



Full wwPDB EM Validation Report ⓘ

Nov 2, 2024 – 06:41 pm GMT

PDB ID : 7Z1T
EMDB ID : EMD-14452
Title : Connexin43 gap junction channel structure in digitonin
Authors : Qi, C.; Korkhov, M.V.
Deposited on : 2022-02-25
Resolution : 2.26 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

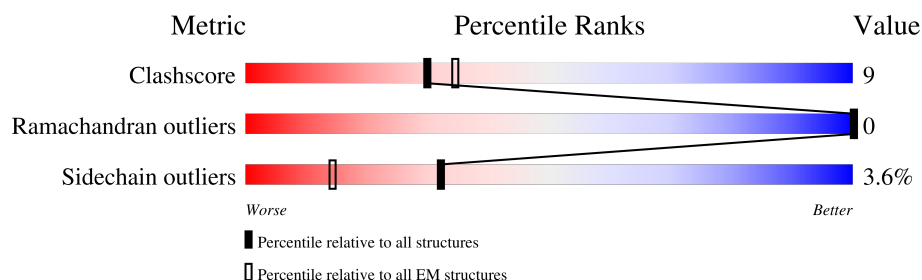
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.26 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	382	
1	B	382	
1	C	382	
1	D	382	
1	E	382	
1	F	382	
1	G	382	
1	H	382	

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Mol	Chain	Length	Quality of chain
1	I	382	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>37%12%51%</div></div>
1	J	382	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>37%12%51%</div></div>
1	K	382	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>36%13%51%</div></div>
1	L	382	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>37%12%51%</div></div>

2 Entry composition

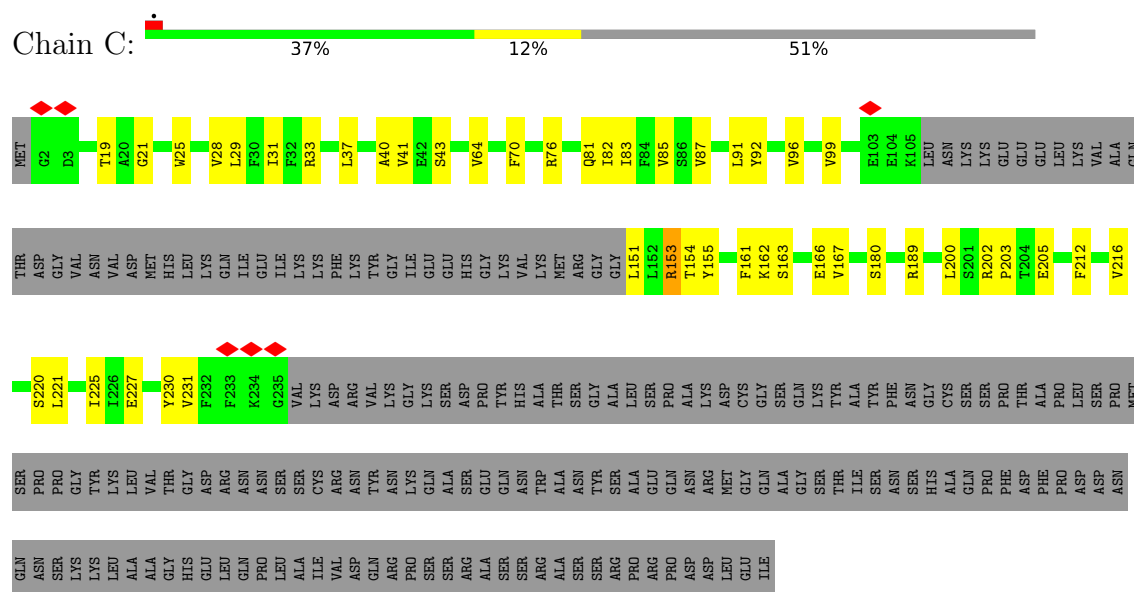
There is only 1 type of molecule in this entry. The entry contains 18492 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

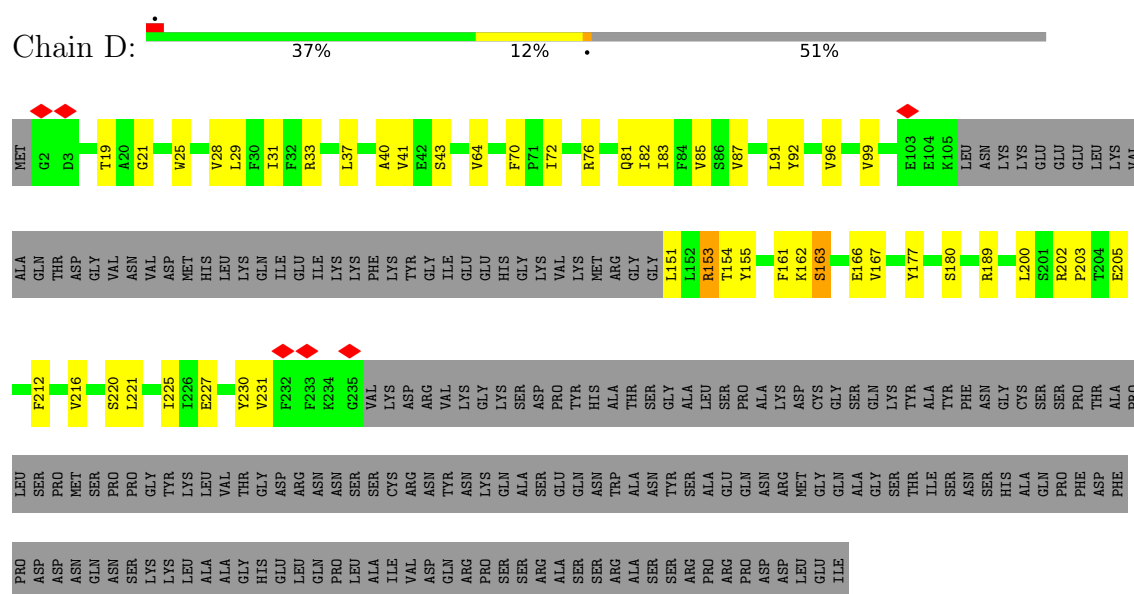
- Molecule 1 is a protein called Gap junction alpha-1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	189	Total	C	N	O	S	0	0
			1541	1033	241	259	8		
1	B	189	Total	C	N	O	S	0	0
			1541	1033	241	259	8		
1	C	189	Total	C	N	O	S	0	0
			1541	1033	241	259	8		
1	D	189	Total	C	N	O	S	0	0
			1541	1033	241	259	8		
1	E	189	Total	C	N	O	S	0	0
			1541	1033	241	259	8		
1	F	189	Total	C	N	O	S	0	0
			1541	1033	241	259	8		
1	G	189	Total	C	N	O	S	0	0
			1541	1033	241	259	8		
1	H	189	Total	C	N	O	S	0	0
			1541	1033	241	259	8		
1	I	189	Total	C	N	O	S	0	0
			1541	1033	241	259	8		
1	J	189	Total	C	N	O	S	0	0
			1541	1033	241	259	8		
1	K	189	Total	C	N	O	S	0	0
			1541	1033	241	259	8		
1	L	189	Total	C	N	O	S	0	0
			1541	1033	241	259	8		

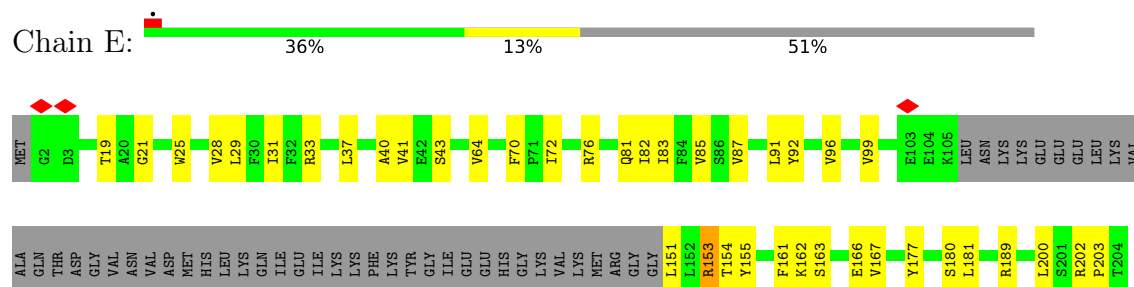
- Molecule 1: Gap junction alpha-1 protein

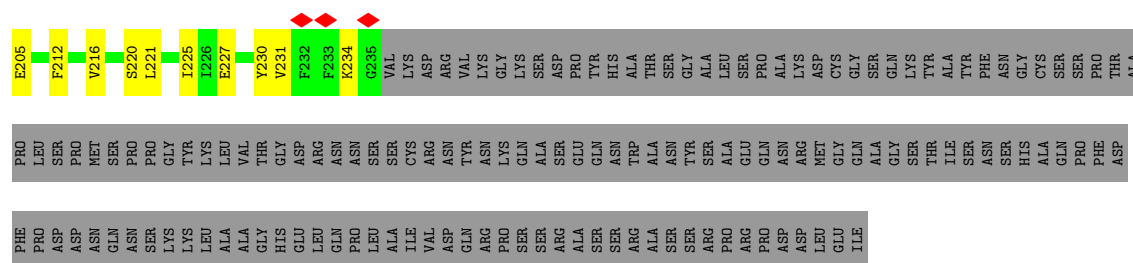


- Molecule 1: Gap junction alpha-1 protein

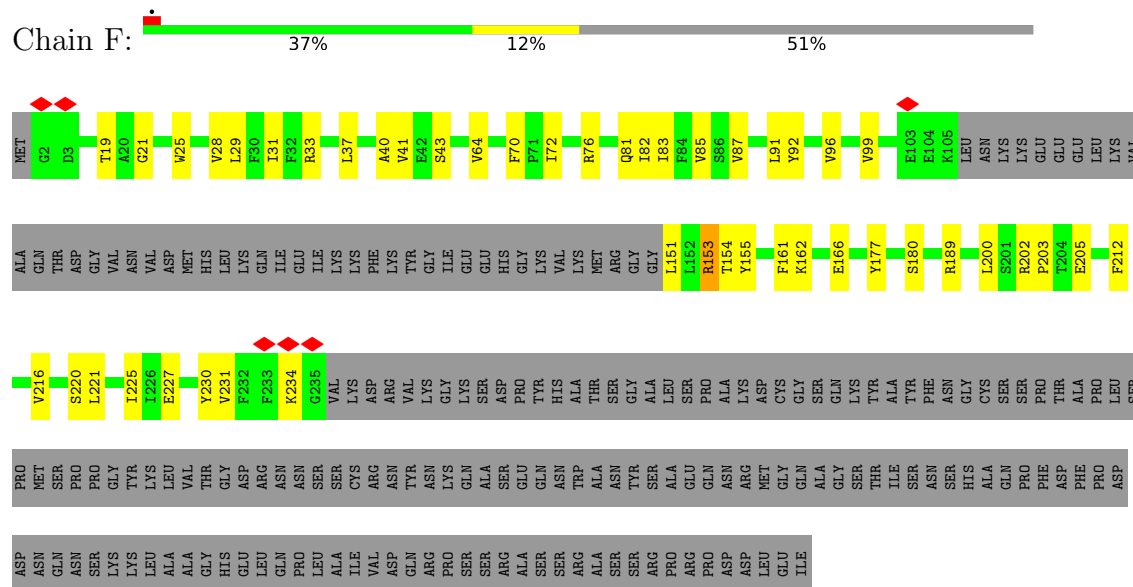


- Molecule 1: Gap junction alpha-1 protein

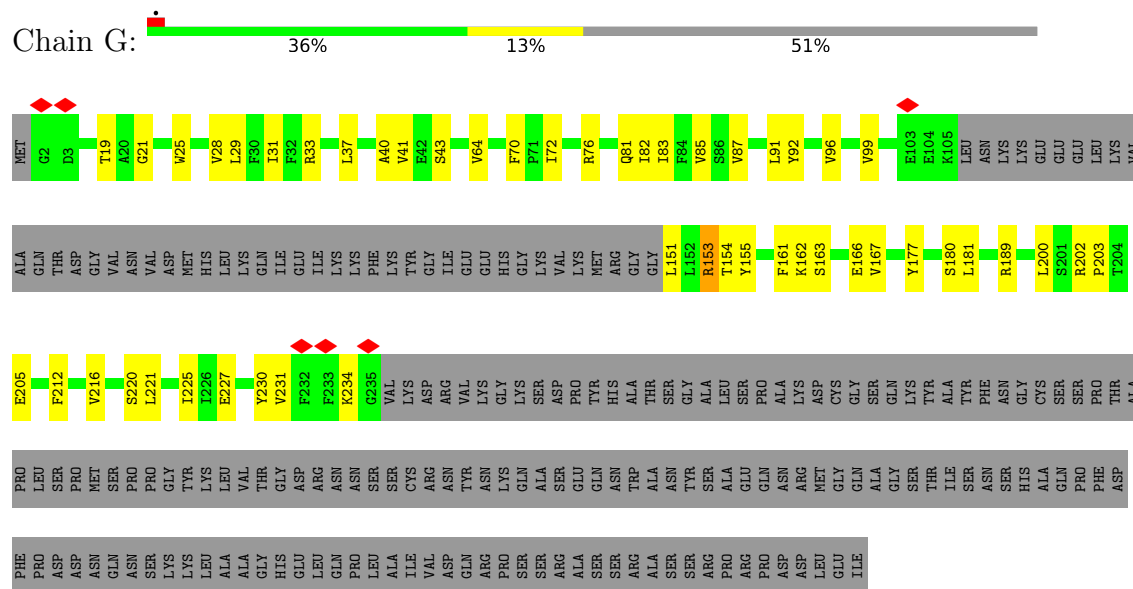




• Molecule 1: Gap junction alpha-1 protein



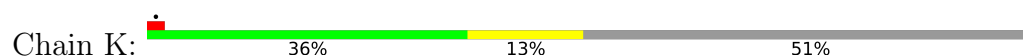
• Molecule 1: Gap junction alpha-1 protein



• Molecule 1: Gap junction alpha-1 protein

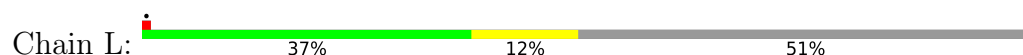
LEU	SER	PRO	ASP	ASP	ASP	GLN	SER	PRO	PRO	GLY	TYR	LEU	LEU	VAL	THR	GLY	ASP	ARG	ASN	ASN	SER	SER	SER	CYS	ILE	VAL	ARG	ASN	TYR	ARG	PRO	LYS	GLN	SER	ALA	ALA	ALA	ASN	TYR	SER	ALA	ALA	GLY	GLN	ASN	GLN	ASP	ASP	ASP	ASP	LEU	GLY	ILE
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• Molecule 1: Gap junction alpha-1 protein



PHE	PRO	PRO	ASP	ASP	ASN	GLN	ASN	SER	PRO	PRO	GLY	LYS	LEU	ALA	ALA	GLY	HIS	GLU	GLU	ASN	GLN	PRO	LEU	ALA	ALA	ILE	VAL	ASP	ASN	GLN	ARG	PRO	SER	SER	ALA	ARG	ALA	GLU	GLN	TYR	ASN	THR	ARG	ALA	SER	SER	ASP	PRO	ARG	ARG	PRO	PRO	ASP	ASP	LEU	GLU	ILE																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
PRO	LEU	SER	PRO	MET	SER	PRO	PRO	GLY	TYR	LYS	LEU	VAL	VAL	THR	THR	GLY	HIS	ASP	ARG	ASN	ASN	SER	VAL	LYS	GLY	LYS	LYS	GLY	ASP	VAL	ASN	GLN	ASN	THR	GLN	ALA	THR	SER	ALA	ALA	GLY	THR	ALA	GLY	GLN	ALA	SER	GLN	GLY	GLY	GLN	ALA	SER	GLN	THR	ILE	ASN	SER	HIS	ALA	GLN	PRO	PHE	ASP																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
E205	F212	V216	S220	L221	L225	I226	E227	Y230	V231	F232	F233	K234	G235	VAL	LYS	ASP	ARG	VAL	LYS	GLY	LYS	PRO	TYR	HIS	ALA	THR	SER	GLY	GLY	ALA	ALA	ALA	THR	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA

• Molecule 1: Gap junction alpha-1 protein



ASP	ASN	GLN	ASN	SER	LYS	LYS	LEU	ALA	ALA	GLY	HIS	GLU	LEU	GLN	PRO	ASN	SER	LEU	ILE	ILE	VAL	ARG	ASN	GLN	ARG	PRO	SER	ALA	GLU	GLN	ASN	ARG	ASP	ASP	LEU	GLU	ILE								
PRO	MET	SER	PRO	PRO	GLY	TYR	LEU	VAL	VAL	THR	GLY	ASP	ARG	ASN	ASN	ASN	GLN	SER	SER	ALA	VAL	ARG	ASN	TYR	ASN	GLN	ALA	ALA	TRP	ASN	GLY	GLN	ASP	ASP	GLU	ILE									
V216	S220	L221	I225	I226	E227	Y230	V231	F232	F233	K234	G235	VAL	LYS	ASP	ARG	VAL	LYS	GLY	LYS	ASP	PRO	TYR	HIS	ALA	SER	ALA	GLY	ALA	LEU	SER	GLN	PRO	ALA	GLY	GLN	ILE									
ALA	THR	ASP	GLY	VAL	ASN	ASP	HIS	LEU	LYS	GLN	ILE	ILE	LYS	LYS	PHE	TYR	GLY	ILE	GLU	HIS	GLY	VAL	LYS	MET	ARG	GLY	L151	L152	R153	T154	Y155	F161	K162	E166	Y177	S180	R189	L200	S201	R202	P203	T204	E205	F212	
MET	G2	D3	T19	A20	G21	V25	V28	L29	F30	I31	F32	R33	L37	A40	V41	E42	S43	V64	F70	F71	I72	R76	Q81	I82	I83	F84	V85	S86	V87	L91	Y92	V96	V99	E103	E104	K105	LEU	ASN	LYS	LYS	GLU	GLU	LEU	LYS	VAL

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50471	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)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.015	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0025	Depositor
Map size (\AA)	251.13599, 251.13599, 251.13599	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.654, 0.654, 0.654	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/1584	0.43	0/2150
1	B	0.26	0/1584	0.43	0/2150
1	C	0.26	0/1584	0.43	0/2150
1	D	0.26	0/1584	0.43	0/2150
1	E	0.26	0/1584	0.43	0/2150
1	F	0.26	0/1584	0.43	0/2150
1	G	0.26	0/1584	0.43	0/2150
1	H	0.26	0/1584	0.43	0/2150
1	I	0.26	0/1584	0.43	0/2150
1	J	0.26	0/1584	0.43	0/2150
1	K	0.26	0/1584	0.43	0/2150
1	L	0.26	0/1584	0.43	0/2150
All	All	0.26	0/19008	0.43	0/25800

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	1541	0	1564	34	0
1	B	1541	0	1564	31	0
1	C	1541	0	1564	29	0
1	D	1541	0	1564	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1541	0	1564	33	0
1	F	1541	0	1564	31	0
1	G	1541	0	1564	33	0
1	H	1541	0	1564	32	0
1	I	1541	0	1564	30	0
1	J	1541	0	1564	31	0
1	K	1541	0	1564	32	0
1	L	1541	0	1564	31	0
All	All	18492	0	18768	330	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 9.

All (330) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:HG3	1:B:216:VAL:HG11	1.79	0.65
1:H:33:ARG:HG3	1:H:216:VAL:HG11	1.79	0.65
1:A:33:ARG:HG3	1:A:216:VAL:HG11	1.79	0.64
1:G:33:ARG:HG3	1:G:216:VAL:HG11	1.79	0.64
1:I:33:ARG:HG3	1:I:216:VAL:HG11	1.80	0.64
1:C:33:ARG:HG3	1:C:216:VAL:HG11	1.80	0.64
1:L:33:ARG:HG3	1:L:216:VAL:HG11	1.80	0.64
1:F:33:ARG:HG3	1:F:216:VAL:HG11	1.80	0.64
1:D:33:ARG:HG3	1:D:216:VAL:HG11	1.79	0.64
1:G:96:VAL:HG22	1:G:151:LEU:HD11	1.80	0.64
1:A:96:VAL:HG22	1:A:151:LEU:HD11	1.80	0.64
1:F:96:VAL:HG22	1:F:151:LEU:HD11	1.80	0.64
1:E:33:ARG:HG3	1:E:216:VAL:HG11	1.80	0.64
1:J:33:ARG:HG3	1:J:216:VAL:HG11	1.79	0.64
1:K:33:ARG:HG3	1:K:216:VAL:HG11	1.80	0.64
1:L:96:VAL:HG22	1:L:151:LEU:HD11	1.80	0.64
1:D:96:VAL:HG22	1:D:151:LEU:HD11	1.80	0.63
1:J:96:VAL:HG22	1:J:151:LEU:HD11	1.80	0.63
1:C:96:VAL:HG22	1:C:151:LEU:HD11	1.80	0.62
1:I:96:VAL:HG22	1:I:151:LEU:HD11	1.80	0.62
1:E:96:VAL:HG22	1:E:151:LEU:HD11	1.80	0.62
1:K:96:VAL:HG22	1:K:151:LEU:HD11	1.80	0.62
1:H:96:VAL:HG22	1:H:151:LEU:HD11	1.80	0.62
1:B:96:VAL:HG22	1:B:151:LEU:HD11	1.80	0.62
1:D:227:GLU:O	1:D:231:VAL:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:GLU:O	1:F:231:VAL:HG23	2.02	0.60
1:J:227:GLU:O	1:J:231:VAL:HG23	2.02	0.60
1:L:227:GLU:O	1:L:231:VAL:HG23	2.02	0.60
1:G:227:GLU:O	1:G:231:VAL:HG23	2.02	0.60
1:A:227:GLU:O	1:A:231:VAL:HG23	2.02	0.60
1:I:227:GLU:O	1:I:231:VAL:HG23	2.02	0.60
1:C:227:GLU:O	1:C:231:VAL:HG23	2.02	0.60
1:E:227:GLU:O	1:E:231:VAL:HG23	2.01	0.59
1:B:227:GLU:O	1:B:231:VAL:HG23	2.01	0.59
1:H:227:GLU:O	1:H:231:VAL:HG23	2.01	0.59
1:K:227:GLU:O	1:K:231:VAL:HG23	2.02	0.59
1:G:221:LEU:O	1:G:225:ILE:HG12	2.04	0.58
1:K:221:LEU:O	1:K:225:ILE:HG12	2.03	0.58
1:A:221:LEU:O	1:A:225:ILE:HG12	2.04	0.58
1:E:221:LEU:O	1:E:225:ILE:HG12	2.04	0.58
1:D:221:LEU:O	1:D:225:ILE:HG12	2.04	0.58
1:J:221:LEU:O	1:J:225:ILE:HG12	2.04	0.58
1:L:221:LEU:O	1:L:225:ILE:HG12	2.04	0.58
1:F:221:LEU:O	1:F:225:ILE:HG12	2.04	0.58
1:C:221:LEU:O	1:C:225:ILE:HG12	2.04	0.57
1:I:221:LEU:O	1:I:225:ILE:HG12	2.04	0.57
1:C:64:VAL:HB	1:C:189:ARG:HG2	1.87	0.57
1:H:221:LEU:O	1:H:225:ILE:HG12	2.04	0.57
1:I:64:VAL:HB	1:I:189:ARG:HG2	1.87	0.57
1:H:64:VAL:HB	1:H:189:ARG:HG2	1.87	0.57
1:B:64:VAL:HB	1:B:189:ARG:HG2	1.87	0.57
1:B:221:LEU:O	1:B:225:ILE:HG12	2.04	0.57
1:J:64:VAL:HB	1:J:189:ARG:HG2	1.87	0.56
1:A:64:VAL:HB	1:A:189:ARG:HG2	1.87	0.56
1:D:64:VAL:HB	1:D:189:ARG:HG2	1.87	0.56
1:G:64:VAL:HB	1:G:189:ARG:HG2	1.87	0.56
1:E:64:VAL:HB	1:E:189:ARG:HG2	1.87	0.56
1:F:64:VAL:HB	1:F:189:ARG:HG2	1.87	0.56
1:K:29:LEU:HD11	1:K:216:VAL:HG13	1.88	0.56
1:K:64:VAL:HB	1:K:189:ARG:HG2	1.87	0.56
1:E:29:LEU:HD11	1:E:216:VAL:HG13	1.88	0.56
1:L:64:VAL:HB	1:L:189:ARG:HG2	1.87	0.56
1:F:29:LEU:HD11	1:F:216:VAL:HG13	1.88	0.56
1:L:29:LEU:HD11	1:L:216:VAL:HG13	1.88	0.56
1:J:29:LEU:HD11	1:J:216:VAL:HG13	1.88	0.55
1:D:29:LEU:HD11	1:D:216:VAL:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:VAL:HG13	1:E:162:LYS:HG3	1.89	0.55
1:K:85:VAL:HG13	1:K:162:LYS:HG3	1.89	0.55
1:L:85:VAL:HG13	1:L:162:LYS:HG3	1.89	0.55
1:A:29:LEU:HD11	1:A:216:VAL:HG13	1.88	0.55
1:C:29:LEU:HD11	1:C:216:VAL:HG13	1.88	0.55
1:F:85:VAL:HG13	1:F:162:LYS:HG3	1.89	0.55
1:I:29:LEU:HD11	1:I:216:VAL:HG13	1.88	0.55
1:B:29:LEU:HD11	1:B:216:VAL:HG13	1.88	0.54
1:G:29:LEU:HD11	1:G:216:VAL:HG13	1.88	0.54
1:H:29:LEU:HD11	1:H:216:VAL:HG13	1.88	0.54
1:A:85:VAL:HG13	1:A:162:LYS:HG3	1.89	0.54
1:C:85:VAL:HG13	1:C:162:LYS:HG3	1.89	0.54
1:G:85:VAL:HG13	1:G:162:LYS:HG3	1.89	0.54
1:I:85:VAL:HG13	1:I:162:LYS:HG3	1.89	0.54
1:D:33:ARG:HD2	1:D:82:ILE:HD13	1.90	0.54
1:J:33:ARG:HD2	1:J:82:ILE:HD13	1.90	0.54
1:D:85:VAL:HG13	1:D:162:LYS:HG3	1.89	0.53
1:J:85:VAL:HG13	1:J:162:LYS:HG3	1.89	0.53
1:G:33:ARG:HD2	1:G:82:ILE:HD13	1.90	0.53
1:A:33:ARG:HD2	1:A:82:ILE:HD13	1.90	0.53
1:B:85:VAL:HG13	1:B:162:LYS:HG3	1.89	0.53
1:H:33:ARG:HD2	1:H:82:ILE:HD13	1.90	0.53
1:H:85:VAL:HG13	1:H:162:LYS:HG3	1.89	0.53
1:L:33:ARG:HD2	1:L:82:ILE:HD13	1.90	0.53
1:B:33:ARG:HD2	1:B:82:ILE:HD13	1.90	0.52
1:F:33:ARG:HD2	1:F:82:ILE:HD13	1.90	0.52
1:H:19:THR:HG22	1:H:230:TYR:CD2	2.45	0.52
1:J:19:THR:HG22	1:J:230:TYR:CD2	2.45	0.52
1:B:19:THR:HG22	1:B:230:TYR:CD2	2.45	0.52
1:D:19:THR:HG22	1:D:230:TYR:CD2	2.45	0.52
1:K:33:ARG:HD2	1:K:82:ILE:HD13	1.90	0.52
1:C:33:ARG:HD2	1:C:82:ILE:HD13	1.90	0.52
1:E:33:ARG:HD2	1:E:82:ILE:HD13	1.90	0.52
1:I:33:ARG:HD2	1:I:82:ILE:HD13	1.90	0.52
1:A:19:THR:HG22	1:A:230:TYR:CD2	2.45	0.52
1:I:19:THR:HG22	1:I:230:TYR:CD2	2.45	0.52
1:C:19:THR:HG22	1:C:230:TYR:CD2	2.45	0.52
1:E:19:THR:HG22	1:E:230:TYR:CD2	2.45	0.52
1:G:19:THR:HG22	1:G:230:TYR:CD2	2.45	0.52
1:K:19:THR:HG22	1:K:230:TYR:CD2	2.45	0.52
1:E:21:GLY:O	1:E:25:TRP:HD1	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ILE:O	1:B:177:TYR:OH	2.16	0.51
1:F:19:THR:HG22	1:F:230:TYR:CD2	2.45	0.51
1:K:21:GLY:O	1:K:25:TRP:HD1	1.93	0.51
1:L:19:THR:HG22	1:L:230:TYR:CD2	2.45	0.51
1:C:21:GLY:O	1:C:25:TRP:HD1	1.94	0.51
1:B:37:LEU:HD12	1:B:41:VAL:HG21	1.93	0.51
1:H:37:LEU:HD12	1:H:41:VAL:HG21	1.93	0.51
1:I:21:GLY:O	1:I:25:TRP:HD1	1.94	0.51
1:B:21:GLY:O	1:B:25:TRP:HD1	1.93	0.51
1:H:21:GLY:O	1:H:25:TRP:HD1	1.93	0.51
1:H:72:ILE:O	1:H:177:TYR:OH	2.16	0.51
1:D:21:GLY:O	1:D:25:TRP:HD1	1.94	0.51
1:E:37:LEU:HD12	1:E:41:VAL:HG21	1.93	0.51
1:J:21:GLY:O	1:J:25:TRP:HD1	1.94	0.51
1:K:37:LEU:HD12	1:K:41:VAL:HG21	1.93	0.51
1:A:37:LEU:HD12	1:A:41:VAL:HG21	1.93	0.50
1:D:37:LEU:HD12	1:D:41:VAL:HG21	1.93	0.50
1:G:37:LEU:HD12	1:G:41:VAL:HG21	1.93	0.50
1:J:37:LEU:HD12	1:J:41:VAL:HG21	1.93	0.50
1:I:37:LEU:HD12	1:I:41:VAL:HG21	1.93	0.50
1:C:37:LEU:HD12	1:C:41:VAL:HG21	1.93	0.50
1:A:21:GLY:O	1:A:25:TRP:HD1	1.94	0.50
1:G:21:GLY:O	1:G:25:TRP:HD1	1.94	0.50
1:F:37:LEU:HD12	1:F:41:VAL:HG21	1.93	0.50
1:L:21:GLY:O	1:L:25:TRP:HD1	1.94	0.49
1:L:37:LEU:HD12	1:L:41:VAL:HG21	1.93	0.49
1:F:21:GLY:O	1:F:25:TRP:HD1	1.94	0.49
1:I:72:ILE:O	1:I:177:TYR:OH	2.16	0.48
1:F:153:ARG:HG3	1:F:154:THR:N	2.29	0.48
1:L:153:ARG:HG3	1:L:154:THR:N	2.29	0.47
1:E:153:ARG:HG3	1:E:154:THR:N	2.29	0.47
1:A:153:ARG:HG3	1:A:154:THR:N	2.29	0.47
1:K:153:ARG:HG3	1:K:154:THR:N	2.29	0.47
1:G:153:ARG:HG3	1:G:154:THR:N	2.29	0.47
1:H:40:ALA:HB1	1:I:76:ARG:HG2	1.97	0.47
1:A:72:ILE:O	1:A:177:TYR:OH	2.16	0.47
1:B:40:ALA:HB1	1:C:76:ARG:HG2	1.97	0.47
1:G:72:ILE:O	1:G:177:TYR:OH	2.16	0.47
1:J:81:GLN:NE2	1:J:166:GLU:OE2	2.48	0.47
1:C:81:GLN:NE2	1:C:166:GLU:OE2	2.48	0.47
1:D:81:GLN:NE2	1:D:166:GLU:OE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:81:GLN:NE2	1:I:166:GLU:OE2	2.48	0.47
1:J:40:ALA:HB1	1:K:76:ARG:HG2	1.97	0.47
1:B:153:ARG:HG3	1:B:154:THR:N	2.29	0.47
1:D:40:ALA:HB1	1:E:76:ARG:HG2	1.97	0.47
1:E:81:GLN:NE2	1:E:166:GLU:OE2	2.48	0.47
1:H:153:ARG:HG3	1:H:154:THR:N	2.29	0.47
1:K:81:GLN:NE2	1:K:166:GLU:OE2	2.48	0.47
1:A:40:ALA:HB1	1:B:76:ARG:HG2	1.97	0.46
1:B:81:GLN:NE2	1:B:166:GLU:OE2	2.48	0.46
1:G:40:ALA:HB1	1:H:76:ARG:HG2	1.97	0.46
1:G:43:SER:HB2	1:H:76:ARG:HH21	1.80	0.46
1:H:81:GLN:NE2	1:H:166:GLU:OE2	2.48	0.46
1:A:81:GLN:NE2	1:A:166:GLU:OE2	2.48	0.46
1:D:99:VAL:HG21	1:D:151:LEU:HD13	1.98	0.46
1:D:153:ARG:HG3	1:D:154:THR:N	2.29	0.46
1:F:81:GLN:NE2	1:F:166:GLU:OE2	2.48	0.46
1:F:99:VAL:HG21	1:F:151:LEU:HD13	1.98	0.46
1:I:99:VAL:HG21	1:I:151:LEU:HD13	1.98	0.46
1:J:99:VAL:HG21	1:J:151:LEU:HD13	1.98	0.46
1:L:99:VAL:HG21	1:L:151:LEU:HD13	1.98	0.46
1:C:99:VAL:HG21	1:C:151:LEU:HD13	1.98	0.46
1:E:99:VAL:HG21	1:E:151:LEU:HD13	1.98	0.46
1:G:81:GLN:NE2	1:G:166:GLU:OE2	2.48	0.46
1:H:43:SER:HB2	1:I:76:ARG:HH21	1.81	0.46
1:K:99:VAL:HG21	1:K:151:LEU:HD13	1.98	0.46
1:L:81:GLN:NE2	1:L:166:GLU:OE2	2.48	0.46
1:E:40:ALA:HB1	1:F:76:ARG:HG2	1.97	0.46
1:G:99:VAL:HG21	1:G:151:LEU:HD13	1.97	0.46
1:J:153:ARG:HG3	1:J:154:THR:N	2.29	0.46
1:A:99:VAL:HG21	1:A:151:LEU:HD13	1.97	0.46
1:B:99:VAL:HG21	1:B:151:LEU:HD13	1.98	0.46
1:E:72:ILE:O	1:E:177:TYR:OH	2.16	0.46
1:H:99:VAL:HG21	1:H:151:LEU:HD13	1.98	0.46
1:B:43:SER:HB2	1:C:76:ARG:HH21	1.81	0.46
1:K:40:ALA:HB1	1:L:76:ARG:HG2	1.98	0.46
1:A:43:SER:HB2	1:B:76:ARG:HH21	1.81	0.46
1:C:153:ARG:HG3	1:C:154:THR:N	2.29	0.46
1:C:28:VAL:O	1:C:31:ILE:HG13	2.16	0.46
1:I:153:ARG:HG3	1:I:154:THR:N	2.29	0.46
1:B:28:VAL:O	1:B:31:ILE:HG13	2.16	0.46
1:D:28:VAL:O	1:D:31:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ILE:O	1:D:177:TYR:OH	2.16	0.46
1:H:28:VAL:O	1:H:31:ILE:HG13	2.16	0.46
1:I:28:VAL:O	1:I:31:ILE:HG13	2.16	0.46
1:F:28:VAL:O	1:F:31:ILE:HG13	2.16	0.45
1:G:76:ARG:HH21	1:L:43:SER:HB2	1.80	0.45
1:J:28:VAL:O	1:J:31:ILE:HG13	2.16	0.45
1:K:72:ILE:O	1:K:177:TYR:OH	2.16	0.45
1:L:28:VAL:O	1:L:31:ILE:HG13	2.16	0.45
1:I:40:ALA:HB1	1:J:76:ARG:HG2	1.97	0.45
1:A:76:ARG:HG2	1:F:40:ALA:HB1	1.97	0.45
1:A:76:ARG:HH21	1:F:43:SER:HB2	1.81	0.45
1:C:40:ALA:HB1	1:D:76:ARG:HG2	1.97	0.45
1:C:43:SER:HB2	1:D:76:ARG:HH21	1.81	0.45
1:G:28:VAL:O	1:G:31:ILE:HG13	2.16	0.45
1:A:28:VAL:O	1:A:31:ILE:HG13	2.16	0.45
1:J:72:ILE:O	1:J:177:TYR:OH	2.16	0.45
1:D:43:SER:HB2	1:E:76:ARG:HH21	1.81	0.45
1:G:76:ARG:HG2	1:L:40:ALA:HB1	1.97	0.45
1:I:43:SER:HB2	1:J:76:ARG:HH21	1.81	0.45
1:G:28:VAL:HG21	1:H:91:LEU:HD23	1.99	0.45
1:E:43:SER:HB2	1:F:76:ARG:HH21	1.80	0.45
1:G:91:LEU:HD23	1:L:28:VAL:HG21	1.99	0.44
1:J:43:SER:HB2	1:K:76:ARG:HH21	1.81	0.44
1:K:43:SER:HB2	1:L:76:ARG:HH21	1.81	0.44
1:B:205:GLU:OE2	1:C:76:ARG:HD2	2.18	0.44
1:H:28:VAL:HG21	1:I:91:LEU:HD23	2.00	0.44
1:J:205:GLU:OE2	1:K:76:ARG:HD2	2.18	0.44
1:A:91:LEU:HD23	1:F:28:VAL:HG21	1.99	0.44
1:C:28:VAL:HG21	1:D:91:LEU:HD23	1.99	0.44
1:H:205:GLU:OE2	1:I:76:ARG:HD2	2.18	0.44
1:A:28:VAL:HG21	1:B:91:LEU:HD23	2.00	0.44
1:A:205:GLU:OE2	1:B:76:ARG:HD2	2.18	0.44
1:I:205:GLU:OE2	1:J:76:ARG:HD2	2.18	0.44
1:K:28:VAL:O	1:K:31:ILE:HG13	2.16	0.44
1:C:205:GLU:OE2	1:D:76:ARG:HD2	2.18	0.44
1:D:205:GLU:OE2	1:E:76:ARG:HD2	2.18	0.44
1:I:28:VAL:HG21	1:J:91:LEU:HD23	2.00	0.44
1:B:28:VAL:HG21	1:C:91:LEU:HD23	2.00	0.44
1:E:28:VAL:O	1:E:31:ILE:HG13	2.16	0.44
1:E:92:TYR:CE2	1:E:155:TYR:HB2	2.53	0.44
1:K:92:TYR:CE2	1:K:155:TYR:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:HD2	1:F:205:GLU:OE2	2.18	0.43
1:H:234:LYS:HD3	1:H:234:LYS:HA	1.90	0.43
1:D:28:VAL:HG21	1:E:91:LEU:HD23	1.99	0.43
1:G:205:GLU:OE2	1:H:76:ARG:HD2	2.18	0.43
1:B:234:LYS:HD3	1:B:234:LYS:HA	1.90	0.43
1:F:92:TYR:CE2	1:F:155:TYR:HB2	2.53	0.43
1:H:92:TYR:CE2	1:H:155:TYR:HB2	2.53	0.43
1:L:92:TYR:CE2	1:L:155:TYR:HB2	2.53	0.43
1:B:92:TYR:CE2	1:B:155:TYR:HB2	2.53	0.43
1:E:28:VAL:HG21	1:F:91:LEU:HD23	1.99	0.43
1:C:92:TYR:CE2	1:C:155:TYR:HB2	2.53	0.43
1:G:92:TYR:CE2	1:G:155:TYR:HB2	2.53	0.43
1:K:28:VAL:HG21	1:L:91:LEU:HD23	1.99	0.43
1:K:205:GLU:OE2	1:L:76:ARG:HD2	2.18	0.43
1:D:92:TYR:CE2	1:D:155:TYR:HB2	2.53	0.43
1:E:205:GLU:OE2	1:F:76:ARG:HD2	2.18	0.43
1:G:76:ARG:HD2	1:L:205:GLU:OE2	2.18	0.43
1:I:92:TYR:CE2	1:I:155:TYR:HB2	2.53	0.43
1:A:92:TYR:CE2	1:A:155:TYR:HB2	2.53	0.43
1:J:92:TYR:CE2	1:J:155:TYR:HB2	2.53	0.43
1:J:28:VAL:HG21	1:K:91:LEU:HD23	2.00	0.43
1:G:234:LYS:HD3	1:G:234:LYS:HA	1.90	0.43
1:L:72:ILE:O	1:L:177:TYR:OH	2.16	0.43
1:B:83:ILE:O	1:B:87:VAL:HG23	2.19	0.42
1:F:72:ILE:O	1:F:177:TYR:OH	2.16	0.42
1:H:83:ILE:O	1:H:87:VAL:HG23	2.19	0.42
1:L:234:LYS:HD3	1:L:234:LYS:HA	1.90	0.42
1:A:234:LYS:HD3	1:A:234:LYS:HA	1.90	0.42
1:C:83:ILE:O	1:C:87:VAL:HG23	2.19	0.42
1:G:83:ILE:O	1:G:87:VAL:HG23	2.19	0.42
1:J:70:PHE:HZ	1:J:200:LEU:HD13	1.84	0.42
1:A:83:ILE:O	1:A:87:VAL:HG23	2.19	0.42
1:D:83:ILE:O	1:D:87:VAL:HG23	2.19	0.42
1:I:83:ILE:O	1:I:87:VAL:HG23	2.19	0.42
1:D:70:PHE:HZ	1:D:200:LEU:HD13	1.84	0.42
1:I:70:PHE:HZ	1:I:200:LEU:HD13	1.84	0.42
1:J:83:ILE:O	1:J:87:VAL:HG23	2.19	0.42
1:C:70:PHE:HZ	1:C:200:LEU:HD13	1.84	0.42
1:E:70:PHE:HZ	1:E:200:LEU:HD13	1.84	0.42
1:E:181:LEU:HD23	1:E:181:LEU:HA	1.90	0.42
1:F:234:LYS:HD3	1:F:234:LYS:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PHE:HZ	1:A:200:LEU:HD13	1.84	0.42
1:E:83:ILE:O	1:E:87:VAL:HG23	2.19	0.42
1:F:70:PHE:HZ	1:F:200:LEU:HD13	1.84	0.42
1:L:70:PHE:HZ	1:L:200:LEU:HD13	1.84	0.42
1:L:83:ILE:O	1:L:87:VAL:HG23	2.19	0.42
1:B:200:LEU:HB2	1:B:203:PRO:HG3	2.02	0.42
1:G:70:PHE:HZ	1:G:200:LEU:HD13	1.84	0.42
1:K:70:PHE:HZ	1:K:200:LEU:HD13	1.84	0.42
1:K:83:ILE:O	1:K:87:VAL:HG23	2.19	0.42
1:F:83:ILE:O	1:F:87:VAL:HG23	2.19	0.41
1:H:200:LEU:HB2	1:H:203:PRO:HG3	2.02	0.41
1:F:200:LEU:HB2	1:F:203:PRO:HG3	2.02	0.41
1:H:23:LYS:H	1:H:23:LYS:HG2	1.70	0.41
1:K:181:LEU:HD23	1:K:181:LEU:HA	1.90	0.41
1:L:200:LEU:HB2	1:L:203:PRO:HG3	2.02	0.41
1:A:200:LEU:HB2	1:A:203:PRO:HG3	2.02	0.41
1:G:200:LEU:HB2	1:G:203:PRO:HG3	2.02	0.41
1:H:70:PHE:HZ	1:H:200:LEU:HD13	1.84	0.41
1:E:200:LEU:HB2	1:E:203:PRO:HG3	2.02	0.41
1:K:200:LEU:HB2	1:K:203:PRO:HG3	2.02	0.41
1:A:92:TYR:CZ	1:A:155:TYR:HB2	2.56	0.41
1:B:70:PHE:HZ	1:B:200:LEU:HD13	1.84	0.41
1:F:37:LEU:HA	1:F:41:VAL:HG22	2.03	0.41
1:F:92:TYR:CZ	1:F:155:TYR:HB2	2.56	0.41
1:G:92:TYR:CZ	1:G:155:TYR:HB2	2.56	0.41
1:K:37:LEU:HA	1:K:41:VAL:HG22	2.03	0.41
1:L:37:LEU:HA	1:L:41:VAL:HG22	2.03	0.41
1:L:92:TYR:CZ	1:L:155:TYR:HB2	2.56	0.41
1:C:200:LEU:HB2	1:C:203:PRO:HG3	2.02	0.41
1:I:200:LEU:HB2	1:I:203:PRO:HG3	2.02	0.41
1:K:234:LYS:HD3	1:K:234:LYS:HA	1.90	0.41
1:A:163:SER:O	1:A:167:VAL:HG13	2.21	0.41
1:B:163:SER:O	1:B:167:VAL:HG13	2.21	0.41
1:D:92:TYR:CZ	1:D:155:TYR:HB2	2.56	0.41
1:E:37:LEU:HA	1:E:41:VAL:HG22	2.03	0.41
1:E:163:SER:O	1:E:167:VAL:HG13	2.21	0.41
1:G:163:SER:O	1:G:167:VAL:HG13	2.21	0.41
1:H:163:SER:O	1:H:167:VAL:HG13	2.21	0.41
1:J:92:TYR:CZ	1:J:155:TYR:HB2	2.56	0.41
1:K:163:SER:O	1:K:167:VAL:HG13	2.21	0.41
1:A:181:LEU:HD23	1:A:181:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:SER:O	1:C:167:VAL:HG13	2.21	0.41
1:E:234:LYS:HD3	1:E:234:LYS:HA	1.90	0.41
1:H:92:TYR:CZ	1:H:155:TYR:HB2	2.56	0.40
1:A:23:LYS:H	1:A:23:LYS:HG2	1.70	0.40
1:A:37:LEU:HA	1:A:41:VAL:HG22	2.03	0.40
1:B:92:TYR:CZ	1:B:155:TYR:HB2	2.56	0.40
1:C:92:TYR:CZ	1:C:155:TYR:HB2	2.56	0.40
1:D:200:LEU:HB2	1:D:203:PRO:HG3	2.02	0.40
1:G:37:LEU:HA	1:G:41:VAL:HG22	2.03	0.40
1:I:163:SER:O	1:I:167:VAL:HG13	2.21	0.40
1:I:92:TYR:CZ	1:I:155:TYR:HB2	2.56	0.40
1:J:200:LEU:HB2	1:J:203:PRO:HG3	2.02	0.40
1:E:92:TYR:CZ	1:E:155:TYR:HB2	2.56	0.40
1:J:37:LEU:HA	1:J:41:VAL:HG22	2.03	0.40
1:J:163:SER:O	1:J:167:VAL:HG13	2.21	0.40
1:D:37:LEU:HA	1:D:41:VAL:HG22	2.03	0.40
1:D:163:SER:O	1:D:167:VAL:HG13	2.21	0.40
1:G:181:LEU:HD23	1:G:181:LEU:HA	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	185/382 (48%)	183 (99%)	2 (1%)	0	100	100
1	B	185/382 (48%)	183 (99%)	2 (1%)	0	100	100
1	C	185/382 (48%)	183 (99%)	2 (1%)	0	100	100
1	D	185/382 (48%)	183 (99%)	2 (1%)	0	100	100
1	E	185/382 (48%)	183 (99%)	2 (1%)	0	100	100
1	F	185/382 (48%)	183 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	185/382 (48%)	183 (99%)	2 (1%)	0	100	100
1	H	185/382 (48%)	183 (99%)	2 (1%)	0	100	100
1	I	185/382 (48%)	183 (99%)	2 (1%)	0	100	100
1	J	185/382 (48%)	183 (99%)	2 (1%)	0	100	100
1	K	185/382 (48%)	183 (99%)	2 (1%)	0	100	100
1	L	185/382 (48%)	183 (99%)	2 (1%)	0	100	100
All	All	2220/4584 (48%)	2196 (99%)	24 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	170/333 (51%)	164 (96%)	6 (4%)	31	38
1	B	170/333 (51%)	164 (96%)	6 (4%)	31	38
1	C	170/333 (51%)	164 (96%)	6 (4%)	31	38
1	D	170/333 (51%)	163 (96%)	7 (4%)	26	30
1	E	170/333 (51%)	164 (96%)	6 (4%)	31	38
1	F	170/333 (51%)	164 (96%)	6 (4%)	31	38
1	G	170/333 (51%)	164 (96%)	6 (4%)	31	38
1	H	170/333 (51%)	164 (96%)	6 (4%)	31	38
1	I	170/333 (51%)	164 (96%)	6 (4%)	31	38
1	J	170/333 (51%)	164 (96%)	6 (4%)	31	38
1	K	170/333 (51%)	164 (96%)	6 (4%)	31	38
1	L	170/333 (51%)	164 (96%)	6 (4%)	31	38
All	All	2040/3996 (51%)	1967 (96%)	73 (4%)	32	37

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	ARG
1	A	161	PHE
1	A	180	SER
1	A	202	ARG
1	A	212	PHE
1	A	220	SER
1	B	153	ARG
1	B	161	PHE
1	B	180	SER
1	B	202	ARG
1	B	212	PHE
1	B	220	SER
1	C	153	ARG
1	C	161	PHE
1	C	180	SER
1	C	202	ARG
1	C	212	PHE
1	C	220	SER
1	D	153	ARG
1	D	161	PHE
1	D	163	SER
1	D	180	SER
1	D	202	ARG
1	D	212	PHE
1	D	220	SER
1	E	153	ARG
1	E	161	PHE
1	E	180	SER
1	E	202	ARG
1	E	212	PHE
1	E	220	SER
1	F	153	ARG
1	F	161	PHE
1	F	180	SER
1	F	202	ARG
1	F	212	PHE
1	F	220	SER
1	G	153	ARG
1	G	161	PHE
1	G	180	SER
1	G	202	ARG
1	G	212	PHE
1	G	220	SER

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Mol	Chain	Res	Type
1	H	153	ARG
1	H	161	PHE
1	H	180	SER
1	H	202	ARG
1	H	212	PHE
1	H	220	SER
1	I	153	ARG
1	I	161	PHE
1	I	180	SER
1	I	202	ARG
1	I	212	PHE
1	I	220	SER
1	J	153	ARG
1	J	161	PHE
1	J	180	SER
1	J	202	ARG
1	J	212	PHE
1	J	220	SER
1	K	153	ARG
1	K	161	PHE
1	K	180	SER
1	K	202	ARG
1	K	212	PHE
1	K	220	SER
1	L	153	ARG
1	L	161	PHE
1	L	180	SER
1	L	202	ARG
1	L	212	PHE
1	L	220	SER

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

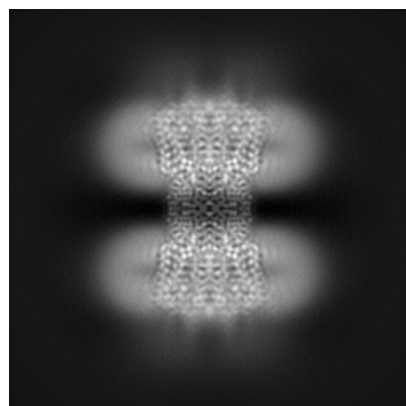
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14452. These allow visual inspection of the internal detail of the map and identification of artifacts.

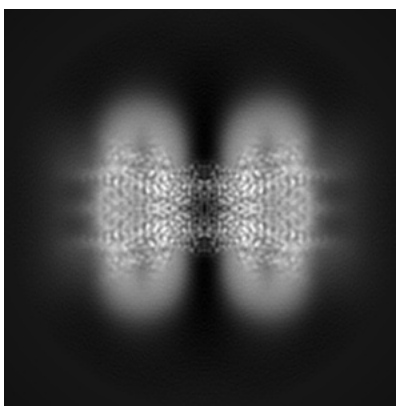
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

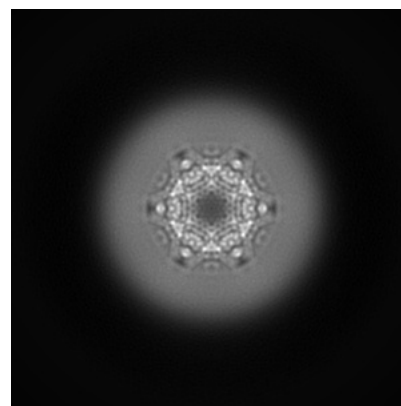
6.1.1 Primary map



X

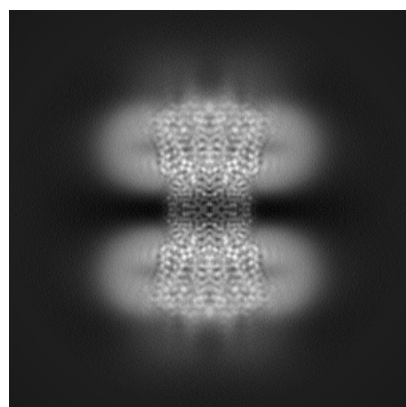


Y

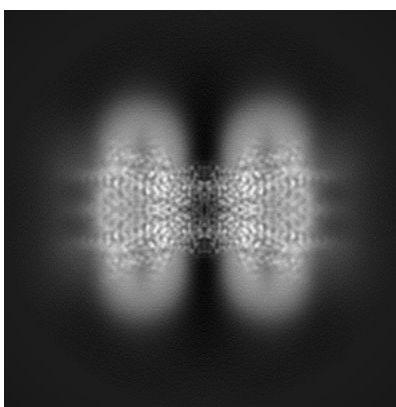


Z

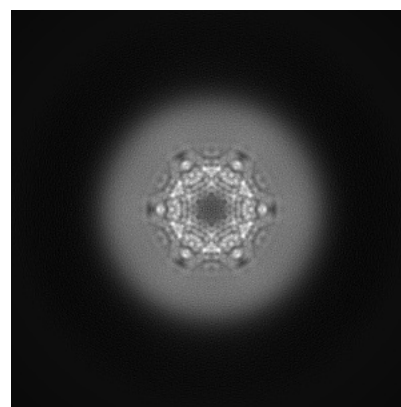
6.1.2 Raw map



X



Y

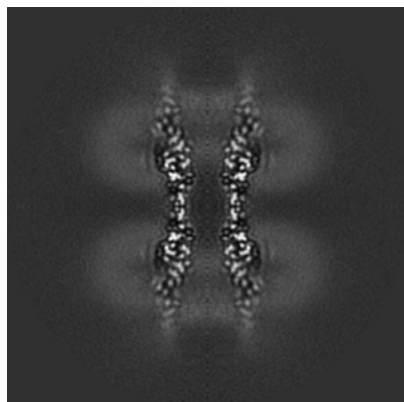


Z

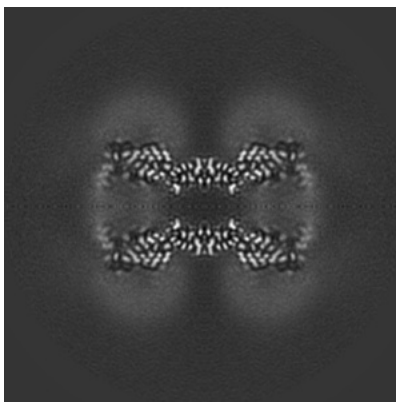
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

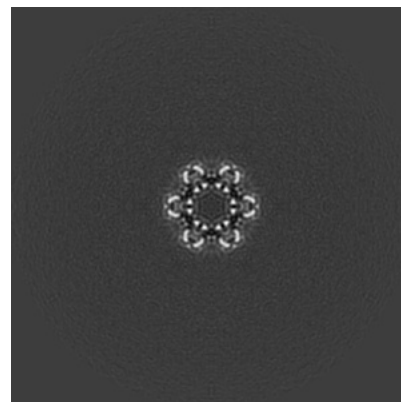
6.2.1 Primary map



X Index: 192

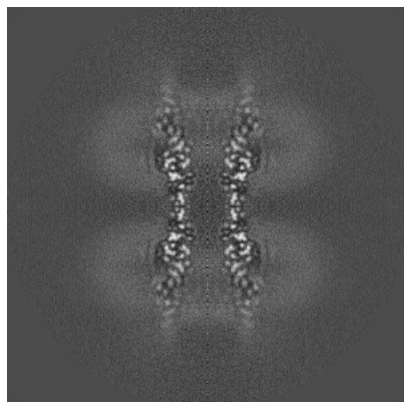


Y Index: 192

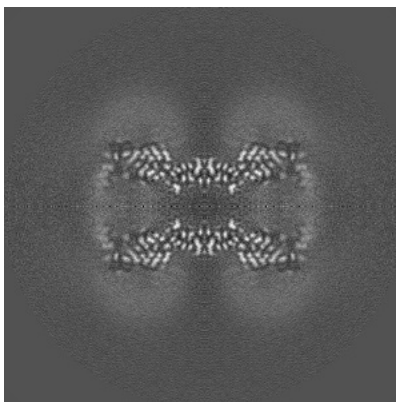


Z Index: 192

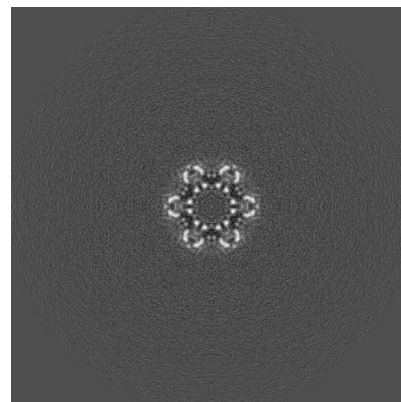
6.2.2 Raw map



X Index: 192



Y Index: 192

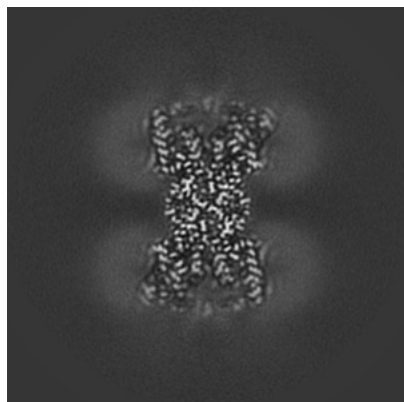


Z Index: 192

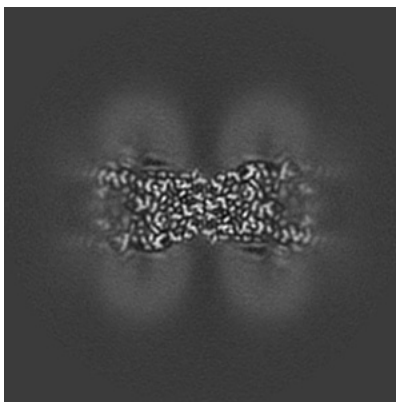
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

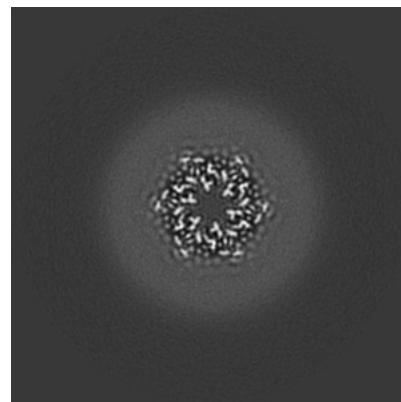
6.3.1 Primary map



X Index: 214

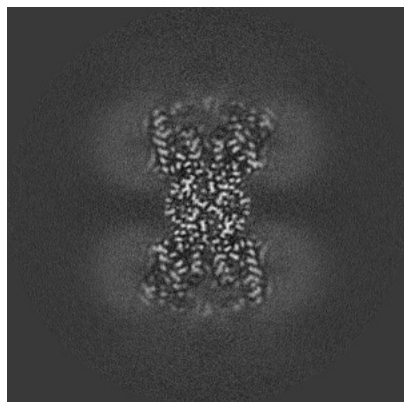


Y Index: 167

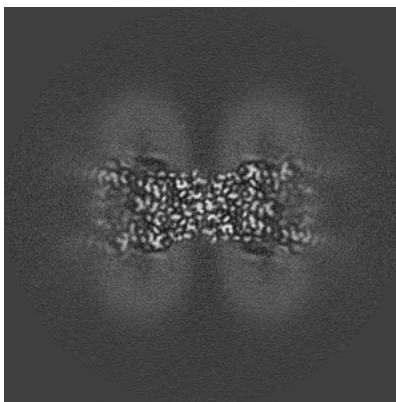


Z Index: 154

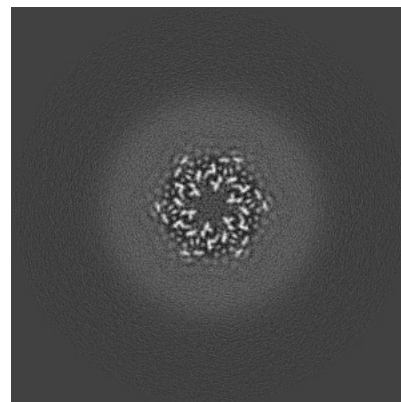
6.3.2 Raw map



X Index: 214



Y Index: 168

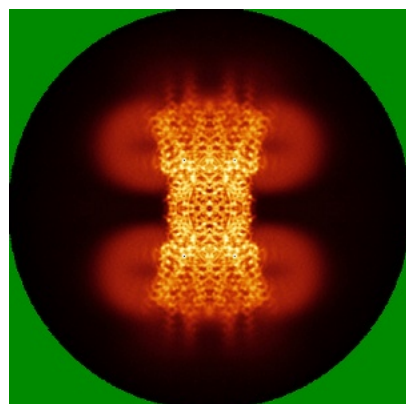


Z Index: 230

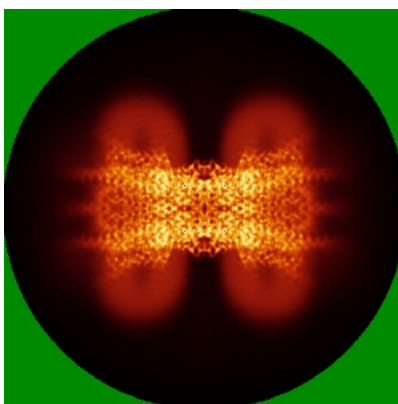
The images above show the largest variance slices of the map in three orthogonal directions.

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

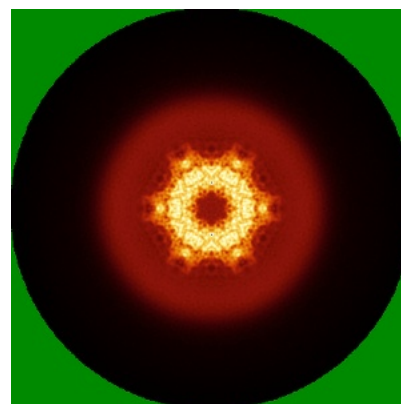
6.4.1 Primary map



X

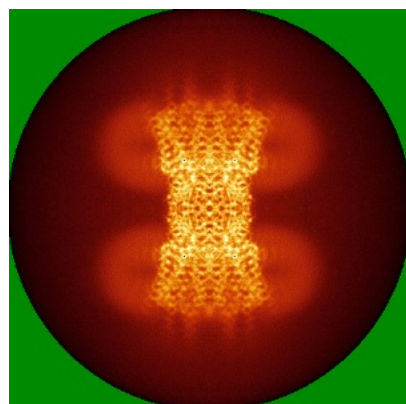


Y

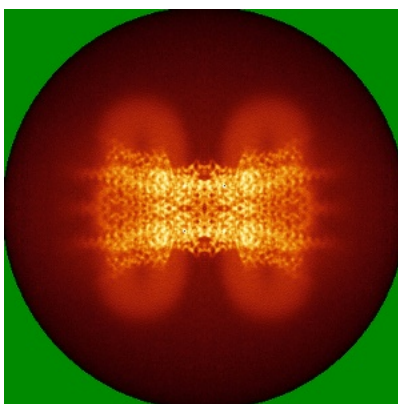


Z

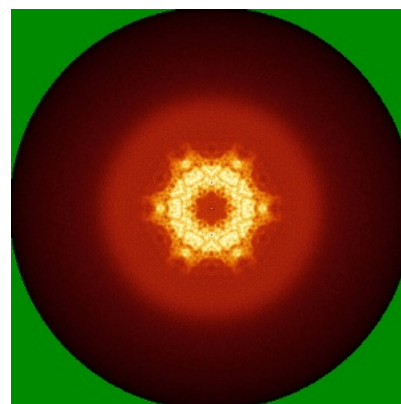
6.4.2 Raw map



X



Y

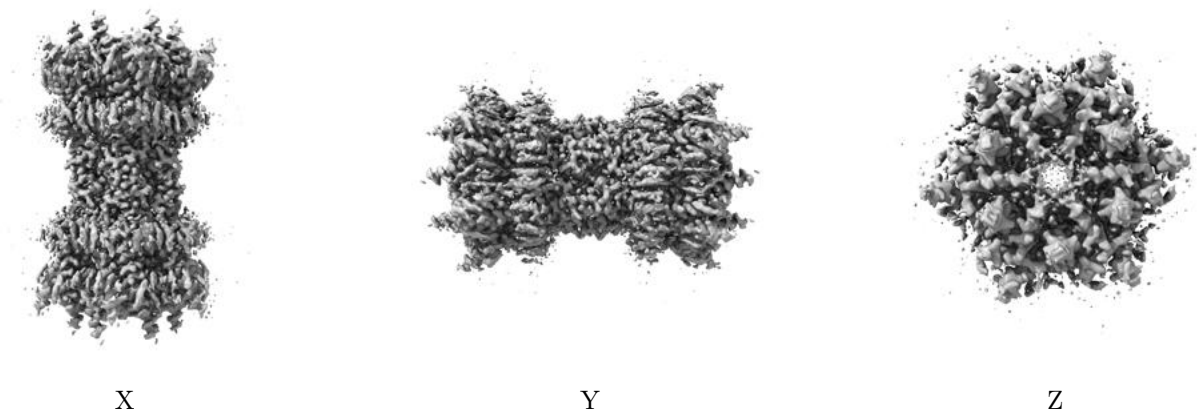


Z

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.

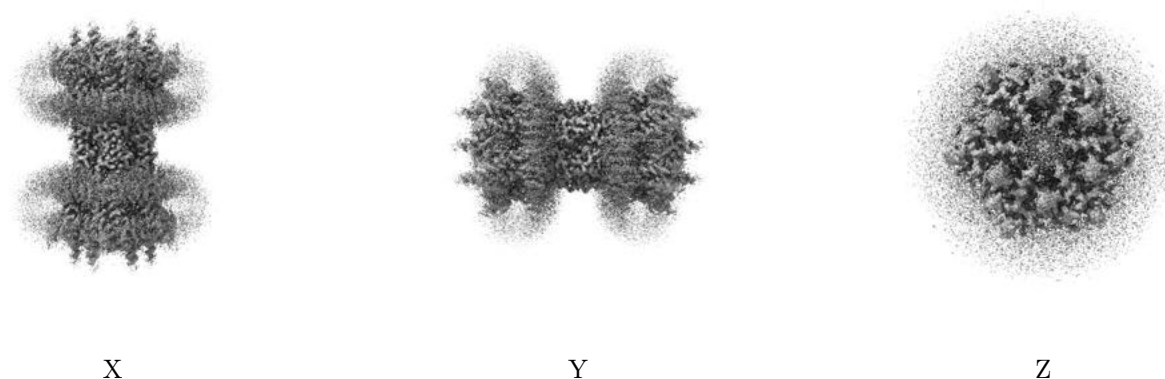
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0025. 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.

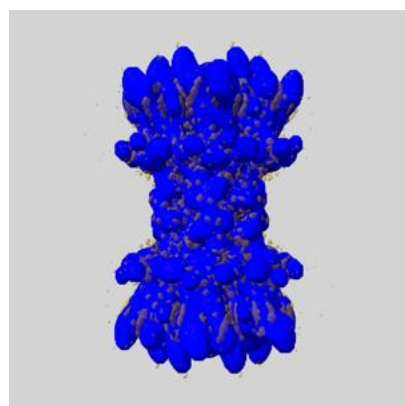
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

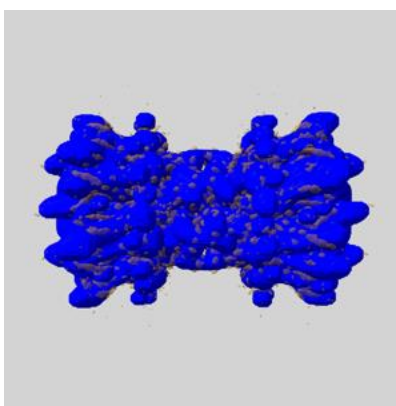
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

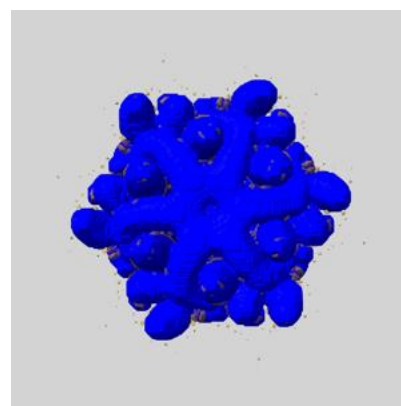
6.6.1 emd_14452_msk_1.map [i](#)



X



Y

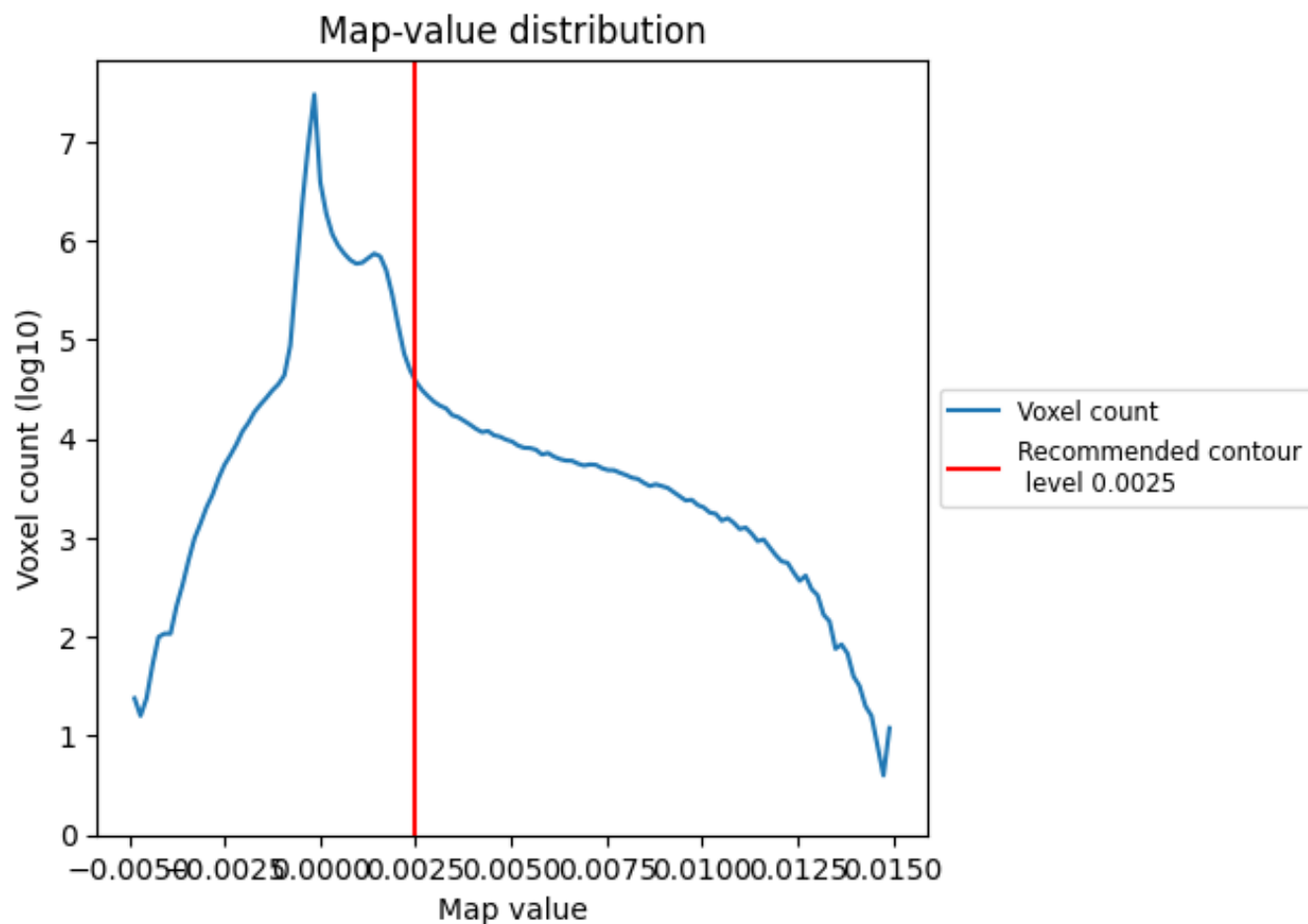


Z

7 Map analysis [i](#)

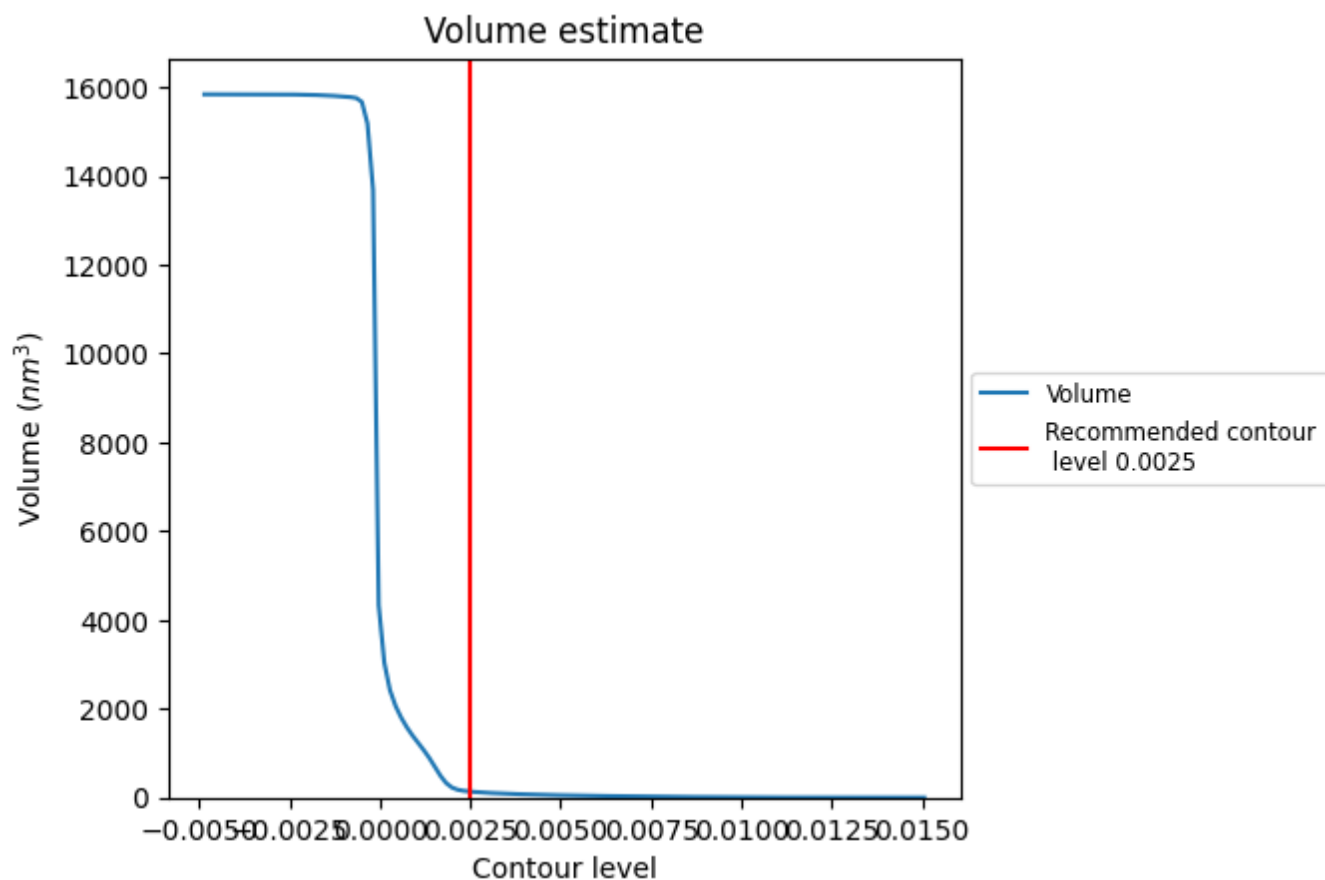
This section contains the results of statistical analysis of the map.

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.

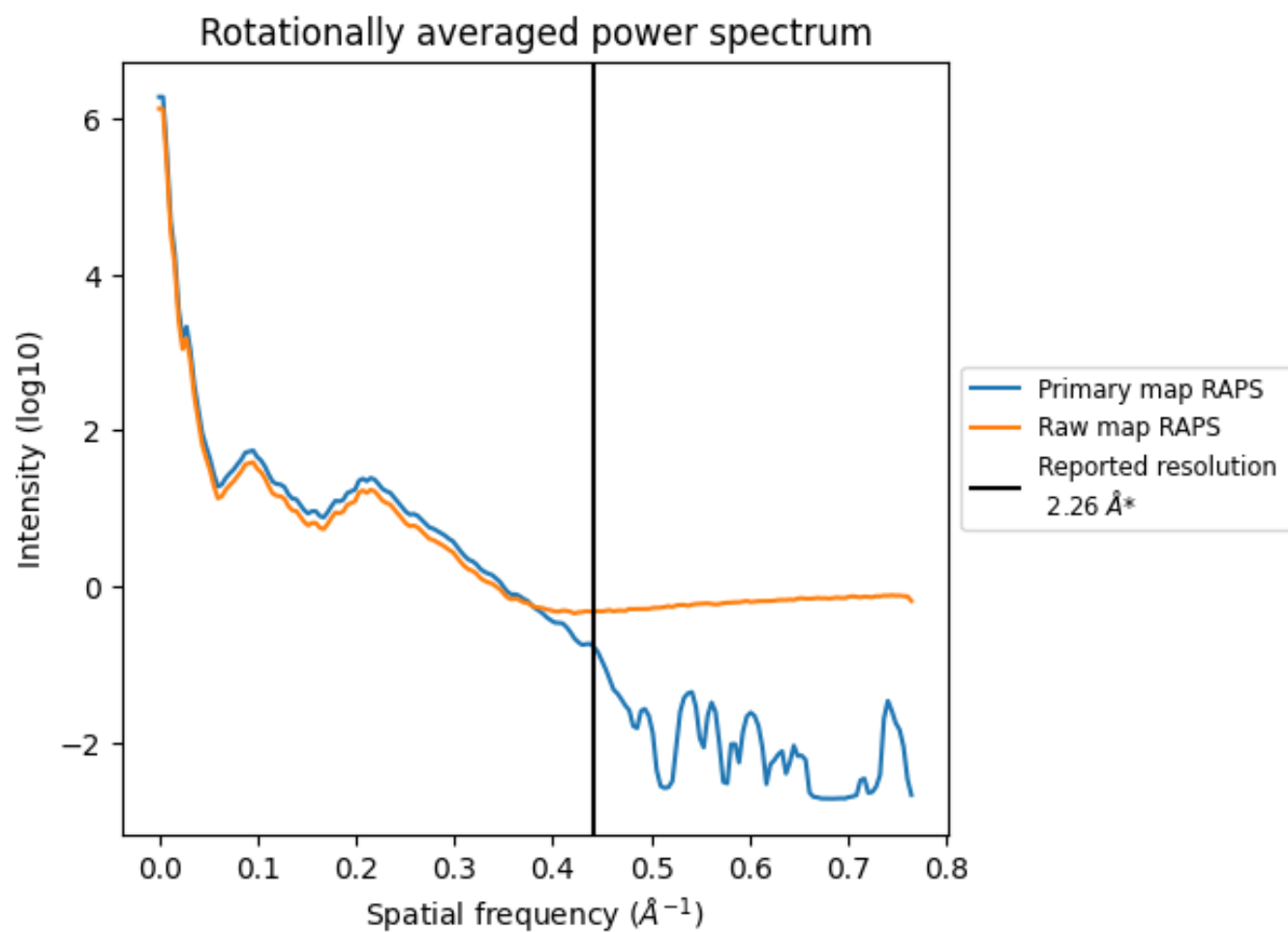
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 135 nm^3 ; this corresponds to an approximate mass of 122 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

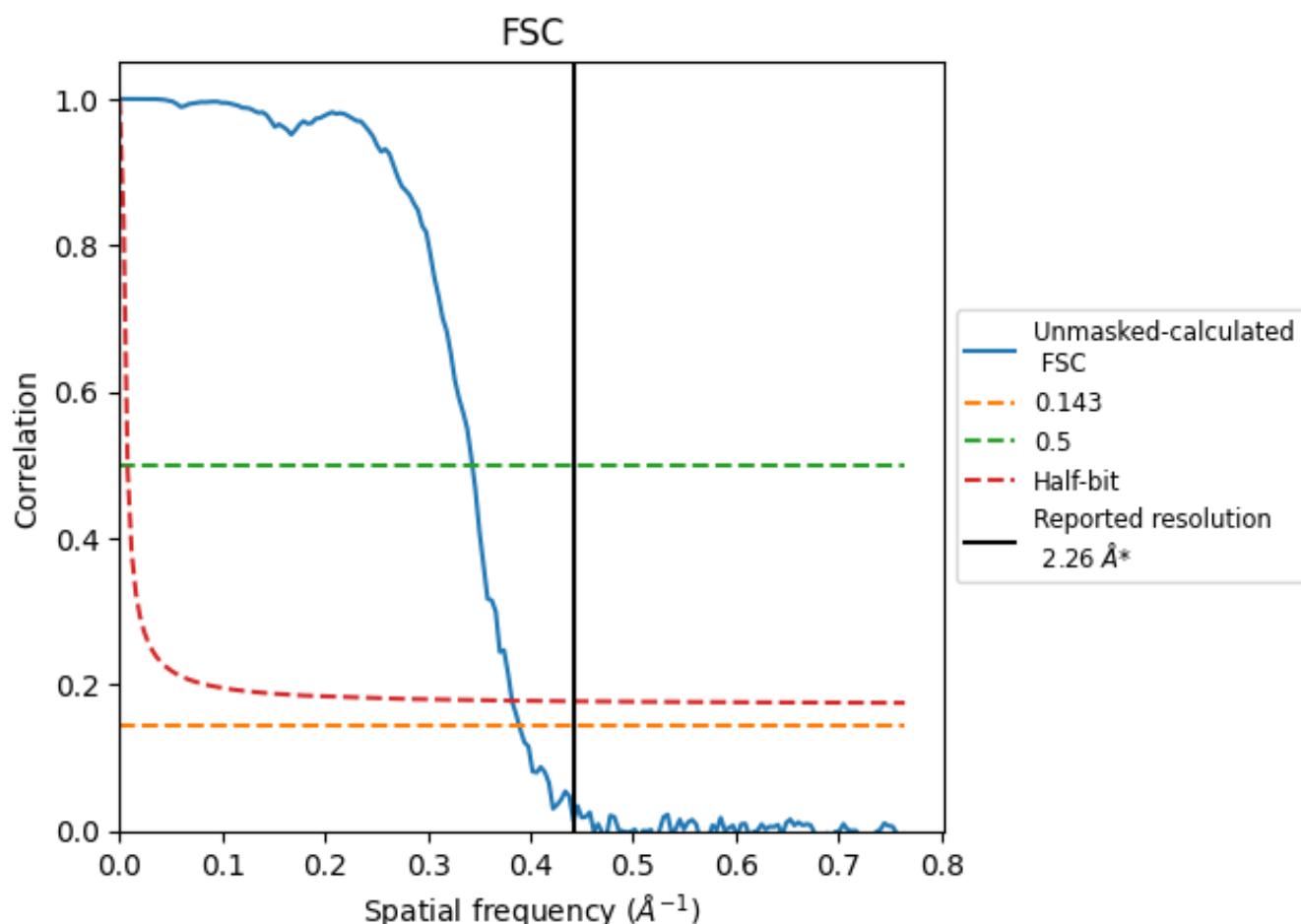


*Reported resolution corresponds to spatial frequency of 0.442 \AA^{-1}

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 0.442 Å⁻¹

8.2 Resolution estimates [i](#)

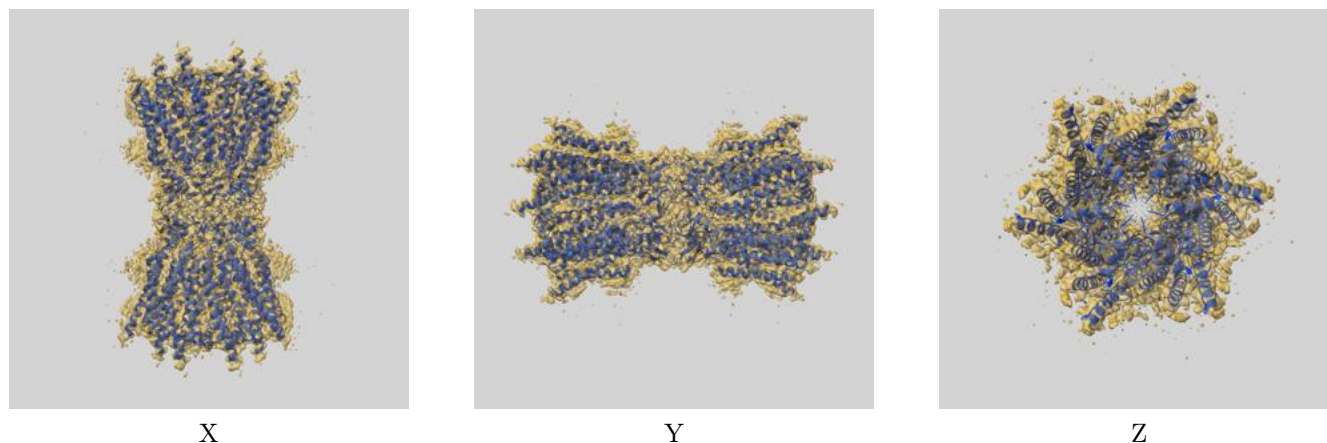
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.26	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.57	2.91	2.62

*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 2.57 differs from the reported value 2.26 by more than 10 %

9 Map-model fit [i](#)

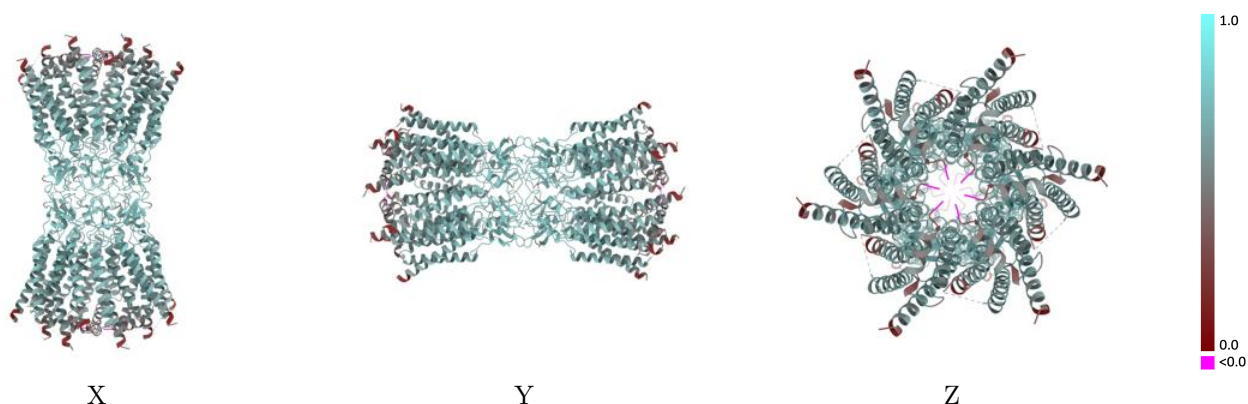
This section contains information regarding the fit between EMDB map EMD-14452 and PDB model 7Z1T. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



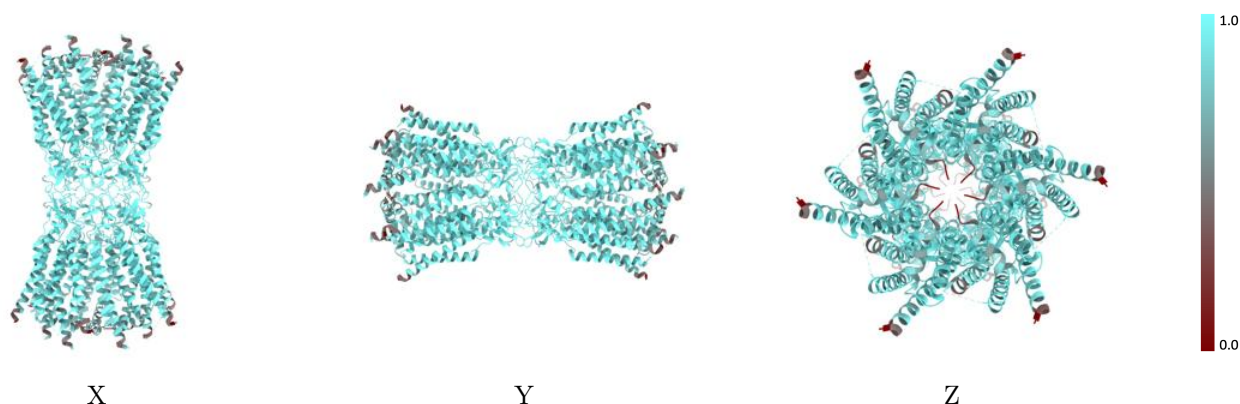
The images above show the 3D surface view of the map at the recommended contour level 0.0025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



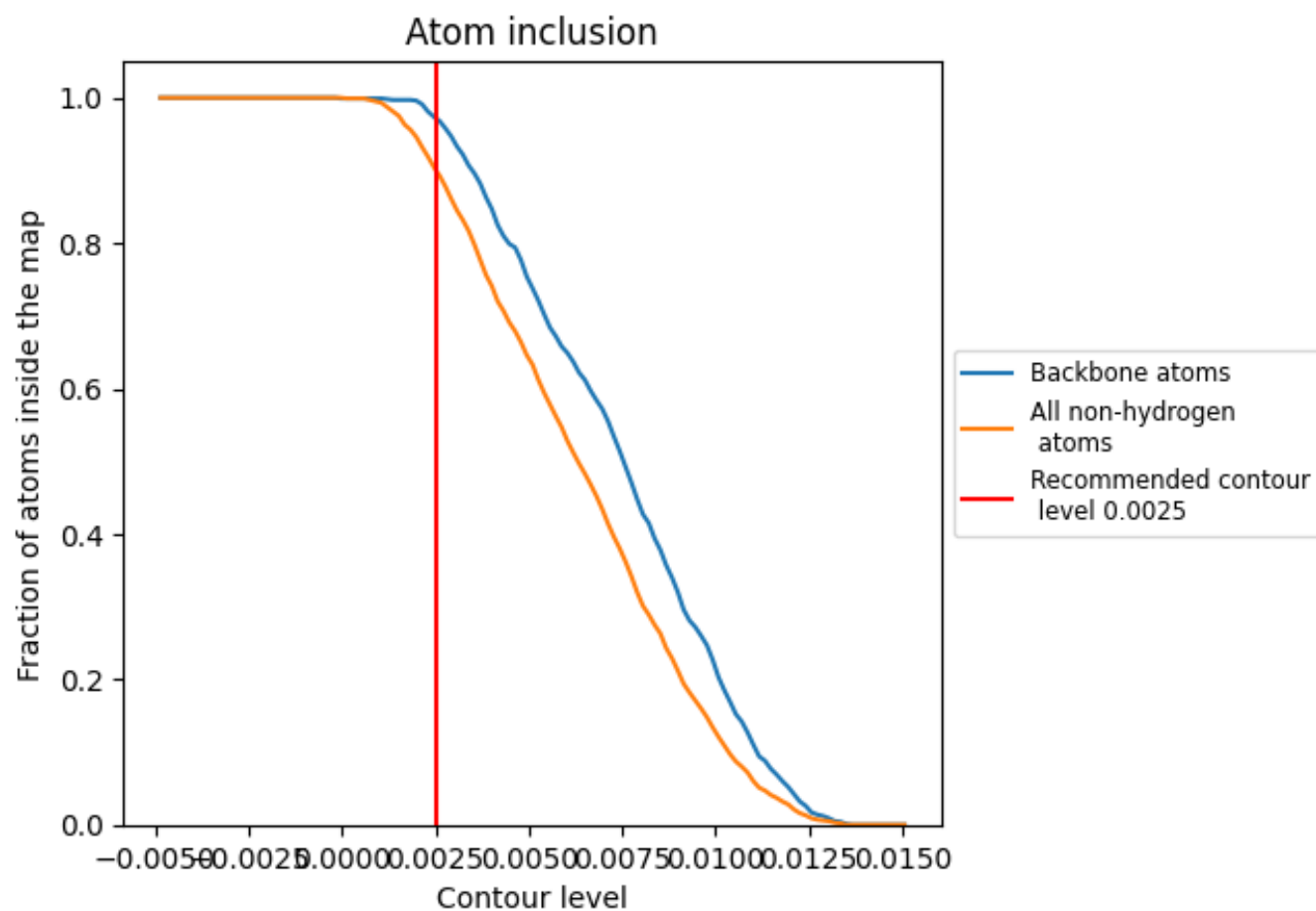
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 90% 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 (0.0025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9010</div>	<div><div></div>0.6050</div>
A	<div><div></div>0.9010</div>	<div><div></div>0.6040</div>
B	<div><div></div>0.9010</div>	<div><div></div>0.6040</div>
C	<div><div></div>0.9010</div>	<div><div></div>0.6060</div>
D	<div><div></div>0.9010</div>	<div><div></div>0.6040</div>
E	<div><div></div>0.9020</div>	<div><div></div>0.6040</div>
F	<div><div></div>0.9010</div>	<div><div></div>0.6040</div>
G	<div><div></div>0.9010</div>	<div><div></div>0.6050</div>
H	<div><div></div>0.9020</div>	<div><div></div>0.6040</div>
I	<div><div></div>0.9010</div>	<div><div></div>0.6050</div>
J	<div><div></div>0.9010</div>	<div><div></div>0.6050</div>
K	<div><div></div>0.9010</div>	<div><div></div>0.6050</div>
L	<div><div></div>0.9010</div>	<div><div></div>0.6040</div>

1.0

0.0

<0.0