 \AA^{-1}

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 0.271 \AA^{-1}

8.2 Resolution estimates [i](#)

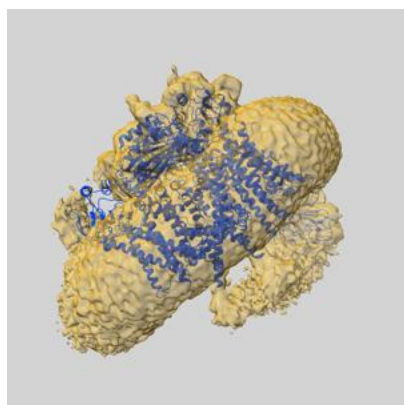
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.69	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.28	7.15	4.35

*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 4.28 differs from the reported value 3.69 by more than 10 %

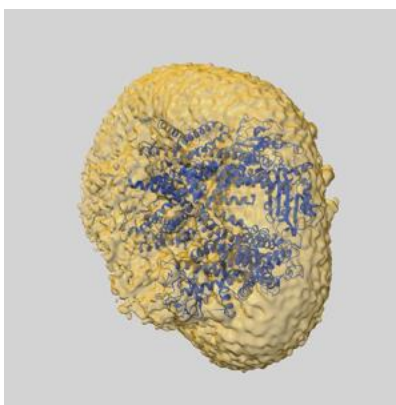
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62726 and PDB model 9L0W. Per-residue inclusion information can be found in section [3](#) on page [8](#).

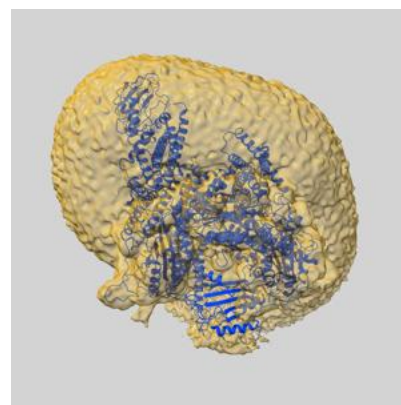
9.1 Map-model overlay [i](#)



X



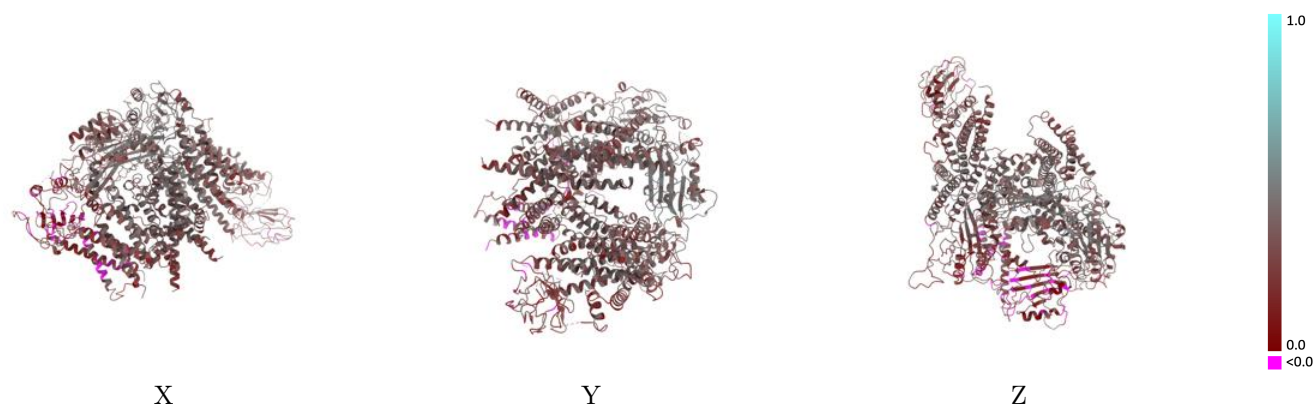
Y



Z

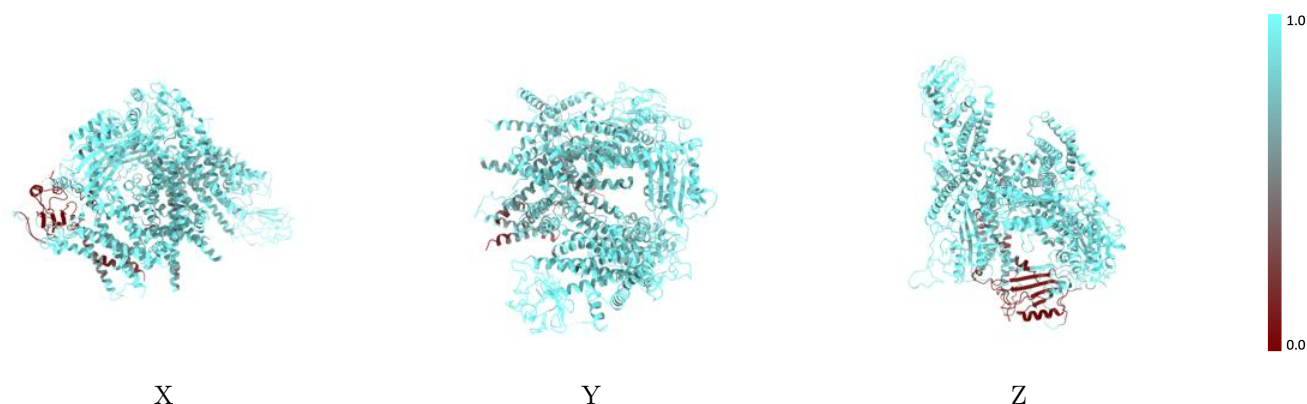
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



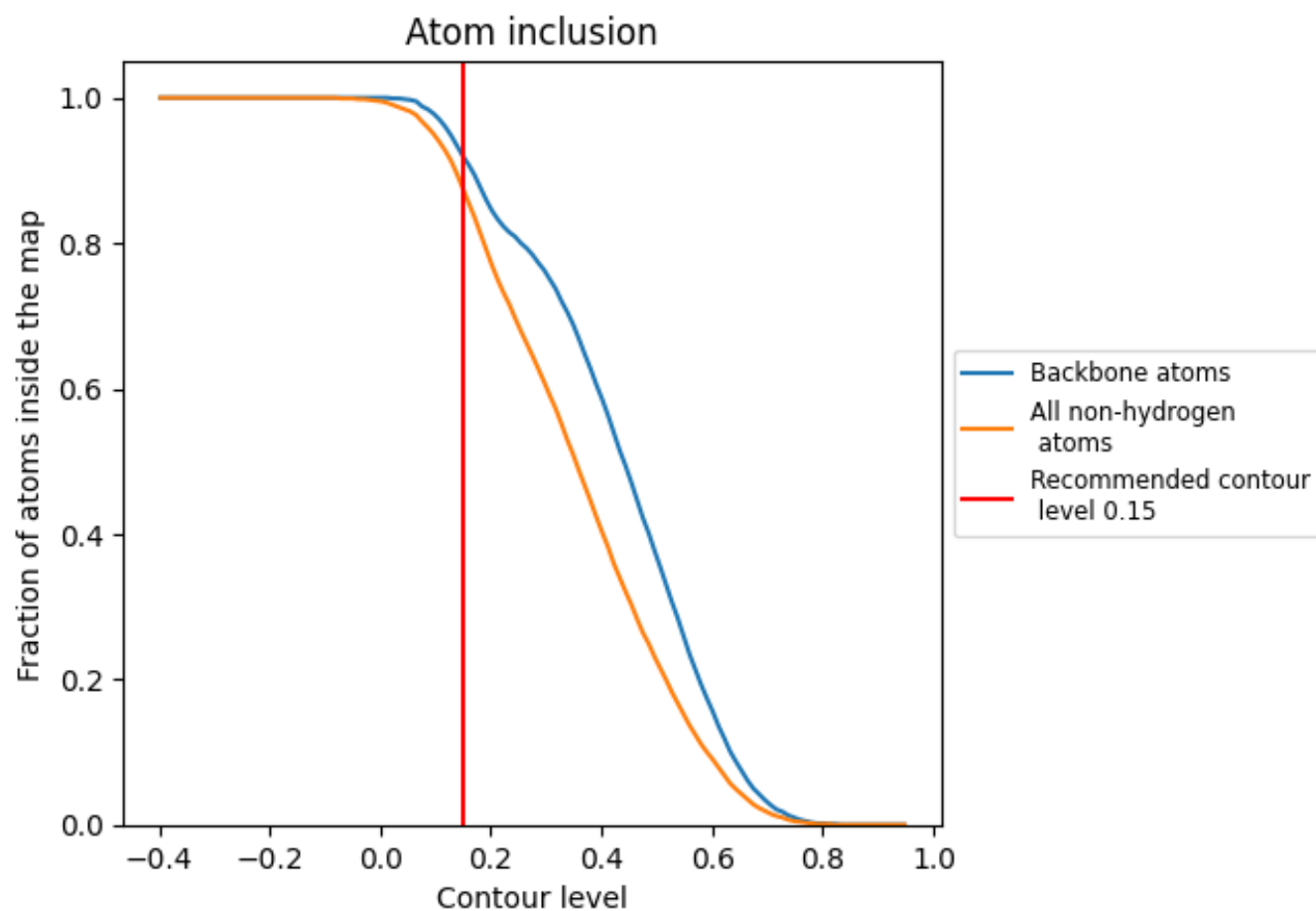
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 87% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8740	<div></div> 0.3230
A	<div></div> 0.9200	<div></div> 0.3020
B	<div></div> 0.9280	<div></div> 0.3820
C	<div></div> 0.9220	<div></div> 0.3640
D	<div></div> 0.6330	<div></div> 0.2170

