



## wwPDB EM Validation Summary Report ⓘ

Oct 23, 2024 – 01:33 am BST

PDB ID : 8RM1  
EMDB ID : EMD-19348  
Title : Cryo-EM structure of a Foamy Virus fusion glycoprotein in the postfusion conformation  
Authors : Fernandez, I.; Backovic, M.  
Deposited on : 2024-01-04  
Resolution : 3.10 Å (reported)  
Based on initial models : 8AEZ, .

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

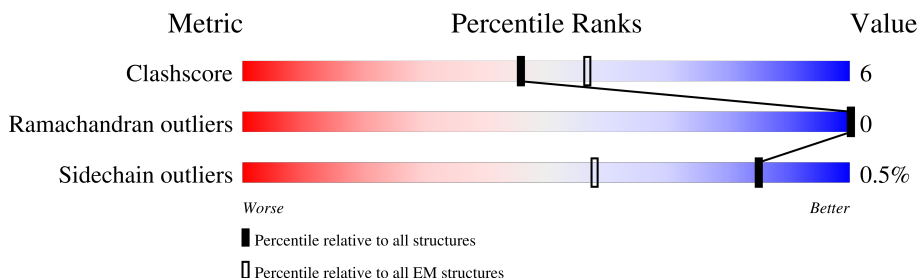
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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  $\geq 3$ , 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	444	<div> <div>7%</div> <div>76%</div> <div>16%</div> <div>8%</div> </div>
1	B	444	<div> <div>7%</div> <div>75%</div> <div>16%</div> <div>8%</div> </div>
1	C	444	<div> <div>7%</div> <div>76%</div> <div>16%</div> <div>8%</div> </div>
2	D	372	<div> <div>74%</div> <div>12%</div> <div>14%</div> </div>
2	E	372	<div> <div>74%</div> <div>12%</div> <div>14%</div> </div>
2	F	372	<div> <div>74%</div> <div>12%</div> <div>14%</div> </div>
3	G	2	<div> <div>100%</div> </div>
3	I	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	K	2	 100%
4	H	3	 67% 33%
4	J	3	 67% 33%
4	L	3	 67% 33%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17913 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 Envelope glycoprotein gp130.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	407	Total	C	N	O	S	0	0
			3329	2131	558	619	21		
1	B	407	Total	C	N	O	S	0	0
			3329	2131	558	619	21		
1	C	407	Total	C	N	O	S	0	0
			3329	2131	558	619	21		

- Molecule 2 is a protein called Envelope glycoprotein gp130.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	321	Total	C	N	O	S	0	0
			2561	1630	442	474	15		
2	E	321	Total	C	N	O	S	0	0
			2561	1630	442	474	15		
2	F	321	Total	C	N	O	S	0	0
			2561	1630	442	474	15		

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	908	ASP	-	expression tag	UNP K7YEW5
D	909	ASP	-	expression tag	UNP K7YEW5
D	910	ASP	-	expression tag	UNP K7YEW5
D	911	ASP	-	expression tag	UNP K7YEW5
D	912	LYS	-	expression tag	UNP K7YEW5
D	913	ALA	-	expression tag	UNP K7YEW5
D	914	GLY	-	expression tag	UNP K7YEW5
D	915	TRP	-	expression tag	UNP K7YEW5
D	916	SER	-	expression tag	UNP K7YEW5
D	917	HIS	-	expression tag	UNP K7YEW5
D	918	PRO	-	expression tag	UNP K7YEW5
D	919	GLN	-	expression tag	UNP K7YEW5
D	920	PHE	-	expression tag	UNP K7YEW5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	921	GLU	-	expression tag	UNP K7YEW5
D	922	LYS	-	expression tag	UNP K7YEW5
D	923	GLY	-	expression tag	UNP K7YEW5
D	924	GLY	-	expression tag	UNP K7YEW5
D	925	GLY	-	expression tag	UNP K7YEW5
D	926	SER	-	expression tag	UNP K7YEW5
D	927	GLY	-	expression tag	UNP K7YEW5
D	928	GLY	-	expression tag	UNP K7YEW5
D	929	GLY	-	expression tag	UNP K7YEW5
D	930	SER	-	expression tag	UNP K7YEW5
D	931	GLY	-	expression tag	UNP K7YEW5
D	932	GLY	-	expression tag	UNP K7YEW5
D	933	GLY	-	expression tag	UNP K7YEW5
D	934	SER	-	expression tag	UNP K7YEW5
D	935	TRP	-	expression tag	UNP K7YEW5
D	936	SER	-	expression tag	UNP K7YEW5
D	937	HIS	-	expression tag	UNP K7YEW5
D	938	PRO	-	expression tag	UNP K7YEW5
D	939	GLN	-	expression tag	UNP K7YEW5
D	940	PHE	-	expression tag	UNP K7YEW5
D	941	GLU	-	expression tag	UNP K7YEW5
D	942	LYS	-	expression tag	UNP K7YEW5
E	908	ASP	-	expression tag	UNP K7YEW5
E	909	ASP	-	expression tag	UNP K7YEW5
E	910	ASP	-	expression tag	UNP K7YEW5
E	911	ASP	-	expression tag	UNP K7YEW5
E	912	LYS	-	expression tag	UNP K7YEW5
E	913	ALA	-	expression tag	UNP K7YEW5
E	914	GLY	-	expression tag	UNP K7YEW5
E	915	TRP	-	expression tag	UNP K7YEW5
E	916	SER	-	expression tag	UNP K7YEW5
E	917	HIS	-	expression tag	UNP K7YEW5
E	918	PRO	-	expression tag	UNP K7YEW5
E	919	GLN	-	expression tag	UNP K7YEW5
E	920	PHE	-	expression tag	UNP K7YEW5
E	921	GLU	-	expression tag	UNP K7YEW5
E	922	LYS	-	expression tag	UNP K7YEW5
E	923	GLY	-	expression tag	UNP K7YEW5
E	924	GLY	-	expression tag	UNP K7YEW5
E	925	GLY	-	expression tag	UNP K7YEW5
E	926	SER	-	expression tag	UNP K7YEW5
E	927	GLY	-	expression tag	UNP K7YEW5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	928	GLY	-	expression tag	UNP K7YEW5
E	929	GLY	-	expression tag	UNP K7YEW5
E	930	SER	-	expression tag	UNP K7YEW5
E	931	GLY	-	expression tag	UNP K7YEW5
E	932	GLY	-	expression tag	UNP K7YEW5
E	933	GLY	-	expression tag	UNP K7YEW5
E	934	SER	-	expression tag	UNP K7YEW5
E	935	TRP	-	expression tag	UNP K7YEW5
E	936	SER	-	expression tag	UNP K7YEW5
E	937	HIS	-	expression tag	UNP K7YEW5
E	938	PRO	-	expression tag	UNP K7YEW5
E	939	GLN	-	expression tag	UNP K7YEW5
E	940	PHE	-	expression tag	UNP K7YEW5
E	941	GLU	-	expression tag	UNP K7YEW5
E	942	LYS	-	expression tag	UNP K7YEW5
F	908	ASP	-	expression tag	UNP K7YEW5
F	909	ASP	-	expression tag	UNP K7YEW5
F	910	ASP	-	expression tag	UNP K7YEW5
F	911	ASP	-	expression tag	UNP K7YEW5
F	912	LYS	-	expression tag	UNP K7YEW5
F	913	ALA	-	expression tag	UNP K7YEW5
F	914	GLY	-	expression tag	UNP K7YEW5
F	915	TRP	-	expression tag	UNP K7YEW5
F	916	SER	-	expression tag	UNP K7YEW5
F	917	HIS	-	expression tag	UNP K7YEW5
F	918	PRO	-	expression tag	UNP K7YEW5
F	919	GLN	-	expression tag	UNP K7YEW5
F	920	PHE	-	expression tag	UNP K7YEW5
F	921	GLU	-	expression tag	UNP K7YEW5
F	922	LYS	-	expression tag	UNP K7YEW5
F	923	GLY	-	expression tag	UNP K7YEW5
F	924	GLY	-	expression tag	UNP K7YEW5
F	925	GLY	-	expression tag	UNP K7YEW5
F	926	SER	-	expression tag	UNP K7YEW5
F	927	GLY	-	expression tag	UNP K7YEW5
F	928	GLY	-	expression tag	UNP K7YEW5
F	929	GLY	-	expression tag	UNP K7YEW5
F	930	SER	-	expression tag	UNP K7YEW5
F	931	GLY	-	expression tag	UNP K7YEW5
F	932	GLY	-	expression tag	UNP K7YEW5
F	933	GLY	-	expression tag	UNP K7YEW5
F	934	SER	-	expression tag	UNP K7YEW5

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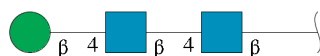
Chain	Residue	Modelled	Actual	Comment	Reference
F	935	TRP	-	expression tag	UNP K7YEW5
F	936	SER	-	expression tag	UNP K7YEW5
F	937	HIS	-	expression tag	UNP K7YEW5
F	938	PRO	-	expression tag	UNP K7YEW5
F	939	GLN	-	expression tag	UNP K7YEW5
F	940	PHE	-	expression tag	UNP K7YEW5
F	941	GLU	-	expression tag	UNP K7YEW5
F	942	LYS	-	expression tag	UNP K7YEW5

- 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	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		

- 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	H	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	L	3	Total	C	N	O	0	0
			39	22	2	15		

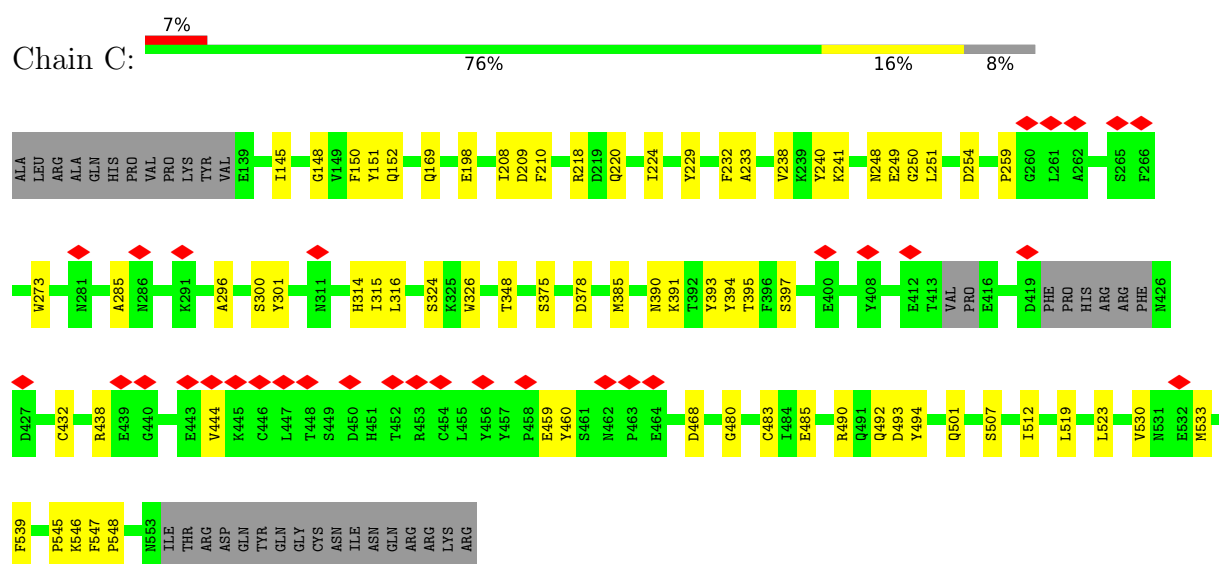
- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



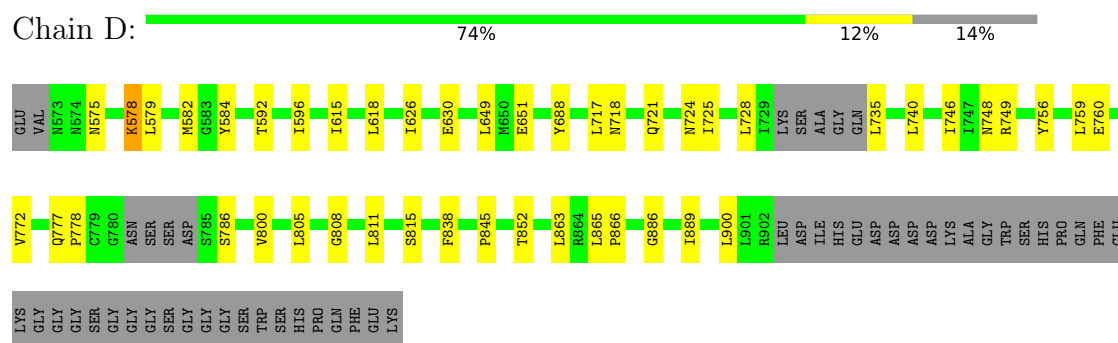
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	



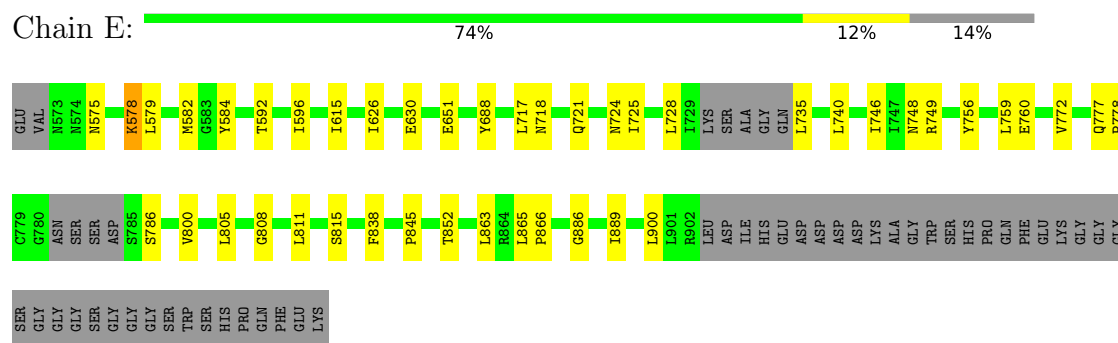




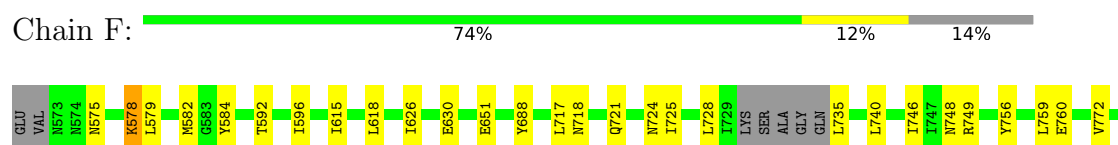
• Molecule 2: Envelope glycoprotein gp130

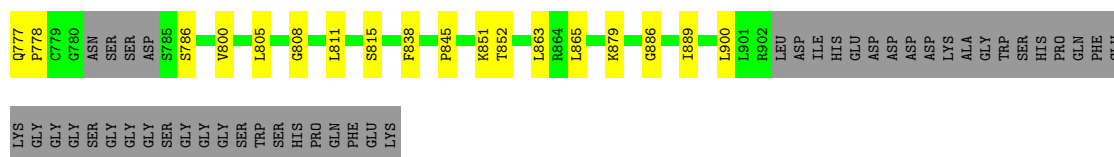


• Molecule 2: Envelope glycoprotein gp130



• Molecule 2: Envelope glycoprotein gp130





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

Chain G:  100%



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

Chain I:  100%



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

Chain K:  100%



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

Chain H:  67% 33%



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

Chain J:  67% 33%



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

Chain L:  67% 33%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98407	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.101	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.00603	Depositor
Map size (Å)	302.72, 302.72, 302.72	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	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	A	0.24	0/3419	0.48	0/4645
1	B	0.24	0/3419	0.48	0/4645
1	C	0.24	0/3419	0.48	0/4645
2	D	0.26	0/2612	0.50	0/3550
2	E	0.26	0/2612	0.50	0/3550
2	F	0.26	0/2612	0.50	0/3550
All	All	0.25	0/18093	0.49	0/24585

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 [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	3329	0	3211	44	0
1	B	3329	0	3211	47	0
1	C	3329	0	3211	44	0
2	D	2561	0	2581	37	0
2	E	2561	0	2581	36	0
2	F	2561	0	2581	39	0
3	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	28	0	25	0	0
3	K	28	0	25	0	0
4	H	39	0	34	1	0
4	J	39	0	34	1	0
4	L	39	0	34	1	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	14	0	13	0	0
All	All	17913	0	17592	212	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 212 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)
2:E:584:TYR:HE1	2:F:900:LEU:HD13	1.47	0.80
2:D:900:LEU:HD13	2:F:584:TYR:HE1	1.47	0.79
2:D:584:TYR:HE1	2:E:900:LEU:HD13	1.46	0.79
2:F:718:ASN:O	2:F:748:ASN:ND2	2.20	0.76
2:E:718:ASN:O	2:E:748:ASN:ND2	2.20	0.75

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	401/444 (90%)	375 (94%)	26 (6%)	0	100	100
1	B	401/444 (90%)	375 (94%)	26 (6%)	0	100	100
1	C	401/444 (90%)	375 (94%)	26 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	315/372 (85%)	305 (97%)	10 (3%)	0	100	100
2	E	315/372 (85%)	305 (97%)	10 (3%)	0	100	100
2	F	315/372 (85%)	305 (97%)	10 (3%)	0	100	100
All	All	2148/2448 (88%)	2040 (95%)	108 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/407 (91%)	367 (100%)	2 (0%)	86	92
1	B	369/407 (91%)	367 (100%)	2 (0%)	86	92
1	C	369/407 (91%)	367 (100%)	2 (0%)	86	92
2	D	291/333 (87%)	290 (100%)	1 (0%)	91	95
2	E	291/333 (87%)	290 (100%)	1 (0%)	91	95
2	F	291/333 (87%)	290 (100%)	1 (0%)	91	95
All	All	1980/2220 (89%)	1971 (100%)	9 (0%)	85	92

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	533	MET
2	F	578	LYS
1	B	198	GLU
1	B	533	MET
2	E	578	LYS

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



### 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 ⓘ

15 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	G	1	1,3	14,14,15	0.28	0	17,19,21	0.39	0
3	NAG	G	2	3	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	H	1	4,2	14,14,15	0.22	0	17,19,21	0.47	0
4	NAG	H	2	4	14,14,15	0.44	0	17,19,21	1.28	2 (11%)
4	BMA	H	3	4	11,11,12	0.53	0	15,15,17	0.85	0
3	NAG	I	1	1,3	14,14,15	0.28	0	17,19,21	0.39	0
3	NAG	I	2	3	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	J	1	4,2	14,14,15	0.22	0	17,19,21	0.47	0
4	NAG	J	2	4	14,14,15	0.45	0	17,19,21	1.28	2 (11%)
4	BMA	J	3	4	11,11,12	0.51	0	15,15,17	0.85	0
3	NAG	K	1	1,3	14,14,15	0.27	0	17,19,21	0.40	0
3	NAG	K	2	3	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	L	1	4,2	14,14,15	0.21	0	17,19,21	0.47	0
4	NAG	L	2	4	14,14,15	0.45	0	17,19,21	1.28	2 (11%)
4	BMA	L	3	4	11,11,12	0.52	0	15,15,17	0.84	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
4	NAG	H	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	4/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
4	NAG	J	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	4/6/23/26	0/1/1/1
4	BMA	J	3	4	-	2/2/19/22	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
4	NAG	L	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	4/6/23/26	0/1/1/1
4	BMA	L	3	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	2	NAG	C2-N2-C7	4.36	129.12	122.90
4	H	2	NAG	C2-N2-C7	4.35	129.10	122.90
4	J	2	NAG	C2-N2-C7	4.34	129.08	122.90
4	H	2	NAG	C1-C2-N2	2.08	114.05	110.49
4	J	2	NAG	C1-C2-N2	2.07	114.02	110.49

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

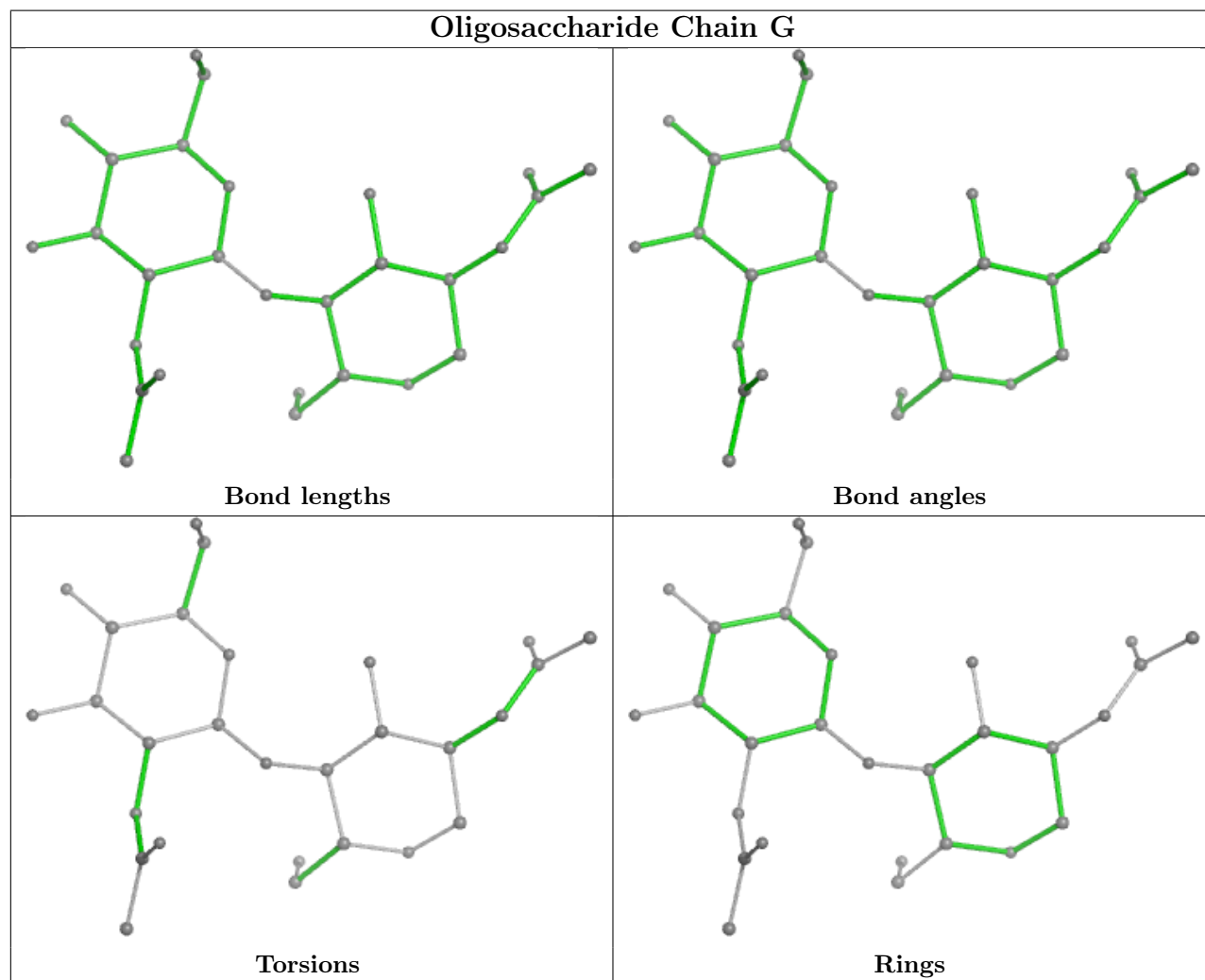
Mol	Chain	Res	Type	Atoms
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	L	2	NAG	C8-C7-N2-C2

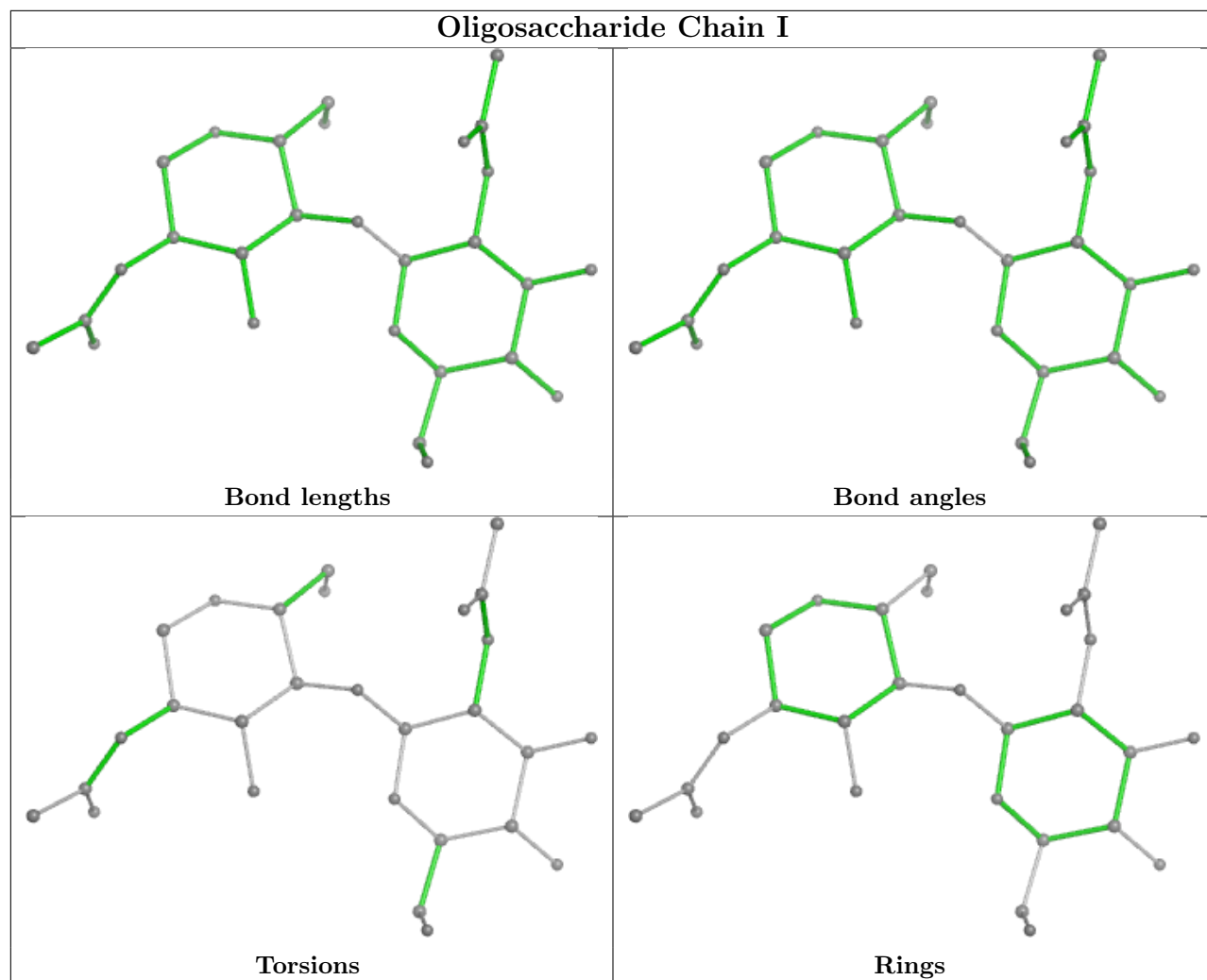
There are no ring outliers.

3 monomers are involved in 3 short contacts:

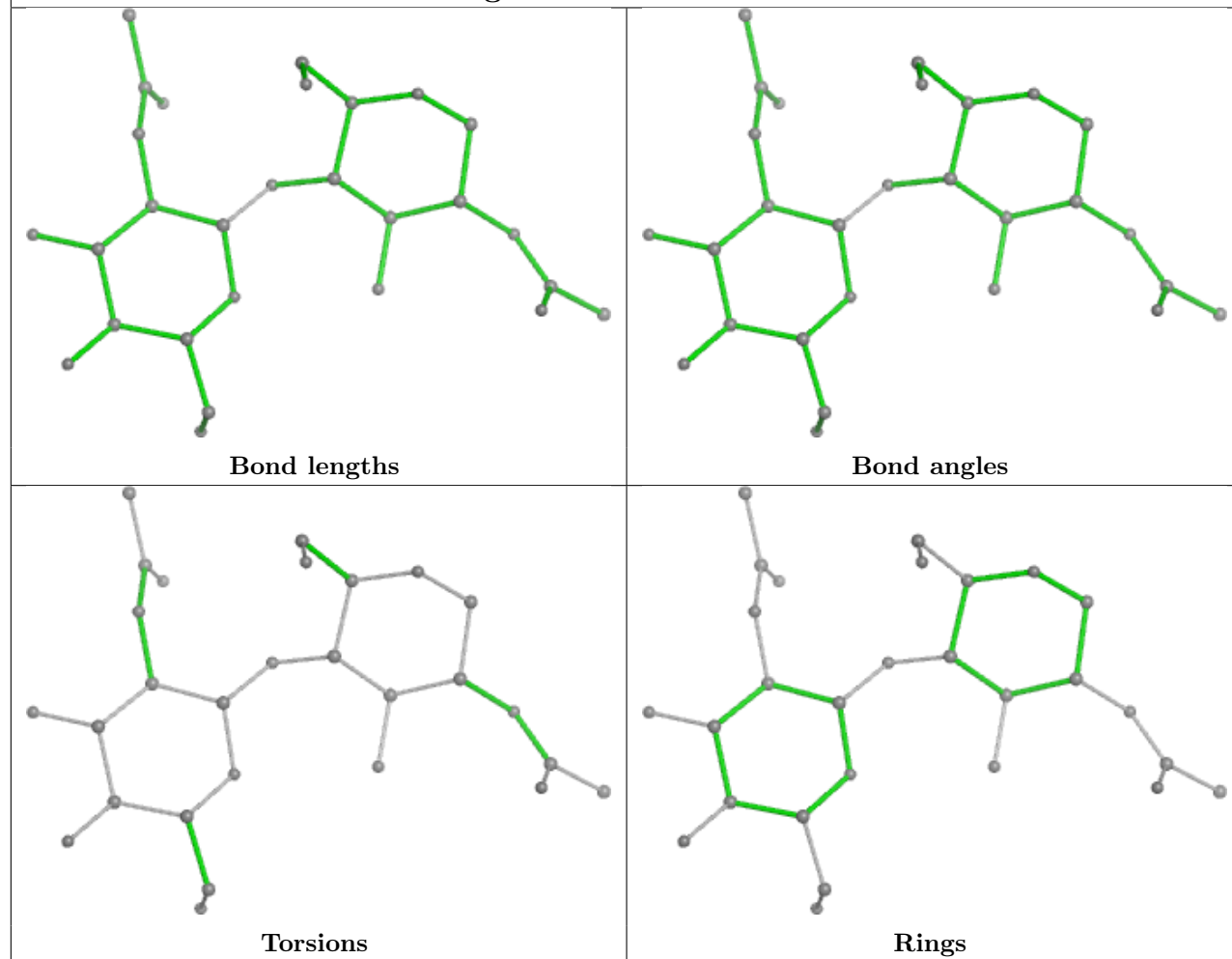
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	2	NAG	1	0
4	J	2	NAG	1	0
4	L	2	NAG	1	0

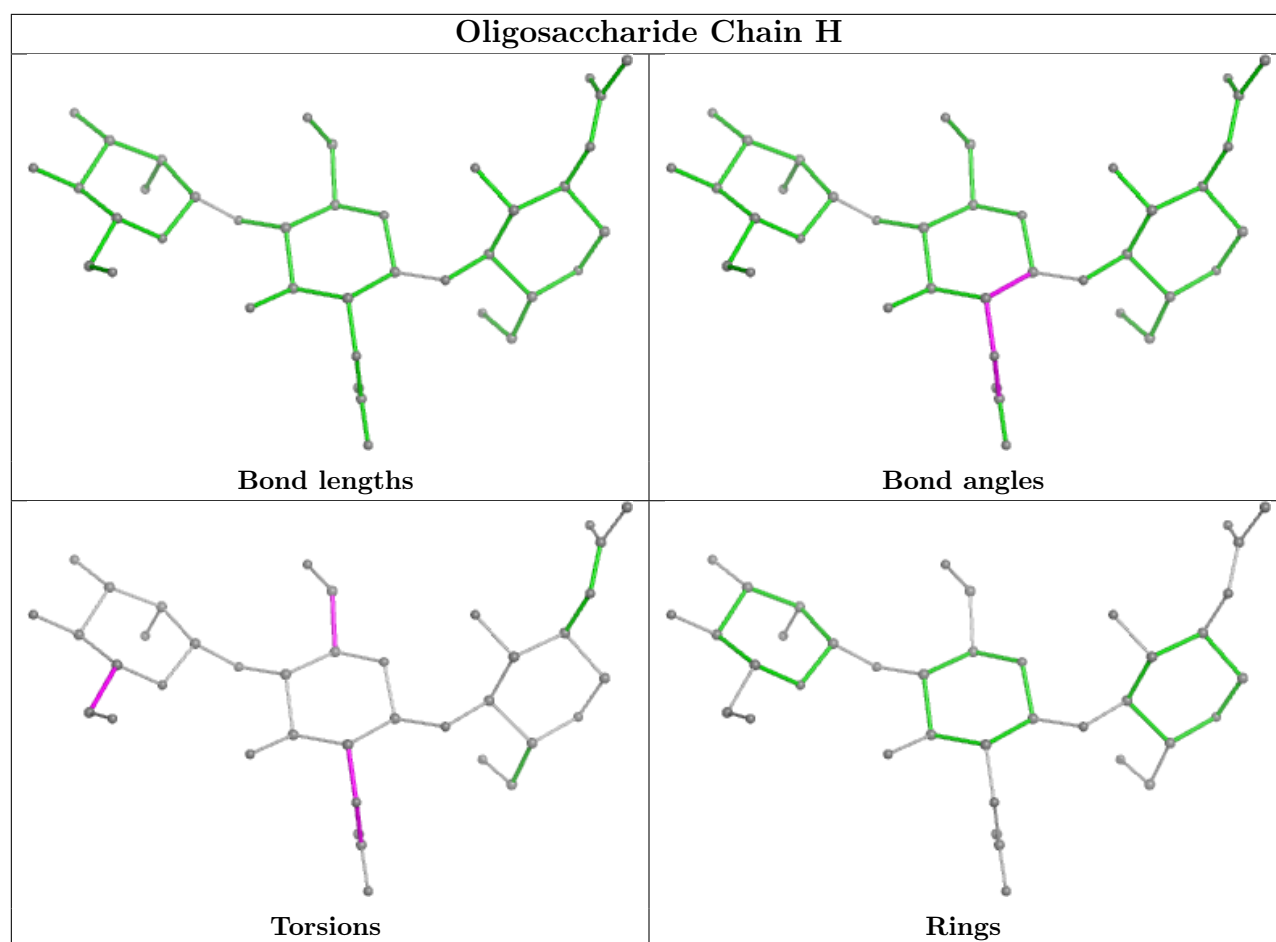
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

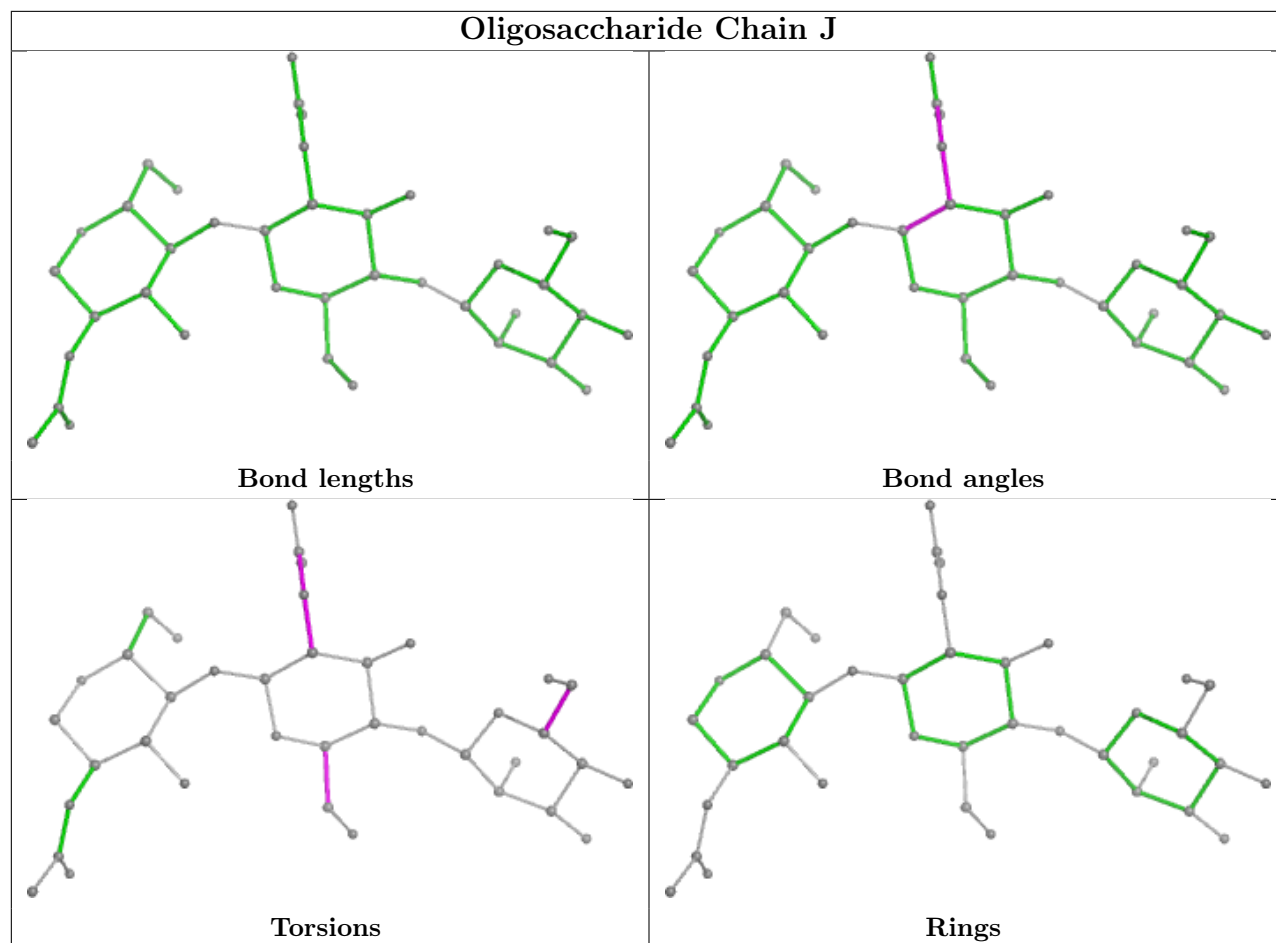


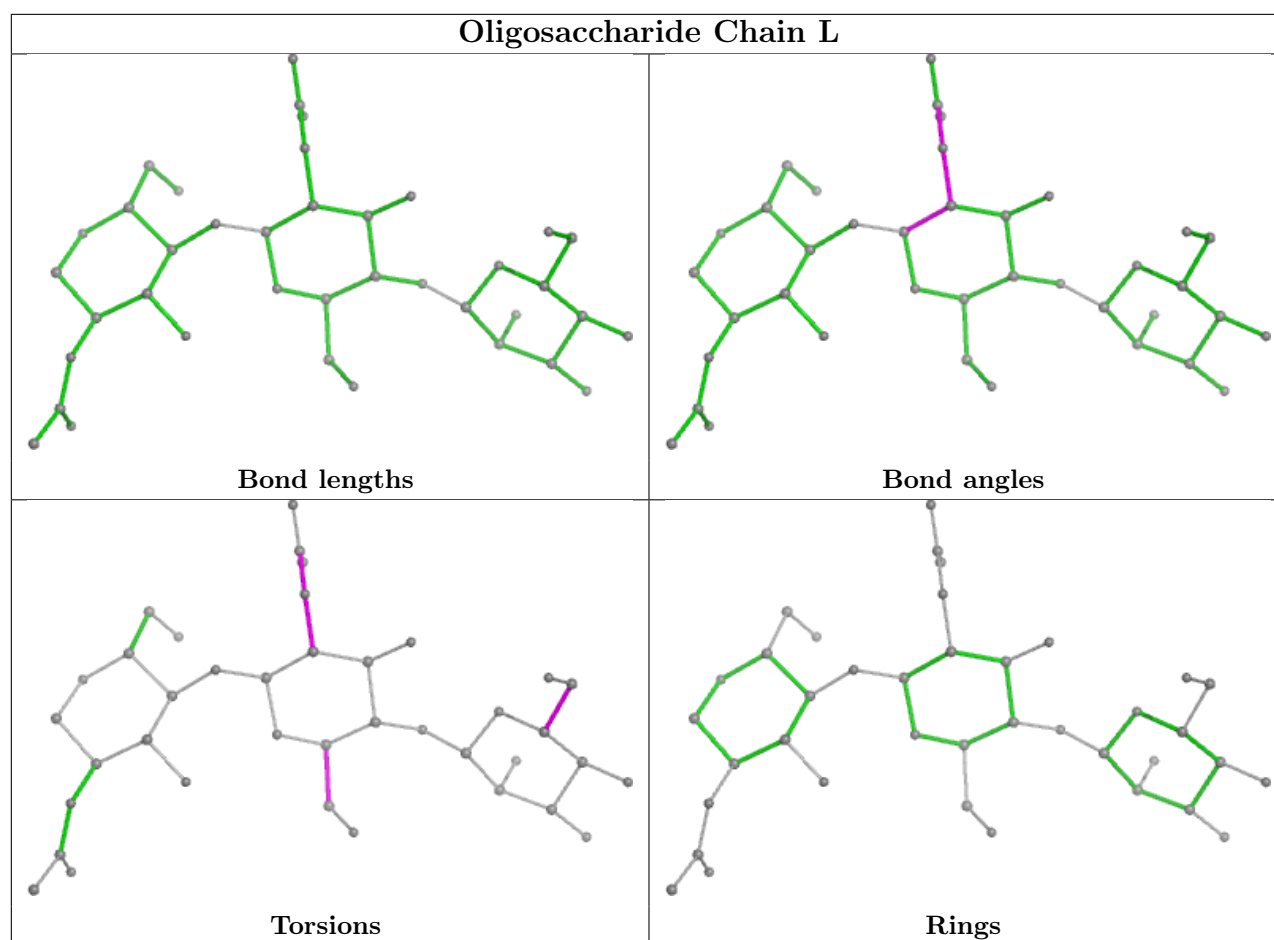


## Oligosaccharide Chain K









## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	A	1001	1	14,14,15	0.28	0	17,19,21	0.45	0
5	NAG	C	1001	1	14,14,15	0.28	0	17,19,21	0.46	0
5	NAG	B	1001	1	14,14,15	0.28	0	17,19,21	0.46	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	A	1001	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1001	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1001	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	NAG	C8-C7-N2-C2
5	A	1001	NAG	O7-C7-N2-C2
5	B	1001	NAG	C8-C7-N2-C2
5	B	1001	NAG	O7-C7-N2-C2
5	C	1001	NAG	C8-C7-N2-C2

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.

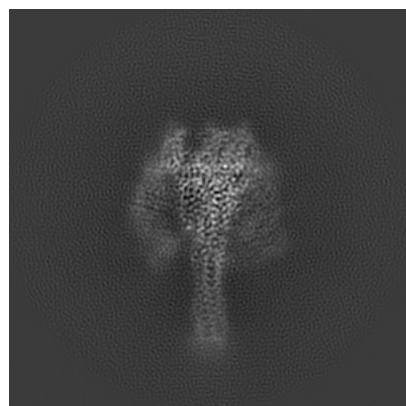
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19348. These allow visual inspection of the internal detail of the map and identification of artifacts.

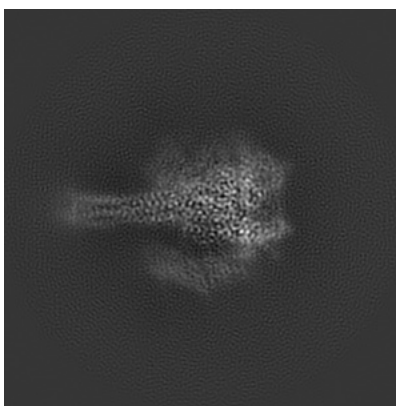
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

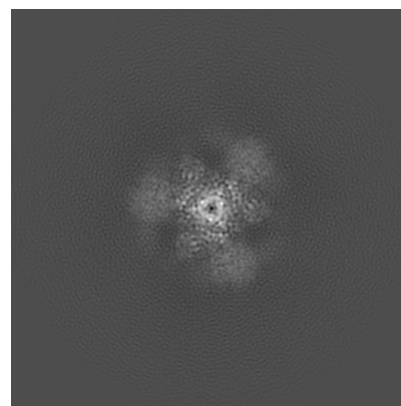
#### 6.1.1 Primary map



X

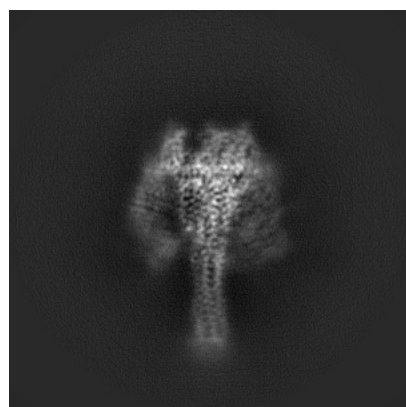


Y

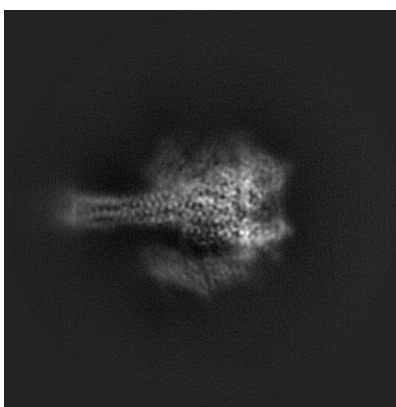


Z

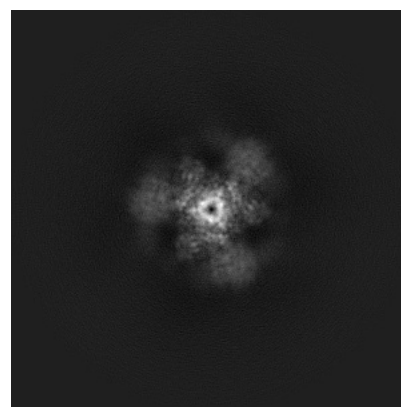
#### 6.1.2 Raw map



X



Y



Z

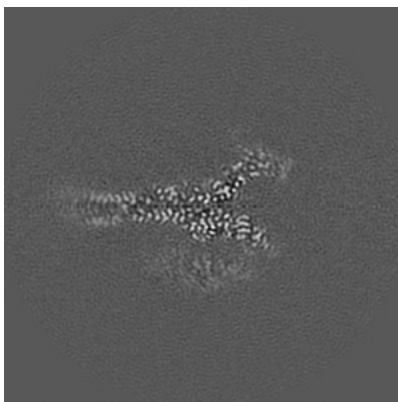
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

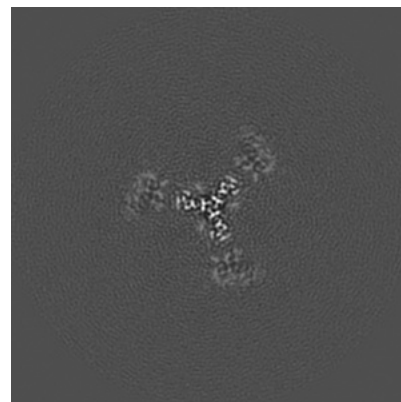
### 6.2.1 Primary map



X Index: 176

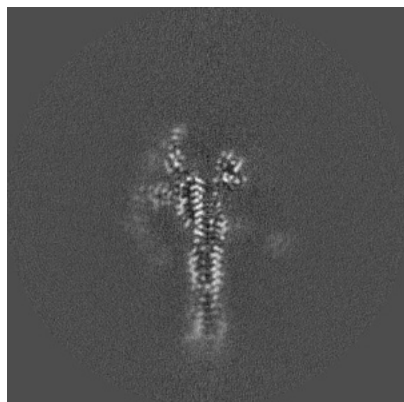


Y Index: 176

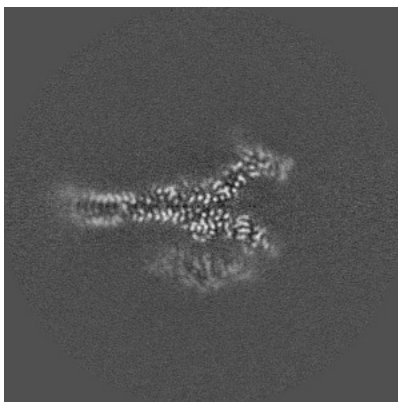


Z Index: 176

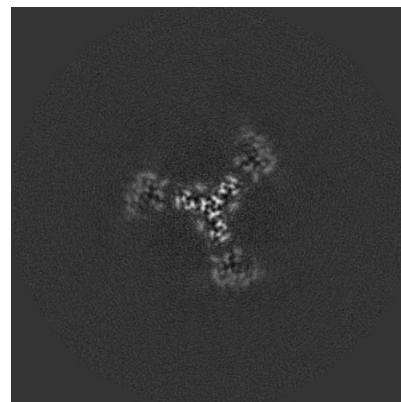
### 6.2.2 Raw map



X Index: 176



Y Index: 176

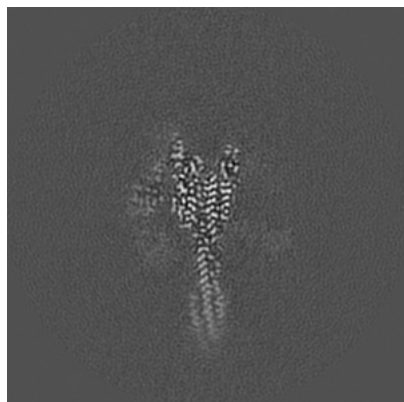


Z Index: 176

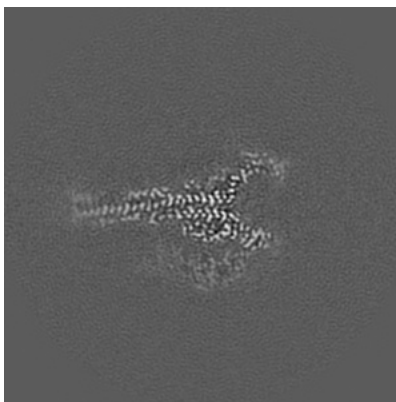
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

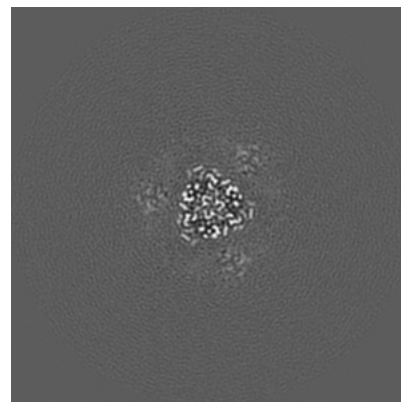
### 6.3.1 Primary map



X Index: 184

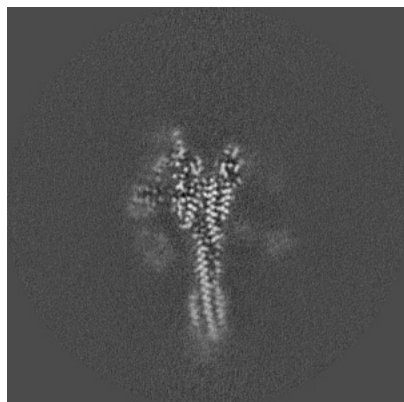


Y Index: 181

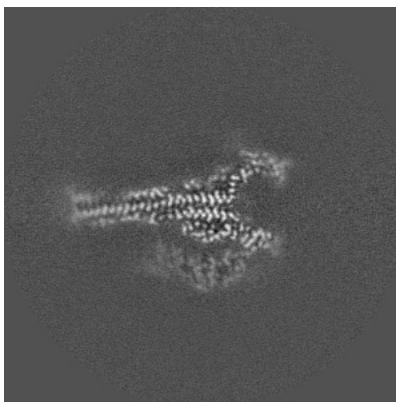


Z Index: 198

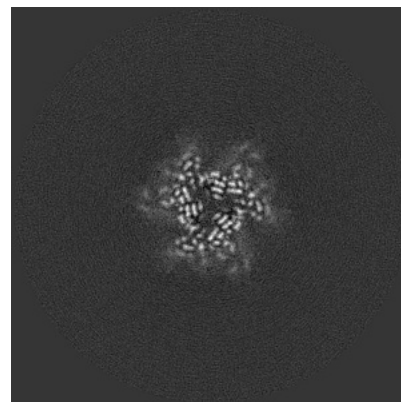
### 6.3.2 Raw map



X Index: 183



Y Index: 181

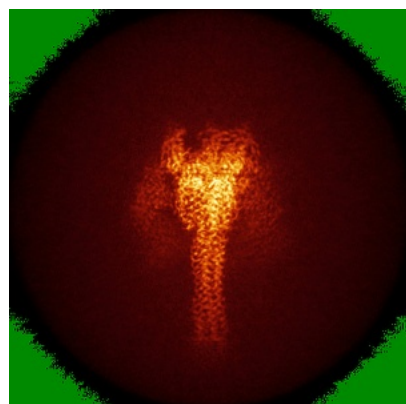


Z Index: 213

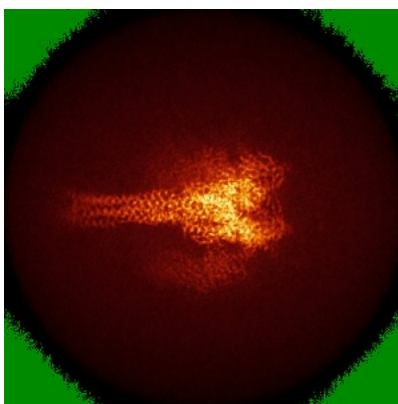
The images above show the largest variance slices of the map in three orthogonal directions.

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

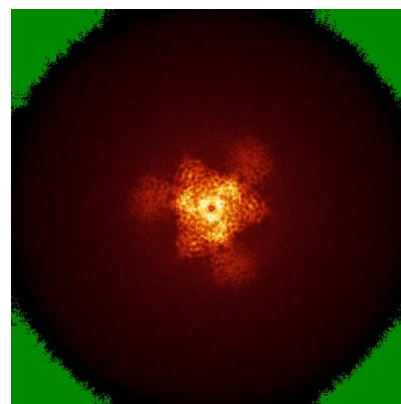
### 6.4.1 Primary map



X

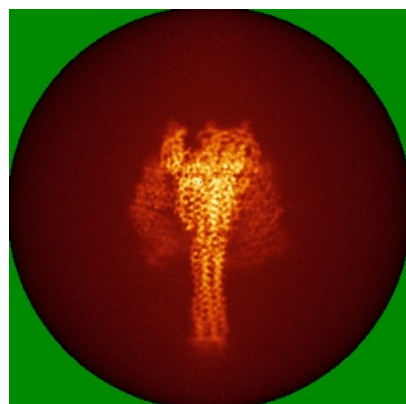


Y

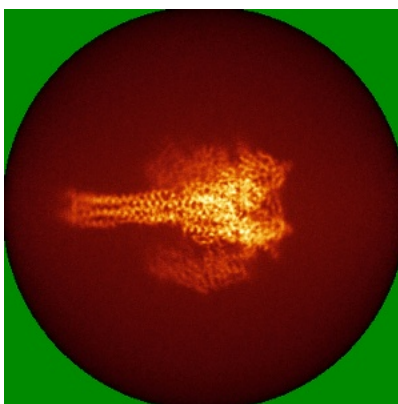


Z

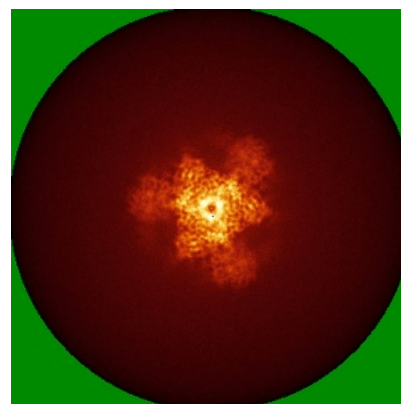
### 6.4.2 Raw map



X



Y



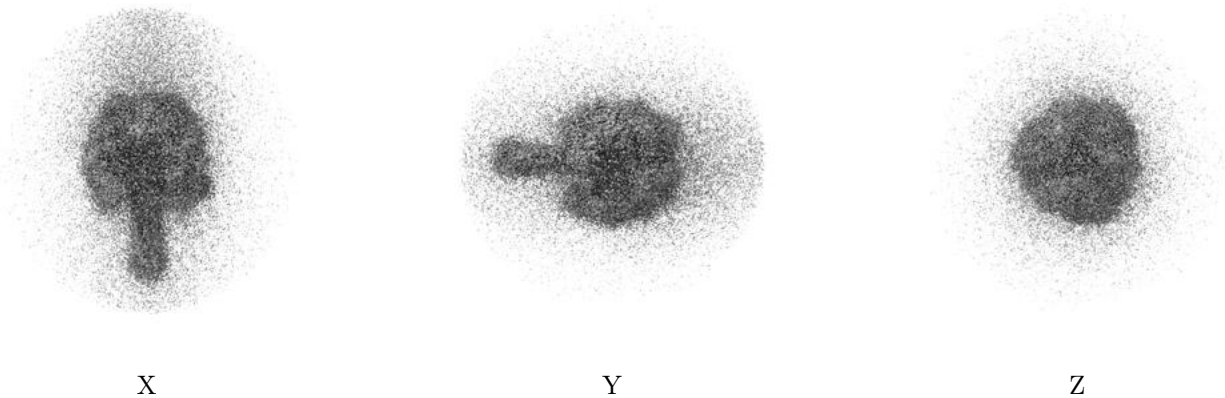
Z

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.



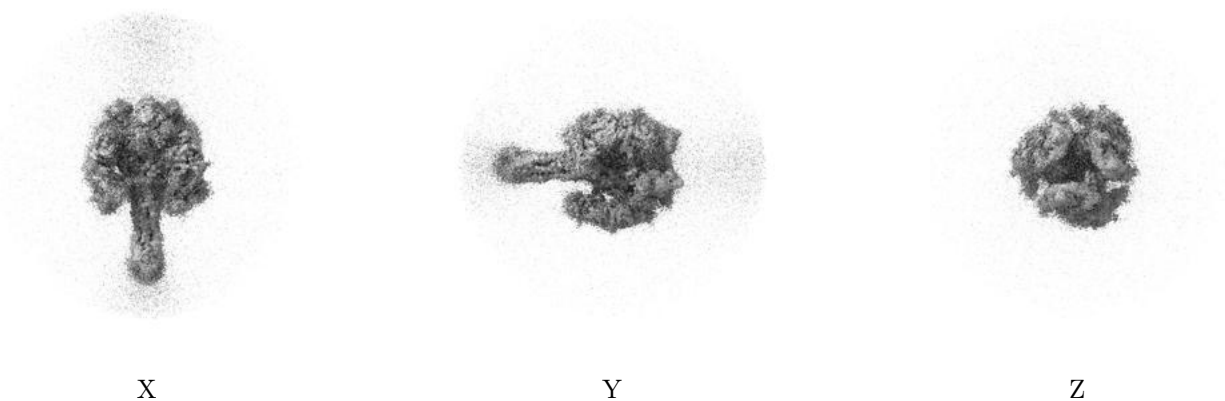
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00603. 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.

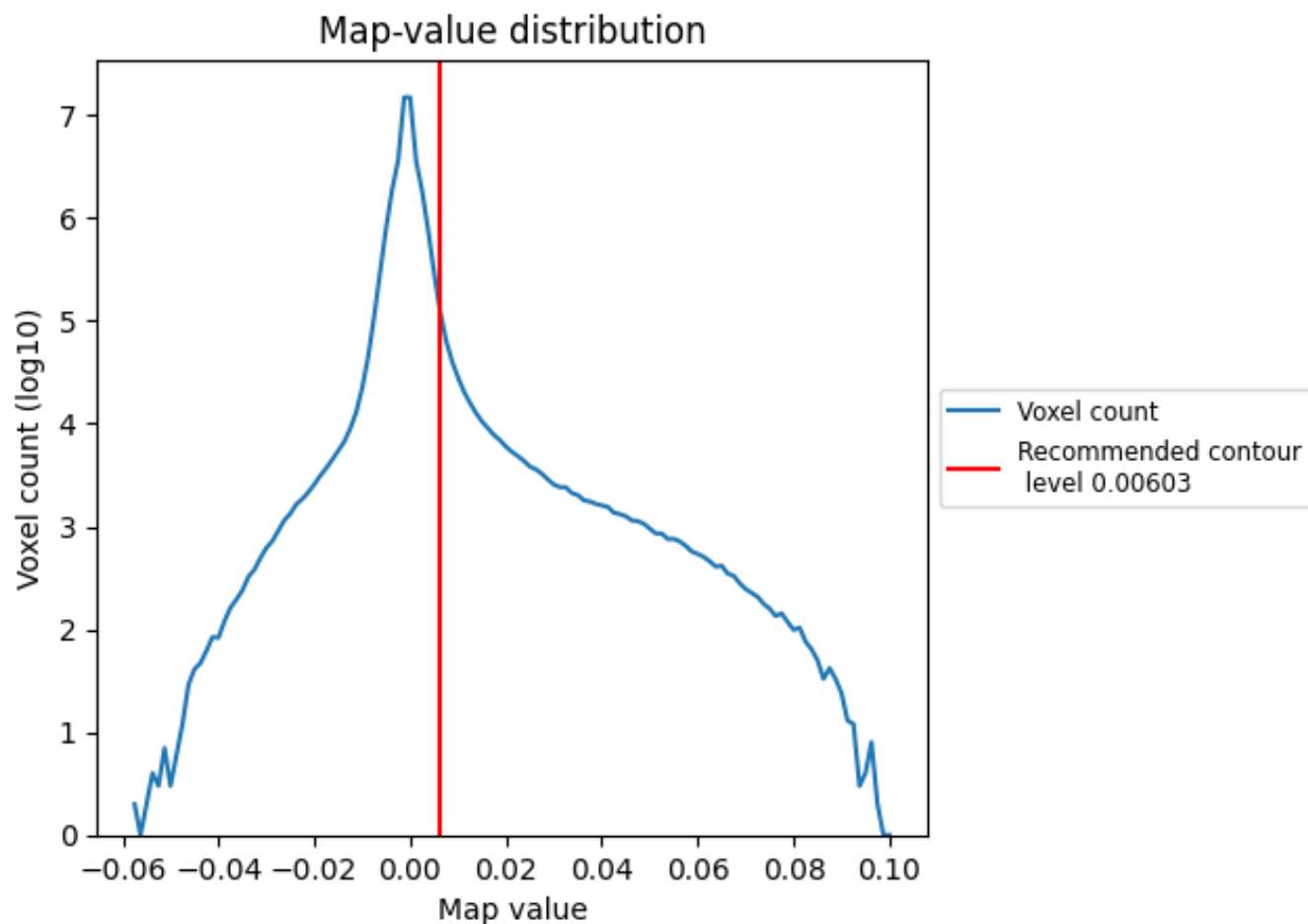
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

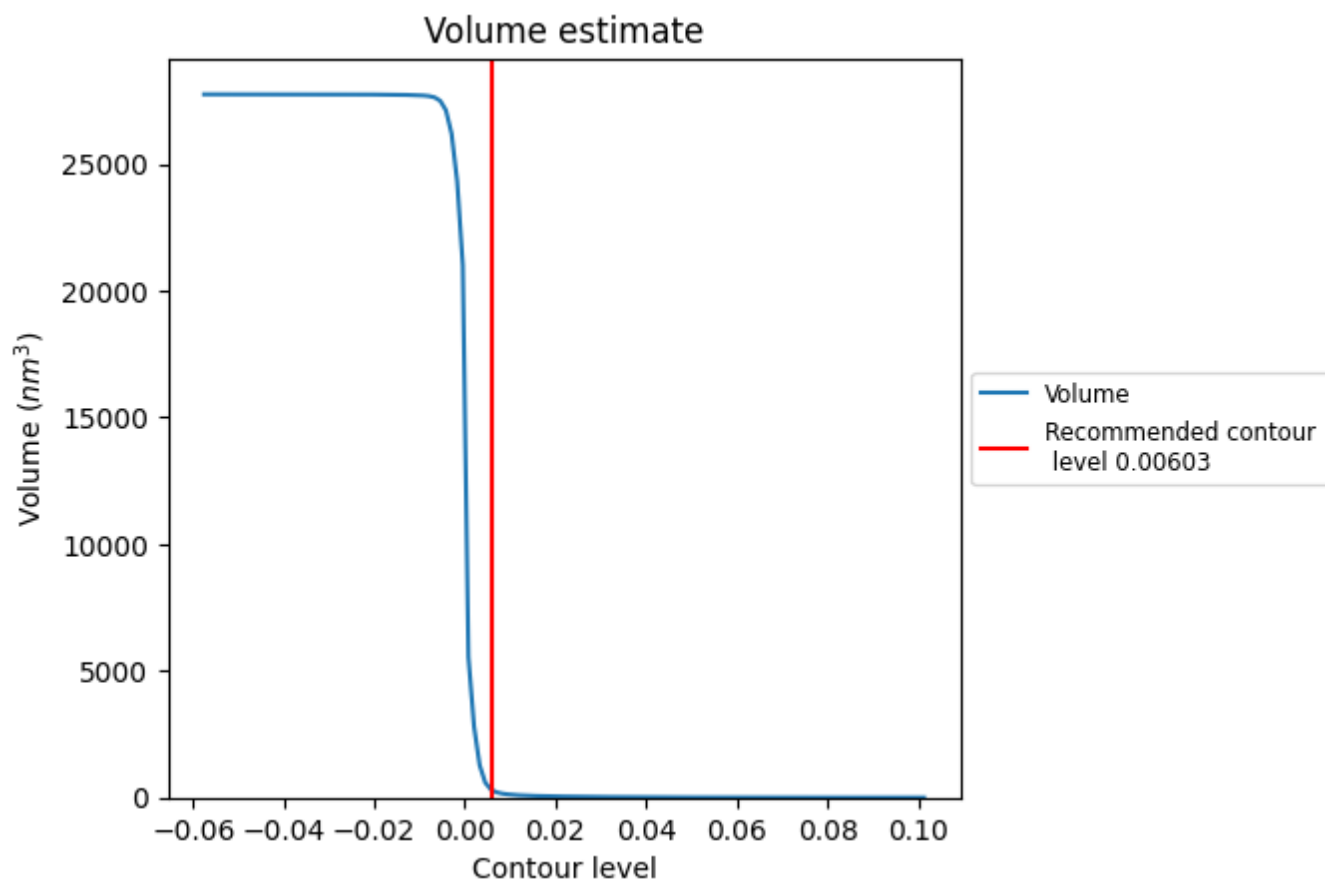
This section contains the results of statistical analysis of the map.

### 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](#)

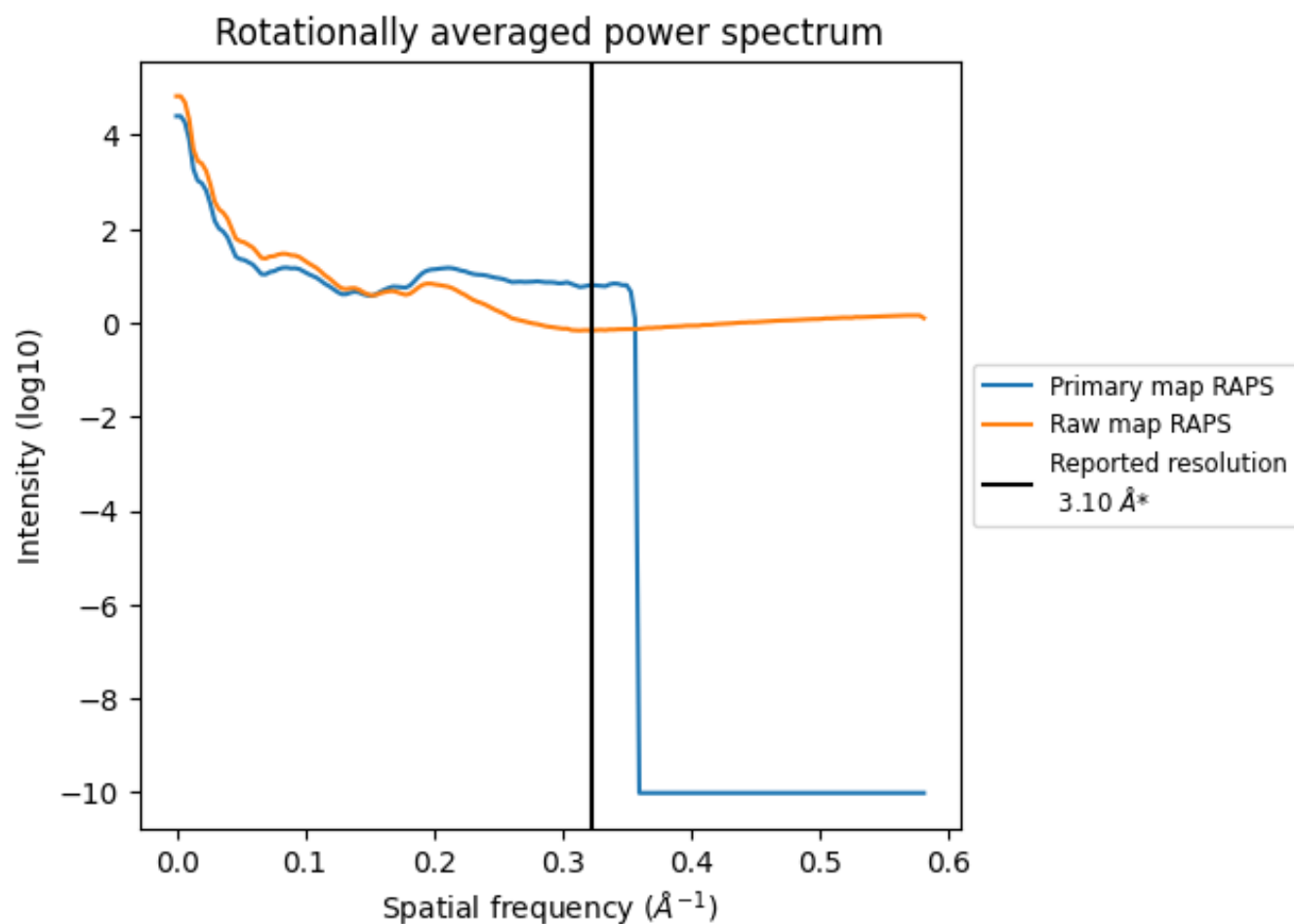


The volume at the recommended contour level is 291 nm<sup>3</sup>; this corresponds to an approximate mass of 263 kDa.

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 ⓘ

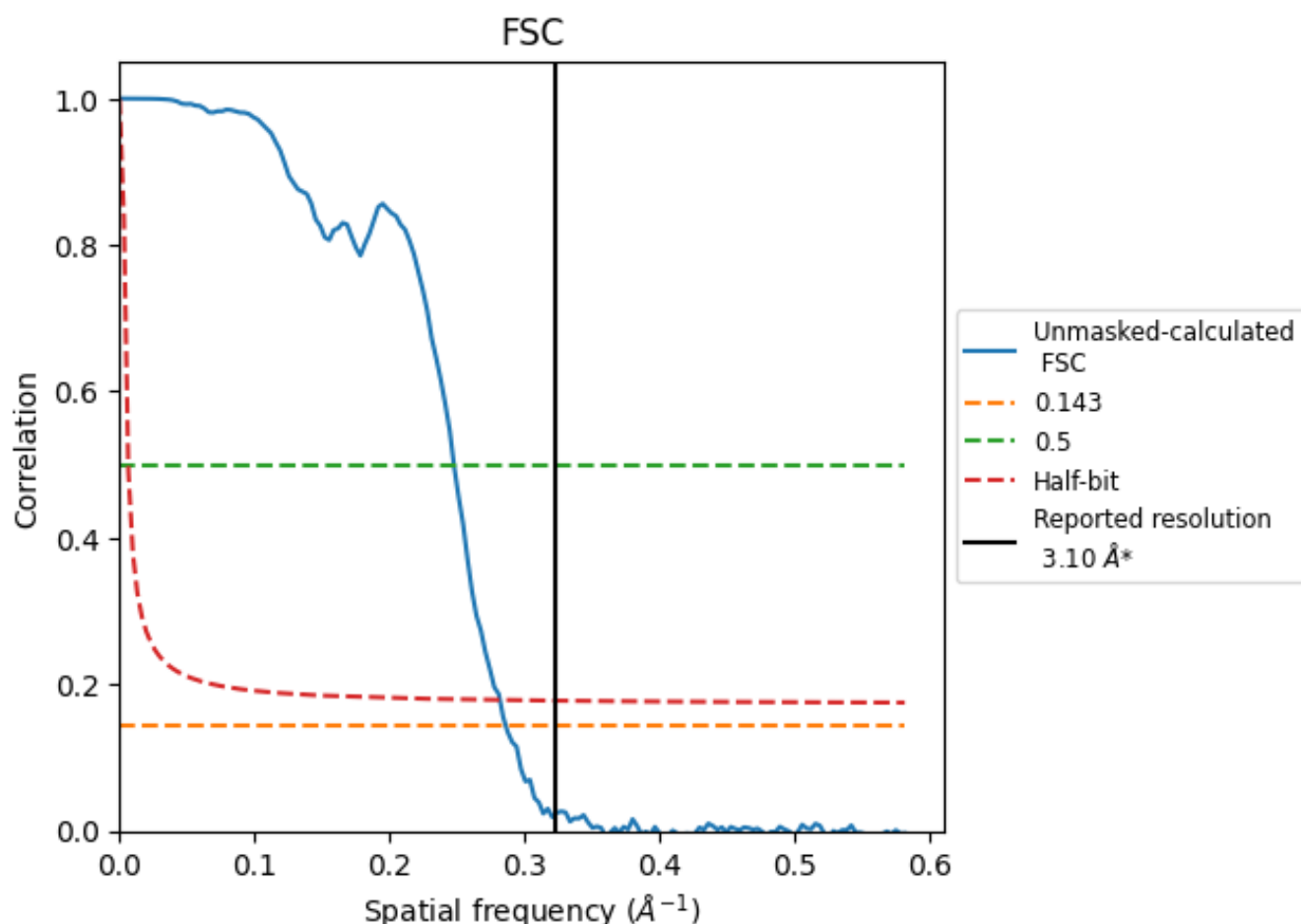


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 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 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

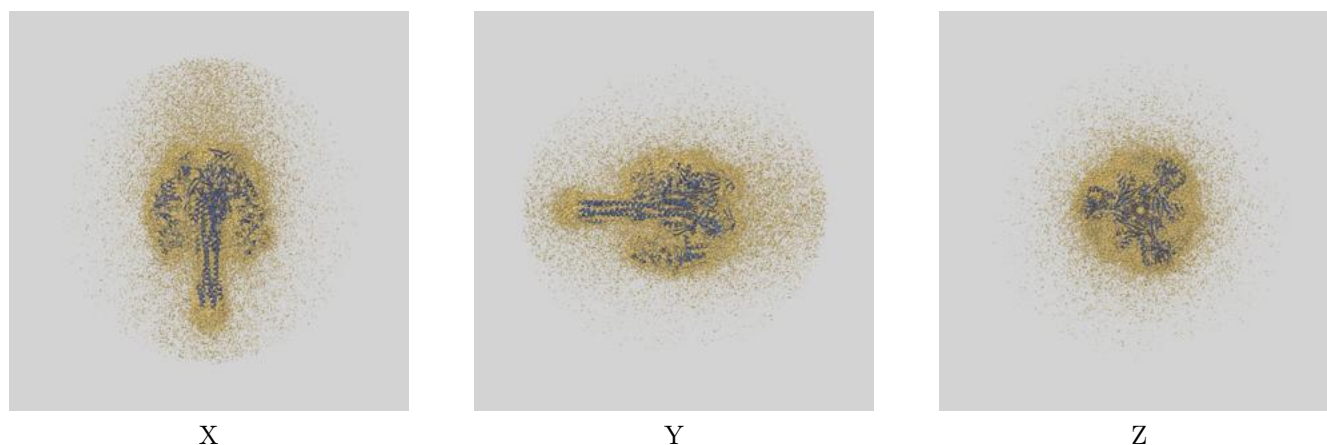
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.50	4.04	3.55

\*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 3.50 differs from the reported value 3.1 by more than 10 %

## 9 Map-model fit [i](#)

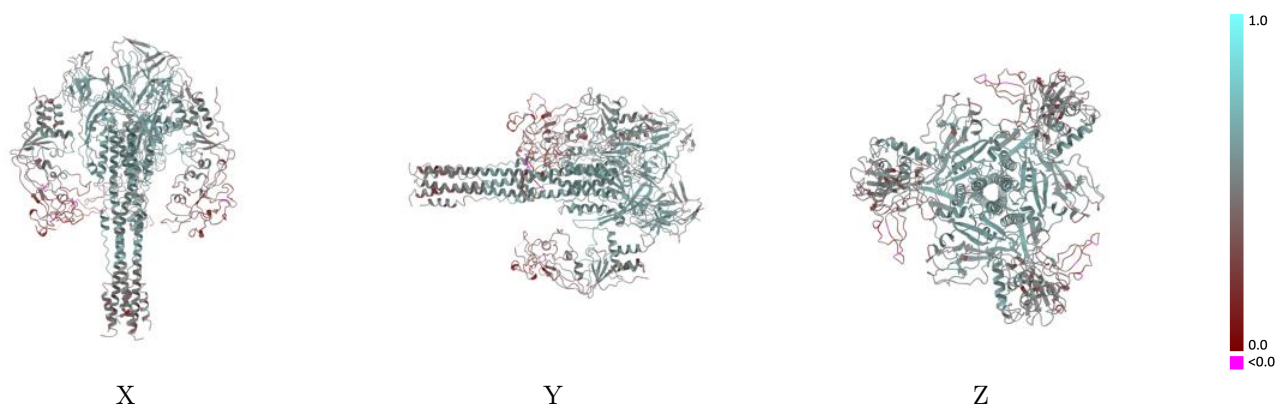
This section contains information regarding the fit between EMDB map EMD-19348 and PDB model 8RM1. Per-residue inclusion information can be found in section [3](#) on page [9](#).

### 9.1 Map-model overlay [i](#)



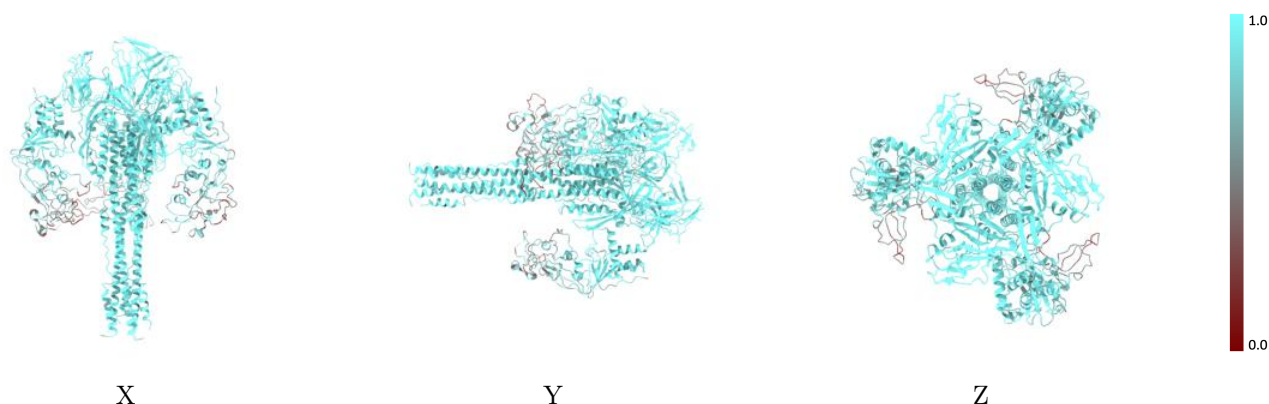
The images above show the 3D surface view of the map at the recommended contour level 0.00603 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



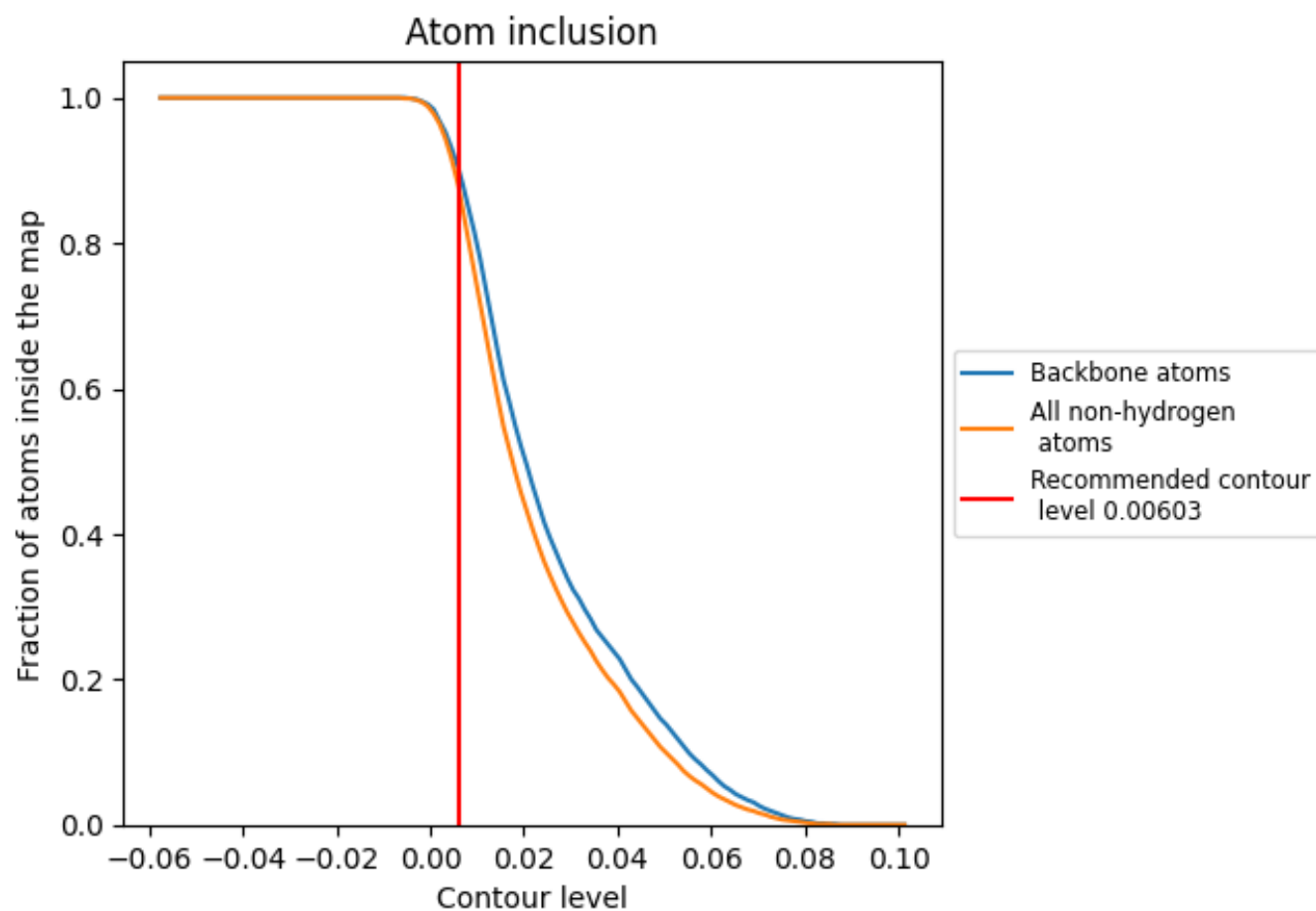
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00603).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 88% 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 (0.00603) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8790</div>	<div><div></div>0.4850</div>
A	<div><div></div>0.8070</div>	<div><div></div>0.4340</div>
B	<div><div></div>0.8070</div>	<div><div></div>0.4350</div>
C	<div><div></div>0.8090</div>	<div><div></div>0.4360</div>
D	<div><div></div>0.9700</div>	<div><div></div>0.5500</div>
E	<div><div></div>0.9710</div>	<div><div></div>0.5500</div>
F	<div><div></div>0.9700</div>	<div><div></div>0.5500</div>
G	<div><div></div>0.8210</div>	<div><div></div>0.4430</div>
H	<div><div></div>0.9740</div>	<div><div></div>0.5150</div>
I	<div><div></div>0.8210</div>	<div><div></div>0.4430</div>
J	<div><div></div>0.9740</div>	<div><div></div>0.5160</div>
K	<div><div></div>0.8210</div>	<div><div></div>0.4460</div>
L	<div><div></div>0.9740</div>	<div><div></div>0.5210</div>

1.0

0.0

<0.0