



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 01:25 PM UTC

PDB ID : 8QKO / pdb_00008qko
EMDB ID : EMD-18468
Title : Connexin-43 gap junction channel in complex with mefloquine
Authors : Lavriha, P.; Korkhov, V.M.; Han, Y.
Deposited on : 2023-09-16
Resolution : 3.73 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
MolProbity : 4-5-2 with Phenix2.0
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

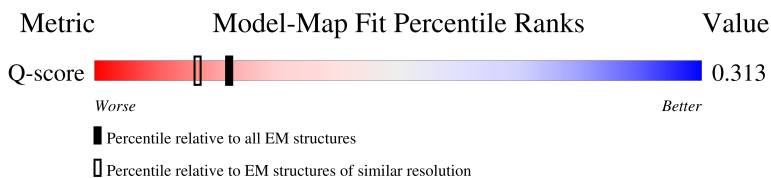
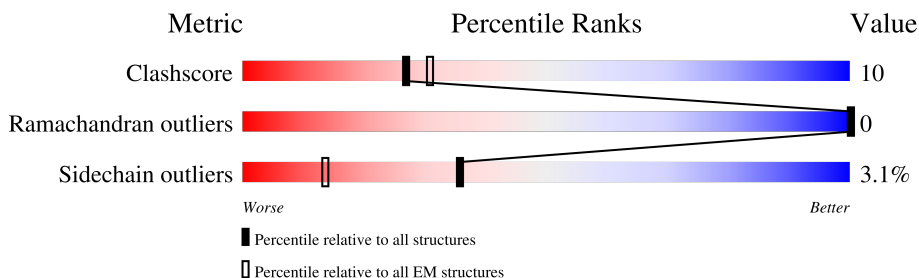
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.73 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	10415 (3.23 - 4.23)

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	

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Mol	Chain	Length	Quality of chain
1	E	382	
1	F	382	
1	G	382	
1	H	382	
1	I	382	
1	J	382	
1	K	382	
1	L	382	

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.

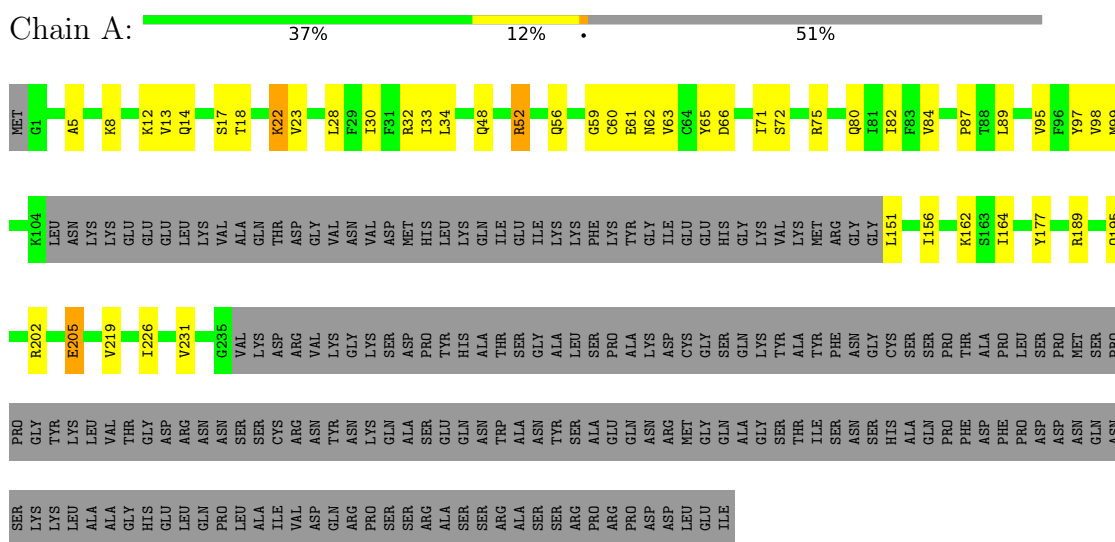
- Molecule 1 is a protein called Gap junction alpha-1 protein.

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

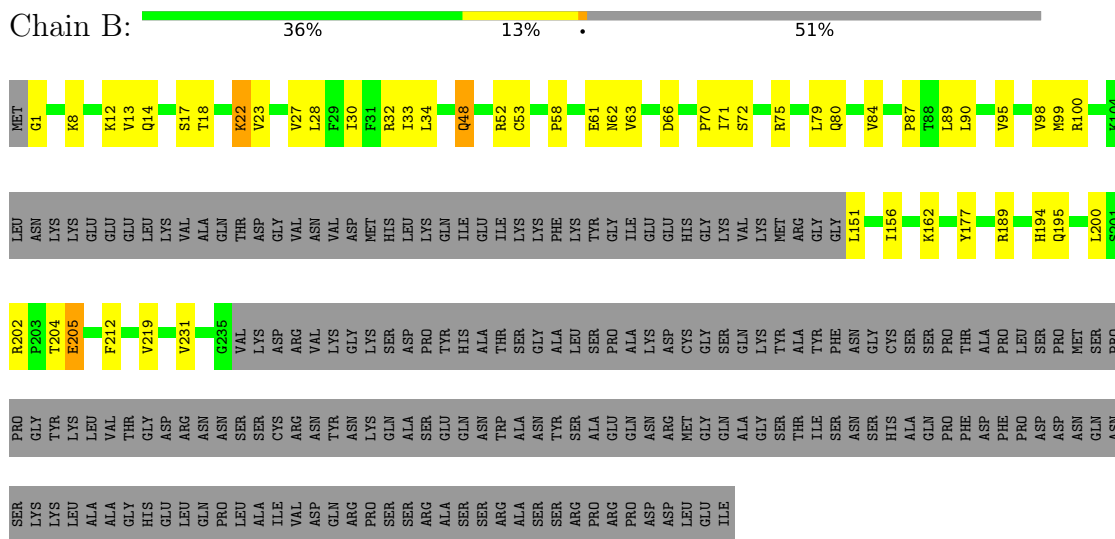
3 Residue-property plots

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: Gap junction alpha-1 protein

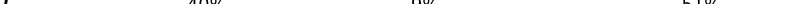


• Molecule 1: Gap junction alpha-1 protein

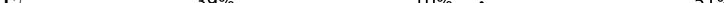


• Molecule 1: Gap junction alpha-1 protein

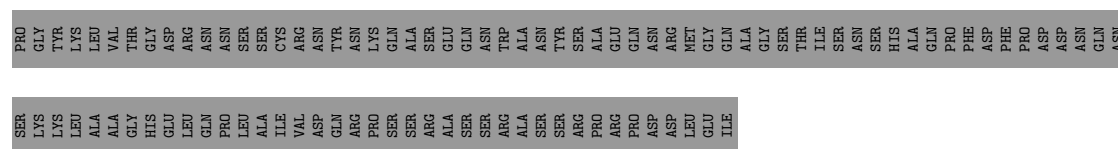
VAL	ARG	ARG	LYS	MET
ASP	ASN	VAL	VAL	G1
GLN	TYR	LYS	ALA	K8
ARG	ASN	GLY	GLN	D11
PRO	LYS	LYS	THR	K12
SER	GLN	SER	ASP	V13
SER	ALA	ASP	GLY	Q14
ARG	SER	PRO	VAL	ASN
ALA	GLU	TYR	ASN	VAL
SER	GLN	HIS	VAL	S17
SER	ASN	ALA	ASP	T18
ARG	TRP	THR	MET	T18
ALA	ALA	SER	HIS	K22
SER	ASN	GLY	LEU	V23
SER	TYR	ALA	LYS	Q22
ARG	SER	LEU	GLN	L28
PRO	ALA	SER	ILE	L28
ARG	GLU	PRO	GLU	R32
PRO	GLN	ALA	ILE	I33
ASP	ASN	LYS	LYS	L34
ASP	ARG	ASP	PHE	R52
LEU	MET	CYS	LYS	R52
GLU	GLY	GLY	THR	Q56
ILE	GLN	SER	GLY	N62
	ALA	GLN	ILE	V63
	GLY	LYS	GLU	D66
	THR	ALA	HIS	I71
	ILE	PHE	GLY	S72
	SER	ASN	LYS	R75
	ASN	CYS	MET	L79
	HIS	SER	ARG	Q80
	ALA	THR	GLY	V84
	GLN	PRO	GLY	P87
	PRO	THR	GLY	T88
	PHE	ALA	L151	L89
	PHE	PRO	I156	V95
	ASP	LEU	I162	F96
	ASP	SER	K162	Y97
	ASN	MET	Y177	V98
	GLN	SER	R189	M99
	ASN	PRO	D190	K104
	SER	GLY	R202	LEU
	LYS	TYR	LYS	ASN
	LEU	LEU	VAL	LYS
	ALA	ALA	E205	GLU
	ALA	THR	V219	GLU
	GLY	GLY	ASP	ASN
	HIS	THR	ARG	LYS
	GLU	ASP	V231	LYS
	LEU	GLN	ASN	GLU
	PRO	PRO	G235	GLU
	LEU	SER	VAL	GLU
	ALA	THR	LYS	TYR
	TYR	CYS	LYS	LEU
	ILE	SER	LYS	TYR

- Chain D: 

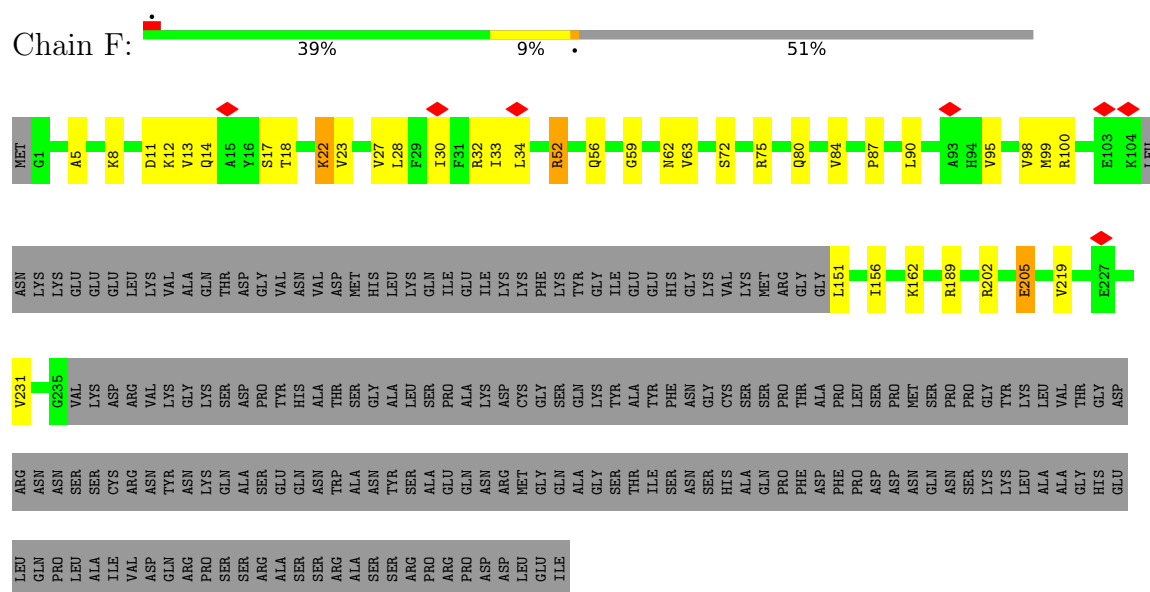
[illegible]

- Chain E:  39% 10% 51%

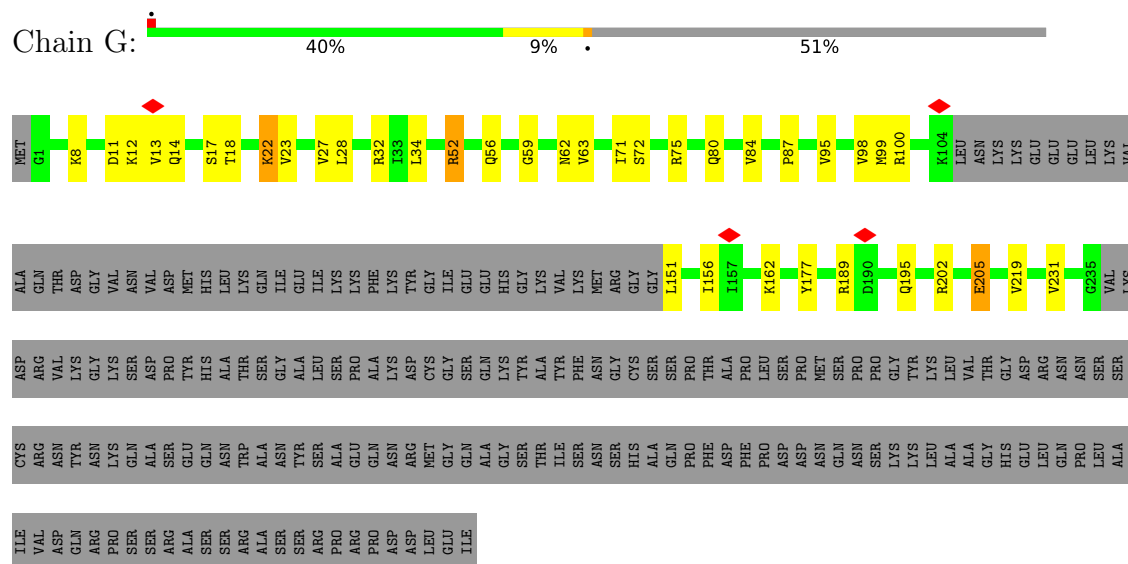
Protein	Category	Score
E205	Protein	0.95
V219	Protein	0.90
L223	Protein	0.85
E227	Protein	0.80
V231	Protein	0.75
G235	Protein	0.70
V231	Protein	0.65
V231	Protein	0.60
V231	Protein	0.55
V231	Protein	0.50
V231	Protein	0.45
V231	Protein	0.40
V231	Protein	0.35
V231	Protein	0.30
V231	Protein	0.25
V231	Protein	0.20
V231	Protein	0.15
V231	Protein	0.10
V231	Protein	0.05
V231	Protein	0.00
V231	Protein	-0.05
V231	Protein	-0.10
V231	Protein	-0.15
V231	Protein	-0.20
V231	Protein	-0.25
V231	Protein	-0.30
V231	Protein	-0.35
V231	Protein	-0.40
V231	Protein	-0.45
V231	Protein	-0.50
V231	Protein	-0.55
V231	Protein	-0.60
V231	Protein	-0.65
V231	Protein	-0.70
V231	Protein	-0.75
V231	Protein	-0.80
V231	Protein	-0.85
V231	Protein	-0.90
V231	Protein	-0.95
V231	Protein	-1.00
V231	Protein	-1.05
V231	Protein	-1.10
V231	Protein	-1.15
V231	Protein	-1.20
V231	Protein	-1.25
V231	Protein	-1.30
V231	Protein	-1.35
V231	Protein	-1.40
V231	Protein	-1.45
V231	Protein	-1.50
V231	Protein	-1.55
V231	Protein	-1.60
V231	Protein	-1.65
V231	Protein	-1.70
V231	Protein	-1.75
V231	Protein	-1.80
V231	Protein	-1.85
V231	Protein	-1.90
V231	Protein	-1.95
V231	Protein	-2.00
V231	Protein	-2.05
V231	Protein	-2.10
V231	Protein	-2.15
V231	Protein	-2.20
V231	Protein	-2.25
V231	Protein	-2.30
V231	Protein	-2.35
V231	Protein	-2.40
V231	Protein	-2.45
V231	Protein	-2.50
V231	Protein	-2.55
V231	Protein	-2.60
V231	Protein	-2.65
V231	Protein	-2.70
V231	Protein	-2.75
V231	Protein	-2.80
V231	Protein	-2.85
V231	Protein	-2.90
V231	Protein	-2.95
V231	Protein	-3.00
V231	Protein	-3.05
V231	Protein	-3.10
V231	Protein	-3.15
V231	Protein	-3.20
V231	Protein	-3.25
V231	Protein	-3.30
V231	Protein	-3.35
V231	Protein	-3.40
V231	Protein	-3.45
V231	Protein	-3.50
V231	Protein	-3.55
V231	Protein	-3.60
V231	Protein	-3.65
V231	Protein	-3.70
V231	Protein	-3.75
V231	Protein	-3.80
V231	Protein	-3.85
V231	Protein	-3.90
V231	Protein	-3.95
V231	Protein	-4.00
V231	Protein	-4.05
V231	Protein	-4.10
V231	Protein	-4.15
V231	Protein	-4.20
V231	Protein	-4.25
V231	Protein	-4.30
V231	Protein	-4.35
V231	Protein	-4.40
V231	Protein	-4.45
V231	Protein	-4.50
V231	Protein	-4.55
V231	Protein	-4.60
V231	Protein	-4.65
V231	Protein	-4.70
V231	Protein	-4.75
V231	Protein	-4.80
V231	Protein	-4.85
V231	Protein	-4.90
V231	Protein	-4.95
V231	Protein	-5.00
V231	Protein	-5.05
V231	Protein	-5.10
V231	Protein	-5.15
V231	Protein	-5.20
V231	Protein	-5.25
V231	Protein	-5.30
V231	Protein	-5.35
V231	Protein	-5.40
V231	Protein	-5.45
V231	Protein	-5.50
V231	Protein	-5.55
V231	Protein	-5.60
V231	Protein	-5.65
V231	Protein	-5.70
V231	Protein	-5.75
V231	Protein	-5.80
V231	Protein	-5.85
V231	Protein	-5.90
V231	Protein	-5.95
V231	Protein	-6



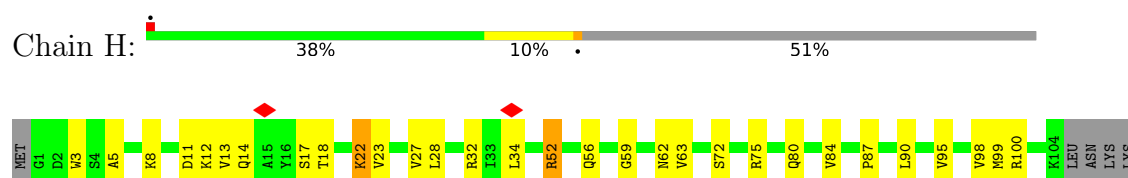
• Molecule 1: Gap junction alpha-1 protein



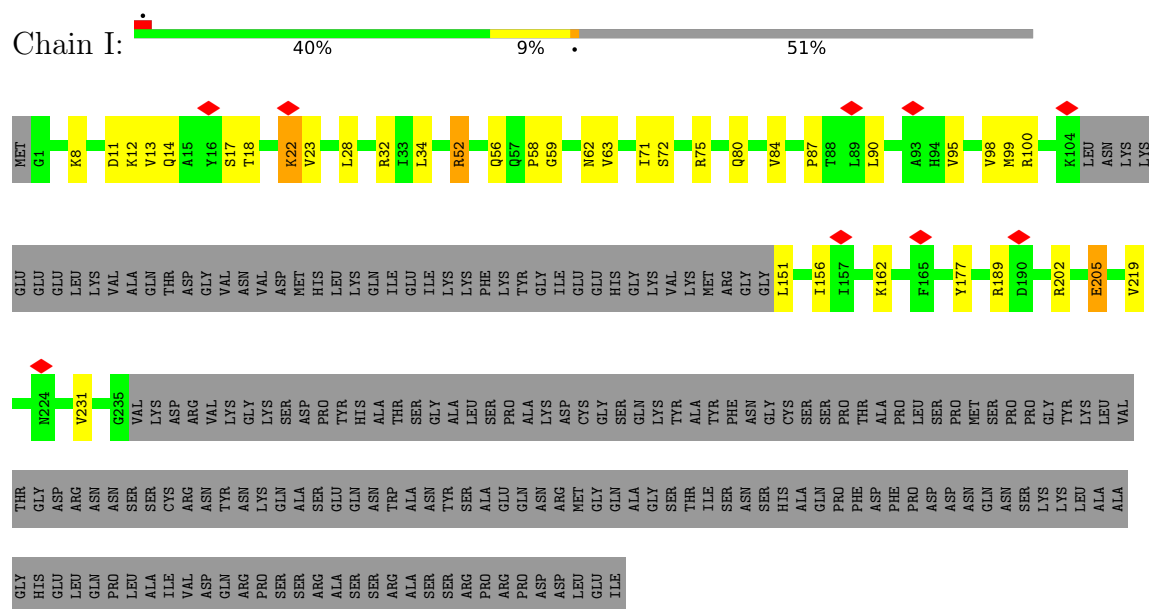
• Molecule 1: Gap junction alpha-1 protein



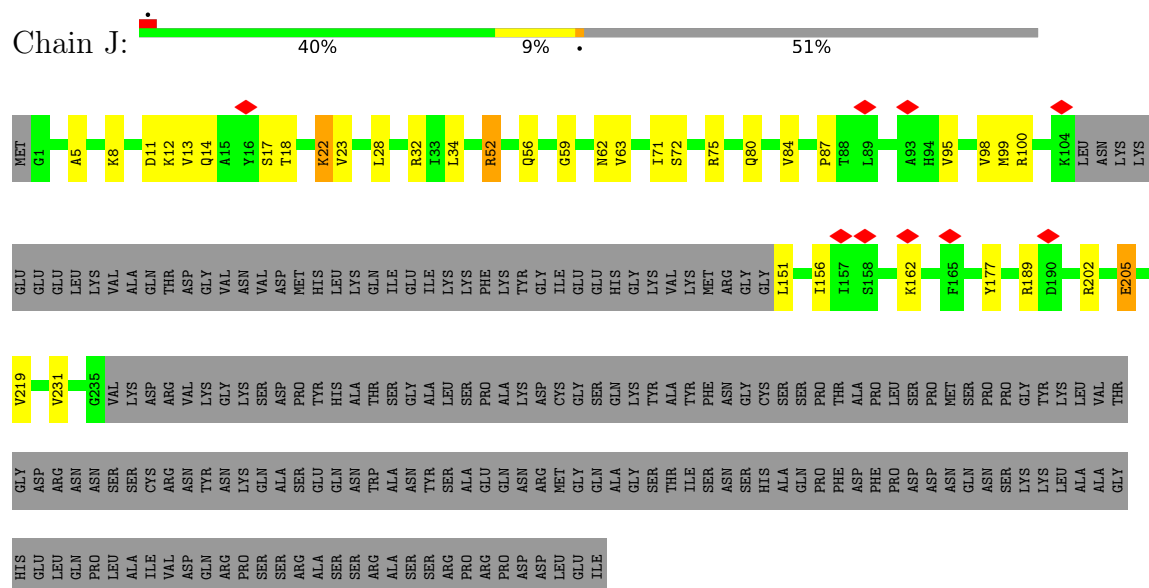
• Molecule 1: Gap junction alpha-1 protein



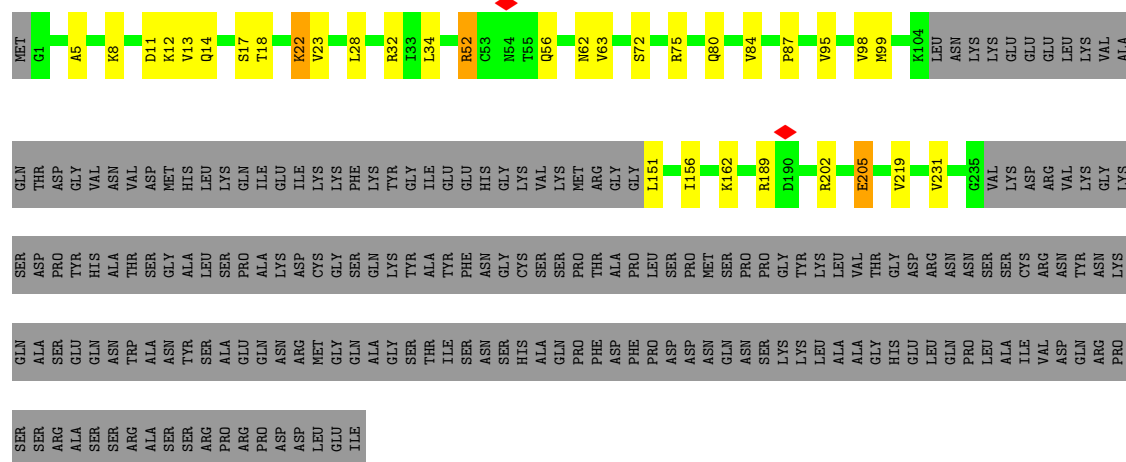
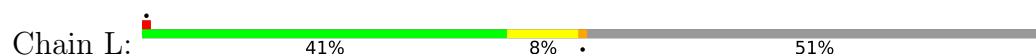
- Molecule 1: Gap junction alpha-1 protein



- Molecule 1: Gap junction alpha-1 protein



Chain K:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28940	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.015	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	249.91118, 249.91118, 249.91118	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.65081036, 0.65081036, 0.65081036	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	0.15	0/1584	0.29	0/2150
1	B	0.15	0/1584	0.28	0/2150
1	C	0.15	0/1584	0.28	0/2150
1	D	0.15	0/1584	0.28	0/2150
1	E	0.15	0/1584	0.28	0/2150
1	F	0.15	0/1584	0.28	0/2150
1	G	0.15	0/1584	0.28	0/2150
1	H	0.15	0/1584	0.28	0/2150
1	I	0.15	0/1584	0.29	0/2150
1	J	0.15	0/1584	0.28	0/2150
1	K	0.15	0/1584	0.28	0/2150
1	L	0.15	0/1584	0.28	0/2150
All	All	0.15	0/19008	0.28	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	1567	64	0
1	B	1541	0	1567	58	0
1	C	1541	0	1567	31	0
1	D	1541	0	1567	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1541	0	1567	34	0
1	F	1541	0	1567	32	0
1	G	1541	0	1567	32	0
1	H	1541	0	1567	53	0
1	I	1541	0	1567	35	0
1	J	1541	0	1567	31	0
1	K	1541	0	1567	65	0
1	L	1541	0	1567	27	0
All	All	18492	0	18804	368	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 10.

All (368) 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:62:ASN:H	1:H:52:ARG:NH2	1.43	1.16
1:B:204:THR:OG1	1:C:66:ASP:OD1	1.74	1.05
1:A:66:ASP:OD1	1:K:204:THR:OG1	1.80	0.98
1:A:62:ASN:ND2	1:K:200:LEU:O	1.96	0.97
1:B:62:ASN:H	1:H:52:ARG:HH21	1.00	0.95
1:B:62:ASN:N	1:H:52:ARG:HH21	1.67	0.91
1:B:62:ASN:N	1:H:52:ARG:NH2	2.19	0.90
1:A:97:TYR:HE2	1:K:22:LYS:HE2	1.37	0.88
1:A:12:LYS:HE3	1:A:99:MET:HG3	1.63	0.81
1:C:12:LYS:HE3	1:C:99:MET:HG3	1.63	0.81
1:H:12:LYS:HE3	1:H:99:MET:HG3	1.63	0.81
1:I:12:LYS:HE3	1:I:99:MET:HG3	1.63	0.81
1:L:12:LYS:HE3	1:L:99:MET:HG3	1.63	0.81
1:D:12:LYS:HE3	1:D:99:MET:HG3	1.63	0.81
1:J:12:LYS:HE3	1:J:99:MET:HG3	1.63	0.81
1:A:59:GLY:H	1:K:52:ARG:NH1	1.80	0.80
1:F:12:LYS:HE3	1:F:99:MET:HG3	1.63	0.80
1:E:12:LYS:HE3	1:E:99:MET:HG3	1.63	0.80
1:K:12:LYS:HE3	1:K:99:MET:HG3	1.63	0.80
1:G:12:LYS:HE3	1:G:99:MET:HG3	1.63	0.80
1:B:12:LYS:HE3	1:B:99:MET:HG3	1.63	0.80
1:A:61:GLU:H	1:K:52:ARG:NH2	1.80	0.80
1:A:61:GLU:N	1:K:52:ARG:NH2	2.31	0.79
1:B:70:PRO:O	1:H:205:GLU:HG2	1.86	0.75
1:B:72:SER:HB3	1:B:75:ARG:HD2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:CYS:N	1:K:52:ARG:HH22	1.85	0.74
1:G:72:SER:HB3	1:G:75:ARG:HD2	1.70	0.74
1:B:100:ARG:NH2	1:H:11:ASP:OD2	2.20	0.73
1:C:72:SER:HB3	1:C:75:ARG:HD2	1.70	0.73
1:I:72:SER:HB3	1:I:75:ARG:HD2	1.70	0.73
1:D:52:ARG:HH12	1:E:59:GLY:H	1.36	0.73
1:C:52:ARG:HH12	1:D:59:GLY:H	1.37	0.73
1:I:52:ARG:HH12	1:J:59:GLY:H	1.37	0.73
1:H:72:SER:HB3	1:H:75:ARG:HD2	1.70	0.73
1:L:72:SER:HB3	1:L:75:ARG:HD2	1.70	0.73
1:J:52:ARG:HH12	1:K:59:GLY:H	1.37	0.72
1:J:72:SER:HB3	1:J:75:ARG:HD2	1.70	0.72
1:D:72:SER:HB3	1:D:75:ARG:HD2	1.70	0.72
1:A:72:SER:HB3	1:A:75:ARG:HD2	1.70	0.72
1:G:52:ARG:HH12	1:I:59:GLY:H	1.37	0.72
1:E:52:ARG:HH12	1:F:59:GLY:H	1.36	0.72
1:E:72:SER:HB3	1:E:75:ARG:HD2	1.70	0.72
1:K:72:SER:HB3	1:K:75:ARG:HD2	1.70	0.72
1:F:72:SER:HB3	1:F:75:ARG:HD2	1.70	0.71
1:F:52:ARG:HH12	1:H:59:GLY:H	1.36	0.70
1:G:59:GLY:H	1:L:52:ARG:HH12	1.36	0.70
1:A:52:ARG:HH21	1:L:62:ASN:CG	1.99	0.70
1:B:156:ILE:HD11	1:B:231:VAL:HG11	1.74	0.70
1:G:156:ILE:HD11	1:G:231:VAL:HG11	1.73	0.70
1:B:58:PRO:HD3	1:I:58:PRO:HD3	1.74	0.70
1:C:156:ILE:HD11	1:C:231:VAL:HG11	1.73	0.70
1:I:156:ILE:HD11	1:I:231:VAL:HG11	1.73	0.69
1:C:18:THR:O	1:C:22:LYS:NZ	2.24	0.69
1:L:18:THR:O	1:L:22:LYS:NZ	2.24	0.69
1:E:156:ILE:HD11	1:E:231:VAL:HG11	1.74	0.69
1:K:156:ILE:HD11	1:K:231:VAL:HG11	1.73	0.69
1:I:18:THR:O	1:I:22:LYS:NZ	2.24	0.69
1:H:156:ILE:HD11	1:H:231:VAL:HG11	1.73	0.69
1:L:156:ILE:HD11	1:L:231:VAL:HG11	1.73	0.69
1:F:156:ILE:HD11	1:F:231:VAL:HG11	1.73	0.69
1:A:156:ILE:HD11	1:A:231:VAL:HG11	1.73	0.69
1:D:156:ILE:HD11	1:D:231:VAL:HG11	1.73	0.69
1:J:156:ILE:HD11	1:J:231:VAL:HG11	1.73	0.69
1:E:18:THR:O	1:E:22:LYS:NZ	2.24	0.68
1:K:18:THR:O	1:K:22:LYS:NZ	2.24	0.68
1:A:59:GLY:HA3	1:K:199:PHE:CD2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LEU:HD21	1:H:27:VAL:HG11	1.75	0.67
1:B:18:THR:O	1:B:22:LYS:NZ	2.24	0.66
1:H:56:GLN:HG3	1:I:56:GLN:HG3	1.77	0.66
1:C:56:GLN:HG3	1:L:56:GLN:HG3	1.77	0.66
1:A:84:VAL:O	1:A:162:LYS:NZ	2.29	0.66
1:E:84:VAL:O	1:E:162:LYS:NZ	2.29	0.66
1:K:84:VAL:O	1:K:162:LYS:NZ	2.29	0.66
1:C:84:VAL:O	1:C:162:LYS:NZ	2.29	0.66
1:F:84:VAL:O	1:F:162:LYS:NZ	2.29	0.66
1:G:18:THR:O	1:G:22:LYS:NZ	2.24	0.66
1:H:84:VAL:O	1:H:162:LYS:NZ	2.29	0.66
1:I:84:VAL:O	1:I:162:LYS:NZ	2.29	0.66
1:J:17:SER:HB3	1:J:22:LYS:HD3	1.77	0.66
1:L:84:VAL:O	1:L:162:LYS:NZ	2.29	0.66
1:A:75:ARG:HH21	1:K:43:ALA:N	1.93	0.66
1:D:17:SER:HB3	1:D:22:LYS:HD3	1.77	0.66
1:H:17:SER:HB3	1:H:22:LYS:HD3	1.77	0.66
1:L:17:SER:HB3	1:L:22:LYS:HD3	1.77	0.66
1:D:84:VAL:O	1:D:162:LYS:NZ	2.29	0.66
1:F:14:GLN:HB2	1:F:22:LYS:HD2	1.78	0.66
1:J:84:VAL:O	1:J:162:LYS:NZ	2.29	0.66
1:A:14:GLN:HB2	1:A:22:LYS:HD2	1.78	0.66
1:B:204:THR:HG23	1:C:66:ASP:OD2	1.96	0.66
1:C:17:SER:HB3	1:C:22:LYS:HD3	1.77	0.65
1:F:56:GLN:HG3	1:J:56:GLN:HG3	1.77	0.65
1:B:84:VAL:O	1:B:162:LYS:NZ	2.29	0.65
1:I:17:SER:HB3	1:I:22:LYS:HD3	1.77	0.65
1:G:84:VAL:O	1:G:162:LYS:NZ	2.29	0.65
1:B:72:SER:N	1:H:205:GLU:OE1	2.25	0.65
1:G:17:SER:HB3	1:G:22:LYS:HD3	1.77	0.65
1:E:14:GLN:HB2	1:E:22:LYS:HD2	1.78	0.65
1:E:56:GLN:HG3	1:K:56:GLN:HG3	1.77	0.65
1:A:61:GLU:H	1:K:52:ARG:HH22	1.44	0.65
1:B:17:SER:HB3	1:B:22:LYS:HD3	1.77	0.65
1:K:14:GLN:HB2	1:K:22:LYS:HD2	1.78	0.65
1:J:14:GLN:HB2	1:J:22:LYS:HD2	1.78	0.65
1:F:17:SER:HB3	1:F:22:LYS:HD3	1.77	0.65
1:A:17:SER:HB3	1:A:22:LYS:HD3	1.77	0.65
1:D:14:GLN:HB2	1:D:22:LYS:HD2	1.78	0.65
1:C:14:GLN:HB2	1:C:22:LYS:HD2	1.78	0.64
1:I:14:GLN:HB2	1:I:22:LYS:HD2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:HIS:HB2	1:G:195:GLN:NE2	2.11	0.64
1:D:18:THR:O	1:D:22:LYS:NZ	2.24	0.64
1:F:18:THR:O	1:F:22:LYS:NZ	2.24	0.64
1:J:18:THR:O	1:J:22:LYS:NZ	2.24	0.64
1:K:17:SER:HB3	1:K:22:LYS:HD3	1.77	0.64
1:E:17:SER:HB3	1:E:22:LYS:HD3	1.77	0.64
1:G:14:GLN:HB2	1:G:22:LYS:HD2	1.78	0.64
1:H:18:THR:O	1:H:22:LYS:NZ	2.24	0.64
1:L:14:GLN:HB2	1:L:22:LYS:HD2	1.78	0.64
1:A:18:THR:O	1:A:22:LYS:NZ	2.24	0.64
1:H:14:GLN:HB2	1:H:22:LYS:HD2	1.78	0.63
1:B:14:GLN:HB2	1:B:22:LYS:HD2	1.78	0.63
1:A:56:GLN:HG3	1:D:56:GLN:HG3	1.82	0.62
1:A:61:GLU:N	1:K:52:ARG:HH22	1.99	0.61
1:A:75:ARG:HB3	1:K:209:PHE:HZ	1.66	0.60
1:G:11:ASP:OD2	1:I:100:ARG:NH2	2.35	0.60
1:A:75:ARG:NH2	1:K:42:SER:OG	2.35	0.60
1:G:100:ARG:NH2	1:L:11:ASP:OD2	2.35	0.60
1:I:11:ASP:OD2	1:J:100:ARG:NH2	2.35	0.60
1:F:11:ASP:OD2	1:H:100:ARG:NH2	2.35	0.60
1:C:11:ASP:OD2	1:D:100:ARG:NH2	2.35	0.59
1:E:11:ASP:OD2	1:F:100:ARG:NH2	2.35	0.59
1:B:66:ASP:OD2	1:H:203:PRO:HD2	2.03	0.59
1:J:11:ASP:OD2	1:K:100:ARG:NH2	2.35	0.59
1:A:75:ARG:HD3	1:K:209:PHE:CE2	2.38	0.58
1:D:11:ASP:OD2	1:E:100:ARG:NH2	2.35	0.58
1:B:53:CYS:O	1:G:56:GLN:OE1	2.22	0.57
1:A:59:GLY:H	1:K:52:ARG:HH12	1.52	0.56
1:A:75:ARG:HH21	1:K:42:SER:C	2.14	0.56
1:A:89:LEU:HD23	1:K:27:VAL:HG23	1.86	0.56
1:A:62:ASN:CG	1:K:200:LEU:O	2.48	0.56
1:A:59:GLY:C	1:K:52:ARG:HH22	2.14	0.56
1:A:59:GLY:HA3	1:K:199:PHE:CE2	2.42	0.55
1:B:62:ASN:HD21	1:H:199:PHE:HB2	1.71	0.55
1:A:75:ARG:HE	1:K:43:ALA:HB2	1.71	0.55
1:B:71:ILE:HA	1:H:205:GLU:CD	2.32	0.54
1:B:90:LEU:CD2	1:H:27:VAL:HG11	2.38	0.54
1:G:71:ILE:O	1:G:177:TYR:OH	2.23	0.54
1:I:71:ILE:O	1:I:177:TYR:OH	2.23	0.54
1:E:98:VAL:HG21	1:E:151:LEU:HD21	1.90	0.53
1:K:98:VAL:HG21	1:K:151:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:LEU:HD23	1:H:27:VAL:HG23	1.91	0.53
1:B:70:PRO:HA	1:H:204:THR:OG1	2.09	0.53
1:H:98:VAL:HG21	1:H:151:LEU:HD21	1.91	0.53
1:L:98:VAL:HG21	1:L:151:LEU:HD21	1.91	0.53
1:A:97:TYR:CE2	1:K:22:LYS:HE2	2.29	0.52
1:A:98:VAL:HG21	1:A:151:LEU:HD21	1.90	0.52
1:B:58:PRO:HG2	1:I:56:GLN:HB3	1.91	0.52
1:B:98:VAL:HG21	1:B:151:LEU:HD21	1.90	0.52
1:A:59:GLY:C	1:K:52:ARG:NH2	2.68	0.52
1:F:98:VAL:HG21	1:F:151:LEU:HD21	1.90	0.52
1:B:200:LEU:O	1:C:62:ASN:ND2	2.43	0.52
1:A:63:VAL:HG12	1:K:183:ALA:HB1	1.91	0.52
1:A:65:TYR:HE2	1:K:202:ARG:CG	2.22	0.52
1:B:62:ASN:CG	1:H:52:ARG:HH21	2.17	0.52
1:G:98:VAL:HG21	1:G:151:LEU:HD21	1.90	0.52
1:C:98:VAL:HG21	1:C:151:LEU:HD21	1.90	0.52
1:D:98:VAL:HG21	1:D:151:LEU:HD21	1.91	0.52
1:I:98:VAL:HG21	1:I:151:LEU:HD21	1.90	0.52
1:J:98:VAL:HG21	1:J:151:LEU:HD21	1.91	0.52
1:B:62:ASN:OD1	1:B:63:VAL:N	2.44	0.51
1:G:62:ASN:OD1	1:G:63:VAL:N	2.44	0.51
1:C:62:ASN:OD1	1:C:63:VAL:N	2.44	0.51
1:I:62:ASN:OD1	1:I:63:VAL:N	2.44	0.51
1:D:62:ASN:OD1	1:D:63:VAL:N	2.44	0.51
1:E:62:ASN:OD1	1:E:63:VAL:N	2.44	0.51
1:J:62:ASN:OD1	1:J:63:VAL:N	2.44	0.51
1:K:62:ASN:OD1	1:K:63:VAL:N	2.44	0.51
1:A:62:ASN:OD1	1:A:63:VAL:N	2.44	0.51
1:D:52:ARG:HH21	1:E:62:ASN:CG	2.20	0.51
1:L:62:ASN:OD1	1:L:63:VAL:N	2.44	0.51
1:B:61:GLU:HB2	1:H:52:ARG:CZ	2.41	0.50
1:H:62:ASN:OD1	1:H:63:VAL:N	2.44	0.50
1:A:97:TYR:HE2	1:K:22:LYS:CE	2.18	0.50
1:B:79:LEU:HD11	1:H:209:PHE:CE1	2.46	0.50
1:E:52:ARG:HH21	1:F:62:ASN:CG	2.19	0.50
1:F:62:ASN:OD1	1:F:63:VAL:N	2.44	0.50
1:C:52:ARG:HH21	1:D:62:ASN:CG	2.20	0.50
1:J:52:ARG:HH21	1:K:62:ASN:CG	2.20	0.50
1:I:52:ARG:HH21	1:J:62:ASN:CG	2.20	0.50
1:F:52:ARG:HH21	1:H:62:ASN:CG	2.20	0.50
1:G:52:ARG:HH21	1:I:62:ASN:CG	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:62:ASN:CG	1:L:52:ARG:HH21	2.20	0.50
1:A:75:ARG:HD3	1:K:209:PHE:HE2	1.76	0.49
1:B:28:LEU:HD11	1:B:219:VAL:HG23	1.95	0.49
1:G:28:LEU:HD11	1:G:219:VAL:HG23	1.95	0.49
1:A:82:ILE:HD11	1:K:31:PHE:HA	1.94	0.49
1:B:75:ARG:HB3	1:H:209:PHE:HZ	1.76	0.49
1:H:63:VAL:O	1:H:189:ARG:NH1	2.46	0.49
1:K:63:VAL:O	1:K:189:ARG:NH1	2.46	0.48
1:L:63:VAL:O	1:L:189:ARG:NH1	2.46	0.48
1:B:61:GLU:N	1:H:52:ARG:HH22	2.11	0.48
1:E:63:VAL:O	1:E:189:ARG:NH1	2.46	0.48
1:H:28:LEU:HD11	1:H:219:VAL:HG23	1.95	0.48
1:L:28:LEU:HD11	1:L:219:VAL:HG23	1.95	0.48
1:B:63:VAL:O	1:B:189:ARG:NH1	2.46	0.48
1:B:72:SER:N	1:H:205:GLU:CD	2.72	0.48
1:I:28:LEU:HD11	1:I:219:VAL:HG23	1.95	0.48
1:G:63:VAL:O	1:G:189:ARG:NH1	2.46	0.48
1:J:63:VAL:O	1:J:189:ARG:NH1	2.46	0.48
1:A:63:VAL:O	1:A:189:ARG:NH1	2.46	0.48
1:D:28:LEU:HD11	1:D:219:VAL:HG23	1.95	0.48
1:D:63:VAL:O	1:D:189:ARG:NH1	2.46	0.48
1:F:63:VAL:O	1:F:189:ARG:NH1	2.46	0.48
1:C:28:LEU:HD11	1:C:219:VAL:HG23	1.95	0.48
1:E:28:LEU:HD11	1:E:219:VAL:HG23	1.95	0.48
1:J:28:LEU:HD11	1:J:219:VAL:HG23	1.95	0.48
1:B:58:PRO:CD	1:I:58:PRO:HD3	2.44	0.48
1:K:28:LEU:HD11	1:K:219:VAL:HG23	1.95	0.48
1:C:63:VAL:O	1:C:189:ARG:NH1	2.46	0.48
1:I:63:VAL:O	1:I:189:ARG:NH1	2.46	0.48
1:B:62:ASN:H	1:H:52:ARG:CZ	2.20	0.48
1:E:13:VAL:HG22	1:E:95:VAL:HG11	1.96	0.47
1:K:13:VAL:HG22	1:K:95:VAL:HG11	1.96	0.47
1:J:13:VAL:HG22	1:J:95:VAL:HG11	1.96	0.47
1:A:75:ARG:NH2	1:K:42:SER:CB	2.78	0.47
1:D:13:VAL:HG22	1:D:95:VAL:HG11	1.96	0.47
1:K:71:ILE:O	1:K:177:TYR:OH	2.23	0.47
1:B:13:VAL:HG22	1:B:95:VAL:HG11	1.96	0.47
1:F:28:LEU:HD11	1:F:219:VAL:HG23	1.95	0.47
1:B:58:PRO:HG2	1:I:56:GLN:O	2.15	0.47
1:E:71:ILE:O	1:E:177:TYR:OH	2.23	0.47
1:G:13:VAL:HG22	1:G:95:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:VAL:HG22	1:F:95:VAL:HG11	1.96	0.47
1:L:13:VAL:HG22	1:L:95:VAL:HG11	1.96	0.47
1:L:84:VAL:O	1:L:87:PRO:HD2	2.15	0.47
1:A:13:VAL:HG22	1:A:95:VAL:HG11	1.96	0.47
1:A:28:LEU:HD11	1:A:219:VAL:HG23	1.95	0.47
1:G:84:VAL:O	1:G:87:PRO:HD2	2.15	0.47
1:H:13:VAL:HG22	1:H:95:VAL:HG11	1.96	0.47
1:C:84:VAL:O	1:C:87:PRO:HD2	2.15	0.47
1:H:84:VAL:O	1:H:87:PRO:HD2	2.15	0.47
1:I:84:VAL:O	1:I:87:PRO:HD2	2.15	0.47
1:B:71:ILE:O	1:B:177:TYR:OH	2.23	0.47
1:B:84:VAL:O	1:B:87:PRO:HD2	2.15	0.47
1:C:13:VAL:HG22	1:C:95:VAL:HG11	1.96	0.47
1:I:13:VAL:HG22	1:I:95:VAL:HG11	1.96	0.47
1:E:84:VAL:O	1:E:87:PRO:HD2	2.15	0.46
1:K:84:VAL:O	1:K:87:PRO:HD2	2.15	0.46
1:A:84:VAL:O	1:A:87:PRO:HD2	2.15	0.46
1:F:84:VAL:O	1:F:87:PRO:HD2	2.15	0.46
1:B:22:LYS:HE2	1:C:97:TYR:HE2	1.80	0.46
1:A:59:GLY:CA	1:K:199:PHE:CD2	2.99	0.46
1:D:84:VAL:O	1:D:87:PRO:HD2	2.15	0.46
1:J:84:VAL:O	1:J:87:PRO:HD2	2.15	0.46
1:A:52:ARG:HH21	1:L:62:ASN:ND2	2.12	0.46
1:A:71:ILE:O	1:A:177:TYR:OH	2.23	0.46
1:B:75:ARG:NH2	1:H:202:ARG:HH22	2.14	0.46
1:C:71:ILE:O	1:C:177:TYR:OH	2.23	0.45
1:D:71:ILE:O	1:D:177:TYR:OH	2.23	0.45
1:J:71:ILE:O	1:J:177:TYR:OH	2.23	0.45
1:A:48:GLN:HG2	1:K:46:ASP:OD2	2.16	0.45
1:A:65:TYR:HE2	1:K:202:ARG:HG3	1.82	0.44
1:B:27:VAL:HG23	1:C:89:LEU:HD23	1.98	0.44
1:B:212:PHE:HE2	1:C:79:LEU:HD22	1.83	0.44
1:A:66:ASP:CG	1:K:204:THR:H	2.25	0.44
1:D:84:VAL:HG13	1:D:162:LYS:HG3	2.00	0.44
1:I:84:VAL:HG13	1:I:162:LYS:HG3	2.00	0.44
1:J:84:VAL:HG13	1:J:162:LYS:HG3	2.00	0.44
1:C:84:VAL:HG13	1:C:162:LYS:HG3	2.00	0.43
1:D:52:ARG:NH1	1:E:59:GLY:H	2.11	0.43
1:E:84:VAL:HG13	1:E:162:LYS:HG3	2.00	0.43
1:J:52:ARG:NH1	1:K:59:GLY:H	2.12	0.43
1:K:84:VAL:HG13	1:K:162:LYS:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:VAL:HG13	1:A:162:LYS:HG3	2.00	0.43
1:C:189:ARG:HD2	1:C:189:ARG:HA	1.91	0.43
1:K:22:LYS:H	1:K:22:LYS:HG2	1.62	0.43
1:B:84:VAL:HG13	1:B:162:LYS:HG3	2.00	0.43
1:E:52:ARG:NH1	1:F:59:GLY:H	2.11	0.43
1:F:84:VAL:HG13	1:F:162:LYS:HG3	2.00	0.43
1:G:84:VAL:HG13	1:G:162:LYS:HG3	2.00	0.43
1:I:189:ARG:HD2	1:I:189:ARG:HA	1.91	0.43
1:H:84:VAL:HG13	1:H:162:LYS:HG3	2.00	0.43
1:L:84:VAL:HG13	1:L:162:LYS:HG3	2.00	0.43
1:D:8:LYS:O	1:D:12:LYS:HG2	2.19	0.42
1:A:189:ARG:HD2	1:A:189:ARG:HA	1.91	0.42
1:B:66:ASP:CG	1:H:203:PRO:HD2	2.43	0.42
1:H:22:LYS:H	1:H:22:LYS:HG2	1.62	0.42
1:J:8:LYS:O	1:J:12:LYS:HG2	2.19	0.42
1:L:22:LYS:H	1:L:22:LYS:HG2	1.62	0.42
1:E:22:LYS:H	1:E:22:LYS:HG2	1.62	0.42
1:B:48:GLN:HA	1:B:48:GLN:HE21	1.83	0.42
1:I:52:ARG:NH1	1:J:59:GLY:H	2.12	0.42
1:B:8:LYS:O	1:B:12:LYS:HG2	2.19	0.42
1:F:52:ARG:NH1	1:H:59:GLY:H	2.11	0.42
1:G:8:LYS:O	1:G:12:LYS:HG2	2.19	0.42
1:H:8:LYS:O	1:H:12:LYS:HG2	2.19	0.42
1:L:8:LYS:O	1:L:12:LYS:HG2	2.19	0.42
1:A:65:TYR:CE2	1:K:202:ARG:HG3	2.55	0.42
1:C:52:ARG:NH1	1:D:59:GLY:H	2.12	0.42
1:A:22:LYS:H	1:A:22:LYS:HG2	1.62	0.42
1:A:75:ARG:CZ	1:K:42:SER:OG	2.67	0.42
1:B:61:GLU:N	1:H:52:ARG:NH2	2.68	0.42
1:A:202:ARG:HB3	1:A:205:GLU:HG3	2.03	0.41
1:F:202:ARG:HB3	1:F:205:GLU:HG3	2.03	0.41
1:K:32:ARG:HH12	1:K:80:GLN:HE21	1.67	0.41
1:B:32:ARG:HH12	1:B:80:GLN:HE21	1.67	0.41
1:E:32:ARG:HH12	1:E:80:GLN:HE21	1.67	0.41
1:G:27:VAL:HG11	1:I:90:LEU:HD21	2.02	0.41
1:K:8:LYS:O	1:K:12:LYS:HG2	2.19	0.41
1:A:75:ARG:CB	1:K:209:PHE:HZ	2.32	0.41
1:C:202:ARG:HB3	1:C:205:GLU:HG3	2.03	0.41
1:G:32:ARG:HH12	1:G:80:GLN:HE21	1.67	0.41
1:J:32:ARG:HH12	1:J:80:GLN:HE21	1.67	0.41
1:D:32:ARG:HH12	1:D:80:GLN:HE21	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:LYS:O	1:E:12:LYS:HG2	2.19	0.41
1:I:202:ARG:HB3	1:I:205:GLU:HG3	2.03	0.41
1:A:8:LYS:O	1:A:12:LYS:HG2	2.19	0.41
1:F:8:LYS:O	1:F:12:LYS:HG2	2.19	0.41
1:I:8:LYS:O	1:I:12:LYS:HG2	2.19	0.41
1:C:8:LYS:O	1:C:12:LYS:HG2	2.19	0.41
1:C:32:ARG:HH12	1:C:80:GLN:HE21	1.67	0.41
1:E:52:ARG:HH22	1:F:59:GLY:C	2.29	0.41
1:F:52:ARG:HH22	1:H:59:GLY:C	2.29	0.41
1:I:32:ARG:HH12	1:I:80:GLN:HE21	1.67	0.41
1:A:164:ILE:HD13	1:A:164:ILE:HA	1.94	0.41
1:B:1:GLY:HA2	1:H:3:TRP:CD1	2.55	0.41
1:D:52:ARG:HH22	1:E:59:GLY:C	2.29	0.41
1:E:189:ARG:HD2	1:E:189:ARG:HA	1.91	0.41
1:E:202:ARG:HB3	1:E:205:GLU:HG3	2.03	0.41
1:F:27:VAL:HG11	1:H:90:LEU:HD21	2.02	0.41
1:H:32:ARG:HH12	1:H:80:GLN:HE21	1.67	0.41
1:K:202:ARG:HB3	1:K:205:GLU:HG3	2.03	0.41
1:L:5:ALA:HA	1:L:8:LYS:HE3	2.03	0.41
1:B:62:ASN:HB3	1:H:52:ARG:HE	1.85	0.41
1:E:27:VAL:HG11	1:F:90:LEU:HD21	2.02	0.41
1:F:5:ALA:HA	1:F:8:LYS:HE3	2.03	0.41
1:F:30:ILE:HA	1:F:33:ILE:HG22	2.03	0.41
1:H:5:ALA:HA	1:H:8:LYS:HE3	2.03	0.41
1:K:30:ILE:HA	1:K:33:ILE:HG22	2.03	0.41
1:L:202:ARG:HB3	1:L:205:GLU:HG3	2.03	0.41
1:D:189:ARG:HD2	1:D:189:ARG:HA	1.91	0.40
1:G:52:ARG:HH22	1:I:59:GLY:C	2.29	0.40
1:G:52:ARG:NH1	1:I:59:GLY:H	2.12	0.40
1:G:189:ARG:HD2	1:G:189:ARG:HA	1.91	0.40
1:H:202:ARG:HB3	1:H:205:GLU:HG3	2.03	0.40
1:L:32:ARG:HH12	1:L:80:GLN:HE21	1.67	0.40
1:A:5:ALA:HA	1:A:8:LYS:HE3	2.03	0.40
1:A:30:ILE:HA	1:A:33:ILE:HG22	2.03	0.40
1:C:52:ARG:HH22	1:D:59:GLY:C	2.30	0.40
1:D:5:ALA:HA	1:D:8:LYS:HE3	2.03	0.40
1:E:30:ILE:HA	1:E:33:ILE:HG22	2.03	0.40
1:I:52:ARG:HH22	1:J:59:GLY:C	2.29	0.40
1:J:5:ALA:HA	1:J:8:LYS:HE3	2.03	0.40
1:J:52:ARG:HH22	1:K:59:GLY:C	2.30	0.40
1:J:202:ARG:HB3	1:J:205:GLU:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ASN:HB2	1:K:201:SER:O	2.21	0.40
1:D:202:ARG:HB3	1:D:205:GLU:HG3	2.03	0.40
1:F:32:ARG:HH12	1:F:80:GLN:HE21	1.67	0.40
1:H:164:ILE:HD13	1:H:164:ILE:HA	1.94	0.40
1:K:189:ARG:HD2	1:K:189:ARG:HA	1.91	0.40
1:A:32:ARG:HH12	1:A:80:GLN:HE21	1.67	0.40
1:B:30:ILE:HA	1:B:33:ILE:HG22	2.03	0.40
1:E:5:ALA:HA	1:E:8:LYS:HE3	2.03	0.40
1:G:59:GLY:H	1:L:52:ARG:NH1	2.11	0.40
1:K:5:ALA:HA	1:K:8:LYS:HE3	2.03	0.40
1:A:226:ILE:HD13	1:A:226:ILE:HA	1.96	0.40
1:B:202:ARG:HB3	1:B:205:GLU:HG3	2.03	0.40
1:G:59:GLY:C	1:L:52:ARG:HH22	2.29	0.40
1:G:202:ARG:HB3	1:G:205:GLU:HG3	2.03	0.40
1:J:189:ARG:HD2	1:J:189:ARG:HA	1.91	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	185/382 (48%)	180 (97%)	5 (3%)	0	100	100
1	B	185/382 (48%)	180 (97%)	5 (3%)	0	100	100
1	C	185/382 (48%)	180 (97%)	5 (3%)	0	100	100
1	D	185/382 (48%)	180 (97%)	5 (3%)	0	100	100
1	E	185/382 (48%)	180 (97%)	5 (3%)	0	100	100
1	F	185/382 (48%)	181 (98%)	4 (2%)	0	100	100
1	G	185/382 (48%)	180 (97%)	5 (3%)	0	100	100
1	H	185/382 (48%)	180 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	185/382 (48%)	180 (97%)	5 (3%)	0	100	100
1	J	185/382 (48%)	180 (97%)	5 (3%)	0	100	100
1	K	185/382 (48%)	180 (97%)	5 (3%)	0	100	100
1	L	185/382 (48%)	180 (97%)	5 (3%)	0	100	100
All	All	2220/4584 (48%)	2161 (97%)	59 (3%)	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%)	32	54
1	B	170/333 (51%)	163 (96%)	7 (4%)	27	52
1	C	170/333 (51%)	165 (97%)	5 (3%)	37	57
1	D	170/333 (51%)	164 (96%)	6 (4%)	32	54
1	E	170/333 (51%)	165 (97%)	5 (3%)	37	57
1	F	170/333 (51%)	165 (97%)	5 (3%)	37	57
1	G	170/333 (51%)	165 (97%)	5 (3%)	37	57
1	H	170/333 (51%)	165 (97%)	5 (3%)	37	57
1	I	170/333 (51%)	165 (97%)	5 (3%)	37	57
1	J	170/333 (51%)	165 (97%)	5 (3%)	37	57
1	K	170/333 (51%)	165 (97%)	5 (3%)	37	57
1	L	170/333 (51%)	165 (97%)	5 (3%)	37	57
All	All	2040/3996 (51%)	1976 (97%)	64 (3%)	36	57

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS

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Mol	Chain	Res	Type
1	A	23	VAL
1	A	34	LEU
1	A	52	ARG
1	A	195	GLN
1	A	205	GLU
1	B	22	LYS
1	B	23	VAL
1	B	34	LEU
1	B	48	GLN
1	B	52	ARG
1	B	195	GLN
1	B	205	GLU
1	C	22	LYS
1	C	23	VAL
1	C	34	LEU
1	C	52	ARG
1	C	205	GLU
1	D	22	LYS
1	D	23	VAL
1	D	34	LEU
1	D	52	ARG
1	D	195	GLN
1	D	205	GLU
1	E	22	LYS
1	E	23	VAL
1	E	34	LEU
1	E	52	ARG
1	E	205	GLU
1	F	22	LYS
1	F	23	VAL
1	F	34	LEU
1	F	52	ARG
1	F	205	GLU
1	G	22	LYS
1	G	23	VAL
1	G	34	LEU
1	G	52	ARG
1	G	205	GLU
1	H	22	LYS
1	H	23	VAL
1	H	34	LEU
1	H	52	ARG

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Mol	Chain	Res	Type
1	H	205	GLU
1	I	22	LYS
1	I	23	VAL
1	I	34	LEU
1	I	52	ARG
1	I	205	GLU
1	J	22	LYS
1	J	23	VAL
1	J	34	LEU
1	J	52	ARG
1	J	205	GLU
1	K	22	LYS
1	K	23	VAL
1	K	34	LEU
1	K	52	ARG
1	K	205	GLU
1	L	22	LYS
1	L	23	VAL
1	L	34	LEU
1	L	52	ARG
1	L	205	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	195	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

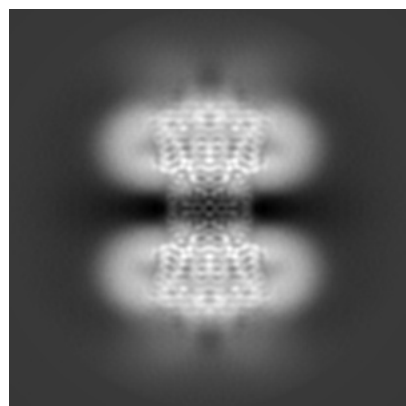
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18468. These allow visual inspection of the internal detail of the map and identification of artifacts.

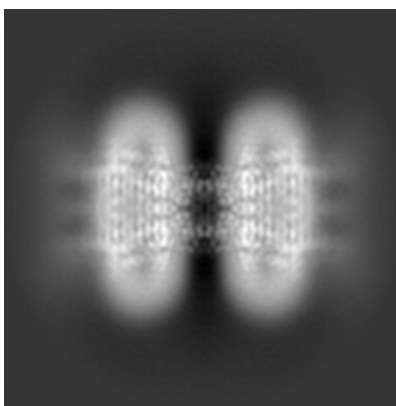
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

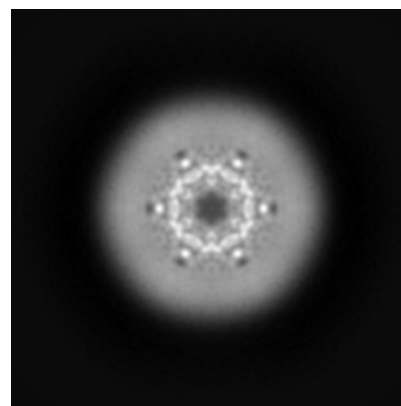
6.1.1 Primary map



X

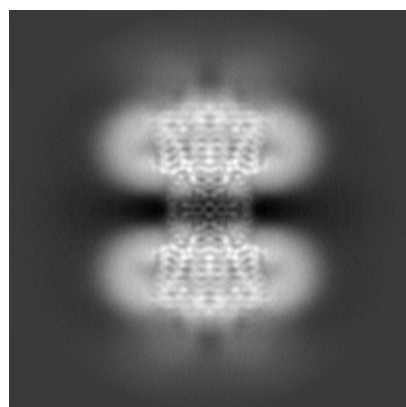


Y

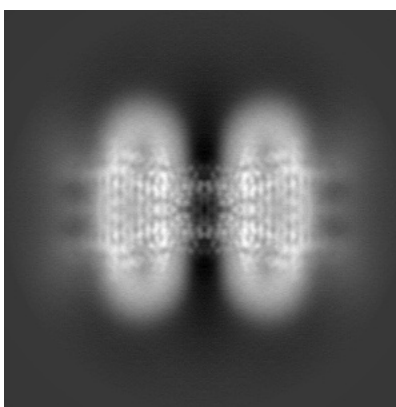


Z

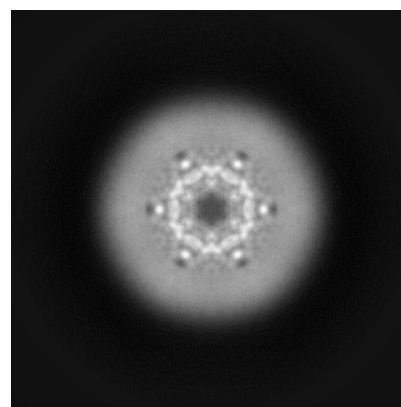
6.1.2 Raw map



X



Y

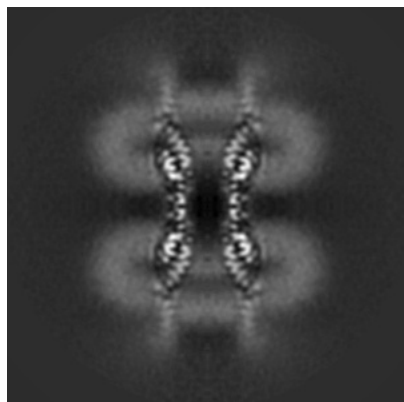


Z

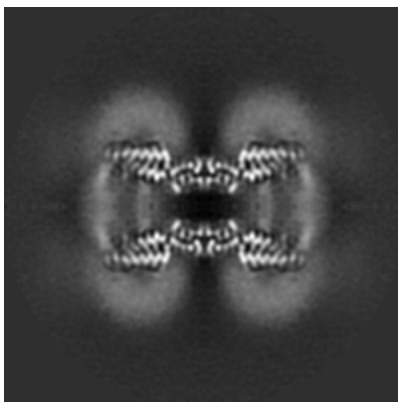
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

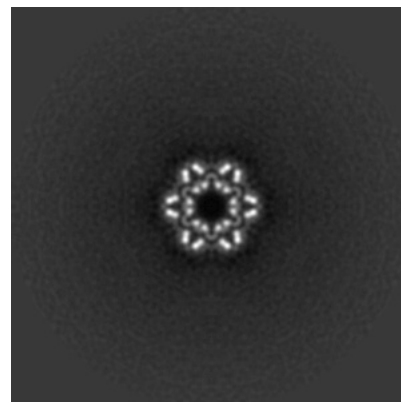
6.2.1 Primary map



X Index: 192

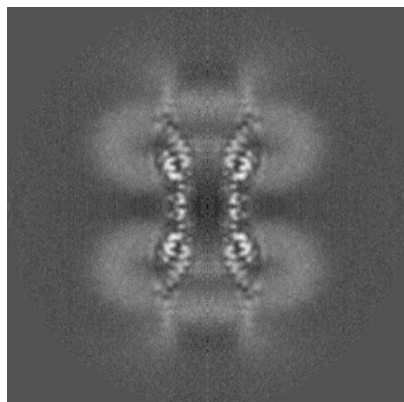


Y Index: 192

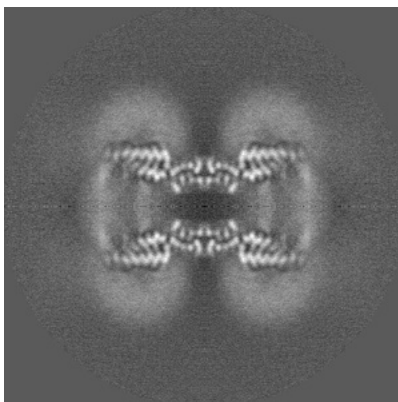


Z Index: 192

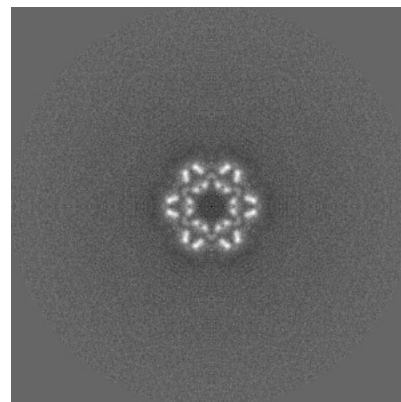
6.2.2 Raw map



X Index: 192



Y Index: 192

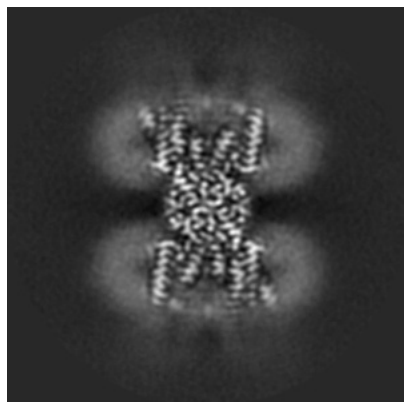


Z Index: 192

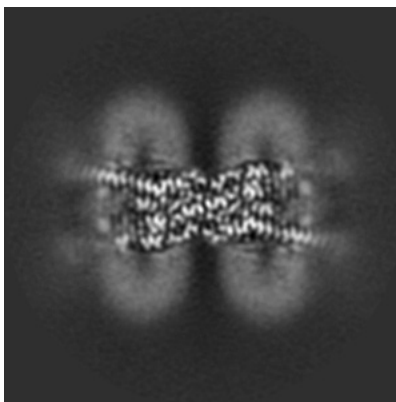
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

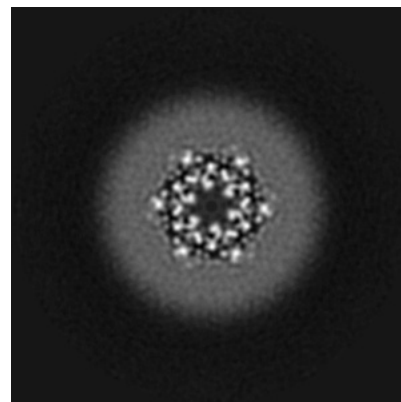
6.3.1 Primary map



X Index: 169

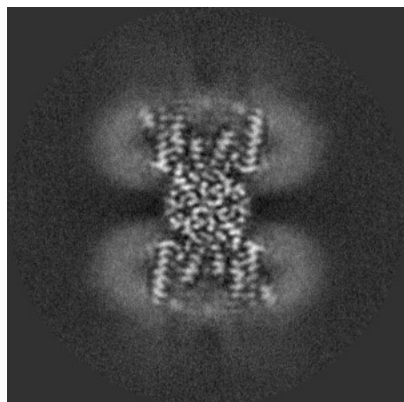


Y Index: 166

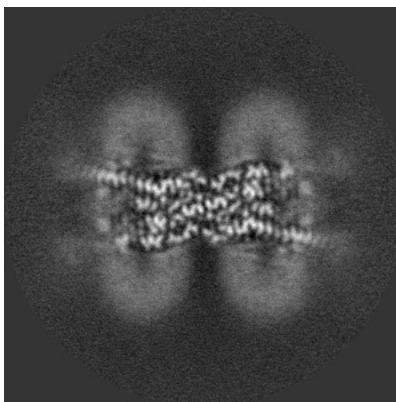


Z Index: 153

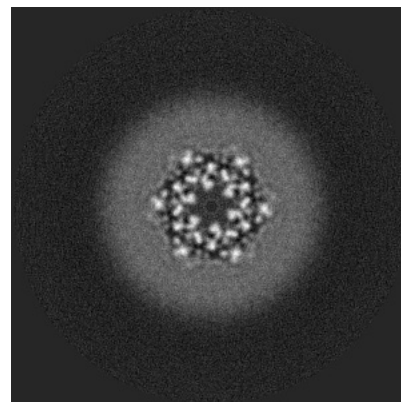
6.3.2 Raw map



X Index: 169



Y Index: 166

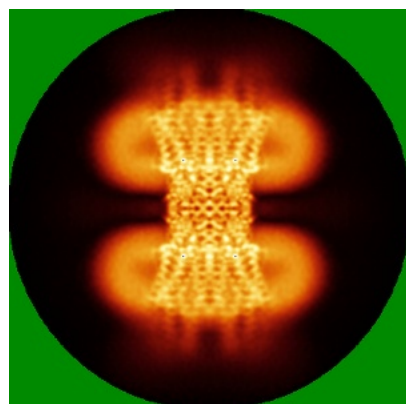


Z Index: 153

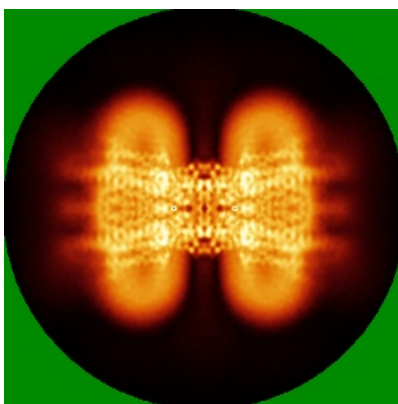
The images above show the largest variance slices of the map in three orthogonal directions.

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

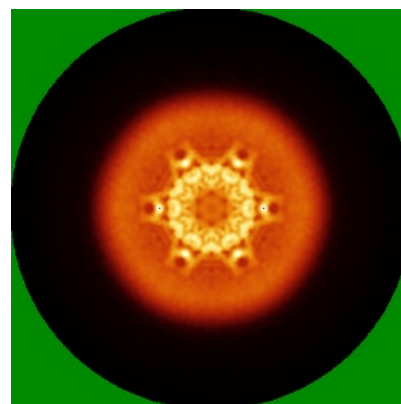
6.4.1 Primary map



X

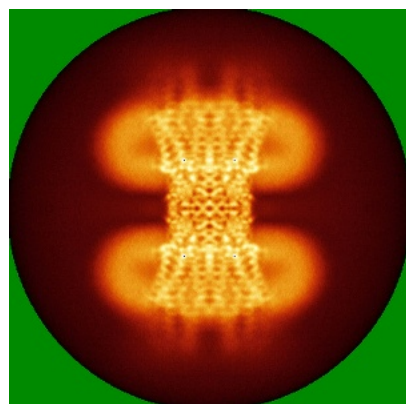


Y

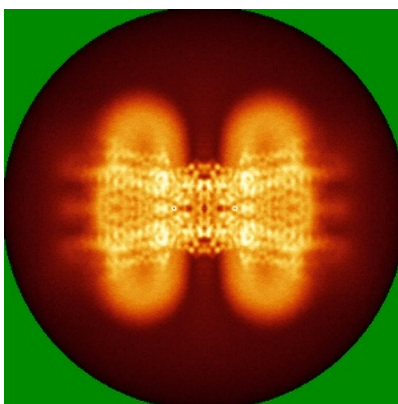


Z

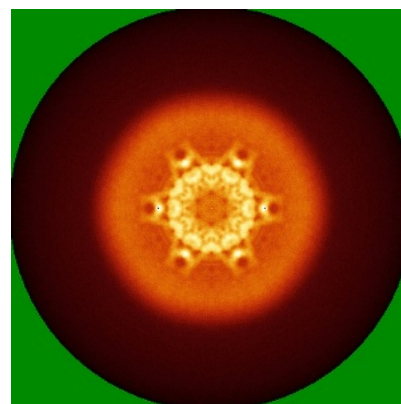
6.4.2 Raw map



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



X



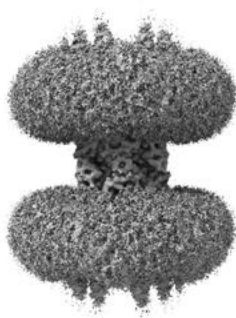
Y



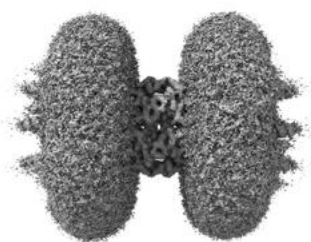
Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

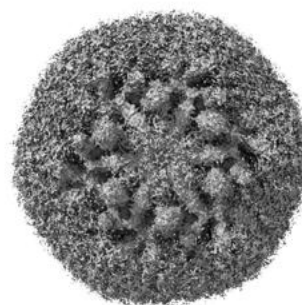
6.5.2 Raw map



X



Y



Z

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.

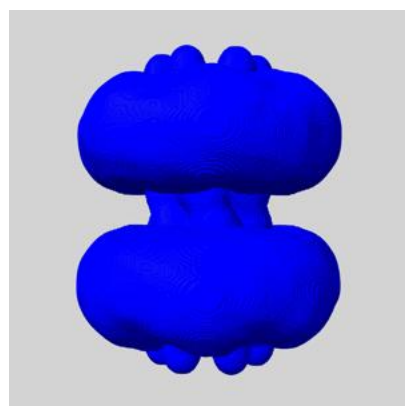
6.6 Mask visualisation [i](#)

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

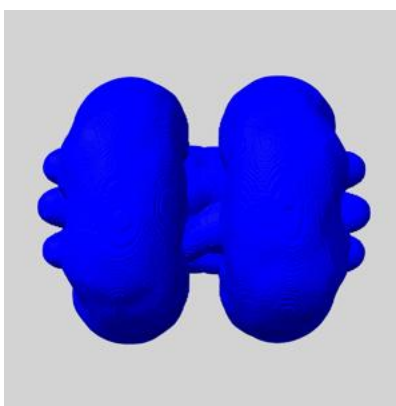
A mask typically either:

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

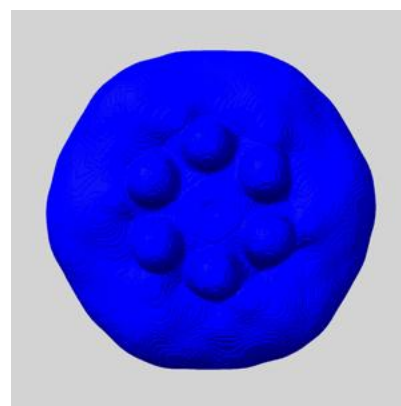
6.6.1 emd_18468_msk_1.map [i](#)



X



Y

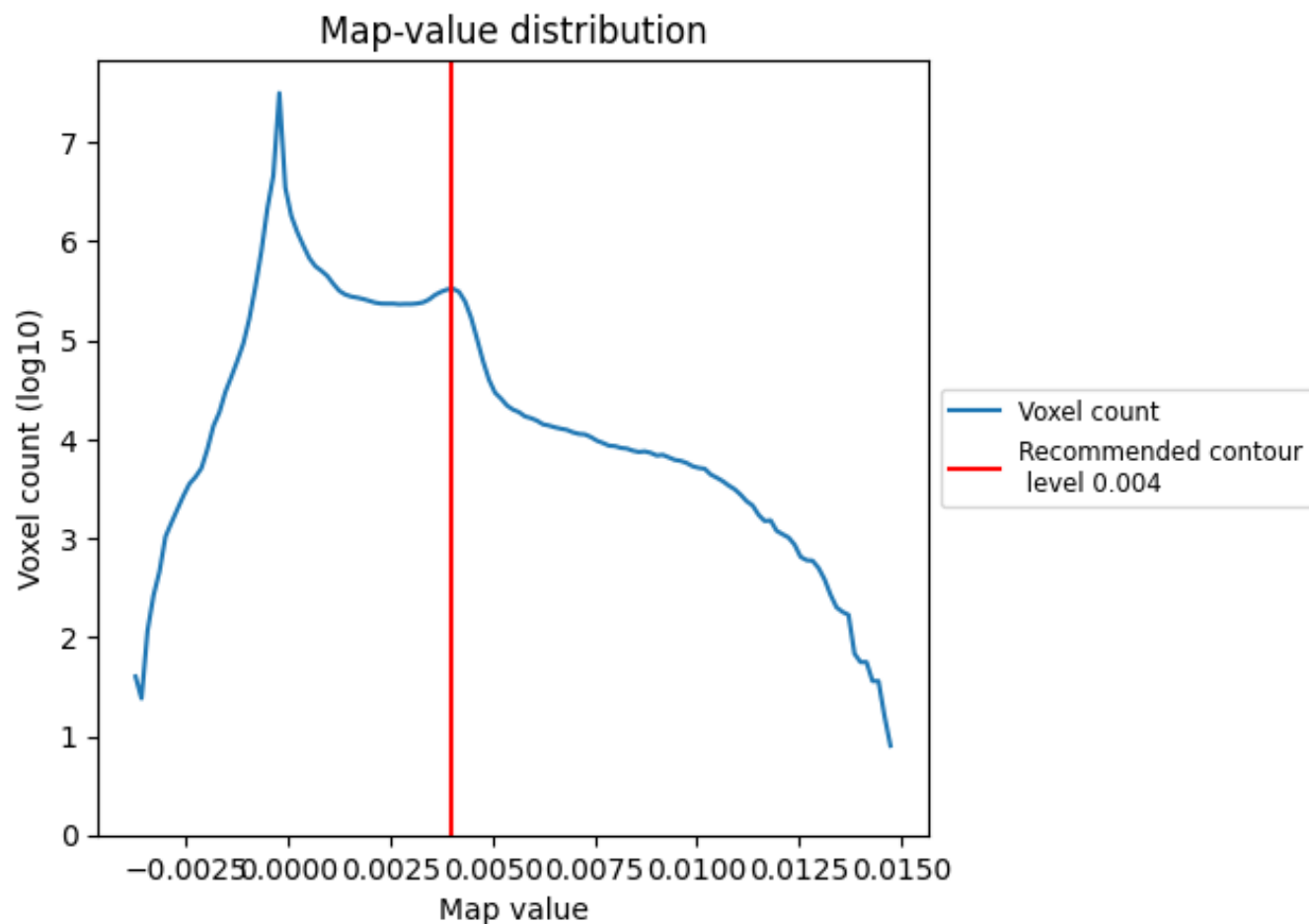


Z

7 Map analysis [i](#)

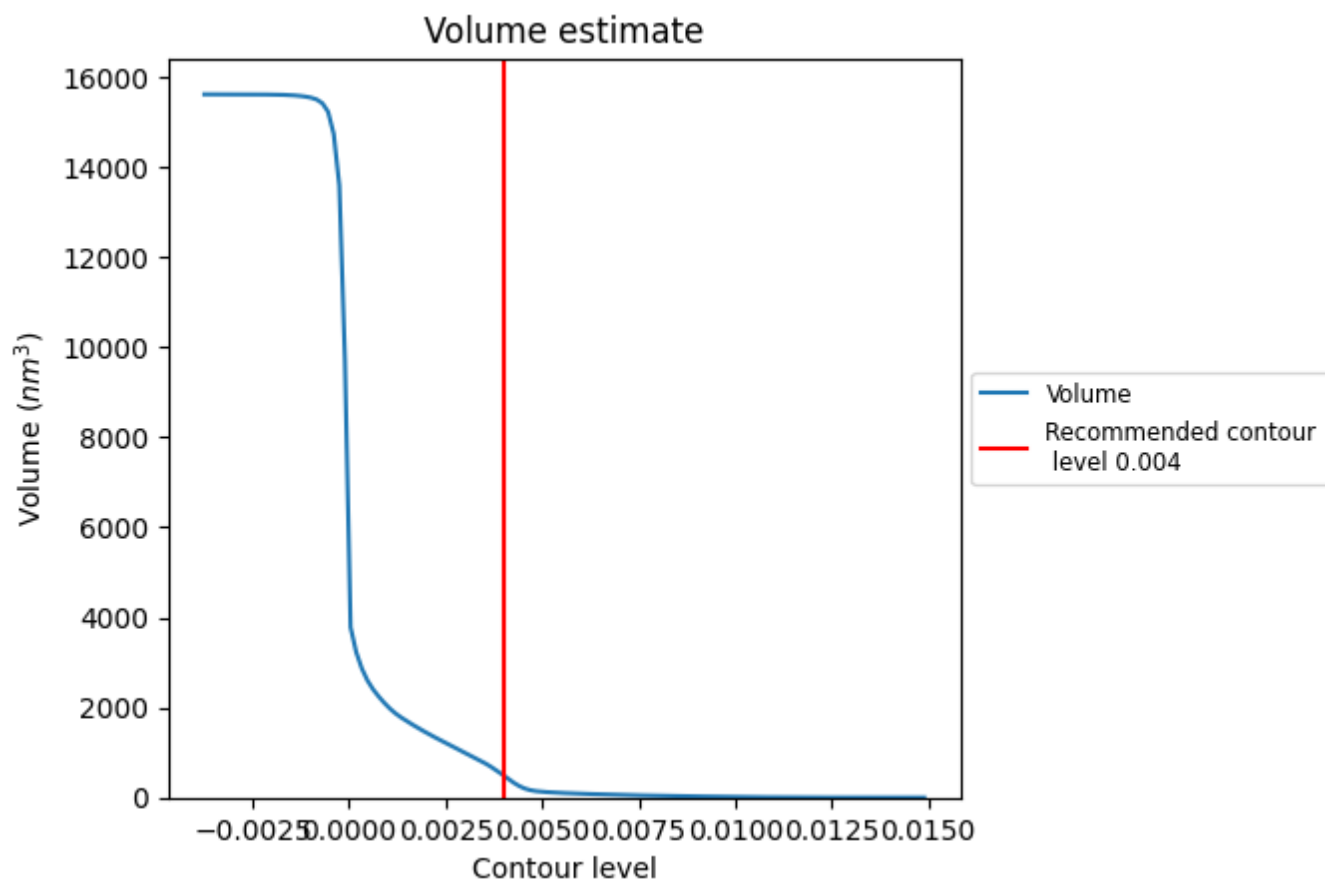
This section contains the results of statistical analysis of the map.

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.

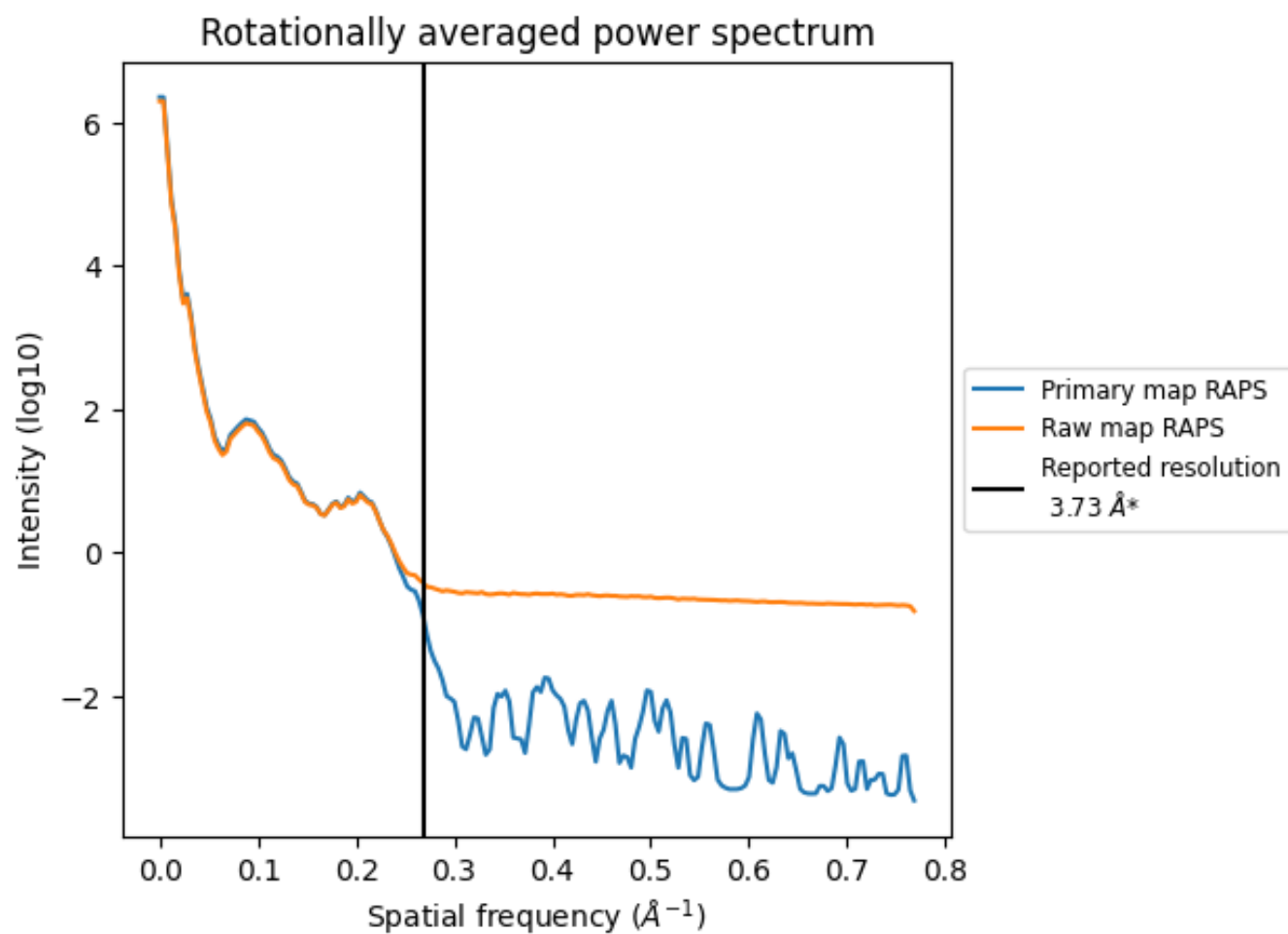
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 494 nm³; this corresponds to an approximate mass of 446 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](#)

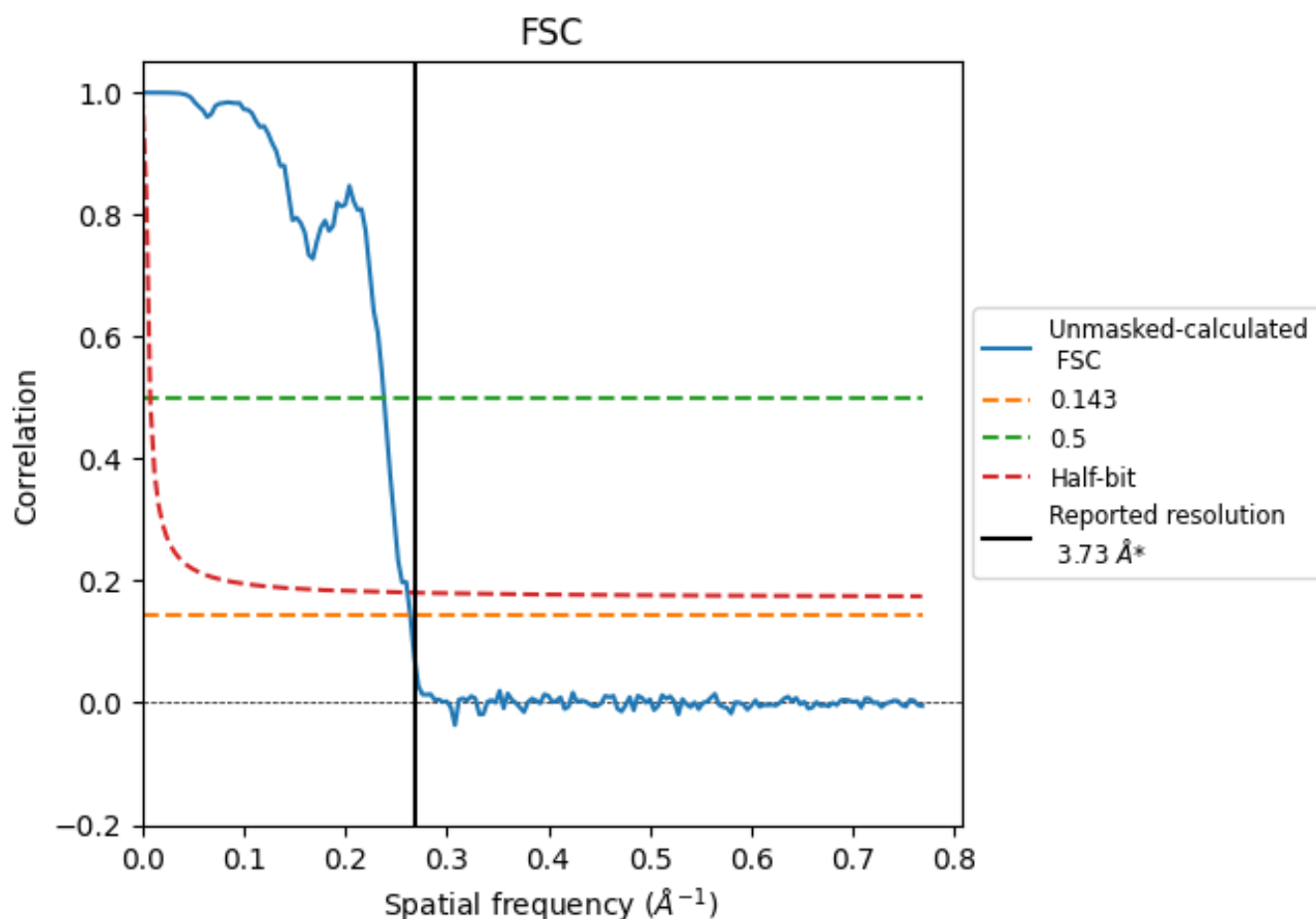


*Reported resolution corresponds to spatial frequency of 0.268 Å⁻¹

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 0.268 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

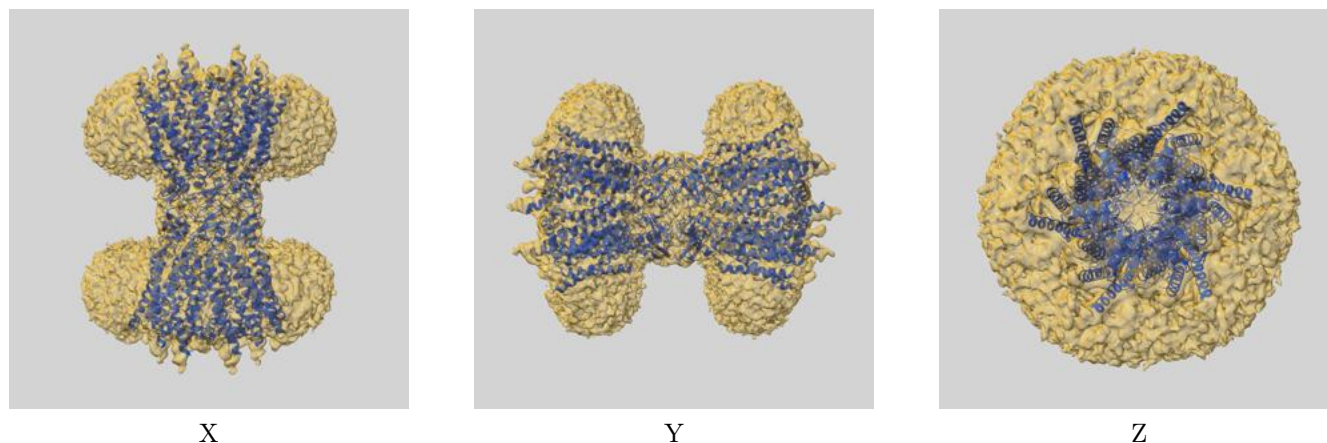
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.73	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.79	4.20	3.83

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

9 Map-model fit [i](#)

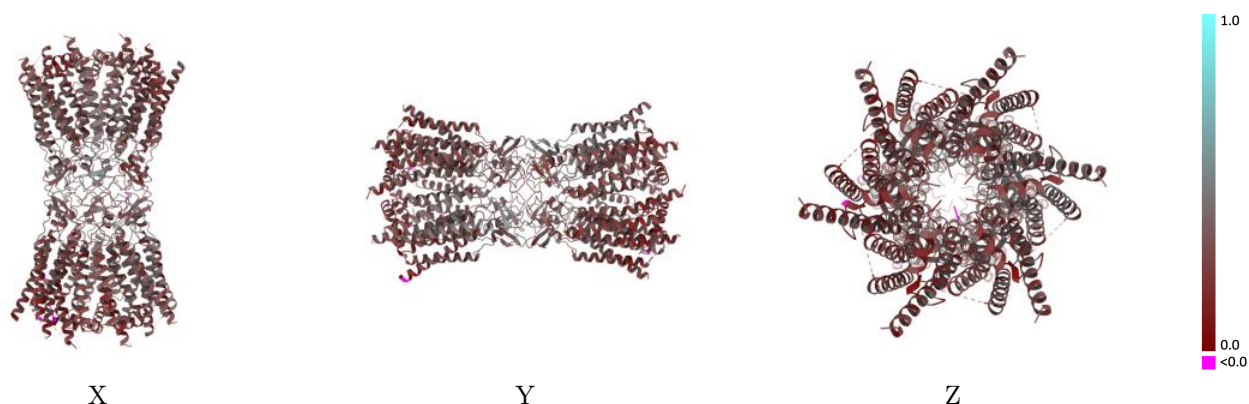
This section contains information regarding the fit between EMDB map EMD-18468 and PDB model 8QKO. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



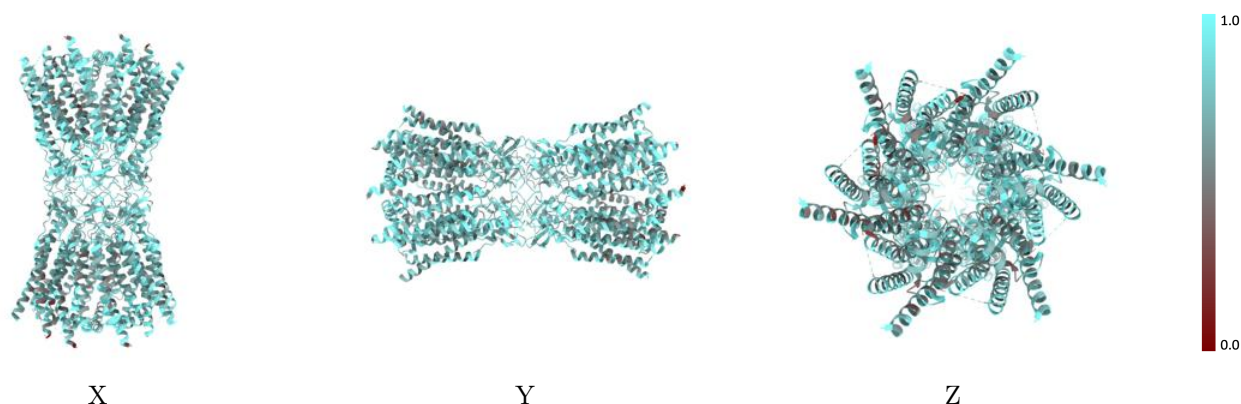
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



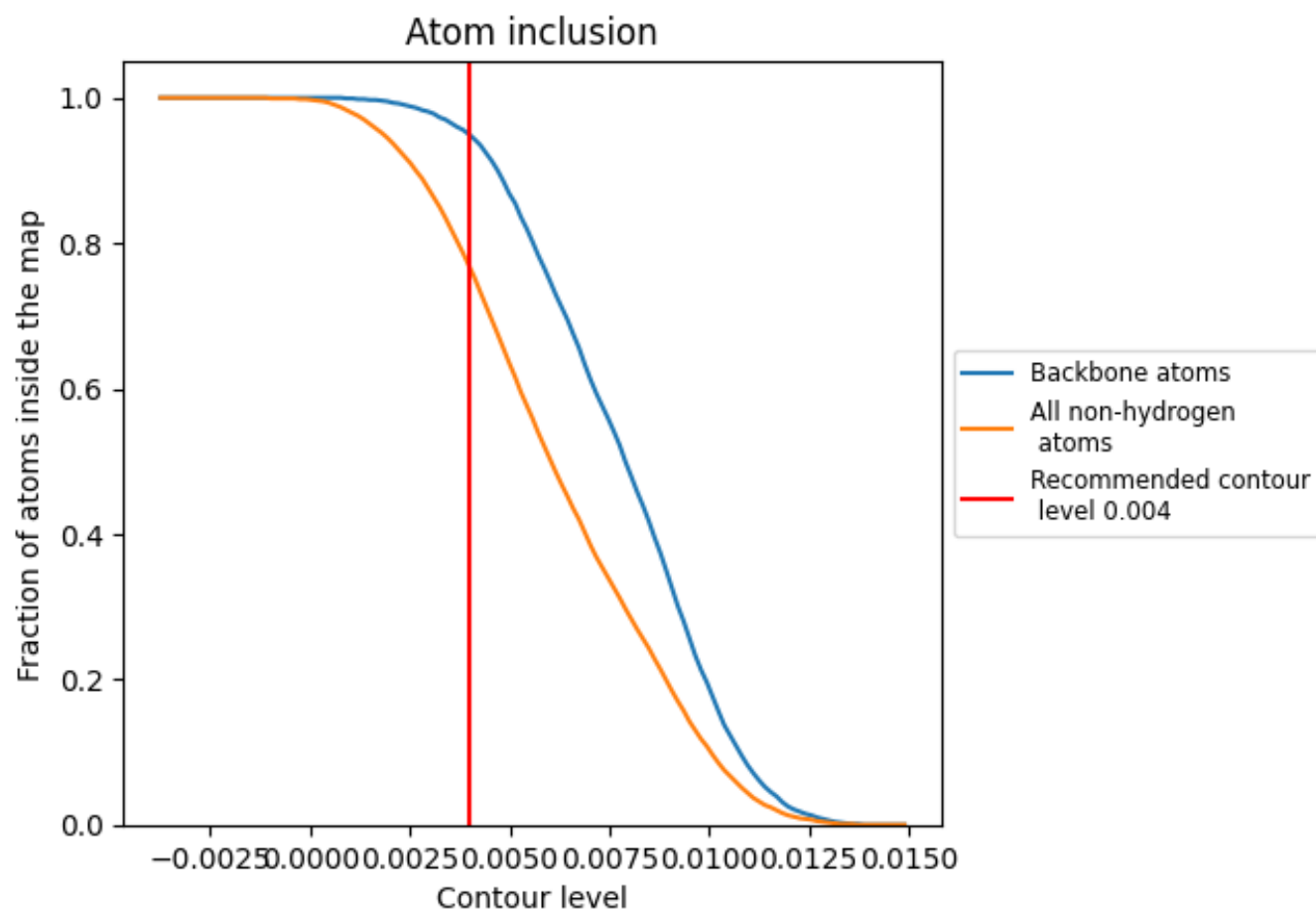
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7670	 0.3130
A	 0.8330	 0.3940
B	 0.8360	 0.3950
C	 0.7810	 0.3040
D	 0.7590	 0.2920
E	 0.7430	 0.2890
F	 0.7630	 0.3070
G	 0.7550	 0.3010
H	 0.7730	 0.3270
I	 0.7320	 0.2760
J	 0.7220	 0.2630
K	 0.7400	 0.2880
L	 0.7710	 0.3170

