



wwPDB EM Validation Summary Report ⓘ

Sep 29, 2026 – 04:35 PM EDT

PDB ID : 9ZY3 / pdb_00009zy3
EMDB ID : EMD-74938
Title : Ca²⁺ bound destabilized open state Connexin-50
Authors : Jarodsky, J.M.; Reichow, S.L.
Deposited on : 2026-01-05
Resolution : 2.20 Å (reported)
Based on initial model : 7jjp

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

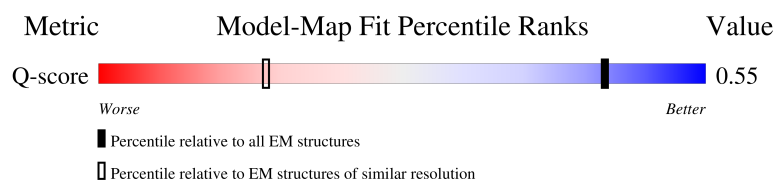
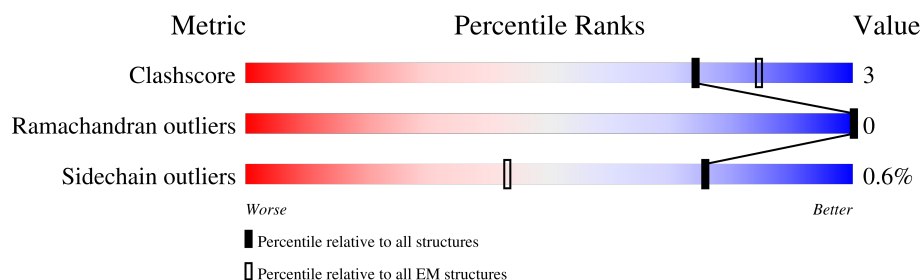
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.2
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.51

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 2.20 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	3184 (1.71 - 2.70)

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	440	
1	B	440	
1	C	440	
1	D	440	

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Mol	Chain	Length	Quality of chain
1	E	440	 40% • 57%
1	F	440	 40% • 57%
1	G	440	 40% • 57%
1	H	440	 40% • 57%
1	I	440	 40% • 57%
1	J	440	 40% • 57%
1	K	440	 40% • 57%
1	L	440	 40% • 57%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 42360 atoms, of which 21636 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-8 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	190	Total 3068	C 1018	H 1525	N 253	O 262	S 10	0	0
1	B	190	Total 3068	C 1018	H 1525	N 253	O 262	S 10	0	0
1	C	190	Total 3068	C 1018	H 1525	N 253	O 262	S 10	0	0
1	D	190	Total 3068	C 1018	H 1525	N 253	O 262	S 10	0	0
1	E	190	Total 3068	C 1018	H 1525	N 253	O 262	S 10	0	0
1	F	190	Total 3068	C 1018	H 1525	N 253	O 262	S 10	0	0
1	G	190	Total 3068	C 1018	H 1525	N 253	O 262	S 10	0	0
1	H	190	Total 3068	C 1018	H 1525	N 253	O 262	S 10	0	0
1	I	190	Total 3068	C 1018	H 1525	N 253	O 262	S 10	0	0
1	J	190	Total 3068	C 1018	H 1525	N 253	O 262	S 10	0	0
1	K	190	Total 3068	C 1018	H 1525	N 253	O 262	S 10	0	0
1	L	190	Total 3068	C 1018	H 1525	N 253	O 262	S 10	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ACE	-	acetylation	UNP P55917
B	1	ACE	-	acetylation	UNP P55917
C	1	ACE	-	acetylation	UNP P55917
D	1	ACE	-	acetylation	UNP P55917
E	1	ACE	-	acetylation	UNP P55917
F	1	ACE	-	acetylation	UNP P55917

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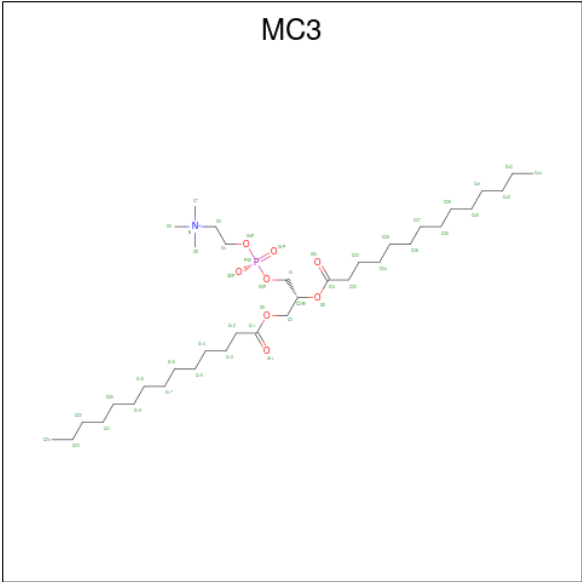
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Chain	Residue	Modelled	Actual	Comment	Reference
G	1	ACE	-	acetylation	UNP P55917
H	1	ACE	-	acetylation	UNP P55917
I	1	ACE	-	acetylation	UNP P55917
J	1	ACE	-	acetylation	UNP P55917
K	1	ACE	-	acetylation	UNP P55917
L	1	ACE	-	acetylation	UNP P55917

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total Ca 1 1	0
2	B	1	Total Ca 1 1	0
2	C	1	Total Ca 1 1	0
2	D	1	Total Ca 1 1	0
2	E	1	Total Ca 1 1	0
2	F	1	Total Ca 1 1	0
2	G	1	Total Ca 1 1	0
2	H	1	Total Ca 1 1	0
2	I	1	Total Ca 1 1	0
2	J	1	Total Ca 1 1	0
2	K	1	Total Ca 1 1	0
2	L	1	Total Ca 1 1	0

- Molecule 3 is 1,2-DIMYRISTOYL-RAC-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: MC3) (formula: C₃₆H₇₂NO₈P).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	H	0
			33	11	22	
3	A	1	Total	C	H	0
			39	13	26	
3	A	1	Total	C	H	0
			30	10	20	
3	A	1	Total	C	H	0
			24	8	16	
3	A	1	Total	C	H	0
			18	6	12	
3	A	1	Total	C	H	0
			24	8	16	
3	A	1	Total	C	H	0
			18	6	12	
3	A	1	Total	C	H	0
			33	11	22	
3	A	1	Total	C	H	0
			33	11	22	
3	A	1	Total	C	H	0
			27	9	18	
3	A	1	Total	C	H	0
			27	9	18	
3	A	1	Total	C	H	0
			18	6	12	
3	A	1	Total	C	H	0
			27	9	18	
3	A	1	Total	C	H	0
			27	9	18	

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Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	H	0
			15	5	10	
3	A	1	Total	C	H	0
			24	8	16	
3	B	1	Total	C	H	0
			33	11	22	
3	B	1	Total	C	H	0
			39	13	26	
3	B	1	Total	C	H	0
			30	10	20	
3	B	1	Total	C	H	0
			24	8	16	
3	B	1	Total	C	H	0
			18	6	12	
3	B	1	Total	C	H	0
			24	8	16	
3	B	1	Total	C	H	0
			18	6	12	
3	B	1	Total	C	H	0
			33	11	22	
3	B	1	Total	C	H	0
			33	11	22	
3	B	1	Total	C	H	0
			27	9	18	
3	B	1	Total	C	H	0
			27	9	18	
3	B	1	Total	C	H	0
			18	6	12	
3	B	1	Total	C	H	0
			27	9	18	
3	B	1	Total	C	H	0
			27	9	18	
3	B	1	Total	C	H	0
			15	5	10	
3	B	1	Total	C	H	0
			24	8	16	
3	C	1	Total	C	H	0
			33	11	22	
3	C	1	Total	C	H	0
			39	13	26	
3	C	1	Total	C	H	0
			30	10	20	

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Mol	Chain	Residues	Atoms			AltConf
3	C	1	Total	C	H	0
			24	8	16	
3	C	1	Total	C	H	0
			18	6	12	
3	C	1	Total	C	H	0
			24	8	16	
3	C	1	Total	C	H	0
			18	6	12	
3	C	1	Total	C	H	0
			33	11	22	
3	C	1	Total	C	H	0
			33	11	22	
3	C	1	Total	C	H	0
			27	9	18	
3	C	1	Total	C	H	0
			27	9	18	
3	C	1	Total	C	H	0
			18	6	12	
3	C	1	Total	C	H	0
			27	9	18	
3	C	1	Total	C	H	0
			27	9	18	
3	C	1	Total	C	H	0
			15	5	10	
3	C	1	Total	C	H	0
			24	8	16	
3	D	1	Total	C	H	0
			33	11	22	
3	D	1	Total	C	H	0
			39	13	26	
3	D	1	Total	C	H	0
			30	10	20	
3	D	1	Total	C	H	0
			24	8	16	
3	D	1	Total	C	H	0
			18	6	12	
3	D	1	Total	C	H	0
			24	8	16	
3	D	1	Total	C	H	0
			18	6	12	
3	D	1	Total	C	H	0
			33	11	22	

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Mol	Chain	Residues	Atoms			AltConf
3	D	1	Total	C	H	0
			33	11	22	
3	D	1	Total	C	H	0
			27	9	18	
3	D	1	Total	C	H	0
			27	9	18	
3	D	1	Total	C	H	0
			18	6	12	
3	D	1	Total	C	H	0
			27	9	18	
3	D	1	Total	C	H	0
			27	9	18	
3	D	1	Total	C	H	0
			15	5	10	
3	D	1	Total	C	H	0
			24	8	16	
3	E	1	Total	C	H	0
			33	11	22	
3	E	1	Total	C	H	0
			39	13	26	
3	E	1	Total	C	H	0
			30	10	20	
3	E	1	Total	C	H	0
			24	8	16	
3	E	1	Total	C	H	0
			18	6	12	
3	E	1	Total	C	H	0
			24	8	16	
3	E	1	Total	C	H	0
			18	6	12	
3	E	1	Total	C	H	0
			33	11	22	
3	E	1	Total	C	H	0
			33	11	22	
3	E	1	Total	C	H	0
			27	9	18	
3	E	1	Total	C	H	0
			27	9	18	
3	E	1	Total	C	H	0
			18	6	12	
3	E	1	Total	C	H	0
			27	9	18	

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Mol	Chain	Residues	Atoms			AltConf
3	E	1	Total	C	H	0
			27	9	18	
3	E	1	Total	C	H	0
			15	5	10	
3	E	1	Total	C	H	0
			24	8	16	
3	F	1	Total	C	H	0
			33	11	22	
3	F	1	Total	C	H	0
			33	11	22	
3	F	1	Total	C	H	0
			27	9	18	
3	F	1	Total	C	H	0
			27	9	18	
3	F	1	Total	C	H	0
			18	6	12	
3	F	1	Total	C	H	0
			27	9	18	
3	F	1	Total	C	H	0
			27	9	18	
3	F	1	Total	C	H	0
			15	5	10	
3	F	1	Total	C	H	0
			24	8	16	
3	F	1	Total	C	H	0
			33	11	22	
3	F	1	Total	C	H	0
			39	13	26	
3	F	1	Total	C	H	0
			30	10	20	
3	F	1	Total	C	H	0
			24	8	16	
3	F	1	Total	C	H	0
			18	6	12	
3	F	1	Total	C	H	0
			24	8	16	
3	F	1	Total	C	H	0
			18	6	12	
3	G	1	Total	C	H	0
			33	11	22	
3	G	1	Total	C	H	0
			39	13	26	

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Mol	Chain	Residues	Atoms			AltConf
3	G	1	Total	C	H	0
			30	10	20	
3	G	1	Total	C	H	0
			24	8	16	
3	G	1	Total	C	H	0
			18	6	12	
3	G	1	Total	C	H	0
			24	8	16	
3	G	1	Total	C	H	0
			18	6	12	
3	G	1	Total	C	H	0
			33	11	22	
3	G	1	Total	C	H	0
			33	11	22	
3	G	1	Total	C	H	0
			27	9	18	
3	G	1	Total	C	H	0
			27	9	18	
3	G	1	Total	C	H	0
			18	6	12	
3	G	1	Total	C	H	0
			27	9	18	
3	G	1	Total	C	H	0
			27	9	18	
3	G	1	Total	C	H	0
			15	5	10	
3	G	1	Total	C	H	0
			24	8	16	
3	H	1	Total	C	H	0
			33	11	22	
3	H	1	Total	C	H	0
			39	13	26	
3	H	1	Total	C	H	0
			30	10	20	
3	H	1	Total	C	H	0
			24	8	16	
3	H	1	Total	C	H	0
			18	6	12	
3	H	1	Total	C	H	0
			24	8	16	
3	H	1	Total	C	H	0
			18	6	12	

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Mol	Chain	Residues	Atoms			AltConf
3	H	1	Total 33	C 11	H 22	0
3	H	1	Total 33	C 11	H 22	0
3	H	1	Total 27	C 9	H 18	0
3	H	1	Total 27	C 9	H 18	0
3	H	1	Total 18	C 6	H 12	0
3	H	1	Total 27	C 9	H 18	0
3	H	1	Total 27	C 9	H 18	0
3	H	1	Total 15	C 5	H 10	0
3	H	1	Total 24	C 8	H 16	0
3	I	1	Total 33	C 11	H 22	0
3	I	1	Total 39	C 13	H 26	0
3	I	1	Total 30	C 10	H 20	0
3	I	1	Total 24	C 8	H 16	0
3	I	1	Total 18	C 6	H 12	0
3	I	1	Total 24	C 8	H 16	0
3	I	1	Total 18	C 6	H 12	0
3	I	1	Total 33	C 11	H 22	0
3	I	1	Total 33	C 11	H 22	0
3	I	1	Total 27	C 9	H 18	0
3	I	1	Total 27	C 9	H 18	0
3	I	1	Total 18	C 6	H 12	0

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Mol	Chain	Residues	Atoms			AltConf
3	I	1	Total	C	H	0
			27	9	18	
3	I	1	Total	C	H	0
			27	9	18	
3	I	1	Total	C	H	0
			15	5	10	
3	I	1	Total	C	H	0
			24	8	16	
3	J	1	Total	C	H	0
			33	11	22	
3	J	1	Total	C	H	0
			39	13	26	
3	J	1	Total	C	H	0
			30	10	20	
3	J	1	Total	C	H	0
			24	8	16	
3	J	1	Total	C	H	0
			18	6	12	
3	J	1	Total	C	H	0
			24	8	16	
3	J	1	Total	C	H	0
			18	6	12	
3	J	1	Total	C	H	0
			33	11	22	
3	J	1	Total	C	H	0
			33	11	22	
3	J	1	Total	C	H	0
			27	9	18	
3	J	1	Total	C	H	0
			27	9	18	
3	J	1	Total	C	H	0
			18	6	12	
3	J	1	Total	C	H	0
			27	9	18	
3	J	1	Total	C	H	0
			27	9	18	
3	J	1	Total	C	H	0
			15	5	10	
3	J	1	Total	C	H	0
			24	8	16	
3	K	1	Total	C	H	0
			33	11	22	

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Mol	Chain	Residues	Atoms			AltConf
3	K	1	Total	C	H	0
			39	13	26	
3	K	1	Total	C	H	0
			30	10	20	
3	K	1	Total	C	H	0
			24	8	16	
3	K	1	Total	C	H	0
			18	6	12	
3	K	1	Total	C	H	0
			24	8	16	
3	K	1	Total	C	H	0
			18	6	12	
3	K	1	Total	C	H	0
			33	11	22	
3	K	1	Total	C	H	0
			33	11	22	
3	K	1	Total	C	H	0
			27	9	18	
3	K	1	Total	C	H	0
			27	9	18	
3	K	1	Total	C	H	0
			18	6	12	
3	K	1	Total	C	H	0
			27	9	18	
3	K	1	Total	C	H	0
			27	9	18	
3	K	1	Total	C	H	0
			15	5	10	
3	K	1	Total	C	H	0
			24	8	16	
3	L	1	Total	C	H	0
			33	11	22	
3	L	1	Total	C	H	0
			33	11	22	
3	L	1	Total	C	H	0
			27	9	18	
3	L	1	Total	C	H	0
			27	9	18	
3	L	1	Total	C	H	0
			18	6	12	
3	L	1	Total	C	H	0
			27	9	18	

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Mol	Chain	Residues	Atoms			AltConf
3	L	1	Total	C	H	0
			27	9	18	
3	L	1	Total	C	H	0
			15	5	10	
3	L	1	Total	C	H	0
			24	8	16	
3	L	1	Total	C	H	0
			33	11	22	
3	L	1	Total	C	H	0
			39	13	26	
3	L	1	Total	C	H	0
			30	10	20	
3	L	1	Total	C	H	0
			24	8	16	
3	L	1	Total	C	H	0
			18	6	12	
3	L	1	Total	C	H	0
			24	8	16	
3	L	1	Total	C	H	0
			18	6	12	

- Molecule 4 is water.

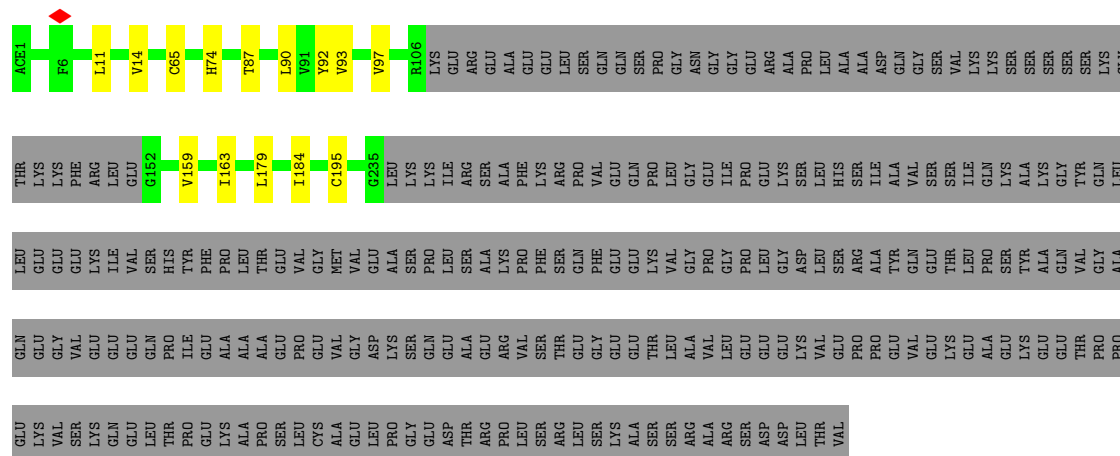
Mol	Chain	Residues	Atoms		AltConf
4	A	44	Total	O	0
			44	44	
4	B	44	Total	O	0
			44	44	
4	C	44	Total	O	0
			44	44	
4	D	44	Total	O	0
			44	44	
4	E	44	Total	O	0
			44	44	
4	F	44	Total	O	0
			44	44	
4	G	44	Total	O	0
			44	44	
4	H	44	Total	O	0
			44	44	
4	I	44	Total	O	0
			44	44	

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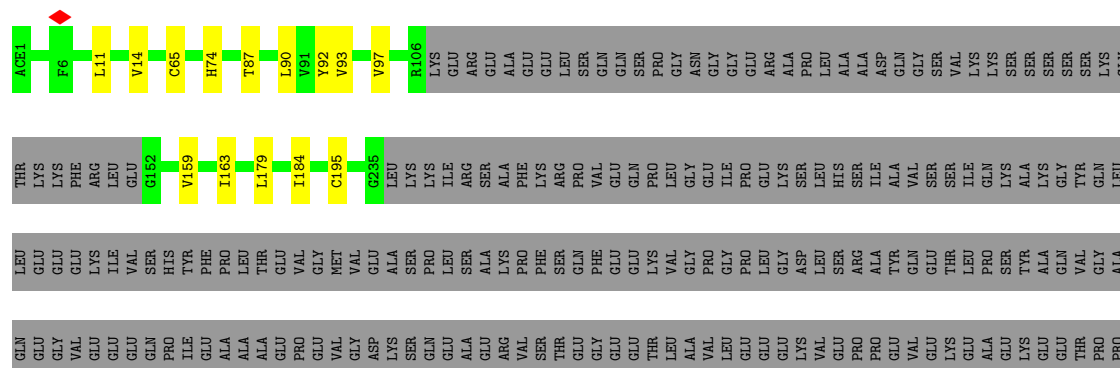
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Mol	Chain	Residues	Atoms		AltConf
4	J	44	Total 44	O 44	0
4	K	44	Total 44	O 44	0
4	L	44	Total 44	O 44	0

- Molecule 1: Gap junction alpha-8 protein



- Molecule 1: Gap junction alpha-8 protein



GLU	LYS	VAL	SER	LYS	GLN	GLU	LEU	THR	PRO	GLU	GLY	ALA	LYS	PRO	SER	CYS	ALA	GLU	LEU	PRO	GLU	GLY	ASP	THR	ARG	PRO	LEU	SER	ARG	LEU	SER	LYS	ALA	SER	SER	ARG	ALA	ASP	ASP	LEU	THR	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 1: Gap junction alpha-8 protein

Chain F:

40%

57%

ACE1	F6	L11	V14	C65	H74	T87	L90	V91	V92	V93	V97	R106	LYS	GLU	ARG	GLU	ALA	GLU	LEU	SER	GLN	GLN	SER	PRO	GLY	ASN	GLY	GLY	GLU	ARG	ALA	PRO	LEU	ALA	ASP	GLN	GLY	SER	LYS	LYS	VAL	GLN	SER	SER	SER	SER	GLY	LYS	GLY
THR	LYS	PHE	LEU	G152	L179	I184	C195	G235	LEU	LYS	ILE	ALA	SER	PHE	LYS	ARG	PRO	VAL	GLN	GLN	LEU	GLY	GLY	ILE	PRO	GLU	LYS	SER	HIS	SER	ALA	ILE	VAL	SER	THR	ILE	PRO	SER	LYS	ALA	LYS	TYR	GLN	LEU	SER	GLY	GLY	GLY	
LYS	ILE	VAL	SER	HIS	TYR	PHE	PRO	LEU	VAL	MET	VAL	GLY	ASP	LYS	SER	GLN	GLU	ALA	SER	PHE	LYS	ARG	PRO	GLY	PRO	GLU	LYS	ASP	LEU	SER	ARG	ALA	TYR	GLN	THR	THR	LEU	PRO	ALA	GLY	VAL	GLY	GLY	GLY	GLY	GLY	GLY	VAL	
GLU	GLU	GLN	PRO	ILE	GLU	ALA	ALA	GLU	PRO	GLU	VAL	GLY	ASP	LYS	SER	GLN	GLU	ALA	ARG	GLU	VAL	THR	GLY	GLU	LEU	VAL	GLY	VAL	GLU	PRO	PRO	GLU	GLY	GLY	VAL	LYS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	SER
LYS	GLN	GLU	LEU	THR	GLU	LYS	ALA	ALA	SER	CYS	ALA	GLU	LEU	PRO	GLY	GLY	ASP	THR	ARG	LYS	LEU	SER	ARG	LEU	SER	LYS	ALA	ARG	ALA	ARG	SER	ASP	ASP	THR	THR	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL

• Molecule 1: Gap junction alpha-8 protein

Chain G:

40%

57%

GLU	LYS	VAL	SER	LYS	GLN	GLU	LEU	THR	PRO	GLU	LYS	THR	PRO	GLN	GLU	VAL	CYS	ALA	GLU	LEU	LEU	PRO	GLY	GLU	GLU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY</
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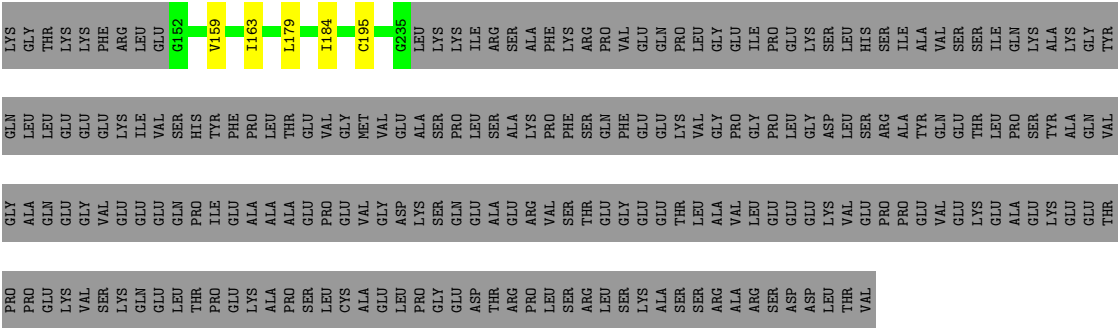
• Molecule 1: Gap junction alpha-8 protein

Chain H:

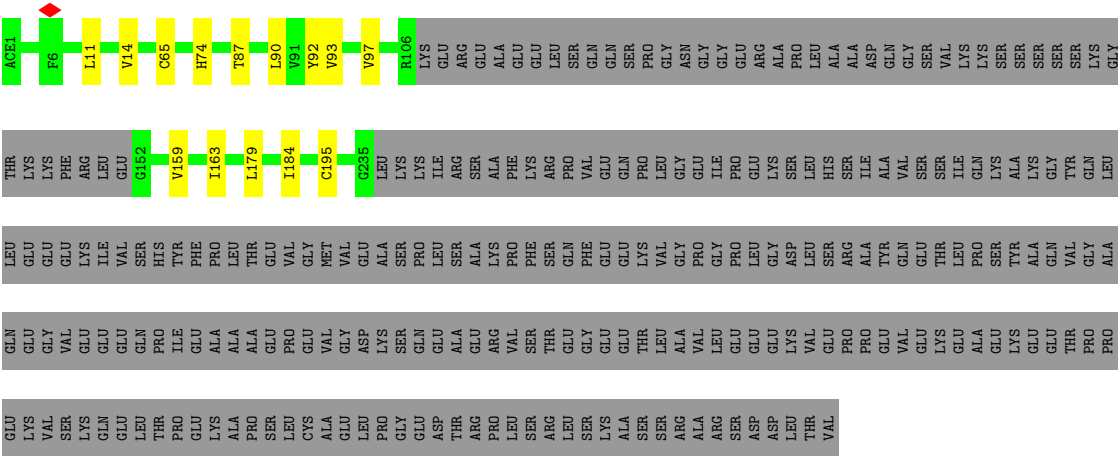
40%

57%

LYS	GLY	THR	LYS	LYS	PHE	ARG	LEU	GLU	G152	V159	I163	L179	I184	C195	G235	LEU	LYS	LYS	ILE	ARG	SER	ALA	SER	VAL	GLN	GLY	PRO	VAL	GLY	ILE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
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● Molecule 1: Gap junction alpha-8 protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D6	Depositor
Number of particles used	242797	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	37	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.010	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0025	Depositor
Map size ($\text{\AA}$)	249.004, 249.004, 249.004	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8893, 0.8893, 0.8893	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, CA, MC3

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	0.38	0/1586	0.52	0/2159
1	B	0.38	0/1586	0.52	0/2159
1	C	0.38	0/1586	0.52	0/2159
1	D	0.38	0/1586	0.52	0/2159
1	E	0.38	0/1586	0.52	0/2159
1	F	0.38	0/1586	0.52	0/2159
1	G	0.38	0/1586	0.52	0/2159
1	H	0.38	0/1586	0.52	0/2159
1	I	0.38	0/1586	0.52	0/2159
1	J	0.38	0/1586	0.52	0/2159
1	K	0.38	0/1586	0.52	0/2159
1	L	0.38	0/1586	0.52	0/2159
All	All	0.38	0/19032	0.52	0/25908

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	1543	1525	1527	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1543	1525	1527	12	0
1	C	1543	1525	1527	12	0
1	D	1543	1525	1527	11	0
1	E	1543	1525	1527	10	0
1	F	1543	1525	1527	10	0
1	G	1543	1525	1527	11	0
1	H	1543	1525	1527	12	0
1	I	1543	1525	1527	12	0
1	J	1543	1525	1527	12	0
1	K	1543	1525	1527	11	0
1	L	1543	1525	1527	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	139	278	220	1	0
3	B	139	278	220	1	0
3	C	139	278	220	1	0
3	D	139	278	220	1	0
3	E	139	278	220	1	0
3	F	139	278	220	1	0
3	G	139	278	220	1	0
3	H	139	278	220	1	0
3	I	139	278	220	1	0
3	J	139	278	220	1	0
3	K	139	278	220	1	0
3	L	139	278	220	1	0
4	A	44	0	0	0	0
4	B	44	0	0	0	0
4	C	44	0	0	0	0
4	D	44	0	0	0	0
4	E	44	0	0	0	0
4	F	44	0	0	0	0
4	G	44	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	44	0	0	0	0
4	I	44	0	0	0	0
4	J	44	0	0	1	0
4	K	44	0	0	0	0
4	L	44	0	0	0	0
All	All	20724	21636	20964	132	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 3.

The worst 5 of 132 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:L:14:VAL:HG22	1:L:93:VAL:HG21	1.56	0.87
1:D:14:VAL:HG22	1:D:93:VAL:HG21	1.56	0.87
1:K:14:VAL:HG22	1:K:93:VAL:HG21	1.56	0.87
1:C:14:VAL:HG22	1:C:93:VAL:HG21	1.56	0.87
1:G:14:VAL:HG22	1:G:93:VAL:HG21	1.56	0.86

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	186/440 (42%)	183 (98%)	3 (2%)	0	100	100
1	B	186/440 (42%)	183 (98%)	3 (2%)	0	100	100
1	C	186/440 (42%)	183 (98%)	3 (2%)	0	100	100
1	D	186/440 (42%)	183 (98%)	3 (2%)	0	100	100
1	E	186/440 (42%)	183 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	186/440 (42%)	183 (98%)	3 (2%)	0	100	100
1	G	186/440 (42%)	183 (98%)	3 (2%)	0	100	100
1	H	186/440 (42%)	183 (98%)	3 (2%)	0	100	100
1	I	186/440 (42%)	183 (98%)	3 (2%)	0	100	100
1	J	186/440 (42%)	183 (98%)	3 (2%)	0	100	100
1	K	186/440 (42%)	183 (98%)	3 (2%)	0	100	100
1	L	186/440 (42%)	183 (98%)	3 (2%)	0	100	100
All	All	2232/5280 (42%)	2196 (98%)	36 (2%)	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	172/384 (45%)	171 (99%)	1 (1%)	78	89
1	B	172/384 (45%)	171 (99%)	1 (1%)	78	89
1	C	172/384 (45%)	171 (99%)	1 (1%)	78	89
1	D	172/384 (45%)	171 (99%)	1 (1%)	78	89
1	E	172/384 (45%)	171 (99%)	1 (1%)	78	89
1	F	172/384 (45%)	171 (99%)	1 (1%)	78	89
1	G	172/384 (45%)	171 (99%)	1 (1%)	78	89
1	H	172/384 (45%)	171 (99%)	1 (1%)	78	89
1	I	172/384 (45%)	171 (99%)	1 (1%)	78	89
1	J	172/384 (45%)	171 (99%)	1 (1%)	78	89
1	K	172/384 (45%)	171 (99%)	1 (1%)	78	89
1	L	172/384 (45%)	171 (99%)	1 (1%)	78	89
All	All	2064/4608 (45%)	2052 (99%)	12 (1%)	76	89

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	87	THR
1	I	87	THR
1	L	87	THR
1	J	87	THR
1	D	87	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	176	HIS
1	I	161	HIS
1	H	74	HIS
1	H	176	HIS
1	J	74	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 204 ligands modelled in this entry, 12 are monoatomic - leaving 192 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MC3	B	515	-	8,8,45	0.33	0	7,7,53	0.78	0
3	MC3	C	515	-	8,8,45	0.33	0	7,7,53	0.79	0
3	MC3	G	512	-	8,8,45	0.34	0	7,7,53	0.79	0
3	MC3	F	508	-	4,4,45	0.37	0	3,3,53	0.57	0
3	MC3	A	509	-	10,10,45	0.30	0	9,9,53	0.81	0
3	MC3	I	505	-	7,7,45	0.35	0	6,6,53	0.72	0
3	MC3	I	506	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	D	510	-	10,10,45	0.31	0	9,9,53	0.82	0
3	MC3	G	504	-	9,9,45	0.35	0	8,8,53	0.73	0
3	MC3	K	511	-	8,8,45	0.34	0	7,7,53	0.78	0
3	MC3	D	507	-	7,7,45	0.35	0	6,6,53	0.74	0
3	MC3	G	505	-	7,7,45	0.35	0	6,6,53	0.72	0
3	MC3	D	512	-	8,8,45	0.33	0	7,7,53	0.78	0
3	MC3	B	506	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	J	506	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	B	513	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	D	516	-	4,4,45	0.37	0	3,3,53	0.57	0
3	MC3	I	503	-	12,12,45	0.31	0	11,11,53	0.83	0
3	MC3	J	509	-	10,10,45	0.29	0	9,9,53	0.81	0
3	MC3	L	508	-	4,4,45	0.37	0	3,3,53	0.57	0
3	MC3	F	509	-	7,7,45	0.34	0	6,6,53	0.74	0
3	MC3	D	513	-	5,5,45	0.36	0	4,4,53	0.62	0
3	MC3	B	502	-	10,10,45	0.29	0	9,9,53	0.79	0
3	MC3	L	505	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	H	515	-	8,8,45	0.33	0	7,7,53	0.78	0
3	MC3	K	515	-	8,8,45	0.33	0	7,7,53	0.79	0
3	MC3	A	503	-	12,12,45	0.31	0	11,11,53	0.83	0
3	MC3	F	507	-	8,8,45	0.33	0	7,7,53	0.78	0
3	MC3	E	515	-	8,8,45	0.33	0	7,7,53	0.78	0
3	MC3	B	508	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	E	514	-	8,8,45	0.34	0	7,7,53	0.78	0
3	MC3	K	510	-	10,10,45	0.31	0	9,9,53	0.83	0
3	MC3	L	516	-	7,7,45	0.35	0	6,6,53	0.74	0
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3	MC3	G	514	-	8,8,45	0.34	0	7,7,53	0.78	0
3	MC3	L	502	-	10,10,45	0.31	0	9,9,53	0.82	0
3	MC3	D	506	-	5,5,45	0.35	0	4,4,53	0.61	0
3	MC3	B	512	-	8,8,45	0.33	0	7,7,53	0.78	0
3	MC3	G	509	-	10,10,45	0.30	0	9,9,53	0.81	0
3	MC3	A	514	-	8,8,45	0.34	0	7,7,53	0.78	0
3	MC3	C	504	-	9,9,45	0.35	0	8,8,53	0.74	0
3	MC3	A	513	-	5,5,45	0.36	0	4,4,53	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MC3	L	512	-	12,12,45	0.31	0	11,11,53	0.84	0
3	MC3	F	513	-	9,9,45	0.35	0	8,8,53	0.73	0
3	MC3	C	507	-	7,7,45	0.34	0	6,6,53	0.74	0
3	MC3	C	512	-	8,8,45	0.33	0	7,7,53	0.78	0
3	MC3	D	517	-	7,7,45	0.34	0	6,6,53	0.74	0
3	MC3	E	513	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	H	511	-	8,8,45	0.34	0	7,7,53	0.77	0
3	MC3	I	512	-	8,8,45	0.34	0	7,7,53	0.78	0
3	MC3	B	509	-	10,10,45	0.30	0	9,9,53	0.81	0
3	MC3	K	517	-	7,7,45	0.35	0	6,6,53	0.74	0
3	MC3	C	511	-	8,8,45	0.34	0	7,7,53	0.78	0
3	MC3	G	503	-	12,12,45	0.31	0	11,11,53	0.84	0
3	MC3	K	504	-	9,9,45	0.35	0	8,8,53	0.74	0
3	MC3	C	506	-	5,5,45	0.35	0	4,4,53	0.61	0
3	MC3	D	503	-	12,12,45	0.31	0	11,11,53	0.83	0
3	MC3	L	513	-	9,9,45	0.35	0	8,8,53	0.74	0
3	MC3	K	507	-	7,7,45	0.35	0	6,6,53	0.74	0
3	MC3	D	508	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	A	508	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	B	503	-	12,12,45	0.31	0	11,11,53	0.84	0
3	MC3	J	516	-	4,4,45	0.37	0	3,3,53	0.57	0
3	MC3	D	505	-	7,7,45	0.35	0	6,6,53	0.72	0
3	MC3	G	516	-	4,4,45	0.37	0	3,3,53	0.57	0
3	MC3	H	503	-	12,12,45	0.31	0	11,11,53	0.83	0
3	MC3	K	506	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	I	508	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	H	508	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	K	513	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	L	503	-	8,8,45	0.34	0	7,7,53	0.77	0
3	MC3	F	502	-	10,10,45	0.31	0	9,9,53	0.82	0
3	MC3	G	515	-	8,8,45	0.33	0	7,7,53	0.78	0
3	MC3	H	504	-	9,9,45	0.35	0	8,8,53	0.74	0
3	MC3	H	516	-	4,4,45	0.37	0	3,3,53	0.57	0
3	MC3	F	517	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	E	504	-	9,9,45	0.35	0	8,8,53	0.74	0
3	MC3	E	509	-	10,10,45	0.30	0	9,9,53	0.81	0
3	MC3	K	503	-	12,12,45	0.31	0	11,11,53	0.84	0
3	MC3	A	515	-	8,8,45	0.33	0	7,7,53	0.78	0
3	MC3	G	506	-	5,5,45	0.35	0	4,4,53	0.61	0
3	MC3	G	513	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	I	502	-	10,10,45	0.29	0	9,9,53	0.79	0
3	MC3	E	505	-	7,7,45	0.34	0	6,6,53	0.71	0
3	MC3	F	501	-	10,10,45	0.30	0	9,9,53	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MC3	L	507	-	8,8,45	0.33	0	7,7,53	0.78	0
3	MC3	A	504	-	9,9,45	0.35	0	8,8,53	0.73	0
3	MC3	J	504	-	9,9,45	0.35	0	8,8,53	0.73	0
3	MC3	A	507	-	7,7,45	0.35	0	6,6,53	0.74	0
3	MC3	C	509	-	10,10,45	0.30	0	9,9,53	0.81	0
3	MC3	E	516	-	4,4,45	0.37	0	3,3,53	0.56	0
3	MC3	C	513	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	F	504	-	8,8,45	0.34	0	7,7,53	0.78	0
3	MC3	C	508	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	K	512	-	8,8,45	0.34	0	7,7,53	0.79	0
3	MC3	F	505	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	K	502	-	10,10,45	0.29	0	9,9,53	0.79	0
3	MC3	K	514	-	8,8,45	0.34	0	7,7,53	0.78	0
3	MC3	L	511	-	10,10,45	0.29	0	9,9,53	0.79	0
3	MC3	A	506	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	G	502	-	10,10,45	0.29	0	9,9,53	0.79	0
3	MC3	I	514	-	8,8,45	0.34	0	7,7,53	0.78	0
3	MC3	D	511	-	8,8,45	0.34	0	7,7,53	0.77	0
3	MC3	F	516	-	7,7,45	0.35	0	6,6,53	0.74	0
3	MC3	D	502	-	10,10,45	0.29	0	9,9,53	0.79	0
3	MC3	H	517	-	7,7,45	0.35	0	6,6,53	0.75	0
3	MC3	J	515	-	8,8,45	0.34	0	7,7,53	0.79	0
3	MC3	K	505	-	7,7,45	0.35	0	6,6,53	0.72	0
3	MC3	A	517	-	7,7,45	0.35	0	6,6,53	0.75	0
3	MC3	E	506	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	B	504	-	9,9,45	0.35	0	8,8,53	0.74	0
3	MC3	F	515	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	C	514	-	8,8,45	0.34	0	7,7,53	0.78	0
3	MC3	A	511	-	8,8,45	0.34	0	7,7,53	0.77	0
3	MC3	D	514	-	8,8,45	0.34	0	7,7,53	0.78	0
3	MC3	D	515	-	8,8,45	0.34	0	7,7,53	0.79	0
3	MC3	J	511	-	8,8,45	0.34	0	7,7,53	0.77	0
3	MC3	J	507	-	7,7,45	0.34	0	6,6,53	0.74	0
3	MC3	G	507	-	7,7,45	0.34	0	6,6,53	0.74	0
3	MC3	E	502	-	10,10,45	0.29	0	9,9,53	0.79	0
3	MC3	L	515	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	H	509	-	10,10,45	0.29	0	9,9,53	0.81	0
3	MC3	L	517	-	5,5,45	0.37	0	4,4,53	0.61	0
3	MC3	E	508	-	5,5,45	0.37	0	4,4,53	0.62	0
3	MC3	B	505	-	7,7,45	0.34	0	6,6,53	0.72	0
3	MC3	H	510	-	10,10,45	0.31	0	9,9,53	0.82	0
3	MC3	L	509	-	7,7,45	0.34	0	6,6,53	0.74	0
3	MC3	C	502	-	10,10,45	0.29	0	9,9,53	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MC3	A	510	-	10,10,45	0.31	0	9,9,53	0.82	0
3	MC3	H	507	-	7,7,45	0.35	0	6,6,53	0.75	0
3	MC3	I	515	-	8,8,45	0.34	0	7,7,53	0.78	0
3	MC3	C	516	-	4,4,45	0.37	0	3,3,53	0.57	0
3	MC3	H	512	-	8,8,45	0.34	0	7,7,53	0.78	0
3	MC3	L	504	-	8,8,45	0.33	0	7,7,53	0.78	0
3	MC3	F	506	-	8,8,45	0.34	0	7,7,53	0.78	0
3	MC3	I	517	-	7,7,45	0.34	0	6,6,53	0.74	0
3	MC3	J	513	-	5,5,45	0.36	0	4,4,53	0.62	0
3	MC3	B	517	-	7,7,45	0.35	0	6,6,53	0.75	0
3	MC3	F	511	-	10,10,45	0.29	0	9,9,53	0.79	0
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3	MC3	C	505	-	7,7,45	0.35	0	6,6,53	0.72	0
3	MC3	A	512	-	8,8,45	0.33	0	7,7,53	0.78	0
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3	MC3	J	502	-	10,10,45	0.30	0	9,9,53	0.79	0
3	MC3	G	517	-	7,7,45	0.34	0	6,6,53	0.74	0
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3	MC3	E	517	-	7,7,45	0.34	0	6,6,53	0.74	0
3	MC3	G	508	-	5,5,45	0.36	0	4,4,53	0.61	0
3	MC3	E	512	-	8,8,45	0.33	0	7,7,53	0.78	0
3	MC3	I	513	-	5,5,45	0.36	0	4,4,53	0.62	0
3	MC3	J	510	-	10,10,45	0.31	0	9,9,53	0.82	0
3	MC3	K	509	-	10,10,45	0.30	0	9,9,53	0.81	0
3	MC3	G	510	-	10,10,45	0.31	0	9,9,53	0.82	0
3	MC3	J	512	-	8,8,45	0.34	0	7,7,53	0.79	0
3	MC3	E	503	-	12,12,45	0.31	0	11,11,53	0.83	0
3	MC3	I	511	-	8,8,45	0.34	0	7,7,53	0.77	0
3	MC3	J	514	-	8,8,45	0.35	0	7,7,53	0.78	0
3	MC3	B	511	-	8,8,45	0.34	0	7,7,53	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MC3	C	517	-	7,7,45	0.34	0	6,6,53	0.74	0
3	MC3	B	510	-	10,10,45	0.31	0	9,9,53	0.82	0
3	MC3	F	512	-	12,12,45	0.31	0	11,11,53	0.84	0
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3	MC3	G	511	-	8,8,45	0.34	0	7,7,53	0.77	0
3	MC3	F	514	-	7,7,45	0.35	0	6,6,53	0.72	0
3	MC3	J	503	-	12,12,45	0.31	0	11,11,53	0.84	0
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3	MC3	I	516	-	4,4,45	0.37	0	3,3,53	0.57	0
3	MC3	E	507	-	7,7,45	0.34	0	6,6,53	0.74	0
3	MC3	B	516	-	4,4,45	0.37	0	3,3,53	0.57	0
3	MC3	H	502	-	10,10,45	0.30	0	9,9,53	0.80	0
3	MC3	H	514	-	8,8,45	0.34	0	7,7,53	0.78	0
3	MC3	I	504	-	9,9,45	0.35	0	8,8,53	0.74	0
3	MC3	C	510	-	10,10,45	0.30	0	9,9,53	0.81	0
3	MC3	B	514	-	8,8,45	0.34	0	7,7,53	0.78	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MC3	B	515	-	-	0/6/6/49	-
3	MC3	C	515	-	-	0/6/6/49	-
3	MC3	G	512	-	-	0/6/6/49	-
3	MC3	F	508	-	-	0/2/2/49	-
3	MC3	A	509	-	-	0/8/8/49	-
3	MC3	I	505	-	-	0/5/5/49	-
3	MC3	I	506	-	-	0/3/3/49	-
3	MC3	D	510	-	-	0/8/8/49	-
3	MC3	G	504	-	-	0/7/7/49	-
3	MC3	K	511	-	-	0/6/6/49	-
3	MC3	D	507	-	-	0/5/5/49	-
3	MC3	G	505	-	-	0/5/5/49	-
3	MC3	D	512	-	-	0/6/6/49	-
3	MC3	B	506	-	-	0/3/3/49	-
3	MC3	J	506	-	-	0/3/3/49	-
3	MC3	B	513	-	-	0/3/3/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MC3	D	516	-	-	0/2/2/49	-
3	MC3	I	503	-	-	0/10/10/49	-
3	MC3	J	509	-	-	0/8/8/49	-
3	MC3	L	508	-	-	0/2/2/49	-
3	MC3	F	509	-	-	0/5/5/49	-
3	MC3	D	513	-	-	0/3/3/49	-
3	MC3	B	502	-	-	0/8/8/49	-
3	MC3	L	505	-	-	0/3/3/49	-
3	MC3	H	515	-	-	0/6/6/49	-
3	MC3	K	515	-	-	0/6/6/49	-
3	MC3	A	503	-	-	0/10/10/49	-
3	MC3	F	507	-	-	0/6/6/49	-
3	MC3	E	515	-	-	0/6/6/49	-
3	MC3	B	508	-	-	0/3/3/49	-
3	MC3	E	514	-	-	0/6/6/49	-
3	MC3	K	510	-	-	0/8/8/49	-
3	MC3	L	516	-	-	0/5/5/49	-
3	MC3	I	507	-	-	0/5/5/49	-
3	MC3	A	516	-	-	0/2/2/49	-
3	MC3	G	514	-	-	0/6/6/49	-
3	MC3	L	502	-	-	0/8/8/49	-
3	MC3	D	506	-	-	0/3/3/49	-
3	MC3	B	512	-	-	0/6/6/49	-
3	MC3	G	509	-	-	0/8/8/49	-
3	MC3	A	514	-	-	0/6/6/49	-
3	MC3	C	504	-	-	0/7/7/49	-
3	MC3	A	513	-	-	0/3/3/49	-
3	MC3	L	512	-	-	0/10/10/49	-
3	MC3	F	513	-	-	0/7/7/49	-
3	MC3	C	507	-	-	0/5/5/49	-
3	MC3	C	512	-	-	0/6/6/49	-
3	MC3	D	517	-	-	0/5/5/49	-
3	MC3	E	513	-	-	0/3/3/49	-
3	MC3	H	511	-	-	0/6/6/49	-
3	MC3	I	512	-	-	0/6/6/49	-
3	MC3	B	509	-	-	0/8/8/49	-
3	MC3	K	517	-	-	0/5/5/49	-
3	MC3	C	511	-	-	0/6/6/49	-
3	MC3	G	503	-	-	0/10/10/49	-
3	MC3	K	504	-	-	0/7/7/49	-
3	MC3	C	506	-	-	0/3/3/49	-
3	MC3	D	503	-	-	0/10/10/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MC3	L	513	-	-	0/7/7/49	-
3	MC3	K	507	-	-	0/5/5/49	-
3	MC3	D	508	-	-	0/3/3/49	-
3	MC3	A	508	-	-	0/3/3/49	-
3	MC3	B	503	-	-	0/10/10/49	-
3	MC3	J	516	-	-	0/2/2/49	-
3	MC3	D	505	-	-	0/5/5/49	-
3	MC3	G	516	-	-	0/2/2/49	-
3	MC3	H	503	-	-	0/10/10/49	-
3	MC3	K	506	-	-	0/3/3/49	-
3	MC3	I	508	-	-	0/3/3/49	-
3	MC3	H	508	-	-	0/3/3/49	-
3	MC3	K	513	-	-	0/3/3/49	-
3	MC3	L	503	-	-	0/6/6/49	-
3	MC3	F	502	-	-	0/8/8/49	-
3	MC3	G	515	-	-	0/6/6/49	-
3	MC3	H	504	-	-	0/7/7/49	-
3	MC3	H	516	-	-	0/2/2/49	-
3	MC3	F	517	-	-	0/3/3/49	-
3	MC3	E	504	-	-	0/7/7/49	-
3	MC3	E	509	-	-	0/8/8/49	-
3	MC3	K	503	-	-	0/10/10/49	-
3	MC3	A	515	-	-	0/6/6/49	-
3	MC3	G	506	-	-	0/3/3/49	-
3	MC3	G	513	-	-	0/3/3/49	-
3	MC3	I	502	-	-	0/8/8/49	-
3	MC3	E	505	-	-	0/5/5/49	-
3	MC3	F	501	-	-	0/8/8/49	-
3	MC3	L	507	-	-	0/6/6/49	-
3	MC3	A	504	-	-	0/7/7/49	-
3	MC3	J	504	-	-	0/7/7/49	-
3	MC3	A	507	-	-	0/5/5/49	-
3	MC3	C	509	-	-	0/8/8/49	-
3	MC3	E	516	-	-	0/2/2/49	-
3	MC3	C	513	-	-	0/3/3/49	-
3	MC3	F	504	-	-	0/6/6/49	-
3	MC3	C	508	-	-	0/3/3/49	-
3	MC3	K	512	-	-	0/6/6/49	-
3	MC3	F	505	-	-	0/3/3/49	-
3	MC3	K	502	-	-	0/8/8/49	-
3	MC3	K	514	-	-	0/6/6/49	-
3	MC3	L	511	-	-	0/8/8/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MC3	A	506	-	-	0/3/3/49	-
3	MC3	G	502	-	-	0/8/8/49	-
3	MC3	I	514	-	-	0/6/6/49	-
3	MC3	D	511	-	-	0/6/6/49	-
3	MC3	F	516	-	-	0/5/5/49	-
3	MC3	D	502	-	-	0/8/8/49	-
3	MC3	H	517	-	-	0/5/5/49	-
3	MC3	J	515	-	-	0/6/6/49	-
3	MC3	K	505	-	-	0/5/5/49	-
3	MC3	A	517	-	-	0/5/5/49	-
3	MC3	E	506	-	-	0/3/3/49	-
3	MC3	B	504	-	-	0/7/7/49	-
3	MC3	F	515	-	-	0/3/3/49	-
3	MC3	C	514	-	-	0/6/6/49	-
3	MC3	A	511	-	-	0/6/6/49	-
3	MC3	D	514	-	-	0/6/6/49	-
3	MC3	D	515	-	-	0/6/6/49	-
3	MC3	J	511	-	-	0/6/6/49	-
3	MC3	J	507	-	-	0/5/5/49	-
3	MC3	G	507	-	-	0/5/5/49	-
3	MC3	E	502	-	-	0/8/8/49	-
3	MC3	L	515	-	-	0/3/3/49	-
3	MC3	H	509	-	-	0/8/8/49	-
3	MC3	L	517	-	-	0/3/3/49	-
3	MC3	E	508	-	-	0/3/3/49	-
3	MC3	B	505	-	-	0/5/5/49	-
3	MC3	H	510	-	-	0/8/8/49	-
3	MC3	L	509	-	-	0/5/5/49	-
3	MC3	C	502	-	-	0/8/8/49	-
3	MC3	A	510	-	-	0/8/8/49	-
3	MC3	H	507	-	-	0/5/5/49	-
3	MC3	I	515	-	-	0/6/6/49	-
3	MC3	C	516	-	-	0/2/2/49	-
3	MC3	H	512	-	-	0/6/6/49	-
3	MC3	L	504	-	-	0/6/6/49	-
3	MC3	F	506	-	-	0/6/6/49	-
3	MC3	I	517	-	-	0/5/5/49	-
3	MC3	J	513	-	-	0/3/3/49	-
3	MC3	B	517	-	-	0/5/5/49	-
3	MC3	F	511	-	-	0/8/8/49	-
3	MC3	K	508	-	-	0/3/3/49	-
3	MC3	J	517	-	-	0/5/5/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MC3	C	505	-	-	0/5/5/49	-
3	MC3	A	512	-	-	0/6/6/49	-
3	MC3	L	514	-	-	0/5/5/49	-
3	MC3	A	502	-	-	0/8/8/49	-
3	MC3	J	502	-	-	0/8/8/49	-
3	MC3	G	517	-	-	0/5/5/49	-
3	MC3	H	506	-	-	0/3/3/49	-
3	MC3	H	513	-	-	0/3/3/49	-
3	MC3	L	506	-	-	0/6/6/49	-
3	MC3	A	505	-	-	0/5/5/49	-
3	MC3	D	509	-	-	0/8/8/49	-
3	MC3	J	505	-	-	0/5/5/49	-
3	MC3	D	504	-	-	0/7/7/49	-
3	MC3	J	508	-	-	0/3/3/49	-
3	MC3	L	501	-	-	0/8/8/49	-
3	MC3	C	503	-	-	0/10/10/49	-
3	MC3	I	509	-	-	0/8/8/49	-
3	MC3	I	510	-	-	0/8/8/49	-
3	MC3	E	517	-	-	0/5/5/49	-
3	MC3	G	508	-	-	0/3/3/49	-
3	MC3	E	512	-	-	0/6/6/49	-
3	MC3	I	513	-	-	0/3/3/49	-
3	MC3	J	510	-	-	0/8/8/49	-
3	MC3	K	509	-	-	0/8/8/49	-
3	MC3	G	510	-	-	0/8/8/49	-
3	MC3	J	512	-	-	0/6/6/49	-
3	MC3	E	503	-	-	0/10/10/49	-
3	MC3	I	511	-	-	0/6/6/49	-
3	MC3	J	514	-	-	0/6/6/49	-
3	MC3	B	511	-	-	0/6/6/49	-
3	MC3	C	517	-	-	0/5/5/49	-
3	MC3	B	510	-	-	0/8/8/49	-
3	MC3	F	512	-	-	0/10/10/49	-
3	MC3	H	505	-	-	0/5/5/49	-
3	MC3	G	511	-	-	0/6/6/49	-
3	MC3	F	514	-	-	0/5/5/49	-
3	MC3	J	503	-	-	0/10/10/49	-
3	MC3	B	507	-	-	0/5/5/49	-
3	MC3	K	516	-	-	0/2/2/49	-
3	MC3	E	510	-	-	0/8/8/49	-
3	MC3	E	511	-	-	0/6/6/49	-
3	MC3	F	503	-	-	0/6/6/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MC3	I	516	-	-	0/2/2/49	-
3	MC3	E	507	-	-	0/5/5/49	-
3	MC3	B	516	-	-	0/2/2/49	-
3	MC3	H	502	-	-	0/8/8/49	-
3	MC3	H	514	-	-	0/6/6/49	-
3	MC3	I	504	-	-	0/7/7/49	-
3	MC3	C	510	-	-	0/8/8/49	-
3	MC3	B	514	-	-	0/6/6/49	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	503	MC3	1	0
3	A	503	MC3	1	0
3	L	512	MC3	1	0
3	G	503	MC3	1	0
3	D	503	MC3	1	0
3	B	503	MC3	1	0
3	H	503	MC3	1	0
3	K	503	MC3	1	0
3	C	503	MC3	1	0
3	E	503	MC3	1	0
3	F	512	MC3	1	0
3	J	503	MC3	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

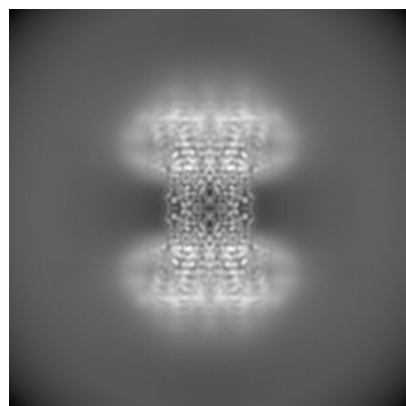
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74938. These allow visual inspection of the internal detail of the map and identification of artifacts.

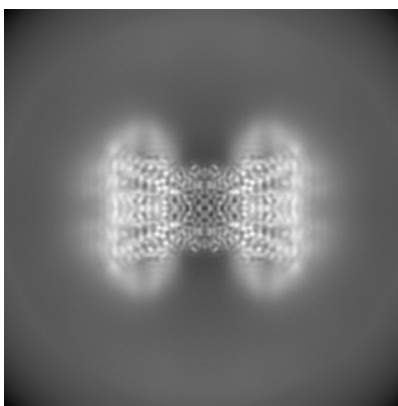
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

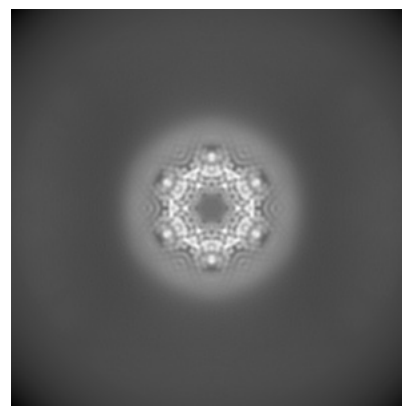
6.1.1 Primary map



X

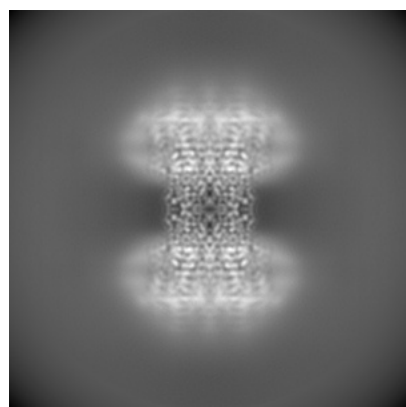


Y

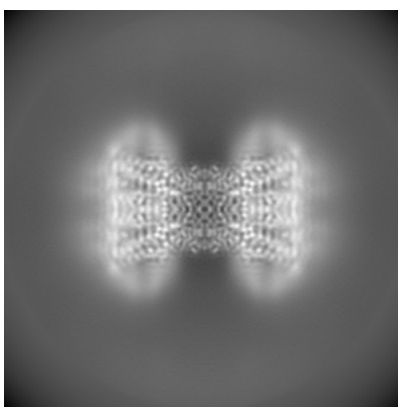


Z

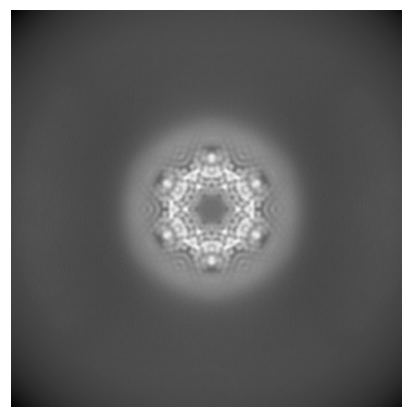
6.1.2 Raw map



X



Y

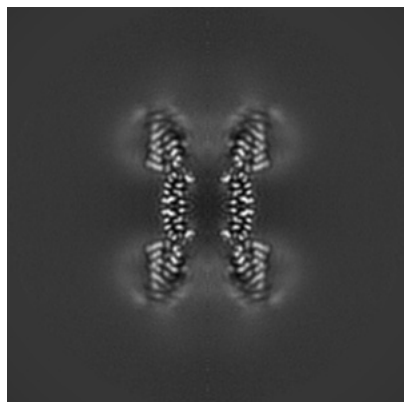


Z

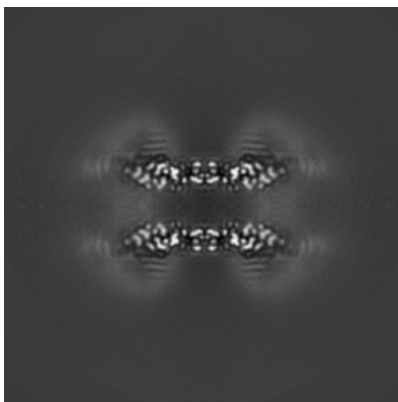
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

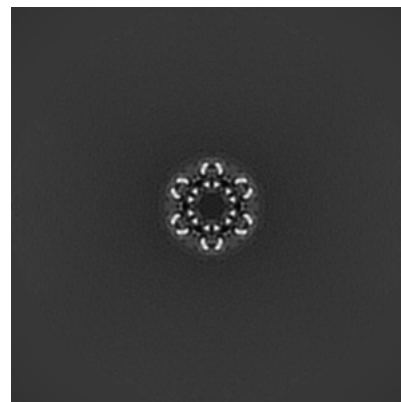
6.2.1 Primary map



X Index: 140

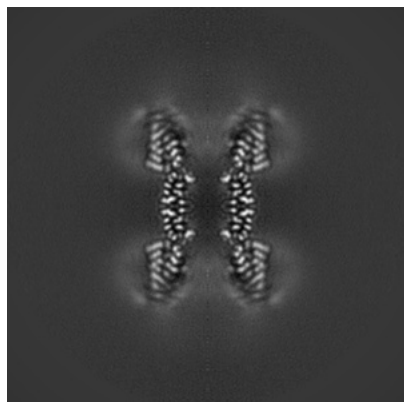


Y Index: 140

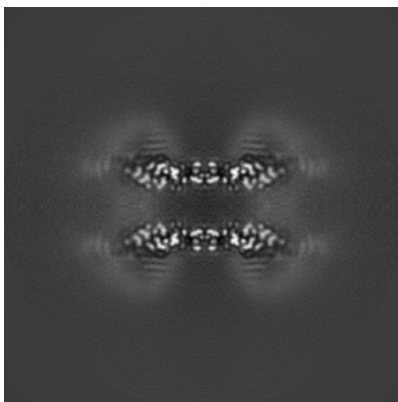


Z Index: 140

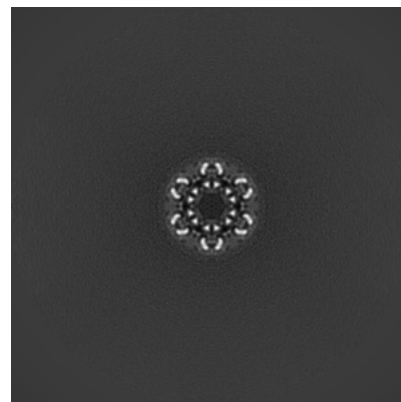
6.2.2 Raw map



X Index: 140



Y Index: 140

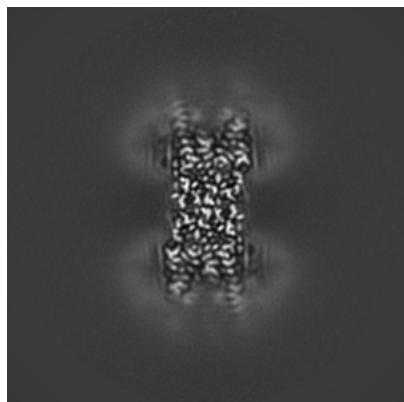


Z Index: 140

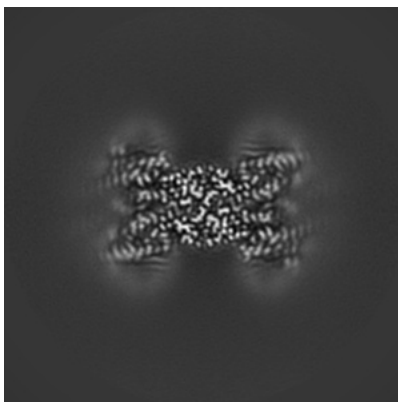
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

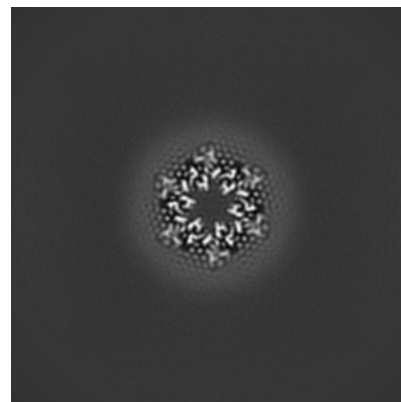
6.3.1 Primary map



X Index: 158

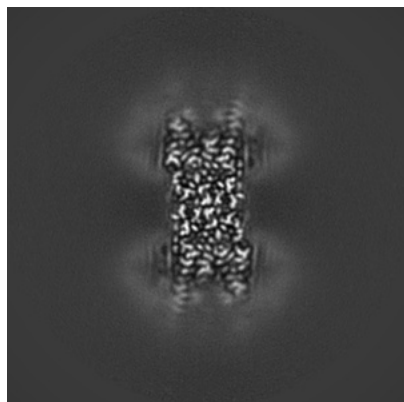


Y Index: 156

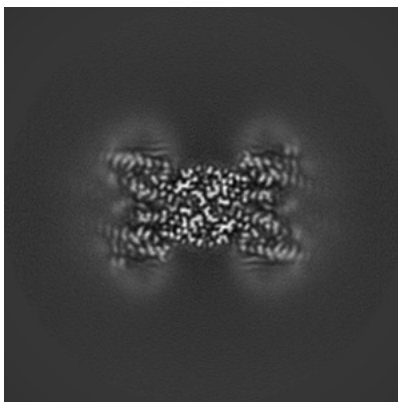


Z Index: 168

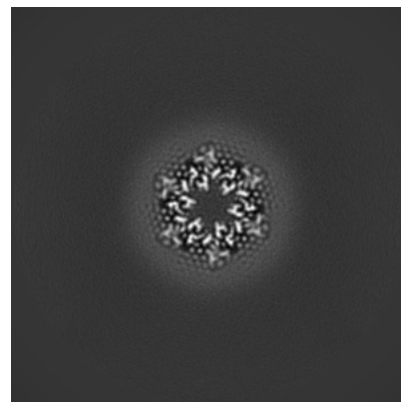
6.3.2 Raw map



X Index: 122



Y Index: 124

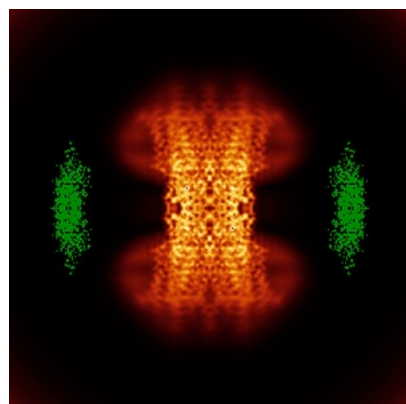


Z Index: 168

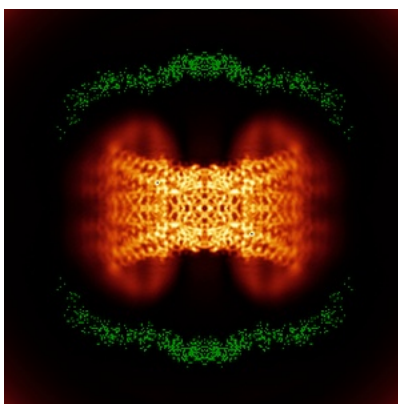
The images above show the largest variance slices of the map in three orthogonal directions.

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

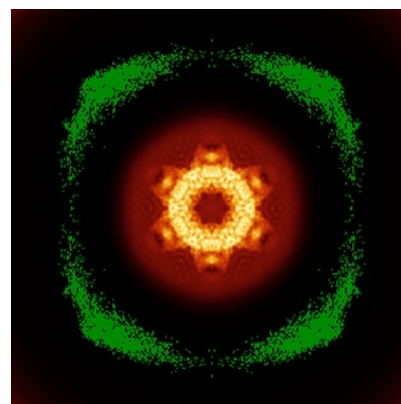
6.4.1 Primary map



X

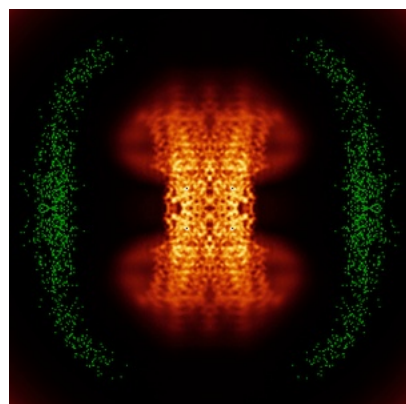


Y

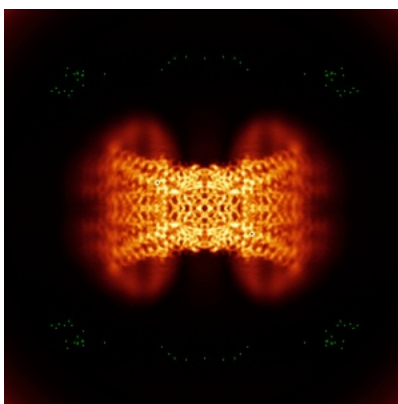


Z

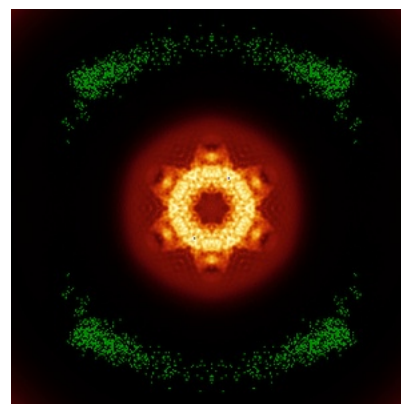
6.4.2 Raw map



X



Y

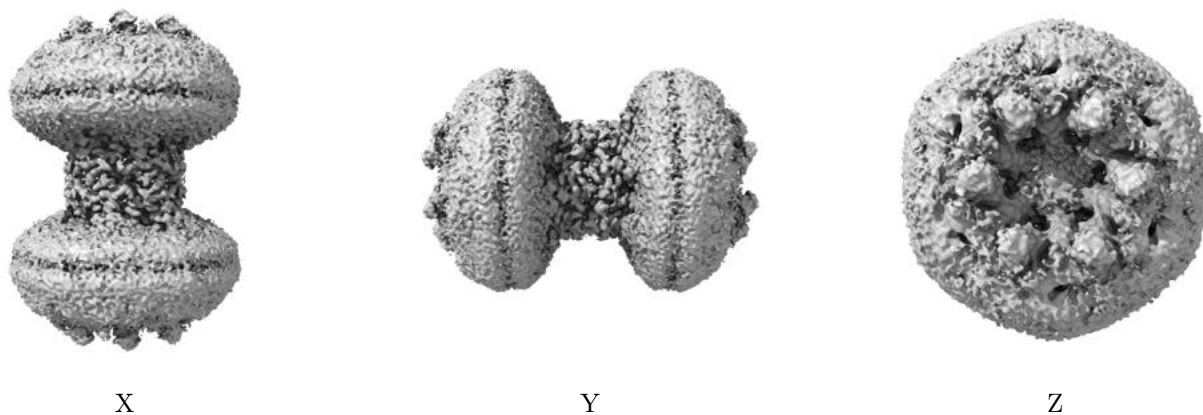


Z

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.

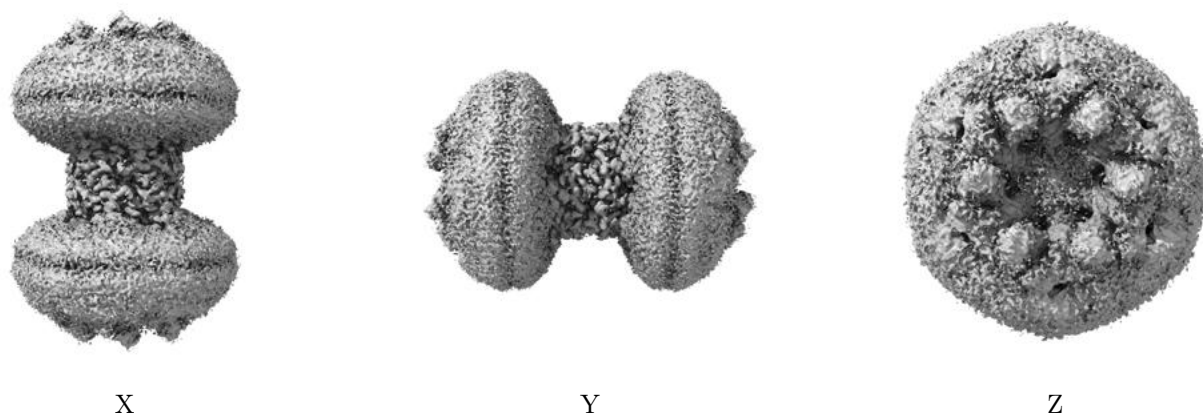
6.5 Orthogonal surface views [i](#)

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.

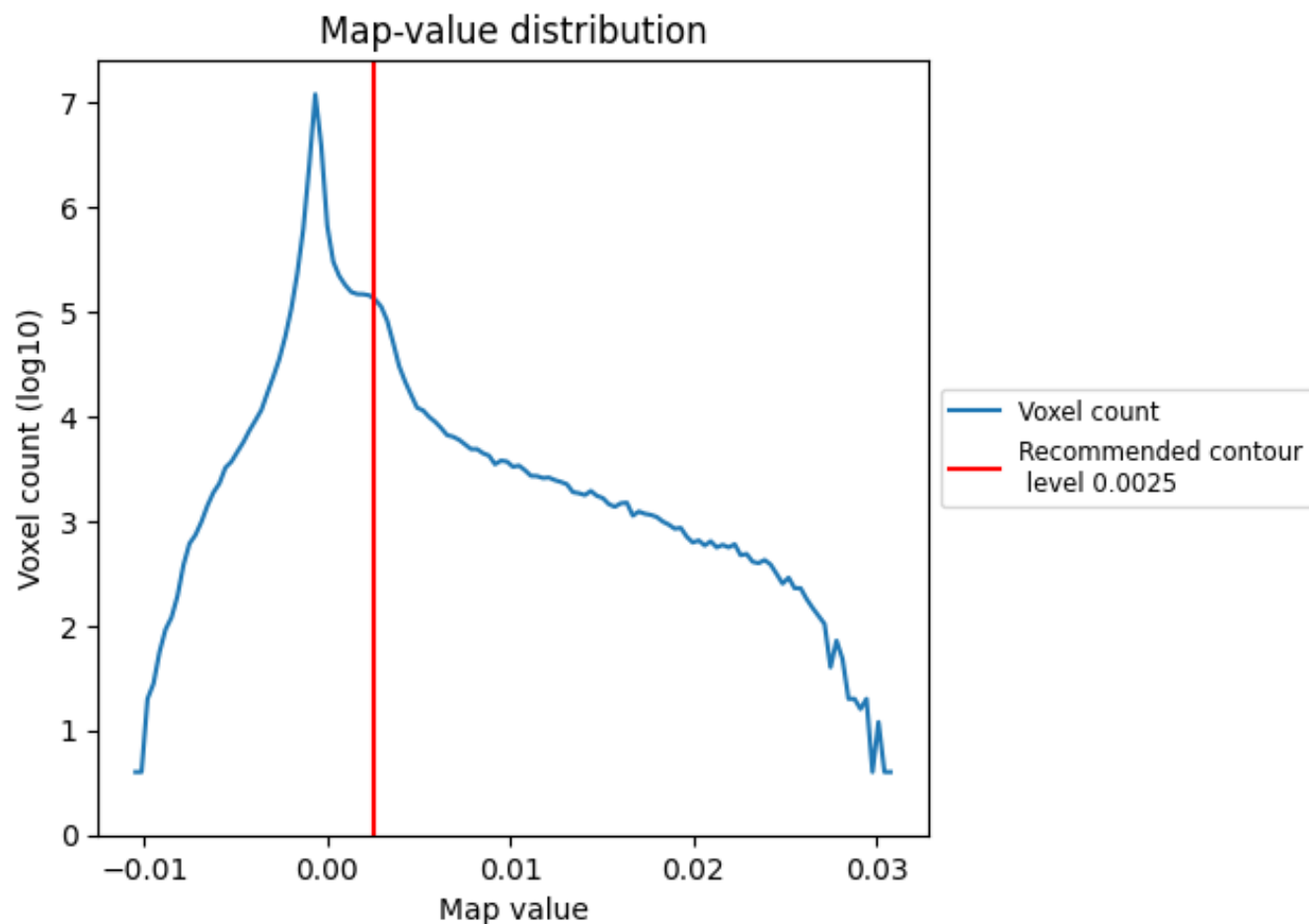
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

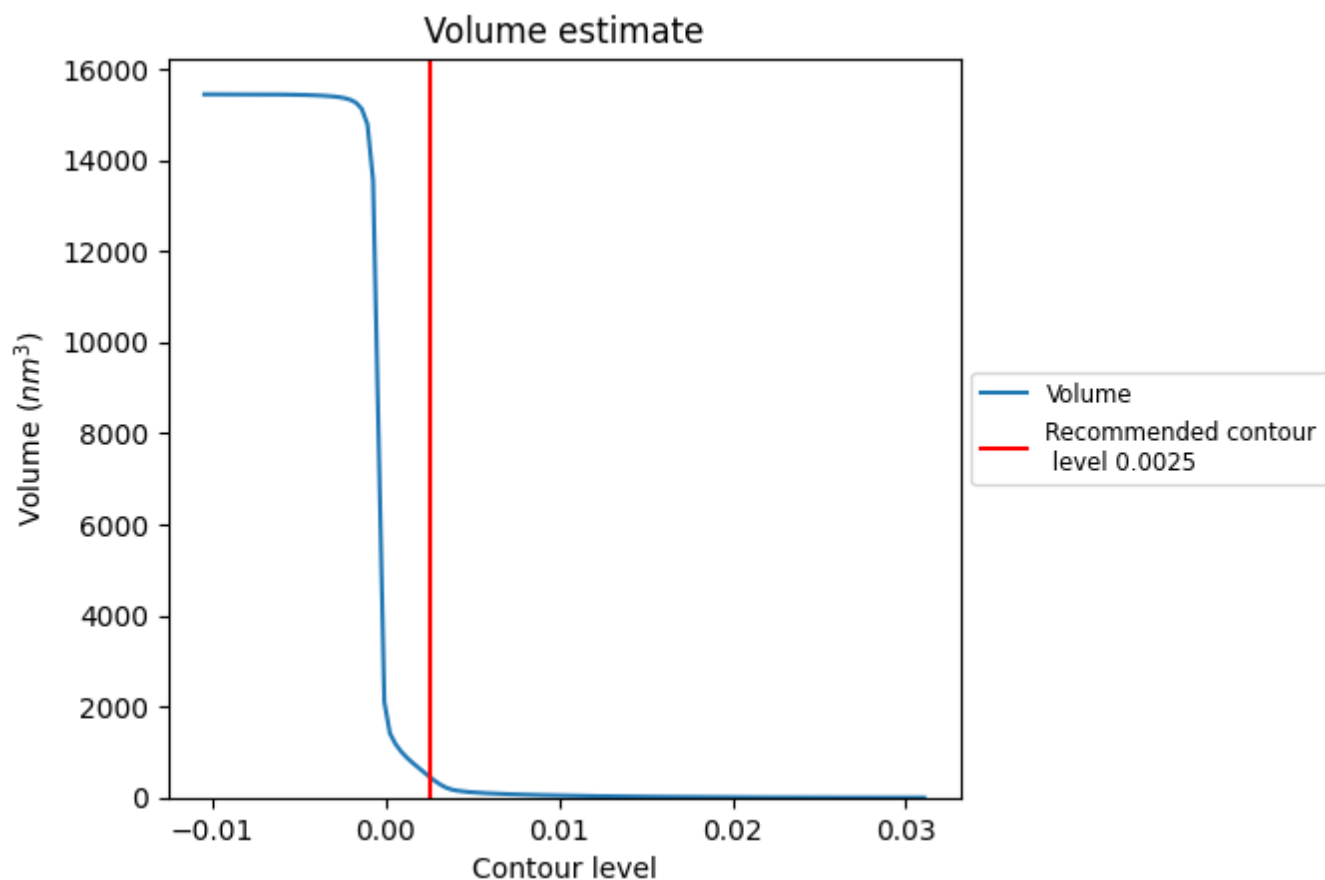
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

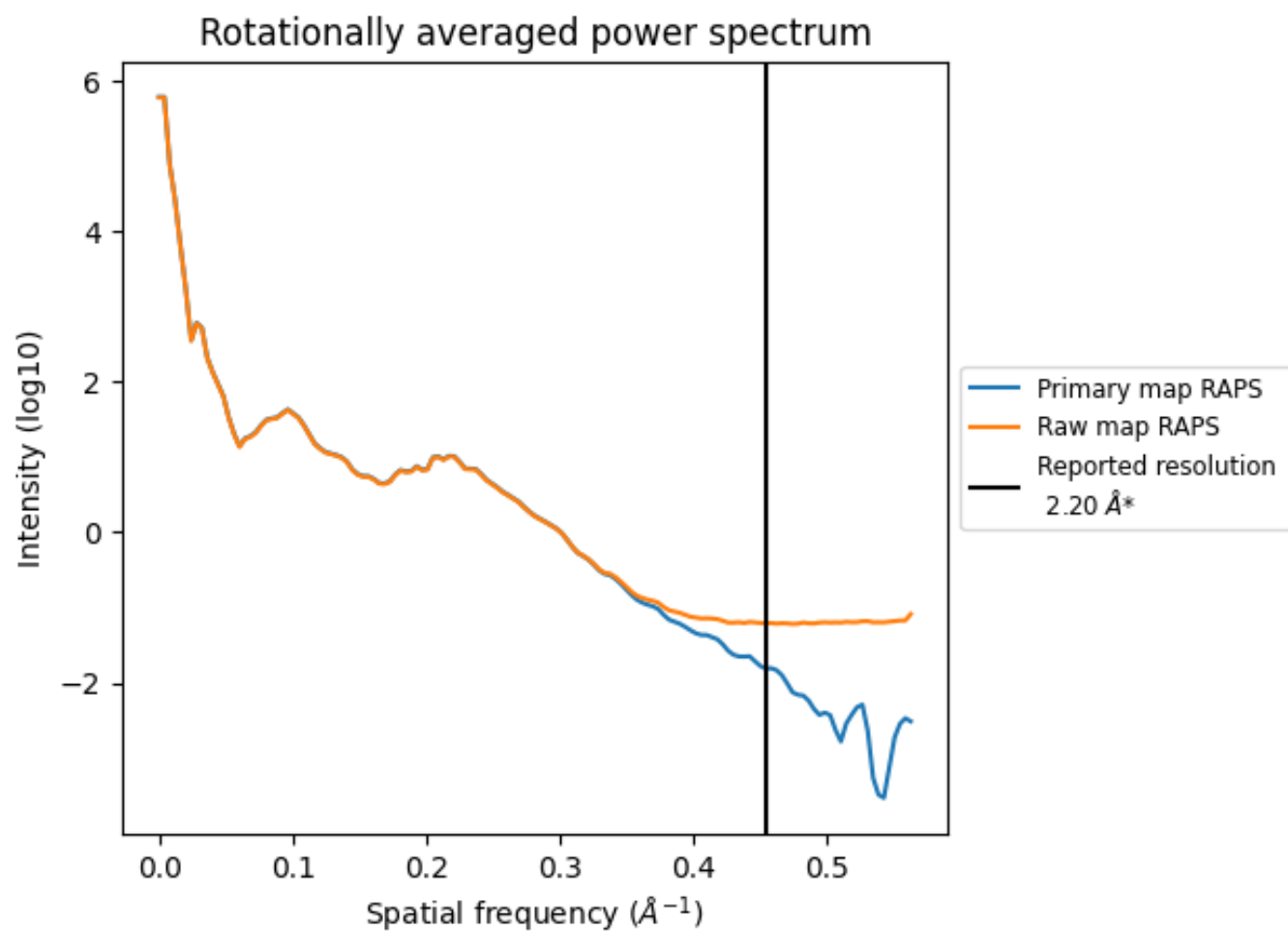
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 463 nm³; this corresponds to an approximate mass of 418 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

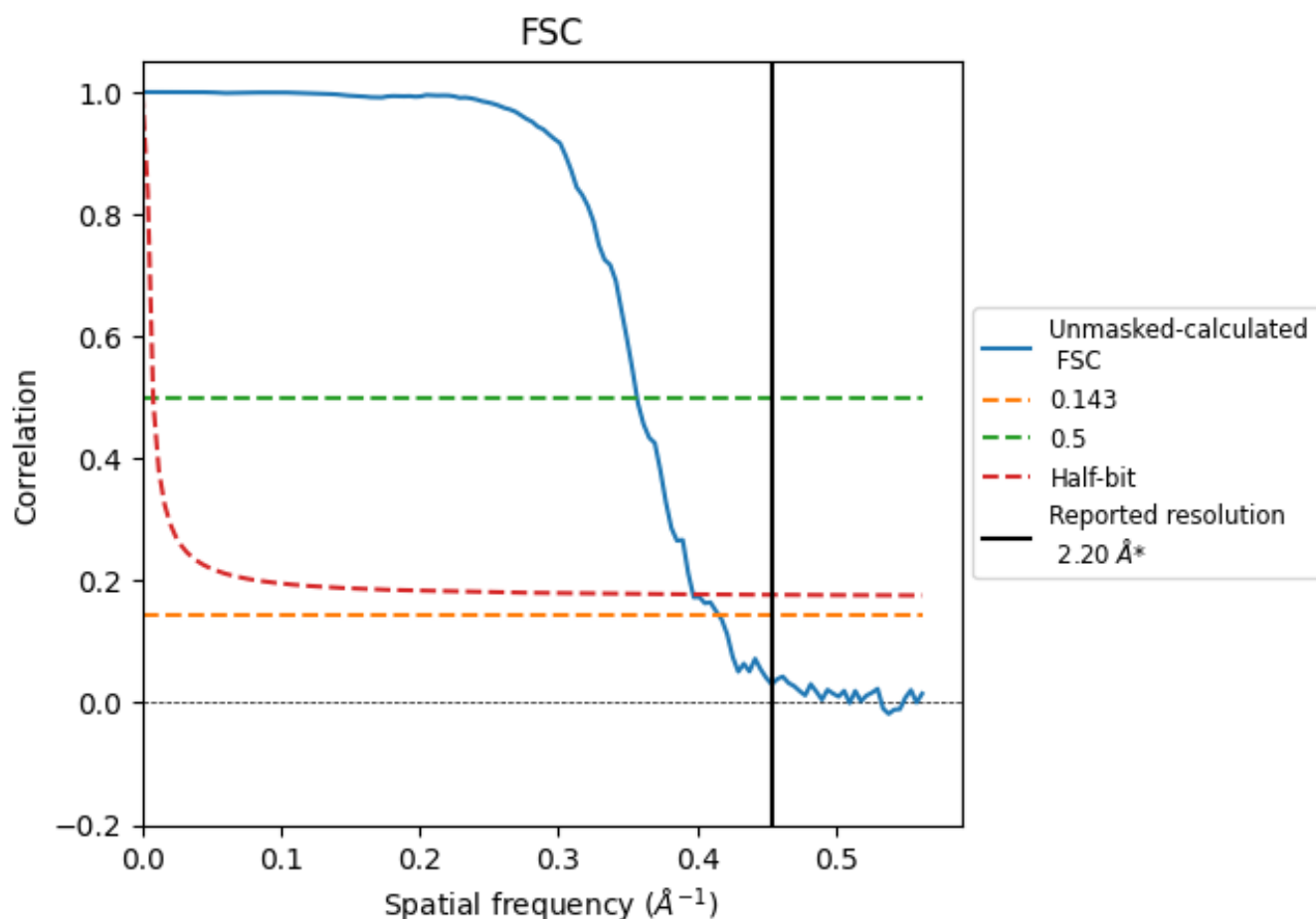


*Reported resolution corresponds to spatial frequency of 0.455 Å⁻¹

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 0.455 Å⁻¹

8.2 Resolution estimates [i](#)

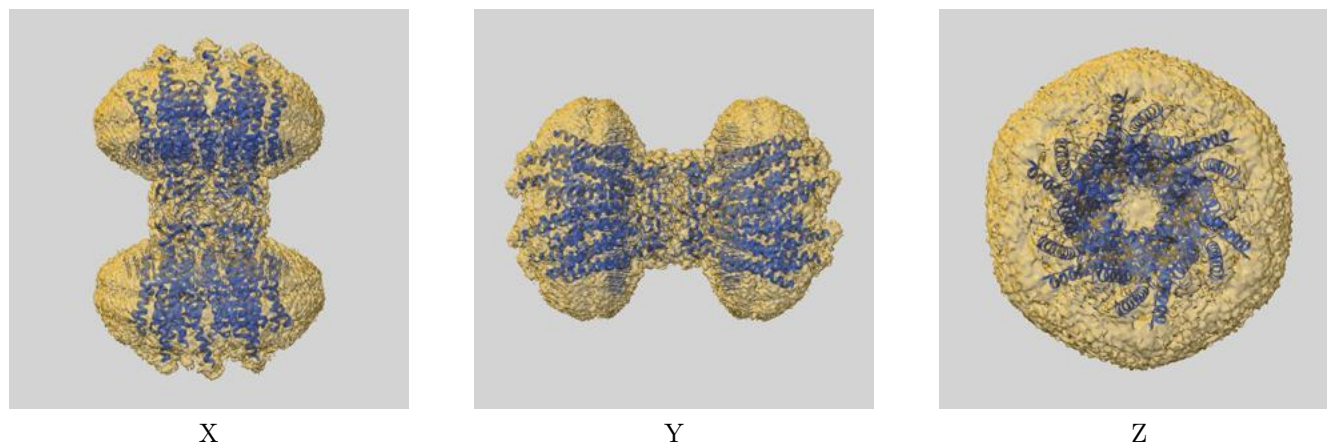
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.41	2.80	2.52

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

9 Map-model fit [i](#)

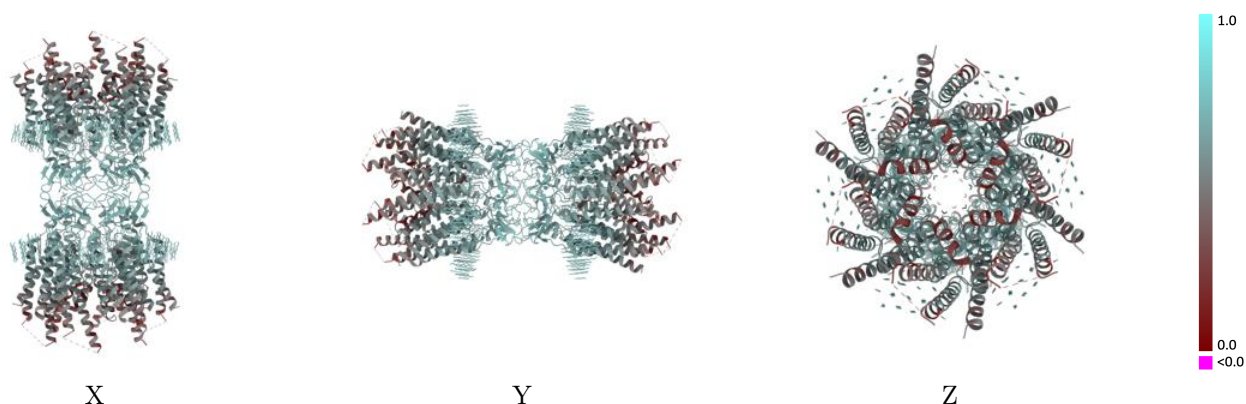
This section contains information regarding the fit between EMDB map EMD-74938 and PDB model 9ZY3. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



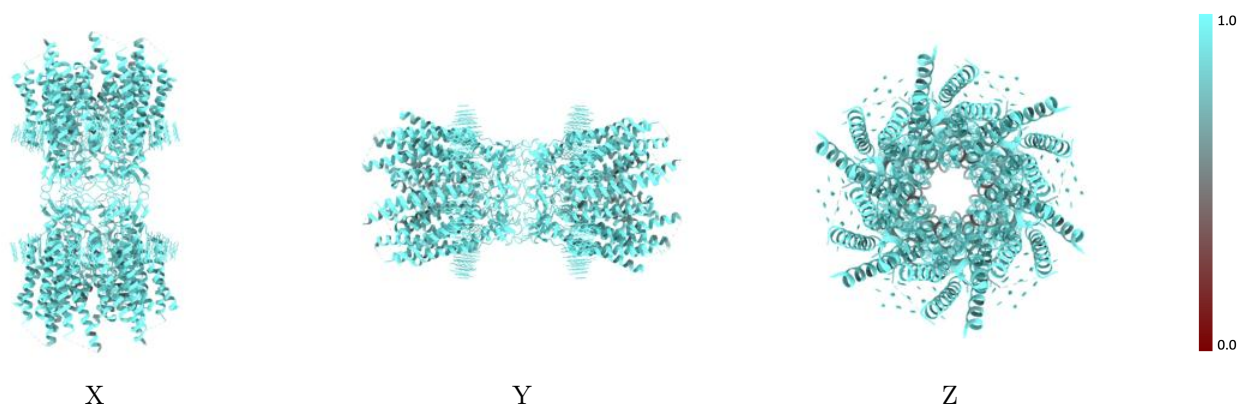
The images above show the 3D surface view of the map at the recommended contour level 0.0025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



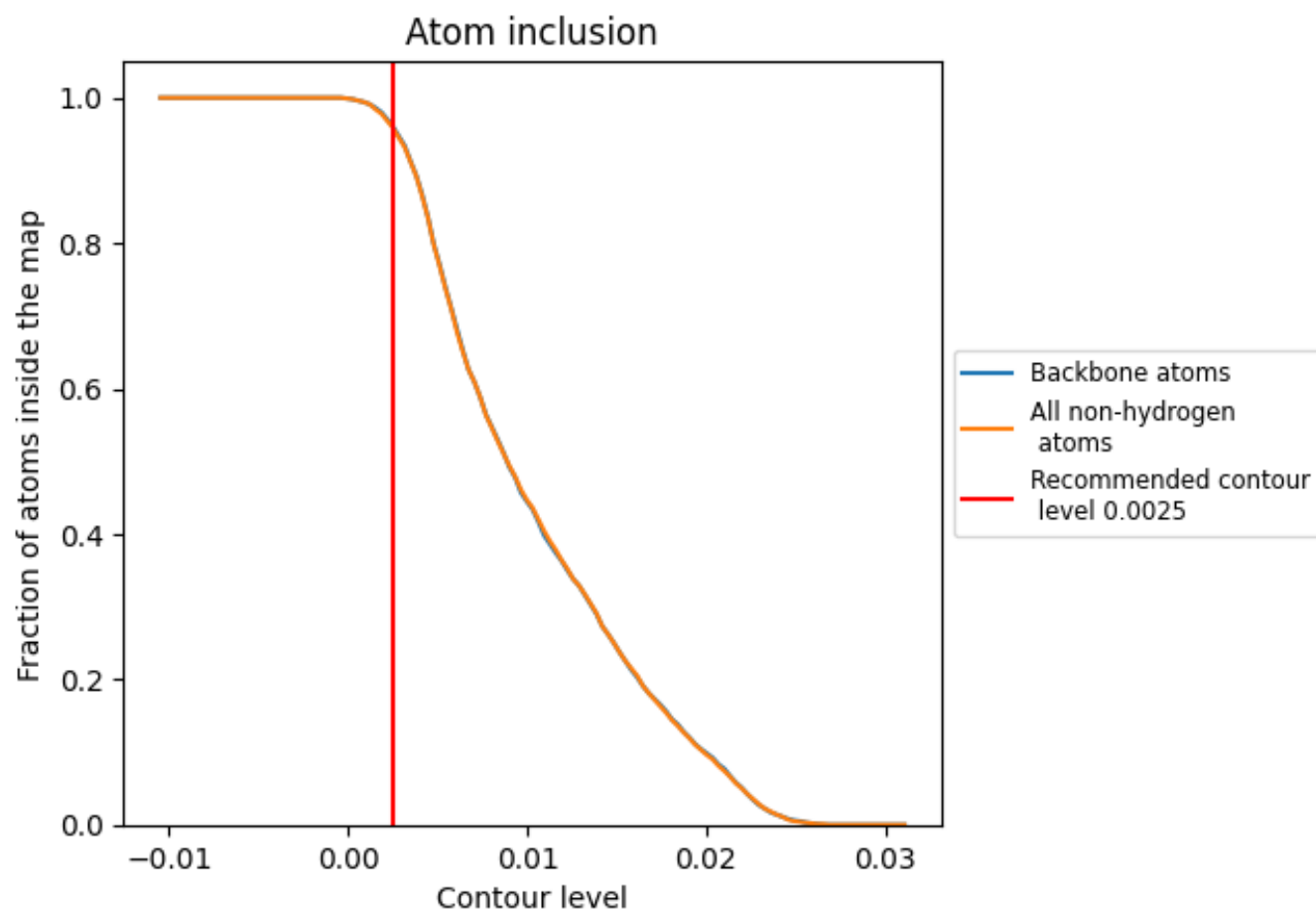
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 96% of all backbone atoms, 96% 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	0.9590	0.5500
A	0.9590	0.5490
B	0.9580	0.5510
C	0.9590	0.5490
D	0.9560	0.5490
E	0.9570	0.5510
F	0.9590	0.5500
G	0.9570	0.5490
H	0.9590	0.5490
I	0.9560	0.5500
J	0.9570	0.5500
K	0.9580	0.5490
L	0.9570	0.5490

1.0

0.0

<0.0