



## Full wwPDB EM Validation Report ⓘ

Jun 3, 2025 – 03:10 PM EDT

PDB ID : 9BTH / pdb\_00009bth  
EMDB ID : EMD-44890  
Title : Rhesus Fab 42056-a.01 in complex with CAP256SU.wk34 RnS SOSIP Env  
Authors : Gorman, J.; Kwong, P.D.  
Deposited on : 2024-05-15  
Resolution : 4.20 Å (reported)  
Based on initial model : 6VTT

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

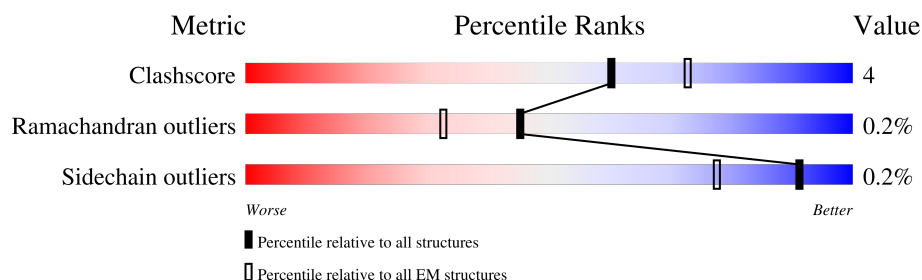
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 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	H	244	
2	L	220	
3	D	471	
3	F	471	
3	G	471	
4	B	154	
4	C	154	
4	E	154	

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Mol	Chain	Length	Quality of chain
5	A	3	<div> <div>33%</div> <div>67%</div> </div>
5	O	3	<div> <div>33%</div> <div>67%</div> </div>
6	I	2	<div> <div>50%</div> <div>50%</div> </div>
6	N	2	<div> <div>50%</div> <div>100%</div> </div>
6	P	2	<div> <div>50%</div> <div>50%</div> </div>
6	R	2	<div> <div>50%</div> <div>50%</div> </div>
6	S	2	<div> <div>50%</div> <div>50%</div> </div>
6	V	2	<div> <div>50%</div> <div>50%</div> </div>
7	J	5	<div> <div>40%</div> <div>60%</div> <div>40%</div> </div>
7	Q	5	<div> <div>40%</div> <div>80%</div> <div>20%</div> </div>
7	T	5	<div> <div>40%</div> <div>100%</div> </div>
8	K	6	<div> <div>100%</div> <div>83%</div> <div>17%</div> </div>
9	M	9	<div> <div>11%</div> <div>22%</div> <div>78%</div> </div>
10	U	7	<div> <div>86%</div> <div>100%</div> </div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 16629 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 Heavy.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	132	Total	C	N	O	S	0	0
			1017	637	168	207	5		

- Molecule 2 is a protein called Light.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	111	Total	C	N	O	S	0	0
			865	541	147	173	4		

- Molecule 3 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	434	Total	C	N	O	S	0	0
			3449	2174	596	653	26		
3	D	432	Total	C	N	O	S	0	0
			3431	2162	594	649	26		
3	F	431	Total	C	N	O	S	0	0
			3422	2156	592	648	26		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	204	ILE	ALA	conflict	UNP A0A0N9FF17
G	302	MET	ASN	conflict	UNP A0A0N9FF17
G	320	LEU	THR	conflict	UNP A0A0N9FF17
G	329	PRO	ALA	conflict	UNP A0A0N9FF17
G	437	PRO	SER	conflict	UNP A0A0N9FF17
G	442	ASN	GLU	conflict	UNP A0A0N9FF17
G	501	CYS	ALA	conflict	UNP A0A0N9FF17
G	502	ASN	ARG	conflict	UNP A0A0N9FF17
G	504	THR	ARG	conflict	UNP A0A0N9FF17
G	508	ARG	LYS	conflict	UNP A0A0N9FF17
G	509	ARG	GLU	conflict	UNP A0A0N9FF17

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Chain	Residue	Modelled	Actual	Comment	Reference
G	510	ARG	LYS	conflict	UNP A0A0N9FF17
G	512	ARG	-	expression tag	UNP A0A0N9FF17
G	513	ARG	-	expression tag	UNP A0A0N9FF17
D	204	ILE	ALA	conflict	UNP A0A0N9FF17
D	302	MET	ASN	conflict	UNP A0A0N9FF17
D	320	LEU	THR	conflict	UNP A0A0N9FF17
D	329	PRO	ALA	conflict	UNP A0A0N9FF17
D	437	PRO	SER	conflict	UNP A0A0N9FF17
D	442	ASN	GLU	conflict	UNP A0A0N9FF17
D	501	CYS	ALA	conflict	UNP A0A0N9FF17
D	502	ASN	ARG	conflict	UNP A0A0N9FF17
D	504	THR	ARG	conflict	UNP A0A0N9FF17
D	508	ARG	LYS	conflict	UNP A0A0N9FF17
D	509	ARG	GLU	conflict	UNP A0A0N9FF17
D	510	ARG	LYS	conflict	UNP A0A0N9FF17
D	512	ARG	-	expression tag	UNP A0A0N9FF17
D	513	ARG	-	expression tag	UNP A0A0N9FF17
F	204	ILE	ALA	conflict	UNP A0A0N9FF17
F	302	MET	ASN	conflict	UNP A0A0N9FF17
F	320	LEU	THR	conflict	UNP A0A0N9FF17
F	329	PRO	ALA	conflict	UNP A0A0N9FF17
F	437	PRO	SER	conflict	UNP A0A0N9FF17
F	442	ASN	GLU	conflict	UNP A0A0N9FF17
F	501	CYS	ALA	conflict	UNP A0A0N9FF17
F	502	ASN	ARG	conflict	UNP A0A0N9FF17
F	504	THR	ARG	conflict	UNP A0A0N9FF17
F	508	ARG	LYS	conflict	UNP A0A0N9FF17
F	509	ARG	GLU	conflict	UNP A0A0N9FF17
F	510	ARG	LYS	conflict	UNP A0A0N9FF17
F	512	ARG	-	expression tag	UNP A0A0N9FF17
F	513	ARG	-	expression tag	UNP A0A0N9FF17

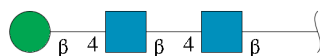
- Molecule 4 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	125	Total	C	N	O	S	0	0
			990	634	164	185	7		
4	E	122	Total	C	N	O	S	0	0
			974	624	161	182	7		
4	B	127	Total	C	N	O	S	0	0
			1008	645	169	187	7		

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	535	ASN	ILE	conflict	UNP A0A0N9FF17
C	559	PRO	ILE	conflict	UNP A0A0N9FF17
C	569	GLY	THR	conflict	UNP A0A0N9FF17
C	573	PHE	ILE	conflict	UNP A0A0N9FF17
C	588	GLU	LYS	conflict	UNP A0A0N9FF17
C	589	VAL	ASP	conflict	UNP A0A0N9FF17
C	605	CYS	THR	conflict	UNP A0A0N9FF17
C	609	PRO	TYR	conflict	UNP A0A0N9FF17
C	636	GLY	ASP	conflict	UNP A0A0N9FF17
C	651	PHE	LYS	conflict	UNP A0A0N9FF17
C	655	ILE	SER	conflict	UNP A0A0N9FF17
C	660	ASN	LEU	conflict	UNP A0A0N9FF17
C	662	THR	ALA	conflict	UNP A0A0N9FF17
E	535	ASN	ILE	conflict	UNP A0A0N9FF17
E	559	PRO	ILE	conflict	UNP A0A0N9FF17
E	569	GLY	THR	conflict	UNP A0A0N9FF17
E	573	PHE	ILE	conflict	UNP A0A0N9FF17
E	588	GLU	LYS	conflict	UNP A0A0N9FF17
E	589	VAL	ASP	conflict	UNP A0A0N9FF17
E	605	CYS	THR	conflict	UNP A0A0N9FF17
E	609	PRO	TYR	conflict	UNP A0A0N9FF17
E	636	GLY	ASP	conflict	UNP A0A0N9FF17
E	651	PHE	LYS	conflict	UNP A0A0N9FF17
E	655	ILE	SER	conflict	UNP A0A0N9FF17
E	660	ASN	LEU	conflict	UNP A0A0N9FF17
E	662	THR	ALA	conflict	UNP A0A0N9FF17
B	535	ASN	ILE	conflict	UNP A0A0N9FF17
B	559	PRO	ILE	conflict	UNP A0A0N9FF17
B	569	GLY	THR	conflict	UNP A0A0N9FF17
B	573	PHE	ILE	conflict	UNP A0A0N9FF17
B	588	GLU	LYS	conflict	UNP A0A0N9FF17
B	589	VAL	ASP	conflict	UNP A0A0N9FF17
B	605	CYS	THR	conflict	UNP A0A0N9FF17
B	609	PRO	TYR	conflict	UNP A0A0N9FF17
B	636	GLY	ASP	conflict	UNP A0A0N9FF17
B	651	PHE	LYS	conflict	UNP A0A0N9FF17
B	655	ILE	SER	conflict	UNP A0A0N9FF17
B	660	ASN	LEU	conflict	UNP A0A0N9FF17
B	662	THR	ALA	conflict	UNP A0A0N9FF17

- Molecule 5 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.



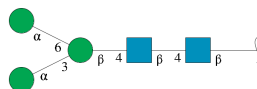
Mol	Chain	Residues	Atoms				AltConf	Trace
5	A	3	Total	C	N	O	0	0
			39	22	2	15		
5	O	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 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
6	I	2	Total	C	N	O	0	0
			28	16	2	10		
6	N	2	Total	C	N	O	0	0
			28	16	2	10		
6	P	2	Total	C	N	O	0	0
			28	16	2	10		
6	R	2	Total	C	N	O	0	0
			28	16	2	10		
6	S	2	Total	C	N	O	0	0
			28	16	2	10		
6	V	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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.



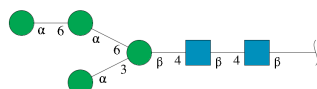
Mol	Chain	Residues	Atoms				AltConf	Trace
7	J	5	Total	C	N	O	0	0
			61	34	2	25		

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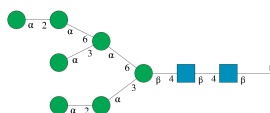
Mol	Chain	Residues	Atoms				AltConf	Trace
7	Q	5	Total	C	N	O	0	0
			61	34	2	25		
7	T	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



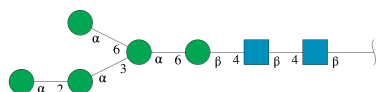
Mol	Chain	Residues	Atoms				AltConf	Trace
8	K	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
9	M	9	Total	C	N	O	0	0
			105	58	2	45		

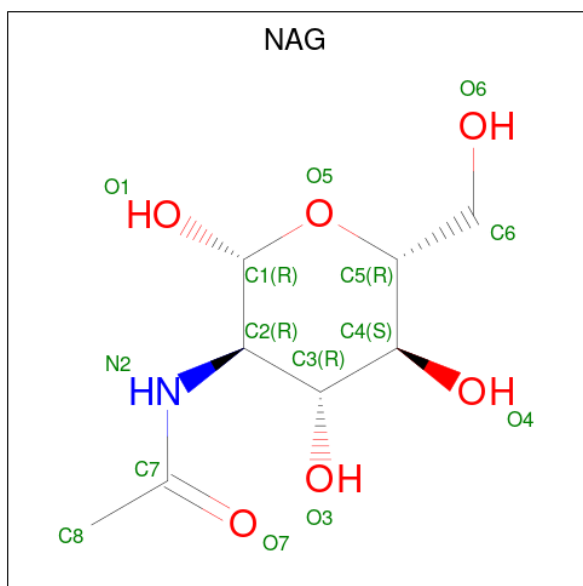
- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





Mol	Chain	Residues	Atoms				AltConf	Trace
10	U	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				AltConf
11	G	1	Total	C	N	O	0
			14	8	1	5	
11	G	1	Total	C	N	O	0
			14	8	1	5	
11	G	1	Total	C	N	O	0
			14	8	1	5	
11	G	1	Total	C	N	O	0
			14	8	1	5	
11	G	1	Total	C	N	O	0
			14	8	1	5	
11	G	1	Total	C	N	O	0
			14	8	1	5	
11	G	1	Total	C	N	O	0
			14	8	1	5	
11	G	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
11	G	1	Total 14	C 8	N 1	O 5	0
11	G	1	Total 14	C 8	N 1	O 5	0
11	G	1	Total 14	C 8	N 1	O 5	0
11	G	1	Total 14	C 8	N 1	O 5	0
11	G	1	Total 14	C 8	N 1	O 5	0
11	G	1	Total 14	C 8	N 1	O 5	0
11	C	1	Total 14	C 8	N 1	O 5	0
11	C	1	Total 14	C 8	N 1	O 5	0
11	D	1	Total 14	C 8	N 1	O 5	0
11	D	1	Total 14	C 8	N 1	O 5	0
11	D	1	Total 14	C 8	N 1	O 5	0
11	D	1	Total 14	C 8	N 1	O 5	0
11	D	1	Total 14	C 8	N 1	O 5	0
11	D	1	Total 14	C 8	N 1	O 5	0
11	D	1	Total 14	C 8	N 1	O 5	0
11	D	1	Total 14	C 8	N 1	O 5	0
11	D	1	Total 14	C 8	N 1	O 5	0
11	D	1	Total 14	C 8	N 1	O 5	0
11	D	1	Total 14	C 8	N 1	O 5	0
11	D	1	Total 14	C 8	N 1	O 5	0
11	D	1	Total 14	C 8	N 1	O 5	0
11	D	1	Total 14	C 8	N 1	O 5	0

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

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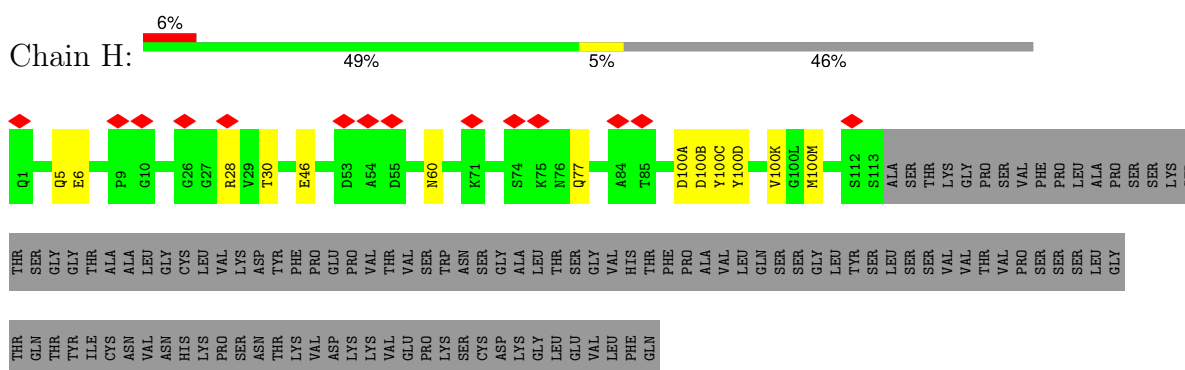
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Mol	Chain	Residues	Atoms				AltConf
11	B	1	Total	C	N	O	0
			14	8	1	5	
11	B	1	Total	C	N	O	0
			14	8	1	5	
11	B	1	Total	C	N	O	0
			14	8	1	5	
11	B	1	Total	C	N	O	0
			14	8	1	5	

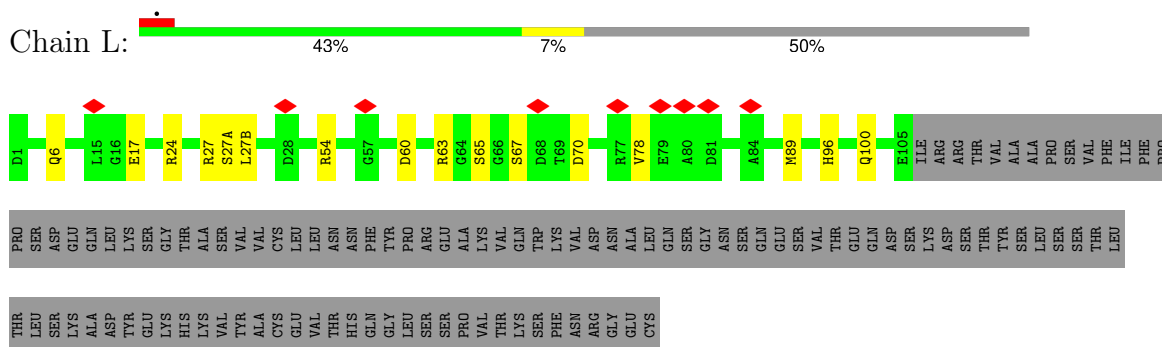
### 3 Residue-property plots [i](#)

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.

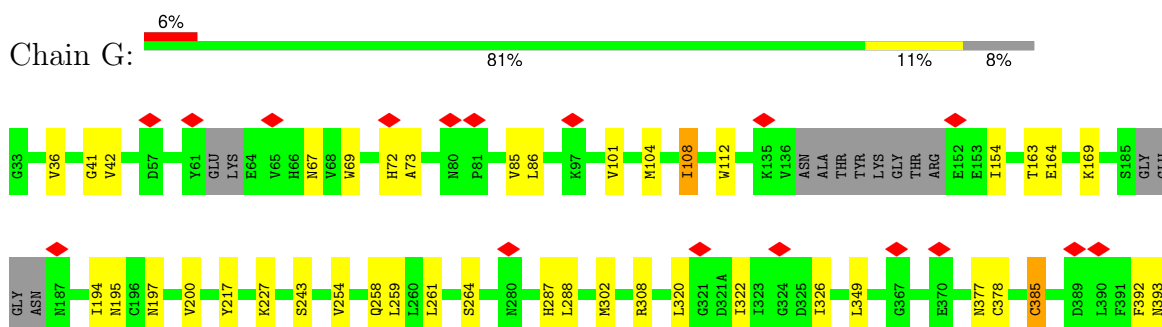
#### • Molecule 1: Heavy



#### • Molecule 2: Light

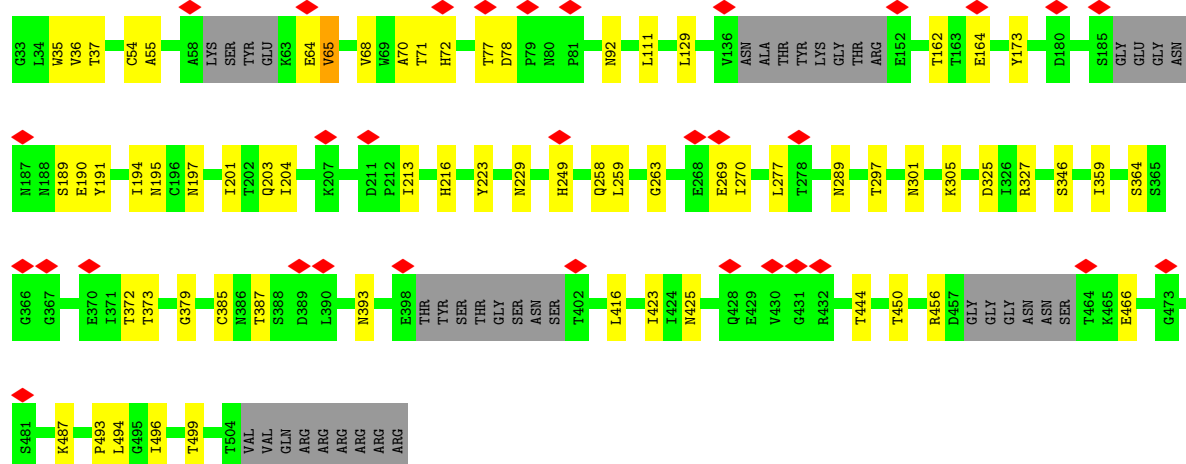
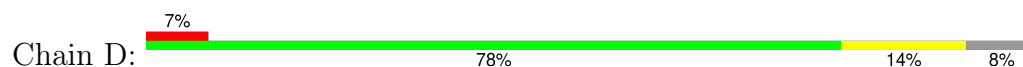


#### • Molecule 3: Envelope glycoprotein gp120

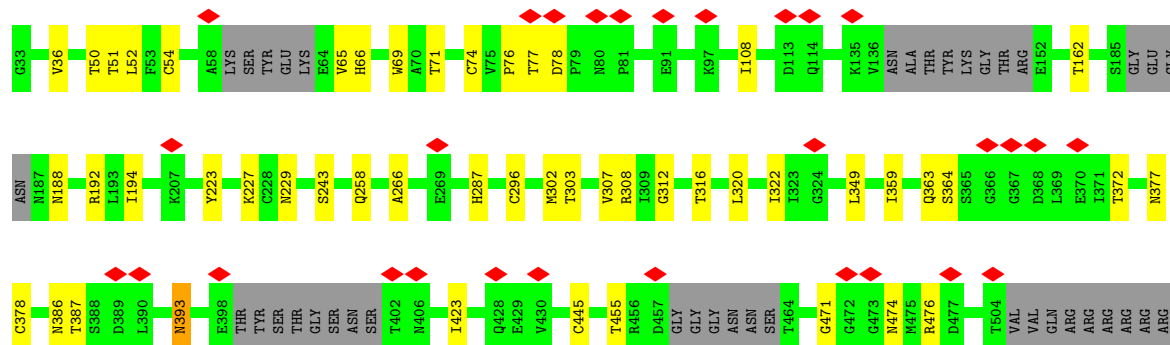
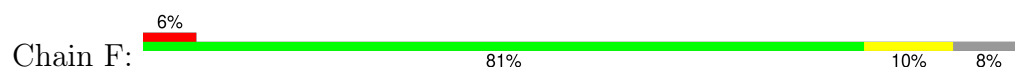




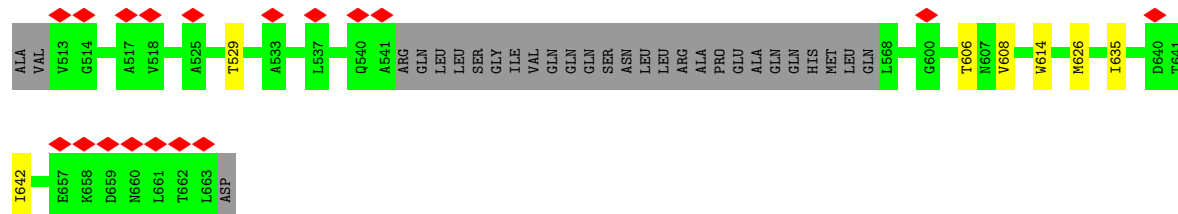
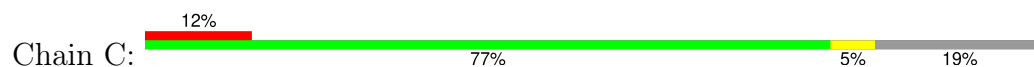
• Molecule 3: Envelope glycoprotein gp120



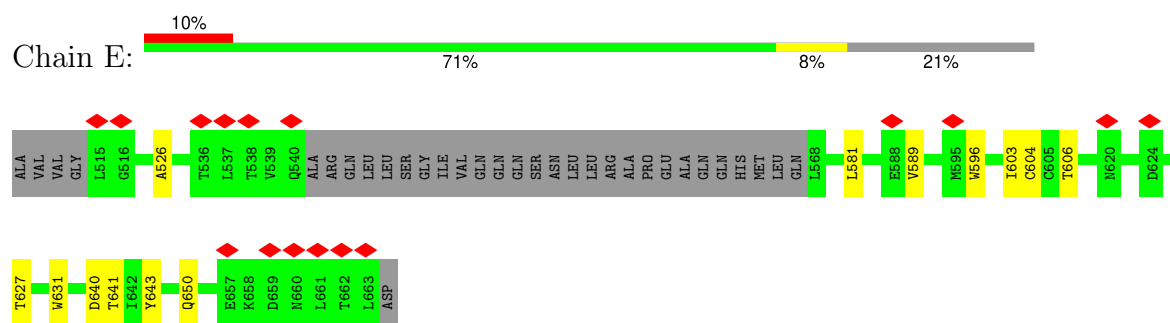
• Molecule 3: Envelope glycoprotein gp120



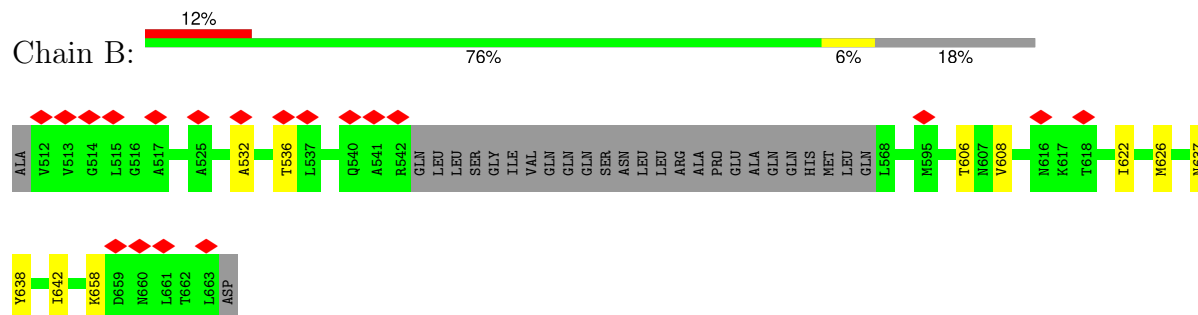
• Molecule 4: Envelope glycoprotein gp41



• Molecule 4: Envelope glycoprotein gp41



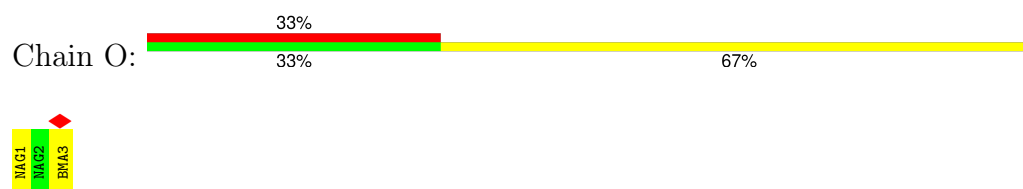
- Molecule 4: Envelope glycoprotein gp41



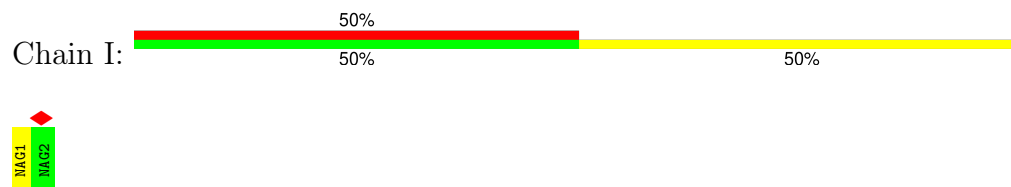
- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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



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



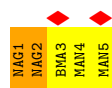
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

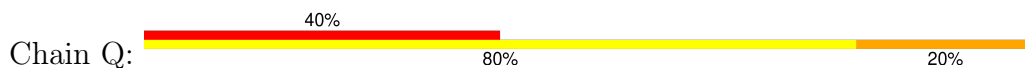


- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





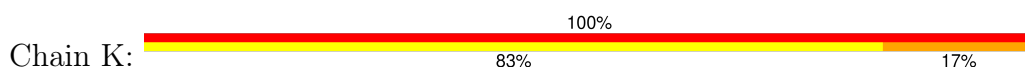
- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-3)-[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



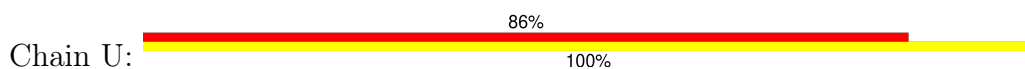
- Molecule 8: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	69264	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	56.03	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.989	Depositor
Minimum map value	-0.903	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.55	Depositor
Map size ( $\text{\AA}$ )	344.32, 344.32, 344.32	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.076, 1.076, 1.076	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: BMA, NAG, MAN, TYS

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	H	0.21	0/1022	0.39	0/1389
2	L	0.14	0/883	0.34	0/1198
3	D	0.16	0/3500	0.42	0/4751
3	F	0.18	0/3491	0.43	0/4740
3	G	0.17	0/3519	0.41	2/4777 (0.0%)
4	B	0.13	0/1029	0.33	0/1396
4	C	0.13	0/1011	0.34	0/1372
4	E	0.13	0/995	0.32	0/1350
All	All	0.16	0/15450	0.40	2/20973 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	385	CYS	CA-C-N	5.03	127.52	120.28
3	G	385	CYS	C-N-CA	5.03	127.52	120.28

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	H	1017	0	979	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	865	0	842	11	0
3	D	3431	0	3359	42	0
3	F	3422	0	3346	35	0
3	G	3449	0	3375	35	0
4	B	1008	0	978	7	0
4	C	990	0	958	5	0
4	E	974	0	939	11	0
5	A	39	0	34	0	0
5	O	39	0	34	0	0
6	I	28	0	25	0	0
6	N	28	0	25	0	0
6	P	28	0	25	1	0
6	R	28	0	25	0	0
6	S	28	0	25	1	0
6	V	28	0	25	0	0
7	J	61	0	52	3	0
7	Q	61	0	52	1	0
7	T	61	0	52	0	0
8	K	72	0	61	1	0
9	M	105	0	88	0	0
10	U	83	0	70	0	0
11	B	56	0	52	0	0
11	C	28	0	26	0	0
11	D	210	0	195	2	0
11	E	56	0	52	0	0
11	F	210	0	195	0	0
11	G	224	0	208	2	0
All	All	16629	0	16097	140	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (140) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:277:LEU:O	3:D:456:ARG:NH1	2.16	0.79
11:G:608:NAG:H83	7:J:1:NAG:H83	1.64	0.79
3:G:36:VAL:O	4:C:606:THR:OG1	2.04	0.75
1:H:5:GLN:NE2	1:H:6:GLU:O	2.20	0.75
3:D:379:GLY:HA3	7:Q:2:NAG:H83	1.68	0.75
3:F:349:LEU:HD11	3:F:359:ILE:HD13	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:307:VAL:O	3:F:316:THR:OG1	2.08	0.71
3:D:270:ILE:HG22	11:D:609:NAG:H81	1.71	0.71
2:L:24:ARG:NH1	2:L:70:ASP:OD1	2.24	0.70
3:D:229:ASN:ND2	6:P:1:NAG:O6	2.26	0.69
3:F:363:GLN:O	3:F:364:SER:OG	2.10	0.68
3:G:264:SER:OG	3:G:482:GLU:OE1	2.10	0.68
3:G:163:THR:OG1	3:G:164:GLU:OE1	2.12	0.67
3:D:36:VAL:O	4:E:606:THR:OG1	2.11	0.67
3:F:194:ILE:HG22	3:F:423:ILE:HD11	1.77	0.66
1:H:46:GLU:OE2	1:H:60:ASN:ND2	2.29	0.66
3:G:101:VAL:HG21	3:G:480:ARG:HG3	1.78	0.65
3:G:477:ASP:OD1	3:G:480:ARG:NH2	2.29	0.65
3:G:104:MET:SD	3:G:217:TYR:OH	2.51	0.63
3:D:325:ASP:O	3:D:327:ARG:NH1	2.33	0.62
3:D:71:THR:HG22	3:D:72:HIS:H	1.63	0.62
3:F:258:GLN:NE2	3:F:372:THR:O	2.33	0.62
3:D:195:ASN:ND2	3:D:425:ASN:OD1	2.33	0.62
2:L:6:GLN:OE1	2:L:100:GLN:N	2.33	0.61
3:F:229:ASN:ND2	6:S:1:NAG:O5	2.34	0.61
2:L:54:ARG:NH1	2:L:60:ASP:OD1	2.34	0.61
1:H:77:GLN:N	1:H:77:GLN:OE1	2.34	0.60
3:D:203:GLN:NE2	3:D:204:ILE:O	2.35	0.60
3:G:169:LYS:HB2	8:K:1:NAG:H82	1.83	0.60
3:F:162:THR:O	3:F:312:GLY:N	2.35	0.59
3:D:373:THR:OG1	3:D:385:CYS:O	2.20	0.58
3:G:287:HIS:C	3:G:288:LEU:HD12	2.29	0.57
3:D:54:CYS:SG	3:D:55:ALA:N	2.77	0.57
3:D:364:SER:OG	3:D:372:THR:OG1	2.23	0.57
3:F:302:MET:HE2	3:F:320:LEU:HB3	1.87	0.57
3:D:64:GLU:O	3:D:65:VAL:HG12	2.04	0.56
3:G:67:ASN:O	3:G:69:TRP:N	2.39	0.56
3:D:92:ASN:O	3:D:487:LYS:NZ	2.38	0.56
3:F:302:MET:SD	3:F:322:ILE:HD13	2.45	0.56
3:F:36:VAL:O	4:B:606:THR:OG1	2.24	0.55
3:F:227:LYS:N	3:F:243:SER:O	2.39	0.55
3:D:189:SER:OG	3:D:190:GLU:OE1	2.20	0.54
3:D:216:HIS:NE2	3:D:249:HIS:O	2.41	0.54
3:G:308:ARG:NH2	3:D:197:ASN:O	2.39	0.54
3:F:36:VAL:HG22	4:B:608:VAL:CG1	2.38	0.54
3:D:269:GLU:OE1	11:D:609:NAG:H82	2.09	0.53
4:E:526:ALA:O	4:E:627:THR:OG1	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:164:GLU:OE1	3:F:192:ARG:NE	2.40	0.53
3:G:302:MET:HE2	3:G:320:LEU:HD23	1.91	0.53
4:E:596:TRP:O	4:E:650:GLN:NE2	2.42	0.53
3:F:194:ILE:CG2	3:F:423:ILE:HD11	2.38	0.52
2:L:67:SER:N	2:L:70:ASP:O	2.39	0.52
3:G:254:VAL:HG21	3:G:261:LEU:O	2.09	0.52
4:C:614:TRP:CH2	4:C:642:ILE:HD13	2.46	0.51
3:D:496:ILE:O	4:E:631:TRP:NE1	2.42	0.51
3:F:393:ASN:O	3:F:393:ASN:ND2	2.39	0.50
1:H:100(K):VAL:HG12	1:H:100(K):VAL:O	2.12	0.50
11:G:608:NAG:H83	7:J:1:NAG:C8	2.40	0.50
3:D:258:GLN:O	3:D:259:LEU:HD12	2.11	0.50
3:D:297:THR:OG1	3:D:444:THR:HG22	2.11	0.50
2:L:63:ARG:NH1	2:L:65:SER:OG	2.44	0.49
3:G:227:LYS:N	3:G:243:SER:O	2.46	0.49
3:F:386:ASN:O	3:F:387:THR:HG22	2.13	0.49
4:B:532:ALA:O	4:B:536:THR:OG1	2.18	0.48
3:D:387:THR:HA	3:D:416:LEU:HD22	1.94	0.48
2:L:89:MET:HE2	2:L:96:HIS:HB3	1.94	0.48
3:D:37:THR:OG1	4:E:604:CYS:O	2.26	0.48
3:D:359:ILE:HG22	3:D:466:GLU:HB3	1.95	0.48
3:D:77:THR:OG1	3:D:78:ASP:N	2.47	0.48
3:G:194:ILE:HG23	3:G:195:ASN:N	2.29	0.48
3:G:397:ASN:OD1	3:G:398:GLU:N	2.47	0.48
3:G:378:CYS:SG	7:J:2:NAG:H83	2.54	0.47
3:F:50:THR:HG21	3:F:223:TYR:HE2	1.79	0.47
3:G:200:VAL:HG13	3:G:200:VAL:O	2.15	0.47
3:D:496:ILE:HD11	4:E:643:TYR:HE1	1.80	0.47
3:G:104:MET:O	3:G:108:ILE:HD12	2.14	0.47
3:G:41:GLY:O	3:G:42:VAL:HG23	2.14	0.47
4:E:640:ASP:OD1	4:E:641:THR:N	2.46	0.47
1:H:100(M):MET:CE	2:L:89:MET:HE1	2.45	0.47
3:D:201:ILE:HD11	3:D:423:ILE:HG23	1.97	0.46
3:G:302:MET:HE1	3:G:322:ILE:HG12	1.98	0.46
3:F:50:THR:HG22	3:F:51:THR:H	1.80	0.46
3:F:455:THR:OG1	3:F:471:GLY:O	2.32	0.46
3:D:346:SER:HB2	3:D:359:ILE:HD11	1.97	0.46
4:B:622:ILE:HD11	4:B:626:MET:SD	2.55	0.46
3:F:349:LEU:CD1	3:F:359:ILE:HG21	2.46	0.46
4:E:603:ILE:HG21	4:B:658:LYS:NZ	2.32	0.45
3:D:173:TYR:O	3:D:305:LYS:NZ	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:27:ARG:O	2:L:27(A):SER:OG	2.35	0.45
3:F:377:ASN:OD1	3:F:378:CYS:N	2.50	0.45
3:D:263:GLY:O	3:D:450:THR:HG21	2.17	0.45
3:G:258:GLN:C	3:G:259:LEU:HD12	2.41	0.45
3:G:302:MET:HE1	3:G:322:ILE:CG1	2.47	0.45
3:D:493:PRO:O	3:D:494:LEU:HD22	2.17	0.44
3:D:201:ILE:CD1	3:D:423:ILE:HG23	2.47	0.44
2:L:17:GLU:O	2:L:78:VAL:HG22	2.17	0.44
4:C:529:THR:HG23	4:C:626:MET:H	1.83	0.44
3:F:65:VAL:HG13	3:F:66:HIS:N	2.32	0.43
3:G:326:ILE:HG23	3:G:326:ILE:O	2.18	0.43
3:D:70:ALA:HB2	3:D:213:ILE:HG21	1.99	0.43
4:E:603:ILE:HG21	4:B:658:LYS:HZ1	1.83	0.43
3:G:108:ILE:O	3:G:112:TRP:N	2.39	0.43
3:F:296:CYS:O	3:F:445:CYS:N	2.52	0.43
1:H:30:THR:O	1:H:30:THR:HG22	2.19	0.42
3:F:54:CYS:HB3	3:F:74:CYS:HB3	1.98	0.42
3:F:71:THR:O	3:F:71:THR:HG22	2.18	0.42
4:B:638:TYR:O	4:B:642:ILE:HD12	2.19	0.42
1:H:100(A):ASP:CB	3:D:162:THR:HG21	2.50	0.42
4:C:635:ILE:HG22	4:C:635:ILE:O	2.19	0.42
1:H:100(B):ASP:O	1:H:100(D):TYR:N	2.49	0.42
3:D:494:LEU:HD21	4:E:589:VAL:HG13	2.01	0.42
3:G:72:HIS:O	3:G:73:ALA:HB3	2.20	0.42
3:G:287:HIS:O	3:G:288:LEU:HD12	2.20	0.42
3:D:68:VAL:O	3:D:111:LEU:HD21	2.19	0.42
2:L:27(A):SER:OG	2:L:27(B):LEU:N	2.53	0.41
3:D:346:SER:CB	3:D:359:ILE:HD11	2.49	0.41
2:L:27:ARG:O	2:L:27(B):LEU:N	2.47	0.41
3:G:154:ILE:HG23	3:G:154:ILE:O	2.20	0.41
3:G:392:PHE:O	3:G:393:ASN:HB3	2.19	0.41
3:F:51:THR:HG22	3:F:52:LEU:N	2.35	0.41
3:G:377:ASN:OD1	3:G:378:CYS:N	2.54	0.41
3:F:302:MET:HE3	3:F:303:THR:O	2.21	0.41
3:G:491:VAL:HG12	3:G:493:PRO:HD3	2.02	0.41
3:F:76:PRO:O	3:F:78:ASP:N	2.50	0.41
1:H:6:GLU:N	1:H:6:GLU:OE1	2.53	0.41
3:F:266:ALA:HB2	3:F:287:HIS:CD2	2.56	0.41
1:H:28:ARG:NH1	3:F:188:ASN:OD1	2.53	0.41
3:G:197:ASN:O	3:F:308:ARG:NH1	2.53	0.41
3:G:36:VAL:HG12	4:C:608:VAL:HG13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:129:LEU:O	3:D:191:TYR:N	2.50	0.41
3:F:69:TRP:HZ3	3:F:108:ILE:HG23	1.85	0.41
3:F:474:ASN:OD1	3:F:476:ARG:N	2.54	0.41
3:G:349:LEU:HD21	3:G:468:PHE:CE2	2.56	0.41
3:D:194:ILE:HG23	3:D:195:ASN:N	2.36	0.41
3:F:77:THR:O	3:F:78:ASP:OD1	2.38	0.41
3:G:85:VAL:HG13	3:G:86:LEU:N	2.35	0.40
3:D:223:TYR:HE2	4:E:581:LEU:HD22	1.86	0.40
3:D:35:TRP:O	3:D:499:THR:N	2.54	0.40
3:F:50:THR:HG22	3:F:51:THR:N	2.35	0.40
3:G:385:CYS:HA	3:G:418:CYS:CB	2.51	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	H	129/244 (53%)	116 (90%)	13 (10%)	0	100	100
2	L	109/220 (50%)	99 (91%)	10 (9%)	0	100	100
3	D	420/471 (89%)	379 (90%)	39 (9%)	2 (0%)	25	62
3	F	419/471 (89%)	388 (93%)	30 (7%)	1 (0%)	44	77
3	G	422/471 (90%)	376 (89%)	45 (11%)	1 (0%)	44	77
4	B	123/154 (80%)	120 (98%)	3 (2%)	0	100	100
4	C	121/154 (79%)	115 (95%)	6 (5%)	0	100	100
4	E	118/154 (77%)	115 (98%)	3 (2%)	0	100	100
All	All	1861/2339 (80%)	1708 (92%)	149 (8%)	4 (0%)	45	77

All (4) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
3	D	65	VAL
3	F	393	ASN
3	D	393	ASN
3	G	108	ILE

### 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	H	112/209 (54%)	112 (100%)	0	100	100
2	L	98/196 (50%)	98 (100%)	0	100	100
3	D	393/424 (93%)	391 (100%)	2 (0%)	86	90
3	F	392/424 (92%)	392 (100%)	0	100	100
3	G	395/424 (93%)	394 (100%)	1 (0%)	91	92
4	B	107/130 (82%)	106 (99%)	1 (1%)	75	83
4	C	105/130 (81%)	105 (100%)	0	100	100
4	E	104/130 (80%)	104 (100%)	0	100	100
All	All	1706/2067 (82%)	1702 (100%)	4 (0%)	91	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	502	ASN
3	D	289	ASN
3	D	301	ASN
4	B	637	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	229	ASN
3	G	478	ASN
4	C	660	ASN

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Mol	Chain	Res	Type
3	D	66	HIS
3	D	229	ASN
3	D	330	HIS
4	E	590	GLN
4	E	650	GLN
3	F	287	HIS
3	F	352	HIS
4	B	535	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\# Z  > 2$
1	TYS	H	100(C)	1	15,16,17	1.59	2 (13%)	15,22,24	0.86	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
1	TYS	H	100(C)	1	-	1/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	100(C)	TYS	OH-S	5.04	1.68	1.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	100(C)	TYS	OH-CZ	-3.19	1.37	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	H	100(C)	TYS	CZ-OH-S-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

55 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	$\# Z  > 2$
5	NAG	A	1	5,3	14,14,15	0.71	0	17,19,21	1.09	1 (5%)
5	NAG	A	2	5	14,14,15	0.70	0	17,19,21	0.87	0
5	BMA	A	3	5	11,11,12	0.83	0	15,15,17	2.52	6 (40%)
6	NAG	I	1	6,3	14,14,15	0.72	0	17,19,21	0.94	1 (5%)
6	NAG	I	2	6	14,14,15	0.70	0	17,19,21	0.88	0
7	NAG	J	1	7,3	14,14,15	0.79	0	17,19,21	1.73	5 (29%)
7	NAG	J	2	7	14,14,15	0.80	0	17,19,21	1.24	1 (5%)
7	BMA	J	3	7	11,11,12	0.87	0	15,15,17	2.23	6 (40%)
7	MAN	J	4	7	11,11,12	0.63	0	15,15,17	1.51	1 (6%)
7	MAN	J	5	7	11,11,12	0.73	0	15,15,17	1.07	1 (6%)
8	NAG	K	1	8,3	14,14,15	0.76	0	17,19,21	1.49	2 (11%)
8	NAG	K	2	8	14,14,15	0.73	0	17,19,21	1.35	2 (11%)
8	BMA	K	3	8	11,11,12	0.81	0	15,15,17	2.77	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	MAN	K	4	8	11,11,12	0.63	0	15,15,17	1.57	1 (6%)
8	MAN	K	5	8	11,11,12	0.68	0	15,15,17	1.07	1 (6%)
8	MAN	K	6	8	11,11,12	0.66	0	15,15,17	1.32	1 (6%)
9	NAG	M	1	9,3	14,14,15	0.73	0	17,19,21	0.85	1 (5%)
9	NAG	M	2	9	14,14,15	0.70	0	17,19,21	1.29	1 (5%)
9	BMA	M	3	9	11,11,12	0.78	0	15,15,17	2.61	5 (33%)
9	MAN	M	4	9	11,11,12	0.79	0	15,15,17	0.86	0
9	MAN	M	5	9	11,11,12	0.77	0	15,15,17	1.00	1 (6%)
9	MAN	M	6	9	11,11,12	0.76	0	15,15,17	0.82	0
9	MAN	M	7	9	11,11,12	0.65	0	15,15,17	1.37	1 (6%)
9	MAN	M	8	9	11,11,12	0.64	0	15,15,17	1.21	1 (6%)
9	MAN	M	9	9	11,11,12	0.68	0	15,15,17	2.81	2 (13%)
6	NAG	N	1	6,3	14,14,15	0.75	0	17,19,21	1.21	1 (5%)
6	NAG	N	2	6	14,14,15	0.70	0	17,19,21	0.95	1 (5%)
5	NAG	O	1	5,3	14,14,15	0.67	0	17,19,21	1.19	2 (11%)
5	NAG	O	2	5	14,14,15	0.69	0	17,19,21	0.89	0
5	BMA	O	3	5	11,11,12	0.86	0	15,15,17	2.30	5 (33%)
6	NAG	P	1	6,3	14,14,15	0.67	0	17,19,21	1.41	3 (17%)
6	NAG	P	2	6	14,14,15	0.71	0	17,19,21	0.90	0
7	NAG	Q	1	7,3	14,14,15	0.80	0	17,19,21	1.40	1 (5%)
7	NAG	Q	2	7	14,14,15	0.82	0	17,19,21	1.36	2 (11%)
7	BMA	Q	3	7	11,11,12	0.84	0	15,15,17	2.25	6 (40%)
7	MAN	Q	4	7	11,11,12	0.65	0	15,15,17	1.61	1 (6%)
7	MAN	Q	5	7	11,11,12	0.76	0	15,15,17	0.97	1 (6%)
6	NAG	R	1	6,3	14,14,15	0.66	0	17,19,21	1.18	2 (11%)
6	NAG	R	2	6	14,14,15	0.72	0	17,19,21	0.88	0
6	NAG	S	1	6,3	14,14,15	0.69	0	17,19,21	0.95	0
6	NAG	S	2	6	14,14,15	0.70	0	17,19,21	0.89	0
7	NAG	T	1	7,3	14,14,15	0.78	0	17,19,21	1.35	1 (5%)
7	NAG	T	2	7	14,14,15	0.71	0	17,19,21	1.53	6 (35%)
7	BMA	T	3	7	11,11,12	0.89	0	15,15,17	2.19	5 (33%)
7	MAN	T	4	7	11,11,12	0.66	0	15,15,17	1.60	1 (6%)
7	MAN	T	5	7	11,11,12	0.75	0	15,15,17	0.98	1 (6%)
10	NAG	U	1	10,3	14,14,15	0.74	0	17,19,21	0.79	1 (5%)
10	NAG	U	2	10	14,14,15	0.69	0	17,19,21	1.31	2 (11%)
10	BMA	U	3	10	11,11,12	0.89	0	15,15,17	2.19	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	MAN	U	4	10	11,11,12	0.68	0	15,15,17	1.10	2 (13%)
10	MAN	U	5	10	11,11,12	0.79	1 (9%)	15,15,17	0.86	0
10	MAN	U	6	10	11,11,12	0.71	0	15,15,17	1.00	1 (6%)
10	MAN	U	7	10	11,11,12	0.66	0	15,15,17	1.32	1 (6%)
6	NAG	V	1	6,3	14,14,15	0.75	0	17,19,21	1.09	1 (5%)
6	NAG	V	2	6	14,14,15	0.72	0	17,19,21	0.92	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	A	2	5	-	0/6/23/26	0/1/1/1
5	BMA	A	3	5	-	0/2/19/22	0/1/1/1
6	NAG	I	1	6,3	-	3/6/23/26	0/1/1/1
6	NAG	I	2	6	-	1/6/23/26	0/1/1/1
7	NAG	J	1	7,3	-	2/6/23/26	0/1/1/1
7	NAG	J	2	7	-	2/6/23/26	0/1/1/1
7	BMA	J	3	7	-	2/2/19/22	0/1/1/1
7	MAN	J	4	7	-	0/2/19/22	0/1/1/1
7	MAN	J	5	7	-	0/2/19/22	0/1/1/1
8	NAG	K	1	8,3	-	2/6/23/26	0/1/1/1
8	NAG	K	2	8	-	0/6/23/26	0/1/1/1
8	BMA	K	3	8	-	1/2/19/22	0/1/1/1
8	MAN	K	4	8	-	1/2/19/22	0/1/1/1
8	MAN	K	5	8	-	0/2/19/22	0/1/1/1
8	MAN	K	6	8	-	1/2/19/22	0/1/1/1
9	NAG	M	1	9,3	-	0/6/23/26	0/1/1/1
9	NAG	M	2	9	-	2/6/23/26	0/1/1/1
9	BMA	M	3	9	-	0/2/19/22	0/1/1/1
9	MAN	M	4	9	-	0/2/19/22	0/1/1/1
9	MAN	M	5	9	-	0/2/19/22	0/1/1/1
9	MAN	M	6	9	-	1/2/19/22	0/1/1/1
9	MAN	M	7	9	-	0/2/19/22	0/1/1/1
9	MAN	M	8	9	-	1/2/19/22	0/1/1/1
9	MAN	M	9	9	-	1/2/19/22	0/1/1/1
6	NAG	N	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	O	1	5,3	-	1/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	BMA	O	3	5	-	1/2/19/22	0/1/1/1
6	NAG	P	1	6,3	-	1/6/23/26	0/1/1/1
6	NAG	P	2	6	-	1/6/23/26	0/1/1/1
7	NAG	Q	1	7,3	-	2/6/23/26	0/1/1/1
7	NAG	Q	2	7	-	2/6/23/26	0/1/1/1
7	BMA	Q	3	7	-	2/2/19/22	0/1/1/1
7	MAN	Q	4	7	-	0/2/19/22	0/1/1/1
7	MAN	Q	5	7	-	0/2/19/22	0/1/1/1
6	NAG	R	1	6,3	-	1/6/23/26	0/1/1/1
6	NAG	R	2	6	-	0/6/23/26	0/1/1/1
6	NAG	S	1	6,3	-	3/6/23/26	0/1/1/1
6	NAG	S	2	6	-	1/6/23/26	0/1/1/1
7	NAG	T	1	7,3	-	2/6/23/26	0/1/1/1
7	NAG	T	2	7	-	2/6/23/26	0/1/1/1
7	BMA	T	3	7	-	2/2/19/22	0/1/1/1
7	MAN	T	4	7	-	0/2/19/22	0/1/1/1
7	MAN	T	5	7	-	0/2/19/22	0/1/1/1
10	NAG	U	1	10,3	-	0/6/23/26	0/1/1/1
10	NAG	U	2	10	-	2/6/23/26	0/1/1/1
10	BMA	U	3	10	-	0/2/19/22	0/1/1/1
10	MAN	U	4	10	-	0/2/19/22	0/1/1/1
10	MAN	U	5	10	-	0/2/19/22	0/1/1/1
10	MAN	U	6	10	-	1/2/19/22	0/1/1/1
10	MAN	U	7	10	-	0/2/19/22	0/1/1/1
6	NAG	V	1	6,3	-	0/6/23/26	0/1/1/1
6	NAG	V	2	6	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	U	5	MAN	O5-C1	-2.09	1.40	1.43

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	9	MAN	C1-O5-C5	9.41	124.80	112.19
8	K	3	BMA	C1-O5-C5	8.32	123.33	112.19
9	M	3	BMA	C1-O5-C5	7.66	122.46	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3	BMA	C1-O5-C5	7.48	122.20	112.19
5	O	3	BMA	C1-O5-C5	6.34	120.68	112.19
10	U	3	BMA	C1-O5-C5	5.43	119.47	112.19
7	Q	3	BMA	C1-O5-C5	5.38	119.40	112.19
7	Q	4	MAN	C1-O5-C5	5.28	119.26	112.19
8	K	4	MAN	C1-O5-C5	5.10	119.02	112.19
7	T	4	MAN	C1-O5-C5	5.04	118.94	112.19
7	J	3	BMA	C1-O5-C5	4.96	118.83	112.19
7	T	3	BMA	C1-O5-C5	4.86	118.70	112.19
7	J	4	MAN	C1-O5-C5	4.59	118.33	112.19
9	M	7	MAN	C1-O5-C5	4.43	118.12	112.19
8	K	2	NAG	O5-C1-C2	-4.38	104.52	111.29
7	J	3	BMA	C3-C4-C5	4.14	117.73	110.23
8	K	6	MAN	C1-O5-C5	4.10	117.68	112.19
7	Q	3	BMA	C3-C4-C5	3.98	117.45	110.23
9	M	9	MAN	C1-C2-C3	3.94	115.39	109.64
7	J	1	NAG	O5-C1-C2	-3.93	105.22	111.29
10	U	7	MAN	C1-O5-C5	3.91	117.43	112.19
10	U	3	BMA	C3-C4-C5	3.90	117.31	110.23
7	T	3	BMA	C3-C4-C5	3.84	117.19	110.23
7	T	1	NAG	O5-C1-C2	-3.75	105.49	111.29
6	N	1	NAG	O5-C1-C2	-3.69	105.58	111.29
7	Q	2	NAG	C4-C3-C2	3.68	116.41	111.02
8	K	3	BMA	C3-C4-C5	3.65	116.85	110.23
9	M	3	BMA	C3-C4-C5	3.65	116.84	110.23
7	Q	1	NAG	O5-C1-C2	-3.53	105.82	111.29
5	A	3	BMA	C3-C4-C5	3.52	116.62	110.23
5	O	3	BMA	C3-C4-C5	3.50	116.58	110.23
8	K	1	NAG	O4-C4-C3	-3.50	102.13	110.38
9	M	8	MAN	C1-O5-C5	3.31	116.63	112.19
6	P	1	NAG	C2-N2-C7	3.30	127.32	122.90
8	K	1	NAG	O5-C1-C2	-3.26	106.25	111.29
9	M	2	NAG	C2-N2-C7	3.04	126.97	122.90
7	J	1	NAG	C1-C2-N2	3.01	115.18	110.43
8	K	5	MAN	C1-O5-C5	2.96	116.16	112.19
10	U	3	BMA	C2-C3-C4	2.93	116.01	110.86
7	J	5	MAN	C1-O5-C5	2.88	116.05	112.19
5	O	3	BMA	C2-C3-C4	2.88	115.92	110.86
7	J	3	BMA	O4-C4-C3	-2.87	103.60	110.38
7	J	3	BMA	C2-C3-C4	2.84	115.86	110.86
7	T	3	BMA	O4-C4-C3	-2.79	103.80	110.38
8	K	3	BMA	O4-C4-C3	-2.79	103.81	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	1	NAG	O5-C1-C2	-2.78	106.98	111.29
7	Q	3	BMA	O4-C4-C3	-2.78	103.82	110.38
5	A	3	BMA	C2-C3-C4	2.74	115.68	110.86
6	R	1	NAG	O5-C1-C2	-2.73	107.07	111.29
10	U	6	MAN	C1-O5-C5	2.71	115.81	112.19
7	T	2	NAG	C3-C4-C5	-2.68	105.37	110.23
10	U	2	NAG	C1-O5-C5	2.68	115.78	112.19
8	K	3	BMA	C2-C3-C4	2.64	115.50	110.86
7	J	1	NAG	C3-C4-C5	2.64	115.01	110.23
5	O	1	NAG	O5-C1-C2	-2.59	107.29	111.29
9	M	3	BMA	O5-C5-C4	2.57	117.09	110.83
9	M	3	BMA	O4-C4-C3	-2.54	104.38	110.38
7	T	2	NAG	C1-O5-C5	2.53	115.58	112.19
8	K	3	BMA	O5-C5-C4	2.53	116.98	110.83
7	T	5	MAN	C1-O5-C5	2.50	115.53	112.19
10	U	3	BMA	O4-C4-C3	-2.49	104.52	110.38
7	Q	5	MAN	C1-O5-C5	2.47	115.50	112.19
6	N	2	NAG	C1-O5-C5	2.47	115.50	112.19
5	O	1	NAG	C2-N2-C7	2.39	126.11	122.90
6	R	1	NAG	C2-N2-C7	2.36	126.06	122.90
6	V	1	NAG	C1-O5-C5	2.36	115.35	112.19
6	I	1	NAG	O5-C1-C2	-2.31	107.72	111.29
7	T	2	NAG	C4-C3-C2	2.29	114.37	111.02
10	U	4	MAN	C1-O5-C5	2.29	115.25	112.19
10	U	4	MAN	O3-C3-C2	-2.29	105.39	110.05
7	Q	3	BMA	O5-C5-C4	2.26	116.34	110.83
9	M	5	MAN	C1-O5-C5	2.25	115.21	112.19
7	T	2	NAG	O3-C3-C2	-2.25	104.73	109.40
5	A	3	BMA	O4-C4-C3	-2.25	105.08	110.38
7	T	2	NAG	C1-C2-N2	2.25	113.97	110.43
7	J	2	NAG	C1-O5-C5	2.24	115.19	112.19
9	M	3	BMA	O6-C6-C5	-2.23	103.72	111.33
9	M	1	NAG	O5-C1-C2	-2.21	107.88	111.29
5	O	3	BMA	O4-C4-C3	-2.19	105.20	110.38
7	Q	3	BMA	C2-C3-C4	2.19	114.71	110.86
7	J	1	NAG	C4-C3-C2	2.17	114.20	111.02
5	O	3	BMA	O3-C3-C2	-2.17	105.63	110.05
7	Q	2	NAG	C2-N2-C7	2.16	125.80	122.90
7	J	3	BMA	O3-C3-C2	-2.14	105.69	110.05
8	K	3	BMA	O3-C3-C2	-2.14	105.69	110.05
5	A	3	BMA	O5-C5-C4	2.13	116.01	110.83
6	P	1	NAG	C1-C2-N2	2.10	113.74	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	U	2	NAG	C3-C4-C5	-2.10	106.43	110.23
5	A	3	BMA	O3-C3-C2	-2.09	105.79	110.05
7	T	3	BMA	O3-C3-C4	2.09	115.30	110.38
7	Q	3	BMA	O3-C3-C2	-2.05	105.86	110.05
10	U	3	BMA	O3-C3-C2	-2.05	105.88	110.05
10	U	1	NAG	O5-C1-C2	-2.04	108.13	111.29
7	T	3	BMA	C1-C2-C3	-2.04	106.67	109.64
7	J	1	NAG	O4-C4-C3	-2.04	105.58	110.38
8	K	2	NAG	O4-C4-C3	-2.03	105.59	110.38
7	T	2	NAG	C2-N2-C7	2.02	125.61	122.90
7	J	3	BMA	O5-C5-C4	2.01	115.71	110.83
5	A	1	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	P	1	NAG	C1-C2-N2-C7
6	R	1	NAG	C1-C2-N2-C7
7	J	1	NAG	C1-C2-N2-C7
7	Q	1	NAG	C1-C2-N2-C7
7	T	1	NAG	C1-C2-N2-C7
9	M	2	NAG	C1-C2-N2-C7
7	J	3	BMA	O5-C5-C6-O6
7	Q	3	BMA	O5-C5-C6-O6
7	T	3	BMA	O5-C5-C6-O6
7	J	3	BMA	C4-C5-C6-O6
7	Q	3	BMA	C4-C5-C6-O6
7	T	3	BMA	C4-C5-C6-O6
8	K	1	NAG	O5-C5-C6-O6
5	O	3	BMA	O5-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
9	M	6	MAN	O5-C5-C6-O6
6	S	1	NAG	O5-C5-C6-O6
9	M	2	NAG	O5-C5-C6-O6
10	U	6	MAN	O5-C5-C6-O6
6	S	2	NAG	O5-C5-C6-O6
6	P	2	NAG	O5-C5-C6-O6
8	K	6	MAN	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
9	M	8	MAN	O5-C5-C6-O6
9	M	9	MAN	O5-C5-C6-O6

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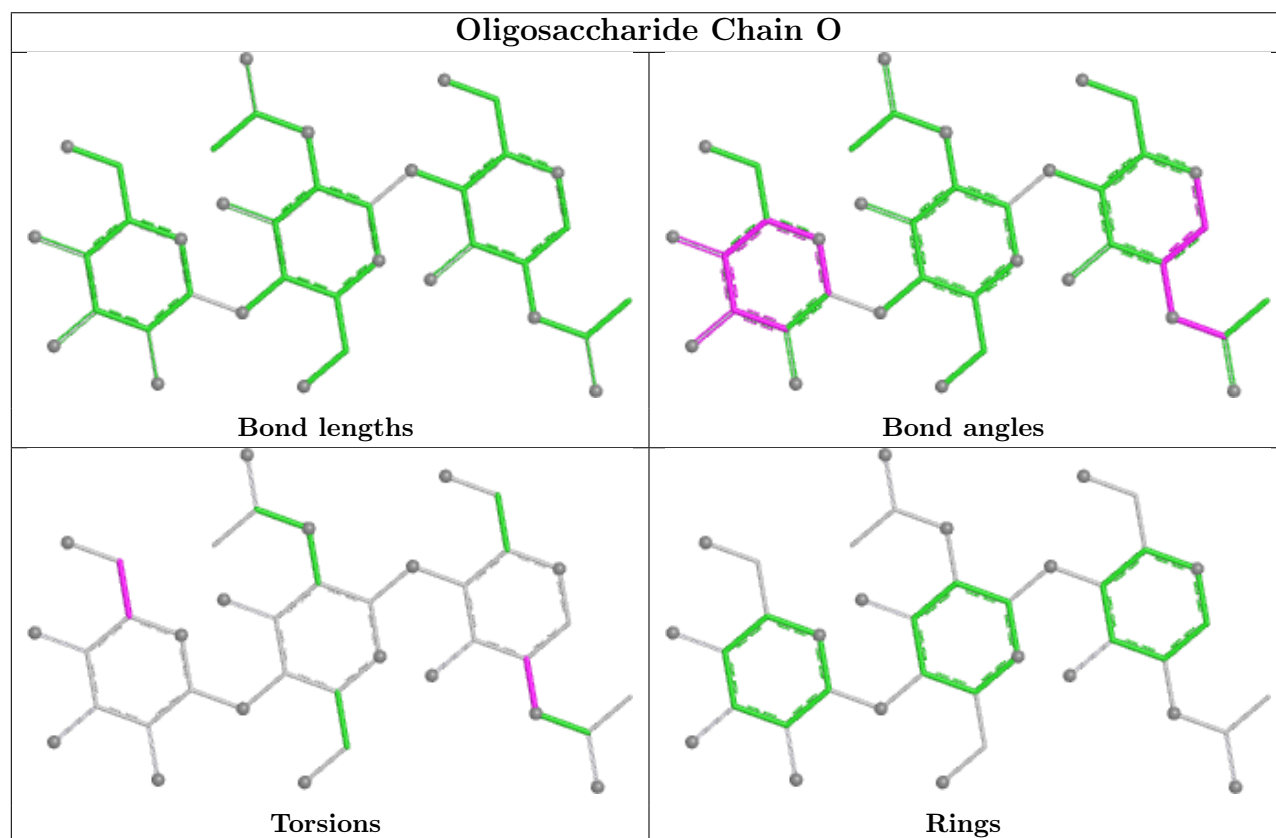
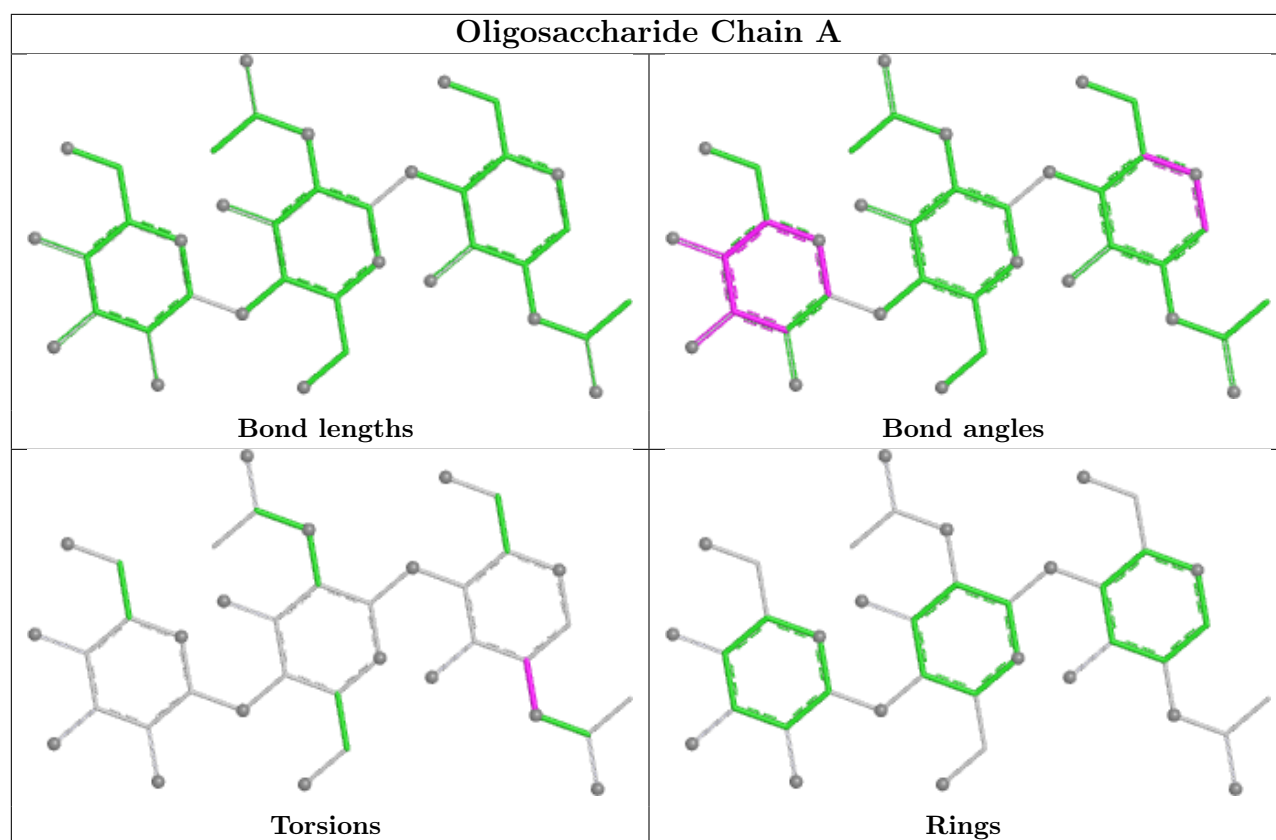
Mol	Chain	Res	Type	Atoms
6	I	1	NAG	O5-C5-C6-O6
8	K	4	MAN	O5-C5-C6-O6
5	O	1	NAG	C3-C2-N2-C7
8	K	3	BMA	O5-C5-C6-O6
5	A	1	NAG	C1-C2-N2-C7
6	I	1	NAG	C1-C2-N2-C7
6	N	1	NAG	C1-C2-N2-C7
6	S	1	NAG	C1-C2-N2-C7
6	V	2	NAG	C1-C2-N2-C7
7	Q	2	NAG	C1-C2-N2-C7
8	K	1	NAG	C4-C5-C6-O6
6	N	1	NAG	C3-C2-N2-C7
6	V	2	NAG	C3-C2-N2-C7
7	J	1	NAG	C3-C2-N2-C7
7	Q	1	NAG	C3-C2-N2-C7
7	T	1	NAG	C3-C2-N2-C7
10	U	2	NAG	C3-C2-N2-C7
7	J	2	NAG	C1-C2-N2-C7
7	T	2	NAG	C1-C2-N2-C7
10	U	2	NAG	C1-C2-N2-C7
5	A	1	NAG	C3-C2-N2-C7
6	I	1	NAG	C3-C2-N2-C7
6	S	1	NAG	C3-C2-N2-C7
7	J	2	NAG	C3-C2-N2-C7
7	Q	2	NAG	C3-C2-N2-C7
7	T	2	NAG	C3-C2-N2-C7

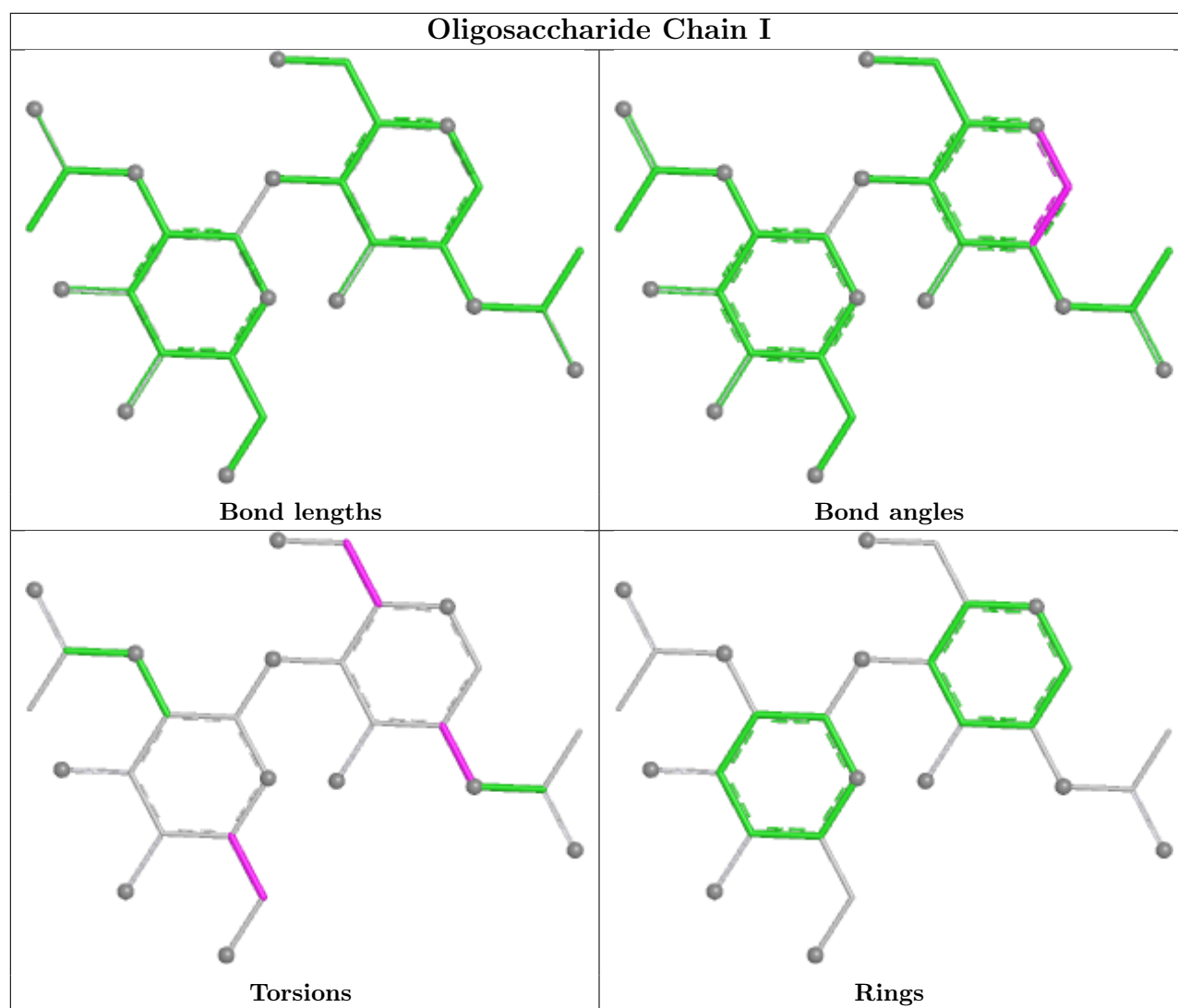
There are no ring outliers.

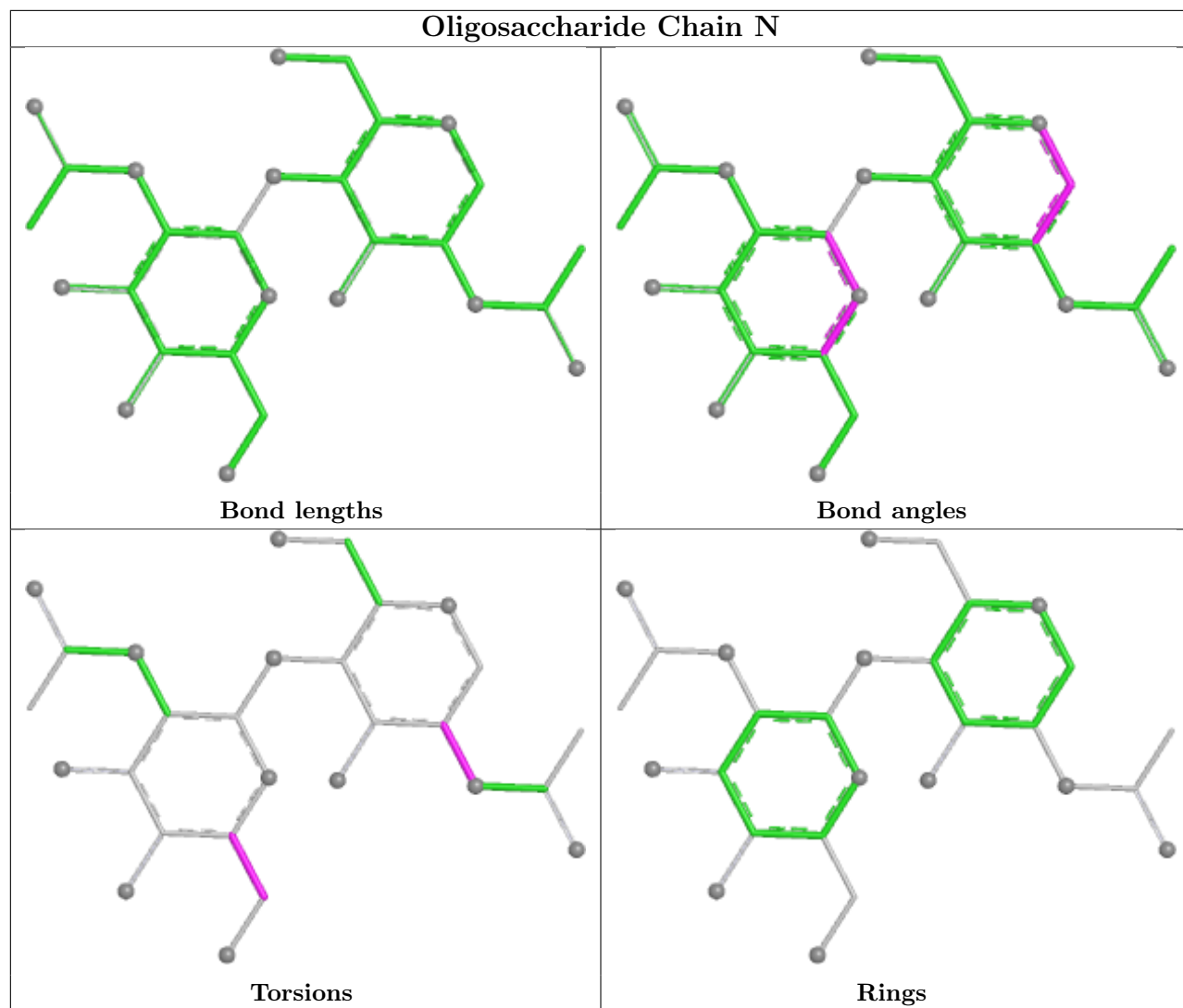
6 monomers are involved in 7 short contacts:

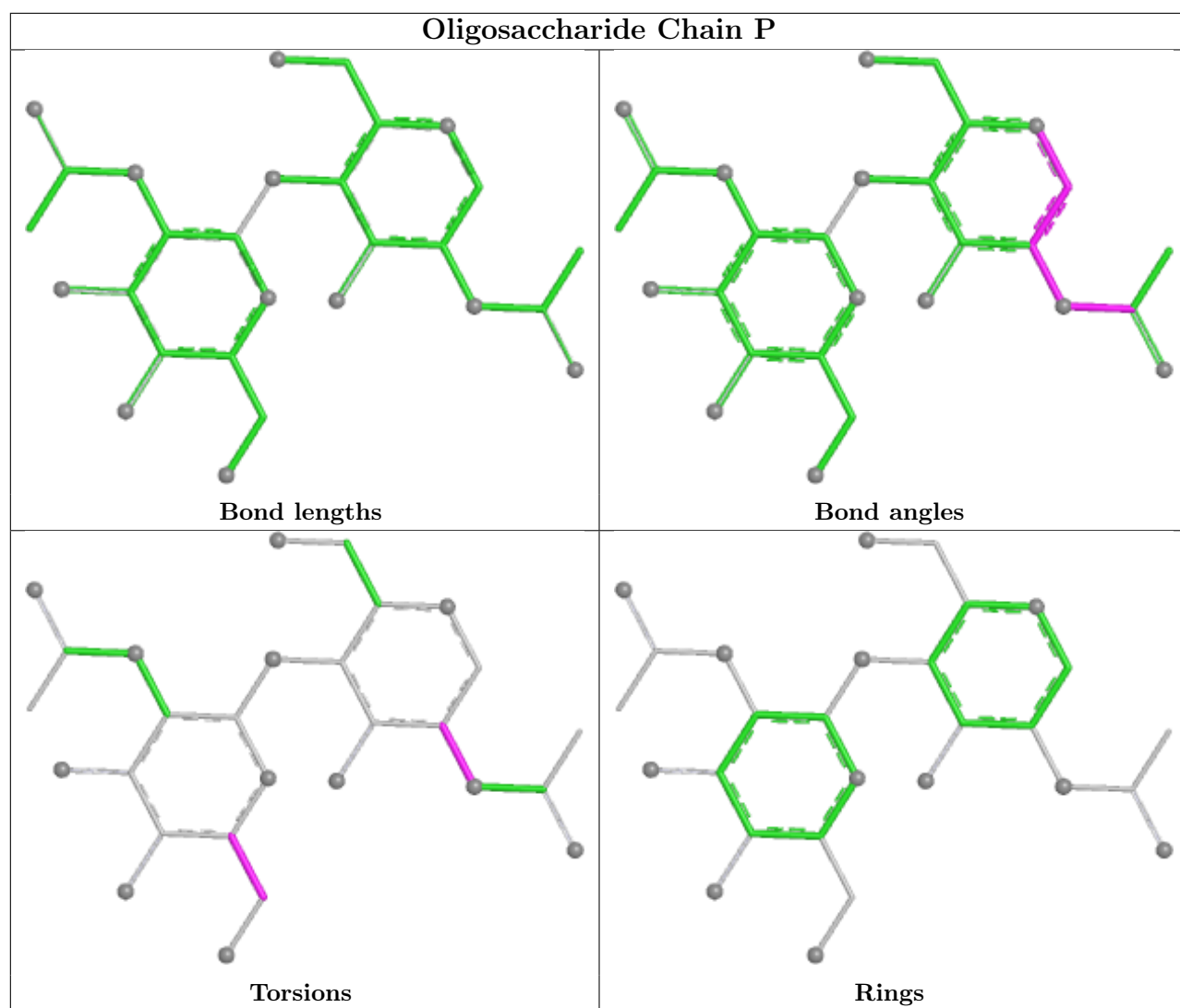
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	S	1	NAG	1	0
7	J	2	NAG	1	0
7	Q	2	NAG	1	0
6	P	1	NAG	1	0
7	J	1	NAG	2	0
8	K	1	NAG	1	0

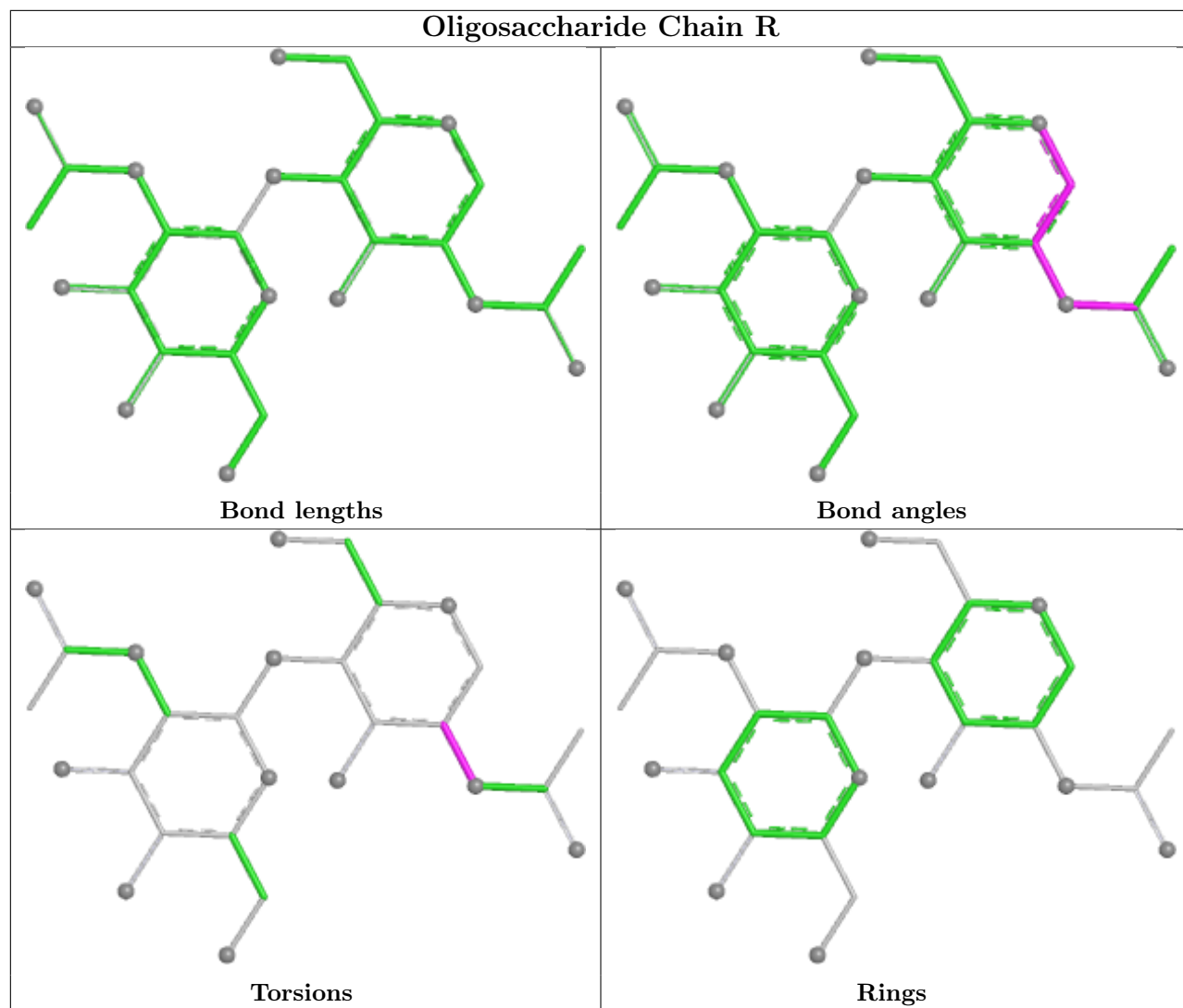
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

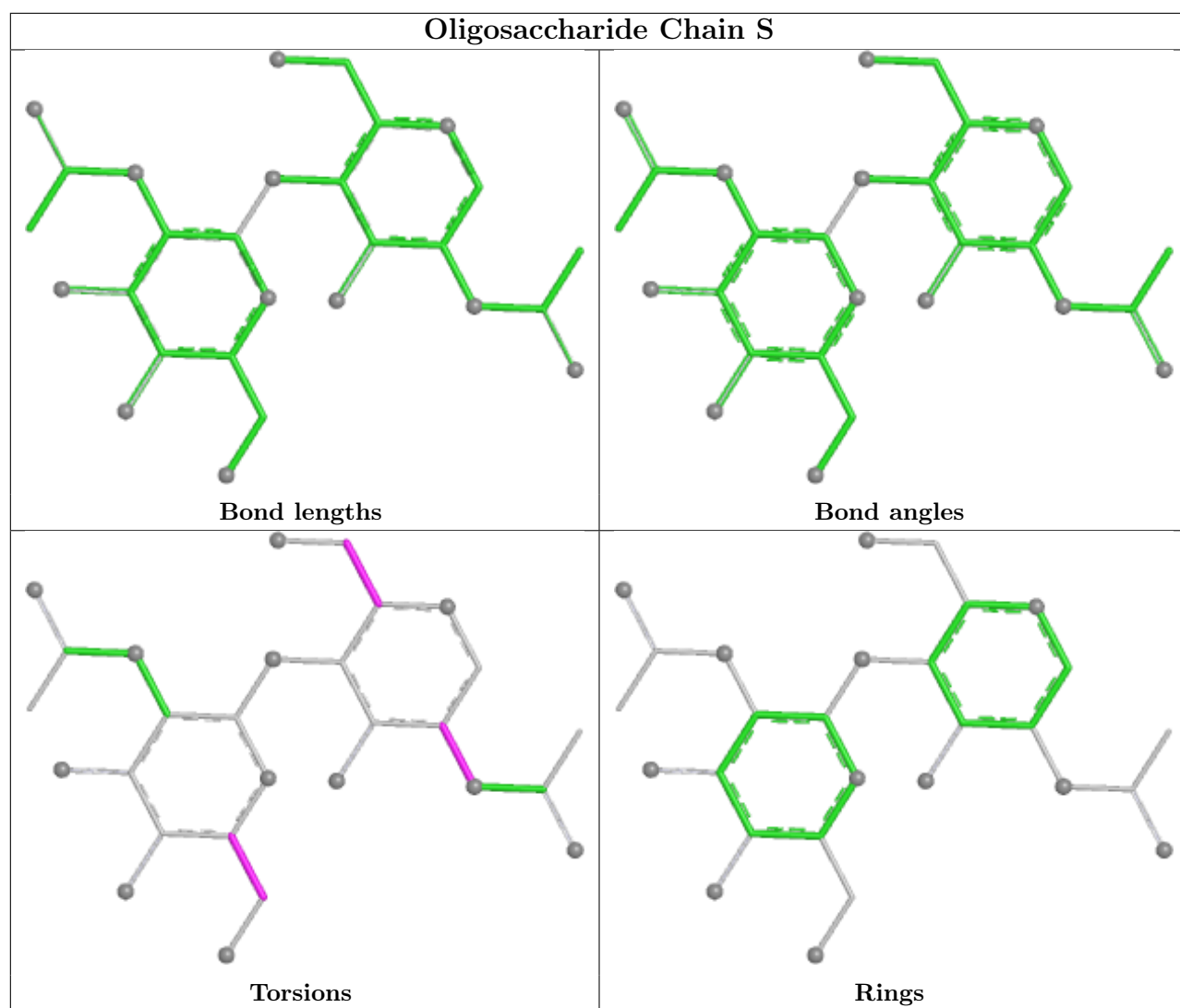




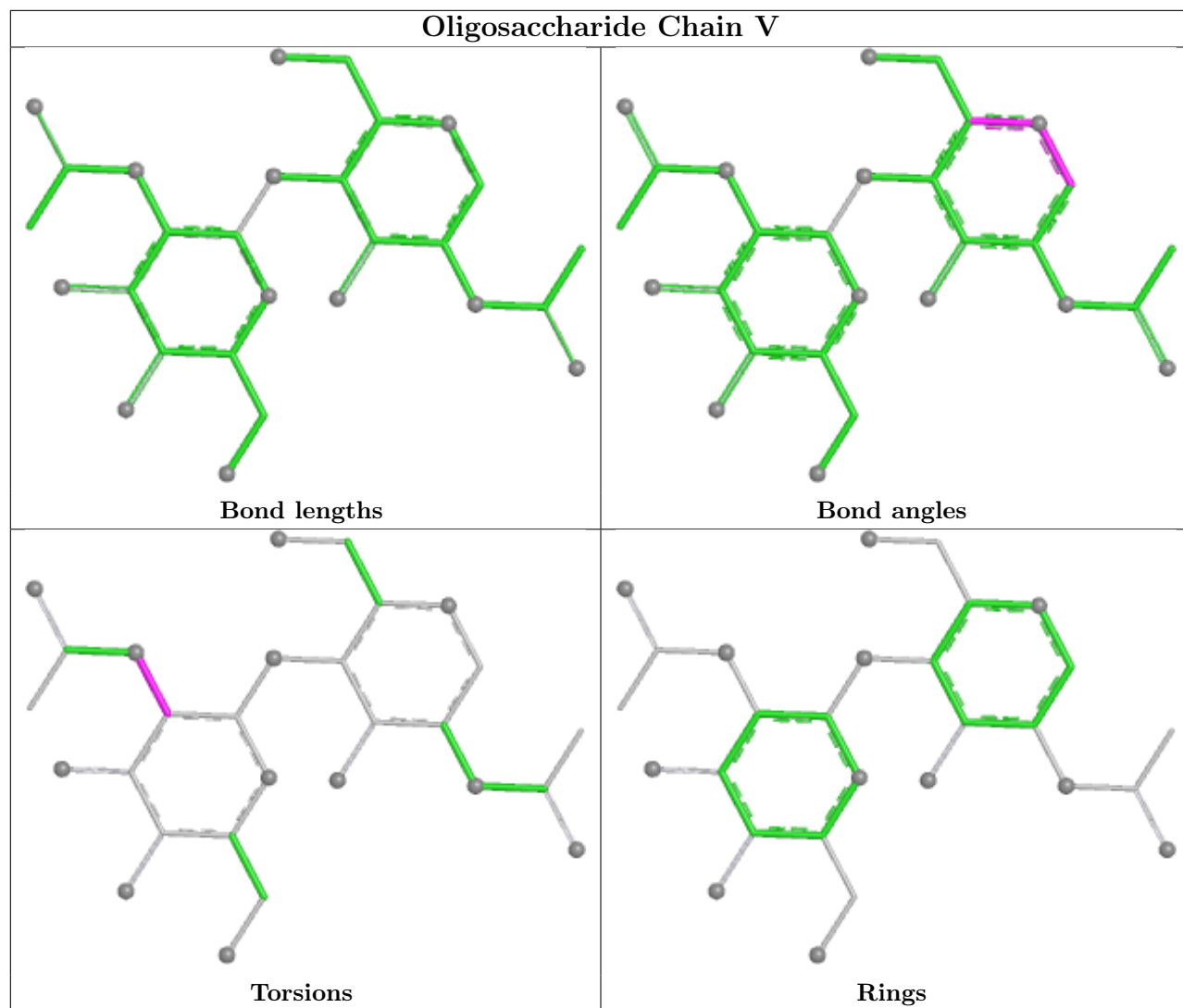


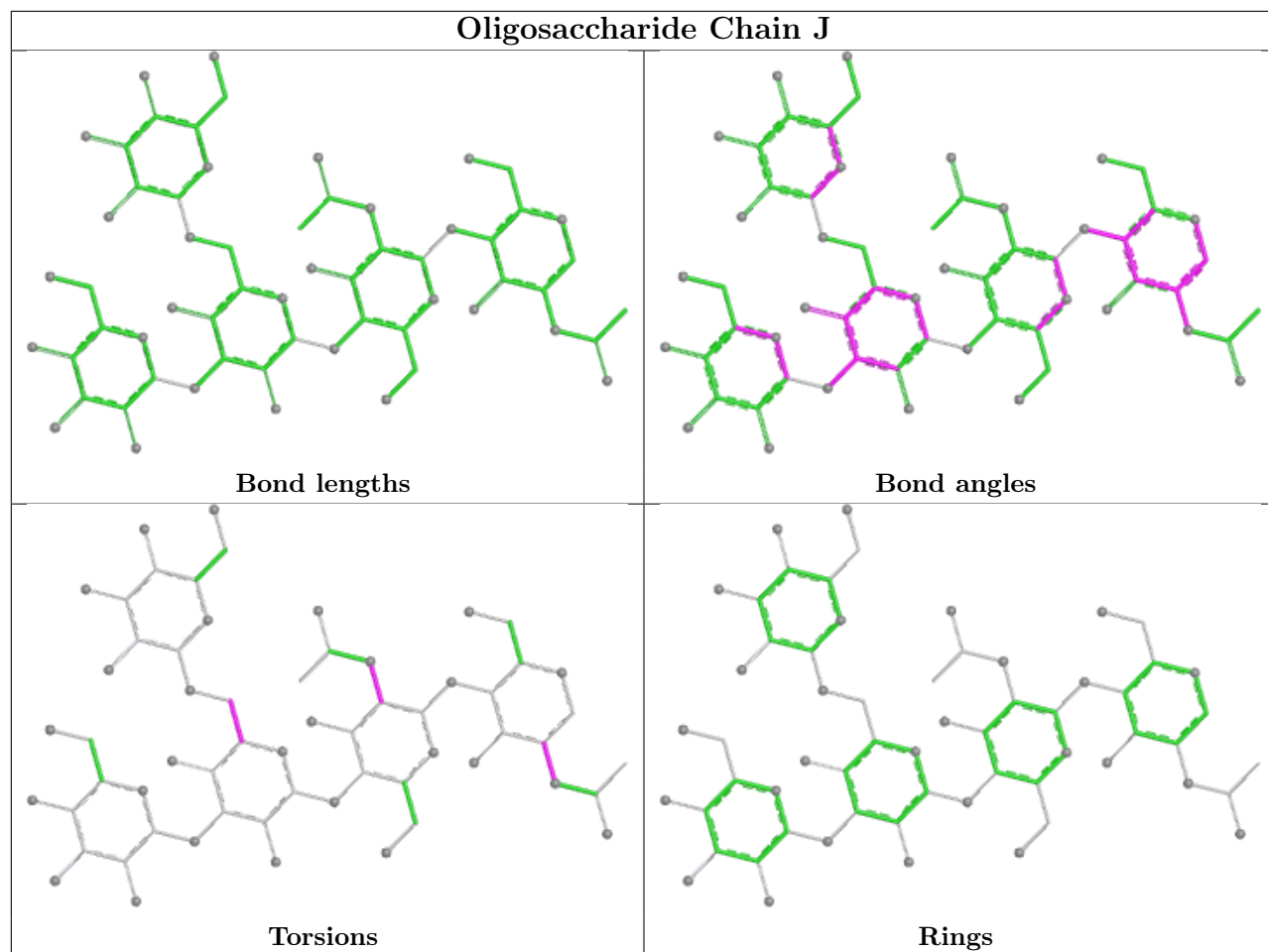


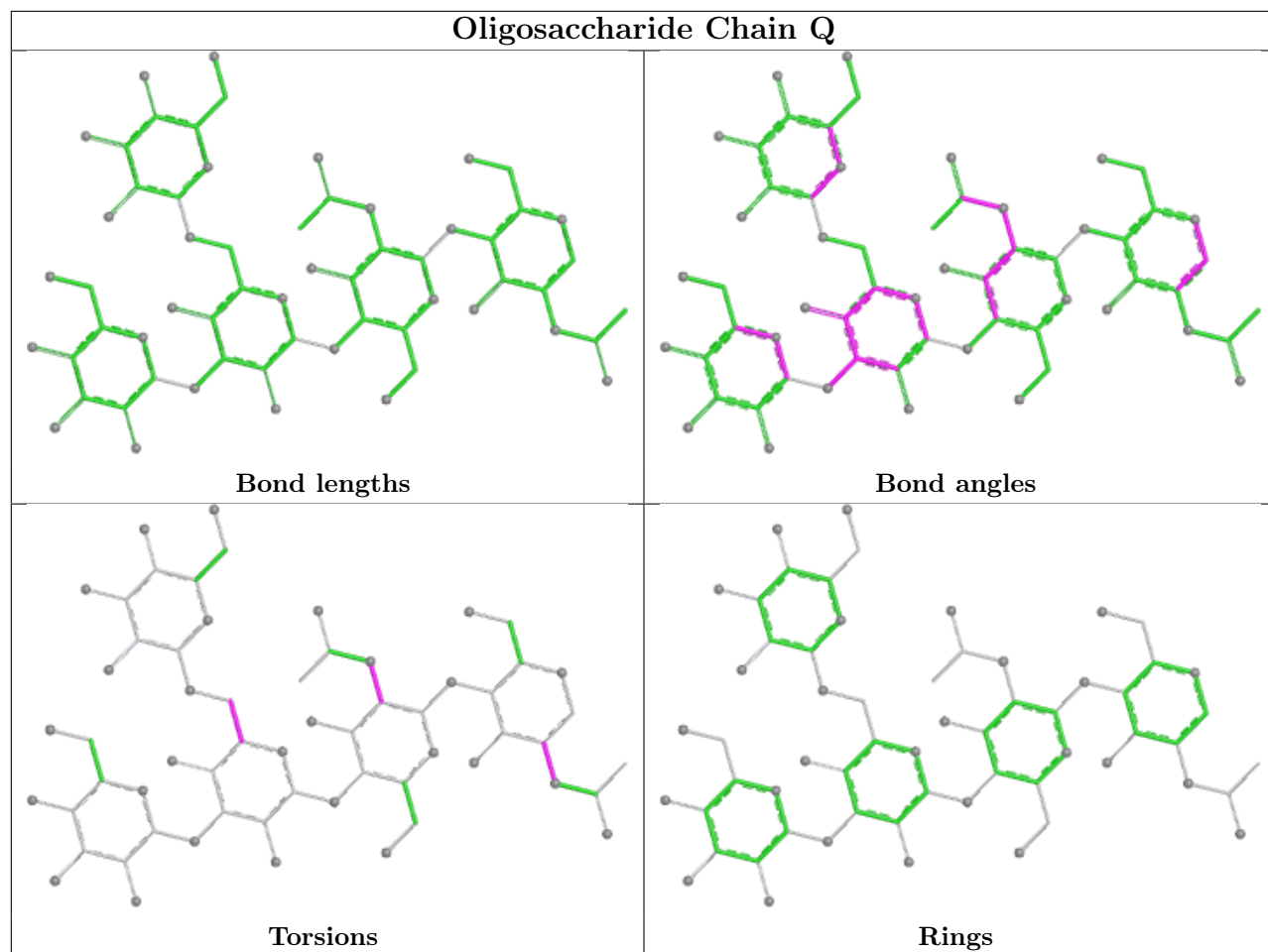


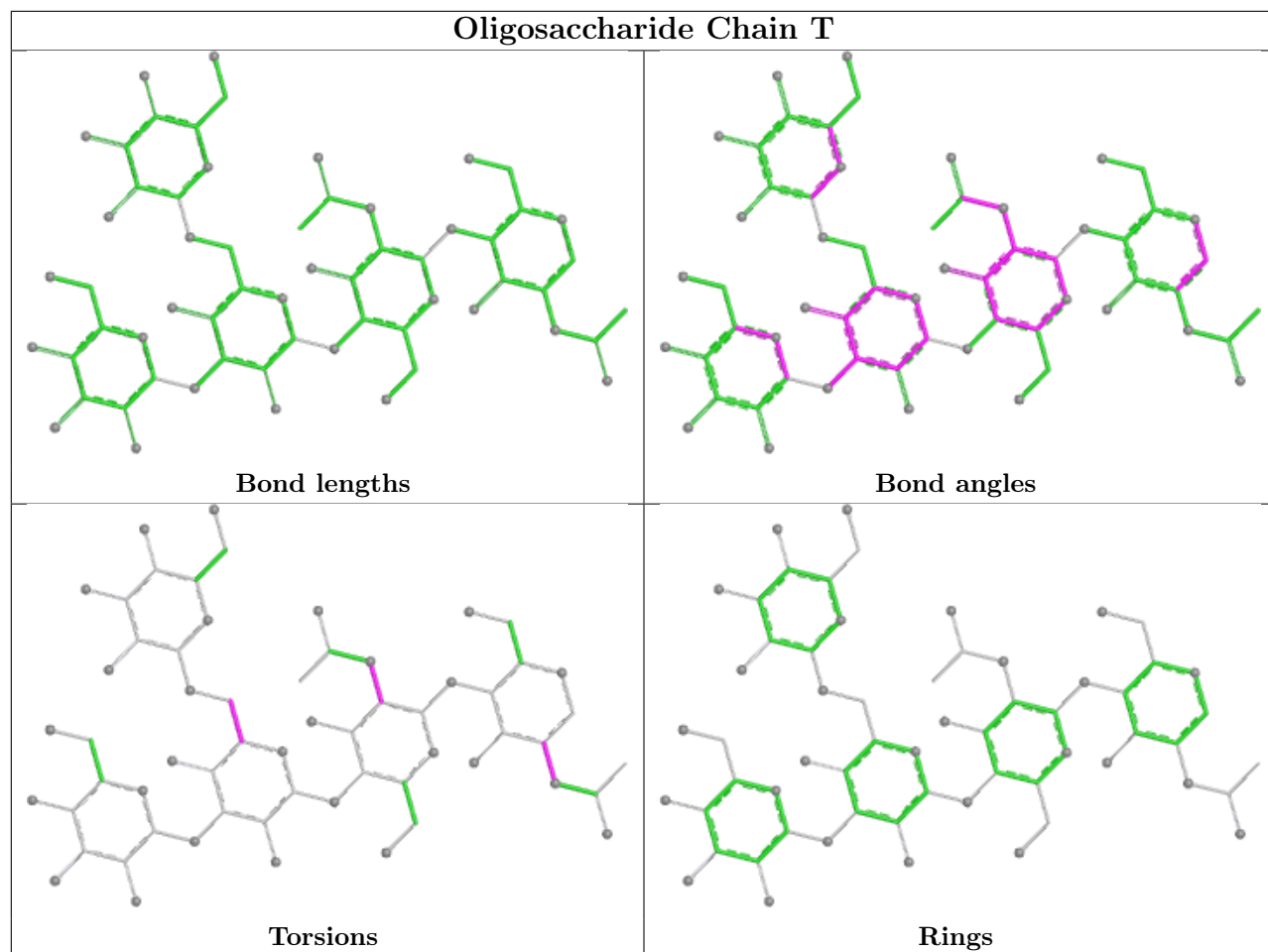


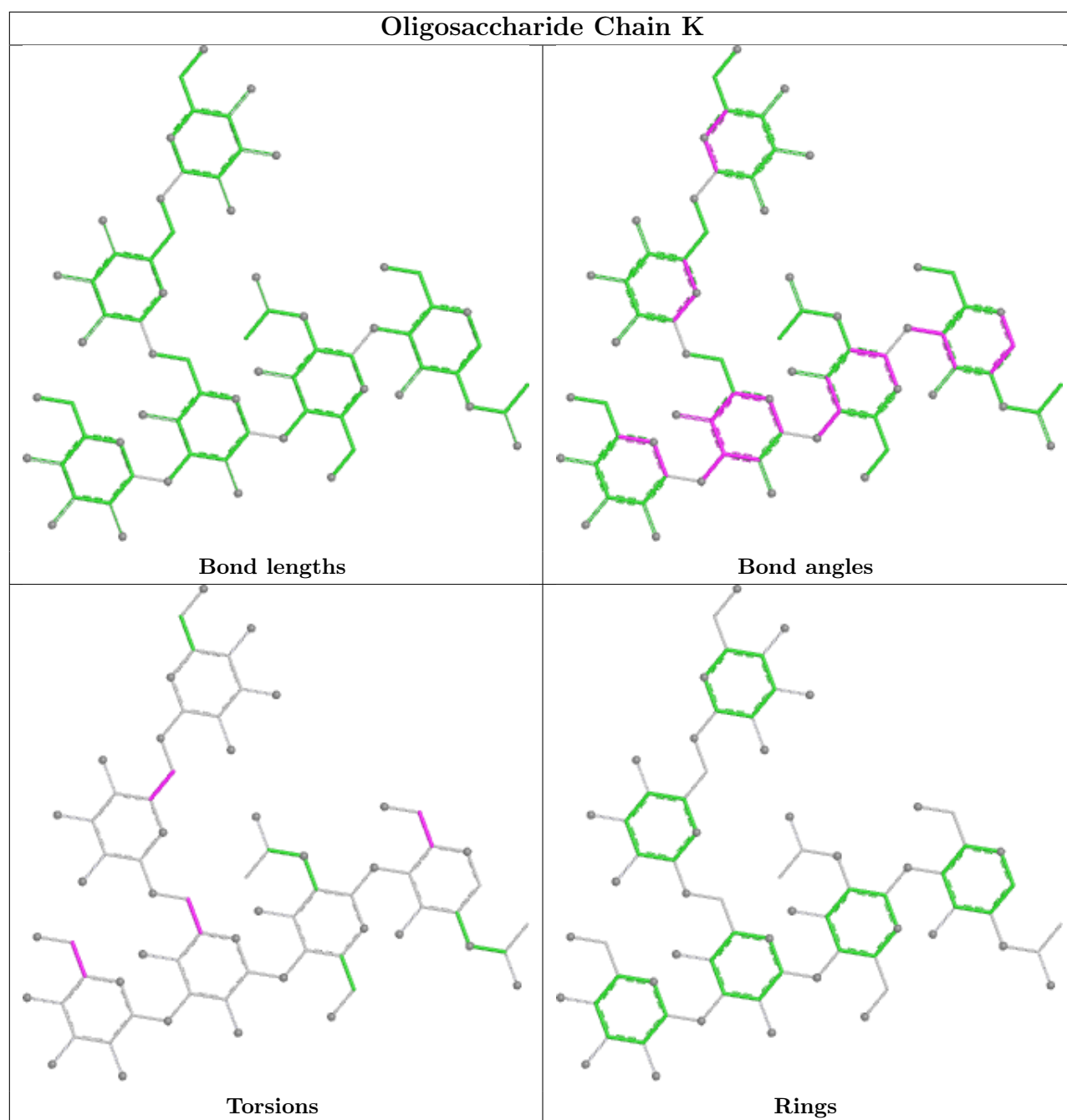


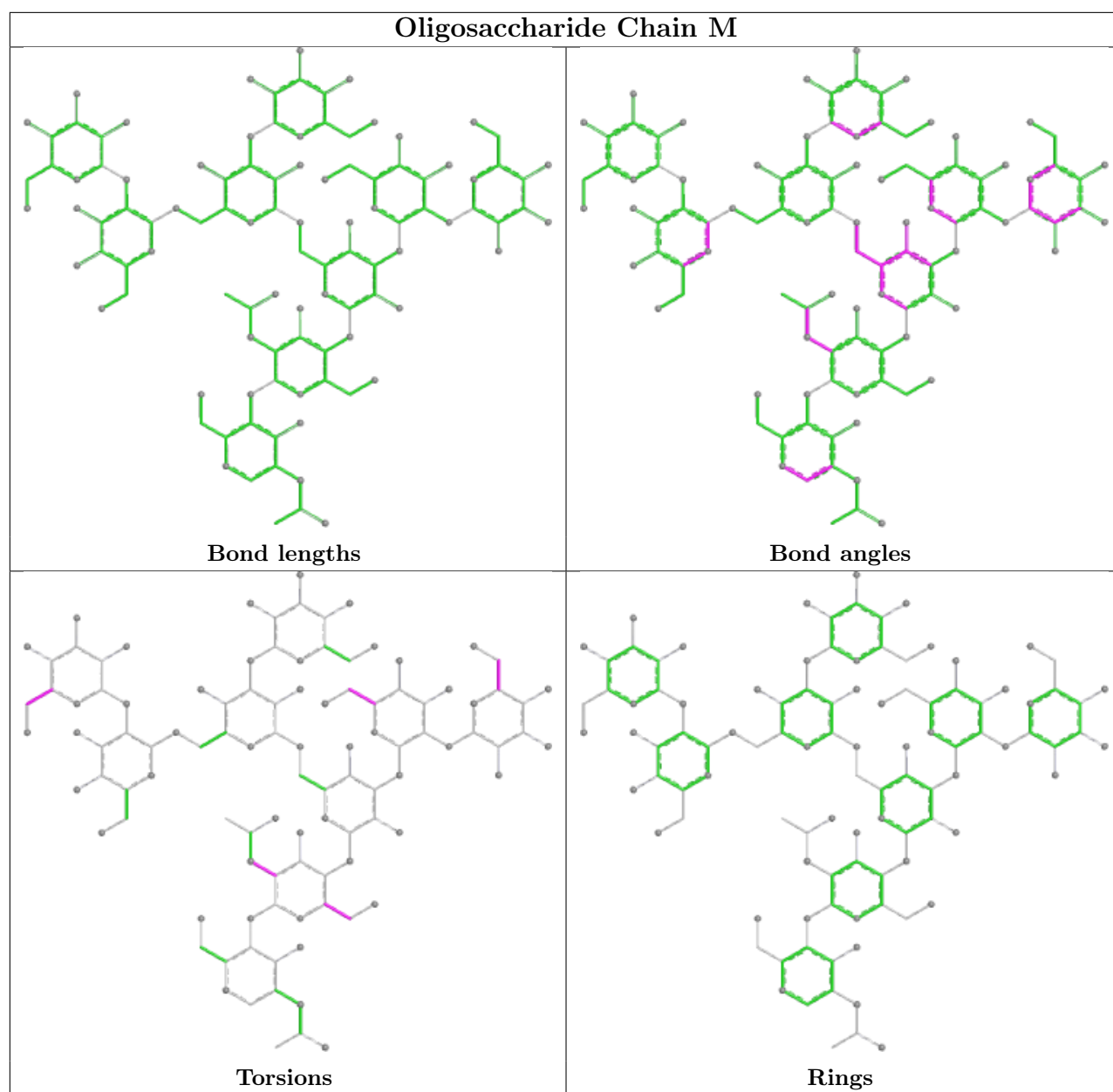


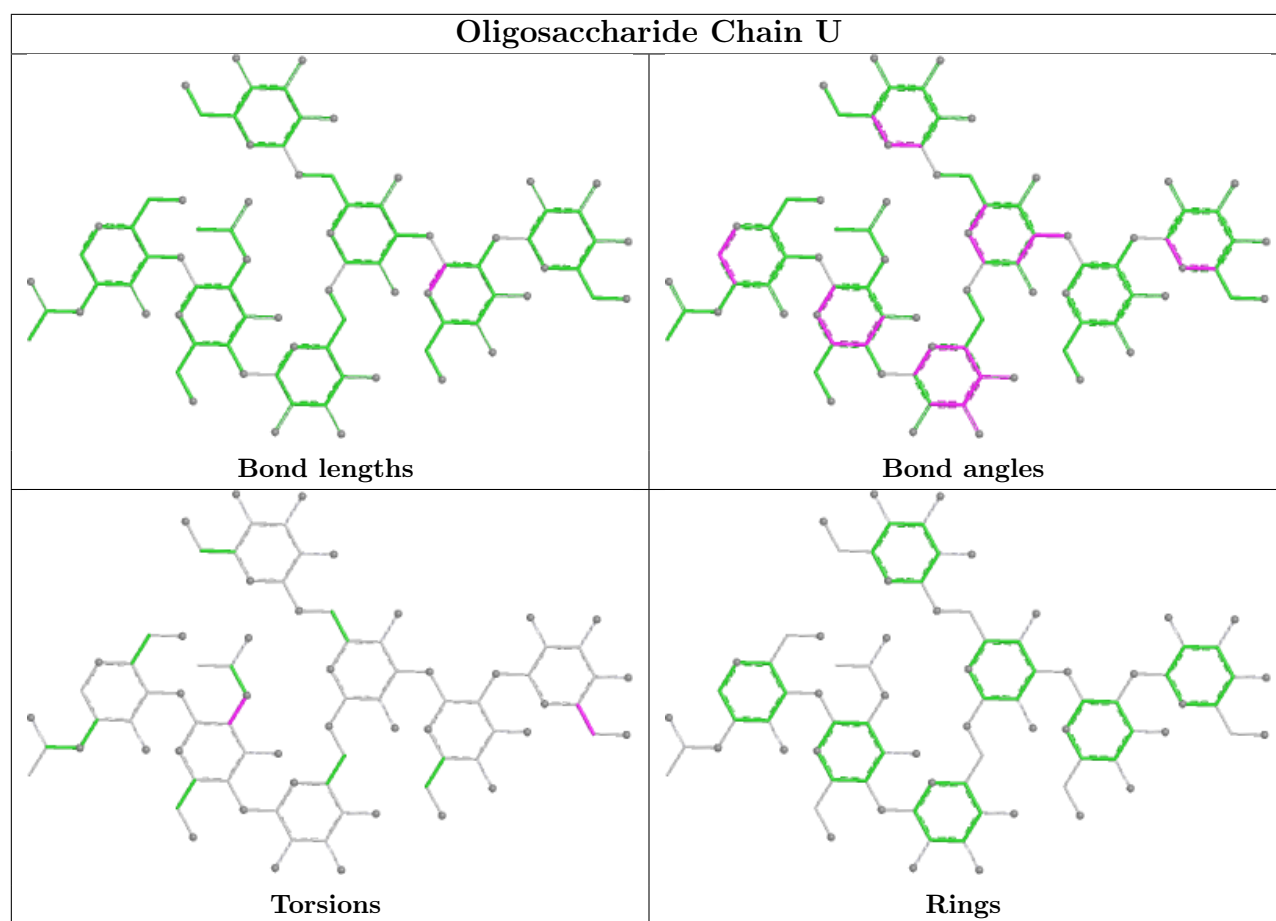












## 5.6 Ligand geometry [i](#)

56 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	$\# Z  > 2$
11	NAG	G	606	3	14,14,15	0.75	0	17,19,21	0.96	0
11	NAG	B	701	4	14,14,15	0.68	0	17,19,21	0.84	0
11	NAG	G	612	3	14,14,15	0.80	0	17,19,21	1.05	0
11	NAG	F	609	3	14,14,15	0.71	0	17,19,21	0.87	0
11	NAG	F	603	3	14,14,15	0.75	0	17,19,21	0.99	1 (5%)
11	NAG	G	609	3	14,14,15	0.80	0	17,19,21	0.83	0
11	NAG	G	603	3	14,14,15	0.70	0	17,19,21	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	NAG	G	607	3	14,14,15	0.69	0	17,19,21	0.85	0
11	NAG	D	602	3	14,14,15	0.70	0	17,19,21	0.83	0
11	NAG	D	605	3	14,14,15	0.80	0	17,19,21	1.12	1 (5%)
11	NAG	D	612	3	14,14,15	0.74	0	17,19,21	0.77	0
11	NAG	D	601	3	14,14,15	0.69	0	17,19,21	0.98	0
11	NAG	F	608	3	14,14,15	0.71	0	17,19,21	0.97	0
11	NAG	F	605	3	14,14,15	0.76	0	17,19,21	1.15	1 (5%)
11	NAG	G	608	3	14,14,15	0.70	0	17,19,21	1.12	2 (11%)
11	NAG	F	614	3	14,14,15	0.76	0	17,19,21	1.57	1 (5%)
11	NAG	G	614	3	14,14,15	0.67	0	17,19,21	0.78	0
11	NAG	E	701	4	14,14,15	0.69	0	17,19,21	0.88	1 (5%)
11	NAG	C	701	4	14,14,15	0.76	0	17,19,21	0.91	0
11	NAG	D	607	3	14,14,15	0.69	0	17,19,21	0.82	0
11	NAG	E	702	4	14,14,15	0.72	0	17,19,21	0.99	1 (5%)
11	NAG	D	606	3	14,14,15	0.70	0	17,19,21	0.88	0
11	NAG	F	601	3	14,14,15	0.70	0	17,19,21	1.17	1 (5%)
11	NAG	D	615	3	14,14,15	0.70	0	17,19,21	1.16	1 (5%)
11	NAG	F	615	3	14,14,15	0.70	0	17,19,21	0.90	0
11	NAG	F	606	3	14,14,15	0.71	0	17,19,21	0.81	0
11	NAG	D	610	3	14,14,15	0.72	0	17,19,21	0.78	0
11	NAG	G	615	3	14,14,15	0.73	0	17,19,21	1.06	1 (5%)
11	NAG	F	602	3	14,14,15	0.69	0	17,19,21	0.77	0
11	NAG	G	602	3	14,14,15	0.71	0	17,19,21	0.85	0
11	NAG	G	605	3	14,14,15	0.70	0	17,19,21	0.81	0
11	NAG	D	603	3	14,14,15	0.68	0	17,19,21	0.90	0
11	NAG	D	604	3	14,14,15	0.72	0	17,19,21	0.82	0
11	NAG	G	611	3	14,14,15	0.69	0	17,19,21	0.94	1 (5%)
11	NAG	F	611	3	14,14,15	0.74	0	17,19,21	0.83	0
11	NAG	G	616	3	14,14,15	0.71	0	17,19,21	0.81	0
11	NAG	D	613	3	14,14,15	0.72	0	17,19,21	0.94	1 (5%)
11	NAG	G	604	3	14,14,15	0.67	0	17,19,21	0.88	0
11	NAG	F	607	3	14,14,15	0.76	0	17,19,21	1.00	0
11	NAG	D	611	3	14,14,15	0.72	0	17,19,21	0.94	0
11	NAG	F	613	3	14,14,15	0.73	0	17,19,21	0.87	0
11	NAG	F	610	3	14,14,15	0.72	0	17,19,21	0.92	1 (5%)
11	NAG	B	704	4	14,14,15	0.71	0	17,19,21	1.01	1 (5%)
11	NAG	G	613	3	14,14,15	0.71	0	17,19,21	0.90	1 (5%)
11	NAG	F	612	3	14,14,15	0.74	0	17,19,21	0.94	0
11	NAG	D	614	3	14,14,15	0.75	0	17,19,21	1.17	1 (5%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	NAG	B	703	4	14,14,15	0.73	0	17,19,21	0.94	0
11	NAG	B	702	4	14,14,15	0.71	0	17,19,21	0.91	0
11	NAG	E	704	4	14,14,15	0.74	0	17,19,21	1.00	0
11	NAG	C	702	4	14,14,15	0.70	0	17,19,21	0.90	0
11	NAG	D	609	3	14,14,15	0.76	0	17,19,21	0.91	0
11	NAG	G	610	3	14,14,15	0.71	0	17,19,21	0.86	0
11	NAG	G	601	3	14,14,15	0.74	0	17,19,21	1.03	1 (5%)
11	NAG	E	703	4	14,14,15	0.72	0	17,19,21	0.78	0
11	NAG	D	608	3	14,14,15	0.70	0	17,19,21	0.93	0
11	NAG	F	604	3	14,14,15	0.70	0	17,19,21	0.83	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
11	NAG	G	606	3	-	1/6/23/26	0/1/1/1
11	NAG	B	701	4	-	1/6/23/26	0/1/1/1
11	NAG	G	612	3	-	0/6/23/26	0/1/1/1
11	NAG	F	609	3	-	1/6/23/26	0/1/1/1
11	NAG	F	603	3	-	1/6/23/26	0/1/1/1
11	NAG	G	609	3	-	0/6/23/26	0/1/1/1
11	NAG	G	603	3	-	1/6/23/26	0/1/1/1
11	NAG	G	607	3	-	0/6/23/26	0/1/1/1
11	NAG	D	602	3	-	1/6/23/26	0/1/1/1
11	NAG	D	605	3	-	0/6/23/26	0/1/1/1
11	NAG	D	612	3	-	0/6/23/26	0/1/1/1
11	NAG	D	601	3	-	3/6/23/26	0/1/1/1
11	NAG	F	608	3	-	0/6/23/26	0/1/1/1
11	NAG	F	605	3	-	1/6/23/26	0/1/1/1
11	NAG	G	608	3	-	1/6/23/26	0/1/1/1
11	NAG	F	614	3	-	0/6/23/26	0/1/1/1
11	NAG	G	614	3	-	0/6/23/26	0/1/1/1
11	NAG	E	701	4	-	0/6/23/26	0/1/1/1
11	NAG	C	701	4	-	0/6/23/26	0/1/1/1
11	NAG	D	607	3	-	0/6/23/26	0/1/1/1
11	NAG	E	702	4	-	0/6/23/26	0/1/1/1
11	NAG	D	606	3	-	1/6/23/26	0/1/1/1
11	NAG	F	601	3	-	2/6/23/26	0/1/1/1
11	NAG	D	615	3	-	0/6/23/26	0/1/1/1
11	NAG	F	615	3	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	F	606	3	-	0/6/23/26	0/1/1/1
11	NAG	D	610	3	-	1/6/23/26	0/1/1/1
11	NAG	G	615	3	-	0/6/23/26	0/1/1/1
11	NAG	F	602	3	-	1/6/23/26	0/1/1/1
11	NAG	G	602	3	-	1/6/23/26	0/1/1/1
11	NAG	G	605	3	-	0/6/23/26	0/1/1/1
11	NAG	D	603	3	-	1/6/23/26	0/1/1/1
11	NAG	D	604	3	-	1/6/23/26	0/1/1/1
11	NAG	G	611	3	-	0/6/23/26	0/1/1/1
11	NAG	F	611	3	-	1/6/23/26	0/1/1/1
11	NAG	G	616	3	-	1/6/23/26	0/1/1/1
11	NAG	D	613	3	-	0/6/23/26	0/1/1/1
11	NAG	G	604	3	-	1/6/23/26	0/1/1/1
11	NAG	F	607	3	-	1/6/23/26	0/1/1/1
11	NAG	D	611	3	-	0/6/23/26	0/1/1/1
11	NAG	F	613	3	-	0/6/23/26	0/1/1/1
11	NAG	F	610	3	-	0/6/23/26	0/1/1/1
11	NAG	B	704	4	-	0/6/23/26	0/1/1/1
11	NAG	G	613	3	-	0/6/23/26	0/1/1/1
11	NAG	F	612	3	-	0/6/23/26	0/1/1/1
11	NAG	D	614	3	-	0/6/23/26	0/1/1/1
11	NAG	B	703	4	-	0/6/23/26	0/1/1/1
11	NAG	B	702	4	-	0/6/23/26	0/1/1/1
11	NAG	E	704	4	-	2/6/23/26	0/1/1/1
11	NAG	C	702	4	-	0/6/23/26	0/1/1/1
11	NAG	D	609	3	-	0/6/23/26	0/1/1/1
11	NAG	G	610	3	-	1/6/23/26	0/1/1/1
11	NAG	G	601	3	-	3/6/23/26	0/1/1/1
11	NAG	E	703	4	-	0/6/23/26	0/1/1/1
11	NAG	D	608	3	-	1/6/23/26	0/1/1/1
11	NAG	F	604	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	614	NAG	C1-O5-C5	5.61	119.70	112.19
11	D	615	NAG	C1-O5-C5	3.72	117.17	112.19
11	D	605	NAG	C1-O5-C5	3.49	116.86	112.19
11	G	608	NAG	O5-C1-C2	-3.26	106.25	111.29
11	G	615	NAG	C1-O5-C5	2.92	116.10	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	601	NAG	C2-N2-C7	2.79	126.64	122.90
11	F	605	NAG	C1-O5-C5	2.65	115.73	112.19
11	F	603	NAG	C1-O5-C5	2.62	115.69	112.19
11	E	702	NAG	C1-O5-C5	2.58	115.64	112.19
11	G	601	NAG	O5-C1-C2	-2.36	107.65	111.29
11	B	704	NAG	O5-C1-C2	-2.25	107.81	111.29
11	D	614	NAG	C2-N2-C7	2.13	125.75	122.90
11	E	701	NAG	O5-C1-C2	-2.12	108.01	111.29
11	G	611	NAG	O5-C1-C2	-2.10	108.05	111.29
11	F	610	NAG	O5-C1-C2	-2.07	108.08	111.29
11	G	608	NAG	C4-C3-C2	-2.06	107.99	111.02
11	D	613	NAG	O5-C1-C2	-2.06	108.10	111.29
11	G	613	NAG	O5-C1-C2	-2.01	108.18	111.29

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	F	601	NAG	C1-C2-N2-C7
11	D	601	NAG	O5-C5-C6-O6
11	G	606	NAG	O5-C5-C6-O6
11	D	608	NAG	O5-C5-C6-O6
11	B	701	NAG	O5-C5-C6-O6
11	G	602	NAG	O5-C5-C6-O6
11	D	603	NAG	O5-C5-C6-O6
11	D	606	NAG	O5-C5-C6-O6
11	D	610	NAG	O5-C5-C6-O6
11	F	605	NAG	O5-C5-C6-O6
11	G	610	NAG	O5-C5-C6-O6
11	G	603	NAG	O5-C5-C6-O6
11	G	608	NAG	O5-C5-C6-O6
11	D	602	NAG	O5-C5-C6-O6
11	F	604	NAG	O5-C5-C6-O6
11	G	604	NAG	O5-C5-C6-O6
11	F	607	NAG	O5-C5-C6-O6
11	G	601	NAG	O5-C5-C6-O6
11	F	603	NAG	O5-C5-C6-O6
11	G	616	NAG	O5-C5-C6-O6
11	F	602	NAG	O5-C5-C6-O6
11	F	609	NAG	O5-C5-C6-O6
11	D	604	NAG	O5-C5-C6-O6
11	F	601	NAG	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
11	F	615	NAG	O5-C5-C6-O6
11	F	611	NAG	O5-C5-C6-O6
11	G	601	NAG	C1-C2-N2-C7
11	D	601	NAG	C1-C2-N2-C7
11	E	704	NAG	C1-C2-N2-C7
11	D	601	NAG	C3-C2-N2-C7
11	G	601	NAG	C3-C2-N2-C7
11	E	704	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	G	608	NAG	2	0
11	D	609	NAG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

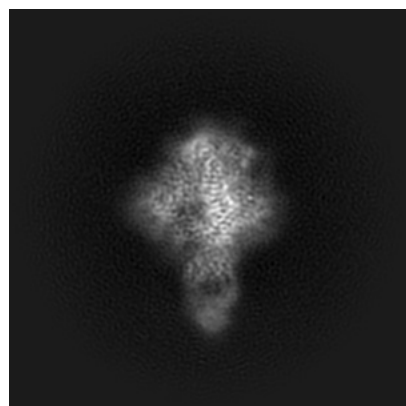
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44890. These allow visual inspection of the internal detail of the map and identification of artifacts.

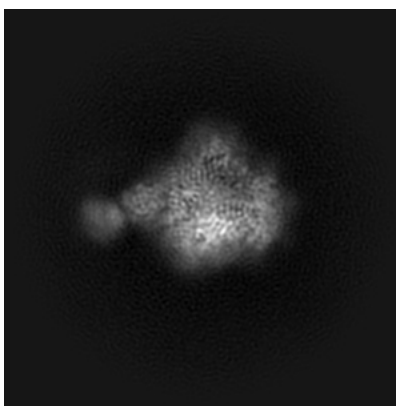
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

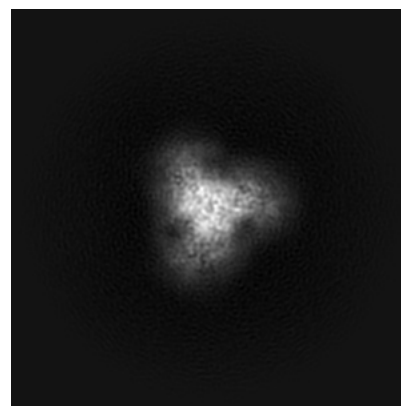
#### 6.1.1 Primary map



X

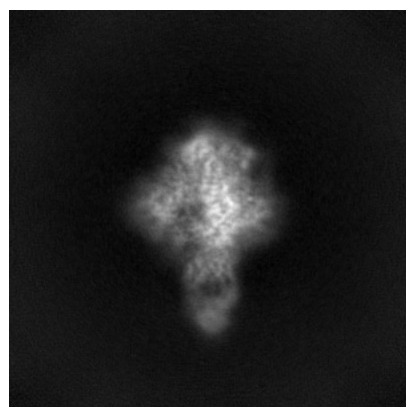


Y

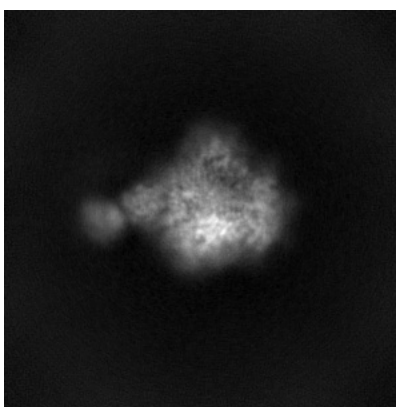


Z

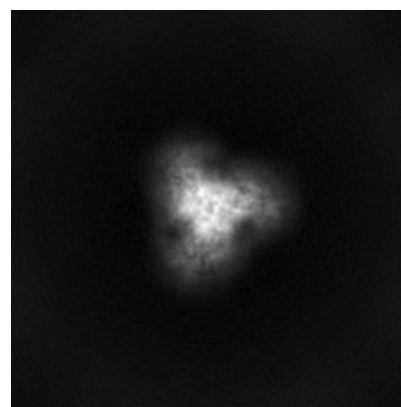
#### 6.1.2 Raw map



X



Y

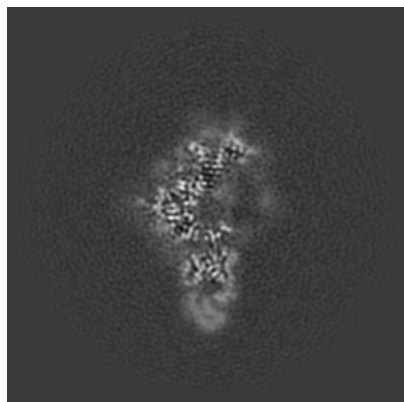


Z

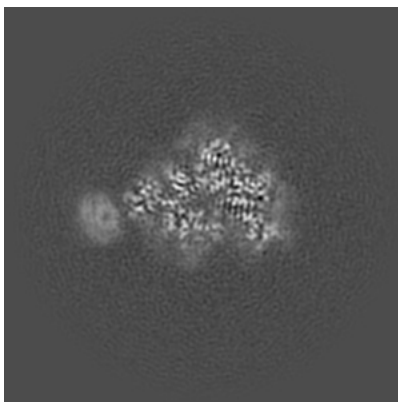
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

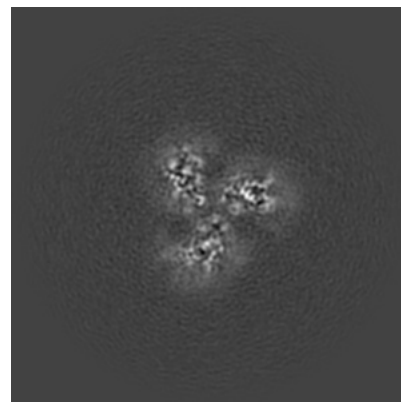
### 6.2.1 Primary map



X Index: 160

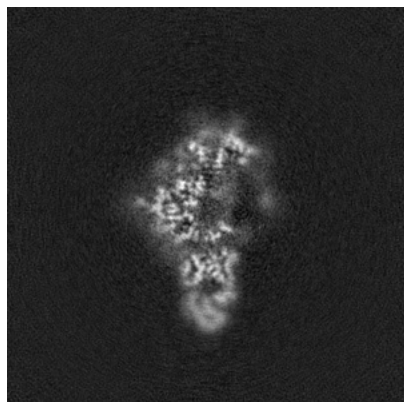


Y Index: 160

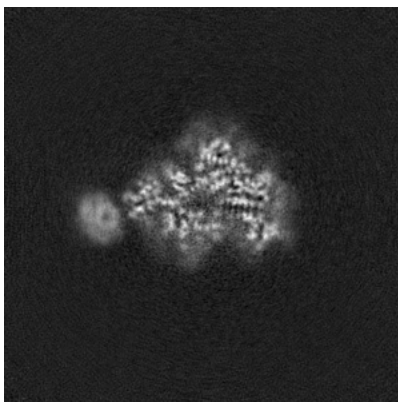


Z Index: 160

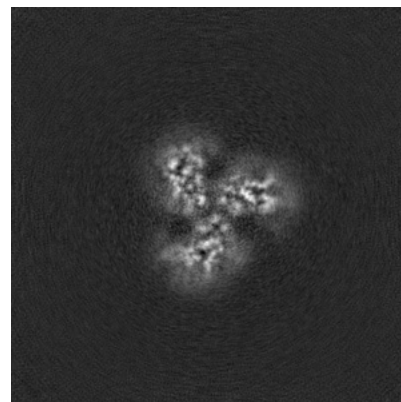
### 6.2.2 Raw map



X Index: 160



Y Index: 160

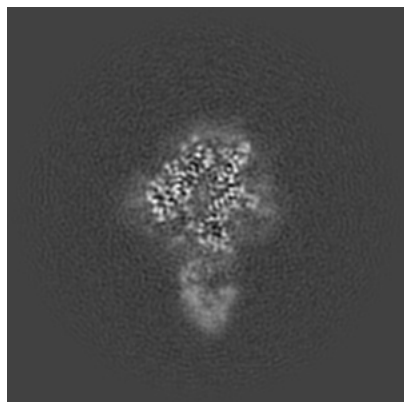


Z Index: 160

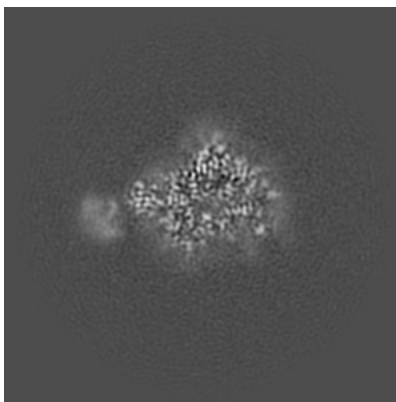
The images above show central slices of the map in three orthogonal directions.

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

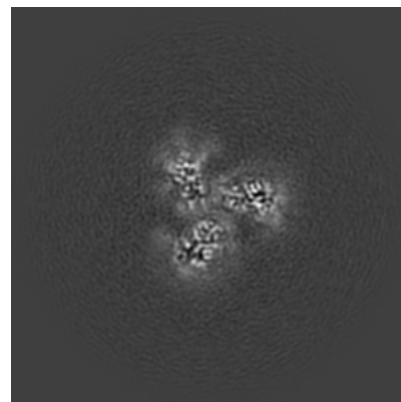
### 6.3.1 Primary map



X Index: 150

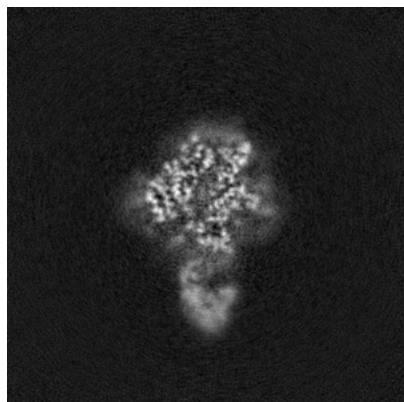


Y Index: 167

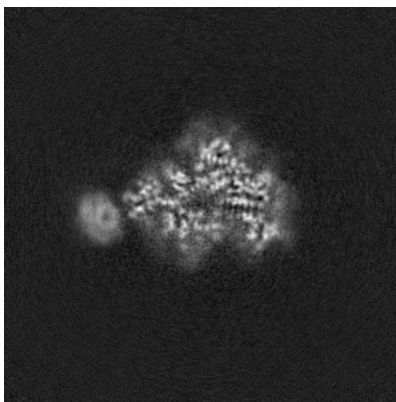


Z Index: 168

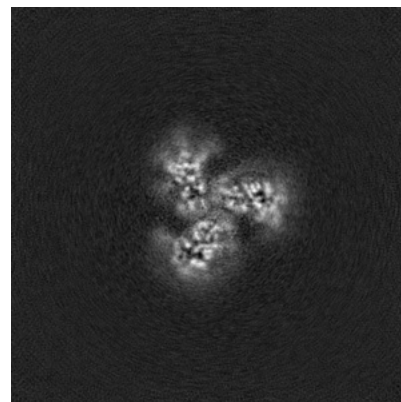
### 6.3.2 Raw map



X Index: 150



Y Index: 160



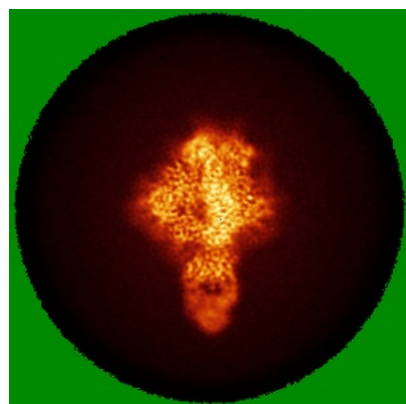
Z Index: 168

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

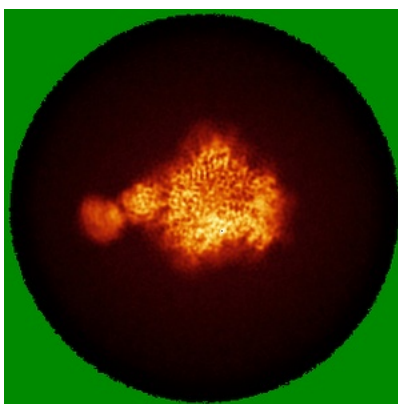


## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

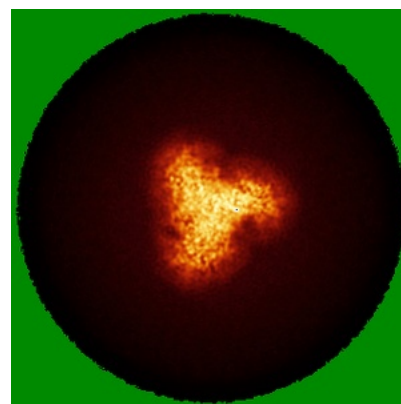
### 6.4.1 Primary map



X

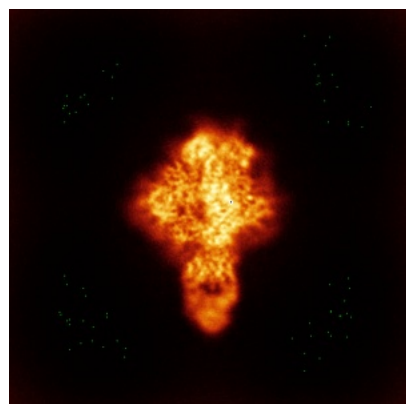


Y

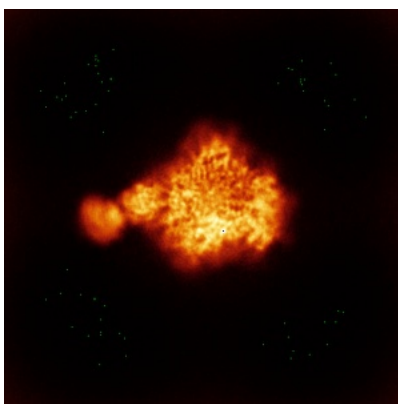


Z

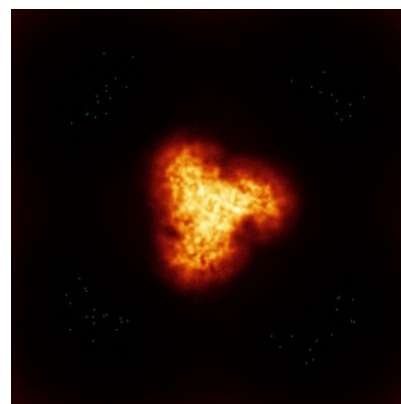
### 6.4.2 Raw map



X



Y



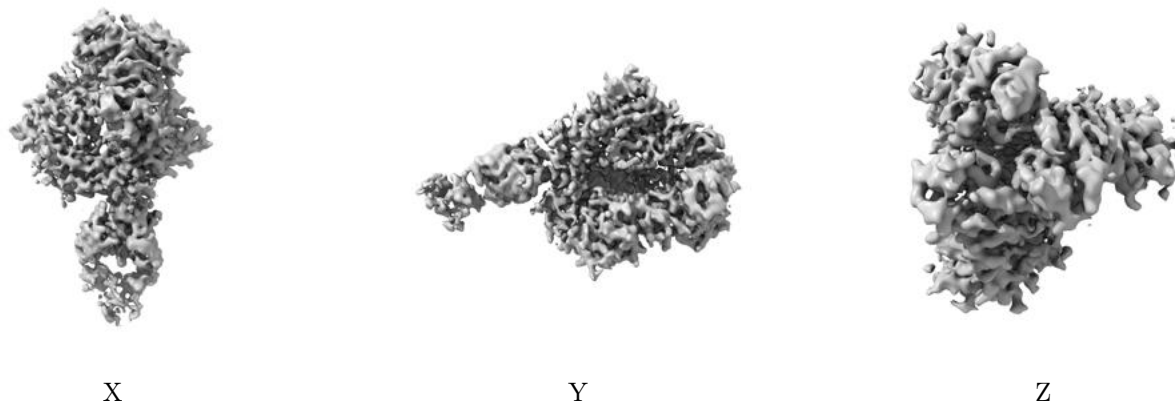
Z

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.



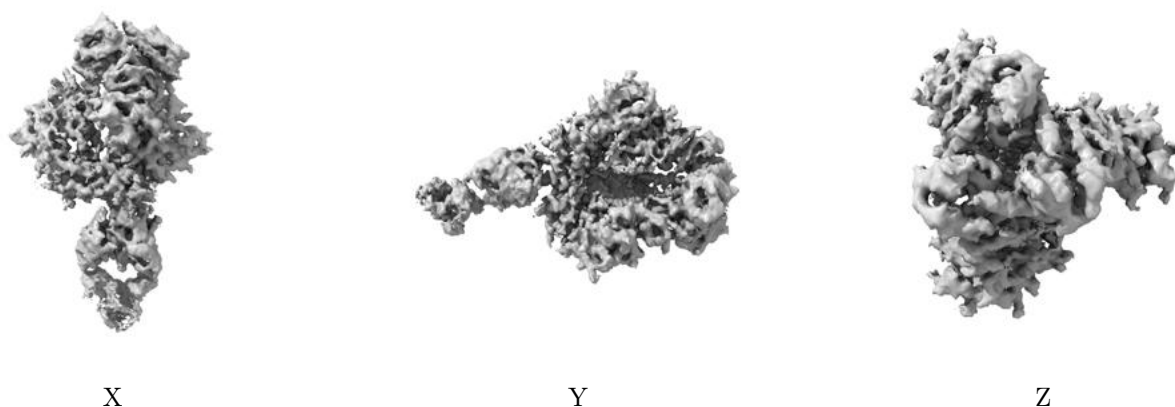
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

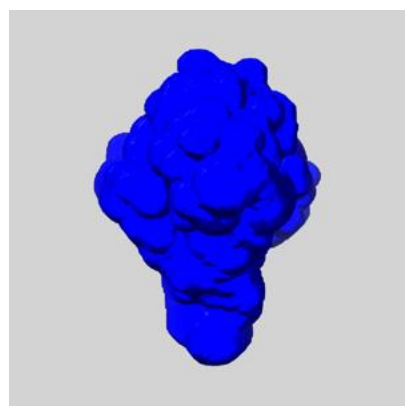
## 6.6 Mask visualisation [i](#)

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

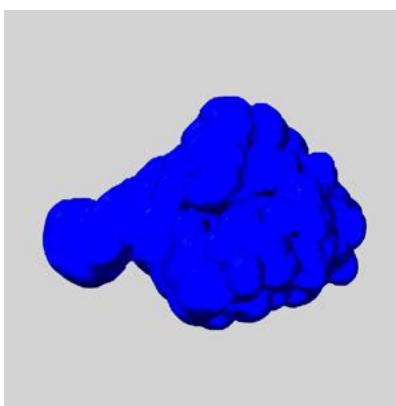
A mask typically either:

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

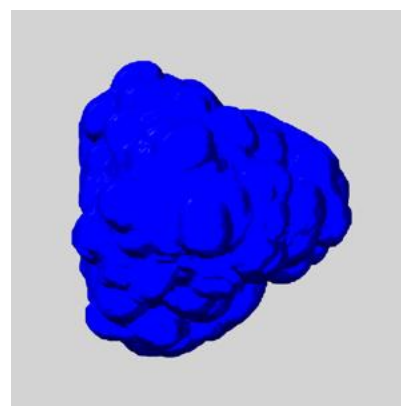
### 6.6.1 emd\_44890\_msk\_1.map [i](#)



X



Y

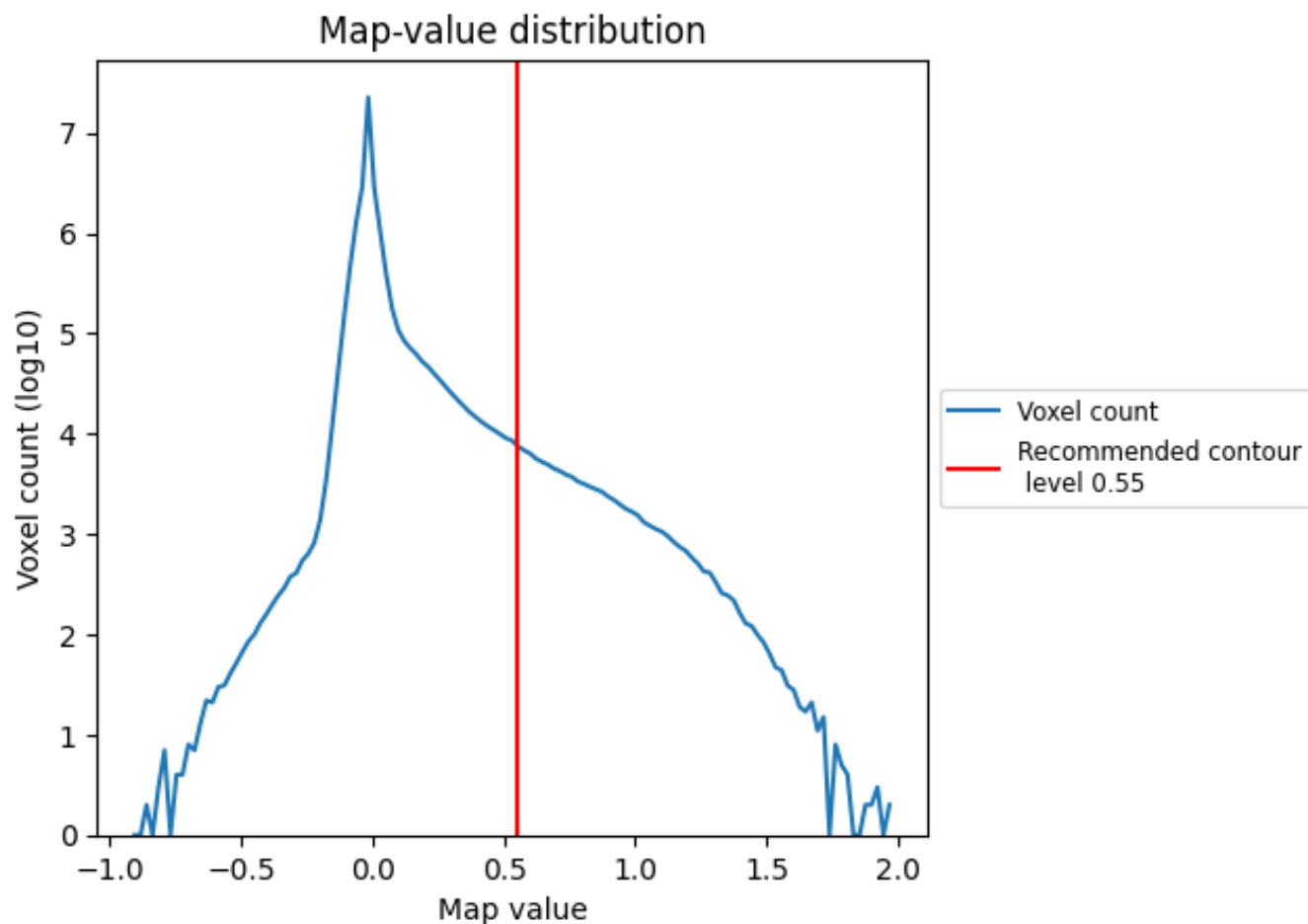


Z

## 7 Map analysis [i](#)

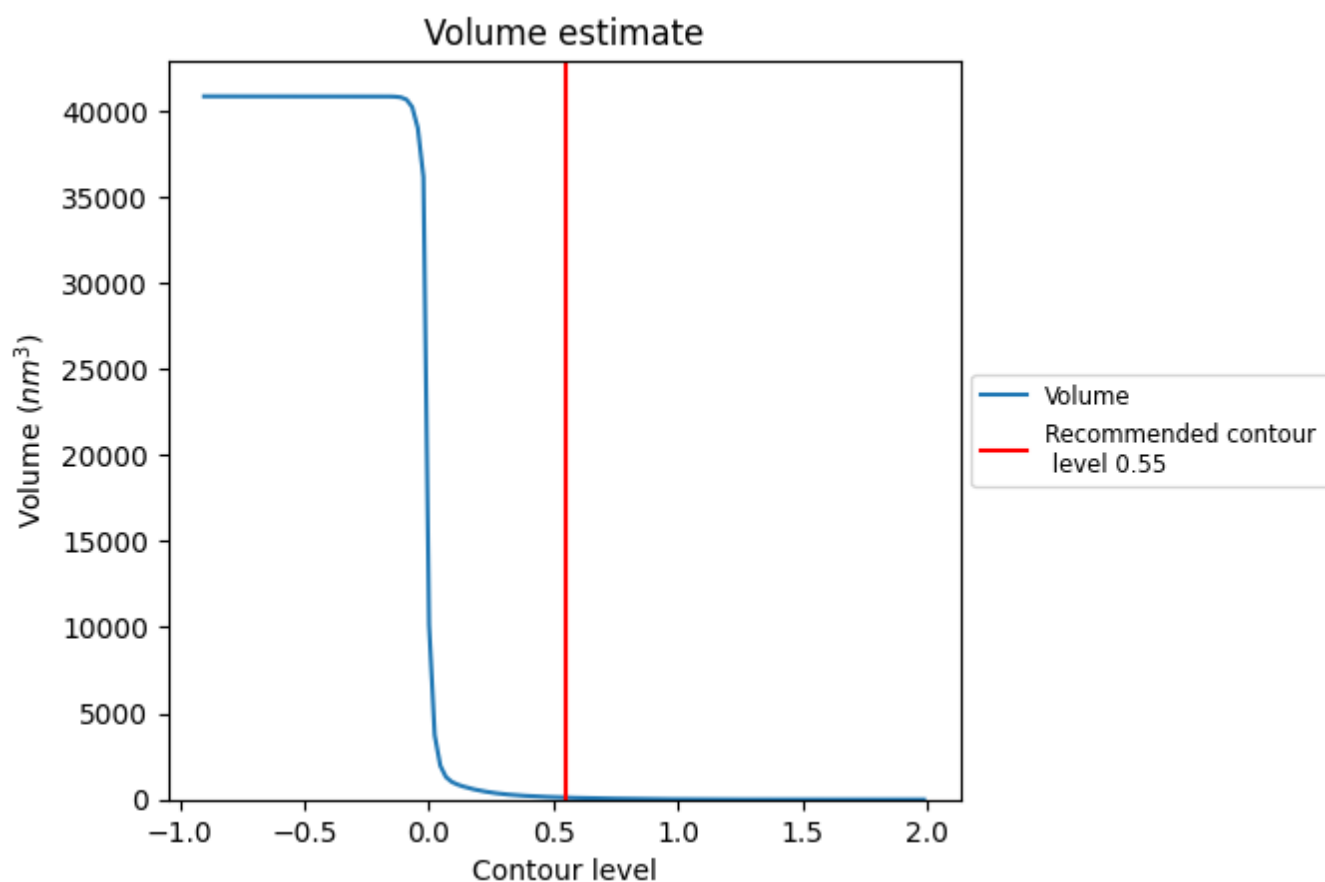
This section contains the results of statistical analysis of the map.

### 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.

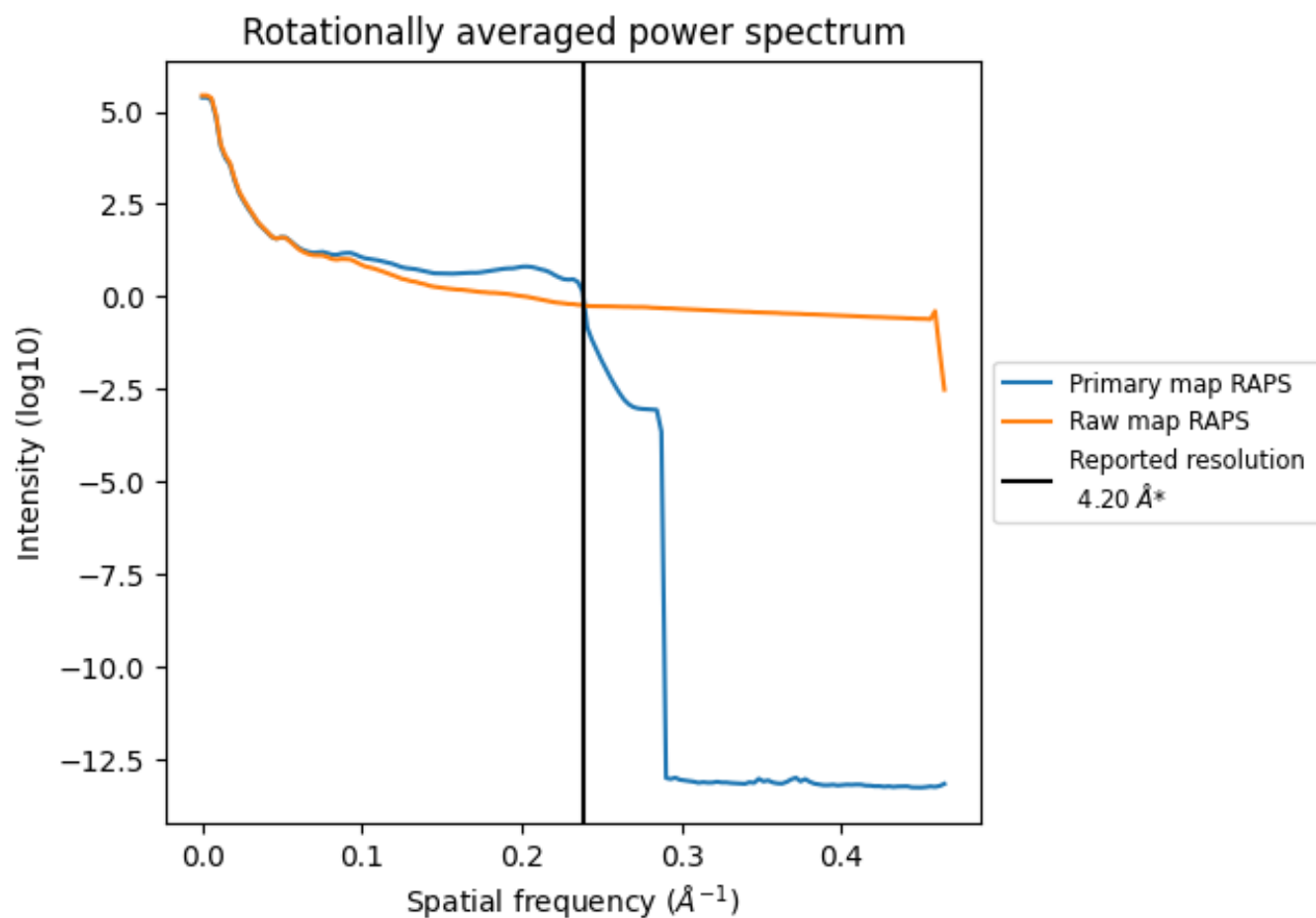
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 116 nm<sup>3</sup>; this corresponds to an approximate mass of 105 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 ⓘ

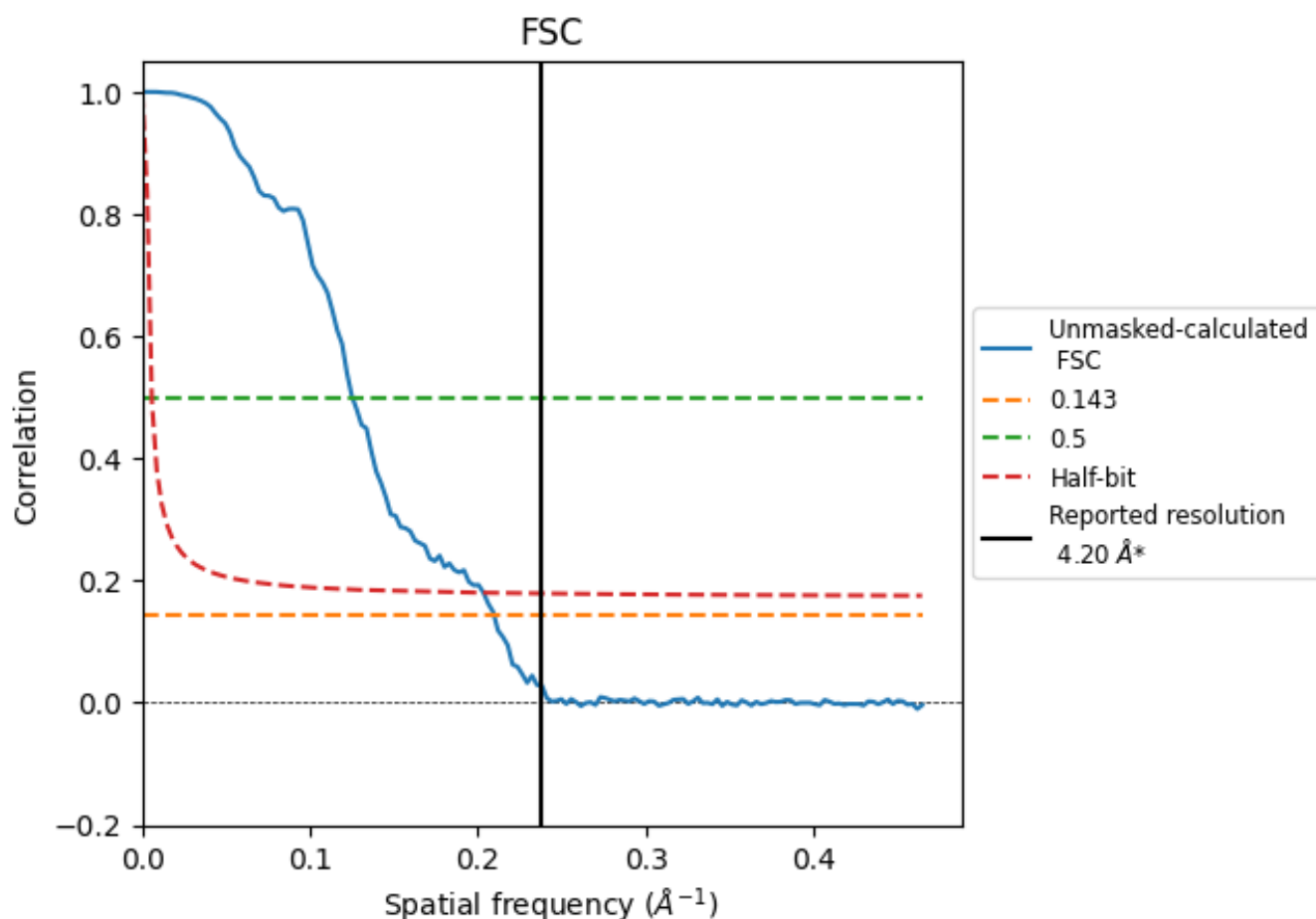


\*Reported resolution corresponds to spatial frequency of 0.238 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

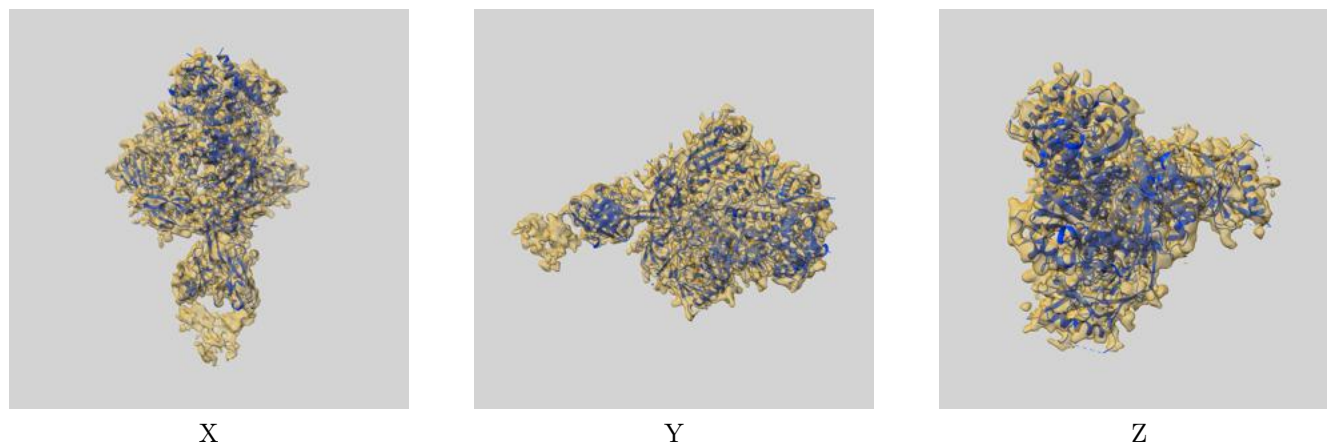
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.77	7.99	4.92

\*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 4.77 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-44890 and PDB model 9BTH. Per-residue inclusion information can be found in section 3 on page 13.

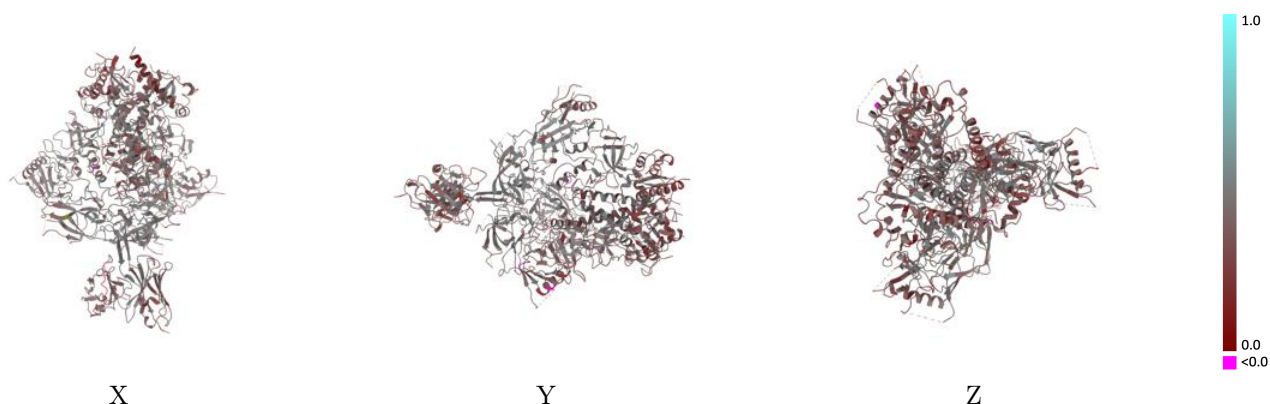
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.55 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.

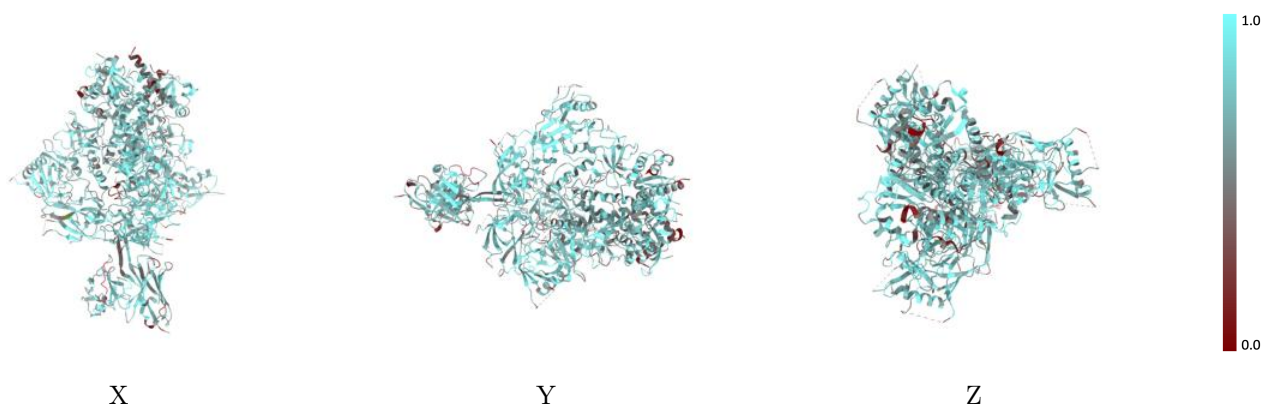


## 9.2 Q-score mapped to coordinate model [i](#)



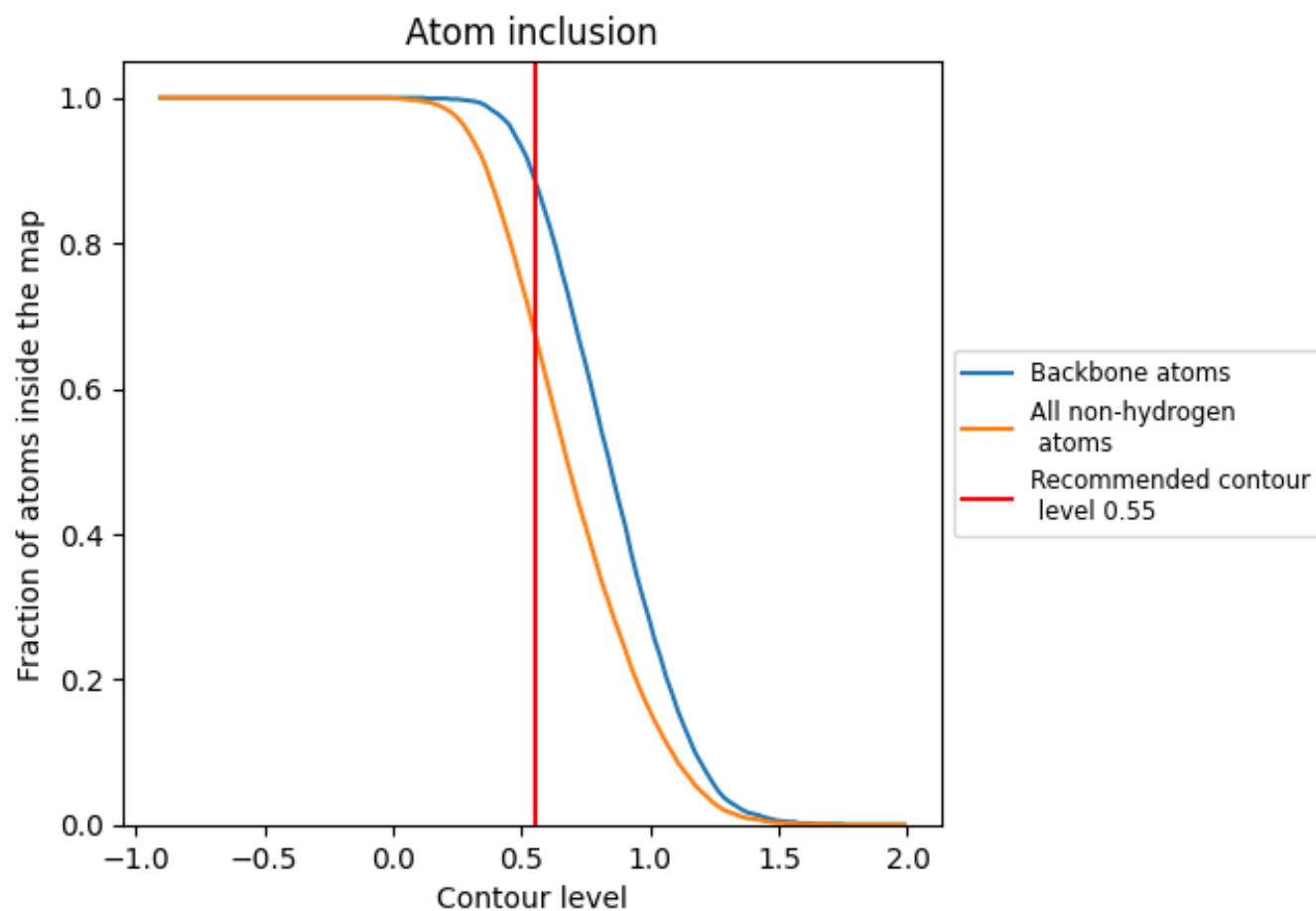
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 68% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6780	 0.3850
A	 0.4100	 0.3950
B	 0.6100	 0.3430
C	 0.6420	 0.3520
D	 0.7170	 0.4070
E	 0.6340	 0.3450
F	 0.7060	 0.3950
G	 0.7120	 0.4000
H	 0.6930	 0.3750
I	 0.6070	 0.4620
J	 0.4590	 0.3540
K	 0.0560	 0.3530
L	 0.6530	 0.3550
M	 0.6380	 0.3880
N	 0.4290	 0.4240
O	 0.3850	 0.3600
P	 0.5000	 0.3710
Q	 0.4260	 0.3810
R	 0.4640	 0.3810
S	 0.4290	 0.3690
T	 0.3770	 0.3230
U	 0.1330	 0.3770
V	 0.2860	 0.3200

