



Full wwPDB EM Validation Report ⓘ

May 19, 2026 – 10:37 AM EDT

PDB ID : 9ZVH / pdb_00009zvh
EMDB ID : EMD-74873
Title : CryoEM structure of H5N1 A/Texas/37/2024 HA bound to Fab H33
Authors : Morano, N.C.; Ho, D.D.; Shapiro, L.; Kwong, P.D.
Deposited on : 2025-12-30
Resolution : 2.93 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

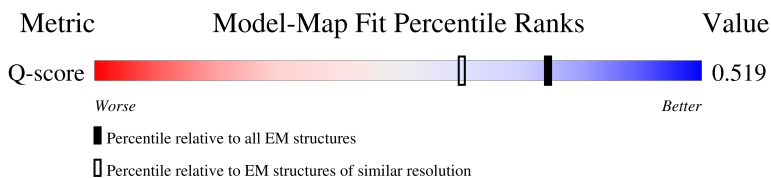
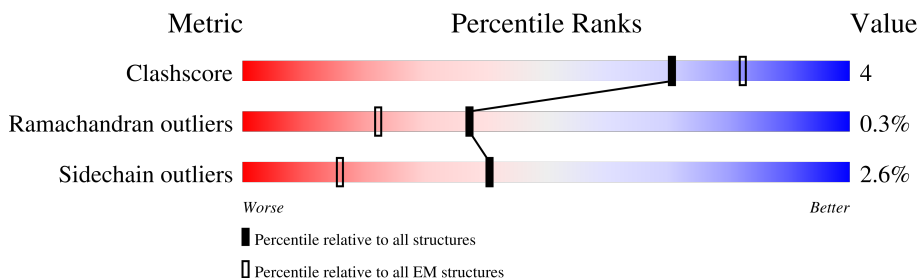
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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





The reported resolution of this entry is 2.93 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	13037 (2.43 - 3.43)

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	118	
1	H	118	
1	I	118	
2	G	107	

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Mol	Chain	Length	Quality of chain
2	K	107	
2	L	107	
3	A	576	
3	B	576	
3	C	576	
4	E	7	
4	F	7	
4	J	7	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 17141 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 H33 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	118	Total	C	N	O	S	0	0
			919	572	163	178	6		
1	I	118	Total	C	N	O	S	0	0
			919	572	163	178	6		
1	D	118	Total	C	N	O	S	0	0
			919	572	163	178	6		

- Molecule 2 is a protein called Fab H33 Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	103	Total	C	N	O	S	0	0
			793	498	128	164	3		
2	K	103	Total	C	N	O	S	0	0
			793	498	128	164	3		
2	G	103	Total	C	N	O	S	0	0
			793	498	128	164	3		

- Molecule 3 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	484	Total	C	N	O	S	0	0
			3864	2433	669	739	23		
3	B	484	Total	C	N	O	S	0	0
			3865	2434	669	739	23		
3	C	484	Total	C	N	O	S	0	0
			3865	2434	669	739	23		

There are 195 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	209	ILE	THR	conflict	UNP A0AAX6NNG0
A	?	-	GLU	deletion	UNP A0AAX6NNG0
A	350	ARG	LYS	conflict	UNP A0AAX6NNG0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	353	ARG	LYS	conflict	UNP A0AAX6NNG0
A	526	GLY	-	expression tag	UNP A0AAX6NNG0
A	527	SER	-	expression tag	UNP A0AAX6NNG0
A	528	SER	-	expression tag	UNP A0AAX6NNG0
A	529	GLY	-	expression tag	UNP A0AAX6NNG0
A	530	SER	-	expression tag	UNP A0AAX6NNG0
A	531	SER	-	expression tag	UNP A0AAX6NNG0
A	532	GLY	-	expression tag	UNP A0AAX6NNG0
A	533	TYR	-	expression tag	UNP A0AAX6NNG0
A	534	ILE	-	expression tag	UNP A0AAX6NNG0
A	535	PRO	-	expression tag	UNP A0AAX6NNG0
A	536	GLU	-	expression tag	UNP A0AAX6NNG0
A	537	ALA	-	expression tag	UNP A0AAX6NNG0
A	538	PRO	-	expression tag	UNP A0AAX6NNG0
A	539	ARG	-	expression tag	UNP A0AAX6NNG0
A	540	ASP	-	expression tag	UNP A0AAX6NNG0
A	541	GLY	-	expression tag	UNP A0AAX6NNG0
A	542	GLN	-	expression tag	UNP A0AAX6NNG0
A	543	ALA	-	expression tag	UNP A0AAX6NNG0
A	544	TYR	-	expression tag	UNP A0AAX6NNG0
A	545	VAL	-	expression tag	UNP A0AAX6NNG0
A	546	ARG	-	expression tag	UNP A0AAX6NNG0
A	547	LYS	-	expression tag	UNP A0AAX6NNG0
A	548	ASP	-	expression tag	UNP A0AAX6NNG0
A	549	GLY	-	expression tag	UNP A0AAX6NNG0
A	550	GLU	-	expression tag	UNP A0AAX6NNG0
A	551	TRP	-	expression tag	UNP A0AAX6NNG0
A	552	VAL	-	expression tag	UNP A0AAX6NNG0
A	553	LEU	-	expression tag	UNP A0AAX6NNG0
A	554	LEU	-	expression tag	UNP A0AAX6NNG0
A	555	SER	-	expression tag	UNP A0AAX6NNG0
A	556	THR	-	expression tag	UNP A0AAX6NNG0
A	557	PHE	-	expression tag	UNP A0AAX6NNG0
A	558	LEU	-	expression tag	UNP A0AAX6NNG0
A	559	GLY	-	expression tag	UNP A0AAX6NNG0
A	560	HIS	-	expression tag	UNP A0AAX6NNG0
A	561	HIS	-	expression tag	UNP A0AAX6NNG0
A	562	HIS	-	expression tag	UNP A0AAX6NNG0
A	563	HIS	-	expression tag	UNP A0AAX6NNG0
A	564	HIS	-	expression tag	UNP A0AAX6NNG0
A	565	HIS	-	expression tag	UNP A0AAX6NNG0
A	566	HIS	-	expression tag	UNP A0AAX6NNG0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	567	HIS	-	expression tag	UNP A0AAX6NNG0
A	568	HIS	-	expression tag	UNP A0AAX6NNG0
A	569	GLY	-	expression tag	UNP A0AAX6NNG0
A	570	GLY	-	expression tag	UNP A0AAX6NNG0
A	571	SER	-	expression tag	UNP A0AAX6NNG0
A	572	GLY	-	expression tag	UNP A0AAX6NNG0
A	573	LEU	-	expression tag	UNP A0AAX6NNG0
A	574	ASN	-	expression tag	UNP A0AAX6NNG0
A	575	ASP	-	expression tag	UNP A0AAX6NNG0
A	576	ILE	-	expression tag	UNP A0AAX6NNG0
A	577	PHE	-	expression tag	UNP A0AAX6NNG0
A	578	GLU	-	expression tag	UNP A0AAX6NNG0
A	579	ALA	-	expression tag	UNP A0AAX6NNG0
A	580	GLN	-	expression tag	UNP A0AAX6NNG0
A	581	LYS	-	expression tag	UNP A0AAX6NNG0
A	582	ILE	-	expression tag	UNP A0AAX6NNG0
A	583	GLU	-	expression tag	UNP A0AAX6NNG0
A	584	TRP	-	expression tag	UNP A0AAX6NNG0
A	585	HIS	-	expression tag	UNP A0AAX6NNG0
A	586	GLU	-	expression tag	UNP A0AAX6NNG0
B	209	ILE	THR	conflict	UNP A0AAX6NNG0
B	?	-	GLU	deletion	UNP A0AAX6NNG0
B	350	ARG	LYS	conflict	UNP A0AAX6NNG0
B	353	ARG	LYS	conflict	UNP A0AAX6NNG0
B	526	GLY	-	expression tag	UNP A0AAX6NNG0
B	527	SER	-	expression tag	UNP A0AAX6NNG0
B	528	SER	-	expression tag	UNP A0AAX6NNG0
B	529	GLY	-	expression tag	UNP A0AAX6NNG0
B	530	SER	-	expression tag	UNP A0AAX6NNG0
B	531	SER	-	expression tag	UNP A0AAX6NNG0
B	532	GLY	-	expression tag	UNP A0AAX6NNG0
B	533	TYR	-	expression tag	UNP A0AAX6NNG0
B	534	ILE	-	expression tag	UNP A0AAX6NNG0
B	535	PRO	-	expression tag	UNP A0AAX6NNG0
B	536	GLU	-	expression tag	UNP A0AAX6NNG0
B	537	ALA	-	expression tag	UNP A0AAX6NNG0
B	538	PRO	-	expression tag	UNP A0AAX6NNG0
B	539	ARG	-	expression tag	UNP A0AAX6NNG0
B	540	ASP	-	expression tag	UNP A0AAX6NNG0
B	541	GLY	-	expression tag	UNP A0AAX6NNG0
B	542	GLN	-	expression tag	UNP A0AAX6NNG0
B	543	ALA	-	expression tag	UNP A0AAX6NNG0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	544	TYR	-	expression tag	UNP A0AAX6NNG0
B	545	VAL	-	expression tag	UNP A0AAX6NNG0
B	546	ARG	-	expression tag	UNP A0AAX6NNG0
B	547	LYS	-	expression tag	UNP A0AAX6NNG0
B	548	ASP	-	expression tag	UNP A0AAX6NNG0
B	549	GLY	-	expression tag	UNP A0AAX6NNG0
B	550	GLU	-	expression tag	UNP A0AAX6NNG0
B	551	TRP	-	expression tag	UNP A0AAX6NNG0
B	552	VAL	-	expression tag	UNP A0AAX6NNG0
B	553	LEU	-	expression tag	UNP A0AAX6NNG0
B	554	LEU	-	expression tag	UNP A0AAX6NNG0
B	555	SER	-	expression tag	UNP A0AAX6NNG0
B	556	THR	-	expression tag	UNP A0AAX6NNG0
B	557	PHE	-	expression tag	UNP A0AAX6NNG0
B	558	LEU	-	expression tag	UNP A0AAX6NNG0
B	559	GLY	-	expression tag	UNP A0AAX6NNG0
B	560	HIS	-	expression tag	UNP A0AAX6NNG0
B	561	HIS	-	expression tag	UNP A0AAX6NNG0
B	562	HIS	-	expression tag	UNP A0AAX6NNG0
B	563	HIS	-	expression tag	UNP A0AAX6NNG0
B	564	HIS	-	expression tag	UNP A0AAX6NNG0
B	565	HIS	-	expression tag	UNP A0AAX6NNG0
B	566	HIS	-	expression tag	UNP A0AAX6NNG0
B	567	HIS	-	expression tag	UNP A0AAX6NNG0
B	568	HIS	-	expression tag	UNP A0AAX6NNG0
B	569	GLY	-	expression tag	UNP A0AAX6NNG0
B	570	GLY	-	expression tag	UNP A0AAX6NNG0
B	571	SER	-	expression tag	UNP A0AAX6NNG0
B	572	GLY	-	expression tag	UNP A0AAX6NNG0
B	573	LEU	-	expression tag	UNP A0AAX6NNG0
B	574	ASN	-	expression tag	UNP A0AAX6NNG0
B	575	ASP	-	expression tag	UNP A0AAX6NNG0
B	576	ILE	-	expression tag	UNP A0AAX6NNG0
B	577	PHE	-	expression tag	UNP A0AAX6NNG0
B	578	GLU	-	expression tag	UNP A0AAX6NNG0
B	579	ALA	-	expression tag	UNP A0AAX6NNG0
B	580	GLN	-	expression tag	UNP A0AAX6NNG0
B	581	LYS	-	expression tag	UNP A0AAX6NNG0
B	582	ILE	-	expression tag	UNP A0AAX6NNG0
B	583	GLU	-	expression tag	UNP A0AAX6NNG0
B	584	TRP	-	expression tag	UNP A0AAX6NNG0
B	585	HIS	-	expression tag	UNP A0AAX6NNG0

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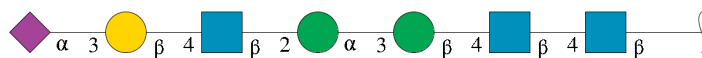
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B	586	GLU	-	expression tag	UNP A0AAX6NNG0
C	209	ILE	THR	conflict	UNP A0AAX6NNG0
C	?	-	GLU	deletion	UNP A0AAX6NNG0
C	350	ARG	LYS	conflict	UNP A0AAX6NNG0
C	353	ARG	LYS	conflict	UNP A0AAX6NNG0
C	526	GLY	-	expression tag	UNP A0AAX6NNG0
C	527	SER	-	expression tag	UNP A0AAX6NNG0
C	528	SER	-	expression tag	UNP A0AAX6NNG0
C	529	GLY	-	expression tag	UNP A0AAX6NNG0
C	530	SER	-	expression tag	UNP A0AAX6NNG0
C	531	SER	-	expression tag	UNP A0AAX6NNG0
C	532	GLY	-	expression tag	UNP A0AAX6NNG0
C	533	TYR	-	expression tag	UNP A0AAX6NNG0
C	534	ILE	-	expression tag	UNP A0AAX6NNG0
C	535	PRO	-	expression tag	UNP A0AAX6NNG0
C	536	GLU	-	expression tag	UNP A0AAX6NNG0
C	537	ALA	-	expression tag	UNP A0AAX6NNG0
C	538	PRO	-	expression tag	UNP A0AAX6NNG0
C	539	ARG	-	expression tag	UNP A0AAX6NNG0
C	540	ASP	-	expression tag	UNP A0AAX6NNG0
C	541	GLY	-	expression tag	UNP A0AAX6NNG0
C	542	GLN	-	expression tag	UNP A0AAX6NNG0
C	543	ALA	-	expression tag	UNP A0AAX6NNG0
C	544	TYR	-	expression tag	UNP A0AAX6NNG0
C	545	VAL	-	expression tag	UNP A0AAX6NNG0
C	546	ARG	-	expression tag	UNP A0AAX6NNG0
C	547	LYS	-	expression tag	UNP A0AAX6NNG0
C	548	ASP	-	expression tag	UNP A0AAX6NNG0
C	549	GLY	-	expression tag	UNP A0AAX6NNG0
C	550	GLU	-	expression tag	UNP A0AAX6NNG0
C	551	TRP	-	expression tag	UNP A0AAX6NNG0
C	552	VAL	-	expression tag	UNP A0AAX6NNG0
C	553	LEU	-	expression tag	UNP A0AAX6NNG0
C	554	LEU	-	expression tag	UNP A0AAX6NNG0
C	555	SER	-	expression tag	UNP A0AAX6NNG0
C	556	THR	-	expression tag	UNP A0AAX6NNG0
C	557	PHE	-	expression tag	UNP A0AAX6NNG0
C	558	LEU	-	expression tag	UNP A0AAX6NNG0
C	559	GLY	-	expression tag	UNP A0AAX6NNG0
C	560	HIS	-	expression tag	UNP A0AAX6NNG0
C	561	HIS	-	expression tag	UNP A0AAX6NNG0
C	562	HIS	-	expression tag	UNP A0AAX6NNG0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	563	HIS	-	expression tag	UNP A0AAX6NNG0
C	564	HIS	-	expression tag	UNP A0AAX6NNG0
C	565	HIS	-	expression tag	UNP A0AAX6NNG0
C	566	HIS	-	expression tag	UNP A0AAX6NNG0
C	567	HIS	-	expression tag	UNP A0AAX6NNG0
C	568	HIS	-	expression tag	UNP A0AAX6NNG0
C	569	GLY	-	expression tag	UNP A0AAX6NNG0
C	570	GLY	-	expression tag	UNP A0AAX6NNG0
C	571	SER	-	expression tag	UNP A0AAX6NNG0
C	572	GLY	-	expression tag	UNP A0AAX6NNG0
C	573	LEU	-	expression tag	UNP A0AAX6NNG0
C	574	ASN	-	expression tag	UNP A0AAX6NNG0
C	575	ASP	-	expression tag	UNP A0AAX6NNG0
C	576	ILE	-	expression tag	UNP A0AAX6NNG0
C	577	PHE	-	expression tag	UNP A0AAX6NNG0
C	578	GLU	-	expression tag	UNP A0AAX6NNG0
C	579	ALA	-	expression tag	UNP A0AAX6NNG0
C	580	GLN	-	expression tag	UNP A0AAX6NNG0
C	581	LYS	-	expression tag	UNP A0AAX6NNG0
C	582	ILE	-	expression tag	UNP A0AAX6NNG0
C	583	GLU	-	expression tag	UNP A0AAX6NNG0
C	584	TRP	-	expression tag	UNP A0AAX6NNG0
C	585	HIS	-	expression tag	UNP A0AAX6NNG0
C	586	GLU	-	expression tag	UNP A0AAX6NNG0

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-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	E	7	Total	C	N	O	0	0
			95	53	4	38		
4	F	7	Total	C	N	O	0	0
			95	53	4	38		
4	J	7	Total	C	N	O	0	0
			95	53	4	38		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



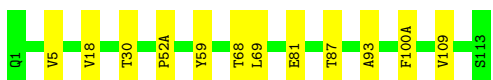
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5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

3 Residue-property plots


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: H33 Fab Heavy Chain

Chain H:  90% 10%




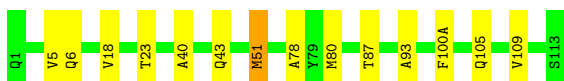
- Molecule 1: H33 Fab Heavy Chain

Chain I:  87% 12%




- Molecule 1: H33 Fab Heavy Chain

Chain D:  88% 11%




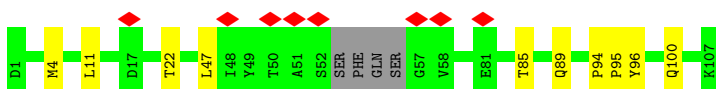
- Molecule 2: Fab H33 Light Chain

Chain L:  7% 91% 6%

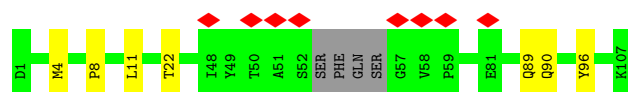
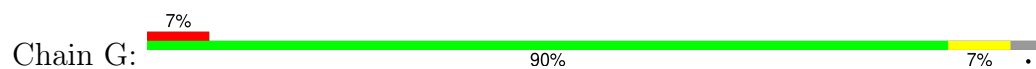


- Molecule 2: Fab H33 Light Chain

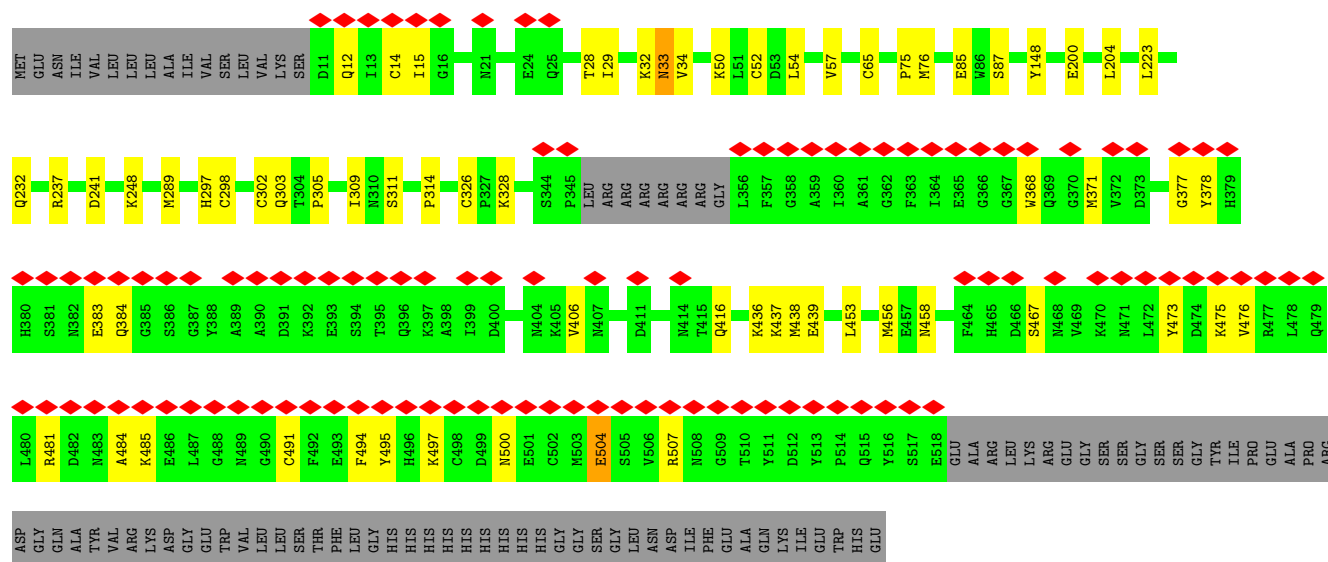
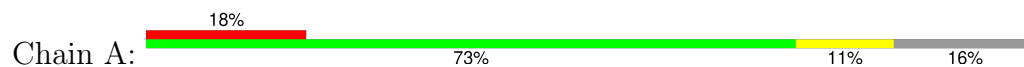
Chain K:  7% 87% 9%



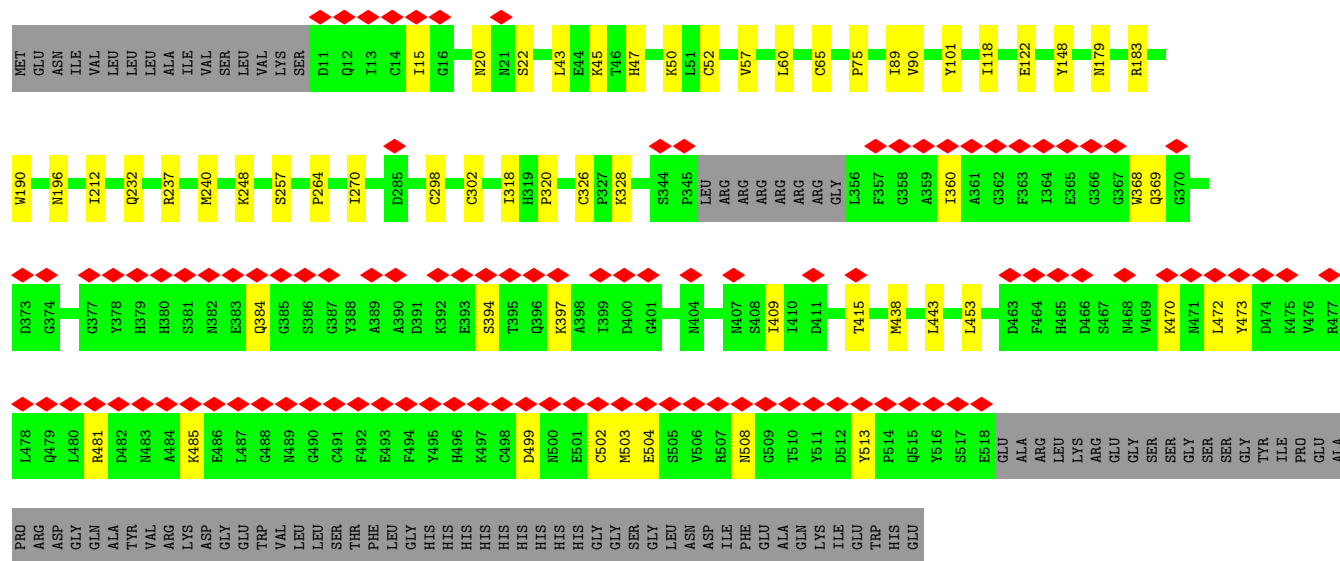
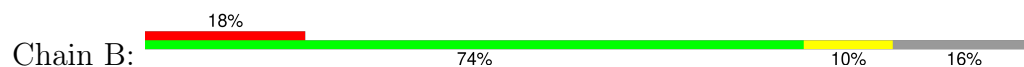
- Molecule 2: Fab H33 Light Chain



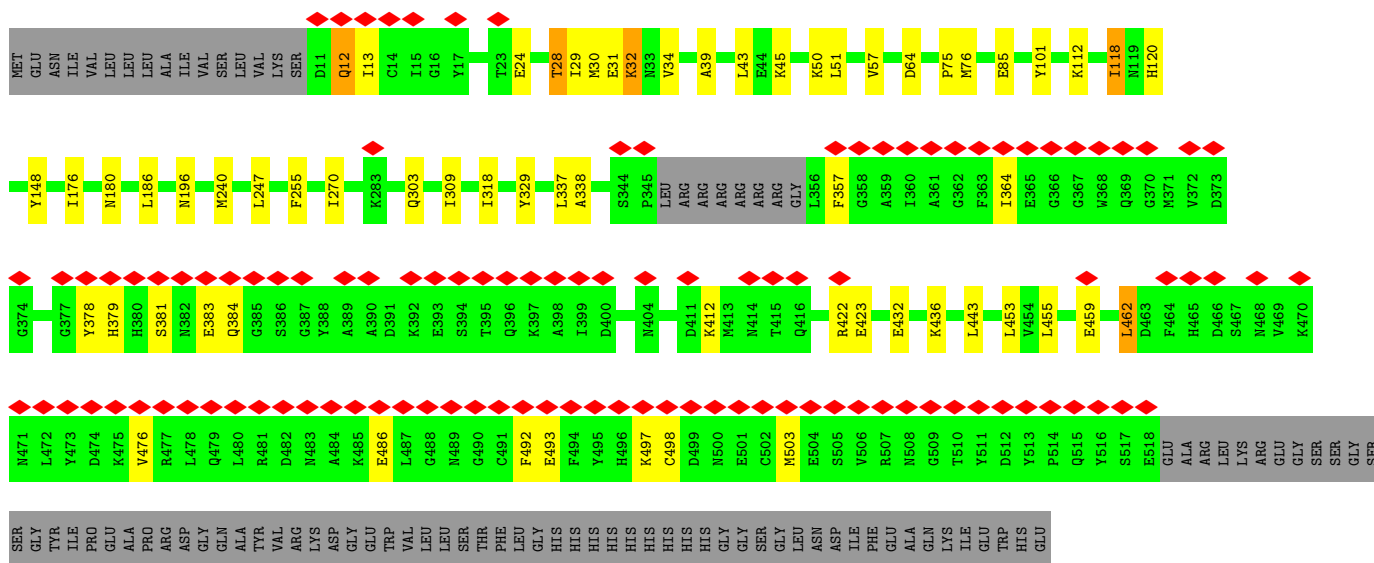
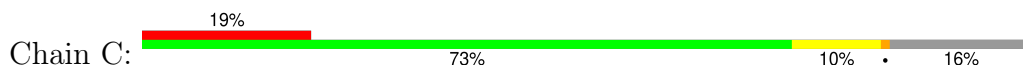
- Molecule 3: Hemagglutinin



- Molecule 3: Hemagglutinin



- Molecule 3: Hemagglutinin



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-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	201510	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.848	Depositor
Minimum map value	-1.319	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.172	Depositor
Map size (\AA)	316.8, 316.8, 316.8	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, BMA, NAG, MAN, GAL

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	0.16	0/940	0.38	0/1275
1	H	0.16	0/940	0.39	0/1275
1	I	0.17	0/940	0.40	0/1275
2	G	0.20	0/812	0.43	0/1109
2	K	0.20	0/812	0.44	0/1109
2	L	0.20	0/812	0.42	0/1109
3	A	0.20	0/3955	0.51	2/5358 (0.0%)
3	B	0.19	0/3956	0.51	3/5360 (0.1%)
3	C	0.18	0/3956	0.47	0/5360
All	All	0.19	0/17123	0.47	5/23230 (0.0%)

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	K	0	1
2	L	0	1
3	A	0	2
All	All	0	4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	MET	CA-CB-CG	7.04	128.18	114.10
3	B	502	CYS	CA-C-N	6.93	134.79	121.54
3	B	502	CYS	C-N-CA	6.93	134.79	121.54
3	A	33	ASN	CA-C-N	6.25	133.22	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	33	ASN	C-N-CA	6.25	133.22	121.97

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	297	HIS	Peptide
3	A	507	ARG	Peptide
2	K	94	PRO	Peptide
2	L	94	PRO	Peptide

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	919	0	870	6	0
1	H	919	0	870	5	0
1	I	919	0	870	9	0
2	G	793	0	753	3	0
2	K	793	0	753	2	0
2	L	793	0	753	0	0
3	A	3864	0	3710	34	0
3	B	3865	0	3715	25	0
3	C	3865	0	3715	34	0
4	E	95	0	80	1	0
4	F	95	0	80	0	0
4	J	95	0	80	1	0
5	A	42	0	39	2	0
5	B	42	0	38	0	0
5	C	42	0	39	1	0
All	All	17141	0	16365	118	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 4.

All (118) 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:B:504:GLU:O	3:B:508:ASN:HB2	1.88	0.74
2:G:4:MET:HE3	2:G:90:GLN:HB3	1.76	0.66
2:G:8:PRO:HG2	2:G:11:LEU:HB3	1.78	0.64
3:C:85:GLU:HA	3:C:120:HIS:HB3	1.83	0.59
3:B:75:PRO:HB3	3:B:148:TYR:HB2	1.85	0.58
3:A:485:LYS:HE3	3:A:495:TYR:HA	1.86	0.58
3:C:34:VAL:HG21	3:C:459:GLU:HG3	1.86	0.58
3:C:32:LYS:HD3	5:C:602:NAG:H82	1.86	0.57
3:C:309:ILE:HG12	3:C:318:ILE:HD12	1.88	0.56
3:B:394:SER:HA	3:B:397:LYS:HD2	1.87	0.56
3:A:309:ILE:HG22	3:A:311:SER:HB2	1.88	0.56
3:B:328:LYS:HG3	3:B:415:THR:HA	1.88	0.54
3:A:28:THR:HG22	3:A:458:ASN:HB3	1.89	0.54
3:A:383:GLU:HG2	3:A:384:GLN:HG3	1.88	0.54
3:C:176:ILE:HG22	3:C:255:PHE:HB2	1.89	0.54
3:C:28:THR:HB	3:C:30:MET:H	1.73	0.54
3:B:43:LEU:HD23	3:B:45:LYS:HE3	1.91	0.52
3:A:75:PRO:HB2	3:A:148:TYR:HB2	1.91	0.52
3:B:232:GLN:HG2	3:B:237:ARG:HG2	1.90	0.52
3:A:371:MET:HE1	3:A:377:GLY:HA3	1.92	0.52
3:A:232:GLN:HG2	3:A:237:ARG:HG2	1.92	0.52
3:C:29:ILE:HG12	3:C:455:LEU:HD21	1.91	0.52
3:C:43:LEU:HD23	3:C:45:LYS:HE3	1.92	0.52
3:A:15:ILE:HG12	3:A:378:TYR:HD1	1.74	0.51
3:B:47:HIS:HB3	3:B:318:ILE:HD13	1.92	0.50
3:A:500:ASN:O	3:A:504:GLU:HB2	2.12	0.50
3:A:473:TYR:HA	3:A:476:VAL:HG22	1.94	0.49
3:C:412:LYS:HB3	3:C:453:LEU:HD11	1.93	0.49
1:I:18:VAL:HG11	1:I:109:VAL:HG11	1.94	0.49
1:D:18:VAL:HG11	1:D:109:VAL:HG11	1.95	0.49
1:H:93:ALA:HB1	1:H:100(A):PHE:HB3	1.95	0.48
2:K:89:GLN:HE21	2:K:96:TYR:HB3	1.78	0.48
2:G:89:GLN:HE21	2:G:96:TYR:HB3	1.78	0.48
3:C:338:ALA:HB1	3:C:462:LEU:HD13	1.95	0.48
3:C:13:ILE:HD11	3:C:378:TYR:HB3	1.95	0.48
1:H:68:THR:HG22	1:H:81:GLU:HB3	1.95	0.48
1:I:80:MET:HE2	1:I:80:MET:HB3	1.73	0.48
3:C:422:ARG:HH21	3:C:432:GLU:HG2	1.79	0.47
1:D:40:ALA:HB3	1:D:43:GLN:HB2	1.97	0.47
1:D:93:ALA:HB1	1:D:100(A):PHE:HB3	1.96	0.47
3:C:118:ILE:HD12	3:C:270:ILE:HG23	1.95	0.47
3:C:486:GLU:HG2	3:C:492:PHE:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:12:GLN:HB2	3:A:491:CYS:HB3	1.96	0.47
3:A:54:LEU:HD12	3:A:87:SER:HB2	1.97	0.47
3:B:302:CYS:HB2	3:B:326:CYS:HB3	1.59	0.47
1:I:93:ALA:HB1	1:I:100(A):PHE:HB3	1.97	0.46
3:B:60:LEU:HD23	3:B:89:ILE:HG12	1.98	0.46
3:C:498:CYS:HB3	3:C:503:MET:HB2	1.98	0.46
1:H:18:VAL:HG11	1:H:109:VAL:HG11	1.97	0.45
1:I:51:MET:HE3	1:I:51:MET:HB3	1.82	0.45
3:C:112:LYS:HE3	3:C:423:GLU:HG2	1.98	0.45
1:H:30:THR:HA	1:H:52(A):PRO:HB2	1.97	0.45
3:B:470:LYS:HD3	3:B:473:TYR:HD2	1.81	0.45
3:A:314:PRO:HG3	3:A:406:VAL:HG13	1.98	0.45
3:A:437:LYS:HA	3:A:437:LYS:HD3	1.83	0.45
1:D:6:GLN:H	1:D:105:GLN:HE21	1.65	0.45
3:A:289:MET:HG2	3:A:305:PRO:HG3	1.98	0.45
3:A:52:CYS:HA	3:A:298:CYS:HB3	1.98	0.45
3:B:101:TYR:CD1	3:B:240:MET:HG3	2.52	0.45
3:B:212:ILE:HG12	3:B:257:SER:HB2	1.99	0.45
1:I:6:GLN:H	1:I:105:GLN:HE21	1.65	0.44
3:B:320:PRO:HB3	3:B:443:LEU:HD21	1.98	0.44
3:C:12:GLN:HA	3:C:493:GLU:HA	1.99	0.44
3:C:101:TYR:CD2	3:C:240:MET:HG3	2.53	0.44
1:I:11:MET:HE2	1:I:11:MET:HB2	1.84	0.44
3:A:76:MET:HE2	3:A:76:MET:HB3	1.89	0.44
3:C:24:GLU:HG2	3:C:39:ALA:HB3	1.99	0.44
3:A:289:MET:HE1	3:A:303:GLN:HG3	2.00	0.44
1:D:51:MET:HE1	1:D:78:ALA:HB1	1.98	0.44
3:A:248:LYS:HD3	3:A:248:LYS:HA	1.77	0.44
1:I:40:ALA:HB3	1:I:43:GLN:HB2	1.99	0.44
3:B:485:LYS:HE2	3:B:485:LYS:HB3	1.87	0.43
3:A:28:THR:O	3:A:29:ILE:HG13	2.18	0.43
3:A:328:LYS:HD2	3:A:416:GLN:HG2	2.00	0.43
3:C:50:LYS:HB2	3:C:50:LYS:HE2	1.83	0.43
1:D:80:MET:HB3	1:D:80:MET:HE2	1.77	0.43
3:B:15:ILE:HD13	3:B:472:LEU:HB3	1.99	0.43
3:A:14:CYS:HB3	3:A:491:CYS:HA	2.00	0.43
3:A:328:LYS:HA	3:A:328:LYS:HD3	1.84	0.43
1:H:59:TYR:HE1	1:H:69:LEU:HG	1.83	0.43
3:A:50:LYS:HE3	3:A:50:LYS:HB2	1.77	0.43
3:B:118:ILE:HG23	3:B:270:ILE:HG23	2.00	0.43
3:C:75:PRO:HB2	3:C:148:TYR:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:438:MET:HE2	3:A:439:GLU:HG2	2.01	0.43
3:C:337:LEU:HD23	3:C:337:LEU:HA	1.92	0.43
1:I:59:TYR:HE1	1:I:69:LEU:HG	1.83	0.42
3:C:383:GLU:HG2	3:C:384:GLN:HG3	2.01	0.42
3:C:51:LEU:HA	3:C:303:GLN:HE22	1.84	0.42
3:A:467:SER:HB2	3:C:357:PHE:HA	2.02	0.42
3:B:190:TRP:HB3	3:B:264:PRO:HG3	2.02	0.42
3:C:329:TYR:HD2	3:C:443:LEU:HD22	1.84	0.42
3:B:481:ARG:HE	3:B:513:TYR:HB2	1.85	0.42
3:A:484:ALA:HA	3:A:494:PHE:HA	2.01	0.42
3:C:180:ASN:HB2	3:C:247:LEU:HD23	2.02	0.42
3:A:302:CYS:HB2	3:A:326:CYS:HB3	1.54	0.41
4:J:6:GAL:H3	4:J:7:SIA:H32	1.94	0.41
3:B:50:LYS:HE3	3:B:50:LYS:HB2	1.78	0.41
3:A:456:MET:SD	3:C:29:ILE:HB	2.60	0.41
3:C:422:ARG:HH22	3:C:436:LYS:HD3	1.86	0.41
3:B:20:ASN:HD21	3:B:22:SER:HB2	1.86	0.41
3:A:32:LYS:HZ2	5:A:603:NAG:HN2	1.69	0.41
3:B:384:GLN:HE21	3:B:499:ASP:HB2	1.84	0.41
3:C:379:HIS:CD2	3:C:381:SER:HB2	2.56	0.41
4:E:6:GAL:H3	4:E:7:SIA:H32	1.92	0.41
3:A:436:LYS:HE3	3:A:436:LYS:HB3	1.92	0.41
3:A:475:LYS:HE2	3:A:475:LYS:HB3	1.91	0.41
3:B:409:ILE:HG12	3:B:453:LEU:HD21	2.03	0.41
3:C:31:GLU:HG2	3:C:34:VAL:HG22	2.03	0.41
3:C:497:LYS:HD3	3:C:497:LYS:HA	1.89	0.41
3:A:32:LYS:NZ	5:A:603:NAG:HN2	2.18	0.41
3:B:470:LYS:HD3	3:B:470:LYS:HA	1.85	0.41
3:C:76:MET:HE2	3:C:76:MET:HB3	1.78	0.41
3:A:200:GLU:HG3	3:A:204:LEU:HD13	2.02	0.40
2:K:4:MET:HB3	2:K:4:MET:HE3	1.81	0.40
3:B:248:LYS:HD3	3:B:248:LYS:HA	1.77	0.40
1:I:6:GLN:HE21	1:I:6:GLN:HB3	1.70	0.40
3:C:364:ILE:HD13	3:C:364:ILE:HA	1.92	0.40
3:B:52:CYS:HB3	3:B:298:CYS:HB2	1.52	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	D	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
1	H	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
1	I	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
2	G	99/107 (92%)	96 (97%)	3 (3%)	0	100	100
2	K	99/107 (92%)	94 (95%)	4 (4%)	1 (1%)	12	31
2	L	99/107 (92%)	94 (95%)	4 (4%)	1 (1%)	12	31
3	A	480/576 (83%)	437 (91%)	41 (8%)	2 (0%)	30	54
3	B	480/576 (83%)	453 (94%)	27 (6%)	0	100	100
3	C	480/576 (83%)	440 (92%)	38 (8%)	2 (0%)	30	54
All	All	2085/2403 (87%)	1951 (94%)	128 (6%)	6 (0%)	37	59

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	34	VAL
3	C	118	ILE
2	L	95	PRO
2	K	95	PRO
3	A	85	GLU
3	C	32	LYS

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	97/97 (100%)	93 (96%)	4 (4%)	27	52
1	H	97/97 (100%)	95 (98%)	2 (2%)	47	70
1	I	97/97 (100%)	94 (97%)	3 (3%)	35	60
2	G	91/95 (96%)	90 (99%)	1 (1%)	65	80
2	K	91/95 (96%)	86 (94%)	5 (6%)	19	41
2	L	91/95 (96%)	87 (96%)	4 (4%)	25	50
3	A	425/502 (85%)	415 (98%)	10 (2%)	43	67
3	B	425/502 (85%)	414 (97%)	11 (3%)	40	65
3	C	425/502 (85%)	417 (98%)	8 (2%)	50	71
All	All	1839/2082 (88%)	1791 (97%)	48 (3%)	41	65

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	5	VAL
1	H	87	THR
2	L	11	LEU
2	L	22	THR
2	L	100	GLN
2	L	106	ILE
3	A	33	ASN
3	A	57	VAL
3	A	65	CYS
3	A	223	LEU
3	A	241	ASP
3	A	368	TRP
3	A	453	LEU
3	A	481	ARG
3	A	497	LYS
3	A	504	GLU
3	B	57	VAL
3	B	65	CYS
3	B	90	VAL
3	B	122	GLU
3	B	179	ASN
3	B	183	ARG
3	B	196	ASN
3	B	360	ILE
3	B	368	TRP
3	B	369	GLN

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Mol	Chain	Res	Type
3	B	438	MET
3	C	12	GLN
3	C	28	THR
3	C	57	VAL
3	C	64	ASP
3	C	186	LEU
3	C	196	ASN
3	C	462	LEU
3	C	476	VAL
1	I	5	VAL
1	I	80	MET
1	I	87	THR
2	K	11	LEU
2	K	22	THR
2	K	47	LEU
2	K	85	THR
2	K	100	GLN
1	D	5	VAL
1	D	23	THR
1	D	51	MET
1	D	87	THR
2	G	22	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	34	ASN
3	A	18	HIS
3	A	97	ASN
3	A	166	ASN
3	A	197	ASN
3	A	254	HIS
3	A	333	ASN
3	A	382	ASN
3	A	407	ASN
3	A	496	HIS
3	B	20	ASN
3	B	379	HIS
3	B	496	HIS
3	B	515	GLN
3	C	20	ASN
3	C	166	ASN

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Mol	Chain	Res	Type
3	C	179	ASN
3	C	196	ASN
3	C	236	GLN
2	K	34	ASN
2	K	37	GLN
2	G	34	ASN
2	G	37	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 ⓘ

21 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	E	1	4	14,14,15	0.72	0	17,19,21	1.23	3 (17%)
4	NAG	E	2	4	14,14,15	0.70	0	17,19,21	1.05	1 (5%)
4	BMA	E	3	4	11,11,12	0.84	0	15,15,17	2.55	6 (40%)
4	MAN	E	4	4	11,11,12	0.63	0	15,15,17	1.53	1 (6%)
4	NAG	E	5	4	14,14,15	0.72	0	17,19,21	1.11	2 (11%)
4	GAL	E	6	4	11,11,12	0.71	0	15,15,17	1.20	1 (6%)
4	SIA	E	7	4	20,20,21	1.49	2 (10%)	21,28,31	1.79	4 (19%)
4	NAG	F	1	4	14,14,15	0.70	0	17,19,21	0.91	0
4	NAG	F	2	4	14,14,15	0.74	0	17,19,21	1.24	2 (11%)
4	BMA	F	3	4	11,11,12	0.87	0	15,15,17	2.38	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	F	4	4	11,11,12	0.70	0	15,15,17	1.12	1 (6%)
4	NAG	F	5	4	14,14,15	0.70	0	17,19,21	1.06	1 (5%)
4	GAL	F	6	4	11,11,12	0.76	0	15,15,17	1.43	3 (20%)
4	SIA	F	7	4	20,20,21	1.53	2 (10%)	21,28,31	1.83	4 (19%)
4	NAG	J	1	4	14,14,15	0.70	0	17,19,21	1.10	1 (5%)
4	NAG	J	2	4	14,14,15	0.72	0	17,19,21	1.31	2 (11%)
4	BMA	J	3	4	11,11,12	0.83	0	15,15,17	2.54	6 (40%)
4	MAN	J	4	4	11,11,12	0.61	0	15,15,17	1.58	1 (6%)
4	NAG	J	5	4	14,14,15	0.73	0	17,19,21	1.11	2 (11%)
4	GAL	J	6	4	11,11,12	0.69	0	15,15,17	1.15	1 (6%)
4	SIA	J	7	4	20,20,21	1.50	2 (10%)	21,28,31	1.90	5 (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	E	1	4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	NAG	E	5	4	-	2/6/23/26	0/1/1/1
4	GAL	E	6	4	-	0/2/19/22	0/1/1/1
4	SIA	E	7	4	-	0/18/34/38	0/1/1/1
4	NAG	F	1	4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	1/2/19/22	0/1/1/1
4	MAN	F	4	4	-	2/2/19/22	0/1/1/1
4	NAG	F	5	4	-	0/6/23/26	0/1/1/1
4	GAL	F	6	4	-	1/2/19/22	0/1/1/1
4	SIA	F	7	4	-	1/18/34/38	0/1/1/1
4	NAG	J	1	4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	BMA	J	3	4	-	0/2/19/22	0/1/1/1
4	MAN	J	4	4	-	2/2/19/22	0/1/1/1
4	NAG	J	5	4	-	2/6/23/26	0/1/1/1
4	GAL	J	6	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SIA	J	7	4	-	1/18/34/38	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	7	SIA	C2-C1	5.47	1.58	1.52
4	J	7	SIA	C2-C1	5.31	1.58	1.52
4	E	7	SIA	C2-C1	5.24	1.58	1.52
4	F	7	SIA	O6-C2	2.06	1.47	1.43
4	E	7	SIA	O6-C2	2.06	1.47	1.43
4	J	7	SIA	O6-C2	2.03	1.47	1.43

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	3	BMA	C1-O5-C5	7.32	122.00	112.19
4	F	3	BMA	C1-O5-C5	7.30	121.97	112.19
4	J	3	BMA	C1-O5-C5	7.28	121.94	112.19
4	J	4	MAN	C1-O5-C5	5.17	119.11	112.19
4	E	4	MAN	C1-O5-C5	4.92	118.77	112.19
4	F	7	SIA	O1A-C1-C2	-4.49	113.16	122.85
4	E	7	SIA	O1A-C1-C2	-4.35	113.46	122.85
4	J	7	SIA	O1A-C1-C2	-4.25	113.66	122.85
4	J	7	SIA	C6-C5-N5	-4.20	104.21	110.91
4	J	7	SIA	O6-C2-C3	-3.76	105.50	110.56
4	F	6	GAL	O3-C3-C2	-3.76	102.39	110.05
4	F	7	SIA	O6-C2-C3	-3.74	105.53	110.56
4	E	3	BMA	C3-C4-C5	3.50	116.58	110.23
4	F	7	SIA	C6-C5-N5	-3.49	105.34	110.91
4	E	7	SIA	O6-C2-C3	-3.46	105.91	110.56
4	E	7	SIA	C6-C5-N5	-3.43	105.43	110.91
4	J	3	BMA	C3-C4-C5	3.43	116.44	110.23
4	E	6	GAL	O3-C3-C2	-3.33	103.25	110.05
4	J	6	GAL	O3-C3-C2	-3.25	103.42	110.05
4	F	4	MAN	C1-O5-C5	3.19	116.46	112.19
4	F	2	NAG	C2-N2-C7	3.06	127.00	122.90
4	J	2	NAG	C2-N2-C7	2.96	126.87	122.90
4	F	5	NAG	O5-C1-C2	-2.93	106.75	111.29
4	E	1	NAG	C2-N2-C7	2.91	126.80	122.90
4	J	5	NAG	C2-N2-C7	2.83	126.69	122.90
4	E	5	NAG	C2-N2-C7	2.81	126.66	122.90
4	J	1	NAG	C2-N2-C7	2.79	126.64	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	3	BMA	C2-C3-C4	2.70	115.61	110.86
4	E	3	BMA	C2-C3-C4	2.64	115.50	110.86
4	J	3	BMA	C2-C3-C4	2.59	115.41	110.86
4	F	3	BMA	C3-C4-C5	2.56	114.88	110.23
4	E	3	BMA	O4-C4-C3	-2.53	104.42	110.38
4	J	3	BMA	O4-C4-C3	-2.51	104.47	110.38
4	J	7	SIA	O1B-C1-O1A	2.50	129.76	124.08
4	E	7	SIA	O1B-C1-O1A	2.50	129.75	124.08
4	F	7	SIA	O1B-C1-O1A	2.37	129.46	124.08
4	J	3	BMA	O3-C3-C4	2.35	115.92	110.38
4	E	3	BMA	O3-C3-C4	2.31	115.83	110.38
4	E	1	NAG	O5-C1-C2	-2.29	107.74	111.29
4	F	6	GAL	C1-C2-C3	2.29	112.98	109.64
4	J	3	BMA	O5-C5-C4	2.29	116.40	110.83
4	J	2	NAG	C1-O5-C5	2.28	115.25	112.19
4	E	3	BMA	O5-C5-C4	2.24	116.27	110.83
4	F	6	GAL	C1-O5-C5	2.21	115.15	112.19
4	E	1	NAG	O4-C4-C3	-2.16	105.28	110.38
4	E	2	NAG	C1-O5-C5	2.14	115.05	112.19
4	E	5	NAG	O5-C1-C2	-2.12	108.01	111.29
4	F	2	NAG	C1-O5-C5	2.09	114.98	112.19
4	J	5	NAG	O5-C1-C2	-2.07	108.08	111.29
4	J	7	SIA	C8-C7-C6	-2.02	109.25	113.05

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	4	MAN	O5-C5-C6-O6
4	F	4	MAN	C4-C5-C6-O6
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	E	5	NAG	C8-C7-N2-C2
4	E	5	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	J	5	NAG	C8-C7-N2-C2
4	J	5	NAG	O7-C7-N2-C2

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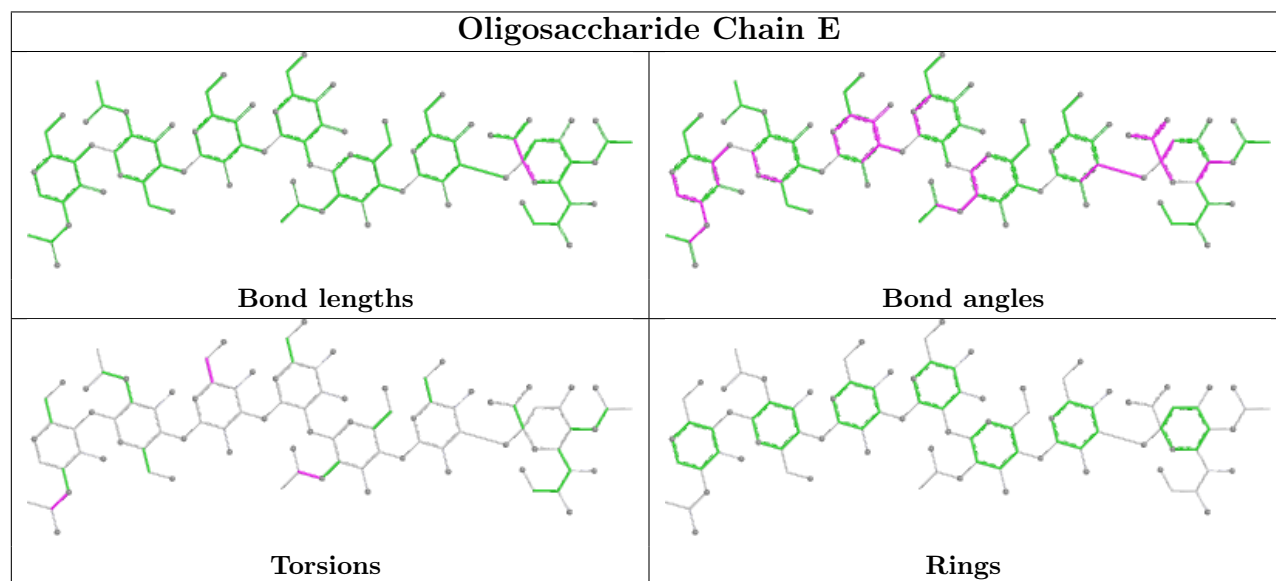
Mol	Chain	Res	Type	Atoms
4	F	6	GAL	O5-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
4	J	4	MAN	C4-C5-C6-O6
4	J	4	MAN	O5-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
4	F	7	SIA	O1A-C1-C2-O6
4	J	7	SIA	C6-C7-C8-O8
4	F	3	BMA	O5-C5-C6-O6

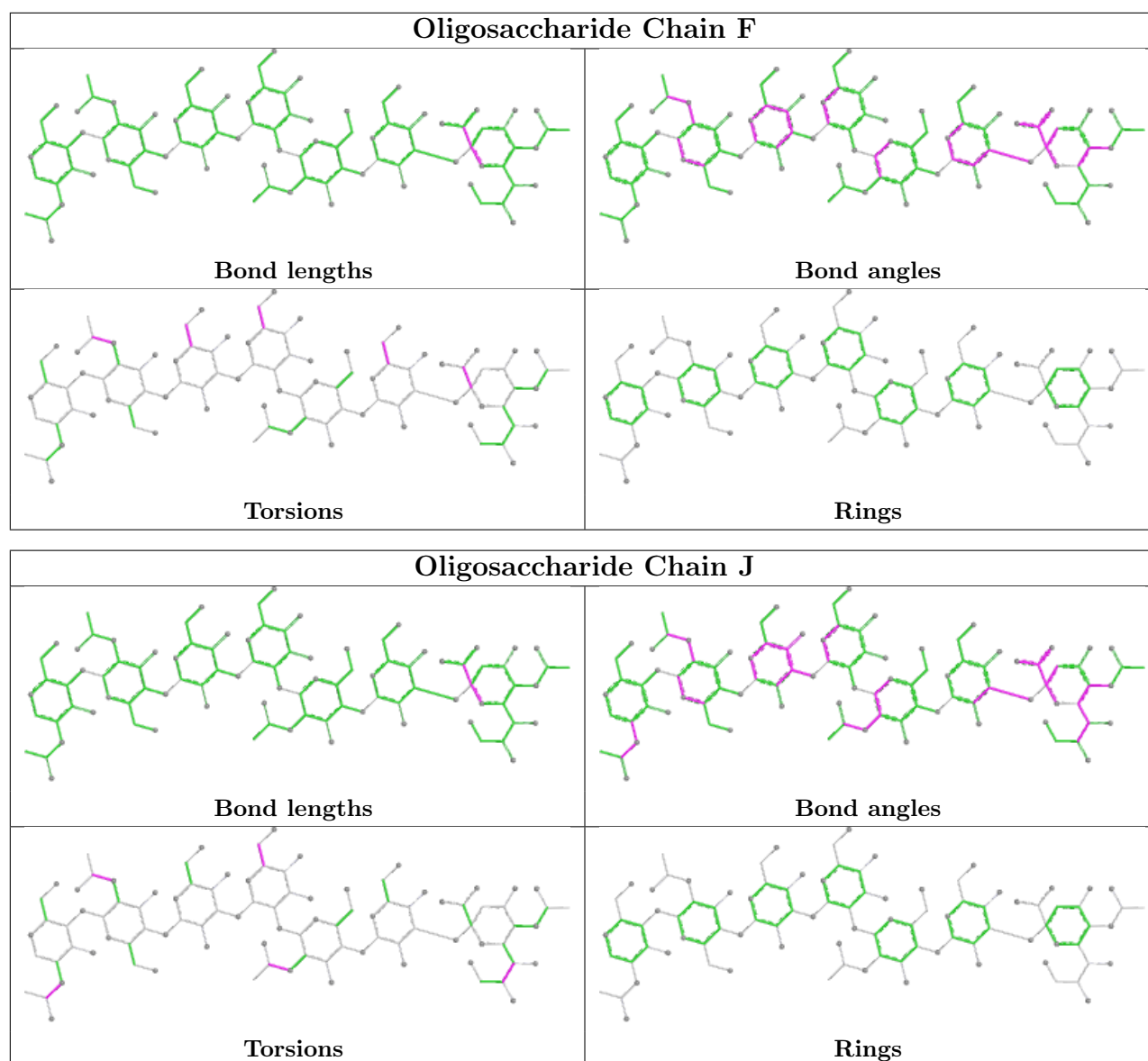
There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	7	SIA	1	0
4	J	6	GAL	1	0
4	E	7	SIA	1	0
4	E	6	GAL	1	0

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





5.6 Ligand geometry [i](#)

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	A	603	3	14,14,15	0.77	0	17,19,21	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	601	3	14,14,15	0.72	0	17,19,21	0.88	0
5	NAG	C	601	3	14,14,15	0.71	0	17,19,21	1.50	2 (11%)
5	NAG	C	603	-	14,14,15	0.70	0	17,19,21	0.73	0
5	NAG	A	601	3	14,14,15	0.74	0	17,19,21	1.23	2 (11%)
5	NAG	B	603	-	14,14,15	1.54	3 (21%)	17,19,21	5.71	11 (64%)
5	NAG	A	602	3	14,14,15	0.75	0	17,19,21	1.61	3 (17%)
5	NAG	B	602	3	14,14,15	0.72	0	17,19,21	1.34	2 (11%)
5	NAG	C	602	3	14,14,15	0.79	0	17,19,21	0.93	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	603	3	-	0/6/23/26	0/1/1/1
5	NAG	B	601	3	-	0/6/23/26	0/1/1/1
5	NAG	C	601	3	-	2/6/23/26	0/1/1/1
5	NAG	C	603	-	-	0/6/23/26	0/1/1/1
5	NAG	A	601	3	-	1/6/23/26	0/1/1/1
5	NAG	B	603	-	-	6/6/23/26	0/1/1/1
5	NAG	A	602	3	-	2/6/23/26	0/1/1/1
5	NAG	B	602	3	-	0/6/23/26	0/1/1/1
5	NAG	C	602	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	603	NAG	C1-C2	3.31	1.56	1.52
5	B	603	NAG	C3-C2	2.95	1.58	1.52
5	B	603	NAG	O5-C1	-2.17	1.40	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	603	NAG	C2-N2-C7	15.98	144.32	122.90
5	B	603	NAG	C1-C2-N2	-10.89	93.28	110.43
5	B	603	NAG	C8-C7-N2	7.17	128.01	116.12
5	B	603	NAG	C4-C3-C2	5.32	118.82	111.02
5	B	603	NAG	C1-O5-C5	-4.73	105.84	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	603	NAG	O7-C7-N2	-4.66	113.75	121.98
5	C	601	NAG	C2-N2-C7	4.47	128.89	122.90
5	A	602	NAG	C2-N2-C7	4.45	128.86	122.90
5	B	603	NAG	O3-C3-C2	3.97	117.65	109.40
5	B	602	NAG	C1-O5-C5	-3.79	107.11	112.19
5	B	603	NAG	O3-C3-C4	-3.76	101.52	110.38
5	A	601	NAG	O5-C1-C2	-3.26	106.25	111.29
5	A	601	NAG	C1-C2-N2	3.00	115.16	110.43
5	A	602	NAG	C1-O5-C5	2.80	115.94	112.19
5	B	603	NAG	O5-C1-C2	2.68	115.44	111.29
5	B	603	NAG	O5-C5-C4	-2.52	104.69	110.83
5	B	602	NAG	C2-N2-C7	2.40	126.11	122.90
5	B	603	NAG	O7-C7-C8	-2.19	118.16	122.05
5	A	603	NAG	O5-C1-C2	-2.19	107.91	111.29
5	A	602	NAG	O7-C7-N2	2.09	125.68	121.98
5	C	601	NAG	O7-C7-N2	2.08	125.66	121.98

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	603	NAG	O5-C5-C6-O6
5	B	603	NAG	C8-C7-N2-C2
5	B	603	NAG	O7-C7-N2-C2
5	B	603	NAG	C4-C5-C6-O6
5	A	601	NAG	O5-C5-C6-O6
5	B	603	NAG	C3-C2-N2-C7
5	B	603	NAG	C1-C2-N2-C7
5	A	602	NAG	C3-C2-N2-C7
5	C	601	NAG	C3-C2-N2-C7
5	A	602	NAG	C1-C2-N2-C7
5	C	601	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
5	A	603	NAG	2	0
5	C	602	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

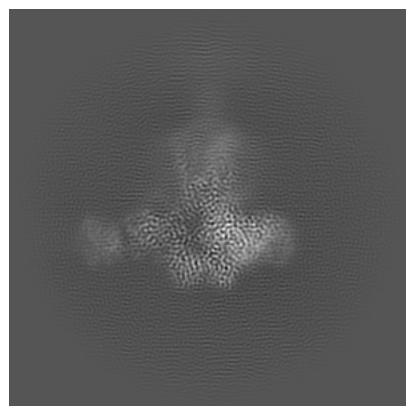
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74873. These allow visual inspection of the internal detail of the map and identification of artifacts.

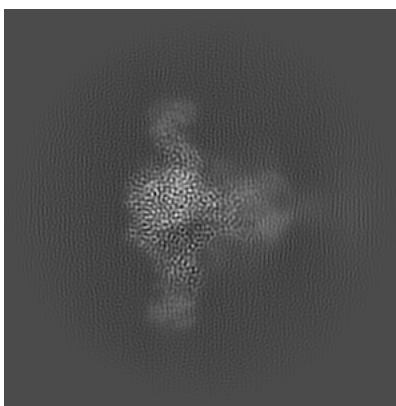
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

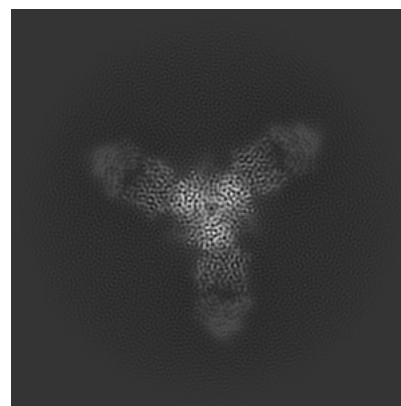
6.1.1 Primary map



X

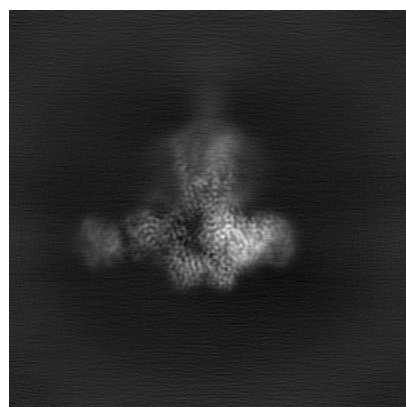


Y

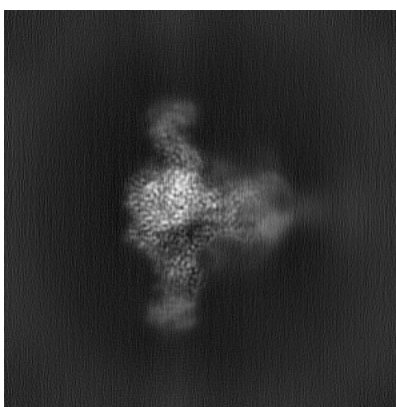


Z

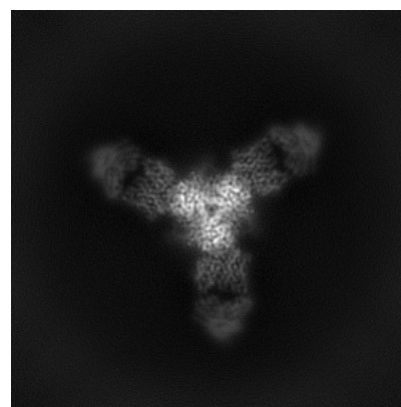
6.1.2 Raw map



X



Y

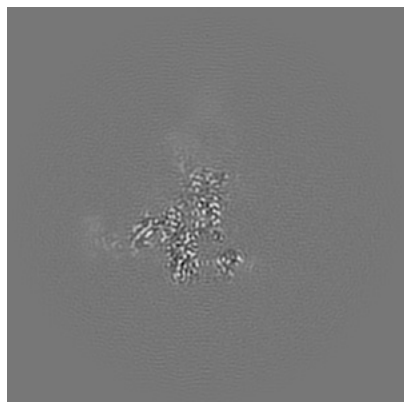


Z

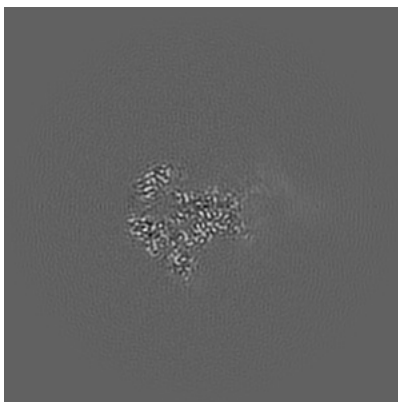
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

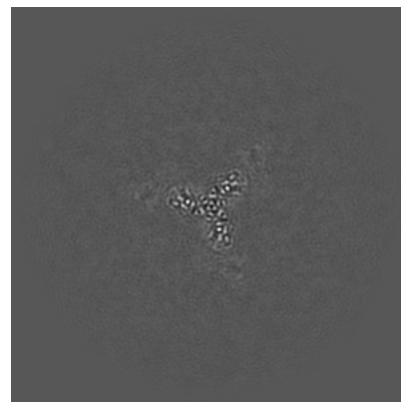
6.2.1 Primary map



X Index: 192

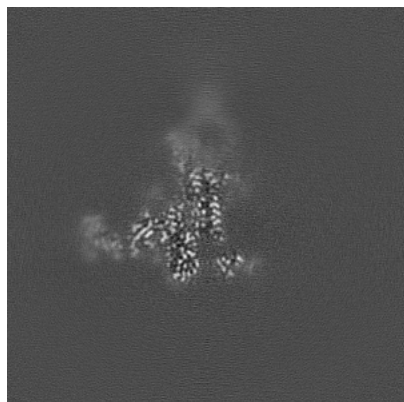


Y Index: 192

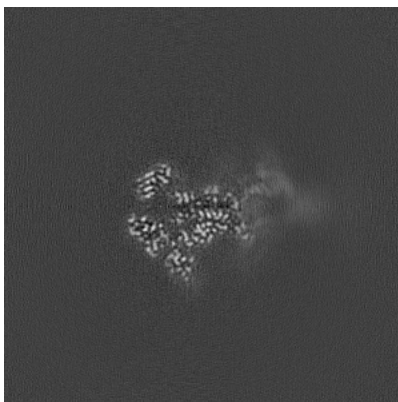


Z Index: 192

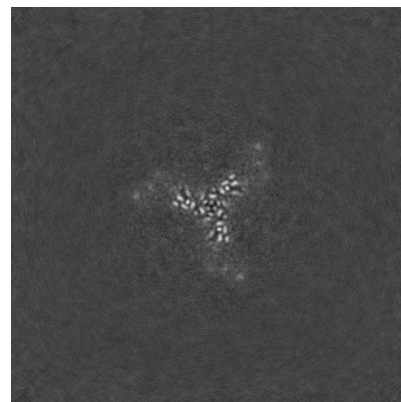
6.2.2 Raw map



X Index: 192



Y Index: 192

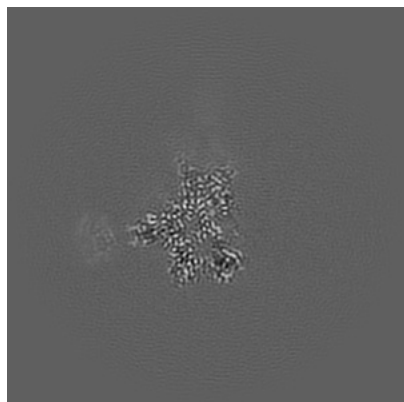


Z Index: 192

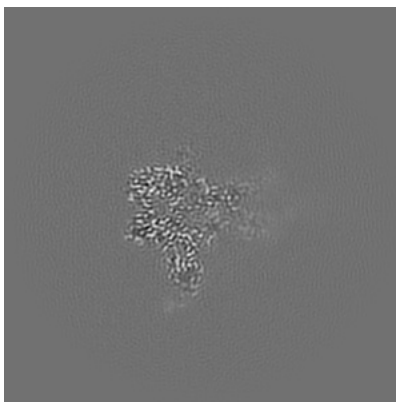
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

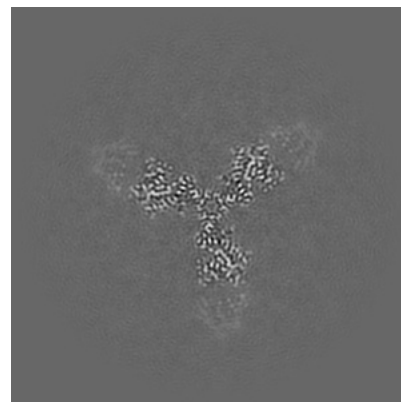
6.3.1 Primary map



X Index: 200

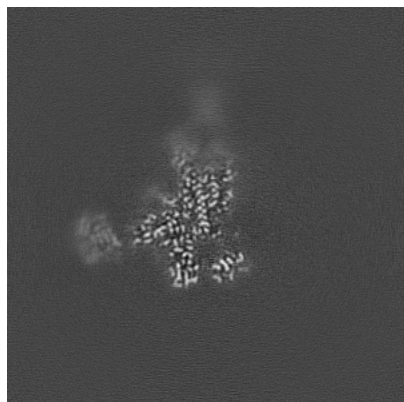


Y Index: 204

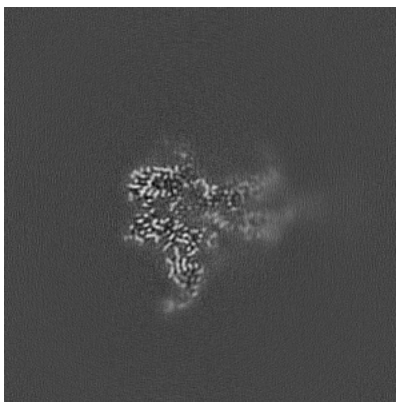


Z Index: 166

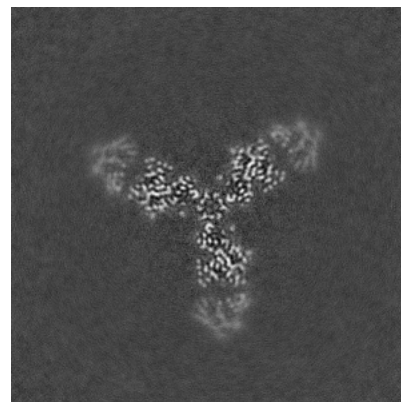
6.3.2 Raw map



X Index: 198



Y Index: 205

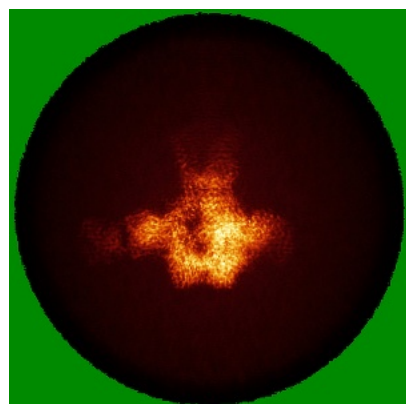


Z Index: 166

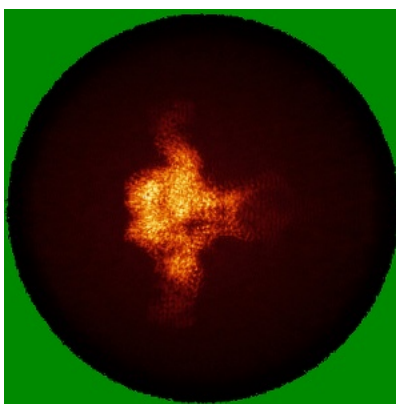
The images above show the largest variance slices of the map in three orthogonal directions.

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

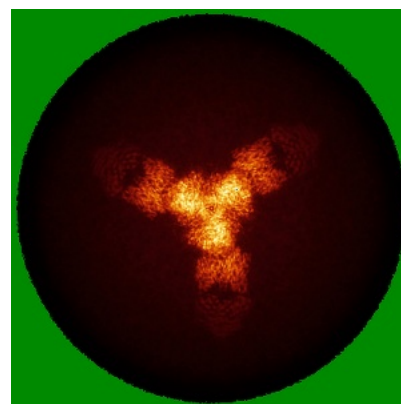
6.4.1 Primary map



X

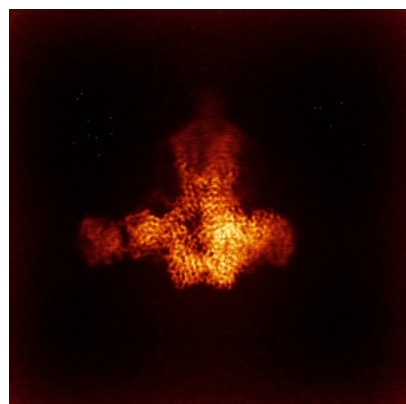


Y

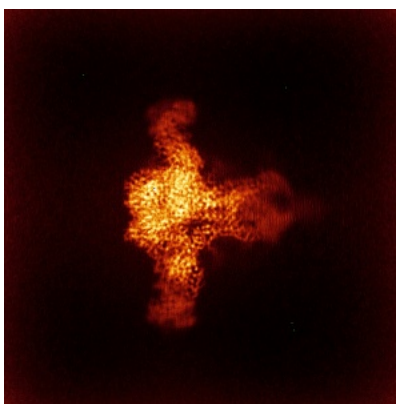


Z

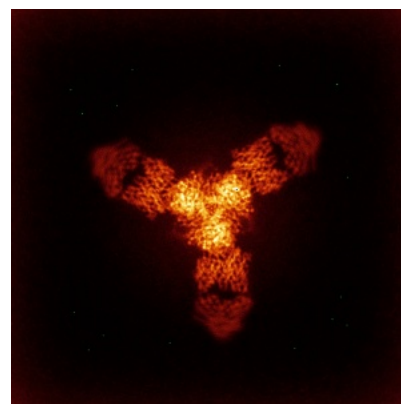
6.4.2 Raw map



X



Y

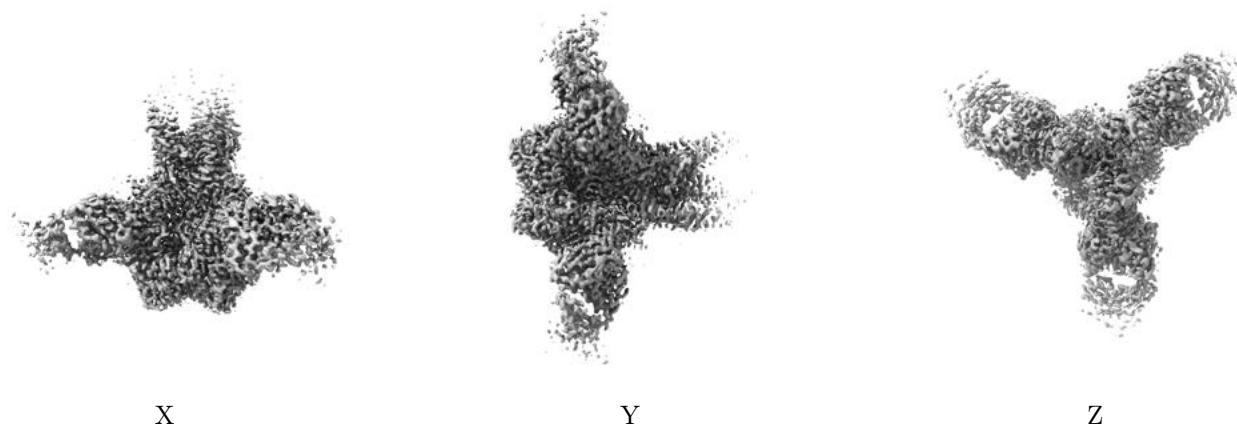


Z

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.

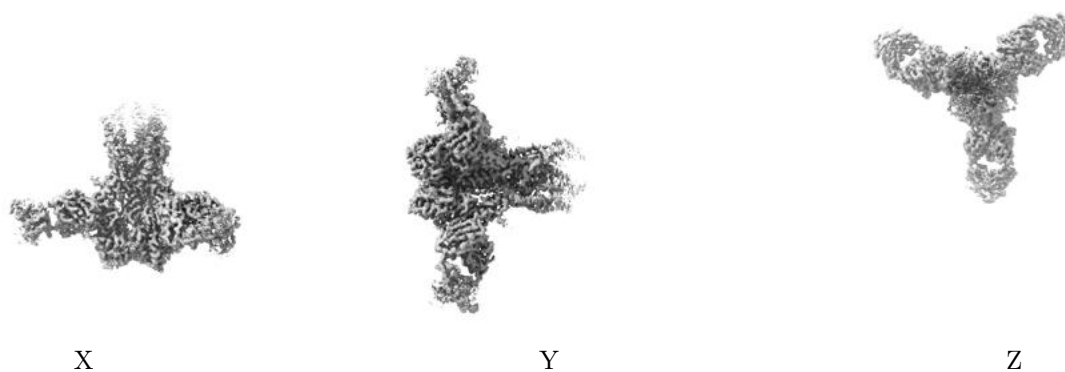
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.172. 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.

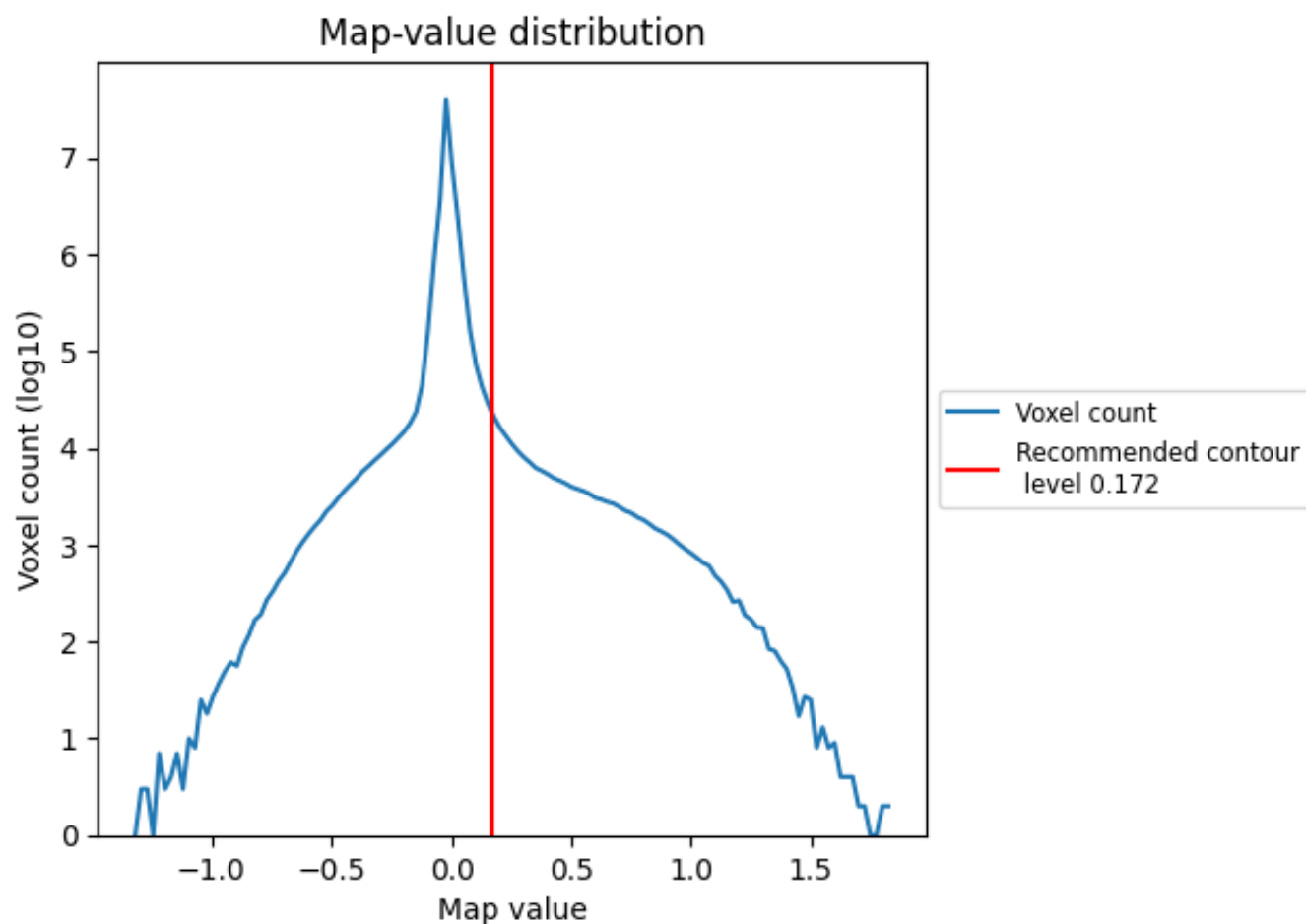
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

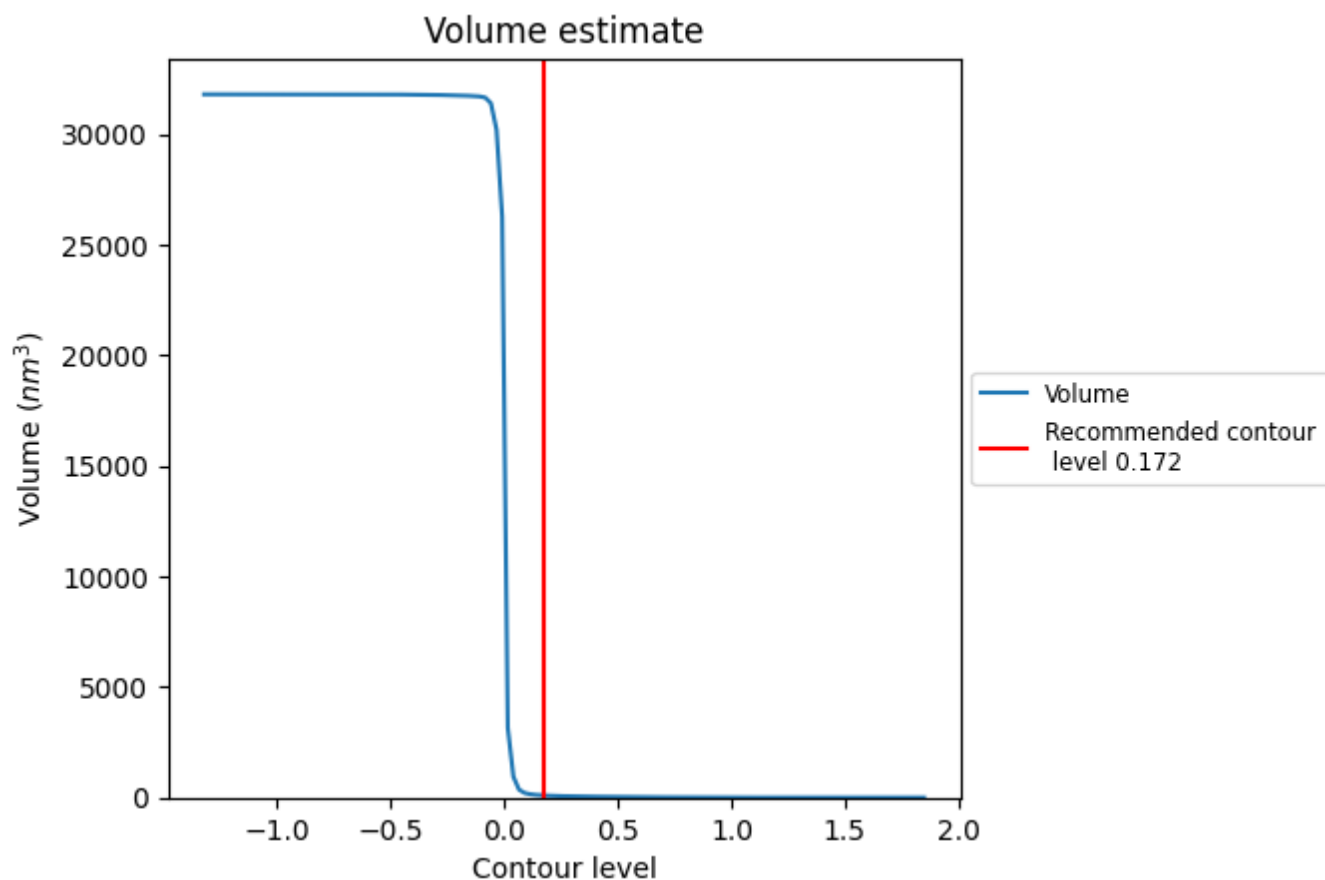
This section contains the results of statistical analysis of the map.

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.

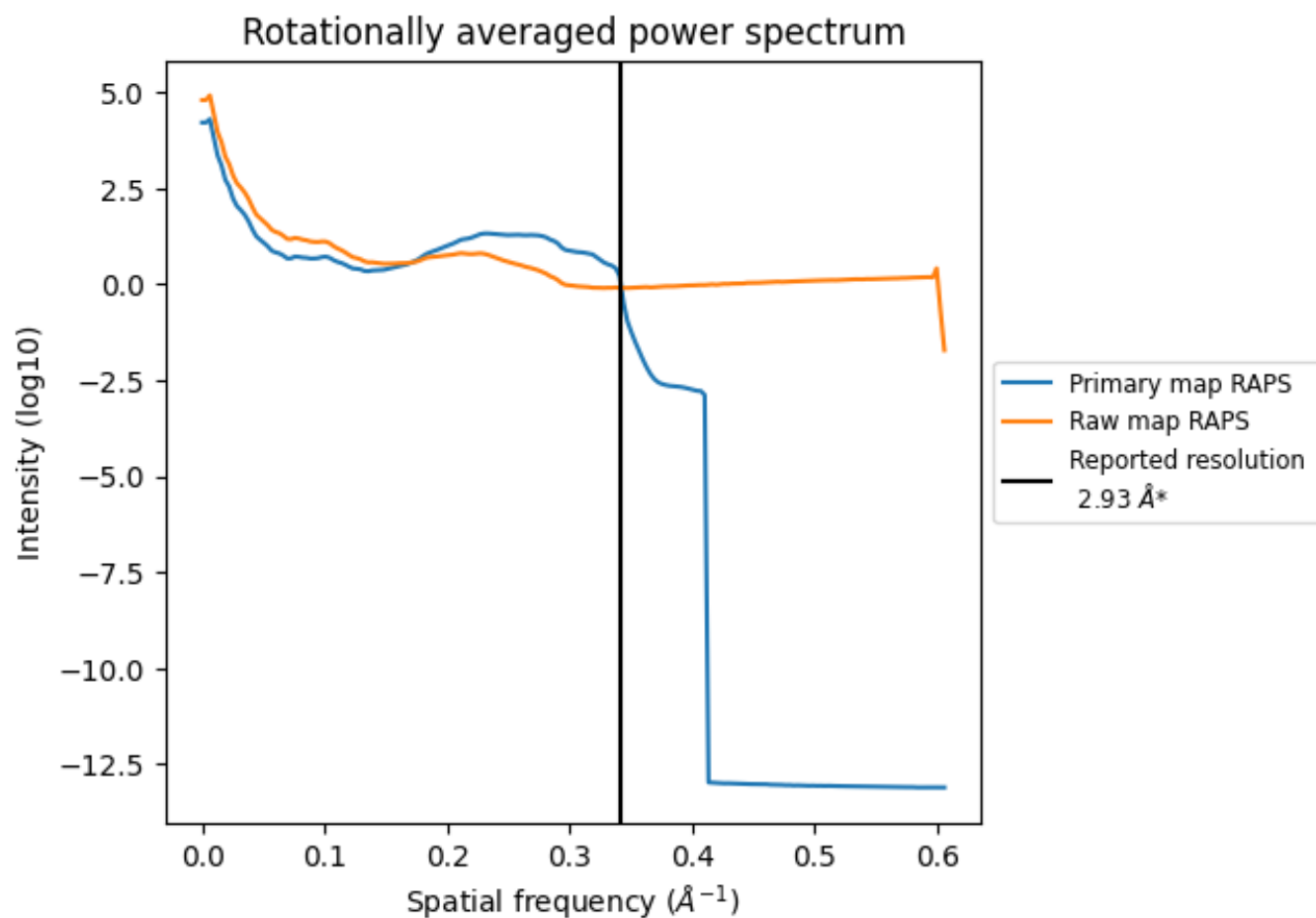
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 98 nm^3 ; this corresponds to an approximate mass of 88 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 ⓘ

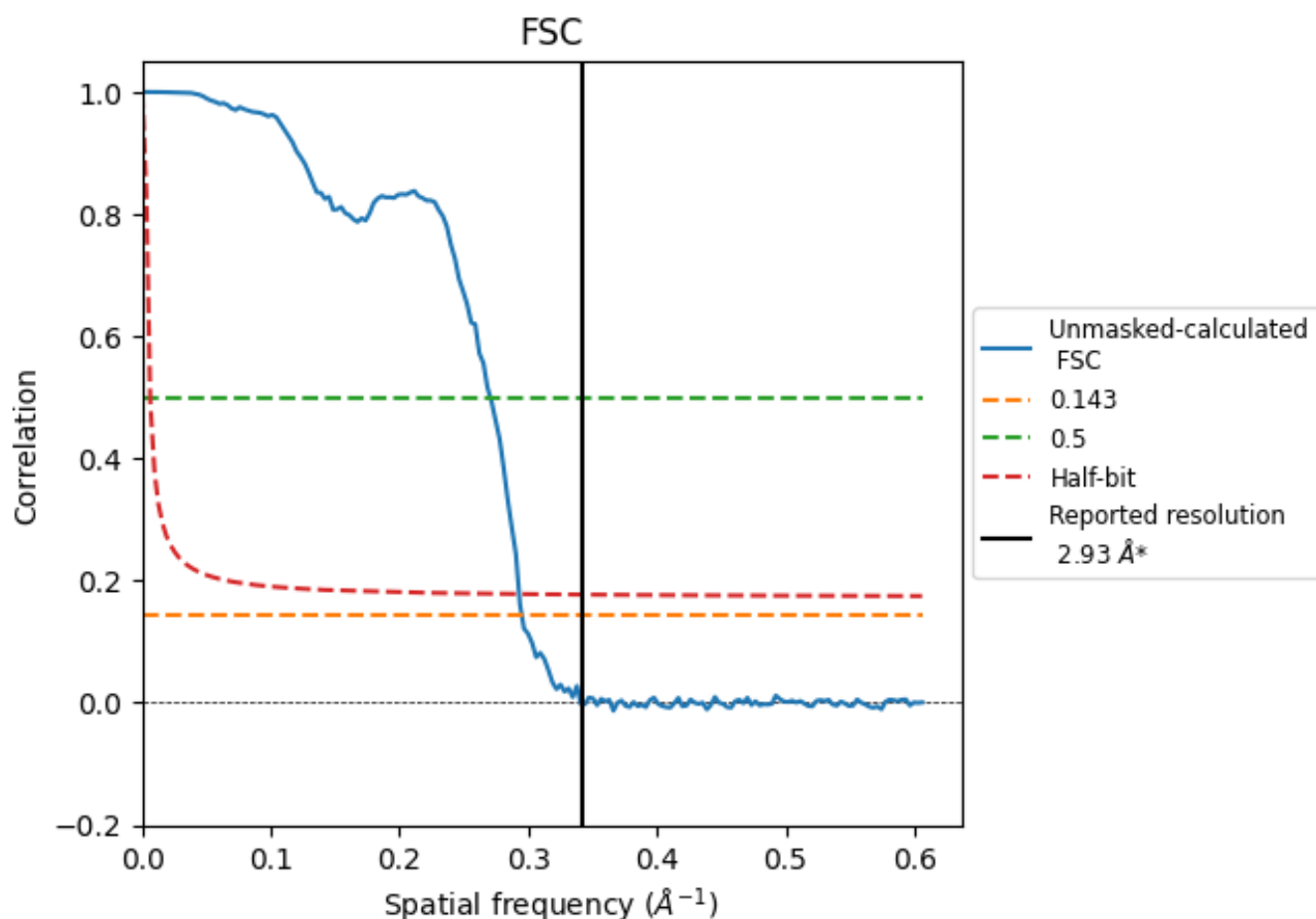


*Reported resolution corresponds to spatial frequency of 0.341 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.341 \AA^{-1}

8.2 Resolution estimates [i](#)

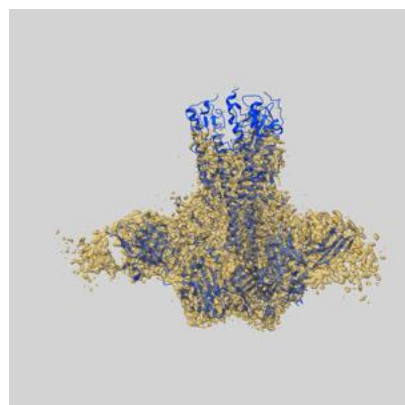
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.93	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.39	3.70	3.41

*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 3.39 differs from the reported value 2.93 by more than 10 %

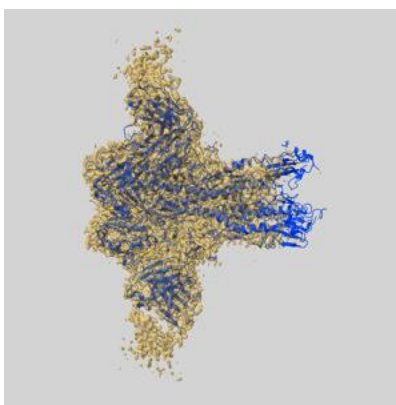
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-74873 and PDB model 9ZVH. Per-residue inclusion information can be found in section 3 on page 11.

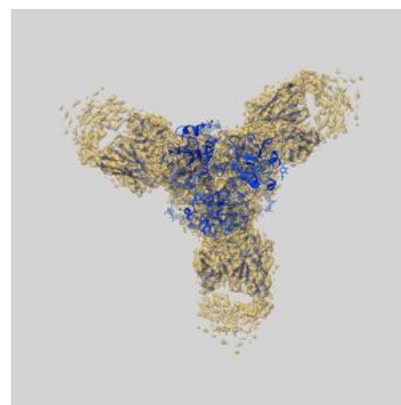
9.1 Map-model overlay [i](#)



X



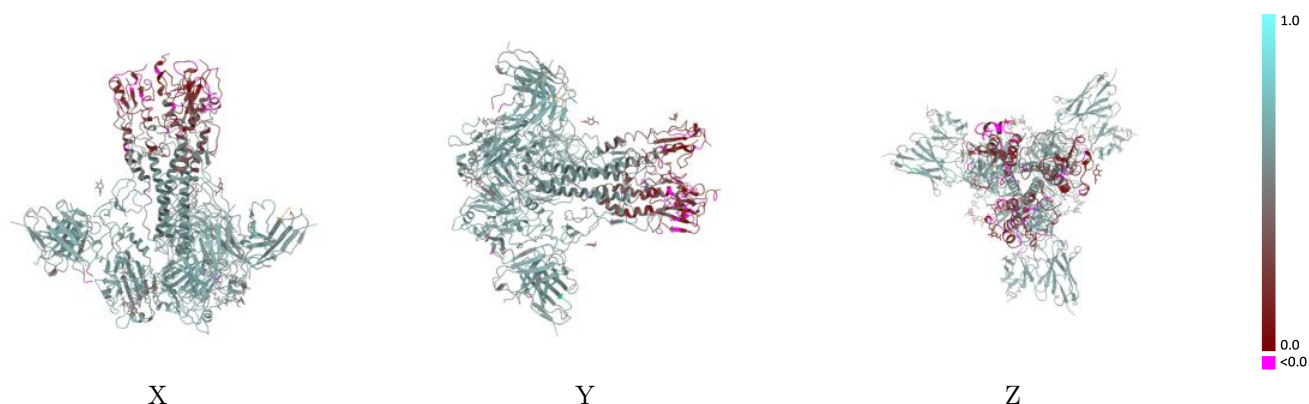
Y



Z

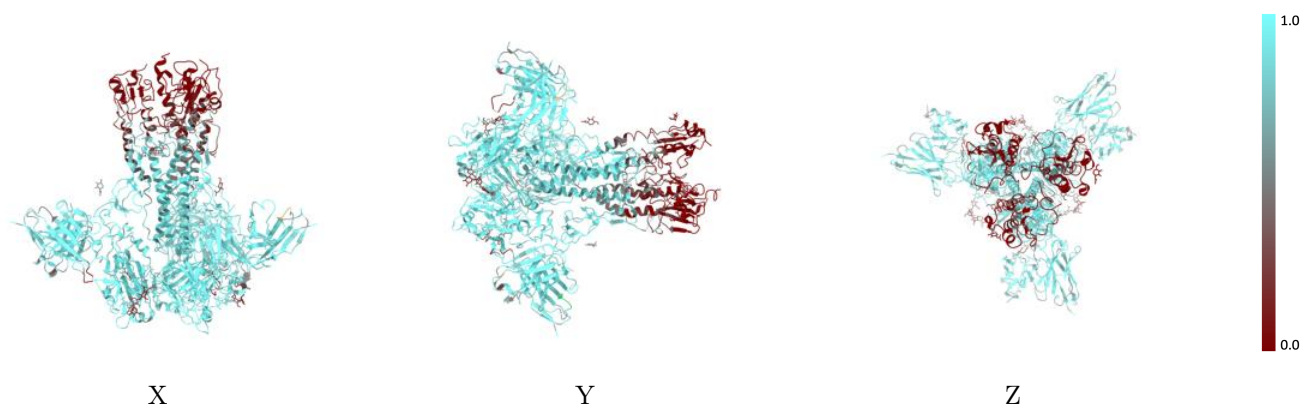
The images above show the 3D surface view of the map at the recommended contour level 0.172 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



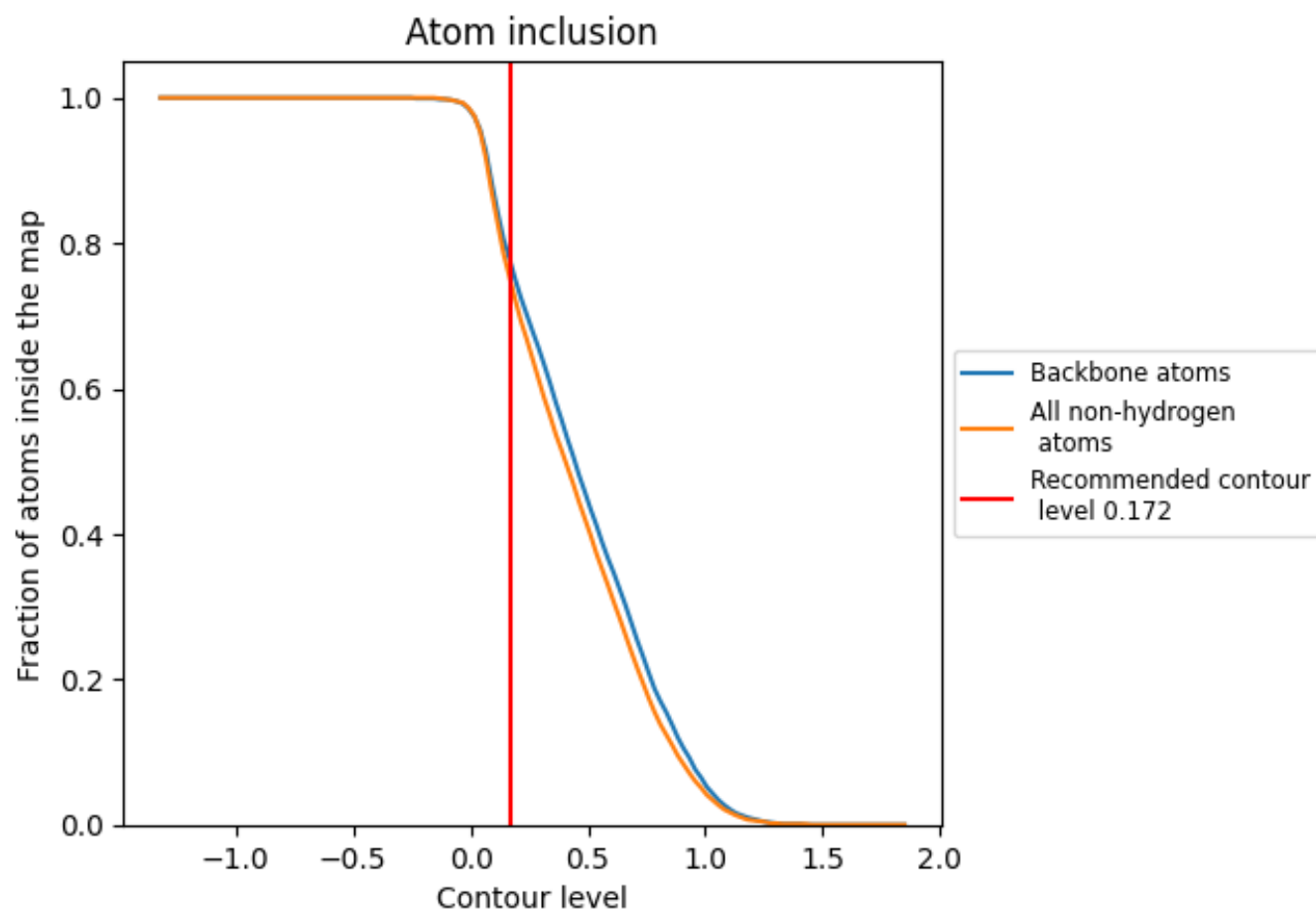
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.172).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 75% 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 (0.172) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7460	 0.5190
A	 0.7100	 0.5040
B	 0.7210	 0.5030
C	 0.7080	 0.4880
D	 0.8790	 0.5870
E	 0.4210	 0.4200
F	 0.4530	 0.4030
G	 0.7870	 0.5540
H	 0.8790	 0.5870
I	 0.8790	 0.5890
J	 0.4320	 0.4250
K	 0.7950	 0.5500
L	 0.7970	 0.5520

