wwPDB EM Validation Summary Report

Oct 13, 2024 – 05:11 am BST

PDB ID	:	8AQT
EMDB ID	:	EMD-15589
Title	:	Beta SARS-CoV-2 Spike bound to mouse ACE2 (local)
Authors	:	Lau, K.; Ni, D.; Beckert, B.; Nazarov, S.; Myasnikov, A.; Pojer, F.; Stahlberg, H.; Uchikawa, E.
Deposited on	:	2022-08-13
Resolution	:	4.40 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:

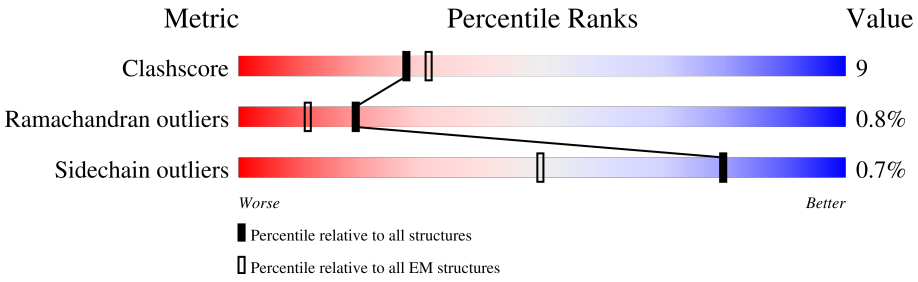
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

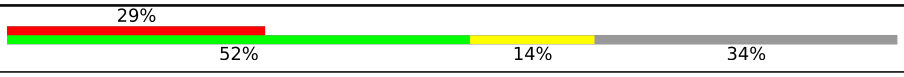
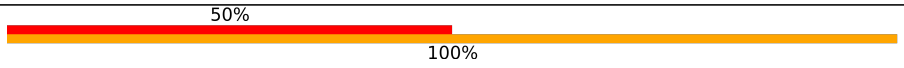
The reported resolution of this entry is 4.40 Å.

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	886	
2	B	1287	
3	C	2	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6321 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 Processed angiotensin-converting enzyme 2,Ig gamma-2A chain C region, membrane-bound form.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	584	Total	C	N	O	S	0	0
			4744	3023	797	895	29		

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP Q8R0I0
A	-14	GLY	-	expression tag	UNP Q8R0I0
A	-13	THR	-	expression tag	UNP Q8R0I0
A	-12	LEU	-	expression tag	UNP Q8R0I0
A	-11	SER	-	expression tag	UNP Q8R0I0
A	-10	ALA	-	expression tag	UNP Q8R0I0
A	-9	PRO	-	expression tag	UNP Q8R0I0
A	-8	PRO	-	expression tag	UNP Q8R0I0
A	-7	CYS	-	expression tag	UNP Q8R0I0
A	-6	THR	-	expression tag	UNP Q8R0I0
A	-5	GLN	-	expression tag	UNP Q8R0I0
A	-4	ARG	-	expression tag	UNP Q8R0I0
A	-3	ILE	-	expression tag	UNP Q8R0I0
A	-2	LYS	-	expression tag	UNP Q8R0I0
A	-1	TRP	-	expression tag	UNP Q8R0I0
A	0	LYS	-	expression tag	UNP Q8R0I0
A	1	GLY	-	expression tag	UNP Q8R0I0
A	2	LEU	-	expression tag	UNP Q8R0I0
A	3	LEU	-	expression tag	UNP Q8R0I0
A	4	LEU	-	expression tag	UNP Q8R0I0
A	5	THR	-	expression tag	UNP Q8R0I0
A	6	ALA	-	expression tag	UNP Q8R0I0
A	7	SER	-	expression tag	UNP Q8R0I0
A	8	LEU	-	expression tag	UNP Q8R0I0
A	9	LEU	-	expression tag	UNP Q8R0I0
A	10	ASN	-	expression tag	UNP Q8R0I0
A	11	PHE	-	expression tag	UNP Q8R0I0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	12	TRP	-	expression tag	UNP Q8R0I0
A	13	ASN	-	expression tag	UNP Q8R0I0
A	14	LEU	-	expression tag	UNP Q8R0I0
A	15	PRO	-	expression tag	UNP Q8R0I0
A	16	THR	-	expression tag	UNP Q8R0I0
A	17	THR	-	expression tag	UNP Q8R0I0
A	18	ALA	-	expression tag	UNP Q8R0I0
A	616	THR	-	linker	UNP Q8R0I0
A	617	GLY	-	linker	UNP Q8R0I0
A	618	LEU	-	linker	UNP Q8R0I0
A	619	GLU	-	linker	UNP Q8R0I0
A	620	VAL	-	linker	UNP Q8R0I0
A	621	LEU	-	linker	UNP Q8R0I0
A	622	PHE	-	linker	UNP Q8R0I0
A	623	GLN	-	linker	UNP Q8R0I0
A	624	GLY	-	linker	UNP Q8R0I0
A	625	PRO	-	linker	UNP Q8R0I0
A	626	MET	-	linker	UNP Q8R0I0
A	627	ASP	-	linker	UNP Q8R0I0
A	860	LYS	-	expression tag	UNP P01865
A	861	HIS	-	expression tag	UNP P01865
A	862	HIS	-	expression tag	UNP P01865
A	863	HIS	-	expression tag	UNP P01865
A	864	HIS	-	expression tag	UNP P01865
A	865	HIS	-	expression tag	UNP P01865
A	866	HIS	-	expression tag	UNP P01865
A	867	HIS	-	expression tag	UNP P01865
A	868	HIS	-	expression tag	UNP P01865
A	869	HIS	-	expression tag	UNP P01865
A	870	HIS	-	expression tag	UNP P01865

- Molecule 2 is a protein called Spike glycoprotein,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	193	Total	C	N	O	S	0	0
			1535	986	255	286	8		

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	83	ALA	ASP	variant	UNP P0DTC2
B	218	GLY	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	ALA	deletion	UNP P0DTC2
B	246	ILE	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	682	GLY	ARG	variant	UNP P0DTC2
B	683	SER	ARG	variant	UNP P0DTC2
B	685	SER	ARG	variant	UNP P0DTC2
B	701	VAL	ALA	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1209	GLY	-	linker	UNP P0DTC2
B	1210	SER	-	linker	UNP P0DTC2
B	1211	GLY	-	linker	UNP P0DTC2
B	1212	TYR	-	linker	UNP P0DTC2
B	1232	LEU	PHE	engineered mutation	UNP P10104
B	1238	GLY	-	expression tag	UNP P10104
B	1239	ARG	-	expression tag	UNP P10104
B	1240	SER	-	expression tag	UNP P10104
B	1241	LEU	-	expression tag	UNP P10104
B	1242	GLU	-	expression tag	UNP P10104
B	1243	VAL	-	expression tag	UNP P10104
B	1244	LEU	-	expression tag	UNP P10104
B	1245	PHE	-	expression tag	UNP P10104
B	1246	GLN	-	expression tag	UNP P10104
B	1247	GLY	-	expression tag	UNP P10104
B	1248	PRO	-	expression tag	UNP P10104
B	1249	GLY	-	expression tag	UNP P10104
B	1250	HIS	-	expression tag	UNP P10104
B	1251	HIS	-	expression tag	UNP P10104
B	1252	HIS	-	expression tag	UNP P10104
B	1253	HIS	-	expression tag	UNP P10104
B	1254	HIS	-	expression tag	UNP P10104
B	1255	HIS	-	expression tag	UNP P10104
B	1256	HIS	-	expression tag	UNP P10104
B	1257	HIS	-	expression tag	UNP P10104
B	1258	HIS	-	expression tag	UNP P10104
B	1259	HIS	-	expression tag	UNP P10104
B	1260	SER	-	expression tag	UNP P10104

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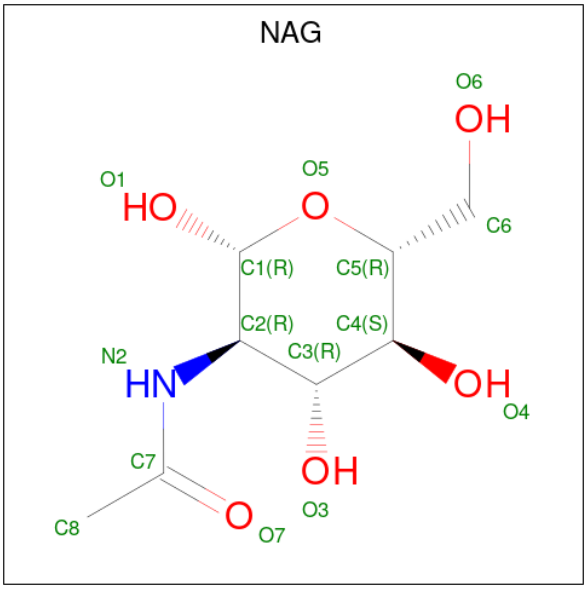
Chain	Residue	Modelled	Actual	Comment	Reference
B	1261	ALA	-	expression tag	UNP P10104
B	1262	TRP	-	expression tag	UNP P10104
B	1263	SER	-	expression tag	UNP P10104
B	1264	HIS	-	expression tag	UNP P10104
B	1265	PRO	-	expression tag	UNP P10104
B	1266	GLN	-	expression tag	UNP P10104
B	1267	PHE	-	expression tag	UNP P10104
B	1268	GLU	-	expression tag	UNP P10104
B	1269	LYS	-	expression tag	UNP P10104
B	1270	GLY	-	expression tag	UNP P10104
B	1271	GLY	-	expression tag	UNP P10104
B	1272	GLY	-	expression tag	UNP P10104
B	1273	SER	-	expression tag	UNP P10104
B	1274	GLY	-	expression tag	UNP P10104
B	1275	GLY	-	expression tag	UNP P10104
B	1276	GLY	-	expression tag	UNP P10104
B	1277	GLY	-	expression tag	UNP P10104
B	1278	SER	-	expression tag	UNP P10104
B	1279	GLY	-	expression tag	UNP P10104
B	1280	GLY	-	expression tag	UNP P10104
B	1281	SER	-	expression tag	UNP P10104
B	1282	ALA	-	expression tag	UNP P10104
B	1283	TRP	-	expression tag	UNP P10104
B	1284	SER	-	expression tag	UNP P10104
B	1285	HIS	-	expression tag	UNP P10104
B	1286	PRO	-	expression tag	UNP P10104
B	1287	GLN	-	expression tag	UNP P10104
B	1288	PHE	-	expression tag	UNP P10104
B	1289	GLU	-	expression tag	UNP P10104
B	1290	LYS	-	expression tag	UNP P10104

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



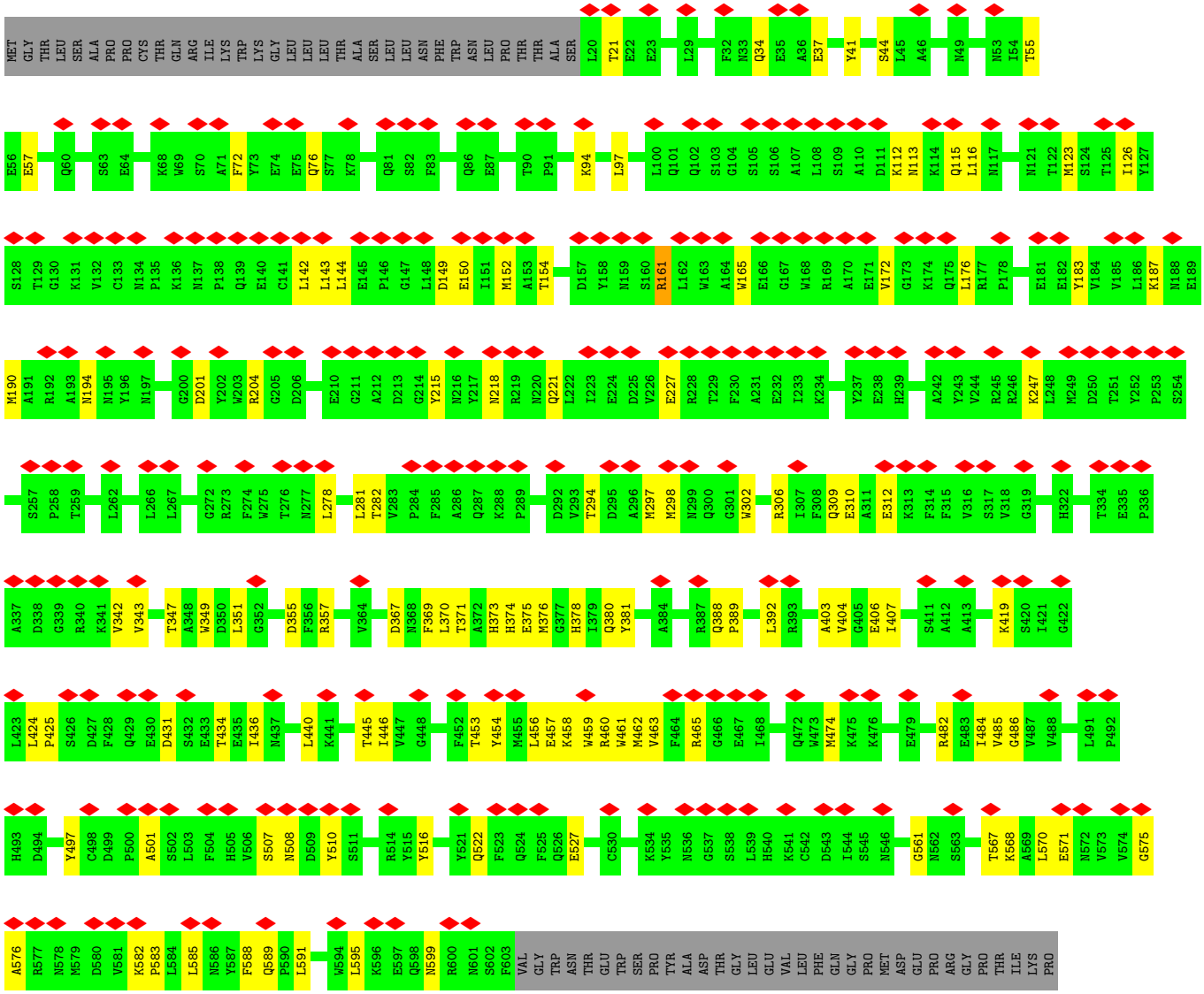
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	B	1	14	8	1	5	0

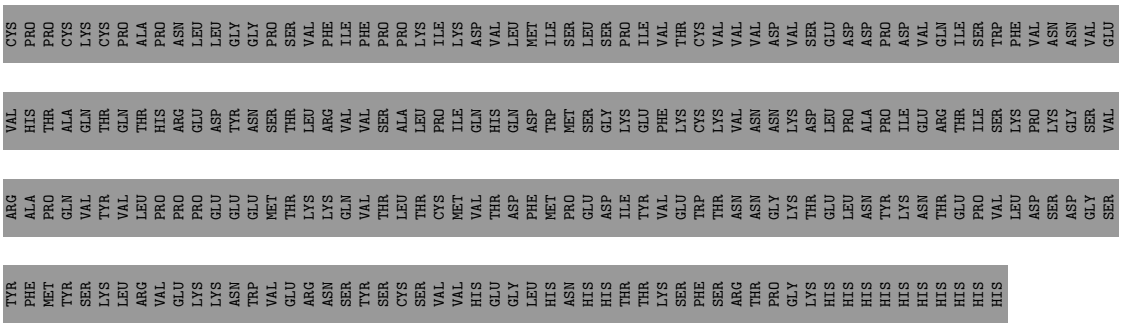
3 Residue-property plots (i)

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: Processed angiotensin-converting enzyme 2,Ig gamma-2A chain C region, membrane-bound form

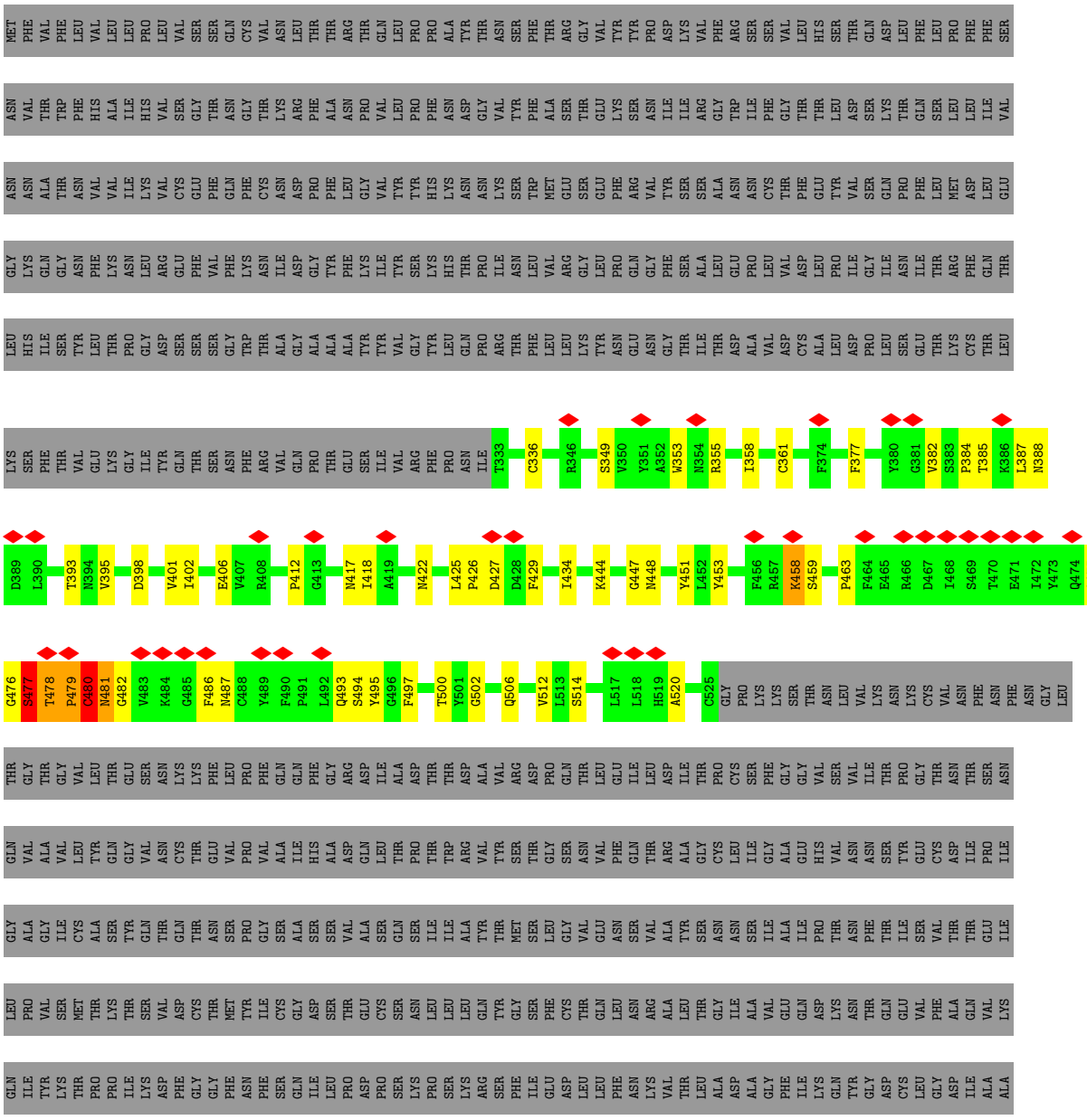
Chain A:





• Molecule 2: Spike glycoprotein,Fibritin

Chain B: 11% 85%



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

ASN GLY ILE GLY VAL THR GLN ASN VAL LEU TYR GLU ASN GLN LYS LEU ILE ALA ASN GLN PHE ASN SER ALA ILE GLY LYS ILE GLN ASP SER LEU LEU SER SER THR ALA SER ALA LEU GLY LYS LEU GLN ASP VAL VAL ASN GLN ASN ALA GLN LEU ALA LEU ASN THR LEU VAL LYS GLN LEU

SER SER ASN PHE GLY ALA ILE SER SER VAL LEU LEU ASN ASP ILE LEU SER ARG LEU ASP PRO PRO GLU ALA GLU VAL GLN ILE ASP ARG LEU ILE THR GLY ARG LEU GLN SER LEU GLN THR TYR VAL THR GLN GLN LEU LEU ILE ARG ALA ALA GLU ILE ARG ALA SER ALA ASN LEU ASP ALA ALA

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

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

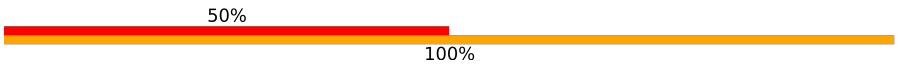
SER PHE LYS GLU GLU LEU ASP LYS TYR PHE LYS ASN HIS THR SER PRO ASP VAL ASP LEU GLY ASP ILE SER GLY ILE ASN ALA SER VAL VAL ASN ILE GLN LYS GLU ILE ASP ARG LEU ASN GLU VAL ALA LYS ASN LEU ASN GLU SER LEU ILE ASP LEU GLN GLU LEU GLY LYS TYR

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

PHE GLU LYS GLY GLY GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52640	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	4.012	Depositor
Minimum map value	-2.446	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.458	Depositor
Map size (Å)	370.83197, 370.83197, 370.83197	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3244, 1.3244, 1.3244	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

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	0.25	0/4873	0.47	0/6612
2	B	0.27	0/1579	0.53	0/2150
All	All	0.25	0/6452	0.49	0/8762

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	A	4744	0	4530	75	0
2	B	1535	0	1452	41	0
3	C	28	0	25	2	0
4	B	14	0	13	0	0
All	All	6321	0	6020	117	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 9.

The worst 5 of 117 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ILE:HG22	1:A:485:VAL:HG13	1.63	0.80
1:A:381:TYR:HB2	1:A:404:VAL:HG11	1.68	0.75
1:A:376:MET:O	1:A:380:GLN:NE2	2.24	0.69
2:B:402:ILE:HD12	2:B:406:GLU:HG3	1.74	0.69
1:A:161:ARG:HH12	1:A:165:TRP:HB3	1.56	0.69

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	582/886 (66%)	550 (94%)	31 (5%)	1 (0%)	44 78
2	B	191/1287 (15%)	175 (92%)	11 (6%)	5 (3%)	4 26
All	All	773/2173 (36%)	725 (94%)	42 (5%)	6 (1%)	19 53

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	389	PRO
2	B	479	PRO
2	B	480	CYS
2	B	478	THR
2	B	481	ASN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	507/789 (64%)	505 (100%)	2 (0%)	89 91
2	B	167/1111 (15%)	164 (98%)	3 (2%)	54 71
All	All	674/1900 (36%)	669 (99%)	5 (1%)	80 87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	161	ARG
2	B	458	LYS
2	B	477	SER
2	B	480	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	368	ASN
1	A	572	ASN
2	B	422	ASN

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)

2 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	$\#\|Z\|>2$
3	NAG	C	1	1,3	14,14,15	0.25	0	17,19,21	0.68	1 (5%)
3	NAG	C	2	3	14,14,15	0.51	0	17,19,21	1.29	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
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2	NAG	C2-N2-C7	4.27	128.99	122.90
3	C	1	NAG	C1-O5-C5	2.08	115.01	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

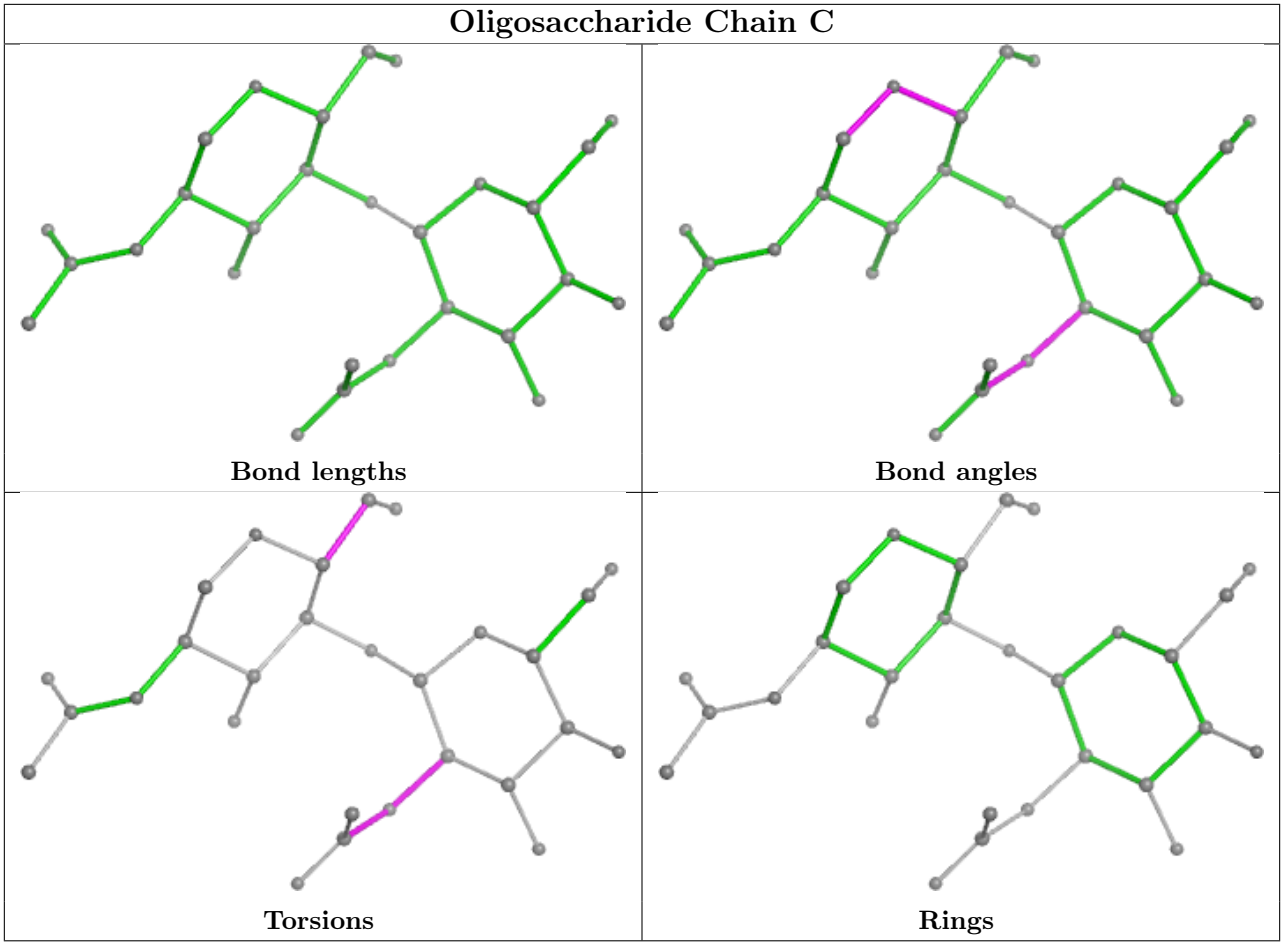
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	C	2	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	NAG	2	0
3	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)

1 ligand is 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	1301	2	14,14,15	0.83	1 (7%)	17,19,21	1.09	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
4	NAG	B	1301	2	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1301	NAG	O5-C1	2.74	1.48	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1301	NAG	C1-O5-C5	4.22	117.91	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

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.

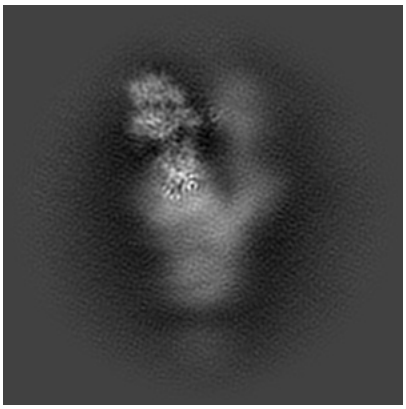
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15589. These allow visual inspection of the internal detail of the map and identification of artifacts.

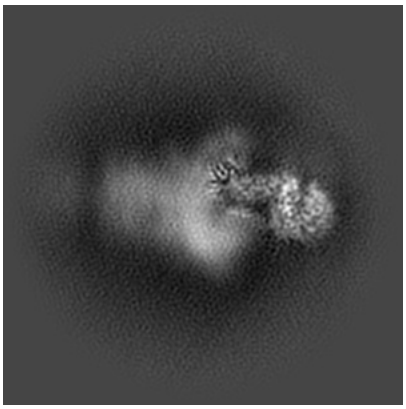
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

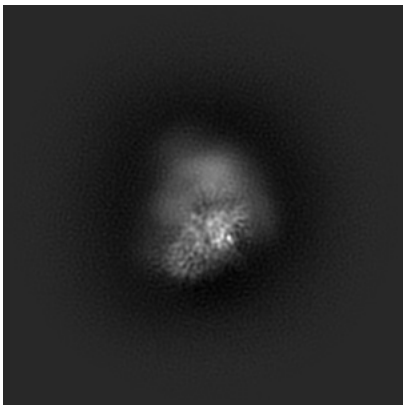
6.1.1 Primary map



X

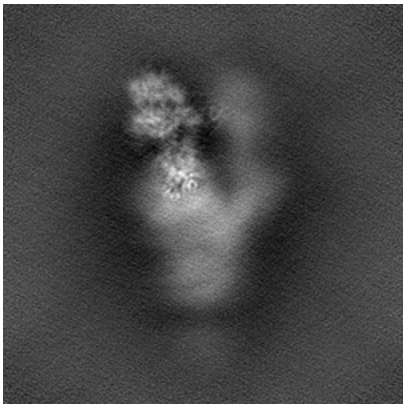


Y

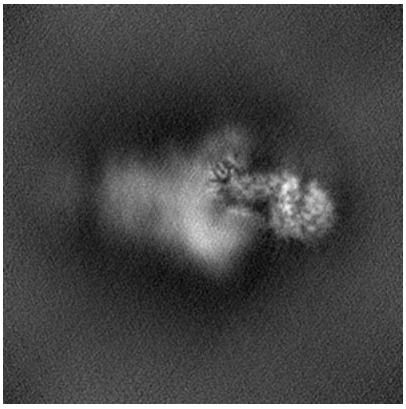


Z

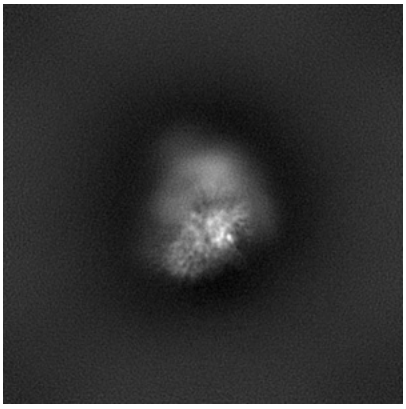
6.1.2 Raw map



X



Y

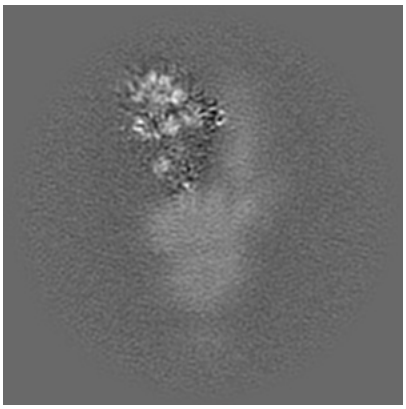


Z

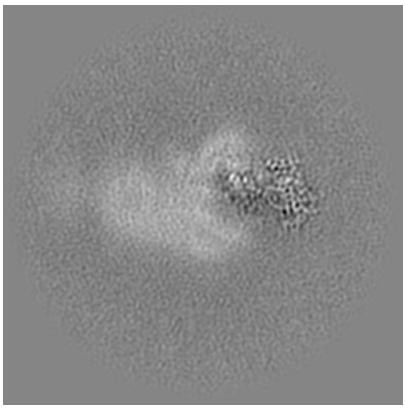
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

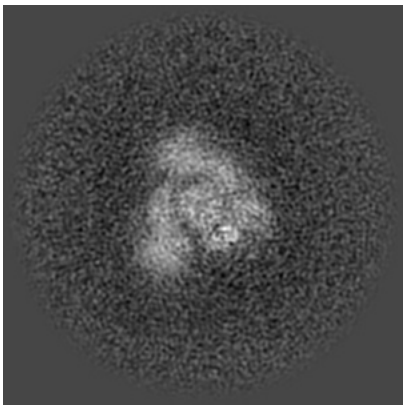
6.2.1 Primary map



X Index: 140

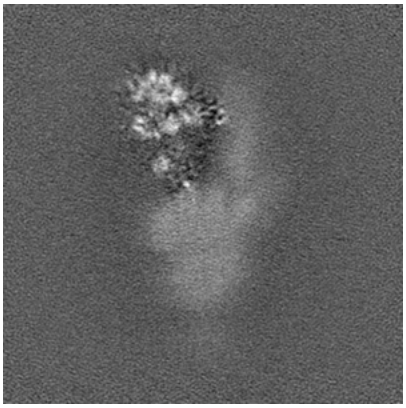


Y Index: 140

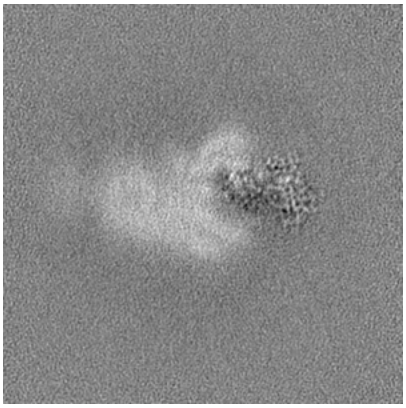


Z Index: 140

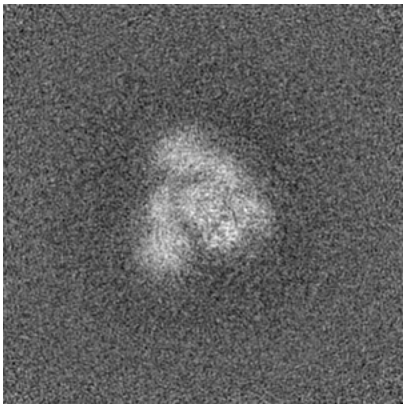
6.2.2 Raw map



X Index: 140



Y Index: 140

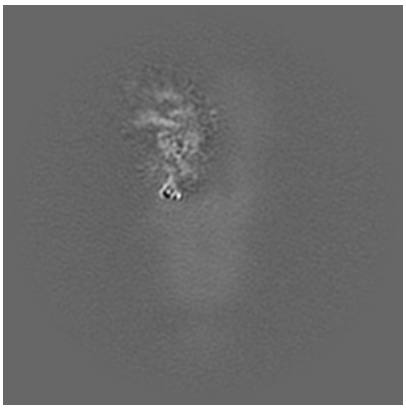


Z Index: 140

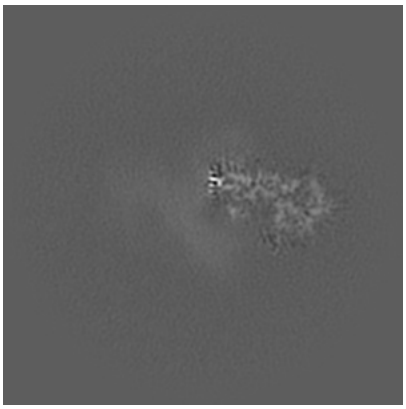
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

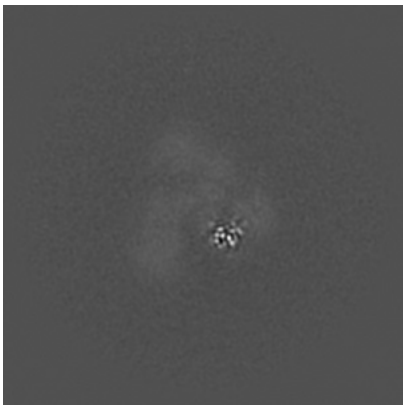
6.3.1 Primary map



X Index: 152

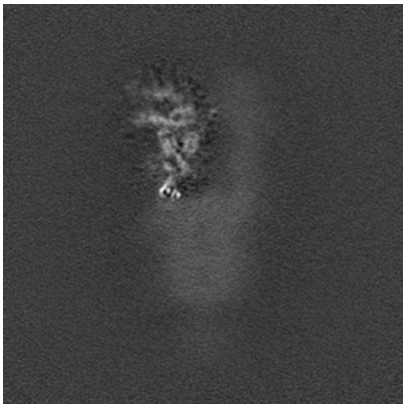


Y Index: 117

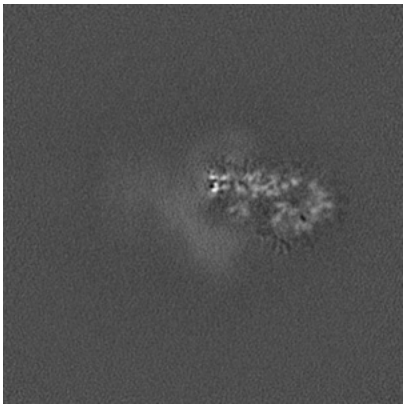


Z Index: 146

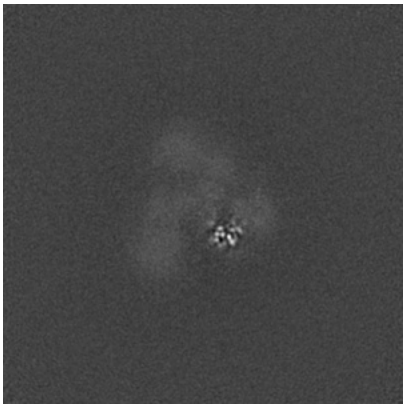
6.3.2 Raw map



X Index: 151



Y Index: 115

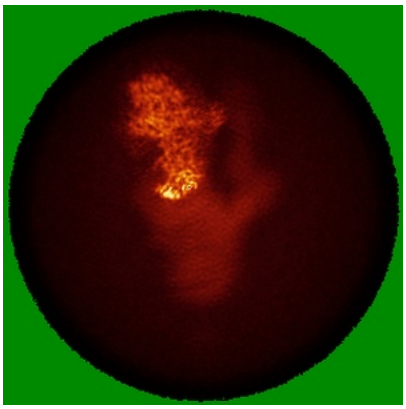


Z Index: 146

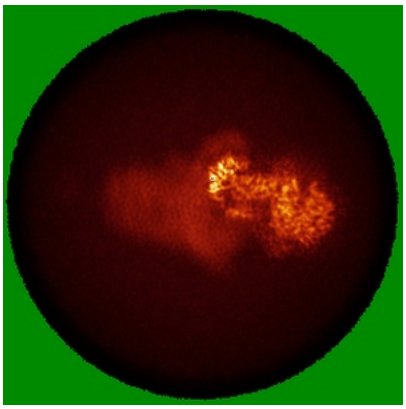
The images above show the largest variance slices of the map in three orthogonal directions.

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

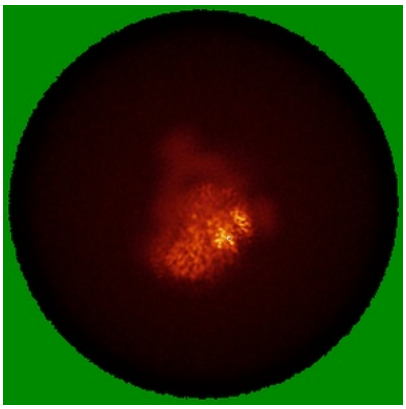
6.4.1 Primary map



X

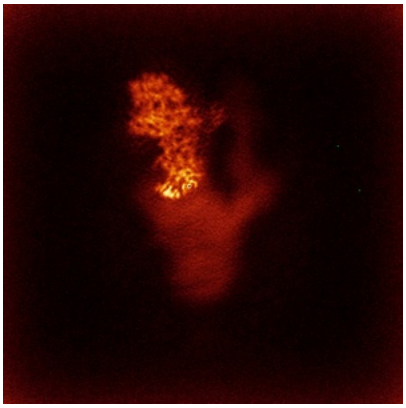


Y

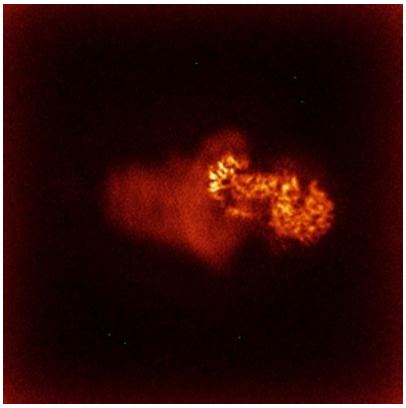


Z

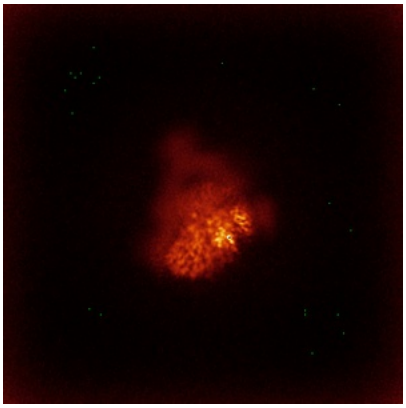
6.4.2 Raw map



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 0.458. 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.

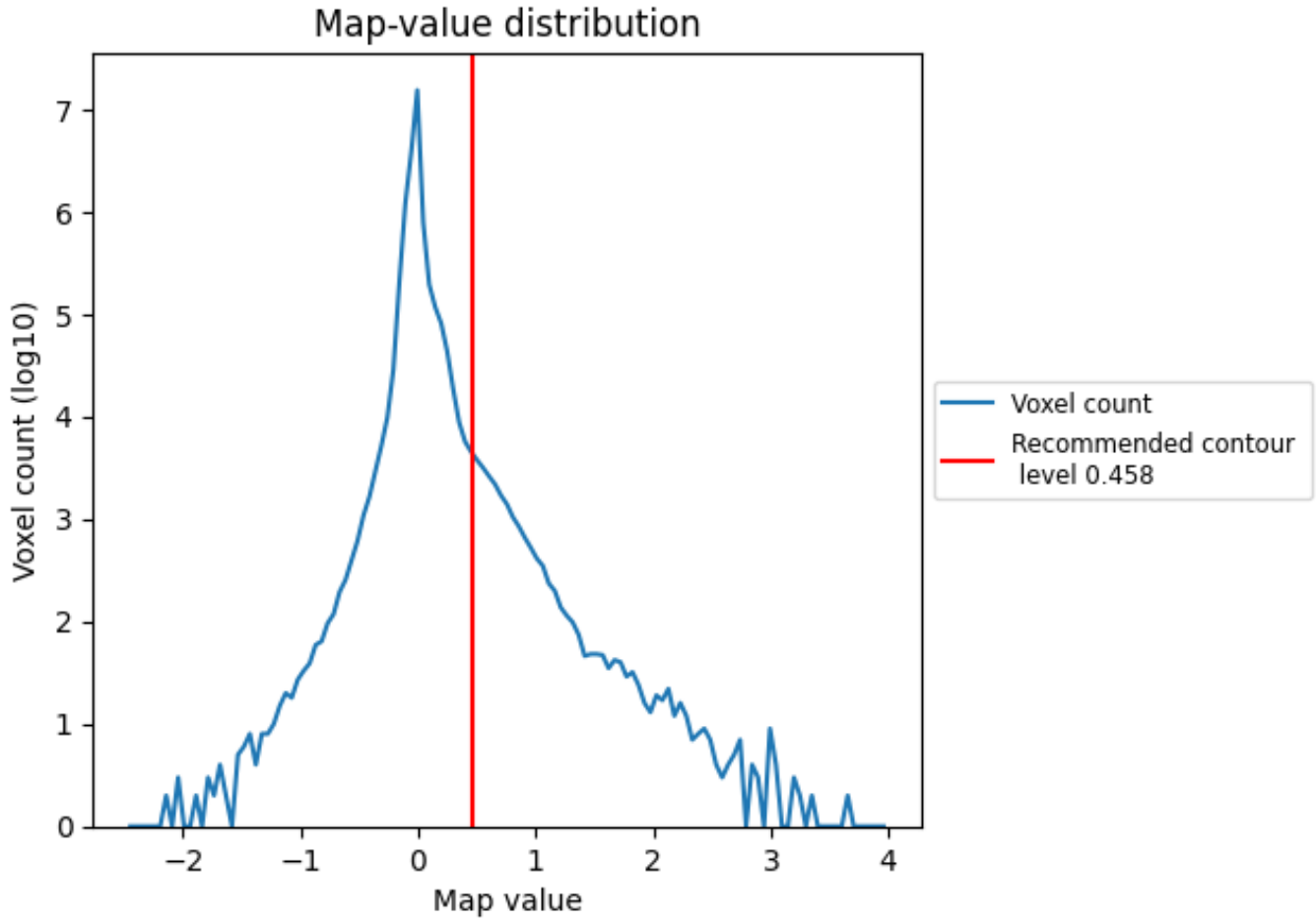
6.6 Mask visualisation (i)

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

7 Map analysis

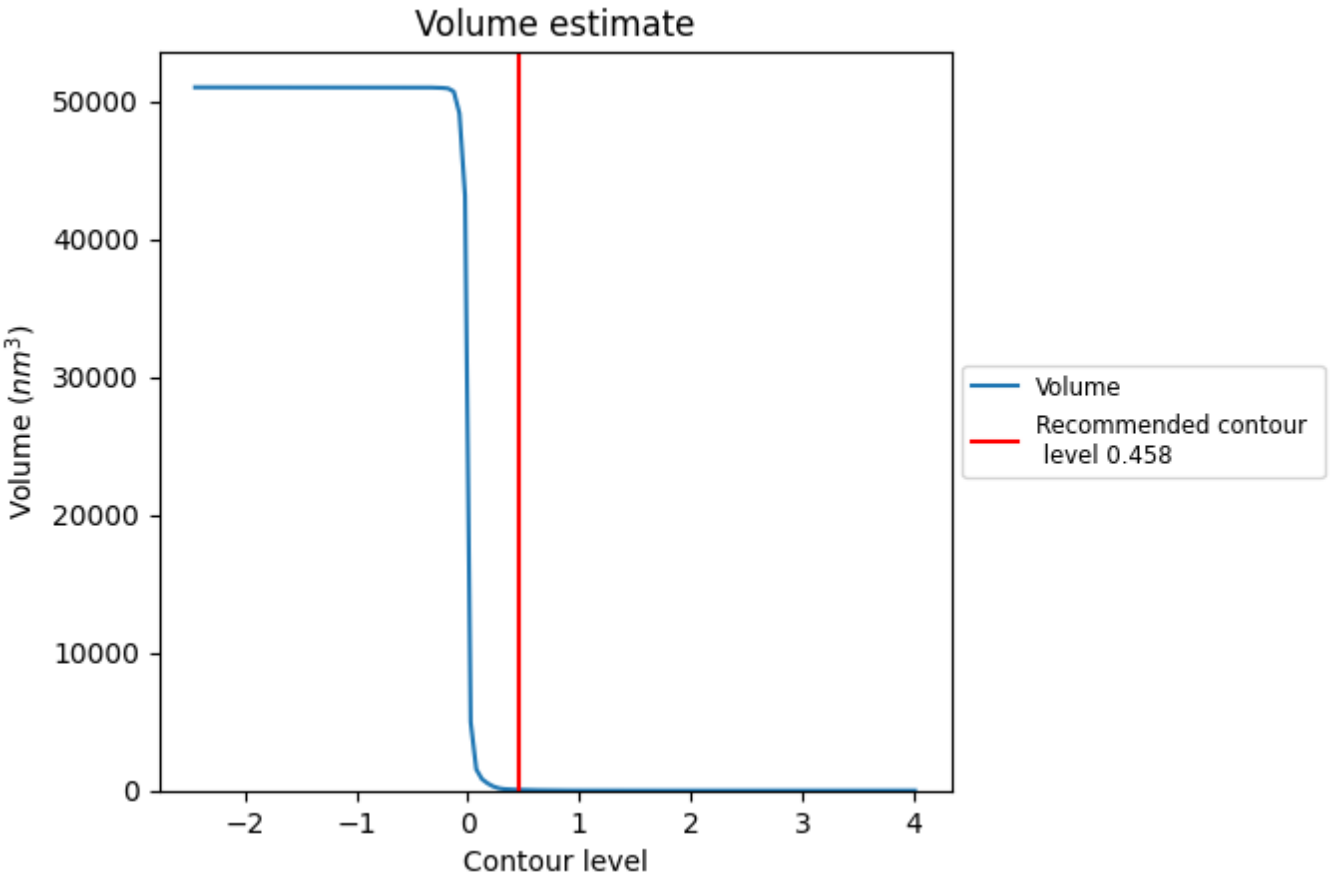
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

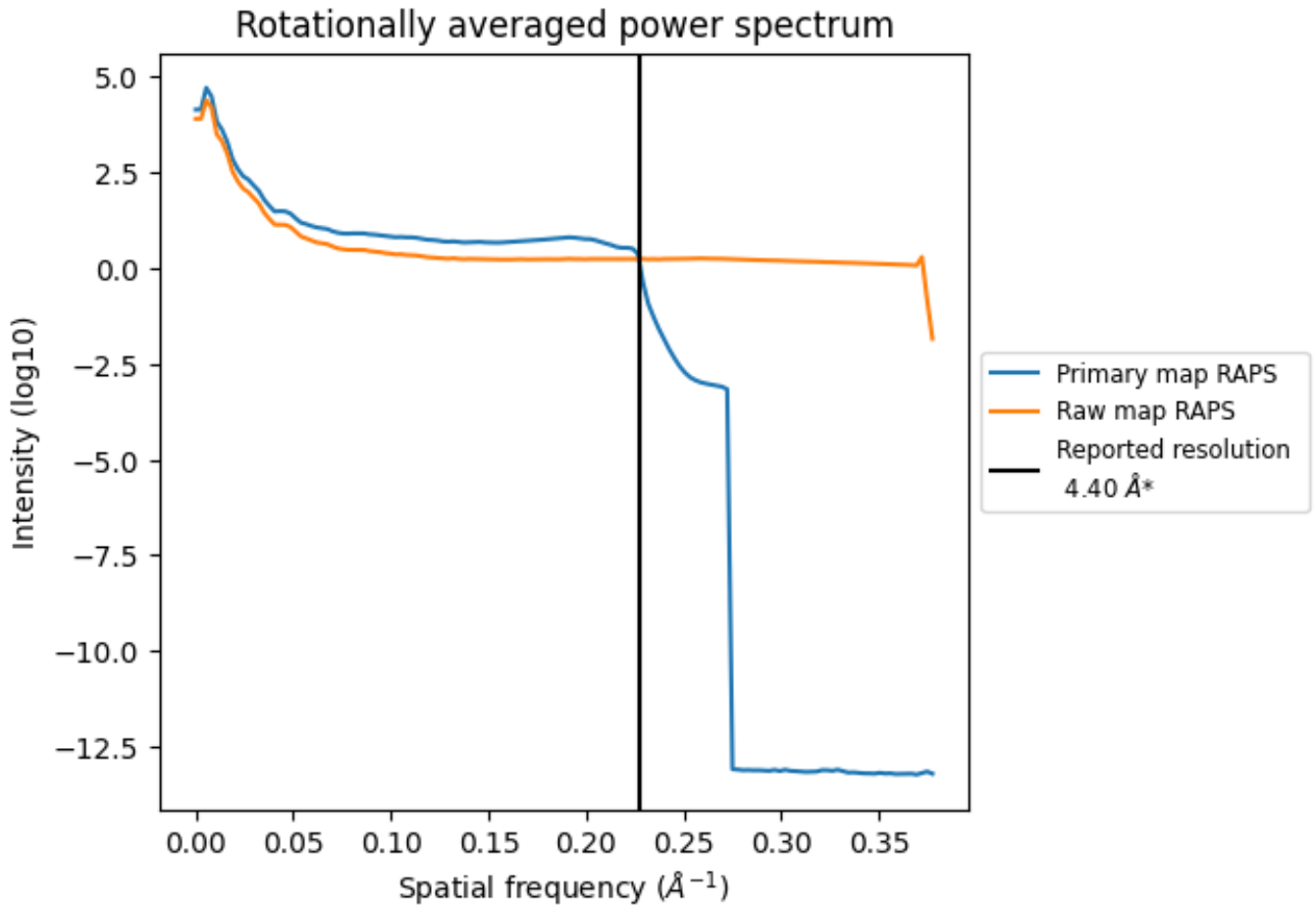
7.2 Volume estimate (i)



The volume at the recommended contour level is 56 nm^3; this corresponds to an approximate mass of 51 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)

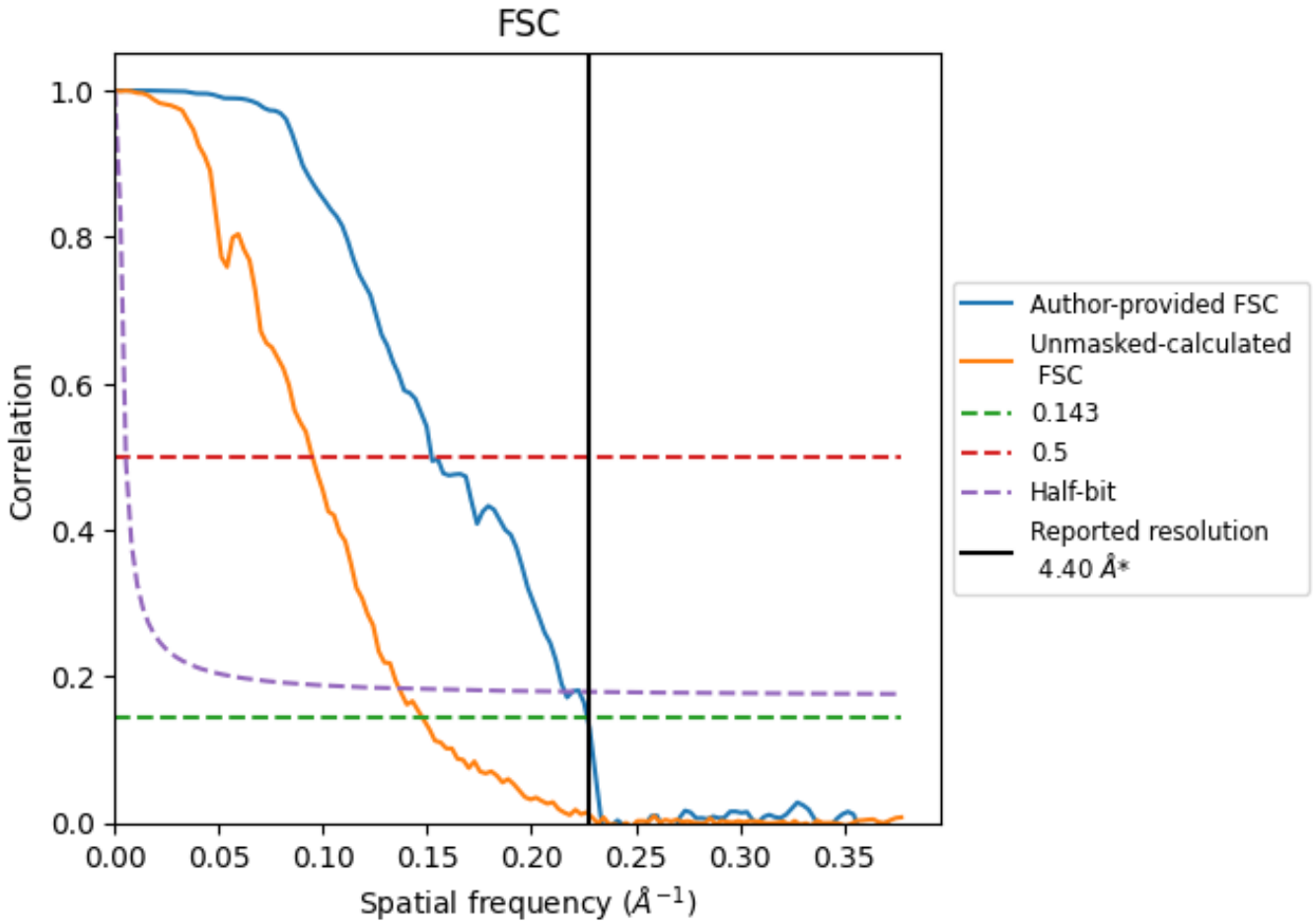


*Reported resolution corresponds to spatial frequency of 0.227 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

8.2 Resolution estimates (i)

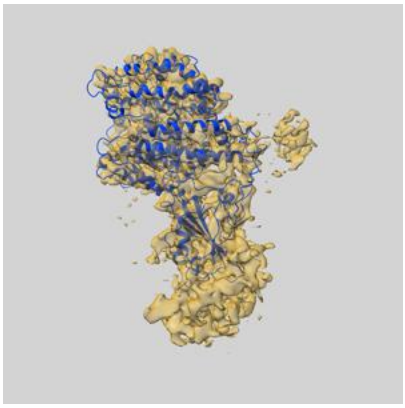
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.41	6.58	4.63
Unmasked-calculated*	6.77	10.55	7.32

*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 6.77 differs from the reported value 4.4 by more than 10 %

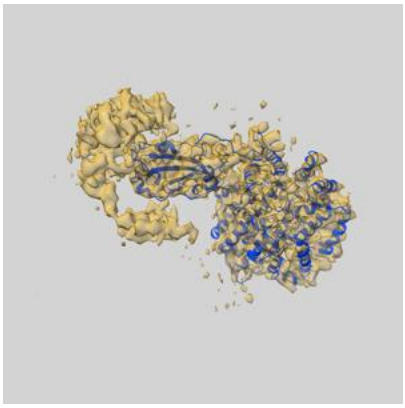
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15589 and PDB model 8AQT. Per-residue inclusion information can be found in section 3 on page 8.

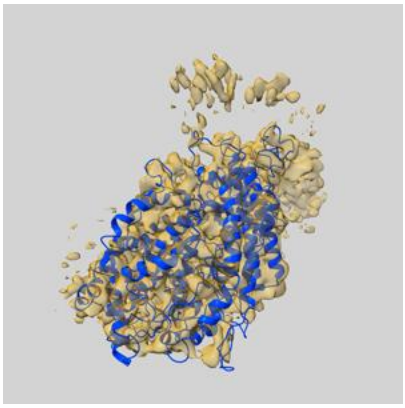
9.1 Map-model overlay



X



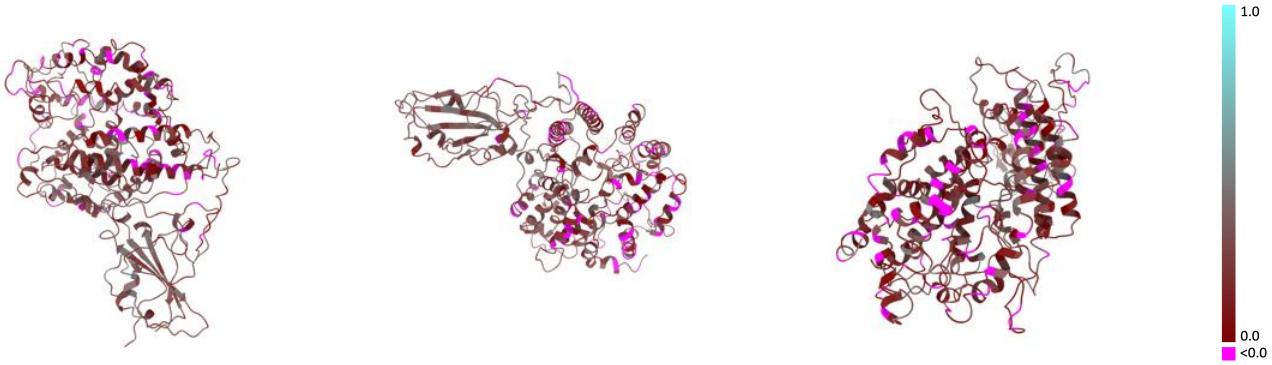
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.458 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.

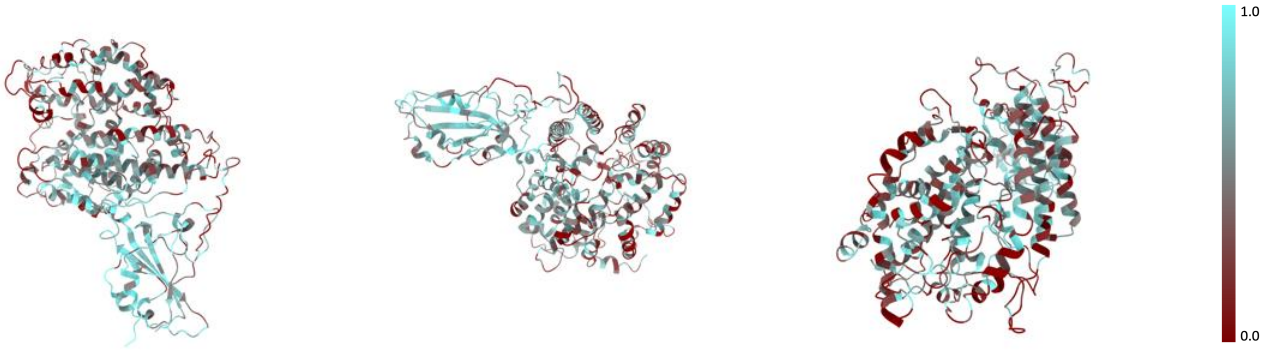
9.2 Q-score mapped to coordinate model (i)



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.

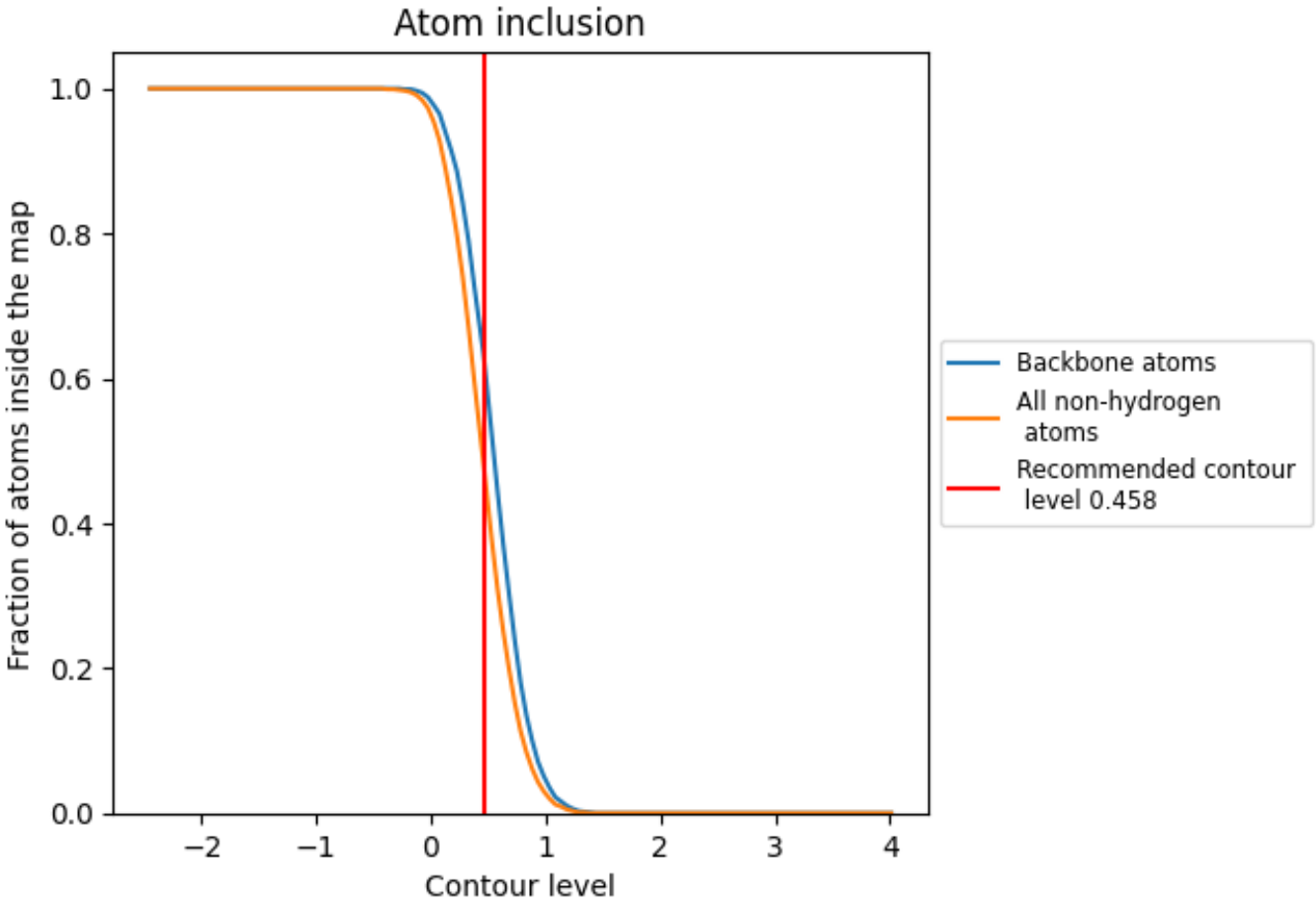
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.458).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 48% 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 (0.458) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4840	0.2120
A	0.4440	0.1860
B	0.6140	0.2960
C	0.2140	-0.0020