



wwPDB EM Validation Summary Report ⓘ

Sep 22, 2026 – 04:18 PM JST

PDB ID : 21BP / pdb_000021bp
EMDB ID : EMD-67557
Title : CryoEM structure of H5N1 A/Texas/37/2024 HA bound to 3BG3 IgG
Authors : Niu, C.; Liu, B.; Li, Z.; Xiong, X.
Deposited on : 2025-12-06
Resolution : 3.06 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

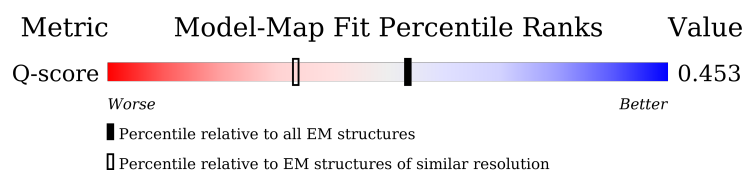
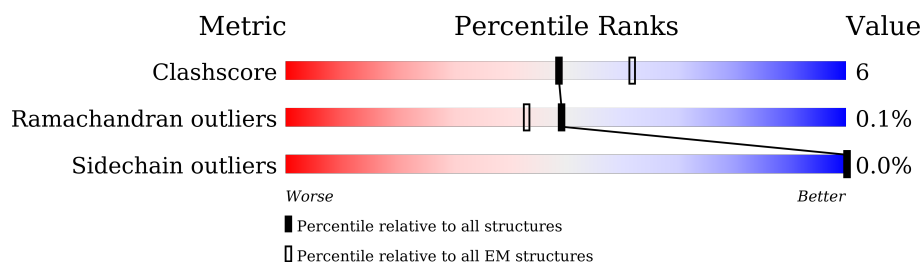
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.06 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.



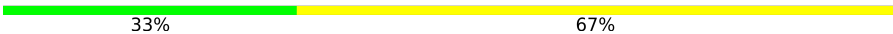
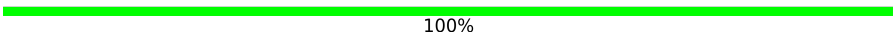
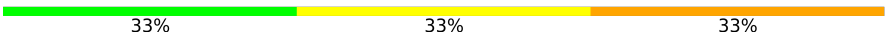
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13976 (2.56 - 3.56)

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	D	452	
1	F	452	
1	H	452	
2	A	552	

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Mol	Chain	Length	Quality of chain
2	B	552	 79% 10% 11%
2	C	552	 77% 11% 11%
3	E	211	 43% 88% 12%
3	G	211	 43% 84% 16%
3	L	211	 42% 84% 15%
4	I	3	 33% 67%
4	J	3	 100%
4	K	3	 33% 33% 33%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21801 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 The heavy chain of 3BG3 IgG.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	226	Total	C	N	O	S	0	0
			1682	1060	282	334	6		
1	F	226	Total	C	N	O	S	0	0
			1682	1060	282	334	6		
1	H	226	Total	C	N	O	S	0	0
			1682	1060	282	334	6		

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	491	Total	C	N	O	S	0	0
			3927	2471	683	750	23		
2	B	491	Total	C	N	O	S	0	0
			3927	2471	683	750	23		
2	A	491	Total	C	N	O	S	0	0
			3927	2471	683	750	23		

There are 147 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	195	ILE	THR	conflict	UNP A0AAX6NN08
C	505	SER	-	expression tag	UNP A0AAX6NN08
C	506	GLY	-	expression tag	UNP A0AAX6NN08
C	507	ARG	-	expression tag	UNP A0AAX6NN08
C	508	GLU	-	expression tag	UNP A0AAX6NN08
C	509	ASN	-	expression tag	UNP A0AAX6NN08
C	510	LEU	-	expression tag	UNP A0AAX6NN08
C	511	TYR	-	expression tag	UNP A0AAX6NN08
C	512	PHE	-	expression tag	UNP A0AAX6NN08
C	513	GLN	-	expression tag	UNP A0AAX6NN08
C	514	GLY	-	expression tag	UNP A0AAX6NN08
C	515	GLY	-	expression tag	UNP A0AAX6NN08
C	516	GLY	-	expression tag	UNP A0AAX6NN08

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Chain	Residue	Modelled	Actual	Comment	Reference
C	517	GLY	-	expression tag	UNP A0AAX6NN08
C	518	SER	-	expression tag	UNP A0AAX6NN08
C	519	GLY	-	expression tag	UNP A0AAX6NN08
C	520	TYR	-	expression tag	UNP A0AAX6NN08
C	521	ILE	-	expression tag	UNP A0AAX6NN08
C	522	PRO	-	expression tag	UNP A0AAX6NN08
C	523	GLU	-	expression tag	UNP A0AAX6NN08
C	524	ALA	-	expression tag	UNP A0AAX6NN08
C	525	PRO	-	expression tag	UNP A0AAX6NN08
C	526	ARG	-	expression tag	UNP A0AAX6NN08
C	527	ASP	-	expression tag	UNP A0AAX6NN08
C	528	GLY	-	expression tag	UNP A0AAX6NN08
C	529	GLN	-	expression tag	UNP A0AAX6NN08
C	530	ALA	-	expression tag	UNP A0AAX6NN08
C	531	TYR	-	expression tag	UNP A0AAX6NN08
C	532	VAL	-	expression tag	UNP A0AAX6NN08
C	533	ARG	-	expression tag	UNP A0AAX6NN08
C	534	LYS	-	expression tag	UNP A0AAX6NN08
C	535	ASP	-	expression tag	UNP A0AAX6NN08
C	536	GLY	-	expression tag	UNP A0AAX6NN08
C	537	GLU	-	expression tag	UNP A0AAX6NN08
C	538	TRP	-	expression tag	UNP A0AAX6NN08
C	539	VAL	-	expression tag	UNP A0AAX6NN08
C	540	LEU	-	expression tag	UNP A0AAX6NN08
C	541	LEU	-	expression tag	UNP A0AAX6NN08
C	542	SER	-	expression tag	UNP A0AAX6NN08
C	543	THR	-	expression tag	UNP A0AAX6NN08
C	544	PHE	-	expression tag	UNP A0AAX6NN08
C	545	LEU	-	expression tag	UNP A0AAX6NN08
C	546	GLY	-	expression tag	UNP A0AAX6NN08
C	547	HIS	-	expression tag	UNP A0AAX6NN08
C	548	HIS	-	expression tag	UNP A0AAX6NN08
C	549	HIS	-	expression tag	UNP A0AAX6NN08
C	550	HIS	-	expression tag	UNP A0AAX6NN08
C	551	HIS	-	expression tag	UNP A0AAX6NN08
C	552	HIS	-	expression tag	UNP A0AAX6NN08
B	195	ILE	THR	conflict	UNP A0AAX6NN08
B	505	SER	-	expression tag	UNP A0AAX6NN08
B	506	GLY	-	expression tag	UNP A0AAX6NN08
B	507	ARG	-	expression tag	UNP A0AAX6NN08
B	508	GLU	-	expression tag	UNP A0AAX6NN08
B	509	ASN	-	expression tag	UNP A0AAX6NN08

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Chain	Residue	Modelled	Actual	Comment	Reference
B	510	LEU	-	expression tag	UNP A0AAX6NN08
B	511	TYR	-	expression tag	UNP A0AAX6NN08
B	512	PHE	-	expression tag	UNP A0AAX6NN08
B	513	GLN	-	expression tag	UNP A0AAX6NN08
B	514	GLY	-	expression tag	UNP A0AAX6NN08
B	515	GLY	-	expression tag	UNP A0AAX6NN08
B	516	GLY	-	expression tag	UNP A0AAX6NN08
B	517	GLY	-	expression tag	UNP A0AAX6NN08
B	518	SER	-	expression tag	UNP A0AAX6NN08
B	519	GLY	-	expression tag	UNP A0AAX6NN08
B	520	TYR	-	expression tag	UNP A0AAX6NN08
B	521	ILE	-	expression tag	UNP A0AAX6NN08
B	522	PRO	-	expression tag	UNP A0AAX6NN08
B	523	GLU	-	expression tag	UNP A0AAX6NN08
B	524	ALA	-	expression tag	UNP A0AAX6NN08
B	525	PRO	-	expression tag	UNP A0AAX6NN08
B	526	ARG	-	expression tag	UNP A0AAX6NN08
B	527	ASP	-	expression tag	UNP A0AAX6NN08
B	528	GLY	-	expression tag	UNP A0AAX6NN08
B	529	GLN	-	expression tag	UNP A0AAX6NN08
B	530	ALA	-	expression tag	UNP A0AAX6NN08
B	531	TYR	-	expression tag	UNP A0AAX6NN08
B	532	VAL	-	expression tag	UNP A0AAX6NN08
B	533	ARG	-	expression tag	UNP A0AAX6NN08
B	534	LYS	-	expression tag	UNP A0AAX6NN08
B	535	ASP	-	expression tag	UNP A0AAX6NN08
B	536	GLY	-	expression tag	UNP A0AAX6NN08
B	537	GLU	-	expression tag	UNP A0AAX6NN08
B	538	TRP	-	expression tag	UNP A0AAX6NN08
B	539	VAL	-	expression tag	UNP A0AAX6NN08
B	540	LEU	-	expression tag	UNP A0AAX6NN08
B	541	LEU	-	expression tag	UNP A0AAX6NN08
B	542	SER	-	expression tag	UNP A0AAX6NN08
B	543	THR	-	expression tag	UNP A0AAX6NN08
B	544	PHE	-	expression tag	UNP A0AAX6NN08
B	545	LEU	-	expression tag	UNP A0AAX6NN08
B	546	GLY	-	expression tag	UNP A0AAX6NN08
B	547	HIS	-	expression tag	UNP A0AAX6NN08
B	548	HIS	-	expression tag	UNP A0AAX6NN08
B	549	HIS	-	expression tag	UNP A0AAX6NN08
B	550	HIS	-	expression tag	UNP A0AAX6NN08
B	551	HIS	-	expression tag	UNP A0AAX6NN08

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Chain	Residue	Modelled	Actual	Comment	Reference
B	552	HIS	-	expression tag	UNP A0AAX6NN08
A	195	ILE	THR	conflict	UNP A0AAX6NN08
A	505	SER	-	expression tag	UNP A0AAX6NN08
A	506	GLY	-	expression tag	UNP A0AAX6NN08
A	507	ARG	-	expression tag	UNP A0AAX6NN08
A	508	GLU	-	expression tag	UNP A0AAX6NN08
A	509	ASN	-	expression tag	UNP A0AAX6NN08
A	510	LEU	-	expression tag	UNP A0AAX6NN08
A	511	TYR	-	expression tag	UNP A0AAX6NN08
A	512	PHE	-	expression tag	UNP A0AAX6NN08
A	513	GLN	-	expression tag	UNP A0AAX6NN08
A	514	GLY	-	expression tag	UNP A0AAX6NN08
A	515	GLY	-	expression tag	UNP A0AAX6NN08
A	516	GLY	-	expression tag	UNP A0AAX6NN08
A	517	GLY	-	expression tag	UNP A0AAX6NN08
A	518	SER	-	expression tag	UNP A0AAX6NN08
A	519	GLY	-	expression tag	UNP A0AAX6NN08
A	520	TYR	-	expression tag	UNP A0AAX6NN08
A	521	ILE	-	expression tag	UNP A0AAX6NN08
A	522	PRO	-	expression tag	UNP A0AAX6NN08
A	523	GLU	-	expression tag	UNP A0AAX6NN08
A	524	ALA	-	expression tag	UNP A0AAX6NN08
A	525	PRO	-	expression tag	UNP A0AAX6NN08
A	526	ARG	-	expression tag	UNP A0AAX6NN08
A	527	ASP	-	expression tag	UNP A0AAX6NN08
A	528	GLY	-	expression tag	UNP A0AAX6NN08
A	529	GLN	-	expression tag	UNP A0AAX6NN08
A	530	ALA	-	expression tag	UNP A0AAX6NN08
A	531	TYR	-	expression tag	UNP A0AAX6NN08
A	532	VAL	-	expression tag	UNP A0AAX6NN08
A	533	ARG	-	expression tag	UNP A0AAX6NN08
A	534	LYS	-	expression tag	UNP A0AAX6NN08
A	535	ASP	-	expression tag	UNP A0AAX6NN08
A	536	GLY	-	expression tag	UNP A0AAX6NN08
A	537	GLU	-	expression tag	UNP A0AAX6NN08
A	538	TRP	-	expression tag	UNP A0AAX6NN08
A	539	VAL	-	expression tag	UNP A0AAX6NN08
A	540	LEU	-	expression tag	UNP A0AAX6NN08
A	541	LEU	-	expression tag	UNP A0AAX6NN08
A	542	SER	-	expression tag	UNP A0AAX6NN08
A	543	THR	-	expression tag	UNP A0AAX6NN08
A	544	PHE	-	expression tag	UNP A0AAX6NN08

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Chain	Residue	Modelled	Actual	Comment	Reference
A	545	LEU	-	expression tag	UNP A0AAX6NN08
A	546	GLY	-	expression tag	UNP A0AAX6NN08
A	547	HIS	-	expression tag	UNP A0AAX6NN08
A	548	HIS	-	expression tag	UNP A0AAX6NN08
A	549	HIS	-	expression tag	UNP A0AAX6NN08
A	550	HIS	-	expression tag	UNP A0AAX6NN08
A	551	HIS	-	expression tag	UNP A0AAX6NN08
A	552	HIS	-	expression tag	UNP A0AAX6NN08

- Molecule 3 is a protein called The light chain of 3BG3 IgG.

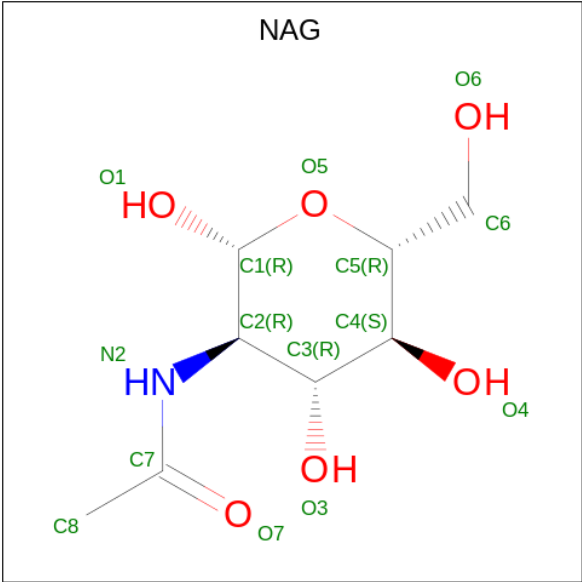
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	211	Total	C	N	O	S	0	0
			1577	985	265	322	5		
3	G	211	Total	C	N	O	S	0	0
			1577	985	265	322	5		
3	L	211	Total	C	N	O	S	0	0
			1577	985	265	322	5		

- 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.

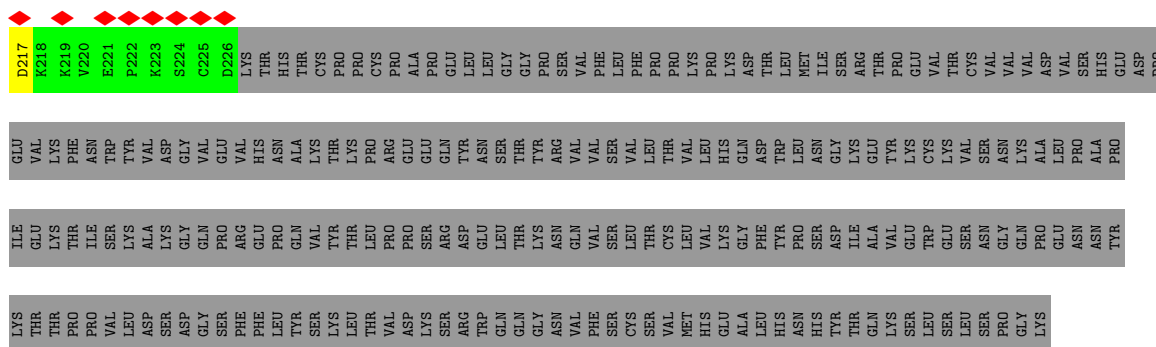


Mol	Chain	Residues	Atoms				AltConf	Trace
4	I	3	Total	C	N	O	0	0
			39	22	2	15		
4	J	3	Total	C	N	O	0	0
			39	22	2	15		
4	K	3	Total	C	N	O	0	0
			39	22	2	15		

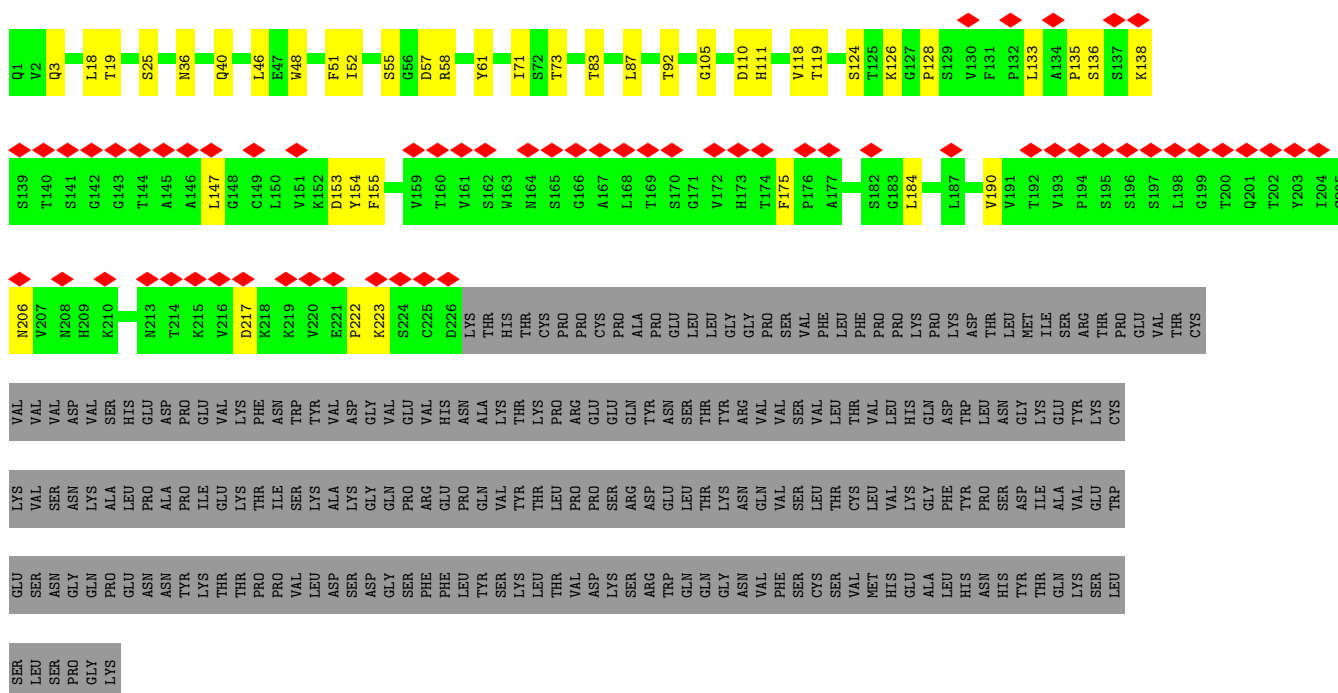
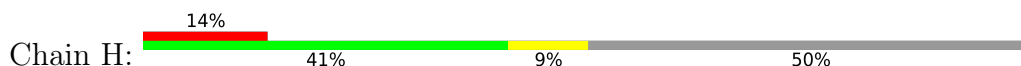
- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



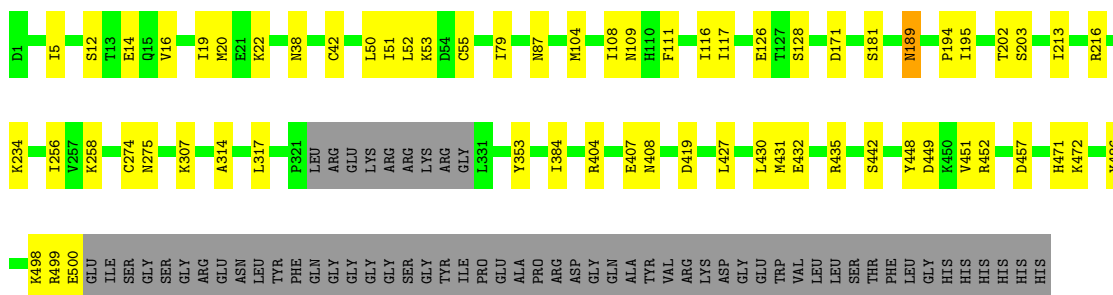
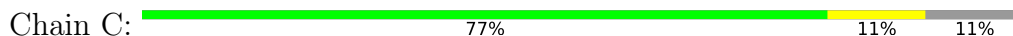
Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5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



- Molecule 1: The heavy chain of 3BG3 IgG

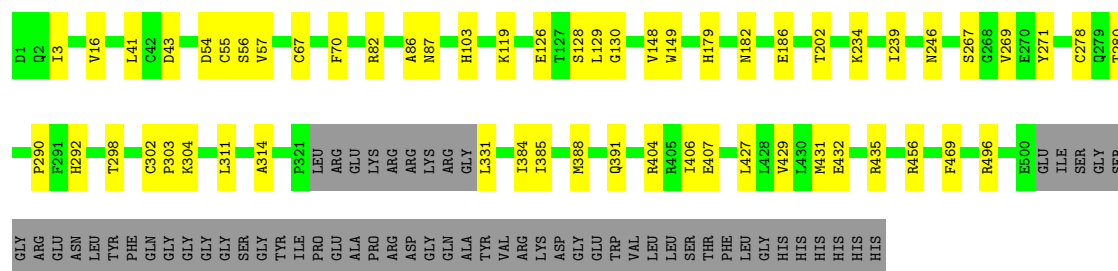


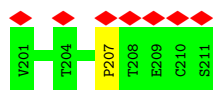
- Molecule 2: Hemagglutinin



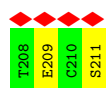
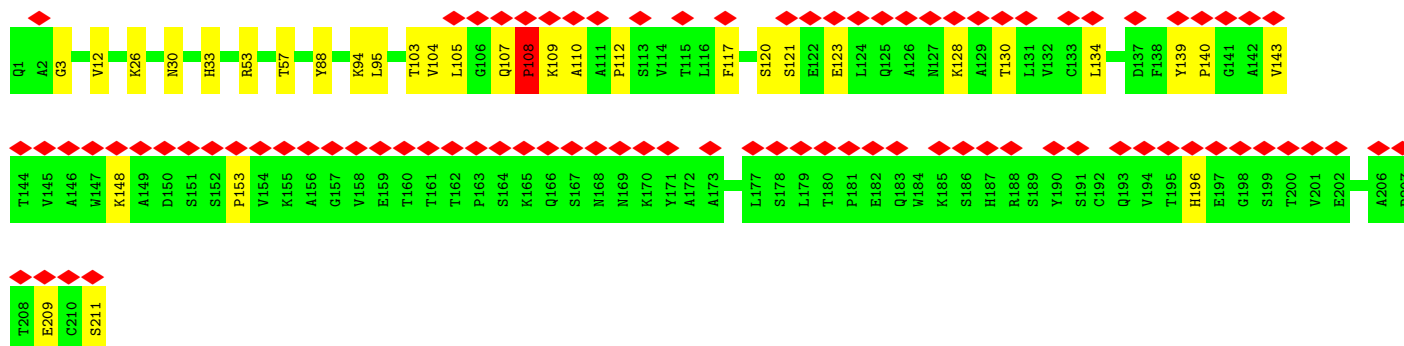
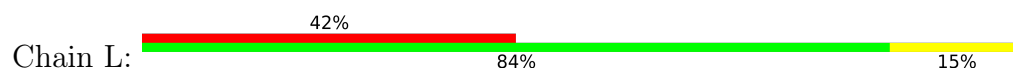
- Molecule 2: Hemagglutinin

Chain B: 

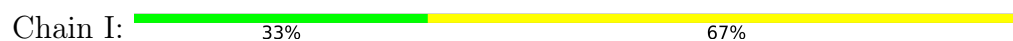




- Molecule 3: The light chain of 3BG3 IgG



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



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



- 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	120969	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.865	Depositor
Minimum map value	-1.680	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	337.92, 337.92, 337.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.32, 1.32, 1.32	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, 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	D	0.21	0/1725	0.35	0/2355
1	F	0.17	0/1725	0.34	0/2355
1	H	0.18	0/1725	0.35	0/2355
2	A	0.18	0/4018	0.36	0/5441
2	B	0.12	0/4018	0.32	0/5441
2	C	0.12	0/4018	0.32	0/5441
3	E	0.23	0/1615	0.35	0/2202
3	G	0.24	0/1615	0.33	0/2202
3	L	0.25	0/1615	0.42	1/2202 (0.0%)
All	All	0.18	0/22074	0.34	1/29994 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	108	PRO	CA-N-CD	-9.49	98.72	112.00

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	D	1682	0	1650	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1682	0	1650	22	0
1	H	1682	0	1650	35	0
2	A	3927	0	3783	46	0
2	B	3927	0	3783	38	0
2	C	3927	0	3783	44	0
3	E	1577	0	1530	19	0
3	G	1577	0	1530	23	0
3	L	1577	0	1530	39	0
4	I	39	0	34	1	0
4	J	39	0	34	0	0
4	K	39	0	34	2	0
5	A	42	0	39	0	0
5	B	42	0	39	0	0
5	C	42	0	39	1	0
All	All	21801	0	21108	247	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 6.

The worst 5 of 247 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:L:108:PRO:HD2	3:L:139:TYR:CE1	1.07	1.59
3:L:108:PRO:CD	3:L:139:TYR:CE1	1.98	1.45
2:B:456:ARG:NH2	2:A:462:LEU:O	1.81	1.12
3:L:108:PRO:CD	3:L:139:TYR:HE1	1.48	1.09
2:B:496:ARG:NH2	2:A:500:GLU:OE1	1.94	1.00

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	D	224/452 (50%)	218 (97%)	6 (3%)	0	100	100
1	F	224/452 (50%)	212 (95%)	12 (5%)	0	100	100
1	H	224/452 (50%)	217 (97%)	7 (3%)	0	100	100
2	A	487/552 (88%)	465 (96%)	22 (4%)	0	100	100
2	B	487/552 (88%)	466 (96%)	21 (4%)	0	100	100
2	C	487/552 (88%)	465 (96%)	22 (4%)	0	100	100
3	E	209/211 (99%)	203 (97%)	4 (2%)	2 (1%)	12	37
3	G	209/211 (99%)	204 (98%)	5 (2%)	0	100	100
3	L	209/211 (99%)	204 (98%)	4 (2%)	1 (0%)	24	52
All	All	2760/3645 (76%)	2654 (96%)	103 (4%)	3 (0%)	49	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	108	PRO
3	E	109	LYS
3	E	108	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	193/402 (48%)	193 (100%)	0	100	100
1	F	193/402 (48%)	193 (100%)	0	100	100
1	H	193/402 (48%)	193 (100%)	0	100	100
2	A	431/479 (90%)	431 (100%)	0	100	100
2	B	431/479 (90%)	431 (100%)	0	100	100
2	C	431/479 (90%)	430 (100%)	1 (0%)	87	87
3	E	175/175 (100%)	175 (100%)	0	100	100
3	G	175/175 (100%)	175 (100%)	0	100	100
3	L	175/175 (100%)	175 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2397/3168 (76%)	2396 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	189	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	218	GLN
3	L	16	GLN
3	G	1	GLN
3	L	183	GLN
2	A	458	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

9 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	I	1	2,4	14,14,15	0.27	0	17,19,21	0.68	0
4	NAG	I	2	4	14,14,15	0.19	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	I	3	4	11,11,12	0.61	0	15,15,17	0.74	0
4	NAG	J	1	2,4	14,14,15	0.30	0	17,19,21	0.68	0
4	NAG	J	2	4	14,14,15	0.24	0	17,19,21	0.44	0
4	BMA	J	3	4	11,11,12	0.63	0	15,15,17	0.74	0
4	NAG	K	1	2,4	14,14,15	0.33	0	17,19,21	0.73	1 (5%)
4	NAG	K	2	4	14,14,15	0.29	0	17,19,21	0.69	0
4	BMA	K	3	4	11,11,12	0.23	0	15,15,17	0.58	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	I	1	2,4	-	3/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	BMA	I	3	4	-	1/2/19/22	0/1/1/1
4	NAG	J	1	2,4	-	3/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
4	NAG	K	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	BMA	K	3	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	1	NAG	C1-O5-C5	2.51	115.60	112.19

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

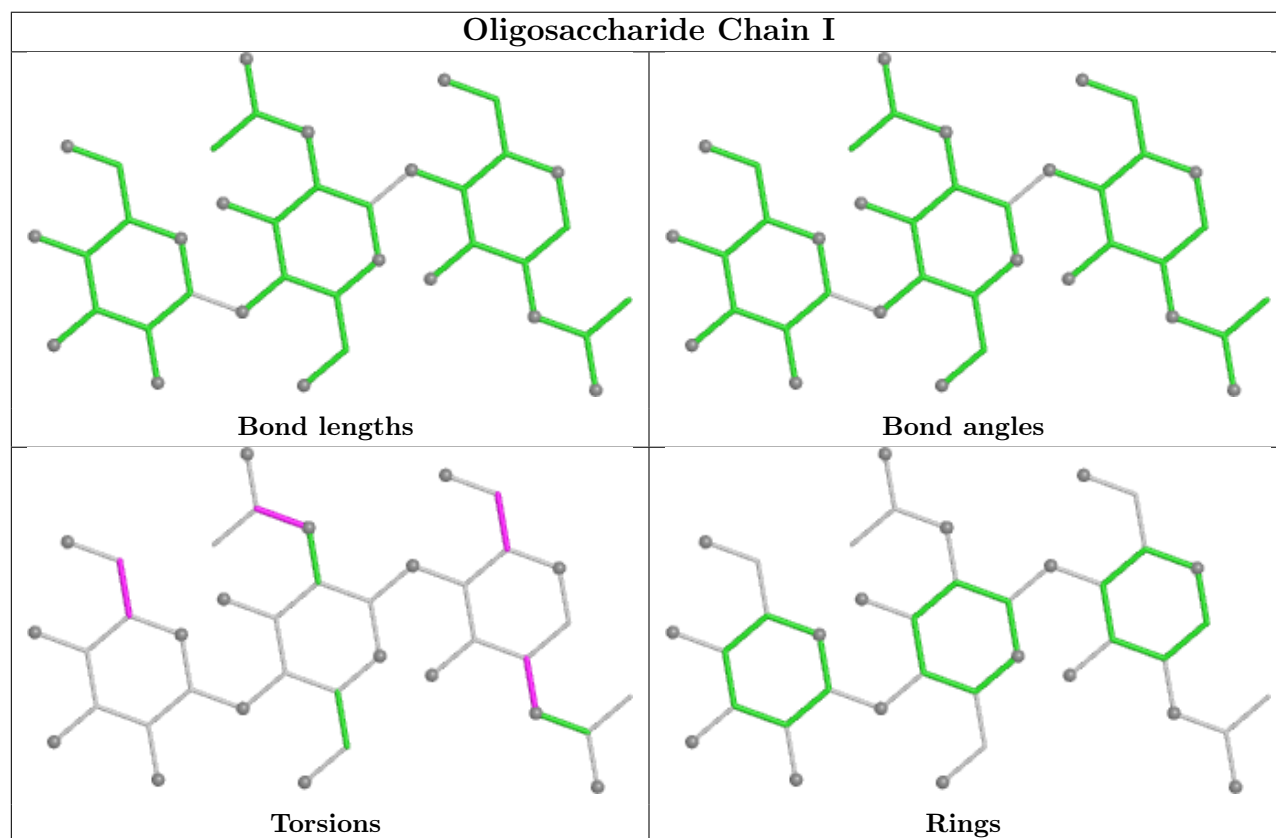
Mol	Chain	Res	Type	Atoms
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
4	I	1	NAG	O5-C5-C6-O6

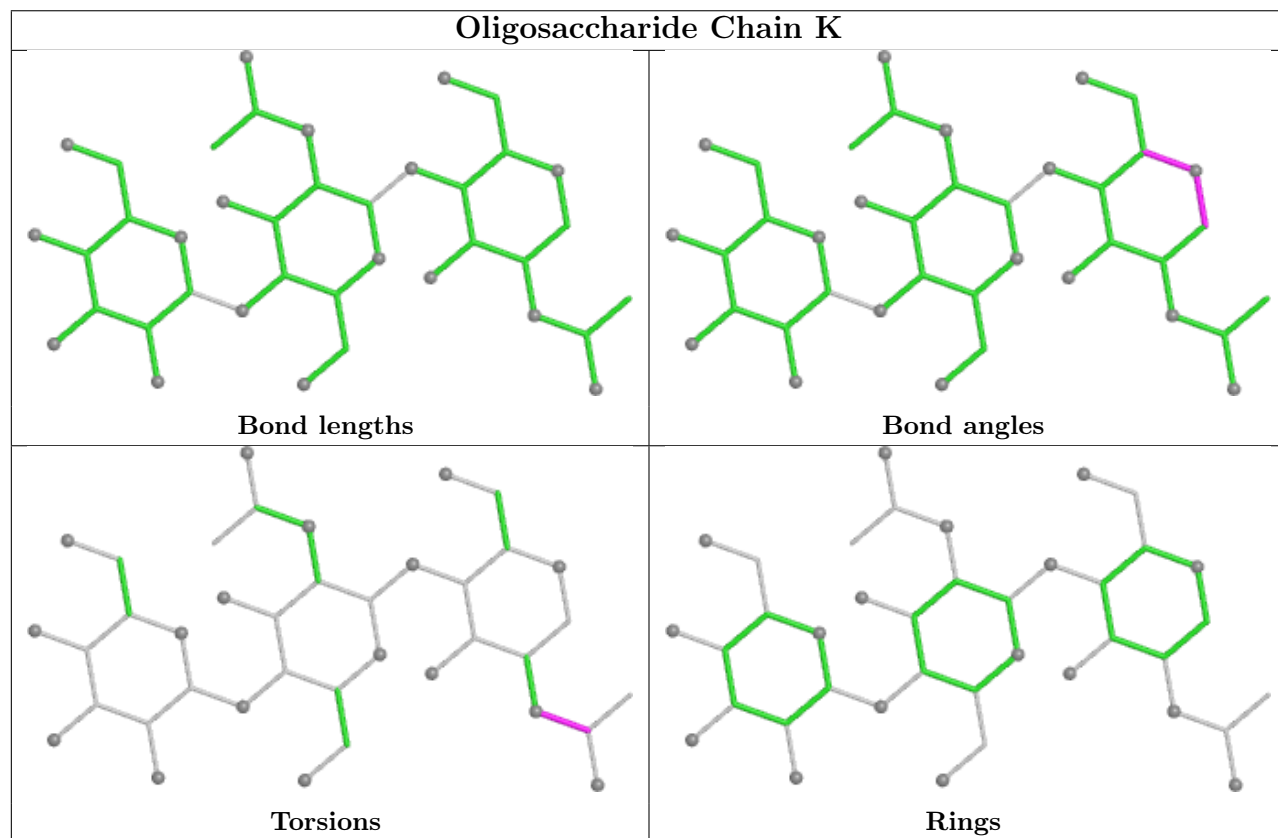
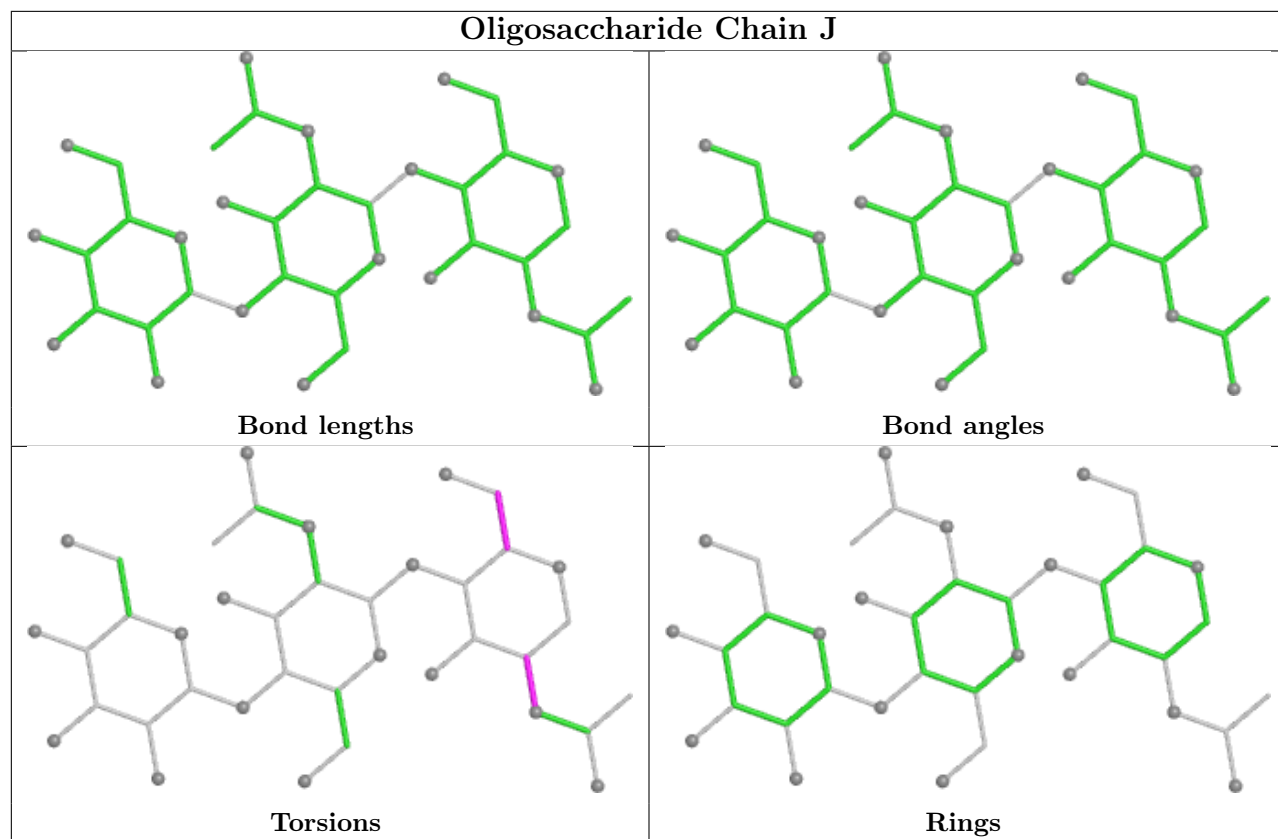
There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	1	NAG	1	0
4	K	1	NAG	2	0
4	K	2	NAG	1	0
4	I	2	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

9 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	B	601	2	14,14,15	0.22	0	17,19,21	0.42	0
5	NAG	C	603	2	14,14,15	0.26	0	17,19,21	0.63	0
5	NAG	A	603	2	14,14,15	0.28	0	17,19,21	0.63	0
5	NAG	B	602	2	14,14,15	0.24	0	17,19,21	0.50	0
5	NAG	A	601	2	14,14,15	0.37	0	17,19,21	0.75	0
5	NAG	B	603	2	14,14,15	0.26	0	17,19,21	0.42	0
5	NAG	A	602	2	14,14,15	0.47	0	17,19,21	0.84	0
5	NAG	C	601	2	14,14,15	0.20	0	17,19,21	0.41	0
5	NAG	C	602	2	14,14,15	0.22	0	17,19,21	0.44	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
5	NAG	B	601	2	-	2/6/23/26	0/1/1/1
5	NAG	C	603	2	-	3/6/23/26	0/1/1/1
5	NAG	A	603	2	-	0/6/23/26	0/1/1/1
5	NAG	B	602	2	-	0/6/23/26	0/1/1/1
5	NAG	A	601	2	-	2/6/23/26	0/1/1/1
5	NAG	B	603	2	-	2/6/23/26	0/1/1/1
5	NAG	A	602	2	-	0/6/23/26	0/1/1/1
5	NAG	C	601	2	-	2/6/23/26	0/1/1/1
5	NAG	C	602	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	601	NAG	C4-C5-C6-O6
5	C	602	NAG	O5-C5-C6-O6
5	B	601	NAG	O5-C5-C6-O6
5	C	601	NAG	C4-C5-C6-O6
5	C	601	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	602	NAG	1	0

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.

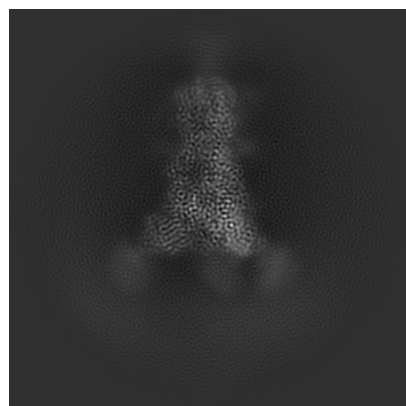
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67557. These allow visual inspection of the internal detail of the map and identification of artifacts.

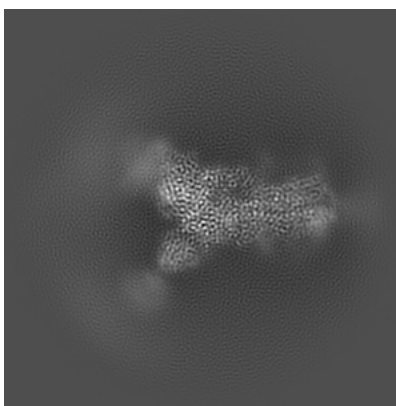
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

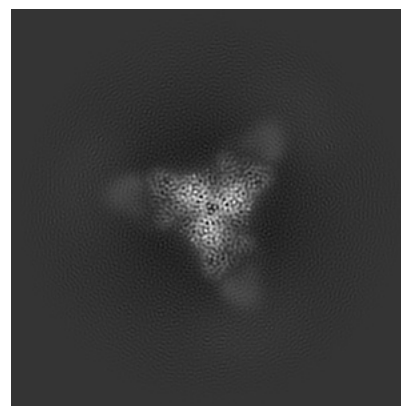
6.1.1 Primary map



X

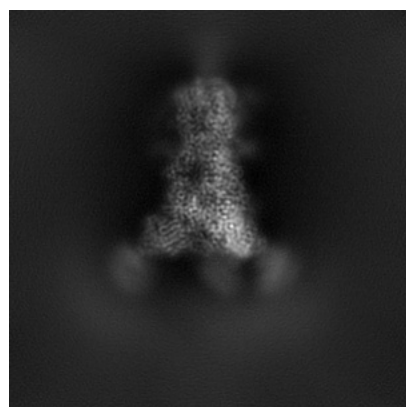


Y

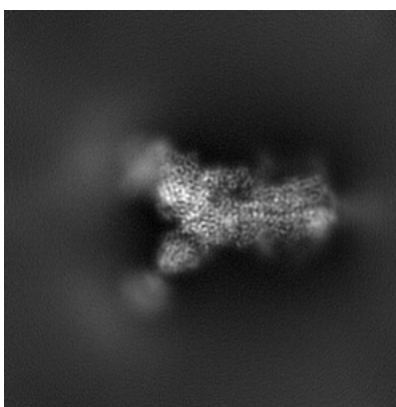


Z

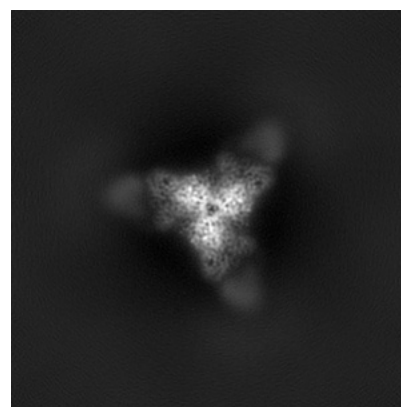
6.1.2 Raw map



X



Y

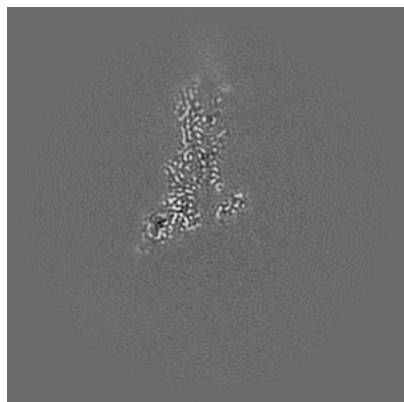


Z

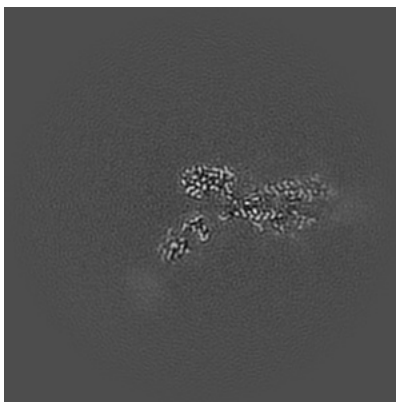
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

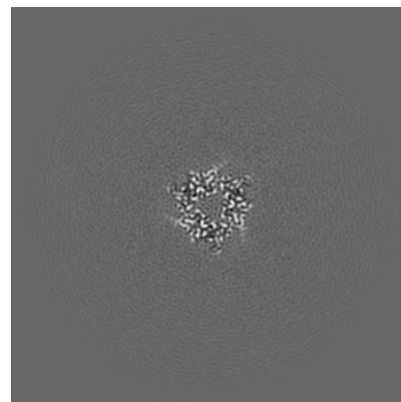
6.2.1 Primary map



X Index: 128

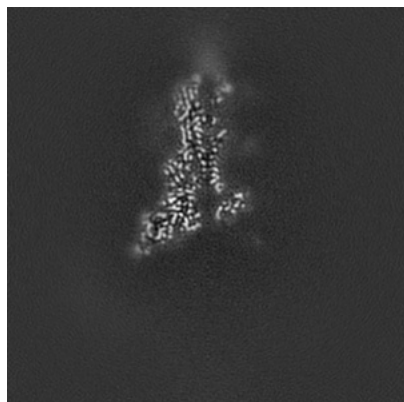


Y Index: 128

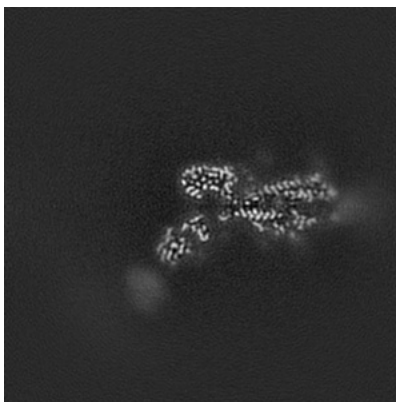


Z Index: 128

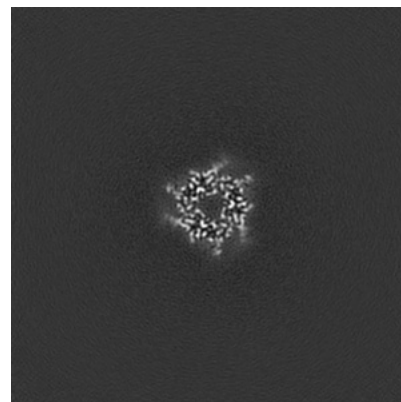
6.2.2 Raw map



X Index: 128



Y Index: 128

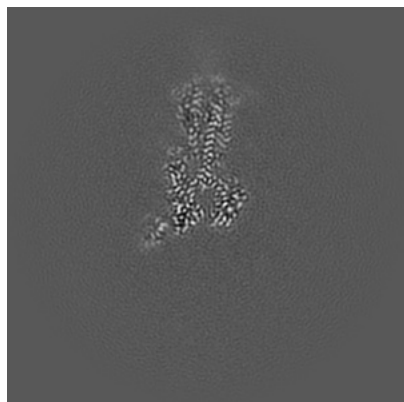


Z Index: 128

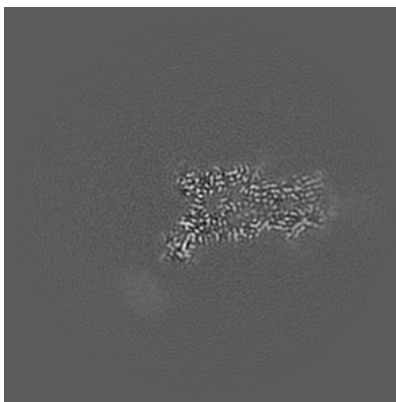
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

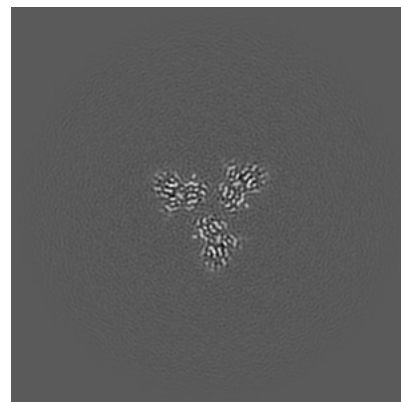
6.3.1 Primary map



X Index: 123

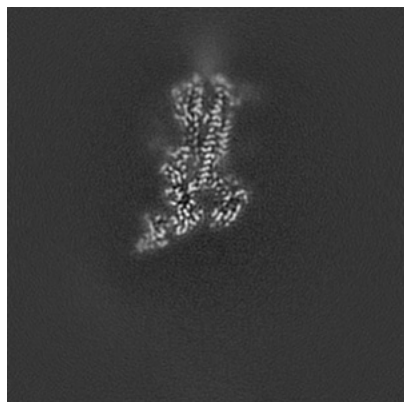


Y Index: 135

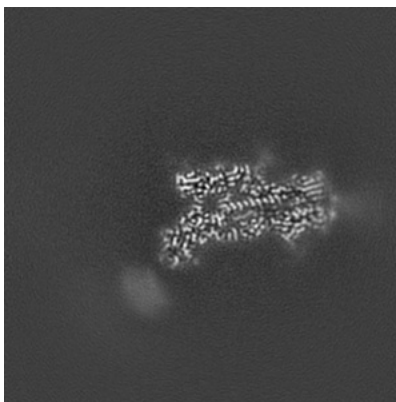


Z Index: 117

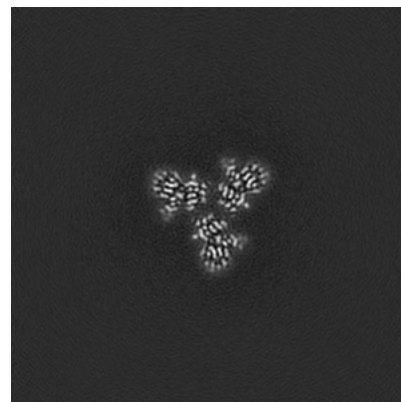
6.3.2 Raw map



X Index: 124



Y Index: 134

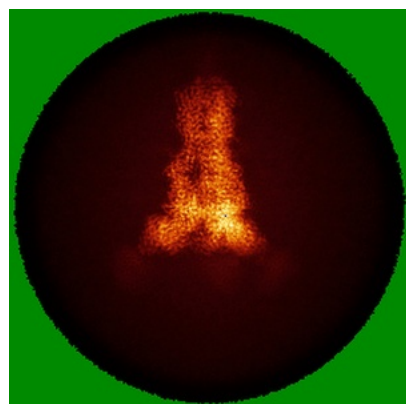


Z Index: 117

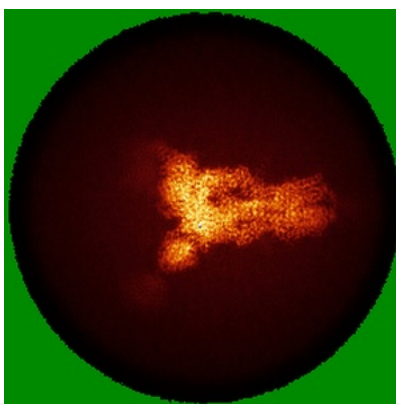
The images above show the largest variance slices of the map in three orthogonal directions.

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

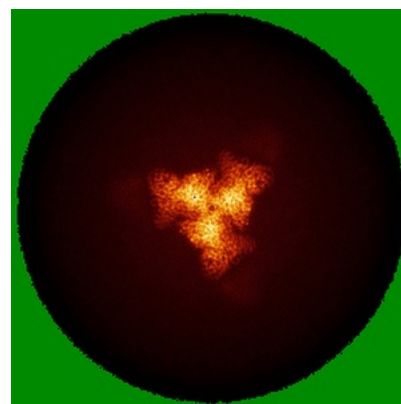
6.4.1 Primary map



X

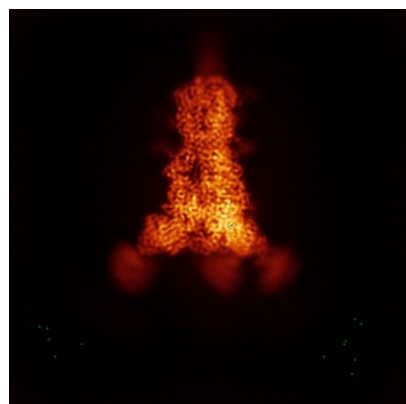


Y

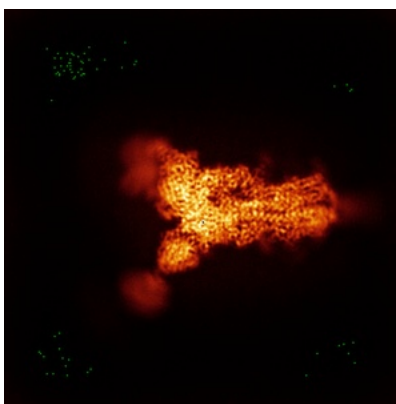


Z

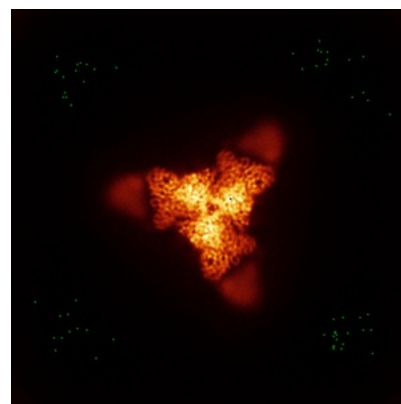
6.4.2 Raw map



X



Y

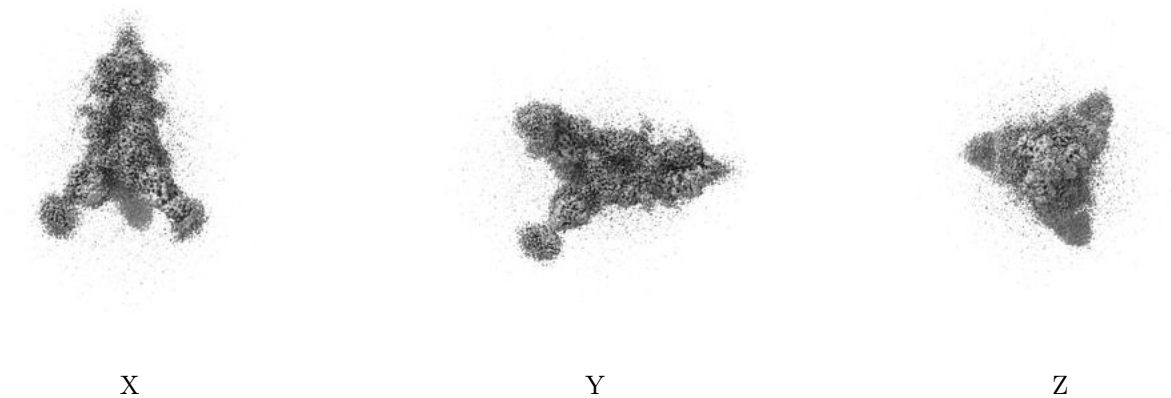


Z

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.

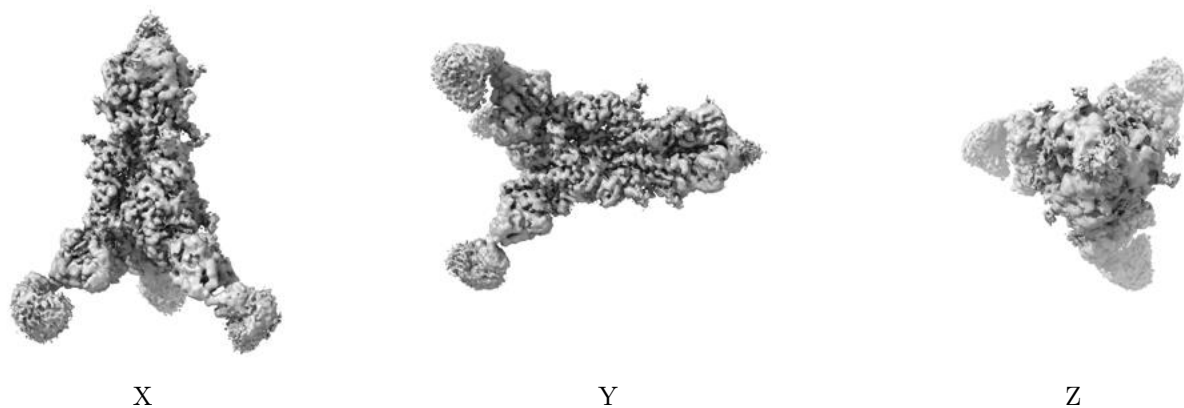
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

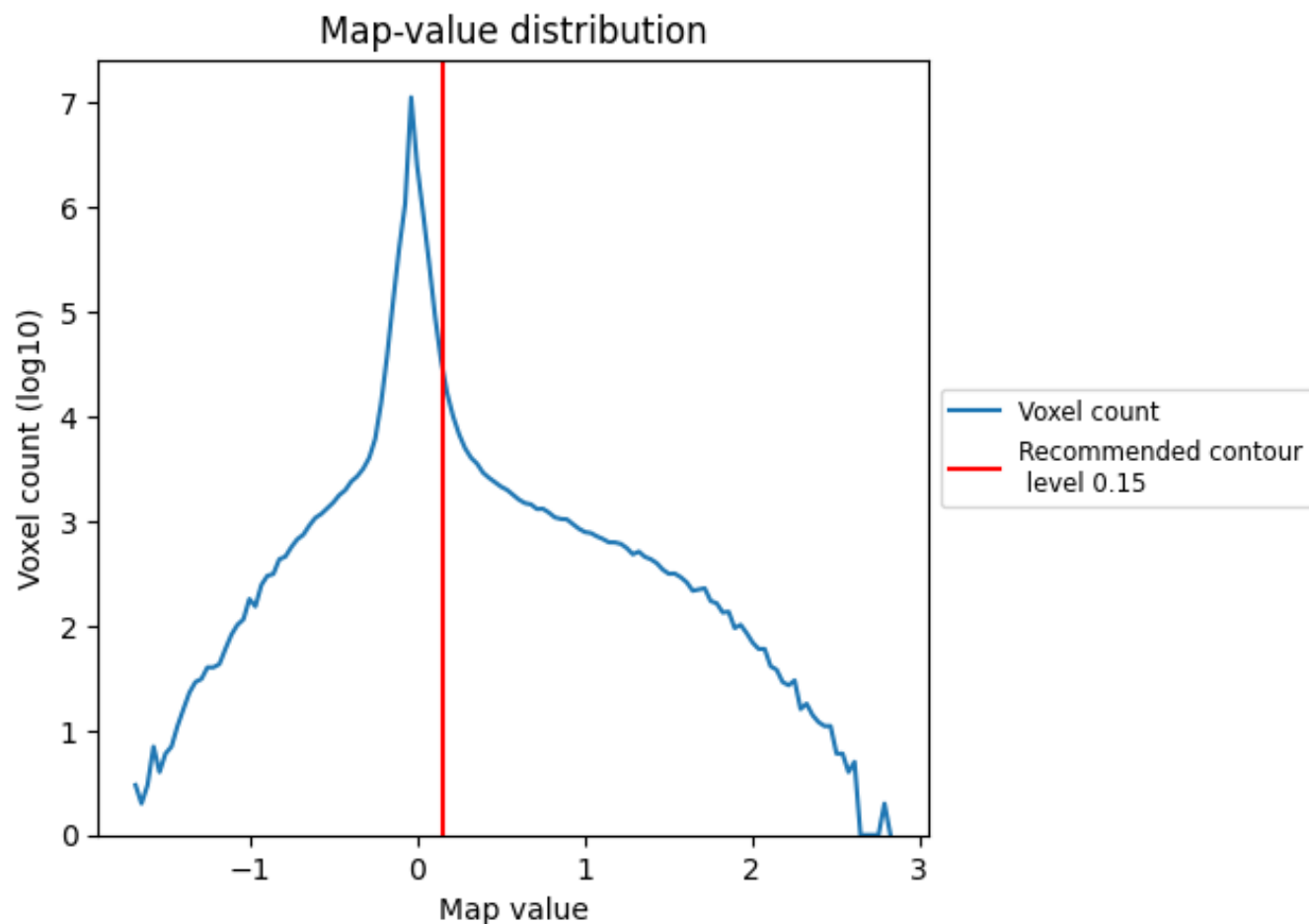
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

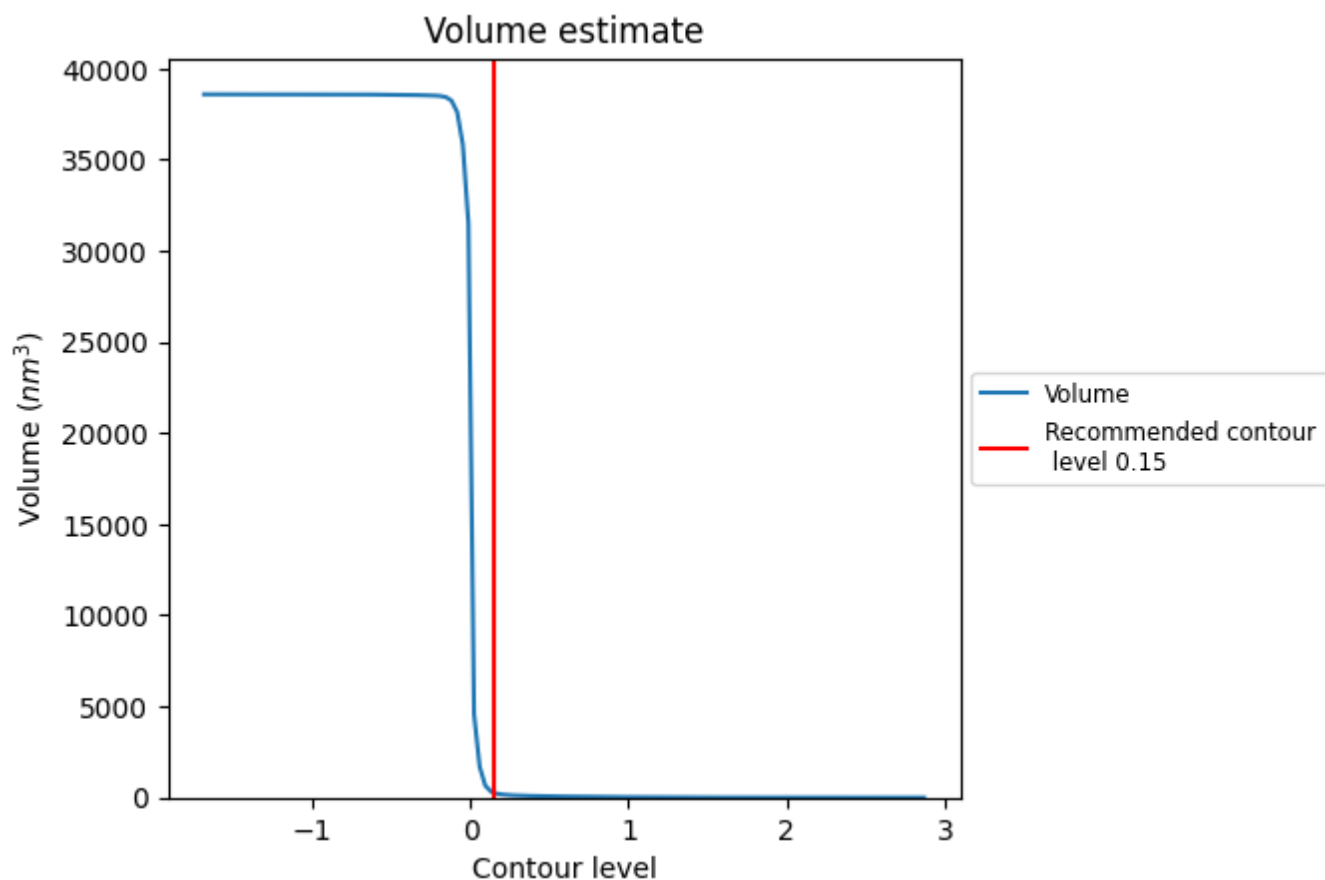
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

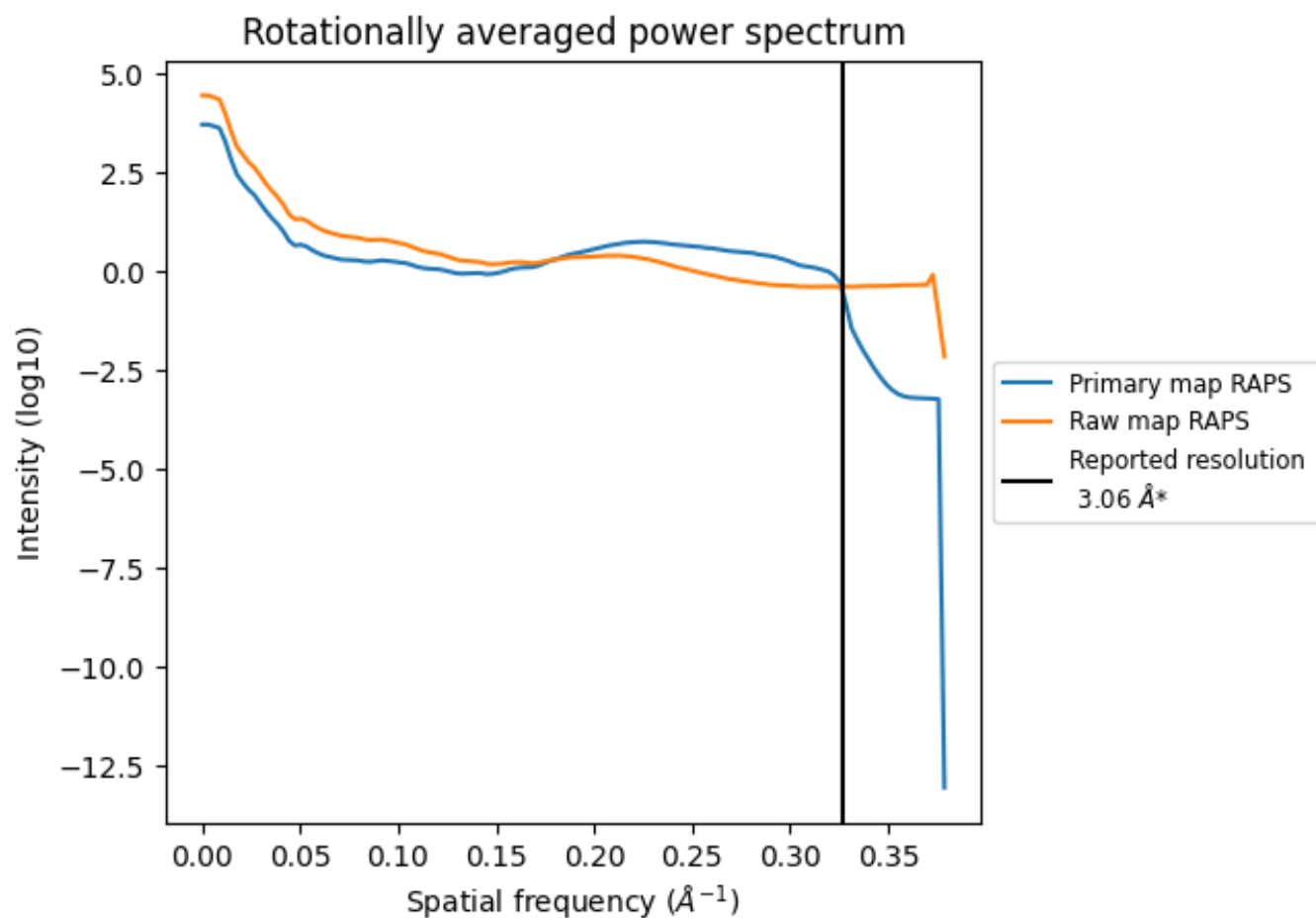
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 270 nm³; this corresponds to an approximate mass of 244 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 ⓘ

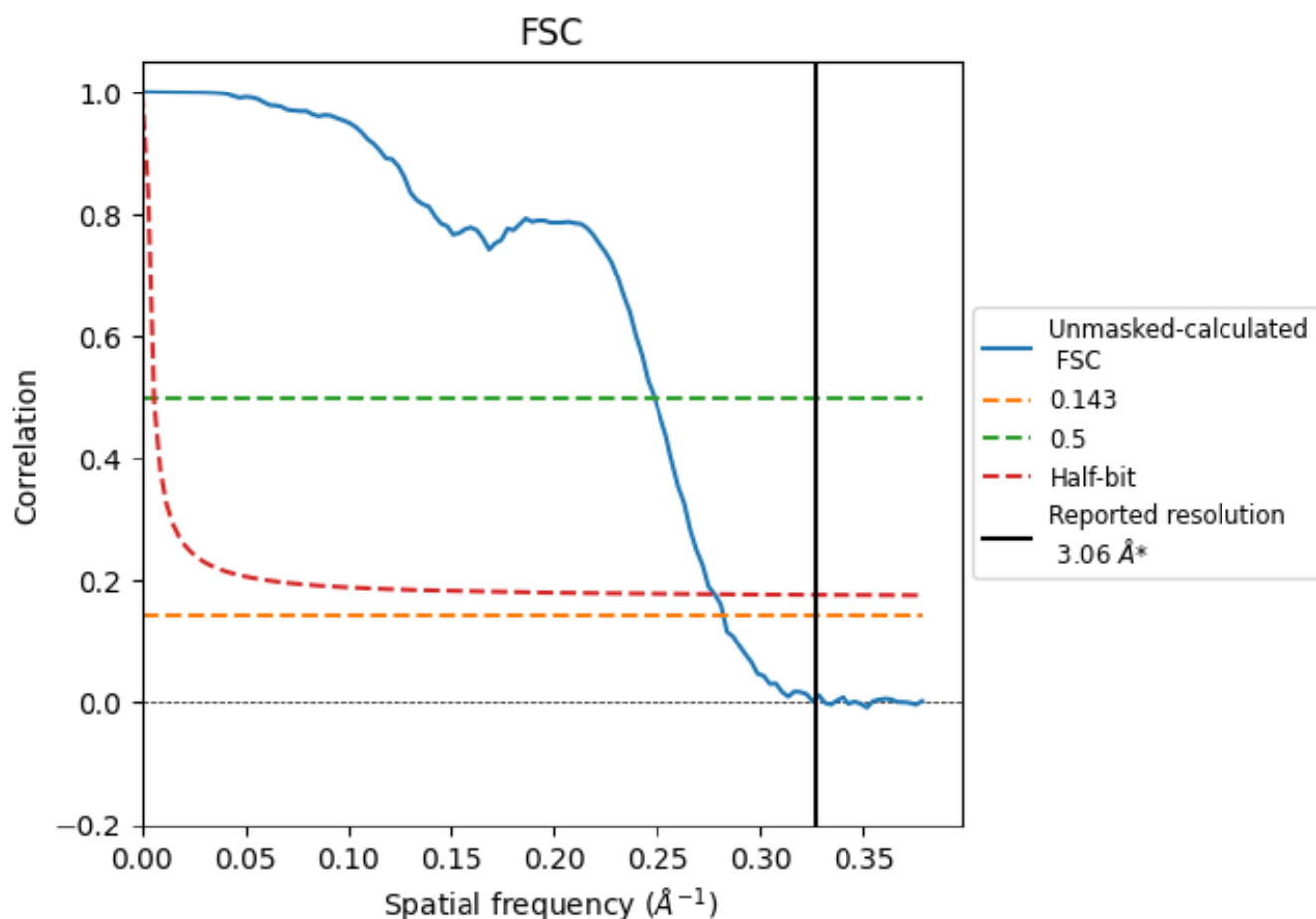


*Reported resolution corresponds to spatial frequency of 0.327 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.327 Å⁻¹

8.2 Resolution estimates [i](#)

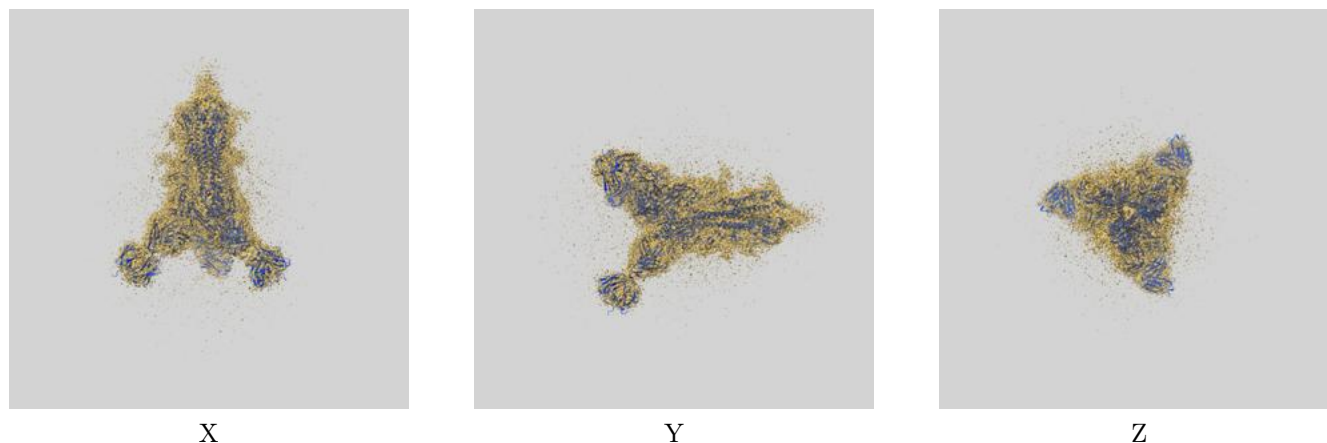
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.54	4.02	3.60

*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 3.54 differs from the reported value 3.06 by more than 10 %

9 Map-model fit [i](#)

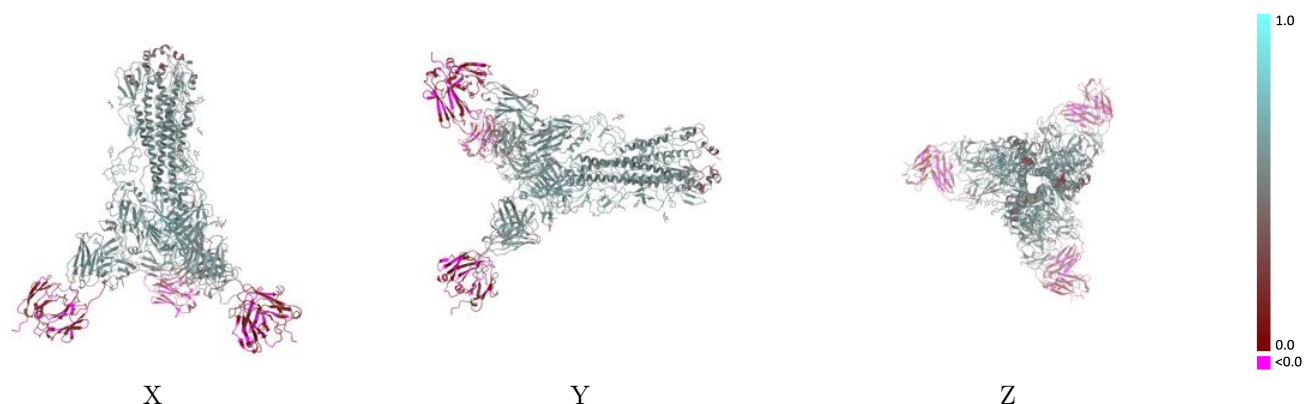
This section contains information regarding the fit between EMDB map EMD-67557 and PDB model 21BP. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



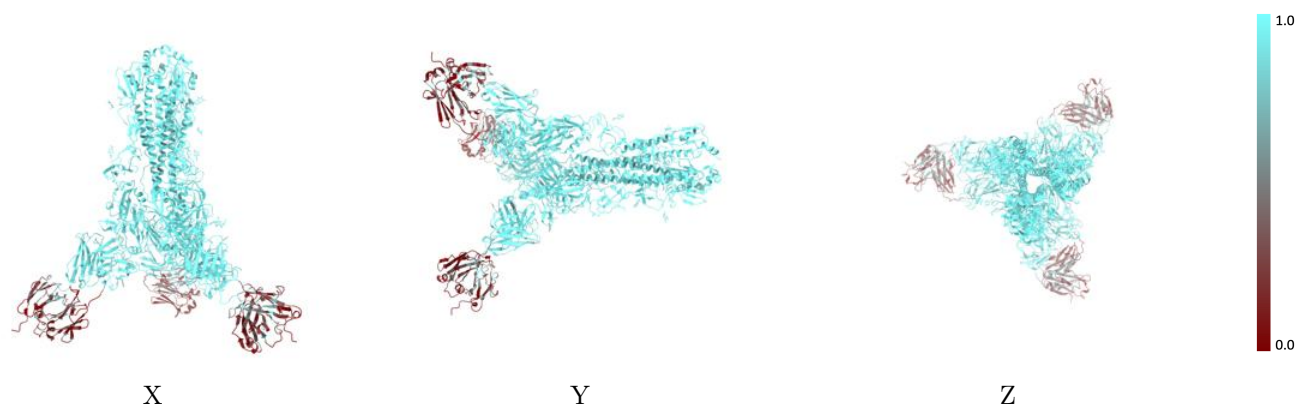
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



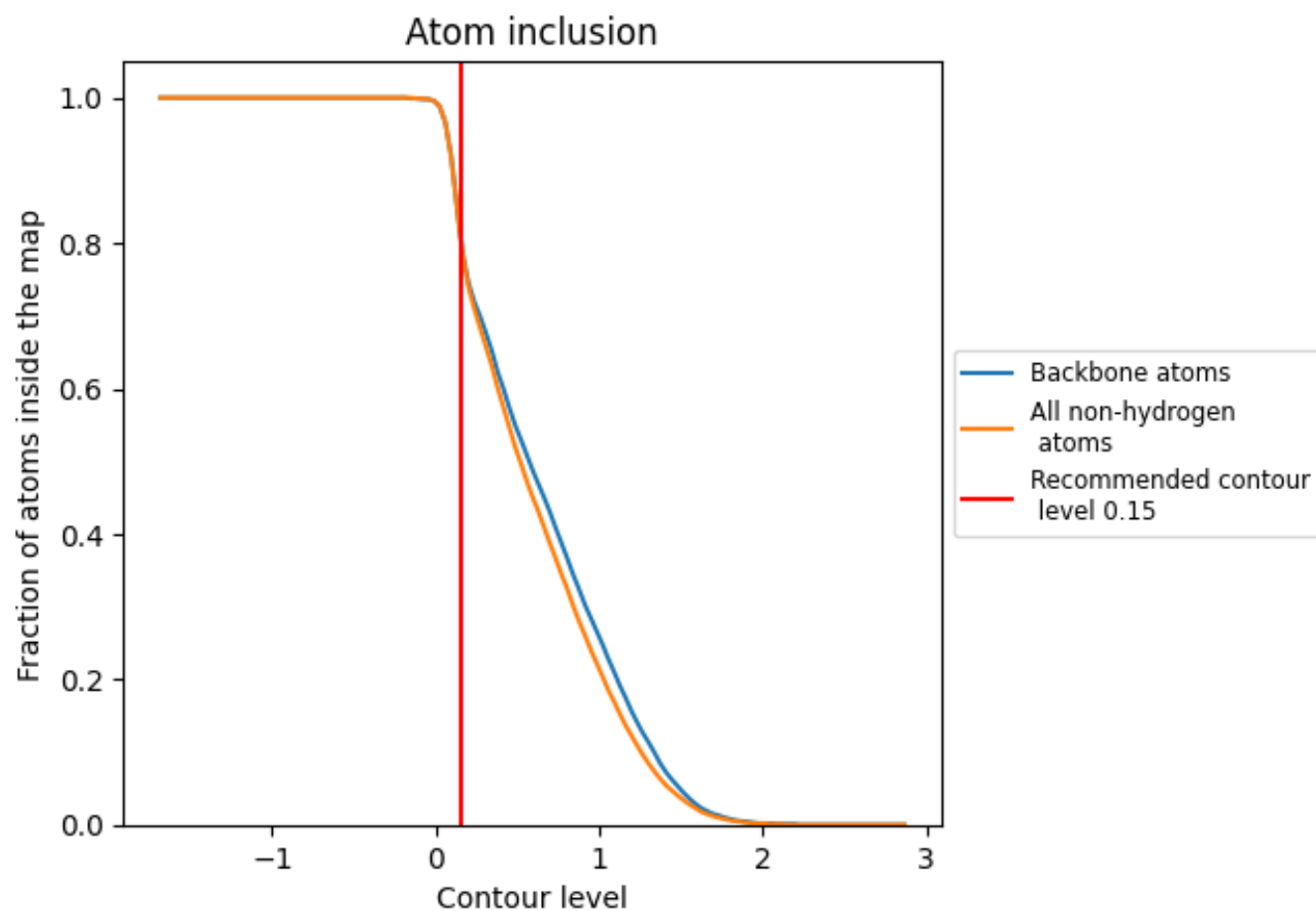
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8120	0.4530
A	0.9670	0.5570
B	0.9680	0.5630
C	0.9690	0.5650
D	0.6830	0.3530
E	0.5610	0.2770
F	0.6810	0.3560
G	0.5490	0.2920
H	0.6800	0.3540
I	0.8720	0.4510
J	0.9740	0.4680
K	0.9230	0.4400
L	0.5620	0.2790

1.0

0.0

<0.0