



wwPDB EM Validation Summary Report ⓘ

Nov 24, 2021 – 11:22 AM EST

PDB ID : 7SOF
EMDB ID : EMD-25269
Title : SARS-CoV-2 S NTD B.1.617.1 kappa variant S2X303 Local Refinement
Authors : McCallum, M.; Veesler, D.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2021-10-29
Resolution : 3.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.0.dev97
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

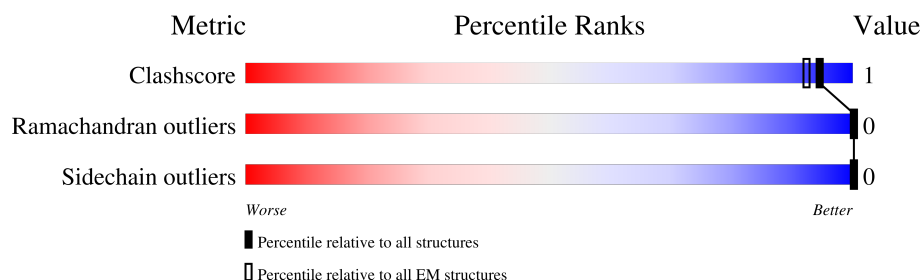
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	L	105	<div> <div>12%</div> <div>98%</div> <div>.</div> </div>
2	H	125	<div> <div>16%</div> <div>100%</div> </div>
3	A	1277	<div> <div>8%</div> <div>19%</div> <div>80%</div> </div>
4	B	3	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3735 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 S2X303 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	105	Total	C	N	O	S	0	0
			730	464	126	138	2		

- Molecule 2 is a protein called S2X303 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	125	Total	C	N	O	S	0	0
			916	598	150	164	4		

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	258	Total	C	N	O	S	0	0
			1966	1294	327	338	7		

There are 85 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	ILE	THR	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	154	LYS	GLU	variant	UNP P0DTC2
A	383	CYS	SER	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	484	GLN	GLU	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	681	ARG	PRO	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	985	CYS	ASP	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2

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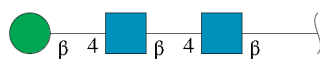
Chain	Residue	Modelled	Actual	Comment	Reference
A	1071	HIS	GLN	variant	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1250	SER	-	expression tag	UNP P0DTC2
A	1251	GLY	-	expression tag	UNP P0DTC2
A	1252	GLY	-	expression tag	UNP P0DTC2
A	1253	LEU	-	expression tag	UNP P0DTC2
A	1254	ASN	-	expression tag	UNP P0DTC2
A	1255	ASP	-	expression tag	UNP P0DTC2
A	1256	ILE	-	expression tag	UNP P0DTC2
A	1257	PHE	-	expression tag	UNP P0DTC2
A	1258	GLU	-	expression tag	UNP P0DTC2
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	GLN	-	expression tag	UNP P0DTC2
A	1261	LYS	-	expression tag	UNP P0DTC2
A	1262	ILE	-	expression tag	UNP P0DTC2
A	1263	GLU	-	expression tag	UNP P0DTC2
A	1264	TRP	-	expression tag	UNP P0DTC2
A	1265	HIS	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	GLY	-	expression tag	UNP P0DTC2
A	1268	SER	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	HIS	-	expression tag	UNP P0DTC2
A	1271	HIS	-	expression tag	UNP P0DTC2
A	1272	HIS	-	expression tag	UNP P0DTC2
A	1273	HIS	-	expression tag	UNP P0DTC2
A	1274	HIS	-	expression tag	UNP P0DTC2
A	1275	HIS	-	expression tag	UNP P0DTC2
A	1276	HIS	-	expression tag	UNP P0DTC2
A	1277	HIS	-	expression tag	UNP P0DTC2

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	84	48	6	30	0
5	A	1	84	48	6	30	0
5	A	1	84	48	6	30	0
5	A	1	84	48	6	30	0
5	A	1	84	48	6	30	0
5	A	1	84	48	6	30	0

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

- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80186	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.899	Depositor
Minimum map value	-3.101	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	431.616, 431.616, 431.616	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.843, 0.843, 0.843	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA

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	L	0.50	0/748	0.58	0/1026
2	H	0.52	0/940	0.56	0/1294
3	A	0.52	0/2023	0.56	0/2761
All	All	0.52	0/3711	0.57	0/5081

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

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	L	730	0	633	1	0
2	H	916	0	871	0	0
3	A	1966	0	1785	7	0
4	B	39	0	34	1	0
5	A	84	0	78	1	0
All	All	3735	0	3401	8	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 1.

The worst 5 of 8 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)
3:A:123:ALA:HB3	4:B:1:NAG:H82	1.90	0.53
3:A:146:HIS:ND1	3:A:147:LYS:N	2.56	0.52
3:A:186:PHE:O	3:A:186:PHE:CG	2.68	0.46
3:A:148:ASN:HA	5:A:1305:NAG:H82	1.98	0.45
3:A:81:ASN:N	3:A:82:PRO:CD	2.81	0.44

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	L	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
2	H	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
3	A	248/1277 (19%)	238 (96%)	10 (4%)	0	100	100
All	All	474/1507 (32%)	458 (97%)	16 (3%)	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	L	61/88 (69%)	61 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	90/110 (82%)	90 (100%)	0	100	100
3	A	189/1112 (17%)	189 (100%)	0	100	100
All	All	340/1310 (26%)	340 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

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	$\# Z > 2$
4	NAG	B	1	4,3	14,14,15	1.15	1 (7%)	17,19,21	1.08	1 (5%)
4	NAG	B	2	4	14,14,15	1.06	1 (7%)	17,19,21	0.97	1 (5%)
4	BMA	B	3	4	11,11,12	1.02	0	15,15,17	0.59	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
4	NAG	B	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1
4	BMA	B	3	4	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	NAG	C1-C2	3.43	1.57	1.52
4	B	2	NAG	C1-C2	2.72	1.56	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	NAG	C8-C7-N2	2.63	120.56	116.10
4	B	2	NAG	C8-C7-N2	2.53	120.39	116.10

There are no chirality outliers.

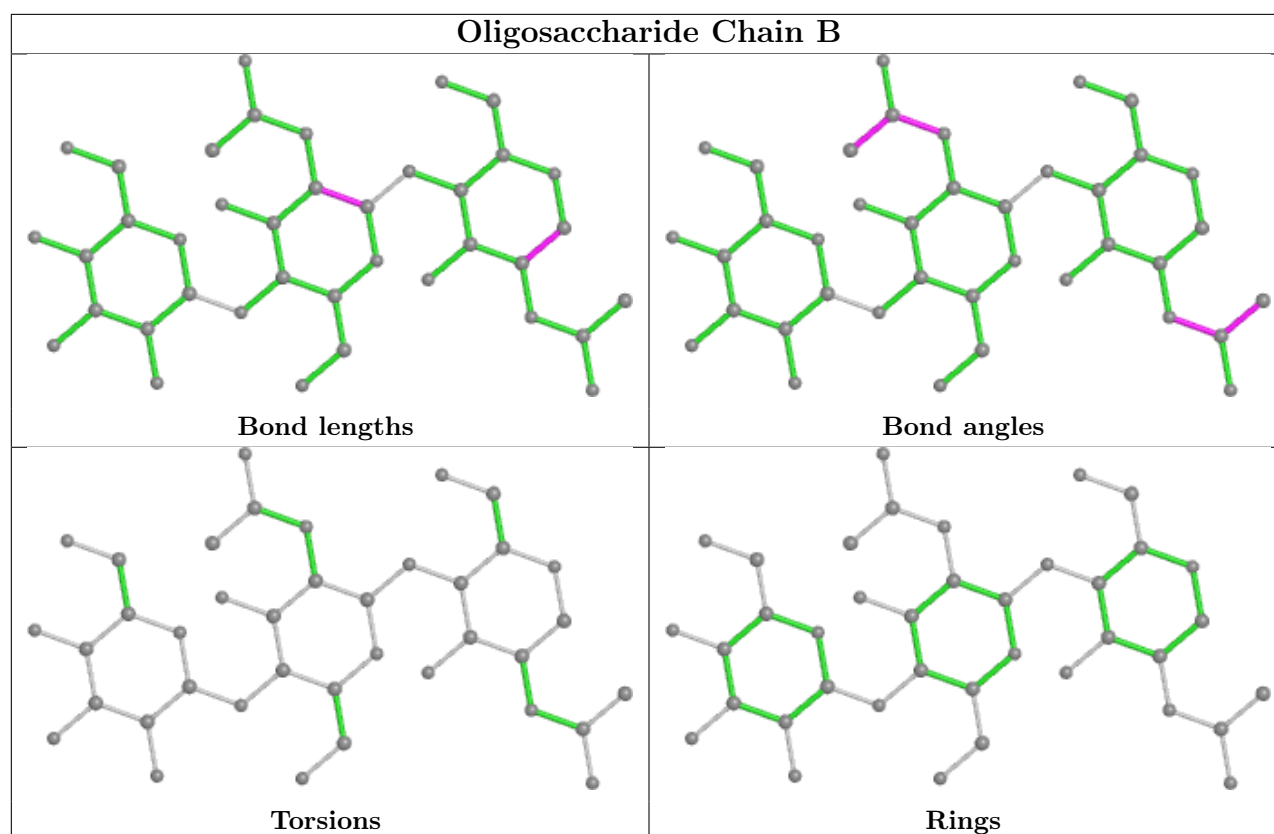
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	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](#)

6 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	$\# Z > 2$
5	NAG	A	1303	3	14,14,15	1.22	1 (7%)	17,19,21	1.08	2 (11%)
5	NAG	A	1302	3	14,14,15	1.14	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	A	1304	3	14,14,15	1.18	1 (7%)	17,19,21	1.06	1 (5%)
5	NAG	A	1306	3	14,14,15	1.14	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	A	1301	3	14,14,15	1.12	1 (7%)	17,19,21	1.05	1 (5%)
5	NAG	A	1305	3	14,14,15	1.21	1 (7%)	17,19,21	1.12	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
5	NAG	A	1303	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1302	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1304	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1306	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1301	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1305	3	-	0/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1305	NAG	C1-C2	3.48	1.57	1.52
5	A	1304	NAG	C1-C2	3.41	1.57	1.52
5	A	1306	NAG	C1-C2	3.29	1.57	1.52
5	A	1303	NAG	C1-C2	3.27	1.57	1.52
5	A	1302	NAG	C1-C2	3.24	1.57	1.52

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1305	NAG	C8-C7-N2	2.78	120.80	116.10
5	A	1306	NAG	C8-C7-N2	2.49	120.31	116.10
5	A	1303	NAG	C2-N2-C7	-2.48	119.38	122.90
5	A	1304	NAG	C8-C7-N2	2.45	120.24	116.10
5	A	1301	NAG	C8-C7-N2	2.44	120.23	116.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1305	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

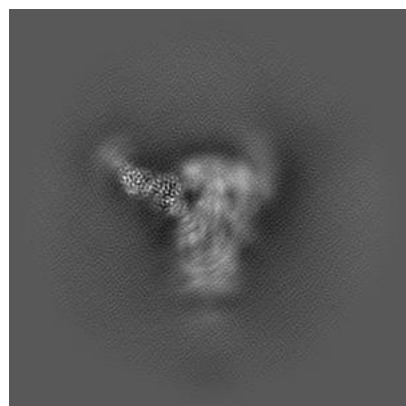
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25269. These allow visual inspection of the internal detail of the map and identification of artifacts.

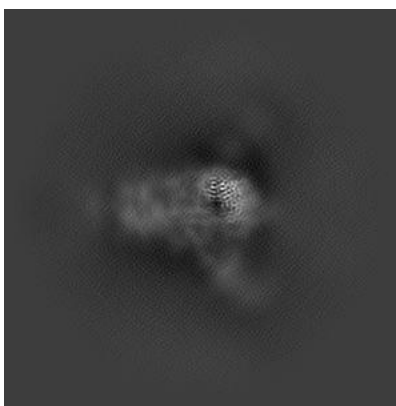
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

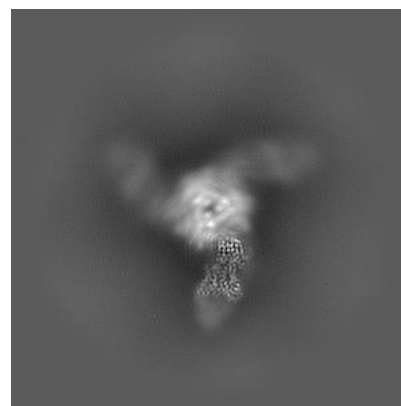
6.1.1 Primary map



X

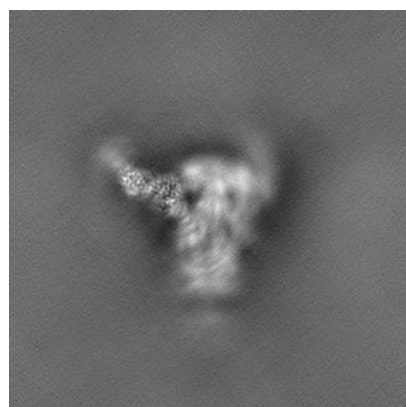


Y

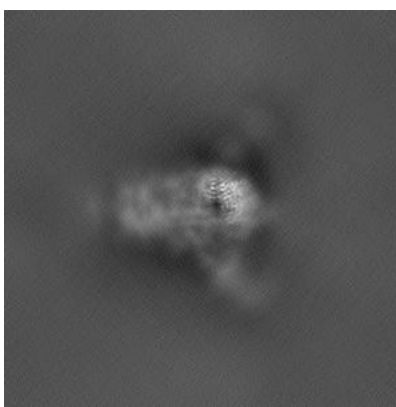


Z

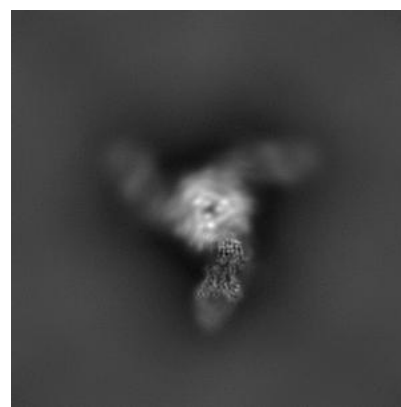
6.1.2 Raw map



X



Y

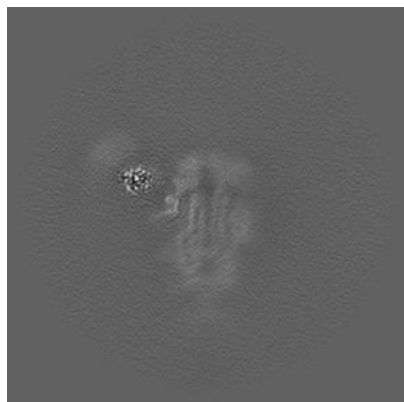


Z

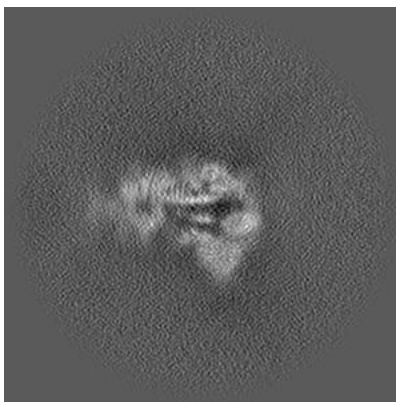
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 256



Y Index: 256

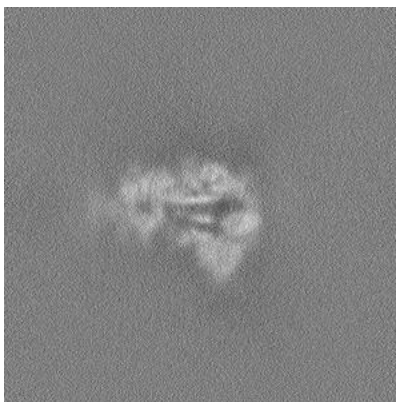


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

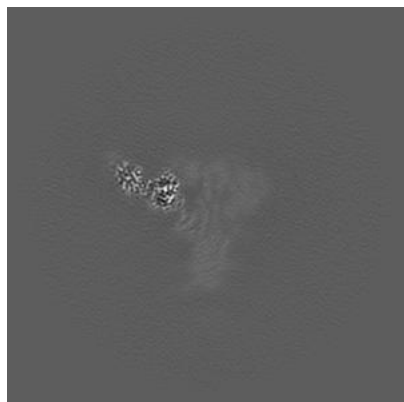


Z Index: 256

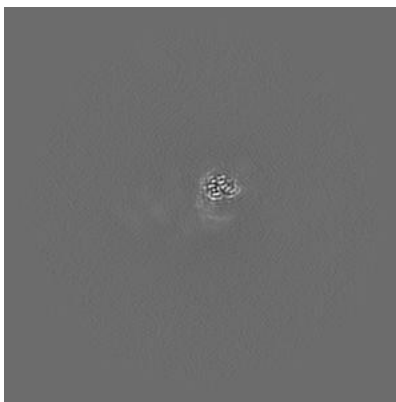
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

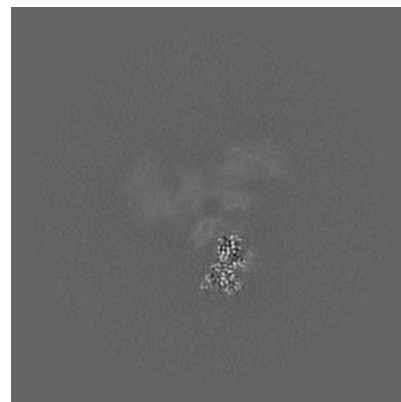
6.3.1 Primary map



X Index: 282

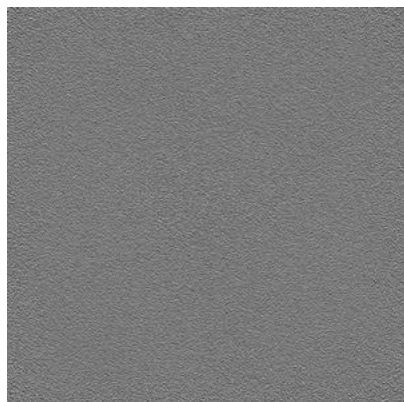


Y Index: 208

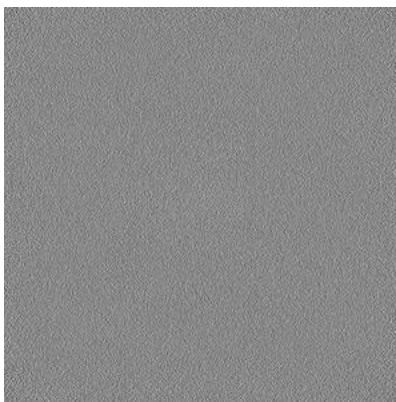


Z Index: 283

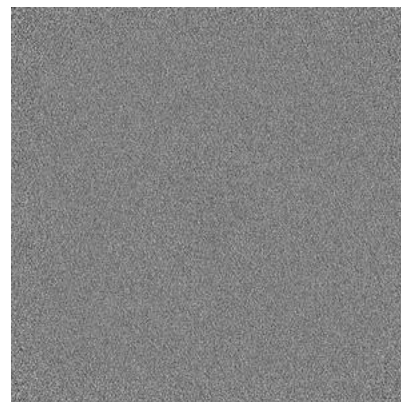
6.3.2 Raw map



X Index: 0



Y Index: 0

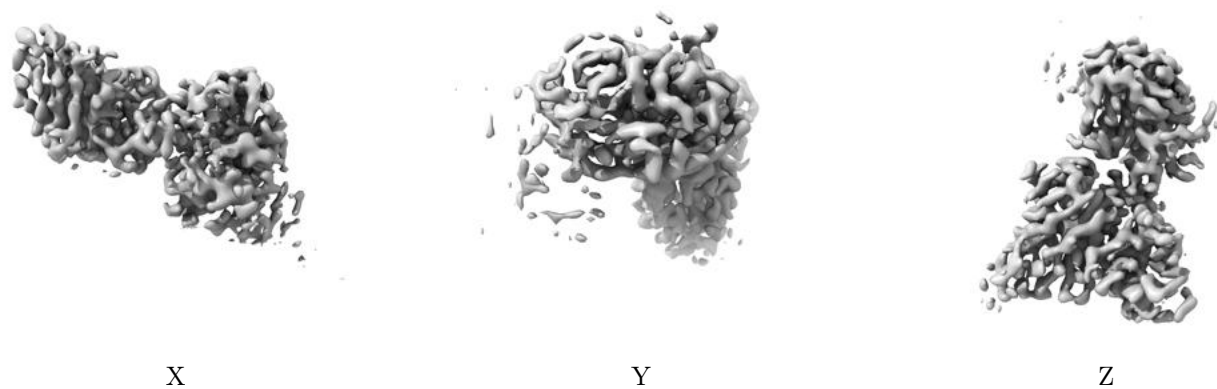


Z Index: 0

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

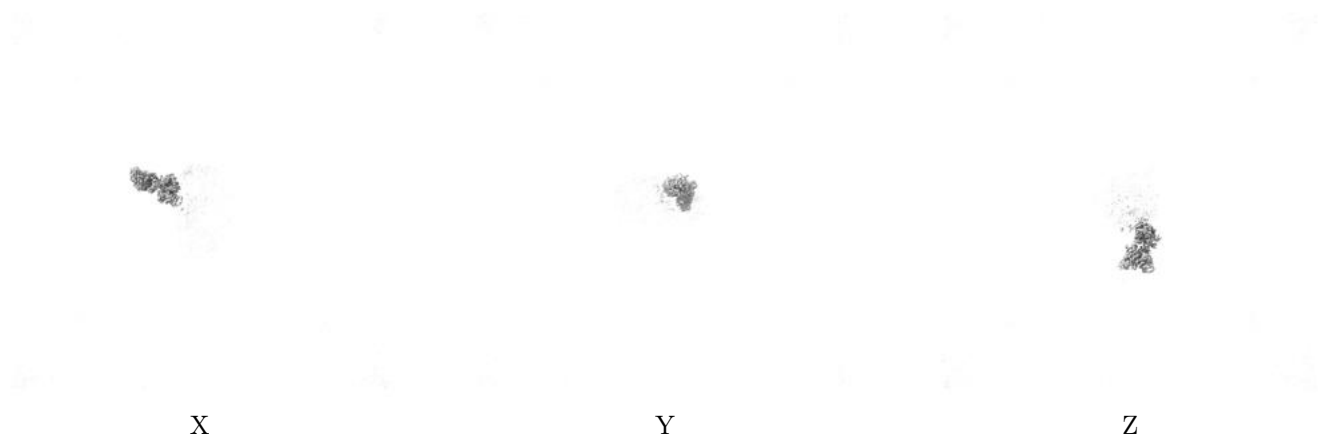
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

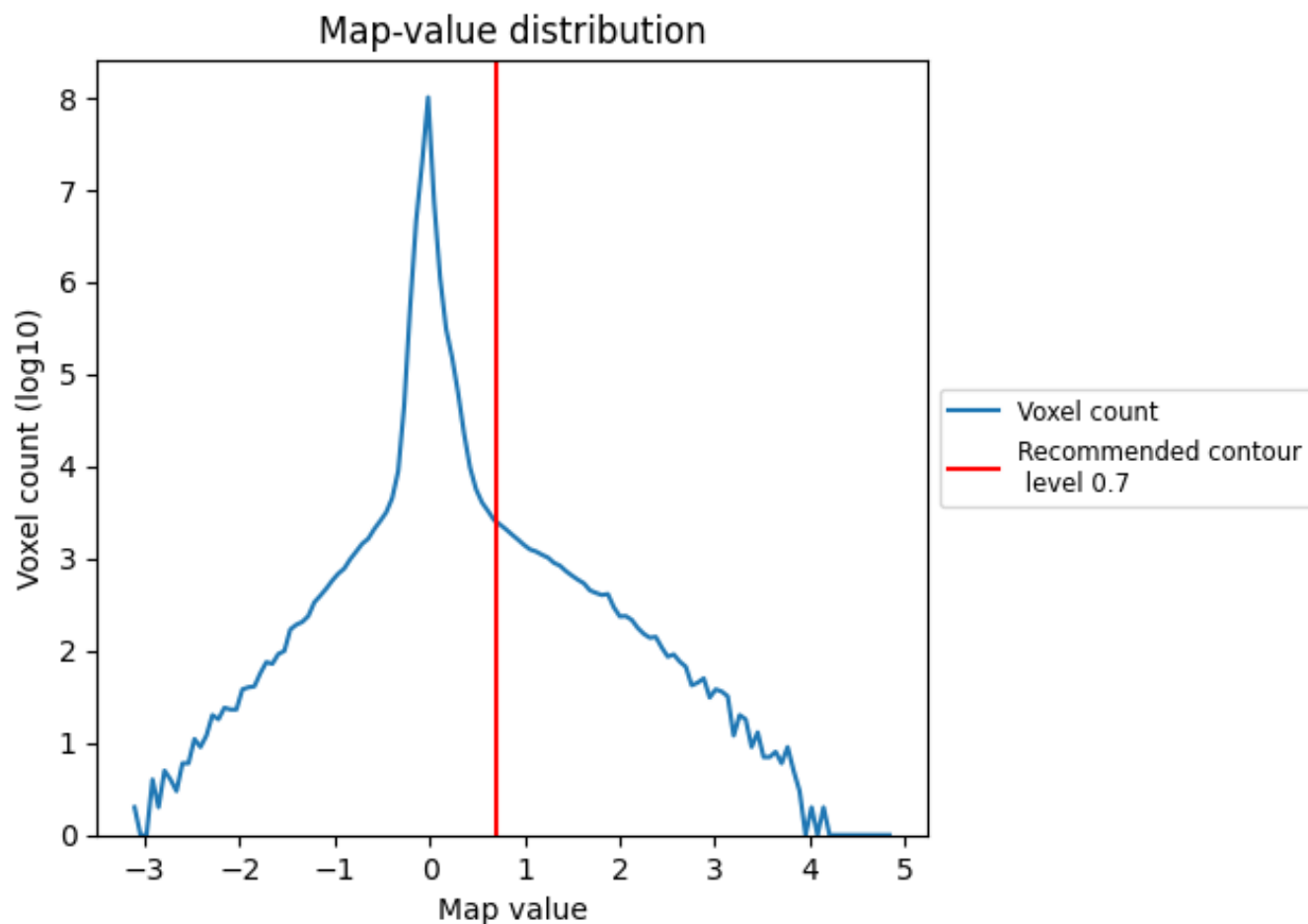
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

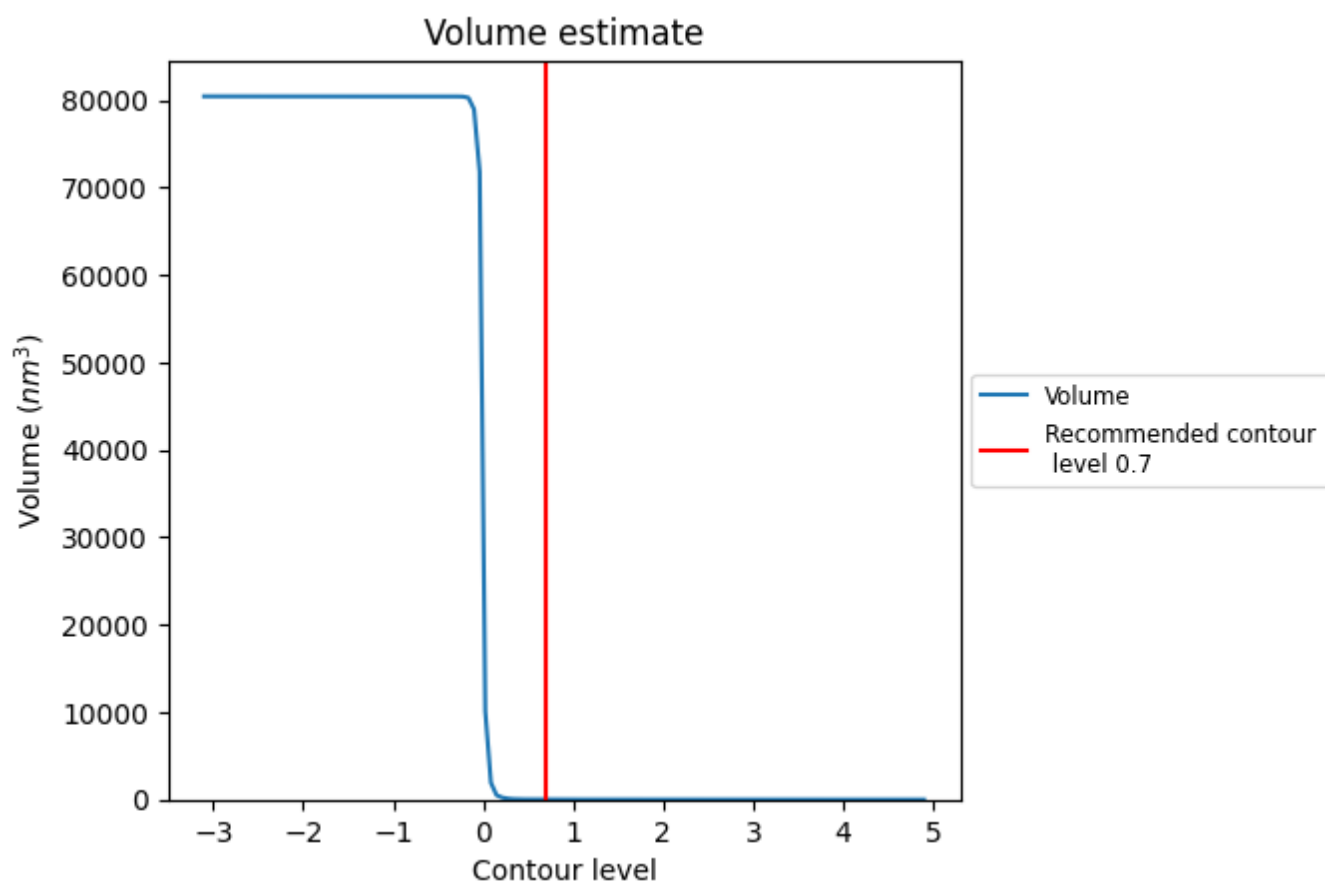
This section contains the results of statistical analysis of the map.

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.

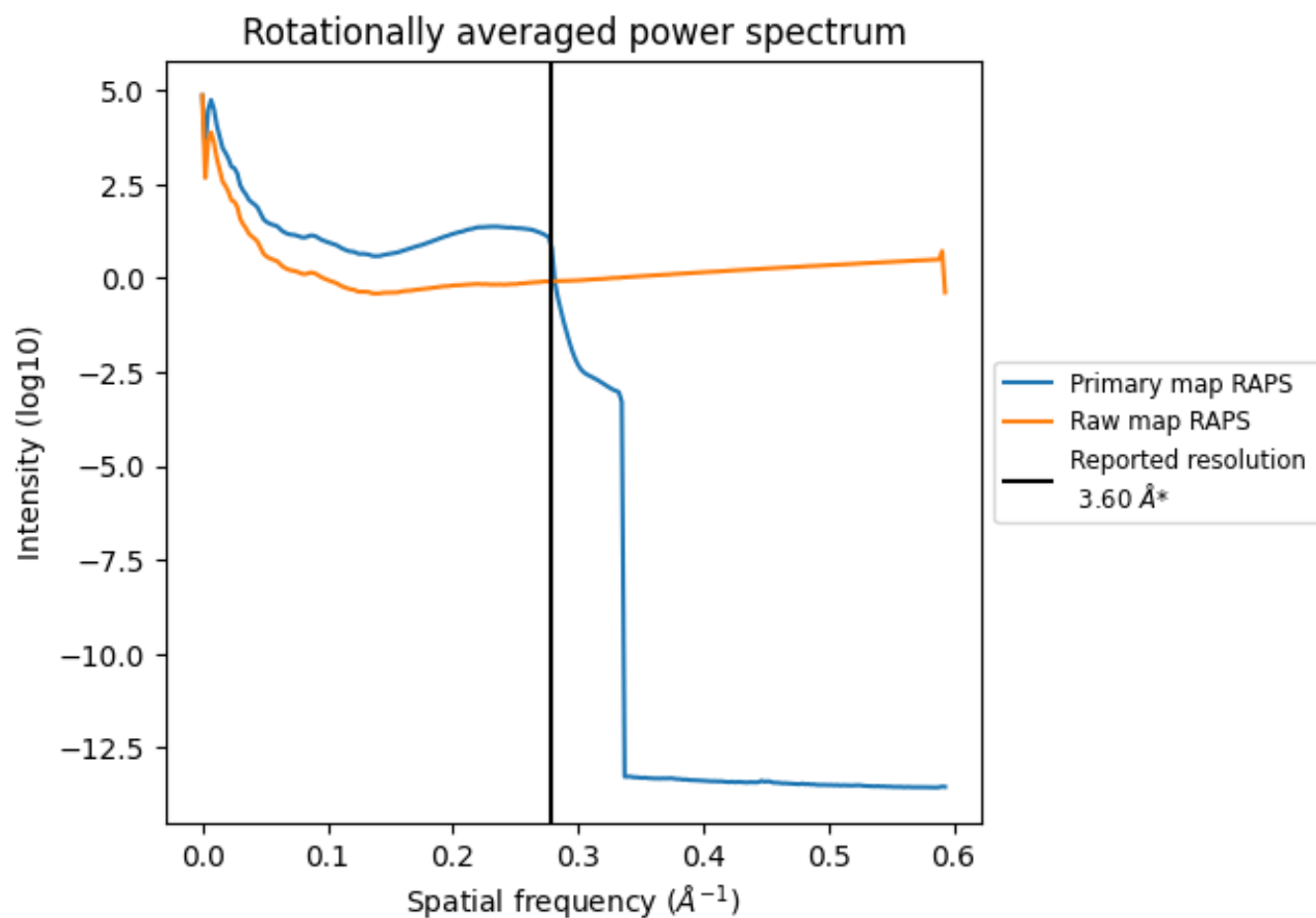
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 14 nm³; this corresponds to an approximate mass of 13 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 ⓘ

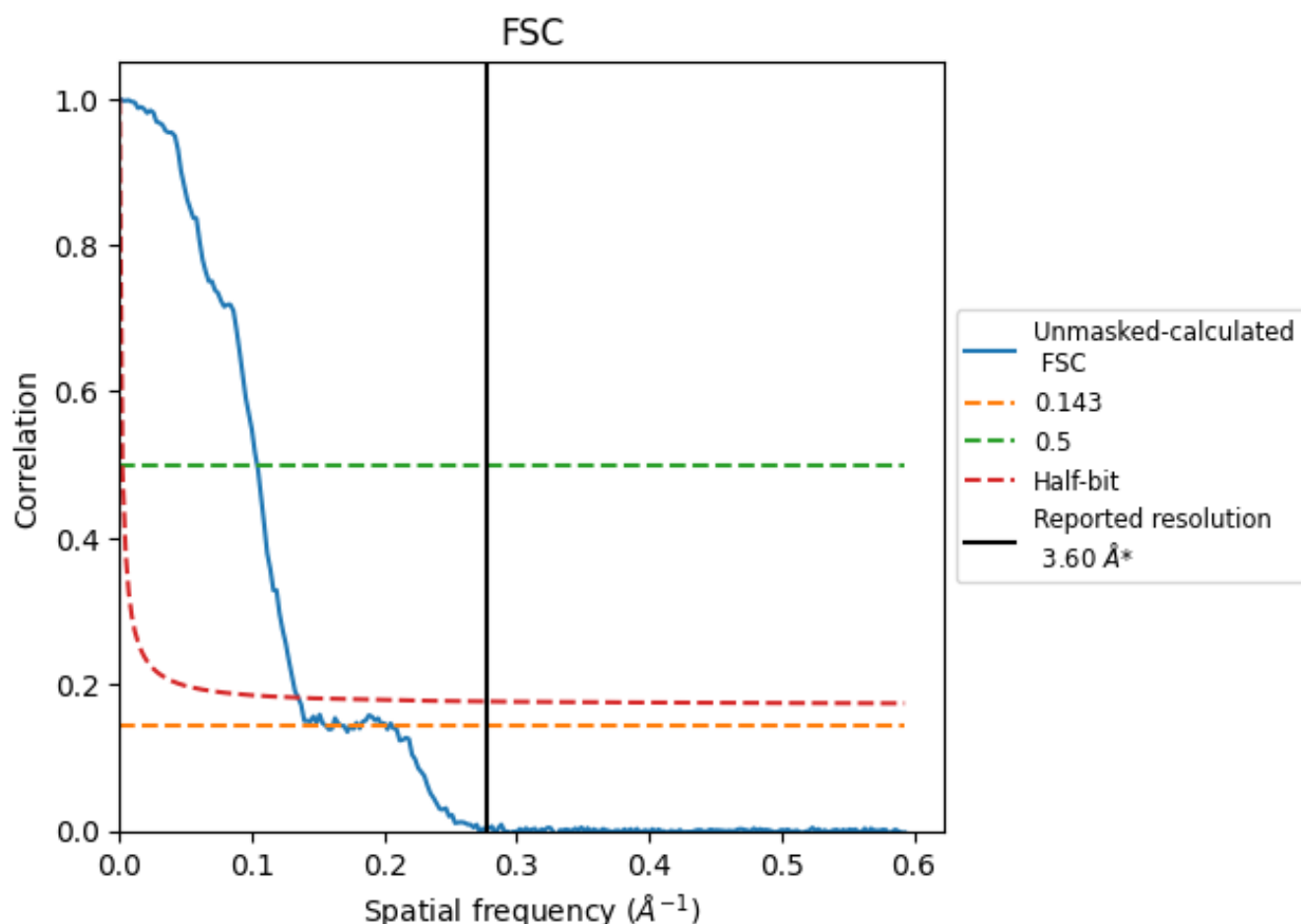


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

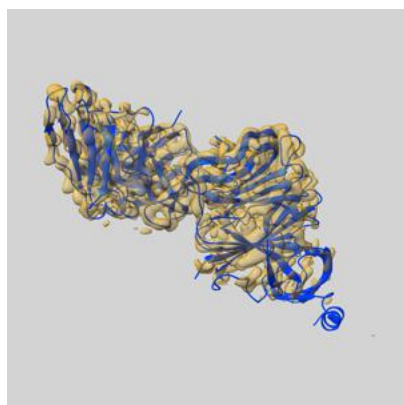
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.41	9.62	7.41

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.41 differs from the reported value 3.6 by more than 10 %

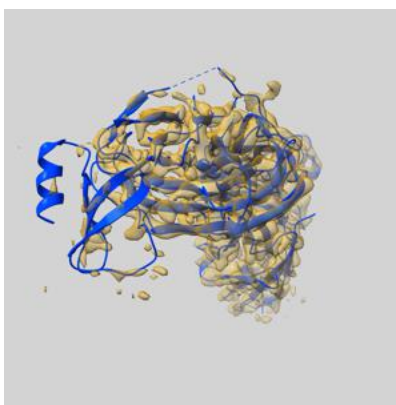
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25269 and PDB model 7SOF. Per-residue inclusion information can be found in section [3](#) on page [7](#).

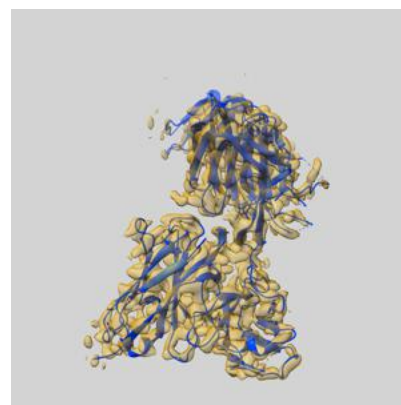
9.1 Map-model overlay [i](#)



X



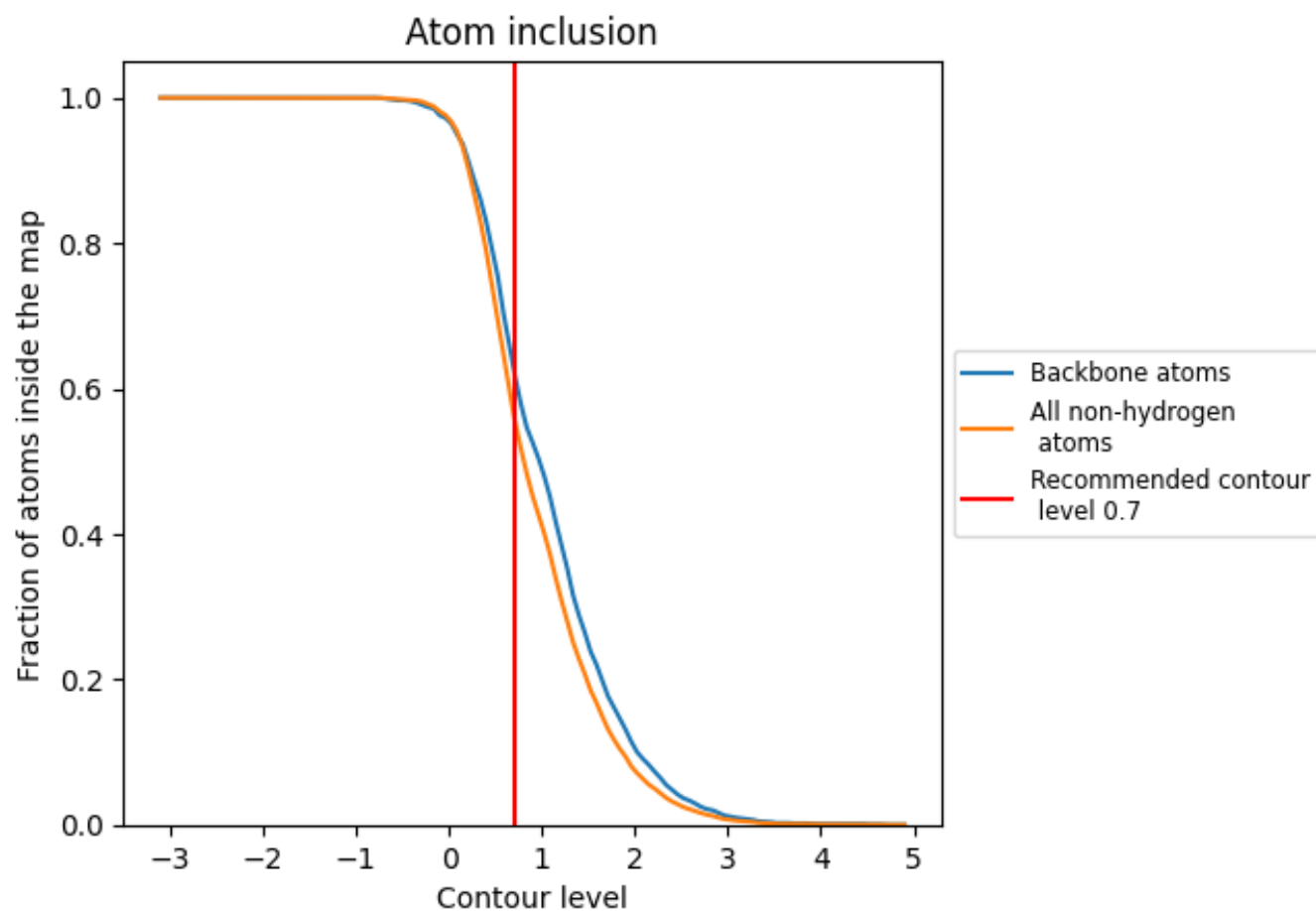
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7 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 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 56% of all non-hydrogen atoms, are inside the map.