



Full wwPDB EM Validation Report ⓘ

May 27, 2026 – 12:15 PM JST

PDB ID : 22BE / pdb_000022be
EMDB ID : EMD-68147
Title : XEN1101 bound KCNQ2/3 heteromer with 3:1 stoichiometry, state 1
Authors : Lu, F.; Fan, X.; Huang, J.
Deposited on : 2026-01-05
Resolution : 2.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

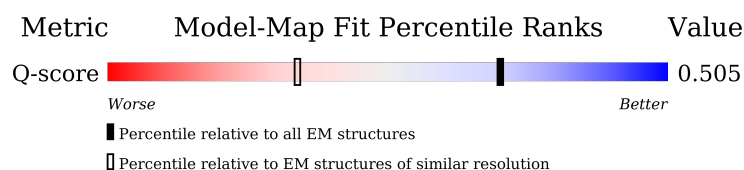
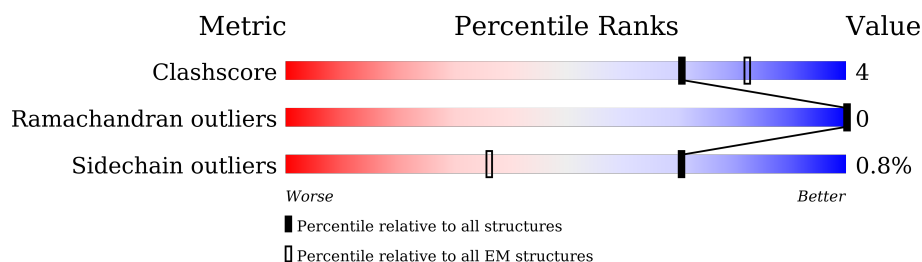
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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	8728 (2.10 - 3.10)

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	872	 25% 71%
2	B	872	 26% 72%
2	C	872	 26% 72%
2	D	872	 25% 71%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8191 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 Potassium voltage-gated channel subfamily KQT member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	251	Total	C	N	O	S	0	0
			2021	1341	337	333	10		

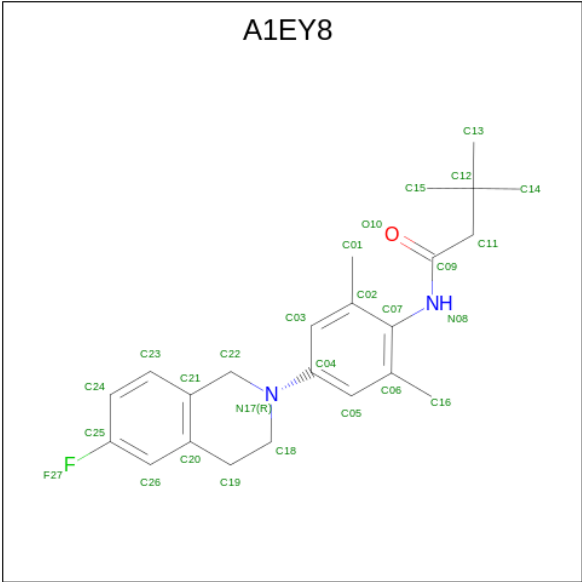
- Molecule 2 is a protein called Potassium voltage-gated channel subfamily KQT member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	248	Total	C	N	O	S	0	0
			2016	1339	339	329	9		
2	C	248	Total	C	N	O	S	0	0
			2016	1339	339	329	9		
2	D	249	Total	C	N	O	S	0	0
			2027	1345	343	330	9		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	K	0
			2	2	
3	D	1	Total	K	0
			1	1	

- Molecule 4 is Azetukalner (CCD ID: A1EY8) (formula: C₂₃H₂₉FN₂O) (labeled as "Ligand of Interest" by depositor).

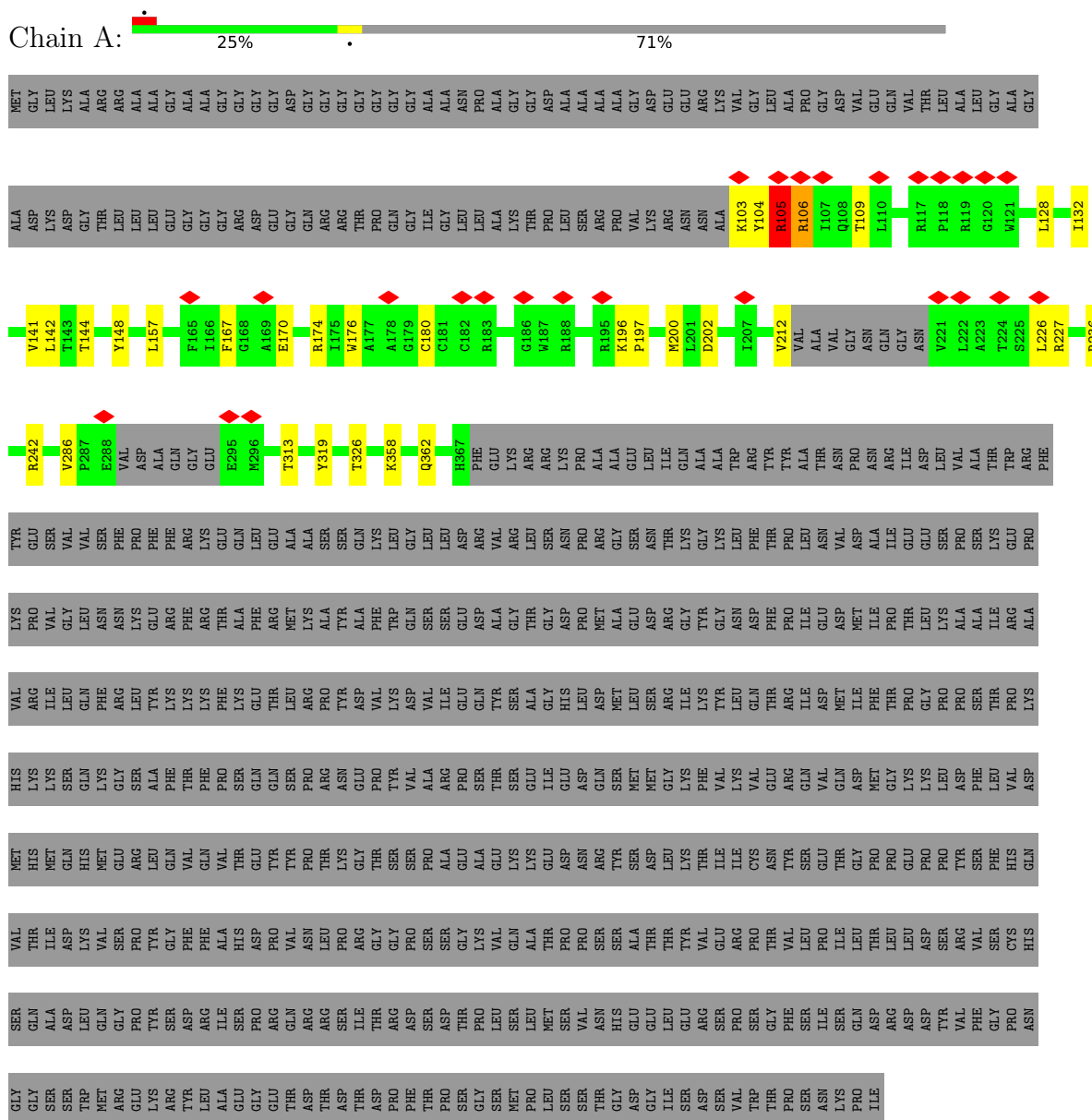


Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	F	N	O	0
			27	23	1	2	1	
4	C	1	Total	C	F	N	O	0
			27	23	1	2	1	
4	D	1	Total	C	F	N	O	0
			27	23	1	2	1	
4	D	1	Total	C	F	N	O	0
			27	23	1	2	1	

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: Potassium voltage-gated channel subfamily KQT member 3



- Molecule 2: Potassium voltage-gated channel subfamily KQT member 2



GLU	GLY	PRO	PHE	GLY	ASP	VAL	TRP	ALA	SER	GLN	GLY	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
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• Molecule 2: Potassium voltage-gated channel subfamily KQT member 2



MET	VAL	GLN	LYS	SER	ARG	ASN	GLY	VAL	THR	PRO	PRO	GLY	SER	GLY	LEU	LYS	LYS	LEU	LYS	VAL	PHE	VAL	GLY	LEU	ASP	PRO	GLY	ALA	PRO	PRO	ASP	SER	THR	ARG	ASP	GLY	GLY	ALA	LEU	LEU	ILE	ALA	GLY	SER	GLU	ALA	PRO	PRO	LYS	ARG	GLY	SER	ILE	LEU	SER	SER	LYS	PRO	ARG	GLY																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
GLY	ALA	GLY	ALA	GLY	LYS	PRO	PRO	ARG	NT1	E86	R87	P88	R89	A97	L101	L109	T114	L126	Y141	R144	I145	R153	K162	V175	A184	ALA	GLY	SER	GLN	GLY	ASN	VAL	PHE	ALA	THR	S195	A196	L197	R198	R201	R207	R210																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
R213	N258	D259	H260	L272	D282	Q286	H328	PHE	GLU	LYS	ARG	ASN	PRO	ALA	ALA	GLY	ILE	GLN	SER	ALA	TRP	ALA	PHE	ARG	LYS	THR	ALA	ASP	THR	ASN	LEU	ARG	THR	ASP	THR	GLY	SER	HIS	THR	VAL	THR	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL

[illegible]

- Molecule 2: Potassium voltage-gated channel subfamily KQT member 2



PRO	THR	GLU	GLY	THR	GLU	PRO	GLU	SER	THR	PHE	GLY	THR	VAL	MET
THR	GLU	THR	ARG	GLY	GLU	ASP	ASP	PRO	ASP	THR	ALA	ALA	VAL	GLY
ALA	ALA	ALA	PRO	ALA	PRO	PRO	PRO	SER	HIS	A196	L197	L198	L199	L200
TRP	TRP	PHE	ILE	ILE	ILE	VAL	VAL	SER	THR	THR	THR	THR	THR	THR
GLN	GLY	GLY	THR	THR	THR	VAL	VAL	PRO	THR	R198	R199	R200	R201	R202
GLN	ALA	ALA	ASP	ASP	ASP	ASP	ASP	CYS	GLN	S196	S197	S198	S199	S200
SER	LYS	LYS	LYS	LYS	LYS	LYS	LYS	CYS	THR	L206	L207	L208	L209	L210
SER	LYS	GLU	ASP	ASP	ASP	ASP	ASP	GLY	THR	R206	R207	R208	R209	R210
HIS	GLY	ALA	THR	THR	THR	THR	THR	PRO	VAL	F206	F207	F208	F209	F210
GLY	GLY	PRO	ALA	ALA	ALA	ALA	ALA	GLY	VAL	M206	M207	M208	M209	M210
THR	THR	THR	GLU	GLU	GLU	GLU	GLU	PRO	THR	R216	R217	R218	R219	R220
SER	SER	SER	ALA	ALA	ALA	ALA	ALA	GLY	MET	Y216	Y217	Y218	Y219	Y220
VAL	VAL	PRO	LEU	LEU	LEU	LEU	LEU	SER	SER	E216	E217	E218	E219	E220
VAL	VAL	GLY	PRO	PRO	PRO	PRO	PRO	GLN	SER	K216	K217	K218	K219	K220
GLY	GLY	ASP	GLU	GLU	GLU	GLU	GLU	ALA	GLN	D216	D217	D218	D219	D220
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	SER	SER	G216	G217	G218	G219	G220
HIS	HIS	HIS	ASP	ASP	ASP	ASP	ASP	GLY	THR	H216	H217	H218	H219	H220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VAL	THR	I216	I217	I218	I219	I220
THR	THR	THR	THR	THR	THR	THR	THR	PRO	VAL	J216	J217	J218	J219	J220
THR	THR	THR	THR	THR	THR	THR	THR	GLY	ALA	L216	L217	L218	L219	L220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ASP	ALA	M216	M217	M218	M219	M220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	N216	N217	N218	N219	N220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	O216	O217	O218	O219	O220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	P216	P217	P218	P219	P220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	Q216	Q217	Q218	Q219	Q220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	R216	R217	R218	R219	R220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	S216	S217	S218	S219	S220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	T216	T217	T218	T219	T220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	U216	U217	U218	U219	U220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	V216	V217	V218	V219	V220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	W216	W217	W218	W219	W220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	X216	X217	X218	X219	X220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	Y216	Y217	Y218	Y219	Y220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	Z216	Z217	Z218	Z219	Z220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	AA216	AA217	AA218	AA219	AA220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	BB216	BB217	BB218	BB219	BB220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	CC216	CC217	CC218	CC219	CC220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	DD216	DD217	DD218	DD219	DD220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	EE216	EE217	EE218	EE219	EE220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	FF216	FF217	FF218	FF219	FF220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GG216	GG217	GG218	GG219	GG220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	HH216	HH217	HH218	HH219	HH220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	II216	II217	II218	II219	II220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	JJ216	JJ217	JJ218	JJ219	JJ220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	KK216	KK217	KK218	KK219	KK220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LL216	LL217	LL218	LL219	LL220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	MM216	MM217	MM218	MM219	MM220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	NN216	NN217	NN218	NN219	NN220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	OO216	OO217	OO218	OO219	OO220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	PP216	PP217	PP218	PP219	PP220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	QQ216	QQ217	QQ218	QQ219	QQ220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	RR216	RR217	RR218	RR219	RR220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	SS216	SS217	SS218	SS219	SS220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	TT216	TT217	TT218	TT219	TT220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	UU216	UU217	UU218	UU219	UU220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VV216	VV217	VV218	VV219	VV220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	WW216	WW217	WW218	WW219	WW220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	XX216	XX217	XX218	XX219	XX220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	YY216	YY217	YY218	YY219	YY220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ZZ216	ZZ217	ZZ218	ZZ219	ZZ220
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	AA221	AA222	AA223	AA224	AA225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	BB221	BB222	BB223	BB224	BB225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	CC221	CC222	CC223	CC224	CC225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	DD221	DD222	DD223	DD224	DD225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	EE221	EE222	EE223	EE224	EE225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	FF221	FF222	FF223	FF224	FF225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GG221	GG222	GG223	GG224	GG225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	HH221	HH222	HH223	HH224	HH225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	II221	II222	II223	II224	II225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	JJ221	JJ222	JJ223	JJ224	JJ225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	KK221	KK222	KK223	KK224	KK225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LL221	LL222	LL223	LL224	LL225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	MM221	MM222	MM223	MM224	MM225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	NN221	NN222	NN223	NN224	NN225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	OO221	OO222	OO223	OO224	OO225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	PP221	PP222	PP223	PP224	PP225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	QQ221	QQ222	QQ223	QQ224	QQ225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	RR221	RR222	RR223	RR224	RR225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	SS221	SS222	SS223	SS224	SS225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	TT221	TT222	TT223	TT224	TT225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	UU221	UU222	UU223	UU224	UU225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	VV221	VV222	VV223	VV224	VV225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	WW221	WW222	WW223	WW224	WW225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	XX221	XX222	XX223	XX224	XX225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	YY221	YY222	YY223	YY224	YY225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ZZ221	ZZ222	ZZ223	ZZ224	ZZ225
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	AA226	AA227	AA228	AA229	AA230
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	BB226	BB227	BB228	BB229	BB230
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	CC226	CC227	CC228	CC229	CC230
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	DD226	DD227	DD228	DD229	DD230
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	EE226	EE227	EE228	EE229	EE230
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	FF226	FF227	FF228	FF229	FF230
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GG226	GG227	GG228	GG229	GG230
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	HH226	HH227	HH228	HH229	HH230
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	II226	II227	II228	II229	II230
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	JJ226	JJ227	JJ228	JJ229	JJ230
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	KK226	KK227	KK228	KK229	KK230
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	LL226	LL227	LL228	LL229	LL230
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	MM226	MM227	MM228	MM229	MM230
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	NN226	NN227	NN228	NN229	NN230
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	OO226	OO227	OO228	OO229	OO230
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	PP226	PP227	PP228	PP229	PP230
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	QQ226	QQ227	QQ228	QQ229	QQ230
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	RR226	RR227	RR228	RR229	RR230
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	SS226	SS227	SS228	SS229	SS230
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	TT226	TT227	TT228	TT229	TT230
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	UU226	UU227	UU228		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171895	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.201	Depositor
Minimum map value	-0.736	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	262.08, 262.08, 262.08	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93599993, 0.93599993, 0.93599993	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, A1EY8

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	0.20	0/2070	0.33	0/2801
2	B	0.14	0/2071	0.26	0/2805
2	C	0.12	0/2071	0.23	0/2805
2	D	0.11	0/2082	0.27	0/2819
All	All	0.15	0/8294	0.27	0/11230

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	2
2	C	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ARG	Sidechain
1	A	106	ARG	Sidechain
2	B	210	ARG	Sidechain
2	B	213	ARG	Sidechain
2	C	213	ARG	Sidechain

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	2021	0	2100	17	0
2	B	2016	0	2053	13	0
2	C	2016	0	2053	14	0
2	D	2027	0	2066	20	0
3	A	2	0	0	0	0
3	D	1	0	0	0	0
4	B	27	0	0	0	0
4	C	27	0	0	0	0
4	D	54	0	0	1	0
All	All	8191	0	8272	58	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 4.

All (58) 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:A:196:LYS:HD2	1:A:197:PRO:HD2	1.76	0.68
2:D:117:GLU:HG3	2:D:118:TYR:HD1	1.63	0.64
1:A:286:VAL:HG11	1:A:326:THR:HG21	1.84	0.60
2:D:117:GLU:HG3	2:D:118:TYR:CD1	2.37	0.60
1:A:142:LEU:HG	1:A:148:TYR:HD2	1.68	0.59
2:C:175:VAL:HG11	2:C:207:ARG:HE	1.71	0.56
2:D:96:HIS:HA	2:D:99:VAL:HG12	1.87	0.55
2:D:100:PHE:HE1	2:D:208:MET:HE3	1.72	0.55
1:A:109:THR:HG22	1:A:180:CYS:SG	2.47	0.55
2:D:325:ARG:HA	2:D:328:HIS:HD2	1.72	0.54
2:D:251:TYR:OH	2:D:255:LYS:NZ	2.39	0.54
2:D:299:LEU:HD12	4:D:903:A1EY8:C03	2.37	0.53
2:D:143:VAL:HA	2:D:146:TRP:HB3	1.91	0.53
2:D:206:LEU:HA	2:D:209:ILE:HD12	1.90	0.53
2:C:109:LEU:HB2	2:C:126:LEU:HD21	1.91	0.53
2:C:153:ARG:CZ	2:C:162:LYS:HE3	2.38	0.52
1:A:358:LYS:O	1:A:362:GLN:HG3	2.10	0.52
1:A:167:PHE:HE2	1:A:236:ARG:HD2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:207:ARG:HA	2:C:210:ARG:HD3	1.92	0.51
1:A:197:PRO:HA	1:A:200:MET:HE2	1.94	0.49
2:B:263:THR:HB	2:C:114:THR:HG22	1.95	0.49
1:A:313:THR:OG1	2:B:280:TYR:OH	2.23	0.48
2:D:133:THR:O	2:D:137:PHE:HB2	2.14	0.48
2:B:299:LEU:HD21	2:C:272:LEU:HD11	1.95	0.48
2:B:81:LEU:HD12	2:B:146:TRP:HZ3	1.78	0.48
2:C:260:HIS:NE2	2:C:282:ASP:O	2.46	0.48
2:C:126:LEU:HD13	2:C:201:ARG:NH1	2.28	0.47
2:D:137:PHE:CE2	2:D:207:ARG:HD3	2.49	0.47
2:C:153:ARG:NH2	2:C:162:LYS:HE3	2.30	0.47
2:B:82:TYR:CE1	2:B:86:GLU:HG3	2.50	0.46
2:D:137:PHE:HE2	2:D:207:ARG:HD3	1.81	0.46
2:C:97:ALA:O	2:C:101:LEU:HG	2.17	0.45
2:D:111:VAL:O	2:D:114:THR:HG22	2.16	0.45
2:D:254:GLU:HG2	2:D:258:ASN:HD22	1.82	0.44
1:A:141:VAL:HG22	2:D:264:TYR:CD2	2.52	0.44
2:B:89:ARG:H	2:B:92:ALA:HB3	1.82	0.44
2:B:162:LYS:HD3	2:B:162:LYS:HA	1.45	0.44
2:D:112:PHE:HD1	2:D:115:ILE:HD12	1.83	0.44
2:C:141:TYR:O	2:C:145:ILE:HG12	2.19	0.43
2:B:133:THR:O	2:B:137:PHE:HB2	2.19	0.43
2:B:86:GLU:C	2:B:87:ARG:HD2	2.44	0.43
1:A:144:THR:HG21	2:D:264:TYR:HB2	2.01	0.43
1:A:212:VAL:HG22	1:A:226:LEU:HD13	2.00	0.43
2:C:88:PRO:O	2:C:89:ARG:HG3	2.20	0.42
2:B:182:VAL:HG22	2:B:197:LEU:HB3	2.02	0.42
2:C:258:ASN:HD21	2:C:286:GLN:HG3	1.84	0.42
2:B:137:PHE:CE2	2:B:207:ARG:HG2	2.55	0.42
1:A:170:GLU:OE2	1:A:174:ARG:NH2	2.53	0.41
1:A:128:LEU:O	1:A:132:ILE:HG12	2.20	0.41
2:D:109:LEU:HD12	2:D:129:LEU:HD12	2.02	0.41
1:A:105:ARG:HA	1:A:105:ARG:HD2	1.69	0.41
2:D:324:HIS:O	2:D:327:LYS:HG3	2.20	0.41
1:A:202:ASP:CG	1:A:242:ARG:HH12	2.29	0.41
2:B:130:GLU:O	2:B:134:ILE:HG12	2.21	0.41
2:C:86:GLU:OE1	2:C:144:ARG:NH1	2.54	0.41
2:B:152:CYS:HA	2:B:155:ARG:HB2	2.03	0.41
1:A:157:LEU:HD12	1:A:227:ARG:HD2	2.03	0.40
1:A:319:TYR:OH	2:D:274:THR:OG1	2.27	0.40

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	245/872 (28%)	243 (99%)	2 (1%)	0	100	100
2	B	244/872 (28%)	244 (100%)	0	0	100	100
2	C	244/872 (28%)	243 (100%)	1 (0%)	0	100	100
2	D	245/872 (28%)	243 (99%)	2 (1%)	0	100	100
All	All	978/3488 (28%)	973 (100%)	5 (0%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/725 (29%)	204 (98%)	5 (2%)	43	70
2	B	207/728 (28%)	205 (99%)	2 (1%)	68	86
2	C	207/728 (28%)	207 (100%)	0	100	100
2	D	208/728 (29%)	208 (100%)	0	100	100
All	All	831/2909 (29%)	824 (99%)	7 (1%)	70	88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	LYS
1	A	104	TYR

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Mol	Chain	Res	Type
1	A	105	ARG
1	A	106	ARG
1	A	176	TRP
2	B	162	LYS
2	B	207	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	362	GLN
2	B	79	ASN
2	B	286	GLN
2	C	258	ASN
2	C	286	GLN
2	C	321	GLN
2	D	79	ASN
2	D	286	GLN
2	D	328	HIS

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 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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
4	A1EY8	C	901	-	29,29,29	0.26	0	43,43,43	0.51	1 (2%)
4	A1EY8	D	903	-	29,29,29	0.26	0	43,43,43	0.51	1 (2%)
4	A1EY8	D	902	-	29,29,29	0.26	0	43,43,43	0.50	1 (2%)
4	A1EY8	B	901	-	29,29,29	0.26	0	43,43,43	0.50	1 (2%)

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
4	A1EY8	C	901	-	-	0/13/22/22	0/3/3/3
4	A1EY8	D	903	-	-	0/13/22/22	0/3/3/3
4	A1EY8	D	902	-	-	0/13/22/22	0/3/3/3
4	A1EY8	B	901	-	-	0/13/22/22	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	903	A1EY8	C18-N17-C04	2.17	123.97	118.09
4	C	901	A1EY8	C18-N17-C04	2.16	123.92	118.09
4	B	901	A1EY8	C18-N17-C04	2.15	123.90	118.09
4	D	902	A1EY8	C18-N17-C04	2.14	123.86	118.09

There are no chirality outliers.

There are no torsion outliers.

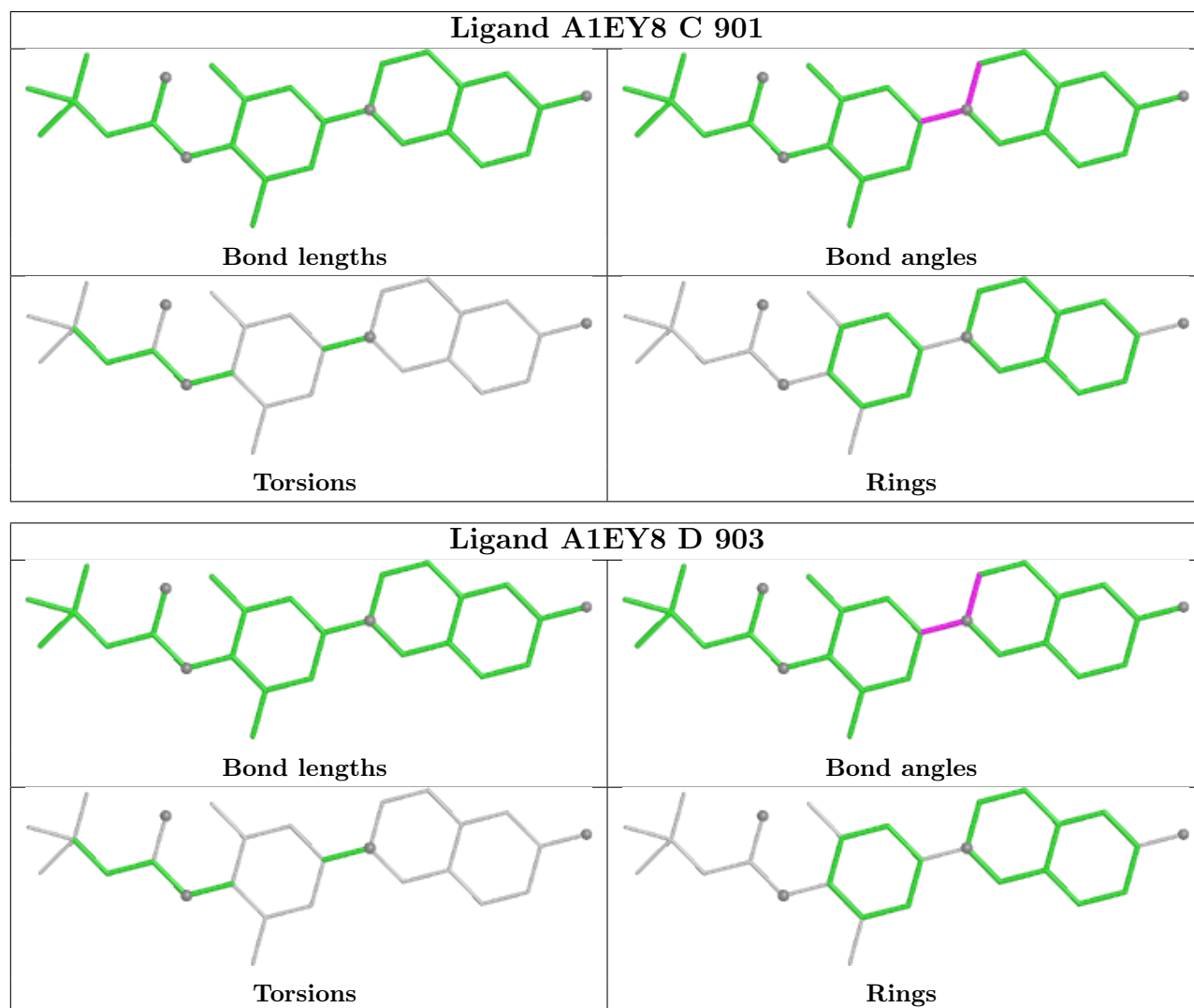
There are no ring outliers.

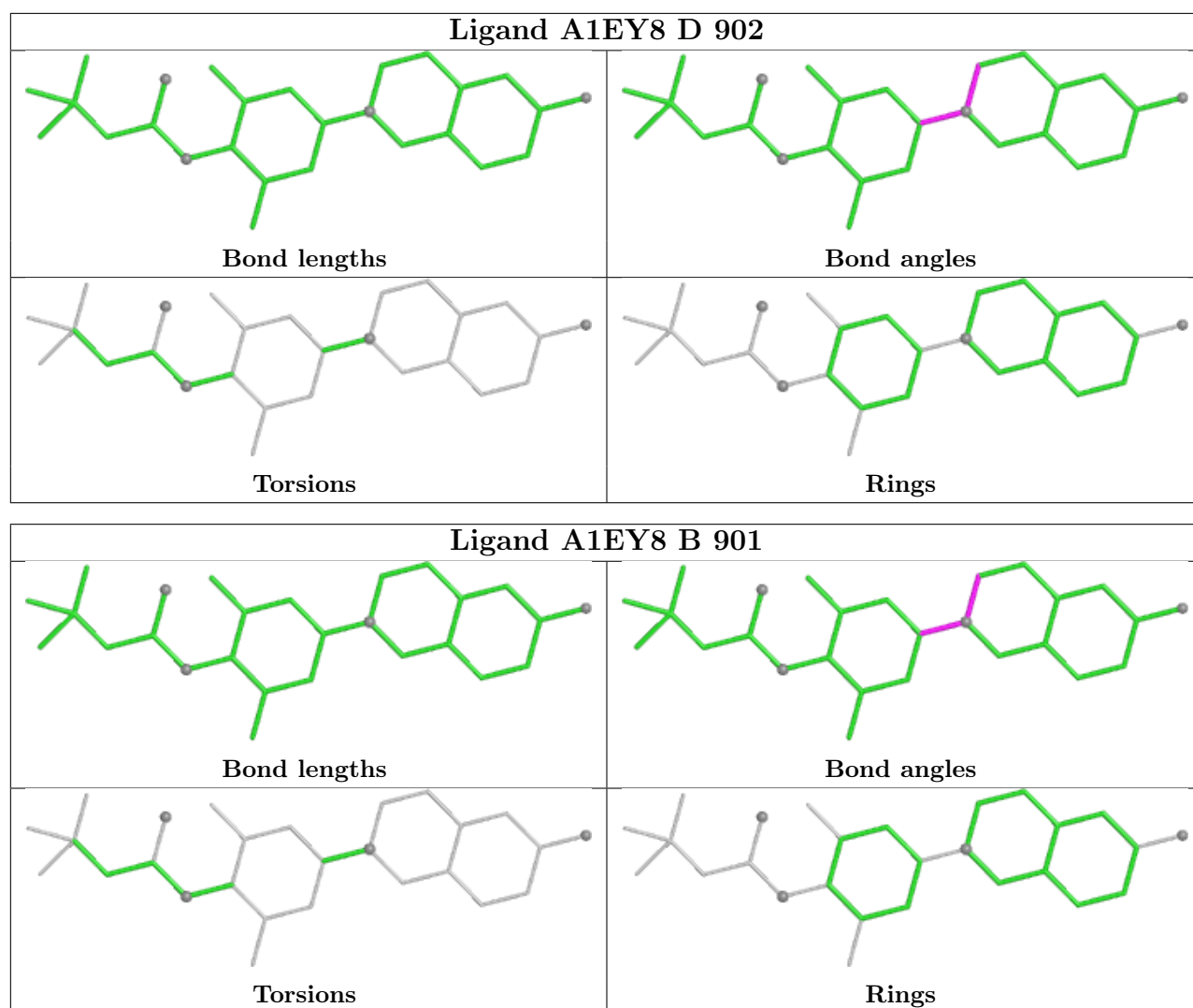
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	903	A1EY8	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.

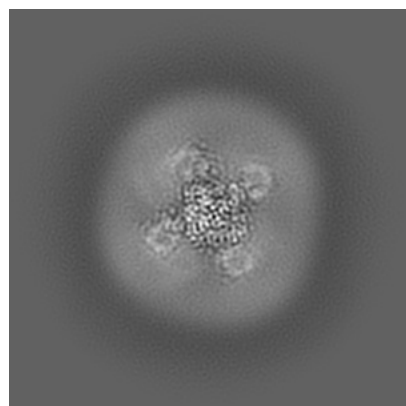
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-68147. These allow visual inspection of the internal detail of the map and identification of artifacts.

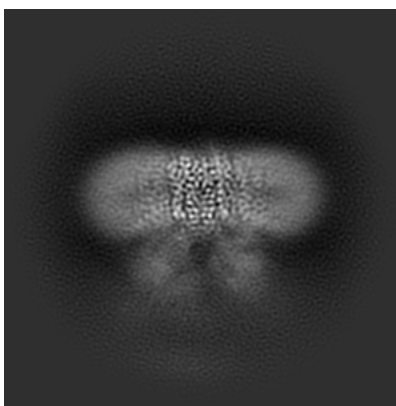
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

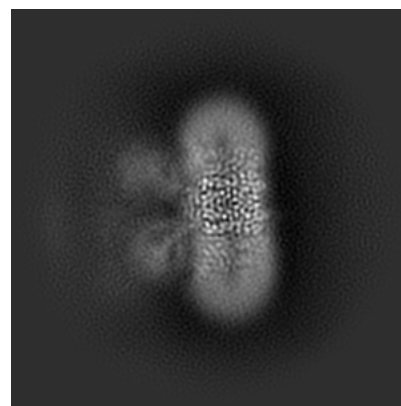
6.1.1 Primary map



X

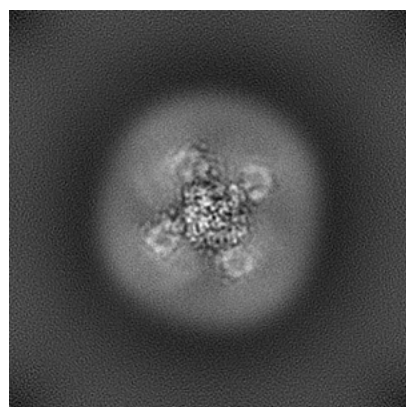


Y

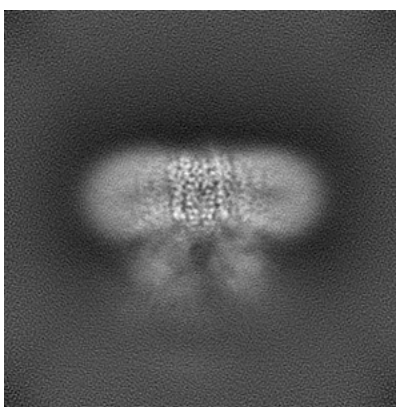


Z

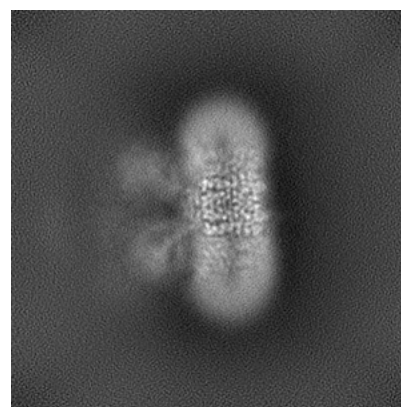
6.1.2 Raw map



X



Y

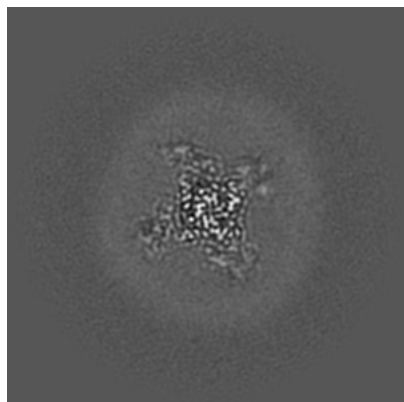


Z

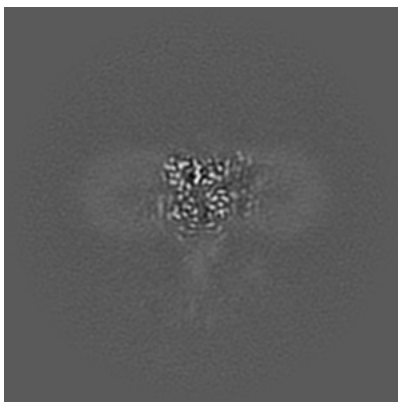
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

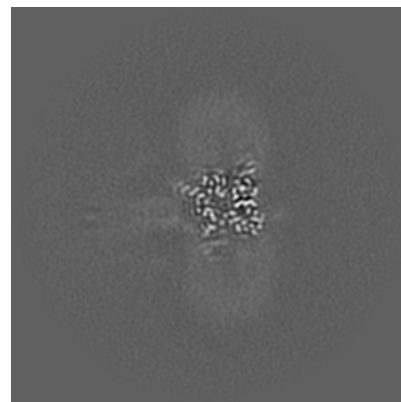
6.2.1 Primary map



X Index: 140

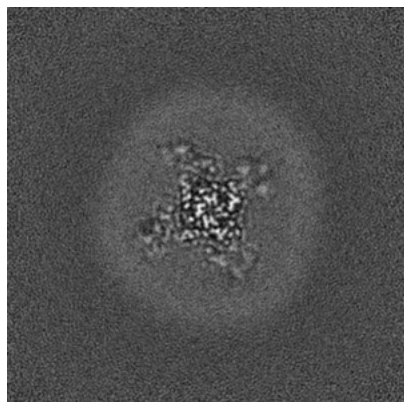


Y Index: 140

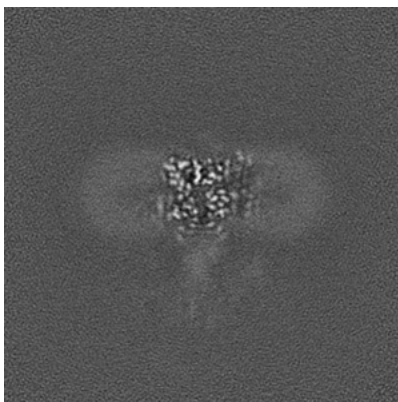


Z Index: 140

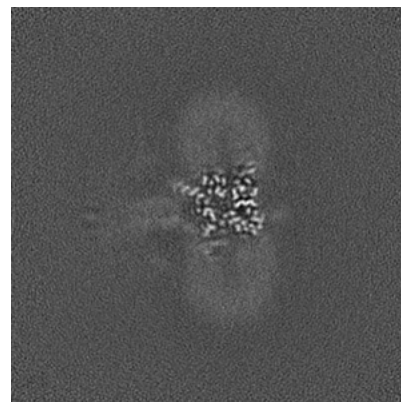
6.2.2 Raw map



X Index: 140



Y Index: 140

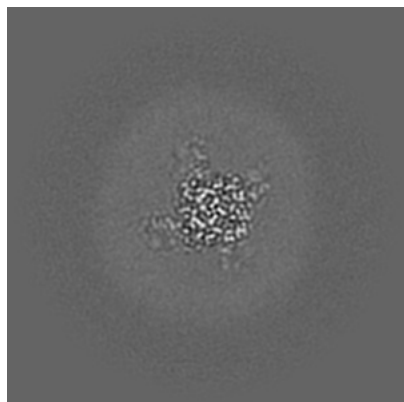


Z Index: 140

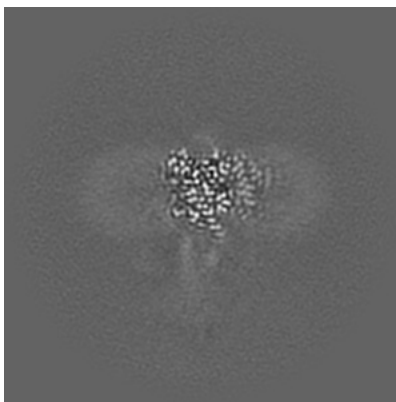
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

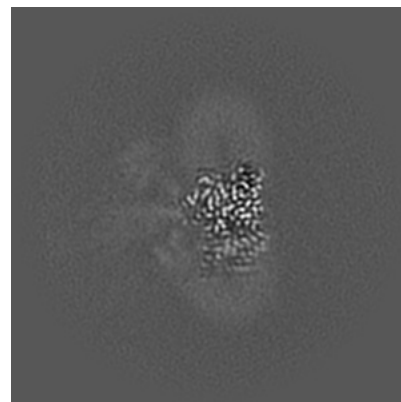
6.3.1 Primary map



X Index: 166

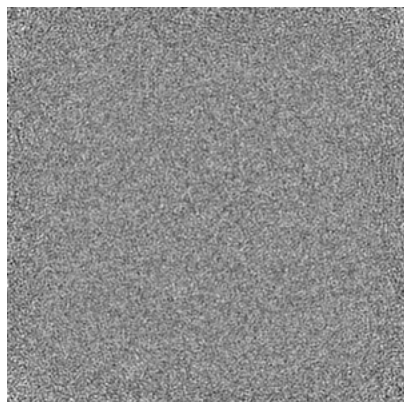


Y Index: 135

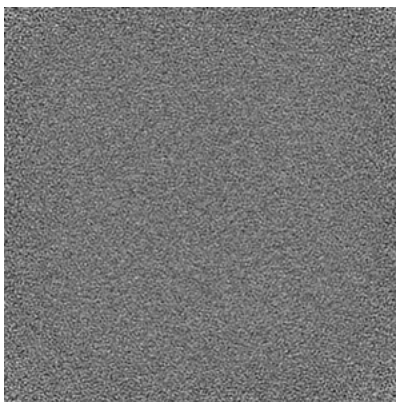


Z Index: 129

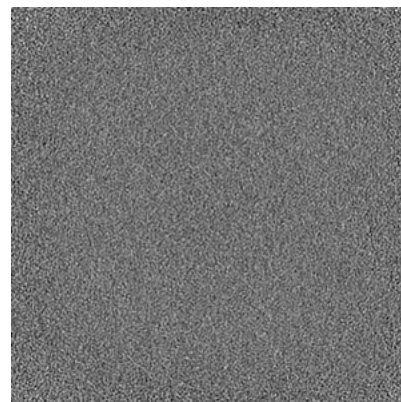
6.3.2 Raw map



X Index: 0



Y Index: 0

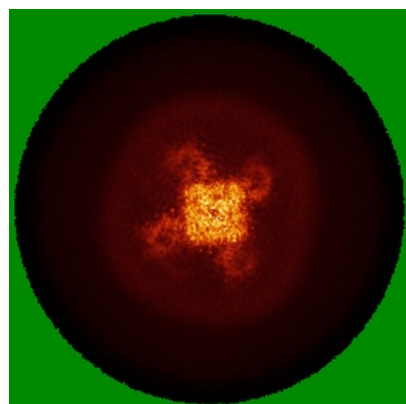


Z Index: 279

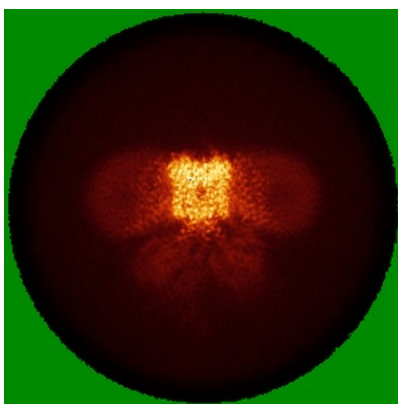
The images above show the largest variance slices of the map in three orthogonal directions.

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

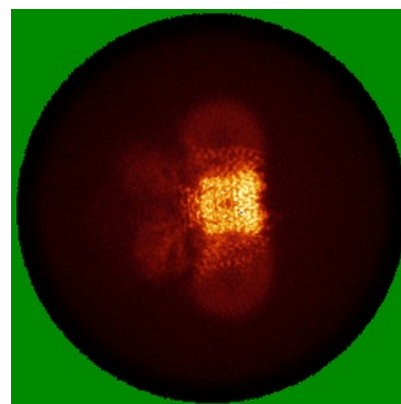
6.4.1 Primary map



X

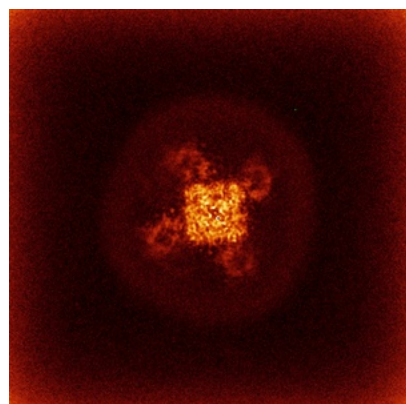


Y

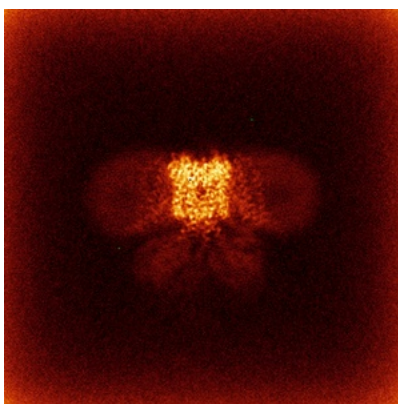


Z

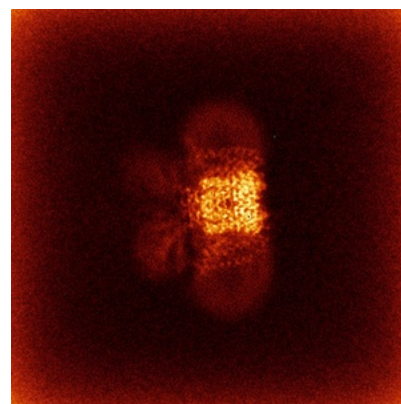
6.4.2 Raw map



X



Y

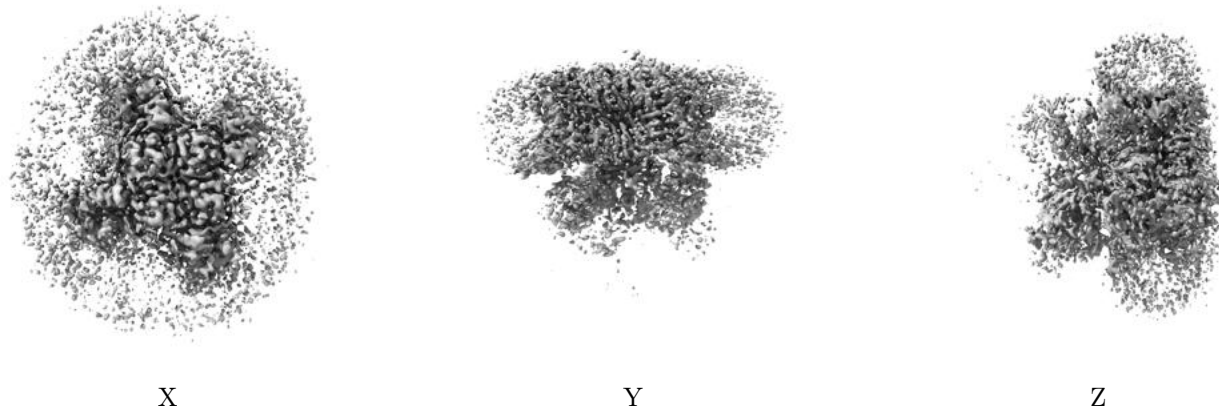


Z

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.

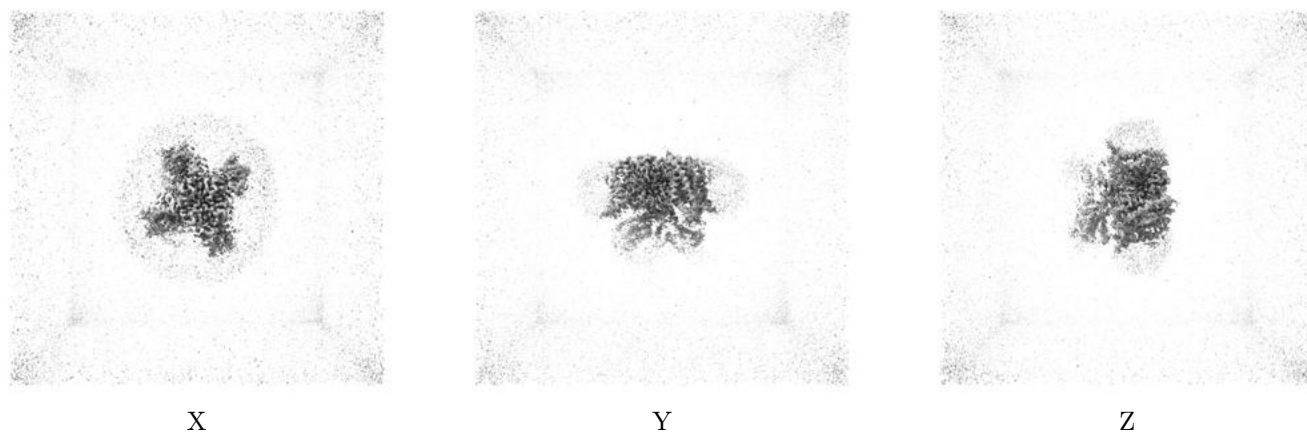
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

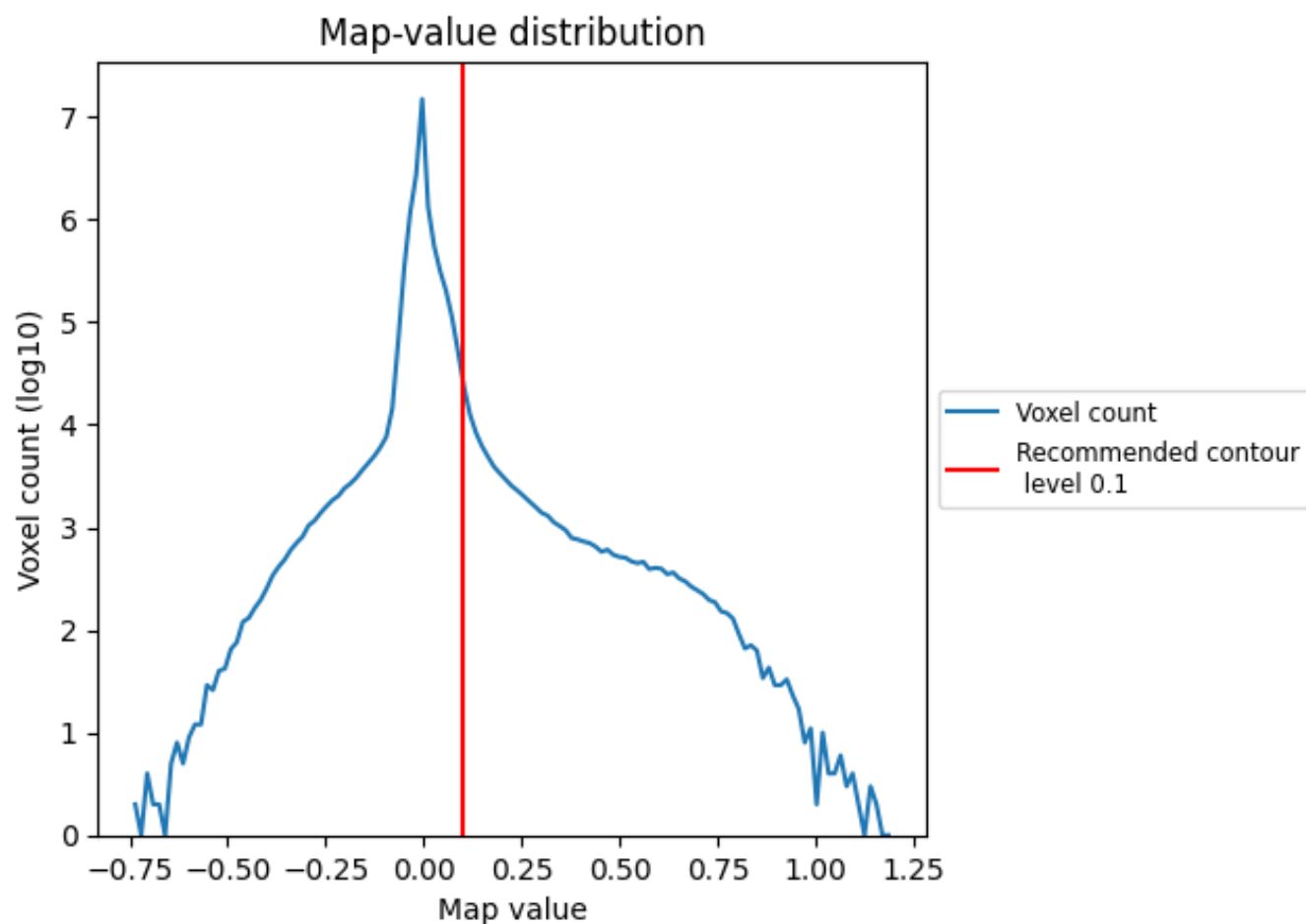
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

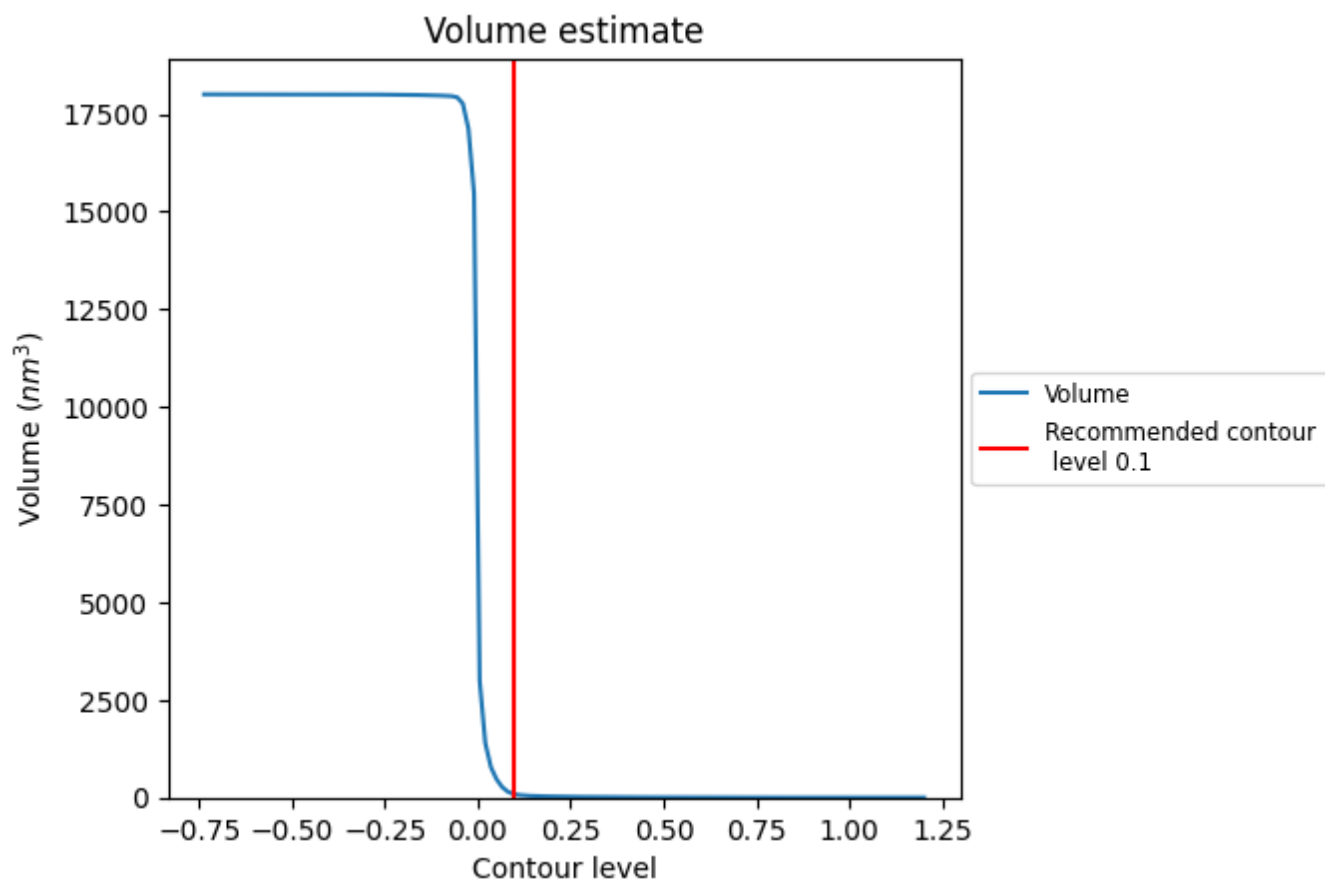
This section contains the results of statistical analysis of the map.

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.

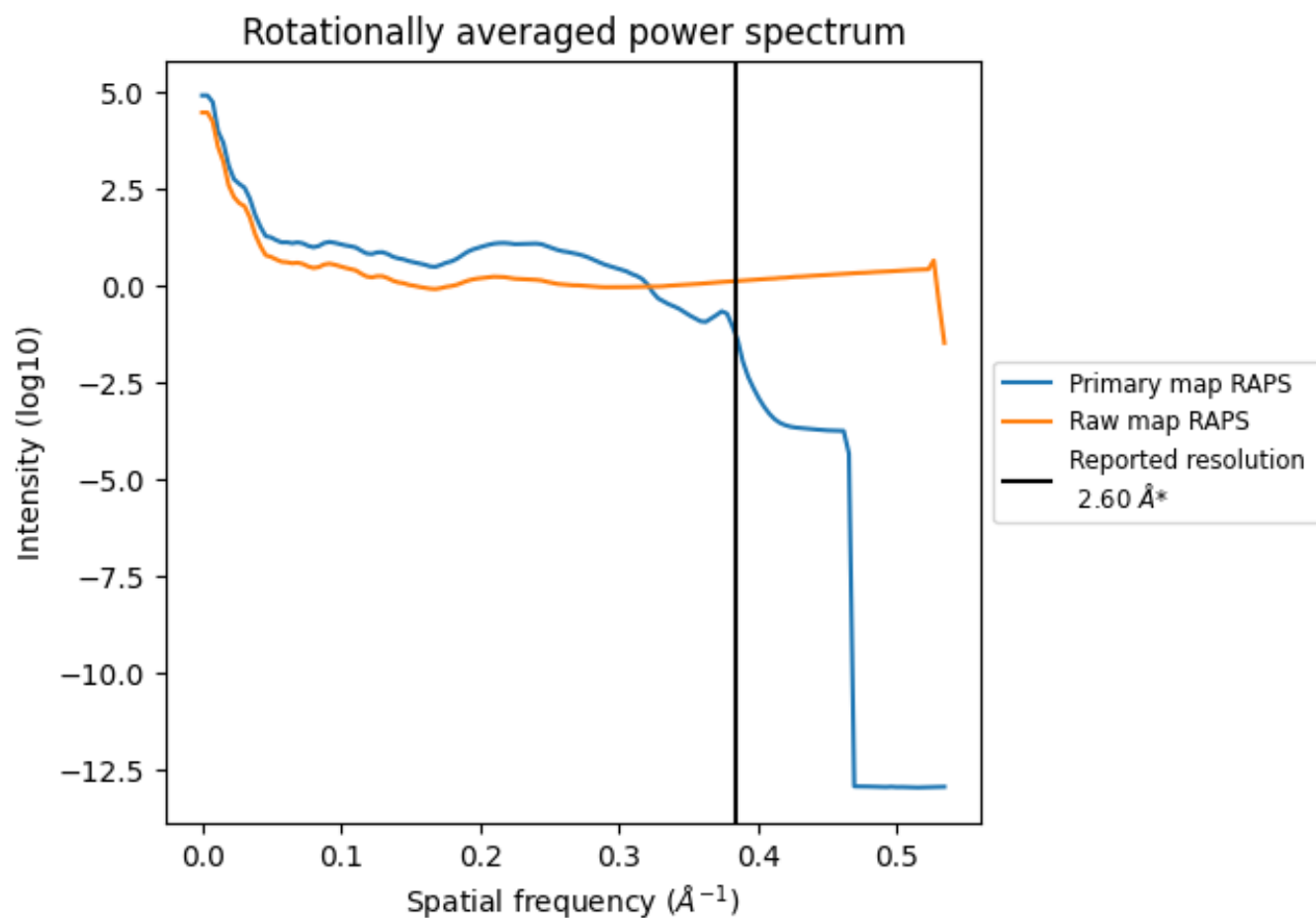
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 84 nm³; this corresponds to an approximate mass of 76 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 ⓘ

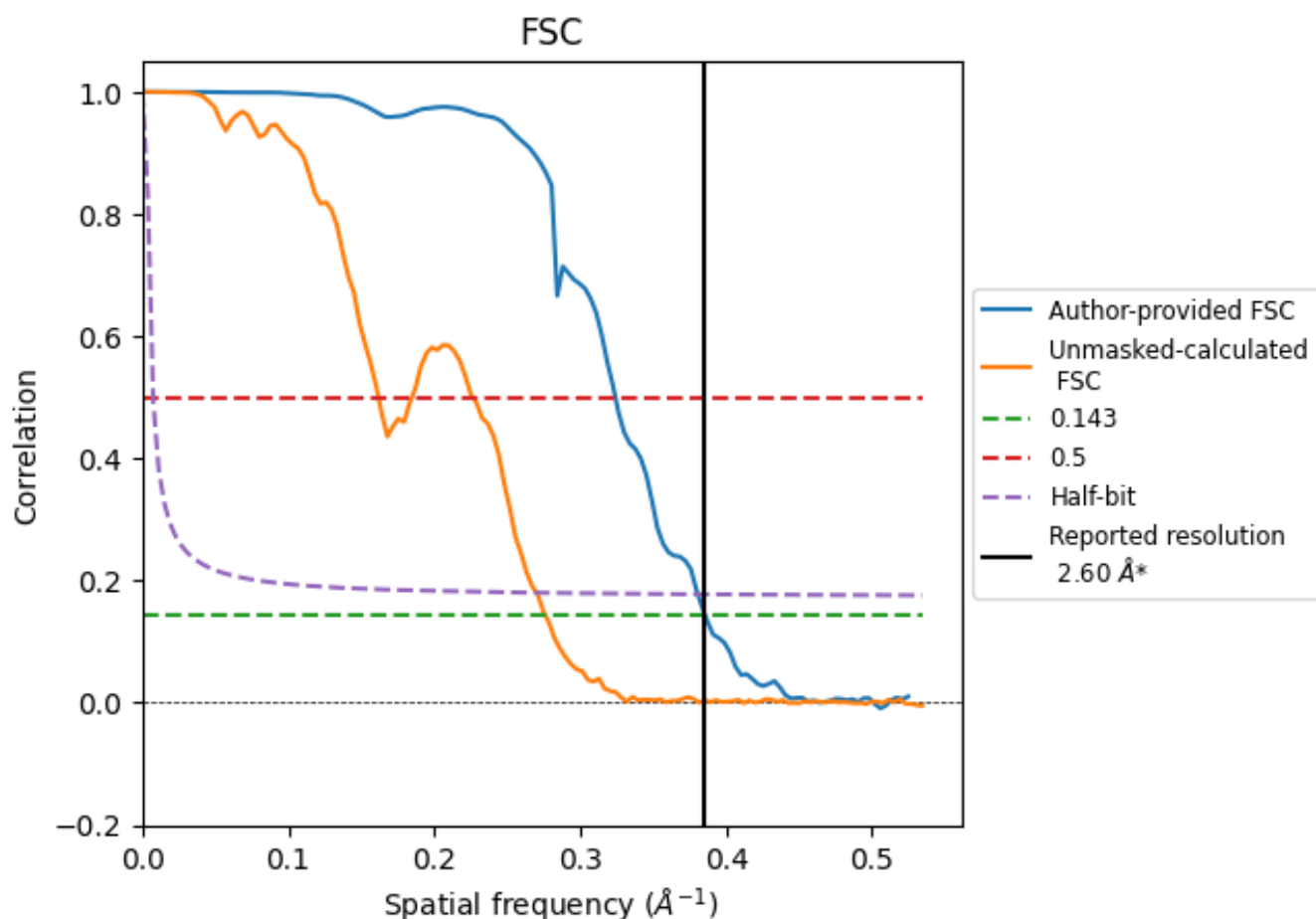


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 Å⁻¹

8.2 Resolution estimates [i](#)

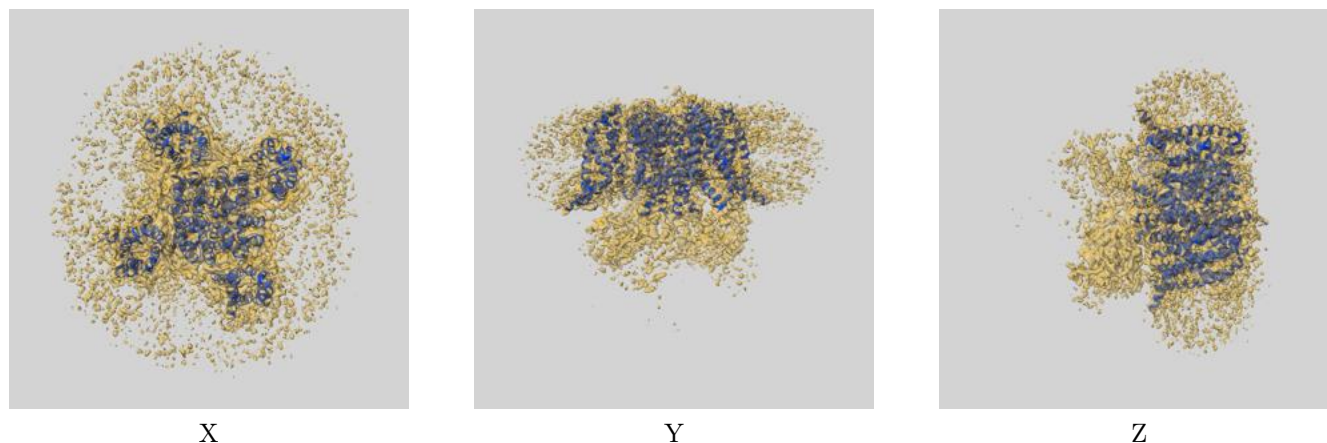
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.59	3.09	2.63
Unmasked-calculated*	3.62	6.18	3.70

*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 3.62 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

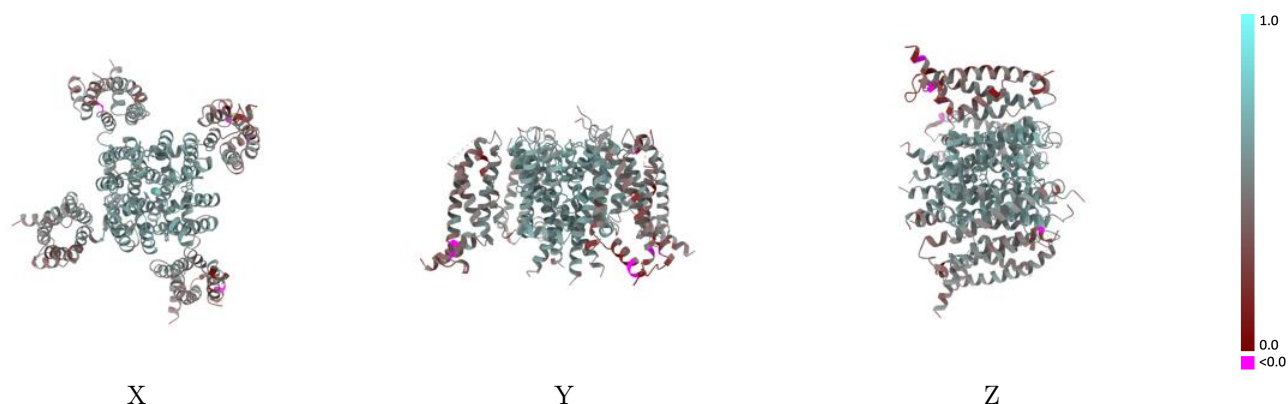
This section contains information regarding the fit between EMDB map EMD-68147 and PDB model 22BE. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



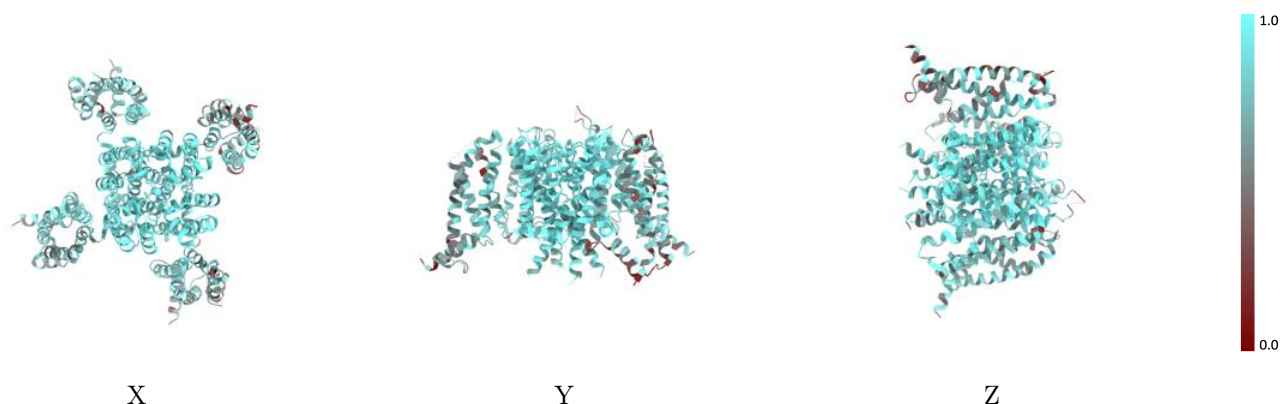
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



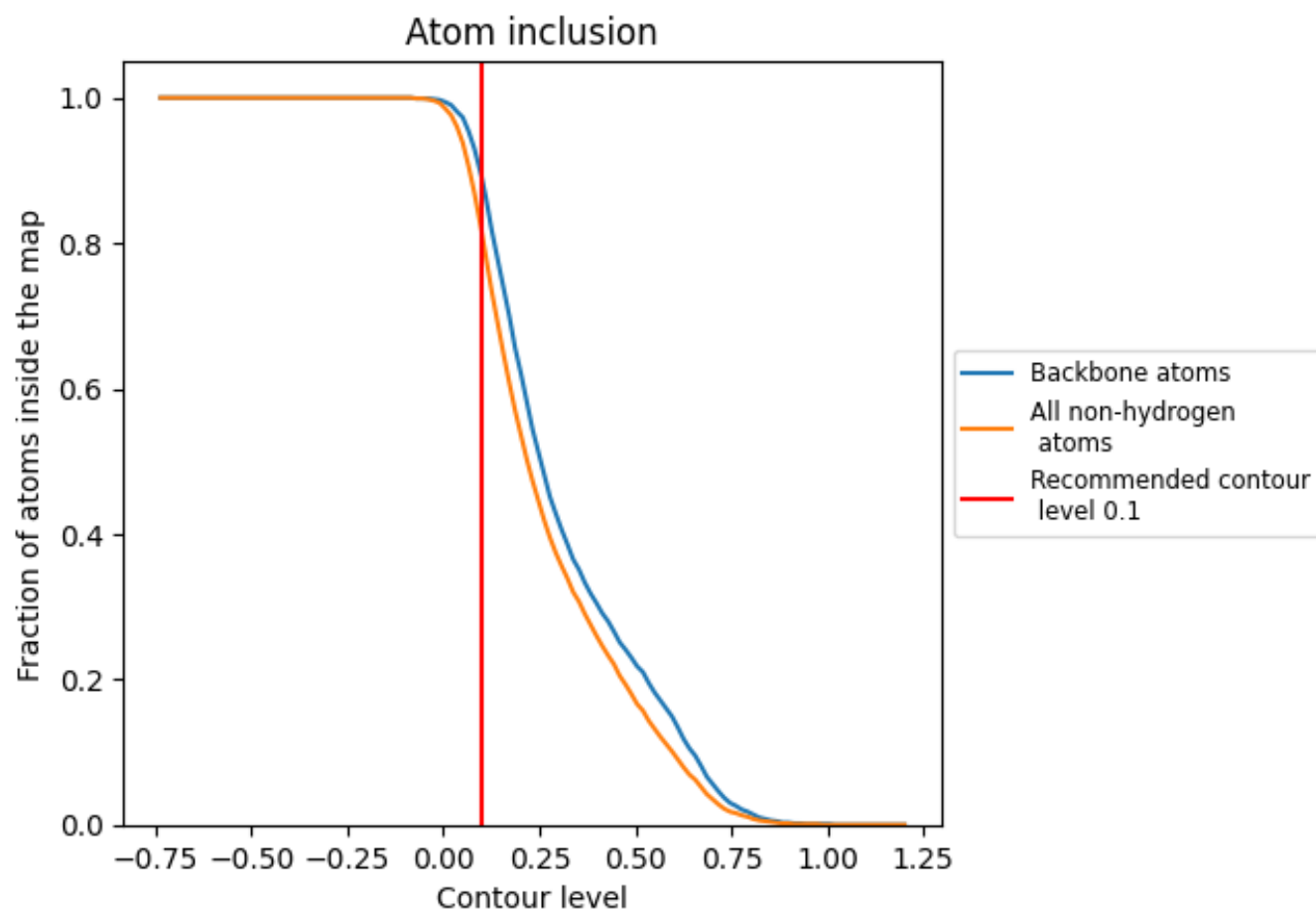
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 82% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8160	<div></div> 0.5050
A	<div></div> 0.7720	<div></div> 0.4680
B	<div></div> 0.8390	<div></div> 0.5250
C	<div></div> 0.8430	<div></div> 0.5250
D	<div></div> 0.8090	<div></div> 0.5040

