wwPDB EM Validation Summary Report (i)

Aug 29, 2026 – 11:37 pm BST

PDB ID	:	9RT2 / pdb_00009rt2
EMDB ID	:	EMD-54238
Title	:	NetF - ANTXR2 structure (C4)
Authors	:	Wang, C.; Iacovache, I.; Zuber, B.
Deposited on	:	2025-07-01
Resolution	:	2.60 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:

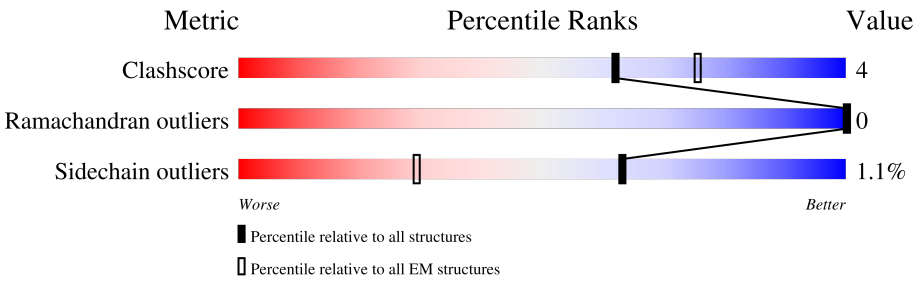
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

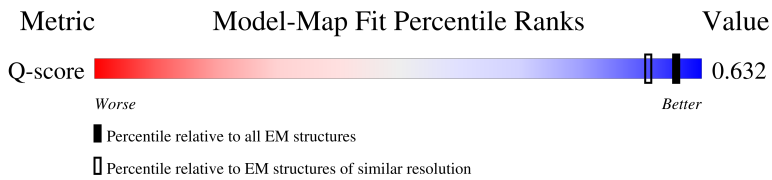
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	N1	289	73% 20% • 7%
1	N2	289	85% 8% 7%
1	N3	289	87% 7% 7%
1	N4	289	85% 8% 7%

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Mol	Chain	Length	Quality of chain
1	N5	289	87% 6% 7%
1	N6	289	85% 8% 7%
1	N7	289	87% 6% 7%
1	N8	289	84% 9% 7%
2	C1	321	73% 13% 13%
2	C2	321	72% 15% 13%
2	C3	321	72% 15% 13%
2	C4	321	72% 15% 13%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 51141 atoms, of which 25393 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 Leukocidin/Hemolysin toxin family.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	N1	269	4243	1367	2089	356	426	5	0	0
1	N2	270	4250	1369	2092	357	427	5	0	0
1	N3	270	4250	1369	2092	357	427	5	0	0
1	N4	270	4250	1369	2092	357	427	5	0	0
1	N5	270	4250	1369	2092	357	427	5	0	0
1	N6	270	4250	1369	2092	357	427	5	0	0
1	N7	270	4250	1369	2092	357	427	5	0	0
1	N8	270	4250	1369	2092	357	427	5	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N1	0	MET	-	initiating methionine	UNP A0A0D3QGV4
N1	1	VAL	-	expression tag	UNP A0A0D3QGV4
N1	2	HIS	-	expression tag	UNP A0A0D3QGV4
N1	3	HIS	-	expression tag	UNP A0A0D3QGV4
N1	4	HIS	-	expression tag	UNP A0A0D3QGV4
N1	5	HIS	-	expression tag	UNP A0A0D3QGV4
N1	6	HIS	-	expression tag	UNP A0A0D3QGV4
N1	7	HIS	-	expression tag	UNP A0A0D3QGV4
N2	1	MET	-	initiating methionine	UNP A0A0D3QGV4
N2	2	VAL	-	expression tag	UNP A0A0D3QGV4
N2	3	HIS	-	expression tag	UNP A0A0D3QGV4
N2	4	HIS	-	expression tag	UNP A0A0D3QGV4
N2	5	HIS	-	expression tag	UNP A0A0D3QGV4
N2	6	HIS	-	expression tag	UNP A0A0D3QGV4

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Chain	Residue	Modelled	Actual	Comment	Reference
N2	7	HIS	-	expression tag	UNP A0A0D3QGV4
N2	8	HIS	-	expression tag	UNP A0A0D3QGV4
N3	1	MET	-	initiating methionine	UNP A0A0D3QGV4
N3	2	VAL	-	expression tag	UNP A0A0D3QGV4
N3	3	HIS	-	expression tag	UNP A0A0D3QGV4
N3	4	HIS	-	expression tag	UNP A0A0D3QGV4
N3	5	HIS	-	expression tag	UNP A0A0D3QGV4
N3	6	HIS	-	expression tag	UNP A0A0D3QGV4
N3	7	HIS	-	expression tag	UNP A0A0D3QGV4
N3	8	HIS	-	expression tag	UNP A0A0D3QGV4
N4	1	MET	-	initiating methionine	UNP A0A0D3QGV4
N4	2	VAL	-	expression tag	UNP A0A0D3QGV4
N4	3	HIS	-	expression tag	UNP A0A0D3QGV4
N4	4	HIS	-	expression tag	UNP A0A0D3QGV4
N4	5	HIS	-	expression tag	UNP A0A0D3QGV4
N4	6	HIS	-	expression tag	UNP A0A0D3QGV4
N4	7	HIS	-	expression tag	UNP A0A0D3QGV4
N4	8	HIS	-	expression tag	UNP A0A0D3QGV4
N5	1	MET	-	initiating methionine	UNP A0A0D3QGV4
N5	2	VAL	-	expression tag	UNP A0A0D3QGV4
N5	3	HIS	-	expression tag	UNP A0A0D3QGV4
N5	4	HIS	-	expression tag	UNP A0A0D3QGV4
N5	5	HIS	-	expression tag	UNP A0A0D3QGV4
N5	6	HIS	-	expression tag	UNP A0A0D3QGV4
N5	7	HIS	-	expression tag	UNP A0A0D3QGV4
N5	8	HIS	-	expression tag	UNP A0A0D3QGV4
N6	1	MET	-	initiating methionine	UNP A0A0D3QGV4
N6	2	VAL	-	expression tag	UNP A0A0D3QGV4
N6	3	HIS	-	expression tag	UNP A0A0D3QGV4
N6	4	HIS	-	expression tag	UNP A0A0D3QGV4
N6	5	HIS	-	expression tag	UNP A0A0D3QGV4
N6	6	HIS	-	expression tag	UNP A0A0D3QGV4
N6	7	HIS	-	expression tag	UNP A0A0D3QGV4
N6	8	HIS	-	expression tag	UNP A0A0D3QGV4
N7	1	MET	-	initiating methionine	UNP A0A0D3QGV4
N7	2	VAL	-	expression tag	UNP A0A0D3QGV4
N7	3	HIS	-	expression tag	UNP A0A0D3QGV4
N7	4	HIS	-	expression tag	UNP A0A0D3QGV4
N7	5	HIS	-	expression tag	UNP A0A0D3QGV4
N7	6	HIS	-	expression tag	UNP A0A0D3QGV4
N7	7	HIS	-	expression tag	UNP A0A0D3QGV4
N7	8	HIS	-	expression tag	UNP A0A0D3QGV4

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Chain	Residue	Modelled	Actual	Comment	Reference
N8	1	MET	-	initiating methionine	UNP A0A0D3QGV4
N8	2	VAL	-	expression tag	UNP A0A0D3QGV4
N8	3	HIS	-	expression tag	UNP A0A0D3QGV4
N8	4	HIS	-	expression tag	UNP A0A0D3QGV4
N8	5	HIS	-	expression tag	UNP A0A0D3QGV4
N8	6	HIS	-	expression tag	UNP A0A0D3QGV4
N8	7	HIS	-	expression tag	UNP A0A0D3QGV4
N8	8	HIS	-	expression tag	UNP A0A0D3QGV4

- Molecule 2 is a protein called Anthrax toxin receptor 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	C1	280	4287	1346	2165	354	413	9	0	0
2	C2	280	4287	1346	2165	354	413	9	0	0
2	C3	280	4287	1346	2165	354	413	9	0	0
2	C4	280	4287	1346	2165	354	413	9	0	0

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C1	286	ARG	-	expression tag	UNP P58335
C1	287	THR	-	expression tag	UNP P58335
C1	288	GLU	-	expression tag	UNP P58335
C1	289	ASN	-	expression tag	UNP P58335
C1	290	LEU	-	expression tag	UNP P58335
C1	291	TYR	-	expression tag	UNP P58335
C1	292	PHE	-	expression tag	UNP P58335
C1	293	GLN	-	expression tag	UNP P58335
C1	294	GLY	-	expression tag	UNP P58335
C1	295	GLY	-	expression tag	UNP P58335
C1	296	ALA	-	expression tag	UNP P58335
C1	297	GLY	-	expression tag	UNP P58335
C1	298	ALA	-	expression tag	UNP P58335
C1	299	ARG	-	expression tag	UNP P58335
C1	300	SER	-	expression tag	UNP P58335
C1	301	ILE	-	expression tag	UNP P58335
C1	302	GLU	-	expression tag	UNP P58335
C1	303	GLY	-	expression tag	UNP P58335

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Chain	Residue	Modelled	Actual	Comment	Reference
C1	304	ARG	-	expression tag	UNP P58335
C1	305	ILE	-	expression tag	UNP P58335
C1	306	VAL	-	expression tag	UNP P58335
C1	307	LYS	-	expression tag	UNP P58335
C1	308	ASP	-	expression tag	UNP P58335
C1	309	TYR	-	expression tag	UNP P58335
C1	310	LYS	-	expression tag	UNP P58335
C1	311	ASP	-	expression tag	UNP P58335
C1	312	ASP	-	expression tag	UNP P58335
C1	313	ASP	-	expression tag	UNP P58335
C1	314	ASP	-	expression tag	UNP P58335
C1	315	LYS	-	expression tag	UNP P58335
C1	316	HIS	-	expression tag	UNP P58335
C1	317	HIS	-	expression tag	UNP P58335
C1	318	HIS	-	expression tag	UNP P58335
C1	319	HIS	-	expression tag	UNP P58335
C1	320	HIS	-	expression tag	UNP P58335
C1	321	HIS	-	expression tag	UNP P58335
C2	286	ARG	-	expression tag	UNP P58335
C2	287	THR	-	expression tag	UNP P58335
C2	288	GLU	-	expression tag	UNP P58335
C2	289	ASN	-	expression tag	UNP P58335
C2	290	LEU	-	expression tag	UNP P58335
C2	291	TYR	-	expression tag	UNP P58335
C2	292	PHE	-	expression tag	UNP P58335
C2	293	GLN	-	expression tag	UNP P58335
C2	294	GLY	-	expression tag	UNP P58335
C2	295	GLY	-	expression tag	UNP P58335
C2	296	ALA	-	expression tag	UNP P58335
C2	297	GLY	-	expression tag	UNP P58335
C2	298	ALA	-	expression tag	UNP P58335
C2	299	ARG	-	expression tag	UNP P58335
C2	300	SER	-	expression tag	UNP P58335
C2	301	ILE	-	expression tag	UNP P58335
C2	302	GLU	-	expression tag	UNP P58335
C2	303	GLY	-	expression tag	UNP P58335
C2	304	ARG	-	expression tag	UNP P58335
C2	305	ILE	-	expression tag	UNP P58335
C2	306	VAL	-	expression tag	UNP P58335
C2	307	LYS	-	expression tag	UNP P58335
C2	308	ASP	-	expression tag	UNP P58335
C2	309	TYR	-	expression tag	UNP P58335

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Chain	Residue	Modelled	Actual	Comment	Reference
C2	310	LYS	-	expression tag	UNP P58335
C2	311	ASP	-	expression tag	UNP P58335
C2	312	ASP	-	expression tag	UNP P58335
C2	313	ASP	-	expression tag	UNP P58335
C2	314	ASP	-	expression tag	UNP P58335
C2	315	LYS	-	expression tag	UNP P58335
C2	316	HIS	-	expression tag	UNP P58335
C2	317	HIS	-	expression tag	UNP P58335
C2	318	HIS	-	expression tag	UNP P58335
C2	319	HIS	-	expression tag	UNP P58335
C2	320	HIS	-	expression tag	UNP P58335
C2	321	HIS	-	expression tag	UNP P58335
C3	286	ARG	-	expression tag	UNP P58335
C3	287	THR	-	expression tag	UNP P58335
C3	288	GLU	-	expression tag	UNP P58335
C3	289	ASN	-	expression tag	UNP P58335
C3	290	LEU	-	expression tag	UNP P58335
C3	291	TYR	-	expression tag	UNP P58335
C3	292	PHE	-	expression tag	UNP P58335
C3	293	GLN	-	expression tag	UNP P58335
C3	294	GLY	-	expression tag	UNP P58335
C3	295	GLY	-	expression tag	UNP P58335
C3	296	ALA	-	expression tag	UNP P58335
C3	297	GLY	-	expression tag	UNP P58335
C3	298	ALA	-	expression tag	UNP P58335
C3	299	ARG	-	expression tag	UNP P58335
C3	300	SER	-	expression tag	UNP P58335
C3	301	ILE	-	expression tag	UNP P58335
C3	302	GLU	-	expression tag	UNP P58335
C3	303	GLY	-	expression tag	UNP P58335
C3	304	ARG	-	expression tag	UNP P58335
C3	305	ILE	-	expression tag	UNP P58335
C3	306	VAL	-	expression tag	UNP P58335
C3	307	LYS	-	expression tag	UNP P58335
C3	308	ASP	-	expression tag	UNP P58335
C3	309	TYR	-	expression tag	UNP P58335
C3	310	LYS	-	expression tag	UNP P58335
C3	311	ASP	-	expression tag	UNP P58335
C3	312	ASP	-	expression tag	UNP P58335
C3	313	ASP	-	expression tag	UNP P58335
C3	314	ASP	-	expression tag	UNP P58335
C3	315	LYS	-	expression tag	UNP P58335

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Chain	Residue	Modelled	Actual	Comment	Reference
C3	316	HIS	-	expression tag	UNP P58335
C3	317	HIS	-	expression tag	UNP P58335
C3	318	HIS	-	expression tag	UNP P58335
C3	319	HIS	-	expression tag	UNP P58335
C3	320	HIS	-	expression tag	UNP P58335
C3	321	HIS	-	expression tag	UNP P58335
C4	286	ARG	-	expression tag	UNP P58335
C4	287	THR	-	expression tag	UNP P58335
C4	288	GLU	-	expression tag	UNP P58335
C4	289	ASN	-	expression tag	UNP P58335
C4	290	LEU	-	expression tag	UNP P58335
C4	291	TYR	-	expression tag	UNP P58335
C4	292	PHE	-	expression tag	UNP P58335
C4	293	GLN	-	expression tag	UNP P58335
C4	294	GLY	-	expression tag	UNP P58335
C4	295	GLY	-	expression tag	UNP P58335
C4	296	ALA	-	expression tag	UNP P58335
C4	297	GLY	-	expression tag	UNP P58335
C4	298	ALA	-	expression tag	UNP P58335
C4	299	ARG	-	expression tag	UNP P58335
C4	300	SER	-	expression tag	UNP P58335
C4	301	ILE	-	expression tag	UNP P58335
C4	302	GLU	-	expression tag	UNP P58335
C4	303	GLY	-	expression tag	UNP P58335
C4	304	ARG	-	expression tag	UNP P58335
C4	305	ILE	-	expression tag	UNP P58335
C4	306	VAL	-	expression tag	UNP P58335
C4	307	LYS	-	expression tag	UNP P58335
C4	308	ASP	-	expression tag	UNP P58335
C4	309	TYR	-	expression tag	UNP P58335
C4	310	LYS	-	expression tag	UNP P58335
C4	311	ASP	-	expression tag	UNP P58335
C4	312	ASP	-	expression tag	UNP P58335
C4	313	ASP	-	expression tag	UNP P58335
C4	314	ASP	-	expression tag	UNP P58335
C4	315	LYS	-	expression tag	UNP P58335
C4	316	HIS	-	expression tag	UNP P58335
C4	317	HIS	-	expression tag	UNP P58335
C4	318	HIS	-	expression tag	UNP P58335
C4	319	HIS	-	expression tag	UNP P58335
C4	320	HIS	-	expression tag	UNP P58335
C4	321	HIS	-	expression tag	UNP P58335

3 Residue-property plots (i)

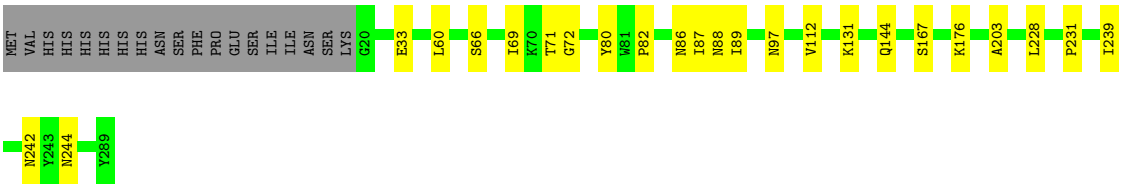
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Leukocidin/Hemolysin toxin family

Chain N1:

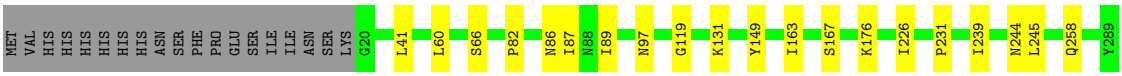
• Molecule 1: Leukocidin/Hemolysin toxin family

Chain N2:



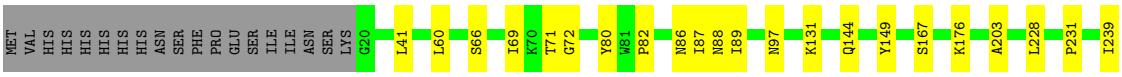
• Molecule 1: Leukocidin/Hemolysin toxin family

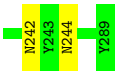
Chain N3:



• Molecule 1: Leukocidin/Hemolysin toxin family

Chain N4:



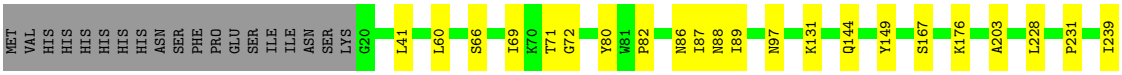


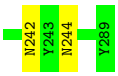
• Molecule 1: Leukocidin/Hemolysin toxin family

Chain N5:

• Molecule 1: Leukocidin/Hemolysin toxin family

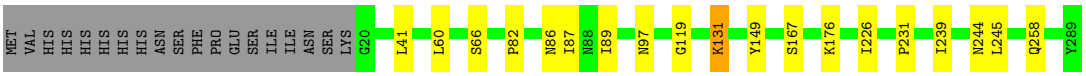
Chain N6:





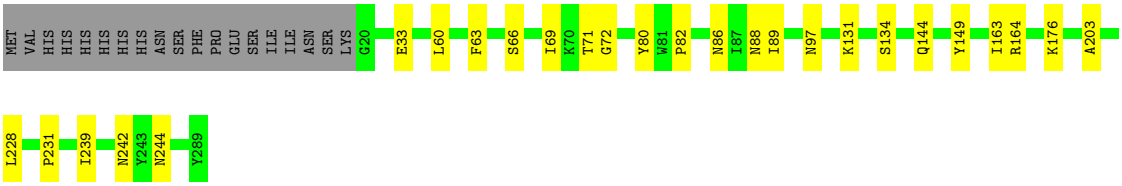
• Molecule 1: Leukocidin/Hemolysin toxin family

Chain N7:



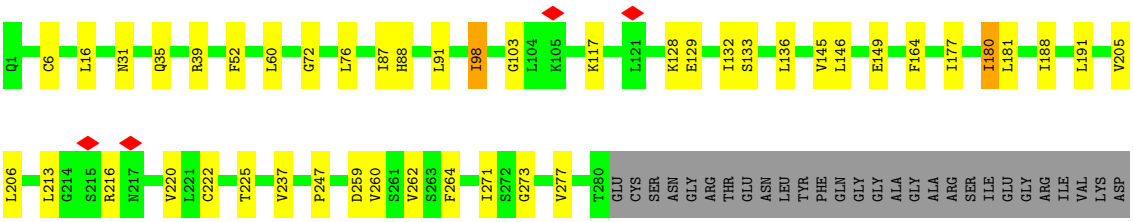
• Molecule 1: Leukocidin/Hemolysin toxin family

Chain N8:



• Molecule 2: Anthrax toxin receptor 2

Chain C1:



TYR LYS ASP ASP ASP ASP LYS HIS HIS HIS HIS HIS HIS

- Molecule 2: Anthrax toxin receptor 2

Chain C2:

Q1 C6 F14 V15 L16 Q34 R39 I50 V51 F52 I58 L73 I87 L91 K92 L93 Q97 K105 K117 L118 L121 V122 P123 S124 K128 E129 I132 L136 V145 L146 E149 Q150 A151 R155 F164 I177 I180 L181

I188 L191 V205 L206 L213 G214 S215 R216 N217 V220 L221 C222 T225 V237 P247 D259 V260 S261 V262 S263 F264 I271 S272 G273 V277 T280 GLU CYS SER ASN GLY ARG THR GLU ASN LEU TYR PHE GLN GLY GLY ALA GLY ALA ARG SER ILE GLU

GLY ARG ILE VAL LYS ASP TYR LYS ASP ASP ASP ASP LYS HIS HIS HIS HIS HIS HIS

- Molecule 2: Anthrax toxin receptor 2

Chain C3:

Q1 C6 F14 V15 L16 Q34 R39 I50 V51 F52 I58 L73 I87 L91 K92 L93 Q97 I98 K105 K117 L118 L121 V122 P123 S124 K128 E129 I132 L136 V145 L146 E149 Q150 A151 R155 F164 I177 I180

L181 I188 L191 V205 L206 L213 G214 S215 R216 N217 V220 L221 C222 T225 V237 P247 D259 V260 S261 V262 S263 F264 I271 S272 G273 V277 T280 GLU CYS SER ASN GLY ARG THR GLU ASN LEU TYR PHE GLN GLY GLY ALA GLY ALA ARG SER ILE

GLU GLY ARG ILE VAL LYS ASP TYR LYS ASP ASP ASP ASP LYS HIS HIS HIS HIS HIS HIS

- Molecule 2: Anthrax toxin receptor 2

Chain C4:

Q1 C6 F14 V15 L16 Q34 R39 I50 V51 F52 I58 L73 I87 L91 K92 L93 Q97 I98 K105 K117 L118 L121 V122 P123 S124 Y125 A126 E127 K128 E129 I132 L136 V145 L146 E149 Q150 A151 R155 F164 I177

I180 L181 I188 L191 V205 L206 L213 G214 S215 R216 N217 V220 L221 C222 T225 V237 P247 D259 V260 S261 V262 S263 F264 I271 S272 G273 V277 T280 GLU CYS SER ASN GLY ARG THR GLU ASN LEU TYR PHE GLN GLY GLY ALA GLY ALA ARG

SER ILE GLU GLY ARG ILE VAL LYS ASP TYR LYS ASP ASP ASP LYS HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67074	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	10000	Depositor
Maximum defocus (nm)	30000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.346	Depositor
Minimum map value	-0.136	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	281.5, 281.5, 281.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.563, 0.563, 0.563	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	N1	0.22	0/2204	0.36	0/2988
1	N2	0.21	0/2208	0.31	0/2993
1	N3	0.20	0/2208	0.30	0/2993
1	N4	0.21	0/2208	0.30	0/2993
1	N5	0.20	0/2208	0.30	0/2993
1	N6	0.21	0/2208	0.30	0/2993
1	N7	0.20	0/2208	0.30	0/2993
1	N8	0.21	0/2208	0.30	0/2993
2	C1	0.13	0/2153	0.29	0/2911
2	C2	0.13	0/2153	0.31	0/2911
2	C3	0.13	0/2153	0.31	0/2911
2	C4	0.13	0/2153	0.31	0/2911
All	All	0.19	0/26272	0.31	0/35583

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	N1	2154	2089	2092	34	0
1	N2	2158	2092	2095	16	0
1	N3	2158	2092	2095	12	0
1	N4	2158	2092	2095	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N5	2158	2092	2095	12	0
1	N6	2158	2092	2095	14	0
1	N7	2158	2092	2095	12	0
1	N8	2158	2092	2095	16	0
2	C1	2122	2165	2166	24	0
2	C2	2122	2165	2166	28	0
2	C3	2122	2165	2166	29	0
2	C4	2122	2165	2166	30	0
All	All	25748	25393	25421	220	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 220 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:N2:131:LYS:H	1:N2:131:LYS:HD3	1.59	0.66
1:N1:93:GLU:O	1:N1:94:LYS:HG2	2.02	0.59
1:N1:85:ASN:HB3	1:N1:243:ASN:HB2	1.84	0.58
1:N6:60:LEU:HD21	1:N6:89:ILE:HB	1.87	0.57
2:C4:52:PHE:CZ	2:C4:87:ILE:HG22	2.40	0.57

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	N1	267/289 (92%)	247 (92%)	20 (8%)	0	100	100
1	N2	268/289 (93%)	260 (97%)	8 (3%)	0	100	100
1	N3	268/289 (93%)	261 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N4	268/289 (93%)	260 (97%)	8 (3%)	0	100	100
1	N5	268/289 (93%)	261 (97%)	7 (3%)	0	100	100
1	N6	268/289 (93%)	260 (97%)	8 (3%)	0	100	100
1	N7	268/289 (93%)	261 (97%)	7 (3%)	0	100	100
1	N8	268/289 (93%)	260 (97%)	8 (3%)	0	100	100
2	C1	278/321 (87%)	263 (95%)	15 (5%)	0	100	100
2	C2	278/321 (87%)	263 (95%)	15 (5%)	0	100	100
2	C3	278/321 (87%)	263 (95%)	15 (5%)	0	100	100
2	C4	278/321 (87%)	263 (95%)	15 (5%)	0	100	100
All	All	3255/3596 (90%)	3122 (96%)	133 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	N1	239/258 (93%)	231 (97%)	8 (3%)	33	61
1	N2	239/258 (93%)	239 (100%)	0	100	100
1	N3	239/258 (93%)	237 (99%)	2 (1%)	73	88
1	N4	239/258 (93%)	238 (100%)	1 (0%)	84	93
1	N5	239/258 (93%)	237 (99%)	2 (1%)	73	88
1	N6	239/258 (93%)	238 (100%)	1 (0%)	84	93
1	N7	239/258 (93%)	237 (99%)	2 (1%)	73	88
1	N8	239/258 (93%)	238 (100%)	1 (0%)	84	93
2	C1	239/273 (88%)	234 (98%)	5 (2%)	47	73
2	C2	239/273 (88%)	236 (99%)	3 (1%)	61	82
2	C3	239/273 (88%)	236 (99%)	3 (1%)	61	82
2	C4	239/273 (88%)	236 (99%)	3 (1%)	61	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2868/3156 (91%)	2837 (99%)	31 (1%)	63 84

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N3	258	GLN
2	C4	180	ILE
2	C2	222	CYS
2	C4	222	CYS
1	N6	131	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	N5	282	ASN
1	N7	200	ASN
2	C3	1	GLN
1	N7	88	ASN
1	N7	258	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.

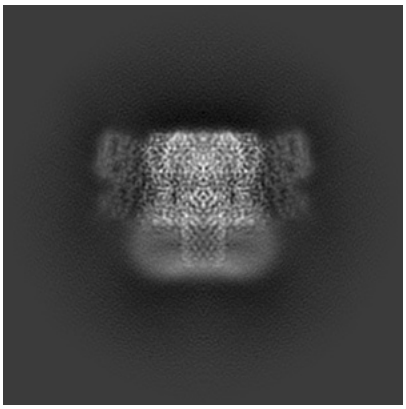
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-54238. These allow visual inspection of the internal detail of the map and identification of artifacts.

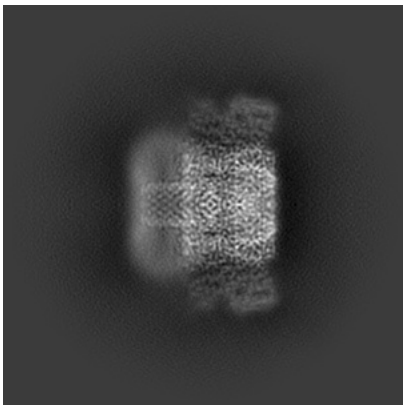
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

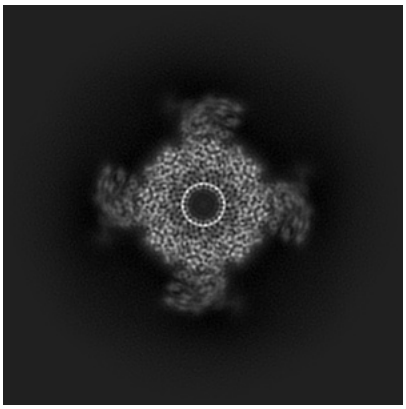
6.1.1 Primary map



X

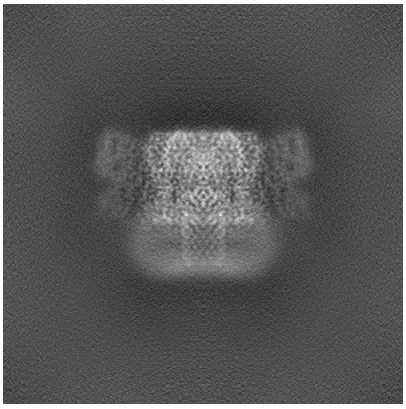


Y

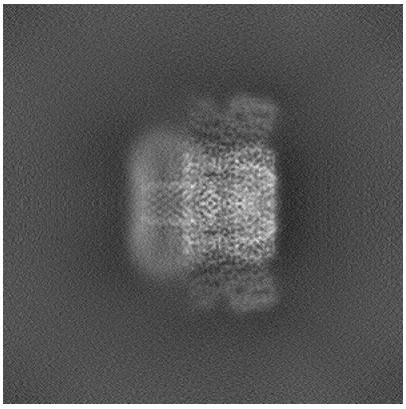


Z

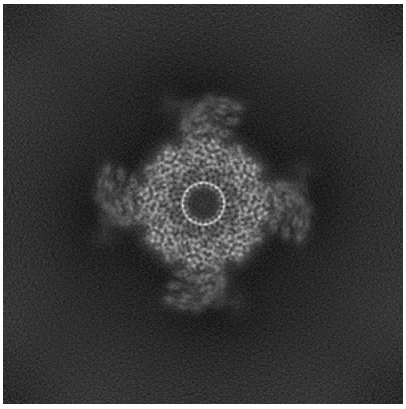
6.1.2 Raw map



X



Y

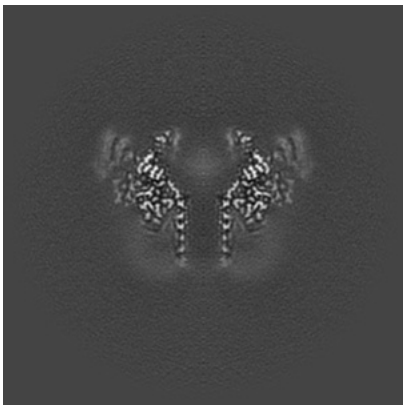


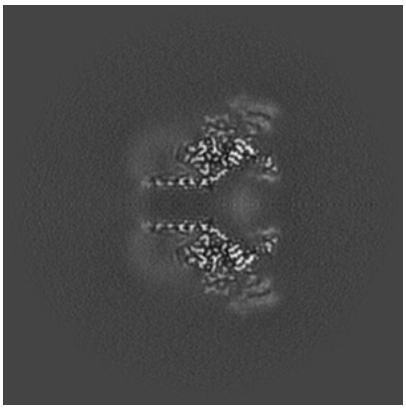
Z

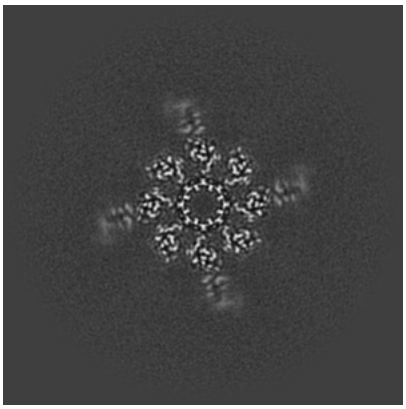
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

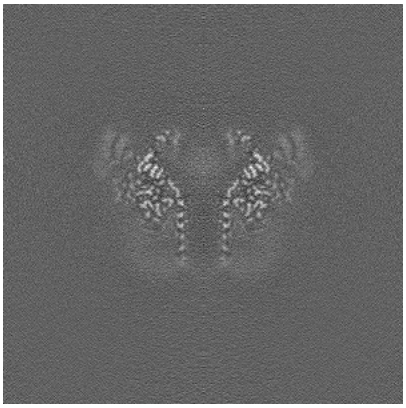
6.2.1 Primary map

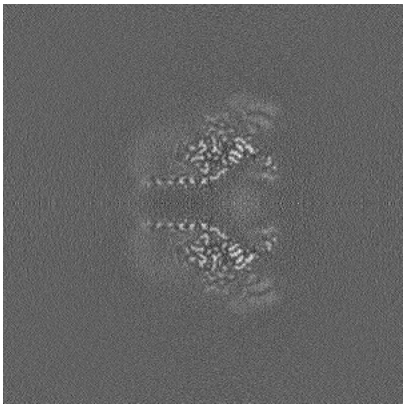

X Index: 250

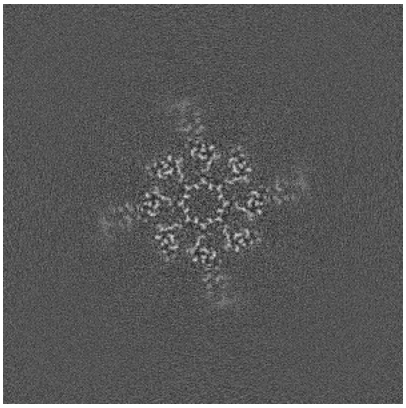

Y Index: 250


Z Index: 250

6.2.2 Raw map


X Index: 250

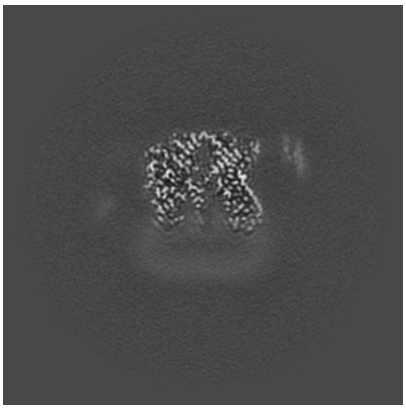

Y Index: 250


Z Index: 250

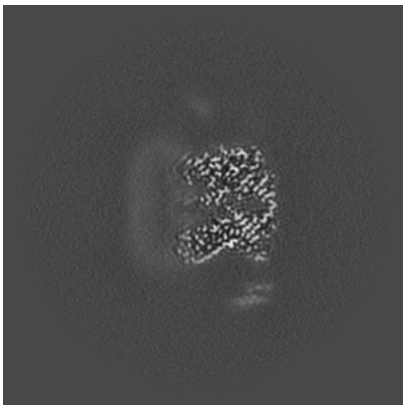
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

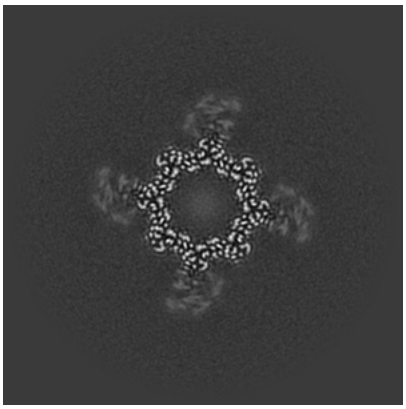
6.3.1 Primary map



X Index: 295

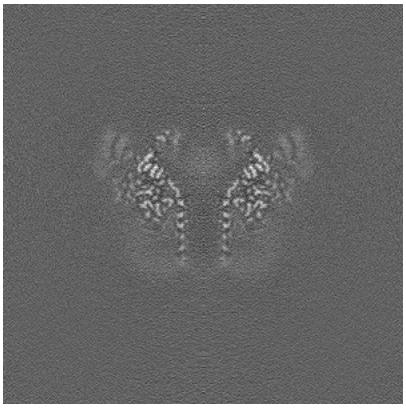


Y Index: 295

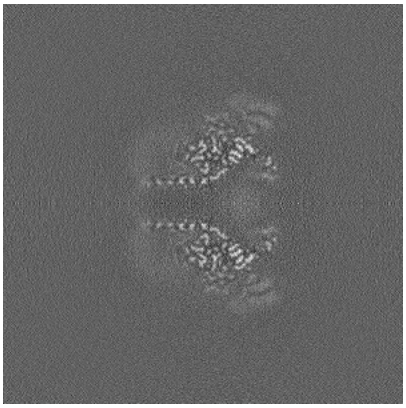


Z Index: 291

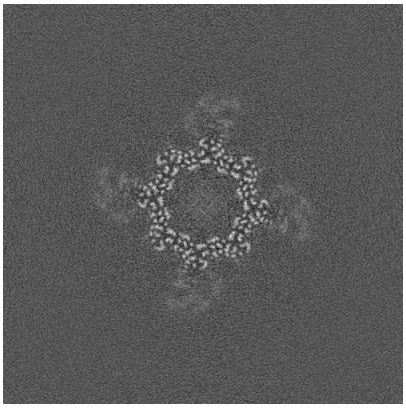
6.3.2 Raw map



X Index: 250



Y Index: 250

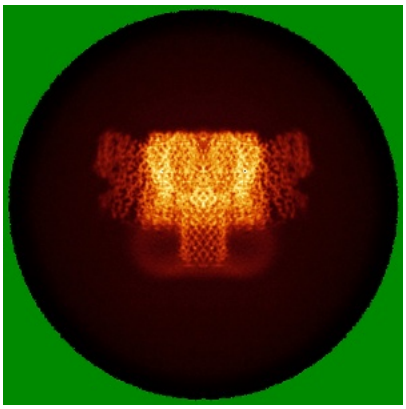


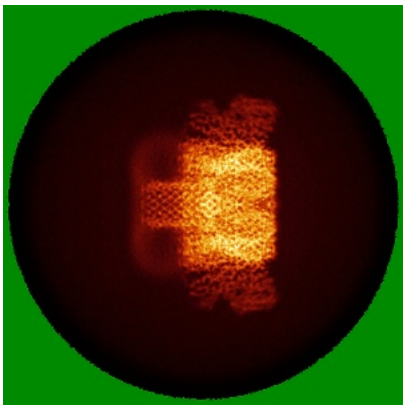
Z Index: 291

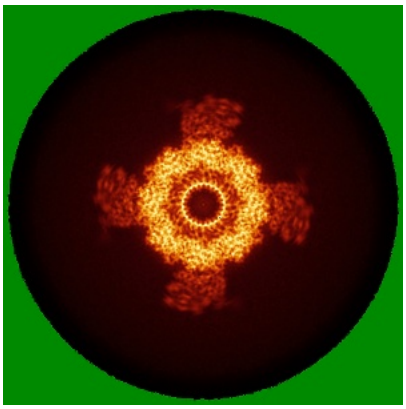
The images above show the largest variance slices of the map in three orthogonal directions.

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

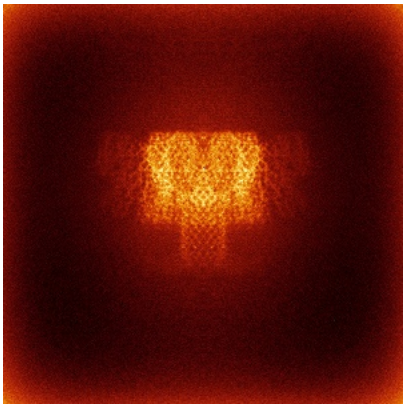
6.4.1 Primary map

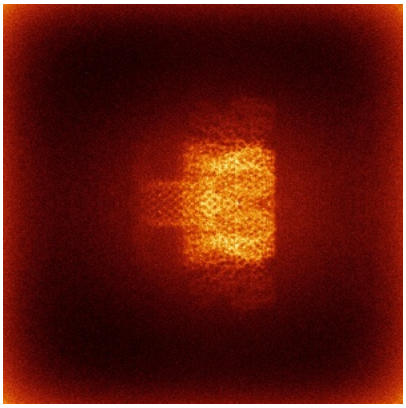

X

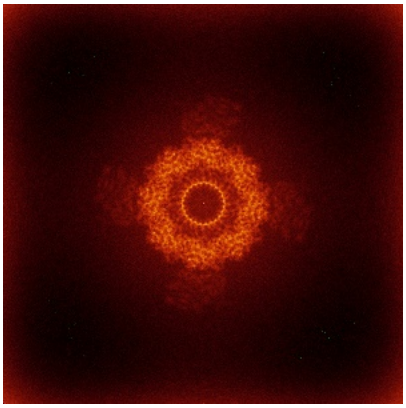

Y


Z

6.4.2 Raw map


X

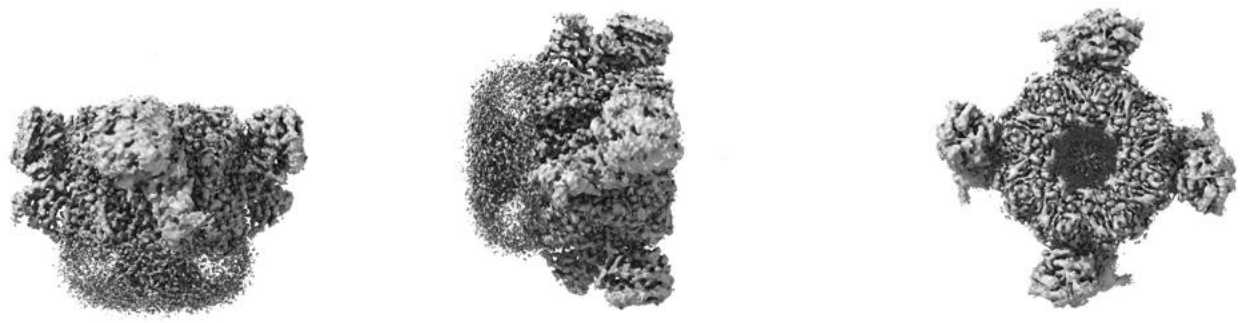

Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

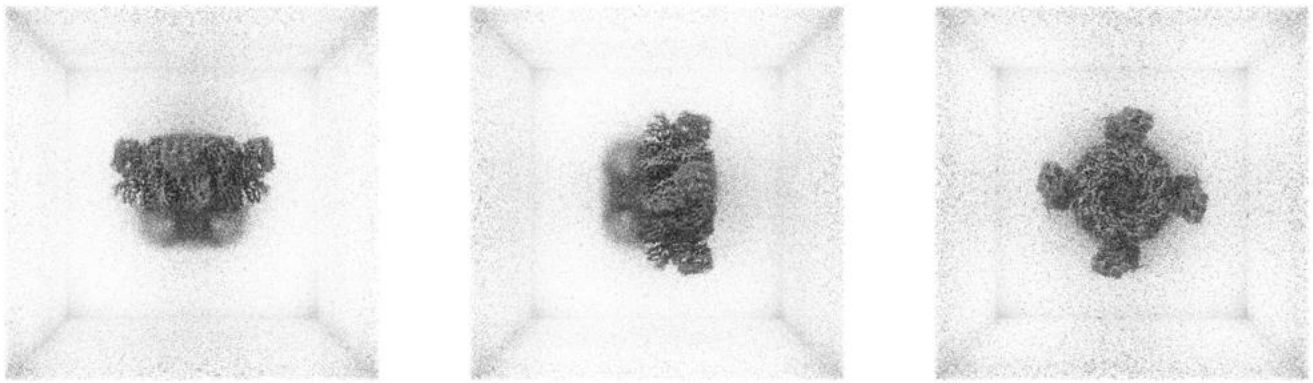
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

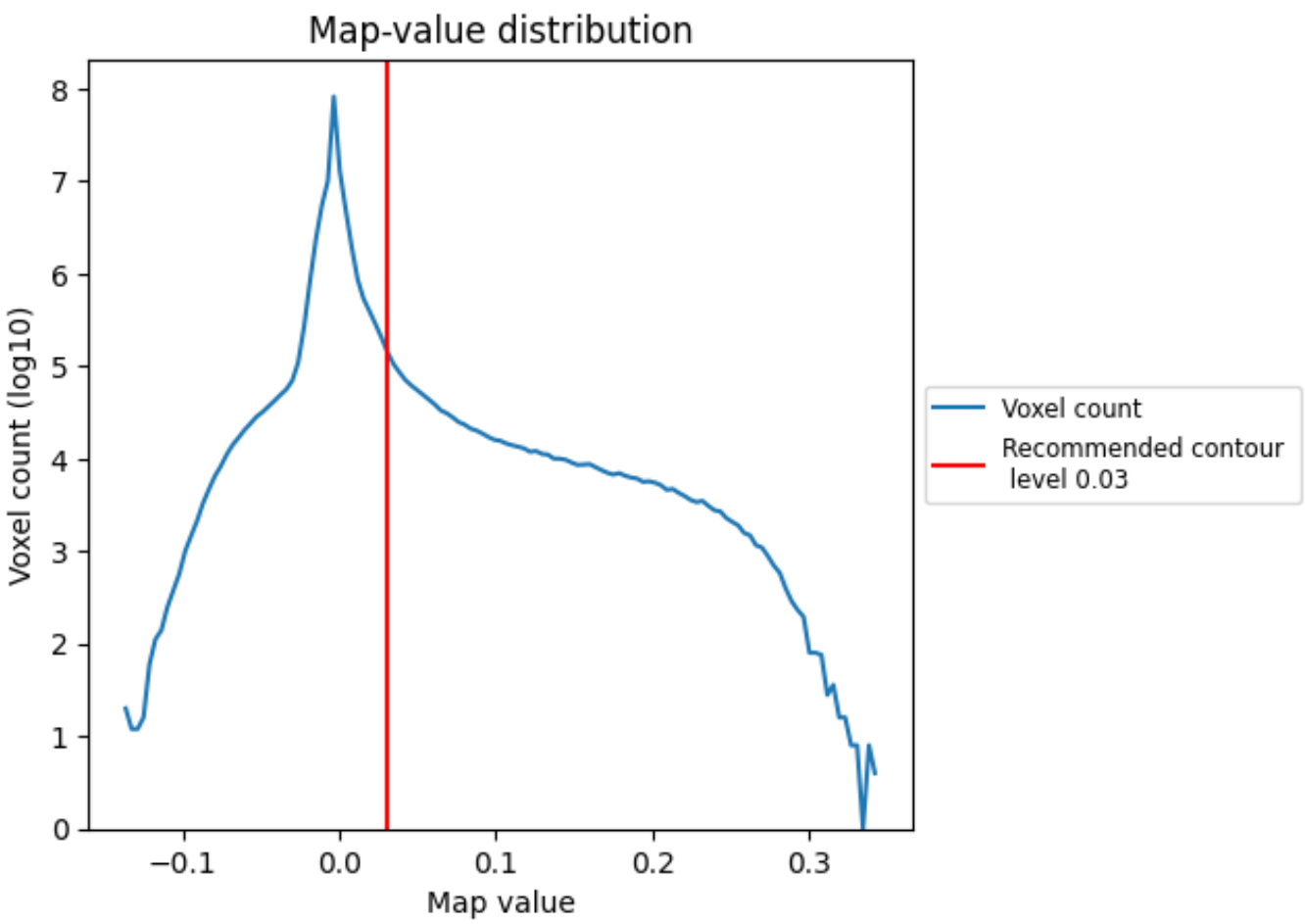
6.6 Mask visualisation (i)

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

7 Map analysis (i)

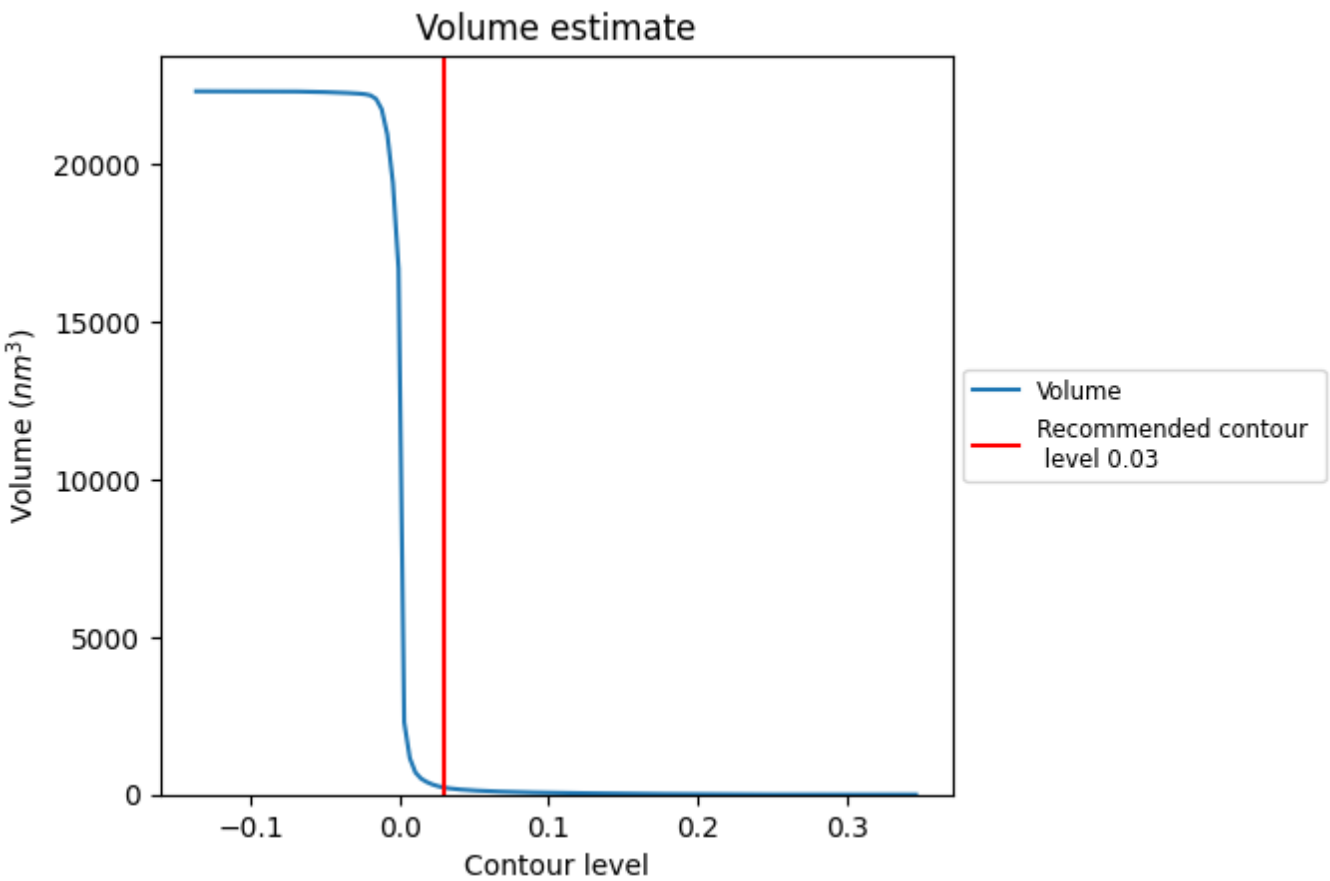
This section contains the results of statistical analysis of the map.

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.

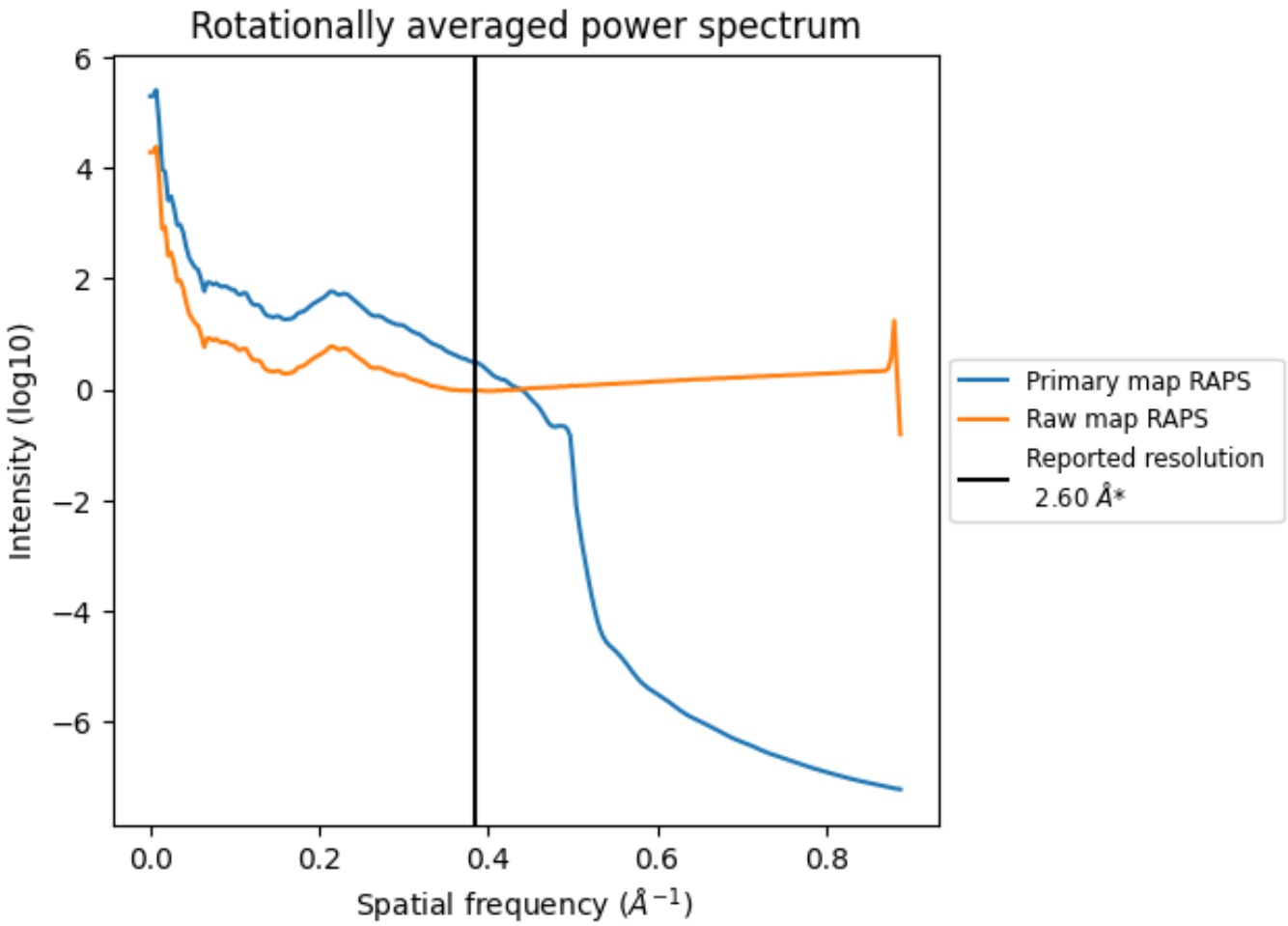
7.2 Volume estimate (i)



The volume at the recommended contour level is 222 nm^3; this corresponds to an approximate mass of 200 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)

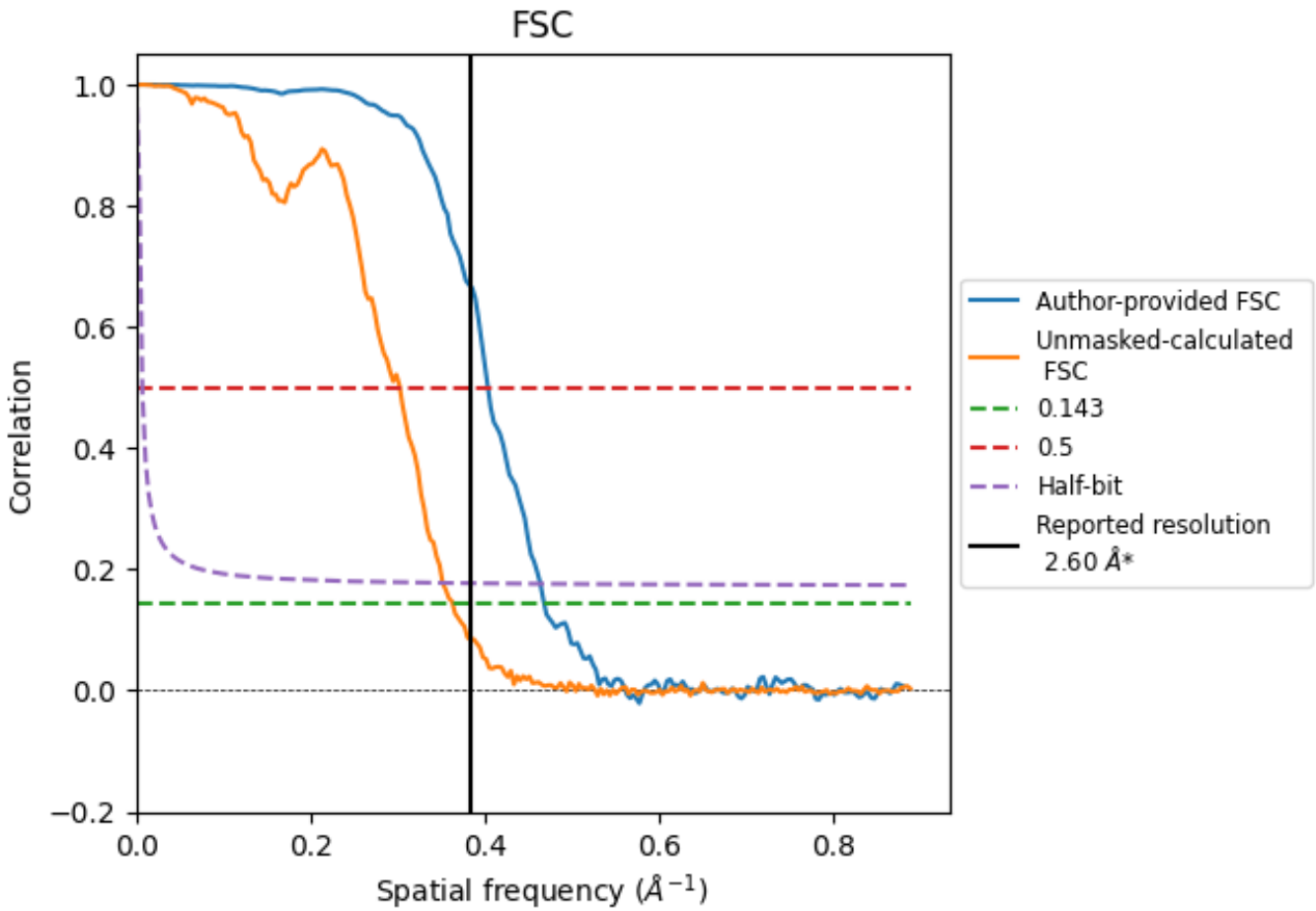


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8.2 Resolution estimates (i)

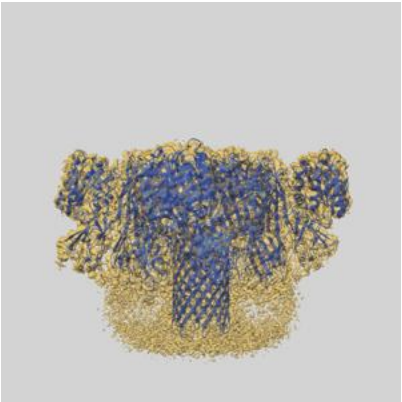
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.14	2.48	2.16
Unmasked-calculated*	2.75	3.31	2.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.14 differs from the reported value 2.6 by more than 10 %

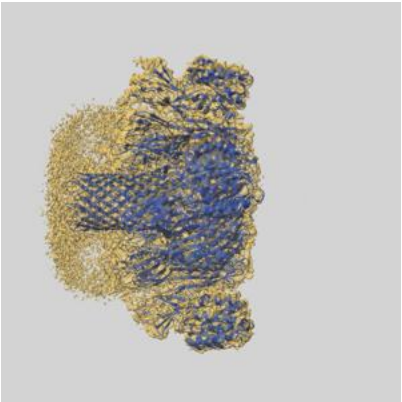
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-54238 and PDB model 9RT2. Per-residue inclusion information can be found in section 3 on page 10.

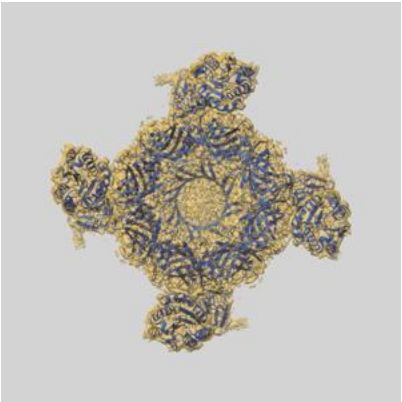
9.1 Map-model overlay (i)



X



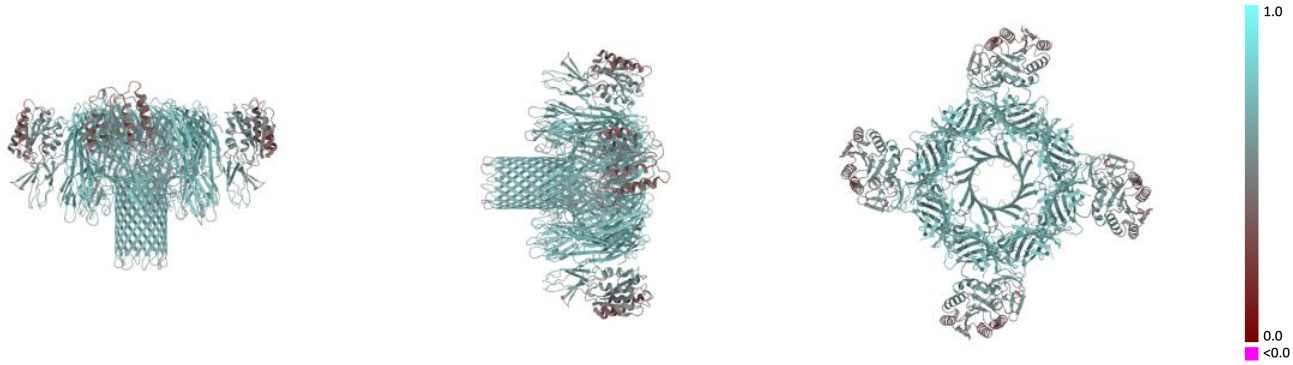
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

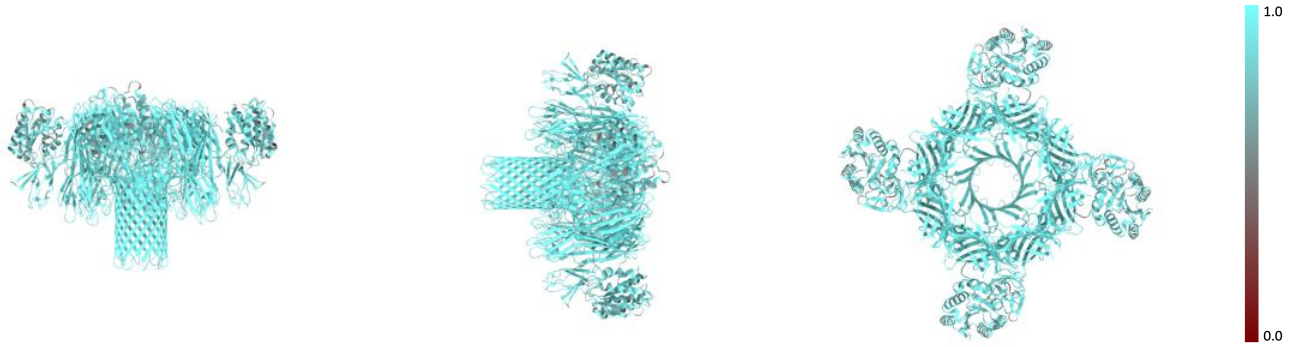
9.2 Q-score mapped to coordinate model (i)



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.

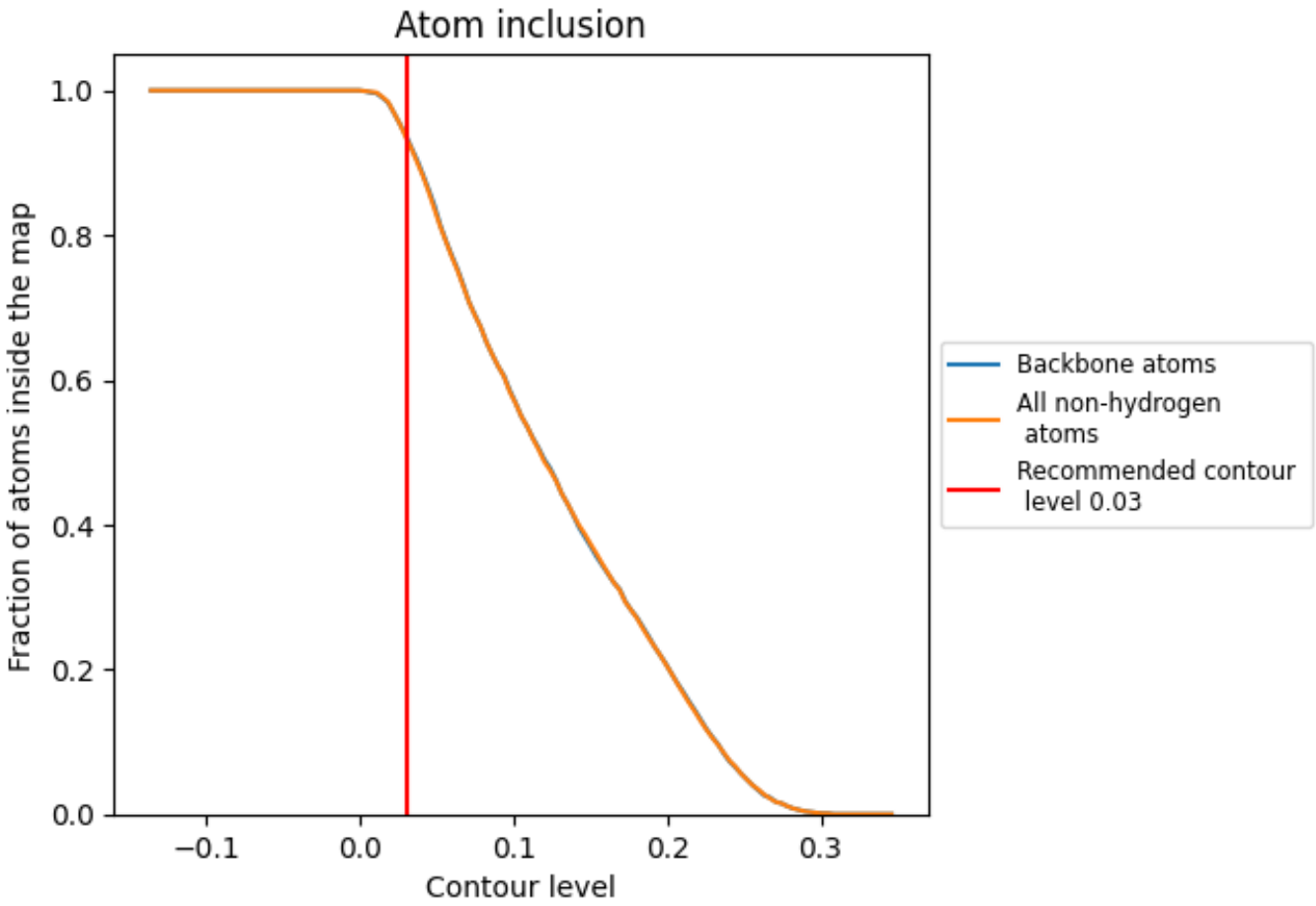
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9340	0.6320
C1	0.8460	0.5130
C2	0.8480	0.5140
C3	0.8490	0.5150
C4	0.8480	0.5150
N1	0.9810	0.6780
N2	0.9860	0.6930
N3	0.9850	0.6900
N4	0.9850	0.6930
N5	0.9850	0.6900
N6	0.9850	0.6940
N7	0.9850	0.6900
N8	0.9850	0.6940