



wwPDB EM Validation Summary Report ⓘ

Mar 29, 2026 – 05:10 AM UTC

PDB ID : 9V6N / pdb_00009v6n
EMDB ID : EMD-64803
Title : Block based reconstruction of RVFV GnGc-Fab140 complex
Authors : Zhang, L.; Meng, K.; Xiang, Y.
Deposited on : 2025-05-27
Resolution : 3.40 Å(reported)

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

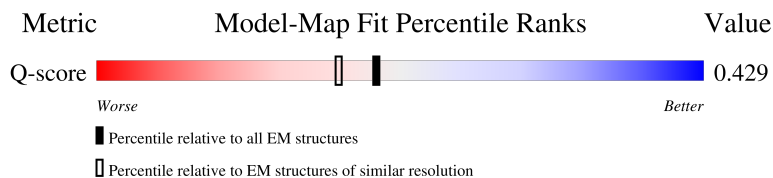
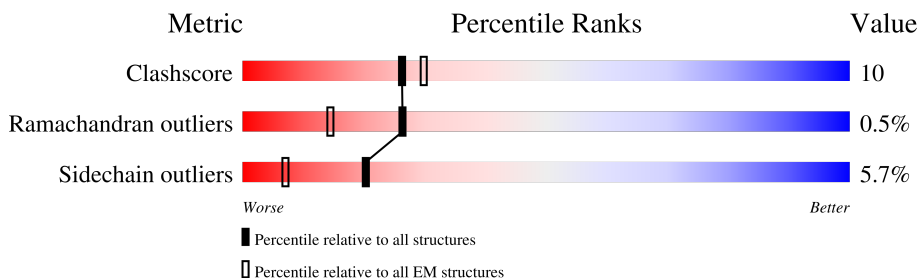
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	1064	
1	B	1064	
2	C	3	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6563 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 Envelopment polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	412	Total	C	N	O	S	0	0
			3119	1941	544	600	34		
1	B	444	Total	C	N	O	S	0	0
			3374	2093	582	671	28		

There are 44 discrepancies between the modelled and reference sequences:

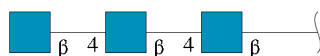
Chain	Residue	Modelled	Actual	Comment	Reference
A	1198	ASP	-	expression tag	UNP A2T069
A	1199	TYR	-	expression tag	UNP A2T069
A	1200	LYS	-	expression tag	UNP A2T069
A	1201	ASP	-	expression tag	UNP A2T069
A	1202	HIS	-	expression tag	UNP A2T069
A	1203	ASP	-	expression tag	UNP A2T069
A	1204	GLY	-	expression tag	UNP A2T069
A	1205	ASP	-	expression tag	UNP A2T069
A	1206	TYR	-	expression tag	UNP A2T069
A	1207	LYS	-	expression tag	UNP A2T069
A	1208	ASP	-	expression tag	UNP A2T069
A	1209	HIS	-	expression tag	UNP A2T069
A	1210	ASP	-	expression tag	UNP A2T069
A	1211	ILE	-	expression tag	UNP A2T069
A	1212	ASP	-	expression tag	UNP A2T069
A	1213	TYR	-	expression tag	UNP A2T069
A	1214	LYS	-	expression tag	UNP A2T069
A	1215	ASP	-	expression tag	UNP A2T069
A	1216	ASP	-	expression tag	UNP A2T069
A	1217	ASP	-	expression tag	UNP A2T069
A	1218	ASP	-	expression tag	UNP A2T069
A	1219	LYS	-	expression tag	UNP A2T069
B	1198	ASP	-	expression tag	UNP A2T069
B	1199	TYR	-	expression tag	UNP A2T069
B	1200	LYS	-	expression tag	UNP A2T069
B	1201	ASP	-	expression tag	UNP A2T069

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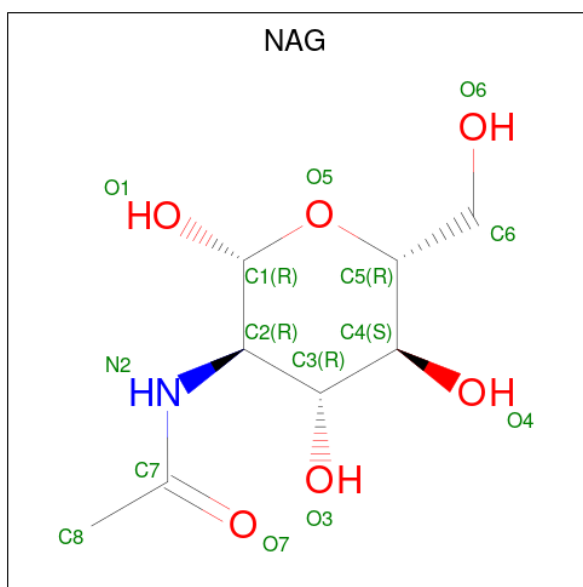
Chain	Residue	Modelled	Actual	Comment	Reference
B	1202	HIS	-	expression tag	UNP A2T069
B	1203	ASP	-	expression tag	UNP A2T069
B	1204	GLY	-	expression tag	UNP A2T069
B	1205	ASP	-	expression tag	UNP A2T069
B	1206	TYR	-	expression tag	UNP A2T069
B	1207	LYS	-	expression tag	UNP A2T069
B	1208	ASP	-	expression tag	UNP A2T069
B	1209	HIS	-	expression tag	UNP A2T069
B	1210	ASP	-	expression tag	UNP A2T069
B	1211	ILE	-	expression tag	UNP A2T069
B	1212	ASP	-	expression tag	UNP A2T069
B	1213	TYR	-	expression tag	UNP A2T069
B	1214	LYS	-	expression tag	UNP A2T069
B	1215	ASP	-	expression tag	UNP A2T069
B	1216	ASP	-	expression tag	UNP A2T069
B	1217	ASP	-	expression tag	UNP A2T069
B	1218	ASP	-	expression tag	UNP A2T069
B	1219	LYS	-	expression tag	UNP A2T069

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
3	A	1	14	8	1	5	0
3	B	1	14	8	1	5	0

[illegible]

- Molecule 1: Envelopment polypotein



PRO	HIS	LEU	ARG	ASN	ARG	PRO	GLY	GLY	LYS	HIS	ASN	TYR	ILE	ASP	GLY	THR	GLN	GLU	ASP	ALA	ALA	THR	THR	CYS	LYS	PRO	VAL	THR	THR	TYR	ALA	ALA	GLY	ALA	CYS	SER	SER	ASP	ASP	VAL	LEU	LEU	LEU	GLU	GLU	LYS	GLY	LYS	PHE	PRO	PRO	PHE	PHE	GLN	SER	TYR	TYR	ALA	HIS	HIS	ARG	THR	THR	LEU	LEU	LEU	GLU	GLU	ALA	PRO
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VAL	HIS	ASP	THR	ILE	LEU	ALA	LYS	ASP	PRO	SER	CYS	ASP	LEU	GLN	SER	ALA	HIS	GLY	ASN	PRO	CYS	LYS	GLU	LYS	LEU	VAL	VAL	LYS	THR	HIS	CYS	PRO	ASN	ASP	TYR	GLN	SER	ALA	ALA	HIS	TYR	LEU	ASN	ASN	ASP	GLY	LYS	MET	ALA	ASP	VAL	LYS	PRO	PRO	LYS	TYR
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GLU	LEU	THR	GLU	ASP	ASN	CYS	PHE	CYS	ARG	GLN	MET	THR	GLY	ALA	ALA	SER	TYR	PRO	LEU	GLN	ASP	PHE	CYS	GLN	SER	GLU	ASP	GLY	SER	LYS	LEU	LYS	THR	LYS	MET	GLY	VAL	CYS	GLU	VAL	GLY	VAL	GLN	ALA	LEU	LYS	LYS	CYS	ASP	GLY
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LEU SER THR HIS GLU VAL VAL PHE LYS ASN SER LYS VAL TYR LEU ASP LYS LEU ASP ASN THR GLU GLU ASN LEU LEU LYS PRO LEU ASP SER PHE CYS PHE GLU HIS LYS GLY GLN TYR LYS GLY THR MET ASP SER GLY CLN THR LYS ARG GLU LEU

[illegible]

CYS	VAL	GLY	TYR	GLU	ARG	VAL	VAL	VAL	LYS	ARG	GLU	LEU	SER	ALA	ALA	PRO	ILE	GLN	ARG	VAL	VAL	GLU	PRO	CYS	THR	THR	ILE	THR	LYS	CYS	GLU	PRO	HIS	GLY	LEU	VAL	VAL	VAL	ARG	SER	SER	SER	ILE	LYS	PHE	GLY	LYS	ILE	SER	SER	ALA	VAL	ALA	CYS	GLY	VAL	VAL	THR	THR	GLY	ASP
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GLN	SER	PRO	THR	GLU	ILE	THR	LEU	LYS	TYR	PRO	GLY	ILE	SER	SER	GLN	SER	SER	SER	ASP	ASP	GLN	SER	VAL	VAL	LYS	ILE	ALA	ALA	HIS	CYS	PRO	PRO	GLN	ASP	PRO	CYS	LEU	VAL	CYS	ALA	HIS	GLY	CYS	ILE	VAL	CYS	LEU	THR
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ASN	TYR	GLN	CYS	HIS	THR	ALA	LEU	SER	ALA	PHE	VAL	VAL	VAL	PHE	PHE	PHE	SER	SER	ILE	ILE	ALA	ILE	ILE	ILE	CYS	LEU	ALA	ALA	VAL	VAL	LEU	LEU	TYR	ARG	VAL	VAL	LEU	LEU	LYS	CYS	CYS	LYS	LYS	VAL	VAL	LEU	ASN	PRO	PRO	LEU	LEU	MET	TRP	TRP	ILE	THR	ALA	ALA	PHE	PHE	ILE	ILE	ARG	ARG	TRP	TRP	LYS	LYS	LYS
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Gene	Chromosome	Position (kb)	Strand	Transcript	Exon	Intron	UTR	Feature
D1121	1	1121	+	R1047	L953	V828	S699	VAL
D1122	1	1122	+	C1048	Y956	T837	R700	ALA
C1049	1	1123	+	C1049	K957	T837	I701	VAL
R1124	1	1124	+	S1081	P958	V842	THR	ALA
E1125	1	1125	+	I1082	M959	V842	THR	ASP
A1126	1	1126	+	T1087	P960	L847	CYS	ASN
V1133	1	1133	+	L1080	D961	K858	T706	ASN
N1134	1	1134	+	S1061	Q962	L859	E707	GLN
P1135	1	1135	+	A1062	L963	L859	G708	VAL
K1136	1	1136	+	H1063	E964	E862	G708	ARG
S1137	1	1137	+	N1064	L969	T864	V709	GLU
K1085	1	1138	+	D1066	P972	D865	N710	ILE
T1087	1	1138	+	K1085	P972	P866	T711	TRP
PHE	1	1138	+	E1076	G979	G968	K712	MET
ASN	1	1138	+	I1071	S980	G968	C713	GLU
PHE	1	1138	+	V1072	L981	S869	R714	GLY
PHE	1	1138	+	L1073	P982	V870	L715	GLY
ASP	1	1138	+	P1074	Q983	S870	S716	GLN
TRP	1	1138	+	S1075	Q983	V870	G717	LEU
PHE	1	1138	+	E1076	P989	I873	I721	VAL
SER	1	1138	+	T1079	F990	D874	R722	LEU
GLY	1	1138	+	K1080	A991	A877	R730	GLY
LEU	1	1138	+	T1089	V999	S880	C731	ASN
MET	1	1138	+	K1081	A1009	R881	L732	PRO
SER	1	1138	+	Q1082	A1009	P882	M733	PRO
PHE	1	1138	+	C1083	T1012	N884	L734	ILE
GLY	1	1138	+	Q1084	T1012	N884	K735	PRO
GLY	1	1138	+	I1085	N1017	N885	G736	ARG
PRO	1	1138	+	T1089	F1018	L890	E739	HIS
LEU	1	1138	+	V1090	E1019	S891	D740	ALA
THR	1	1138	+	E1094	V1020	L392	Q741	ILE
ILE	1	1138	+	F1097	F1021	D893	K746	PRO
LEU	1	1138	+	M1098	F1022	A894	I747	ARG
LEU	1	1138	+	Y1099	V1023	E995	K748	THR
CYS	1	1138	+	S1100	G1024	G896	C771	TVR
TVR	1	1138	+	C1101	A1025	I897	E782	LEU
VAL	1	1138	+	D1102	A1026	S898	E782	MET
ALA	1	1138	+	G1103	C1029	S900	V785	LEU
LEU	1	1138	+	D1104	D1030	Y913	R792	LEU
SER	1	1138	+	P1107	A1031	A914	D793	ILE
ILE	1	1138	+	L1108	L1034	I915	N794	VAL
PHE	1	1138	+	L1109	H1035	Q926	S797	SER
PHE	1	1138	+	V1110	T1037	G927	K798	TVR
LEU	1	1138	+	K1111	G1038	E931	E799	ALA
LEU	1	1138	+	G1112	C1039	E931	E799	SER
TVR	1	1138	+	T1113	Y1040	H944	M809	ALA
LEU	1	1138	+	A1116	S1041	E945	R810	SER
GLY	1	1138	+	I1117	C1042	S946	E811	C691
THR	1	1138	+	D1118	G1045	S946	N812	E993
GLY	1	1138	+	P1119	F1120	R949	C818	Q996

SER
LYS
MET
TRP
LEU
ALA
ALA
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GLY
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- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
MAG3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	811329	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.085	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	175.664, 175.664, 175.664	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	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: NAG

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	0.16	0/3186	0.31	0/4300
1	B	0.27	0/3435	0.45	1/4640 (0.0%)
All	All	0.22	0/6621	0.39	1/8940 (0.0%)

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	1107	PRO	CA-N-CD	-6.78	102.51	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	LYS	Peptide
1	B	792	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	3119	0	3055	42	0
1	B	3374	0	3243	94	0
2	C	42	0	37	1	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
All	All	6563	0	6361	130	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 130 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1039:CYS:CB	1:B:1117:ILE:HD11	1.87	1.03
1:B:1039:CYS:HB2	1:B:1117:ILE:HD11	1.52	0.92
1:B:1039:CYS:HB2	1:B:1117:ILE:CD1	2.08	0.84
1:B:1039:CYS:SG	1:B:1117:ILE:HD11	2.20	0.80
1:A:511:CYS:HB2	1:B:1133:VAL:HG11	1.62	0.80

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	410/1064 (38%)	394 (96%)	15 (4%)	1 (0%)	43 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	440/1064 (41%)	406 (92%)	31 (7%)	3 (1%)	18	47
All	All	850/2128 (40%)	800 (94%)	46 (5%)	4 (0%)	26	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1121	ASP
1	B	982	PRO
1	A	228	SER
1	B	980	SER

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	352/912 (39%)	332 (94%)	20 (6%)	18	45
1	B	381/912 (42%)	359 (94%)	22 (6%)	18	45
All	All	733/1824 (40%)	691 (94%)	42 (6%)	20	45

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	828	VAL
1	B	960	ILE
1	B	842	VAL
1	B	893	ASP
1	B	981	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1043	ASN
1	B	986	ASN

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Mol	Chain	Res	Type
1	A	408	HIS
1	A	401	GLN
1	B	817	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

3 monosaccharides are modelled in this entry.

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	$\# Z > 2$
2	NAG	C	1	1,2	14,14,15	0.45	0	17,19,21	1.53	3 (17%)
2	NAG	C	2	2	14,14,15	0.39	0	17,19,21	1.35	2 (11%)
2	NAG	C	3	2	14,14,15	0.32	0	17,19,21	0.91	1 (5%)

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
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	NAG	C	3	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	C1-O5-C5	-3.77	107.14	112.19
2	C	1	NAG	C4-C3-C2	3.26	115.79	111.02
2	C	1	NAG	C3-C4-C5	2.86	115.41	110.23
2	C	1	NAG	C1-O5-C5	-2.75	108.50	112.19
2	C	3	NAG	C2-N2-C7	-2.38	119.71	122.90

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

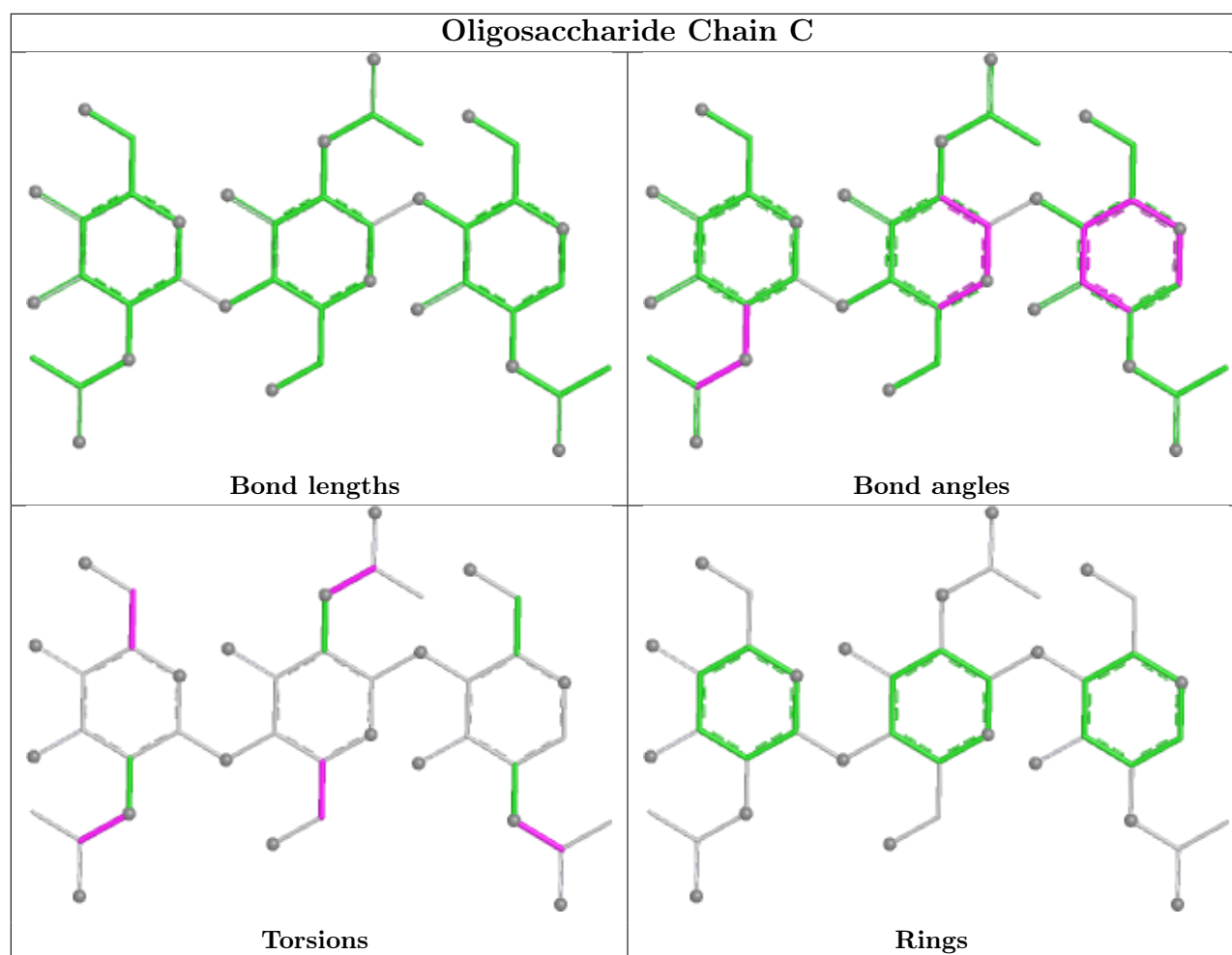
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	C	3	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	3	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	NAG	B	1301	1	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	A	1301	1	14,14,15	0.24	0	17,19,21	0.41	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	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

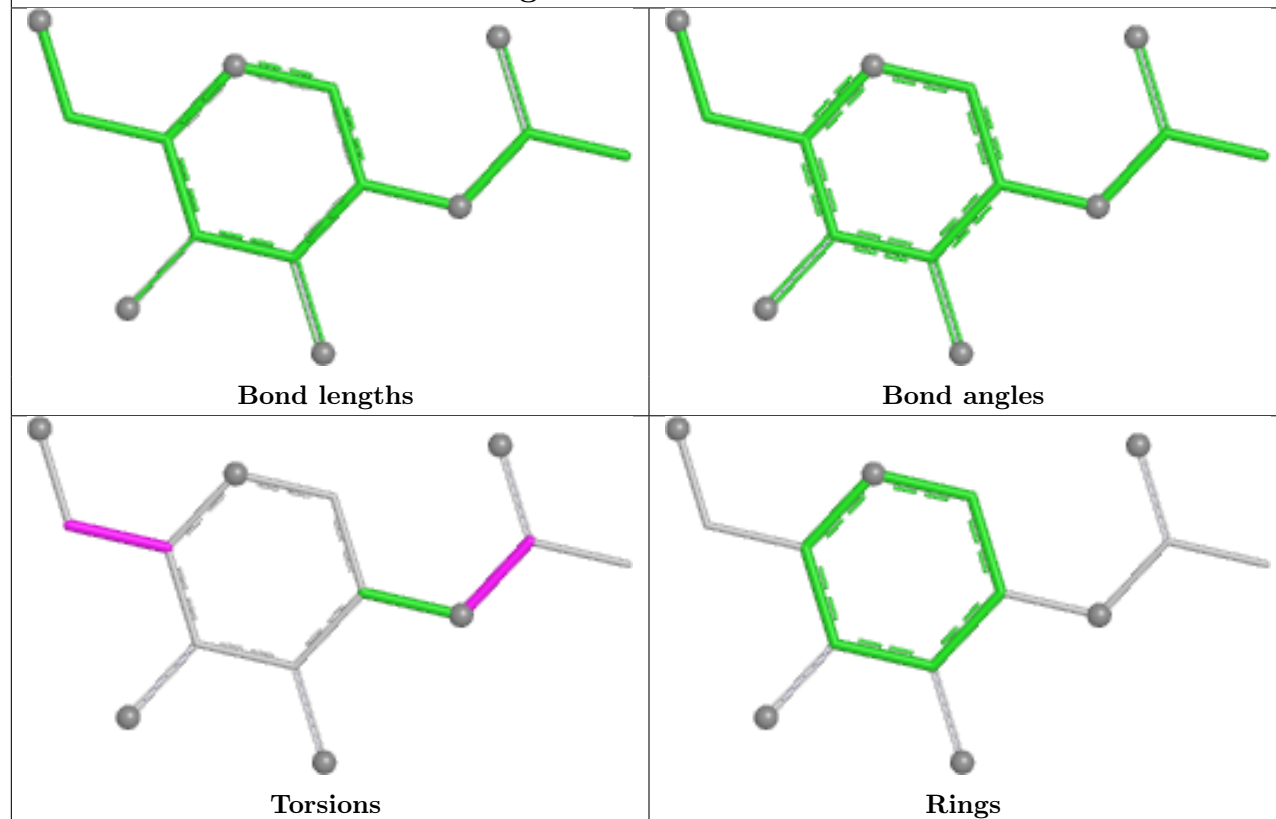
Mol	Chain	Res	Type	Atoms
3	B	1301	NAG	O5-C5-C6-O6
3	B	1301	NAG	C4-C5-C6-O6
3	A	1301	NAG	C8-C7-N2-C2
3	A	1301	NAG	O7-C7-N2-C2
3	B	1301	NAG	C8-C7-N2-C2

There are no ring outliers.

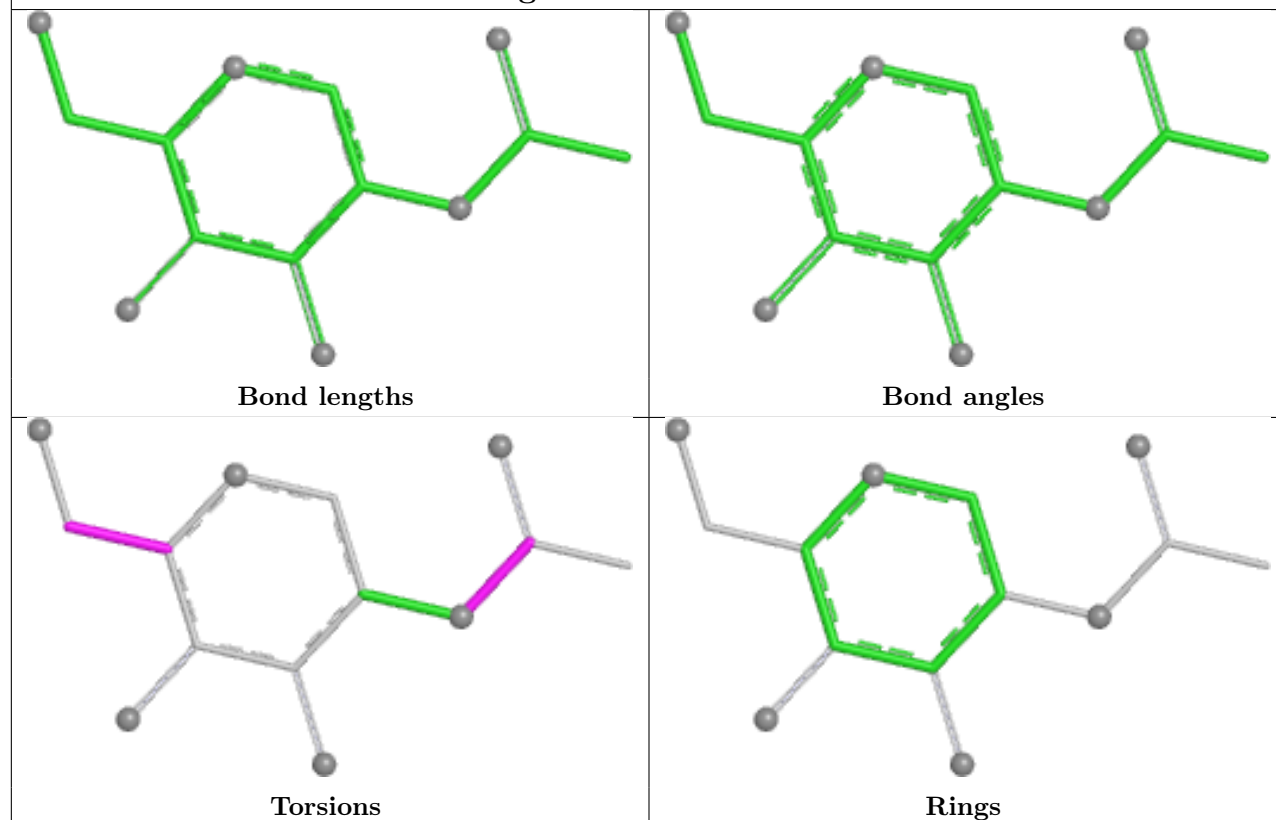
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand NAG B 1301



Ligand NAG A 1301



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.

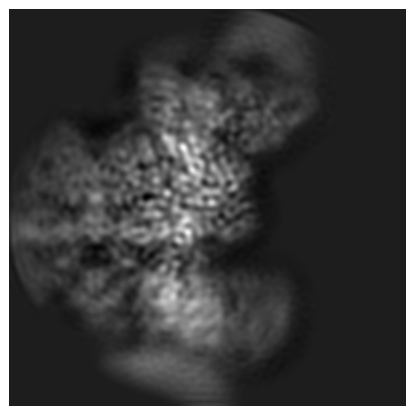
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64803. These allow visual inspection of the internal detail of the map and identification of artifacts.

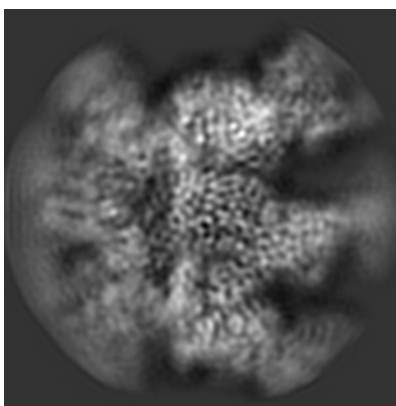
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

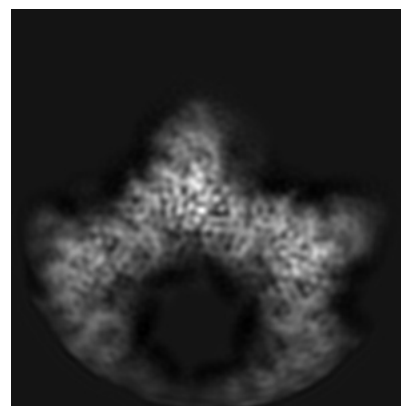
6.1.1 Primary map



X

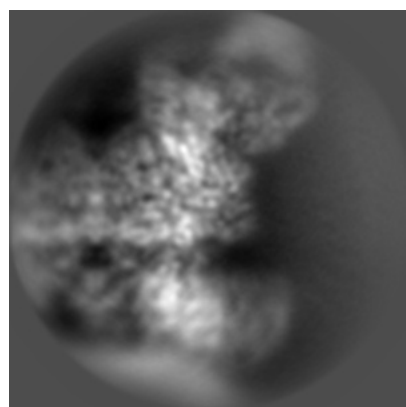


Y

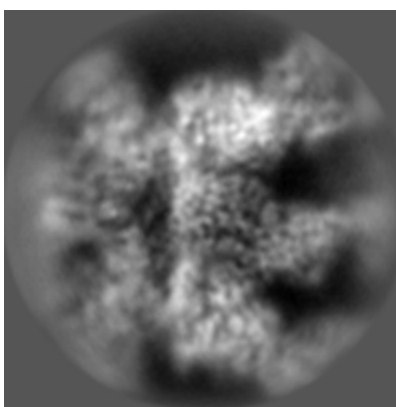


Z

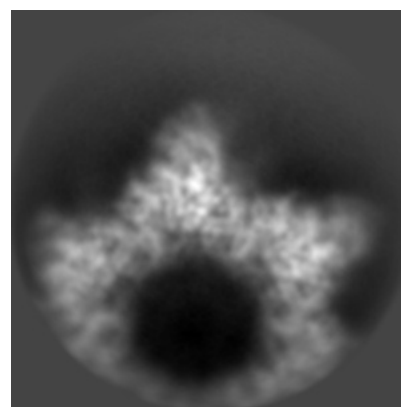
6.1.2 Raw map



X



Y

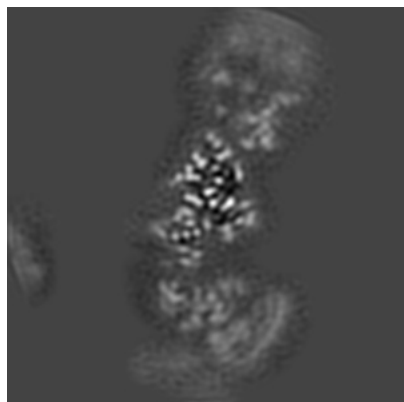


Z

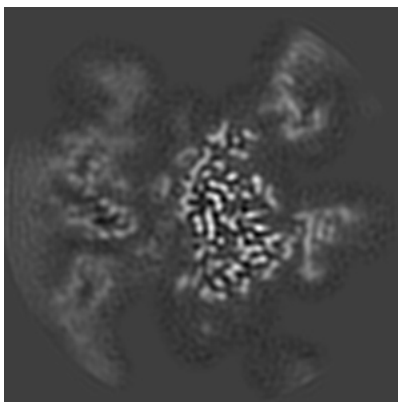
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

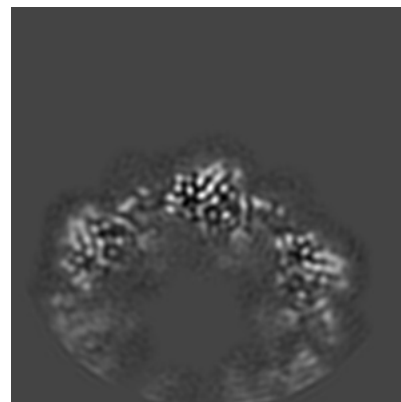
6.2.1 Primary map



X Index: 80

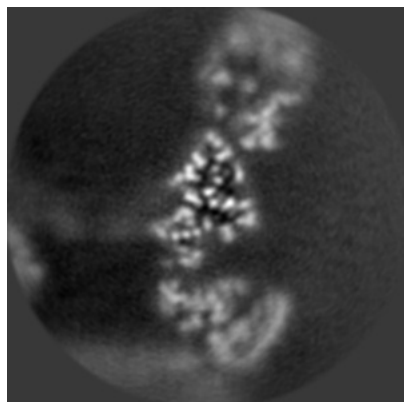


Y Index: 80

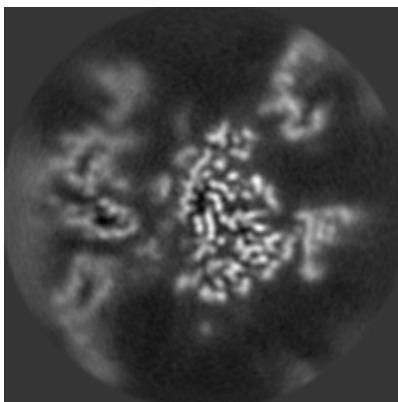


Z Index: 80

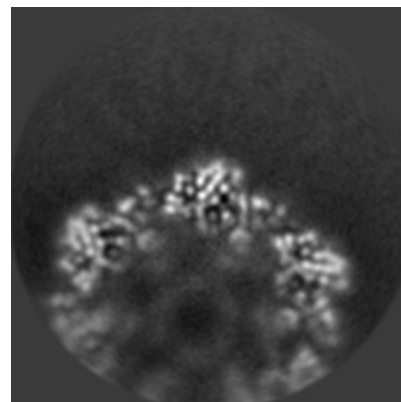
6.2.2 Raw map



X Index: 80



Y Index: 80

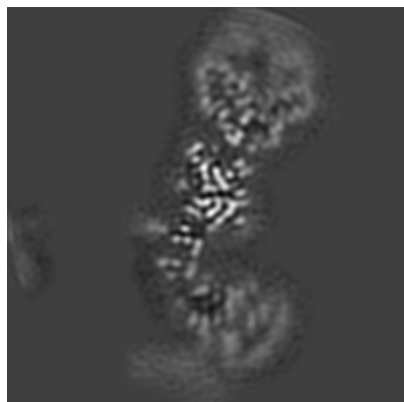


Z Index: 80

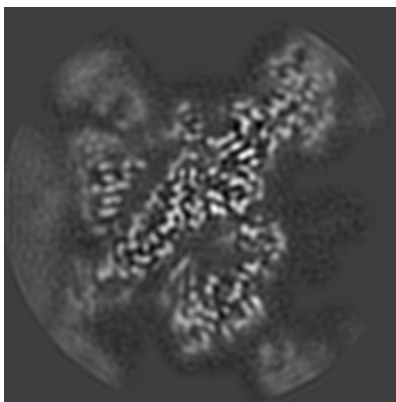
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

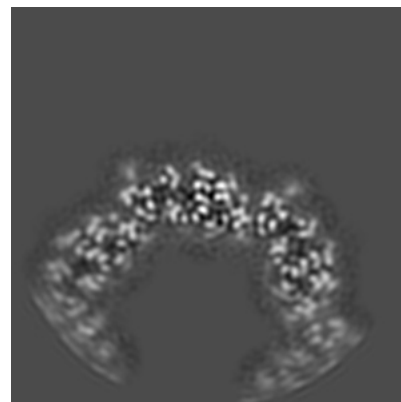
6.3.1 Primary map



X Index: 75

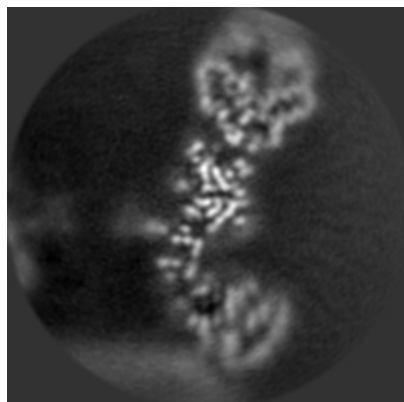


Y Index: 72

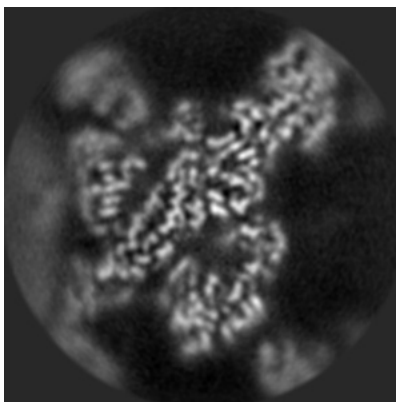


Z Index: 93

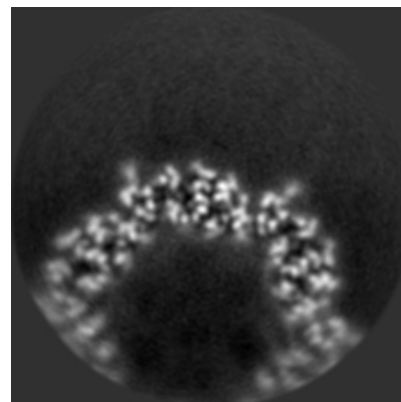
6.3.2 Raw map



X Index: 75



Y Index: 72

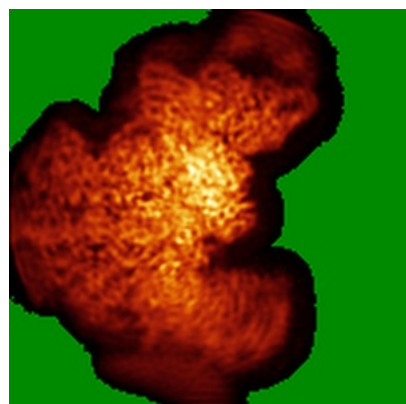


Z Index: 93

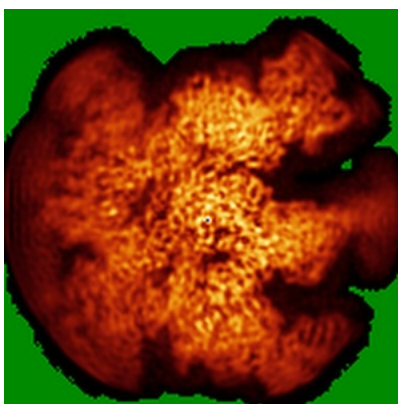
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

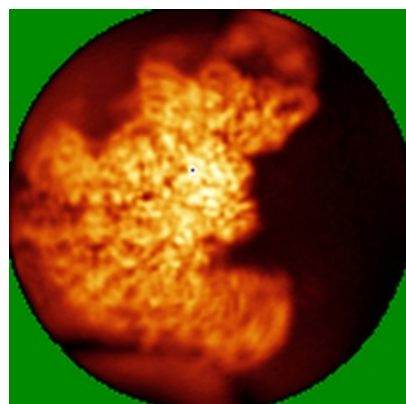


Y

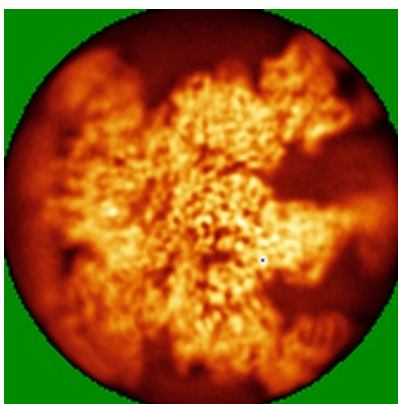


Z

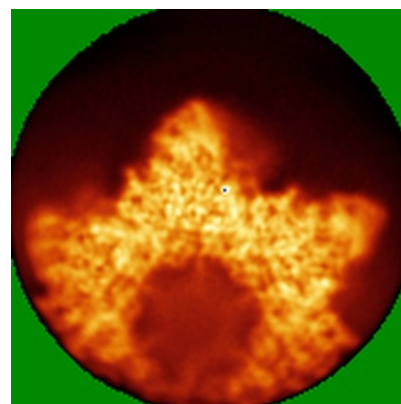
6.4.2 Raw map



X



Y

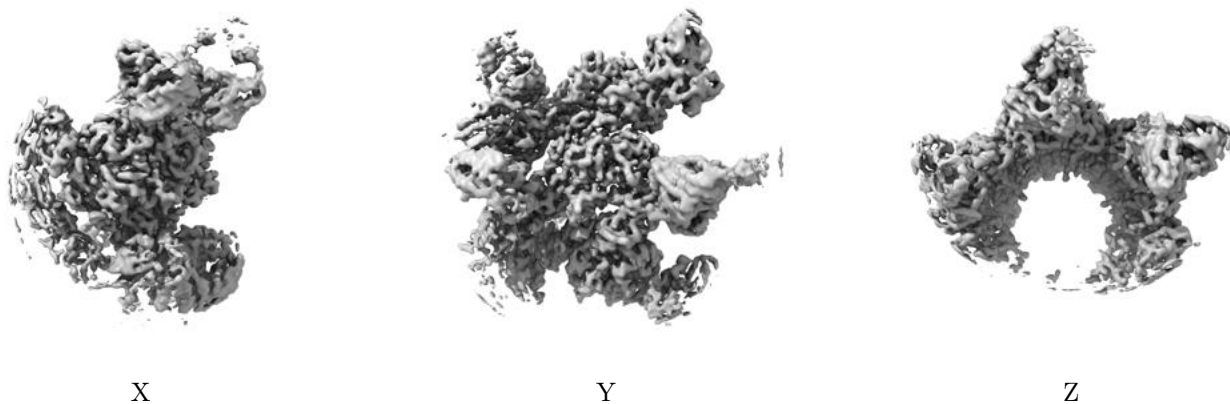


Z

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.

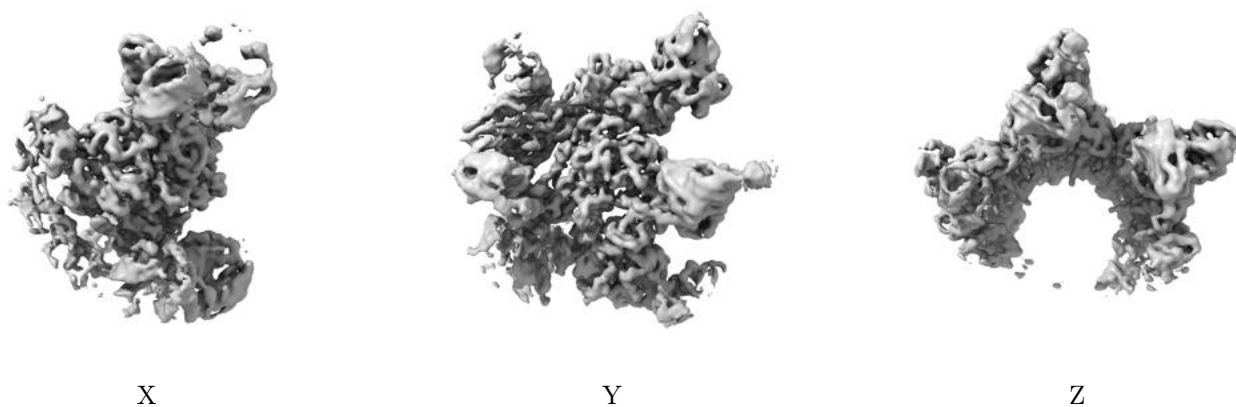
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. 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.

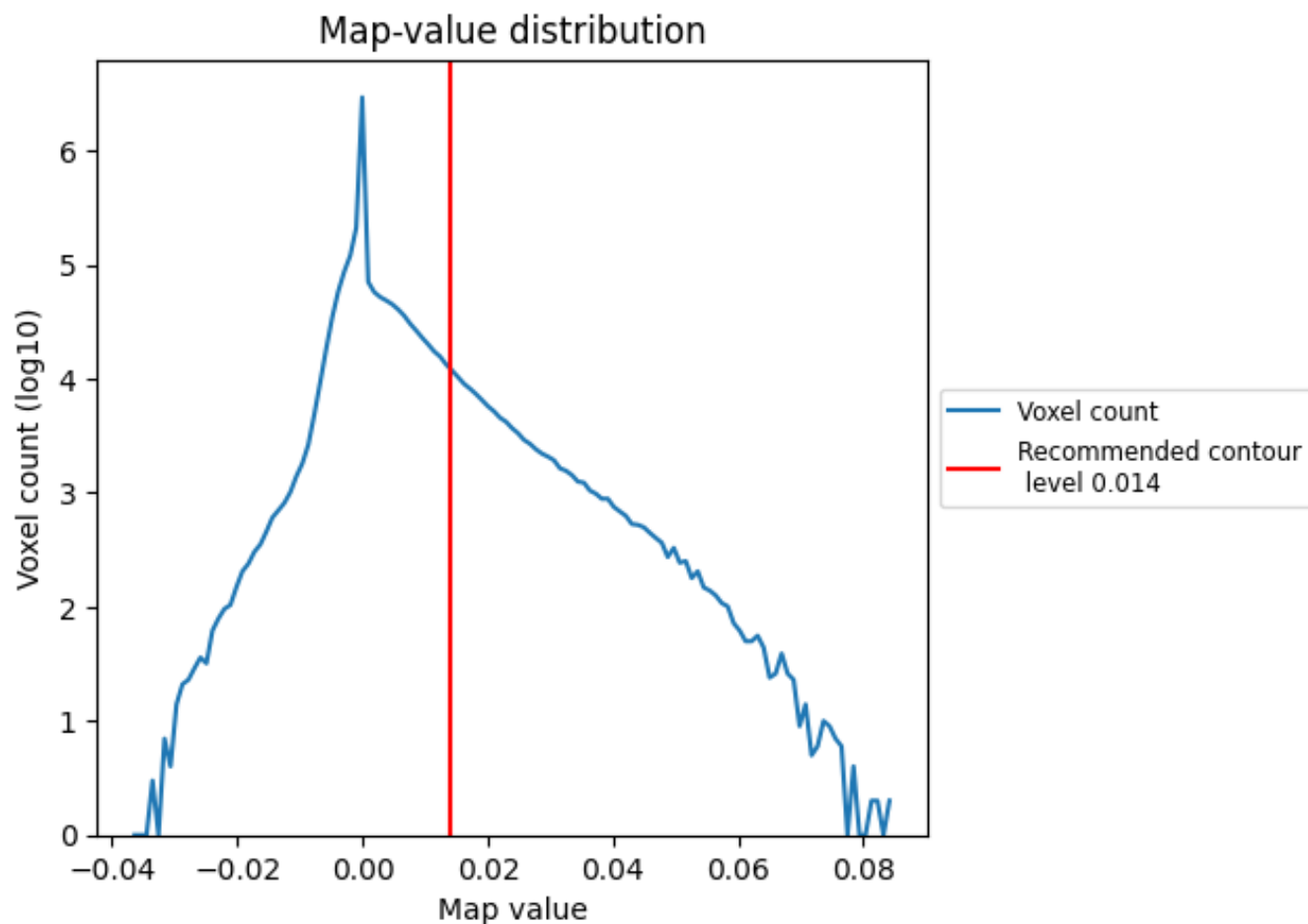
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

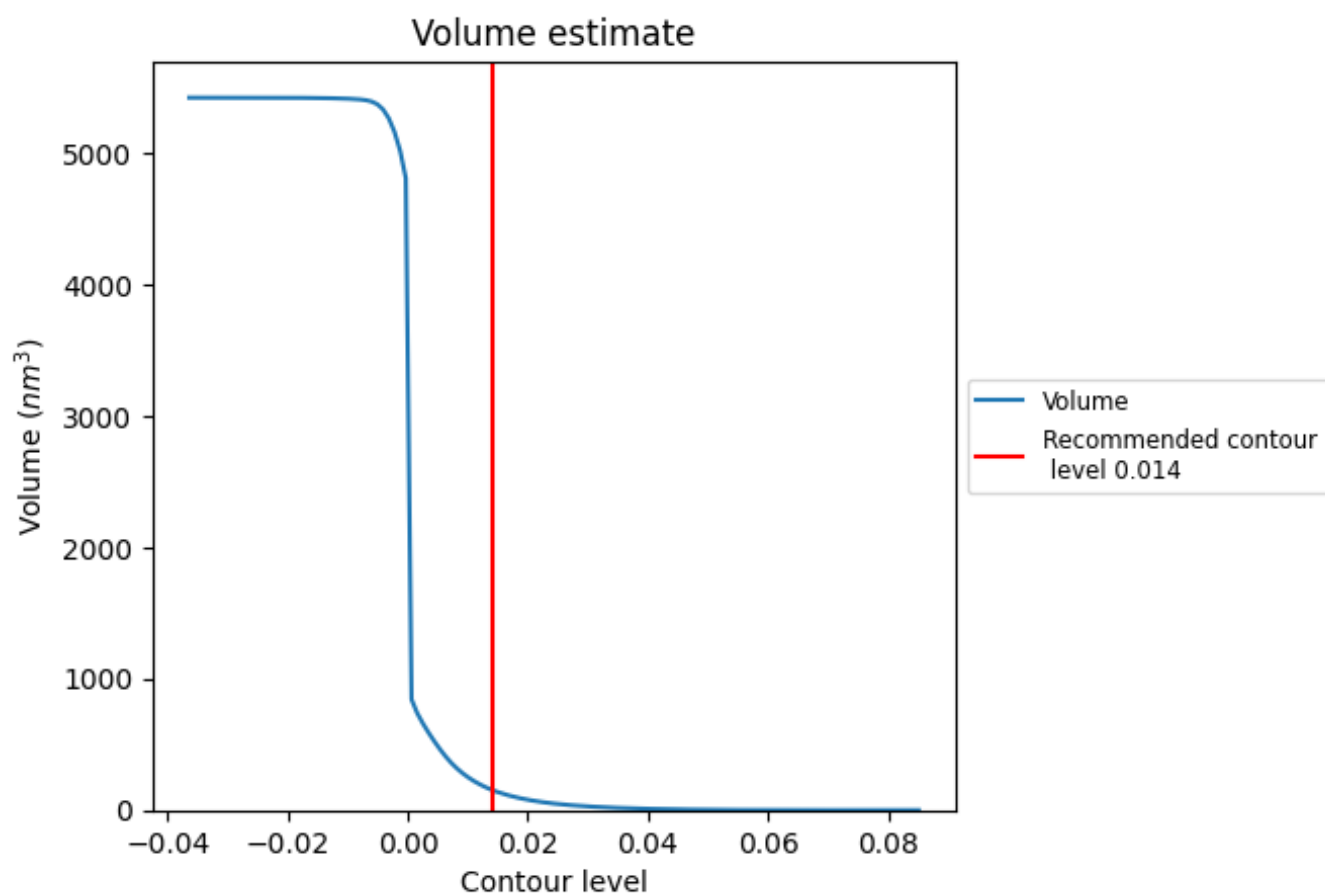
This section contains the results of statistical analysis of the map.

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.

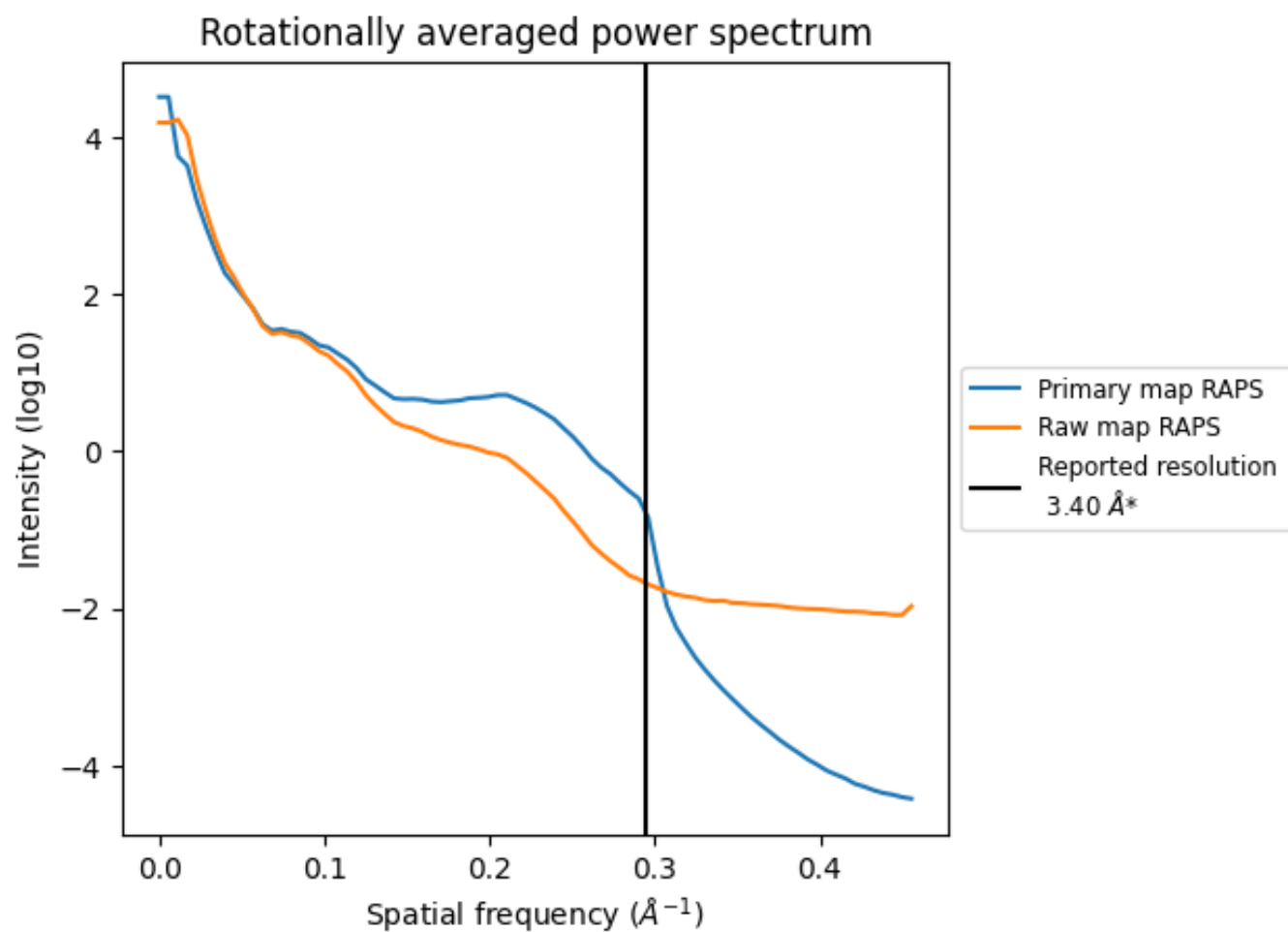
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 154 nm³; this corresponds to an approximate mass of 139 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 ⓘ

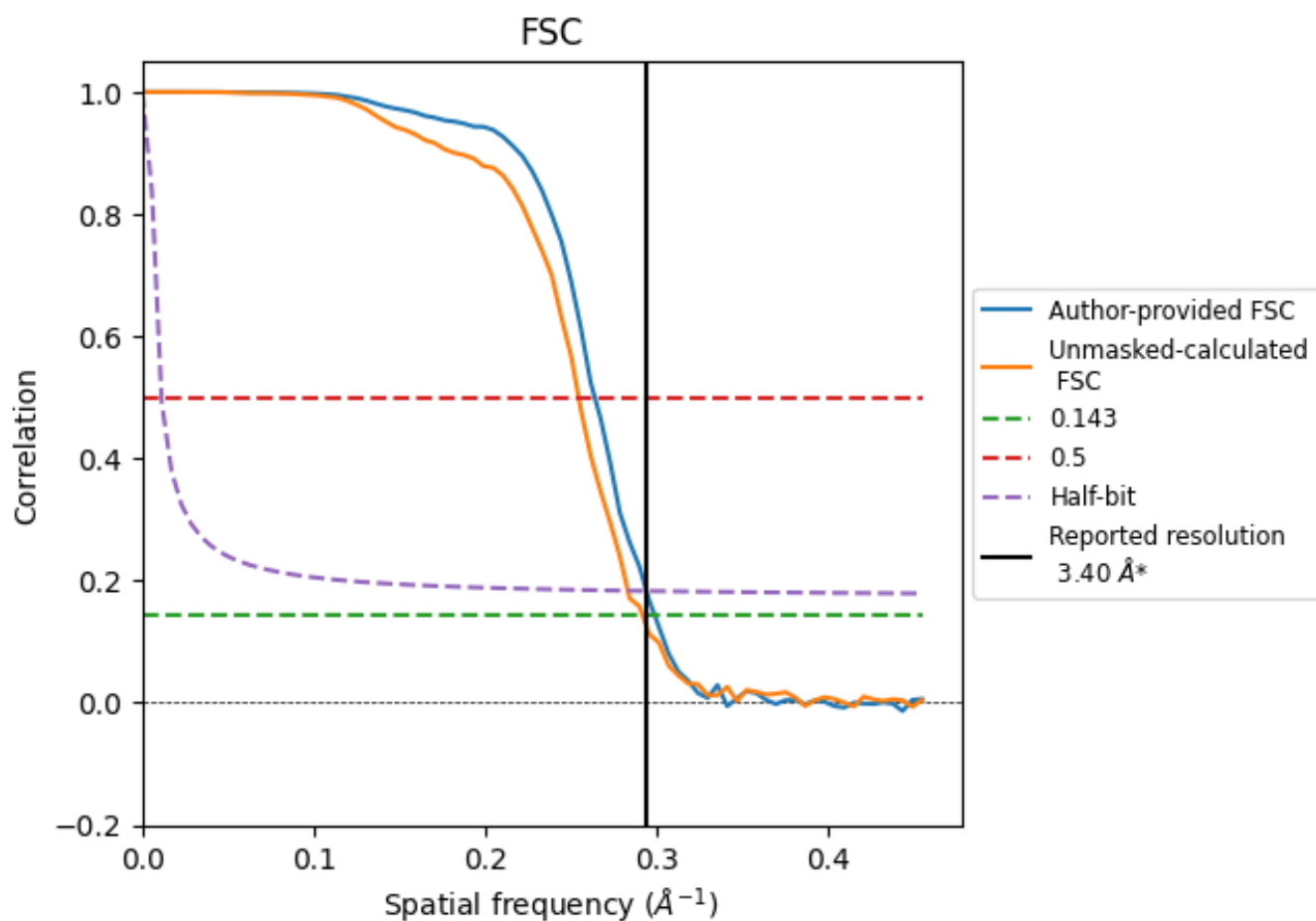


*Reported resolution corresponds to spatial frequency of $0.294 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

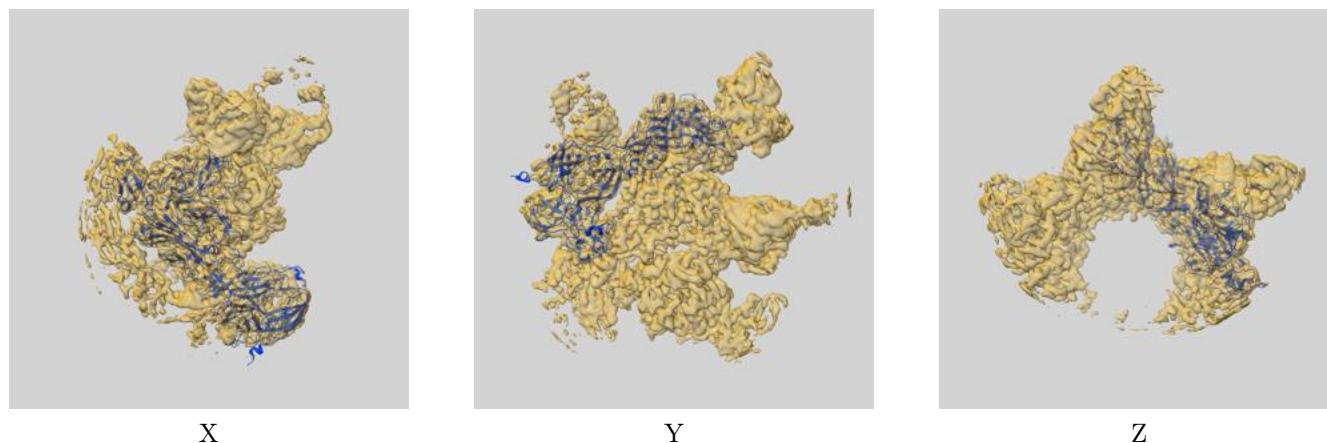
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.34	3.79	3.40
Unmasked-calculated*	3.42	3.92	3.53

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

9 Map-model fit [i](#)

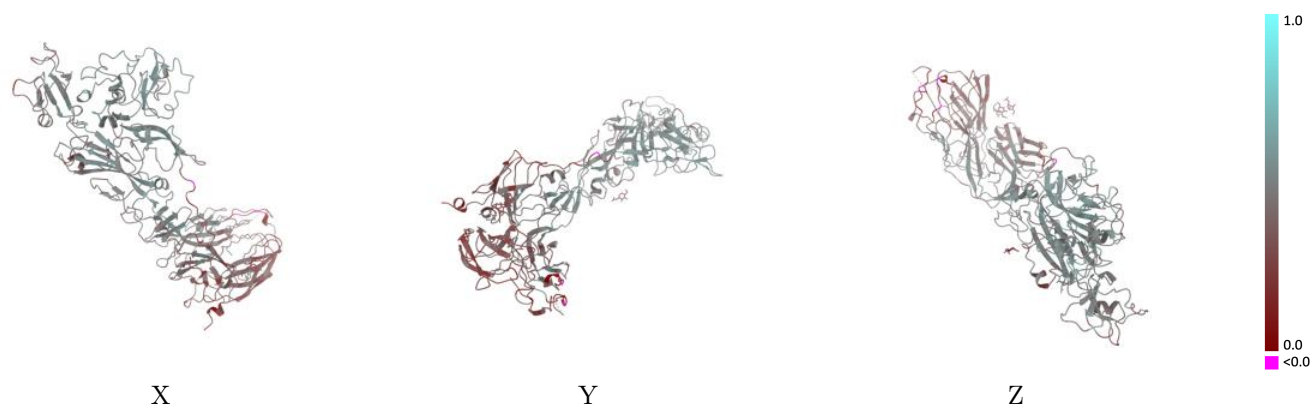
This section contains information regarding the fit between EMDB map EMD-64803 and PDB model 9V6N. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



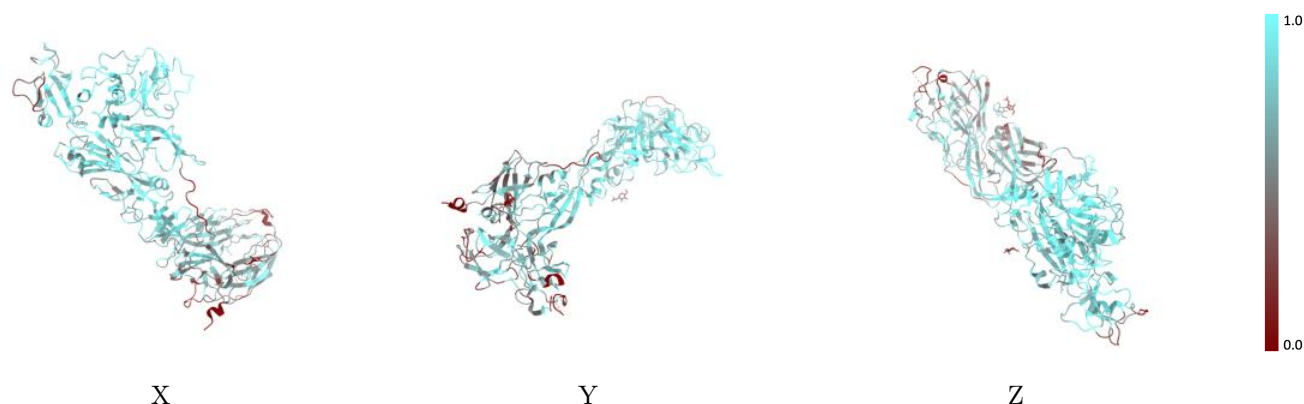
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



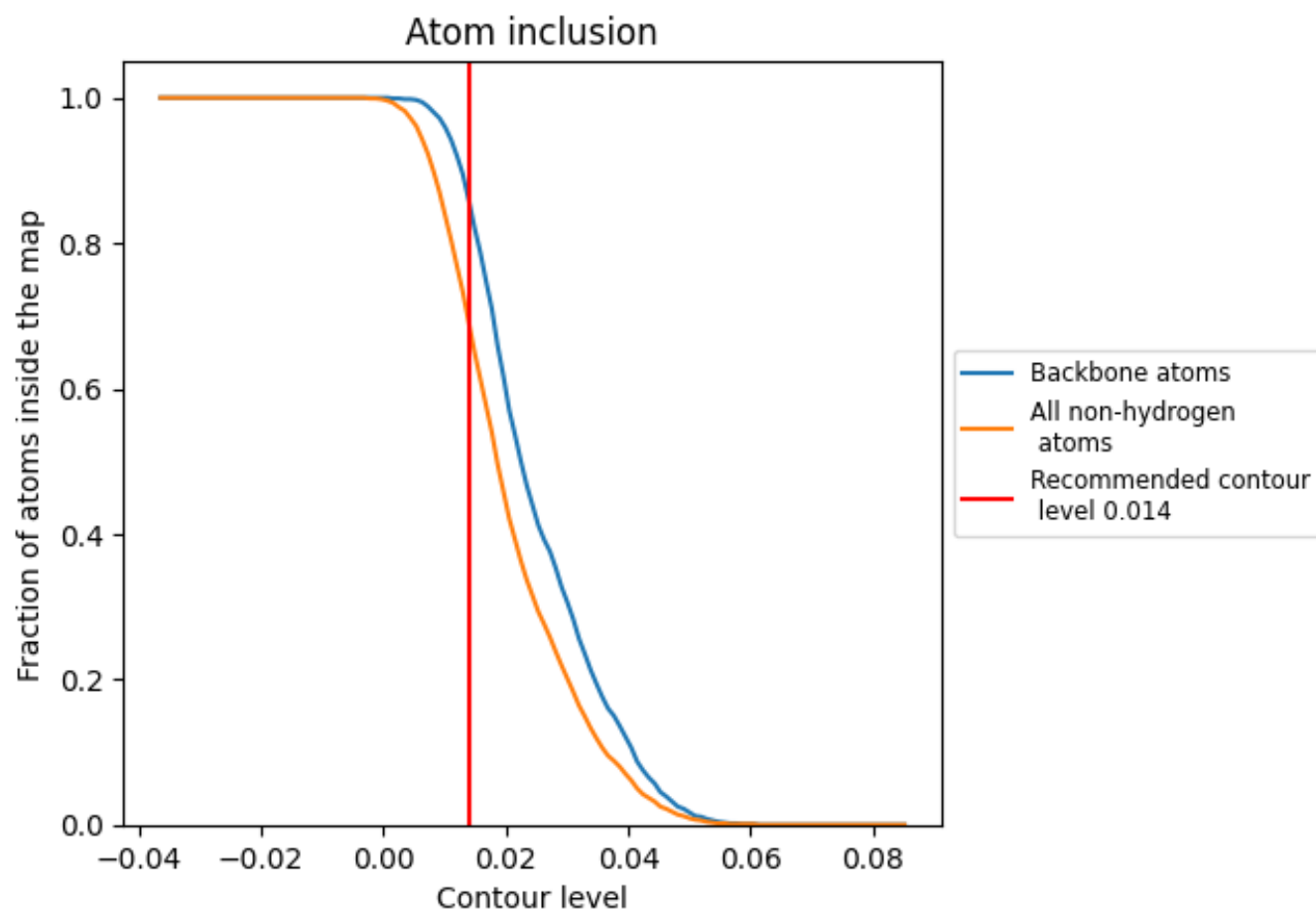
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 69% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6890	0.4290
A	0.7270	0.4590
B	0.6580	0.4030
C	0.4290	0.3370

