



## Full wwPDB EM Validation Report ⓘ

May 19, 2025 – 03:13 PM EDT

PDB ID : 9CB1 / pdb\_00009cb1  
EMDB ID : EMD-45412  
Title : Cryo-EM Structure of the Human Neutralizing Antibody 5-1 in Complex with  
Prefusion Human Metapneumovirus F Glycoprotein  
Authors : Guo, L.Q.; McLellan, J.S.  
Deposited on : 2024-06-18  
Resolution : 4.24 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](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.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
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) : 2.43.1

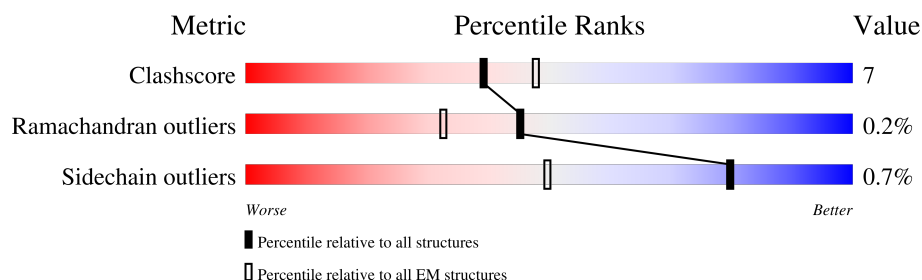
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.24 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.






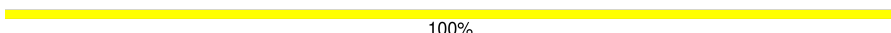
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	219	
1	B	219	
1	C	219	
2	D	214	
2	E	214	
2	F	214	
3	G	551	
3	H	551	

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Mol	Chain	Length	Quality of chain
3	I	551	
4	J	2	
4	K	2	
4	L	2	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15105 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 5-1 Fab Heavy Chain Variable Domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	119	Total	C	N	O	S	0	0
			911	575	157	173	6		
1	B	119	Total	C	N	O	S	0	0
			911	575	157	173	6		
1	C	119	Total	C	N	O	S	0	0
			911	575	157	173	6		

- Molecule 2 is a protein called 5-1 Fab Light Chain Variable Domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	108	Total	C	N	O	S	0	0
			841	524	145	168	4		
2	E	108	Total	C	N	O	S	0	0
			841	524	145	168	4		
2	F	108	Total	C	N	O	S	0	0
			841	524	145	168	4		

- Molecule 3 is a protein called Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	429	Total	C	N	O	S	0	0
			3255	2039	559	626	31		
3	H	429	Total	C	N	O	S	0	0
			3255	2039	559	626	31		
3	I	429	Total	C	N	O	S	0	0
			3255	2039	559	626	31		

There are 231 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	84	CYS	VAL	engineered mutation	UNP H6X1Z1
G	100	ARG	GLN	engineered mutation	UNP H6X1Z1
G	101	ARG	SER	engineered mutation	UNP H6X1Z1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	110	CYS	LEU	engineered mutation	UNP H6X1Z1
G	127	CYS	THR	engineered mutation	UNP H6X1Z1
G	140	CYS	ALA	engineered mutation	UNP H6X1Z1
G	147	CYS	ALA	engineered mutation	UNP H6X1Z1
G	153	CYS	ASN	engineered mutation	UNP H6X1Z1
G	185	PRO	ALA	engineered mutation	UNP H6X1Z1
G	219	LYS	LEU	engineered mutation	UNP H6X1Z1
G	231	ILE	VAL	engineered mutation	UNP H6X1Z1
G	249	CYS	ALA	engineered mutation	UNP H6X1Z1
G	322	CYS	ASN	engineered mutation	UNP H6X1Z1
G	365	CYS	THR	engineered mutation	UNP H6X1Z1
G	453	GLN	GLU	engineered mutation	UNP H6X1Z1
G	463	CYS	VAL	engineered mutation	UNP H6X1Z1
G	491	GLY	-	expression tag	UNP H6X1Z1
G	492	GLY	-	expression tag	UNP H6X1Z1
G	493	GLY	-	expression tag	UNP H6X1Z1
G	494	SER	-	expression tag	UNP H6X1Z1
G	495	GLY	-	expression tag	UNP H6X1Z1
G	496	TYR	-	expression tag	UNP H6X1Z1
G	497	ILE	-	expression tag	UNP H6X1Z1
G	498	PRO	-	expression tag	UNP H6X1Z1
G	499	GLU	-	expression tag	UNP H6X1Z1
G	500	ALA	-	expression tag	UNP H6X1Z1
G	501	PRO	-	expression tag	UNP H6X1Z1
G	502	ARG	-	expression tag	UNP H6X1Z1
G	503	ASP	-	expression tag	UNP H6X1Z1
G	504	GLY	-	expression tag	UNP H6X1Z1
G	505	GLN	-	expression tag	UNP H6X1Z1
G	506	ALA	-	expression tag	UNP H6X1Z1
G	507	TYR	-	expression tag	UNP H6X1Z1
G	508	VAL	-	expression tag	UNP H6X1Z1
G	509	ARG	-	expression tag	UNP H6X1Z1
G	510	LYS	-	expression tag	UNP H6X1Z1
G	511	ASP	-	expression tag	UNP H6X1Z1
G	512	GLY	-	expression tag	UNP H6X1Z1
G	513	GLU	-	expression tag	UNP H6X1Z1
G	514	TRP	-	expression tag	UNP H6X1Z1
G	515	VAL	-	expression tag	UNP H6X1Z1
G	516	LEU	-	expression tag	UNP H6X1Z1
G	517	LEU	-	expression tag	UNP H6X1Z1
G	518	SER	-	expression tag	UNP H6X1Z1
G	519	THR	-	expression tag	UNP H6X1Z1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	520	PHE	-	expression tag	UNP H6X1Z1
G	521	LEU	-	expression tag	UNP H6X1Z1
G	522	GLY	-	expression tag	UNP H6X1Z1
G	523	ARG	-	expression tag	UNP H6X1Z1
G	524	SER	-	expression tag	UNP H6X1Z1
G	525	LEU	-	expression tag	UNP H6X1Z1
G	526	GLU	-	expression tag	UNP H6X1Z1
G	527	VAL	-	expression tag	UNP H6X1Z1
G	528	LEU	-	expression tag	UNP H6X1Z1
G	529	PHE	-	expression tag	UNP H6X1Z1
G	530	GLN	-	expression tag	UNP H6X1Z1
G	531	GLY	-	expression tag	UNP H6X1Z1
G	532	PRO	-	expression tag	UNP H6X1Z1
G	533	GLY	-	expression tag	UNP H6X1Z1
G	534	HIS	-	expression tag	UNP H6X1Z1
G	535	HIS	-	expression tag	UNP H6X1Z1
G	536	HIS	-	expression tag	UNP H6X1Z1
G	537	HIS	-	expression tag	UNP H6X1Z1
G	538	HIS	-	expression tag	UNP H6X1Z1
G	539	HIS	-	expression tag	UNP H6X1Z1
G	540	HIS	-	expression tag	UNP H6X1Z1
G	541	HIS	-	expression tag	UNP H6X1Z1
G	542	SER	-	expression tag	UNP H6X1Z1
G	543	ALA	-	expression tag	UNP H6X1Z1
G	544	TRP	-	expression tag	UNP H6X1Z1
G	545	SER	-	expression tag	UNP H6X1Z1
G	546	HIS	-	expression tag	UNP H6X1Z1
G	547	PRO	-	expression tag	UNP H6X1Z1
G	548	GLN	-	expression tag	UNP H6X1Z1
G	549	PHE	-	expression tag	UNP H6X1Z1
G	550	GLU	-	expression tag	UNP H6X1Z1
G	551	LYS	-	expression tag	UNP H6X1Z1
H	84	CYS	VAL	engineered mutation	UNP H6X1Z1
H	100	ARG	GLN	engineered mutation	UNP H6X1Z1
H	101	ARG	SER	engineered mutation	UNP H6X1Z1
H	110	CYS	LEU	engineered mutation	UNP H6X1Z1
H	127	CYS	THR	engineered mutation	UNP H6X1Z1
H	140	CYS	ALA	engineered mutation	UNP H6X1Z1
H	147	CYS	ALA	engineered mutation	UNP H6X1Z1
H	153	CYS	ASN	engineered mutation	UNP H6X1Z1
H	185	PRO	ALA	engineered mutation	UNP H6X1Z1
H	219	LYS	LEU	engineered mutation	UNP H6X1Z1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	231	ILE	VAL	engineered mutation	UNP H6X1Z1
H	249	CYS	ALA	engineered mutation	UNP H6X1Z1
H	322	CYS	ASN	engineered mutation	UNP H6X1Z1
H	365	CYS	THR	engineered mutation	UNP H6X1Z1
H	453	GLN	GLU	engineered mutation	UNP H6X1Z1
H	463	CYS	VAL	engineered mutation	UNP H6X1Z1
H	491	GLY	-	expression tag	UNP H6X1Z1
H	492	GLY	-	expression tag	UNP H6X1Z1
H	493	GLY	-	expression tag	UNP H6X1Z1
H	494	SER	-	expression tag	UNP H6X1Z1
H	495	GLY	-	expression tag	UNP H6X1Z1
H	496	TYR	-	expression tag	UNP H6X1Z1
H	497	ILE	-	expression tag	UNP H6X1Z1
H	498	PRO	-	expression tag	UNP H6X1Z1
H	499	GLU	-	expression tag	UNP H6X1Z1
H	500	ALA	-	expression tag	UNP H6X1Z1
H	501	PRO	-	expression tag	UNP H6X1Z1
H	502	ARG	-	expression tag	UNP H6X1Z1
H	503	ASP	-	expression tag	UNP H6X1Z1
H	504	GLY	-	expression tag	UNP H6X1Z1
H	505	GLN	-	expression tag	UNP H6X1Z1
H	506	ALA	-	expression tag	UNP H6X1Z1
H	507	TYR	-	expression tag	UNP H6X1Z1
H	508	VAL	-	expression tag	UNP H6X1Z1
H	509	ARG	-	expression tag	UNP H6X1Z1
H	510	LYS	-	expression tag	UNP H6X1Z1
H	511	ASP	-	expression tag	UNP H6X1Z1
H	512	GLY	-	expression tag	UNP H6X1Z1
H	513	GLU	-	expression tag	UNP H6X1Z1
H	514	TRP	-	expression tag	UNP H6X1Z1
H	515	VAL	-	expression tag	UNP H6X1Z1
H	516	LEU	-	expression tag	UNP H6X1Z1
H	517	LEU	-	expression tag	UNP H6X1Z1
H	518	SER	-	expression tag	UNP H6X1Z1
H	519	THR	-	expression tag	UNP H6X1Z1
H	520	PHE	-	expression tag	UNP H6X1Z1
H	521	LEU	-	expression tag	UNP H6X1Z1
H	522	GLY	-	expression tag	UNP H6X1Z1
H	523	ARG	-	expression tag	UNP H6X1Z1
H	524	SER	-	expression tag	UNP H6X1Z1
H	525	LEU	-	expression tag	UNP H6X1Z1
H	526	GLU	-	expression tag	UNP H6X1Z1

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Chain	Residue	Modelled	Actual	Comment	Reference
H	527	VAL	-	expression tag	UNP H6X1Z1
H	528	LEU	-	expression tag	UNP H6X1Z1
H	529	PHE	-	expression tag	UNP H6X1Z1
H	530	GLN	-	expression tag	UNP H6X1Z1
H	531	GLY	-	expression tag	UNP H6X1Z1
H	532	PRO	-	expression tag	UNP H6X1Z1
H	533	GLY	-	expression tag	UNP H6X1Z1
H	534	HIS	-	expression tag	UNP H6X1Z1
H	535	HIS	-	expression tag	UNP H6X1Z1
H	536	HIS	-	expression tag	UNP H6X1Z1
H	537	HIS	-	expression tag	UNP H6X1Z1
H	538	HIS	-	expression tag	UNP H6X1Z1
H	539	HIS	-	expression tag	UNP H6X1Z1
H	540	HIS	-	expression tag	UNP H6X1Z1
H	541	HIS	-	expression tag	UNP H6X1Z1
H	542	SER	-	expression tag	UNP H6X1Z1
H	543	ALA	-	expression tag	UNP H6X1Z1
H	544	TRP	-	expression tag	UNP H6X1Z1
H	545	SER	-	expression tag	UNP H6X1Z1
H	546	HIS	-	expression tag	UNP H6X1Z1
H	547	PRO	-	expression tag	UNP H6X1Z1
H	548	GLN	-	expression tag	UNP H6X1Z1
H	549	PHE	-	expression tag	UNP H6X1Z1
H	550	GLU	-	expression tag	UNP H6X1Z1
H	551	LYS	-	expression tag	UNP H6X1Z1
I	84	CYS	VAL	engineered mutation	UNP H6X1Z1
I	100	ARG	GLN	engineered mutation	UNP H6X1Z1
I	101	ARG	SER	engineered mutation	UNP H6X1Z1
I	110	CYS	LEU	engineered mutation	UNP H6X1Z1
I	127	CYS	THR	engineered mutation	UNP H6X1Z1
I	140	CYS	ALA	engineered mutation	UNP H6X1Z1
I	147	CYS	ALA	engineered mutation	UNP H6X1Z1
I	153	CYS	ASN	engineered mutation	UNP H6X1Z1
I	185	PRO	ALA	engineered mutation	UNP H6X1Z1
I	219	LYS	LEU	engineered mutation	UNP H6X1Z1
I	231	ILE	VAL	engineered mutation	UNP H6X1Z1
I	249	CYS	ALA	engineered mutation	UNP H6X1Z1
I	322	CYS	ASN	engineered mutation	UNP H6X1Z1
I	365	CYS	THR	engineered mutation	UNP H6X1Z1
I	453	GLN	GLU	engineered mutation	UNP H6X1Z1
I	463	CYS	VAL	engineered mutation	UNP H6X1Z1
I	491	GLY	-	expression tag	UNP H6X1Z1

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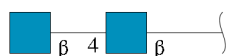
Chain	Residue	Modelled	Actual	Comment	Reference
I	492	GLY	-	expression tag	UNP H6X1Z1
I	493	GLY	-	expression tag	UNP H6X1Z1
I	494	SER	-	expression tag	UNP H6X1Z1
I	495	GLY	-	expression tag	UNP H6X1Z1
I	496	TYR	-	expression tag	UNP H6X1Z1
I	497	ILE	-	expression tag	UNP H6X1Z1
I	498	PRO	-	expression tag	UNP H6X1Z1
I	499	GLU	-	expression tag	UNP H6X1Z1
I	500	ALA	-	expression tag	UNP H6X1Z1
I	501	PRO	-	expression tag	UNP H6X1Z1
I	502	ARG	-	expression tag	UNP H6X1Z1
I	503	ASP	-	expression tag	UNP H6X1Z1
I	504	GLY	-	expression tag	UNP H6X1Z1
I	505	GLN	-	expression tag	UNP H6X1Z1
I	506	ALA	-	expression tag	UNP H6X1Z1
I	507	TYR	-	expression tag	UNP H6X1Z1
I	508	VAL	-	expression tag	UNP H6X1Z1
I	509	ARG	-	expression tag	UNP H6X1Z1
I	510	LYS	-	expression tag	UNP H6X1Z1
I	511	ASP	-	expression tag	UNP H6X1Z1
I	512	GLY	-	expression tag	UNP H6X1Z1
I	513	GLU	-	expression tag	UNP H6X1Z1
I	514	TRP	-	expression tag	UNP H6X1Z1
I	515	VAL	-	expression tag	UNP H6X1Z1
I	516	LEU	-	expression tag	UNP H6X1Z1
I	517	LEU	-	expression tag	UNP H6X1Z1
I	518	SER	-	expression tag	UNP H6X1Z1
I	519	THR	-	expression tag	UNP H6X1Z1
I	520	PHE	-	expression tag	UNP H6X1Z1
I	521	LEU	-	expression tag	UNP H6X1Z1
I	522	GLY	-	expression tag	UNP H6X1Z1
I	523	ARG	-	expression tag	UNP H6X1Z1
I	524	SER	-	expression tag	UNP H6X1Z1
I	525	LEU	-	expression tag	UNP H6X1Z1
I	526	GLU	-	expression tag	UNP H6X1Z1
I	527	VAL	-	expression tag	UNP H6X1Z1
I	528	LEU	-	expression tag	UNP H6X1Z1
I	529	PHE	-	expression tag	UNP H6X1Z1
I	530	GLN	-	expression tag	UNP H6X1Z1
I	531	GLY	-	expression tag	UNP H6X1Z1
I	532	PRO	-	expression tag	UNP H6X1Z1
I	533	GLY	-	expression tag	UNP H6X1Z1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	534	HIS	-	expression tag	UNP H6X1Z1
I	535	HIS	-	expression tag	UNP H6X1Z1
I	536	HIS	-	expression tag	UNP H6X1Z1
I	537	HIS	-	expression tag	UNP H6X1Z1
I	538	HIS	-	expression tag	UNP H6X1Z1
I	539	HIS	-	expression tag	UNP H6X1Z1
I	540	HIS	-	expression tag	UNP H6X1Z1
I	541	HIS	-	expression tag	UNP H6X1Z1
I	542	SER	-	expression tag	UNP H6X1Z1
I	543	ALA	-	expression tag	UNP H6X1Z1
I	544	TRP	-	expression tag	UNP H6X1Z1
I	545	SER	-	expression tag	UNP H6X1Z1
I	546	HIS	-	expression tag	UNP H6X1Z1
I	547	PRO	-	expression tag	UNP H6X1Z1
I	548	GLN	-	expression tag	UNP H6X1Z1
I	549	PHE	-	expression tag	UNP H6X1Z1
I	550	GLU	-	expression tag	UNP H6X1Z1
I	551	LYS	-	expression tag	UNP H6X1Z1

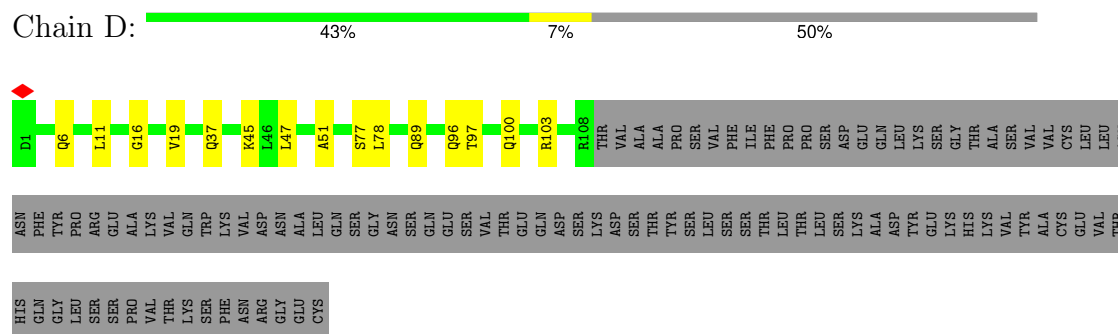
- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



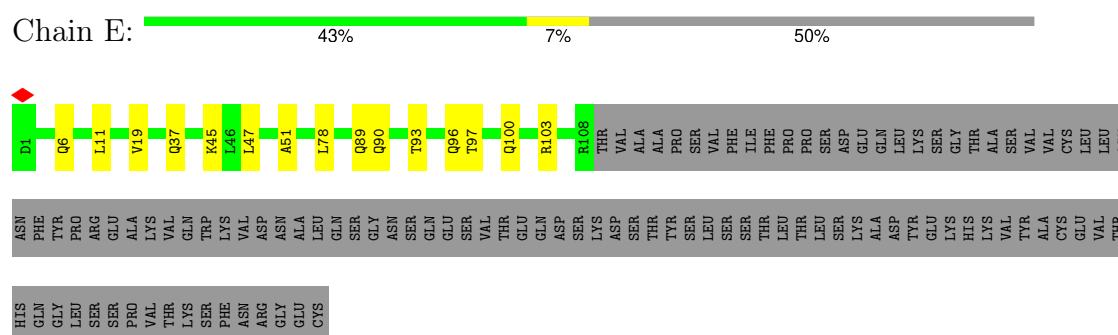
Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		



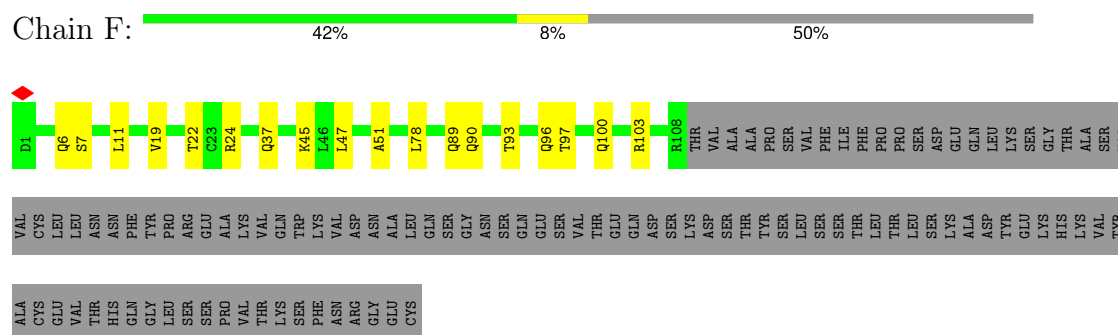
- Molecule 2: 5-1 Fab Light Chain Variable Domain



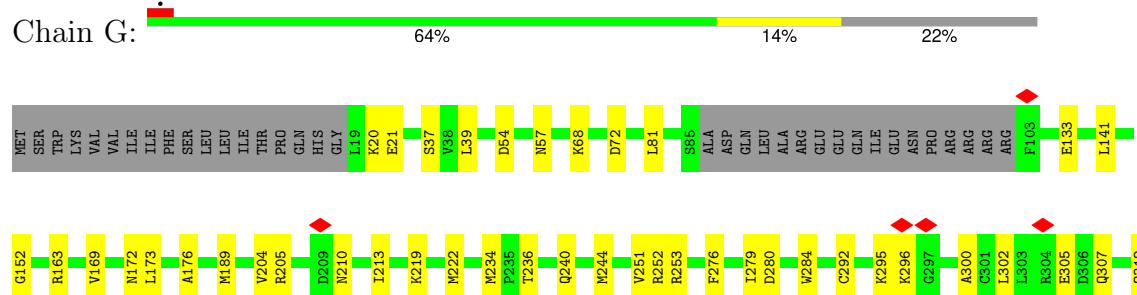
- Molecule 2: 5-1 Fab Light Chain Variable Domain

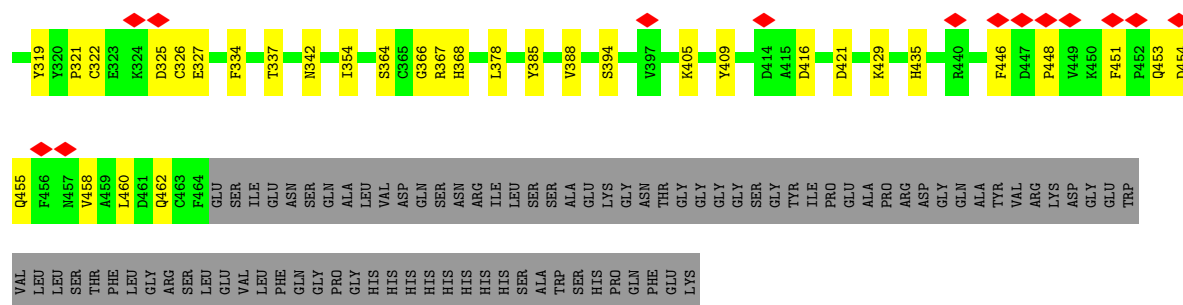


- Molecule 2: 5-1 Fab Light Chain Variable Domain

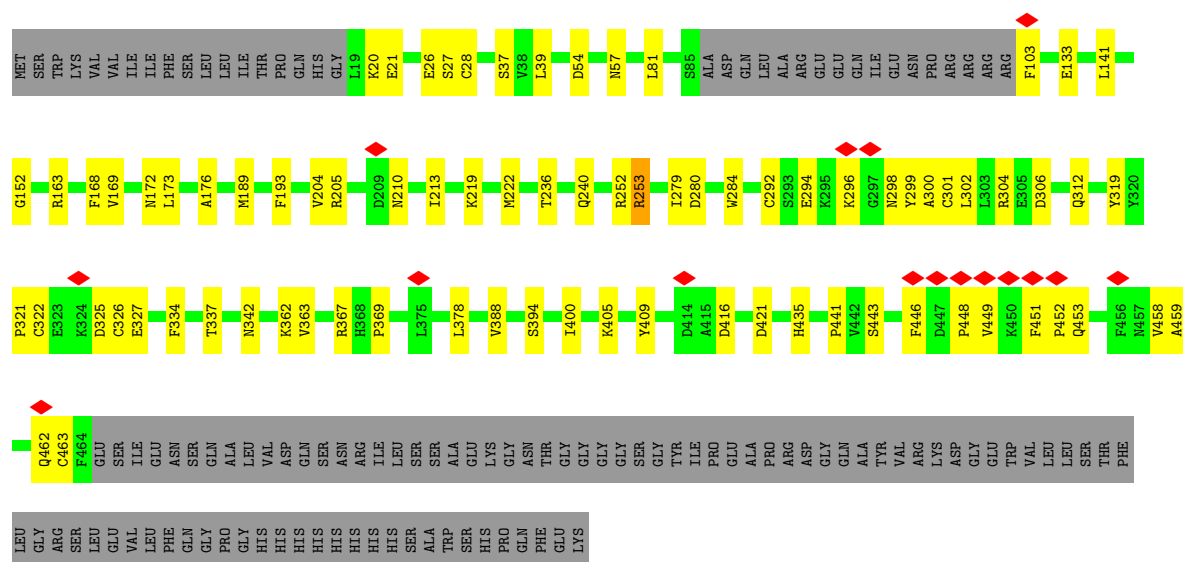


- Molecule 3: Fusion glycoprotein F0

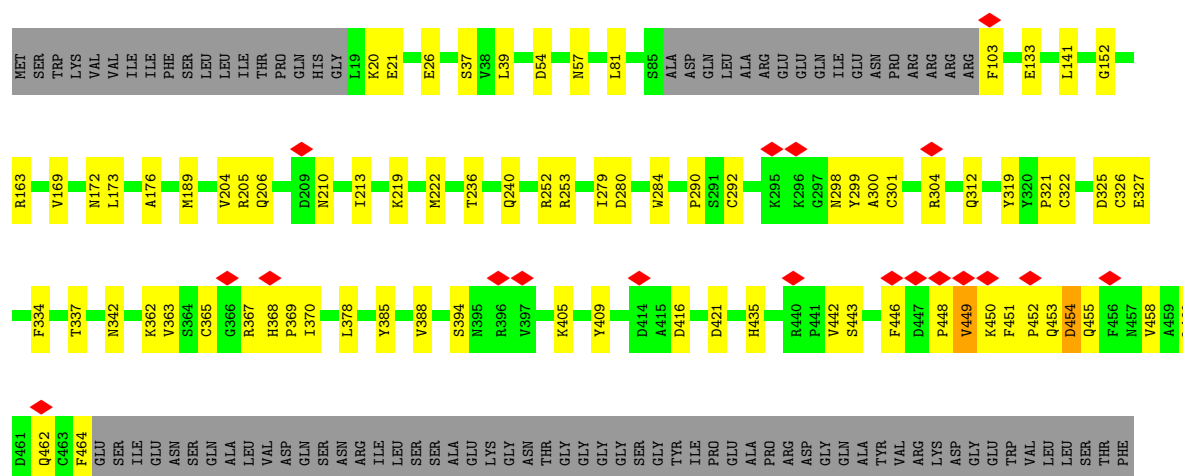




### • Molecule 3: Fusion glycoprotein F0



### • Molecule 3: Fusion glycoprotein F0



LEU	GLY	ARG	SER	LEU	GLU	VAL	LEU	PHE	GLN	GLY	PRO	GLY	HIS	HIS	HIS	HIS	HIS	HIS	HIS	SER	ALA	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS
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● Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



NAG1
NAG2

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



NAG1
NAG2

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



NAG1
NAG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18483	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	48.64	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	150000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.023	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0251	Depositor
Map size ( $\text{\AA}$ )	338.4, 338.4, 338.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.94, 0.94, 0.94	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.15	0/937	0.45	0/1279
1	B	0.14	0/937	0.46	0/1279
1	C	0.15	0/937	0.46	0/1279
2	D	0.14	0/860	0.46	0/1166
2	E	0.21	0/860	0.49	0/1166
2	F	0.22	0/860	0.49	0/1166
3	G	0.46	0/3303	0.61	0/4471
3	H	0.47	0/3303	0.63	0/4471
3	I	0.46	0/3303	0.62	0/4471
All	All	0.39	0/15300	0.57	0/20748

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
2	E	0	1
2	F	0	2
3	H	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
2	D	103	ARG	Sidechain
2	E	103	ARG	Sidechain
2	F	103	ARG	Sidechain
2	F	24	ARG	Sidechain
3	H	253	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	911	0	874	12	0
1	B	911	0	874	13	0
1	C	911	0	874	12	0
2	D	841	0	808	6	0
2	E	841	0	808	6	0
2	F	841	0	808	7	0
3	G	3255	0	3262	49	0
3	H	3255	0	3262	54	0
3	I	3255	0	3262	59	0
4	J	28	0	25	0	0
4	K	28	0	25	3	0
4	L	28	0	25	0	0
All	All	15105	0	14907	209	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 7.

All (209) 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:I:300:ALA:HA	3:I:367:ARG:HA	1.44	0.99
3:H:300:ALA:HB2	3:H:448:PRO:HD3	1.58	0.85
3:G:219:LYS:HE3	3:I:205:ARG:HA	1.70	0.74
3:G:205:ARG:HA	3:H:219:LYS:HE3	1.70	0.73
1:A:87:THR:HG23	1:A:110:THR:HA	1.71	0.73
1:B:87:THR:HG23	1:B:110:THR:HA	1.72	0.70
3:H:388:VAL:O	3:H:405:LYS:NZ	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:172:ASN:HB3	3:G:189:MET:HE1	1.75	0.67
3:H:172:ASN:HB3	3:H:189:MET:HE1	1.77	0.67
1:C:87:THR:HG23	1:C:110:THR:HA	1.75	0.67
3:H:296:LYS:HD2	3:H:449:VAL:HG21	1.76	0.67
1:C:94:ARG:NH2	1:C:101:ASP:OD2	2.27	0.66
3:H:362:LYS:HE3	3:I:368:HIS:HB2	1.77	0.66
3:H:362:LYS:HD3	3:H:459:ALA:HB2	1.79	0.65
3:I:298:ASN:HD21	3:I:452:PRO:HG2	1.61	0.65
3:H:205:ARG:HA	3:I:219:LYS:HE3	1.77	0.65
3:G:222:MET:O	3:G:252:ARG:NH2	2.28	0.64
3:I:388:VAL:O	3:I:405:LYS:NZ	2.31	0.64
1:B:94:ARG:NH2	1:B:101:ASP:OD2	2.30	0.63
1:A:94:ARG:NH2	1:A:101:ASP:OD2	2.30	0.63
3:G:388:VAL:O	3:G:405:LYS:NZ	2.32	0.62
3:G:133:GLU:OE2	3:G:152:GLY:N	2.33	0.62
3:H:304:ARG:HA	3:H:363:VAL:HG12	1.81	0.61
3:I:133:GLU:OE2	3:I:152:GLY:N	2.33	0.61
3:I:141:LEU:O	3:I:163:ARG:NH2	2.33	0.61
3:H:133:GLU:OE2	3:H:152:GLY:N	2.35	0.60
3:H:302:LEU:HB2	3:H:446:PHE:HE2	1.67	0.59
3:H:141:LEU:O	3:H:163:ARG:NH2	2.34	0.59
2:D:6:GLN:O	2:D:100:GLN:NE2	2.36	0.58
3:I:253:ARG:NH1	3:I:327:GLU:OE1	2.36	0.58
3:I:169:VAL:HG13	3:I:173:LEU:HD23	1.86	0.58
4:K:1:NAG:H61	4:K:2:NAG:C7	2.33	0.58
3:I:304:ARG:HA	3:I:363:VAL:HG12	1.84	0.58
3:I:292:CYS:HA	3:I:301:CYS:HA	1.86	0.58
2:D:19:VAL:HG21	2:D:78:LEU:HD13	1.86	0.57
3:G:141:LEU:O	3:G:163:ARG:NH2	2.37	0.57
3:G:21:GLU:HB2	3:G:378:LEU:HD12	1.87	0.57
3:H:103:PHE:HE2	3:I:290:PRO:HB3	1.70	0.57
3:I:455:GLN:HB3	3:I:458:VAL:HG21	1.87	0.57
3:I:322:CYS:HB2	3:I:325:ASP:OD2	2.06	0.56
3:G:322:CYS:HB2	3:G:325:ASP:OD2	2.06	0.56
3:G:366:GLY:C	3:G:368:HIS:H	2.14	0.55
3:I:21:GLU:HB2	3:I:378:LEU:HD12	1.88	0.55
3:H:169:VAL:HG13	3:H:173:LEU:HD23	1.89	0.55
3:H:253:ARG:NH1	3:H:327:GLU:OE1	2.40	0.55
3:H:322:CYS:HB2	3:H:325:ASP:OD2	2.05	0.55
3:I:301:CYS:SG	3:I:369:PRO:HA	2.46	0.55
3:I:367:ARG:HH11	3:I:453:GLN:H	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:169:VAL:HG13	3:G:173:LEU:HD23	1.87	0.55
3:I:443:SER:HA	3:I:446:PHE:HB3	1.89	0.55
1:B:6:GLN:O	1:B:105:GLN:NE2	2.39	0.55
2:E:6:GLN:O	2:E:100:GLN:NE2	2.35	0.54
2:E:19:VAL:HG21	2:E:78:LEU:HD13	1.89	0.54
1:B:50:TRP:CH2	1:B:52:SER:HB2	2.42	0.54
3:H:21:GLU:HB2	3:H:378:LEU:HD12	1.89	0.54
3:G:455:GLN:HB3	3:G:458:VAL:HG21	1.90	0.54
1:C:50:TRP:CH2	1:C:52:SER:HB2	2.44	0.53
2:F:19:VAL:HG21	2:F:78:LEU:HD13	1.90	0.53
3:I:363:VAL:HG21	3:I:460:LEU:HG	1.90	0.53
3:H:342:ASN:ND2	3:I:421:ASP:OD2	2.42	0.53
3:H:81:LEU:HD13	3:H:204:VAL:HG13	1.91	0.53
3:G:448:PRO:HA	3:G:451:PHE:CZ	2.44	0.52
3:H:21:GLU:OE2	3:H:409:TYR:OH	2.26	0.52
3:H:292:CYS:HB3	3:H:299:TYR:HD1	1.74	0.52
3:G:302:LEU:HD11	3:G:460:LEU:HD12	1.91	0.52
3:G:366:GLY:HA2	3:G:454:ASP:H	1.73	0.52
2:F:6:GLN:O	2:F:100:GLN:NE2	2.37	0.52
3:G:37:SER:O	3:G:280:ASP:N	2.43	0.52
3:I:222:MET:O	3:I:252:ARG:NH2	2.36	0.51
3:G:253:ARG:NH1	3:G:327:GLU:OE1	2.44	0.51
3:G:21:GLU:OE2	3:G:409:TYR:OH	2.28	0.51
3:H:27:SER:O	3:H:28:CYS:C	2.53	0.51
3:G:421:ASP:OD2	3:I:342:ASN:ND2	2.44	0.51
3:H:176:ALA:HB2	3:H:189:MET:HE3	1.92	0.51
1:A:6:GLN:O	1:A:105:GLN:NE2	2.42	0.51
3:G:81:LEU:HD13	3:G:204:VAL:HG13	1.93	0.51
3:G:176:ALA:HB2	3:G:189:MET:HE3	1.93	0.51
3:H:37:SER:O	3:H:280:ASP:N	2.44	0.51
1:A:50:TRP:CH2	1:A:52:SER:HB2	2.45	0.50
3:H:300:ALA:HB1	3:H:446:PHE:HB2	1.93	0.50
1:B:46:GLU:OE2	1:B:62:ASN:ND2	2.44	0.50
3:I:292:CYS:HB2	3:I:385:TYR:CE1	2.46	0.50
2:F:37:GLN:O	2:F:45:LYS:N	2.34	0.50
3:I:37:SER:O	3:I:280:ASP:N	2.44	0.50
3:I:26:GLU:HG2	3:I:442:VAL:HG23	1.93	0.50
3:H:103:PHE:CZ	3:I:301:CYS:HB2	2.47	0.50
3:H:319:TYR:CE2	3:H:321:PRO:HB3	2.46	0.50
3:G:284:TRP:HH2	3:G:312:GLN:HG3	1.77	0.50
3:G:54:ASP:OD2	3:G:57:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:319:TYR:CE2	3:I:321:PRO:HB3	2.47	0.49
1:C:6:GLN:O	1:C:105:GLN:NE2	2.43	0.49
3:I:81:LEU:HD13	3:I:204:VAL:HG13	1.94	0.49
3:G:354:ILE:HG12	3:G:460:LEU:HD22	1.95	0.49
3:I:172:ASN:HB3	3:I:189:MET:HE1	1.95	0.49
3:H:54:ASP:OD2	3:H:57:ASN:ND2	2.45	0.49
2:E:37:GLN:HB2	2:E:47:LEU:HD11	1.94	0.48
3:I:284:TRP:CH2	3:I:312:GLN:HG3	2.48	0.48
3:G:284:TRP:CH2	3:G:312:GLN:HG3	2.48	0.48
3:G:342:ASN:ND2	3:H:421:ASP:OD2	2.47	0.48
3:I:169:VAL:HA	3:I:173:LEU:HB3	1.96	0.48
3:G:319:TYR:CE2	3:G:321:PRO:HB3	2.49	0.48
3:G:251:VAL:HG22	3:G:276:PHE:HE2	1.78	0.47
3:I:292:CYS:SG	3:I:369:PRO:HA	2.55	0.47
3:I:206:GLN:O	3:I:210:ASN:ND2	2.40	0.47
2:F:37:GLN:HB2	2:F:47:LEU:HD11	1.96	0.47
3:I:284:TRP:HH2	3:I:312:GLN:HG3	1.79	0.47
3:H:39:LEU:HB3	3:H:337:THR:CG2	2.45	0.47
3:H:459:ALA:O	3:H:463:CYS:SG	2.73	0.47
3:I:365:CYS:HB3	3:I:446:PHE:HE2	1.80	0.46
3:H:222:MET:O	3:H:252:ARG:NH2	2.42	0.46
3:G:39:LEU:HB3	3:G:337:THR:CG2	2.45	0.46
1:B:36:TRP:CE2	1:B:80:MET:HB2	2.51	0.46
2:D:37:GLN:O	2:D:45:LYS:N	2.35	0.46
3:G:292:CYS:HB2	3:G:385:TYR:CZ	2.51	0.46
3:G:305:GLU:C	3:G:307:GLN:H	2.23	0.46
3:H:394:SER:HA	3:H:416:ASP:HB2	1.97	0.46
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.98	0.46
3:I:20:LYS:HE3	3:I:435:HIS:CD2	2.50	0.46
3:I:453:GLN:O	3:I:454:ASP:C	2.57	0.46
1:B:35:THR:HG21	1:B:100(D):TYR:CE2	2.51	0.46
1:B:2:GLY:HA2	1:B:26:ALA:HB3	1.96	0.45
3:G:300:ALA:HB1	3:G:446:PHE:CG	2.51	0.45
3:I:362:LYS:HD3	3:I:362:LYS:HA	1.82	0.45
3:G:20:LYS:HE3	3:G:435:HIS:CD2	2.52	0.45
1:A:35:THR:HG21	1:A:100(D):TYR:CE2	2.51	0.45
1:A:46:GLU:OE2	1:A:62:ASN:ND2	2.49	0.45
2:F:89:GLN:NE2	2:F:96:GLN:HB3	2.32	0.45
3:G:295:LYS:HE2	3:G:296:LYS:HE3	1.98	0.45
3:I:39:LEU:HB3	3:I:337:THR:CG2	2.47	0.45
3:G:366:GLY:C	3:G:368:HIS:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:443:SER:HA	3:H:446:PHE:CD2	2.52	0.45
2:E:89:GLN:NE2	2:E:96:GLN:HB3	2.31	0.45
3:H:20:LYS:HE3	3:H:435:HIS:CD2	2.52	0.45
3:I:54:ASP:OD2	3:I:57:ASN:ND2	2.49	0.45
3:I:450:LYS:O	3:I:451:PHE:C	2.59	0.45
3:G:240:GLN:HA	3:G:279:ILE:HD13	1.99	0.45
3:I:240:GLN:HA	3:I:279:ILE:HD13	1.99	0.45
3:G:462:GLN:HG2	3:H:367:ARG:HH22	1.82	0.44
3:I:455:GLN:HE22	3:I:462:GLN:HB3	1.82	0.44
4:K:1:NAG:H61	4:K:2:NAG:N2	2.32	0.44
3:H:451:PHE:CE1	3:H:453:GLN:HB2	2.53	0.44
1:A:36:TRP:CE2	1:A:80:MET:HB2	2.52	0.44
1:B:6:GLN:H	1:B:105:GLN:CD	2.25	0.44
3:I:176:ALA:HB2	3:I:189:MET:HE3	2.00	0.44
3:G:292:CYS:HB2	3:G:385:TYR:CE1	2.53	0.44
3:H:103:PHE:HD2	3:I:370:ILE:HD12	1.83	0.44
2:E:37:GLN:O	2:E:45:LYS:N	2.35	0.43
3:H:326:CYS:HA	3:H:334:PHE:O	2.18	0.43
3:H:363:VAL:H	3:H:459:ALA:HA	1.83	0.43
3:I:446:PHE:HA	3:I:464:PHE:HE1	1.83	0.43
3:G:416:ASP:OD1	3:G:429:LYS:NZ	2.50	0.43
1:C:36:TRP:CE2	1:C:80:MET:HB2	2.53	0.43
3:H:39:LEU:HB3	3:H:337:THR:HG23	2.00	0.43
1:A:33:GLY:O	1:A:95:GLY:N	2.51	0.43
3:H:298:ASN:HB3	3:H:448:PRO:HB2	2.01	0.43
2:E:90:GLN:NE2	2:E:93:THR:OG1	2.52	0.43
3:H:304:ARG:HB3	3:H:306:ASP:OD1	2.18	0.43
3:I:448:PRO:O	3:I:449:VAL:C	2.62	0.43
4:K:1:NAG:H61	4:K:2:NAG:H82	2.00	0.43
1:C:22:CYS:N	1:C:78:GLY:O	2.49	0.43
1:C:46:GLU:OE2	1:C:62:ASN:ND2	2.50	0.43
3:G:394:SER:HA	3:G:416:ASP:HB2	2.01	0.43
3:I:21:GLU:OE2	3:I:409:TYR:OH	2.26	0.43
1:C:2:GLY:HA2	1:C:26:ALA:HB3	2.01	0.42
1:A:27:TYR:CE1	1:A:29:PHE:HA	2.55	0.42
2:D:89:GLN:NE2	2:D:96:GLN:HB3	2.35	0.42
3:I:452:PRO:O	3:I:455:GLN:HG3	2.19	0.42
1:A:50:TRP:CZ2	1:A:52:SER:HB2	2.55	0.42
1:A:6:GLN:H	1:A:105:GLN:CD	2.28	0.42
1:C:6:GLN:H	1:C:105:GLN:CD	2.27	0.42
3:G:210:ASN:HB3	3:G:213:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:236:THR:HB	3:H:240:GLN:OE1	2.19	0.42
3:G:68:LYS:NZ	3:G:72:ASP:OD2	2.37	0.42
3:G:234:MET:HE1	3:G:244:MET:HE1	2.01	0.42
1:A:11:VAL:HG22	1:A:110:THR:HB	2.02	0.42
3:G:172:ASN:O	3:G:173:LEU:C	2.63	0.42
3:H:367:ARG:HE	3:H:452:PRO:C	2.27	0.42
3:G:326:CYS:HA	3:G:334:PHE:O	2.20	0.42
3:G:364:SER:HB3	3:I:103:PHE:HB2	2.02	0.42
3:I:326:CYS:HA	3:I:334:PHE:O	2.20	0.42
3:H:210:ASN:HB3	3:H:213:ILE:O	2.20	0.41
3:I:394:SER:HA	3:I:416:ASP:HB2	2.02	0.41
3:H:394:SER:HB3	3:H:400:ILE:HD11	2.01	0.41
1:C:35:THR:HG21	1:C:100(D):TYR:CZ	2.55	0.41
3:H:284:TRP:CH2	3:H:312:GLN:HG3	2.55	0.41
1:B:27:TYR:CE1	1:B:29:PHE:HA	2.55	0.41
3:I:210:ASN:HB3	3:I:213:ILE:O	2.20	0.41
3:I:443:SER:HA	3:I:446:PHE:CD1	2.55	0.41
1:C:50:TRP:CZ2	1:C:52:SER:HB2	2.55	0.41
2:F:90:GLN:NE2	2:F:93:THR:OG1	2.52	0.41
3:H:168:PHE:CE2	3:H:193:PHE:HA	2.55	0.41
3:H:458:VAL:HB	3:H:462:GLN:HB2	2.03	0.41
1:B:4:LEU:HD23	1:B:24:ALA:HA	2.02	0.41
3:G:236:THR:HB	3:G:240:GLN:OE1	2.20	0.41
3:H:301:CYS:SG	3:H:369:PRO:HA	2.61	0.41
3:I:39:LEU:HB3	3:I:337:THR:HG23	2.02	0.41
1:C:35:THR:HG21	1:C:100(D):TYR:CE2	2.56	0.41
2:F:7:SER:O	2:F:22:THR:OG1	2.33	0.41
3:H:26:GLU:O	3:H:441:PRO:HA	2.21	0.41
3:H:240:GLN:HA	3:H:279:ILE:HD13	2.03	0.41
3:G:367:ARG:HD2	3:G:453:GLN:HE21	1.86	0.40
3:H:294:GLU:HB2	3:H:299:TYR:CZ	2.56	0.40
1:B:35:THR:HG21	1:B:100(D):TYR:CZ	2.56	0.40
1:B:33:GLY:O	1:B:95:GLY:N	2.51	0.40
3:I:446:PHE:HA	3:I:464:PHE:CE1	2.57	0.40
2:D:16:GLY:HA2	2:D:77:SER:OG	2.21	0.40
3:G:39:LEU:HB3	3:G:337:THR:HG23	2.04	0.40
3:I:236:THR:HB	3:I:240:GLN:OE1	2.21	0.40
3:I:385:TYR:O	3:I:388:VAL:HG22	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	117/219 (53%)	115 (98%)	2 (2%)	0	100	100
1	B	117/219 (53%)	114 (97%)	3 (3%)	0	100	100
1	C	117/219 (53%)	115 (98%)	2 (2%)	0	100	100
2	D	106/214 (50%)	102 (96%)	3 (3%)	1 (1%)	14	50
2	E	106/214 (50%)	102 (96%)	3 (3%)	1 (1%)	14	50
2	F	106/214 (50%)	102 (96%)	3 (3%)	1 (1%)	14	50
3	G	425/551 (77%)	406 (96%)	19 (4%)	0	100	100
3	H	425/551 (77%)	406 (96%)	19 (4%)	0	100	100
3	I	425/551 (77%)	411 (97%)	14 (3%)	0	100	100
All	All	1944/2952 (66%)	1873 (96%)	68 (4%)	3 (0%)	45	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	51	ALA
2	E	51	ALA
2	F	51	ALA

### 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	98/184 (53%)	97 (99%)	1 (1%)	73	82

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	98/184 (53%)	97 (99%)	1 (1%)	73	82
1	C	98/184 (53%)	97 (99%)	1 (1%)	73	82
2	D	94/189 (50%)	92 (98%)	2 (2%)	48	67
2	E	94/189 (50%)	92 (98%)	2 (2%)	48	67
2	F	94/189 (50%)	92 (98%)	2 (2%)	48	67
3	G	366/469 (78%)	366 (100%)	0	100	100
3	H	366/469 (78%)	366 (100%)	0	100	100
3	I	366/469 (78%)	363 (99%)	3 (1%)	79	85
All	All	1674/2526 (66%)	1662 (99%)	12 (1%)	80	87

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	THR
1	B	35	THR
1	C	35	THR
2	D	11	LEU
2	D	97	THR
2	E	11	LEU
2	E	97	THR
2	F	11	LEU
2	F	97	THR
3	I	299	TYR
3	I	449	VAL
3	I	454	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	B	31	ASN
1	C	31	ASN
2	D	38	HIS
2	E	38	HIS
2	F	38	HIS
3	G	195	GLN
3	G	435	HIS
3	G	453	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	H	195	GLN
3	H	435	HIS
3	I	195	GLN
3	I	435	HIS
3	I	455	GLN

### 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 ⓘ

6 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	J	1	3,4	14,14,15	0.39	0	17,19,21	0.46	0
4	NAG	J	2	4	14,14,15	0.40	0	17,19,21	2.01	4 (23%)
4	NAG	K	1	3,4	14,14,15	0.40	0	17,19,21	0.75	0
4	NAG	K	2	4	14,14,15	0.41	0	17,19,21	2.00	4 (23%)
4	NAG	L	1	3,4	14,14,15	0.42	0	17,19,21	1.00	2 (11%)
4	NAG	L	2	4	14,14,15	0.39	0	17,19,21	2.00	4 (23%)

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	J	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	1/6/23/26	0/1/1/1
4	NAG	K	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	K	2	4	-	1/6/23/26	0/1/1/1
4	NAG	L	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	2	NAG	O5-C5-C6	6.54	120.39	107.66
4	L	2	NAG	O5-C5-C6	6.52	120.36	107.66
4	K	2	NAG	O5-C5-C6	6.51	120.33	107.66
4	L	1	NAG	C2-N2-C7	2.92	126.81	122.90
4	L	2	NAG	C4-C3-C2	2.73	115.03	111.02
4	K	2	NAG	C4-C3-C2	2.73	115.02	111.02
4	J	2	NAG	C4-C3-C2	2.72	115.01	111.02
4	J	2	NAG	O3-C3-C4	2.47	116.20	110.38
4	L	2	NAG	O3-C3-C4	2.46	116.16	110.38
4	K	2	NAG	O3-C3-C4	2.45	116.16	110.38
4	L	1	NAG	C1-C2-N2	2.33	114.11	110.43
4	J	2	NAG	O4-C4-C5	2.06	114.41	109.32
4	K	2	NAG	O4-C4-C5	2.05	114.36	109.32
4	L	2	NAG	O4-C4-C5	2.04	114.35	109.32

There are no chirality outliers.

All (6) torsion outliers are listed below:

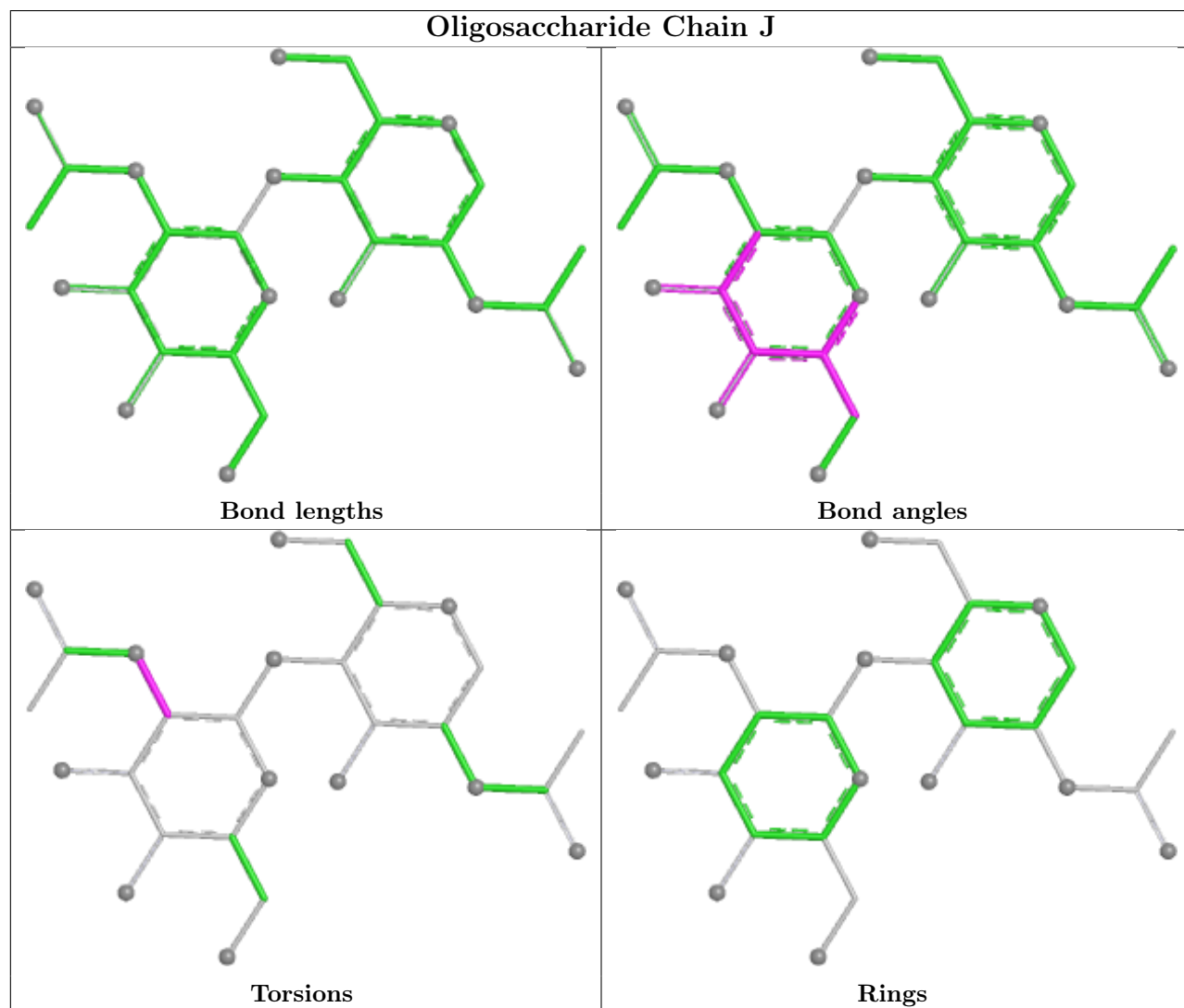
Mol	Chain	Res	Type	Atoms
4	L	1	NAG	C1-C2-N2-C7
4	L	1	NAG	C3-C2-N2-C7
4	J	2	NAG	C1-C2-N2-C7
4	K	1	NAG	C1-C2-N2-C7
4	K	2	NAG	C1-C2-N2-C7
4	L	2	NAG	C1-C2-N2-C7

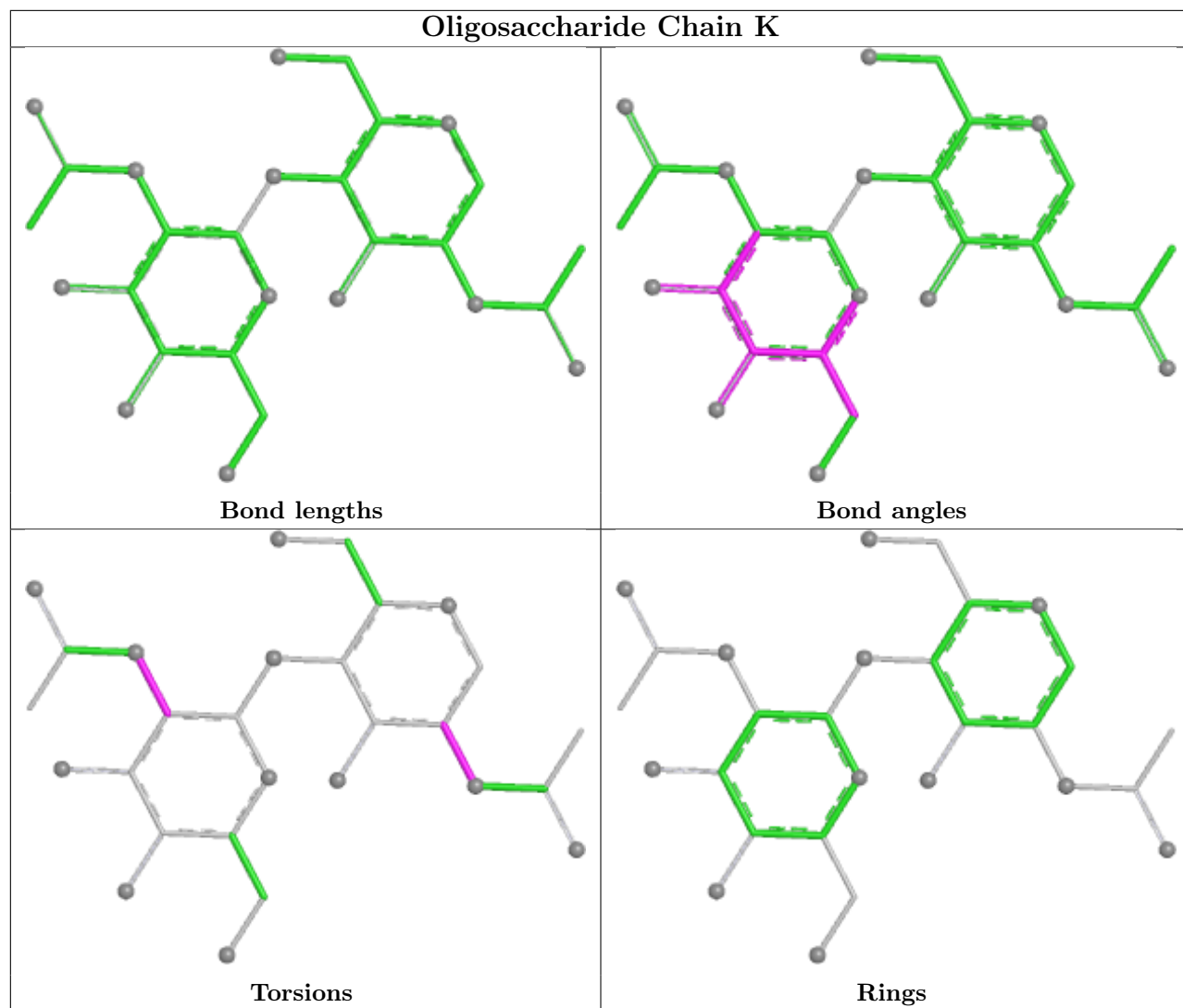
There are no ring outliers.

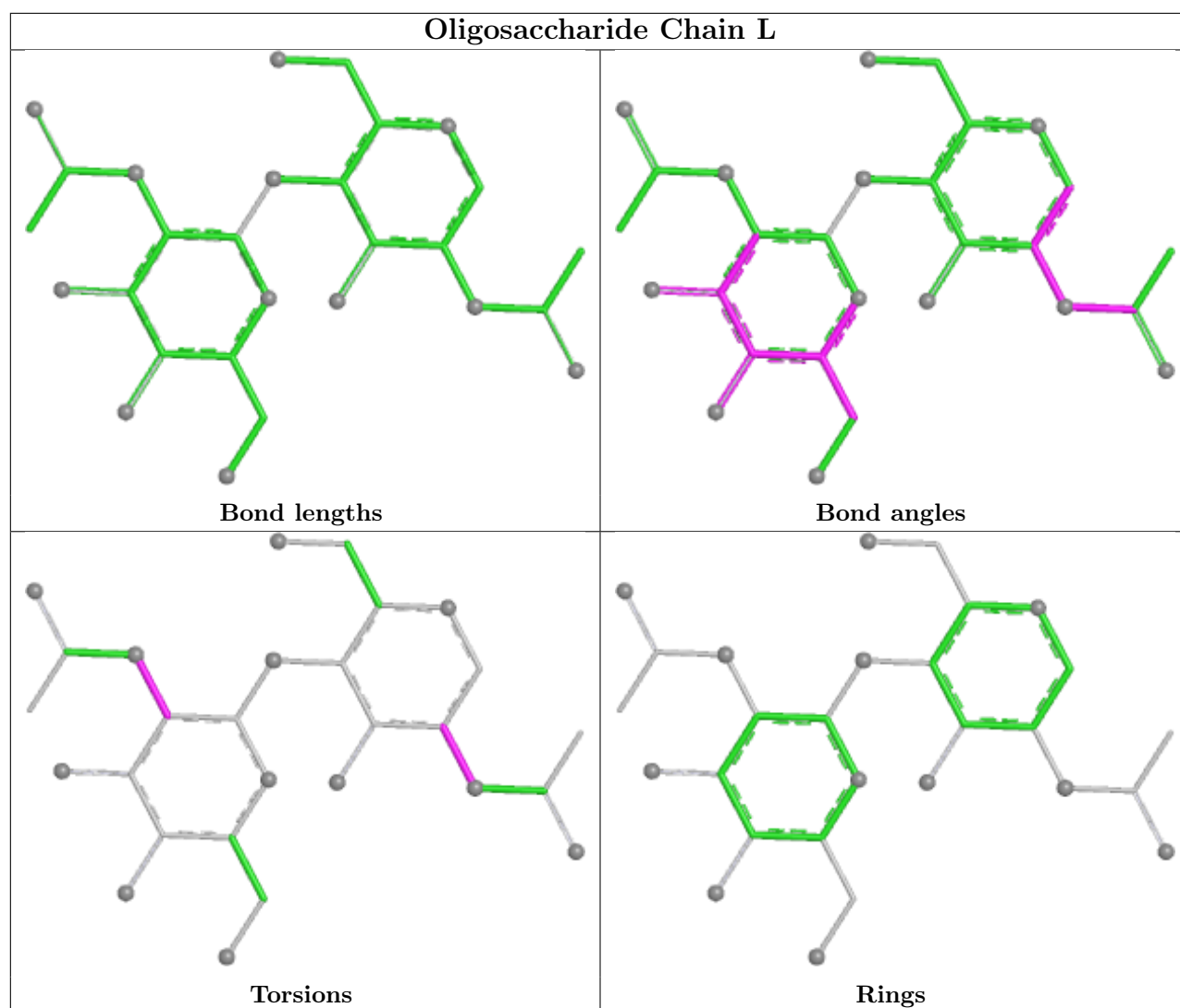
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1	NAG	3	0
4	K	2	NAG	3	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](#)

There are no ligands in this entry.

## 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.

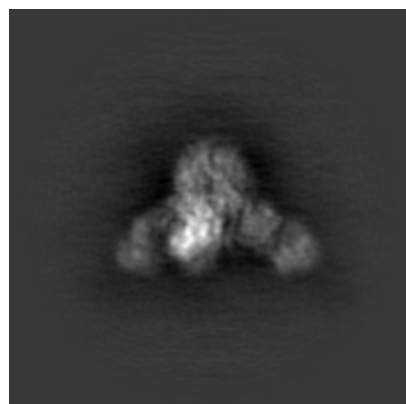
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45412. These allow visual inspection of the internal detail of the map and identification of artifacts.

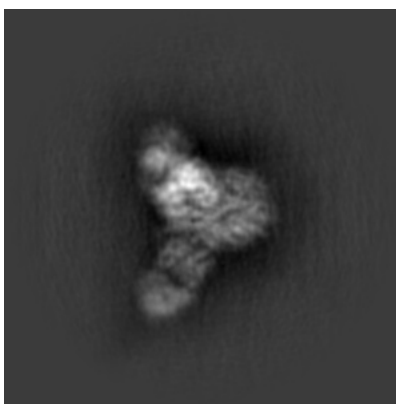
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

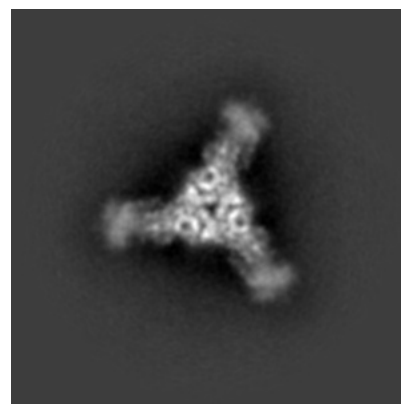
#### 6.1.1 Primary map



X

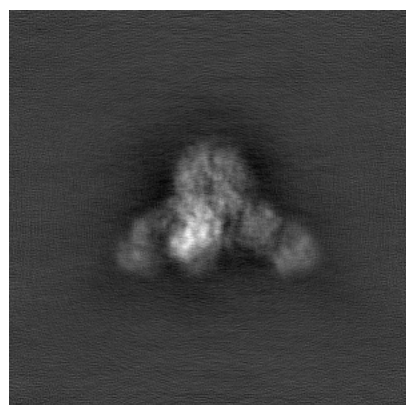


Y

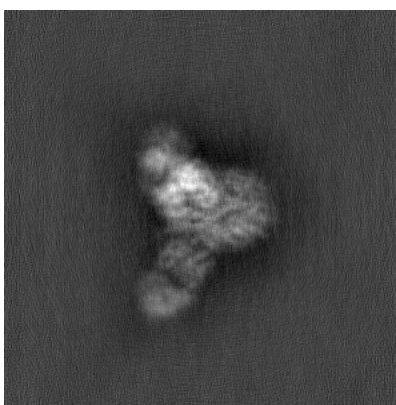


Z

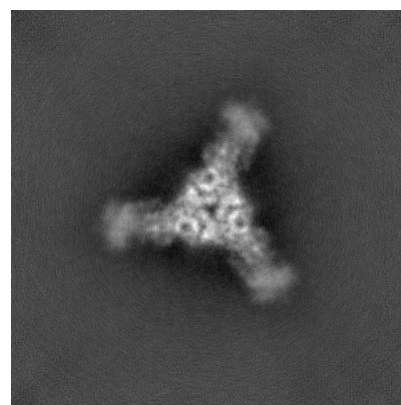
#### 6.1.2 Raw map



X



Y

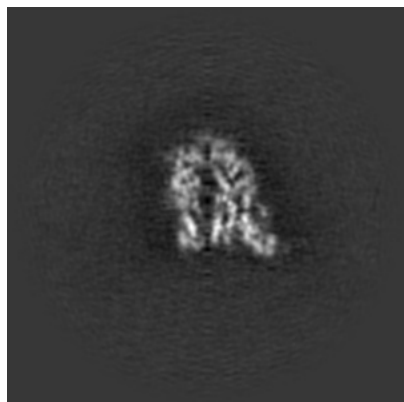


Z

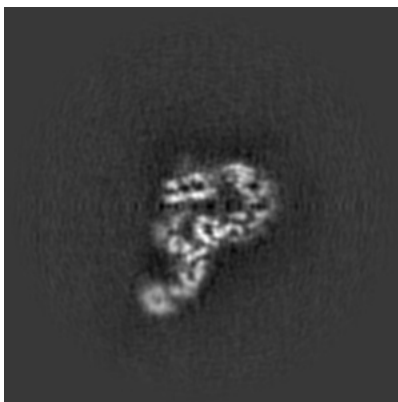
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

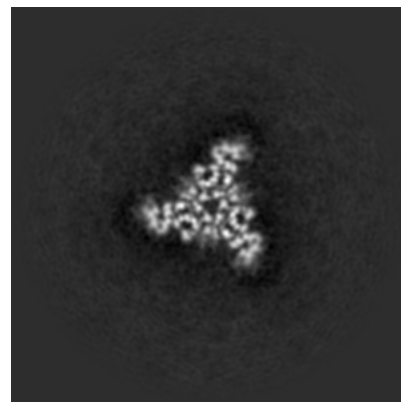
### 6.2.1 Primary map



X Index: 180

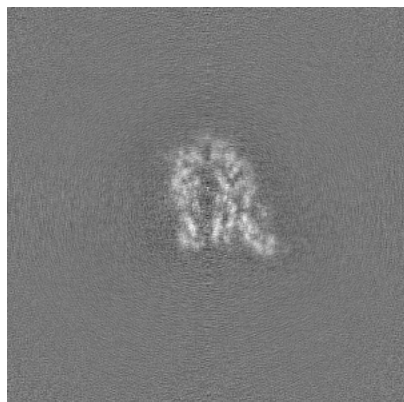


Y Index: 180

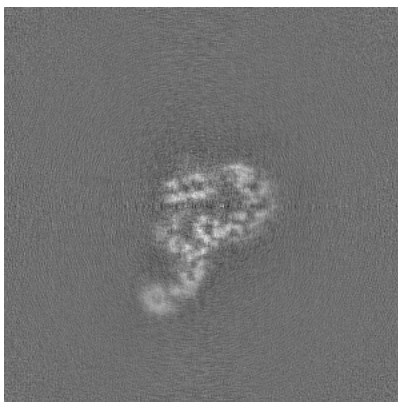


Z Index: 180

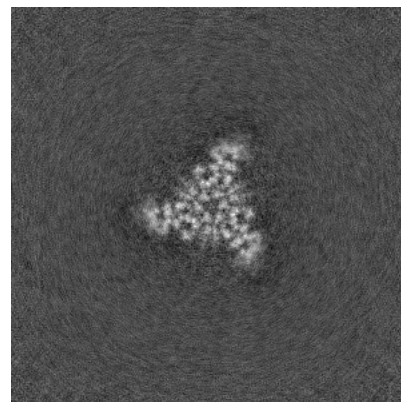
### 6.2.2 Raw map



X Index: 180



Y Index: 180



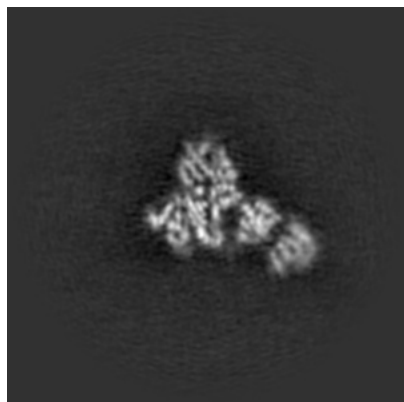
Z Index: 180

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

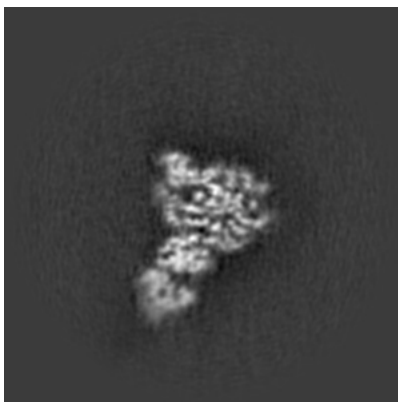


## 6.3 Largest variance slices [i](#)

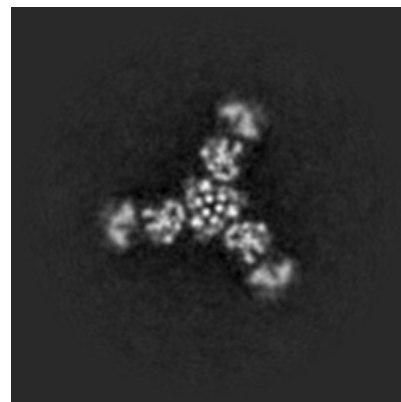
### 6.3.1 Primary map



X Index: 200

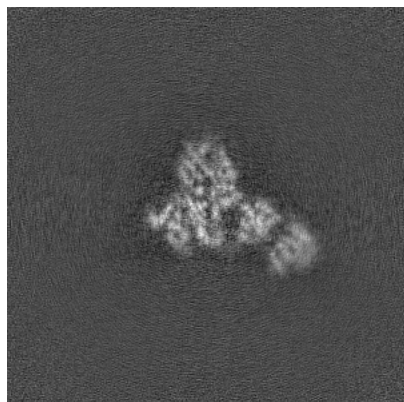


Y Index: 162

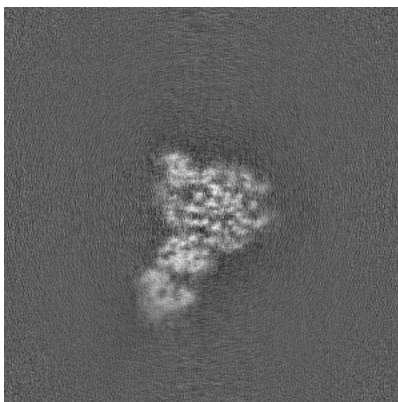


Z Index: 154

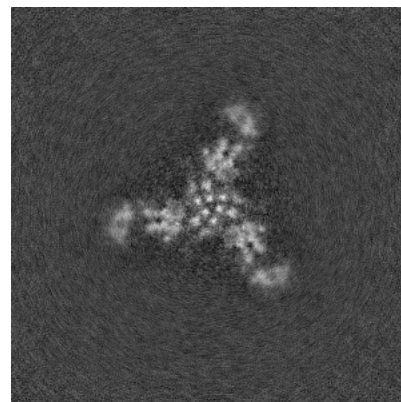
### 6.3.2 Raw map



X Index: 200



Y Index: 162



Z Index: 157

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

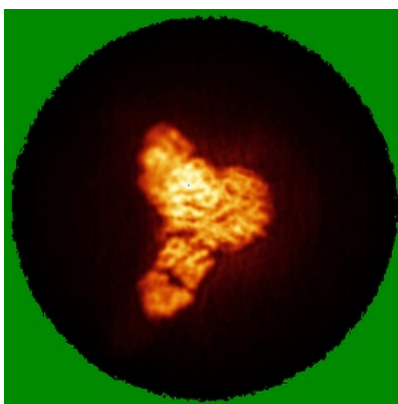


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

### 6.4.1 Primary map



X

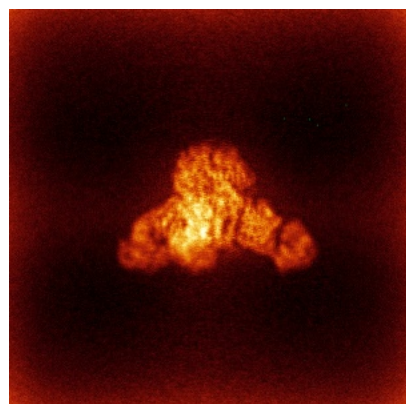


Y

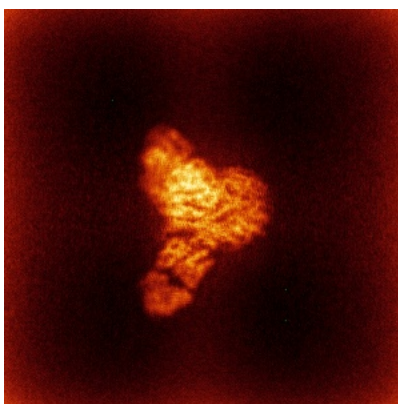


Z

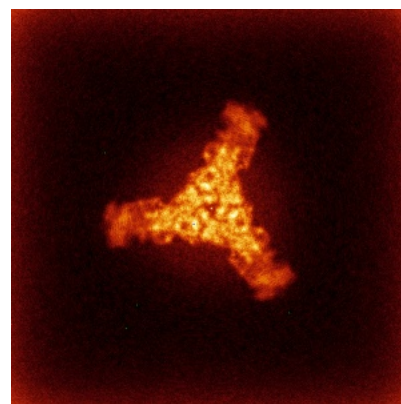
### 6.4.2 Raw map



X



Y

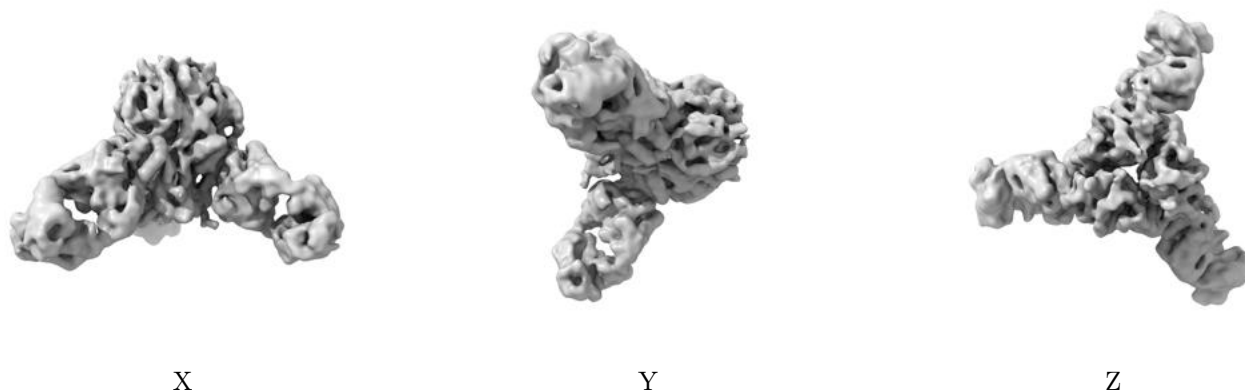


Z

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.

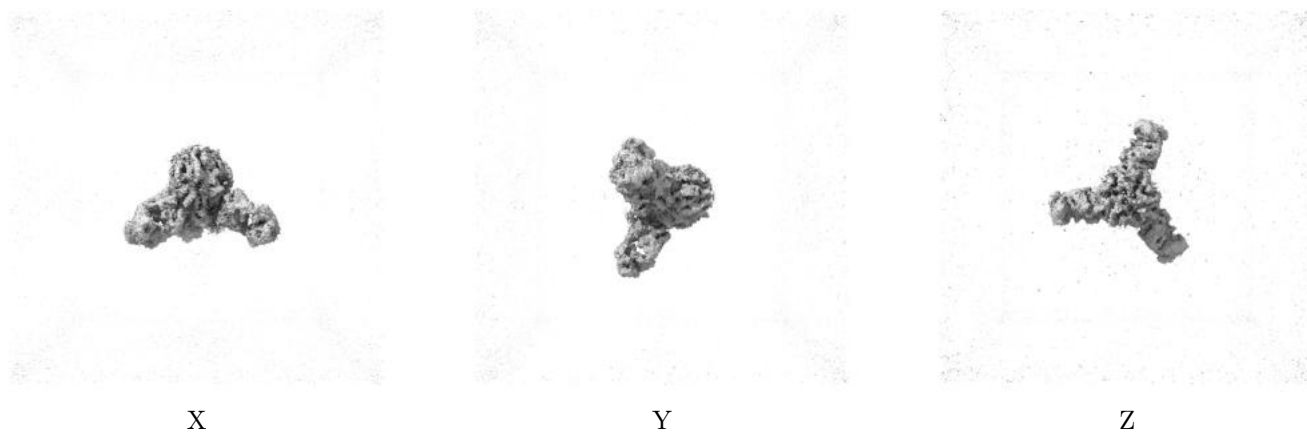
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0251. 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.

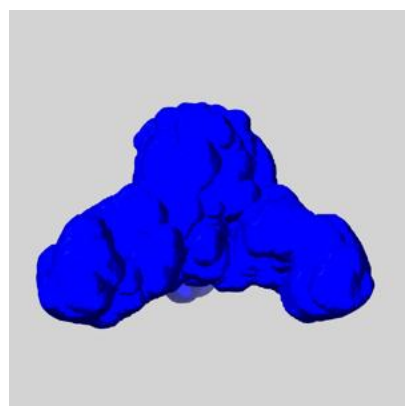
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

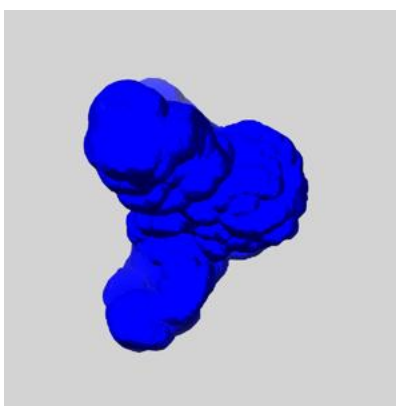
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

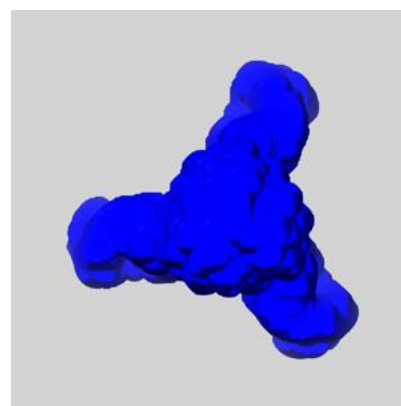
### 6.6.1 emd\_45412\_msk\_1.map [i](#)



X



Y

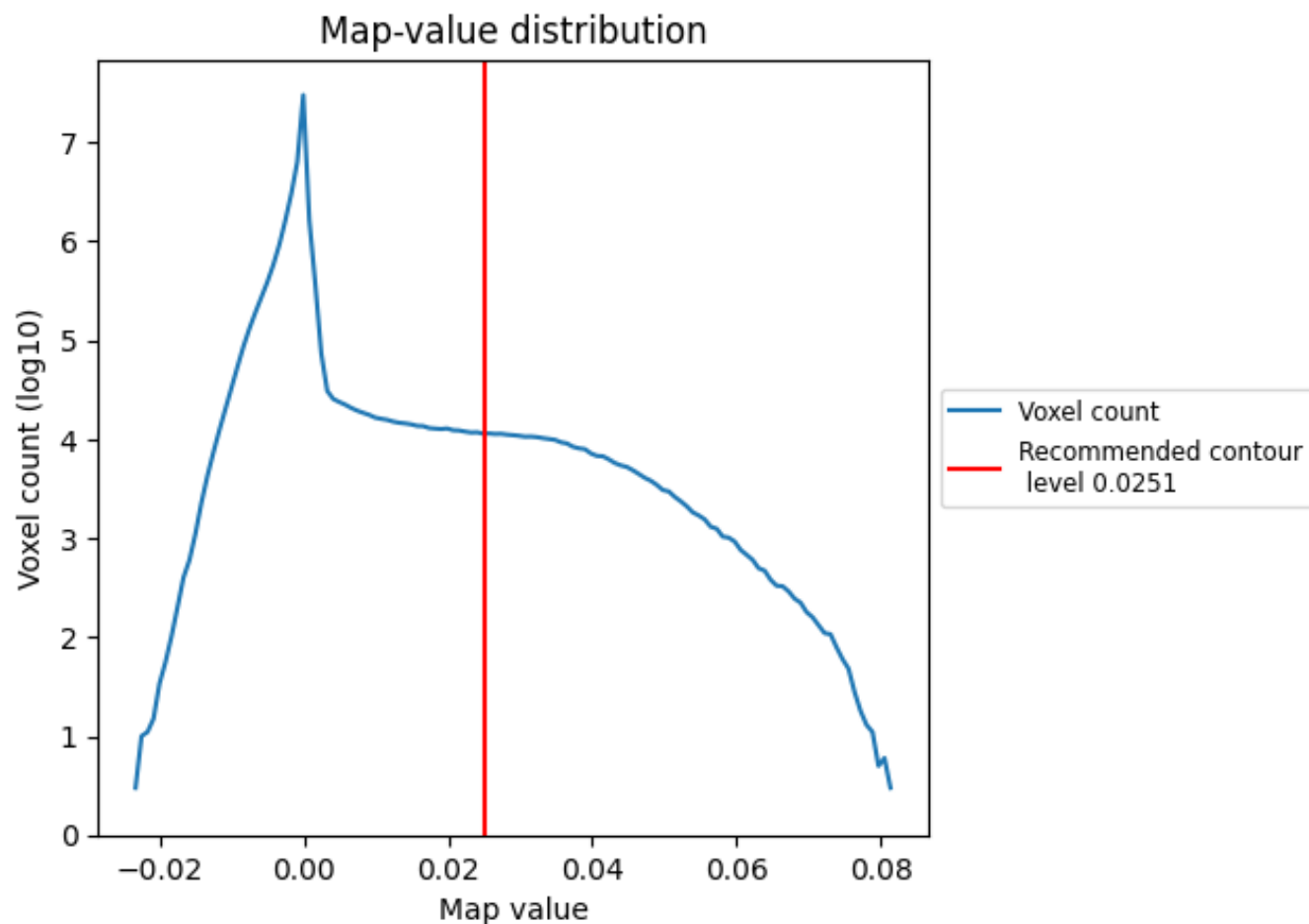


Z

## 7 Map analysis [i](#)

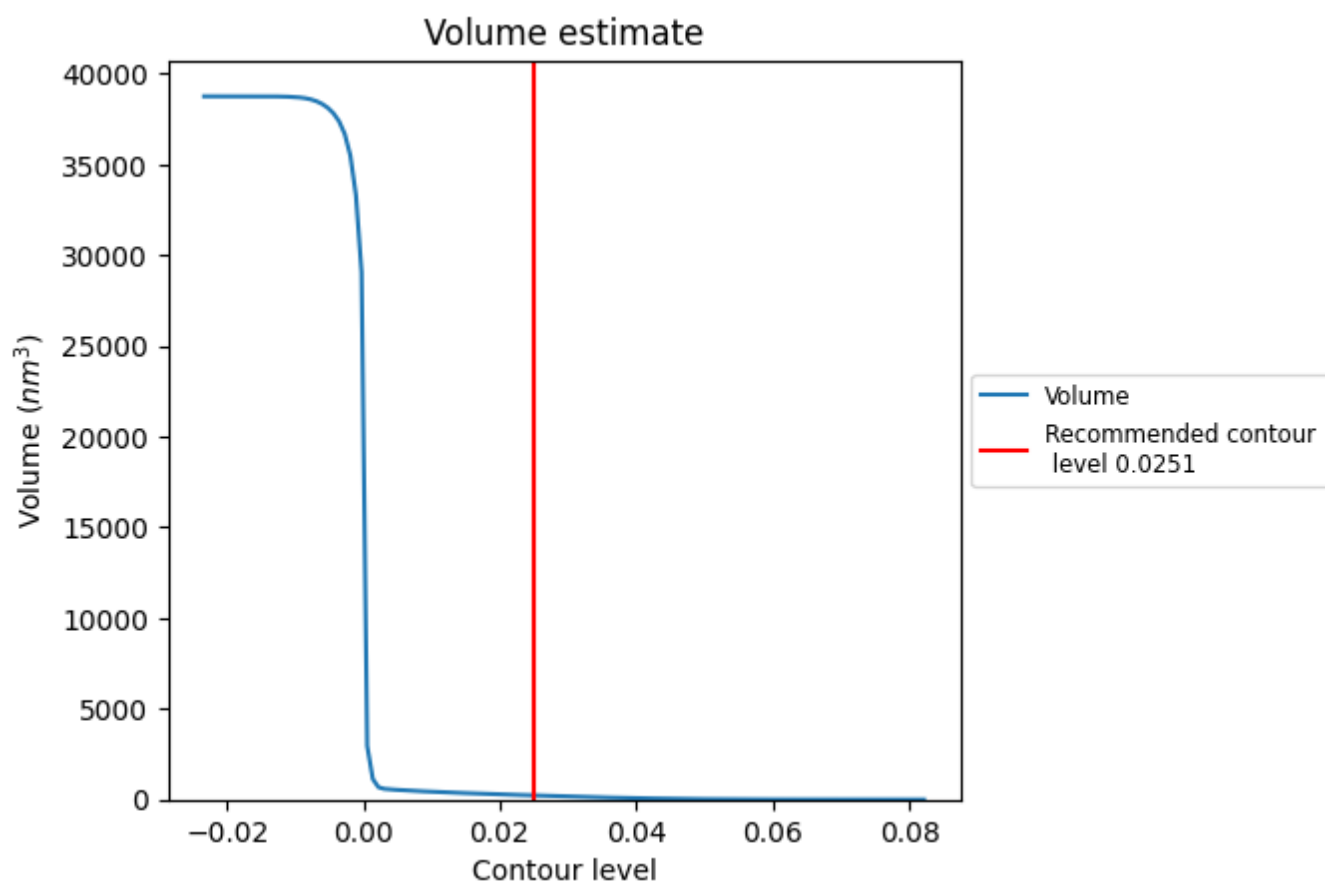
This section contains the results of statistical analysis of the map.

### 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.

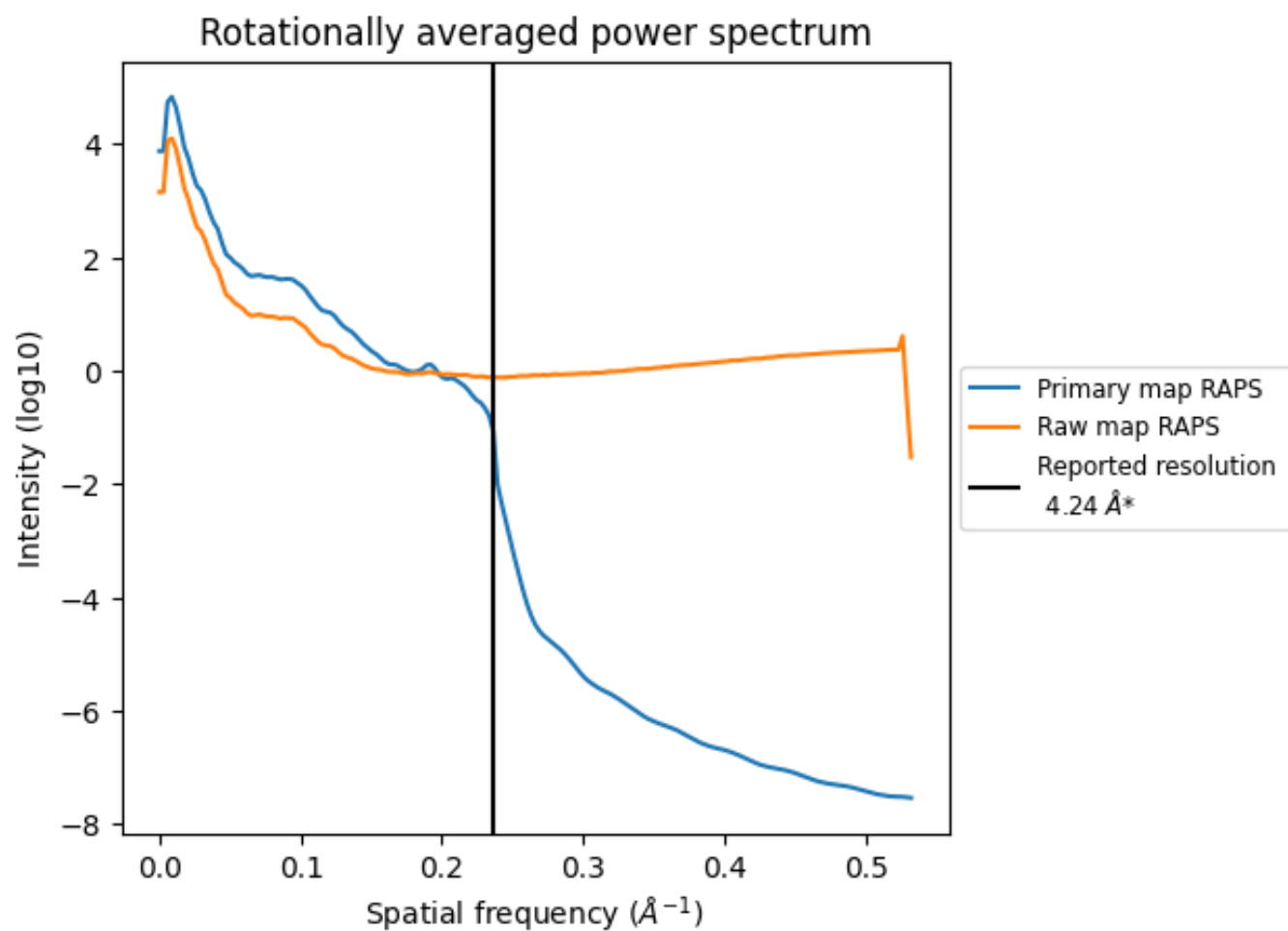
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 227 nm<sup>3</sup>; this corresponds to an approximate mass of 205 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 ⓘ

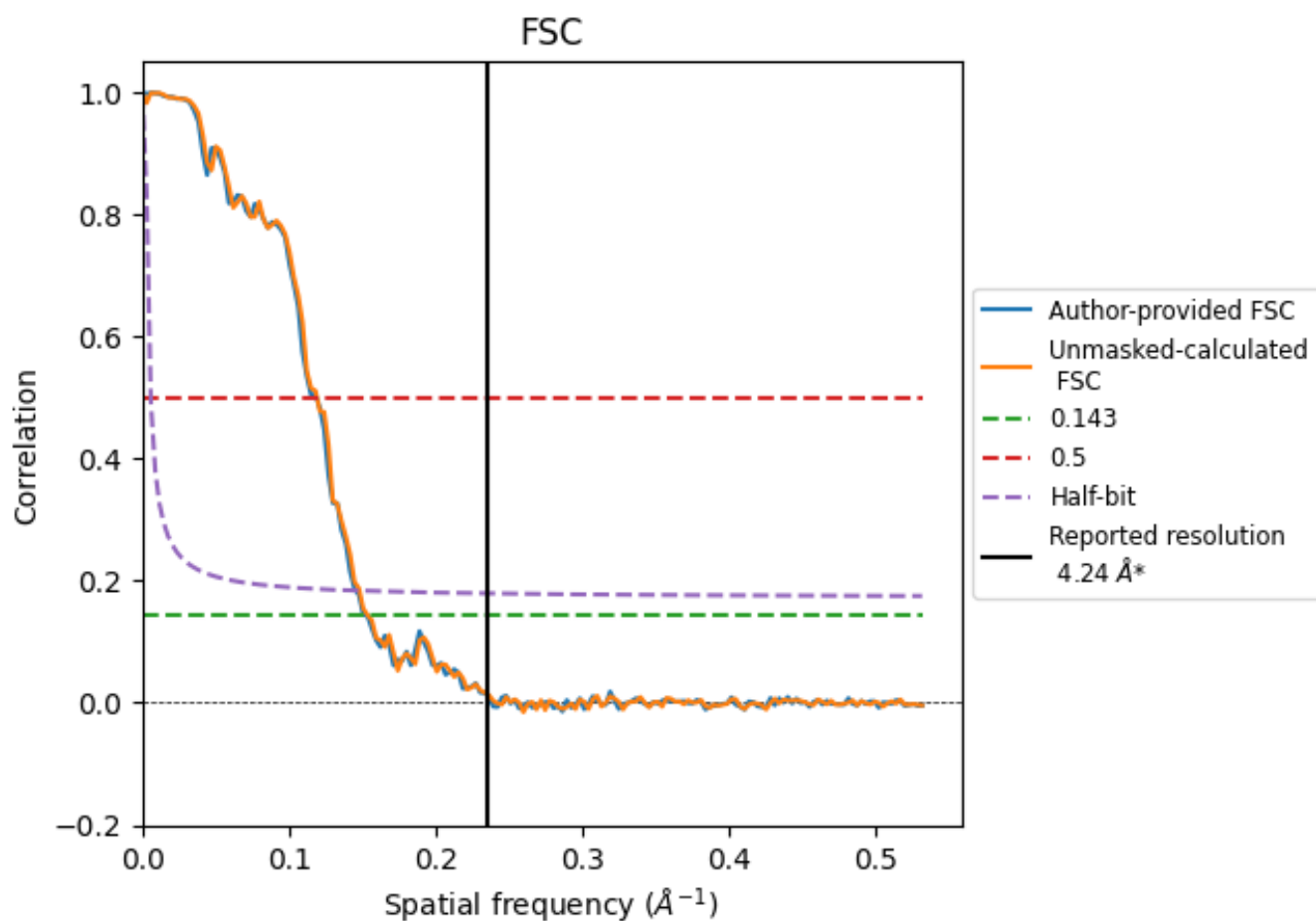


\*Reported resolution corresponds to spatial frequency of 0.236  $\text{\AA}^{-1}$

## 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  $0.236 \text{ \AA}^{-1}$

## 8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.24	-	-
Author-provided FSC curve	6.57	8.42	6.86
Unmasked-calculated*	6.50	8.39	6.75

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.57 differs from the reported value 4.24 by more than 10 %

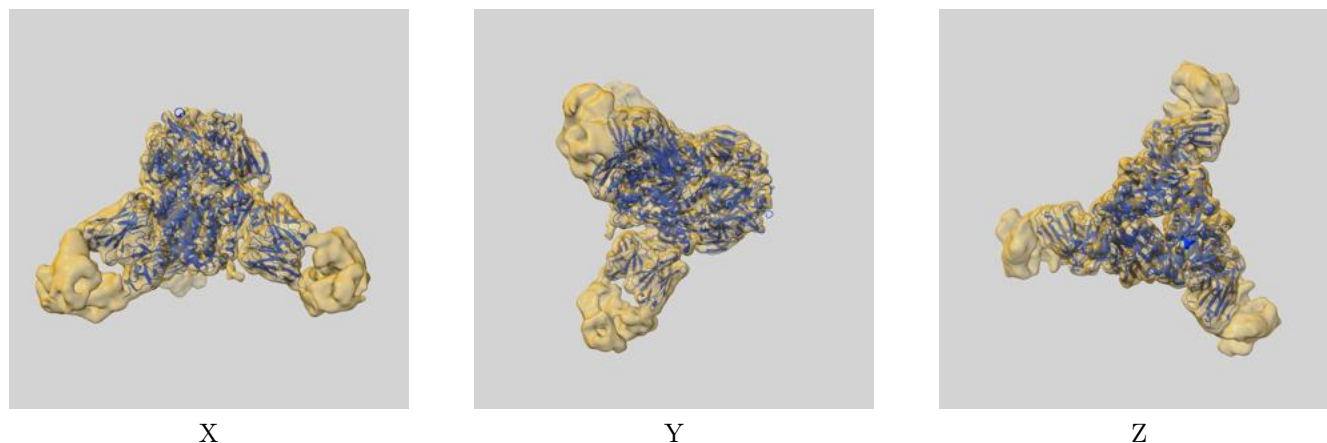
The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.50 differs from the reported value 4.24 by more than 10 %



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

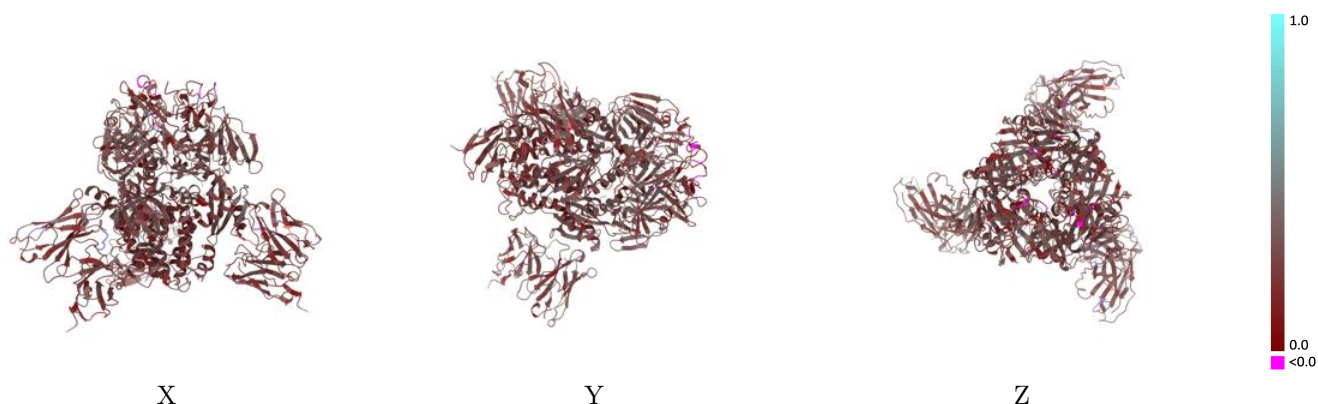
This section contains information regarding the fit between EMDB map EMD-45412 and PDB model 9CB1. Per-residue inclusion information can be found in section 3 on page 11.

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



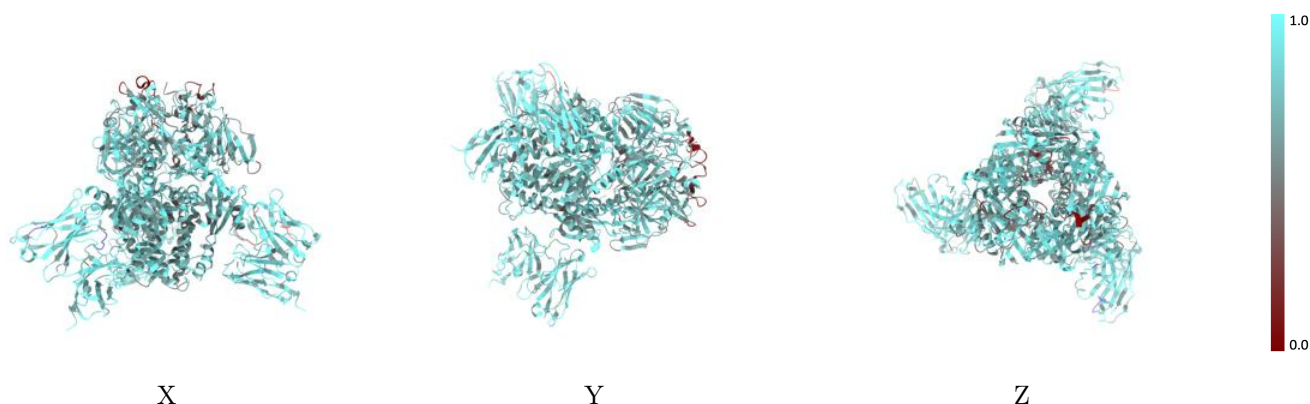
The images above show the 3D surface view of the map at the recommended contour level 0.0251 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



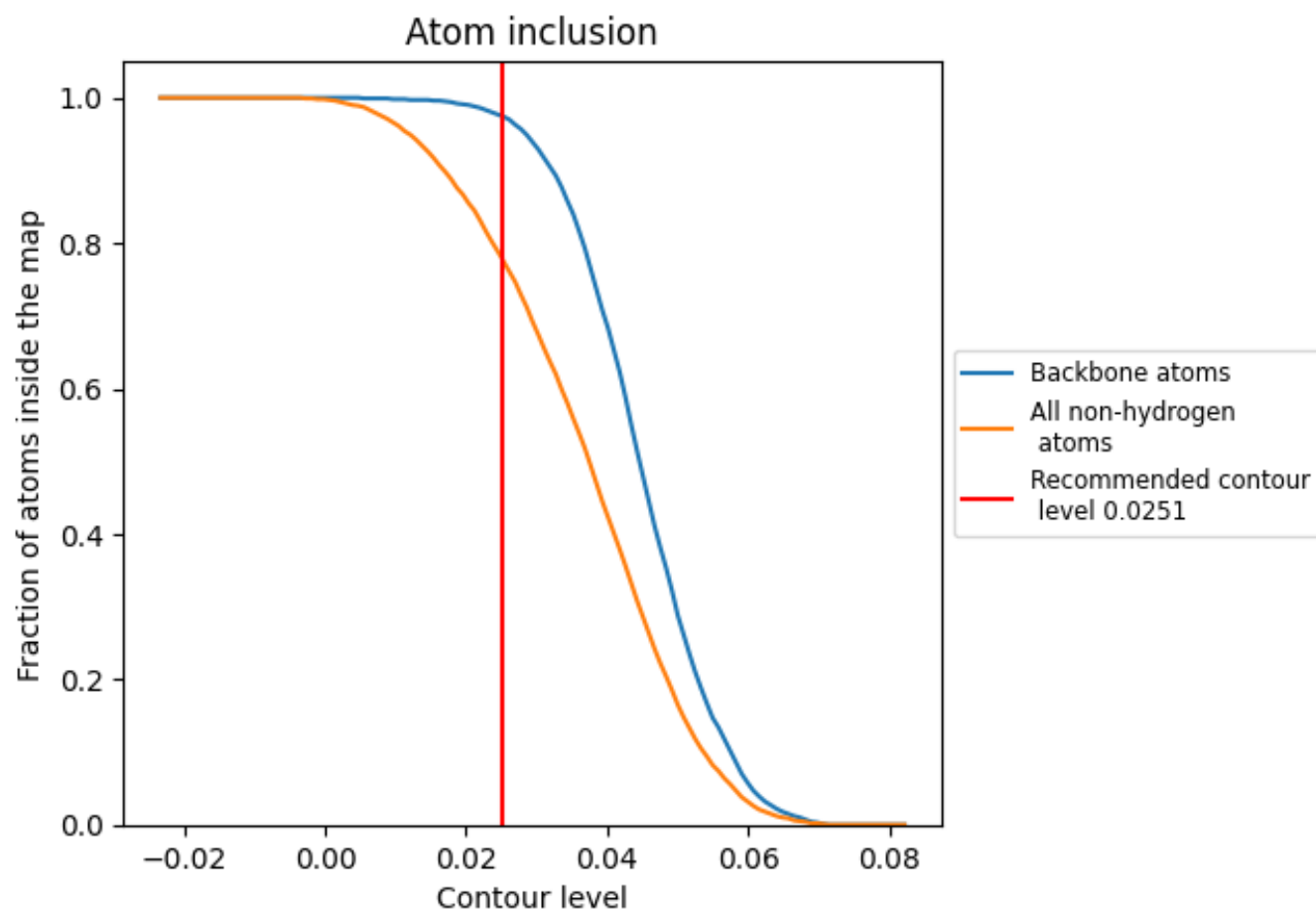
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0251).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 78% 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 (0.0251) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7790	<div></div> 0.2700
A	<div></div> 0.8670	<div></div> 0.2800
B	<div></div> 0.8660	<div></div> 0.2790
C	<div></div> 0.8660	<div></div> 0.2800
D	<div></div> 0.8520	<div></div> 0.2720
E	<div></div> 0.8550	<div></div> 0.2720
F	<div></div> 0.8610	<div></div> 0.2680
G	<div></div> 0.7340	<div></div> 0.2680
H	<div></div> 0.7370	<div></div> 0.2670
I	<div></div> 0.7400	<div></div> 0.2680
J	<div></div> 0.6070	<div></div> 0.2290
K	<div></div> 0.5710	<div></div> 0.2470
L	<div></div> 0.5360	<div></div> 0.1990

