



Full wwPDB EM Validation Report ⓘ

Aug 13, 2026 – 04:22 PM EDT

PDB ID : 9ZTJ / pdb_00009ztj
EMDB ID : EMD-74755
Title : CryoEM structure of H5N1 A/Texas/37/2024 HA bound to Fab H91
Authors : Morano, N.C.; Ho, D.D.; Shapiro, L.; Kwong, P.D.
Deposited on : 2025-12-23
Resolution : 3.08 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.dev133
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) : 2.50

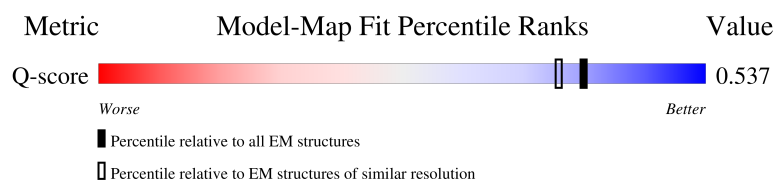
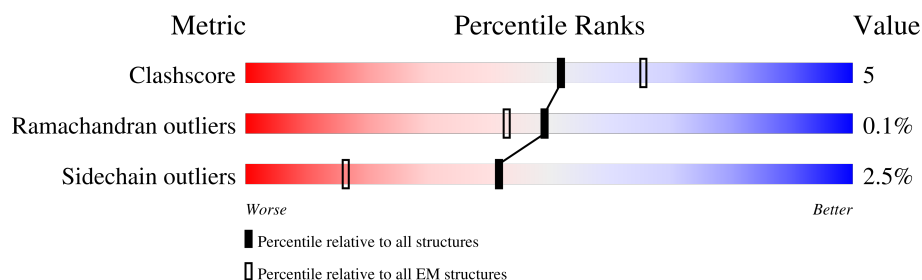
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.08 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.



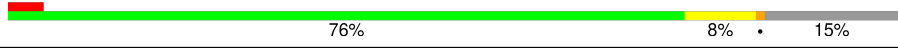
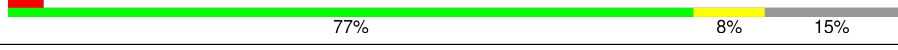
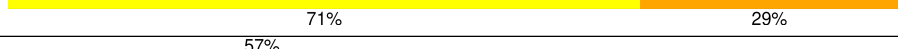
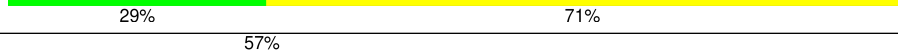
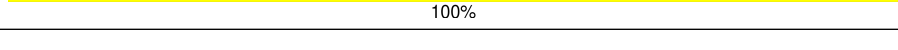
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14000 (2.58 - 3.58)

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	253	 39% 7% 53%
1	G	253	 40% 6% 53%
1	H	253	 40% 6% 53%
2	I	234	 40% 5% 55%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	234	
2	L	234	
3	A	576	
3	B	576	
3	C	576	
4	E	7	
4	F	7	
4	J	7	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	604	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 17466 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 H91 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	119	Total	C	N	O	S	0	0
			923	587	161	172	3		
1	D	119	Total	C	N	O	S	0	0
			923	587	161	172	3		
1	G	119	Total	C	N	O	S	0	0
			923	587	161	172	3		

- Molecule 2 is a protein called H91 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	106	Total	C	N	O	S	0	0
			824	514	143	164	3		
2	I	106	Total	C	N	O	S	0	0
			824	514	143	164	3		
2	K	106	Total	C	N	O	S	0	0
			824	514	143	164	3		

- Molecule 3 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	490	Total	C	N	O	S	0	0
			3918	2466	681	748	23		
3	B	491	Total	C	N	O	S	0	0
			3927	2471	683	750	23		
3	C	491	Total	C	N	O	S	0	0
			3927	2471	683	750	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	349	ARG	LYS	conflict	UNP A0AAX6NNG0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	352	ARG	LYS	conflict	UNP A0AAX6NNG0
A	525	GLY	-	expression tag	UNP A0AAX6NNG0
A	526	SER	-	expression tag	UNP A0AAX6NNG0
A	527	SER	-	expression tag	UNP A0AAX6NNG0
A	528	GLY	-	expression tag	UNP A0AAX6NNG0
A	529	SER	-	expression tag	UNP A0AAX6NNG0
A	530	SER	-	expression tag	UNP A0AAX6NNG0
A	531	GLY	-	expression tag	UNP A0AAX6NNG0
A	532	TYR	-	expression tag	UNP A0AAX6NNG0
A	533	ILE	-	expression tag	UNP A0AAX6NNG0
A	534	PRO	-	expression tag	UNP A0AAX6NNG0
A	535	GLU	-	expression tag	UNP A0AAX6NNG0
A	536	ALA	-	expression tag	UNP A0AAX6NNG0
A	537	PRO	-	expression tag	UNP A0AAX6NNG0
A	538	ARG	-	expression tag	UNP A0AAX6NNG0
A	539	ASP	-	expression tag	UNP A0AAX6NNG0
A	540	GLY	-	expression tag	UNP A0AAX6NNG0
A	541	GLN	-	expression tag	UNP A0AAX6NNG0
A	542	ALA	-	expression tag	UNP A0AAX6NNG0
A	543	TYR	-	expression tag	UNP A0AAX6NNG0
A	544	VAL	-	expression tag	UNP A0AAX6NNG0
A	545	ARG	-	expression tag	UNP A0AAX6NNG0
A	546	LYS	-	expression tag	UNP A0AAX6NNG0
A	547	ASP	-	expression tag	UNP A0AAX6NNG0
A	548	GLY	-	expression tag	UNP A0AAX6NNG0
A	549	GLU	-	expression tag	UNP A0AAX6NNG0
A	550	TRP	-	expression tag	UNP A0AAX6NNG0
A	551	VAL	-	expression tag	UNP A0AAX6NNG0
A	552	LEU	-	expression tag	UNP A0AAX6NNG0
A	553	LEU	-	expression tag	UNP A0AAX6NNG0
A	554	SER	-	expression tag	UNP A0AAX6NNG0
A	555	THR	-	expression tag	UNP A0AAX6NNG0
A	556	PHE	-	expression tag	UNP A0AAX6NNG0
A	557	LEU	-	expression tag	UNP A0AAX6NNG0
A	558	GLY	-	expression tag	UNP A0AAX6NNG0
A	559	HIS	-	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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	566	HIS	-	expression tag	UNP A0AAX6NNG0
A	567	HIS	-	expression tag	UNP A0AAX6NNG0
A	568	GLY	-	expression tag	UNP A0AAX6NNG0
A	569	GLY	-	expression tag	UNP A0AAX6NNG0
A	570	SER	-	expression tag	UNP A0AAX6NNG0
A	571	GLY	-	expression tag	UNP A0AAX6NNG0
A	572	LEU	-	expression tag	UNP A0AAX6NNG0
A	573	ASN	-	expression tag	UNP A0AAX6NNG0
A	574	ASP	-	expression tag	UNP A0AAX6NNG0
A	575	ILE	-	expression tag	UNP A0AAX6NNG0
A	576	PHE	-	expression tag	UNP A0AAX6NNG0
A	577	GLU	-	expression tag	UNP A0AAX6NNG0
A	578	ALA	-	expression tag	UNP A0AAX6NNG0
A	579	GLN	-	expression tag	UNP A0AAX6NNG0
A	580	LYS	-	expression tag	UNP A0AAX6NNG0
A	581	ILE	-	expression tag	UNP A0AAX6NNG0
A	582	GLU	-	expression tag	UNP A0AAX6NNG0
A	583	TRP	-	expression tag	UNP A0AAX6NNG0
A	584	HIS	-	expression tag	UNP A0AAX6NNG0
A	585	GLU	-	expression tag	UNP A0AAX6NNG0
B	199	ILE	THR	conflict	UNP A0AAX6NNG0
B	?	-	GLU	deletion	UNP A0AAX6NNG0
B	338	ARG	LYS	conflict	UNP A0AAX6NNG0
B	341	ARG	LYS	conflict	UNP A0AAX6NNG0
B	514	GLY	-	expression tag	UNP A0AAX6NNG0
B	515	SER	-	expression tag	UNP A0AAX6NNG0
B	516	SER	-	expression tag	UNP A0AAX6NNG0
B	517	GLY	-	expression tag	UNP A0AAX6NNG0
B	518	SER	-	expression tag	UNP A0AAX6NNG0
B	519	SER	-	expression tag	UNP A0AAX6NNG0
B	520	GLY	-	expression tag	UNP A0AAX6NNG0
B	521	TYR	-	expression tag	UNP A0AAX6NNG0
B	522	ILE	-	expression tag	UNP A0AAX6NNG0
B	523	PRO	-	expression tag	UNP A0AAX6NNG0
B	524	GLU	-	expression tag	UNP A0AAX6NNG0
B	525	ALA	-	expression tag	UNP A0AAX6NNG0
B	526	PRO	-	expression tag	UNP A0AAX6NNG0
B	527	ARG	-	expression tag	UNP A0AAX6NNG0
B	528	ASP	-	expression tag	UNP A0AAX6NNG0
B	529	GLY	-	expression tag	UNP A0AAX6NNG0
B	530	GLN	-	expression tag	UNP A0AAX6NNG0
B	531	ALA	-	expression tag	UNP A0AAX6NNG0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	532	TYR	-	expression tag	UNP A0AAX6NNG0
B	533	VAL	-	expression tag	UNP A0AAX6NNG0
B	534	ARG	-	expression tag	UNP A0AAX6NNG0
B	535	LYS	-	expression tag	UNP A0AAX6NNG0
B	536	ASP	-	expression tag	UNP A0AAX6NNG0
B	537	GLY	-	expression tag	UNP A0AAX6NNG0
B	538	GLU	-	expression tag	UNP A0AAX6NNG0
B	539	TRP	-	expression tag	UNP A0AAX6NNG0
B	540	VAL	-	expression tag	UNP A0AAX6NNG0
B	541	LEU	-	expression tag	UNP A0AAX6NNG0
B	542	LEU	-	expression tag	UNP A0AAX6NNG0
B	543	SER	-	expression tag	UNP A0AAX6NNG0
B	544	THR	-	expression tag	UNP A0AAX6NNG0
B	545	PHE	-	expression tag	UNP A0AAX6NNG0
B	546	LEU	-	expression tag	UNP A0AAX6NNG0
B	547	GLY	-	expression tag	UNP A0AAX6NNG0
B	548	HIS	-	expression tag	UNP A0AAX6NNG0
B	549	HIS	-	expression tag	UNP A0AAX6NNG0
B	550	HIS	-	expression tag	UNP A0AAX6NNG0
B	551	HIS	-	expression tag	UNP A0AAX6NNG0
B	552	HIS	-	expression tag	UNP A0AAX6NNG0
B	553	HIS	-	expression tag	UNP A0AAX6NNG0
B	554	HIS	-	expression tag	UNP A0AAX6NNG0
B	555	HIS	-	expression tag	UNP A0AAX6NNG0
B	556	HIS	-	expression tag	UNP A0AAX6NNG0
B	557	GLY	-	expression tag	UNP A0AAX6NNG0
B	558	GLY	-	expression tag	UNP A0AAX6NNG0
B	559	SER	-	expression tag	UNP A0AAX6NNG0
B	560	GLY	-	expression tag	UNP A0AAX6NNG0
B	561	LEU	-	expression tag	UNP A0AAX6NNG0
B	562	ASN	-	expression tag	UNP A0AAX6NNG0
B	563	ASP	-	expression tag	UNP A0AAX6NNG0
B	564	ILE	-	expression tag	UNP A0AAX6NNG0
B	565	PHE	-	expression tag	UNP A0AAX6NNG0
B	566	GLU	-	expression tag	UNP A0AAX6NNG0
B	567	ALA	-	expression tag	UNP A0AAX6NNG0
B	568	GLN	-	expression tag	UNP A0AAX6NNG0
B	569	LYS	-	expression tag	UNP A0AAX6NNG0
B	570	ILE	-	expression tag	UNP A0AAX6NNG0
B	571	GLU	-	expression tag	UNP A0AAX6NNG0
B	572	TRP	-	expression tag	UNP A0AAX6NNG0
B	573	HIS	-	expression tag	UNP A0AAX6NNG0

Continued on next page...

Continued from previous page...

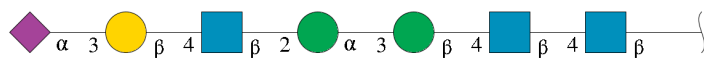
Chain	Residue	Modelled	Actual	Comment	Reference
B	574	GLU	-	expression tag	UNP A0AAX6NNG0
C	209	ILE	THR	conflict	UNP A0AAX6NNG0
C	?	-	GLU	deletion	UNP A0AAX6NNG0
C	350	ARG	LYS	conflict	UNP A0AAX6NNG0
C	353	ARG	LYS	conflict	UNP A0AAX6NNG0
C	526	GLY	-	expression tag	UNP A0AAX6NNG0
C	527	SER	-	expression 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

Continued on next page...

Continued from previous page...

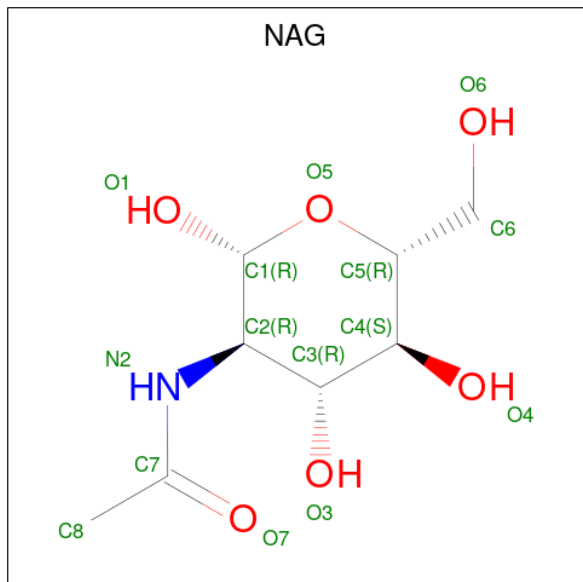
Chain	Residue	Modelled	Actual	Comment	Reference
C	563	HIS	-	expression tag	UNP A0AAX6NNG0
C	564	HIS	-	expression tag	UNP A0AAX6NNG0
C	565	HIS	-	expression tag	UNP A0AAX6NNG0
C	566	HIS	-	expression tag	UNP A0AAX6NNG0
C	567	HIS	-	expression tag	UNP A0AAX6NNG0
C	568	HIS	-	expression tag	UNP A0AAX6NNG0
C	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.

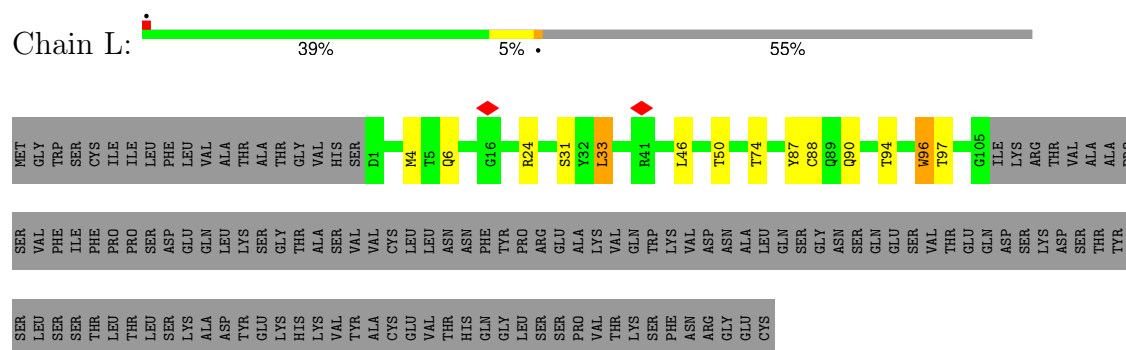


Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	7	Total	C	N	O	0	0
			95	53	4	38		
4	F	7	Total	C	N	O	0	0
			95	53	4	38		
4	J	7	Total	C	N	O	0	0
			95	53	4	38		

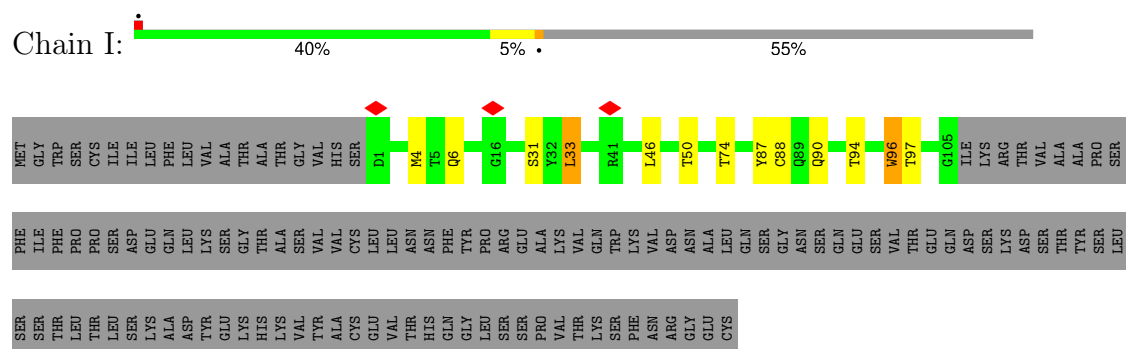
- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



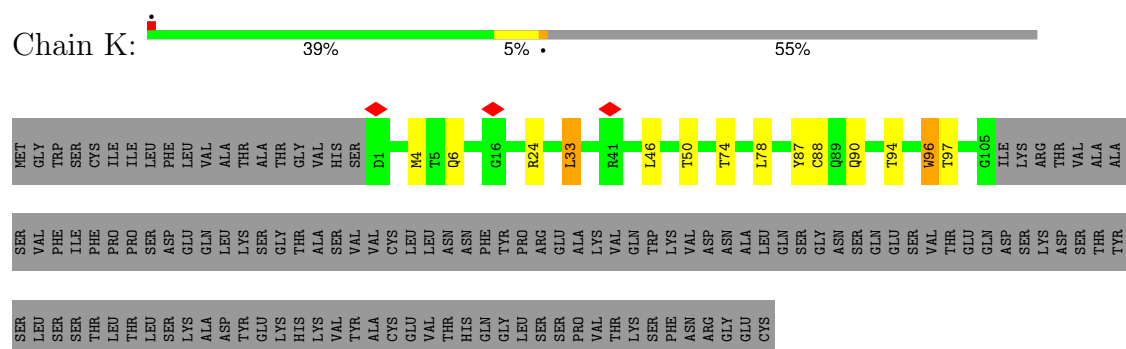
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5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



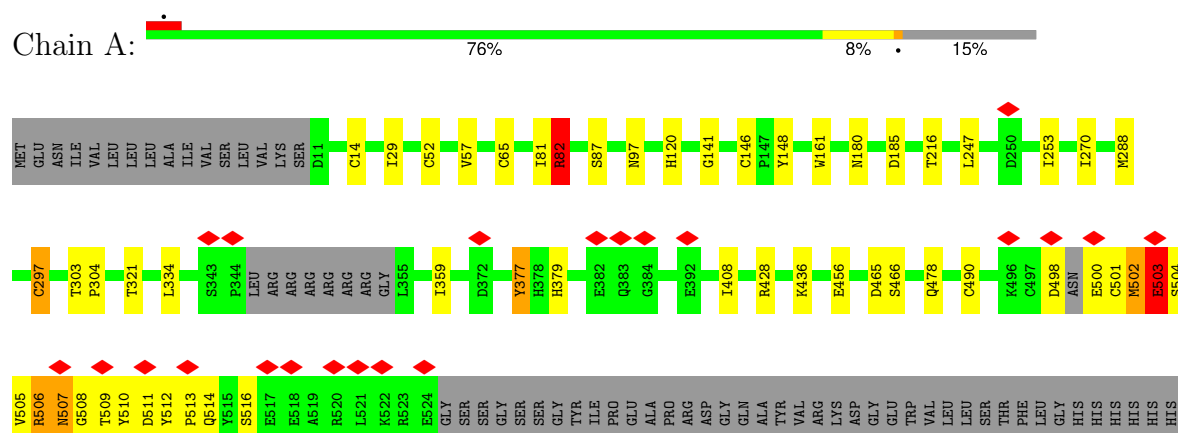
- Molecule 2: H91 Fab Light Chain



- Molecule 2: H91 Fab Light Chain



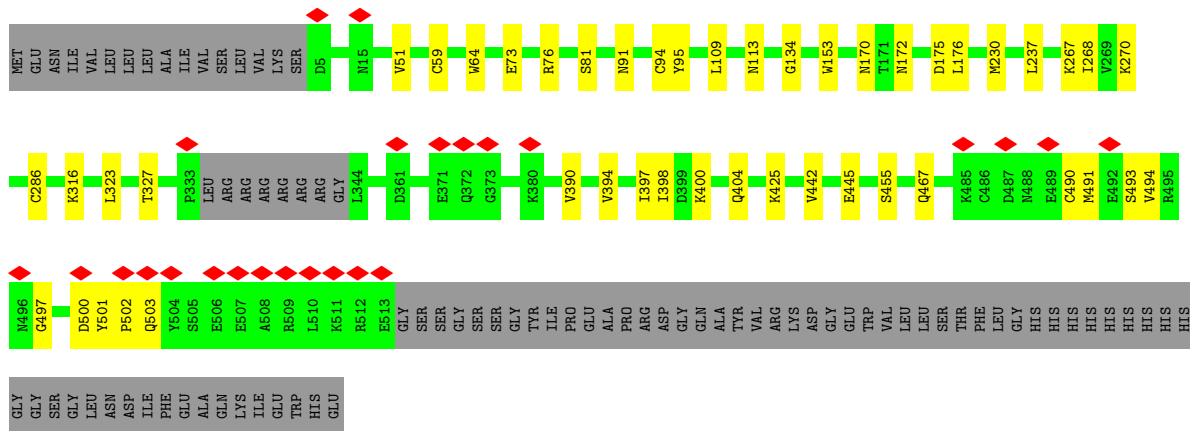
- Molecule 3: Hemagglutinin



HIS
HIS
HIS
GLY
GLY
SER
SER
LEU
LEU
ASN
ASP
ILE
PHE
GLU
ALA
GLN
LYS
ILE
GLU
TRP
HIS
GLU

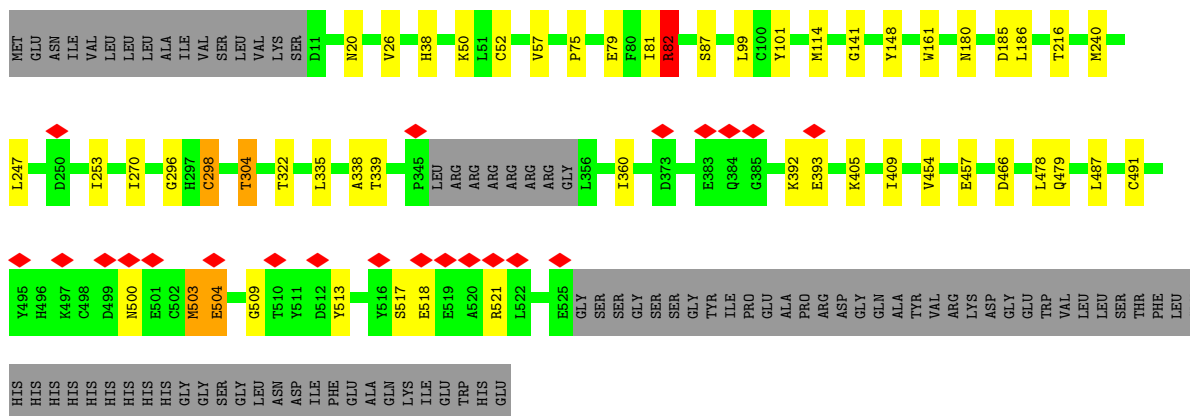
• Molecule 3: Hemagglutinin

Chain B:



• Molecule 3: Hemagglutinin

Chain C:

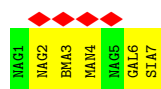


• Molecule 4: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



• 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	105159	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	1.351	Depositor
Minimum map value	-0.923	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.134	Depositor
Map size ($\text{\AA}$)	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 ($\text{\AA}$)	0.825, 0.825, 0.825	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.25	0/948	0.63	0/1292
1	G	0.25	0/948	0.63	0/1292
1	H	0.25	0/948	0.63	0/1292
2	I	0.26	0/843	0.64	2/1144 (0.2%)
2	K	0.26	0/843	0.64	2/1144 (0.2%)
2	L	0.26	0/843	0.64	2/1144 (0.2%)
3	A	0.31	2/4008 (0.0%)	0.60	12/5425 (0.2%)
3	B	0.24	0/4018	0.49	1/5441 (0.0%)
3	C	0.26	1/4018 (0.0%)	0.53	6/5441 (0.1%)
All	All	0.27	3/17417 (0.0%)	0.57	25/23615 (0.1%)

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
3	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	GLU	C-O	-11.64	1.10	1.24
3	C	82	ARG	C-N	-5.50	1.29	1.33
3	A	82	ARG	C-N	-5.02	1.29	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	GLU	CB-CA-C	10.25	126.97	110.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	MET	CA-C-N	-9.04	108.68	120.44
3	A	502	MET	C-N-CA	-9.04	108.68	120.44
3	A	82	ARG	CB-CA-C	8.63	126.44	109.35
3	C	82	ARG	CB-CA-C	8.54	126.27	109.35
3	A	503	GLU	CA-C-O	-7.92	112.50	120.82
3	C	81	ILE	CA-C-N	-7.89	109.95	122.73
3	C	81	ILE	C-N-CA	-7.89	109.95	122.73
3	A	81	ILE	CA-C-N	-7.58	110.45	122.73
3	A	81	ILE	C-N-CA	-7.58	110.45	122.73
3	A	503	GLU	N-CA-C	-6.76	103.83	111.07
3	B	491	MET	N-CA-C	-6.43	104.27	111.28
2	I	50	THR	CA-C-N	6.30	133.57	121.54
2	I	50	THR	C-N-CA	6.30	133.57	121.54
2	L	50	THR	CA-C-N	6.29	133.56	121.54
2	L	50	THR	C-N-CA	6.29	133.56	121.54
2	K	50	THR	CA-C-N	6.26	133.49	121.54
2	K	50	THR	C-N-CA	6.26	133.49	121.54
3	C	503	MET	N-CA-C	-5.88	104.05	111.11
3	A	506	ARG	N-CA-C	-5.85	105.64	112.89
3	C	82	ARG	CA-C-N	5.40	128.03	123.33
3	C	82	ARG	C-N-CA	5.40	128.03	123.33
3	A	507	ASN	CA-CB-CG	5.30	117.90	112.60
3	A	82	ARG	CA-C-N	5.07	127.74	123.33
3	A	82	ARG	C-N-CA	5.07	127.74	123.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	503	GLU	Mainchain

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	D	923	0	892	14	0
1	G	923	0	892	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	923	0	892	11	0
2	I	824	0	784	8	0
2	K	824	0	784	8	0
2	L	824	0	784	8	0
3	A	3918	0	3769	85	0
3	B	3927	0	3780	22	0
3	C	3927	0	3780	28	0
4	E	95	0	80	1	0
4	F	95	0	80	0	0
4	J	95	0	80	0	0
5	A	56	0	52	50	0
5	B	56	0	52	0	0
5	C	56	0	52	0	0
All	All	17466	0	16753	186	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 5.

All (186) 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:A:504:SER:H	5:A:604:NAG:C6	1.40	1.34
5:A:604:NAG:C6	5:A:604:NAG:O6	1.75	1.33
3:A:503:GLU:N	5:A:604:NAG:C6	1.95	1.29
3:A:501:CYS:C	5:A:604:NAG:H61	1.58	1.27
3:A:501:CYS:C	5:A:604:NAG:C6	2.09	1.25
1:H:2:VAL:O	1:H:23:PRO:O	1.59	1.21
3:A:500:GLU:O	5:A:604:NAG:C6	1.88	1.21
3:A:504:SER:N	5:A:604:NAG:C6	2.02	1.20
3:A:500:GLU:O	5:A:604:NAG:H5	1.40	1.19
3:A:502:MET:C	5:A:604:NAG:H62	1.67	1.18
1:D:2:VAL:O	1:D:23:PRO:O	1.59	1.17
1:G:2:VAL:O	1:G:23:PRO:O	1.59	1.16
3:A:503:GLU:N	5:A:604:NAG:H62	1.62	1.09
3:A:501:CYS:CA	5:A:604:NAG:H61	1.92	1.00
3:A:503:GLU:HB3	5:A:604:NAG:C5	1.94	0.97
3:A:503:GLU:HB3	5:A:604:NAG:H4	1.49	0.95
3:A:503:GLU:N	5:A:604:NAG:O6	1.99	0.93
3:A:504:SER:N	5:A:604:NAG:H62	1.87	0.88
3:A:502:MET:N	5:A:604:NAG:C6	2.37	0.87
3:A:503:GLU:C	5:A:604:NAG:H62	1.99	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:500:GLU:O	5:A:604:NAG:H61	1.77	0.85
3:A:503:GLU:C	5:A:604:NAG:C6	2.50	0.84
3:A:503:GLU:HB3	5:A:604:NAG:C4	2.08	0.84
3:A:500:GLU:O	5:A:604:NAG:C5	2.24	0.83
3:A:500:GLU:C	5:A:604:NAG:C6	2.52	0.82
3:A:504:SER:N	5:A:604:NAG:C5	2.43	0.81
3:A:502:MET:C	5:A:604:NAG:C6	2.42	0.79
3:A:500:GLU:C	5:A:604:NAG:O6	2.26	0.78
3:A:503:GLU:H	5:A:604:NAG:C6	1.94	0.77
5:A:604:NAG:C6	5:A:604:NAG:C5	2.63	0.75
3:A:503:GLU:CA	5:A:604:NAG:C6	2.66	0.73
3:A:500:GLU:HA	5:A:604:NAG:O4	1.87	0.73
3:B:500:ASP:HB3	3:B:503:GLN:HB3	1.69	0.73
3:A:503:GLU:H	5:A:604:NAG:HO6	1.37	0.72
3:A:502:MET:N	5:A:604:NAG:O6	2.23	0.71
3:A:503:GLU:CB	5:A:604:NAG:C5	2.70	0.69
3:A:504:SER:H	5:A:604:NAG:C5	2.06	0.69
3:A:505:VAL:CG1	3:A:510:TYR:HB2	2.23	0.67
3:A:505:VAL:HG12	3:A:510:TYR:HB2	1.75	0.67
3:A:501:CYS:O	5:A:604:NAG:C6	2.42	0.67
3:A:501:CYS:O	5:A:604:NAG:H61	1.93	0.66
3:A:503:GLU:CA	5:A:604:NAG:H62	2.28	0.63
3:A:501:CYS:HA	5:A:604:NAG:H61	1.81	0.60
3:A:503:GLU:O	3:A:506:ARG:N	2.33	0.60
3:A:65:CYS:HA	3:A:97:ASN:HB2	1.86	0.57
3:C:479:GLN:HE22	3:C:509:GLY:HA2	1.68	0.57
3:A:503:GLU:HB3	5:A:604:NAG:O5	2.04	0.57
1:H:3:GLN:C	1:H:5:GLN:H	2.13	0.56
1:G:3:GLN:C	1:G:5:GLN:H	2.13	0.56
1:H:33:GLY:HA2	1:H:97:ILE:HD12	1.88	0.56
1:D:33:GLY:HA2	1:D:97:ILE:HD12	1.88	0.56
1:G:33:GLY:HA2	1:G:97:ILE:HD12	1.88	0.56
3:A:501:CYS:C	5:A:604:NAG:H62	2.20	0.56
1:D:3:GLN:C	1:D:5:GLN:H	2.13	0.56
2:K:94:THR:HA	2:K:96:TRP:HZ3	1.72	0.55
2:I:90:GLN:HE21	2:I:97:THR:HG22	1.72	0.55
2:I:94:THR:HA	2:I:96:TRP:HZ3	1.72	0.55
1:H:97:ILE:HG23	3:C:82:ARG:HB3	1.87	0.54
3:C:216:THR:HG22	3:C:253:ILE:HA	1.88	0.54
3:C:487:LEU:HD12	3:C:491:CYS:HB2	1.90	0.54
2:L:90:GLN:HE21	2:L:97:THR:HG22	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:59:CYS:HA	3:B:91:ASN:HB2	1.90	0.54
2:L:94:THR:HA	2:L:96:TRP:HZ3	1.72	0.53
2:K:33:LEU:HD21	2:K:88:CYS:HB3	1.90	0.53
2:K:90:GLN:HE21	2:K:97:THR:HG22	1.72	0.53
3:C:409:ILE:HD11	3:C:457:GLU:HG3	1.90	0.53
2:L:33:LEU:HD21	2:L:88:CYS:HB3	1.90	0.52
3:A:503:GLU:C	5:A:604:NAG:C5	2.82	0.52
3:A:503:GLU:CB	5:A:604:NAG:H4	2.31	0.52
2:I:33:LEU:HD21	2:I:88:CYS:HB3	1.90	0.52
3:A:303:THR:HG22	3:A:321:THR:HG22	1.92	0.52
3:A:379:HIS:HB3	3:A:506:ARG:HH12	1.75	0.52
3:C:101:TYR:CD1	3:C:240:MET:HG3	2.45	0.52
1:H:40:PRO:HB2	1:H:43:LYS:HB2	1.93	0.51
3:A:216:THR:HG22	3:A:253:ILE:HA	1.91	0.51
1:G:40:PRO:HB2	1:G:43:LYS:HB2	1.93	0.51
1:D:40:PRO:HB2	1:D:43:LYS:HB2	1.92	0.49
3:A:141:GLY:HA3	3:A:161:TRP:HB3	1.93	0.49
1:H:39:GLN:HB2	1:H:45:LEU:HD23	1.95	0.49
3:A:498:ASP:O	3:A:502:MET:HG2	2.12	0.49
3:A:503:GLU:CA	5:A:604:NAG:C5	2.90	0.49
3:B:134:GLY:HA3	3:B:153:TRP:HB3	1.93	0.49
3:A:502:MET:CA	5:A:604:NAG:C6	2.90	0.49
5:A:604:NAG:C6	5:A:604:NAG:H5	2.42	0.49
3:A:502:MET:O	3:A:506:ARG:HG3	2.12	0.49
3:B:172:ASN:HB3	3:B:267:LYS:HE3	1.95	0.49
1:D:39:GLN:HB2	1:D:45:LEU:HD23	1.95	0.48
2:I:6:GLN:HE22	2:I:87:TYR:HA	1.78	0.48
2:K:6:GLN:HE22	2:K:87:TYR:HA	1.78	0.48
3:C:141:GLY:HA3	3:C:161:TRP:HB3	1.95	0.48
3:A:504:SER:N	5:A:604:NAG:O5	2.47	0.48
3:B:175:ASP:HB2	3:B:268:ILE:HD12	1.95	0.48
3:B:113:ASN:HB2	3:B:270:LYS:HG2	1.95	0.48
3:C:500:ASN:O	3:C:504:GLU:HB3	2.14	0.48
2:L:6:GLN:HE22	2:L:87:TYR:HA	1.78	0.48
1:G:39:GLN:HB2	1:G:45:LEU:HD23	1.95	0.47
3:B:95:TYR:CD1	3:B:230:MET:HG3	2.49	0.47
3:A:501:CYS:O	5:A:604:NAG:H62	2.13	0.47
3:A:503:GLU:C	5:A:604:NAG:O5	2.58	0.47
3:C:304:THR:HG22	3:C:322:THR:HG22	1.96	0.47
1:H:3:GLN:O	1:H:5:GLN:N	2.47	0.47
3:A:359:ILE:HD12	3:A:465:ASP:HA	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:504:SER:HA	3:A:507:ASN:OD1	2.14	0.46
1:D:3:GLN:O	1:D:5:GLN:N	2.47	0.46
1:D:97:ILE:HG23	3:A:82:ARG:HB3	1.98	0.46
3:B:316:LYS:HD2	3:B:404:GLN:HB2	1.97	0.46
1:H:97:ILE:O	3:C:82:ARG:HB2	2.16	0.46
3:A:502:MET:CA	5:A:604:NAG:H62	2.44	0.46
3:C:513:TYR:O	3:C:517:SER:N	2.50	0.45
3:A:185:ASP:HB2	3:A:270:ILE:HD12	1.97	0.45
3:A:500:GLU:C	5:A:604:NAG:H61	2.33	0.45
3:A:478:GLN:HE22	3:A:508:GLY:HA2	1.81	0.45
3:B:170:ASN:HB2	3:B:237:LEU:HD23	1.98	0.45
3:C:75:PRO:HB2	3:C:148:TYR:HB2	1.99	0.45
3:B:394:VAL:O	3:B:398:ILE:HD12	2.16	0.45
3:B:425:LYS:HD3	3:B:425:LYS:HA	1.66	0.45
3:C:57:VAL:HB	3:C:87:SER:HB3	1.99	0.45
3:C:518:GLU:HA	3:C:521:ARG:HH12	1.82	0.44
3:A:57:VAL:HB	3:A:87:SER:HB3	2.00	0.44
3:B:397:ILE:HD11	3:B:445:GLU:HG3	1.99	0.44
1:G:3:GLN:O	1:G:5:GLN:N	2.47	0.44
3:A:511:ASP:HB3	3:A:514:GLN:HB2	2.00	0.44
3:A:512:TYR:O	3:A:516:SER:N	2.51	0.44
3:B:501:TYR:N	3:B:502:PRO:HD2	2.33	0.44
3:B:51:VAL:HB	3:B:81:SER:HB3	1.99	0.43
3:C:335:LEU:HG	3:C:454:VAL:HG21	2.00	0.43
3:B:490:CYS:HA	3:B:493:SER:HB3	1.99	0.43
3:A:428:ARG:HA	3:A:428:ARG:HD2	1.81	0.43
3:C:180:ASN:HB2	3:C:247:LEU:HD23	1.99	0.43
3:A:377:TYR:CD1	3:A:506:ARG:HG2	2.54	0.43
3:A:504:SER:O	3:A:509:THR:N	2.48	0.43
3:C:405:LYS:HD3	3:C:457:GLU:HB3	2.00	0.43
2:I:31:SER:CB	3:A:148:TYR:OH	2.67	0.43
1:D:97:ILE:HG12	3:A:82:ARG:HB3	2.01	0.43
3:B:400:LYS:HD3	3:B:400:LYS:HA	1.82	0.43
3:A:379:HIS:HB3	3:A:506:ARG:NH1	2.33	0.42
3:A:288:MET:HG3	3:A:304:PRO:HG3	2.02	0.42
2:L:4:MET:HE3	2:L:4:MET:HB3	1.88	0.42
2:I:4:MET:HE3	2:I:4:MET:HB3	1.88	0.42
3:C:26:VAL:HG11	3:C:338:ALA:HB2	2.02	0.42
3:C:52:CYS:HB3	3:C:298:CYS:HB2	1.76	0.42
3:C:114:MET:HE2	3:C:114:MET:HB3	1.84	0.42
2:I:31:SER:OG	3:A:148:TYR:OH	2.30	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:502:MET:O	3:A:503:GLU:O	2.38	0.42
3:B:323:LEU:HG	3:B:442:VAL:HG21	2.00	0.42
3:C:99:LEU:HD23	3:C:99:LEU:HA	1.87	0.42
2:L:94:THR:HA	2:L:96:TRP:CZ3	2.53	0.42
1:D:53:TYR:HE1	3:A:120:HIS:CE1	2.38	0.42
1:D:97:ILE:O	3:A:82:ARG:HB2	2.18	0.42
3:C:360:ILE:HD12	3:C:466:ASP:HA	2.02	0.42
3:A:436:LYS:HD3	3:A:436:LYS:HA	1.71	0.42
3:B:64:TRP:HZ3	3:B:109:LEU:HD21	1.85	0.42
3:C:185:ASP:HB2	3:C:270:ILE:HD12	2.00	0.42
2:K:4:MET:HE3	2:K:4:MET:HB3	1.88	0.41
4:E:6:GAL:H3	4:E:7:SIA:H32	1.96	0.41
1:D:28:SER:HB3	1:D:35(A):TRP:CZ2	2.55	0.41
3:A:502:MET:O	3:A:503:GLU:C	2.61	0.41
3:A:52:CYS:HB3	3:A:297:CYS:HB2	1.73	0.41
3:B:73:GLU:H	3:B:73:GLU:HG2	1.68	0.41
3:B:327:THR:HG23	3:B:390:VAL:HG11	2.01	0.41
3:C:38:HIS:HB3	3:C:339:THR:HG23	2.02	0.41
1:H:97:ILE:HG12	3:C:82:ARG:HB3	2.01	0.41
2:I:94:THR:HA	2:I:96:TRP:CZ3	2.53	0.41
3:A:14:CYS:HA	3:A:490:CYS:HA	2.03	0.41
3:A:513:PRO:O	3:A:514:GLN:C	2.64	0.41
2:K:24:ARG:HB2	2:K:24:ARG:NH1	2.36	0.41
3:B:76:ARG:HE	3:B:76:ARG:HB2	1.75	0.41
1:D:87:THR:HB	1:D:111:VAL:HG22	2.04	0.40
1:G:28:SER:HB3	1:G:35(A):TRP:CZ2	2.55	0.40
2:K:94:THR:HA	2:K:96:TRP:CZ3	2.53	0.40
2:L:24:ARG:HB2	2:L:24:ARG:NH1	2.36	0.40
1:D:3:GLN:C	1:D:5:GLN:N	2.77	0.40
1:G:87:THR:HB	1:G:111:VAL:HG22	2.03	0.40
2:K:78:LEU:HD12	2:K:78:LEU:HA	1.86	0.40
1:H:28:SER:HB3	1:H:35(A):TRP:CZ2	2.55	0.40
1:H:34:TYR:CD2	1:H:94:ARG:HD3	2.56	0.40
1:D:34:TYR:CD2	1:D:94:ARG:HD3	2.57	0.40
3:A:29:ILE:HD13	3:A:29:ILE:HA	2.00	0.40
3:A:180:ASN:HB2	3:A:247:LEU:HD23	2.02	0.40
3:A:334:LEU:HD12	3:A:334:LEU:HA	1.90	0.40
3:A:501:CYS:CA	5:A:604:NAG:C6	2.72	0.40
3:B:467:GLN:OE1	3:B:497:GLY:HA2	2.21	0.40
3:C:50:LYS:HD2	3:C:296:GLY:HA3	2.03	0.40
2:L:31:SER:CB	3:C:148:TYR:OH	2.70	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:408:ILE:HD11	3:A:456:GLU:HG3	2.04	0.40
3:C:392:LYS:O	3:C:393:GLU:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	117/253 (46%)	112 (96%)	4 (3%)	1 (1%)	14	41
1	G	117/253 (46%)	112 (96%)	4 (3%)	1 (1%)	14	41
1	H	117/253 (46%)	112 (96%)	4 (3%)	1 (1%)	14	41
2	I	104/234 (44%)	101 (97%)	3 (3%)	0	100	100
2	K	104/234 (44%)	101 (97%)	3 (3%)	0	100	100
2	L	104/234 (44%)	101 (97%)	3 (3%)	0	100	100
3	A	484/576 (84%)	462 (96%)	22 (4%)	0	100	100
3	B	487/576 (84%)	466 (96%)	21 (4%)	0	100	100
3	C	487/576 (84%)	469 (96%)	18 (4%)	0	100	100
All	All	2121/3189 (66%)	2036 (96%)	82 (4%)	3 (0%)	49	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	4	LEU
1	D	4	LEU
1	G	4	LEU

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	99/216 (46%)	94 (95%)	5 (5%)	21	50
1	G	99/216 (46%)	94 (95%)	5 (5%)	21	50
1	H	99/216 (46%)	94 (95%)	5 (5%)	21	50
2	I	92/206 (45%)	88 (96%)	4 (4%)	26	55
2	K	92/206 (45%)	88 (96%)	4 (4%)	26	55
2	L	92/206 (45%)	88 (96%)	4 (4%)	26	55
3	A	430/502 (86%)	424 (99%)	6 (1%)	59	73
3	B	431/502 (86%)	426 (99%)	5 (1%)	63	75
3	C	431/502 (86%)	422 (98%)	9 (2%)	47	68
All	All	1865/2772 (67%)	1818 (98%)	47 (2%)	42	66

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	2	VAL
1	H	67	VAL
1	H	72	ASP
1	H	87	THR
1	H	97	ILE
2	L	33	LEU
2	L	46	LEU
2	L	74	THR
2	L	96	TRP
1	D	2	VAL
1	D	67	VAL
1	D	72	ASP
1	D	87	THR
1	D	97	ILE
2	I	33	LEU
2	I	46	LEU
2	I	74	THR
2	I	96	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	2	VAL
1	G	67	VAL
1	G	72	ASP
1	G	87	THR
1	G	97	ILE
2	K	33	LEU
2	K	46	LEU
2	K	74	THR
2	K	96	TRP
3	A	82	ARG
3	A	146	CYS
3	A	297	CYS
3	A	377	TYR
3	A	466	SER
3	A	503	GLU
3	B	94	CYS
3	B	176	LEU
3	B	286	CYS
3	B	455	SER
3	B	494	VAL
3	C	20	ASN
3	C	79	GLU
3	C	82	ARG
3	C	186	LEU
3	C	298	CYS
3	C	304	THR
3	C	478	LEU
3	C	503	MET
3	C	504	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	39	GLN
2	L	6	GLN
2	L	38	GLN
1	D	100	ASN
2	I	6	GLN
1	G	39	GLN
2	K	6	GLN
2	K	38	GLN
3	A	38	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	47	HIS
3	A	136	HIS
3	A	197	ASN
3	A	478	GLN
3	A	495	HIS
3	B	158	ASN
3	B	224	ASN
3	B	370	ASN
3	B	372	GLN
3	B	402	ASN
3	B	471	ASN
3	C	20	ASN
3	C	47	HIS
3	C	136	HIS
3	C	166	ASN
3	C	483	ASN
3	C	489	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	0.71	0	17,19,21	1.15	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	E	2	4	14,14,15	0.75	0	17,19,21	1.35	2 (11%)
4	BMA	E	3	4	11,11,12	0.84	0	15,15,17	2.51	5 (33%)
4	MAN	E	4	4	11,11,12	0.67	0	15,15,17	1.44	1 (6%)
4	NAG	E	5	4	14,14,15	0.73	0	17,19,21	1.11	1 (5%)
4	GAL	E	6	4	11,11,12	0.71	0	15,15,17	1.39	3 (20%)
4	SIA	E	7	4	20,20,21	1.53	2 (10%)	21,28,31	1.74	4 (19%)
4	NAG	F	1	4	14,14,15	0.70	0	17,19,21	1.10	0
4	NAG	F	2	4	14,14,15	0.76	0	17,19,21	1.41	2 (11%)
4	BMA	F	3	4	11,11,12	0.85	0	15,15,17	2.41	4 (26%)
4	MAN	F	4	4	11,11,12	0.69	0	15,15,17	1.19	1 (6%)
4	NAG	F	5	4	14,14,15	0.72	0	17,19,21	0.90	0
4	GAL	F	6	4	11,11,12	0.73	0	15,15,17	1.47	3 (20%)
4	SIA	F	7	4	20,20,21	1.51	2 (10%)	21,28,31	1.82	4 (19%)
4	NAG	J	1	4	14,14,15	0.69	0	17,19,21	1.28	3 (17%)
4	NAG	J	2	4	14,14,15	0.74	0	17,19,21	1.41	3 (17%)
4	BMA	J	3	4	11,11,12	0.84	0	15,15,17	2.40	5 (33%)
4	MAN	J	4	4	11,11,12	0.68	0	15,15,17	1.24	1 (6%)
4	NAG	J	5	4	14,14,15	0.73	0	17,19,21	1.08	1 (5%)
4	GAL	J	6	4	11,11,12	0.74	0	15,15,17	1.57	3 (20%)
4	SIA	J	7	4	20,20,21	1.52	2 (10%)	21,28,31	1.80	4 (19%)

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	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1
4	NAG	E	5	4	-	3/6/23/26	0/1/1/1
4	GAL	E	6	4	-	0/2/19/22	0/1/1/1
4	SIA	E	7	4	-	1/18/34/38	0/1/1/1
4	NAG	F	1	4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	4/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	NAG	F	5	4	-	1/6/23/26	0/1/1/1
4	GAL	F	6	4	-	0/2/19/22	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	-	0/2/19/22	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
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	E	7	SIA	C2-C1	5.45	1.58	1.52
4	F	7	SIA	C2-C1	5.43	1.58	1.52
4	J	7	SIA	C2-C1	5.42	1.58	1.52
4	E	7	SIA	O6-C2	2.15	1.47	1.43
4	J	7	SIA	O6-C2	2.13	1.47	1.43
4	F	7	SIA	O6-C2	2.11	1.47	1.43

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	3	BMA	C1-O5-C5	7.43	122.14	112.19
4	F	3	BMA	C1-O5-C5	7.38	122.07	112.19
4	J	3	BMA	C1-O5-C5	7.26	121.91	112.19
4	J	7	SIA	O1A-C1-C2	-4.65	112.79	122.85
4	E	7	SIA	O1A-C1-C2	-4.53	113.06	122.85
4	E	4	MAN	C1-O5-C5	4.47	118.18	112.19
4	F	7	SIA	O1A-C1-C2	-4.45	113.23	122.85
4	J	6	GAL	O3-C3-C2	-3.98	101.94	110.05
4	F	6	GAL	O3-C3-C2	-3.85	102.19	110.05
4	F	7	SIA	O6-C2-C3	-3.79	105.46	110.56
4	J	4	MAN	C1-O5-C5	3.72	117.17	112.19
4	E	6	GAL	O3-C3-C2	-3.67	102.57	110.05
4	J	7	SIA	O6-C2-C3	-3.64	105.66	110.56
4	F	4	MAN	C1-O5-C5	3.54	116.92	112.19
4	F	7	SIA	C6-C5-N5	-3.51	105.31	110.91
4	E	7	SIA	O6-C2-C3	-3.50	105.85	110.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	7	SIA	C6-C5-N5	-3.41	105.47	110.91
4	F	2	NAG	C2-N2-C7	3.28	127.30	122.90
4	E	3	BMA	C3-C4-C5	3.22	116.08	110.23
4	J	2	NAG	C2-N2-C7	3.20	127.19	122.90
4	E	7	SIA	C6-C5-N5	-3.11	105.94	110.91
4	E	2	NAG	C2-N2-C7	3.11	127.06	122.90
4	E	5	NAG	C2-N2-C7	2.94	126.84	122.90
4	J	1	NAG	O5-C1-C2	-2.93	106.76	111.29
4	J	6	GAL	C1-C2-C3	2.82	113.75	109.64
4	J	5	NAG	C2-N2-C7	2.80	126.65	122.90
4	J	3	BMA	C3-C4-C5	2.78	115.27	110.23
4	F	3	BMA	C3-C4-C5	2.71	115.14	110.23
4	E	3	BMA	C2-C3-C4	2.67	115.56	110.86
4	F	3	BMA	C2-C3-C4	2.57	115.39	110.86
4	J	3	BMA	C2-C3-C4	2.52	115.29	110.86
4	J	1	NAG	C2-N2-C7	2.51	126.26	122.90
4	F	6	GAL	C1-C2-C3	2.50	113.29	109.64
4	E	1	NAG	O5-C1-C2	-2.43	107.54	111.29
4	E	2	NAG	C1-O5-C5	2.42	115.43	112.19
4	E	3	BMA	O4-C4-C3	-2.42	104.68	110.38
4	J	7	SIA	O1B-C1-O1A	2.41	129.55	124.08
4	E	1	NAG	C2-N2-C7	2.41	126.13	122.90
4	E	7	SIA	O1B-C1-O1A	2.39	129.49	124.08
4	F	7	SIA	O1B-C1-O1A	2.36	129.43	124.08
4	J	6	GAL	C1-O5-C5	2.34	115.33	112.19
4	J	2	NAG	O4-C4-C3	-2.23	105.11	110.38
4	F	6	GAL	C1-O5-C5	2.19	115.12	112.19
4	E	6	GAL	C1-C2-C3	2.17	112.81	109.64
4	J	1	NAG	O4-C4-C3	-2.16	105.29	110.38
4	F	3	BMA	O4-C4-C3	-2.12	105.38	110.38
4	J	3	BMA	O3-C3-C2	-2.11	105.75	110.05
4	J	2	NAG	C1-O5-C5	2.10	115.00	112.19
4	J	3	BMA	O4-C4-C3	-2.09	105.44	110.38
4	E	3	BMA	O5-C5-C4	2.07	115.88	110.83
4	F	2	NAG	O4-C4-C3	-2.07	105.50	110.38
4	E	6	GAL	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

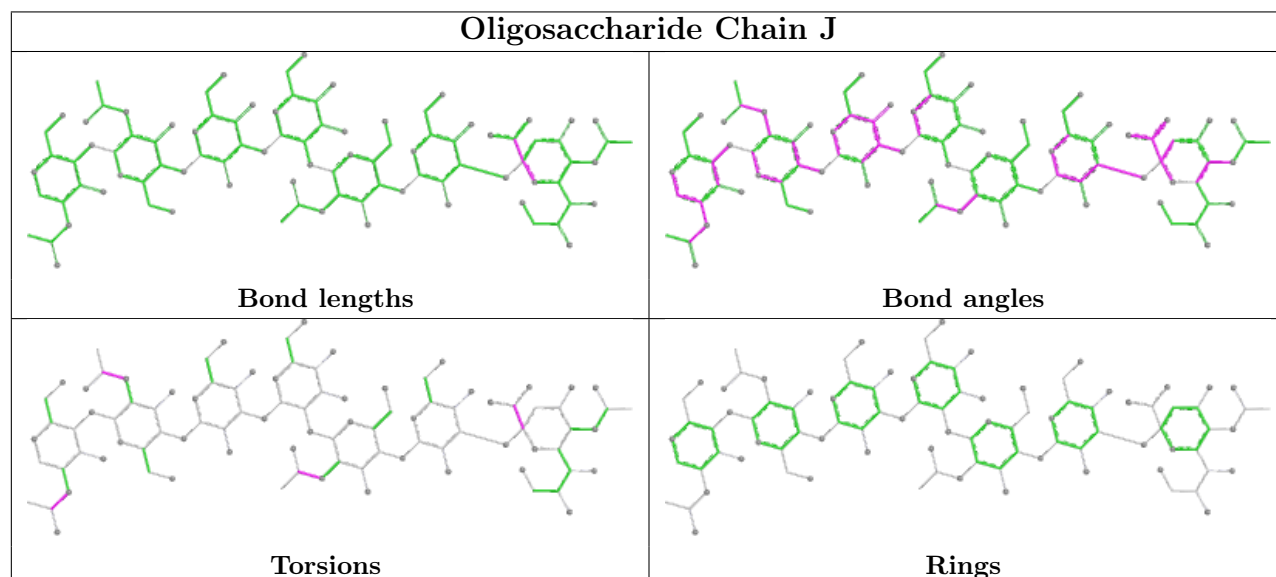
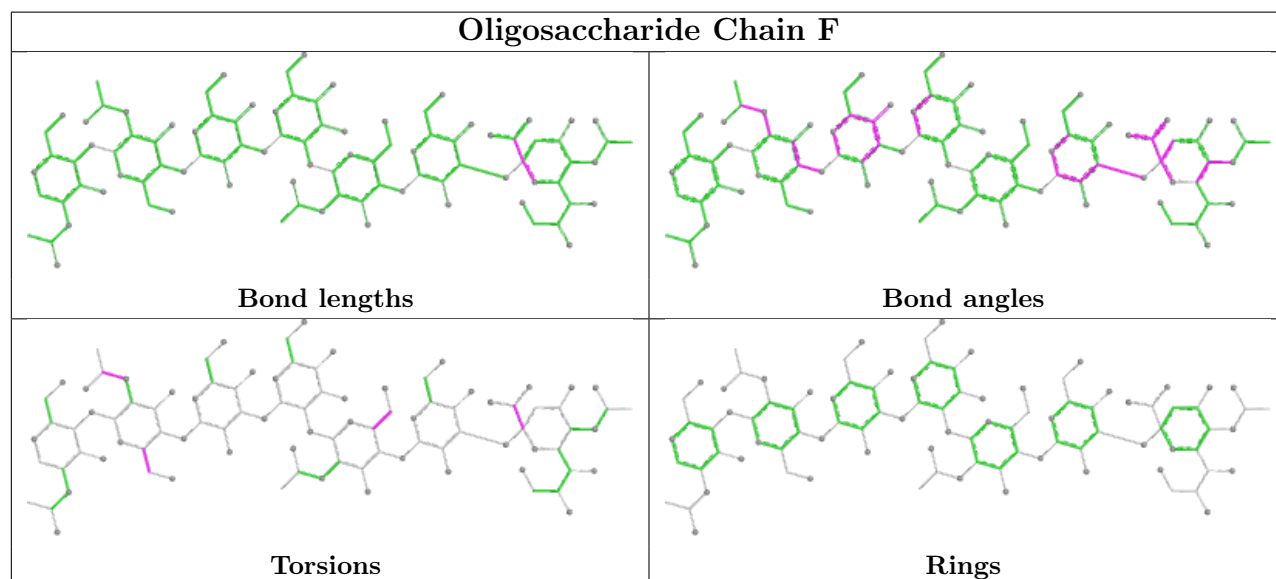
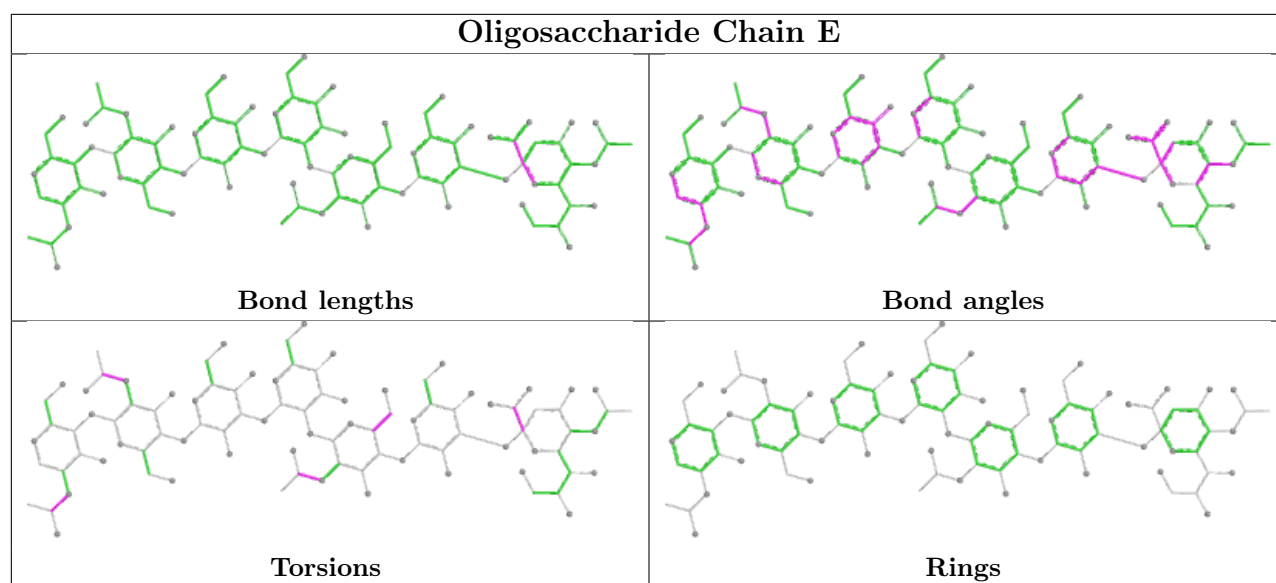
Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	E	5	NAG	C8-C7-N2-C2
4	E	5	NAG	O7-C7-N2-C2
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	J	5	NAG	C8-C7-N2-C2
4	J	5	NAG	O7-C7-N2-C2
4	F	2	NAG	C4-C5-C6-O6
4	E	5	NAG	O5-C5-C6-O6
4	F	5	NAG	O5-C5-C6-O6
4	E	7	SIA	O1A-C1-C2-O6
4	F	7	SIA	O1A-C1-C2-O6
4	J	7	SIA	O1A-C1-C2-O6

There are no ring outliers.

2 monomers are involved in 1 short contact:

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

12 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	602	3	14,14,15	0.69	0	17,19,21	0.86	0
5	NAG	C	603	3	14,14,15	0.31	0	17,19,21	0.54	0
5	NAG	A	603	3	14,14,15	0.30	0	17,19,21	0.57	0
5	NAG	B	601	3	14,14,15	0.72	0	17,19,21	0.82	0
5	NAG	B	602	3	14,14,15	0.69	0	17,19,21	0.93	1 (5%)
5	NAG	B	603	3	14,14,15	0.31	0	17,19,21	0.58	0
5	NAG	C	604	3	14,14,15	0.30	0	17,19,21	0.88	1 (5%)
5	NAG	A	601	3	14,14,15	0.76	0	17,19,21	0.81	0
5	NAG	C	601	3	14,14,15	0.76	0	17,19,21	0.83	0
5	NAG	B	604	3	14,14,15	0.30	0	17,19,21	0.71	0
5	NAG	C	602	3	14,14,15	0.69	0	17,19,21	0.92	1 (5%)
5	NAG	A	604	3	14,14,15	9.24	4 (28%)	17,19,21	5.27	7 (41%)

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	602	3	-	0/6/23/26	0/1/1/1
5	NAG	C	603	3	-	2/6/23/26	0/1/1/1
5	NAG	A	603	3	-	2/6/23/26	0/1/1/1
5	NAG	B	601	3	-	0/6/23/26	0/1/1/1
5	NAG	B	602	3	-	0/6/23/26	0/1/1/1
5	NAG	B	603	3	-	0/6/23/26	0/1/1/1
5	NAG	C	604	3	-	3/6/23/26	0/1/1/1
5	NAG	A	601	3	-	0/6/23/26	0/1/1/1
5	NAG	C	601	3	-	0/6/23/26	0/1/1/1
5	NAG	B	604	3	-	2/6/23/26	0/1/1/1
5	NAG	C	602	3	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	604	3	-	5/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	604	NAG	C6-C5	33.31	2.63	1.51
5	A	604	NAG	O6-C6	7.90	1.75	1.42
5	A	604	NAG	C4-C5	3.51	1.60	1.53
5	A	604	NAG	O5-C5	2.31	1.47	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	604	NAG	C1-O5-C5	13.01	129.62	112.19
5	A	604	NAG	C6-C5-C4	10.54	138.91	113.02
5	A	604	NAG	O5-C1-C2	-7.90	99.07	111.29
5	A	604	NAG	O6-C6-C5	-6.18	90.29	111.33
5	A	604	NAG	O5-C5-C4	-5.88	96.52	110.83
5	A	604	NAG	O5-C5-C6	5.33	118.04	107.66
5	A	604	NAG	O4-C4-C5	4.69	120.87	109.32
5	C	604	NAG	C1-O5-C5	2.94	116.13	112.19
5	C	602	NAG	O5-C1-C2	-2.69	107.12	111.29
5	B	602	NAG	O5-C1-C2	-2.65	107.20	111.29

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	604	NAG	C1-C2-N2-C7
5	A	604	NAG	C8-C7-N2-C2
5	A	604	NAG	O7-C7-N2-C2
5	B	604	NAG	C8-C7-N2-C2
5	B	604	NAG	O7-C7-N2-C2
5	C	603	NAG	C8-C7-N2-C2
5	C	603	NAG	O7-C7-N2-C2
5	C	604	NAG	C8-C7-N2-C2
5	C	604	NAG	O7-C7-N2-C2
5	A	604	NAG	C4-C5-C6-O6
5	A	603	NAG	C8-C7-N2-C2
5	A	603	NAG	O7-C7-N2-C2
5	A	604	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	604	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	NAG	50	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

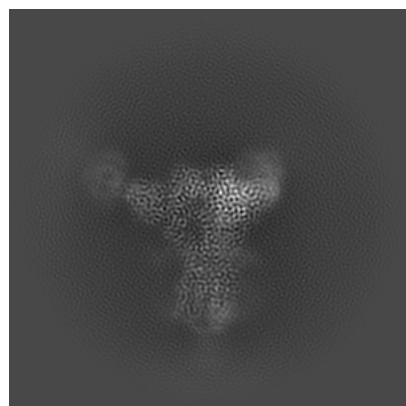
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74755. These allow visual inspection of the internal detail of the map and identification of artifacts.

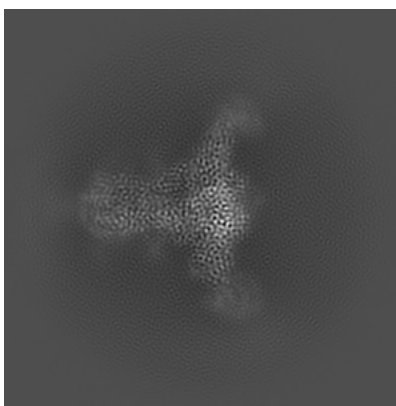
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

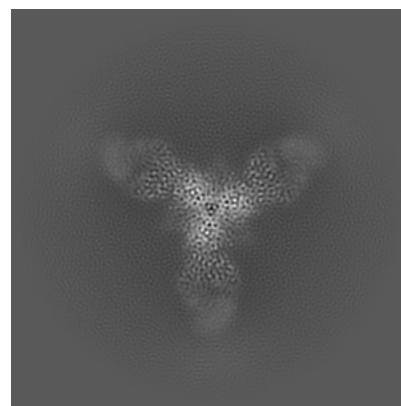
6.1.1 Primary map



X

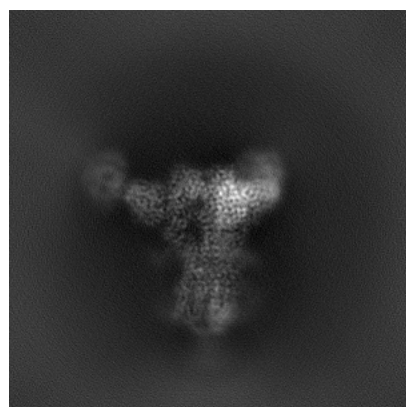


Y

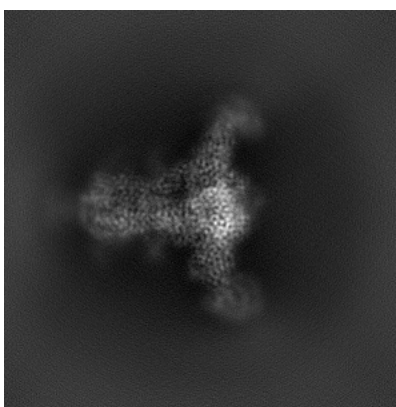


Z

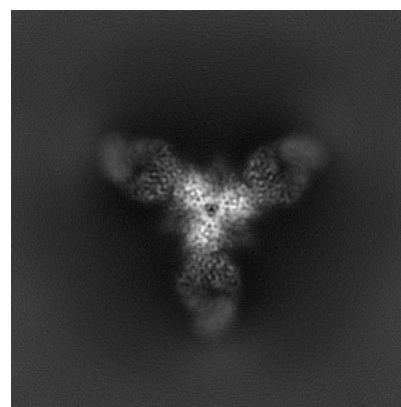
6.1.2 Raw map



X



Y

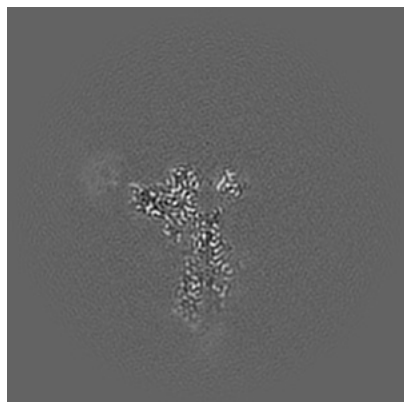


Z

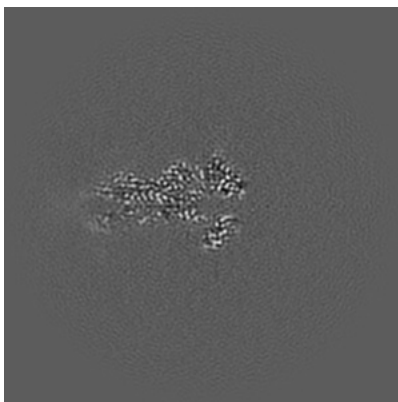
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

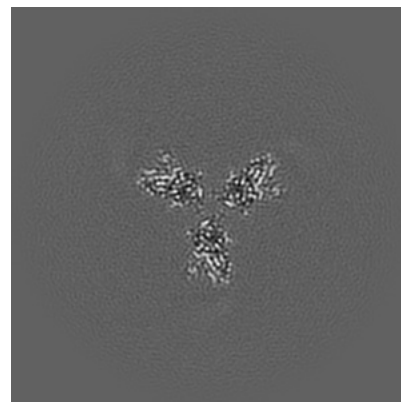
6.2.1 Primary map



X Index: 192

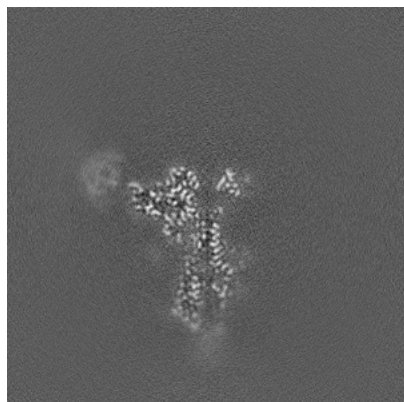


Y Index: 192

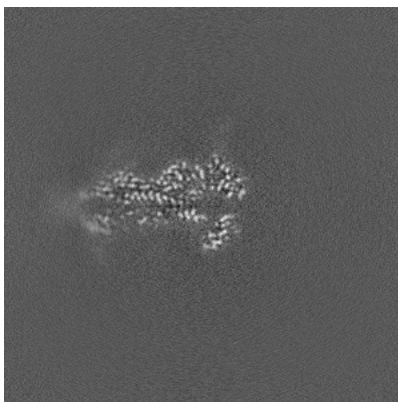


Z Index: 192

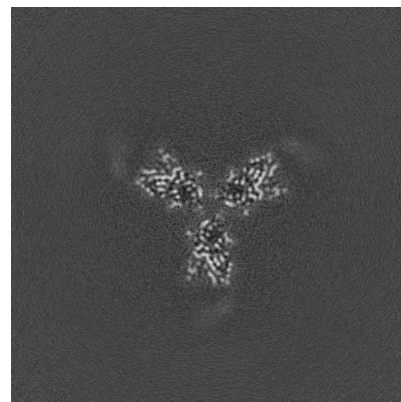
6.2.2 Raw map



X Index: 192



Y Index: 192

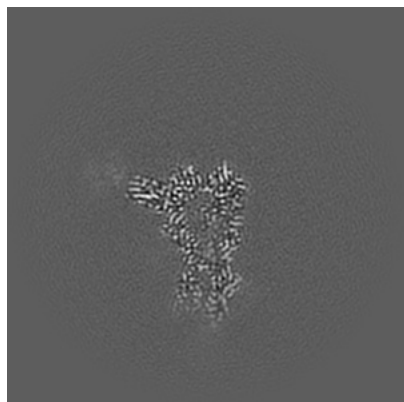


Z Index: 192

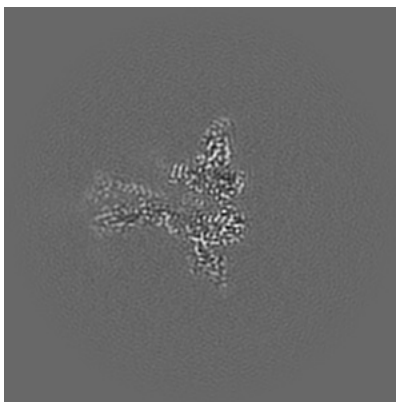
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

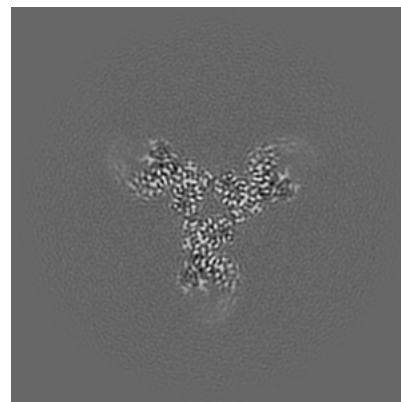
6.3.1 Primary map



X Index: 179

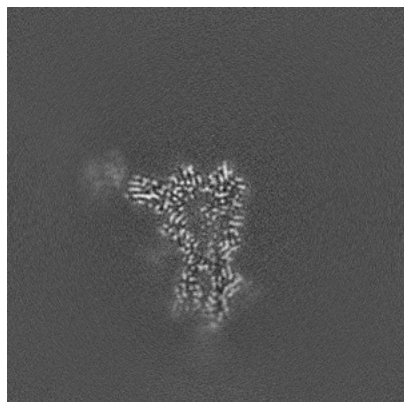


Y Index: 206

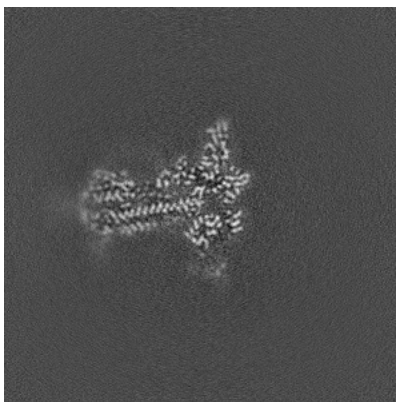


Z Index: 204

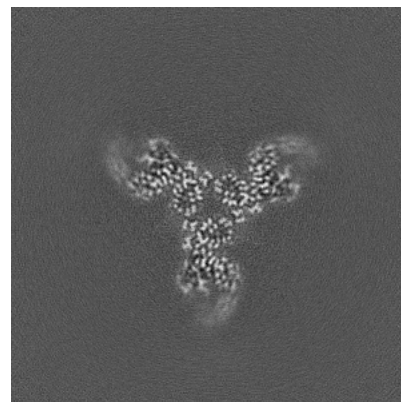
6.3.2 Raw map



X Index: 179



Y Index: 200

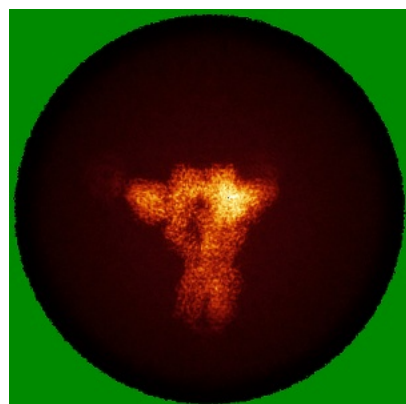


Z Index: 204

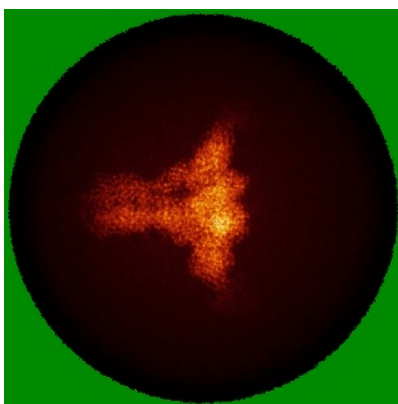
The images above show the largest variance slices of the map in three orthogonal directions.

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

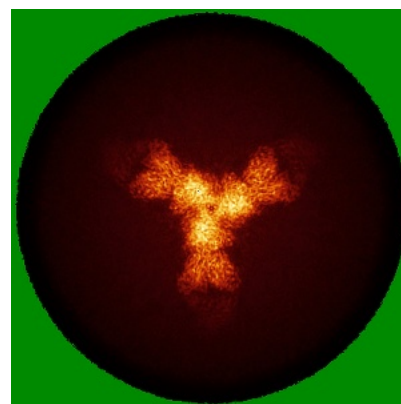
6.4.1 Primary map



X

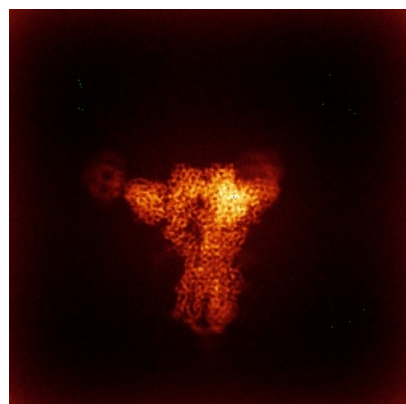


Y

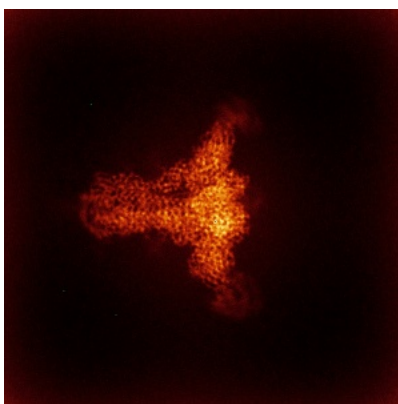


Z

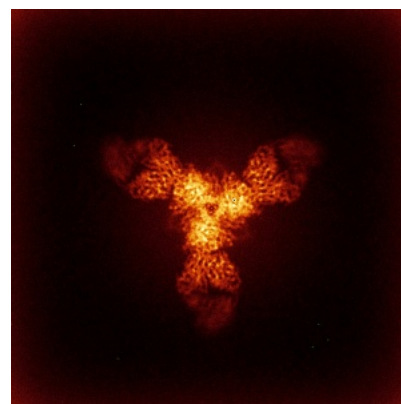
6.4.2 Raw map



X



Y

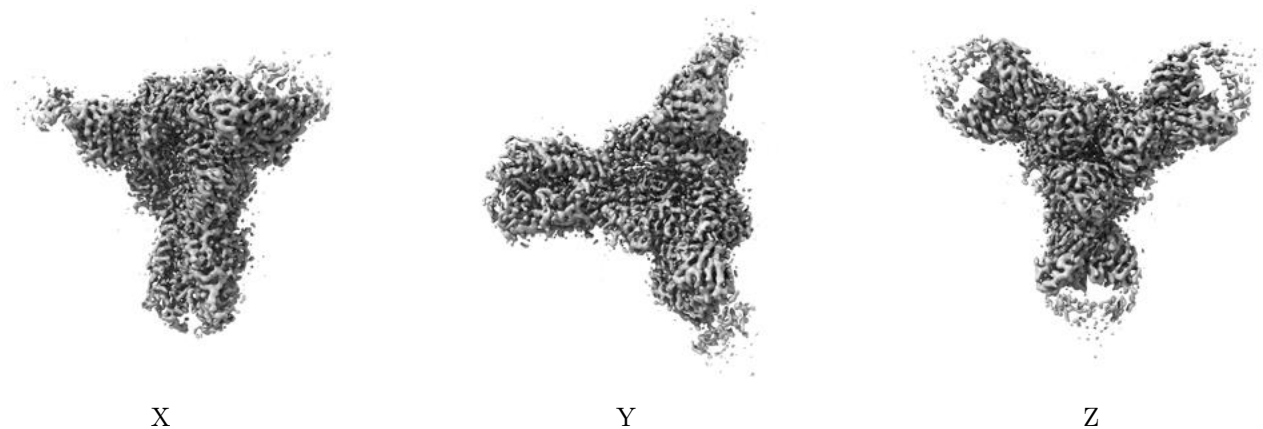


Z

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.

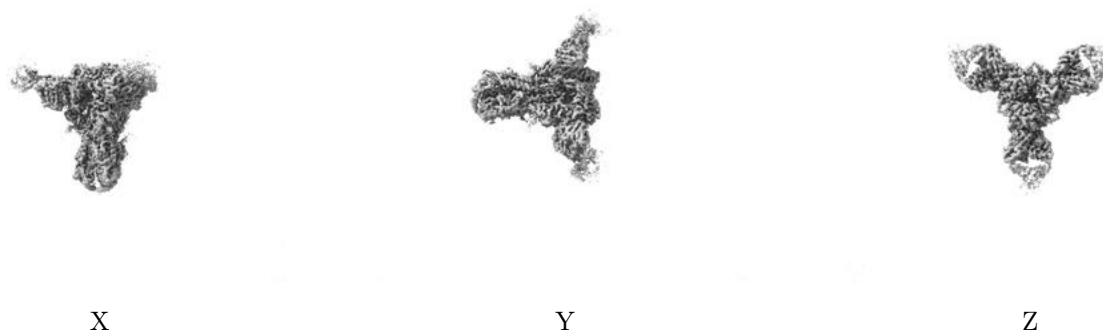
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.134. 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.

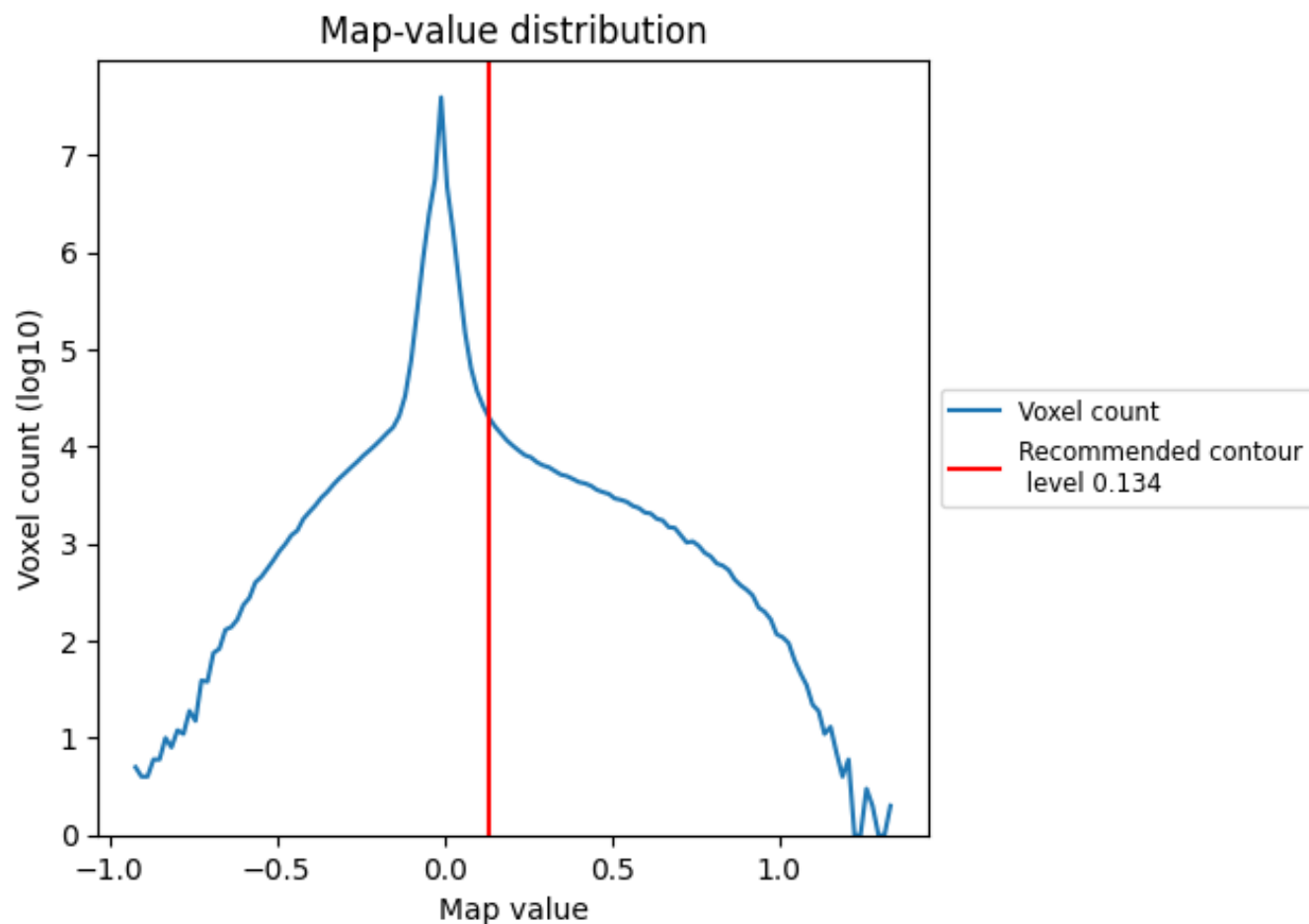
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

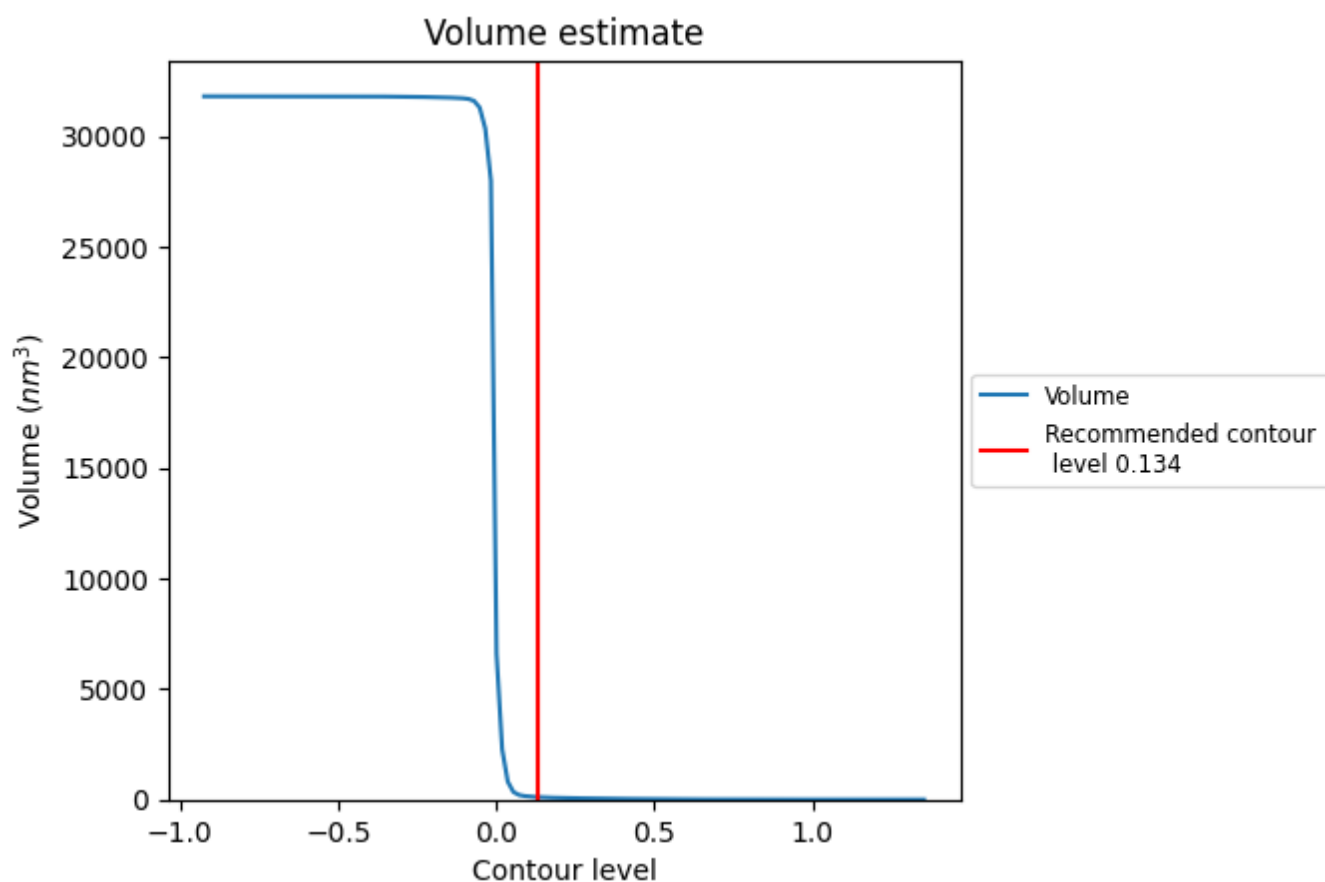
This section contains the results of statistical analysis of the map.

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.

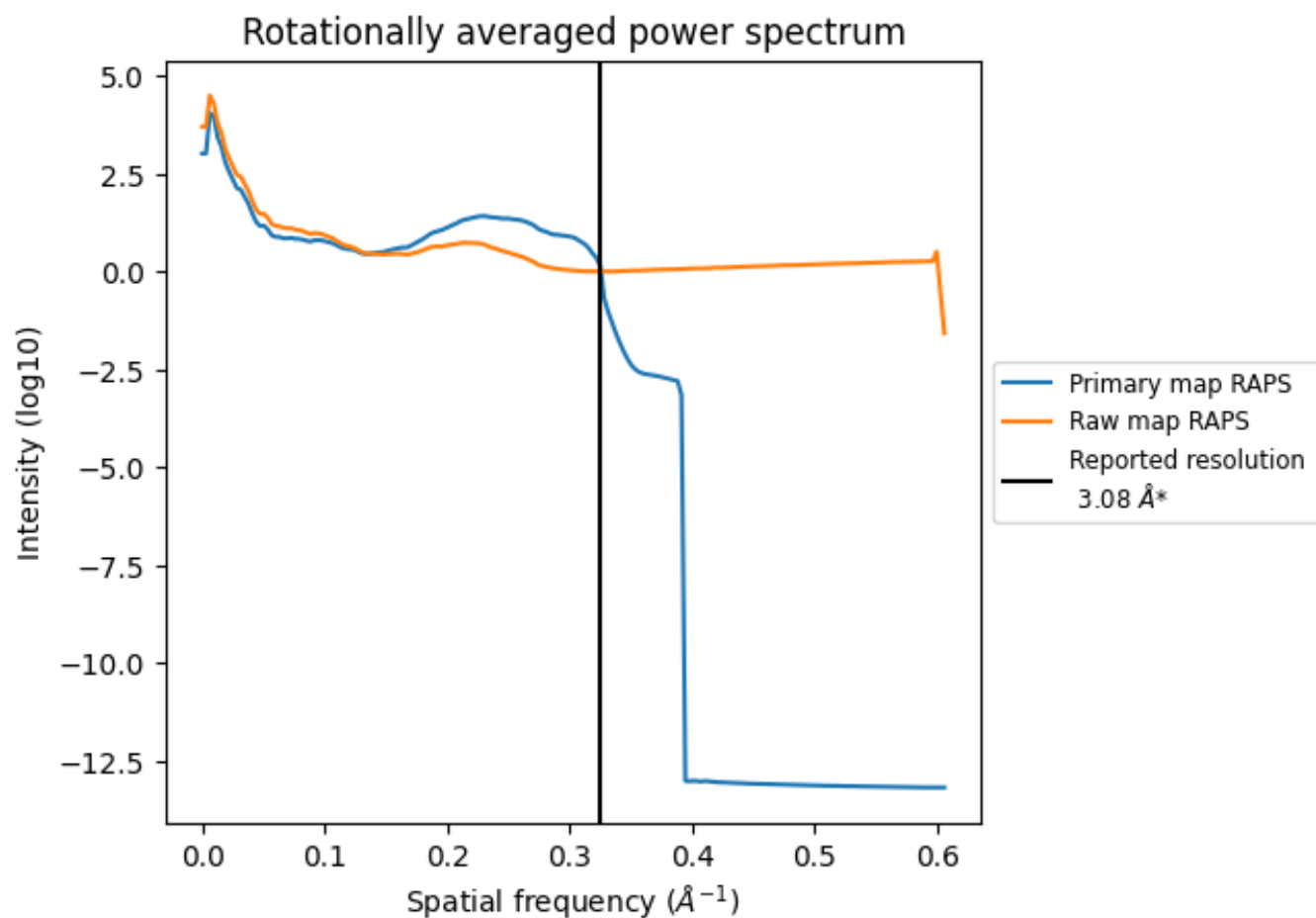
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 109 nm³; this corresponds to an approximate mass of 98 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 ⓘ

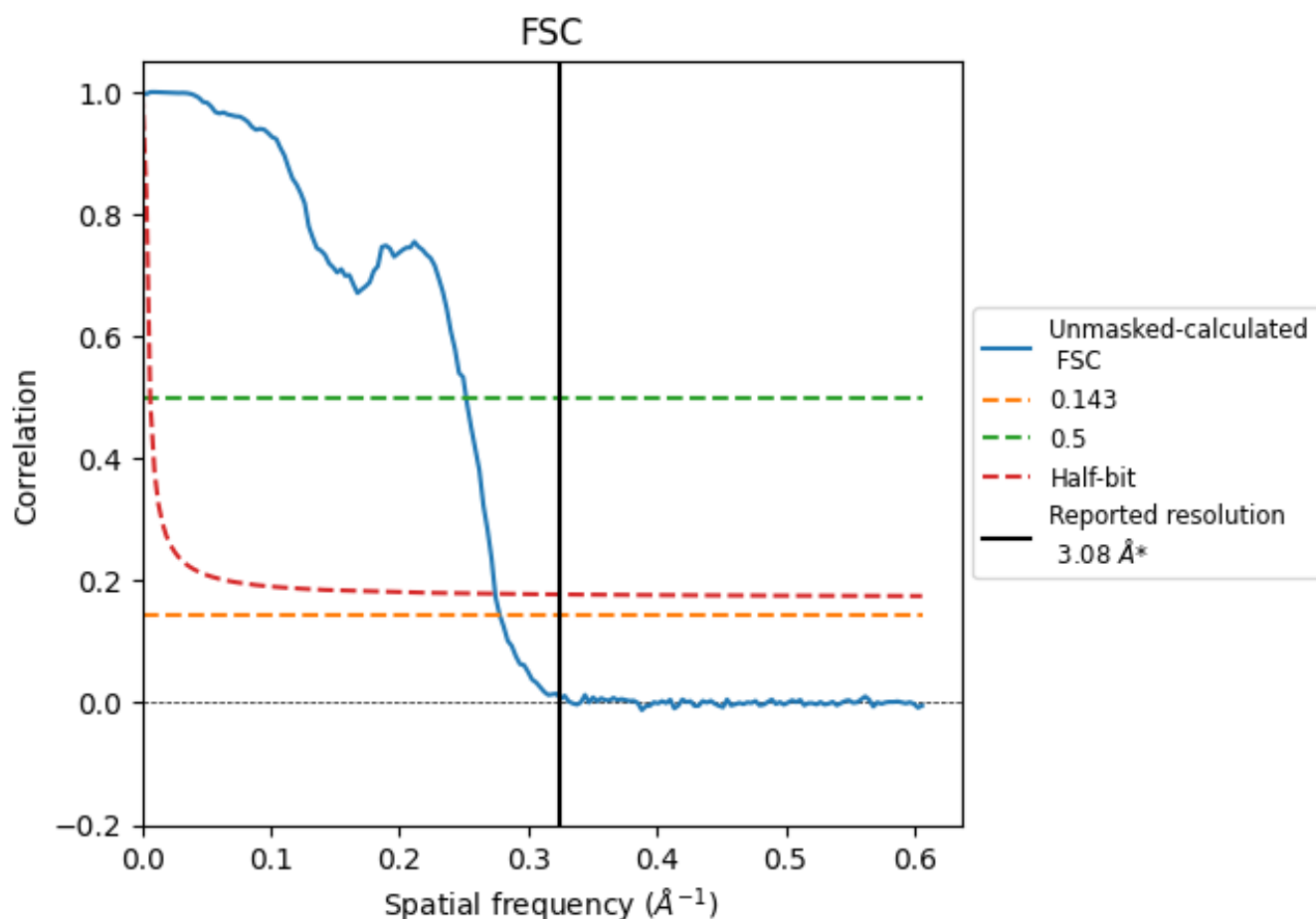


*Reported resolution corresponds to spatial frequency of 0.325 Å⁻¹

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 0.325 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

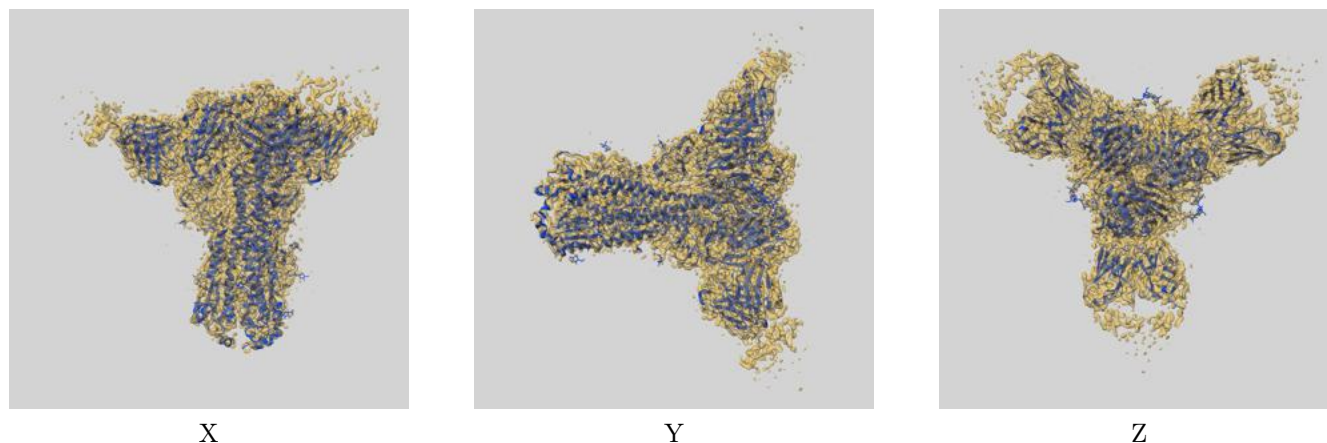
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.60	3.97	3.65

*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 3.60 differs from the reported value 3.08 by more than 10 %

9 Map-model fit [i](#)

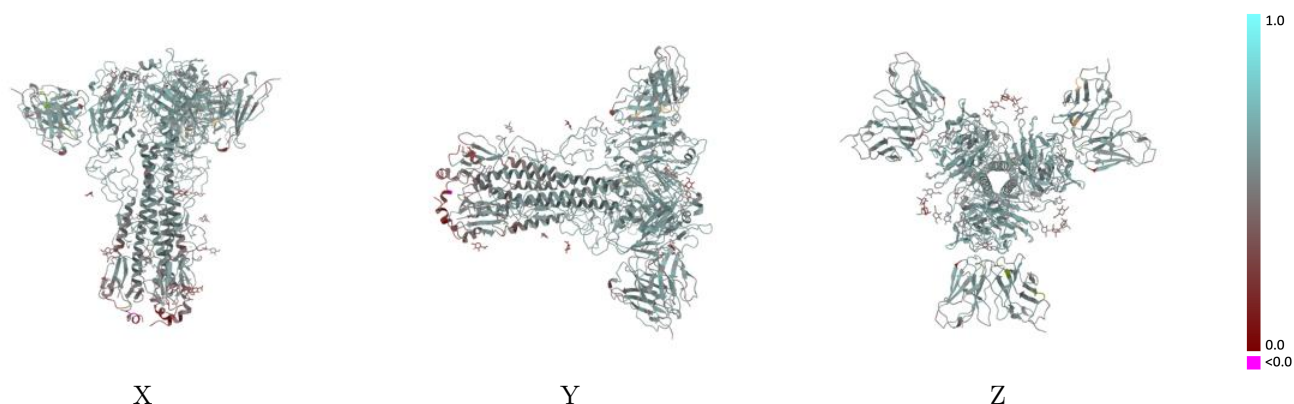
This section contains information regarding the fit between EMDB map EMD-74755 and PDB model 9ZTJ. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



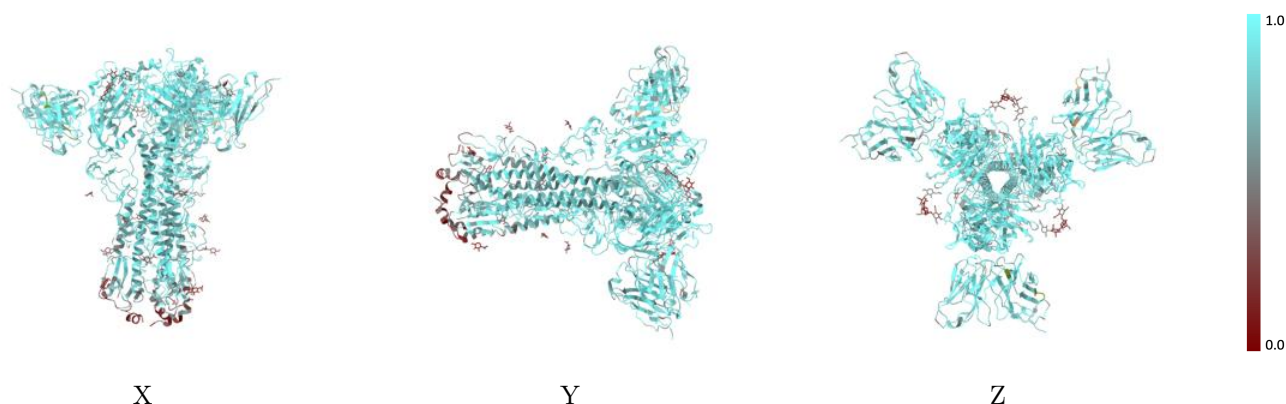
The images above show the 3D surface view of the map at the recommended contour level 0.134 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



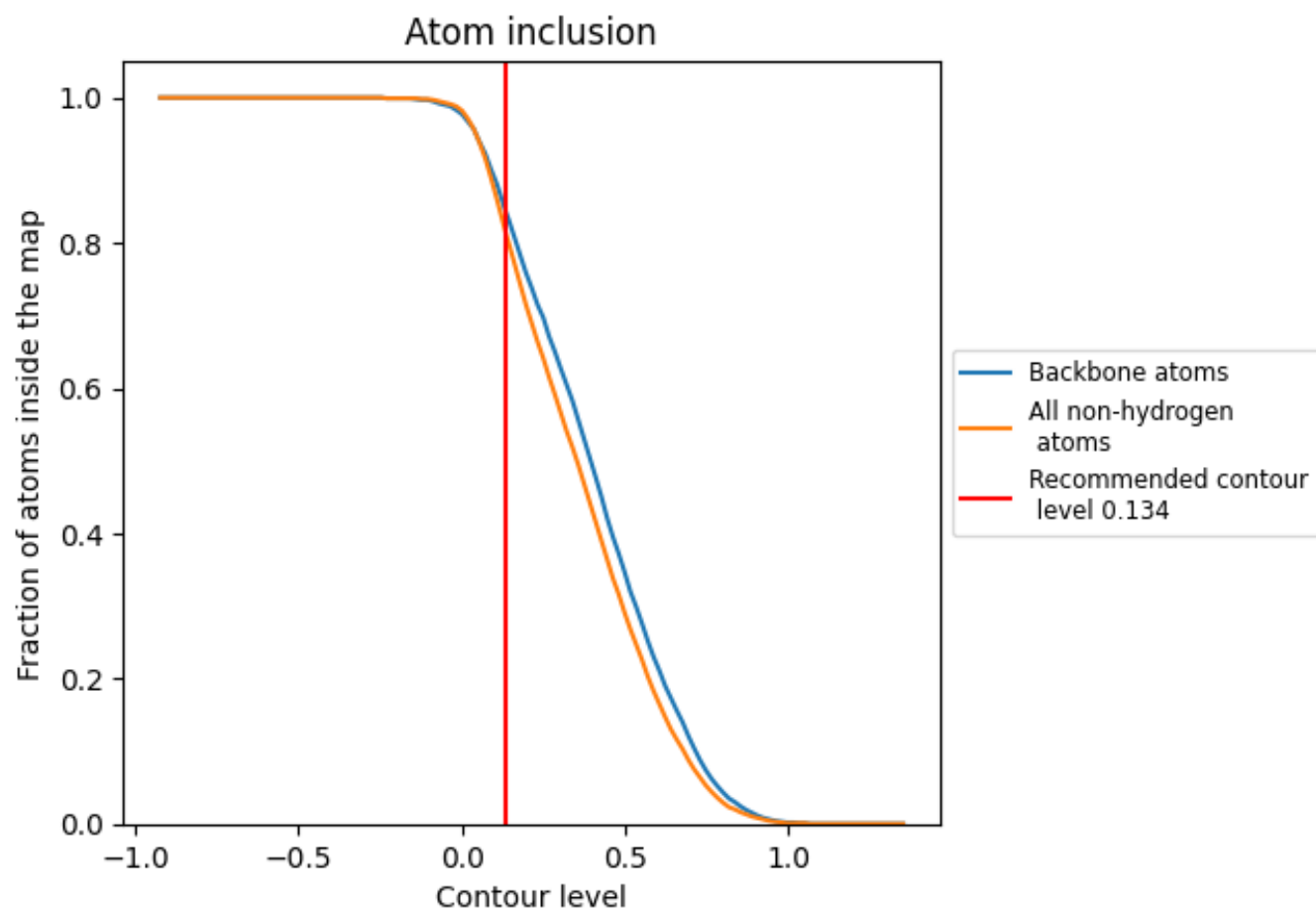
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.134).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 82% 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 (0.134) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8150	0.5370
A	0.8200	0.5370
B	0.8150	0.5390
C	0.8150	0.5360
D	0.8420	0.5480
E	0.4840	0.4260
F	0.4950	0.4170
G	0.8380	0.5470
H	0.8390	0.5460
I	0.8160	0.5370
J	0.4840	0.4010
K	0.8210	0.5380
L	0.8190	0.5350

