



## Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 05:42 PM EDT

PDB ID : 9Q26 / pdb\_00009q26  
EMDB ID : EMD-72151  
Title : Structure of the Measles virus Fusion glycoprotein ectodomain in complex with two neutralizing antibodies 4F09 and 3A12  
Authors : Zyla, D.; Acciani, M.; Niemeyer, G.; Saphire, E.O.  
Deposited on : 2025-08-14  
Resolution : 2.30 Å(reported)  
Based on initial model : 8UUT

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

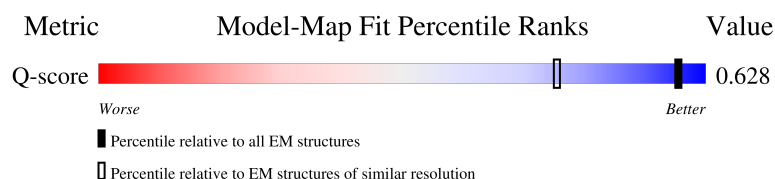
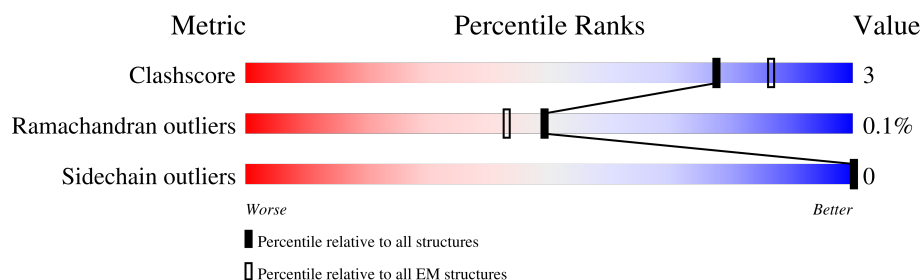
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 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*




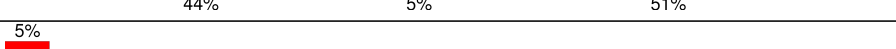
The reported resolution of this entry is 2.30 Å.

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.






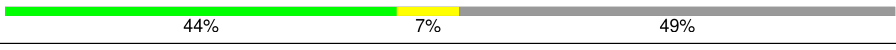

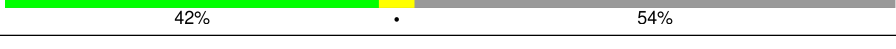

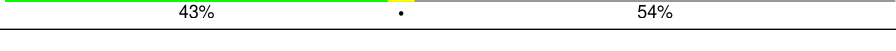
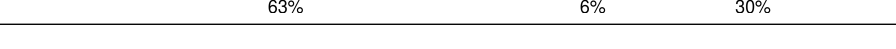
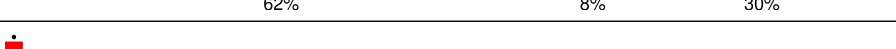
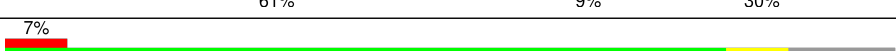


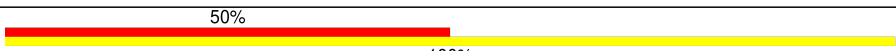
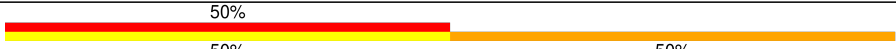
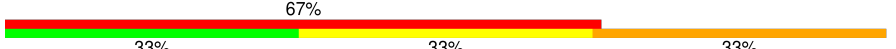


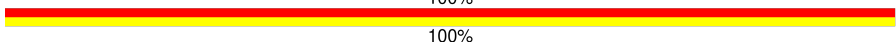

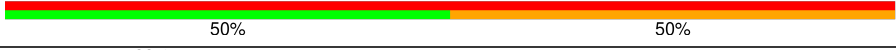


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4254 ( 1.80 - 2.80 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	D	252	
1	H	252	
1	L	252	
2	E	236	

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Mol	Chain	Length	Quality of chain
2	I	236	
2	M	236	
3	F	259	
3	J	259	
3	N	259	
4	G	236	
4	K	236	
4	O	236	
5	a	112	
5	b	112	
5	c	112	
6	A	420	
6	B	420	
6	C	420	
7	P	4	
7	V	4	
8	Q	3	
8	S	3	
8	W	3	
9	R	2	
9	T	2	
9	X	2	
10	U	3	

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 21446 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 3A12 Fab Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	122	Total	C	N	O	S	0	0
			934	591	160	181	2		
1	H	123	Total	C	N	O	S	0	0
			940	594	161	183	2		
1	L	123	Total	C	N	O	S	0	0
			937	592	160	183	2		

- Molecule 2 is a protein called 3A12 Fab Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	108	Total	C	N	O	S	0	0
			833	523	139	167	4		
2	I	108	Total	C	N	O	S	0	0
			833	523	139	167	4		
2	M	108	Total	C	N	O	S	0	0
			833	523	139	167	4		

- Molecule 3 is a protein called 4F09 Fab Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	131	Total	C	N	O	S	0	0
			1023	656	168	197	2		
3	J	131	Total	C	N	O	S	0	0
			1021	655	168	196	2		
3	N	131	Total	C	N	O	S	0	0
			1021	655	168	196	2		

- Molecule 4 is a protein called 4F09 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	108	Total	C	N	O	S	0	0
			837	530	140	164	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	108	Total	C	N	O	S	0	0
			837	530	140	164	3		
4	O	108	Total	C	N	O	S	0	0
			837	530	140	164	3		

- Molecule 5 is a protein called Fusion glycoprotein F2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	78	Total	C	N	O	S	0	0
			615	387	116	108	4		
5	b	78	Total	C	N	O	S	0	0
			615	387	116	108	4		
5	c	78	Total	C	N	O	S	0	0
			615	387	116	108	4		

- Molecule 6 is a protein called Fusion glycoprotein F1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	370	Total	C	N	O	S	0	0
			2789	1761	471	543	14		
6	B	370	Total	C	N	O	S	0	0
			2789	1761	471	543	14		
6	C	370	Total	C	N	O	S	0	0
			2789	1761	471	543	14		

There are 117 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	GLY	GLU	engineered mutation	UNP Q786F3
A	455	GLY	GLU	engineered mutation	UNP Q786F3
A	496	GLY	-	expression tag	UNP Q786F3
A	497	VAL	-	expression tag	UNP Q786F3
A	498	ASP	-	expression tag	UNP Q786F3
A	499	ASP	-	expression tag	UNP Q786F3
A	500	ASP	-	expression tag	UNP Q786F3
A	501	ASP	-	expression tag	UNP Q786F3
A	502	LYS	-	expression tag	UNP Q786F3
A	503	ALA	-	expression tag	UNP Q786F3
A	504	GLY	-	expression tag	UNP Q786F3
A	505	TRP	-	expression tag	UNP Q786F3
A	506	SER	-	expression tag	UNP Q786F3
A	507	HIS	-	expression tag	UNP Q786F3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	508	PRO	-	expression tag	UNP Q786F3
A	509	GLN	-	expression tag	UNP Q786F3
A	510	PHE	-	expression tag	UNP Q786F3
A	511	GLU	-	expression tag	UNP Q786F3
A	512	LYS	-	expression tag	UNP Q786F3
A	513	GLY	-	expression tag	UNP Q786F3
A	514	GLY	-	expression tag	UNP Q786F3
A	515	GLY	-	expression tag	UNP Q786F3
A	516	SER	-	expression tag	UNP Q786F3
A	517	GLY	-	expression tag	UNP Q786F3
A	518	GLY	-	expression tag	UNP Q786F3
A	519	GLY	-	expression tag	UNP Q786F3
A	520	SER	-	expression tag	UNP Q786F3
A	521	GLY	-	expression tag	UNP Q786F3
A	522	GLY	-	expression tag	UNP Q786F3
A	523	GLY	-	expression tag	UNP Q786F3
A	524	SER	-	expression tag	UNP Q786F3
A	525	TRP	-	expression tag	UNP Q786F3
A	526	SER	-	expression tag	UNP Q786F3
A	527	HIS	-	expression tag	UNP Q786F3
A	528	PRO	-	expression tag	UNP Q786F3
A	529	GLN	-	expression tag	UNP Q786F3
A	530	PHE	-	expression tag	UNP Q786F3
A	531	GLU	-	expression tag	UNP Q786F3
A	532	LYS	-	expression tag	UNP Q786F3
B	170	GLY	GLU	engineered mutation	UNP Q786F3
B	455	GLY	GLU	engineered mutation	UNP Q786F3
B	496	GLY	-	expression tag	UNP Q786F3
B	497	VAL	-	expression tag	UNP Q786F3
B	498	ASP	-	expression tag	UNP Q786F3
B	499	ASP	-	expression tag	UNP Q786F3
B	500	ASP	-	expression tag	UNP Q786F3
B	501	ASP	-	expression tag	UNP Q786F3
B	502	LYS	-	expression tag	UNP Q786F3
B	503	ALA	-	expression tag	UNP Q786F3
B	504	GLY	-	expression tag	UNP Q786F3
B	505	TRP	-	expression tag	UNP Q786F3
B	506	SER	-	expression tag	UNP Q786F3
B	507	HIS	-	expression tag	UNP Q786F3
B	508	PRO	-	expression tag	UNP Q786F3
B	509	GLN	-	expression tag	UNP Q786F3
B	510	PHE	-	expression tag	UNP Q786F3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	511	GLU	-	expression tag	UNP Q786F3
B	512	LYS	-	expression tag	UNP Q786F3
B	513	GLY	-	expression tag	UNP Q786F3
B	514	GLY	-	expression tag	UNP Q786F3
B	515	GLY	-	expression tag	UNP Q786F3
B	516	SER	-	expression tag	UNP Q786F3
B	517	GLY	-	expression tag	UNP Q786F3
B	518	GLY	-	expression tag	UNP Q786F3
B	519	GLY	-	expression tag	UNP Q786F3
B	520	SER	-	expression tag	UNP Q786F3
B	521	GLY	-	expression tag	UNP Q786F3
B	522	GLY	-	expression tag	UNP Q786F3
B	523	GLY	-	expression tag	UNP Q786F3
B	524	SER	-	expression tag	UNP Q786F3
B	525	TRP	-	expression tag	UNP Q786F3
B	526	SER	-	expression tag	UNP Q786F3
B	527	HIS	-	expression tag	UNP Q786F3
B	528	PRO	-	expression tag	UNP Q786F3
B	529	GLN	-	expression tag	UNP Q786F3
B	530	PHE	-	expression tag	UNP Q786F3
B	531	GLU	-	expression tag	UNP Q786F3
B	532	LYS	-	expression tag	UNP Q786F3
C	170	GLY	GLU	engineered mutation	UNP Q786F3
C	455	GLY	GLU	engineered mutation	UNP Q786F3
C	496	GLY	-	expression tag	UNP Q786F3
C	497	VAL	-	expression tag	UNP Q786F3
C	498	ASP	-	expression tag	UNP Q786F3
C	499	ASP	-	expression tag	UNP Q786F3
C	500	ASP	-	expression tag	UNP Q786F3
C	501	ASP	-	expression tag	UNP Q786F3
C	502	LYS	-	expression tag	UNP Q786F3
C	503	ALA	-	expression tag	UNP Q786F3
C	504	GLY	-	expression tag	UNP Q786F3
C	505	TRP	-	expression tag	UNP Q786F3
C	506	SER	-	expression tag	UNP Q786F3
C	507	HIS	-	expression tag	UNP Q786F3
C	508	PRO	-	expression tag	UNP Q786F3
C	509	GLN	-	expression tag	UNP Q786F3
C	510	PHE	-	expression tag	UNP Q786F3
C	511	GLU	-	expression tag	UNP Q786F3
C	512	LYS	-	expression tag	UNP Q786F3
C	513	GLY	-	expression tag	UNP Q786F3

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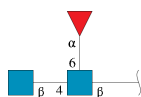
Chain	Residue	Modelled	Actual	Comment	Reference
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C	515	GLY	-	expression tag	UNP Q786F3
C	516	SER	-	expression tag	UNP Q786F3
C	517	GLY	-	expression tag	UNP Q786F3
C	518	GLY	-	expression tag	UNP Q786F3
C	519	GLY	-	expression tag	UNP Q786F3
C	520	SER	-	expression tag	UNP Q786F3
C	521	GLY	-	expression tag	UNP Q786F3
C	522	GLY	-	expression tag	UNP Q786F3
C	523	GLY	-	expression tag	UNP Q786F3
C	524	SER	-	expression tag	UNP Q786F3
C	525	TRP	-	expression tag	UNP Q786F3
C	526	SER	-	expression tag	UNP Q786F3
C	527	HIS	-	expression tag	UNP Q786F3
C	528	PRO	-	expression tag	UNP Q786F3
C	529	GLN	-	expression tag	UNP Q786F3
C	530	PHE	-	expression tag	UNP Q786F3
C	531	GLU	-	expression tag	UNP Q786F3
C	532	LYS	-	expression tag	UNP Q786F3

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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
7	P	4	Total	C	N	O	0	0
			50	28	2	20		
7	V	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.





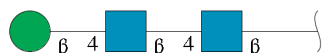
Mol	Chain	Residues	Atoms				AltConf	Trace
8	Q	3	Total	C	N	O	0	0
			38	22	2	14		
8	S	3	Total	C	N	O	0	0
			38	22	2	14		
8	W	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



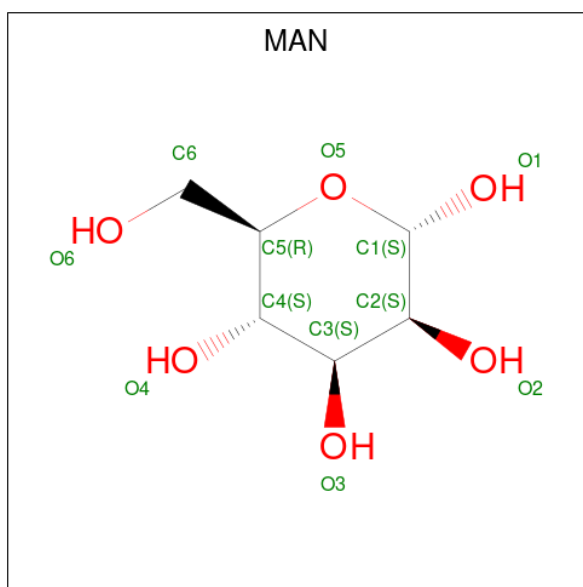
Mol	Chain	Residues	Atoms				AltConf	Trace
9	R	2	Total	C	N	O	0	0
			28	16	2	10		
9	T	2	Total	C	N	O	0	0
			28	16	2	10		
9	X	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 10 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
10	U	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 11 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).

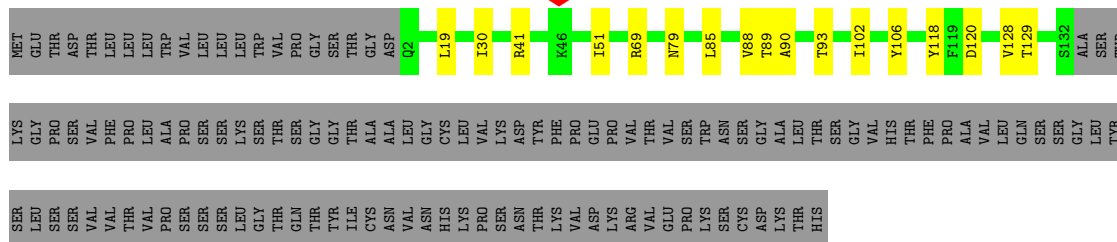
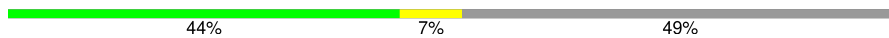


Mol	Chain	Residues	Atoms			AltConf
11	F	1	Total	C	O	0
			11	6	5	

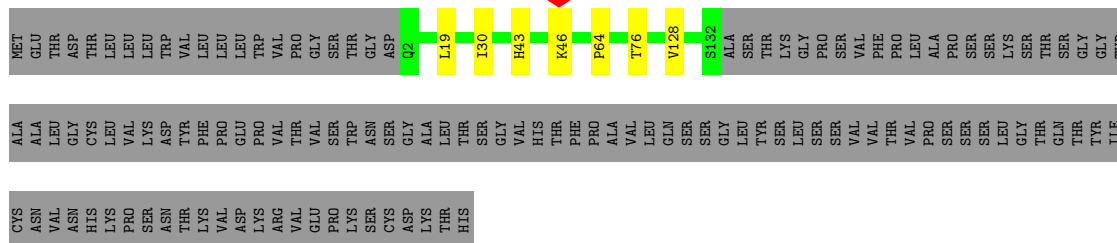




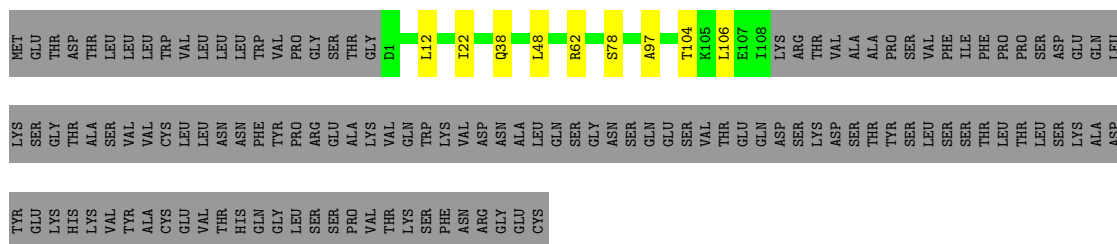
Chain J:



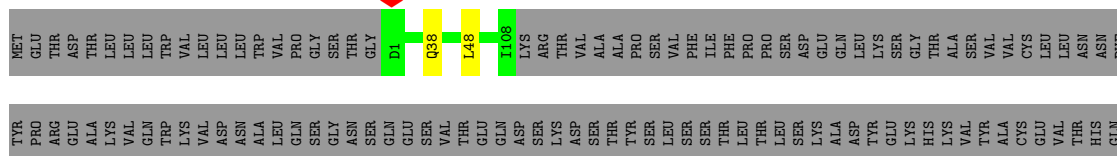
Chain N:



Chain G:



Chain K:



GLY  
LEU  
SER  
SER  
PRO  
VAL  
THR  
LYS  
SER  
PHE  
ASN  
ARG  
GLY  
GLU  
CYS

• Molecule 4: 4F09 Fab Light Chain

Chain O:  43% 54%

MET GLU THR ASP THR LEU LEU LEU TRP VAL LEU LEU LEU TRP VAL PRO GLY SER THR GLY D1 T6 Q38 L48 L79 A97 Q102 L106 E107 I108 LYS ARG THR THR VAL ALA ALA PRO SER SER PHE ILE THR PHE LEU PRO PRO SER ASP GLU GLN ALA LEU LYS GLY THR

ALA SER VAL VAL CYS LEU LEU ASN ASN PHE THR LEU LEU LEU ARG GLU VAL VAL GLY VAL GLN THR LYS VAL ASP ASN ALA LEU GLN SER GLY SER ASN GLN SER GLU VAL THR GLU GLN ASP SER LYS ASP VAL ALA ALA TYR SER SER LEU VAL PHE SER SER THR THR LEU THR PRO LEU SER LYS GLU ASP TYR LYS GLY HIS

LYS VAL TYR ALA CYS GLU VAL THR HIS GLN GLY PHE LEU LEU SER SER PRO VAL THR THR SER PHE ASN ARG GLY GLU CYS

• Molecule 5: Fusion glycoprotein F2

Chain a:  63% 6% 30%

MET GLY LEU LYS VAL ASN VAL SER ALA ILE PHE MET MET ALA VAL LEU LEU THR LEU LEU GLN THR PRO THR GLY Q24 R48 V55 N66 T69 R70 T95 I98 V101 GLN SER VAL VAL SER SER ARG ARG HIS LYS ARG

• Molecule 5: Fusion glycoprotein F2

Chain b:  62% 8% 30%


MET GLY LEU LYS VAL ASN VAL SER ALA ILE PHE MET MET ALA VAL LEU LEU THR LEU LEU GLN THR PRO THR GLY Q24 R48 V55 K57 L58 M59 T63 L64 T69 Y76 L80 V101 GLN SER VAL ALA SER SER ARG ARG HIS LYS ARG

• Molecule 5: Fusion glycoprotein F2

Chain c:  61% 9% 30%

MET GLY LEU LYS VAL ASN VAL SER ALA ILE PHE MET MET ALA VAL LEU LEU THR LEU LEU GLN THR PRO THR GLY Q24 M46 T47 R48 V55 T63 L64 T69 Y76 L80 R81 T95 I98 V101 GLN SER VAL ALA SER SER ARG ARG HIS LYS ARG

• Molecule 6: Fusion glycoprotein F1

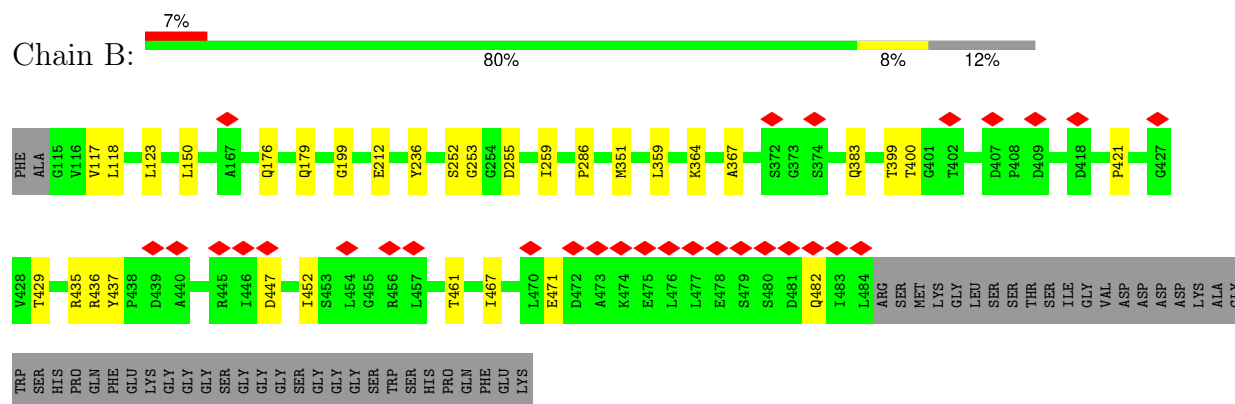
Chain A:  7% 81% 7% 12%

PHE ALA G115 V116 V117 L118 L123 L150 R151 E155 G199 E212 L216 L234 S235 Y236 G253 G258 E261 P266 M337 M351 L354 L359 K364 S372 G373 S374 R378 L386 I393 K396 I403 D407 P408 D409

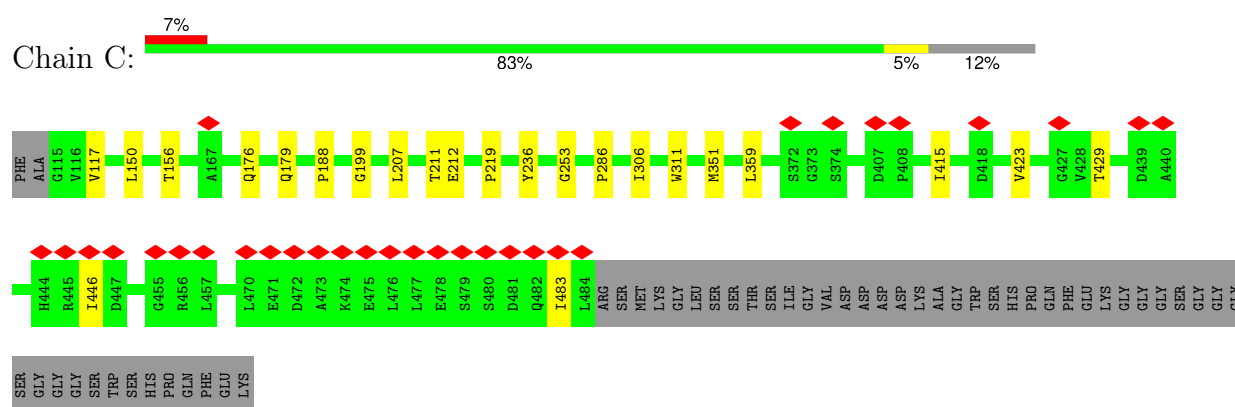
D418 V423 G427 V428 T429 R435 R436 Y437 P438 D439 A440 R445 I446 D447 L454 Q455 R456 L470 E471 D472 A473 K474 E475 L476 L477 E478 S479 S480 D481 Q482 I483 L484 ARG SER MET LYS GLY LEU SER SER THR SER ILE GLY VAL ASP ASP ASP ASP LYS ALA GLY TRP SER

HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY TRP SER HIS PRO GLN PHE GLU LYS

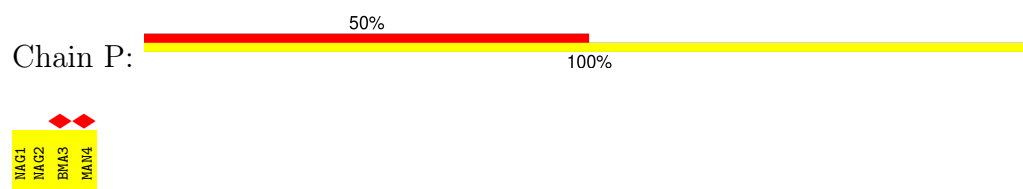
- Molecule 6: Fusion glycoprotein F1



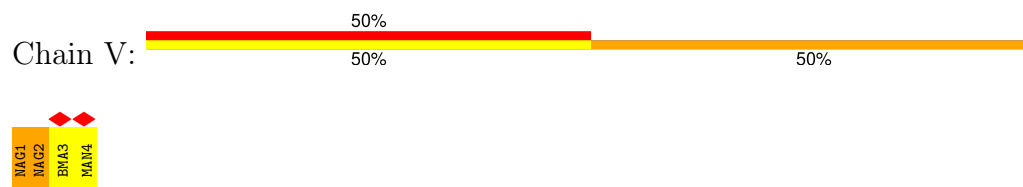
- Molecule 6: Fusion glycoprotein F1



- Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: 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, C3	Depositor
Number of particles used	196000	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 ( $e^-/\text{\AA}^2$ )	70	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.934	Depositor
Minimum map value	-0.583	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.094	Depositor
Map size (Å)	337.932, 337.932, 337.932	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9387, 0.9387, 0.9387	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: MAN, NAG, FUC, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	D	0.08	0/958	0.25	0/1305
1	H	0.10	0/964	0.27	0/1313
1	L	0.09	0/961	0.27	0/1309
2	E	0.09	0/851	0.30	0/1154
2	I	0.08	0/851	0.26	0/1154
2	M	0.07	0/851	0.25	0/1154
3	F	0.09	0/1057	0.28	0/1445
3	J	0.10	0/1055	0.27	0/1442
3	N	0.09	0/1055	0.26	0/1442
4	G	0.10	0/857	0.30	0/1164
4	K	0.10	0/857	0.28	0/1164
4	O	0.11	0/857	0.30	0/1164
5	a	0.10	0/623	0.26	0/843
5	b	0.09	0/623	0.26	0/843
5	c	0.09	0/623	0.26	0/843
6	A	0.08	0/2830	0.24	0/3844
6	B	0.08	0/2830	0.23	0/3844
6	C	0.08	0/2830	0.23	0/3844
All	All	0.09	0/21533	0.26	0/29271

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	934	0	905	6	0
1	H	940	0	910	7	0
1	L	937	0	907	7	0
2	E	833	0	813	4	0
2	I	833	0	813	8	0
2	M	833	0	813	1	0
3	F	1023	0	965	7	0
3	J	1021	0	963	11	0
3	N	1021	0	963	4	0
4	G	837	0	814	5	0
4	K	837	0	814	1	0
4	O	837	0	814	4	0
5	a	615	0	649	6	0
5	b	615	0	649	6	0
5	c	615	0	649	8	0
6	A	2789	0	2823	21	0
6	B	2789	0	2823	24	0
6	C	2789	0	2823	20	0
7	P	50	0	43	0	0
7	V	50	0	43	2	0
8	Q	38	0	34	2	0
8	S	38	0	34	0	0
8	W	38	0	34	0	0
9	R	28	0	25	0	0
9	T	28	0	25	0	0
9	X	28	0	25	1	0
10	U	39	0	34	0	0
11	F	11	0	10	0	0
All	All	21446	0	21217	124	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 3.

All (124) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:95:THR:HG22	6:C:253:GLY:H	1.39	0.86
5:b:69:THR:HG22	6:B:199:GLY:HA2	1.73	0.70
5:a:69:THR:HG22	6:A:199:GLY:HA2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:104:LYS:HG3	1:H:105:ASP:H	1.60	0.67
5:c:69:THR:HG22	6:C:199:GLY:HA2	1.77	0.65
3:F:43:HIS:HB2	3:F:46:LYS:HB2	1.77	0.65
6:C:415:ILE:HG21	6:C:423:VAL:HG11	1.81	0.63
6:B:399:THR:HG21	6:B:421:PRO:HD2	1.81	0.62
6:B:399:THR:HG23	6:B:400:THR:HG23	1.82	0.62
2:E:95:THR:HG22	6:B:253:GLY:H	1.65	0.60
4:G:22:ILE:HD12	4:G:104:THR:HG21	1.85	0.59
6:C:351:MET:HE1	6:C:359:LEU:HD12	1.85	0.59
5:a:48:ARG:HA	6:A:286:PRO:HA	1.84	0.59
6:A:351:MET:HE1	6:A:359:LEU:HD12	1.85	0.58
1:H:14:LYS:HG2	1:H:15:PRO:HD2	1.86	0.58
5:a:66:ASN:HA	8:Q:1:NAG:H82	1.87	0.57
2:I:95:THR:HG22	6:C:253:GLY:N	2.17	0.57
3:N:43:HIS:HB2	3:N:46:LYS:HB2	1.86	0.57
6:A:258:GLY:HA2	6:A:337:MET:HE3	1.87	0.56
4:G:38:GLN:HB2	4:G:48:LEU:HD11	1.87	0.56
1:L:41:ARG:HB2	1:L:51:ILE:HD11	1.87	0.56
5:a:55:VAL:HG21	6:A:150:LEU:HD21	1.88	0.54
6:B:351:MET:HE1	6:B:359:LEU:HD12	1.89	0.54
1:H:93:SER:HB3	1:H:123:VAL:HG23	1.90	0.53
5:b:48:ARG:HA	6:B:286:PRO:HA	1.89	0.53
5:b:55:VAL:HG21	6:B:150:LEU:HD21	1.90	0.53
6:A:378:ARG:HD3	6:A:393:ILE:HG23	1.90	0.52
6:C:156:THR:HB	7:V:2:NAG:H61	1.90	0.52
4:K:38:GLN:HB2	4:K:48:LEU:HD11	1.92	0.52
1:H:62:TYR:HD2	1:H:67:LYS:HG3	1.75	0.52
3:F:89:THR:HG22	3:F:90:ALA:H	1.76	0.50
6:A:117:VAL:HG23	6:B:429:THR:HG22	1.94	0.50
4:O:38:GLN:HB2	4:O:48:LEU:HD11	1.93	0.50
6:B:176:GLN:HG3	6:B:179:GLN:HB2	1.93	0.50
3:J:89:THR:HG22	3:J:90:ALA:H	1.77	0.49
1:D:50:TRP:HZ2	1:D:53:TYR:HD1	1.61	0.49
6:A:212:GLU:HG3	6:A:236:TYR:CG	2.48	0.49
6:B:364:LYS:HB3	6:B:447:ASP:HB3	1.94	0.49
2:M:95:THR:HG22	6:A:253:GLY:HA3	1.95	0.48
6:A:386:LEU:HD22	6:A:423:VAL:HG21	1.95	0.48
6:C:212:GLU:HG3	6:C:236:TYR:CD1	2.48	0.48
6:B:212:GLU:HG3	6:B:236:TYR:CG	2.47	0.48
5:c:55:VAL:HG21	6:C:150:LEU:HD21	1.96	0.48
5:c:63:THR:HB	7:V:1:NAG:H82	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:107:SER:HA	2:I:33:TYR:CE1	2.48	0.47
6:A:364:LYS:HG3	6:A:447:ASP:HB3	1.97	0.47
3:N:19:LEU:HD11	3:N:128:VAL:HG11	1.96	0.47
6:C:176:GLN:HG3	6:C:179:GLN:HB2	1.96	0.47
3:J:41:ARG:HB3	3:J:51:ILE:HD11	1.97	0.47
1:L:14:LYS:HB3	1:L:17:HIS:CD2	2.50	0.46
6:A:435:ARG:HH12	6:A:439:ASP:HB2	1.81	0.46
5:c:63:THR:HG23	5:c:64:LEU:HD12	1.98	0.46
4:O:6:THR:HA	4:O:102:GLN:HE22	1.81	0.46
6:C:446:ILE:HG12	9:X:1:NAG:H81	1.98	0.46
3:F:19:LEU:HD11	3:F:128:VAL:HG11	1.98	0.45
1:D:22:THR:HG23	1:D:80:GLN:HG3	1.99	0.45
3:J:106:TYR:CE2	6:C:188:PRO:HG3	2.52	0.45
5:b:57:LYS:HE2	5:b:59:MET:O	2.17	0.45
2:I:48:LEU:HB3	2:I:49:ILE:HD12	1.98	0.45
6:B:482:GLN:HE22	6:C:483:ILE:HG22	1.80	0.45
3:F:30:ILE:HG23	3:F:37:TRP:NE1	2.32	0.45
6:B:118:LEU:HD11	6:B:123:LEU:HD22	1.99	0.45
3:F:89:THR:HG22	3:F:90:ALA:N	2.32	0.45
3:J:19:LEU:HD11	3:J:128:VAL:HG11	1.99	0.44
5:c:95:THR:HA	5:c:98:ILE:HD12	1.99	0.44
1:L:50:TRP:HZ2	1:L:53:TYR:HD2	1.64	0.44
6:A:118:LEU:HD11	6:A:123:LEU:HD22	2.00	0.44
1:H:50:TRP:HZ2	1:H:53:TYR:HD1	1.65	0.44
2:I:12:LEU:HD11	2:I:106:VAL:HG22	1.99	0.44
1:D:30:ILE:HG13	1:D:37:TRP:CE2	2.53	0.44
3:J:69:ARG:HH21	3:J:85:LEU:HG	1.83	0.44
2:I:4:ARG:HE	2:I:4:ARG:HB3	1.66	0.44
2:I:34:LEU:HD22	2:I:72:PHE:CG	2.53	0.44
5:c:46:MET:HB3	6:C:286:PRO:HB3	1.99	0.43
4:G:62:ARG:HD2	4:G:78:SER:O	2.19	0.43
3:J:19:LEU:HB2	3:J:88:VAL:HG11	1.99	0.43
3:N:30:ILE:HD11	3:N:76:THR:HA	1.99	0.43
6:B:435:ARG:HD2	6:B:437:TYR:O	2.18	0.43
3:F:64:PRO:HG2	4:G:97:ALA:HB2	1.99	0.43
1:H:30:ILE:HD11	1:H:81:PHE:HD1	1.83	0.43
6:A:212:GLU:HG3	6:A:236:TYR:CD1	2.54	0.43
5:b:63:THR:HG23	5:b:64:LEU:HD22	2.00	0.43
3:J:102:ILE:HD11	3:J:120:ASP:CG	2.42	0.43
5:b:76:TYR:CZ	5:b:80:LEU:HD11	2.54	0.43
5:c:76:TYR:CZ	5:c:80:LEU:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:ARG:HD2	6:B:252:SER:O	2.19	0.43
3:J:89:THR:HG22	3:J:90:ALA:N	2.33	0.43
6:A:354:LEU:HD23	6:B:461:THR:HG22	2.01	0.43
6:A:261:GLU:HG3	6:C:219:PRO:HG2	2.01	0.43
6:B:212:GLU:HG3	6:B:236:TYR:CD1	2.54	0.43
6:B:117:VAL:HG23	6:C:429:THR:HG22	2.01	0.42
2:E:95:THR:HG22	6:B:253:GLY:N	2.32	0.42
2:I:40:LYS:HD3	2:I:85:ALA:HB2	2.00	0.42
6:B:383:GLN:HB3	6:B:436:ARG:HD2	2.02	0.42
3:J:102:ILE:HD13	3:J:118:TYR:CE2	2.54	0.42
4:O:79:LEU:HD11	4:O:106:LEU:HD21	2.00	0.42
6:A:216:LEU:HD13	6:A:234:LEU:HD23	2.02	0.42
6:B:367:ALA:HB1	6:B:452:ILE:HG12	2.02	0.42
3:J:30:ILE:HG23	3:J:79:ASN:OD1	2.20	0.42
1:L:30:ILE:HG13	1:L:37:TRP:CE2	2.55	0.42
6:C:176:GLN:CG	6:C:179:GLN:HB2	2.50	0.42
6:C:207:LEU:O	6:C:211:THR:HG23	2.20	0.42
1:L:62:TYR:HB2	1:L:67:LYS:HG3	2.02	0.42
3:J:93:THR:HG23	3:J:129:THR:HA	2.00	0.42
6:A:396:LYS:HG3	6:A:403:ILE:HG12	2.02	0.42
5:c:81:ARG:HD2	5:c:81:ARG:HA	1.73	0.42
6:A:429:THR:HG22	6:C:117:VAL:HG23	2.02	0.41
2:E:95:THR:HG23	6:B:255:ASP:HB2	2.02	0.41
5:a:70:ARG:NH2	8:Q:3:FUC:H5	2.35	0.41
6:A:435:ARG:HD2	6:A:437:TYR:O	2.20	0.41
5:a:95:THR:HA	5:a:98:ILE:HD12	2.02	0.41
6:C:306:ILE:HD12	6:C:311:TRP:CD1	2.55	0.41
6:B:467:ILE:O	6:B:471:GLU:HG2	2.21	0.41
3:N:64:PRO:HD2	4:O:97:ALA:HA	2.03	0.41
6:A:151:ARG:O	6:A:155:GLU:HG2	2.21	0.41
6:C:212:GLU:HG3	6:C:236:TYR:CG	2.55	0.41
1:D:21:LEU:HD11	1:D:96:TYR:HD2	1.86	0.41
3:F:46:LYS:HA	3:F:46:LYS:HD3	1.85	0.41
4:G:12:LEU:HB3	4:G:106:LEU:HD23	2.02	0.41
6:B:255:ASP:HB3	6:B:259:ILE:HD12	2.02	0.41
1:L:46:LYS:HG3	1:L:47:GLY:H	1.85	0.40
1:L:14:LYS:HB3	1:L:17:HIS:HD2	1.86	0.40
2:E:80:GLN:HB3	2:E:82:GLU:HG2	2.03	0.40
1:D:62:TYR:HD2	1:D:67:LYS:HG3	1.87	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	120/252 (48%)	116 (97%)	4 (3%)	0	100	100
1	H	121/252 (48%)	117 (97%)	4 (3%)	0	100	100
1	L	121/252 (48%)	115 (95%)	6 (5%)	0	100	100
2	E	106/236 (45%)	101 (95%)	4 (4%)	1 (1%)	14	17
2	I	106/236 (45%)	100 (94%)	5 (5%)	1 (1%)	14	17
2	M	106/236 (45%)	100 (94%)	6 (6%)	0	100	100
3	F	129/259 (50%)	126 (98%)	3 (2%)	0	100	100
3	J	129/259 (50%)	127 (98%)	2 (2%)	0	100	100
3	N	129/259 (50%)	128 (99%)	1 (1%)	0	100	100
4	G	106/236 (45%)	102 (96%)	4 (4%)	0	100	100
4	K	106/236 (45%)	102 (96%)	4 (4%)	0	100	100
4	O	106/236 (45%)	99 (93%)	7 (7%)	0	100	100
5	a	76/112 (68%)	75 (99%)	1 (1%)	0	100	100
5	b	76/112 (68%)	75 (99%)	1 (1%)	0	100	100
5	c	76/112 (68%)	75 (99%)	1 (1%)	0	100	100
6	A	368/420 (88%)	362 (98%)	6 (2%)	0	100	100
6	B	368/420 (88%)	363 (99%)	5 (1%)	0	100	100
6	C	368/420 (88%)	360 (98%)	8 (2%)	0	100	100
All	All	2717/4545 (60%)	2643 (97%)	72 (3%)	2 (0%)	49	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	69	GLN
2	I	69	GLN



### 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	103/217 (48%)	103 (100%)	0	100	100
1	H	104/217 (48%)	104 (100%)	0	100	100
1	L	104/217 (48%)	104 (100%)	0	100	100
2	E	94/209 (45%)	94 (100%)	0	100	100
2	I	94/209 (45%)	94 (100%)	0	100	100
2	M	94/209 (45%)	94 (100%)	0	100	100
3	F	110/222 (50%)	110 (100%)	0	100	100
3	J	110/222 (50%)	110 (100%)	0	100	100
3	N	110/222 (50%)	110 (100%)	0	100	100
4	G	92/207 (44%)	92 (100%)	0	100	100
4	K	92/207 (44%)	92 (100%)	0	100	100
4	O	92/207 (44%)	92 (100%)	0	100	100
5	a	70/99 (71%)	70 (100%)	0	100	100
5	b	70/99 (71%)	70 (100%)	0	100	100
5	c	70/99 (71%)	70 (100%)	0	100	100
6	A	307/343 (90%)	307 (100%)	0	100	100
6	B	307/343 (90%)	307 (100%)	0	100	100
6	C	307/343 (90%)	307 (100%)	0	100	100
All	All	2330/3891 (60%)	2330 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
6	C	389	ASN
6	C	406	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 ⓘ

26 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	$\# Z  > 2$
7	NAG	P	1	5,7	14,14,15	0.72	0	17,19,21	1.60	1 (5%)
7	NAG	P	2	7	14,14,15	0.72	0	17,19,21	1.15	2 (11%)
7	BMA	P	3	7	11,11,12	0.83	0	15,15,17	1.97	3 (20%)
7	MAN	P	4	7	11,11,12	0.73	0	15,15,17	1.02	1 (6%)
8	NAG	Q	1	5,8	14,14,15	0.72	0	17,19,21	1.16	1 (5%)
8	NAG	Q	2	8	14,14,15	0.72	0	17,19,21	0.82	0
8	FUC	Q	3	8	10,10,11	0.79	0	14,14,16	0.89	0
9	NAG	R	1	5,9	14,14,15	0.76	0	17,19,21	1.28	1 (5%)
9	NAG	R	2	9	14,14,15	0.72	0	17,19,21	1.19	1 (5%)
8	NAG	S	1	5,8	14,14,15	0.73	0	17,19,21	0.95	0
8	NAG	S	2	8	14,14,15	0.71	0	17,19,21	0.88	0
8	FUC	S	3	8	10,10,11	0.79	0	14,14,16	0.91	0
9	NAG	T	1	5,9	14,14,15	0.74	0	17,19,21	1.06	1 (5%)
9	NAG	T	2	9	14,14,15	0.72	0	17,19,21	0.84	0
10	NAG	U	1	5,10	14,14,15	0.74	0	17,19,21	1.35	1 (5%)
10	NAG	U	2	10	14,14,15	0.73	0	17,19,21	0.87	0
10	BMA	U	3	10	11,11,12	0.84	0	15,15,17	2.06	3 (20%)
7	NAG	V	1	5,7	14,14,15	0.78	0	17,19,21	2.47	2 (11%)
7	NAG	V	2	7	14,14,15	0.73	0	17,19,21	0.95	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BMA	V	3	7	11,11,12	0.86	0	15,15,17	2.10	3 (20%)
7	MAN	V	4	7	11,11,12	0.71	0	15,15,17	1.07	1 (6%)
8	NAG	W	1	5,8	14,14,15	0.72	0	17,19,21	0.98	1 (5%)
8	NAG	W	2	8	14,14,15	0.70	0	17,19,21	1.17	1 (5%)
8	FUC	W	3	8	10,10,11	0.79	0	14,14,16	0.86	0
9	NAG	X	1	5,9	14,14,15	0.73	0	17,19,21	0.99	1 (5%)
9	NAG	X	2	9	14,14,15	0.71	0	17,19,21	0.80	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
7	NAG	P	1	5,7	-	1/6/23/26	0/1/1/1
7	NAG	P	2	7	-	0/6/23/26	0/1/1/1
7	BMA	P	3	7	-	2/2/19/22	0/1/1/1
7	MAN	P	4	7	-	0/2/19/22	0/1/1/1
8	NAG	Q	1	5,8	-	0/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	0/6/23/26	0/1/1/1
8	FUC	Q	3	8	-	-	0/1/1/1
9	NAG	R	1	5,9	-	2/6/23/26	0/1/1/1
9	NAG	R	2	9	-	3/6/23/26	0/1/1/1
8	NAG	S	1	5,8	-	0/6/23/26	0/1/1/1
8	NAG	S	2	8	-	2/6/23/26	0/1/1/1
8	FUC	S	3	8	-	-	0/1/1/1
9	NAG	T	1	5,9	-	0/6/23/26	0/1/1/1
9	NAG	T	2	9	-	0/6/23/26	0/1/1/1
10	NAG	U	1	5,10	-	2/6/23/26	0/1/1/1
10	NAG	U	2	10	-	0/6/23/26	0/1/1/1
10	BMA	U	3	10	-	1/2/19/22	0/1/1/1
7	NAG	V	1	5,7	-	4/6/23/26	0/1/1/1
7	NAG	V	2	7	-	3/6/23/26	0/1/1/1
7	BMA	V	3	7	-	2/2/19/22	0/1/1/1
7	MAN	V	4	7	-	0/2/19/22	0/1/1/1
8	NAG	W	1	5,8	-	3/6/23/26	0/1/1/1
8	NAG	W	2	8	-	2/6/23/26	0/1/1/1
8	FUC	W	3	8	-	-	0/1/1/1
9	NAG	X	1	5,9	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	X	2	9	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	V	1	NAG	C2-N2-C7	8.87	134.79	122.90
7	V	3	BMA	C1-O5-C5	6.37	120.72	112.19
10	U	3	BMA	C1-O5-C5	6.23	120.54	112.19
7	P	3	BMA	C1-O5-C5	5.79	119.94	112.19
7	P	1	NAG	C2-N2-C7	4.81	129.35	122.90
10	U	1	NAG	C2-N2-C7	3.72	127.88	122.90
9	R	2	NAG	C2-N2-C7	3.16	127.14	122.90
8	W	2	NAG	C2-N2-C7	3.08	127.03	122.90
8	Q	1	NAG	C1-O5-C5	3.03	116.25	112.19
9	R	1	NAG	C2-N2-C7	3.03	126.96	122.90
7	V	4	MAN	C1-O5-C5	2.96	116.15	112.19
7	P	4	MAN	C1-O5-C5	2.78	115.92	112.19
7	P	2	NAG	O5-C1-C2	-2.76	107.03	111.29
7	V	1	NAG	C8-C7-N2	2.58	120.40	116.12
7	P	2	NAG	O4-C4-C3	-2.43	104.66	110.38
9	X	1	NAG	O5-C1-C2	-2.41	107.57	111.29
9	T	1	NAG	C1-O5-C5	2.33	115.31	112.19
7	V	3	BMA	C2-C3-C4	2.32	114.94	110.86
7	V	2	NAG	C2-N2-C7	2.31	126.00	122.90
7	V	3	BMA	C3-C4-C5	2.30	114.39	110.23
10	U	3	BMA	C2-C3-C4	2.27	114.85	110.86
10	U	3	BMA	C3-C4-C5	2.24	114.29	110.23
7	P	3	BMA	C3-C4-C5	2.22	114.26	110.23
7	P	3	BMA	C2-C3-C4	2.12	114.59	110.86
8	W	1	NAG	C2-N2-C7	2.09	125.70	122.90

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	P	1	NAG	C3-C2-N2-C7
7	V	3	BMA	O5-C5-C6-O6
7	P	3	BMA	C4-C5-C6-O6
7	P	3	BMA	O5-C5-C6-O6
7	V	1	NAG	C8-C7-N2-C2

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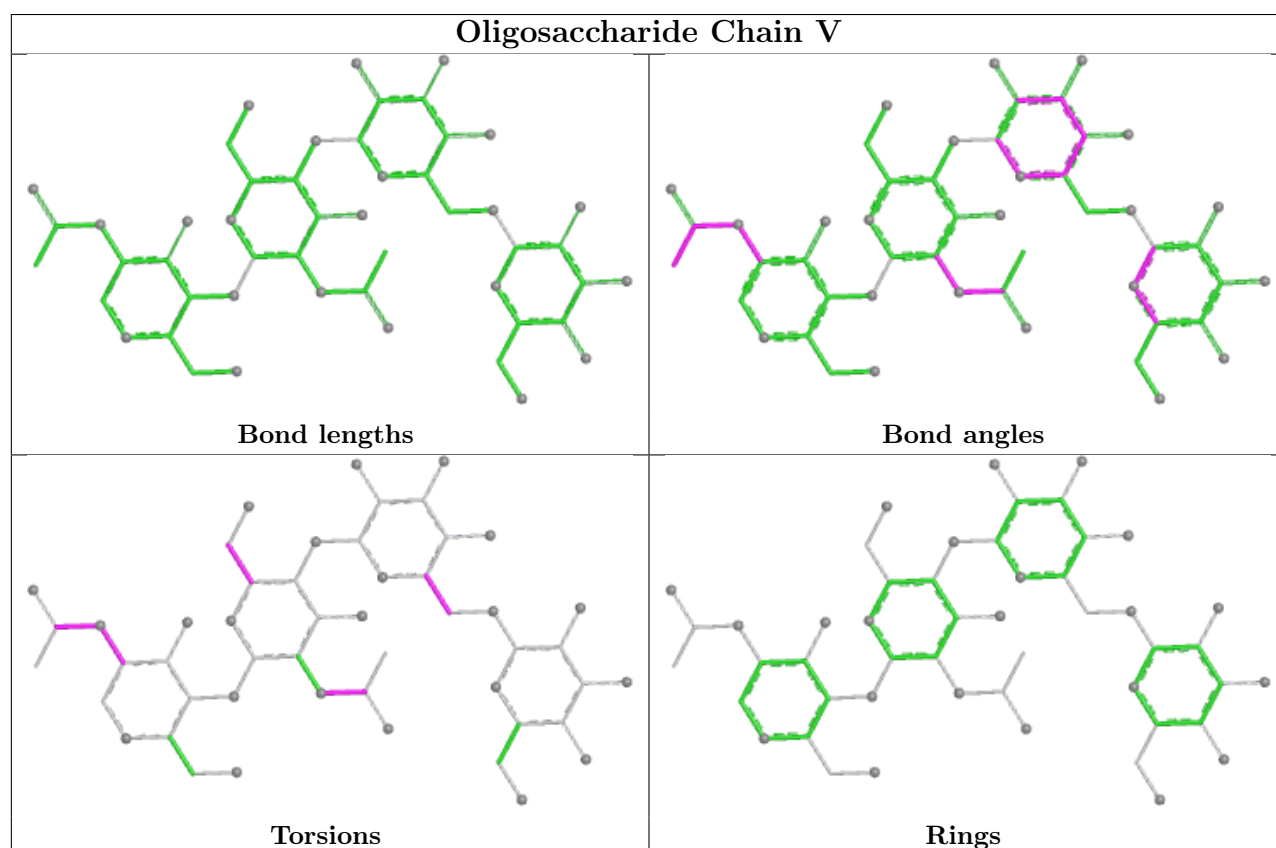
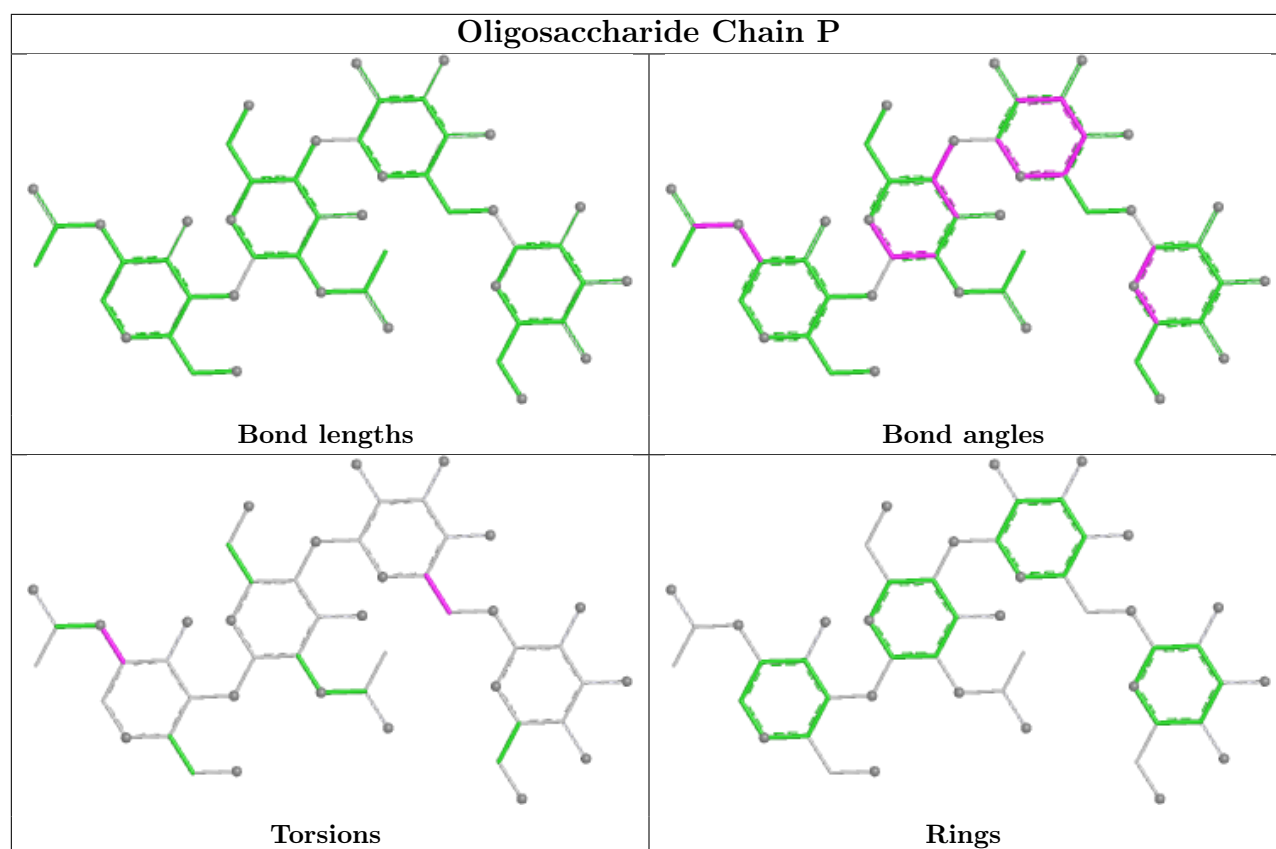
Mol	Chain	Res	Type	Atoms
7	V	1	NAG	O7-C7-N2-C2
7	V	2	NAG	C8-C7-N2-C2
7	V	2	NAG	O7-C7-N2-C2
8	S	2	NAG	C8-C7-N2-C2
8	S	2	NAG	O7-C7-N2-C2
8	W	1	NAG	C8-C7-N2-C2
8	W	1	NAG	O7-C7-N2-C2
9	R	1	NAG	C8-C7-N2-C2
9	R	1	NAG	O7-C7-N2-C2
9	X	1	NAG	C8-C7-N2-C2
9	X	1	NAG	O7-C7-N2-C2
9	X	1	NAG	O5-C5-C6-O6
7	V	3	BMA	C4-C5-C6-O6
10	U	3	BMA	O5-C5-C6-O6
7	V	2	NAG	O5-C5-C6-O6
9	R	2	NAG	O5-C5-C6-O6
8	W	2	NAG	C1-C2-N2-C7
9	R	2	NAG	C1-C2-N2-C7
7	V	1	NAG	C3-C2-N2-C7
8	W	2	NAG	C3-C2-N2-C7
10	U	1	NAG	C3-C2-N2-C7
7	V	1	NAG	C1-C2-N2-C7
10	U	1	NAG	C1-C2-N2-C7
9	R	2	NAG	C3-C2-N2-C7
8	W	1	NAG	C4-C5-C6-O6

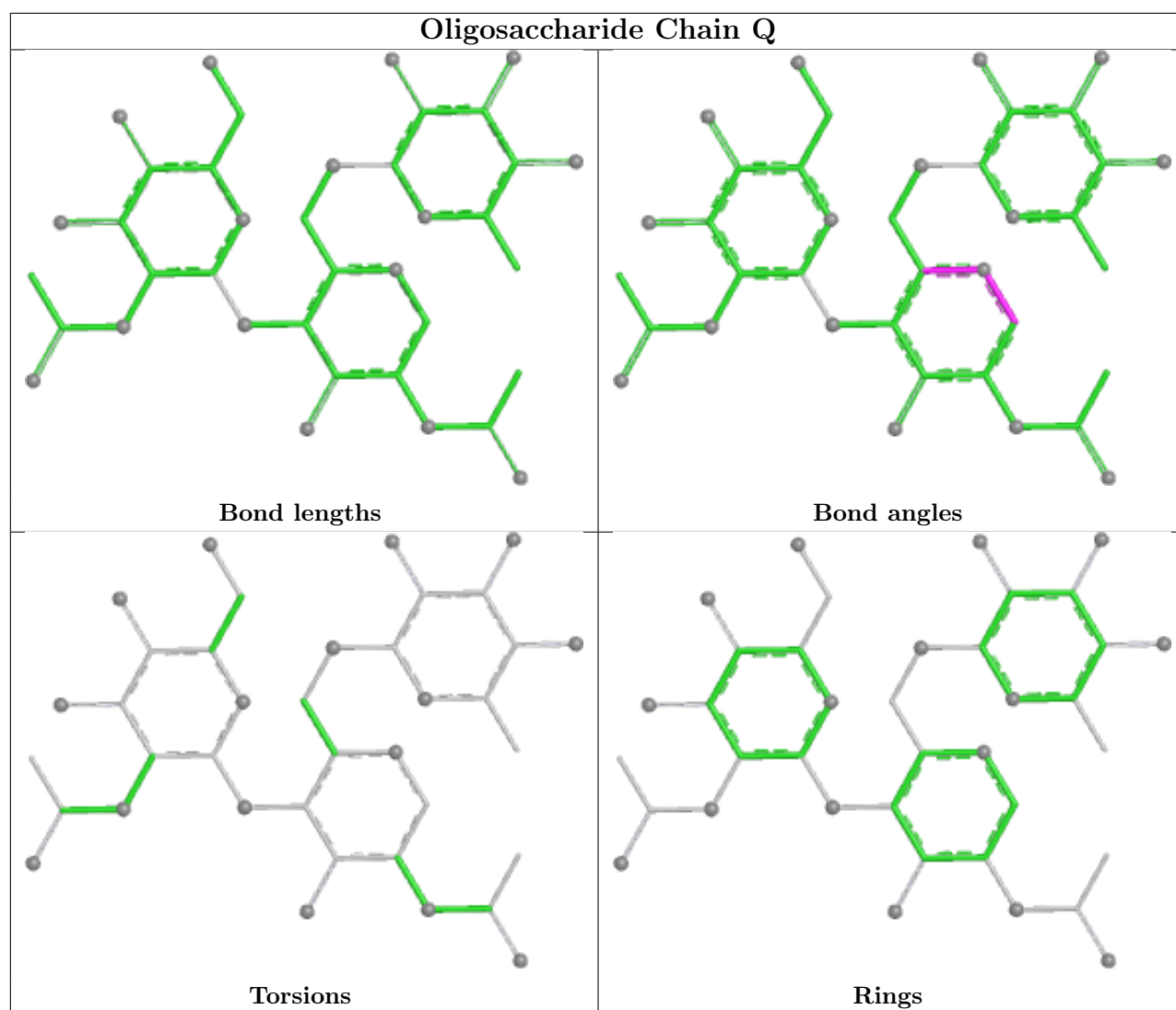
There are no ring outliers.

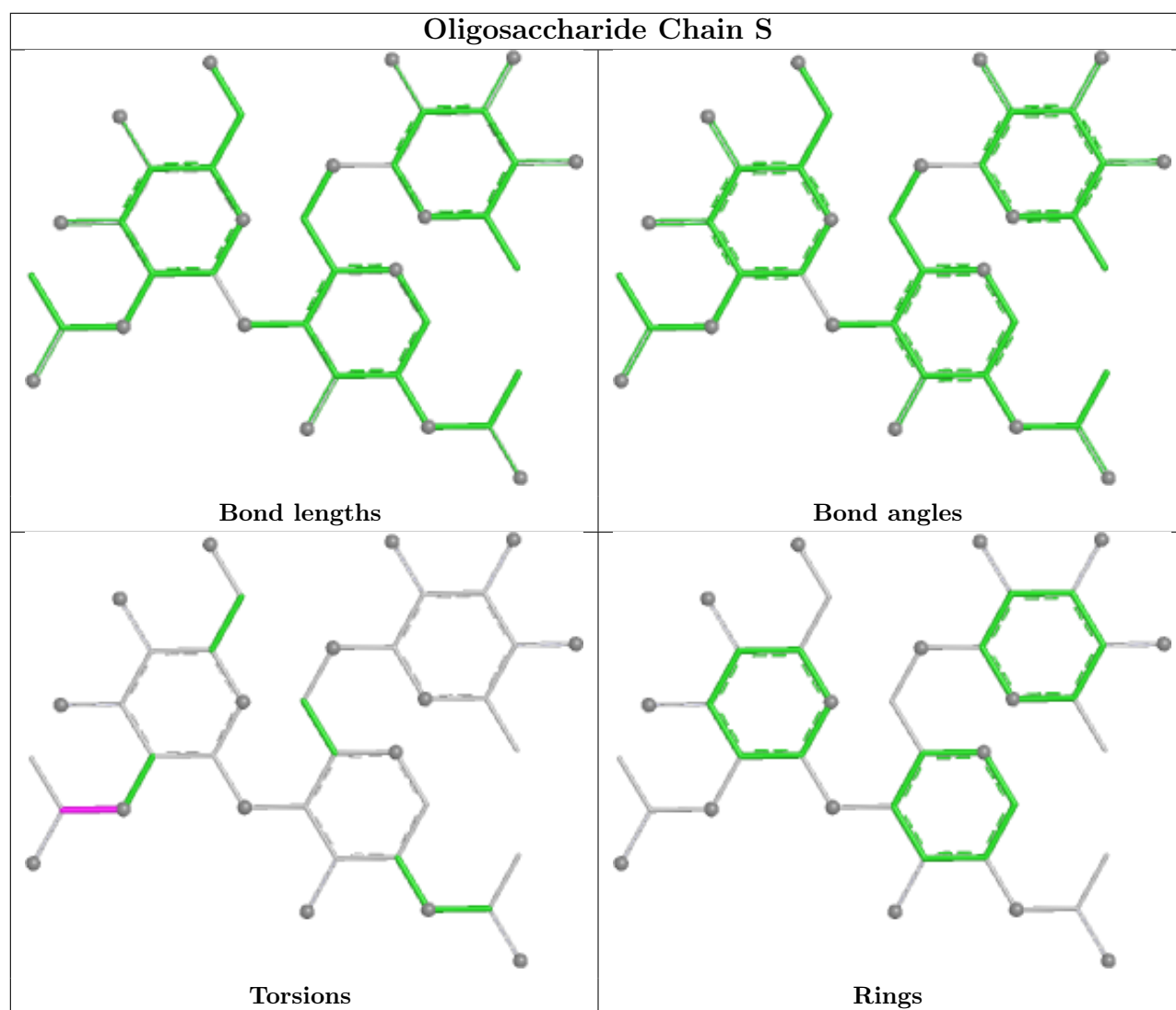
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	V	1	NAG	1	0
8	Q	3	FUC	1	0
9	X	1	NAG	1	0
7	V	2	NAG	1	0
8	Q	1	NAG	1	0

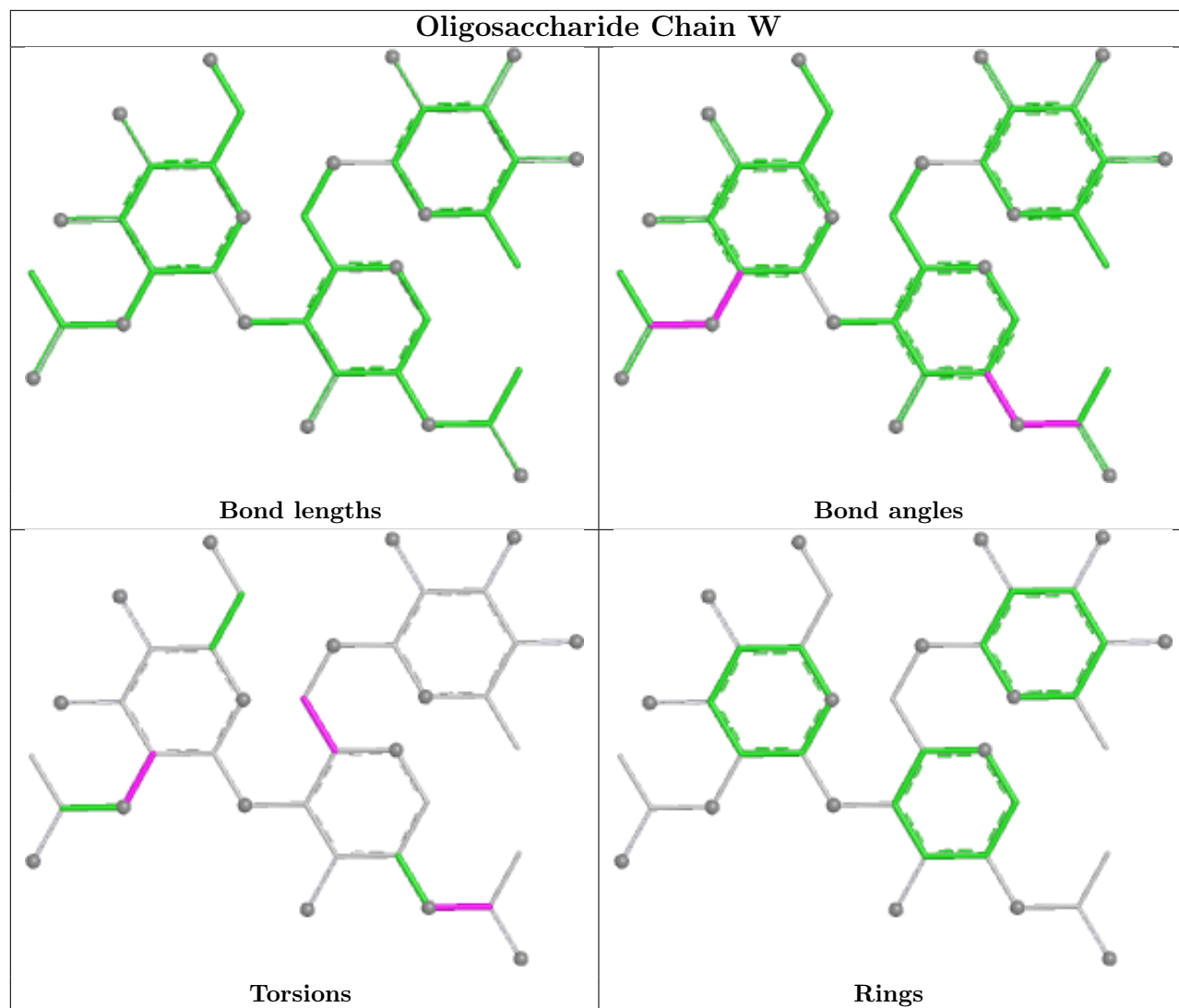
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

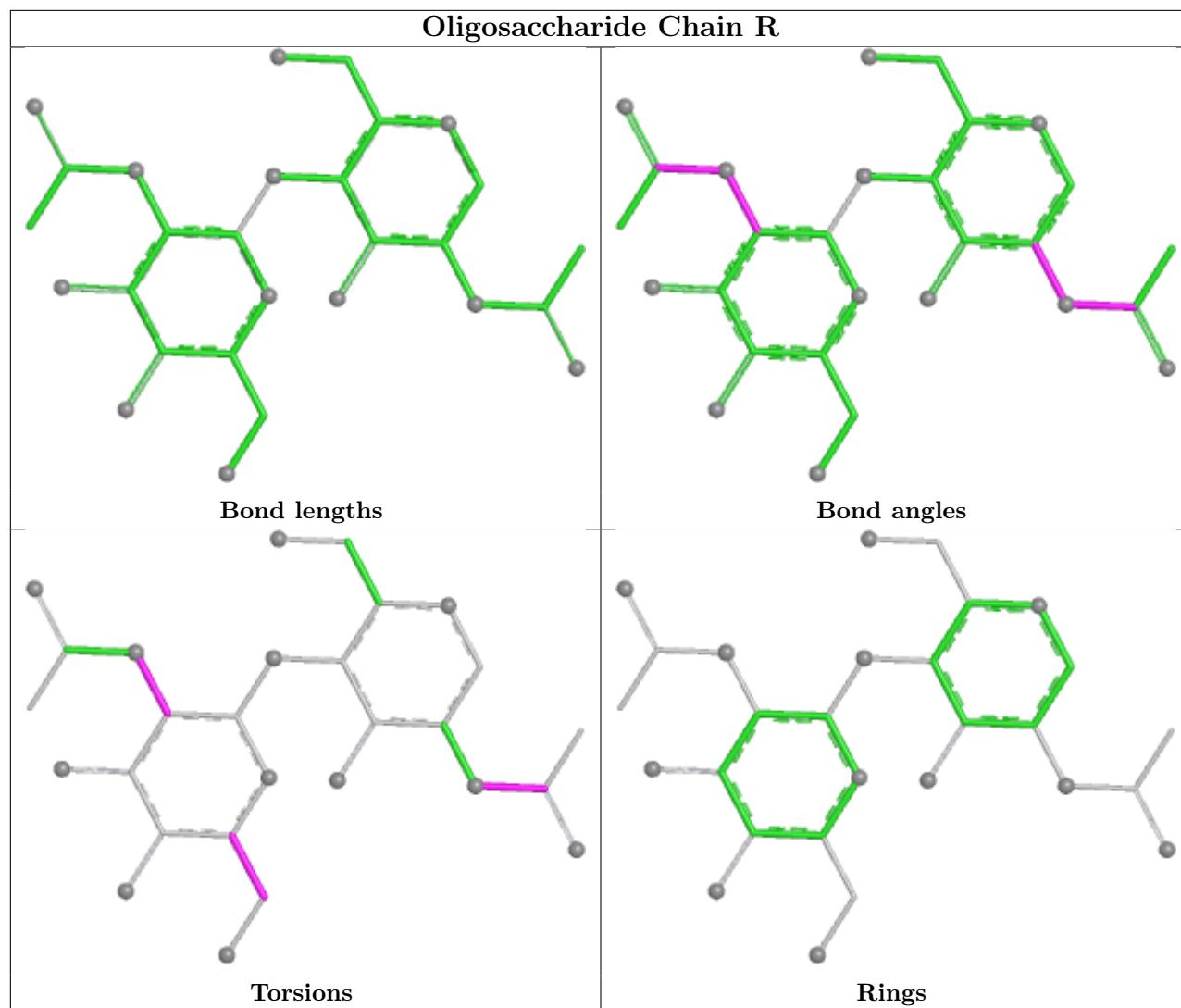


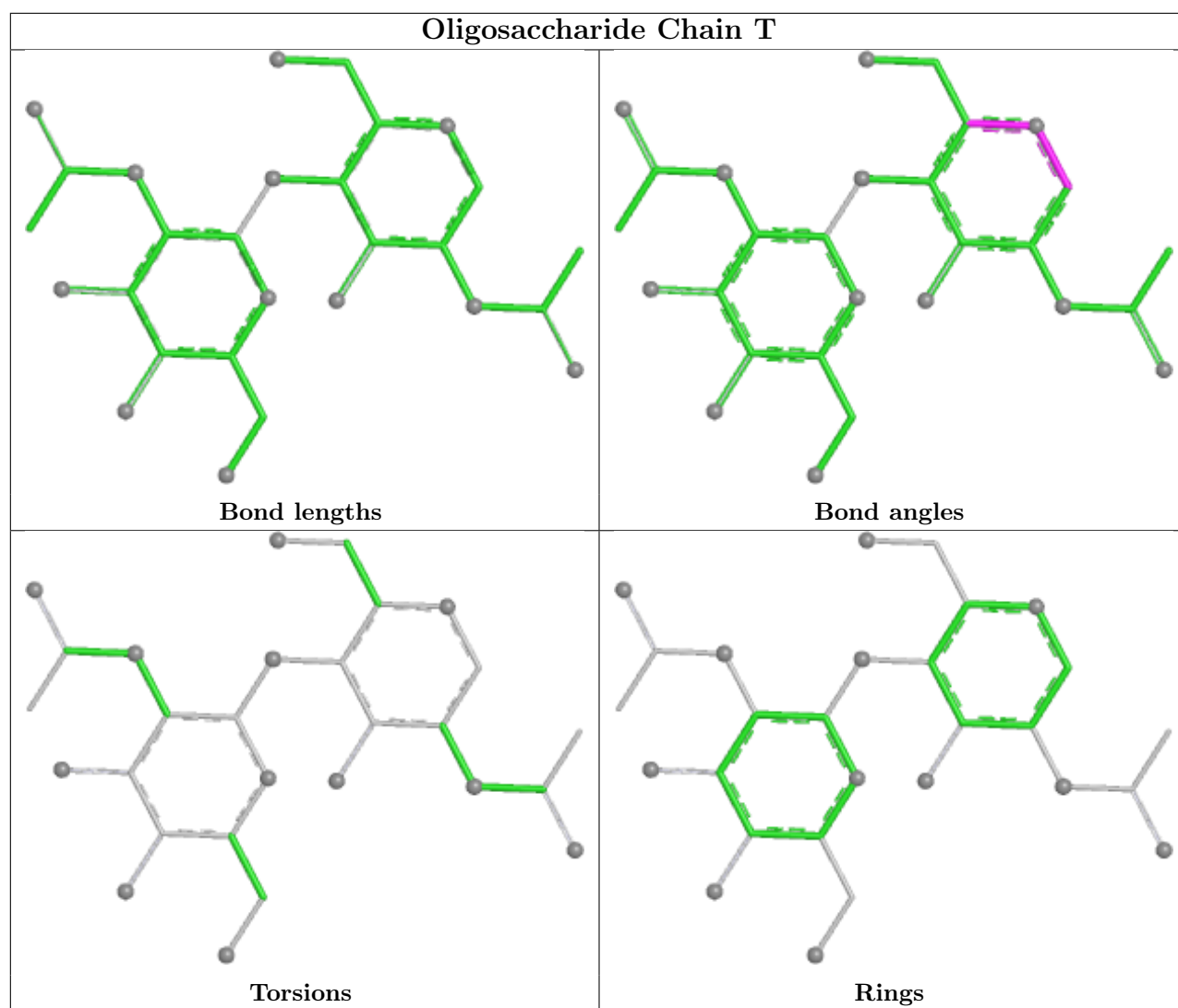


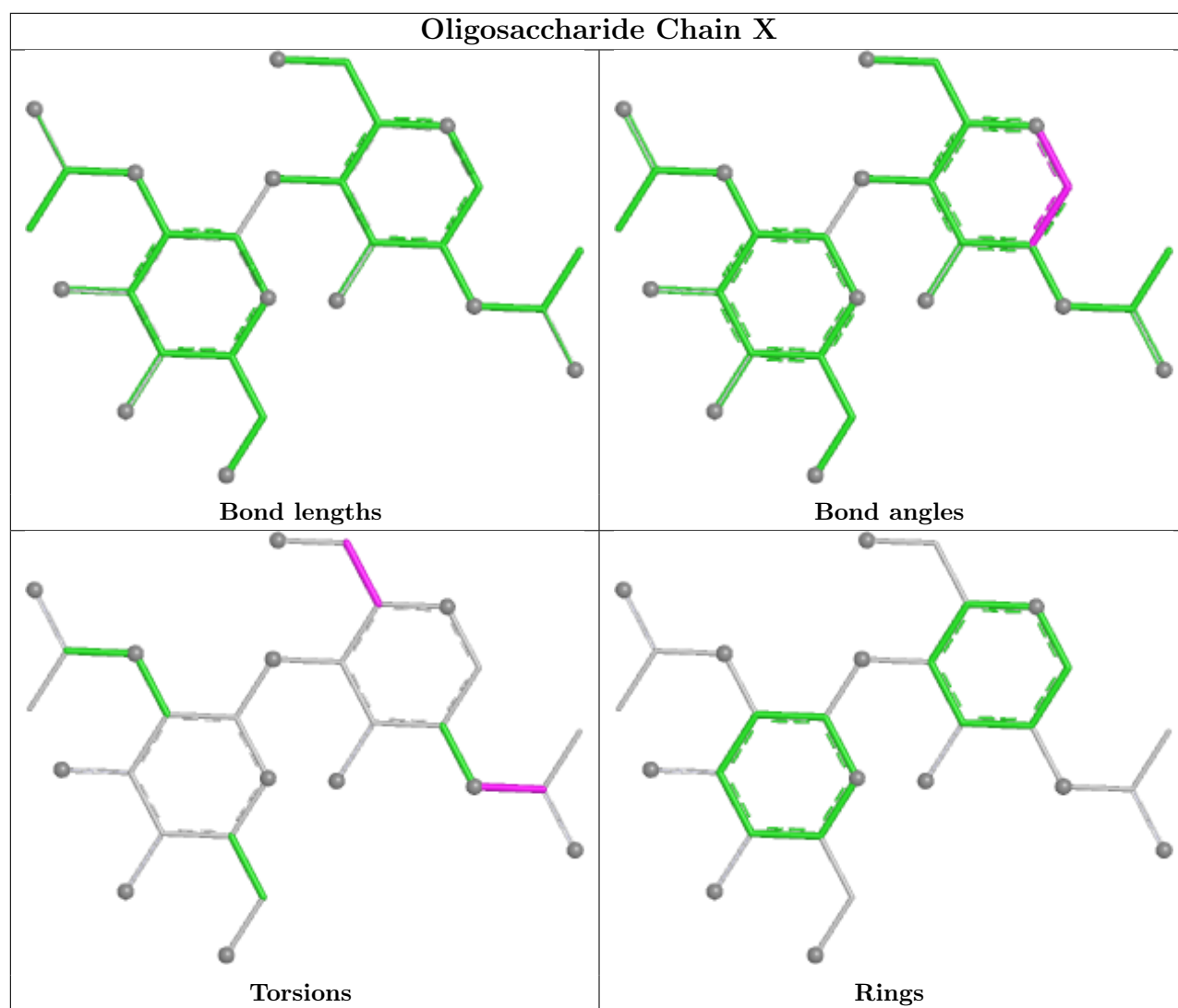


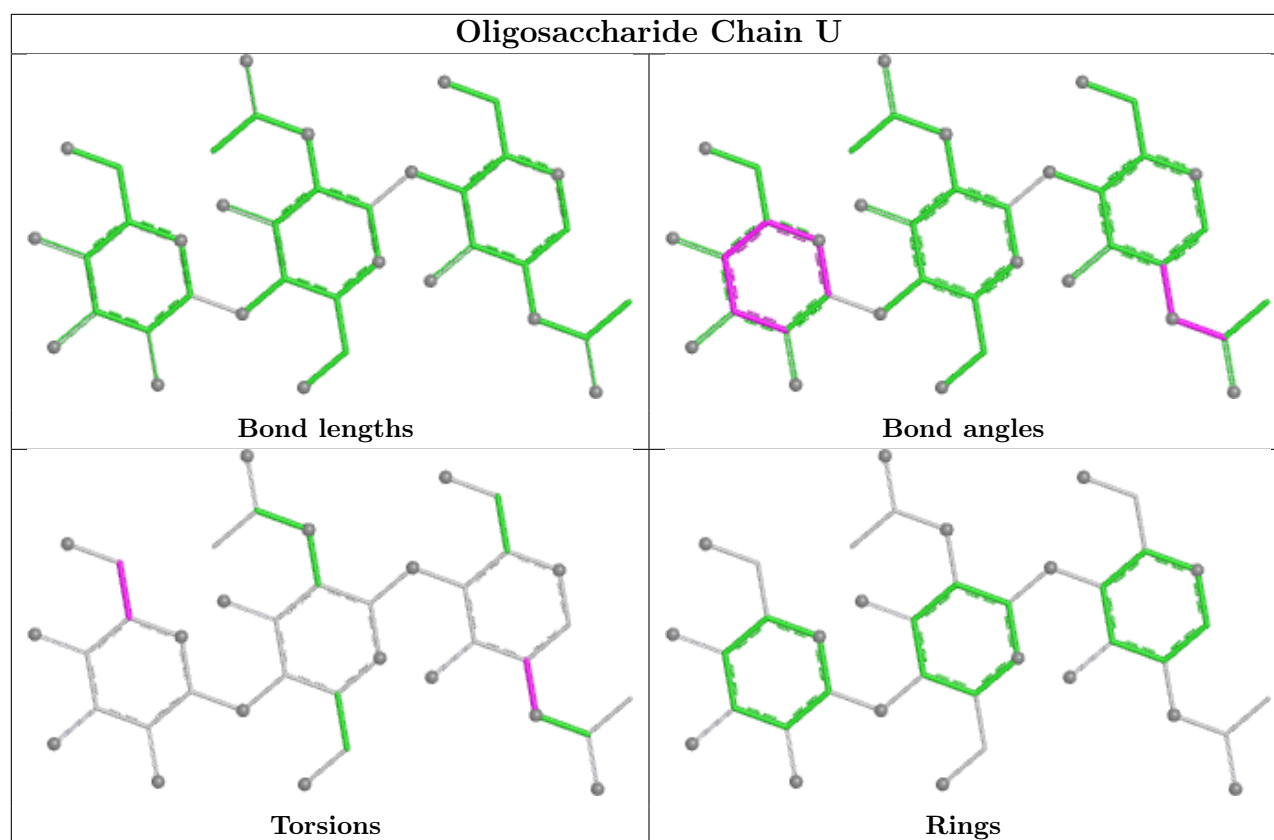












## 5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z  > 2$
11	MAN	F	501	-	11,11,12	0.78	0	15,15,17	1.04	1 (6%)

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
11	MAN	F	501	-	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
11	F	501	MAN	C1-O5-C5	2.79	115.92	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	F	501	MAN	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

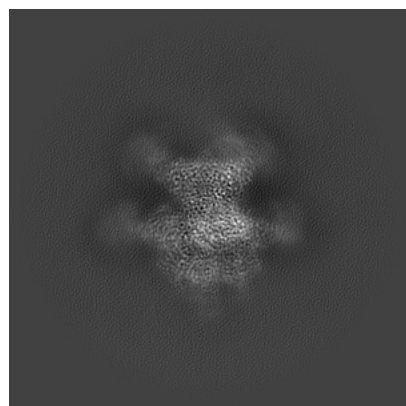
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72151. These allow visual inspection of the internal detail of the map and identification of artifacts.

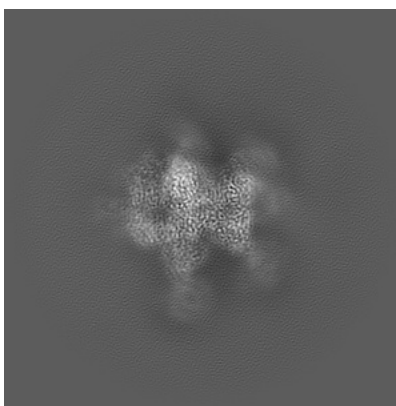
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

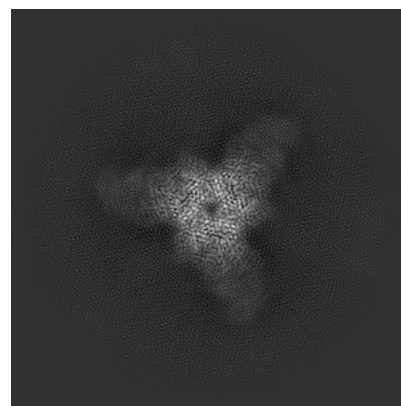
#### 6.1.1 Primary map



X

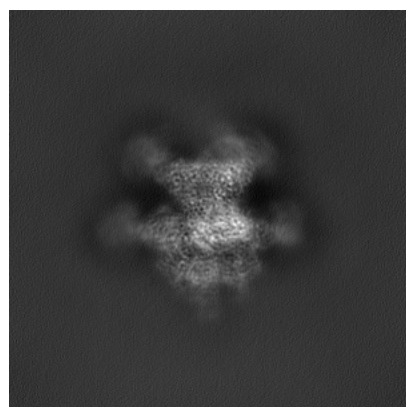


Y

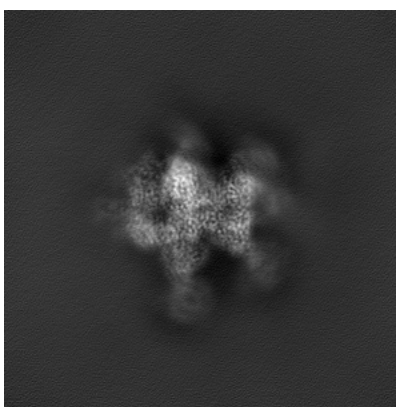


Z

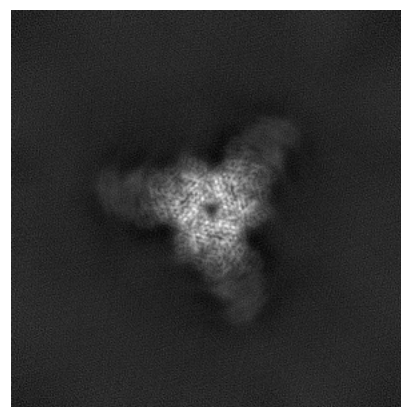
#### 6.1.2 Raw map



X



Y

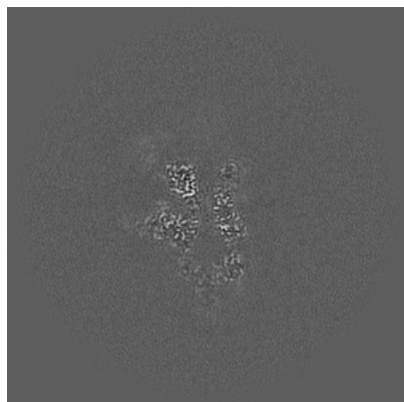


Z

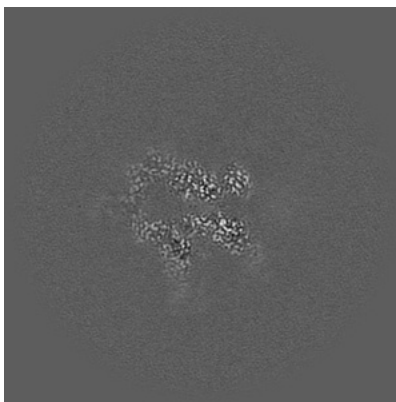
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

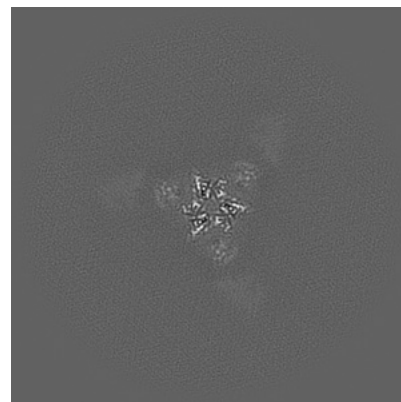
### 6.2.1 Primary map



X Index: 180

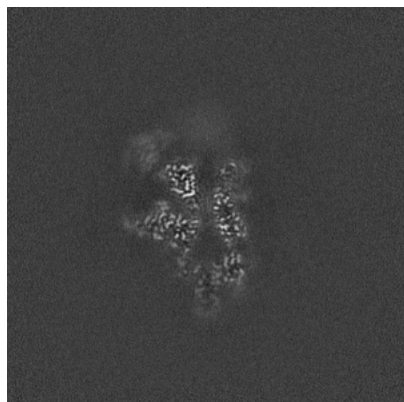


Y Index: 180

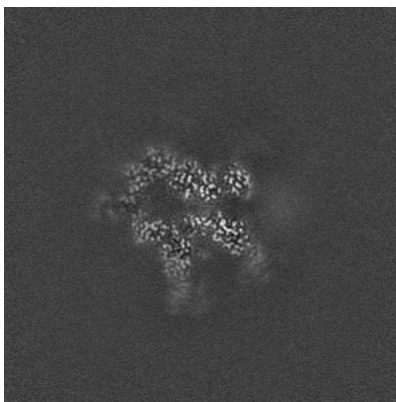


Z Index: 180

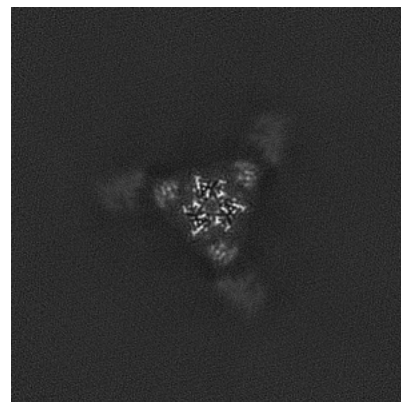
### 6.2.2 Raw map



X Index: 180



Y Index: 180



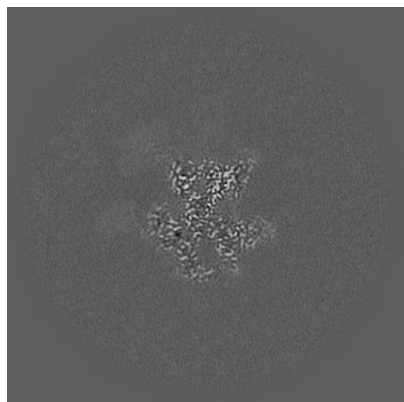
Z Index: 180

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

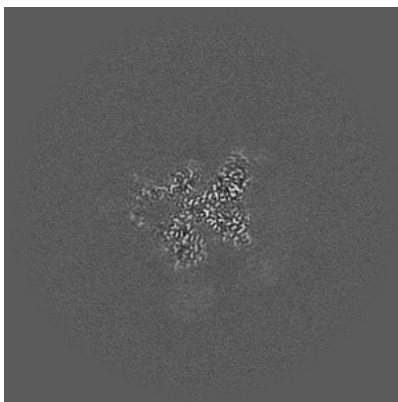


## 6.3 Largest variance slices [i](#)

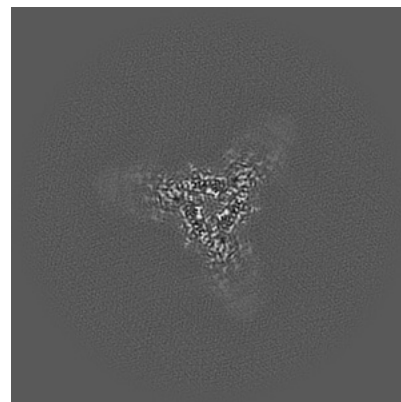
### 6.3.1 Primary map



X Index: 196

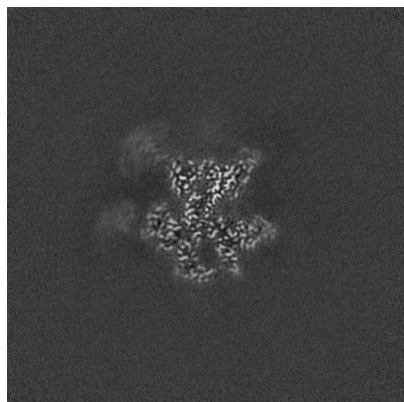


Y Index: 191

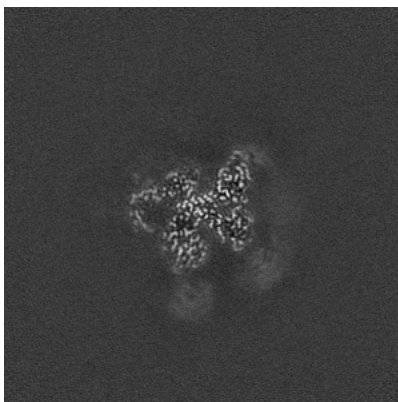


Z Index: 168

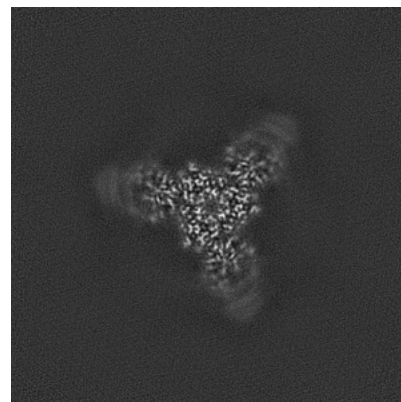
### 6.3.2 Raw map



X Index: 196



Y Index: 193

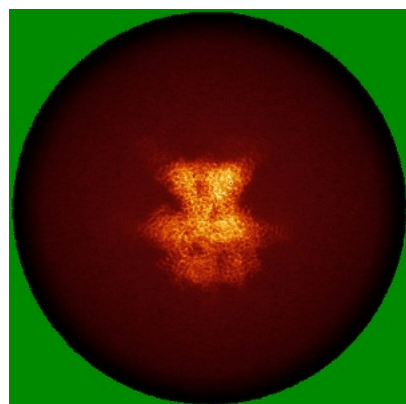


Z Index: 167

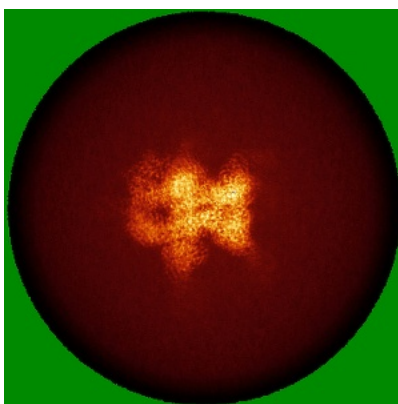
The images above show the largest variance slices of the map in three orthogonal directions.

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

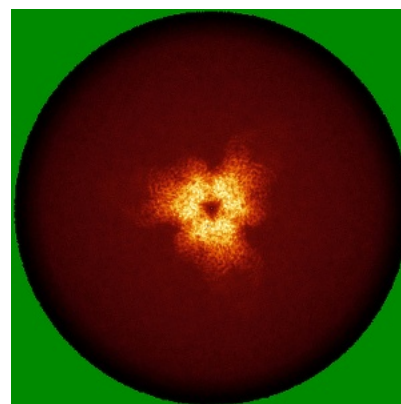
### 6.4.1 Primary map



X

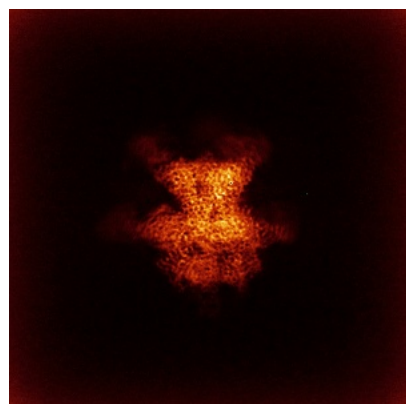


Y

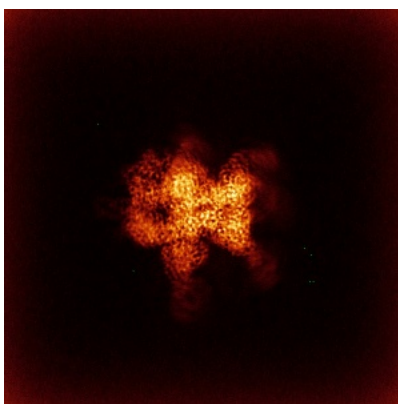


Z

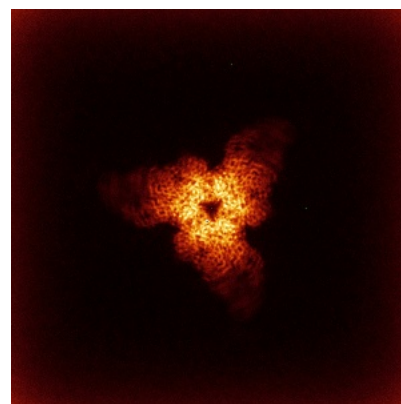
### 6.4.2 Raw map



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](#)

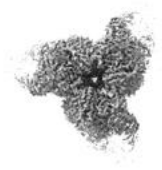
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.094. 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



X



Y



Z

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

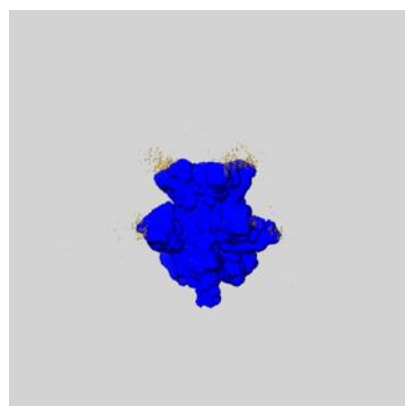
## 6.6 Mask visualisation [i](#)

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

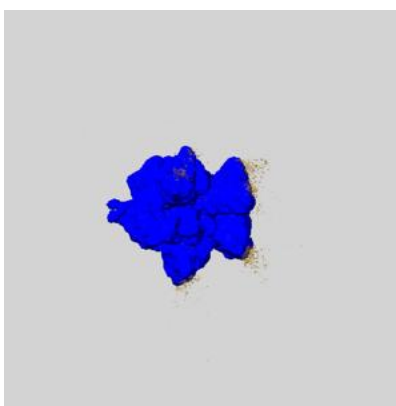
A mask typically either:

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

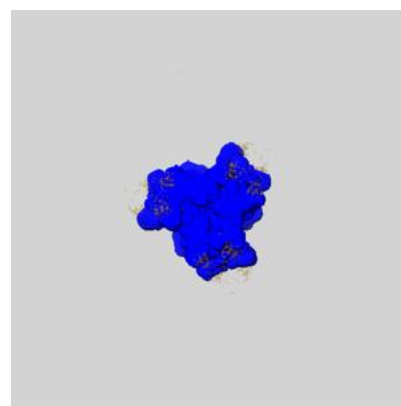
### 6.6.1 emd\_72151\_msk\_1.map [i](#)



X



Y

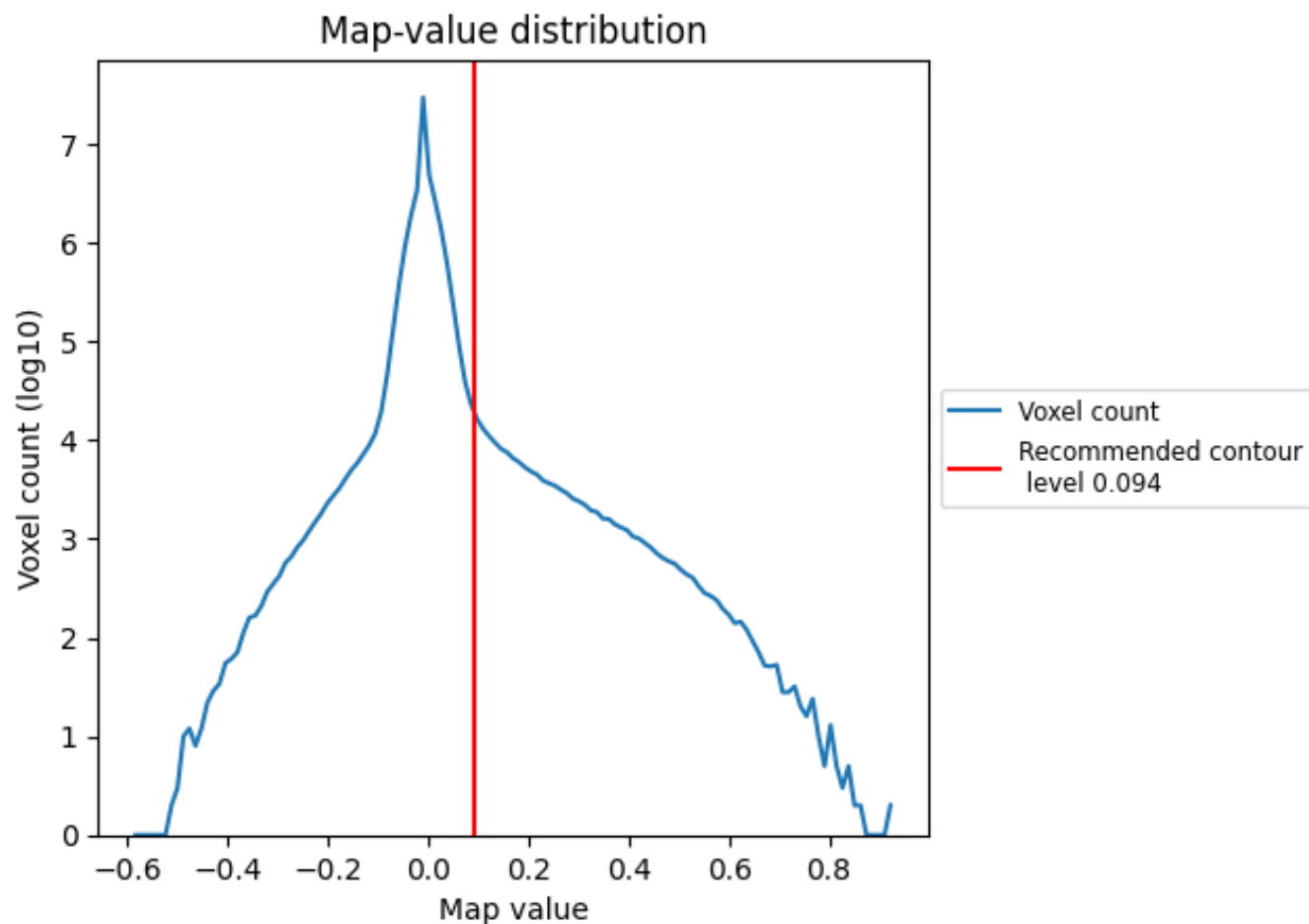


Z

## 7 Map analysis [i](#)

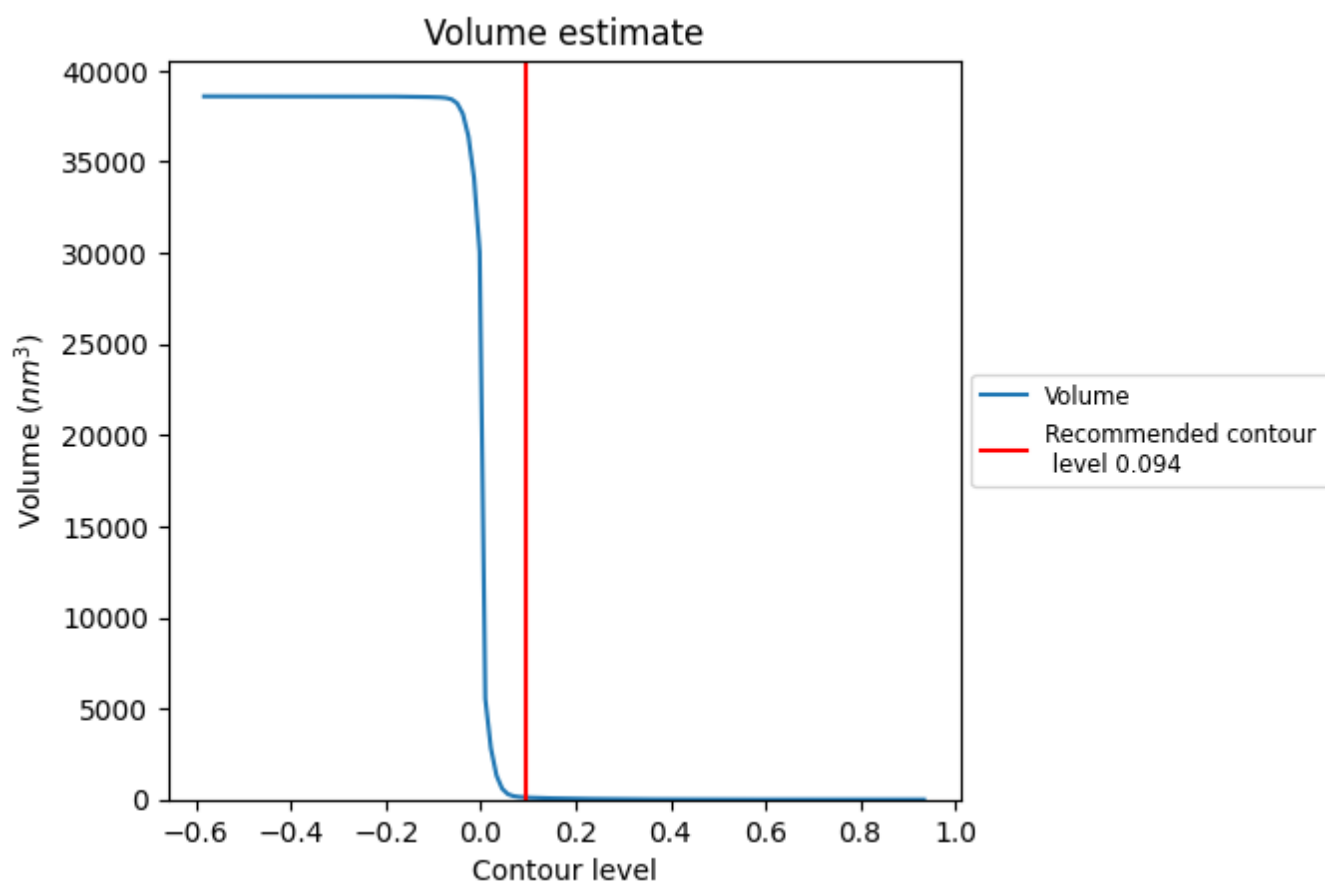
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

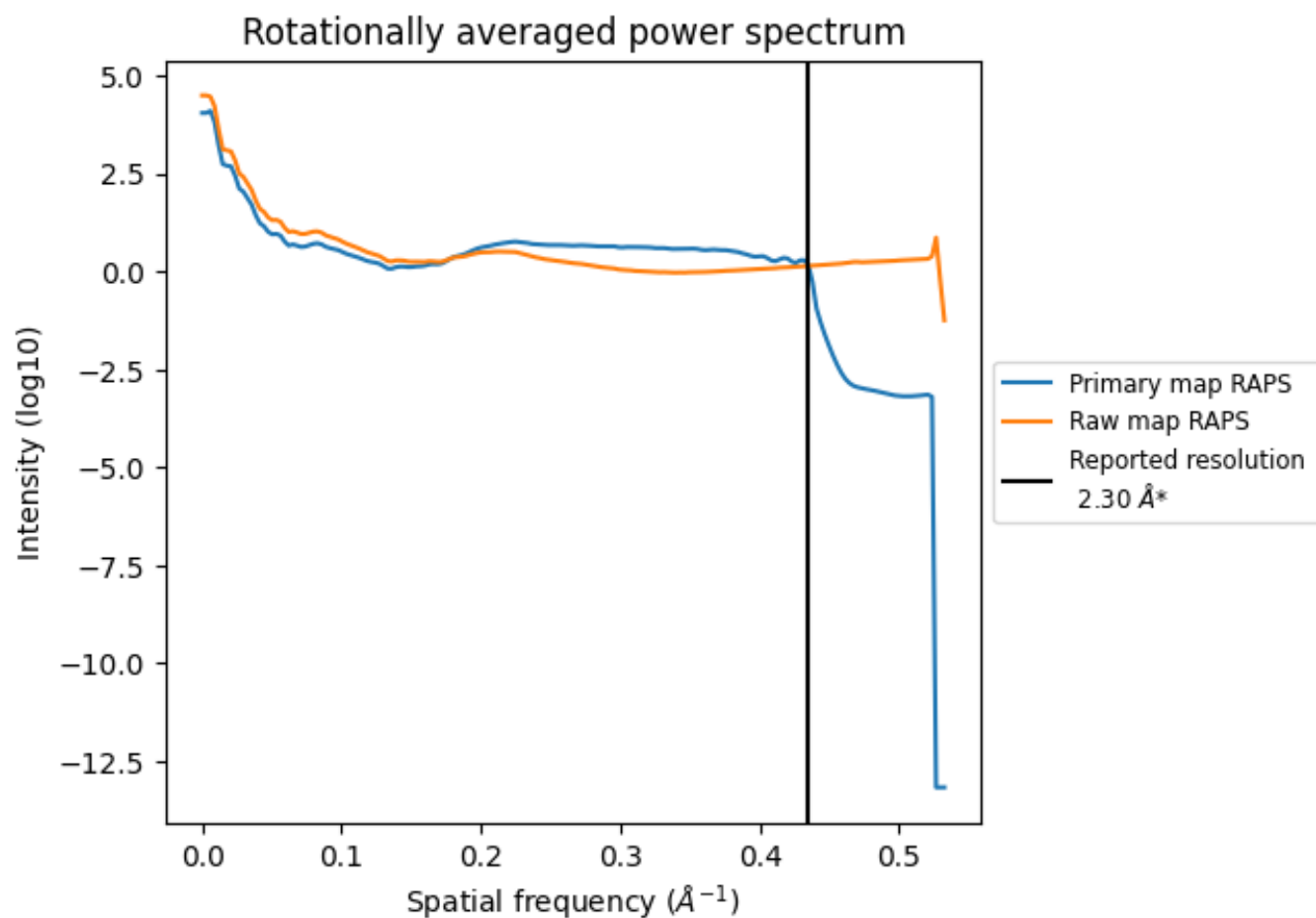
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 120 nm<sup>3</sup>; this corresponds to an approximate mass of 108 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 ⓘ

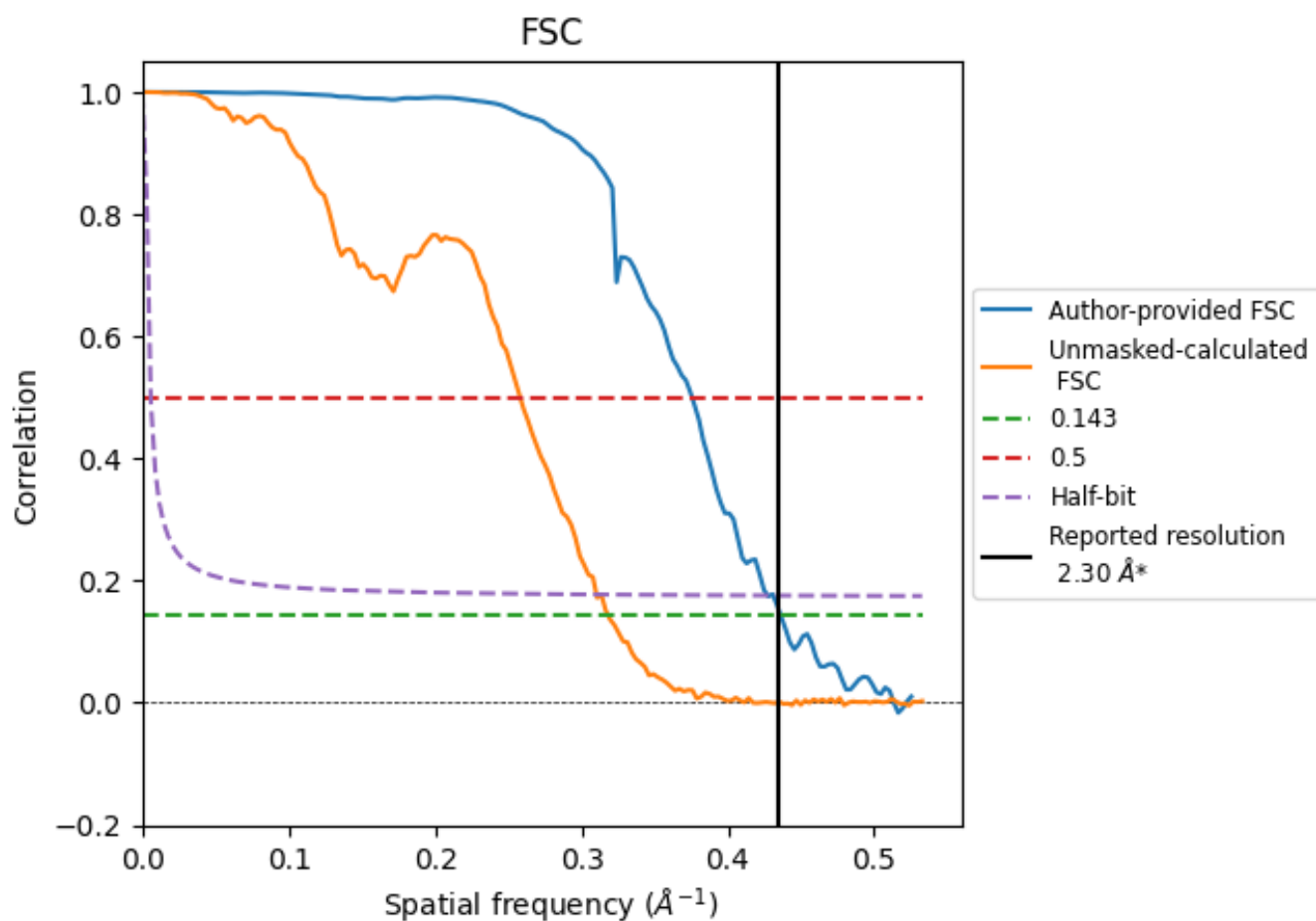


\*Reported resolution corresponds to spatial frequency of 0.435 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.435 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

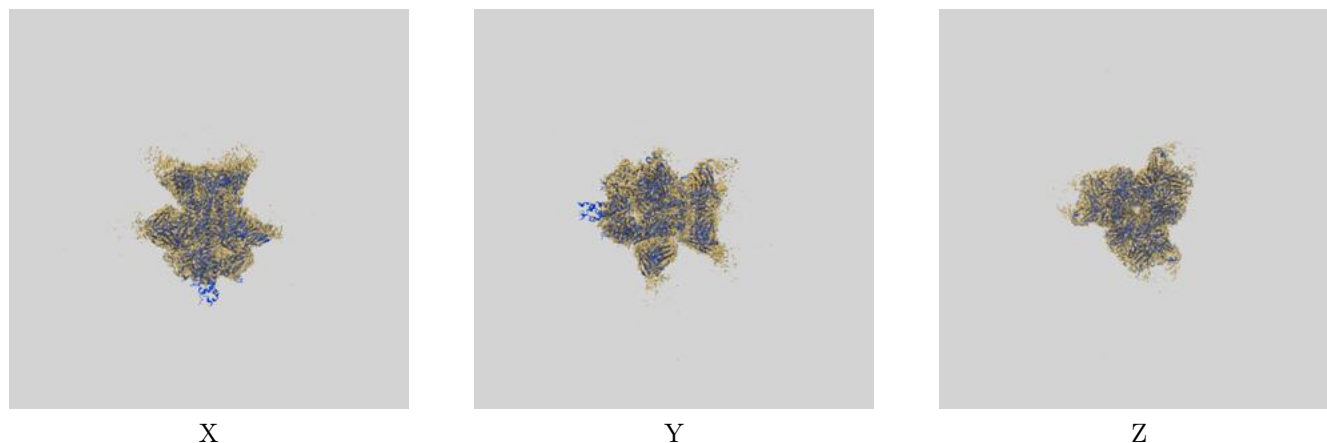
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.29	2.66	2.34
Unmasked-calculated*	3.14	3.87	3.22

\*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 3.14 differs from the reported value 2.3 by more than 10 %

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

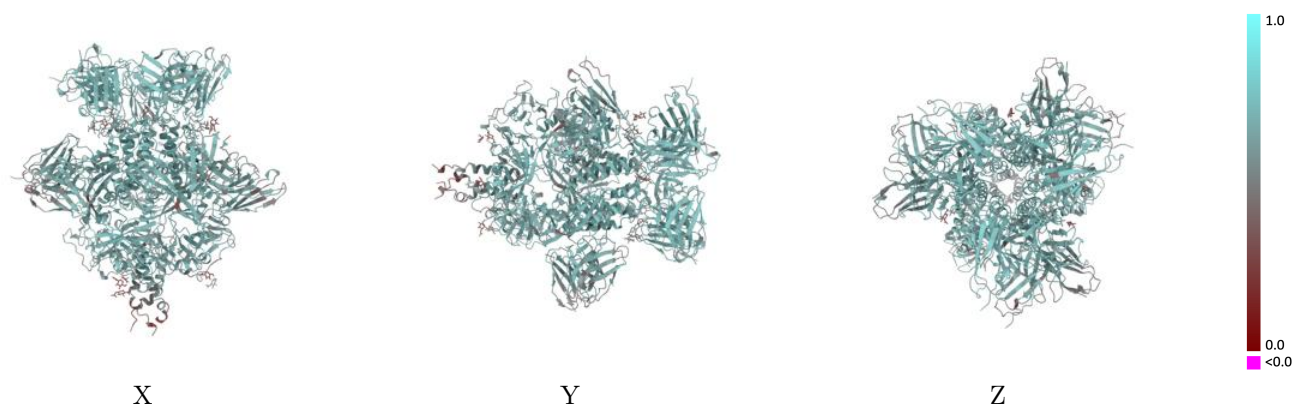
This section contains information regarding the fit between EMDB map EMD-72151 and PDB model 9Q26. Per-residue inclusion information can be found in section [3](#) on page [11](#).

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



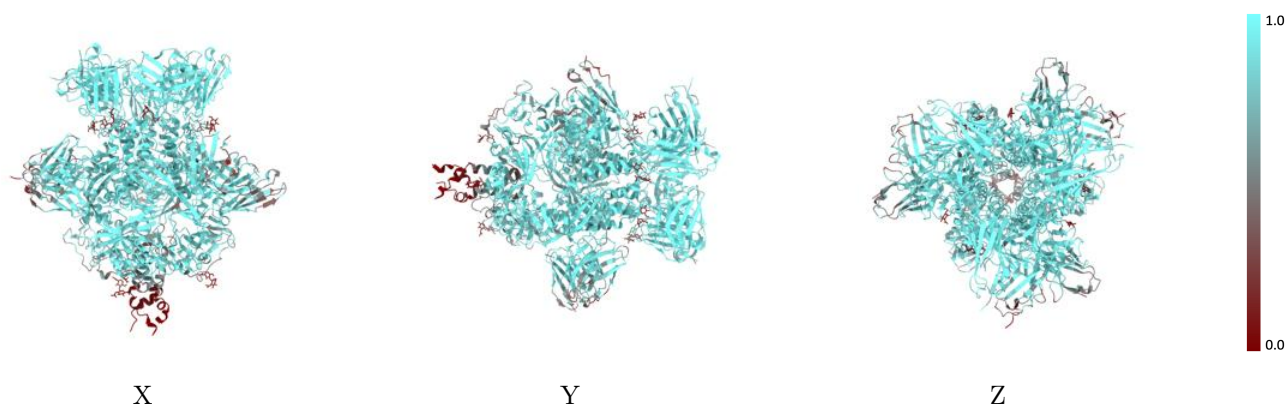
The images above show the 3D surface view of the map at the recommended contour level 0.094 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



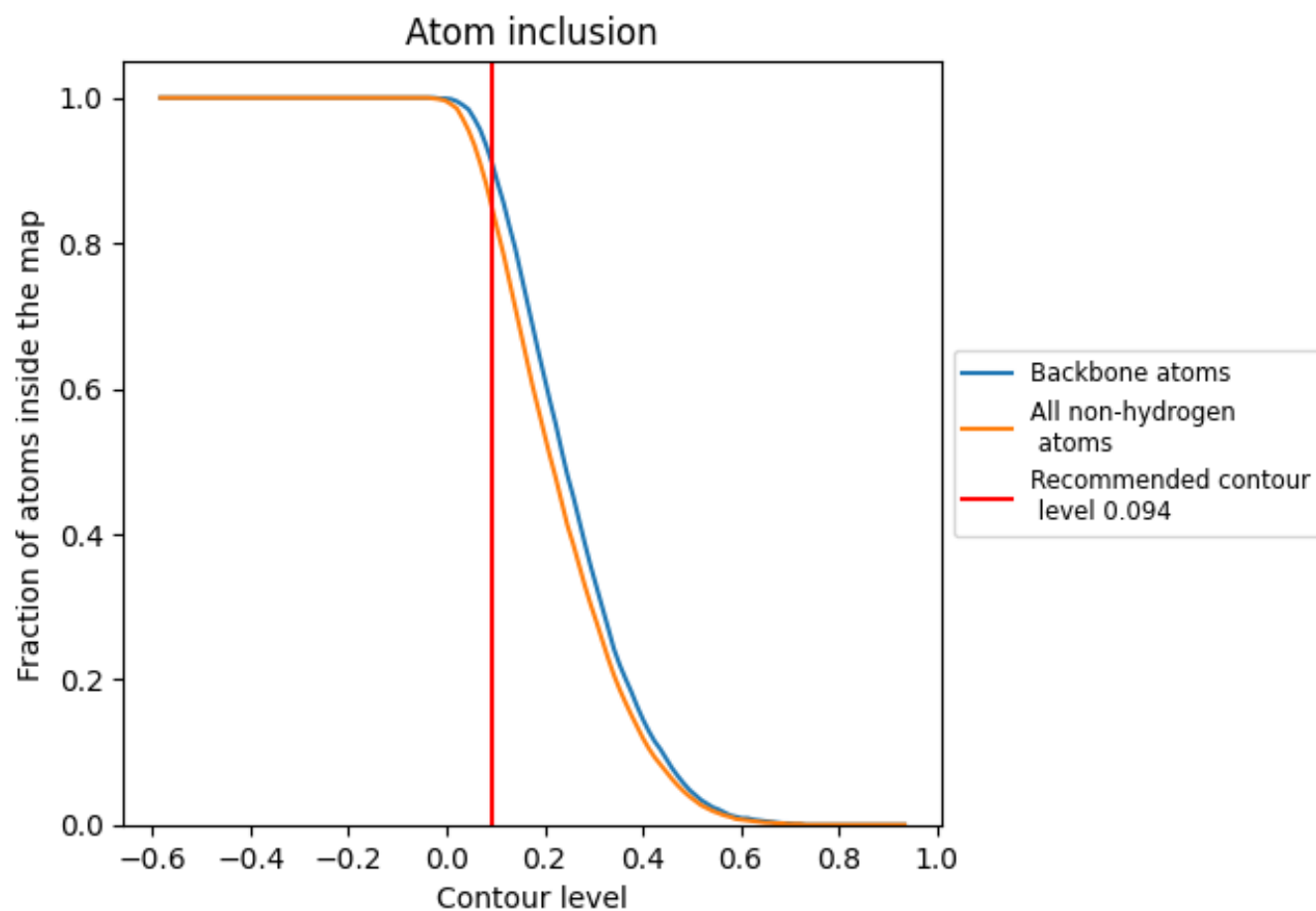
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.094).

























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 85% 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 (0.094) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8460	 0.6280
A	 0.8370	 0.6320
B	 0.8360	 0.6360
C	 0.8350	 0.6330
D	 0.7860	 0.5910
E	 0.7720	 0.5890
F	 0.9160	 0.6560
G	 0.9270	 0.6610
H	 0.7830	 0.5920
I	 0.7780	 0.5920
J	 0.9240	 0.6560
K	 0.9280	 0.6590
L	 0.7790	 0.5940
M	 0.7780	 0.5840
N	 0.9280	 0.6630
O	 0.9290	 0.6600
P	 0.5400	 0.5360
Q	 0.3680	 0.4120
R	 0.1070	 0.2410
S	 0.2890	 0.3660
T	 0.1430	 0.2330
U	 0.6920	 0.5800
V	 0.5000	 0.4950
W	 0.2630	 0.3920
X	 0.0360	 0.3370
a	 0.9330	 0.6590
b	 0.9350	 0.6580
c	 0.9300	 0.6580

