



## wwPDB EM Validation Summary Report ⓘ

Oct 20, 2024 – 07:03 PM EDT

PDB ID : 7UGP  
EMDB ID : EMD-26493  
Title : Cryo-EM structure of BG24 Fabs with an inferred germline light chain and 10-1074 Fabs in complex with HIV-1 Env immunogen BG505-SOSIPv4.1-GT1 containing the N276 gp120 glycan- Class 1  
Authors : Dam, K.A.; Bjorkman, P.J.  
Deposited on : 2022-03-25  
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

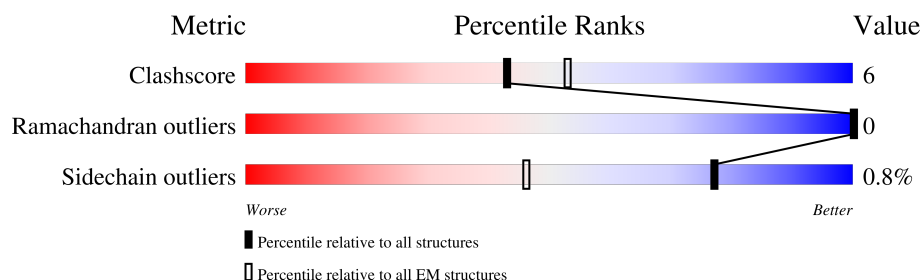
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	A	443	
1	B	443	
1	C	443	
2	D	128	
2	E	128	
2	F	128	
3	M	133	
3	N	133	

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Mol	Chain	Length	Quality of chain
3	O	133	
4	G	120	
4	H	120	
4	I	120	
5	P	107	
5	Q	107	
5	R	107	
6	J	105	
6	K	105	
6	L	105	
7	S	6	
7	V	6	
7	Z	6	
8	T	2	
8	W	2	
8	a	2	
9	U	3	
9	X	3	
9	Y	3	

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 25047 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	443	Total	C	N	O	S	0	0
			3488	2195	616	650	27		
1	B	443	Total	C	N	O	S	0	0
			3488	2195	616	650	27		
1	C	443	Total	C	N	O	S	0	0
			3488	2195	616	650	27		

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP Q2N0S5
A	?	-	LYS	deletion	UNP Q2N0S5
A	?	-	ALA	deletion	UNP Q2N0S5
A	?	-	TYR	deletion	UNP Q2N0S5
A	?	-	GLU	deletion	UNP Q2N0S5
A	?	-	THR	deletion	UNP Q2N0S5
A	64	LYS	GLU	conflict	UNP Q2N0S5
A	?	-	THR	deletion	UNP Q2N0S5
A	?	-	ASP	deletion	UNP Q2N0S5
A	?	-	ASP	deletion	UNP Q2N0S5
A	?	-	MET	deletion	UNP Q2N0S5
A	?	-	ARG	deletion	UNP Q2N0S5
A	169	ARG	LYS	conflict	UNP Q2N0S5
A	173	HIS	TYR	conflict	UNP Q2N0S5
A	174	ALA	SER	conflict	UNP Q2N0S5
A	178	LYS	ARG	conflict	UNP Q2N0S5
A	181	ILE	VAL	conflict	UNP Q2N0S5
A	183	PRO	GLN	conflict	UNP Q2N0S5
A	?	-	GLY	deletion	UNP Q2N0S5
A	?	-	ASN	deletion	UNP Q2N0S5
A	?	-	ARG	deletion	UNP Q2N0S5
A	?	-	SER	deletion	UNP Q2N0S5
A	?	-	ASN	deletion	UNP Q2N0S5
A	?	-	ASN	deletion	UNP Q2N0S5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP Q2N0S5
A	189	THR	LYS	conflict	UNP Q2N0S5
A	190	SER	GLU	conflict	UNP Q2N0S5
A	199	ALA	SER	conflict	UNP Q2N0S5
A	316	TRP	ALA	conflict	UNP Q2N0S5
A	332	ASN	THR	conflict	UNP Q2N0S5
A	386	ASP	ASN	conflict	UNP Q2N0S5
A	?	-	ASN	deletion	UNP Q2N0S5
A	?	-	THR	deletion	UNP Q2N0S5
A	?	-	SER	deletion	UNP Q2N0S5
A	?	-	VAL	deletion	UNP Q2N0S5
A	?	-	GLN	deletion	UNP Q2N0S5
A	?	-	GLY	deletion	UNP Q2N0S5
A	?	-	SER	deletion	UNP Q2N0S5
A	?	-	ASN	deletion	UNP Q2N0S5
A	?	-	SER	deletion	UNP Q2N0S5
A	?	-	THR	deletion	UNP Q2N0S5
A	?	-	GLY	deletion	UNP Q2N0S5
A	?	-	SER	deletion	UNP Q2N0S5
A	462	ASP	ASN	conflict	UNP Q2N0S5
A	471	SER	GLY	conflict	UNP Q2N0S5
A	501	CYS	ALA	conflict	UNP Q2N0S5
B	?	-	ALA	deletion	UNP Q2N0S5
B	?	-	LYS	deletion	UNP Q2N0S5
B	?	-	ALA	deletion	UNP Q2N0S5
B	?	-	TYR	deletion	UNP Q2N0S5
B	?	-	GLU	deletion	UNP Q2N0S5
B	?	-	THR	deletion	UNP Q2N0S5
B	64	LYS	GLU	conflict	UNP Q2N0S5
B	?	-	THR	deletion	UNP Q2N0S5
B	?	-	ASP	deletion	UNP Q2N0S5
B	?	-	ASP	deletion	UNP Q2N0S5
B	?	-	MET	deletion	UNP Q2N0S5
B	?	-	ARG	deletion	UNP Q2N0S5
B	169	ARG	LYS	conflict	UNP Q2N0S5
B	173	HIS	TYR	conflict	UNP Q2N0S5
B	174	ALA	SER	conflict	UNP Q2N0S5
B	178	LYS	ARG	conflict	UNP Q2N0S5
B	181	ILE	VAL	conflict	UNP Q2N0S5
B	183	PRO	GLN	conflict	UNP Q2N0S5
B	?	-	GLY	deletion	UNP Q2N0S5
B	?	-	ASN	deletion	UNP Q2N0S5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ARG	deletion	UNP Q2N0S5
B	?	-	SER	deletion	UNP Q2N0S5
B	?	-	ASN	deletion	UNP Q2N0S5
B	?	-	ASN	deletion	UNP Q2N0S5
B	?	-	SER	deletion	UNP Q2N0S5
B	189	THR	LYS	conflict	UNP Q2N0S5
B	190	SER	GLU	conflict	UNP Q2N0S5
B	199	ALA	SER	conflict	UNP Q2N0S5
B	316	TRP	ALA	conflict	UNP Q2N0S5
B	332	ASN	THR	conflict	UNP Q2N0S5
B	386	ASP	ASN	conflict	UNP Q2N0S5
B	?	-	ASN	deletion	UNP Q2N0S5
B	?	-	THR	deletion	UNP Q2N0S5
B	?	-	SER	deletion	UNP Q2N0S5
B	?	-	VAL	deletion	UNP Q2N0S5
B	?	-	GLN	deletion	UNP Q2N0S5
B	?	-	GLY	deletion	UNP Q2N0S5
B	?	-	SER	deletion	UNP Q2N0S5
B	?	-	ASN	deletion	UNP Q2N0S5
B	?	-	SER	deletion	UNP Q2N0S5
B	?	-	THR	deletion	UNP Q2N0S5
B	?	-	GLY	deletion	UNP Q2N0S5
B	?	-	SER	deletion	UNP Q2N0S5
B	462	ASP	ASN	conflict	UNP Q2N0S5
B	471	SER	GLY	conflict	UNP Q2N0S5
B	501	CYS	ALA	conflict	UNP Q2N0S5
C	?	-	ALA	deletion	UNP Q2N0S5
C	?	-	LYS	deletion	UNP Q2N0S5
C	?	-	ALA	deletion	UNP Q2N0S5
C	?	-	TYR	deletion	UNP Q2N0S5
C	?	-	GLU	deletion	UNP Q2N0S5
C	?	-	THR	deletion	UNP Q2N0S5
C	64	LYS	GLU	conflict	UNP Q2N0S5
C	?	-	THR	deletion	UNP Q2N0S5
C	?	-	ASP	deletion	UNP Q2N0S5
C	?	-	ASP	deletion	UNP Q2N0S5
C	?	-	MET	deletion	UNP Q2N0S5
C	?	-	ARG	deletion	UNP Q2N0S5
C	169	ARG	LYS	conflict	UNP Q2N0S5
C	173	HIS	TYR	conflict	UNP Q2N0S5
C	174	ALA	SER	conflict	UNP Q2N0S5
C	178	LYS	ARG	conflict	UNP Q2N0S5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	181	ILE	VAL	conflict	UNP Q2N0S5
C	183	PRO	GLN	conflict	UNP Q2N0S5
C	?	-	GLY	deletion	UNP Q2N0S5
C	?	-	ASN	deletion	UNP Q2N0S5
C	?	-	ARG	deletion	UNP Q2N0S5
C	?	-	SER	deletion	UNP Q2N0S5
C	?	-	ASN	deletion	UNP Q2N0S5
C	?	-	ASN	deletion	UNP Q2N0S5
C	?	-	SER	deletion	UNP Q2N0S5
C	189	THR	LYS	conflict	UNP Q2N0S5
C	190	SER	GLU	conflict	UNP Q2N0S5
C	199	ALA	SER	conflict	UNP Q2N0S5
C	316	TRP	ALA	conflict	UNP Q2N0S5
C	332	ASN	THR	conflict	UNP Q2N0S5
C	386	ASP	ASN	conflict	UNP Q2N0S5
C	?	-	ASN	deletion	UNP Q2N0S5
C	?	-	THR	deletion	UNP Q2N0S5
C	?	-	SER	deletion	UNP Q2N0S5
C	?	-	VAL	deletion	UNP Q2N0S5
C	?	-	GLN	deletion	UNP Q2N0S5
C	?	-	GLY	deletion	UNP Q2N0S5
C	?	-	SER	deletion	UNP Q2N0S5
C	?	-	ASN	deletion	UNP Q2N0S5
C	?	-	SER	deletion	UNP Q2N0S5
C	?	-	THR	deletion	UNP Q2N0S5
C	?	-	GLY	deletion	UNP Q2N0S5
C	?	-	SER	deletion	UNP Q2N0S5
C	462	ASP	ASN	conflict	UNP Q2N0S5
C	471	SER	GLY	conflict	UNP Q2N0S5
C	501	CYS	ALA	conflict	UNP Q2N0S5

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	124	Total	C	N	O	S	0	0
			986	622	171	188	5		
2	E	124	Total	C	N	O	S	0	0
			989	624	171	188	6		
2	F	124	Total	C	N	O	S	0	0
			989	624	171	188	6		

- Molecule 3 is a protein called 10-1074 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		
3	N	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		
3	O	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		

- Molecule 4 is a protein called BG24 mature Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	120	Total	C	N	O	S	0	0
			940	591	169	174	6		
4	H	120	Total	C	N	O	S	0	0
			940	591	169	174	6		
4	I	120	Total	C	N	O	S	0	0
			940	591	169	174	6		

- Molecule 5 is a protein called 10-1074 Fab light chain.

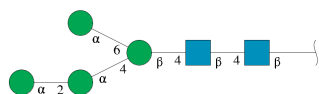
Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	107	Total	C	N	O	S	0	0
			824	515	152	154	3		
5	Q	107	Total	C	N	O	S	0	0
			824	515	152	154	3		
5	R	107	Total	C	N	O	S	0	0
			815	509	149	154	3		

- Molecule 6 is a protein called BG24 mature Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	105	Total	C	N	O	S	0	0
			778	483	129	163	3		
6	K	105	Total	C	N	O	S	0	0
			778	483	129	163	3		
6	L	105	Total	C	N	O	S	0	0
			778	483	129	163	3		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-4)-[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.





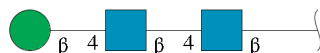
Mol	Chain	Residues	Atoms				AltConf	Trace
7	S	6	Total	C	N	O	0	0
			72	40	2	30		
7	V	6	Total	C	N	O	0	0
			72	40	2	30		
7	Z	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 8 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
8	T	2	Total	C	N	O	0	0
			28	16	2	10		
8	W	2	Total	C	N	O	0	0
			28	16	2	10		
8	a	2	Total	C	N	O	0	0
			28	16	2	10		

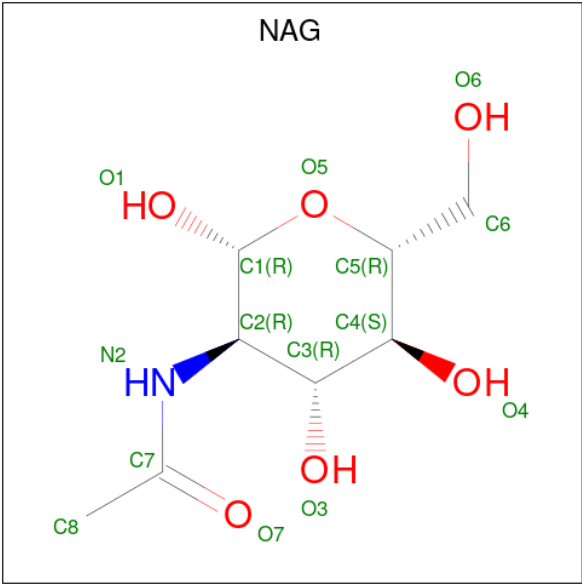
- Molecule 9 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG)

(formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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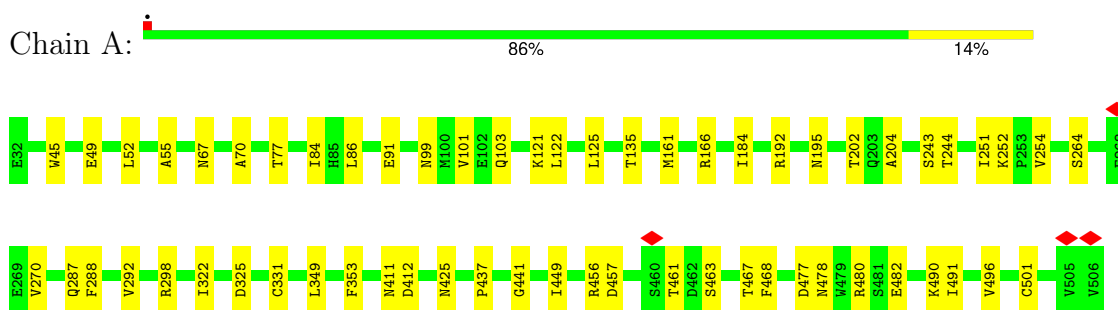
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Mol	Chain	Residues	Atoms				AltConf
10	B	1	Total 14	C 8	N 1	O 5	0
10	B	1	Total 14	C 8	N 1	O 5	0
10	B	1	Total 14	C 8	N 1	O 5	0
10	B	1	Total 14	C 8	N 1	O 5	0
10	B	1	Total 14	C 8	N 1	O 5	0
10	B	1	Total 14	C 8	N 1	O 5	0
10	B	1	Total 14	C 8	N 1	O 5	0
10	C	1	Total 14	C 8	N 1	O 5	0
10	C	1	Total 14	C 8	N 1	O 5	0
10	C	1	Total 14	C 8	N 1	O 5	0
10	C	1	Total 14	C 8	N 1	O 5	0
10	C	1	Total 14	C 8	N 1	O 5	0
10	C	1	Total 14	C 8	N 1	O 5	0
10	C	1	Total 14	C 8	N 1	O 5	0
10	C	1	Total 14	C 8	N 1	O 5	0
10	C	1	Total 14	C 8	N 1	O 5	0
10	D	1	Total 14	C 8	N 1	O 5	0
10	E	1	Total 14	C 8	N 1	O 5	0
10	F	1	Total 14	C 8	N 1	O 5	0
10	Y	1	Total 14	C 8	N 1	O 5	0

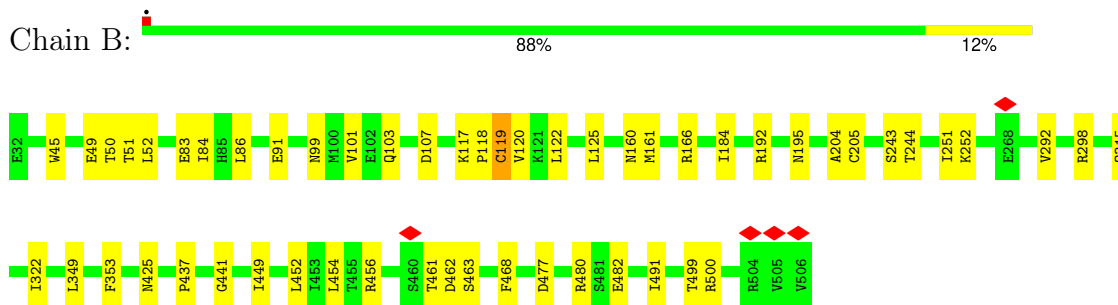
### 3 Residue-property plots

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

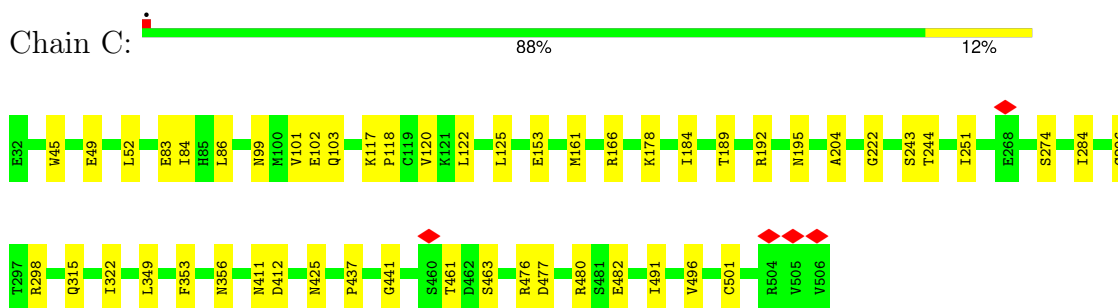
- Molecule 1: Envelope glycoprotein gp120



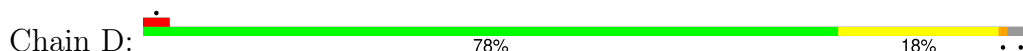
- Molecule 1: Envelope glycoprotein gp120

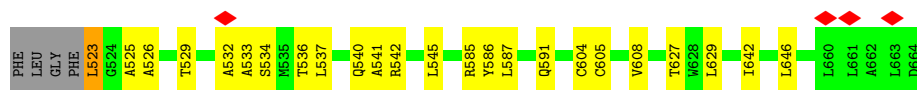


- Molecule 1: Envelope glycoprotein gp120

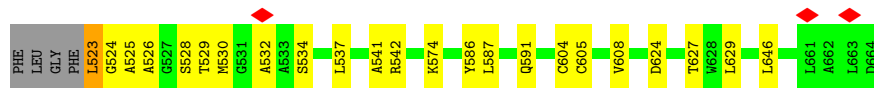
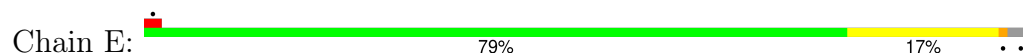


- Molecule 2: Envelope glycoprotein gp41

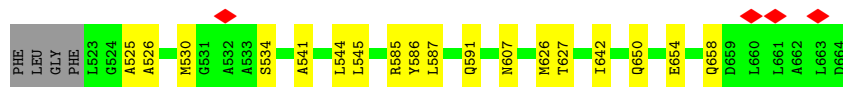
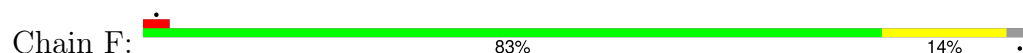




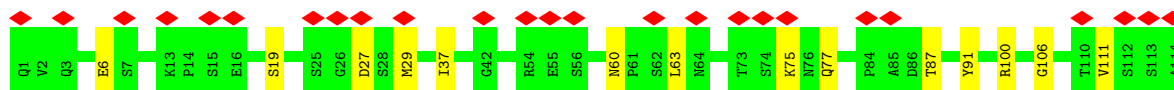
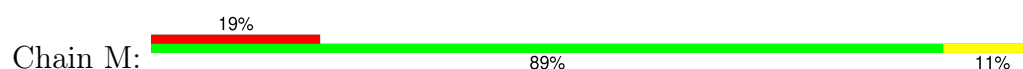
- Molecule 2: Envelope glycoprotein gp41



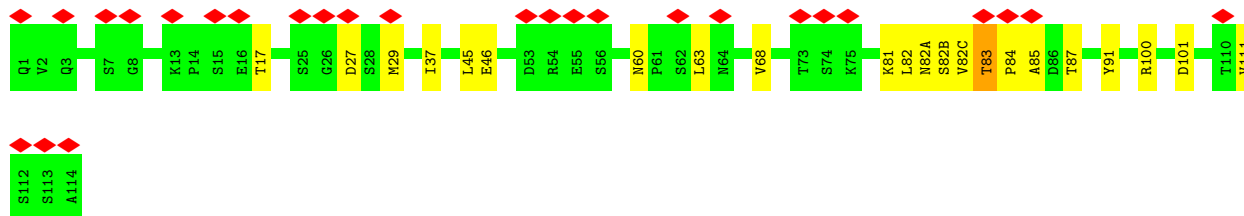
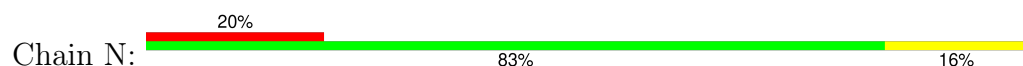
- Molecule 2: Envelope glycoprotein gp41



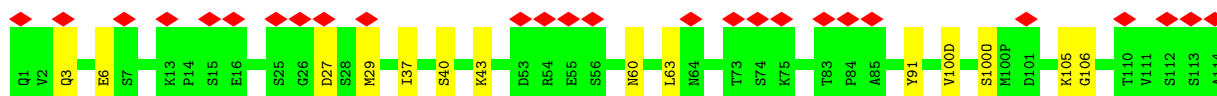
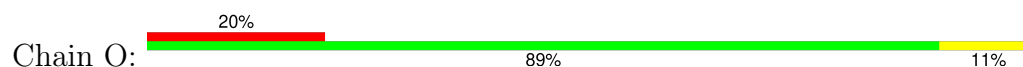
- Molecule 3: 10-1074 Fab heavy chain



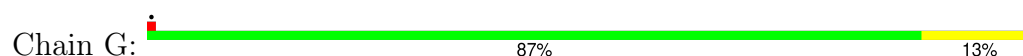
- Molecule 3: 10-1074 Fab heavy chain



- Molecule 3: 10-1074 Fab heavy chain

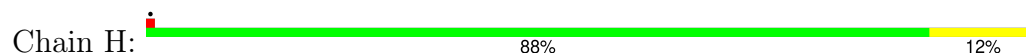


- Molecule 4: BG24 mature Fab heavy chain

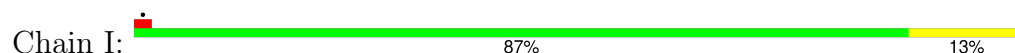




- Molecule 4: BG24 mature Fab heavy chain



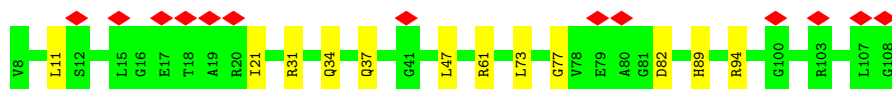
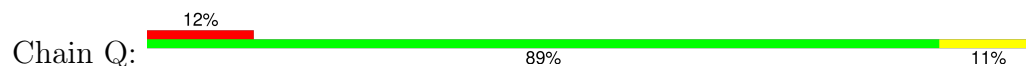
- Molecule 4: BG24 mature Fab heavy chain



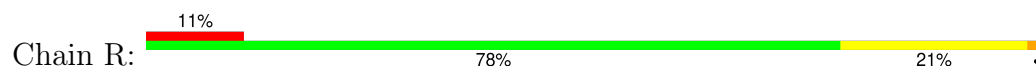
- Molecule 5: 10-1074 Fab light chain



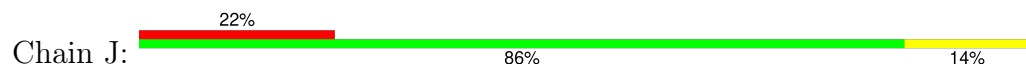
- Molecule 5: 10-1074 Fab light chain



- Molecule 5: 10-1074 Fab light chain

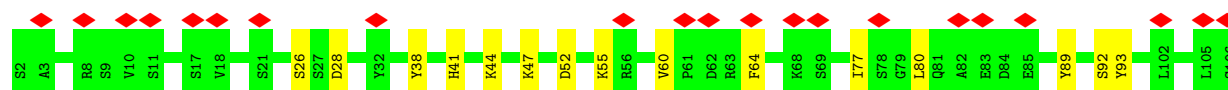
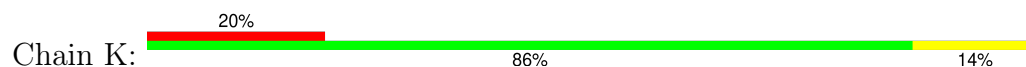


- Molecule 6: BG24 mature Fab light chain

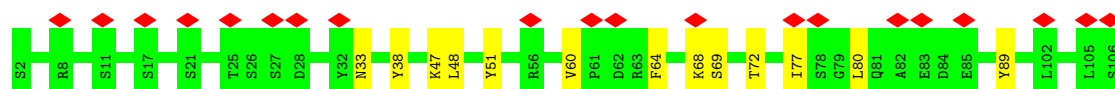
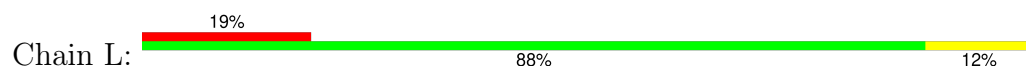




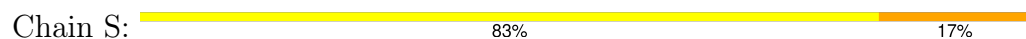
- Molecule 6: BG24 mature Fab light chain



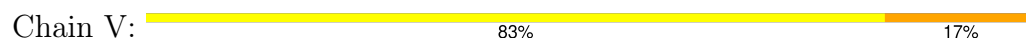
- Molecule 6: BG24 mature Fab light chain



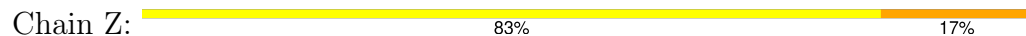
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-4)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



MAG1  
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%

MAG1  
MAG2

- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  100%

MAG1  
MAG2

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

Chain U:  67% 33%


MAG1  
MAG2  
BMA3

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

Chain X:  67% 33%

MAG1  
MAG2  
BMA3

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

Chain Y:  67% 33%

MAG1  
MAG2  
BMA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23830	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.057	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0122	Depositor
Map size ( $\text{\AA}$ )	312.84, 312.84, 312.84	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.869, 0.869, 0.869	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.31	0/3563	0.58	0/4841
1	B	0.31	0/3563	0.58	0/4841
1	C	0.31	0/3563	0.57	0/4841
2	D	0.27	0/1002	0.49	0/1360
2	E	0.27	0/1005	0.51	0/1363
2	F	0.27	0/1005	0.50	0/1363
3	M	0.30	0/1066	0.55	0/1451
3	N	0.30	0/1066	0.55	0/1451
3	O	0.31	0/1066	0.57	0/1451
4	G	0.28	0/964	0.50	0/1310
4	H	0.28	0/964	0.50	0/1310
4	I	0.29	0/964	0.51	0/1310
5	P	0.29	0/845	0.52	0/1148
5	Q	0.29	0/845	0.52	0/1148
5	R	0.29	0/836	0.53	0/1137
6	J	0.31	0/796	0.55	0/1080
6	K	0.31	0/796	0.53	0/1080
6	L	0.32	0/796	0.53	0/1080
All	All	0.30	0/24705	0.55	0/33565

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3488	0	3432	40	0
1	B	3488	0	3433	47	0
1	C	3488	0	3432	45	0
2	D	986	0	972	28	0
2	E	989	0	979	28	0
2	F	989	0	979	33	0
3	M	1041	0	1005	8	0
3	N	1041	0	1005	29	0
3	O	1041	0	1005	16	0
4	G	940	0	904	8	0
4	H	940	0	904	7	0
4	I	940	0	904	9	0
5	P	824	0	790	7	0
5	Q	824	0	790	8	0
5	R	815	0	770	39	0
6	J	778	0	736	7	0
6	K	778	0	736	7	0
6	L	778	0	736	6	0
7	S	72	0	61	1	0
7	V	72	0	61	1	0
7	Z	72	0	61	1	0
8	T	28	0	25	0	0
8	W	28	0	25	0	0
8	a	28	0	23	0	0
9	U	39	0	34	1	0
9	X	39	0	34	1	0
9	Y	39	0	24	0	0
10	A	140	0	130	0	0
10	B	140	0	130	0	0
10	C	126	0	117	0	0
10	D	14	0	13	0	0
10	E	14	0	13	0	0
10	F	14	0	13	0	0
10	Y	14	0	23	0	0
All	All	25047	0	24299	317	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 317 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)
1:A:86:LEU:CD1	2:D:525:ALA:HB1	1.56	1.33
5:R:49:TYR:O	5:R:53:ASP:HB3	1.24	1.30
3:N:82:LEU:HG	3:N:82(C):VAL:CG1	1.64	1.27
2:E:526:ALA:O	2:E:627:THR:HG23	1.29	1.27
3:N:83:THR:OG1	3:N:84:PRO:HD2	1.31	1.25

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/443 (98%)	402 (92%)	33 (8%)	0	100	100
1	B	435/443 (98%)	405 (93%)	30 (7%)	0	100	100
1	C	435/443 (98%)	407 (94%)	28 (6%)	0	100	100
2	D	120/128 (94%)	118 (98%)	2 (2%)	0	100	100
2	E	120/128 (94%)	117 (98%)	3 (2%)	0	100	100
2	F	120/128 (94%)	116 (97%)	4 (3%)	0	100	100
3	M	131/133 (98%)	125 (95%)	6 (5%)	0	100	100
3	N	131/133 (98%)	128 (98%)	3 (2%)	0	100	100
3	O	131/133 (98%)	125 (95%)	6 (5%)	0	100	100
4	G	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
4	H	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
4	I	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
5	P	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
5	Q	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
5	R	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
6	J	103/105 (98%)	85 (82%)	18 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	K	103/105 (98%)	86 (84%)	17 (16%)	0	100	100
6	L	103/105 (98%)	84 (82%)	19 (18%)	0	100	100
All	All	3036/3108 (98%)	2834 (93%)	202 (7%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	396/397 (100%)	393 (99%)	3 (1%)	79	84
1	B	396/397 (100%)	395 (100%)	1 (0%)	91	92
1	C	396/397 (100%)	393 (99%)	3 (1%)	79	84
2	D	107/111 (96%)	106 (99%)	1 (1%)	75	83
2	E	108/111 (97%)	107 (99%)	1 (1%)	75	83
2	F	108/111 (97%)	108 (100%)	0	100	100
3	M	116/116 (100%)	115 (99%)	1 (1%)	75	83
3	N	116/116 (100%)	114 (98%)	2 (2%)	56	72
3	O	116/116 (100%)	115 (99%)	1 (1%)	75	83
4	G	99/99 (100%)	98 (99%)	1 (1%)	73	81
4	H	99/99 (100%)	98 (99%)	1 (1%)	73	81
4	I	99/99 (100%)	98 (99%)	1 (1%)	73	81
5	P	85/85 (100%)	85 (100%)	0	100	100
5	Q	85/85 (100%)	85 (100%)	0	100	100
5	R	83/85 (98%)	81 (98%)	2 (2%)	44	63
6	J	87/87 (100%)	86 (99%)	1 (1%)	70	79
6	K	87/87 (100%)	86 (99%)	1 (1%)	70	79
6	L	87/87 (100%)	86 (99%)	1 (1%)	70	79
All	All	2670/2685 (99%)	2649 (99%)	21 (1%)	77	84

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	71	ARG
5	R	51	ASN
6	L	47	LYS
6	J	47	LYS
5	R	47	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
3	N	64	ASN
4	G	6	GLN
3	O	76	ASN
4	G	39	GLN
1	B	103	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 ⓘ

34 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	S	1	1,7	14,14,15	0.56	0	17,19,21	0.86	1 (5%)
7	NAG	S	2	7	14,14,15	0.42	0	17,19,21	1.26	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BMA	S	3	7	11,11,12	1.80	3 (27%)	15,15,17	1.32	3 (20%)
7	MAN	S	4	7	11,11,12	1.78	4 (36%)	15,15,17	1.67	2 (13%)
7	MAN	S	5	7	11,11,12	1.17	1 (9%)	15,15,17	1.41	2 (13%)
7	MAN	S	6	7	11,11,12	1.39	2 (18%)	15,15,17	1.40	2 (13%)
8	NAG	T	1	1,8	14,14,15	0.74	0	17,19,21	1.65	3 (17%)
8	NAG	T	2	8	14,14,15	0.82	1 (7%)	17,19,21	1.13	2 (11%)
9	NAG	U	1	1,9	14,14,15	0.75	0	17,19,21	1.75	5 (29%)
9	NAG	U	2	9	14,14,15	0.63	0	17,19,21	1.52	2 (11%)
9	BMA	U	3	9	11,11,12	1.65	3 (27%)	15,15,17	0.94	1 (6%)
7	NAG	V	1	1,7	14,14,15	0.60	0	17,19,21	0.89	1 (5%)
7	NAG	V	2	7	14,14,15	0.42	0	17,19,21	1.23	2 (11%)
7	BMA	V	3	7	11,11,12	1.80	3 (27%)	15,15,17	1.34	3 (20%)
7	MAN	V	4	7	11,11,12	1.79	4 (36%)	15,15,17	1.69	2 (13%)
7	MAN	V	5	7	11,11,12	1.20	2 (18%)	15,15,17	1.45	2 (13%)
7	MAN	V	6	7	11,11,12	1.33	2 (18%)	15,15,17	1.47	2 (13%)
8	NAG	W	1	1,8	14,14,15	0.63	0	17,19,21	0.78	1 (5%)
8	NAG	W	2	8	14,14,15	0.73	1 (7%)	17,19,21	0.80	1 (5%)
9	NAG	X	1	1,9	14,14,15	0.82	0	17,19,21	1.51	3 (17%)
9	NAG	X	2	9	14,14,15	0.78	1 (7%)	17,19,21	1.43	3 (17%)
9	BMA	X	3	9	11,11,12	1.15	1 (9%)	15,15,17	1.32	1 (6%)
9	NAG	Y	1	1,9	14,14,15	0.98	0	17,19,21	3.52	6 (35%)
9	NAG	Y	2	10,9	14,14,15	0.69	0	17,19,21	1.60	3 (17%)
10	BMA	Y	3	9	11,11,12	1.36	2 (18%)	15,15,17	0.87	0
10	NAG	Y	3	1	14,14,15	1.54	2 (14%)	17,19,21	2.78	3 (17%)
7	NAG	Z	1	1,7	14,14,15	0.66	1 (7%)	17,19,21	0.83	1 (5%)
7	NAG	Z	2	7	14,14,15	0.43	0	17,19,21	1.21	2 (11%)
7	BMA	Z	3	7	11,11,12	1.71	3 (27%)	15,15,17	1.23	2 (13%)
7	MAN	Z	4	7	11,11,12	2.34	3 (27%)	15,15,17	2.40	2 (13%)
7	MAN	Z	5	7	11,11,12	1.50	2 (18%)	15,15,17	1.63	2 (13%)
7	MAN	Z	6	7	11,11,12	1.36	2 (18%)	15,15,17	1.39	2 (13%)
8	NAG	a	1	1,8	14,14,15	1.10	1 (7%)	17,19,21	2.93	4 (23%)
8	NAG	a	2	8	14,14,15	0.72	1 (7%)	17,19,21	0.77	1 (5%)

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	S	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	S	2	7	-	4/6/23/26	0/1/1/1
7	BMA	S	3	7	-	2/2/19/22	0/1/1/1
7	MAN	S	4	7	-	1/2/19/22	1/1/1/1
7	MAN	S	5	7	-	2/2/19/22	0/1/1/1
7	MAN	S	6	7	-	0/2/19/22	1/1/1/1
8	NAG	T	1	1,8	-	3/6/23/26	0/1/1/1
8	NAG	T	2	8	-	4/6/23/26	0/1/1/1
9	NAG	U	1	1,9	-	4/6/23/26	0/1/1/1
9	NAG	U	2	9	-	4/6/23/26	0/1/1/1
9	BMA	U	3	9	-	1/2/19/22	0/1/1/1
7	NAG	V	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	V	2	7	-	4/6/23/26	0/1/1/1
7	BMA	V	3	7	-	2/2/19/22	0/1/1/1
7	MAN	V	4	7	-	1/2/19/22	1/1/1/1
7	MAN	V	5	7	-	2/2/19/22	0/1/1/1
7	MAN	V	6	7	-	0/2/19/22	1/1/1/1
8	NAG	W	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	W	2	8	-	2/6/23/26	0/1/1/1
9	NAG	X	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	X	2	9	-	4/6/23/26	0/1/1/1
9	BMA	X	3	9	-	1/2/19/22	0/1/1/1
9	NAG	Y	1	1,9	-	4/6/23/26	0/1/1/1
9	NAG	Y	2	10,9	-	4/6/23/26	0/1/1/1
10	BMA	Y	3	9	-	1/2/19/22	0/1/1/1
10	NAG	Y	3	1	-	5/6/23/26	0/1/1/1
7	NAG	Z	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	4/6/23/26	0/1/1/1
7	BMA	Z	3	7	-	2/2/19/22	0/1/1/1
7	MAN	Z	4	7	-	0/2/19/22	0/1/1/1
7	MAN	Z	5	7	-	1/2/19/22	1/1/1/1
7	MAN	Z	6	7	-	0/2/19/22	1/1/1/1
8	NAG	a	1	1,8	-	4/6/23/26	0/1/1/1
8	NAG	a	2	8	-	0/6/23/26	0/1/1/1

The worst 5 of 45 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Z	4	MAN	C1-C2	5.10	1.64	1.52
7	Z	4	MAN	O5-C1	4.78	1.51	1.43
10	Y	3	NAG	C1-C2	4.64	1.58	1.52
7	Z	3	BMA	C4-C5	3.50	1.60	1.53
7	V	3	BMA	C4-C5	3.43	1.60	1.53

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Y	1	NAG	C2-N2-C7	10.27	136.66	122.90
8	a	1	NAG	C2-N2-C7	10.04	136.36	122.90
10	Y	3	NAG	C2-N2-C7	9.95	136.24	122.90
7	Z	4	MAN	C1-O5-C5	8.00	122.90	112.19
9	Y	1	NAG	C1-C2-N2	6.27	120.31	110.43

There are no chirality outliers.

5 of 74 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	V	3	BMA	O5-C5-C6-O6
7	Z	3	BMA	O5-C5-C6-O6
9	U	1	NAG	O5-C5-C6-O6
7	S	3	BMA	O5-C5-C6-O6
9	U	2	NAG	O5-C5-C6-O6

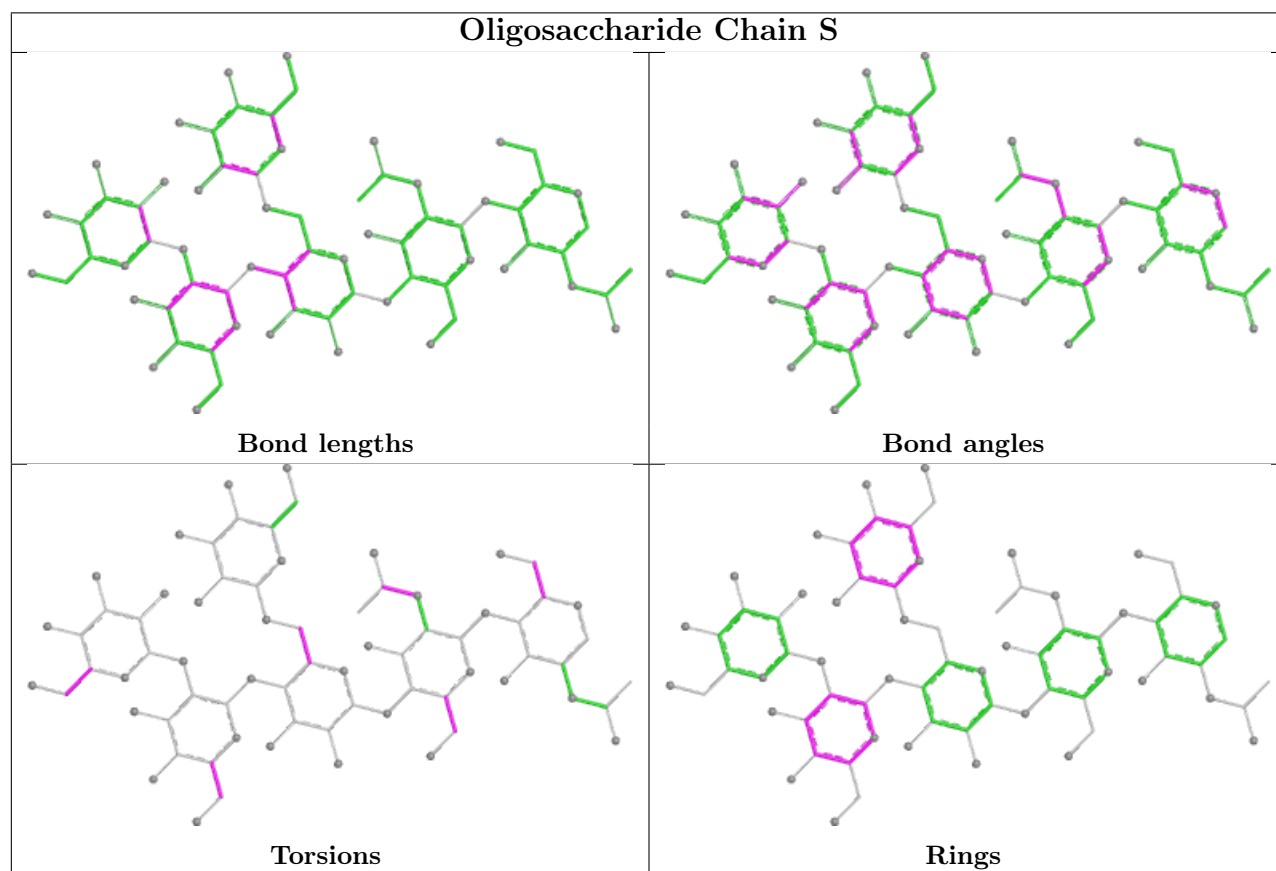
5 of 6 ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	Z	6	MAN	C1-C2-C3-C4-C5-O5
7	S	6	MAN	C1-C2-C3-C4-C5-O5
7	V	4	MAN	C1-C2-C3-C4-C5-O5
7	S	4	MAN	C1-C2-C3-C4-C5-O5
7	Z	5	MAN	C1-C2-C3-C4-C5-O5

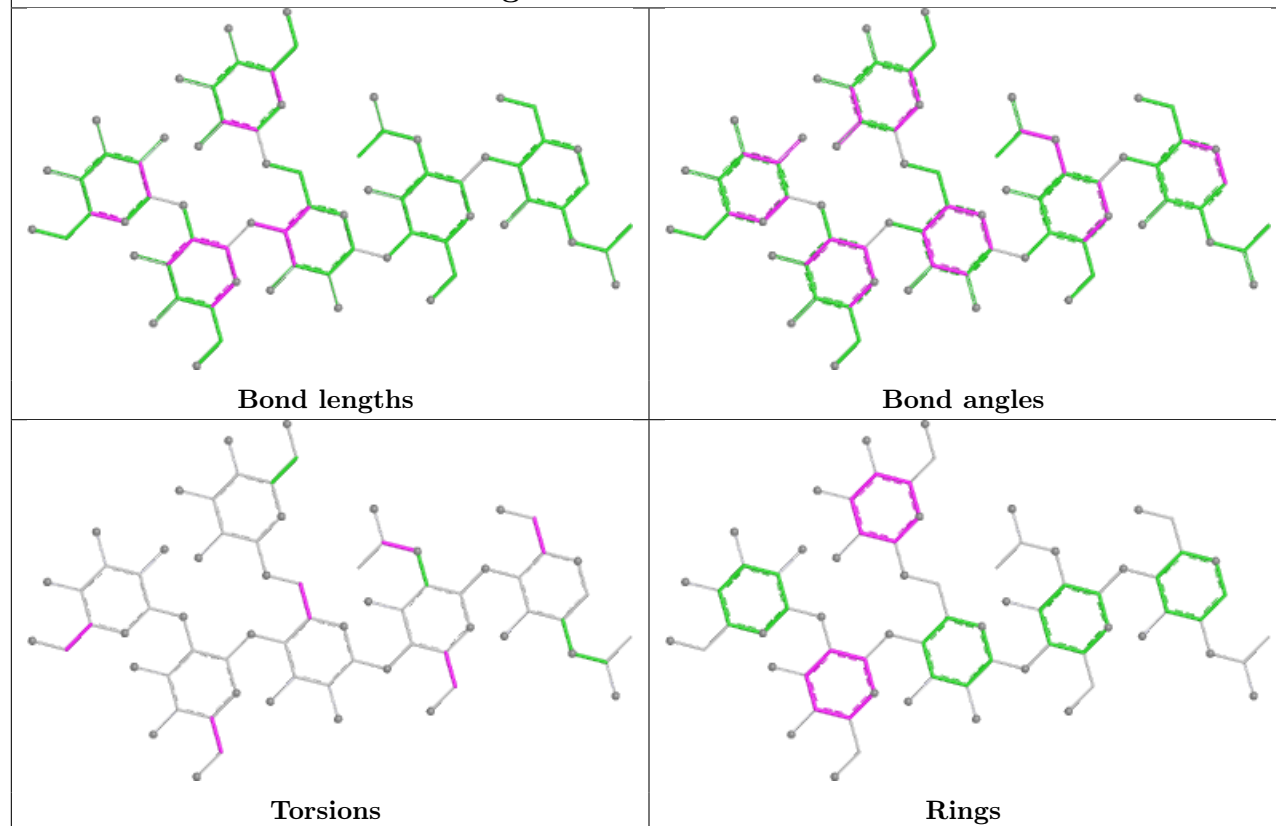
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	U	1	NAG	1	0
7	Z	2	NAG	1	0
7	S	4	MAN	1	0
7	V	4	MAN	1	0
9	X	1	NAG	1	0

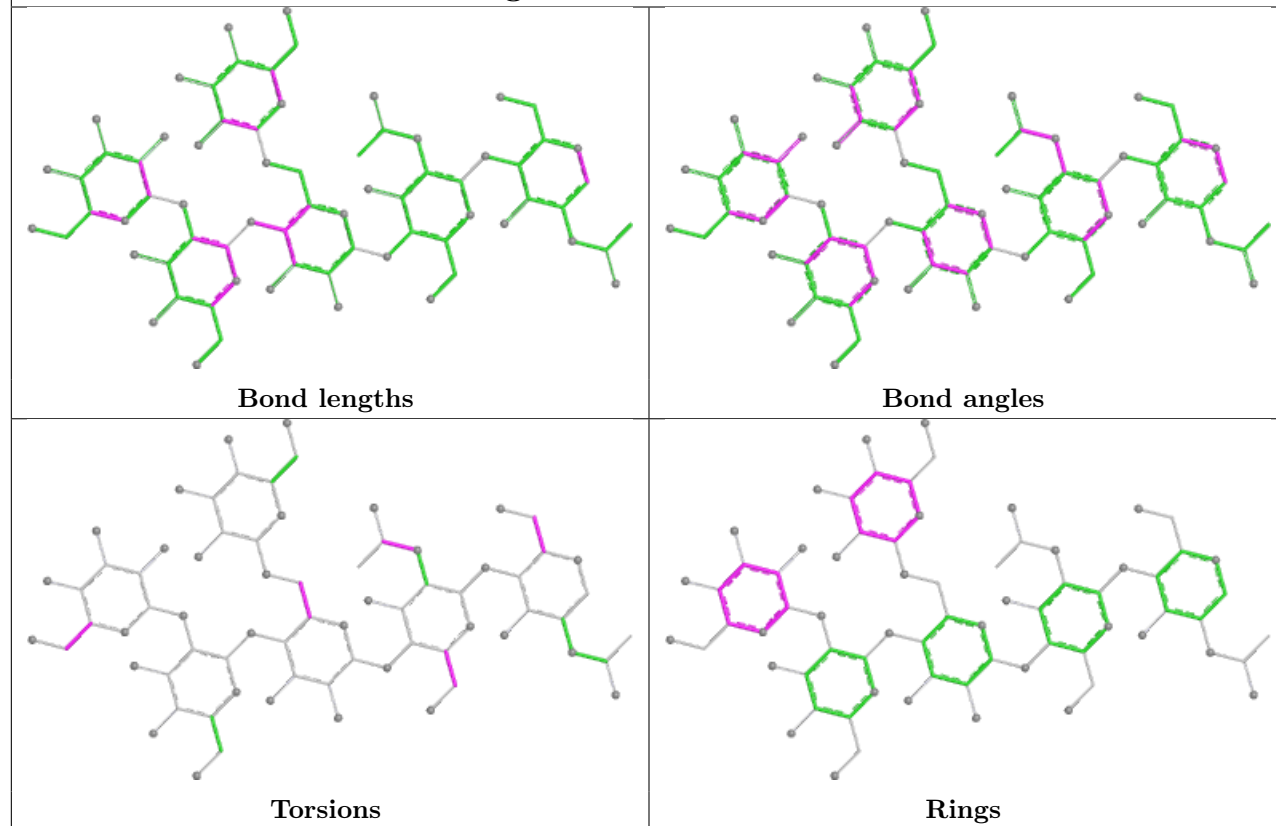
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

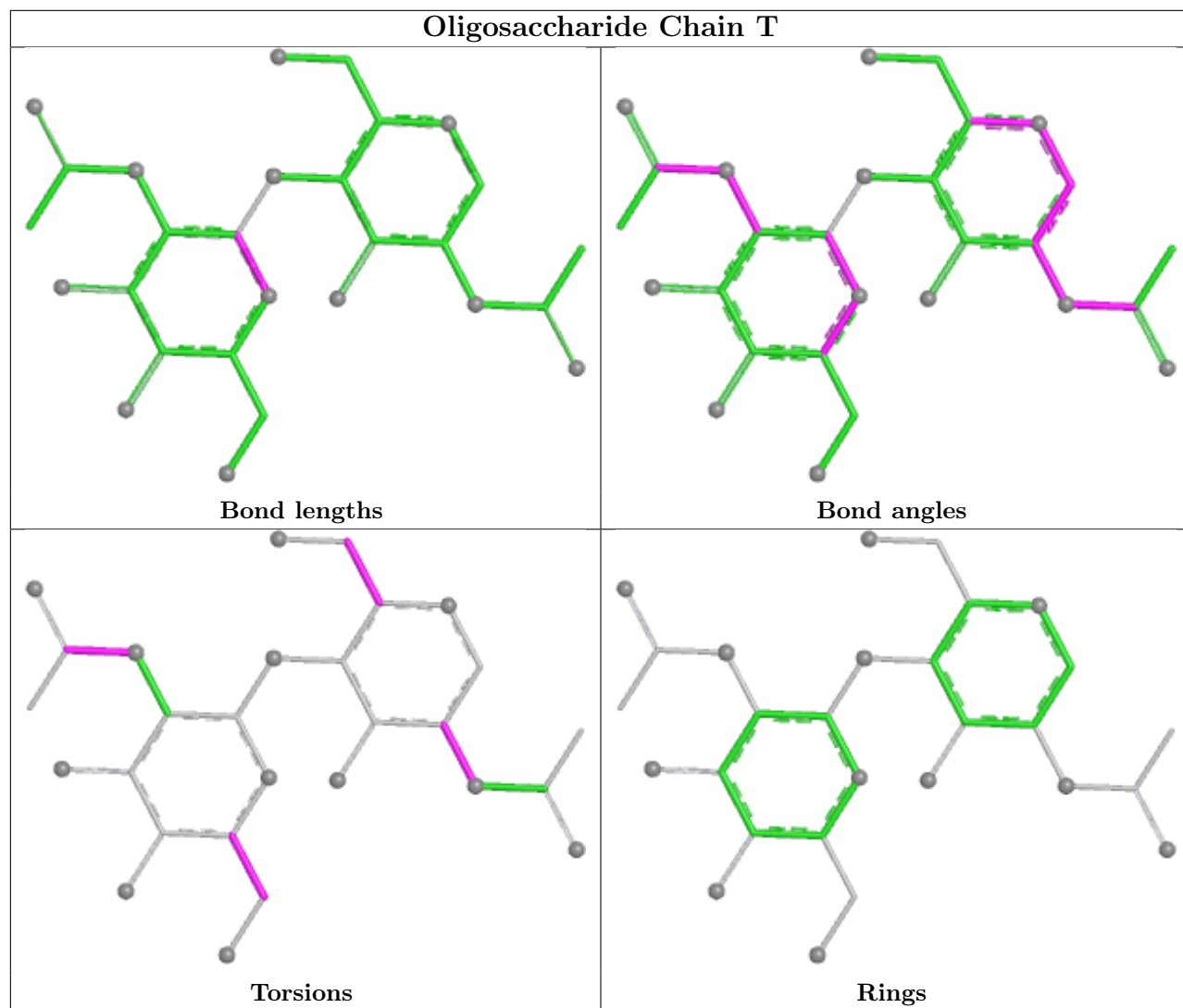


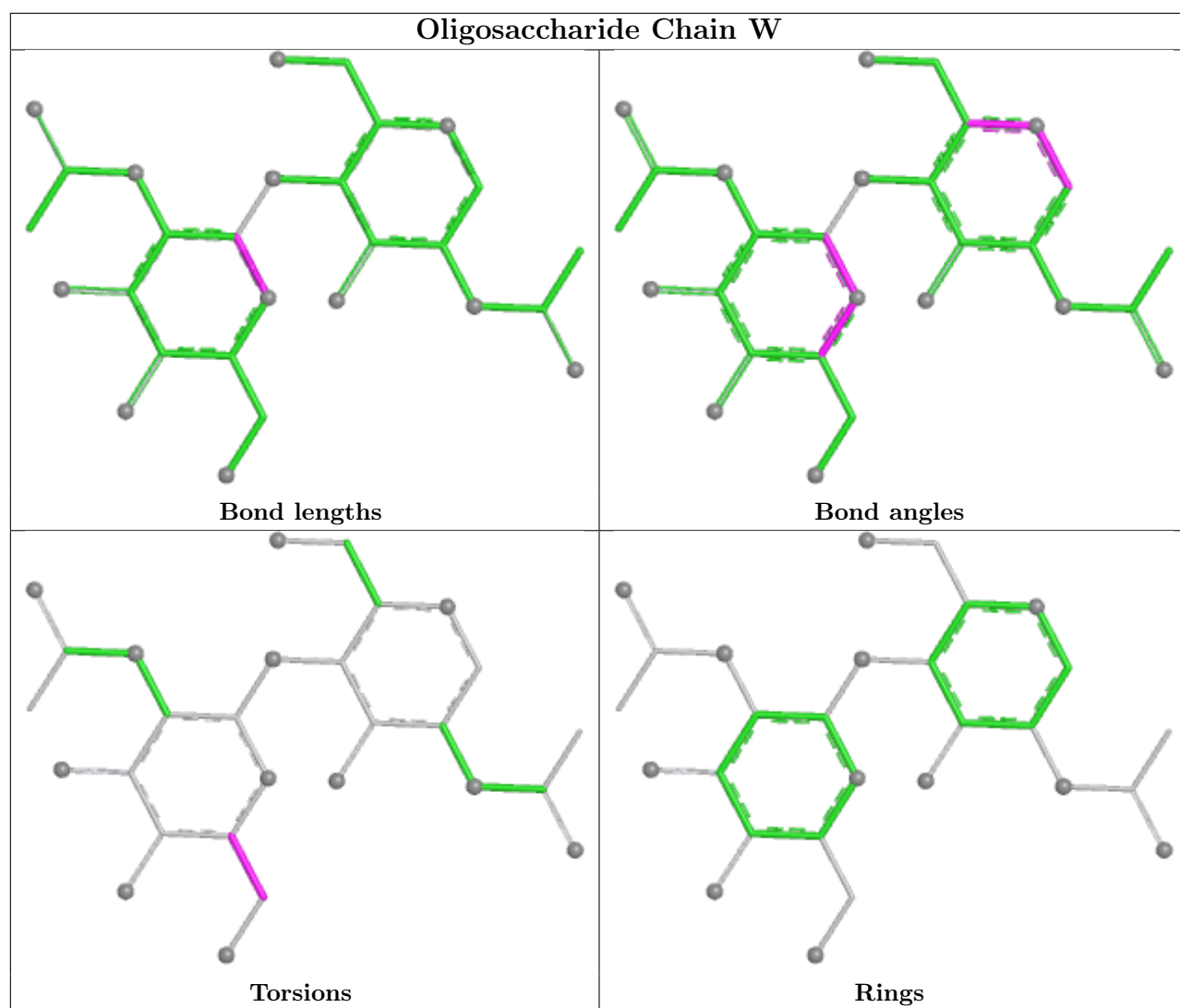
## Oligosaccharide Chain V

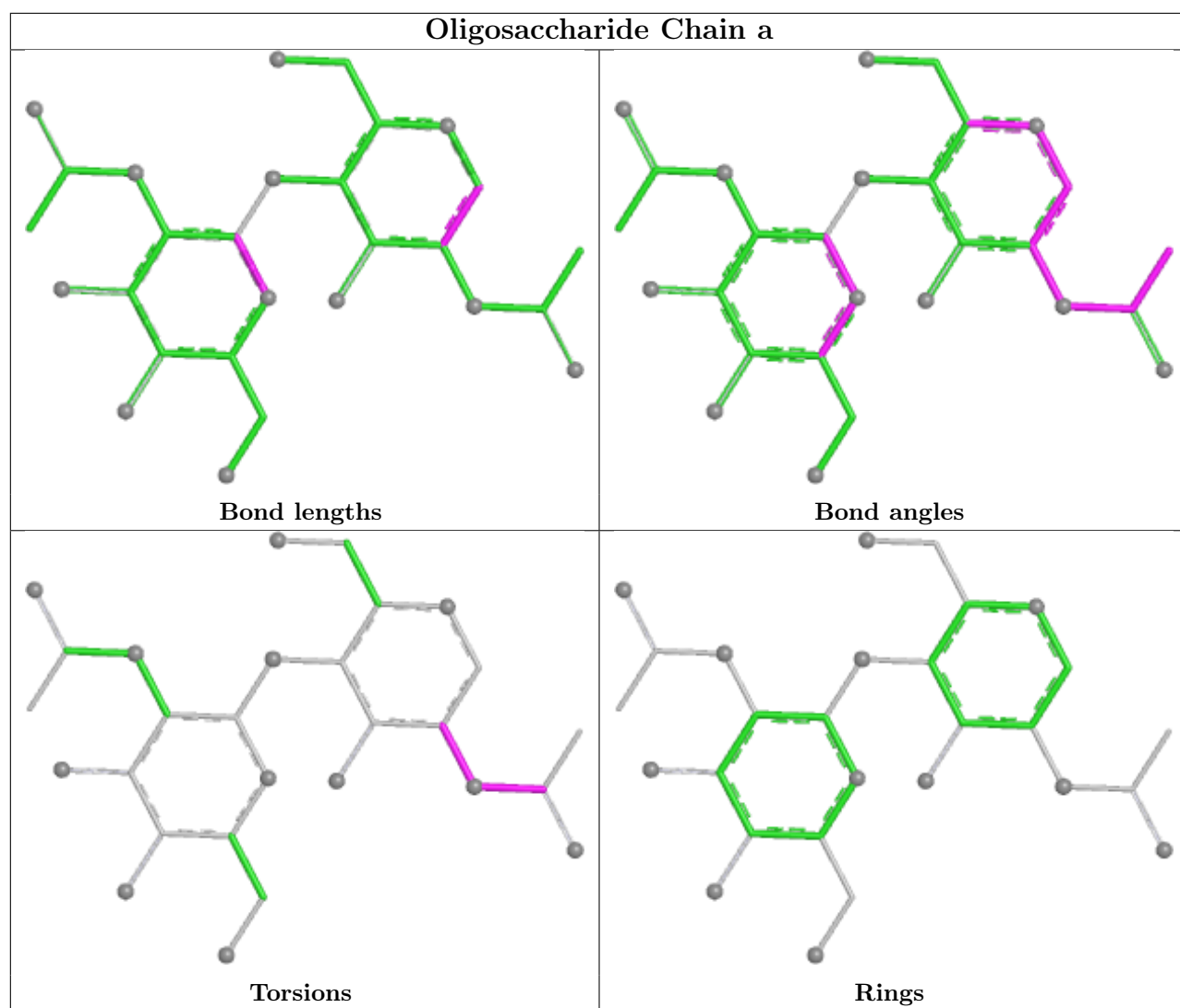


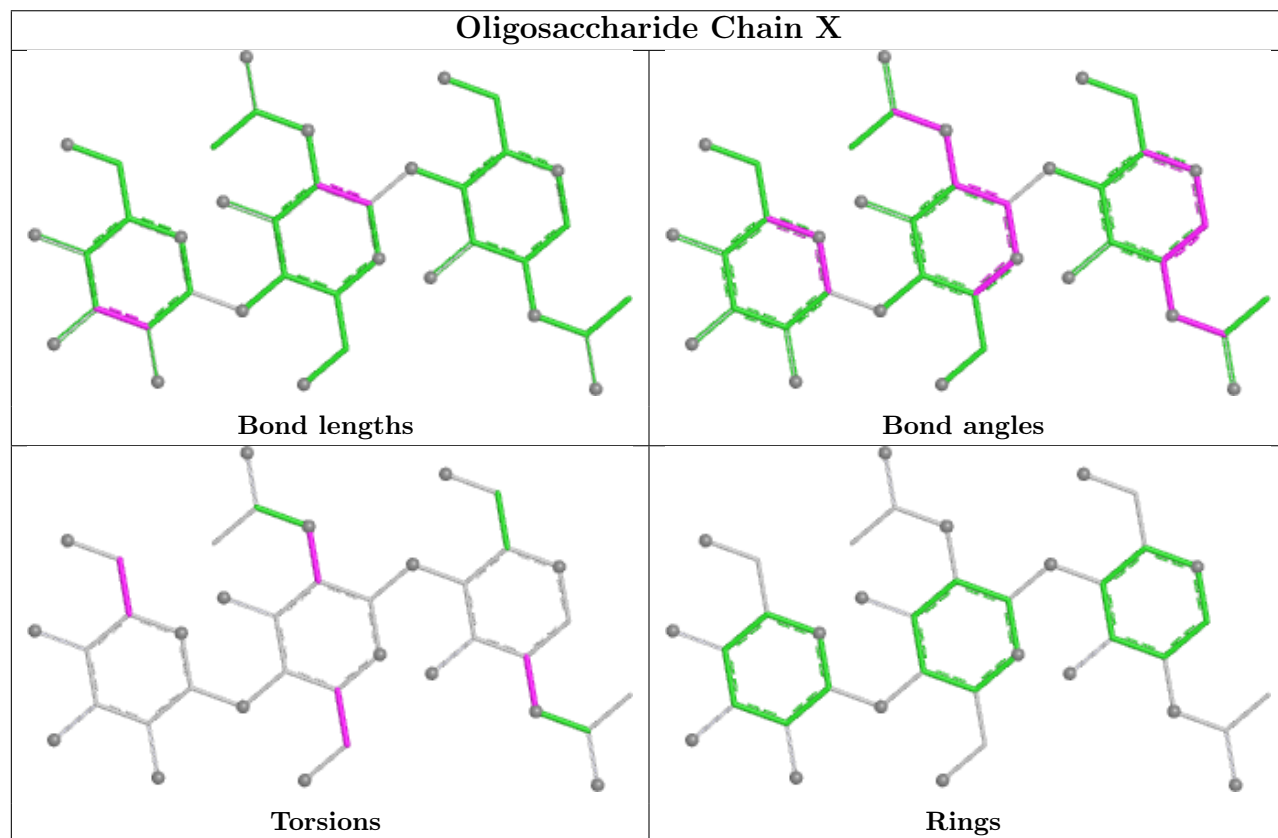
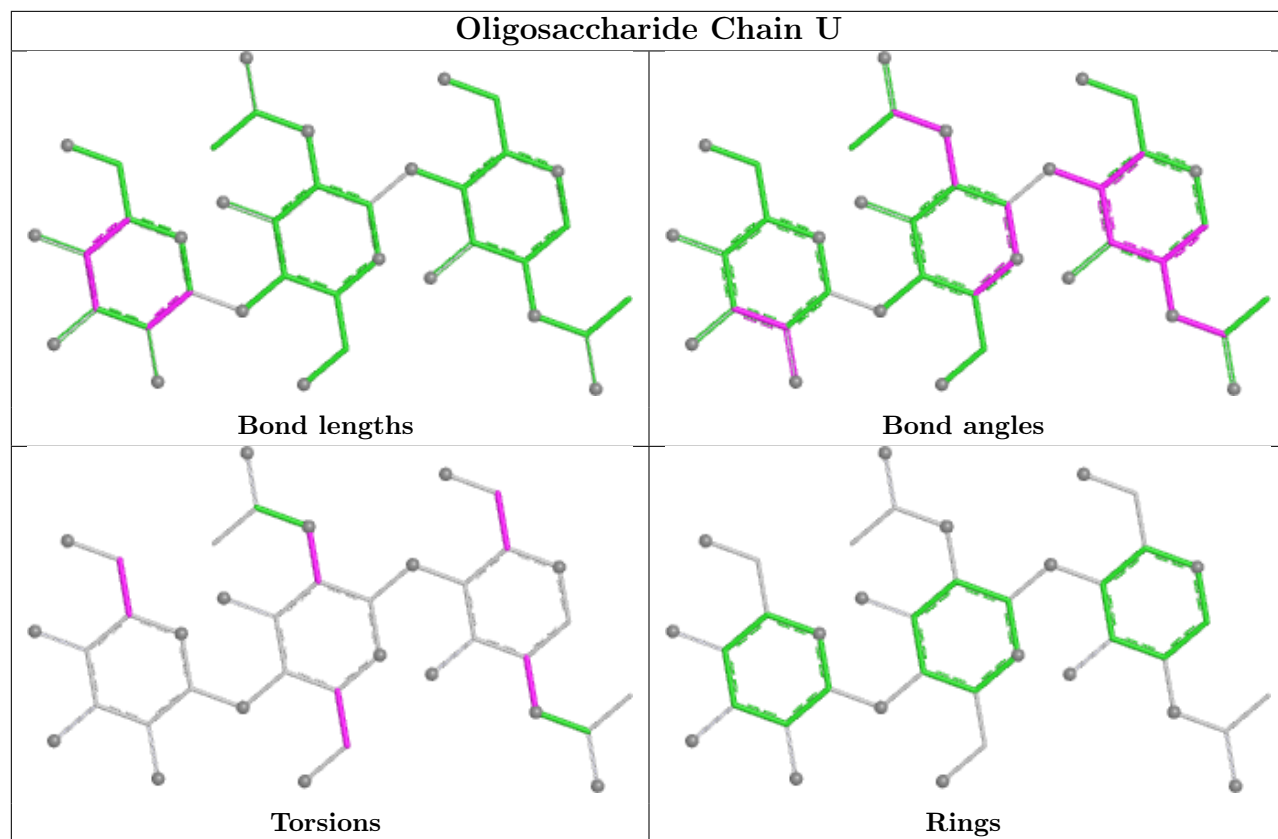
## Oligosaccharide Chain Z

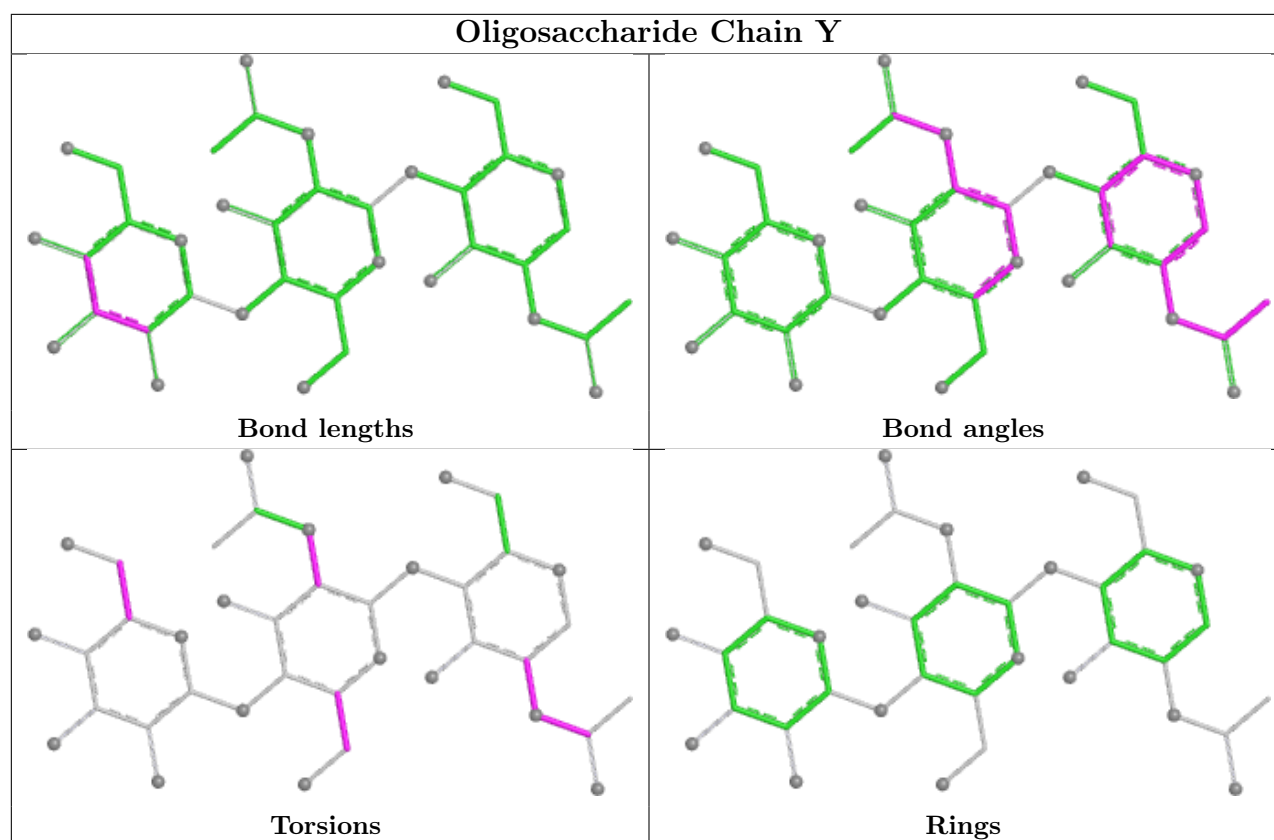












## 5.6 Ligand geometry [i](#)

34 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$
10	NAG	B	601	1	14,14,15	1.03	2 (14%)	17,19,21	0.63	1 (5%)
10	NAG	A	606	1	14,14,15	0.81	1 (7%)	17,19,21	0.74	1 (5%)
10	NAG	A	605	1	14,14,15	0.90	1 (7%)	17,19,21	0.92	2 (11%)
10	NAG	A	602	1	14,14,15	0.88	1 (7%)	17,19,21	0.58	0
10	NAG	A	608	1	14,14,15	0.98	2 (14%)	17,19,21	1.45	3 (17%)
10	NAG	Y	3	1	14,14,15	1.54	2 (14%)	17,19,21	2.78	3 (17%)
10	NAG	A	610	1	14,14,15	0.86	1 (7%)	17,19,21	0.97	2 (11%)
10	NAG	D	701	2	14,14,15	0.85	1 (7%)	17,19,21	0.92	2 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	NAG	A	607	1	14,14,15	0.94	2 (14%)	17,19,21	1.43	3 (17%)
10	NAG	C	602	-	14,14,15	0.77	1 (7%)	17,19,21	0.74	1 (5%)
10	NAG	B	606	1	14,14,15	0.80	1 (7%)	17,19,21	0.71	1 (5%)
10	NAG	B	602	1	14,14,15	0.84	1 (7%)	17,19,21	0.58	0
10	NAG	C	603	1	14,14,15	1.12	2 (14%)	17,19,21	0.65	0
10	NAG	A	604	1	14,14,15	0.82	1 (7%)	17,19,21	0.63	1 (5%)
10	NAG	C	604	1	14,14,15	0.95	1 (7%)	17,19,21	0.95	2 (11%)
10	NAG	B	608	1	14,14,15	0.91	1 (7%)	17,19,21	1.06	2 (11%)
10	NAG	B	609	1	14,14,15	0.80	1 (7%)	17,19,21	0.67	1 (5%)
10	NAG	B	607	1	14,14,15	0.93	2 (14%)	17,19,21	1.44	3 (17%)
10	NAG	E	701	2	14,14,15	0.85	1 (7%)	17,19,21	0.94	2 (11%)
10	NAG	F	701	2	14,14,15	0.84	1 (7%)	17,19,21	0.93	2 (11%)
10	NAG	A	609	1	14,14,15	0.75	1 (7%)	17,19,21	0.71	1 (5%)
10	NAG	B	610	1	14,14,15	0.84	1 (7%)	17,19,21	0.98	2 (11%)
10	NAG	C	606	1	14,14,15	0.94	2 (14%)	17,19,21	1.45	3 (17%)
10	NAG	B	604	1	14,14,15	1.26	2 (14%)	17,19,21	2.92	4 (23%)
10	BMA	Y	3	9	11,11,12	1.36	2 (18%)	15,15,17	0.87	0
10	NAG	C	605	1	14,14,15	0.81	1 (7%)	17,19,21	0.73	1 (5%)
10	NAG	B	603	1	14,14,15	1.24	2 (14%)	17,19,21	1.15	1 (5%)
10	NAG	C	607	1	14,14,15	1.17	2 (14%)	17,19,21	2.90	3 (17%)
10	NAG	C	601	1	14,14,15	0.96	2 (14%)	17,19,21	0.72	1 (5%)
10	NAG	A	601	1	14,14,15	0.82	1 (7%)	17,19,21	0.75	1 (5%)
10	NAG	A	603	1	14,14,15	1.13	2 (14%)	17,19,21	1.13	1 (5%)
10	NAG	B	605	1	14,14,15	0.88	1 (7%)	17,19,21	0.95	2 (11%)
10	NAG	C	608	1	14,14,15	0.91	1 (7%)	17,19,21	1.45	3 (17%)
10	NAG	C	609	1	14,14,15	0.82	1 (7%)	17,19,21	1.02	2 (11%)

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
10	NAG	B	601	1	-	1/6/23/26	0/1/1/1
10	NAG	A	606	1	-	2/6/23/26	0/1/1/1
10	NAG	A	605	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	A	602	1	-	0/6/23/26	0/1/1/1
10	NAG	A	608	1	-	4/6/23/26	0/1/1/1
10	NAG	Y	3	1	-	5/6/23/26	0/1/1/1
10	NAG	A	610	1	-	2/6/23/26	0/1/1/1
10	NAG	D	701	2	-	4/6/23/26	0/1/1/1
10	NAG	A	607	1	-	2/6/23/26	0/1/1/1
10	NAG	C	602	-	-	2/6/23/26	0/1/1/1
10	NAG	B	606	1	-	2/6/23/26	0/1/1/1
10	NAG	B	602	1	-	0/6/23/26	0/1/1/1
10	NAG	C	603	1	-	2/6/23/26	0/1/1/1
10	NAG	A	604	1	-	2/6/23/26	0/1/1/1
10	NAG	C	604	1	-	2/6/23/26	0/1/1/1
10	NAG	B	608	1	-	4/6/23/26	0/1/1/1
10	NAG	B	609	1	-	2/6/23/26	0/1/1/1
10	NAG	B	607	1	-	2/6/23/26	0/1/1/1
10	NAG	E	701	2	-	4/6/23/26	0/1/1/1
10	NAG	F	701	2	-	4/6/23/26	0/1/1/1
10	NAG	A	609	1	-	2/6/23/26	0/1/1/1
10	NAG	B	610	1	-	4/6/23/26	0/1/1/1
10	NAG	C	606	1	-	2/6/23/26	0/1/1/1
10	NAG	B	604	1	-	6/6/23/26	0/1/1/1
10	BMA	Y	3	9	-	1/2/19/22	0/1/1/1
10	NAG	C	605	1	-	2/6/23/26	0/1/1/1
10	NAG	B	603	1	-	2/6/23/26	0/1/1/1
10	NAG	C	607	1	-	5/6/23/26	0/1/1/1
10	NAG	C	601	1	-	0/6/23/26	0/1/1/1
10	NAG	A	601	1	-	2/6/23/26	0/1/1/1
10	NAG	A	603	1	-	2/6/23/26	0/1/1/1
10	NAG	B	605	1	-	3/6/23/26	0/1/1/1
10	NAG	C	608	1	-	4/6/23/26	0/1/1/1
10	NAG	C	609	1	-	4/6/23/26	0/1/1/1

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Y	3	NAG	C1-C2	4.64	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	603	NAG	C1-C2	3.31	1.56	1.52
10	B	604	NAG	C1-C2	3.27	1.56	1.52
10	B	603	NAG	O5-C1	3.15	1.49	1.43
10	C	603	NAG	C1-C2	3.13	1.56	1.52

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	607	NAG	C2-N2-C7	10.07	136.40	122.90
10	B	604	NAG	C2-N2-C7	10.07	136.39	122.90
10	Y	3	NAG	C2-N2-C7	9.95	136.24	122.90
10	B	604	NAG	C1-C2-N2	5.15	118.55	110.43
10	C	607	NAG	C1-C2-N2	5.05	118.39	110.43

There are no chirality outliers.

5 of 87 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	608	NAG	C4-C5-C6-O6
10	C	605	NAG	O5-C5-C6-O6
10	E	701	NAG	O5-C5-C6-O6
10	B	606	NAG	O5-C5-C6-O6
10	A	601	NAG	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	3
1	C	3
1	A	3

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Mol	Chain	Number of breaks
2	F	1
2	E	1
2	D	1

The worst 5 of 12 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	397:SER	C	411:ASN	N	25.12
1	C	397:SER	C	411:ASN	N	24.97
1	A	397:SER	C	411:ASN	N	24.77
1	F	546:SER	C	565:LEU	N	23.15
1	E	546:SER	C	565:LEU	N	23.07

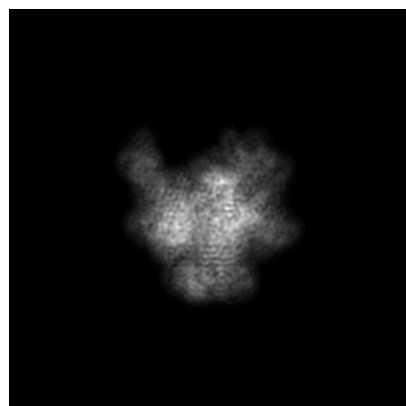
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26493. These allow visual inspection of the internal detail of the map and identification of artifacts.

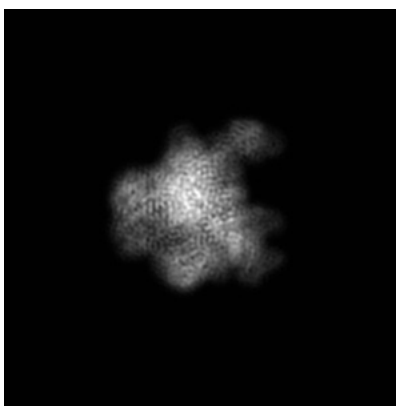
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

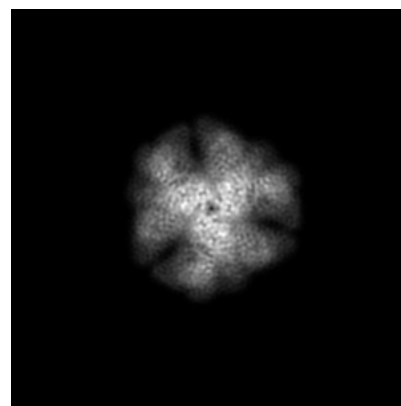
#### 6.1.1 Primary map



X

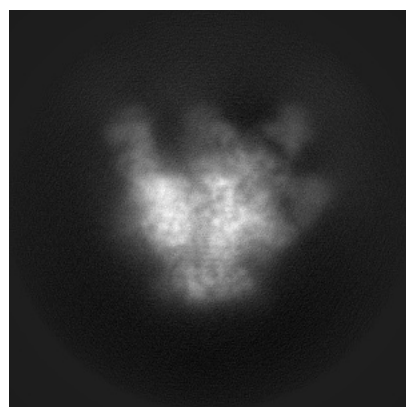


Y

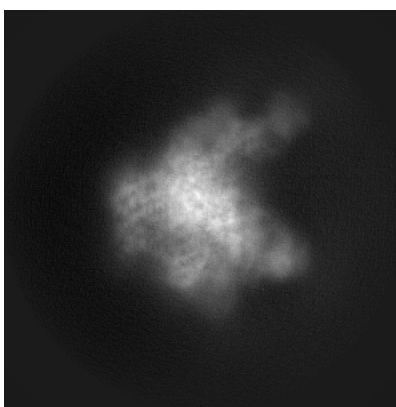


Z

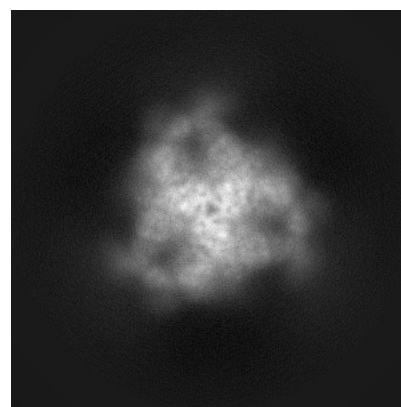
#### 6.1.2 Raw map



X



Y

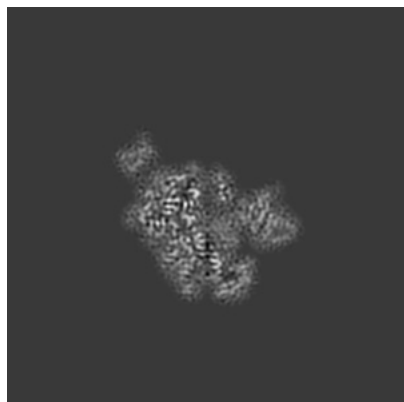


Z

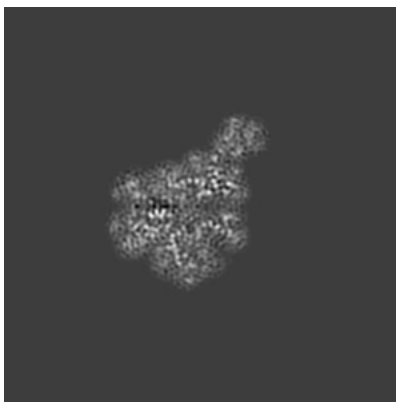
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

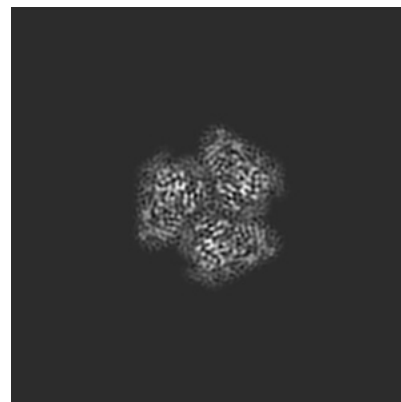
### 6.2.1 Primary map



X Index: 180

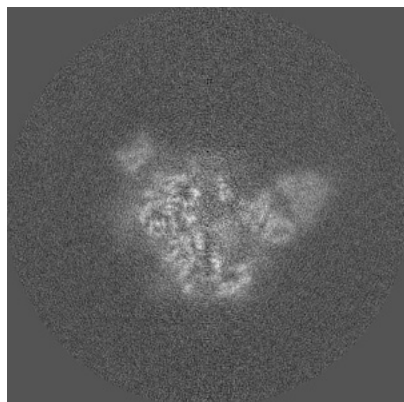


Y Index: 180

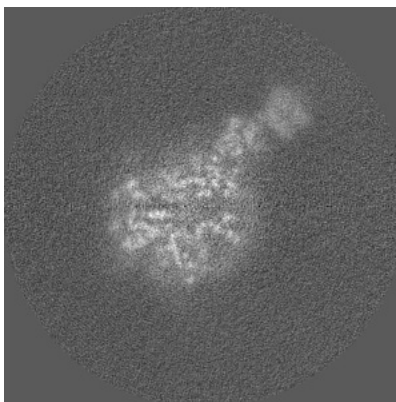


Z Index: 180

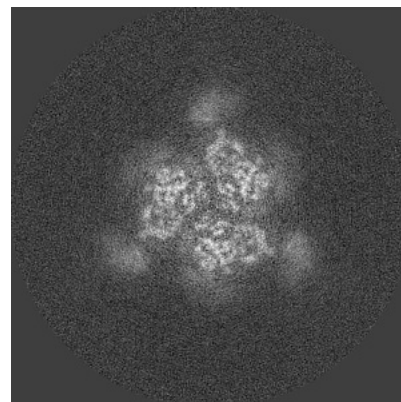
### 6.2.2 Raw map



X Index: 180



Y Index: 180

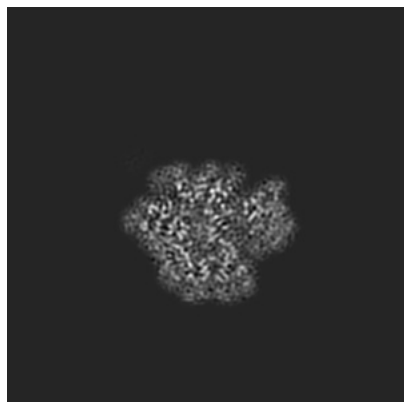


Z Index: 180

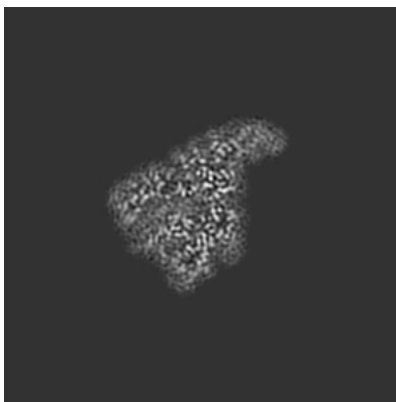
The images above show central slices of the map in three orthogonal directions.

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

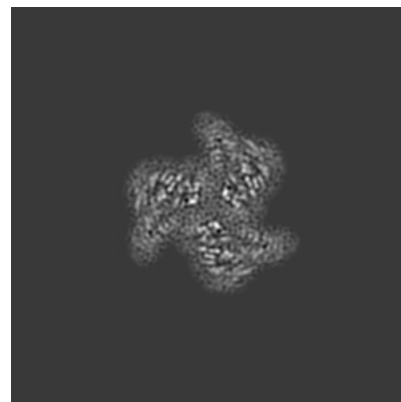
### 6.3.1 Primary map



X Index: 190

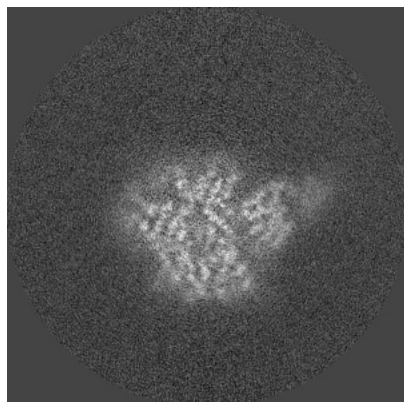


Y Index: 196

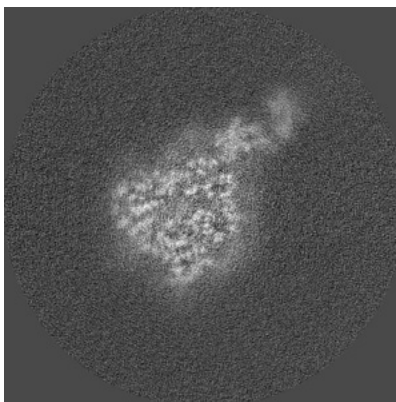


Z Index: 166

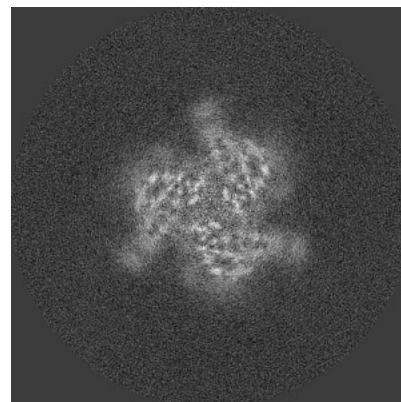
### 6.3.2 Raw map



X Index: 191



Y Index: 190



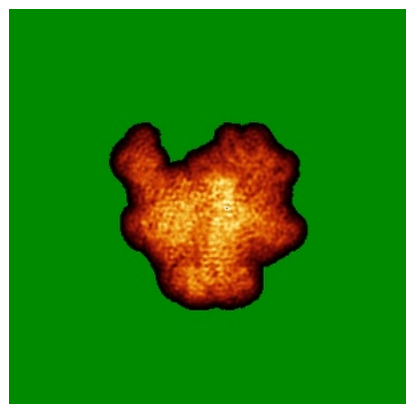
Z Index: 167

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

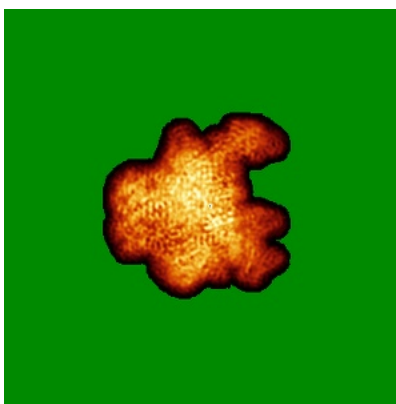


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

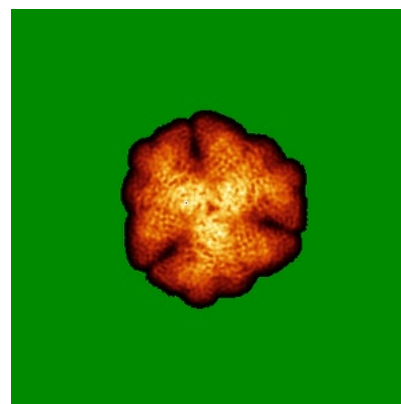
### 6.4.1 Primary map



X

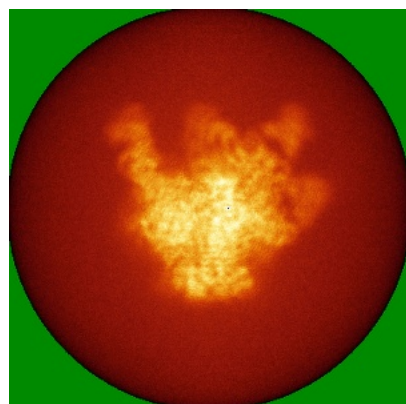


Y

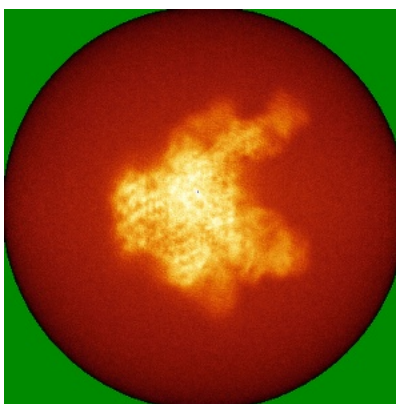


Z

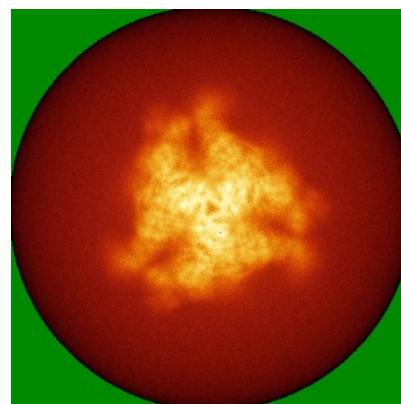
### 6.4.2 Raw map



X



Y



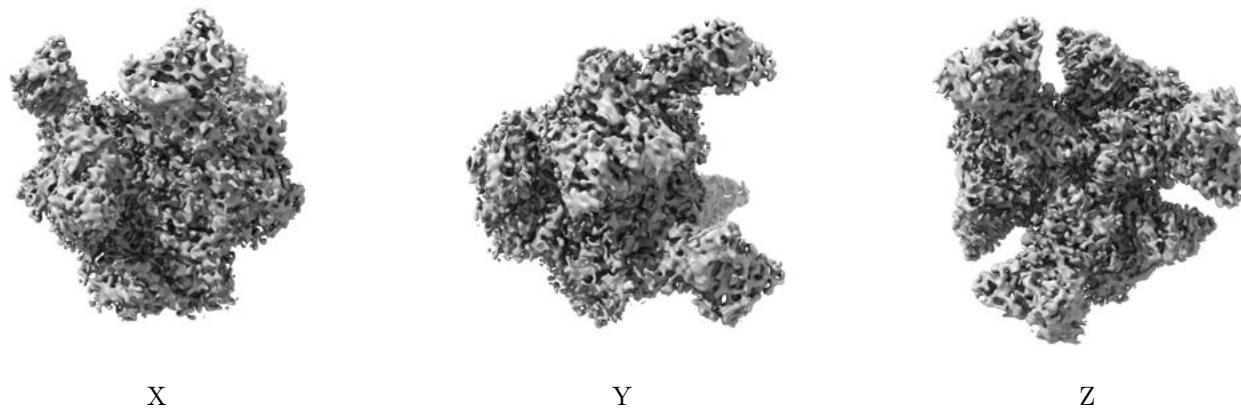
Z

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.



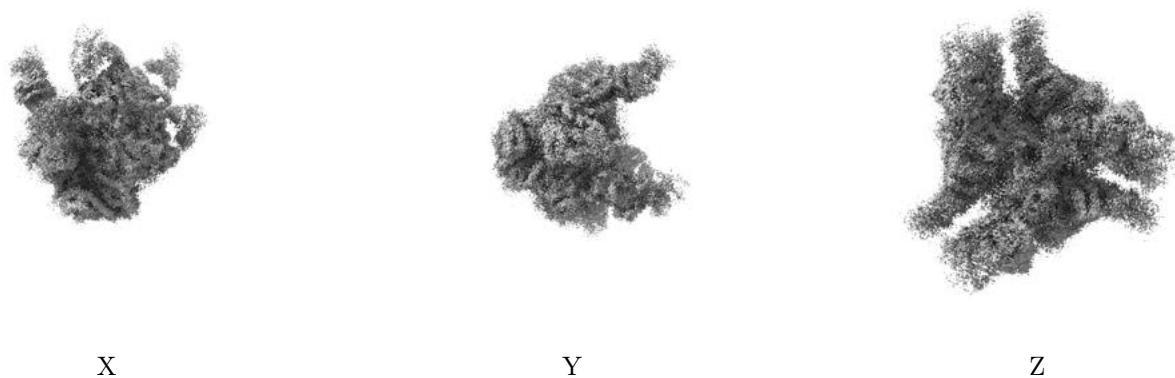
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0122. 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.

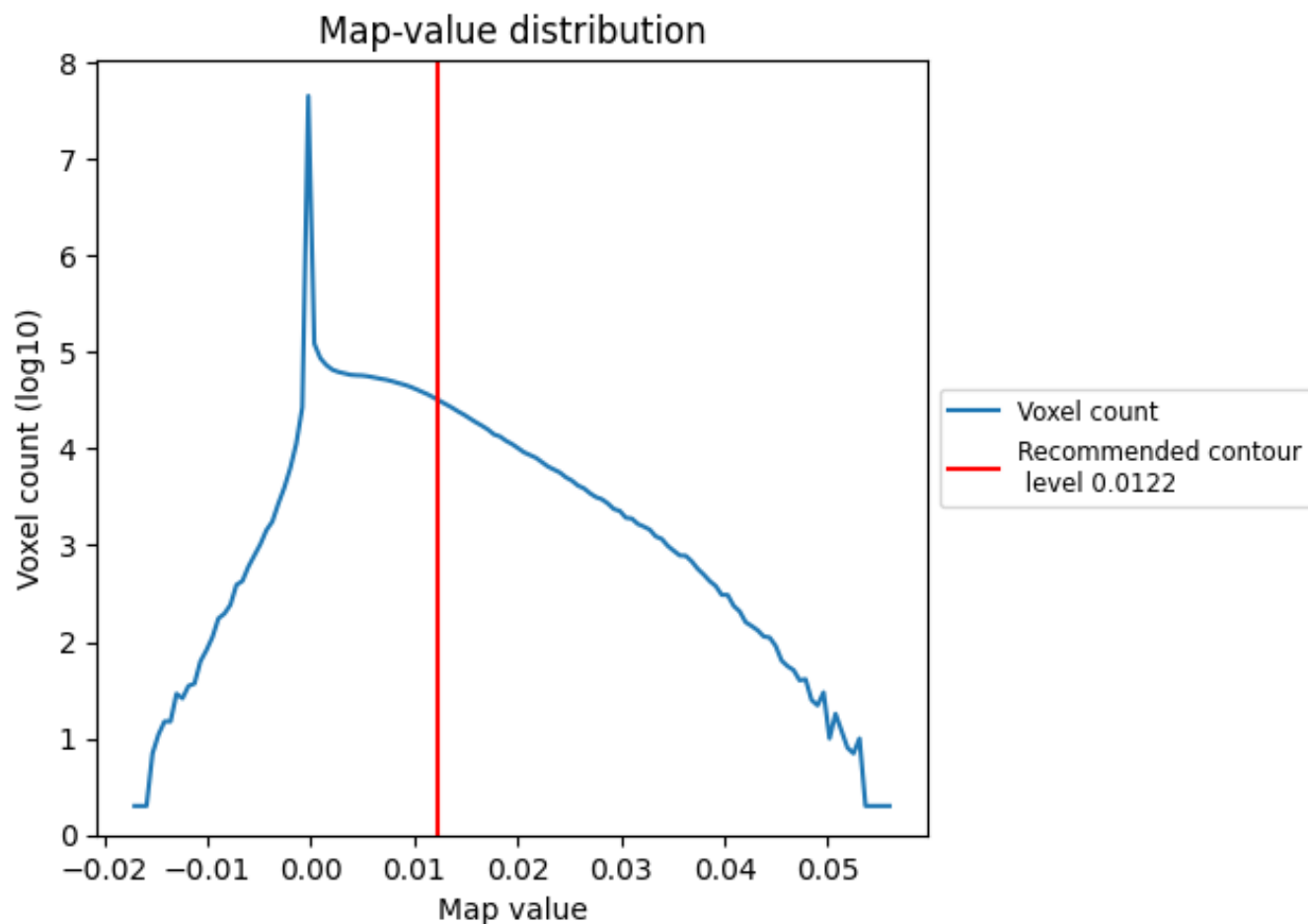
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

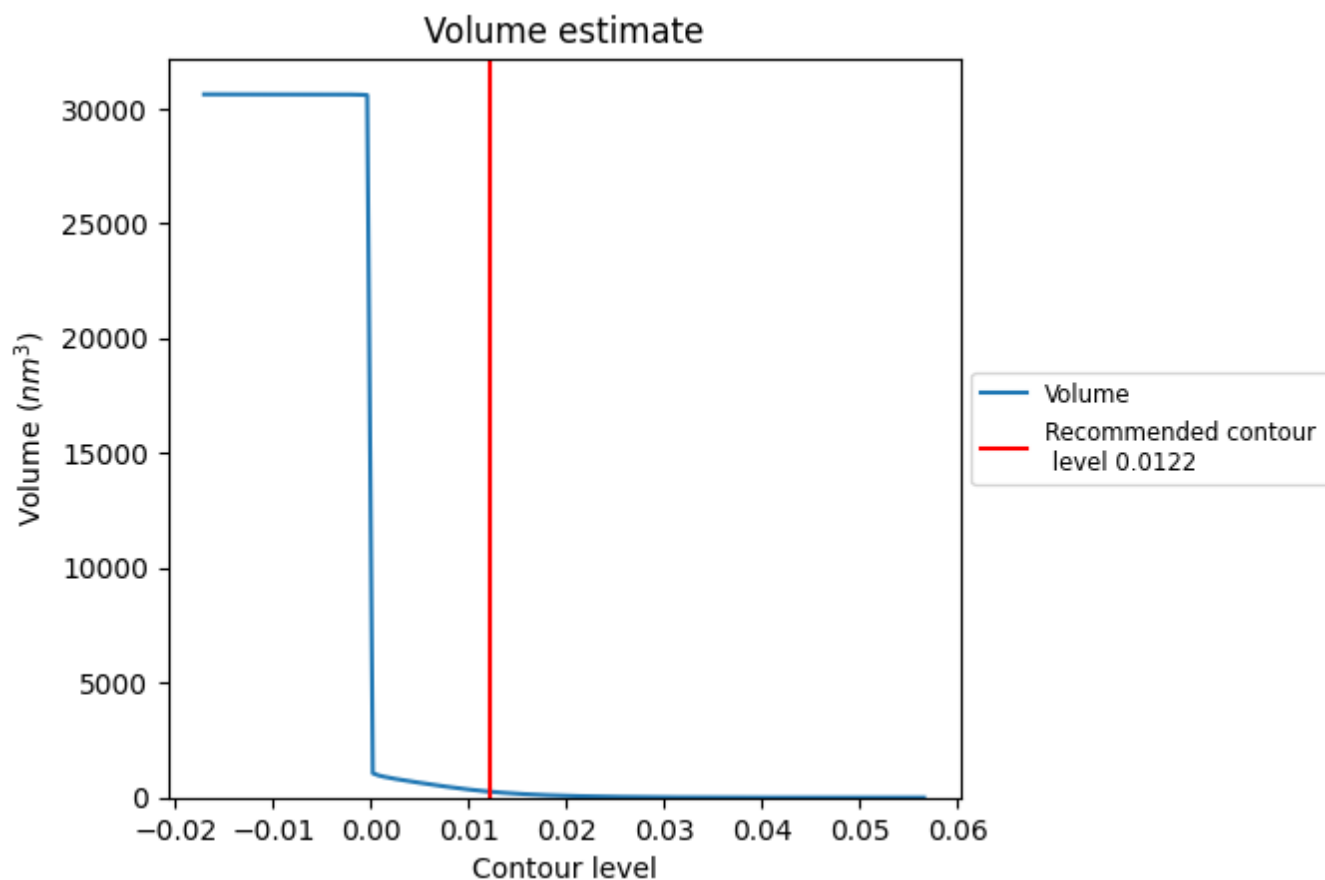
This section contains the results of statistical analysis of the map.

### 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.

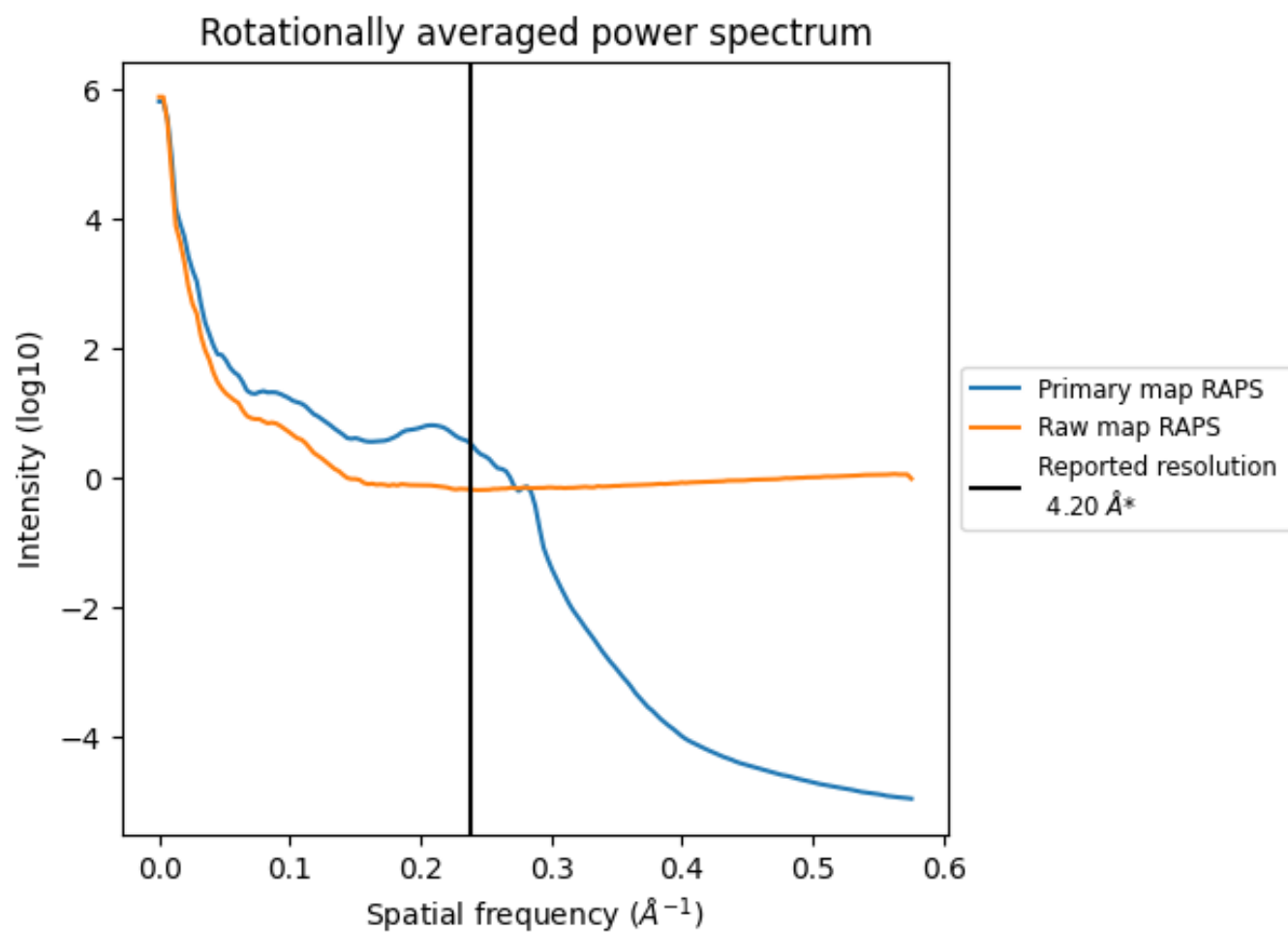
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 256 nm<sup>3</sup>; this corresponds to an approximate mass of 231 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 ⓘ

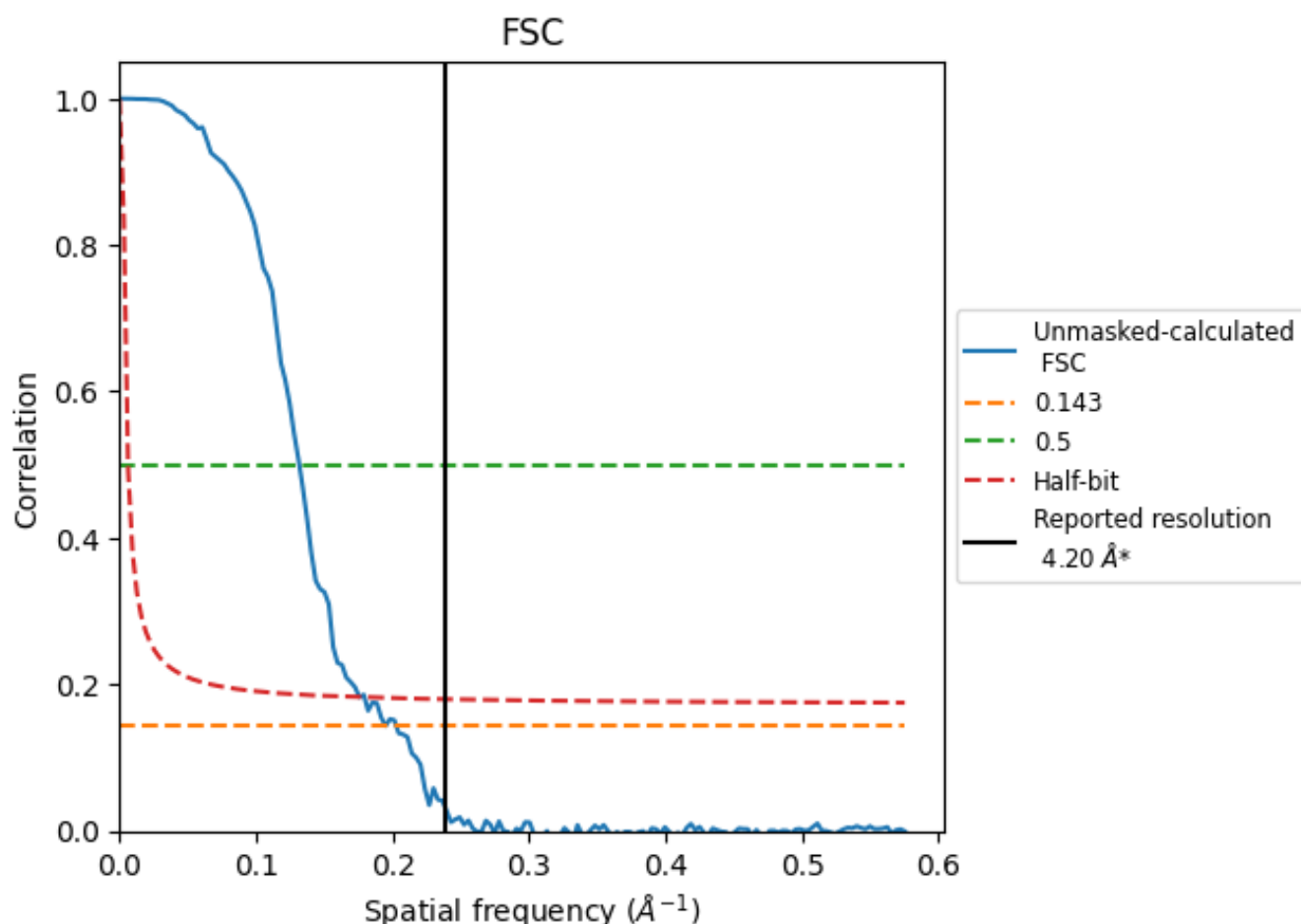


\*Reported resolution corresponds to spatial frequency of 0.238  $\text{\AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.238 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

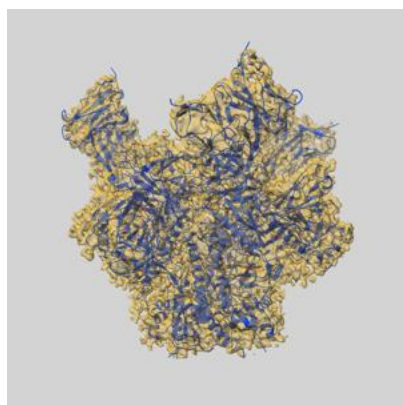
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.93	7.59	5.57

\*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 4.93 differs from the reported value 4.2 by more than 10 %

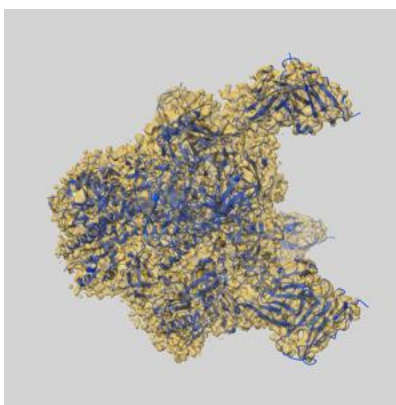
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26493 and PDB model 7UGP. Per-residue inclusion information can be found in section [3](#) on page [12](#).

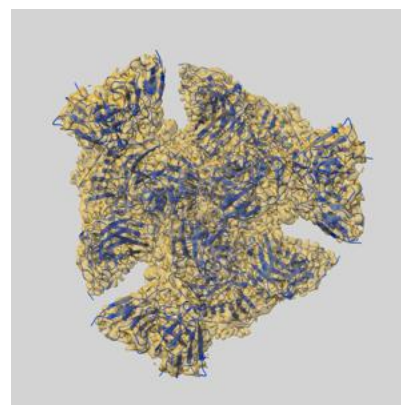
### 9.1 Map-model overlay [i](#)



X



Y



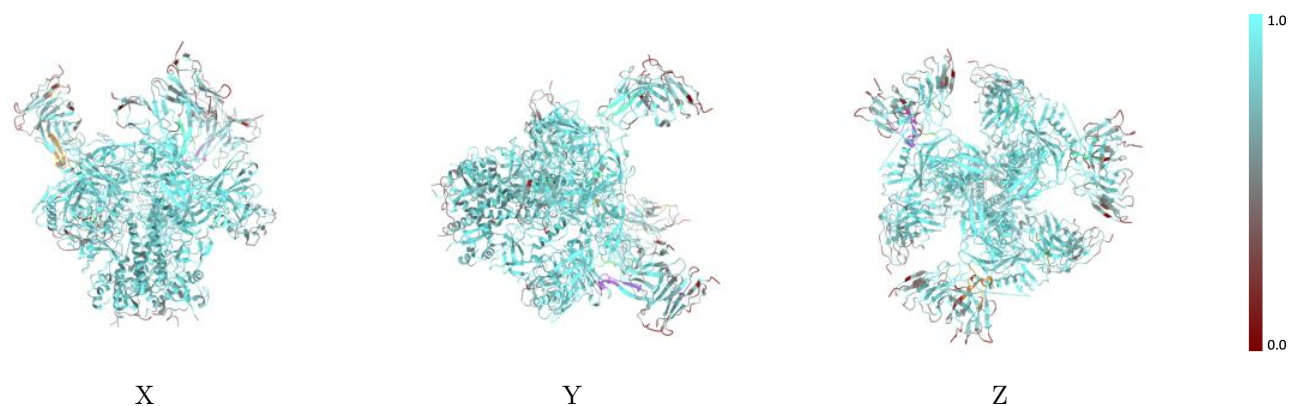
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0122 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](#)

This section was not generated.

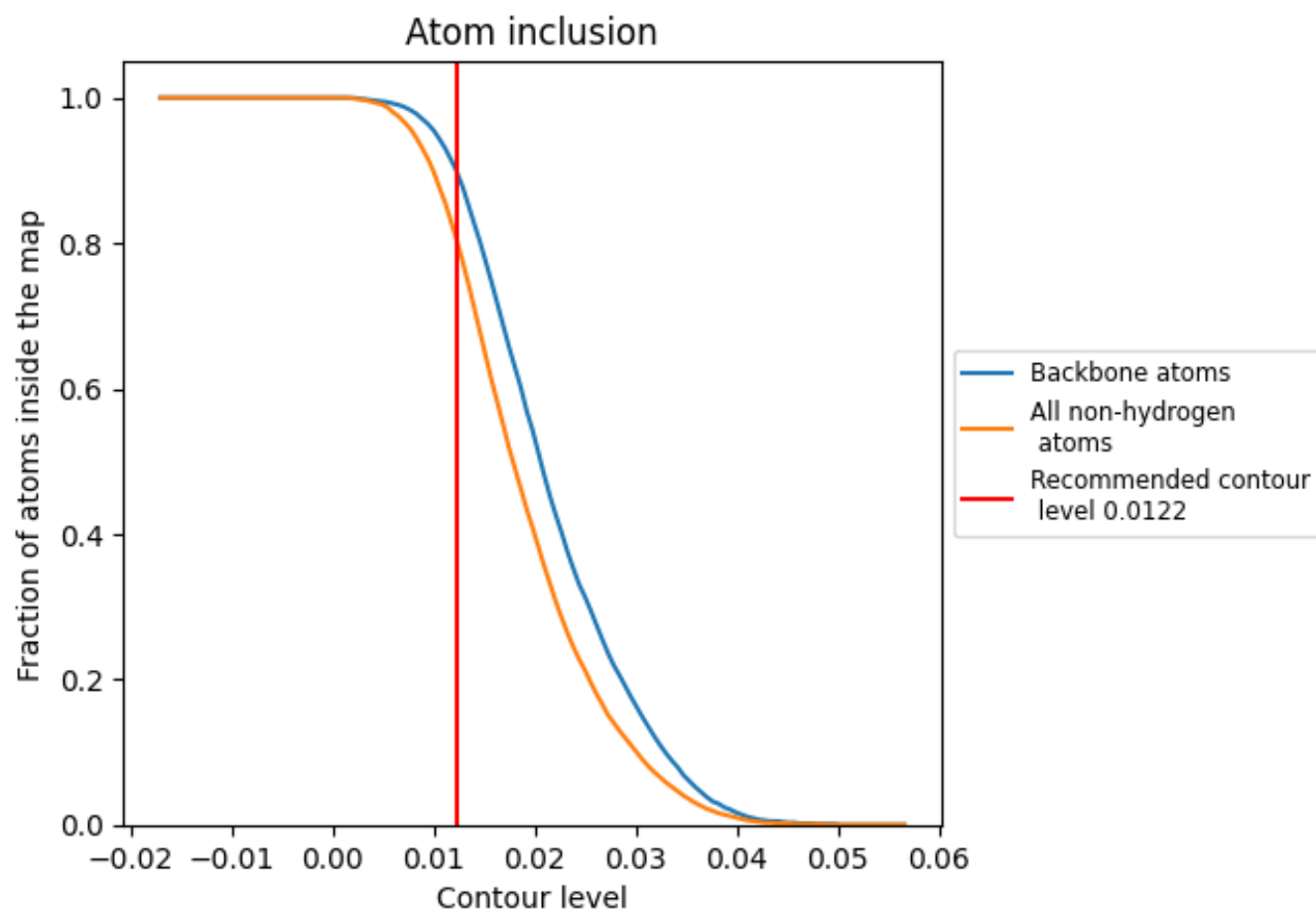
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.0122).































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 81% 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 (0.0122) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	 0.8080
A	 0.8840
B	 0.8850
C	 0.8850
D	 0.8160
E	 0.8180
F	 0.8160
G	 0.8610
H	 0.8610
I	 0.8690
J	 0.6490
K	 0.6500
L	 0.6510
M	 0.6400
N	 0.6430
O	 0.6350
P	 0.7550
Q	 0.7520
R	 0.7610
S	 0.9030
T	 0.5360
U	 0.8210
V	 0.9170
W	 0.6430
X	 0.7440
Y	 0.7740
Z	 0.9170
a	 0.6430

