



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:46 PM UTC

PDB ID : 8AQT / pdb_00008aqt
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 Full wwPDB EM Validation 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
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

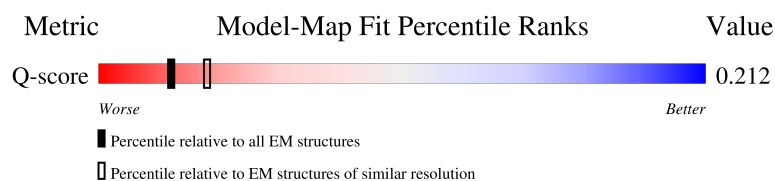
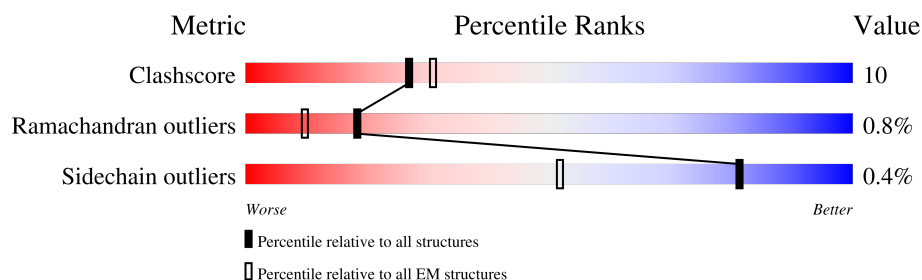
1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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	886	29% 52% 14% 34%
2	B	1287	11% 85%
3	C	2	50% 100%

2 Entry composition

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
			Total	C	N	O	S		
1	A	584	4744	3023	797	895	29	0	0

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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

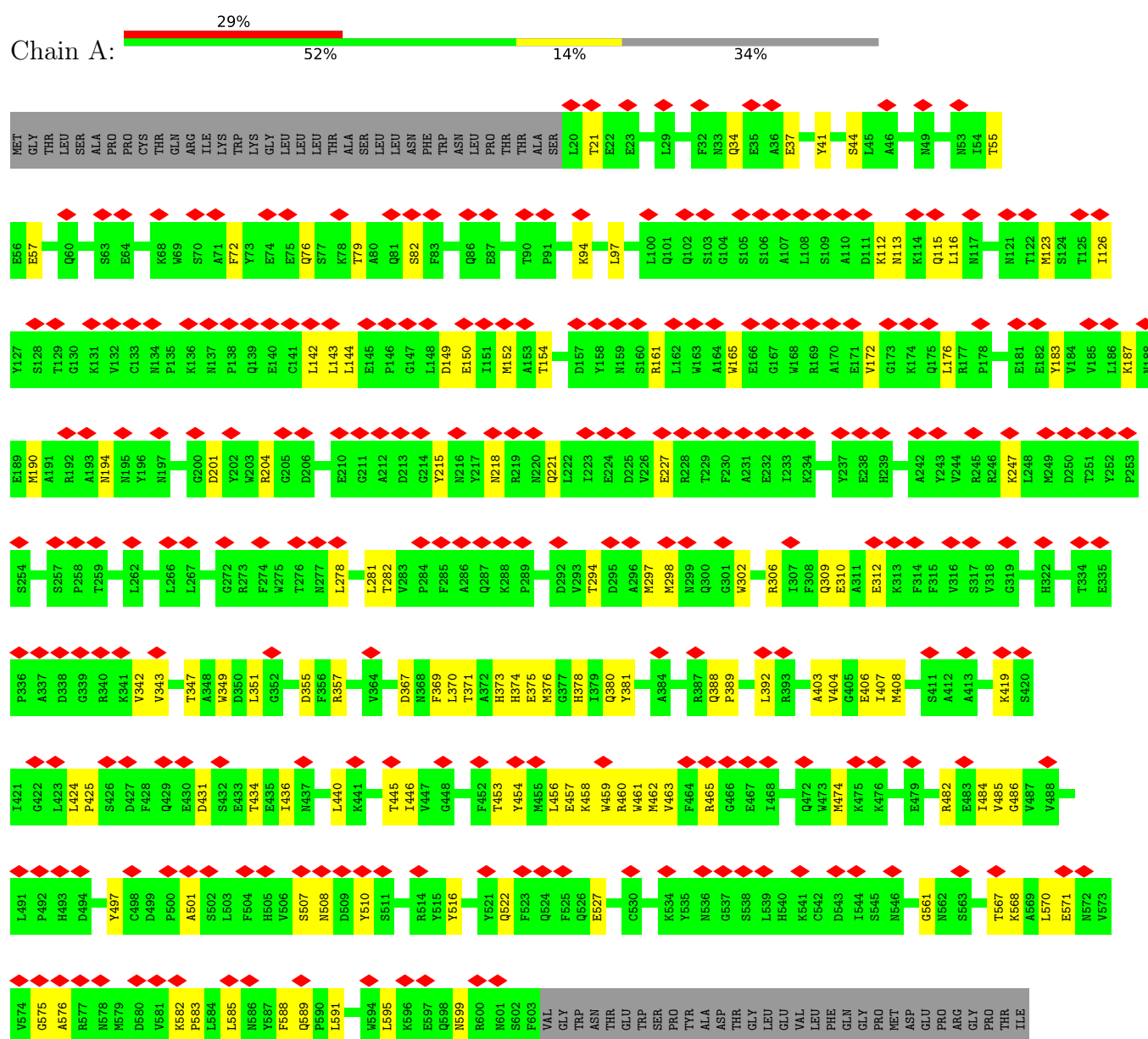


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	B	1	14	8	1	5	0

3 Residue-property plots

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



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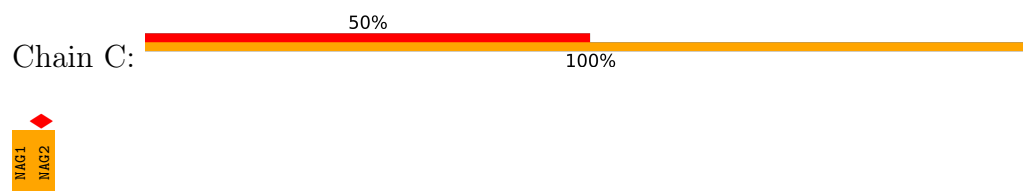
- Molecule 2: Spike glycoprotein, Fibrin



VAL	GLU	PRO	SER	GLY	Q474	L387	LYS	LEU	GLY	ASN	ASN	MET
LYS	ILE	ILE	ASN	LEU	A475	N388	SER	HIS	LYS	VAL	ASN	PHE
GLN	LEU	GLY	GLN	THR	G476	D389	PHE	SER	GLN	ALA	ASN	THR
ILE	PRO	ALA	VAL	GLY	S477	L390	THR	THR	ASN	THR	GLN	THR
TYR	VAL	GLY	ALA	THR	T478	L393	VAL	TYR	PHE	PHE	VAL	HIS
LYS	SER	ILE	VAL	GLY	P479	N394	GLY	LEU	LYS	VAL	VAL	VAL
THR	MET	CYS	LEU	VAL	C480	V395	ILE	PRO	ASN	ILE	ILE	LEU
PRO	PRO	ALA	THR	LEU	N481	V395	GLY	GLY	LEU	HIS	HIS	PRO
PRO	LYS	SER	GLN	THR	G482	D398	TYR	ASP	ARG	VAL	VAL	LEU
ASN	THR	THR	VAL	SER	W483	L401	GLN	SER	GLY	CYS	CYS	VAL
GLN	VAL	GLN	ASN	ASN	K484	V401	THR	SER	PHE	GLY	GLY	SER
ASP	ASP	THR	CYS	LYS	K484	I402	SER	SER	VAL	THR	THR	SER
PHE	CYS	THR	THR	LYS	G485	E406	ASN	GLY	PHE	GLN	GLN	CYS
GLY	GLY	THR	THR	PHE	F486	E406	PHE	TRP	THR	THR	THR	GLY
GLY	THR	ASN	GLY	LEU	N487	V407	ARG	THR	ALA	ILE	LYS	ASN
ASN	ASN	PRO	PRO	PRO	C488	R408	VAL	ALA	ASP	ASP	ASN	LEU
PHE	ILE	VAL	VAL	PHE	Y489	P412	GLN	GLY	GLY	PRO	ARG	THR
CYS	CYS	SER	ALA	GLN	F490	G413	THR	ALA	ALA	TYR	PHE	THR
GLN	GLY	ILE	ILE	PHE	P491	L492	GLY	ALA	ALA	PHE	ALA	THR
ILE	ASP	SER	HIS	GLY	L492	I417	GLY	TYR	GLY	ARG	ASN	ARG
PRO	VAL	VAL	ASP	ARG	Q493	I418	ILE	TYR	ILE	VAL	VAL	GLN
ALA	ALA	ALA	GLN	ASP	S494	A419	VAL	VAL	SER	TYR	TYR	LEU
THR	GLU	SER	LEU	ILE	Y495	A419	ARG	GLY	THR	PRO	PRO	PRO
CYS	CYS	SER	LEU	ALA	G496	N422	PHE	TYR	HIS	PHE	ASN	ASN
SER	ASN	SER	PRO	ASP	F497	L425	PRO	LEU	LYS	ALA	ASN	ALA
LYS	ASN	SER	THR	THR	T500	P426	ILE	GLN	PRO	ASN	ASP	TYR
PRO	LEU	ILE	THR	THR	Y601	D427	THR	PRO	ASN	GLY	GLY	THR
SER	LEU	THR	THR	THR	G602	F429	ARG	GLN	THR	VAL	VAL	ASN
LYS	LEU	ALA	ARG	ASP	Q606	D429	THR	ARG	ILE	THR	THR	THR
ARG	GLN	VAL	VAL	ALA	Q606	I434	THR	THR	ASN	THR	THR	THR
PHE	GLY	THR	GLY	GLY	V512	L513	GLY	LYS	GLY	GLY	GLY	GLY
GLU	PHE	GLY	GLY	PRO	I513	S514	THR	TYR	LEU	LEU	GLY	GLY
ASP	CYS	GLY	SER	GLN	S514	K444	ASN	ASN	PRO	TYR	TYR	VAL
LEU	LEU	VAL	ASN	THR	S514	L444	GLY	GLY	GLY	GLY	GLY	GLY
LEU	GLN	GLU	PHE	LEU	L517	G447	ASN	GLY	GLY	ARG	ARG	THR
LEU	ASN	ASN	VAL	GLY	L518	N448	ASN	GLY	THR	ASN	ASN	PRO
LYS	ASN	SER	GLN	ILE	L518	W448	THR	THR	PHE	THR	THR	ASN
ASN	ASN	VAL	THR	LEU	H519	A520	VAL	ILE	ALA	ARG	ARG	VAL
VAL	ALA	ALA	ARG	ASP	A520	Y451	ALA	THR	ALA	SER	SER	VAL
THR	THR	THR	GLY	ILE	C525	L452	THR	ASP	LEU	GLY	GLY	PHE
LEU	LEU	SER	ALA	ILE	C525	Y453	ASN	ASP	LEU	ALA	ALA	THR
LEU	GLY	CYS	CYS	PRO	PRO	F456	GLY	ALA	GLY	THR	THR	THR
ASP	ILE	ILE	ILE	SER	LYS	R457	THR	VAL	VAL	ILE	ILE	THR
ALA	ALA	SER	THR	PHE	LYS	K458	GLY	CYS	ASP	THR	THR	THR
ALA	VAL	ILE	GLY	GLY	THR	S459	THR	THR	THR	THR	THR	THR
PHE	GLU	ILE	ALA	ALA	SER	W459	GLY	LEU	THR	THR	THR	THR
GLY	VAL	ALA	ALA	PHE	THR	A463	VAL	LEU	VAL	THR	THR	THR
GLY	VAL	THR	ASN	ILE	VAL	F464	VAL	SER	ASN	THR	THR	THR
ASP	GLN	THR	ASN	THR	LYS	E465	ASN	GLU	ILE	GLN	GLN	PHE
CYS	GLY	ILE	SER	THR	ASN	R466	LYS	THR	ILE	THR	THR	THR
GLY	VAL	SER	TYR	GLY	LYS	D467	LYS	LYS	THR	GLN	GLN	THR
LEU	PHE	VAL	CYS	GLY	THR	D467	CYS	CYS	ARG	THR	THR	THR
GLY	GLY	VAL	GLY	THR	THR	I468	THR	THR	PHE	ASP	ASP	PHE
THR	THR	THR	VAL	THR	ASN	C469	THR	THR	GLN	THR	THR	THR
THR	GLN	THR	THR	THR	ASN	C469	THR	THR	THR	THR	THR	THR

[illegible]

- Molecule 3: 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	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 ($e^-/\text{\AA}^2$)	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 ($\text{\AA}$)	370.83197, 370.83197, 370.83197	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3244, 1.3244, 1.3244	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	0.14	0/4873	0.39	0/6612
2	B	0.17	0/1579	0.44	1/2150 (0.0%)
All	All	0.15	0/6452	0.40	1/8762 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	479	PRO	CB-CA-C	-6.86	100.23	111.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4744	0	4530	79	0
2	B	1535	0	1452	42	0
3	C	28	0	25	2	0
4	B	14	0	13	0	0
All	All	6321	0	6020	122	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.

All (122) 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
2:B:476:GLY:O	2:B:477:SER:C	2.33	0.71
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
1:A:370:LEU:O	1:A:374:HIS:ND1	2.16	0.68
1:A:527:GLU:HG3	1:A:583:PRO:HB3	1.76	0.67
1:A:247:LYS:NZ	1:A:281:LEU:O	2.24	0.67
2:B:479:PRO:C	2:B:481:ASN:N	2.49	0.66
2:B:398:ASP:HB3	2:B:512:VAL:HB	1.76	0.66
1:A:459:TRP:O	1:A:463:VAL:HG13	1.97	0.65
2:B:412:PRO:HB3	2:B:427:ASP:HA	1.79	0.64
1:A:457:GLU:OE2	1:A:461:TRP:NE1	2.30	0.64
1:A:445:THR:HG23	1:A:446:ILE:HG23	1.80	0.64
1:A:570:LEU:HB3	1:A:576:ALA:HB3	1.80	0.63
2:B:447:GLY:HA2	2:B:497:PHE:H	1.63	0.62
3:C:2:NAG:H3	3:C:2:NAG:H83	1.82	0.61
1:A:407:ILE:HD11	1:A:522:GLN:HA	1.83	0.61
2:B:479:PRO:HB2	2:B:481:ASN:H	1.67	0.59
2:B:477:SER:HB3	2:B:486:PHE:HB2	1.85	0.59
2:B:398:ASP:O	2:B:512:VAL:N	2.32	0.59
2:B:478:THR:HB	2:B:479:PRO:HD3	1.84	0.59
1:A:376:MET:SD	1:A:380:GLN:NE2	2.76	0.59
1:A:149:ASP:HA	1:A:152:MET:HG3	1.84	0.59
1:A:453:THR:HG21	1:A:516:TYR:HB2	1.84	0.58
2:B:480:CYS:O	2:B:482:GLY:N	2.37	0.57
1:A:41:TYR:OH	2:B:500:THR:OG1	2.22	0.57
1:A:94:LYS:HA	1:A:97:LEU:HD12	1.87	0.57
1:A:294:THR:HA	1:A:297:MET:HE2	1.87	0.57
2:B:479:PRO:C	2:B:481:ASN:H	2.13	0.56
1:A:351:LEU:HB2	1:A:355:ASP:HB3	1.88	0.56
1:A:113:ASN:HA	1:A:116:LEU:HB3	1.87	0.56
1:A:355:ASP:OD2	1:A:357:ARG:NH2	2.40	0.55
2:B:453:TYR:HE1	2:B:493:GLN:HB2	1.72	0.55
1:A:571:GLU:HA	1:A:575:GLY:HA2	1.88	0.54
1:A:72:PHE:O	1:A:76:GLN:HG2	2.06	0.54
2:B:479:PRO:O	2:B:481:ASN:N	2.40	0.54
1:A:392:LEU:HD23	1:A:561:GLY:HA3	1.88	0.54
2:B:377:PHE:HD1	2:B:434:ILE:HG12	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:MET:O	1:A:194:ASN:HB3	2.08	0.54
2:B:418:ILE:HA	2:B:422:ASN:HD22	1.72	0.54
1:A:227:GLU:N	1:A:227:GLU:OE1	2.40	0.54
2:B:382:VAL:HB	2:B:387:LEU:HD21	1.90	0.52
1:A:582:LYS:HG3	1:A:583:PRO:HD3	1.90	0.52
1:A:143:LEU:HD12	1:A:144:LEU:H	1.74	0.52
1:A:369:PHE:O	1:A:373:HIS:ND1	2.42	0.52
2:B:479:PRO:O	2:B:480:CYS:C	2.50	0.52
1:A:44:SER:HB2	1:A:351:LEU:HD22	1.90	0.52
1:A:278:LEU:O	1:A:282:THR:OG1	2.24	0.52
1:A:431:ASP:OD2	1:A:434:THR:OG1	2.27	0.52
1:A:367:ASP:O	1:A:371:THR:HG23	2.10	0.52
2:B:385:THR:O	2:B:388:ASN:ND2	2.43	0.52
1:A:183:TYR:O	1:A:187:LYS:HG2	2.09	0.51
1:A:218:ASN:HB2	1:A:221:GLN:HB2	1.91	0.51
1:A:436:ILE:O	1:A:440:LEU:HG	2.11	0.51
1:A:419:LYS:NZ	1:A:425:PRO:O	2.44	0.51
2:B:417:ASN:OD1	2:B:418:ILE:N	2.42	0.51
2:B:426:PRO:HD3	2:B:463:PRO:HB3	1.93	0.51
2:B:476:GLY:HA2	2:B:480:CYS:HB2	1.91	0.51
1:A:501:ALA:O	1:A:507:SER:OG	2.25	0.50
1:A:342:VAL:HG22	1:A:343:VAL:H	1.76	0.50
2:B:358:ILE:HB	2:B:395:VAL:HB	1.92	0.50
2:B:425:LEU:HD12	2:B:426:PRO:HD2	1.93	0.50
3:C:1:NAG:H3	3:C:2:NAG:H82	1.94	0.50
2:B:384:PRO:HA	2:B:387:LEU:HD12	1.95	0.49
1:A:310:GLU:OE2	1:A:373:HIS:NE2	2.46	0.48
1:A:227:GLU:OE2	1:A:454:TYR:OH	2.23	0.48
1:A:462:MET:HA	1:A:465:ARG:HH11	1.79	0.48
2:B:444:LYS:HE2	2:B:448:ASN:HB2	1.95	0.48
2:B:349:SER:O	2:B:353:TRP:HB3	2.14	0.47
2:B:401:VAL:HG11	2:B:451:TYR:CE2	2.49	0.47
1:A:508:ASN:HB2	1:A:510:TYR:CE1	2.49	0.47
2:B:453:TYR:CE1	2:B:493:GLN:HB2	2.49	0.47
1:A:347:THR:HB	1:A:349:TRP:HE1	1.80	0.47
1:A:375:GLU:HA	1:A:378:HIS:ND1	2.30	0.47
1:A:431:ASP:OD1	1:A:431:ASP:N	2.46	0.47
1:A:172:VAL:O	1:A:176:LEU:HD23	2.15	0.46
1:A:297:MET:HB2	1:A:302:TRP:CE3	2.51	0.46
1:A:302:TRP:HD1	1:A:306:ARG:HG3	1.81	0.46
1:A:34:GLN:O	1:A:37:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLU:O	1:A:154:THR:OG1	2.29	0.46
1:A:388:GLN:HB3	1:A:392:LEU:HB2	1.97	0.46
1:A:458:LYS:O	1:A:462:MET:HG2	2.16	0.45
2:B:475:ALA:HB1	2:B:487:ASN:ND2	2.31	0.45
1:A:309:GLN:HA	1:A:312:GLU:OE2	2.15	0.45
1:A:482:ARG:HA	1:A:486:GLY:HA2	1.98	0.45
1:A:294:THR:HA	1:A:297:MET:HG2	1.99	0.45
2:B:494:SER:OG	2:B:495:TYR:N	2.49	0.45
1:A:142:LEU:HD23	1:A:143:LEU:N	2.32	0.45
2:B:478:THR:H	2:B:479:PRO:CD	2.29	0.45
1:A:376:MET:HE3	1:A:376:MET:HB3	1.81	0.44
1:A:403:ALA:HA	1:A:406:GLU:HG2	2.00	0.44
1:A:585:LEU:O	1:A:589:GLN:HG2	2.17	0.44
2:B:458:LYS:HD2	2:B:459:SER:HB3	2.00	0.44
1:A:347:THR:HB	1:A:349:TRP:NE1	2.33	0.44
2:B:429:PHE:CZ	2:B:514:SER:HA	2.53	0.43
2:B:479:PRO:HD2	2:B:480:CYS:H	1.82	0.43
1:A:407:ILE:HG22	1:A:408:MET:HE2	1.99	0.43
2:B:393:THR:HG21	2:B:520:ALA:HB3	2.01	0.43
2:B:336:CYS:HB2	2:B:361:CYS:HB3	1.71	0.43
1:A:79:THR:O	1:A:82:SER:OG	2.33	0.43
1:A:55:THR:HG23	1:A:57:GLU:HG2	1.99	0.43
1:A:201:ASP:HA	1:A:204:ARG:HG2	2.01	0.43
1:A:595:LEU:O	1:A:599:ASN:ND2	2.43	0.43
1:A:112:LYS:O	1:A:115:GLN:NE2	2.51	0.43
1:A:343:VAL:HG13	1:A:343:VAL:O	2.19	0.43
1:A:123:MET:O	1:A:126:ILE:HG12	2.19	0.42
1:A:419:LYS:NZ	1:A:424:LEU:HB3	2.34	0.42
2:B:502:GLY:O	2:B:506:GLN:HG2	2.20	0.42
1:A:456:LEU:HD22	1:A:460:ARG:HH21	1.82	0.42
1:A:474:MET:HB3	1:A:497:TYR:OH	2.20	0.42
1:A:567:THR:O	1:A:571:GLU:HG2	2.20	0.42
1:A:294:THR:O	1:A:298:MET:HG2	2.19	0.42
1:A:456:LEU:HD22	1:A:460:ARG:NH2	2.35	0.42
2:B:363:ALA:H	2:B:525:CYS:C	2.27	0.42
1:A:215:TYR:CZ	1:A:568:LYS:HE2	2.54	0.42
2:B:479:PRO:HB2	2:B:481:ASN:HB2	2.02	0.41
1:A:588:PHE:HD1	1:A:591:LEU:HD12	1.84	0.41
1:A:112:LYS:HD3	1:A:112:LYS:HA	1.85	0.41
2:B:353:TRP:HH2	2:B:355:ARG:CZ	2.34	0.40
1:A:161:ARG:NH1	1:A:165:TRP:HB3	2.32	0.40

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%)	43	77
2	B	191/1287 (15%)	175 (92%)	11 (6%)	5 (3%)	4	25
All	All	773/2173 (36%)	725 (94%)	42 (5%)	6 (1%)	18	52

All (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
2	B	477	SER

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%)	506 (100%)	1 (0%)	87	85
2	B	167/1111 (15%)	165 (99%)	2 (1%)	63	73
All	All	674/1900 (36%)	671 (100%)	3 (0%)	81	82

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
2	B	477	SER
2	B	480	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	98	GLN
1	A	175	GLN
1	A	330	ASN
1	A	368	ASN
1	A	380	GLN
1	A	401	HIS
1	A	442	GLN
1	A	540	HIS
1	A	572	ASN
1	A	589	GLN
2	B	334	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	0.26	0	17,19,21	0.69	1 (5%)
3	NAG	C	2	3	14,14,15	0.54	0	17,19,21	1.37	2 (11%)

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	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C2-N2-C7	4.54	128.99	122.90
3	C	1	NAG	C1-O5-C5	2.11	115.01	112.19
3	C	2	NAG	C1-C2-N2	2.08	113.71	110.43

There are no chirality outliers.

All (6) torsion outliers are listed below:

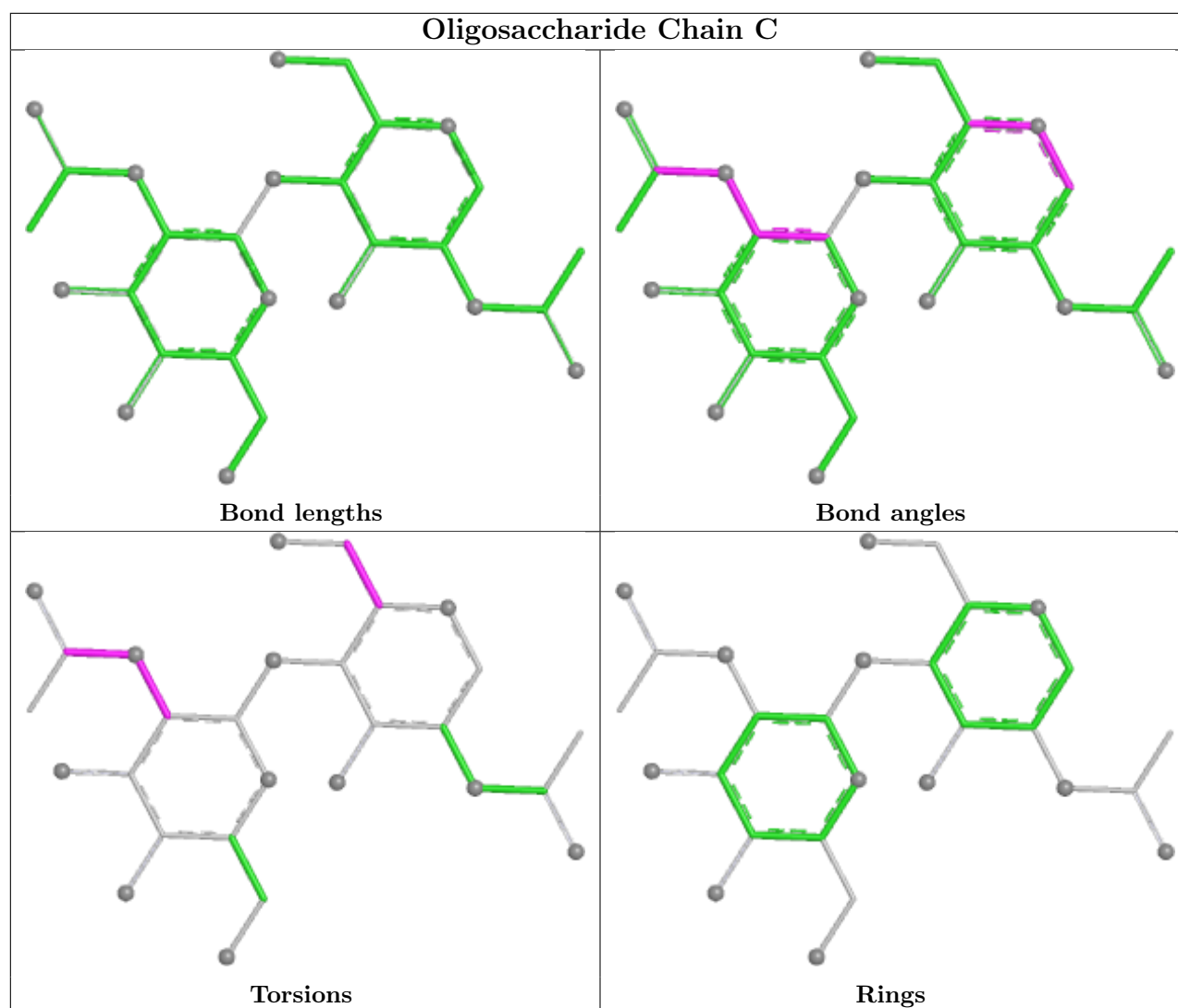
Mol	Chain	Res	Type	Atoms
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	C	2	NAG	C3-C2-N2-C7
3	C	2	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	1	0
3	C	2	NAG	2	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	0.82	1 (7%)	17,19,21	1.11	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	2.62	1.48	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1301	NAG	C1-O5-C5	4.27	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.

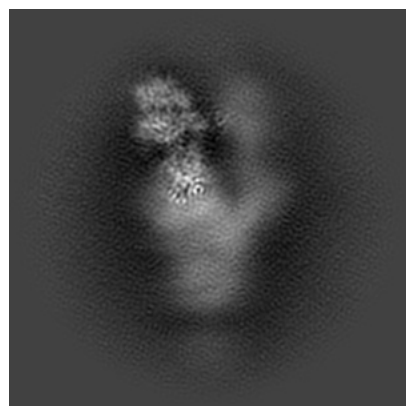
6 Map visualisation [i](#)

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.

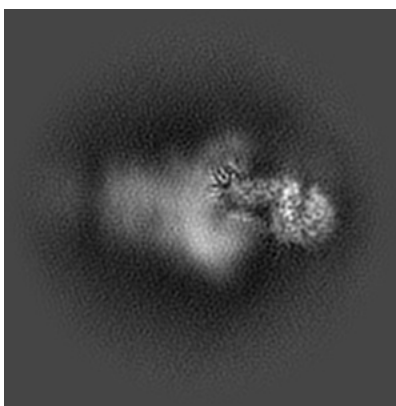
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

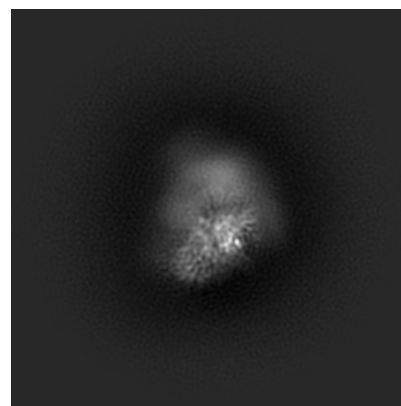
6.1.1 Primary map



X

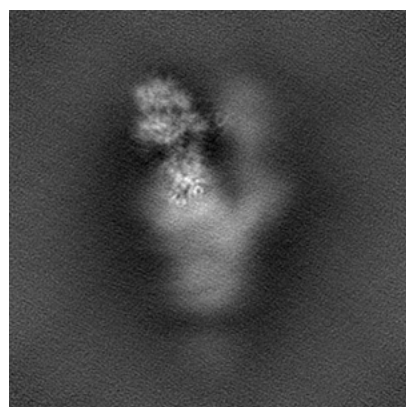


Y

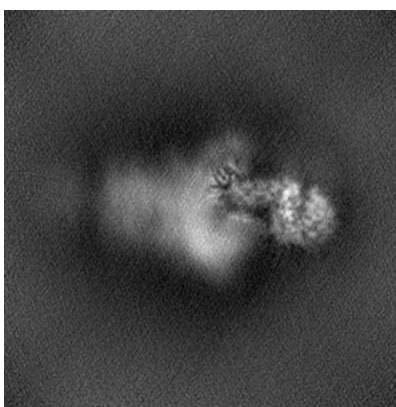


Z

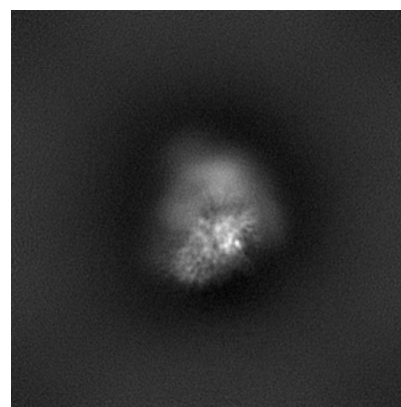
6.1.2 Raw map



X



Y

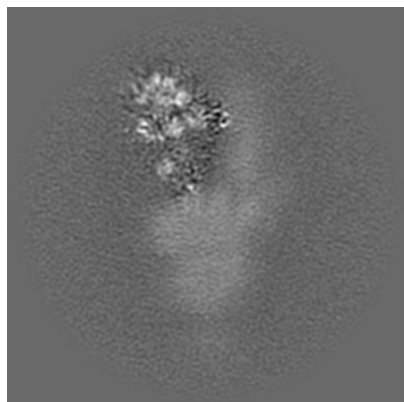


Z

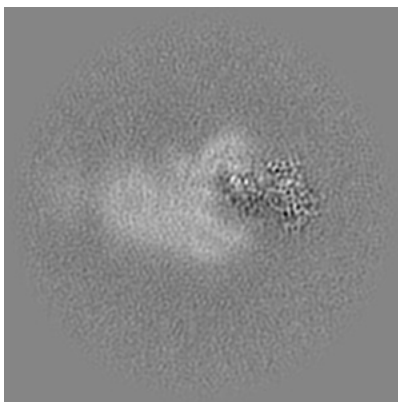
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

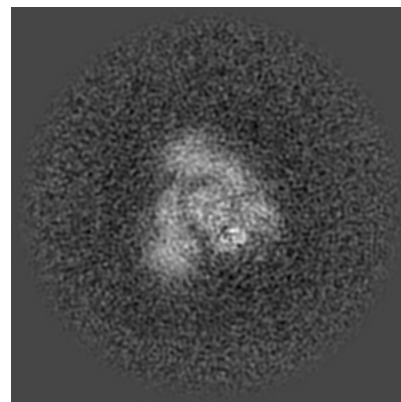
6.2.1 Primary map



X Index: 140

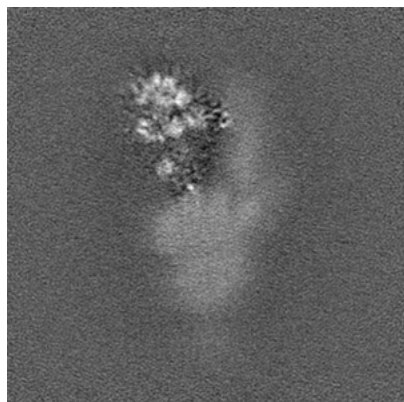


Y Index: 140

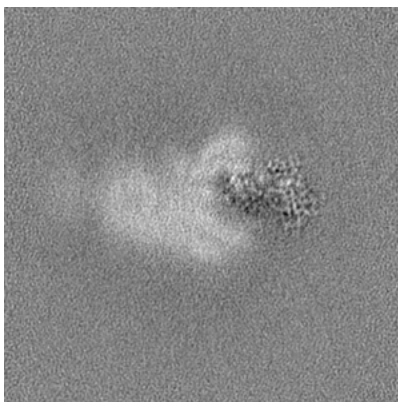


Z Index: 140

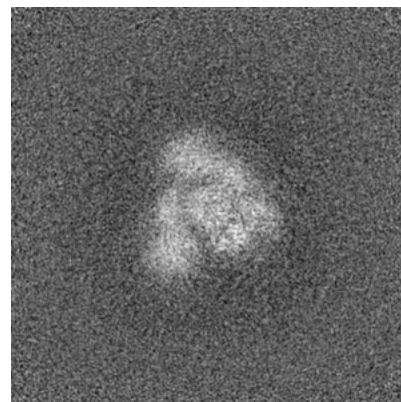
6.2.2 Raw map



X Index: 140



Y Index: 140



Z Index: 140

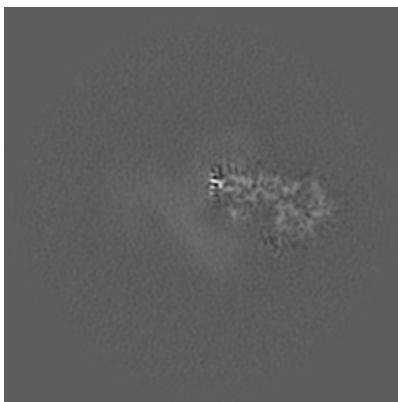
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

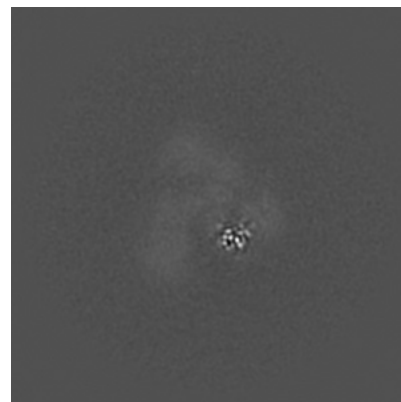
6.3.1 Primary map



X Index: 152

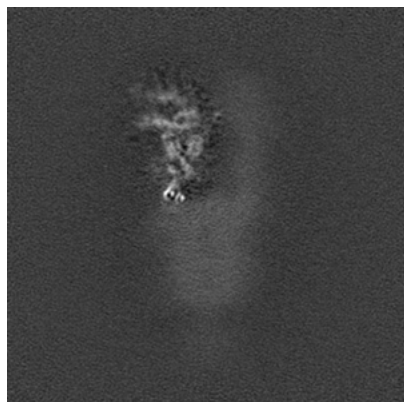


Y Index: 117

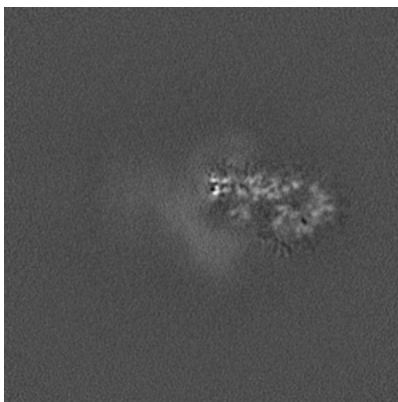


Z Index: 146

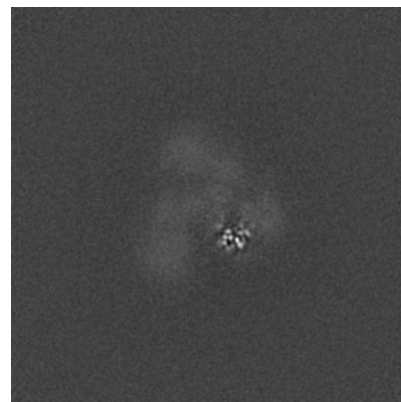
6.3.2 Raw map



X Index: 151



Y Index: 115

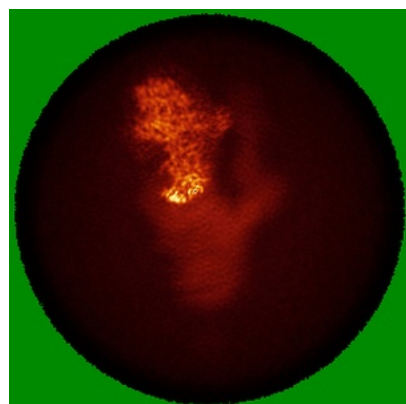


Z Index: 146

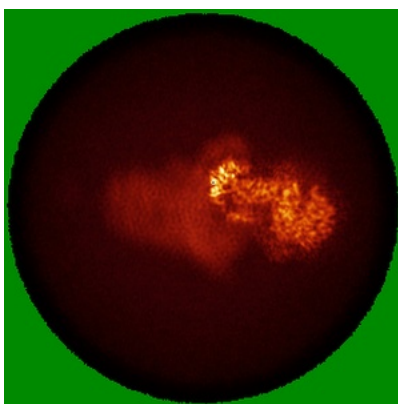
The images above show the largest variance slices of the map in three orthogonal directions.

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

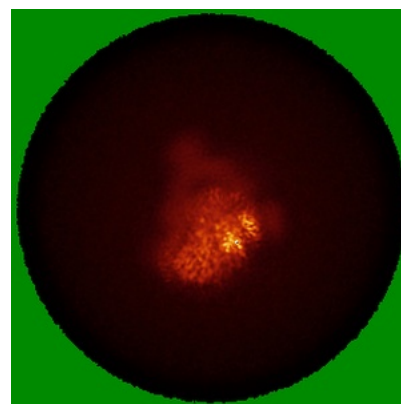
6.4.1 Primary map



X

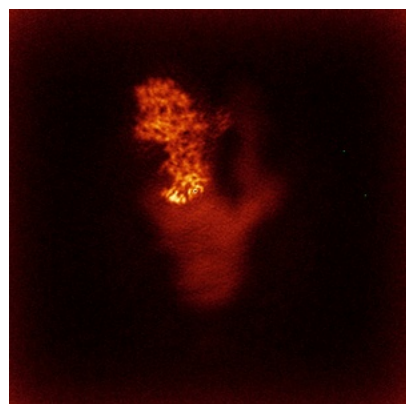


Y

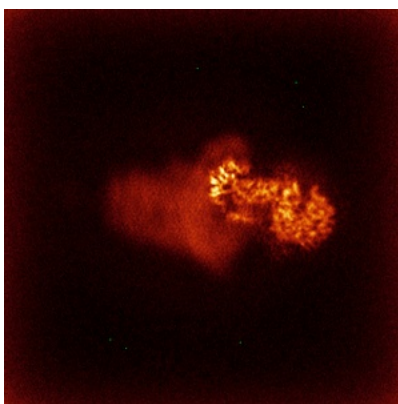


Z

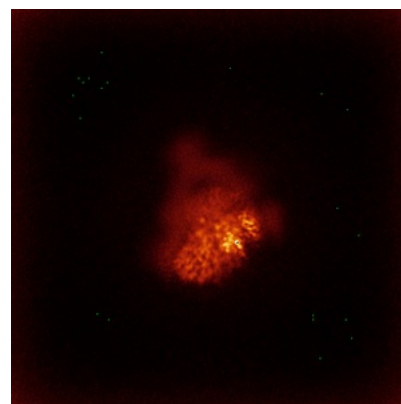
6.4.2 Raw map



X



Y

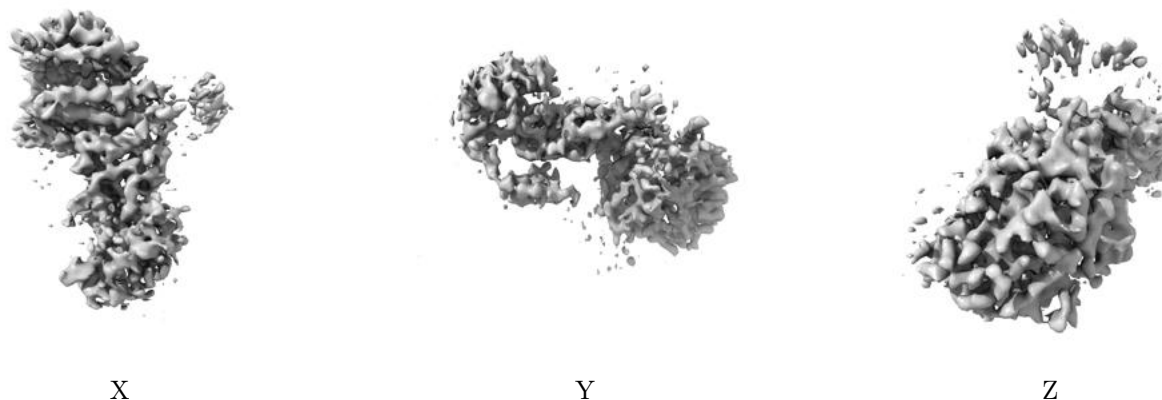


Z

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



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.

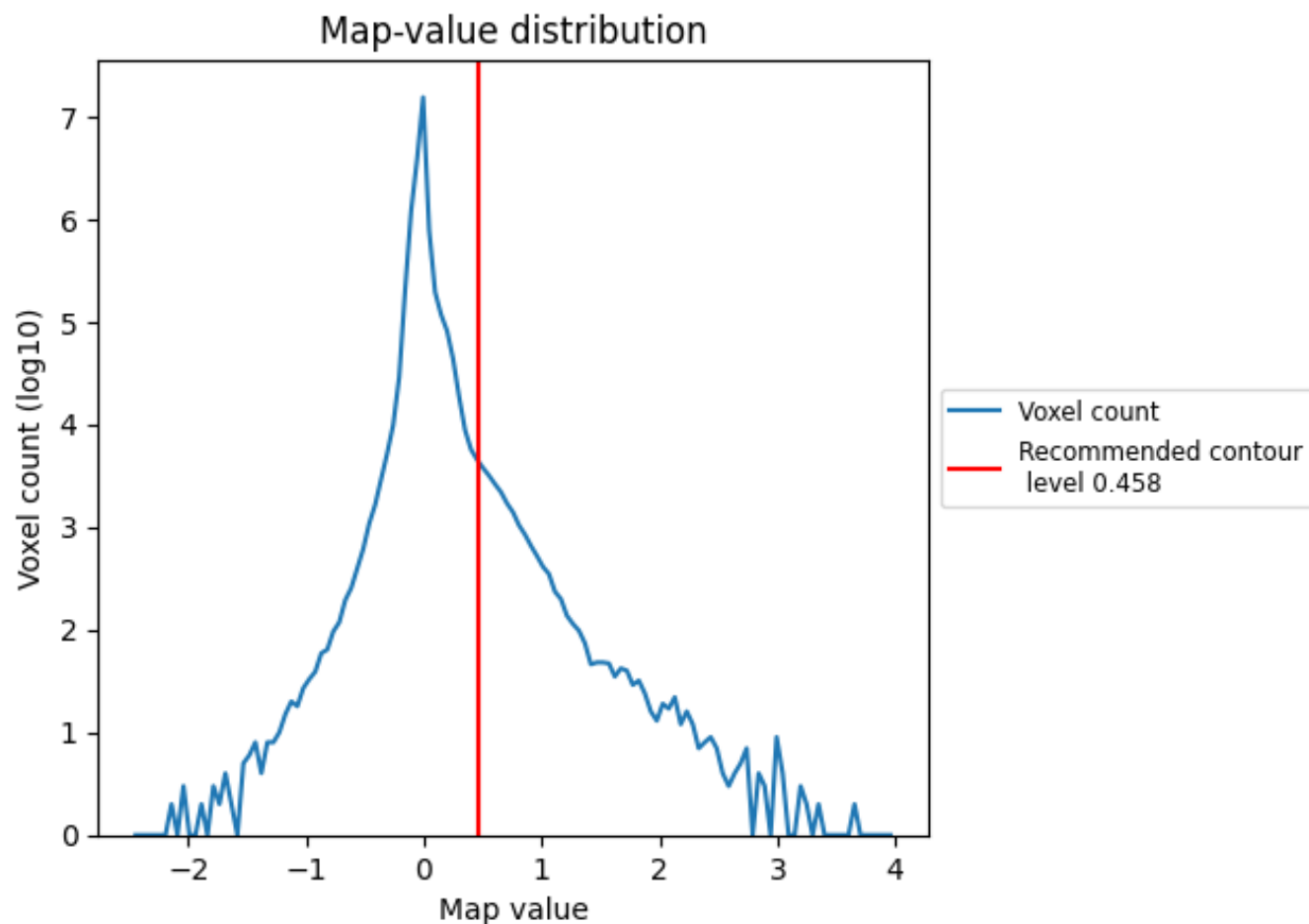
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

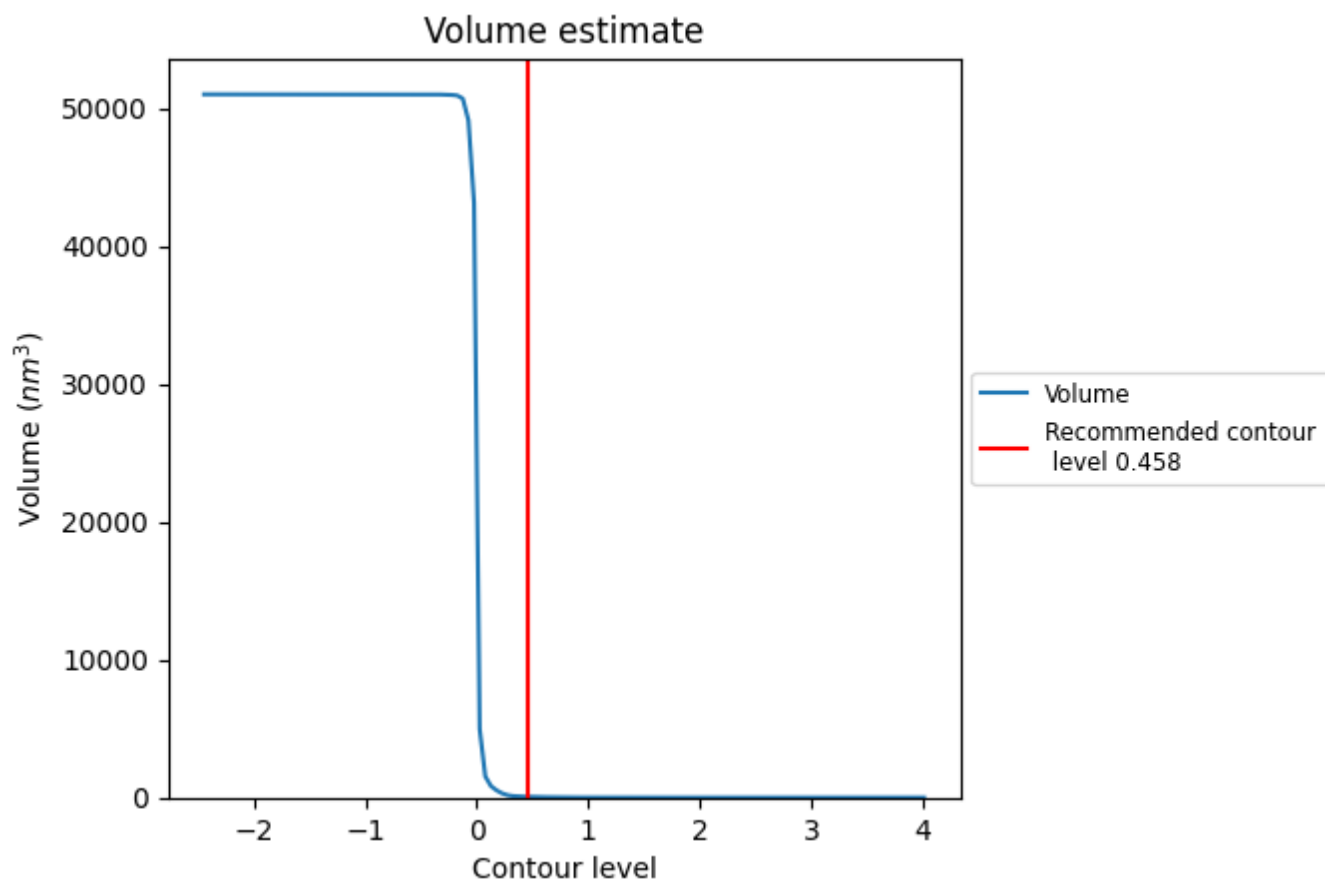
This section contains the results of statistical analysis of the map.

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.

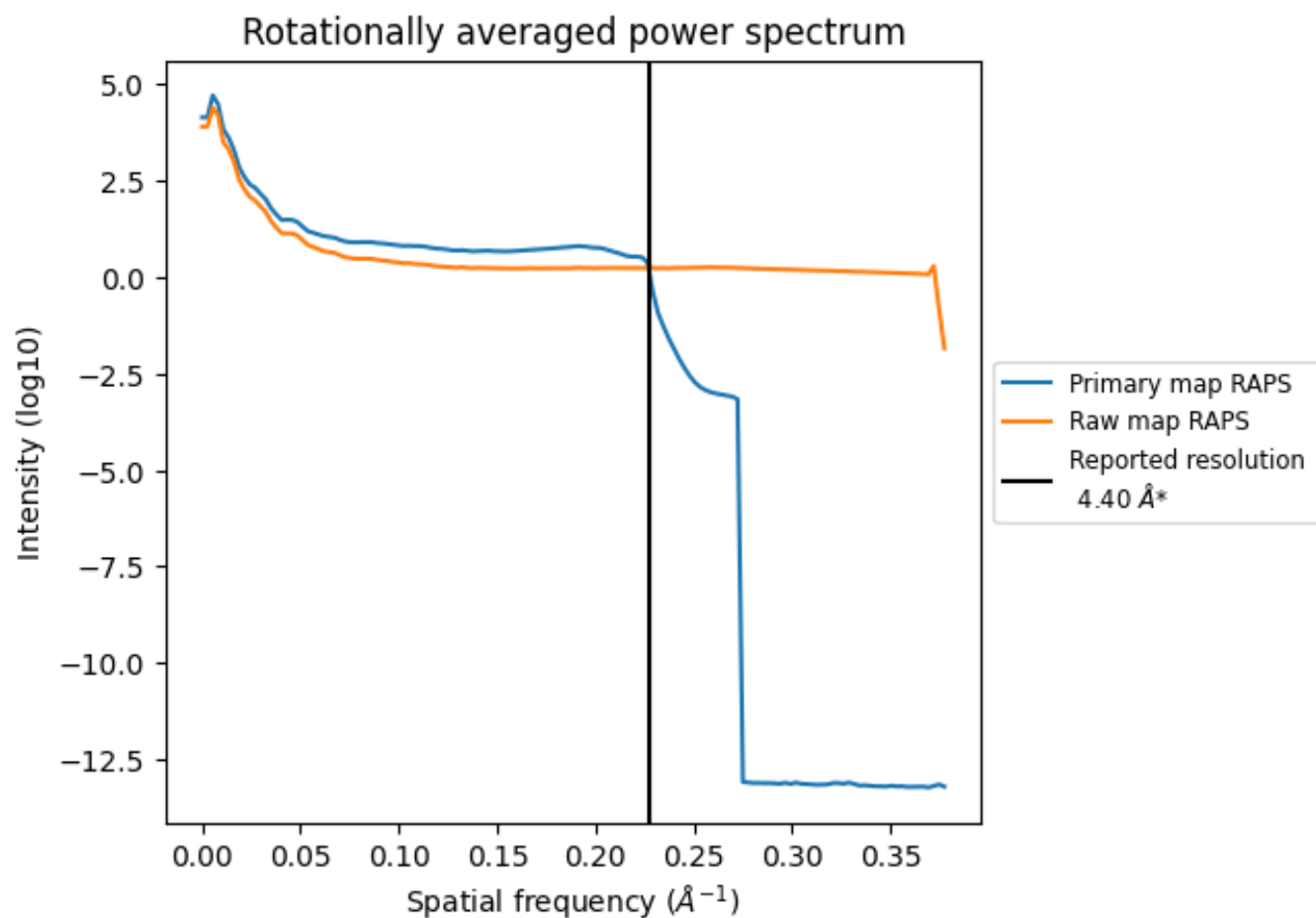
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 56 nm³; 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 ⓘ

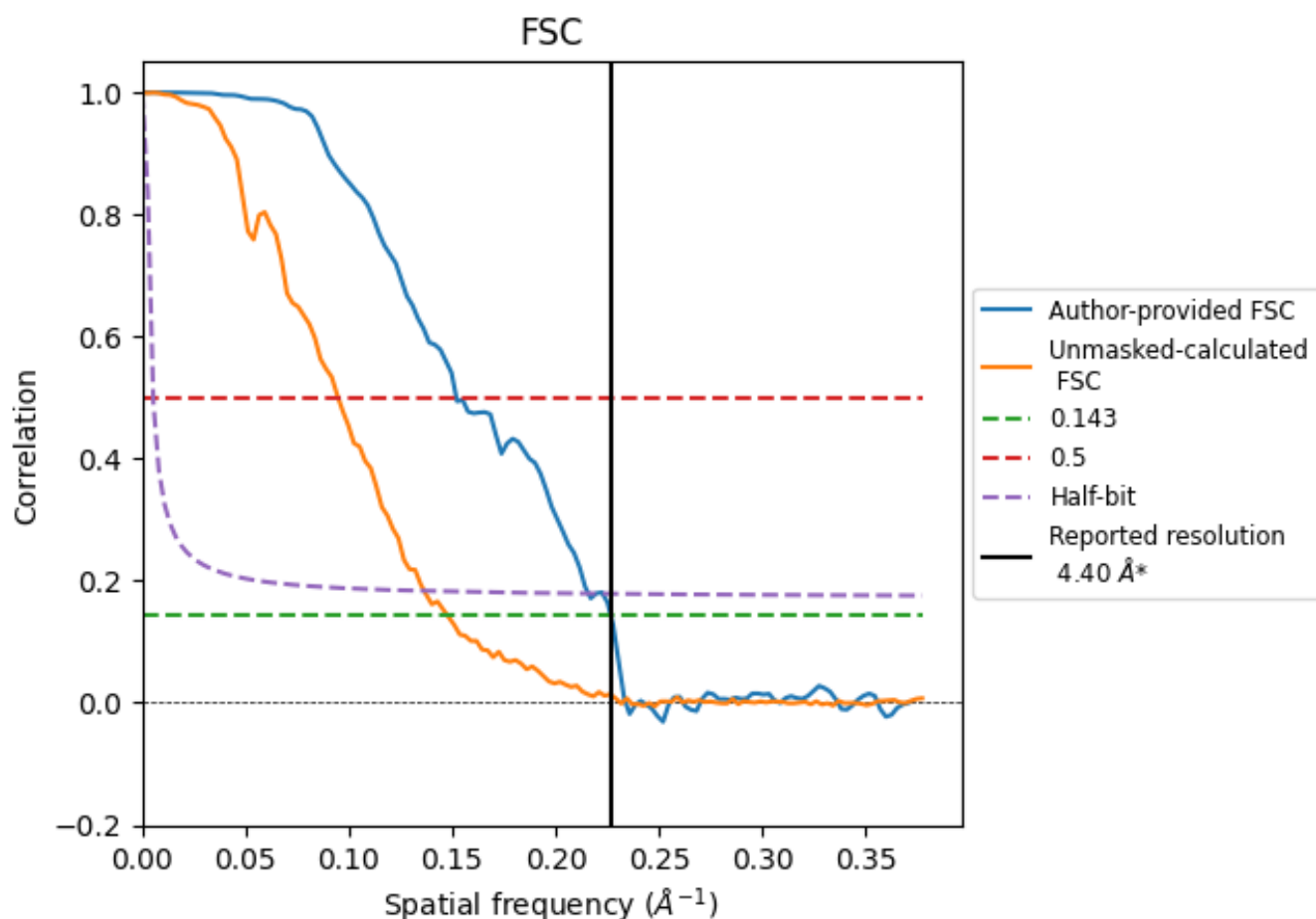


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

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 0.227 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	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 [i](#)

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 [i](#)

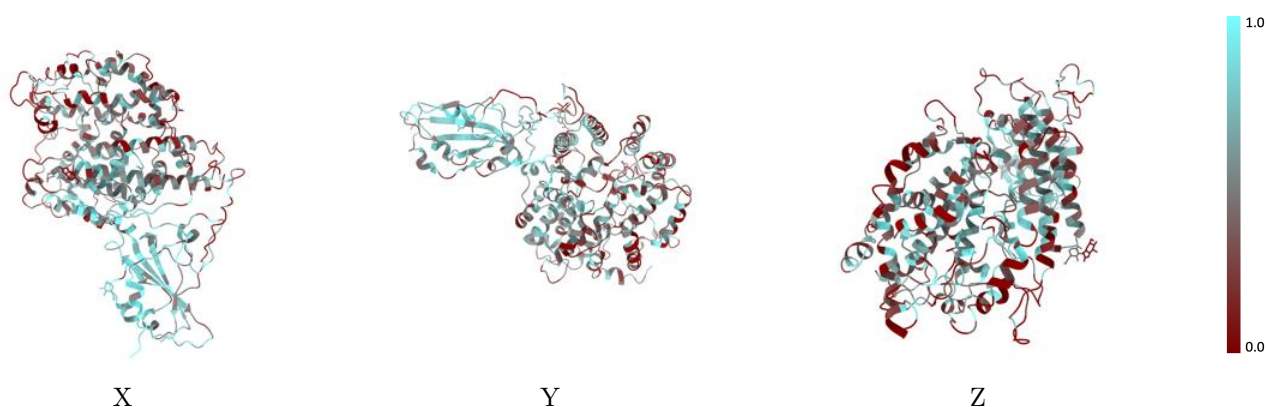
This section was not generated.

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



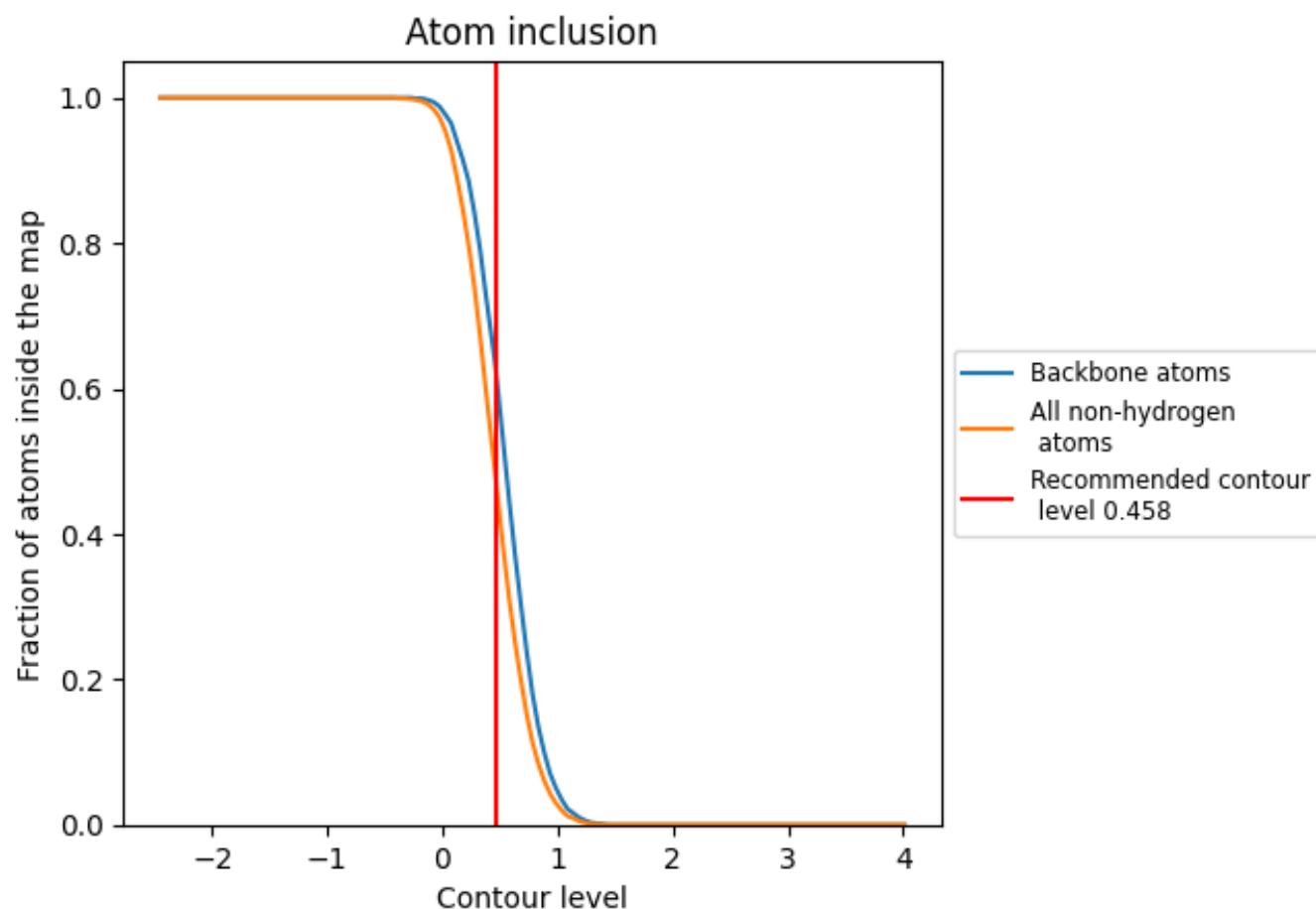
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.458).

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

