wwPDB EM Validation Summary Report (i)

Aug 29, 2026 – 12:31 PM EDT

PDB ID	:	11SO / pdb_000011so
EMDB ID	:	EMD-76009
Title	:	EcMscM lacking the first periplasmic helical bundle in NaCl in a closed conformation
Authors	:	Hiotis, G.; Walz, T.
Deposited on	:	2026-03-11
Resolution	:	4.30 Å(reported)
Based on initial model	:	.

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 (i) 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 (i)) were used in the production of this report:

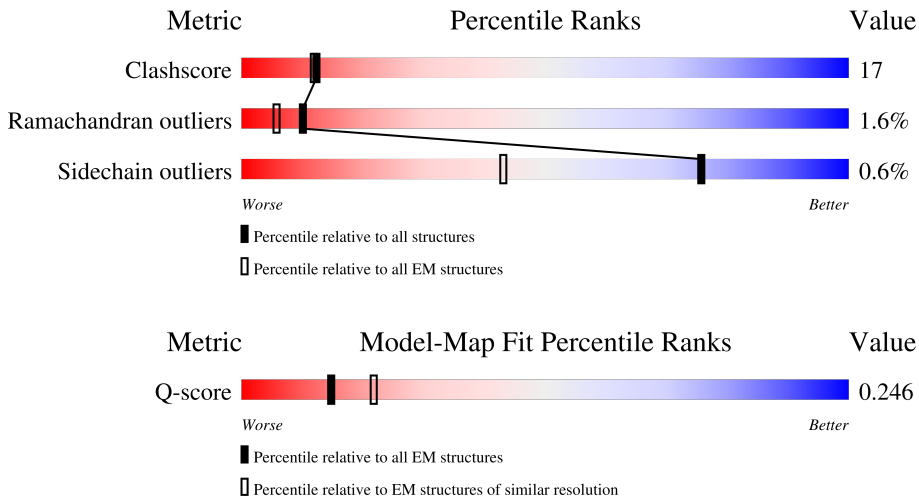
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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	4585 (3.80 - 4.80)

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 <=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	901	12% 73% 14% • 11%
1	B	901	12% 73% 14% • 11%
1	C	901	12% 74% 14% • 11%
1	D	901	12% 73% 14% • 11%

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Mol	Chain	Length	Quality of chain
1	E	901	12% 73% 14% • 11%
1	F	901	12% 73% 14% • 11%
1	G	901	13% 73% 14% • 11%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 31598 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 Miniconductance mechanosensitive channel MscM.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	804	4514	2761	867	881	5	0	0
1	B	804	4514	2761	867	881	5	0	0
1	C	804	4514	2761	867	881	5	0	0
1	D	804	4514	2761	867	881	5	0	0
1	E	804	4514	2761	867	881	5	0	0
1	F	804	4514	2761	867	881	5	0	0
1	G	804	4514	2761	867	881	5	0	0

There are 322 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	MET	-	initiating methionine	UNP P39285
A	214	ARG	-	expression tag	UNP P39285
A	215	LEU	-	expression tag	UNP P39285
A	216	ILE	-	expression tag	UNP P39285
A	217	ILE	-	expression tag	UNP P39285
A	218	THR	-	expression tag	UNP P39285
A	219	PHE	-	expression tag	UNP P39285
A	220	LEU	-	expression tag	UNP P39285
A	221	MET	-	expression tag	UNP P39285
A	222	ALA	-	expression tag	UNP P39285
A	223	TRP	-	expression tag	UNP P39285
A	224	CYS	-	expression tag	UNP P39285
A	225	LEU	-	expression tag	UNP P39285
A	226	SER	-	expression tag	UNP P39285
A	227	TRP	-	expression tag	UNP P39285
A	228	GLY	-	expression tag	UNP P39285

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Chain	Residue	Modelled	Actual	Comment	Reference
A	229	ALA	-	expression tag	UNP P39285
A	230	TYR	-	expression tag	UNP P39285
A	231	ALA	-	expression tag	UNP P39285
A	232	ALA	-	expression tag	UNP P39285
A	233	THR	-	expression tag	UNP P39285
A	234	ALA	-	expression tag	UNP P39285
A	235	PRO	-	expression tag	UNP P39285
A	236	ASP	-	expression tag	UNP P39285
A	237	SER	-	expression tag	UNP P39285
A	238	LYS	-	expression tag	UNP P39285
A	239	GLN	-	expression tag	UNP P39285
A	240	ILE	-	expression tag	UNP P39285
A	241	THR	-	expression tag	UNP P39285
A	242	GLN	-	expression tag	UNP P39285
A	243	GLU	-	expression tag	UNP P39285
A	244	LEU	-	expression tag	UNP P39285
A	245	GLU	-	expression tag	UNP P39285
A	246	GLN	-	expression tag	UNP P39285
A	247	ALA	-	expression tag	UNP P39285
A	248	LYS	-	expression tag	UNP P39285
A	249	ALA	-	expression tag	UNP P39285
A	250	ALA	-	expression tag	UNP P39285
A	251	LYS	-	expression tag	UNP P39285
A	252	PRO	-	expression tag	UNP P39285
A	1108	LEU	-	expression tag	UNP P39285
A	1109	GLU	-	expression tag	UNP P39285
A	1110	VAL	-	expression tag	UNP P39285
A	1111	LEU	-	expression tag	UNP P39285
A	1112	PHE	-	expression tag	UNP P39285
A	1113	GLN	-	expression tag	UNP P39285
B	213	MET	-	initiating methionine	UNP P39285
B	214	ARG	-	expression tag	UNP P39285
B	215	LEU	-	expression tag	UNP P39285
B	216	ILE	-	expression tag	UNP P39285
B	217	ILE	-	expression tag	UNP P39285
B	218	THR	-	expression tag	UNP P39285
B	219	PHE	-	expression tag	UNP P39285
B	220	LEU	-	expression tag	UNP P39285
B	221	MET	-	expression tag	UNP P39285
B	222	ALA	-	expression tag	UNP P39285
B	223	TRP	-	expression tag	UNP P39285
B	224	CYS	-	expression tag	UNP P39285

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Chain	Residue	Modelled	Actual	Comment	Reference
B	225	LEU	-	expression tag	UNP P39285
B	226	SER	-	expression tag	UNP P39285
B	227	TRP	-	expression tag	UNP P39285
B	228	GLY	-	expression tag	UNP P39285
B	229	ALA	-	expression tag	UNP P39285
B	230	TYR	-	expression tag	UNP P39285
B	231	ALA	-	expression tag	UNP P39285
B	232	ALA	-	expression tag	UNP P39285
B	233	THR	-	expression tag	UNP P39285
B	234	ALA	-	expression tag	UNP P39285
B	235	PRO	-	expression tag	UNP P39285
B	236	ASP	-	expression tag	UNP P39285
B	237	SER	-	expression tag	UNP P39285
B	238	LYS	-	expression tag	UNP P39285
B	239	GLN	-	expression tag	UNP P39285
B	240	ILE	-	expression tag	UNP P39285
B	241	THR	-	expression tag	UNP P39285
B	242	GLN	-	expression tag	UNP P39285
B	243	GLU	-	expression tag	UNP P39285
B	244	LEU	-	expression tag	UNP P39285
B	245	GLU	-	expression tag	UNP P39285
B	246	GLN	-	expression tag	UNP P39285
B	247	ALA	-	expression tag	UNP P39285
B	248	LYS	-	expression tag	UNP P39285
B	249	ALA	-	expression tag	UNP P39285
B	250	ALA	-	expression tag	UNP P39285
B	251	LYS	-	expression tag	UNP P39285
B	252	PRO	-	expression tag	UNP P39285
B	1108	LEU	-	expression tag	UNP P39285
B	1109	GLU	-	expression tag	UNP P39285
B	1110	VAL	-	expression tag	UNP P39285
B	1111	LEU	-	expression tag	UNP P39285
B	1112	PHE	-	expression tag	UNP P39285
B	1113	GLN	-	expression tag	UNP P39285
C	213	MET	-	initiating methionine	UNP P39285
C	214	ARG	-	expression tag	UNP P39285
C	215	LEU	-	expression tag	UNP P39285
C	216	ILE	-	expression tag	UNP P39285
C	217	ILE	-	expression tag	UNP P39285
C	218	THR	-	expression tag	UNP P39285
C	219	PHE	-	expression tag	UNP P39285
C	220	LEU	-	expression tag	UNP P39285

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Chain	Residue	Modelled	Actual	Comment	Reference
C	221	MET	-	expression tag	UNP P39285
C	222	ALA	-	expression tag	UNP P39285
C	223	TRP	-	expression tag	UNP P39285
C	224	CYS	-	expression tag	UNP P39285
C	225	LEU	-	expression tag	UNP P39285
C	226	SER	-	expression tag	UNP P39285
C	227	TRP	-	expression tag	UNP P39285
C	228	GLY	-	expression tag	UNP P39285
C	229	ALA	-	expression tag	UNP P39285
C	230	TYR	-	expression tag	UNP P39285
C	231	ALA	-	expression tag	UNP P39285
C	232	ALA	-	expression tag	UNP P39285
C	233	THR	-	expression tag	UNP P39285
C	234	ALA	-	expression tag	UNP P39285
C	235	PRO	-	expression tag	UNP P39285
C	236	ASP	-	expression tag	UNP P39285
C	237	SER	-	expression tag	UNP P39285
C	238	LYS	-	expression tag	UNP P39285
C	239	GLN	-	expression tag	UNP P39285
C	240	ILE	-	expression tag	UNP P39285
C	241	THR	-	expression tag	UNP P39285
C	242	GLN	-	expression tag	UNP P39285
C	243	GLU	-	expression tag	UNP P39285
C	244	LEU	-	expression tag	UNP P39285
C	245	GLU	-	expression tag	UNP P39285
C	246	GLN	-	expression tag	UNP P39285
C	247	ALA	-	expression tag	UNP P39285
C	248	LYS	-	expression tag	UNP P39285
C	249	ALA	-	expression tag	UNP P39285
C	250	ALA	-	expression tag	UNP P39285
C	251	LYS	-	expression tag	UNP P39285
C	252	PRO	-	expression tag	UNP P39285
C	1108	LEU	-	expression tag	UNP P39285
C	1109	GLU	-	expression tag	UNP P39285
C	1110	VAL	-	expression tag	UNP P39285
C	1111	LEU	-	expression tag	UNP P39285
C	1112	PHE	-	expression tag	UNP P39285
C	1113	GLN	-	expression tag	UNP P39285
D	213	MET	-	initiating methionine	UNP P39285
D	214	ARG	-	expression tag	UNP P39285
D	215	LEU	-	expression tag	UNP P39285
D	216	ILE	-	expression tag	UNP P39285

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Chain	Residue	Modelled	Actual	Comment	Reference
D	217	ILE	-	expression tag	UNP P39285
D	218	THR	-	expression tag	UNP P39285
D	219	PHE	-	expression tag	UNP P39285
D	220	LEU	-	expression tag	UNP P39285
D	221	MET	-	expression tag	UNP P39285
D	222	ALA	-	expression tag	UNP P39285
D	223	TRP	-	expression tag	UNP P39285
D	224	CYS	-	expression tag	UNP P39285
D	225	LEU	-	expression tag	UNP P39285
D	226	SER	-	expression tag	UNP P39285
D	227	TRP	-	expression tag	UNP P39285
D	228	GLY	-	expression tag	UNP P39285
D	229	ALA	-	expression tag	UNP P39285
D	230	TYR	-	expression tag	UNP P39285
D	231	ALA	-	expression tag	UNP P39285
D	232	ALA	-	expression tag	UNP P39285
D	233	THR	-	expression tag	UNP P39285
D	234	ALA	-	expression tag	UNP P39285
D	235	PRO	-	expression tag	UNP P39285
D	236	ASP	-	expression tag	UNP P39285
D	237	SER	-	expression tag	UNP P39285
D	238	LYS	-	expression tag	UNP P39285
D	239	GLN	-	expression tag	UNP P39285
D	240	ILE	-	expression tag	UNP P39285
D	241	THR	-	expression tag	UNP P39285
D	242	GLN	-	expression tag	UNP P39285
D	243	GLU	-	expression tag	UNP P39285
D	244	LEU	-	expression tag	UNP P39285
D	245	GLU	-	expression tag	UNP P39285
D	246	GLN	-	expression tag	UNP P39285
D	247	ALA	-	expression tag	UNP P39285
D	248	LYS	-	expression tag	UNP P39285
D	249	ALA	-	expression tag	UNP P39285
D	250	ALA	-	expression tag	UNP P39285
D	251	LYS	-	expression tag	UNP P39285
D	252	PRO	-	expression tag	UNP P39285
D	1108	LEU	-	expression tag	UNP P39285
D	1109	GLU	-	expression tag	UNP P39285
D	1110	VAL	-	expression tag	UNP P39285
D	1111	LEU	-	expression tag	UNP P39285
D	1112	PHE	-	expression tag	UNP P39285
D	1113	GLN	-	expression tag	UNP P39285

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Chain	Residue	Modelled	Actual	Comment	Reference
E	213	MET	-	initiating methionine	UNP P39285
E	214	ARG	-	expression tag	UNP P39285
E	215	LEU	-	expression tag	UNP P39285
E	216	ILE	-	expression tag	UNP P39285
E	217	ILE	-	expression tag	UNP P39285
E	218	THR	-	expression tag	UNP P39285
E	219	PHE	-	expression tag	UNP P39285
E	220	LEU	-	expression tag	UNP P39285
E	221	MET	-	expression tag	UNP P39285
E	222	ALA	-	expression tag	UNP P39285
E	223	TRP	-	expression tag	UNP P39285
E	224	CYS	-	expression tag	UNP P39285
E	225	LEU	-	expression tag	UNP P39285
E	226	SER	-	expression tag	UNP P39285
E	227	TRP	-	expression tag	UNP P39285
E	228	GLY	-	expression tag	UNP P39285
E	229	ALA	-	expression tag	UNP P39285
E	230	TYR	-	expression tag	UNP P39285
E	231	ALA	-	expression tag	UNP P39285
E	232	ALA	-	expression tag	UNP P39285
E	233	THR	-	expression tag	UNP P39285
E	234	ALA	-	expression tag	UNP P39285
E	235	PRO	-	expression tag	UNP P39285
E	236	ASP	-	expression tag	UNP P39285
E	237	SER	-	expression tag	UNP P39285
E	238	LYS	-	expression tag	UNP P39285
E	239	GLN	-	expression tag	UNP P39285
E	240	ILE	-	expression tag	UNP P39285
E	241	THR	-	expression tag	UNP P39285
E	242	GLN	-	expression tag	UNP P39285
E	243	GLU	-	expression tag	UNP P39285
E	244	LEU	-	expression tag	UNP P39285
E	245	GLU	-	expression tag	UNP P39285
E	246	GLN	-	expression tag	UNP P39285
E	247	ALA	-	expression tag	UNP P39285
E	248	LYS	-	expression tag	UNP P39285
E	249	ALA	-	expression tag	UNP P39285
E	250	ALA	-	expression tag	UNP P39285
E	251	LYS	-	expression tag	UNP P39285
E	252	PRO	-	expression tag	UNP P39285
E	1108	LEU	-	expression tag	UNP P39285
E	1109	GLU	-	expression tag	UNP P39285

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1110	VAL	-	expression tag	UNP P39285
E	1111	LEU	-	expression tag	UNP P39285
E	1112	PHE	-	expression tag	UNP P39285
E	1113	GLN	-	expression tag	UNP P39285
F	213	MET	-	initiating methionine	UNP P39285
F	214	ARG	-	expression tag	UNP P39285
F	215	LEU	-	expression tag	UNP P39285
F	216	ILE	-	expression tag	UNP P39285
F	217	ILE	-	expression tag	UNP P39285
F	218	THR	-	expression tag	UNP P39285
F	219	PHE	-	expression tag	UNP P39285
F	220	LEU	-	expression tag	UNP P39285
F	221	MET	-	expression tag	UNP P39285
F	222	ALA	-	expression tag	UNP P39285
F	223	TRP	-	expression tag	UNP P39285
F	224	CYS	-	expression tag	UNP P39285
F	225	LEU	-	expression tag	UNP P39285
F	226	SER	-	expression tag	UNP P39285
F	227	TRP	-	expression tag	UNP P39285
F	228	GLY	-	expression tag	UNP P39285
F	229	ALA	-	expression tag	UNP P39285
F	230	TYR	-	expression tag	UNP P39285
F	231	ALA	-	expression tag	UNP P39285
F	232	ALA	-	expression tag	UNP P39285
F	233	THR	-	expression tag	UNP P39285
F	234	ALA	-	expression tag	UNP P39285
F	235	PRO	-	expression tag	UNP P39285
F	236	ASP	-	expression tag	UNP P39285
F	237	SER	-	expression tag	UNP P39285
F	238	LYS	-	expression tag	UNP P39285
F	239	GLN	-	expression tag	UNP P39285
F	240	ILE	-	expression tag	UNP P39285
F	241	THR	-	expression tag	UNP P39285
F	242	GLN	-	expression tag	UNP P39285
F	243	GLU	-	expression tag	UNP P39285
F	244	LEU	-	expression tag	UNP P39285
F	245	GLU	-	expression tag	UNP P39285
F	246	GLN	-	expression tag	UNP P39285
F	247	ALA	-	expression tag	UNP P39285
F	248	LYS	-	expression tag	UNP P39285
F	249	ALA	-	expression tag	UNP P39285
F	250	ALA	-	expression tag	UNP P39285

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Chain	Residue	Modelled	Actual	Comment	Reference
F	251	LYS	-	expression tag	UNP P39285
F	252	PRO	-	expression tag	UNP P39285
F	1108	LEU	-	expression tag	UNP P39285
F	1109	GLU	-	expression tag	UNP P39285
F	1110	VAL	-	expression tag	UNP P39285
F	1111	LEU	-	expression tag	UNP P39285
F	1112	PHE	-	expression tag	UNP P39285
F	1113	GLN	-	expression tag	UNP P39285
G	213	MET	-	initiating methionine	UNP P39285
G	214	ARG	-	expression tag	UNP P39285
G	215	LEU	-	expression tag	UNP P39285
G	216	ILE	-	expression tag	UNP P39285
G	217	ILE	-	expression tag	UNP P39285
G	218	THR	-	expression tag	UNP P39285
G	219	PHE	-	expression tag	UNP P39285
G	220	LEU	-	expression tag	UNP P39285
G	221	MET	-	expression tag	UNP P39285
G	222	ALA	-	expression tag	UNP P39285
G	223	TRP	-	expression tag	UNP P39285
G	224	CYS	-	expression tag	UNP P39285
G	225	LEU	-	expression tag	UNP P39285
G	226	SER	-	expression tag	UNP P39285
G	227	TRP	-	expression tag	UNP P39285
G	228	GLY	-	expression tag	UNP P39285
G	229	ALA	-	expression tag	UNP P39285
G	230	TYR	-	expression tag	UNP P39285
G	231	ALA	-	expression tag	UNP P39285
G	232	ALA	-	expression tag	UNP P39285
G	233	THR	-	expression tag	UNP P39285
G	234	ALA	-	expression tag	UNP P39285
G	235	PRO	-	expression tag	UNP P39285
G	236	ASP	-	expression tag	UNP P39285
G	237	SER	-	expression tag	UNP P39285
G	238	LYS	-	expression tag	UNP P39285
G	239	GLN	-	expression tag	UNP P39285
G	240	ILE	-	expression tag	UNP P39285
G	241	THR	-	expression tag	UNP P39285
G	242	GLN	-	expression tag	UNP P39285
G	243	GLU	-	expression tag	UNP P39285
G	244	LEU	-	expression tag	UNP P39285
G	245	GLU	-	expression tag	UNP P39285
G	246	GLN	-	expression tag	UNP P39285

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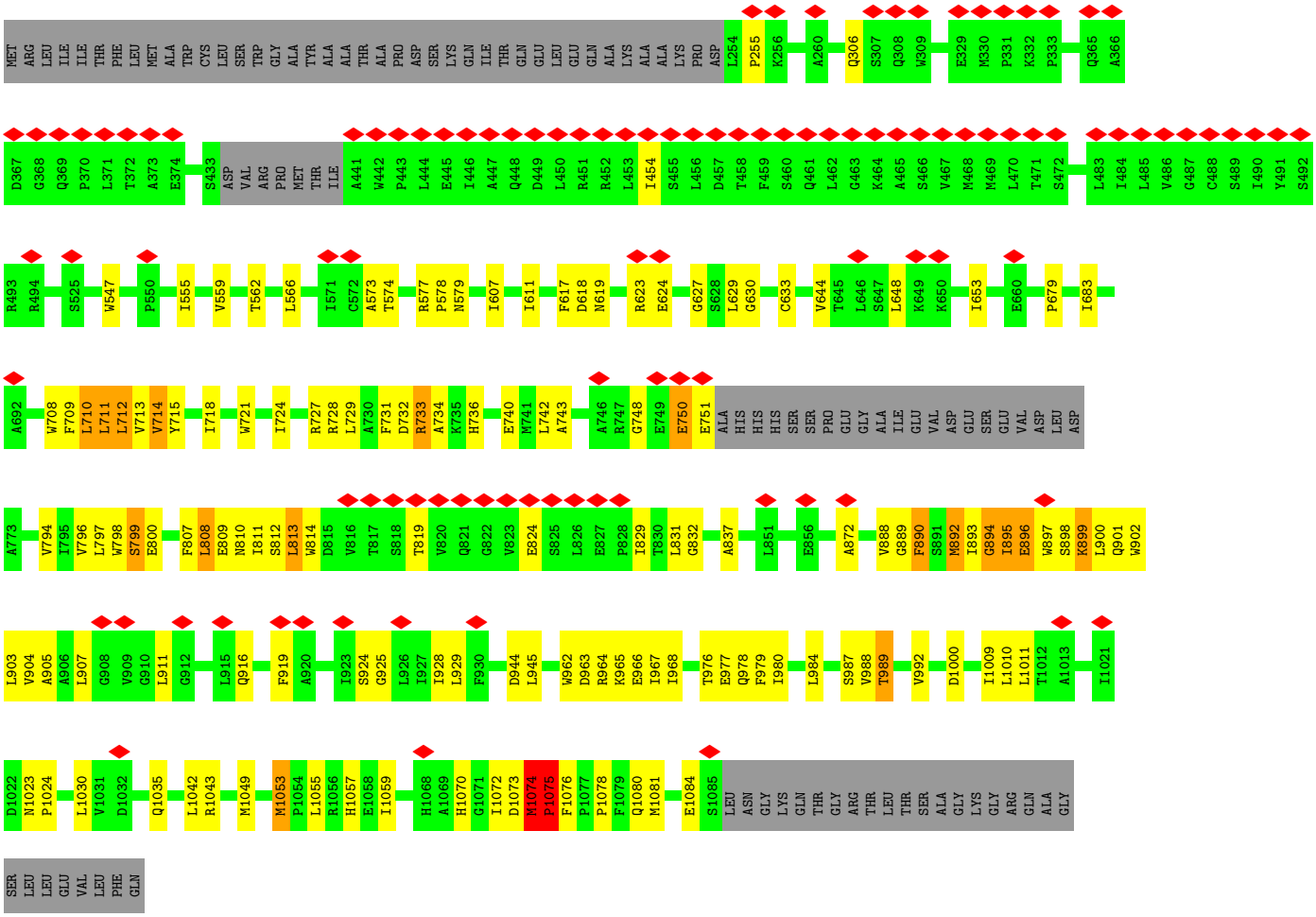
Chain	Residue	Modelled	Actual	Comment	Reference
G	247	ALA	-	expression tag	UNP P39285
G	248	LYS	-	expression tag	UNP P39285
G	249	ALA	-	expression tag	UNP P39285
G	250	ALA	-	expression tag	UNP P39285
G	251	LYS	-	expression tag	UNP P39285
G	252	PRO	-	expression tag	UNP P39285
G	1108	LEU	-	expression tag	UNP P39285
G	1109	GLU	-	expression tag	UNP P39285
G	1110	VAL	-	expression tag	UNP P39285
G	1111	LEU	-	expression tag	UNP P39285
G	1112	PHE	-	expression tag	UNP P39285
G	1113	GLN	-	expression tag	UNP P39285

3 Residue-property plots (i)

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.

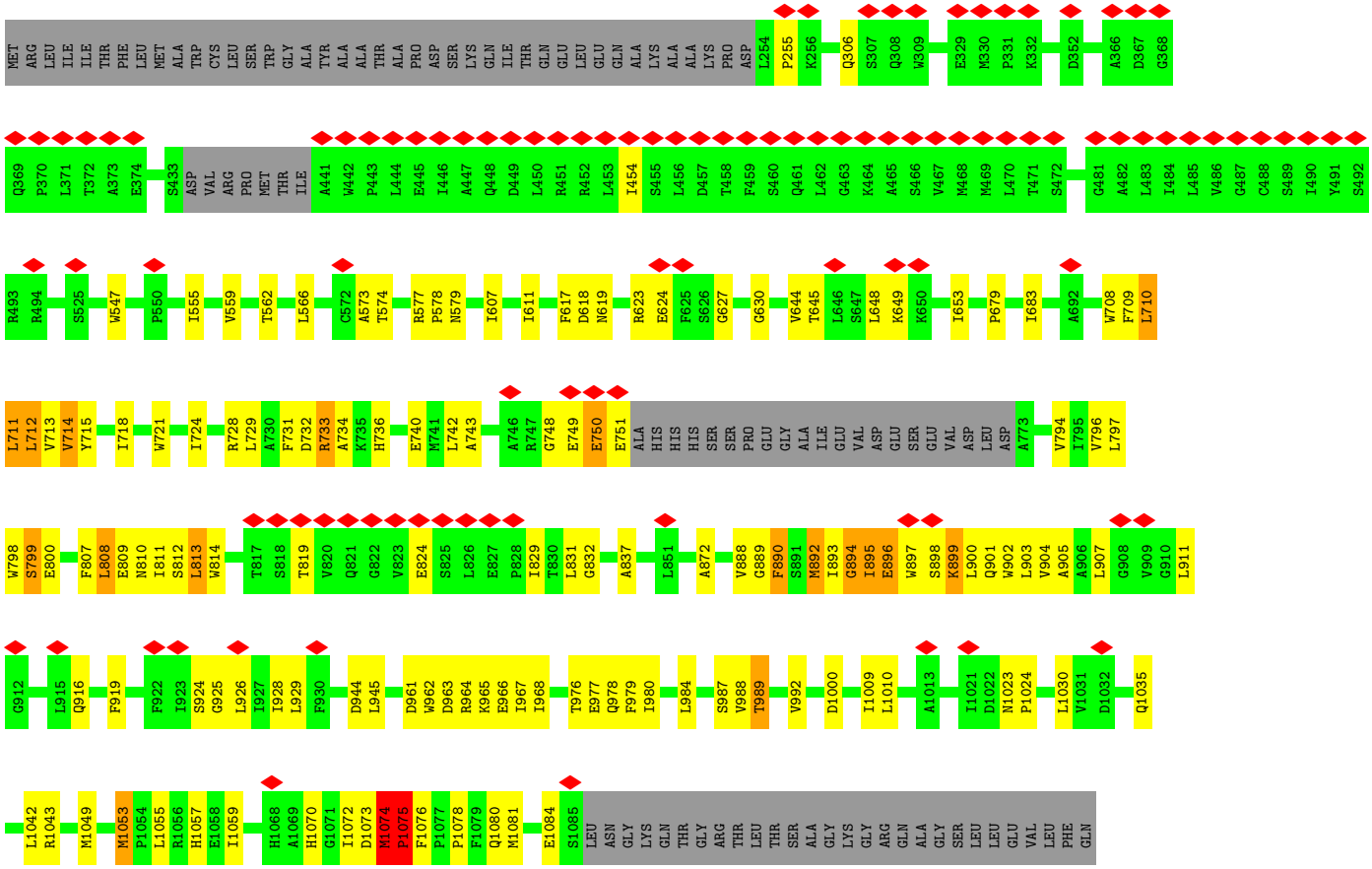
• Molecule 1: Miniconductance mechanosensitive channel MscM

Chain A:



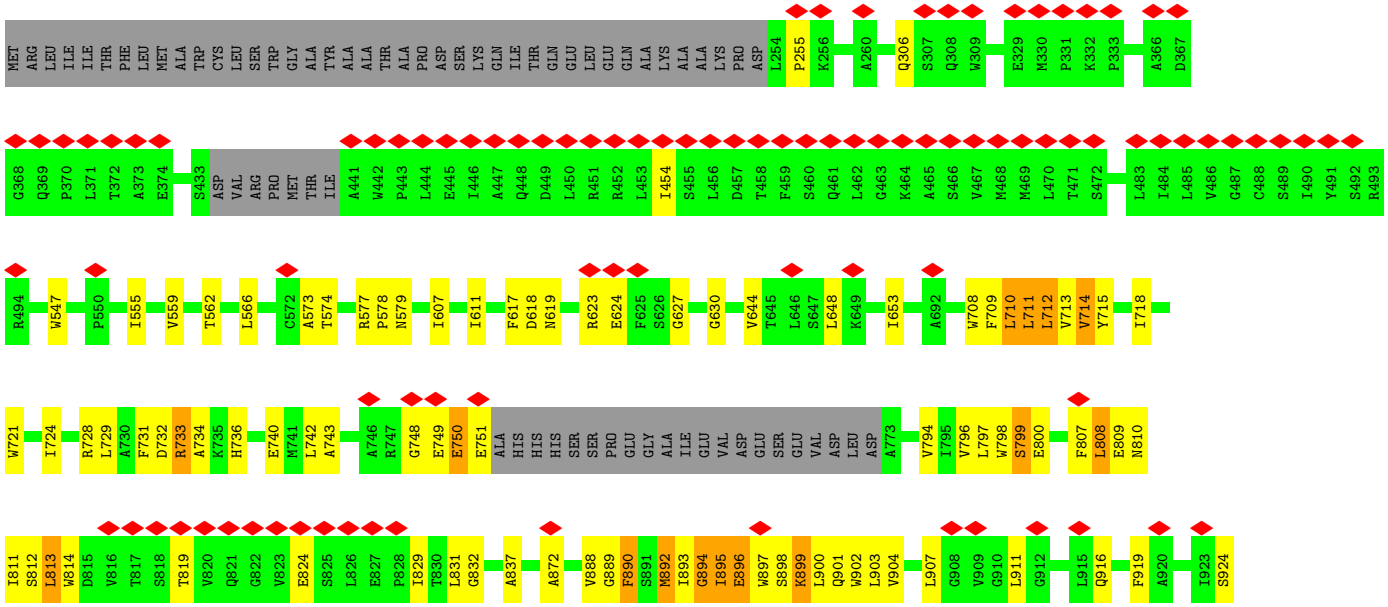
• Molecule 1: Miniconductance mechanosensitive channel MscM

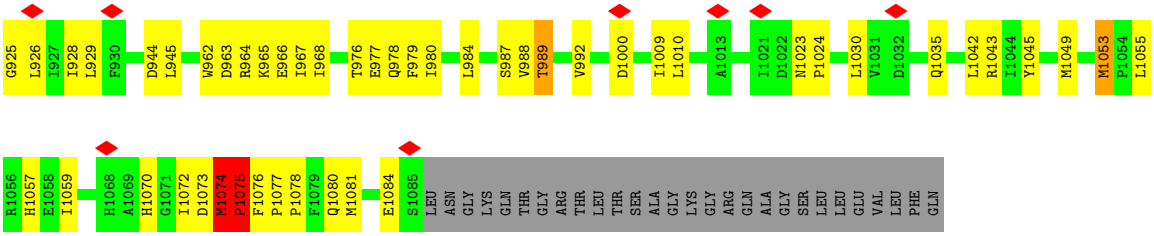
Chain B:



• Molecule 1: Miniconductance mechanosensitive channel MscM

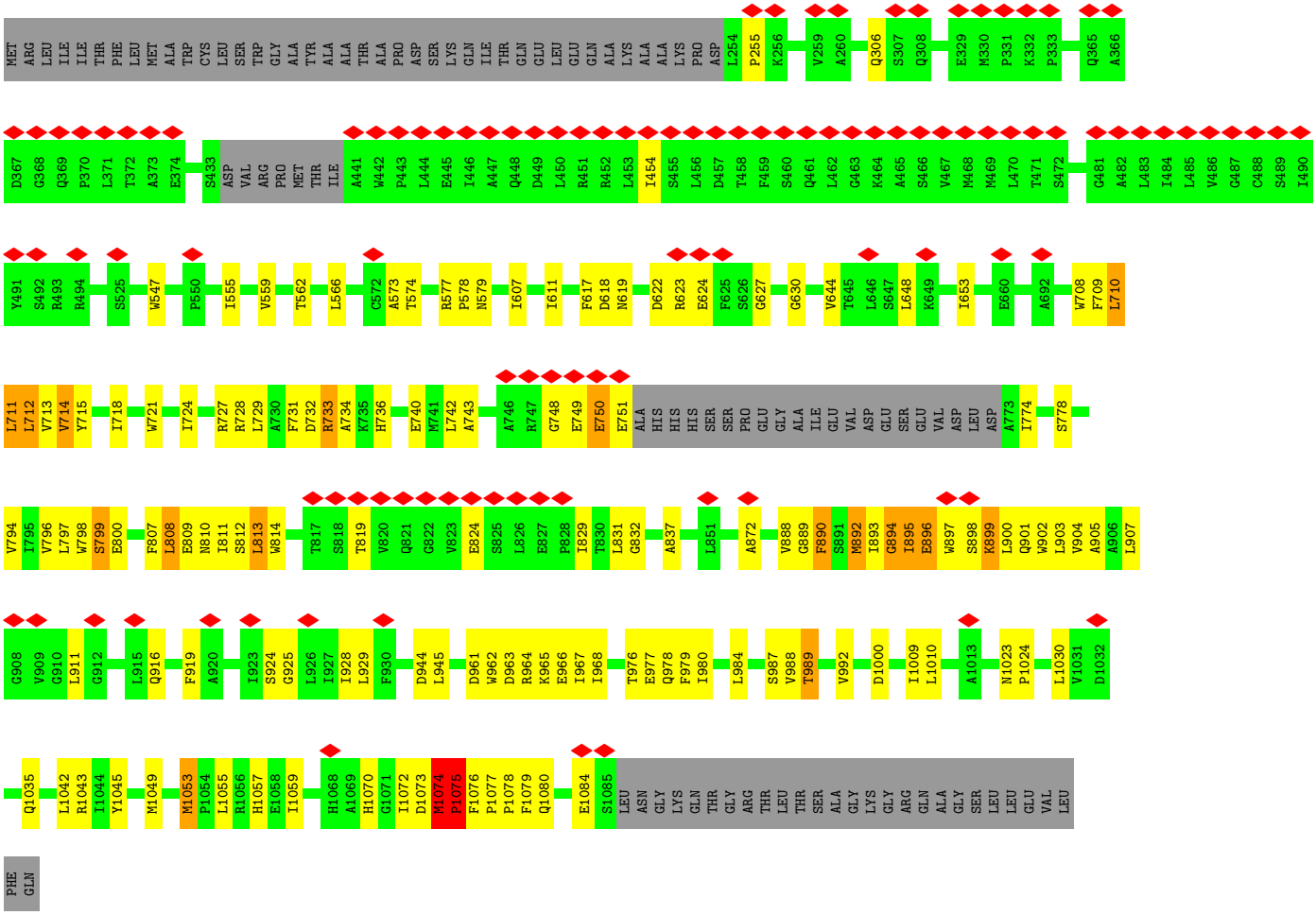
Chain C:





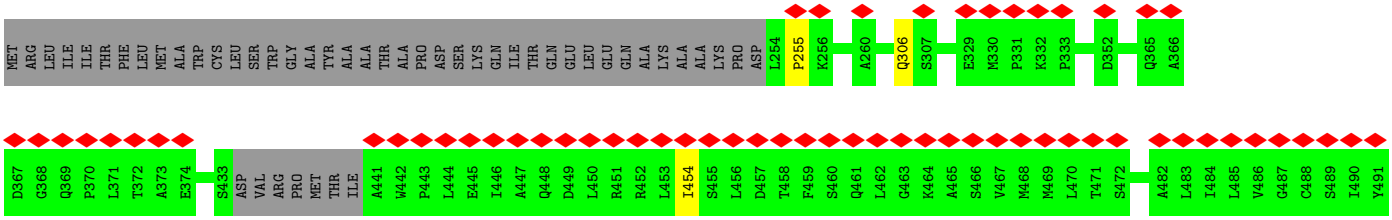
- Molecule 1: Miniconductance mechanosensitive channel MscM

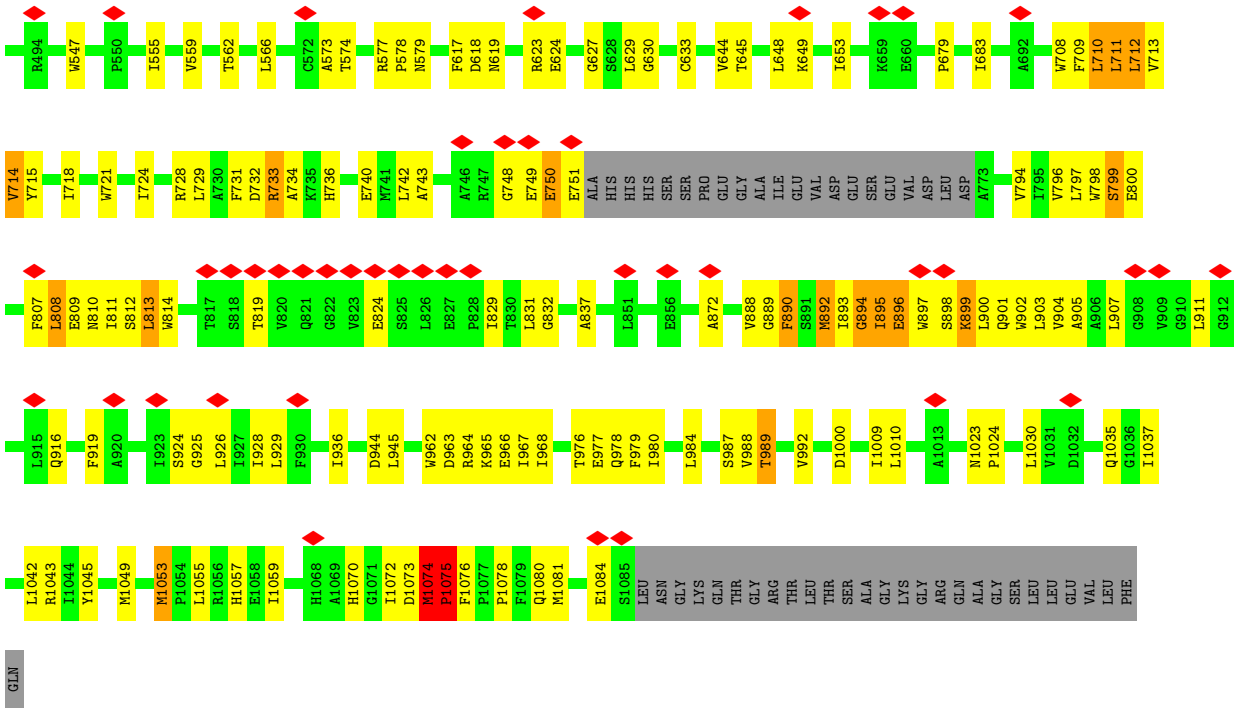
Chain D:



- Molecule 1: Miniconductance mechanosensitive channel MscM

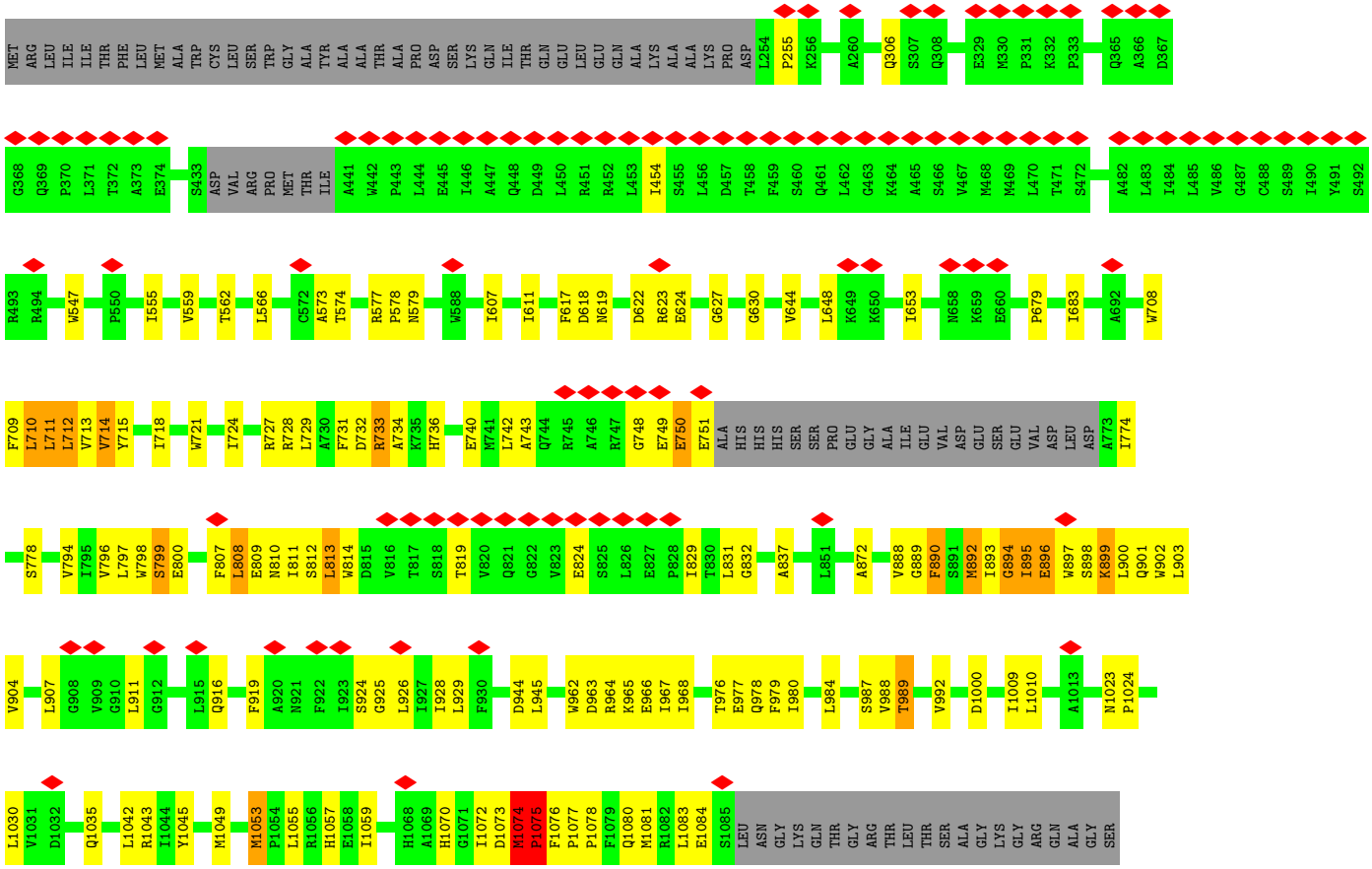
Chain E:





- Molecule 1: Miniconductance mechanosensitive channel MscM

Chain F:



LEU LEU GLU VAL LEU PHE GLN

• Molecule 1: Miniconductance mechanosensitive channel MscM

Chain G: 13% 73% 14% • 11%

MET ARG LEU ILE ILE THR PHE LEU MET ALA TRP CYS LEU SER TRP GLY ALA TYR ALA ALA THR ALA PRO ASP SER LYS GLN ILE THR GLN GLU LEU GLU GLN ALA LYS ALA ALA LYS PRO ASP L254 P255 K256 A260 Q306 S307 Q308 W309 E329 M330 P331 K332 P333 Q365 A366

D367 G368 Q369 P370 L371 T372 A373 E374 S433 ASP VAL ARG PRO MET THR ILE A441 W442 P443 L444 E445 I446 A447 Q448 D449 L450 R451 R452 L453 I454 S455 L456 D457 T458 F459 S460 Q461 L462 G463 K464 A465 S466 V467 M468 M469 L470 T471 S472 A482 L483 I484 L485 V486 G487 C488 S489 I490 Y491

S492 R493 R494 S525 W547 P550 I555 V559 T562 L566 C572 A573 T574 R577 P578 N579 I607 I611 F617 D618 N619 D622 R623 E624 F625 S626 G627 G630 V644 T645 L646 S647 L648 K649 K650 A651 G652 I653 F654 L655 N658 K659 E660

P679 I683 A692 W708 F709 L710 L711 L712 V713 V714 Y715 I718 W721 I724 R728 L729 A730 F731 D732 R733 A734 K735 H736 E740 M741 L742 A743 A746 R747 G748 E749 E750 E751 ALA HIS HIS HIS SER SER PRO GLU GLY ALA ILE GLU VAL ASP GLU SER GLU VAL

ASP LEU ASP A773 V794 I795 V796 L797 W798 S799 E800 F807 L808 E809 N810 I811 S812 L813 W814 D815 V816 T817 S818 T819 V820 Q821 G822 V823 E824 S825 L826 E827 P828 I829 T830 L831 G832 A837 L851 E856 A872 V888 G889 F890 S891 M892 I893 G894 I895 E896 W897 S898 K899

L900 Q901 W902 L903 V904 A905 A906 L907 G908 V909 G910 L911 G912 L915 Q916 F919 A920 I923 S924 G925 L926 I927 I928 L929 F930 D944 L945 W962 D963 R964 K965 E966 I967 I968 T976 E977 Q978 F979 I980 L984 S987 V988 T989 V992 D1000 I1009 L1010 A1013

N1023 P1024 L1030 V1031 D1032 Q1035 L1042 R1043 M1049 M1053 P1054 L1055 R1056 H1057 E1058 I1059 H1068 A1069 H1070 G1071 I1072 D1073 M1074 P1075 F1076 P1077 P1078 F1079 D1963 Q1080 M1081 E1084 S1085 LEU ASN GLY LYS GLN THR GLY ARG THR LEU THR SER ALA GLY LYS GLY ARG GLN ALA GLY

SER LEU LEU GLU VAL LEU PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	58387	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	46.84	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	12.012	Depositor
Minimum map value	-0.124	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.404	Depositor
Recommended contour level	2.1	Depositor
Map size (Å)	381.15, 381.15, 381.15	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.847, 0.847, 0.847	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	0.66	7/4544 (0.2%)	0.81	29/6279 (0.5%)
1	B	0.66	6/4544 (0.1%)	0.81	29/6279 (0.5%)
1	C	0.66	6/4544 (0.1%)	0.81	29/6279 (0.5%)
1	D	0.66	7/4544 (0.2%)	0.81	29/6279 (0.5%)
1	E	0.66	6/4544 (0.1%)	0.81	29/6279 (0.5%)
1	F	0.66	7/4544 (0.2%)	0.81	29/6279 (0.5%)
1	G	0.66	6/4544 (0.1%)	0.81	29/6279 (0.5%)
All	All	0.66	45/31808 (0.1%)	0.81	203/43953 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
1	E	0	3
1	F	0	3
1	G	0	3
All	All	0	21

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	711	LEU	CA-C	-6.38	1.44	1.52
1	F	711	LEU	CA-C	-6.38	1.44	1.52
1	B	711	LEU	CA-C	-6.37	1.44	1.52
1	E	711	LEU	CA-C	-6.36	1.44	1.52
1	A	711	LEU	CA-C	-6.34	1.44	1.52

The worst 5 of 203 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	963	ASP	N-CA-C	-13.31	96.55	112.92
1	C	963	ASP	N-CA-C	-13.30	96.56	112.92
1	B	963	ASP	N-CA-C	-13.29	96.58	112.92
1	E	963	ASP	N-CA-C	-13.28	96.58	112.92
1	A	963	ASP	N-CA-C	-13.28	96.59	112.92

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1072	ILE	Mainchain
1	A	573	ALA	Peptide
1	A	799	SER	Mainchain
1	B	573	ALA	Peptide
1	B	799	SER	Mainchain

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	4514	0	2901	156	0
1	B	4514	0	2901	155	0
1	C	4514	0	2901	154	0
1	D	4514	0	2901	159	0
1	E	4514	0	2901	158	0
1	F	4514	0	2901	161	0
1	G	4514	0	2901	158	0
All	All	31598	0	20307	884	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 17.

The worst 5 of 884 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:980:ILE:HG22	1:G:967:ILE:HG23	1.14	1.14
1:A:967:ILE:HG23	1:B:980:ILE:HG22	1.13	1.12
1:E:964:ARG:HE	1:F:984:LEU:HD11	1.16	1.10
1:B:967:ILE:HG23	1:C:980:ILE:HG22	1.14	1.10
1:D:967:ILE:HG23	1:E:980:ILE:HG22	1.11	1.08

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	798/901 (89%)	774 (97%)	11 (1%)	13 (2%)	7	37
1	B	798/901 (89%)	774 (97%)	11 (1%)	13 (2%)	7	37
1	C	798/901 (89%)	774 (97%)	11 (1%)	13 (2%)	7	37
1	D	798/901 (89%)	774 (97%)	11 (1%)	13 (2%)	7	37
1	E	798/901 (89%)	774 (97%)	11 (1%)	13 (2%)	7	37
1	F	798/901 (89%)	774 (97%)	11 (1%)	13 (2%)	7	37
1	G	798/901 (89%)	774 (97%)	11 (1%)	13 (2%)	7	37
All	All	5586/6307 (89%)	5418 (97%)	77 (1%)	91 (2%)	10	37

5 of 91 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	PRO
1	A	454	ILE
1	A	547	TRP
1	A	578	PRO
1	A	618	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	158/762 (21%)	157 (99%)	1 (1%)	78	80
1	B	158/762 (21%)	157 (99%)	1 (1%)	78	80
1	C	158/762 (21%)	157 (99%)	1 (1%)	78	80
1	D	158/762 (21%)	157 (99%)	1 (1%)	78	80
1	E	158/762 (21%)	157 (99%)	1 (1%)	78	80
1	F	158/762 (21%)	157 (99%)	1 (1%)	78	80
1	G	158/762 (21%)	157 (99%)	1 (1%)	78	80
All	All	1106/5334 (21%)	1099 (99%)	7 (1%)	76	80

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1075	PRO
1	E	1075	PRO
1	G	1075	PRO
1	F	1075	PRO
1	C	1075	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	978	GLN
1	F	978	GLN
1	E	1061	GLN
1	F	1035	GLN
1	B	1061	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation (i)

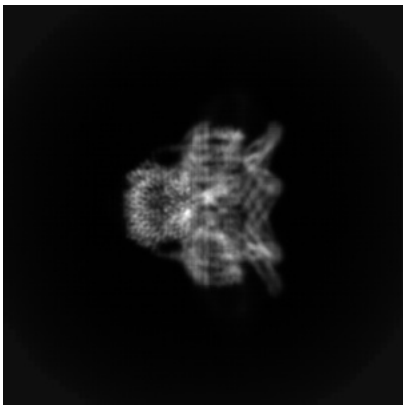
This section contains visualisations of the EMDB entry EMD-76009. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

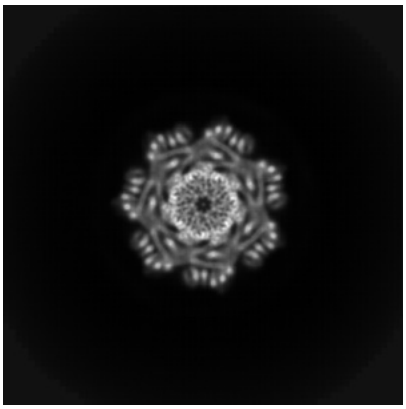
6.1 Orthogonal projections (i)

6.1.1 Primary map

X

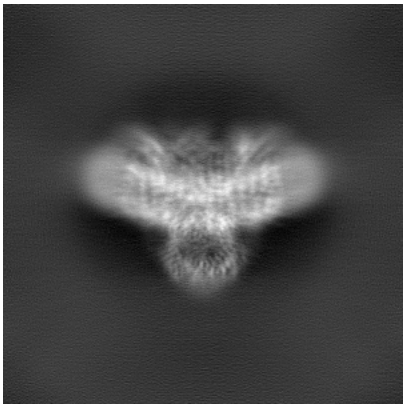


Y

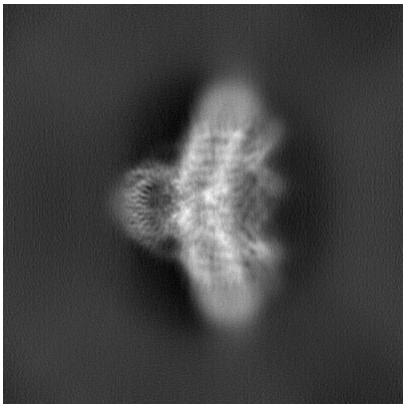


Z

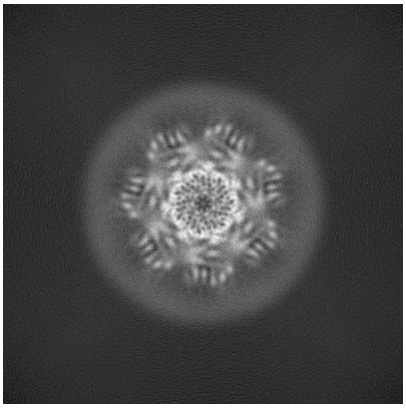
6.1.2 Raw map



X



Y



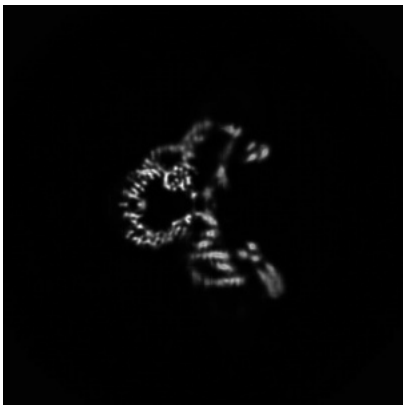
Z

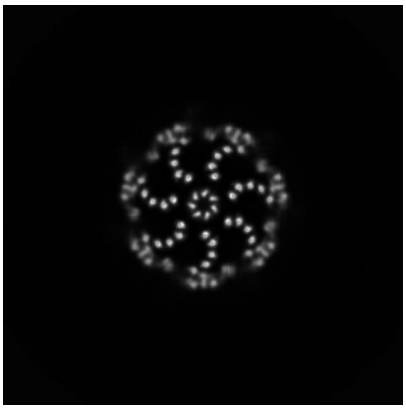
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

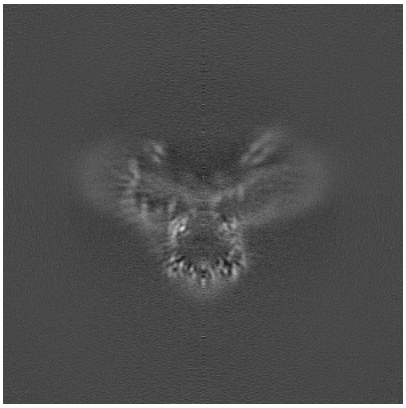
6.2.1 Primary map

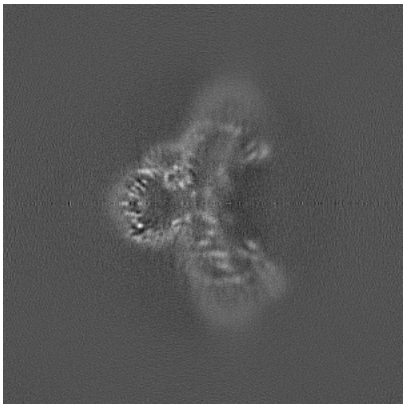
X Index: 225

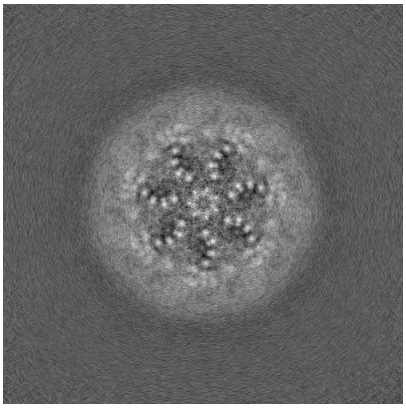

Y Index: 225


Z Index: 225

6.2.2 Raw map


X Index: 225


Y Index: 225

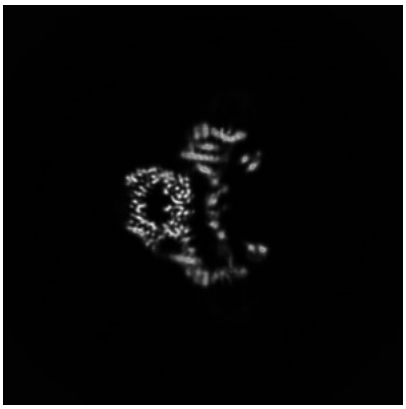

Z Index: 225

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

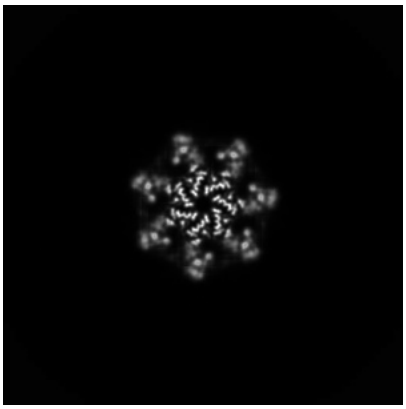
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 237

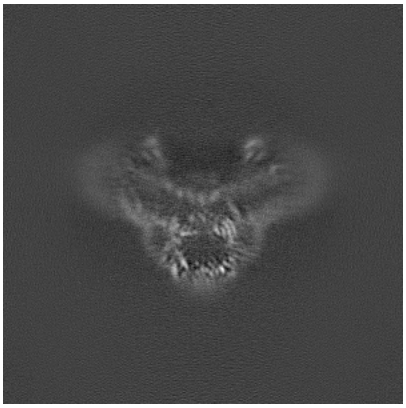


Y Index: 245

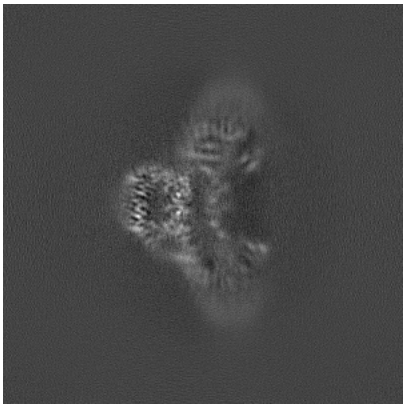


Z Index: 207

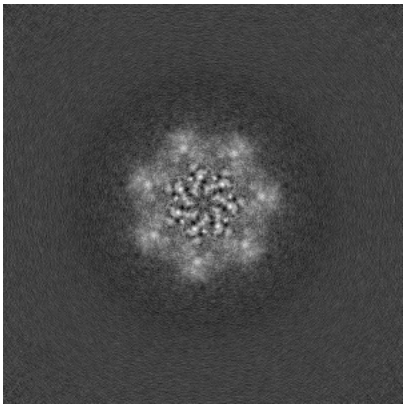
6.3.2 Raw map



X Index: 211



Y Index: 246



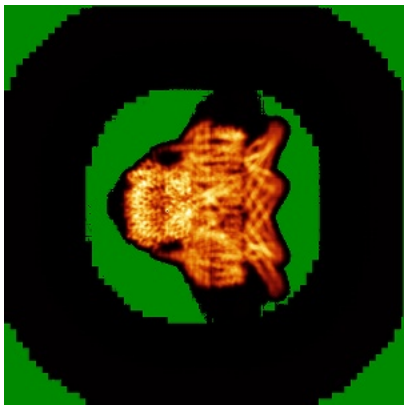
Z Index: 207

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

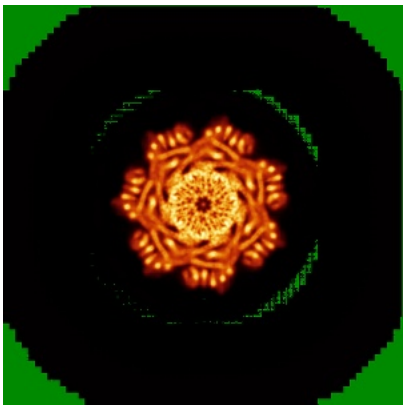
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X



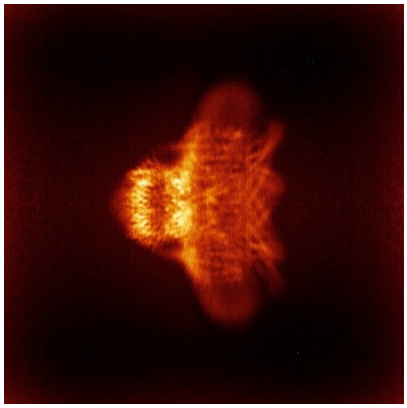
Y



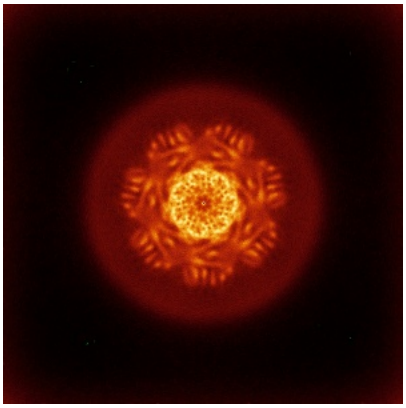
Z

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 2.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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.

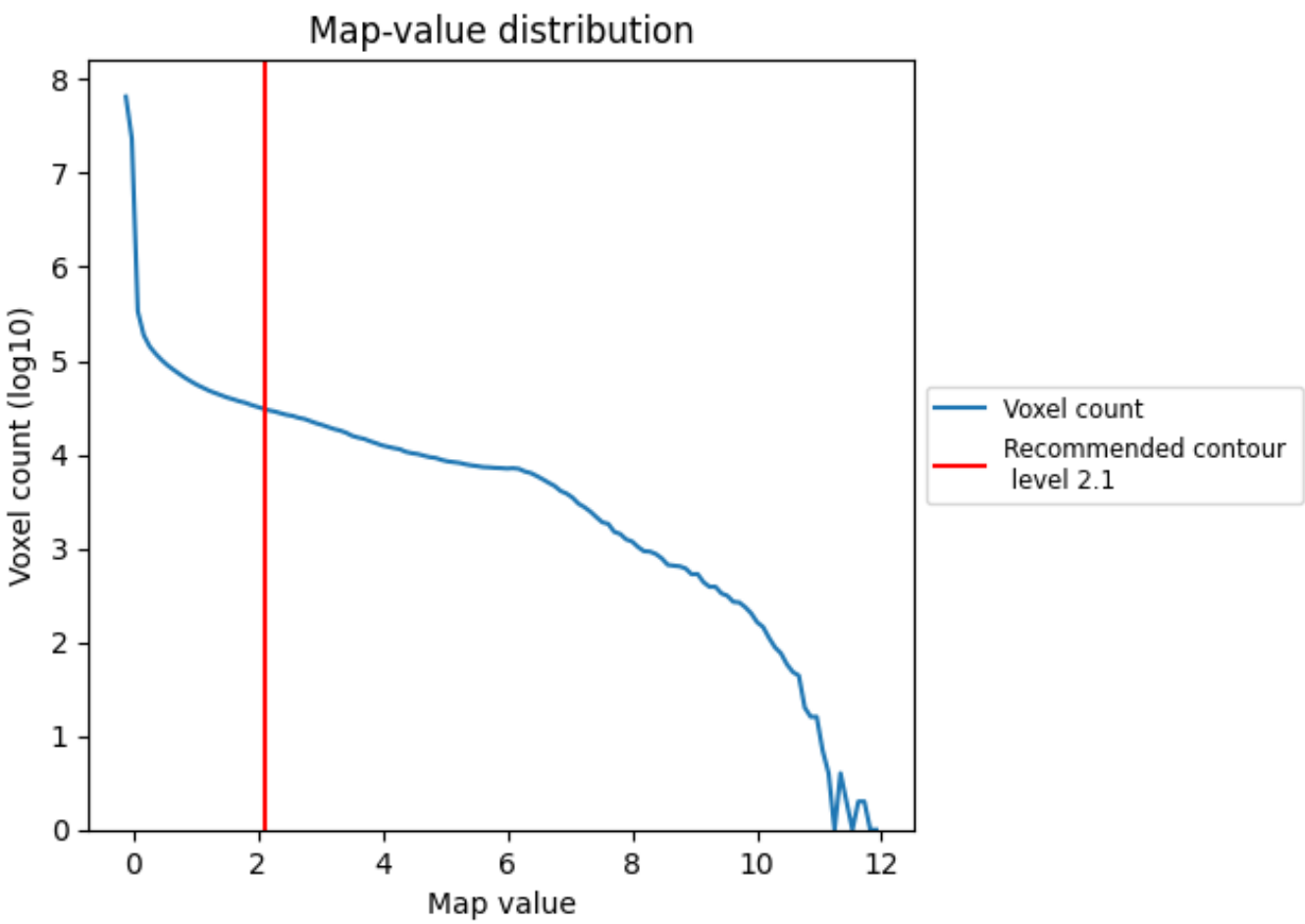
6.6 Mask visualisation (i)

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

7 Map analysis (i)

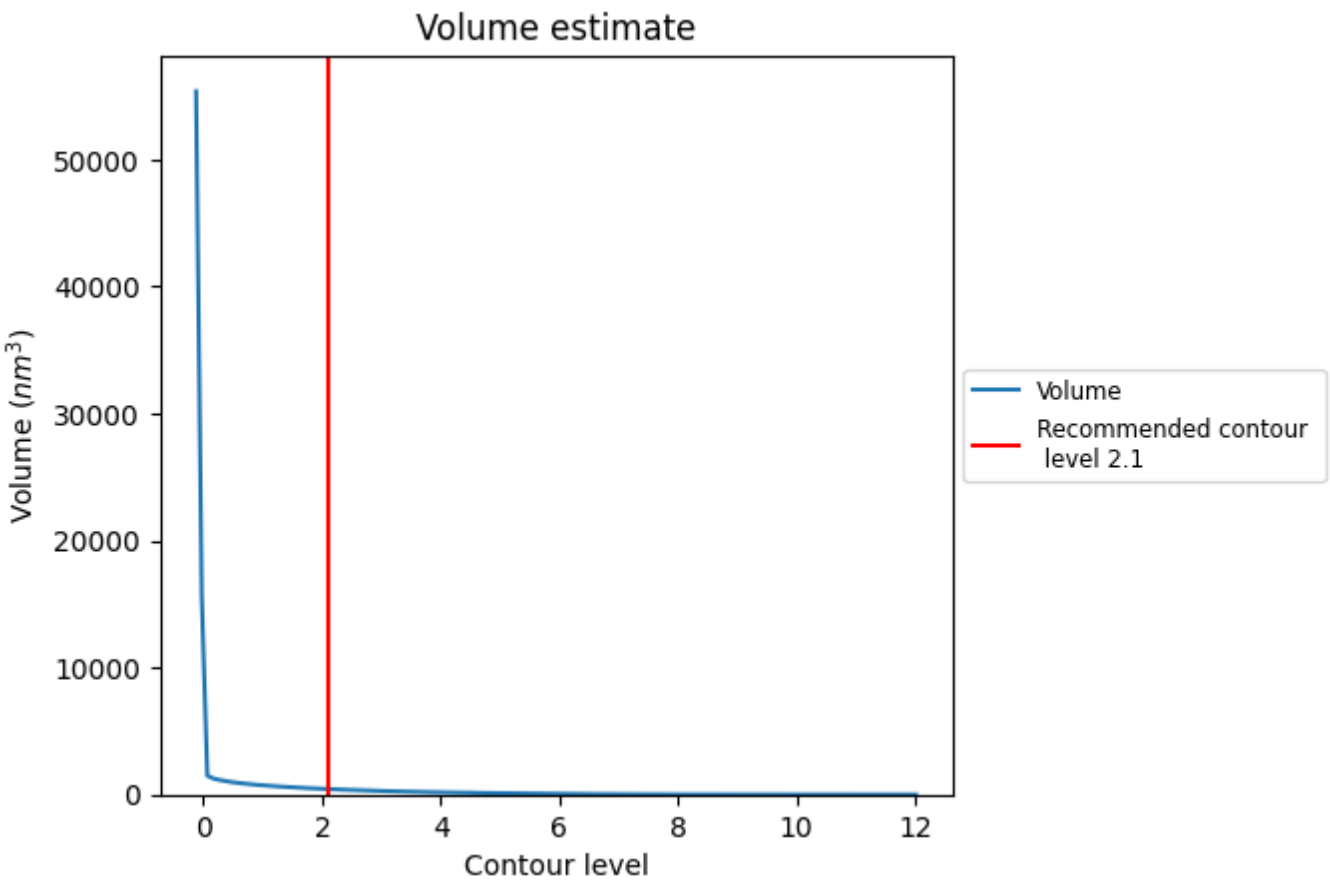
This section contains the results of statistical analysis of the map.

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.

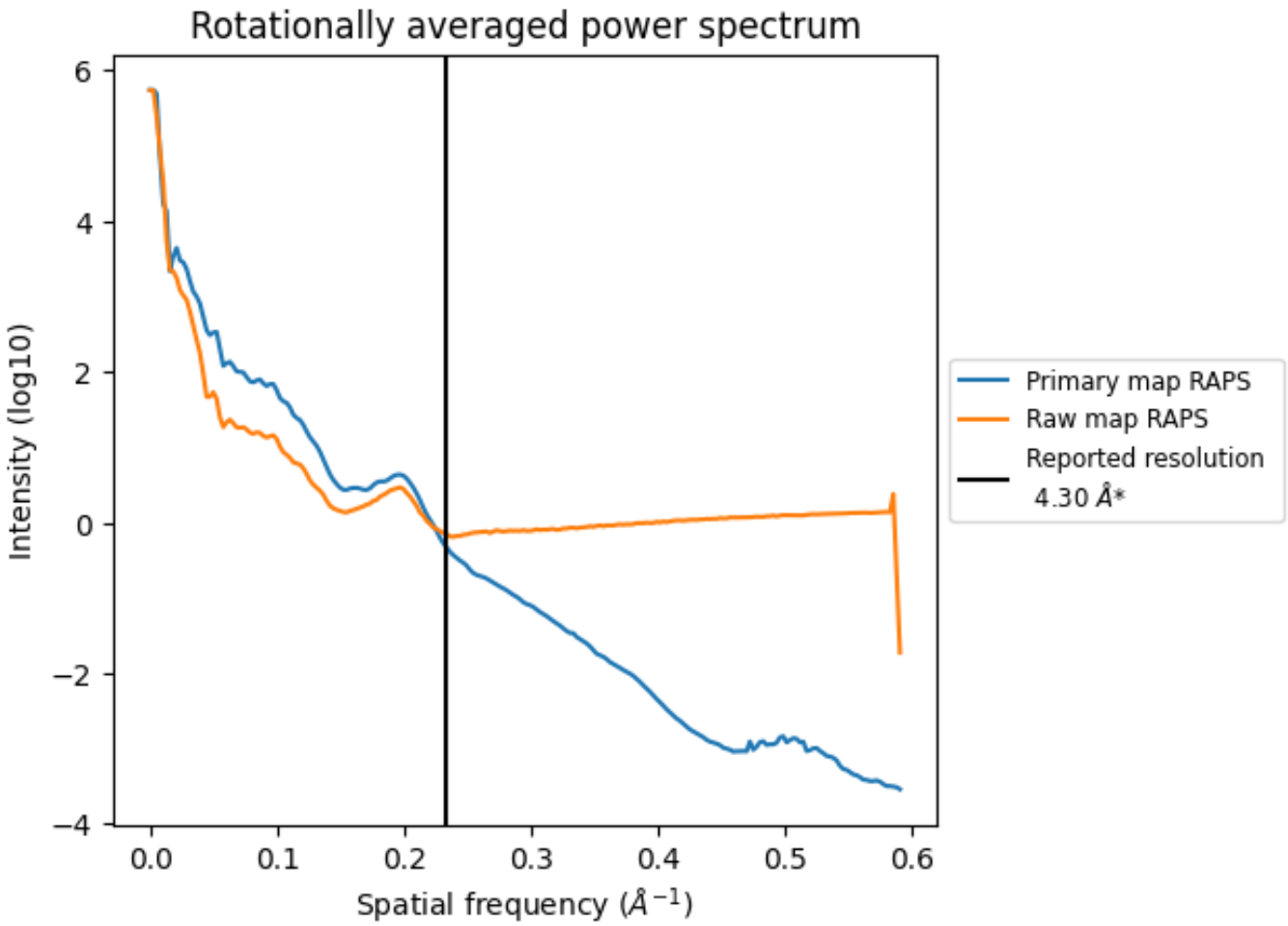
7.2 Volume estimate (i)



The volume at the recommended contour level is 432 nm^3; this corresponds to an approximate mass of 390 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)

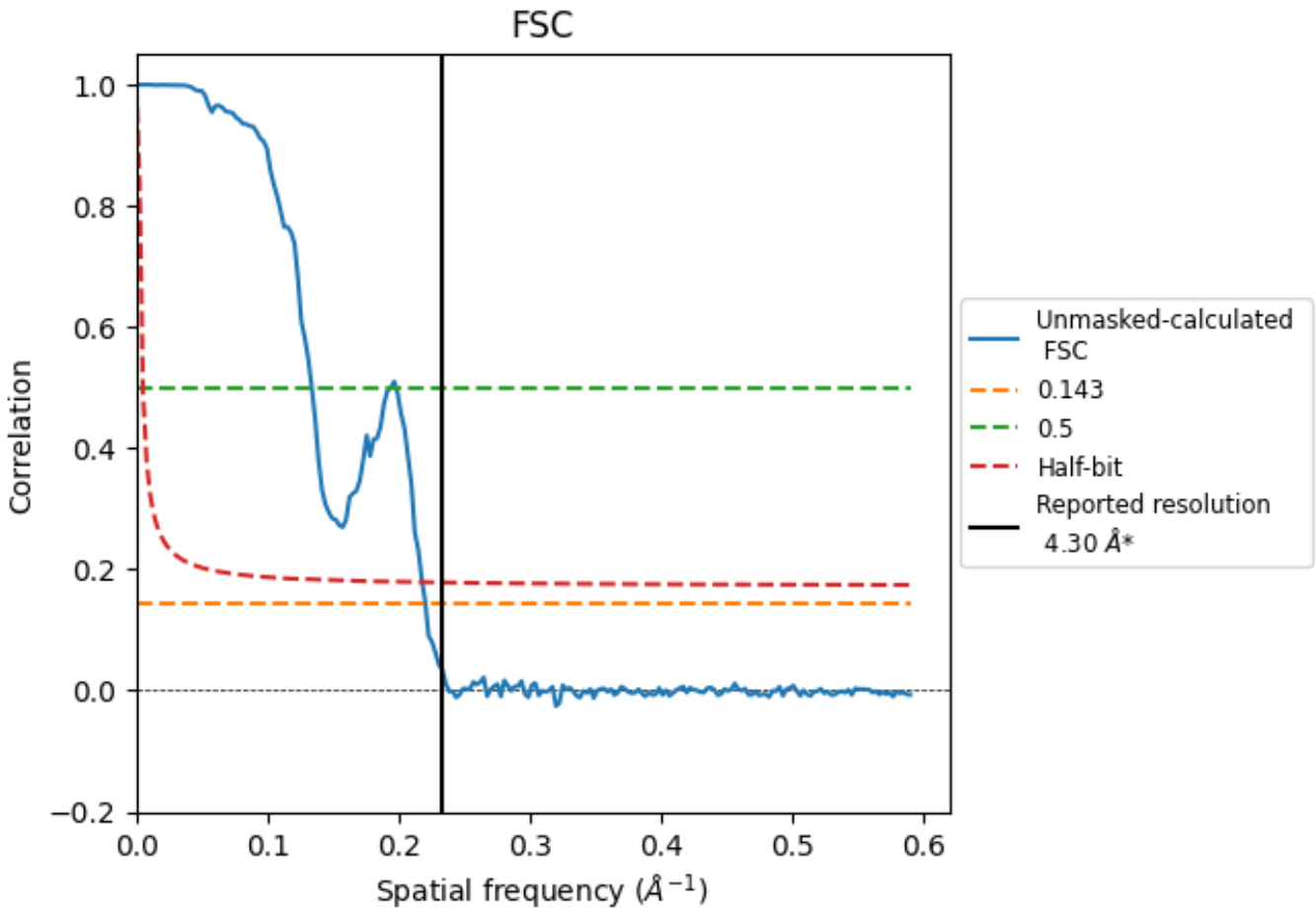


*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

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 0.233 Å^{-1}

8.2 Resolution estimates (i)

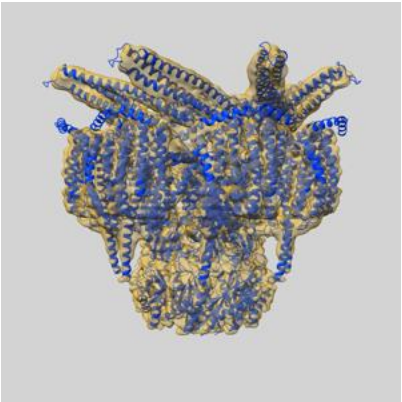
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.53	7.47	4.59

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

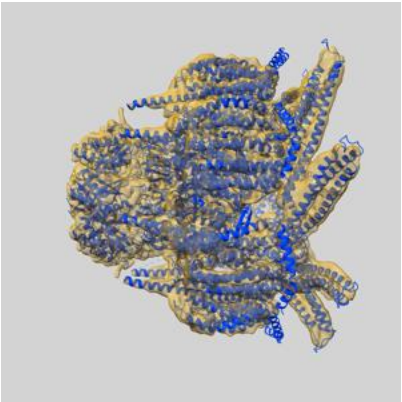
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-76009 and PDB model 11SO. Per-residue inclusion information can be found in section 3 on page 13.

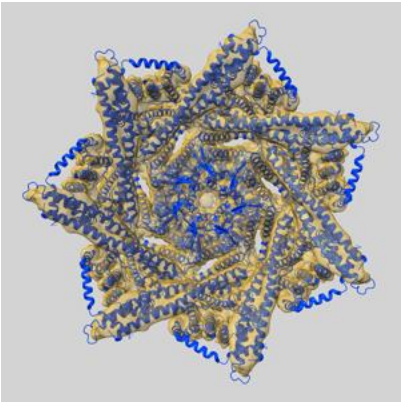
9.1 Map-model overlay (i)



X



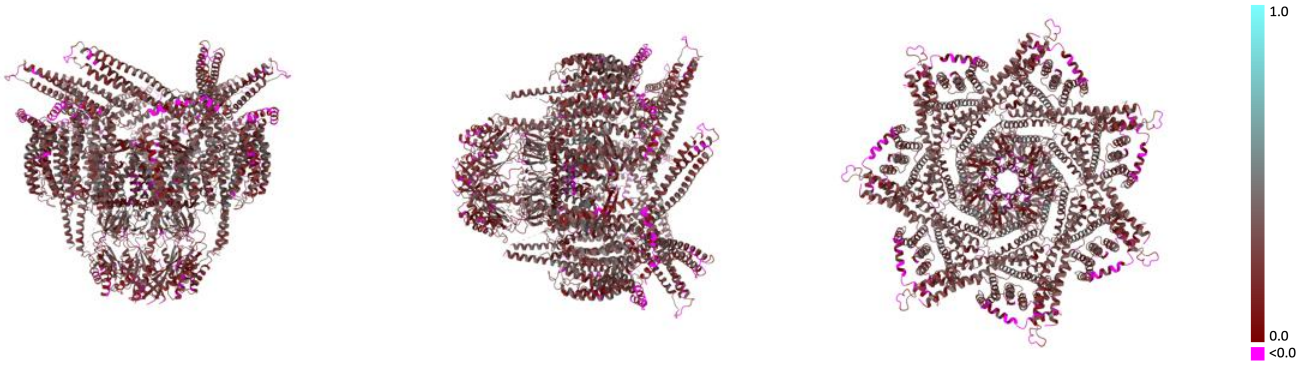
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

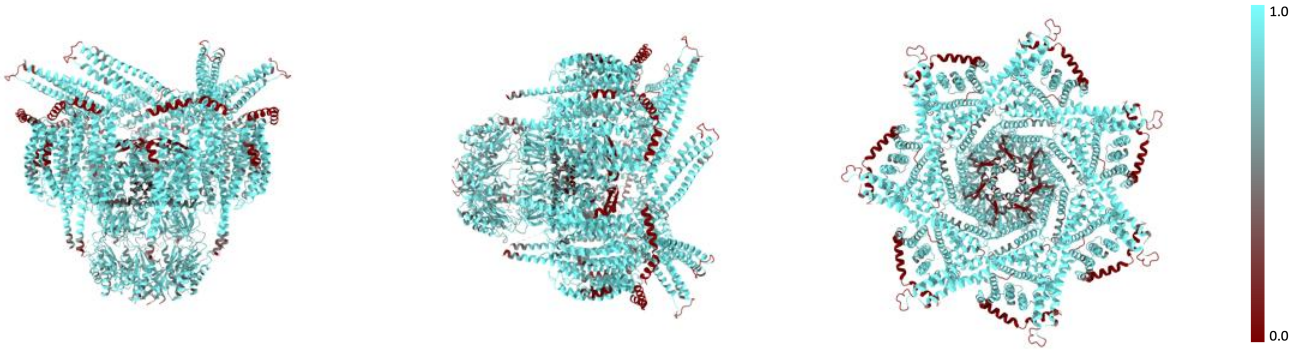
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

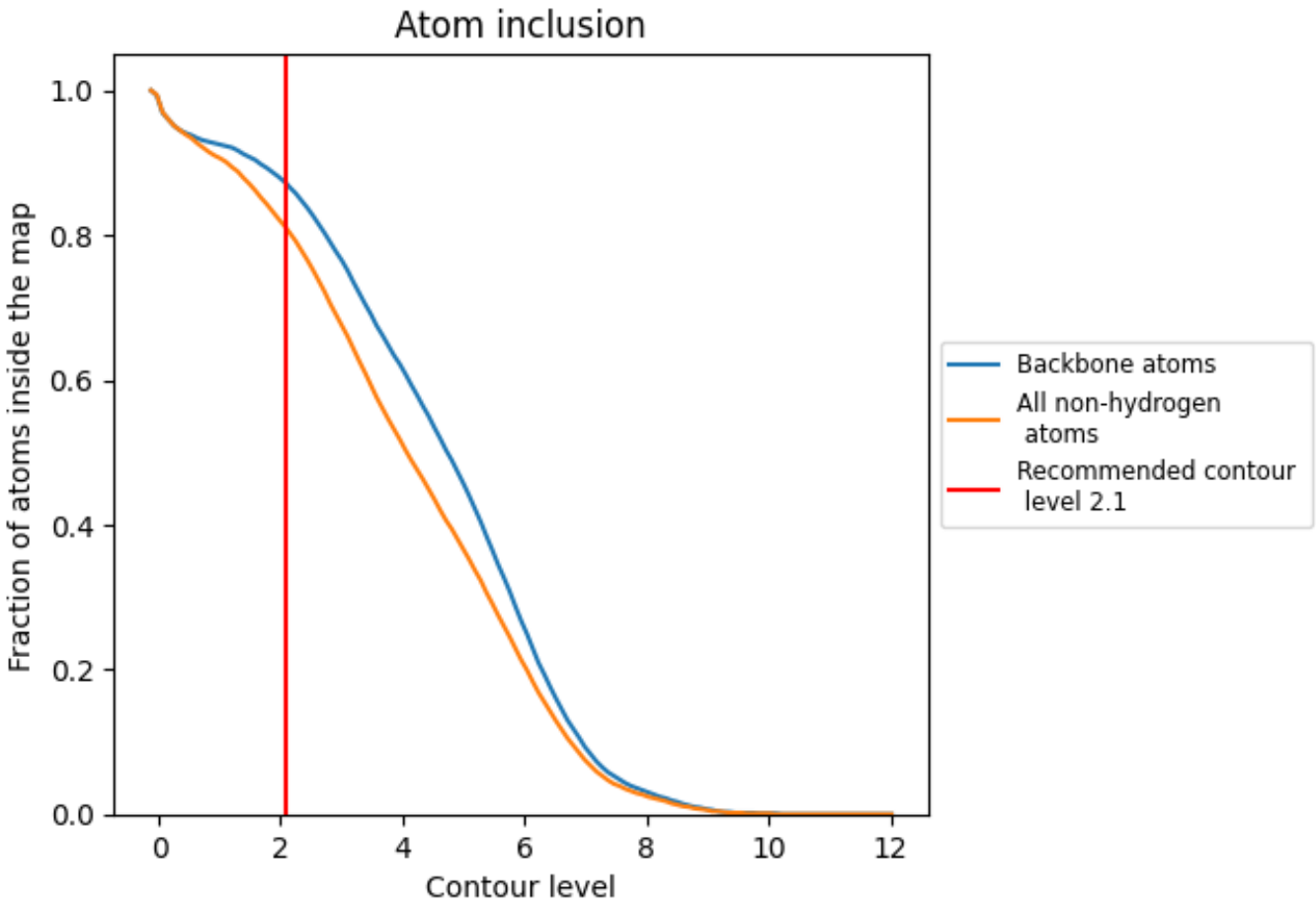
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (2.1).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (2.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8090	0.2460
A	0.8080	0.2470
B	0.8100	0.2450
C	0.8140	0.2480
D	0.8070	0.2460
E	0.8110	0.2450
F	0.8090	0.2450
G	0.8030	0.2470