



## Full wwPDB EM Validation Report ⓘ

Aug 28, 2025 – 10:28 AM EDT

PDB ID : 9MLA / pdb\_00009mla  
EMDB ID : EMD-48351  
Title : Pre-fusion HERV-K Envelope Protein Trimer Ectodomain in complex with Kenv-6 Fab  
Authors : Shek, J.; Sun, C.; Hastie, K.; Saphire, E.O.  
Deposited on : 2024-12-18  
Resolution : 2.24 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.dev126  
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) : 2.45.1

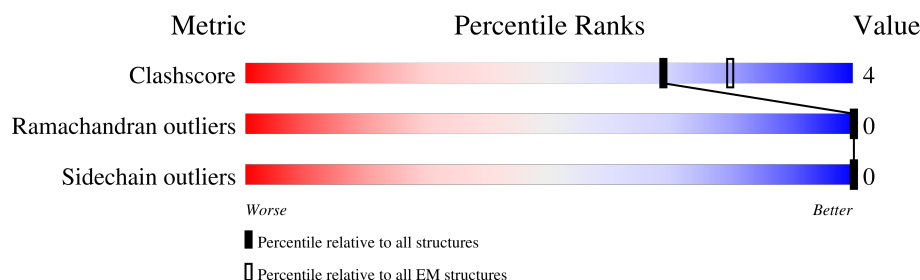
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.24 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	369	
1	B	369	
1	C	369	
2	D	253	
2	E	253	
2	F	253	
3	G	119	
3	H	119	

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Mol	Chain	Length	Quality of chain
3	I	119	
4	J	107	
4	K	107	
4	L	107	
5	M	5	
5	R	5	
5	W	5	
6	N	2	
6	O	2	
6	P	2	
6	Q	2	
6	S	2	
6	T	2	
6	U	2	
6	V	2	
6	X	2	
6	Y	2	
6	Z	2	
6	a	2	
7	b	3	
7	c	3	
7	e	3	
7	f	3	
7	h	3	
7	i	3	

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Mol	Chain	Length	Quality of chain
8	d	4	<div><div><div>75%</div><div>50%</div><div>50%</div></div></div>
8	g	4	<div><div><div>75%</div><div>50%</div><div>50%</div></div></div>
8	j	4	<div><div><div>75%</div><div>50%</div><div>50%</div></div></div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18633 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 Surface protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	360	Total	C	N	O	S	0	0
			2882	1846	495	521	20		
1	B	360	Total	C	N	O	S	0	0
			2882	1846	495	521	20		
1	C	360	Total	C	N	O	S	0	0
			2882	1846	495	521	20		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	167	ARG	THR	conflict	UNP P61570
A	185	THR	ILE	conflict	UNP P61570
A	328	ILE	VAL	conflict	UNP P61570
A	437	CYS	VAL	engineered mutation	UNP P61570
A	463	ARG	SER	engineered mutation	UNP P61570
A	464	ARG	LYS	engineered mutation	UNP P61570
B	167	ARG	THR	conflict	UNP P61570
B	185	THR	ILE	conflict	UNP P61570
B	328	ILE	VAL	conflict	UNP P61570
B	437	CYS	VAL	engineered mutation	UNP P61570
B	463	ARG	SER	engineered mutation	UNP P61570
B	464	ARG	LYS	engineered mutation	UNP P61570
C	167	ARG	THR	conflict	UNP P61570
C	185	THR	ILE	conflict	UNP P61570
C	328	ILE	VAL	conflict	UNP P61570
C	437	CYS	VAL	engineered mutation	UNP P61570
C	463	ARG	SER	engineered mutation	UNP P61570
C	464	ARG	LYS	engineered mutation	UNP P61570

- Molecule 2 is a protein called Transmembrane protein,Fibrinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	155	Total	C	N	O	S	0	0
			1230	772	219	232	7		
2	E	155	Total	C	N	O	S	0	0
			1230	772	219	232	7		
2	F	155	Total	C	N	O	S	0	0
			1230	772	219	232	7		

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	484	ALA	GLY	conflict	UNP P61570
D	498	CYS	VAL	engineered mutation	UNP P61570
D	599	GLU	LYS	conflict	UNP P61570
D	633	ASP	-	linker	UNP P61570
D	634	ASP	-	linker	UNP P61570
D	635	ASP	-	linker	UNP P61570
D	636	ASP	-	linker	UNP P61570
D	637	LYS	-	linker	UNP P61570
D	638	ALA	-	linker	UNP P61570
D	639	GLY	-	linker	UNP P61570
D	640	GLY	-	linker	UNP P61570
D	641	SER	-	linker	UNP P61570
D	642	GLY	-	linker	UNP P61570
D	643	GLY	-	linker	UNP P61570
D	644	SER	-	linker	UNP P61570
D	645	GLY	-	linker	UNP P61570
D	646	GLY	-	linker	UNP P61570
D	647	SER	-	linker	UNP P61570
D	648	GLY	-	linker	UNP P61570
D	649	GLY	-	linker	UNP P61570
D	650	GLY	-	linker	UNP P61570
D	671	LEU	PHE	conflict	UNP P10104
D	677	ALA	-	expression tag	UNP P10104
D	678	SER	-	expression tag	UNP P10104
D	679	GLY	-	expression tag	UNP P10104
D	680	LEU	-	expression tag	UNP P10104
D	681	GLU	-	expression tag	UNP P10104
D	682	VAL	-	expression tag	UNP P10104
D	683	LEU	-	expression tag	UNP P10104
D	684	PHE	-	expression tag	UNP P10104
D	685	GLN	-	expression tag	UNP P10104
D	686	GLY	-	expression tag	UNP P10104
D	687	PRO	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
D	688	GLY	-	expression tag	UNP P10104
D	689	ALA	-	expression tag	UNP P10104
D	690	GLY	-	expression tag	UNP P10104
D	691	TRP	-	expression tag	UNP P10104
D	692	SER	-	expression tag	UNP P10104
D	693	HIS	-	expression tag	UNP P10104
D	694	PRO	-	expression tag	UNP P10104
D	695	GLN	-	expression tag	UNP P10104
D	696	PHE	-	expression tag	UNP P10104
D	697	GLU	-	expression tag	UNP P10104
D	698	LYS	-	expression tag	UNP P10104
D	699	GLY	-	expression tag	UNP P10104
D	700	GLY	-	expression tag	UNP P10104
D	701	GLY	-	expression tag	UNP P10104
D	702	SER	-	expression tag	UNP P10104
D	703	GLY	-	expression tag	UNP P10104
D	704	GLY	-	expression tag	UNP P10104
D	705	GLY	-	expression tag	UNP P10104
D	706	SER	-	expression tag	UNP P10104
D	707	GLY	-	expression tag	UNP P10104
D	708	GLY	-	expression tag	UNP P10104
D	709	GLY	-	expression tag	UNP P10104
D	710	SER	-	expression tag	UNP P10104
D	711	TRP	-	expression tag	UNP P10104
D	712	SER	-	expression tag	UNP P10104
D	713	HIS	-	expression tag	UNP P10104
D	714	PRO	-	expression tag	UNP P10104
D	715	GLN	-	expression tag	UNP P10104
D	716	PHE	-	expression tag	UNP P10104
D	717	GLU	-	expression tag	UNP P10104
D	718	LYS	-	expression tag	UNP P10104
E	484	ALA	GLY	conflict	UNP P61570
E	498	CYS	VAL	engineered mutation	UNP P61570
E	599	GLU	LYS	conflict	UNP P61570
E	633	ASP	-	linker	UNP P61570
E	634	ASP	-	linker	UNP P61570
E	635	ASP	-	linker	UNP P61570
E	636	ASP	-	linker	UNP P61570
E	637	LYS	-	linker	UNP P61570
E	638	ALA	-	linker	UNP P61570
E	639	GLY	-	linker	UNP P61570
E	640	GLY	-	linker	UNP P61570

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Chain	Residue	Modelled	Actual	Comment	Reference
E	641	SER	-	linker	UNP P61570
E	642	GLY	-	linker	UNP P61570
E	643	GLY	-	linker	UNP P61570
E	644	SER	-	linker	UNP P61570
E	645	GLY	-	linker	UNP P61570
E	646	GLY	-	linker	UNP P61570
E	647	SER	-	linker	UNP P61570
E	648	GLY	-	linker	UNP P61570
E	649	GLY	-	linker	UNP P61570
E	650	GLY	-	linker	UNP P61570
E	671	LEU	PHE	conflict	UNP P10104
E	677	ALA	-	expression tag	UNP P10104
E	678	SER	-	expression tag	UNP P10104
E	679	GLY	-	expression tag	UNP P10104
E	680	LEU	-	expression tag	UNP P10104
E	681	GLU	-	expression tag	UNP P10104
E	682	VAL	-	expression tag	UNP P10104
E	683	LEU	-	expression tag	UNP P10104
E	684	PHE	-	expression tag	UNP P10104
E	685	GLN	-	expression tag	UNP P10104
E	686	GLY	-	expression tag	UNP P10104
E	687	PRO	-	expression tag	UNP P10104
E	688	GLY	-	expression tag	UNP P10104
E	689	ALA	-	expression tag	UNP P10104
E	690	GLY	-	expression tag	UNP P10104
E	691	TRP	-	expression tag	UNP P10104
E	692	SER	-	expression tag	UNP P10104
E	693	HIS	-	expression tag	UNP P10104
E	694	PRO	-	expression tag	UNP P10104
E	695	GLN	-	expression tag	UNP P10104
E	696	PHE	-	expression tag	UNP P10104
E	697	GLU	-	expression tag	UNP P10104
E	698	LYS	-	expression tag	UNP P10104
E	699	GLY	-	expression tag	UNP P10104
E	700	GLY	-	expression tag	UNP P10104
E	701	GLY	-	expression tag	UNP P10104
E	702	SER	-	expression tag	UNP P10104
E	703	GLY	-	expression tag	UNP P10104
E	704	GLY	-	expression tag	UNP P10104
E	705	GLY	-	expression tag	UNP P10104
E	706	SER	-	expression tag	UNP P10104
E	707	GLY	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
E	708	GLY	-	expression tag	UNP P10104
E	709	GLY	-	expression tag	UNP P10104
E	710	SER	-	expression tag	UNP P10104
E	711	TRP	-	expression tag	UNP P10104
E	712	SER	-	expression tag	UNP P10104
E	713	HIS	-	expression tag	UNP P10104
E	714	PRO	-	expression tag	UNP P10104
E	715	GLN	-	expression tag	UNP P10104
E	716	PHE	-	expression tag	UNP P10104
E	717	GLU	-	expression tag	UNP P10104
E	718	LYS	-	expression tag	UNP P10104
F	484	ALA	GLY	conflict	UNP P61570
F	498	CYS	VAL	engineered mutation	UNP P61570
F	599	GLU	LYS	conflict	UNP P61570
F	633	ASP	-	linker	UNP P61570
F	634	ASP	-	linker	UNP P61570
F	635	ASP	-	linker	UNP P61570
F	636	ASP	-	linker	UNP P61570
F	637	LYS	-	linker	UNP P61570
F	638	ALA	-	linker	UNP P61570
F	639	GLY	-	linker	UNP P61570
F	640	GLY	-	linker	UNP P61570
F	641	SER	-	linker	UNP P61570
F	642	GLY	-	linker	UNP P61570
F	643	GLY	-	linker	UNP P61570
F	644	SER	-	linker	UNP P61570
F	645	GLY	-	linker	UNP P61570
F	646	GLY	-	linker	UNP P61570
F	647	SER	-	linker	UNP P61570
F	648	GLY	-	linker	UNP P61570
F	649	GLY	-	linker	UNP P61570
F	650	GLY	-	linker	UNP P61570
F	671	LEU	PHE	conflict	UNP P10104
F	677	ALA	-	expression tag	UNP P10104
F	678	SER	-	expression tag	UNP P10104
F	679	GLY	-	expression tag	UNP P10104
F	680	LEU	-	expression tag	UNP P10104
F	681	GLU	-	expression tag	UNP P10104
F	682	VAL	-	expression tag	UNP P10104
F	683	LEU	-	expression tag	UNP P10104
F	684	PHE	-	expression tag	UNP P10104
F	685	GLN	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
F	686	GLY	-	expression tag	UNP P10104
F	687	PRO	-	expression tag	UNP P10104
F	688	GLY	-	expression tag	UNP P10104
F	689	ALA	-	expression tag	UNP P10104
F	690	GLY	-	expression tag	UNP P10104
F	691	TRP	-	expression tag	UNP P10104
F	692	SER	-	expression tag	UNP P10104
F	693	HIS	-	expression tag	UNP P10104
F	694	PRO	-	expression tag	UNP P10104
F	695	GLN	-	expression tag	UNP P10104
F	696	PHE	-	expression tag	UNP P10104
F	697	GLU	-	expression tag	UNP P10104
F	698	LYS	-	expression tag	UNP P10104
F	699	GLY	-	expression tag	UNP P10104
F	700	GLY	-	expression tag	UNP P10104
F	701	GLY	-	expression tag	UNP P10104
F	702	SER	-	expression tag	UNP P10104
F	703	GLY	-	expression tag	UNP P10104
F	704	GLY	-	expression tag	UNP P10104
F	705	GLY	-	expression tag	UNP P10104
F	706	SER	-	expression tag	UNP P10104
F	707	GLY	-	expression tag	UNP P10104
F	708	GLY	-	expression tag	UNP P10104
F	709	GLY	-	expression tag	UNP P10104
F	710	SER	-	expression tag	UNP P10104
F	711	TRP	-	expression tag	UNP P10104
F	712	SER	-	expression tag	UNP P10104
F	713	HIS	-	expression tag	UNP P10104
F	714	PRO	-	expression tag	UNP P10104
F	715	GLN	-	expression tag	UNP P10104
F	716	PHE	-	expression tag	UNP P10104
F	717	GLU	-	expression tag	UNP P10104
F	718	LYS	-	expression tag	UNP P10104

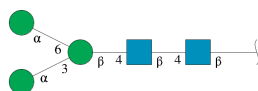
- Molecule 3 is a protein called Kenv-6 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	119	Total	C	N	O	S	0	0
			950	620	147	179	4		
3	H	119	Total	C	N	O	S	0	0
			950	620	147	179	4		
3	I	119	Total	C	N	O	S	0	0
			950	620	147	179	4		

- Molecule 4 is a protein called Kenv-6 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	107	Total	C	N	O	S	0	0
			821	516	138	164	3		
4	K	107	Total	C	N	O	S	0	0
			821	516	138	164	3		
4	L	107	Total	C	N	O	S	0	0
			821	516	138	164	3		

- Molecule 5 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
5	M	5	Total	C	N	O	0	0
			61	34	2	25		
5	R	5	Total	C	N	O	0	0
			61	34	2	25		
5	W	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



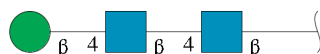
Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	2	Total	C	N	O	0	0
			28	16	2	10		
6	O	2	Total	C	N	O	0	0
			28	16	2	10		
6	P	2	Total	C	N	O	0	0
			28	16	2	10		
6	Q	2	Total	C	N	O	0	0
			28	16	2	10		
6	S	2	Total	C	N	O	0	0
			28	16	2	10		

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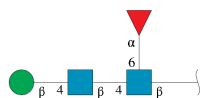
Mol	Chain	Residues	Atoms				AltConf	Trace
6	T	2	Total	C	N	O	0	0
			28	16	2	10		
6	U	2	Total	C	N	O	0	0
			28	16	2	10		
6	V	2	Total	C	N	O	0	0
			28	16	2	10		
6	X	2	Total	C	N	O	0	0
			28	16	2	10		
6	Y	2	Total	C	N	O	0	0
			28	16	2	10		
6	Z	2	Total	C	N	O	0	0
			28	16	2	10		
6	a	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 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
7	b	3	Total	C	N	O	0	0
			39	22	2	15		
7	c	3	Total	C	N	O	0	0
			39	22	2	15		
7	e	3	Total	C	N	O	0	0
			39	22	2	15		
7	f	3	Total	C	N	O	0	0
			39	22	2	15		
7	h	3	Total	C	N	O	0	0
			39	22	2	15		
7	i	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
8	d	4	Total	C	N	O	0	0
			49	28	2	19		
8	g	4	Total	C	N	O	0	0
			49	28	2	19		
8	j	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).

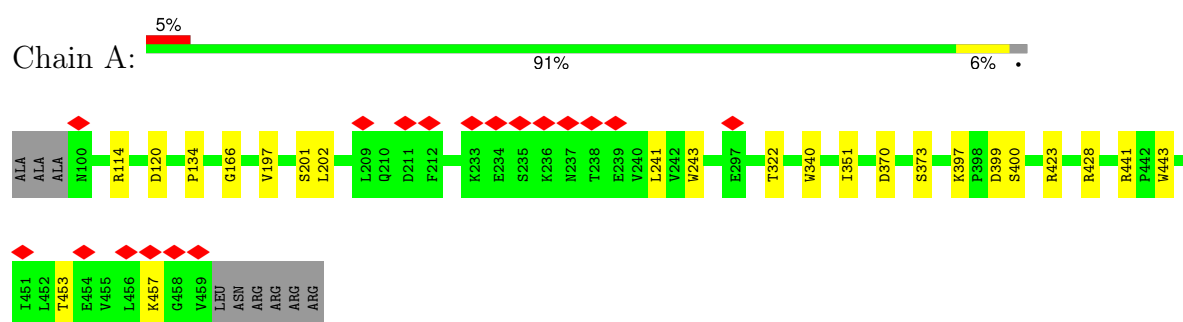


Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	B	1	Total	C	N	O	0
			14	8	1	5	
9	C	1	Total	C	N	O	0
			14	8	1	5	
9	D	1	Total	C	N	O	0
			14	8	1	5	
9	E	1	Total	C	N	O	0
			14	8	1	5	
9	F	1	Total	C	N	O	0
			14	8	1	5	

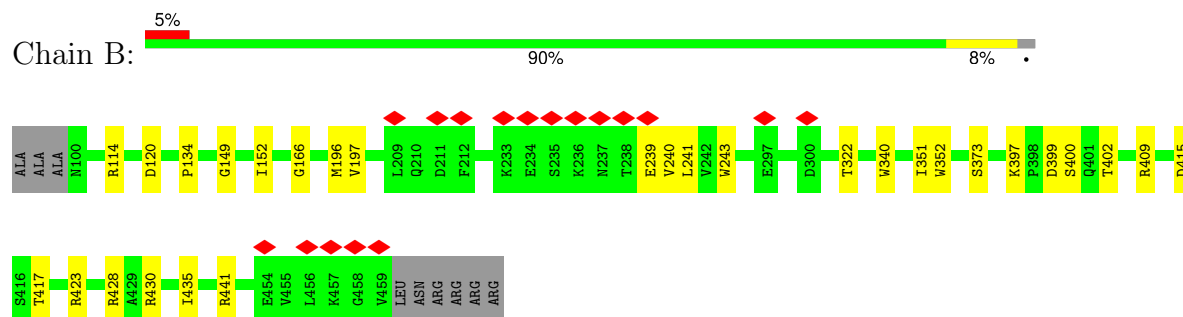
### 3 Residue-property plots [i](#)

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.

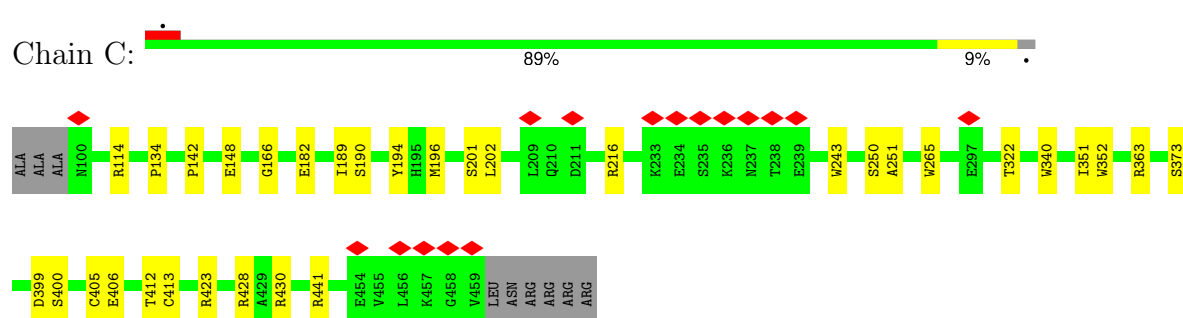
- Molecule 1: Surface protein



- Molecule 1: Surface protein



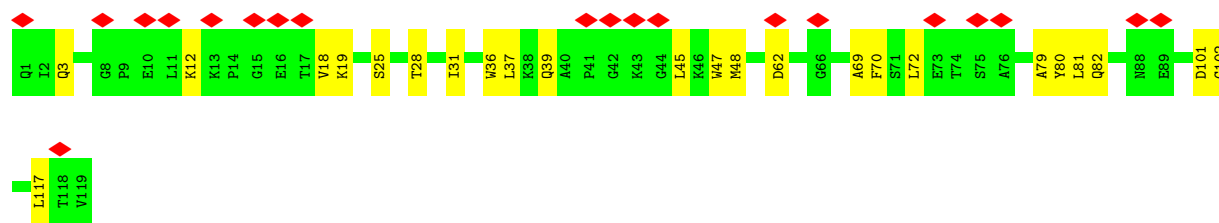
- Molecule 1: Surface protein



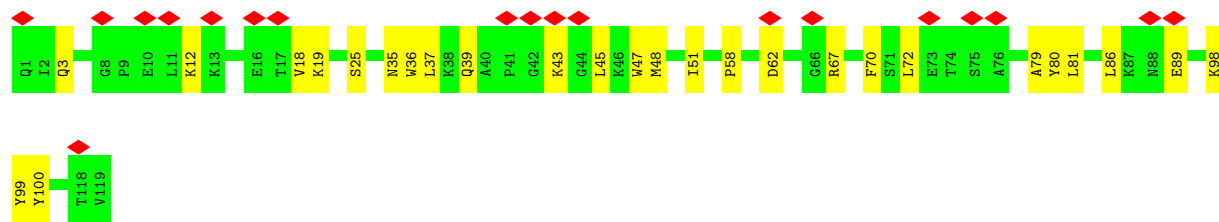
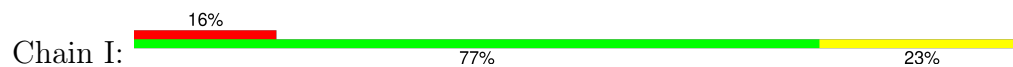
- Molecule 2: Transmembrane protein,Fibrin



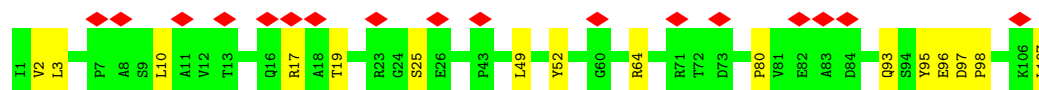
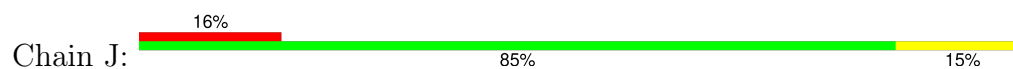




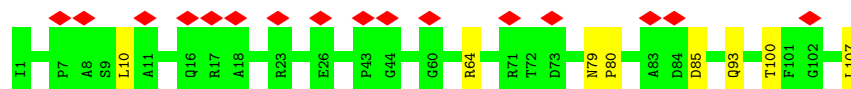
• Molecule 3: Kenv-6 Fab heavy chain



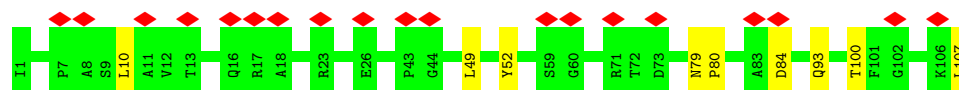
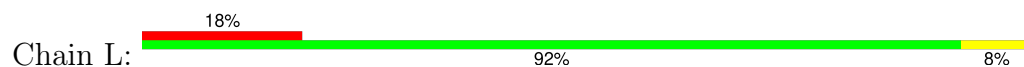
• Molecule 4: Kenv-6 Fab light chain



• Molecule 4: Kenv-6 Fab light chain



• Molecule 4: Kenv-6 Fab light chain



• Molecule 5: 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 5: 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

Chain R: 



- Molecule 5: 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

Chain W: 



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

Chain N: 



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

Chain O: 



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

Chain P: 



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

Chain Q: 



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



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



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



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



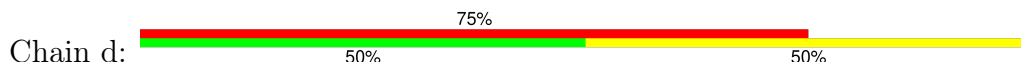
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



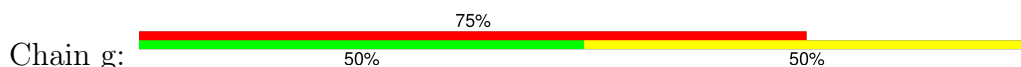
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



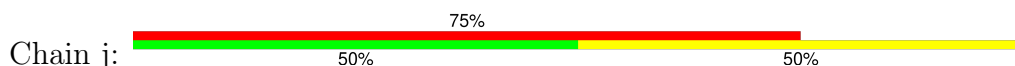
- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



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





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	479625	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.890	Depositor
Minimum map value	-0.351	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.16	Depositor
Map size ( $\text{\AA}$ )	422.40128, 422.40128, 422.40128	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.94286, 0.94286, 0.94286	Depositor

## 5 Model quality [i](#)

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

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

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	0.12	0/2974	0.28	0/4070
1	B	0.12	0/2974	0.27	0/4070
1	C	0.12	0/2974	0.27	0/4070
2	D	0.10	0/1254	0.24	0/1702
2	E	0.11	0/1254	0.25	0/1702
2	F	0.11	0/1254	0.25	0/1702
3	G	0.09	0/980	0.24	0/1332
3	H	0.09	0/980	0.25	0/1332
3	I	0.09	0/980	0.25	0/1332
4	J	0.11	0/841	0.34	0/1144
4	K	0.10	0/841	0.31	0/1144
4	L	0.10	0/841	0.31	0/1144
All	All	0.11	0/18147	0.27	0/24744

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	2882	0	2817	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2882	0	2817	17	0
1	C	2882	0	2817	20	0
2	D	1230	0	1194	6	0
2	E	1230	0	1194	9	0
2	F	1230	0	1194	7	0
3	G	950	0	904	16	0
3	H	950	0	904	13	0
3	I	950	0	904	17	0
4	J	821	0	787	10	0
4	K	821	0	787	4	0
4	L	821	0	787	5	0
5	M	61	0	52	0	0
5	R	61	0	52	0	0
5	W	61	0	52	0	0
6	N	28	0	25	0	0
6	O	28	0	25	1	0
6	P	28	0	25	0	0
6	Q	28	0	25	0	0
6	S	28	0	25	0	0
6	T	28	0	25	0	0
6	U	28	0	25	0	0
6	V	28	0	25	0	0
6	X	28	0	25	0	0
6	Y	28	0	25	0	0
6	Z	28	0	25	0	0
6	a	28	0	25	0	0
7	b	39	0	34	0	0
7	c	39	0	34	1	0
7	e	39	0	34	0	0
7	f	39	0	34	1	0
7	h	39	0	34	0	0
7	i	39	0	34	1	0
8	d	49	0	43	0	0
8	g	49	0	43	0	0
8	j	49	0	43	0	0
9	A	14	0	13	0	0
9	B	14	0	13	0	0
9	C	14	0	13	0	0
9	D	14	0	13	0	0
9	E	14	0	13	0	0
9	F	14	0	13	0	0
All	All	18633	0	17973	128	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 (128) 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:441:ARG:HE	7:c:1:NAG:H81	1.57	0.70
1:B:441:ARG:HE	7:f:1:NAG:H81	1.57	0.69
1:C:441:ARG:HE	7:i:1:NAG:H81	1.57	0.68
2:F:584:ASP:OD1	2:F:587:THR:OG1	2.11	0.68
2:E:584:ASP:OD1	2:E:587:THR:OG1	2.12	0.67
3:H:3:GLN:HB2	3:H:25:SER:HB3	1.76	0.66
4:K:64:ARG:NH1	4:K:85:ASP:OD2	2.31	0.63
3:G:12:LYS:HG3	3:G:18:VAL:HG22	1.80	0.63
3:G:35:ASN:HD21	3:G:99:TYR:HD2	1.47	0.62
3:G:19:LYS:HD2	3:G:80:TYR:HB3	1.81	0.62
3:I:35:ASN:HD21	3:I:99:TYR:HD2	1.46	0.62
3:G:36:TRP:HB3	3:G:48:MET:HE3	1.82	0.61
1:B:166:GLY:HA3	1:B:423:ARG:HG3	1.83	0.59
2:D:584:ASP:OD1	2:D:587:THR:OG1	2.16	0.59
4:J:17:ARG:NH1	4:J:19:THR:OG1	2.36	0.59
3:H:19:LYS:HD2	3:H:80:TYR:HB3	1.85	0.58
3:H:36:TRP:HB3	3:H:48:MET:HE3	1.86	0.57
3:I:19:LYS:HD2	3:I:80:TYR:HB3	1.87	0.57
4:J:93:GLN:HE21	4:J:95:TYR:HB3	1.70	0.56
3:I:39:GLN:HB2	3:I:45:LEU:HD23	1.86	0.56
2:D:603:ALA:HA	2:D:607:LEU:HD23	1.88	0.56
3:I:36:TRP:HB3	3:I:48:MET:HE3	1.88	0.56
1:C:182:GLU:HG2	1:C:194:TYR:HE1	1.70	0.56
3:I:3:GLN:HB2	3:I:25:SER:HB3	1.88	0.56
3:I:37:LEU:HD23	3:I:47:TRP:HA	1.88	0.55
3:H:12:LYS:HG3	3:H:18:VAL:HG22	1.87	0.55
1:A:120:ASP:OD1	2:E:520:GLN:NE2	2.40	0.54
3:H:39:GLN:HB2	3:H:45:LEU:HD23	1.88	0.54
3:G:39:GLN:HB2	3:G:45:LEU:HD23	1.88	0.54
4:K:93:GLN:HE21	4:K:100:THR:H	1.55	0.54
3:H:28:THR:HG23	3:H:31:ILE:HG12	1.90	0.53
2:F:590:ILE:HG22	2:F:594:LYS:HD2	1.90	0.53
3:G:37:LEU:HD23	3:G:47:TRP:HA	1.90	0.53
1:A:399:ASP:OD1	1:A:400:SER:N	2.42	0.53
1:B:397:LYS:HE2	1:B:402:THR:HB	1.90	0.53
3:I:12:LYS:HG3	3:I:18:VAL:HG22	1.91	0.53
1:C:322:THR:HG21	1:C:340:TRP:CZ2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:79:ASN:HB2	4:K:80:PRO:HD3	1.91	0.52
4:J:10:LEU:HB3	4:J:107:LEU:HD12	1.91	0.52
4:J:3:LEU:HD11	4:J:93:GLN:HB2	1.90	0.52
4:L:79:ASN:HB2	4:L:80:PRO:HD3	1.90	0.52
1:A:166:GLY:HA3	1:A:423:ARG:HG3	1.90	0.52
3:G:73:GLU:OE1	3:G:80:TYR:OH	2.28	0.52
3:I:67:ARG:NH2	3:I:89:GLU:OE2	2.41	0.52
1:B:399:ASP:OD1	1:B:400:SER:N	2.42	0.52
1:C:430:ARG:NH1	2:F:579:LEU:O	2.44	0.51
3:G:72:LEU:HA	3:G:79:ALA:HA	1.93	0.51
3:H:62:ASP:N	3:H:62:ASP:OD1	2.42	0.51
1:C:216:ARG:HE	1:C:250:SER:HB3	1.75	0.51
1:C:134:PRO:HD3	1:C:243:TRP:CD1	2.46	0.51
1:C:166:GLY:HA3	1:C:423:ARG:HG3	1.92	0.51
3:G:2:ILE:HG22	3:G:110:VAL:HG11	1.94	0.50
4:J:49:LEU:HD21	4:J:52:TYR:HB3	1.92	0.50
3:I:98:LYS:NZ	3:I:99:TYR:O	2.42	0.49
3:G:17:THR:HG22	3:G:84:ASN:HA	1.94	0.49
1:C:399:ASP:OD1	1:C:400:SER:N	2.46	0.49
1:A:322:THR:HG21	1:A:340:TRP:CZ2	2.48	0.49
1:A:134:PRO:HD3	1:A:243:TRP:CD1	2.47	0.49
3:H:70:PHE:HE1	3:H:81:LEU:HD13	1.77	0.49
2:D:544:GLU:OE1	2:E:539:ARG:NH2	2.31	0.48
3:H:101:ASP:OD1	3:H:102:GLY:N	2.40	0.48
3:I:62:ASP:N	3:I:62:ASP:OD1	2.43	0.48
3:H:37:LEU:HD23	3:H:47:TRP:HA	1.94	0.48
3:I:51:ILE:HD11	3:I:72:LEU:HD22	1.94	0.48
3:H:69:ALA:HB3	3:H:82:GLN:HB3	1.95	0.48
1:A:201:SER:OG	1:A:202:LEU:N	2.47	0.48
1:C:363:ARG:NH1	3:I:100:TYR:OH	2.46	0.48
2:E:584:ASP:OD1	2:E:584:ASP:N	2.45	0.48
1:B:134:PRO:HD3	1:B:243:TRP:CD1	2.49	0.48
3:I:70:PHE:HE1	3:I:81:LEU:HD13	1.80	0.47
1:B:239:GLU:HG2	1:B:240:VAL:HG23	1.96	0.47
1:C:351:ILE:O	1:C:373:SER:OG	2.25	0.46
4:J:2:VAL:HG12	4:J:25:SER:HB3	1.97	0.46
4:L:93:GLN:HE21	4:L:100:THR:H	1.63	0.46
3:G:62:ASP:N	3:G:62:ASP:OD1	2.45	0.46
3:H:72:LEU:HA	3:H:79:ALA:HA	1.98	0.46
1:B:152:ILE:HD12	2:E:482:ALA:HA	1.96	0.46
3:G:70:PHE:HE1	3:G:81:LEU:HD13	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:49:LEU:HD21	4:L:52:TYR:HB3	1.98	0.46
4:K:10:LEU:HB3	4:K:107:LEU:HD12	1.98	0.46
4:J:93:GLN:NE2	4:J:95:TYR:HB3	2.31	0.46
1:C:196:MET:HB3	1:C:352:TRP:HB2	1.98	0.46
4:J:64:ARG:HD2	4:J:80:PRO:HG2	1.99	0.45
1:B:322:THR:HG21	1:B:340:TRP:CZ2	2.51	0.45
3:I:58:PRO:HB3	3:I:70:PHE:HB2	1.98	0.45
1:C:430:ARG:HH12	2:F:579:LEU:C	2.25	0.45
1:A:114:ARG:HH21	1:A:428:ARG:NH2	2.15	0.45
1:B:120:ASP:OD1	2:F:520:GLN:NE2	2.50	0.45
3:G:58:PRO:HB3	3:G:70:PHE:HB2	1.98	0.45
1:A:453:THR:HG22	1:A:457:LYS:HE2	2.00	0.44
1:C:142:PRO:HG3	1:C:413:CYS:SG	2.57	0.44
1:C:182:GLU:HG2	1:C:194:TYR:CE1	2.53	0.44
1:A:397:LYS:HE2	1:A:397:LYS:HB2	1.84	0.44
1:B:114:ARG:HH21	1:B:428:ARG:NH2	2.16	0.44
1:B:196:MET:HB3	1:B:352:TRP:HB2	1.98	0.44
1:C:148:GLU:OE2	1:C:412:THR:OG1	2.28	0.44
3:H:18:VAL:HG21	3:H:117:LEU:HD11	2.00	0.44
1:C:251:ALA:HB2	1:C:265:TRP:CE2	2.53	0.44
1:B:435:ILE:HD12	2:E:579:LEU:HD11	1.99	0.43
1:C:405:CYS:SG	1:C:406:GLU:N	2.91	0.43
2:D:590:ILE:HG22	2:D:594:LYS:HD2	1.99	0.43
3:I:72:LEU:HA	3:I:79:ALA:HA	2.00	0.43
1:C:201:SER:OG	1:C:202:LEU:N	2.51	0.43
3:G:35:ASN:ND2	3:G:99:TYR:HD2	2.16	0.43
4:J:93:GLN:HE22	4:J:96:GLU:N	2.16	0.43
4:L:10:LEU:HB3	4:L:107:LEU:HD12	1.99	0.43
2:F:584:ASP:OD1	2:F:584:ASP:N	2.48	0.43
1:B:149:GLY:HA2	1:B:409:ARG:HB3	2.01	0.43
4:J:97:ASP:OD1	4:J:98:PRO:HA	2.19	0.43
4:L:84:ASP:OD1	4:L:84:ASP:N	2.51	0.43
1:B:197:VAL:HG21	1:B:241:LEU:HD22	2.00	0.42
2:E:590:ILE:HG22	2:E:594:LYS:HD2	2.02	0.42
1:B:430:ARG:HH12	2:E:579:LEU:C	2.27	0.42
2:E:619:ASP:OD1	2:E:620:GLY:N	2.53	0.42
1:C:114:ARG:HH21	1:C:428:ARG:NH2	2.18	0.42
1:B:351:ILE:O	1:B:373:SER:OG	2.27	0.41
1:B:415:ASP:OD1	1:B:417:THR:OG1	2.38	0.41
2:D:619:ASP:OD1	2:D:620:GLY:N	2.53	0.41
1:C:189:ILE:HG13	1:C:190:SER:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ILE:O	1:A:373:SER:OG	2.29	0.41
3:I:18:VAL:HG23	3:I:86:LEU:HD11	2.02	0.41
1:A:443:TRP:CZ3	2:D:606:ASN:HB3	2.56	0.41
3:G:29:PHE:HE2	3:G:72:LEU:HD12	1.86	0.41
2:F:619:ASP:OD1	2:F:620:GLY:N	2.53	0.40
3:G:43:LYS:HD2	3:G:43:LYS:HA	1.76	0.40
1:A:197:VAL:HG21	1:A:241:LEU:HD22	2.03	0.40
1:A:370:ASP:HB3	6:O:1:NAG:H62	2.04	0.40
3:I:43:LYS:HD2	3:I:43:LYS:HA	1.77	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	A	358/369 (97%)	345 (96%)	13 (4%)	0	100	100
1	B	358/369 (97%)	348 (97%)	10 (3%)	0	100	100
1	C	358/369 (97%)	347 (97%)	11 (3%)	0	100	100
2	D	153/253 (60%)	151 (99%)	2 (1%)	0	100	100
2	E	153/253 (60%)	150 (98%)	3 (2%)	0	100	100
2	F	153/253 (60%)	150 (98%)	3 (2%)	0	100	100
3	G	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
3	H	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
3	I	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
4	J	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
4	K	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
4	L	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
All	All	2199/2544 (86%)	2120 (96%)	79 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	328/336 (98%)	328 (100%)	0	100	100
1	B	328/336 (98%)	328 (100%)	0	100	100
1	C	328/336 (98%)	328 (100%)	0	100	100
2	D	135/203 (66%)	135 (100%)	0	100	100
2	E	135/203 (66%)	135 (100%)	0	100	100
2	F	135/203 (66%)	135 (100%)	0	100	100
3	G	97/97 (100%)	97 (100%)	0	100	100
3	H	97/97 (100%)	97 (100%)	0	100	100
3	I	97/97 (100%)	97 (100%)	0	100	100
4	J	90/90 (100%)	90 (100%)	0	100	100
4	K	90/90 (100%)	90 (100%)	0	100	100
4	L	90/90 (100%)	90 (100%)	0	100	100
All	All	1950/2178 (90%)	1950 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	GLN
1	A	210	GLN
1	A	280	GLN
1	B	280	GLN
1	C	210	GLN
1	C	270	GLN
1	C	422	HIS
2	D	563	GLN
2	D	570	HIS

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Mol	Chain	Res	Type
2	E	513	ASN
2	E	563	GLN
2	E	570	HIS
2	E	596	GLN
2	F	570	HIS
3	G	39	GLN
3	G	84	ASN
3	H	3	GLN
3	H	39	GLN
4	J	41	GLN
4	J	93	GLN
4	K	33	ASN
4	K	41	GLN
4	L	33	ASN
4	L	56	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

69 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	M	1	5,1	14,14,15	0.80	0	17,19,21	1.04	2 (11%)
5	NAG	M	2	5	14,14,15	0.74	0	17,19,21	0.98	1 (5%)
5	BMA	M	3	5	11,11,12	0.84	0	15,15,17	2.14	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MAN	M	4	5	11,11,12	0.71	0	15,15,17	1.17	1 (6%)
5	MAN	M	5	5	11,11,12	0.71	0	15,15,17	1.04	1 (6%)
6	NAG	N	1	1,6	14,14,15	0.75	0	17,19,21	0.95	0
6	NAG	N	2	6	14,14,15	0.72	0	17,19,21	0.84	0
6	NAG	O	1	1,6	14,14,15	0.74	0	17,19,21	1.02	1 (5%)
6	NAG	O	2	6	14,14,15	0.72	0	17,19,21	0.84	0
6	NAG	P	1	1,6	14,14,15	0.76	0	17,19,21	1.04	0
6	NAG	P	2	6	14,14,15	0.71	0	17,19,21	1.17	1 (5%)
6	NAG	Q	1	1,6	14,14,15	0.75	0	17,19,21	2.46	4 (23%)
6	NAG	Q	2	6	14,14,15	0.79	0	17,19,21	2.36	3 (17%)
5	NAG	R	1	5,1	14,14,15	0.77	0	17,19,21	0.98	1 (5%)
5	NAG	R	2	5	14,14,15	0.76	0	17,19,21	1.03	1 (5%)
5	BMA	R	3	5	11,11,12	0.84	0	15,15,17	2.01	2 (13%)
5	MAN	R	4	5	11,11,12	0.75	0	15,15,17	1.08	1 (6%)
5	MAN	R	5	5	11,11,12	0.71	0	15,15,17	1.10	1 (6%)
6	NAG	S	1	1,6	14,14,15	0.70	0	17,19,21	0.86	0
6	NAG	S	2	6	14,14,15	0.70	0	17,19,21	0.91	1 (5%)
6	NAG	T	1	1,6	14,14,15	0.75	0	17,19,21	1.02	1 (5%)
6	NAG	T	2	6	14,14,15	0.73	0	17,19,21	0.85	0
6	NAG	U	1	1,6	14,14,15	0.75	0	17,19,21	0.99	0
6	NAG	U	2	6	14,14,15	0.69	0	17,19,21	1.15	1 (5%)
6	NAG	V	1	1,6	14,14,15	0.76	0	17,19,21	2.46	5 (29%)
6	NAG	V	2	6	14,14,15	0.78	0	17,19,21	2.35	3 (17%)
5	NAG	W	1	5,1	14,14,15	0.81	0	17,19,21	1.01	2 (11%)
5	NAG	W	2	5	14,14,15	0.71	0	17,19,21	1.05	1 (5%)
5	BMA	W	3	5	11,11,12	0.87	0	15,15,17	1.88	2 (13%)
5	MAN	W	4	5	11,11,12	0.75	0	15,15,17	1.18	1 (6%)
5	MAN	W	5	5	11,11,12	0.77	0	15,15,17	1.17	1 (6%)
6	NAG	X	1	1,6	14,14,15	0.71	0	17,19,21	0.79	0
6	NAG	X	2	6	14,14,15	0.69	0	17,19,21	0.77	0
6	NAG	Y	1	1,6	14,14,15	0.76	0	17,19,21	1.02	1 (5%)
6	NAG	Y	2	6	14,14,15	0.73	0	17,19,21	0.85	0
6	NAG	Z	1	1,6	14,14,15	0.76	0	17,19,21	1.07	0
6	NAG	Z	2	6	14,14,15	0.70	0	17,19,21	1.17	1 (5%)
6	NAG	a	1	1,6	14,14,15	0.75	0	17,19,21	2.46	4 (23%)
6	NAG	a	2	6	14,14,15	0.79	0	17,19,21	2.36	3 (17%)
7	NAG	b	1	7,2	14,14,15	0.75	0	17,19,21	1.04	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	b	2	7	14,14,15	0.72	0	17,19,21	0.94	0
7	BMA	b	3	7	11,11,12	0.84	0	15,15,17	2.06	3 (20%)
7	NAG	c	1	7,2	14,14,15	0.74	0	17,19,21	0.82	0
7	NAG	c	2	7	14,14,15	0.73	0	17,19,21	0.86	0
7	BMA	c	3	7	11,11,12	0.83	0	15,15,17	2.11	3 (20%)
8	NAG	d	1	8,2	14,14,15	0.78	0	17,19,21	1.17	1 (5%)
8	NAG	d	2	8	14,14,15	0.72	0	17,19,21	0.79	0
8	BMA	d	3	8	11,11,12	0.85	0	15,15,17	2.14	3 (20%)
8	FUC	d	4	8	10,10,11	0.80	0	14,14,16	0.92	0
7	NAG	e	1	7,2	14,14,15	0.74	0	17,19,21	1.10	2 (11%)
7	NAG	e	2	7	14,14,15	0.72	0	17,19,21	0.91	0
7	BMA	e	3	7	11,11,12	0.84	0	15,15,17	2.06	3 (20%)
7	NAG	f	1	7,2	14,14,15	0.77	0	17,19,21	0.85	0
7	NAG	f	2	7	14,14,15	0.73	0	17,19,21	0.91	0
7	BMA	f	3	7	11,11,12	0.82	0	15,15,17	2.09	3 (20%)
8	NAG	g	1	8,2	14,14,15	0.76	0	17,19,21	1.16	2 (11%)
8	NAG	g	2	8	14,14,15	0.72	0	17,19,21	0.79	0
8	BMA	g	3	8	11,11,12	0.84	0	15,15,17	2.14	3 (20%)
8	FUC	g	4	8	10,10,11	0.81	0	14,14,16	0.92	0
7	NAG	h	1	7,2	14,14,15	0.74	0	17,19,21	1.06	2 (11%)
7	NAG	h	2	7	14,14,15	0.72	0	17,19,21	0.89	0
7	BMA	h	3	7	11,11,12	0.84	0	15,15,17	2.08	3 (20%)
7	NAG	i	1	7,2	14,14,15	0.75	0	17,19,21	0.83	0
7	NAG	i	2	7	14,14,15	0.72	0	17,19,21	0.92	1 (5%)
7	BMA	i	3	7	11,11,12	0.84	0	15,15,17	2.09	3 (20%)
8	NAG	j	1	8,2	14,14,15	0.78	0	17,19,21	1.18	2 (11%)
8	NAG	j	2	8	14,14,15	0.73	0	17,19,21	0.78	0
8	BMA	j	3	8	11,11,12	0.86	0	15,15,17	2.14	3 (20%)
8	FUC	j	4	8	10,10,11	0.81	0	14,14,16	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	M	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	BMA	M	3	5	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	M	4	5	-	2/2/19/22	0/1/1/1
5	MAN	M	5	5	-	0/2/19/22	0/1/1/1
6	NAG	N	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	2/6/23/26	0/1/1/1
6	NAG	O	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	O	2	6	-	0/6/23/26	0/1/1/1
6	NAG	P	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	P	2	6	-	2/6/23/26	0/1/1/1
6	NAG	Q	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	4/6/23/26	0/1/1/1
5	NAG	R	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	R	2	5	-	3/6/23/26	0/1/1/1
5	BMA	R	3	5	-	2/2/19/22	0/1/1/1
5	MAN	R	4	5	-	2/2/19/22	0/1/1/1
5	MAN	R	5	5	-	2/2/19/22	0/1/1/1
6	NAG	S	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	S	2	6	-	0/6/23/26	0/1/1/1
6	NAG	T	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	0/6/23/26	0/1/1/1
6	NAG	U	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	U	2	6	-	2/6/23/26	0/1/1/1
6	NAG	V	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	V	2	6	-	4/6/23/26	0/1/1/1
5	NAG	W	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
5	BMA	W	3	5	-	1/2/19/22	0/1/1/1
5	MAN	W	4	5	-	0/2/19/22	0/1/1/1
5	MAN	W	5	5	-	2/2/19/22	0/1/1/1
6	NAG	X	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	X	2	6	-	1/6/23/26	0/1/1/1
6	NAG	Y	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	0/6/23/26	0/1/1/1
6	NAG	Z	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	2/6/23/26	0/1/1/1
6	NAG	a	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	a	2	6	-	4/6/23/26	0/1/1/1
7	NAG	b	1	7,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	b	2	7	-	2/6/23/26	0/1/1/1
7	BMA	b	3	7	-	0/2/19/22	0/1/1/1
7	NAG	c	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	c	2	7	-	0/6/23/26	0/1/1/1
7	BMA	c	3	7	-	1/2/19/22	0/1/1/1
8	NAG	d	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	d	2	8	-	0/6/23/26	0/1/1/1
8	BMA	d	3	8	-	1/2/19/22	0/1/1/1
8	FUC	d	4	8	-	-	0/1/1/1
7	NAG	e	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	e	2	7	-	2/6/23/26	0/1/1/1
7	BMA	e	3	7	-	1/2/19/22	0/1/1/1
7	NAG	f	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	f	2	7	-	0/6/23/26	0/1/1/1
7	BMA	f	3	7	-	1/2/19/22	0/1/1/1
8	NAG	g	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	g	2	8	-	0/6/23/26	0/1/1/1
8	BMA	g	3	8	-	1/2/19/22	0/1/1/1
8	FUC	g	4	8	-	-	0/1/1/1
7	NAG	h	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	h	2	7	-	2/6/23/26	0/1/1/1
7	BMA	h	3	7	-	1/2/19/22	0/1/1/1
7	NAG	i	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	i	2	7	-	0/6/23/26	0/1/1/1
7	BMA	i	3	7	-	1/2/19/22	0/1/1/1
8	NAG	j	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	j	2	8	-	0/6/23/26	0/1/1/1
8	BMA	j	3	8	-	1/2/19/22	0/1/1/1
8	FUC	j	4	8	-	-	0/1/1/1

There are no bond length outliers.

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	V	1	NAG	C2-N2-C7	8.68	134.53	122.90
6	Q	1	NAG	C2-N2-C7	8.65	134.50	122.90
6	a	1	NAG	C2-N2-C7	8.59	134.41	122.90
6	a	2	NAG	C2-N2-C7	8.31	134.03	122.90
6	Q	2	NAG	C2-N2-C7	8.28	133.99	122.90
6	V	2	NAG	C2-N2-C7	8.26	133.97	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	3	BMA	C1-O5-C5	6.73	121.21	112.19
8	j	3	BMA	C1-O5-C5	6.69	121.15	112.19
8	g	3	BMA	C1-O5-C5	6.68	121.14	112.19
8	d	3	BMA	C1-O5-C5	6.66	121.12	112.19
7	c	3	BMA	C1-O5-C5	6.55	120.97	112.19
7	i	3	BMA	C1-O5-C5	6.47	120.86	112.19
7	f	3	BMA	C1-O5-C5	6.43	120.80	112.19
7	h	3	BMA	C1-O5-C5	6.40	120.76	112.19
7	e	3	BMA	C1-O5-C5	6.29	120.62	112.19
7	b	3	BMA	C1-O5-C5	6.21	120.50	112.19
5	R	3	BMA	C1-O5-C5	6.15	120.43	112.19
5	W	3	BMA	C1-O5-C5	5.33	119.34	112.19
5	M	4	MAN	C1-O5-C5	3.47	116.83	112.19
5	W	4	MAN	C1-O5-C5	3.38	116.71	112.19
5	R	5	MAN	C1-O5-C5	3.25	116.55	112.19
5	W	5	MAN	C1-O5-C5	3.24	116.52	112.19
6	Z	2	NAG	C2-N2-C7	3.16	127.14	122.90
6	P	2	NAG	C2-N2-C7	3.16	127.14	122.90
6	U	2	NAG	C2-N2-C7	3.11	127.07	122.90
8	d	1	NAG	C2-N2-C7	2.98	126.89	122.90
6	a	1	NAG	C1-C2-N2	2.94	115.06	110.43
8	g	1	NAG	C2-N2-C7	2.92	126.81	122.90
8	j	1	NAG	C2-N2-C7	2.91	126.80	122.90
6	Q	1	NAG	C1-C2-N2	2.87	114.96	110.43
5	R	4	MAN	C1-O5-C5	2.87	116.03	112.19
5	M	5	MAN	C1-O5-C5	2.80	115.94	112.19
6	V	1	NAG	C1-C2-N2	2.70	114.69	110.43
6	V	2	NAG	C8-C7-N2	2.60	120.42	116.12
6	Q	2	NAG	C8-C7-N2	2.59	120.42	116.12
6	a	2	NAG	C8-C7-N2	2.56	120.37	116.12
5	R	1	NAG	C2-N2-C7	2.51	126.26	122.90
6	V	1	NAG	C8-C7-N2	2.49	120.25	116.12
6	Q	2	NAG	C1-C2-N2	2.49	114.36	110.43
6	V	2	NAG	C1-C2-N2	2.48	114.34	110.43
6	a	1	NAG	O5-C1-C2	-2.48	107.45	111.29
6	Q	1	NAG	C8-C7-N2	2.48	120.23	116.12
6	a	1	NAG	C8-C7-N2	2.47	120.21	116.12
5	M	1	NAG	C1-O5-C5	2.45	115.46	112.19
6	a	2	NAG	C1-C2-N2	2.45	114.29	110.43
6	S	2	NAG	O5-C1-C2	-2.35	107.66	111.29
6	V	1	NAG	O5-C1-C2	-2.33	107.68	111.29
7	b	3	BMA	C3-C4-C5	2.33	114.46	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	1	NAG	O5-C1-C2	-2.33	107.69	111.29
7	h	1	NAG	C2-N2-C7	2.32	126.01	122.90
7	e	1	NAG	C2-N2-C7	2.31	125.99	122.90
5	W	3	BMA	C3-C4-C5	2.30	114.39	110.23
7	c	3	BMA	C2-C3-C4	2.29	114.89	110.86
7	h	3	BMA	C3-C4-C5	2.28	114.37	110.23
5	R	2	NAG	C2-N2-C7	2.25	125.92	122.90
7	b	1	NAG	C2-N2-C7	2.24	125.91	122.90
8	d	3	BMA	C3-C4-C5	2.24	114.30	110.23
8	d	3	BMA	C2-C3-C4	2.24	114.80	110.86
5	M	3	BMA	C2-C3-C4	2.23	114.79	110.86
8	g	3	BMA	C2-C3-C4	2.23	114.78	110.86
7	b	3	BMA	C2-C3-C4	2.22	114.77	110.86
8	j	3	BMA	C2-C3-C4	2.22	114.77	110.86
7	e	3	BMA	C3-C4-C5	2.21	114.24	110.23
8	g	3	BMA	C3-C4-C5	2.21	114.23	110.23
8	j	3	BMA	C3-C4-C5	2.18	114.19	110.23
7	f	3	BMA	C2-C3-C4	2.18	114.70	110.86
7	i	3	BMA	C2-C3-C4	2.17	114.68	110.86
6	Y	1	NAG	C2-N2-C7	2.17	125.81	122.90
7	e	1	NAG	O4-C4-C3	-2.17	105.27	110.38
6	O	1	NAG	C2-N2-C7	2.15	125.78	122.90
6	T	1	NAG	C2-N2-C7	2.15	125.78	122.90
5	W	1	NAG	C1-O5-C5	2.14	115.05	112.19
7	f	3	BMA	C3-C4-C5	2.13	114.10	110.23
5	M	3	BMA	C3-C4-C5	2.13	114.08	110.23
5	R	3	BMA	C2-C3-C4	2.12	114.60	110.86
7	e	3	BMA	C2-C3-C4	2.12	114.59	110.86
7	h	3	BMA	C2-C3-C4	2.12	114.59	110.86
7	i	3	BMA	C3-C4-C5	2.11	114.06	110.23
7	h	1	NAG	O4-C4-C3	-2.09	105.45	110.38
5	W	2	NAG	C1-O5-C5	2.08	114.98	112.19
5	M	2	NAG	C1-O5-C5	2.08	114.97	112.19
5	W	1	NAG	O5-C1-C2	-2.08	108.08	111.29
7	i	2	NAG	O5-C1-C2	-2.07	108.09	111.29
8	j	1	NAG	O4-C4-C3	-2.05	105.55	110.38
7	b	1	NAG	O4-C4-C3	-2.04	105.57	110.38
7	c	3	BMA	C3-C4-C5	2.04	113.92	110.23
5	M	1	NAG	O5-C1-C2	-2.02	108.16	111.29
8	g	1	NAG	O4-C4-C3	-2.01	105.64	110.38
6	V	1	NAG	O7-C7-C8	-2.00	118.49	122.05

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	R	5	MAN	C4-C5-C6-O6
5	W	5	MAN	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	M	4	MAN	O5-C5-C6-O6
5	R	3	BMA	O5-C5-C6-O6
5	W	1	NAG	O5-C5-C6-O6
5	M	4	MAN	C4-C5-C6-O6
5	R	5	MAN	O5-C5-C6-O6
5	M	2	NAG	C8-C7-N2-C2
5	M	2	NAG	O7-C7-N2-C2
5	R	1	NAG	C8-C7-N2-C2
5	R	1	NAG	O7-C7-N2-C2
5	R	2	NAG	C8-C7-N2-C2
5	R	2	NAG	O7-C7-N2-C2
5	W	2	NAG	C8-C7-N2-C2
5	W	2	NAG	O7-C7-N2-C2
6	N	1	NAG	C8-C7-N2-C2
6	N	1	NAG	O7-C7-N2-C2
6	N	2	NAG	C8-C7-N2-C2
6	N	2	NAG	O7-C7-N2-C2
6	O	1	NAG	C8-C7-N2-C2
6	O	1	NAG	O7-C7-N2-C2
6	Q	1	NAG	C8-C7-N2-C2
6	Q	1	NAG	O7-C7-N2-C2
6	Q	2	NAG	C8-C7-N2-C2
6	Q	2	NAG	O7-C7-N2-C2
6	T	1	NAG	C8-C7-N2-C2
6	T	1	NAG	O7-C7-N2-C2
6	V	1	NAG	C8-C7-N2-C2
6	V	1	NAG	O7-C7-N2-C2
6	V	2	NAG	C8-C7-N2-C2
6	V	2	NAG	O7-C7-N2-C2
6	Y	1	NAG	C8-C7-N2-C2
6	Y	1	NAG	O7-C7-N2-C2
6	a	1	NAG	C8-C7-N2-C2
6	a	1	NAG	O7-C7-N2-C2
6	a	2	NAG	C8-C7-N2-C2
6	a	2	NAG	O7-C7-N2-C2
7	b	2	NAG	C8-C7-N2-C2
7	b	2	NAG	O7-C7-N2-C2
7	c	1	NAG	C8-C7-N2-C2
7	c	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
7	e	2	NAG	C8-C7-N2-C2
7	e	2	NAG	O7-C7-N2-C2
7	f	1	NAG	C8-C7-N2-C2
7	f	1	NAG	O7-C7-N2-C2
7	h	2	NAG	C8-C7-N2-C2
7	h	2	NAG	O7-C7-N2-C2
7	i	1	NAG	C8-C7-N2-C2
7	i	1	NAG	O7-C7-N2-C2
8	d	1	NAG	C8-C7-N2-C2
8	d	1	NAG	O7-C7-N2-C2
8	g	1	NAG	C8-C7-N2-C2
8	g	1	NAG	O7-C7-N2-C2
8	j	1	NAG	C8-C7-N2-C2
8	j	1	NAG	O7-C7-N2-C2
5	W	5	MAN	C4-C5-C6-O6
5	W	3	BMA	O5-C5-C6-O6
5	M	3	BMA	O5-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
7	h	3	BMA	O5-C5-C6-O6
7	c	3	BMA	O5-C5-C6-O6
7	i	3	BMA	O5-C5-C6-O6
7	f	3	BMA	O5-C5-C6-O6
5	W	1	NAG	C4-C5-C6-O6
5	R	4	MAN	C4-C5-C6-O6
5	R	3	BMA	C4-C5-C6-O6
6	X	2	NAG	O5-C5-C6-O6
7	e	3	BMA	O5-C5-C6-O6
6	Q	1	NAG	C1-C2-N2-C7
5	R	4	MAN	O5-C5-C6-O6
8	g	3	BMA	O5-C5-C6-O6
6	P	2	NAG	C3-C2-N2-C7
6	Q	1	NAG	C3-C2-N2-C7
6	U	2	NAG	C3-C2-N2-C7
6	Z	2	NAG	C3-C2-N2-C7
6	a	1	NAG	C3-C2-N2-C7
8	j	3	BMA	O5-C5-C6-O6
8	d	3	BMA	O5-C5-C6-O6
6	P	2	NAG	C1-C2-N2-C7
6	Q	2	NAG	C1-C2-N2-C7
6	U	2	NAG	C1-C2-N2-C7
6	V	1	NAG	C1-C2-N2-C7
6	V	2	NAG	C1-C2-N2-C7

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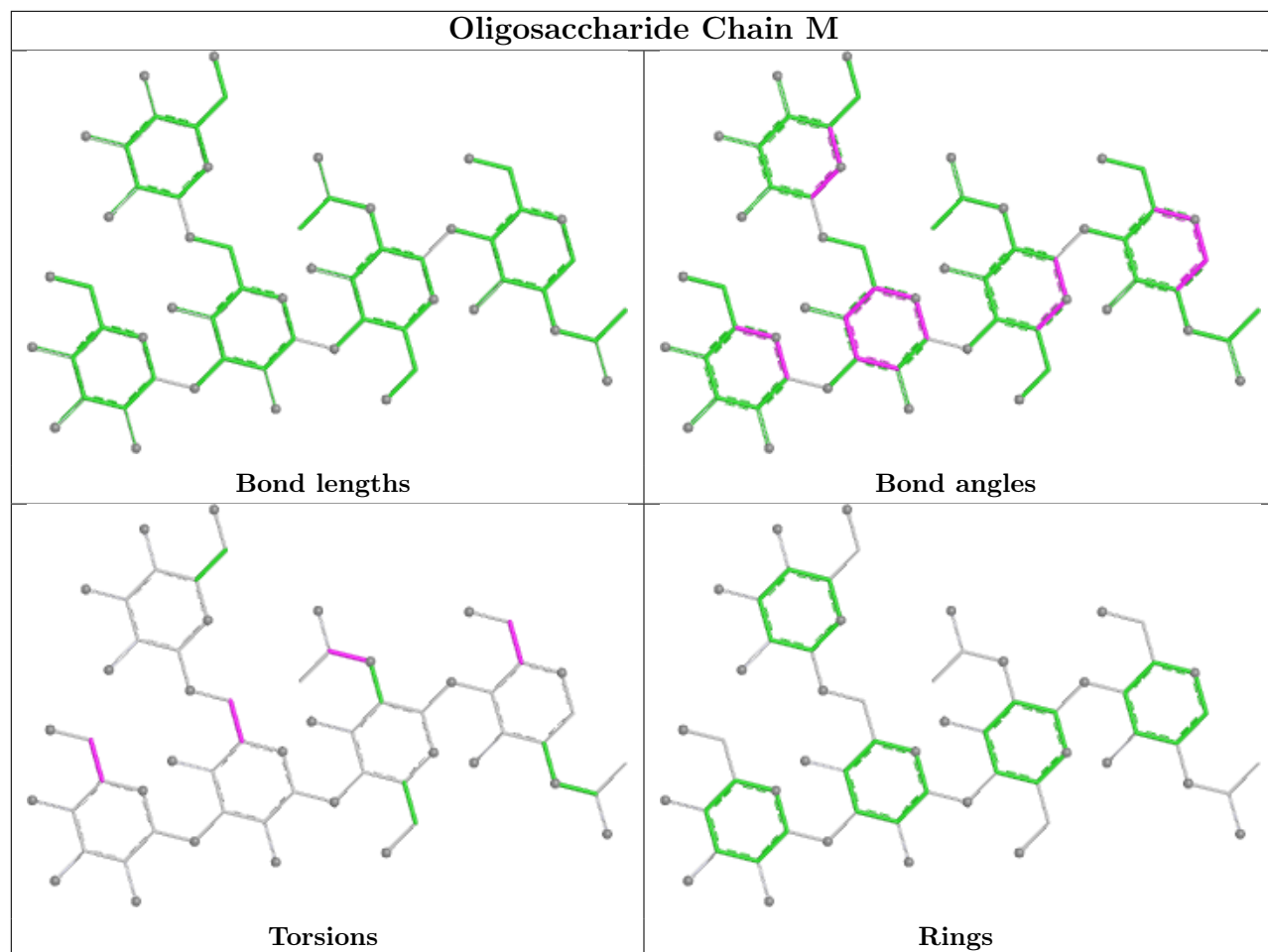
Mol	Chain	Res	Type	Atoms
6	Z	2	NAG	C1-C2-N2-C7
6	a	1	NAG	C1-C2-N2-C7
6	a	2	NAG	C1-C2-N2-C7
6	Q	2	NAG	C3-C2-N2-C7
6	V	1	NAG	C3-C2-N2-C7
6	V	2	NAG	C3-C2-N2-C7
6	a	2	NAG	C3-C2-N2-C7
5	R	2	NAG	C4-C5-C6-O6

There are no ring outliers.

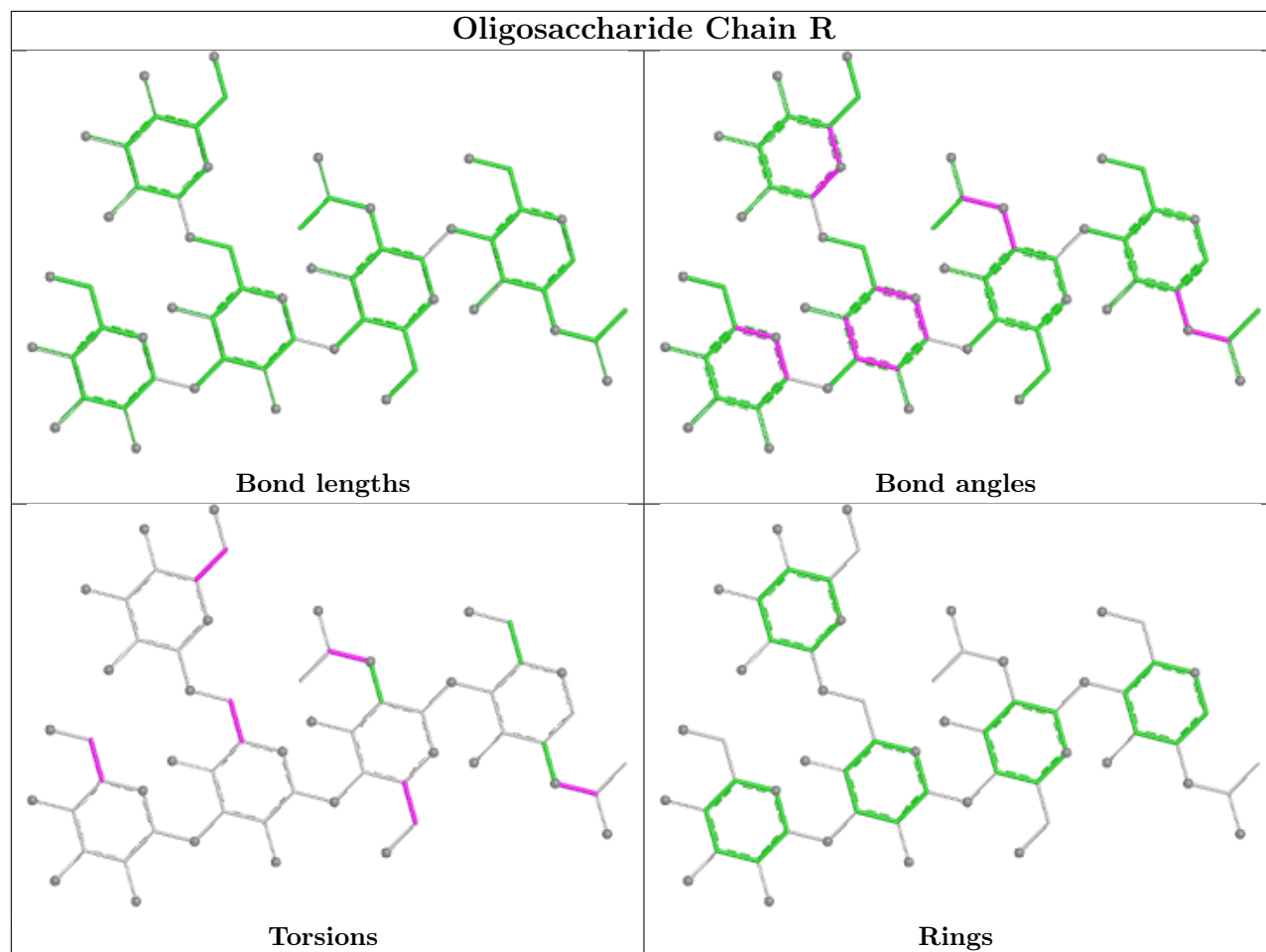
4 monomers are involved in 4 short contacts:

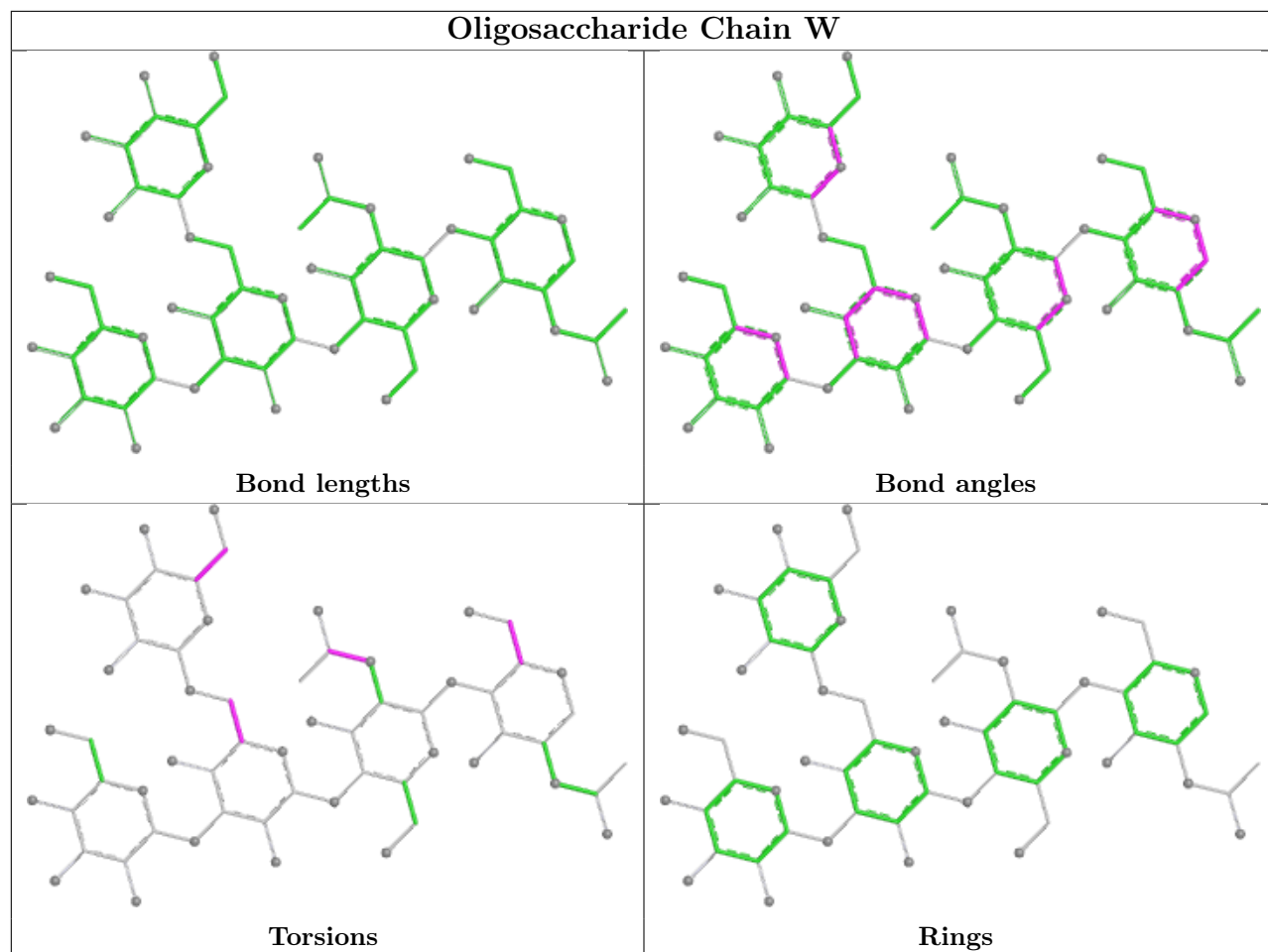
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	f	1	NAG	1	0
6	O	1	NAG	1	0
7	c	1	NAG	1	0
7	i	1	NAG	1	0

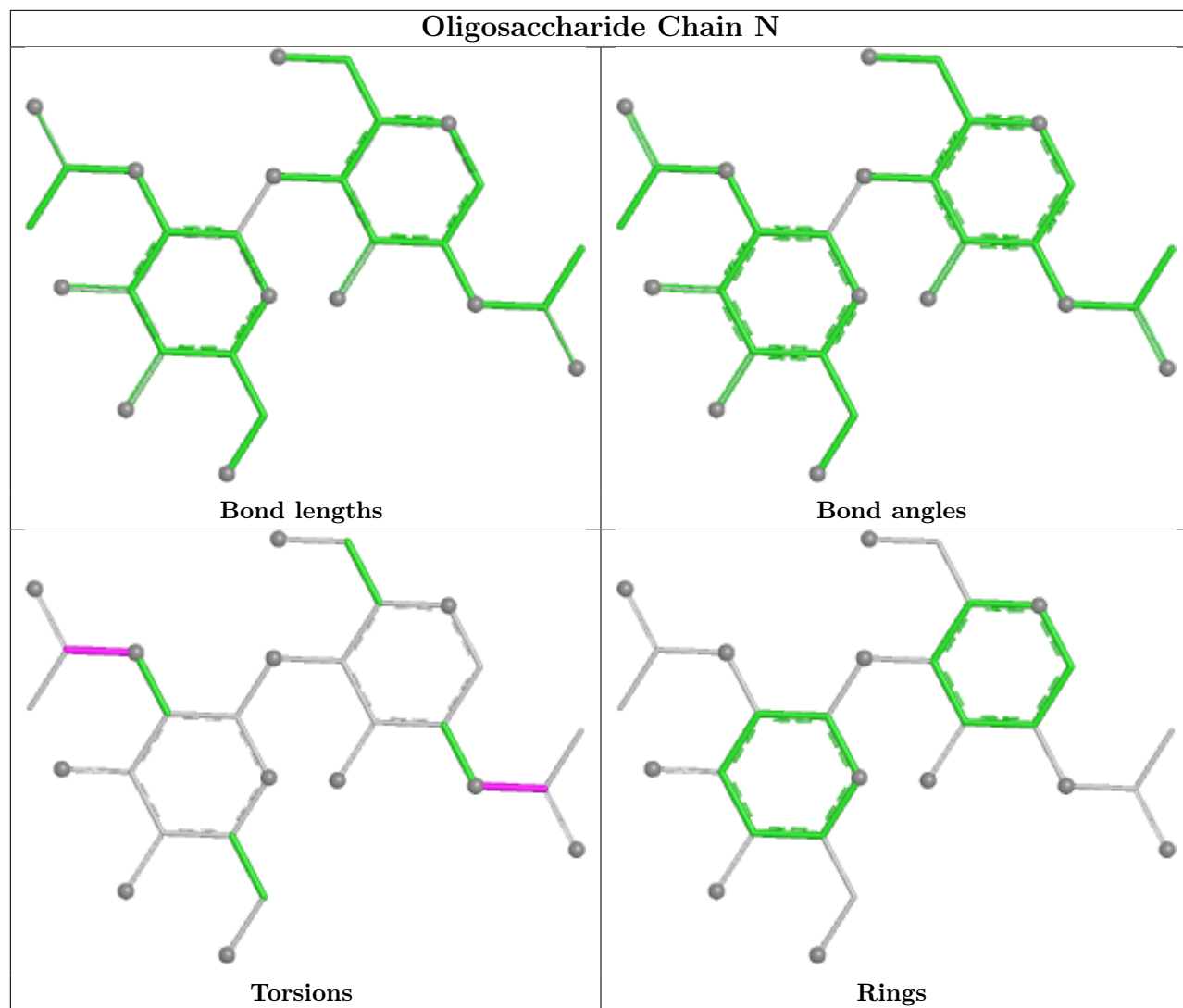
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

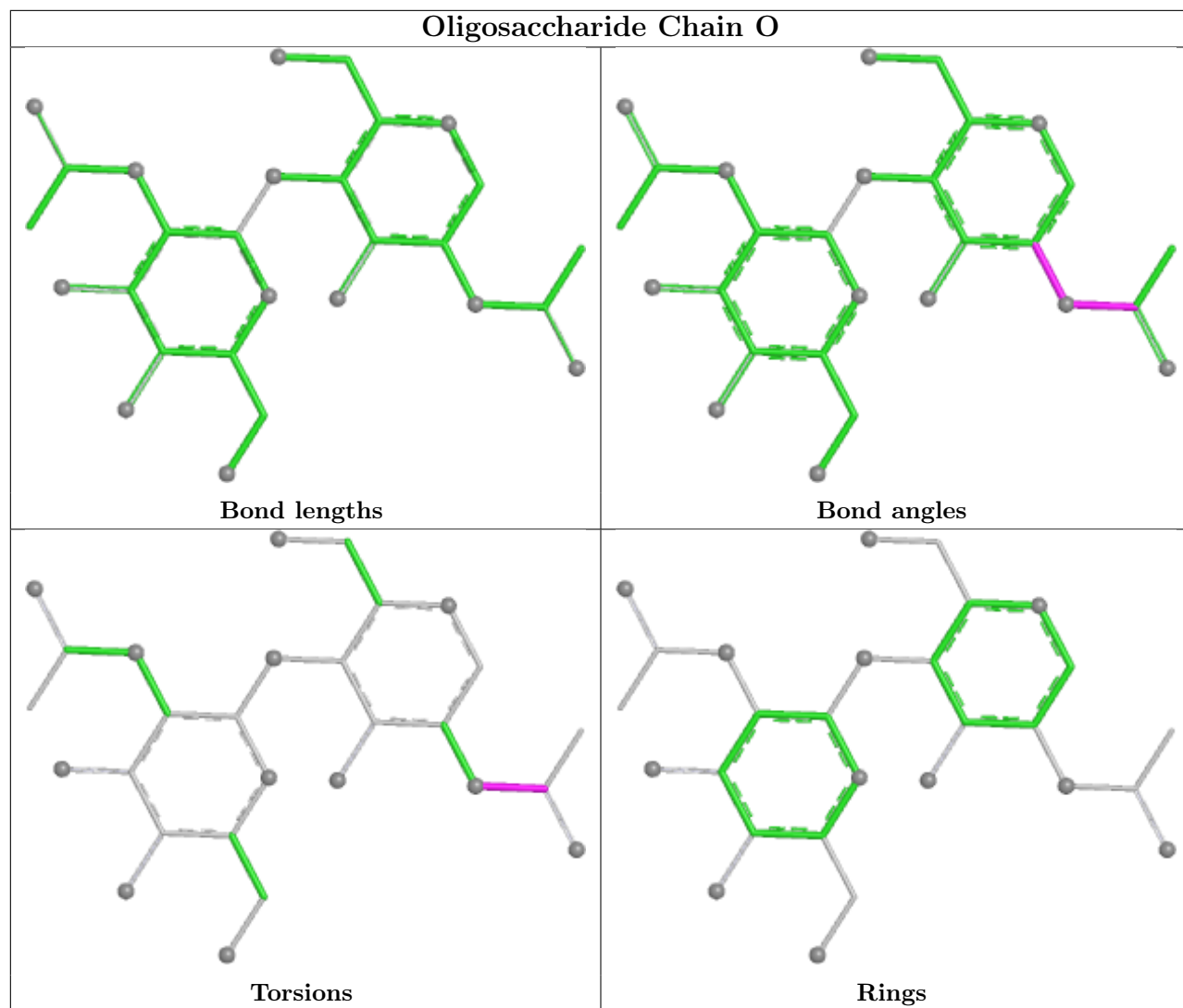


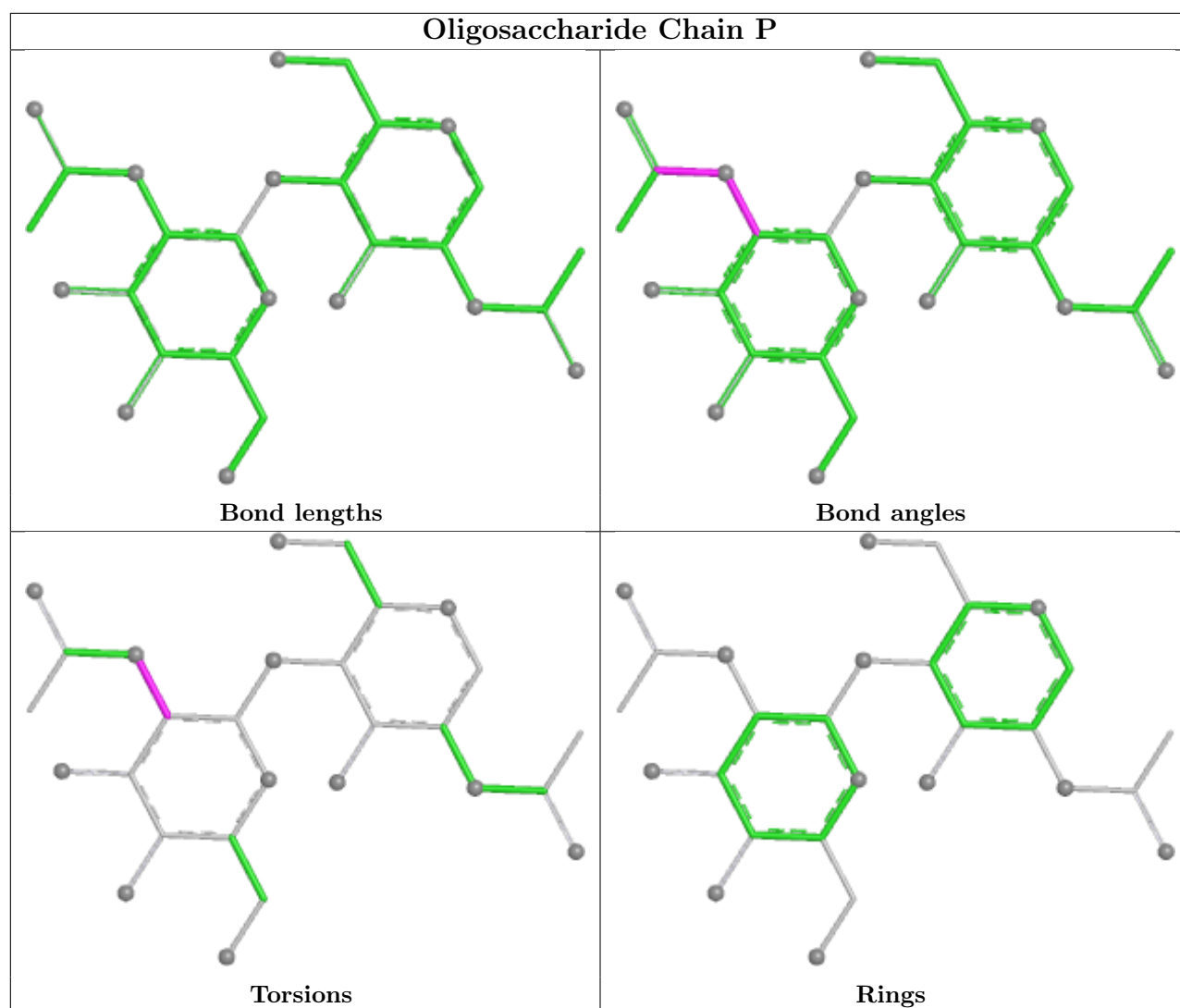


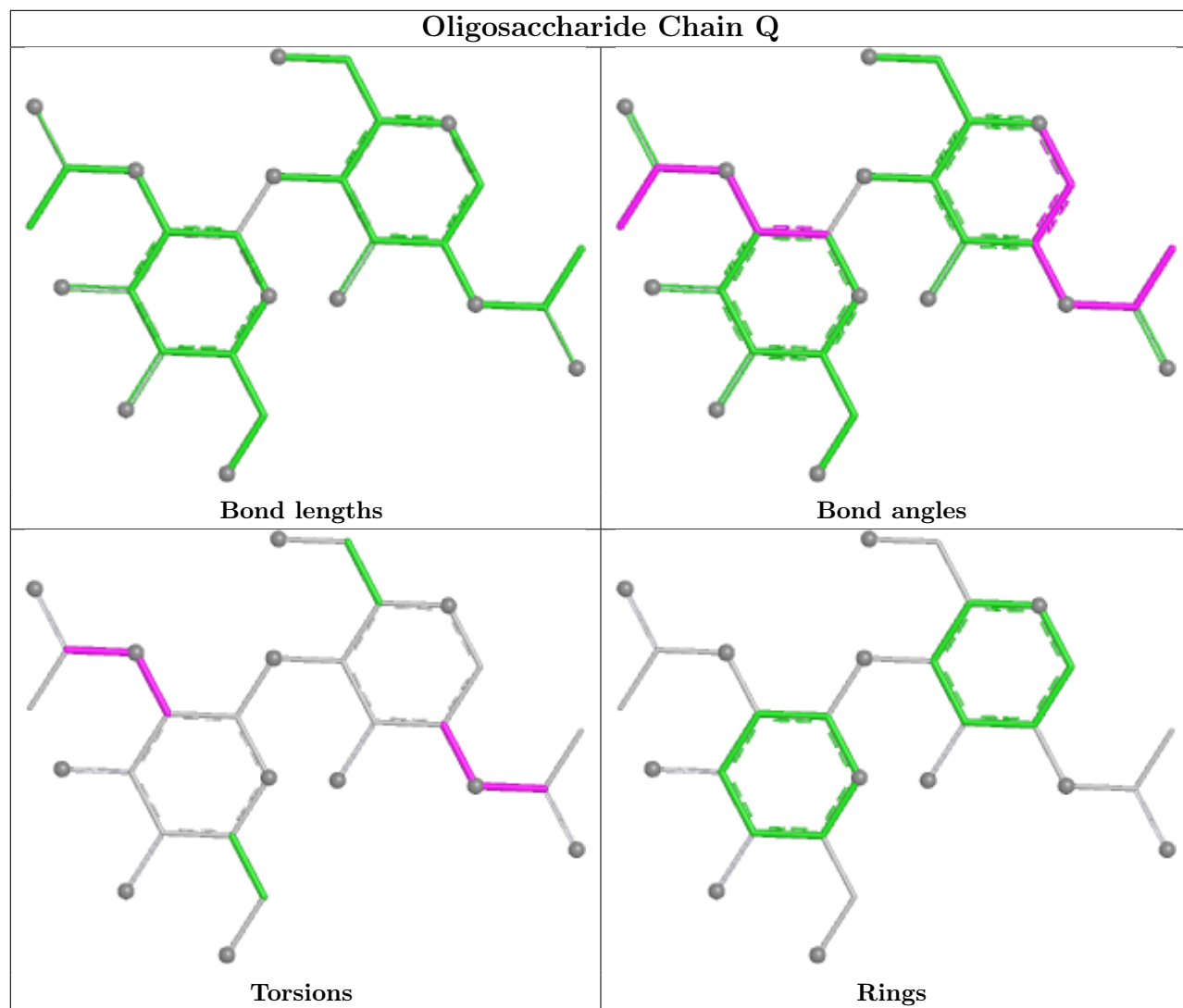


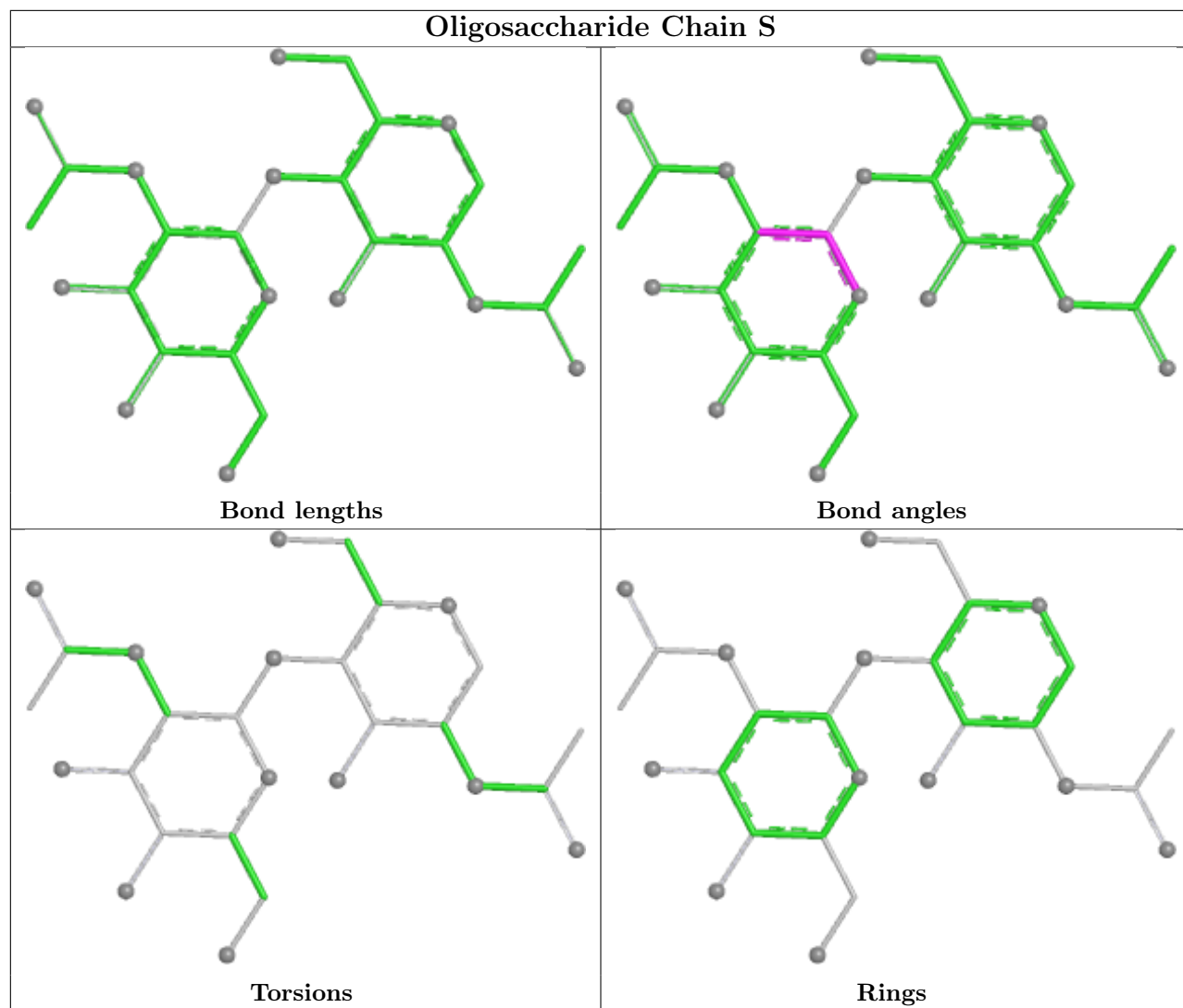


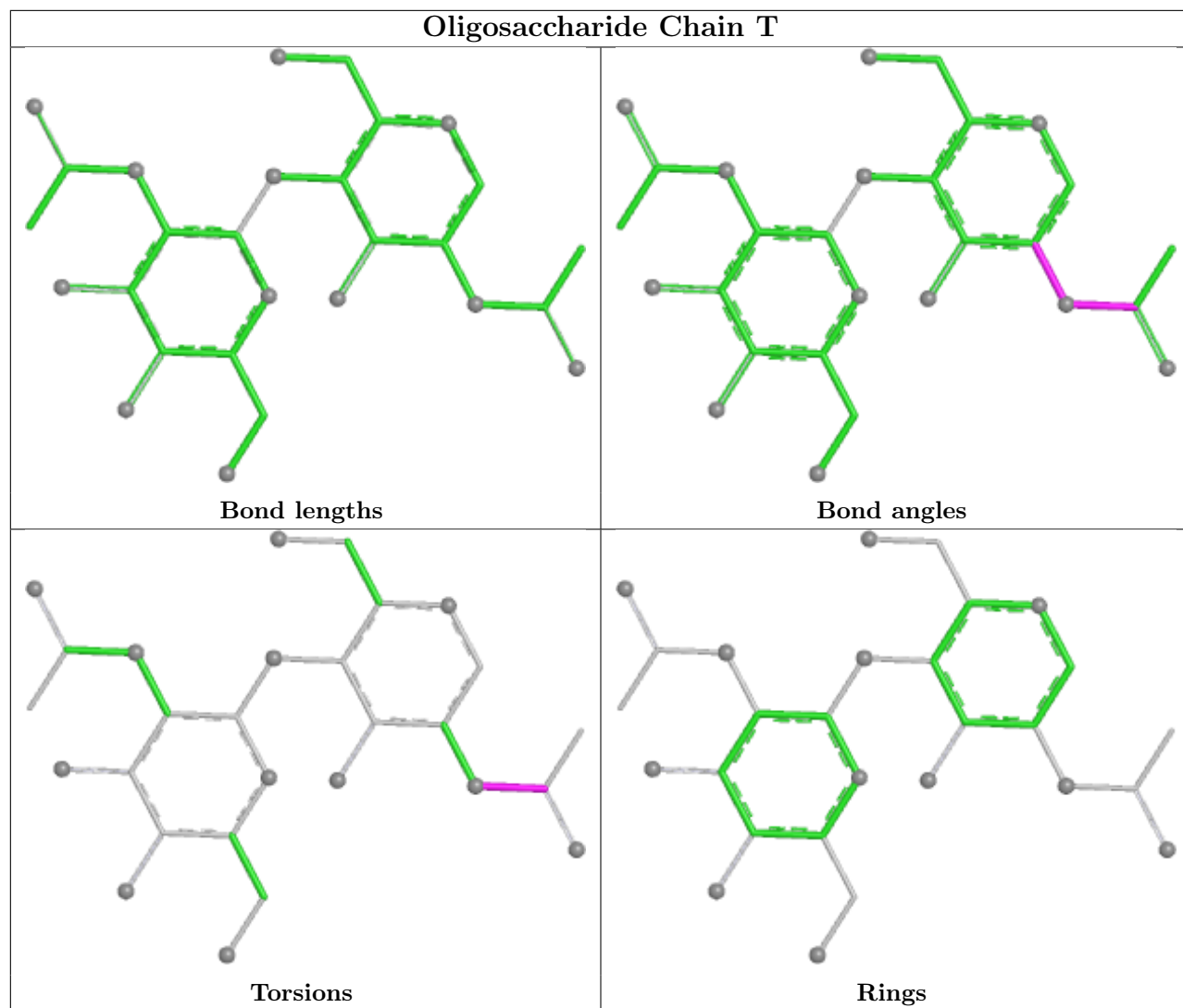




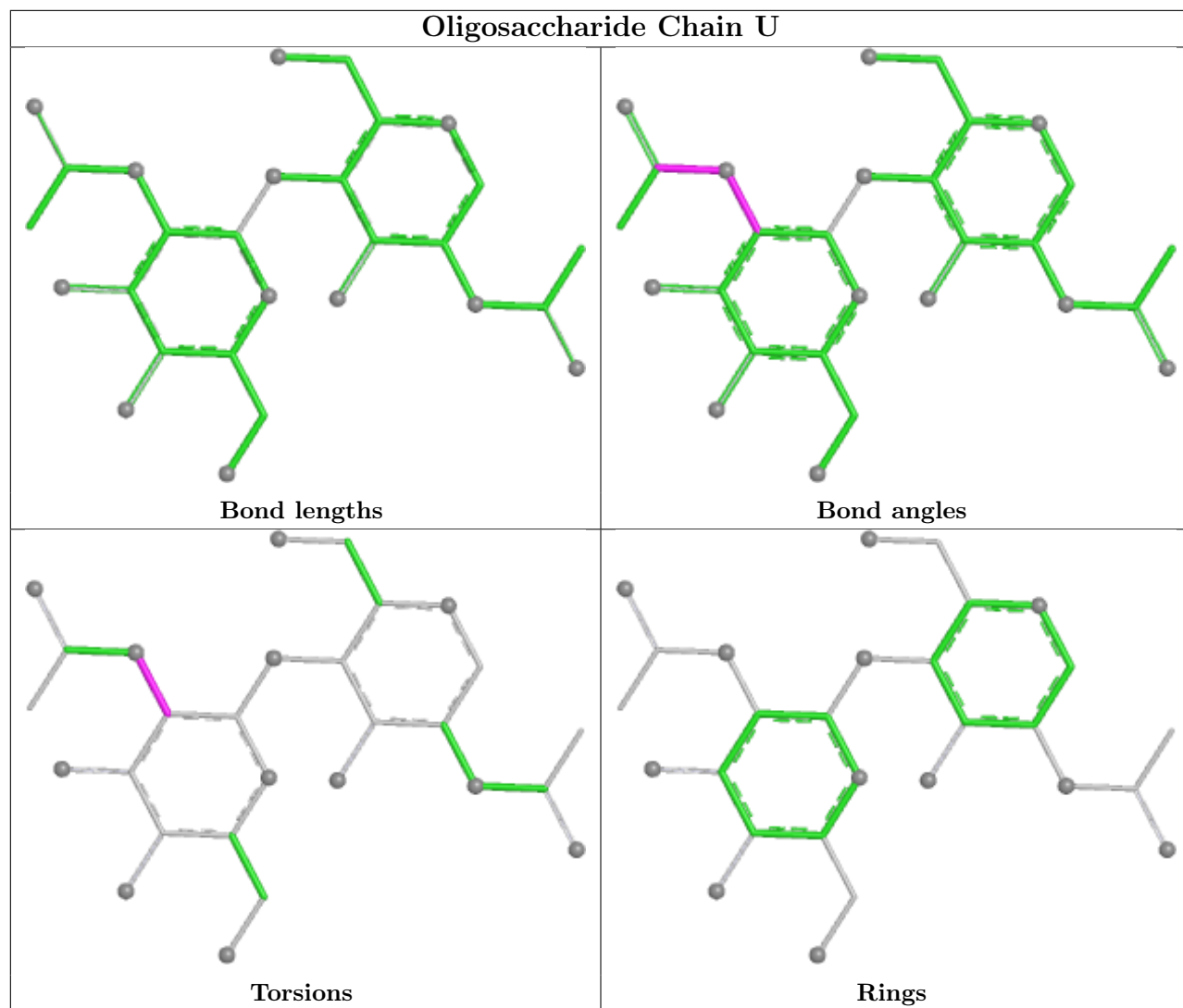


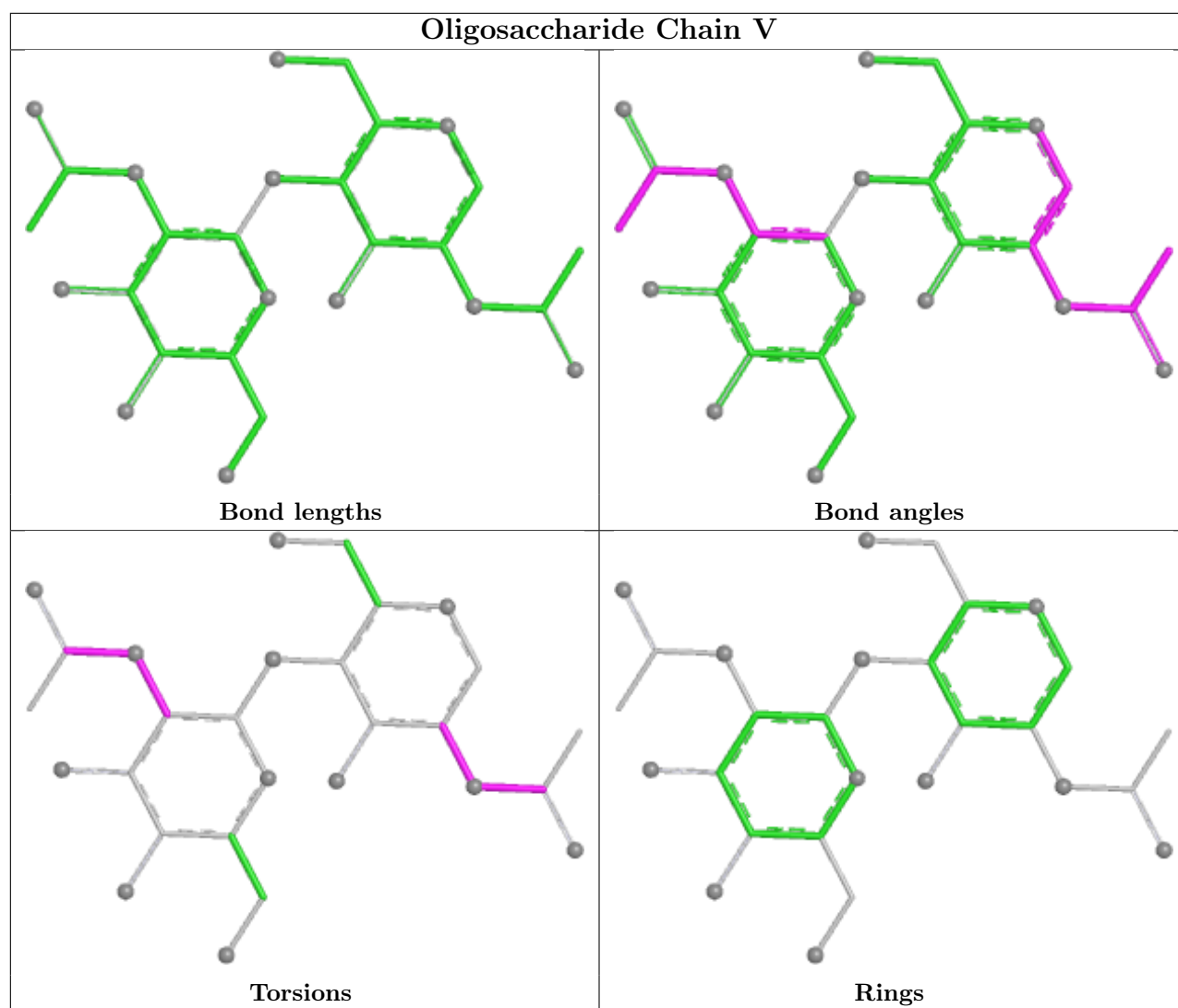


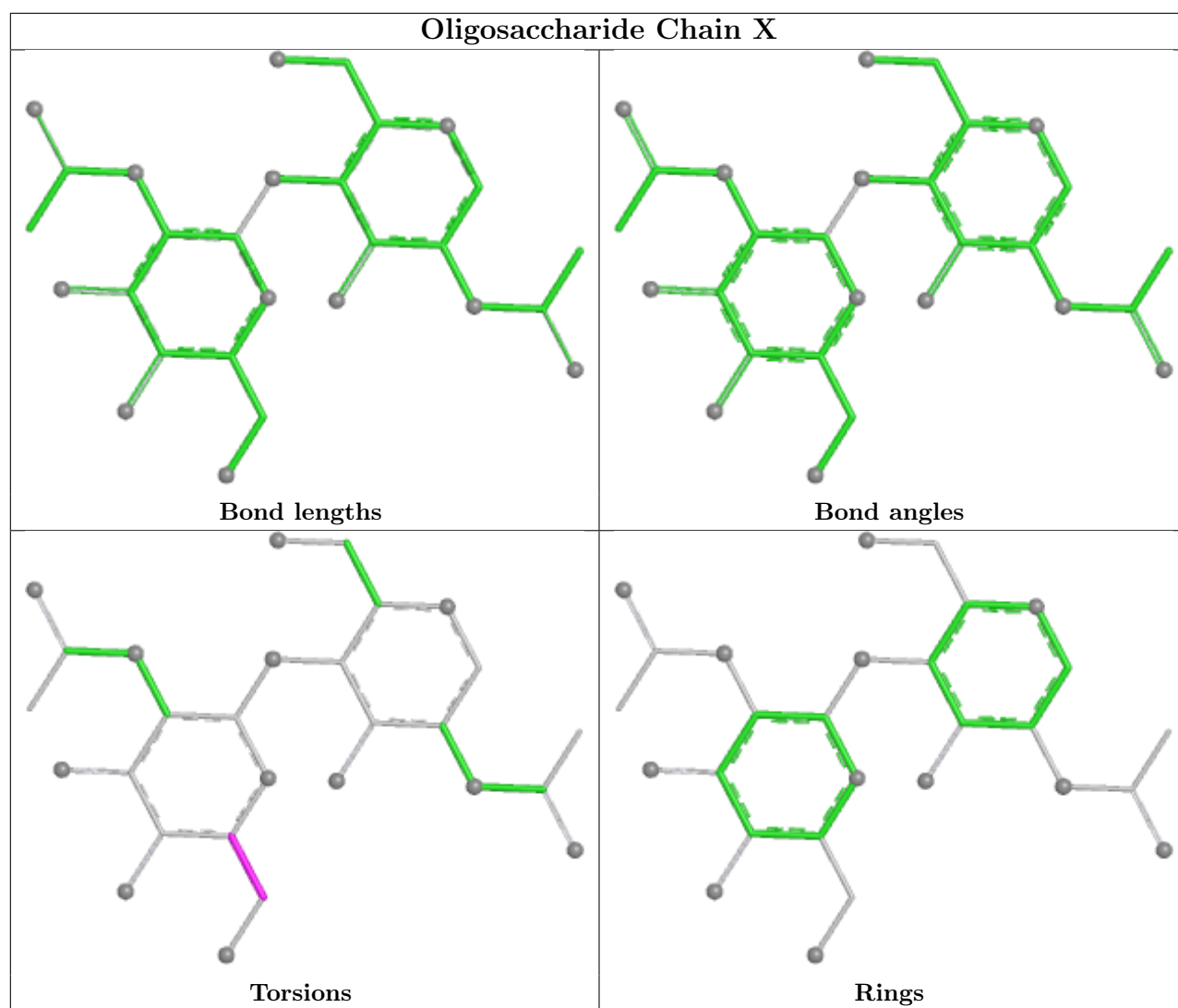


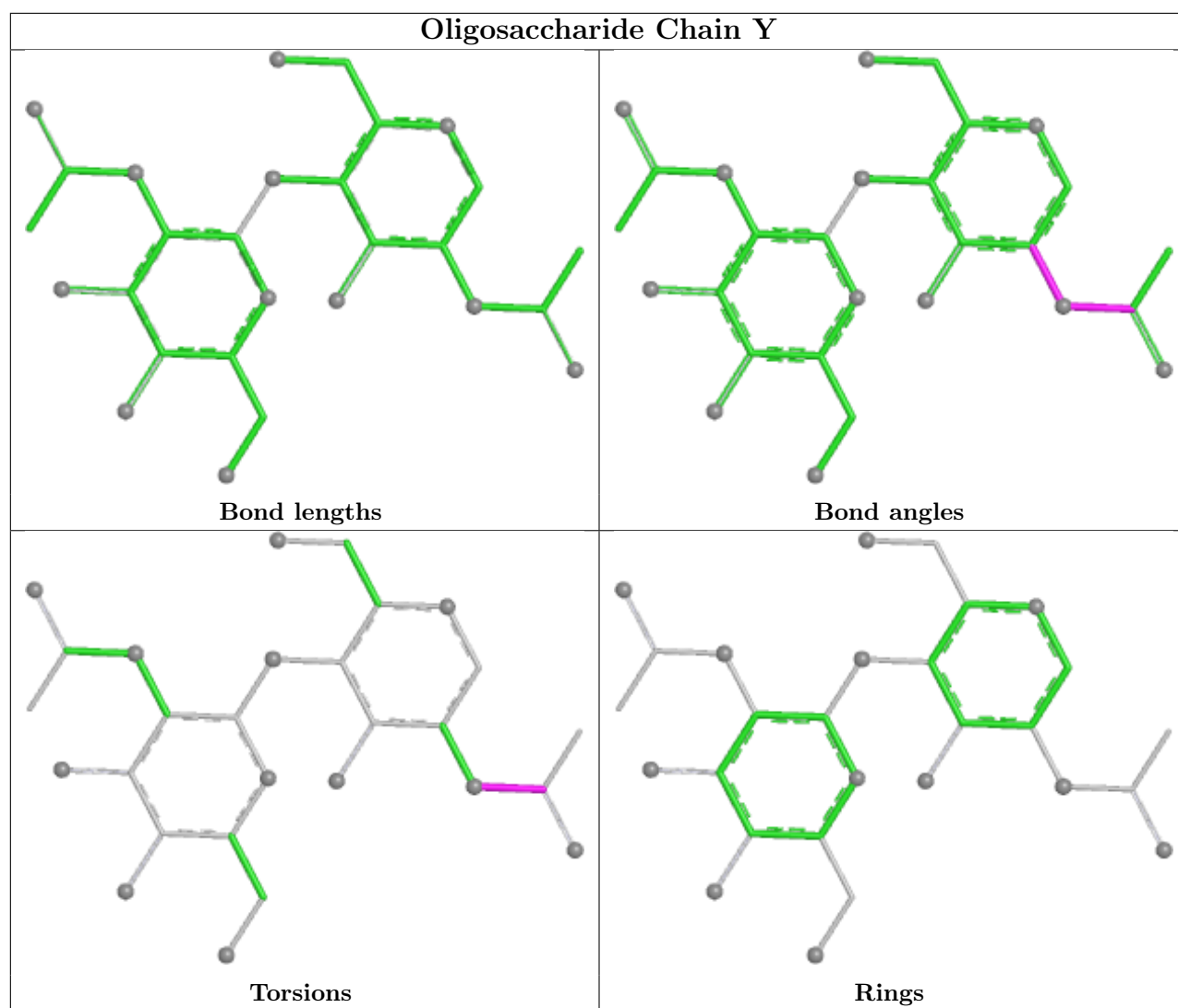


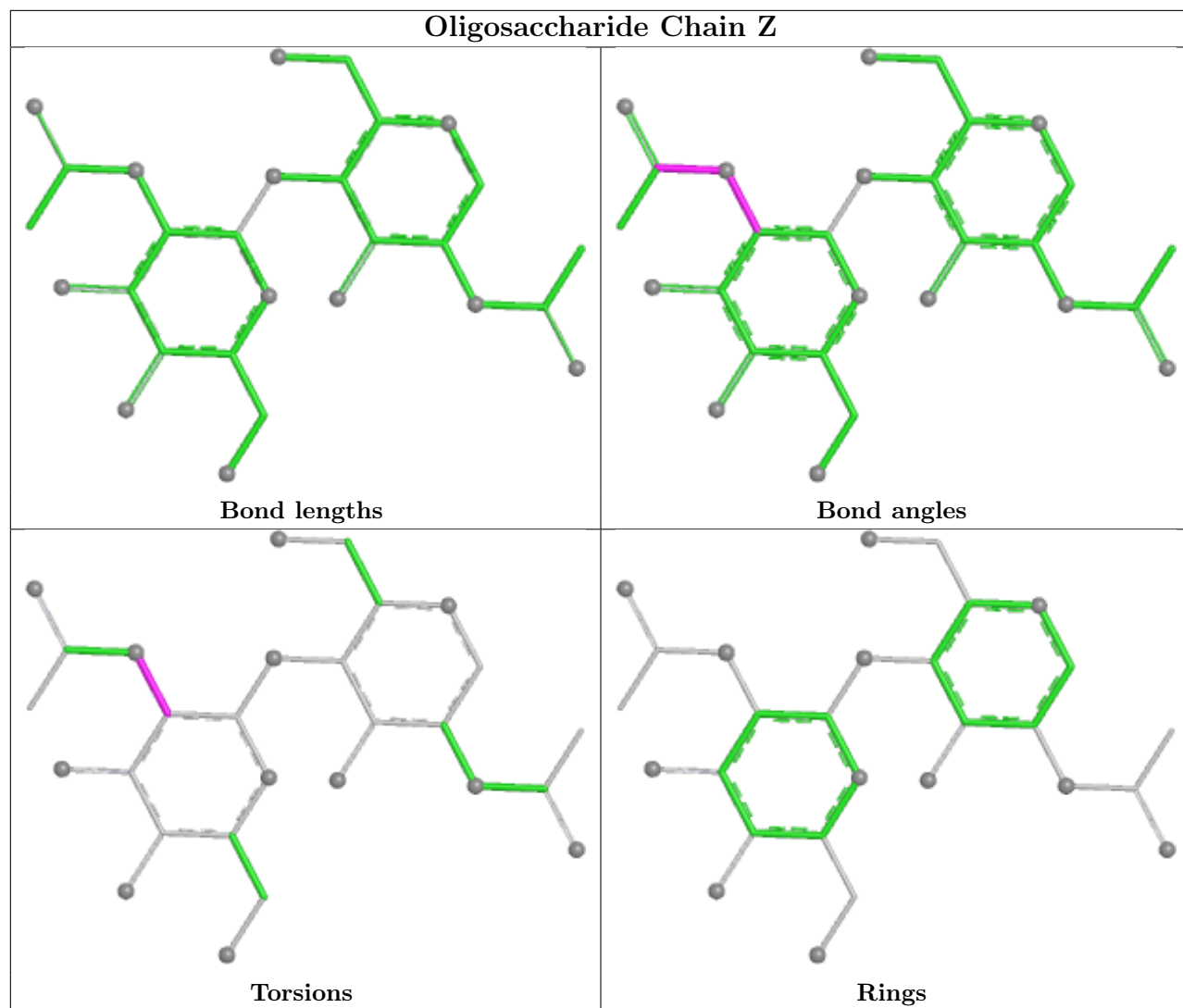


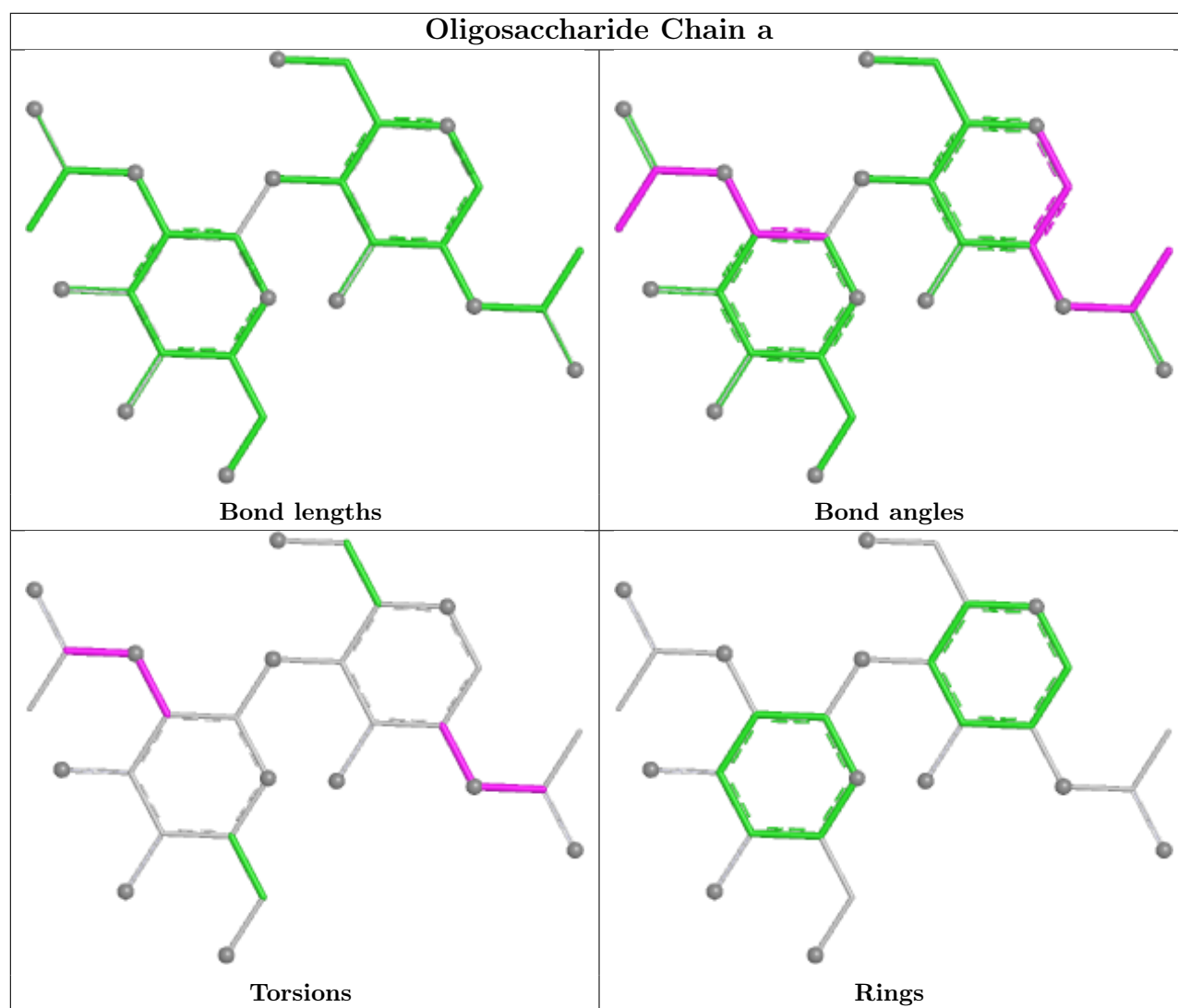


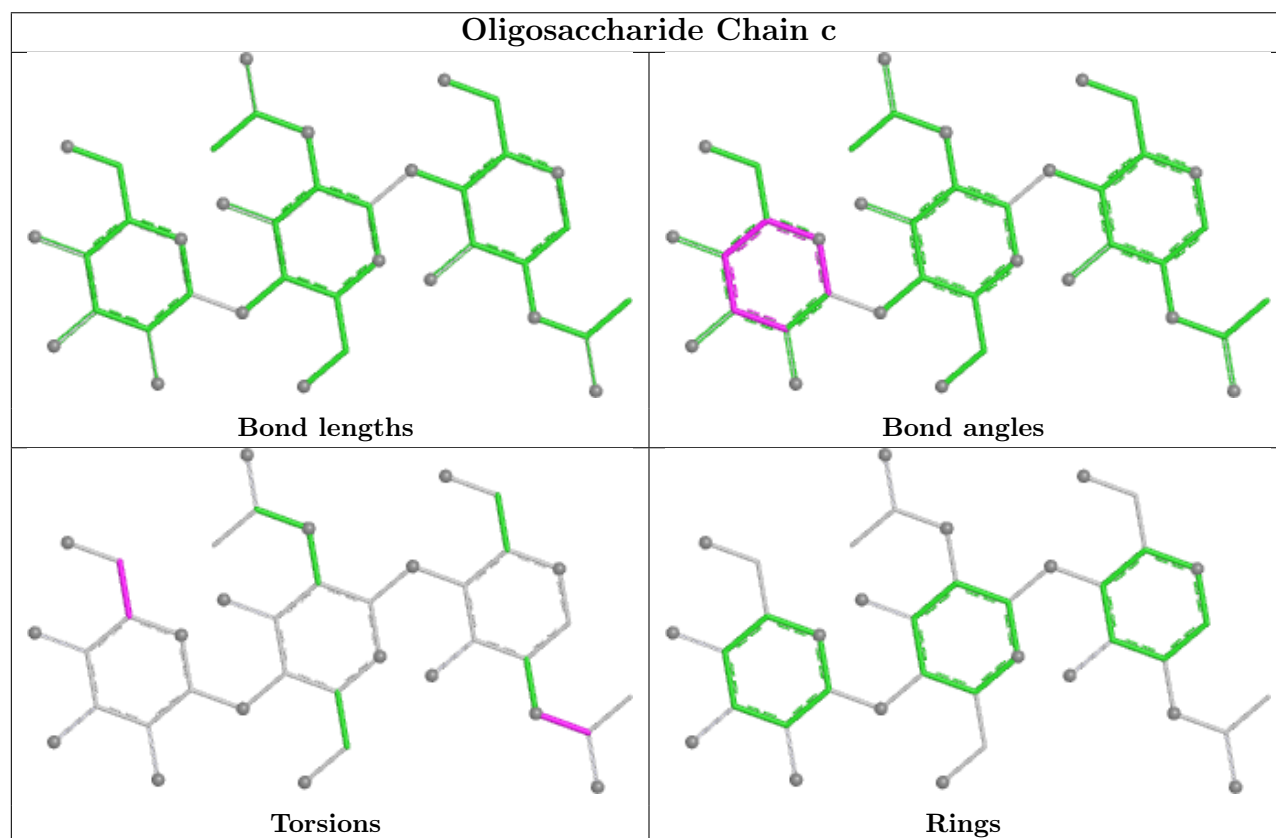
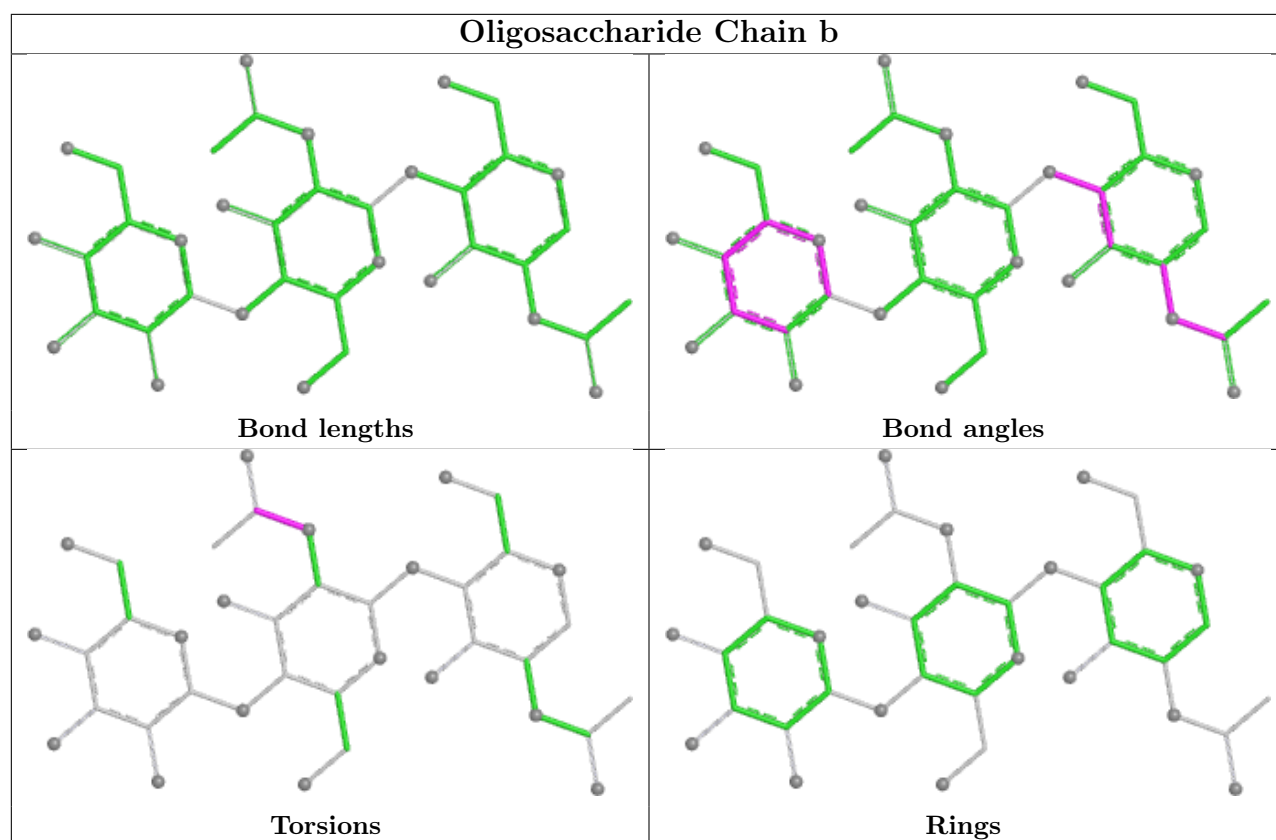


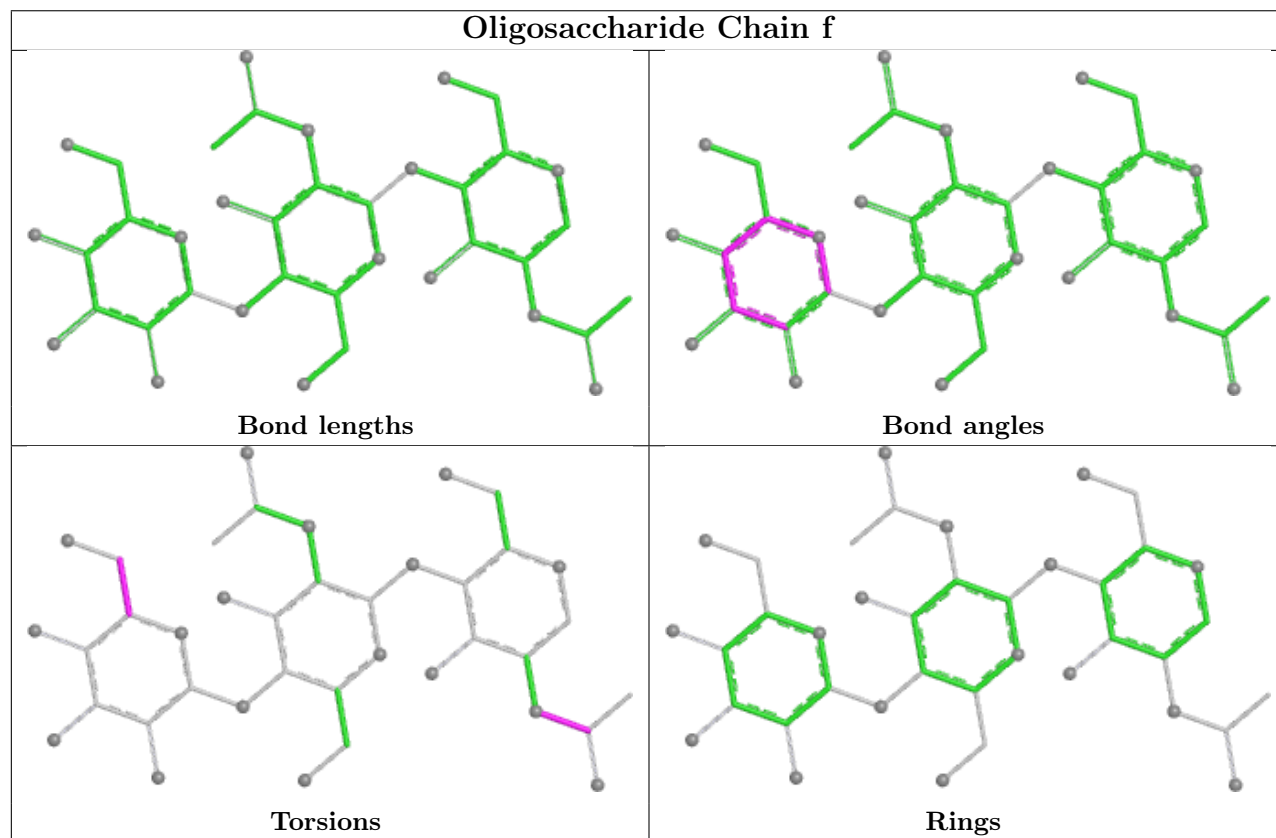
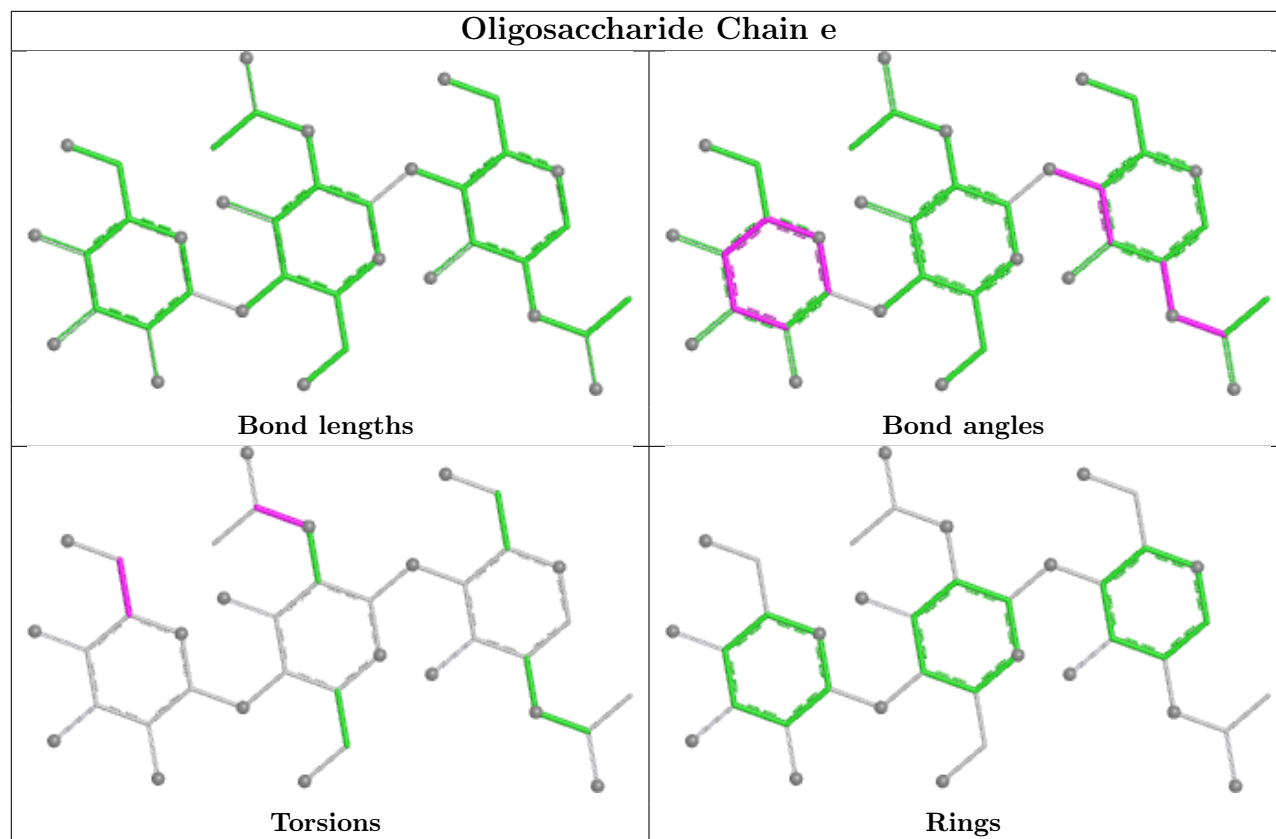




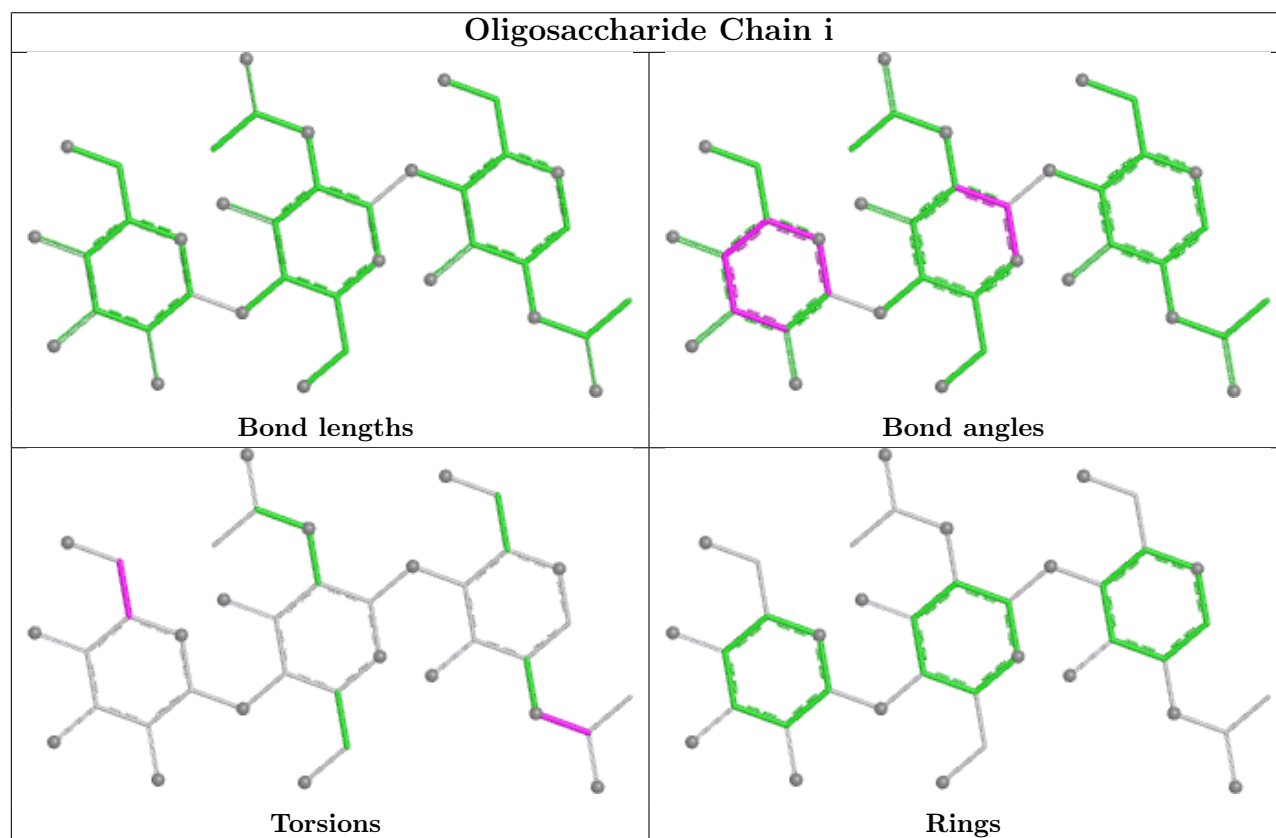
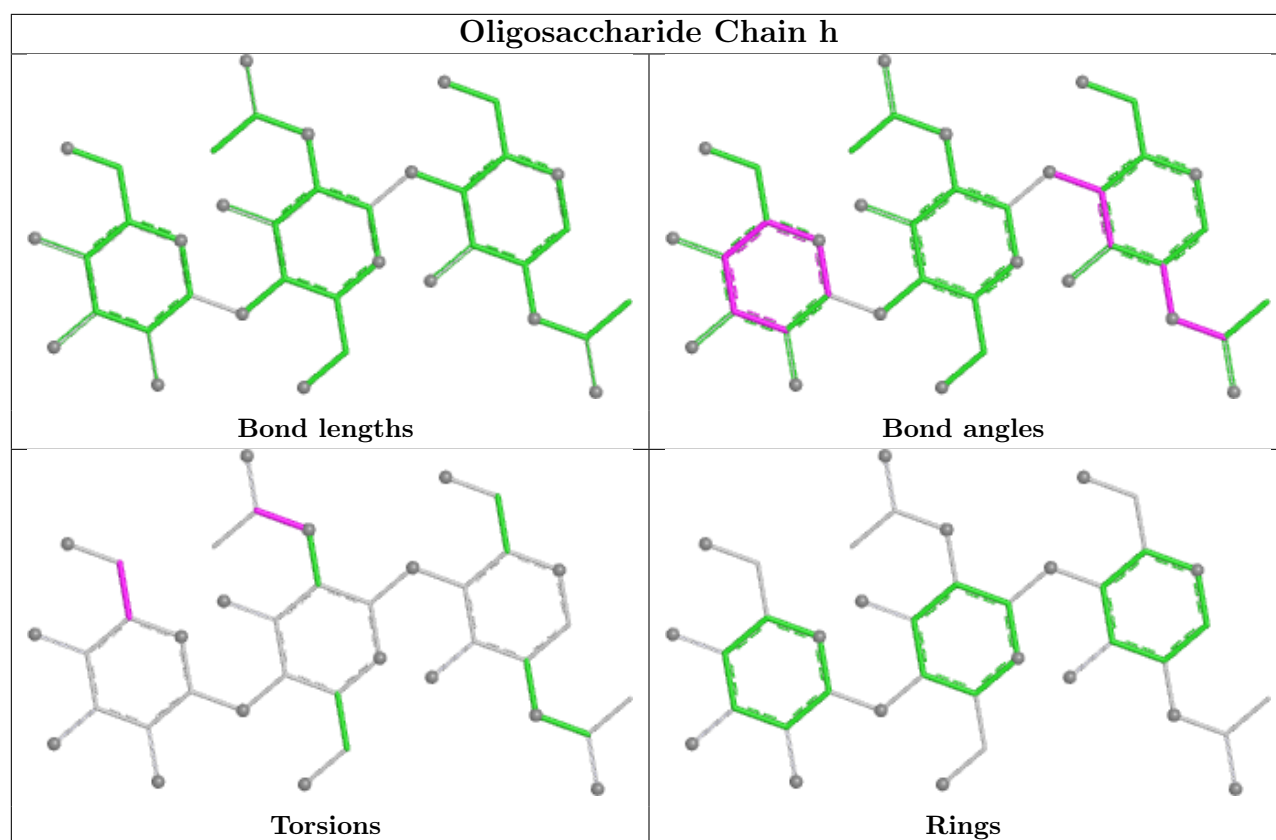


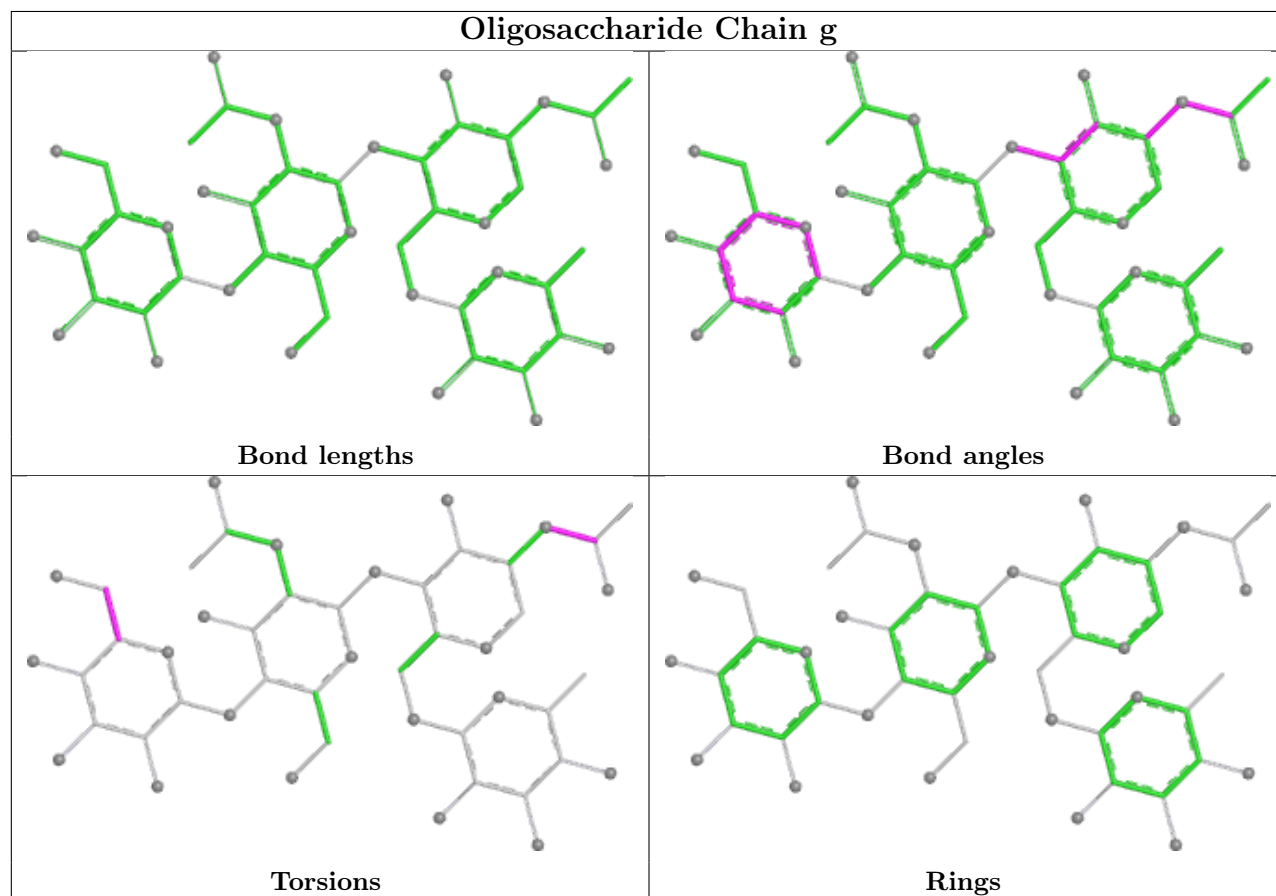
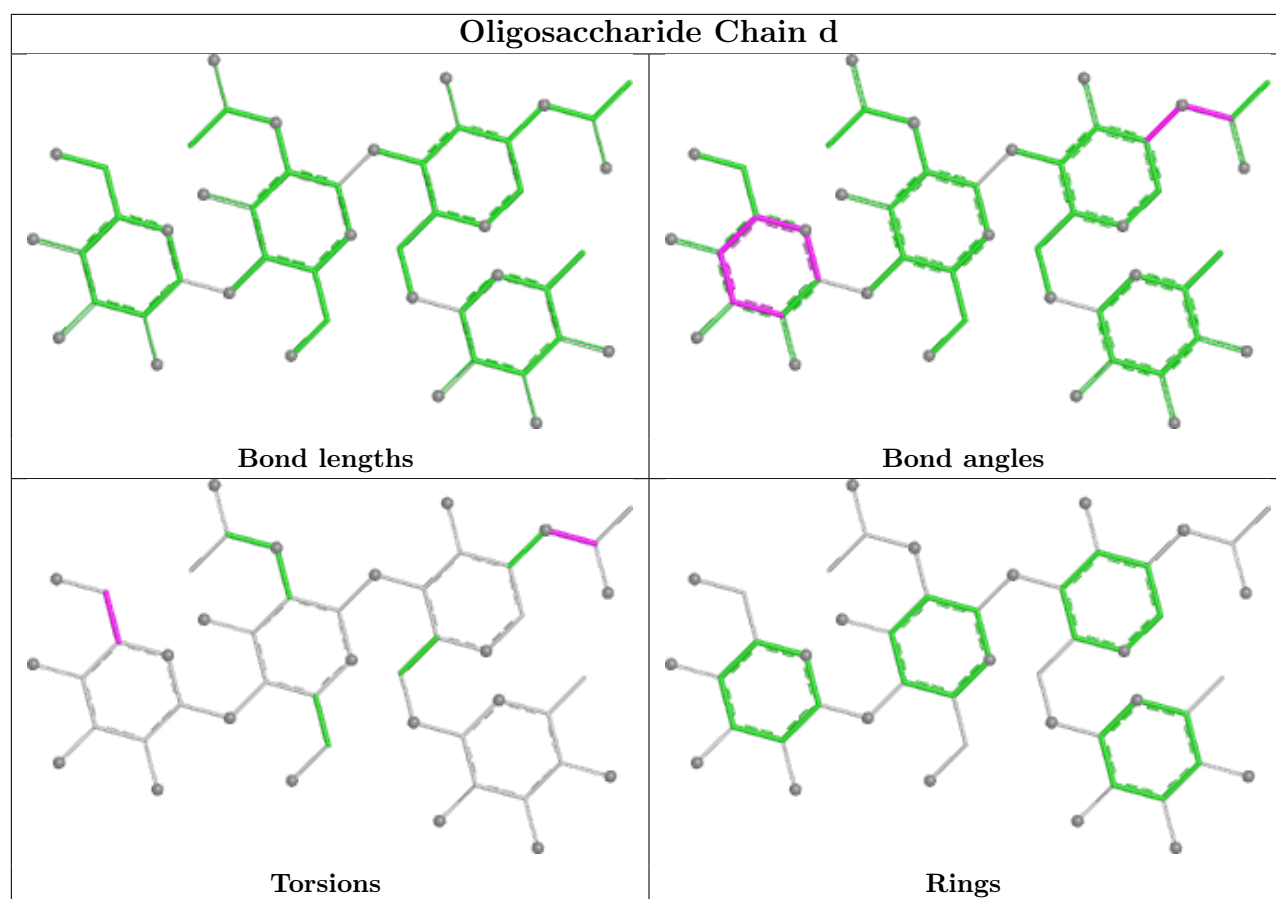


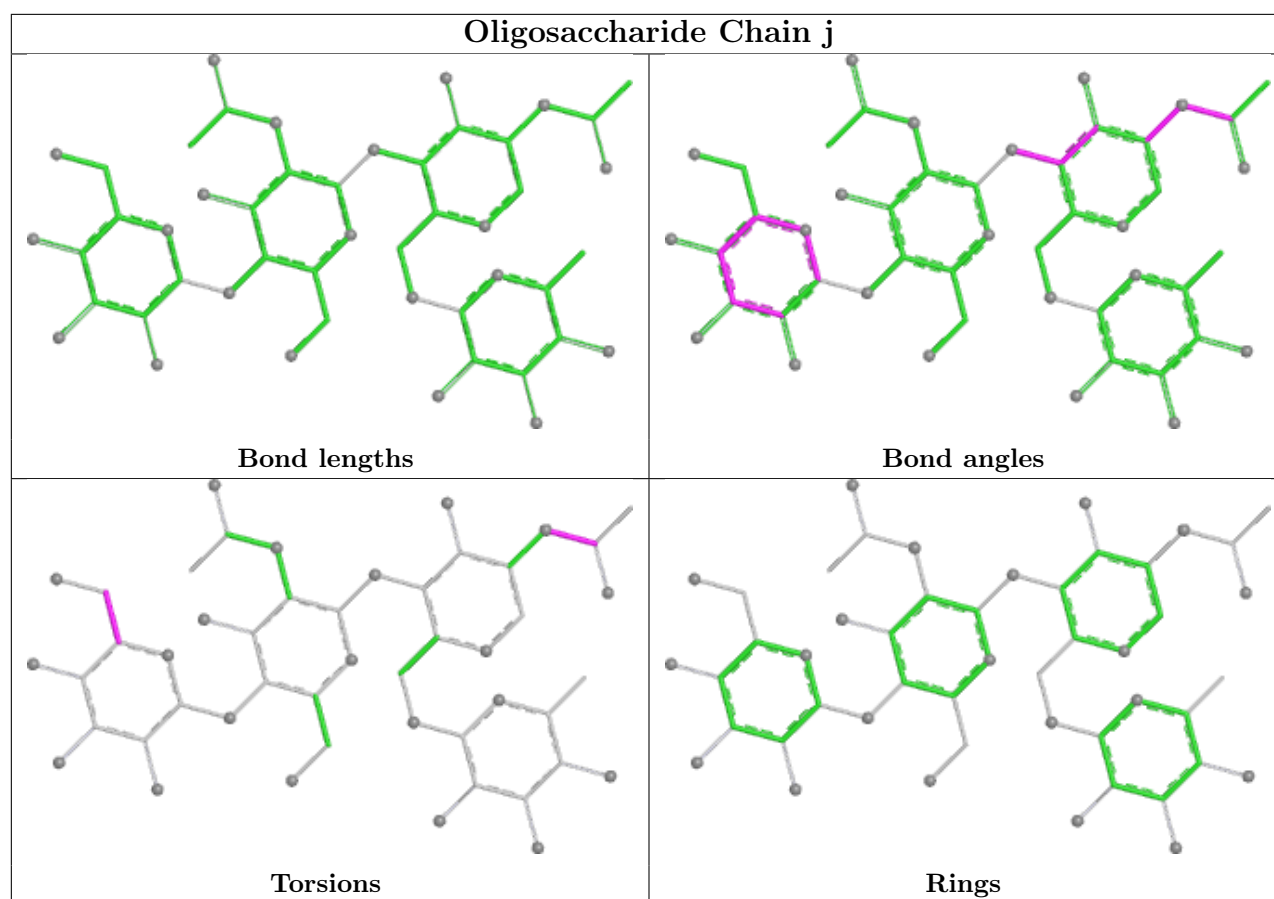












## 5.6 Ligand geometry [i](#)

6 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	$\# Z  > 2$
9	NAG	B	501	1	14,14,15	0.72	0	17,19,21	0.96	1 (5%)
9	NAG	F	801	2	14,14,15	0.71	0	17,19,21	0.91	0
9	NAG	E	801	2	14,14,15	0.71	0	17,19,21	0.91	0
9	NAG	D	801	2	14,14,15	0.71	0	17,19,21	0.91	1 (5%)
9	NAG	A	501	1	14,14,15	0.73	0	17,19,21	0.78	0
9	NAG	C	501	1	14,14,15	0.69	0	17,19,21	0.85	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
9	NAG	B	501	1	-	2/6/23/26	0/1/1/1
9	NAG	F	801	2	-	3/6/23/26	0/1/1/1
9	NAG	E	801	2	-	3/6/23/26	0/1/1/1
9	NAG	D	801	2	-	3/6/23/26	0/1/1/1
9	NAG	A	501	1	-	0/6/23/26	0/1/1/1
9	NAG	C	501	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	NAG	C2-N2-C7	2.22	125.88	122.90
9	D	801	NAG	C2-N2-C7	2.01	125.60	122.90

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	501	NAG	C8-C7-N2-C2
9	B	501	NAG	O7-C7-N2-C2
9	C	501	NAG	C8-C7-N2-C2
9	C	501	NAG	O7-C7-N2-C2
9	D	801	NAG	C8-C7-N2-C2
9	D	801	NAG	O7-C7-N2-C2
9	E	801	NAG	C8-C7-N2-C2
9	E	801	NAG	O7-C7-N2-C2
9	F	801	NAG	C8-C7-N2-C2
9	F	801	NAG	O7-C7-N2-C2
9	D	801	NAG	O5-C5-C6-O6
9	E	801	NAG	O5-C5-C6-O6
9	C	501	NAG	O5-C5-C6-O6
9	F	801	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

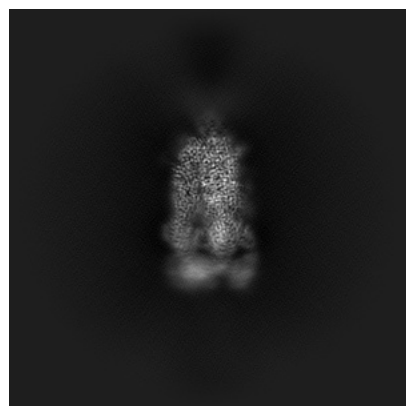
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-48351. These allow visual inspection of the internal detail of the map and identification of artifacts.

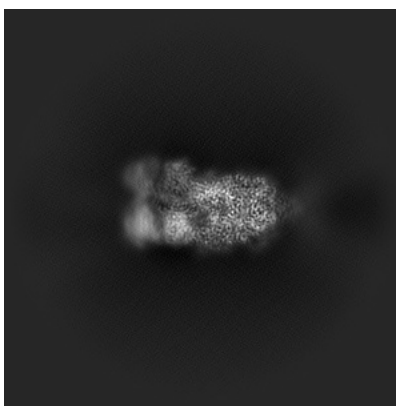
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

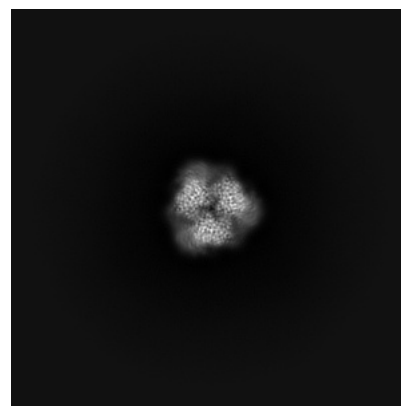
#### 6.1.1 Primary map



X

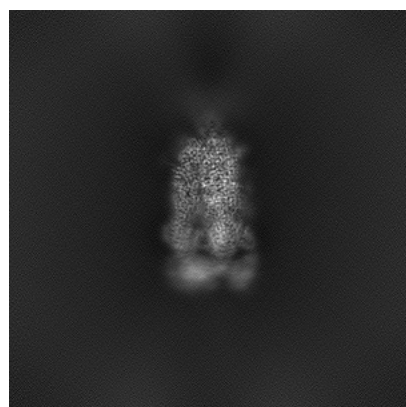


Y

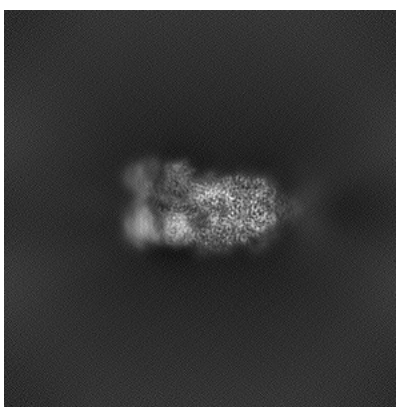


Z

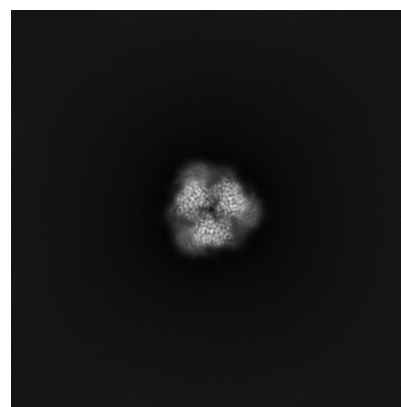
#### 6.1.2 Raw map



X



Y

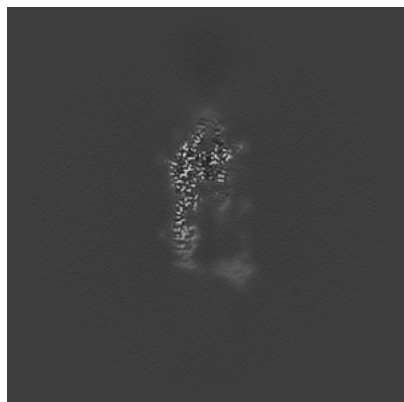


Z

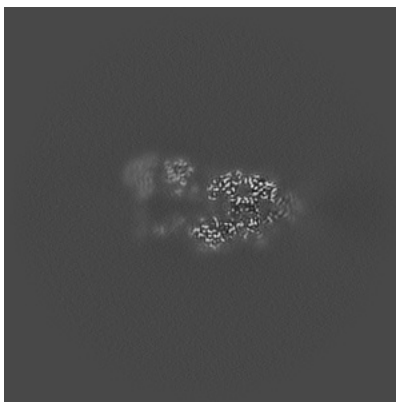
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

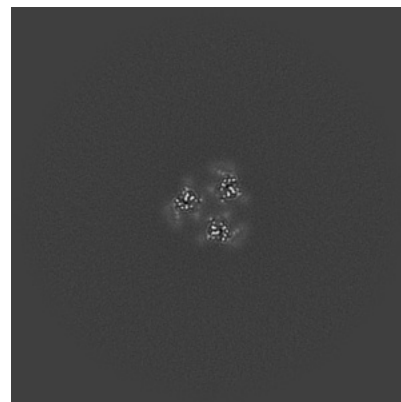
### 6.2.1 Primary map



X Index: 224

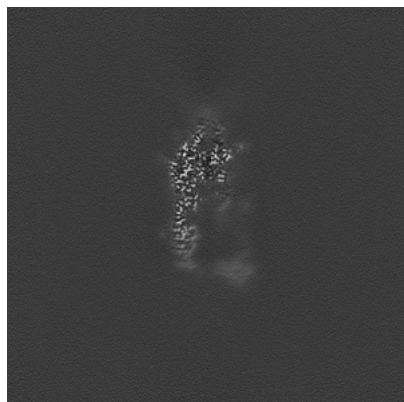


Y Index: 224

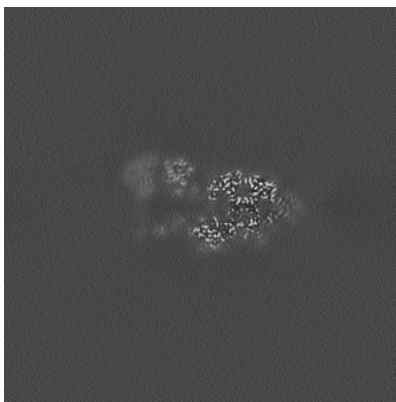


Z Index: 224

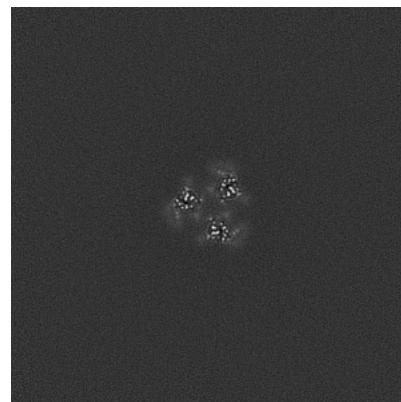
### 6.2.2 Raw map



X Index: 224



Y Index: 224



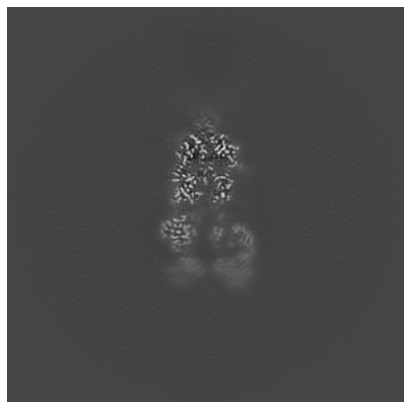
Z Index: 224

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

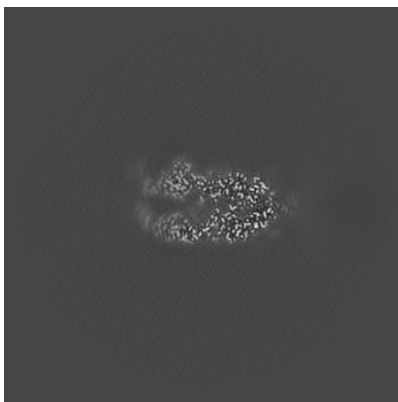


## 6.3 Largest variance slices [i](#)

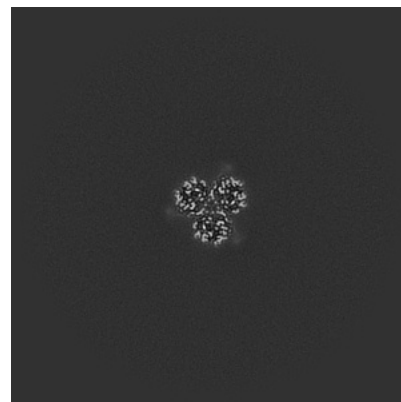
### 6.3.1 Primary map



X Index: 215

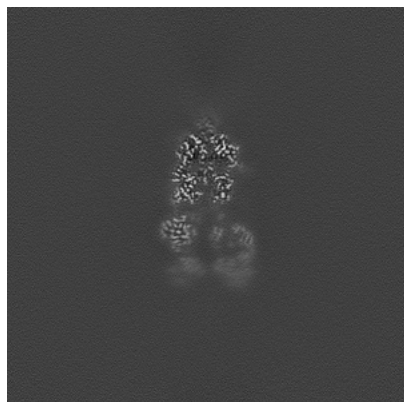


Y Index: 237

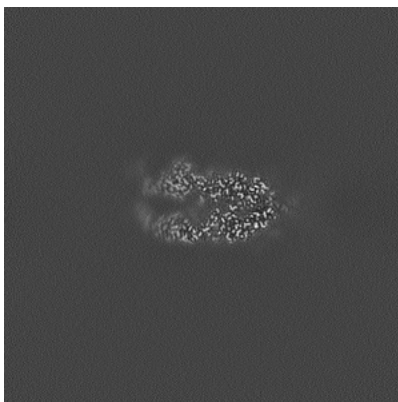


Z Index: 253

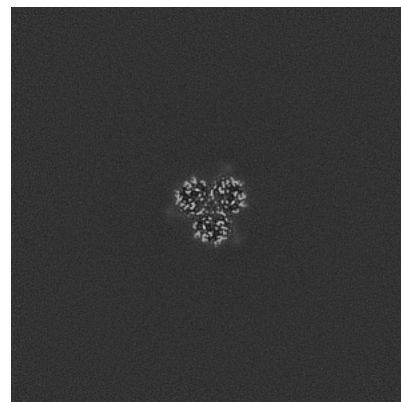
### 6.3.2 Raw map



X Index: 215



Y Index: 237



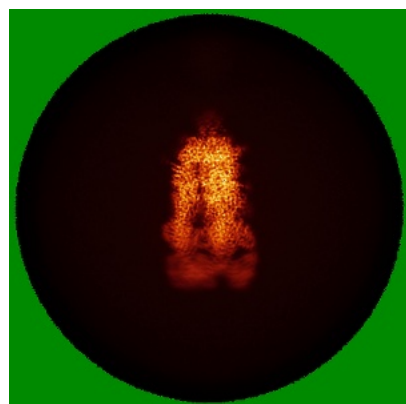
Z Index: 253

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

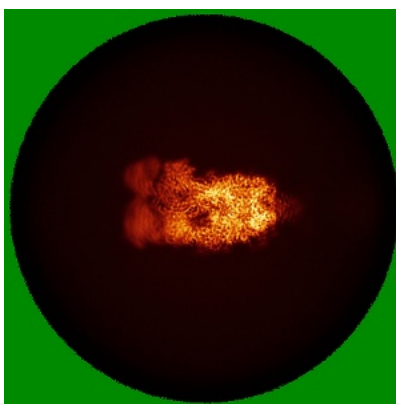


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

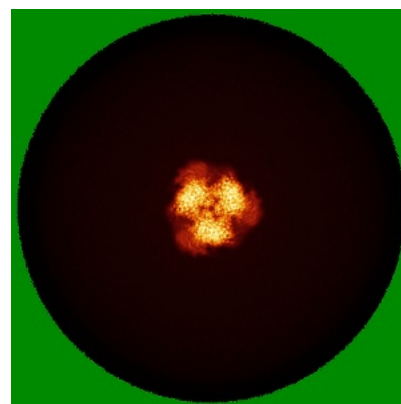
### 6.4.1 Primary map



X

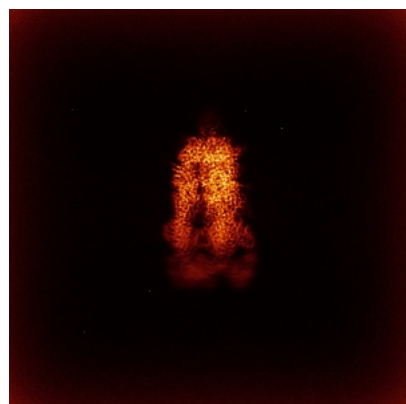


Y

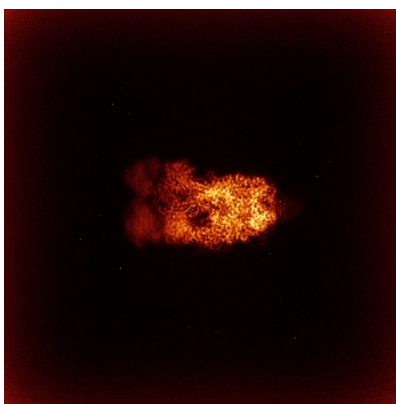


Z

### 6.4.2 Raw map



X



Y

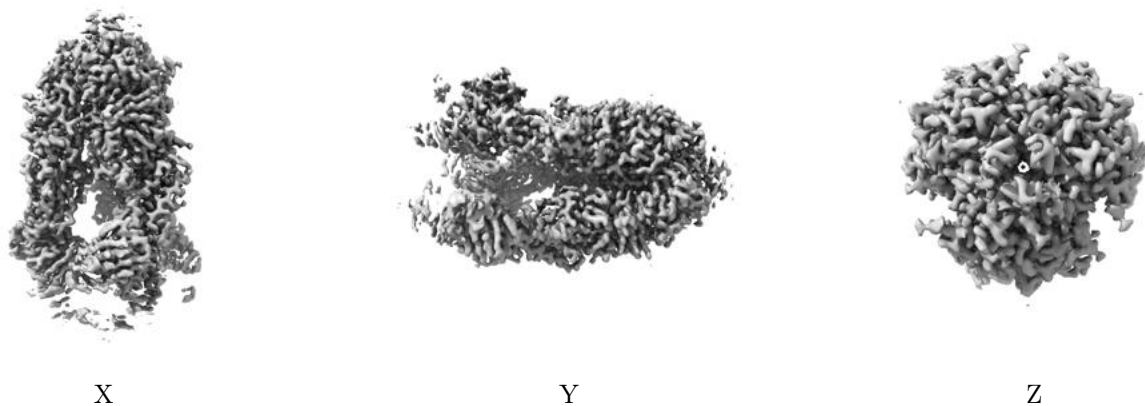


Z

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.

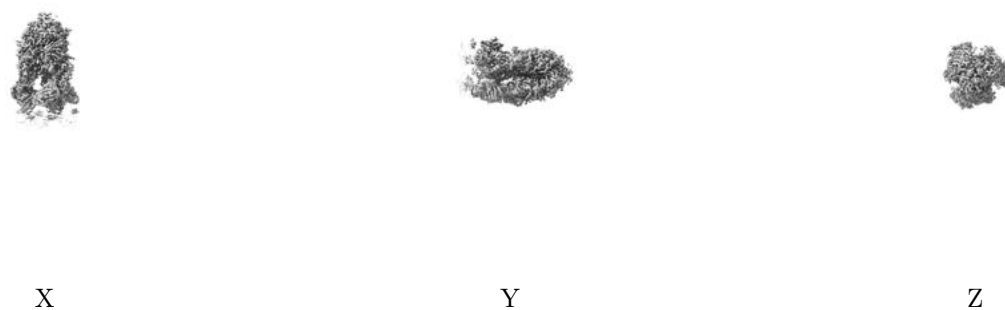
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. 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.

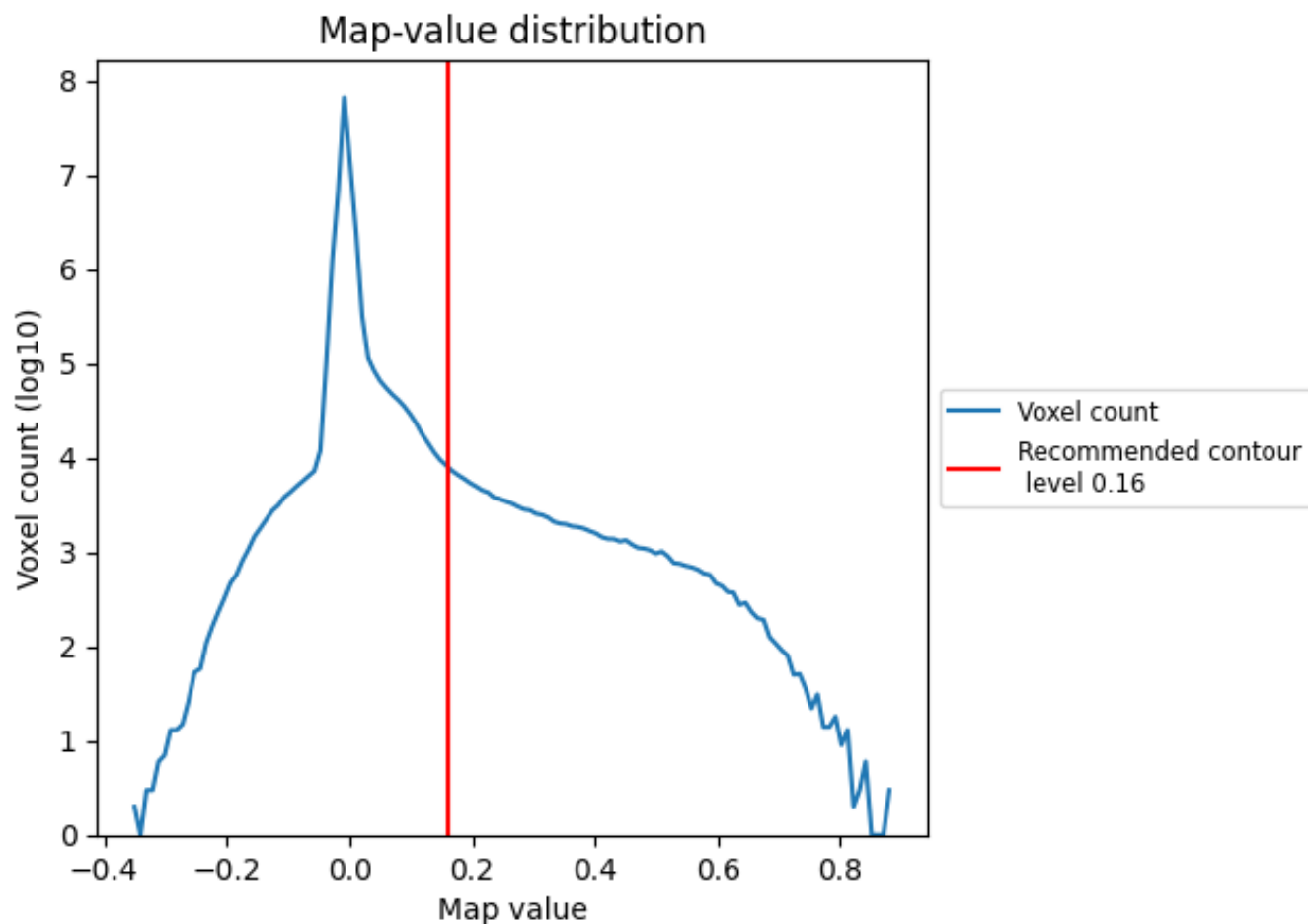
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

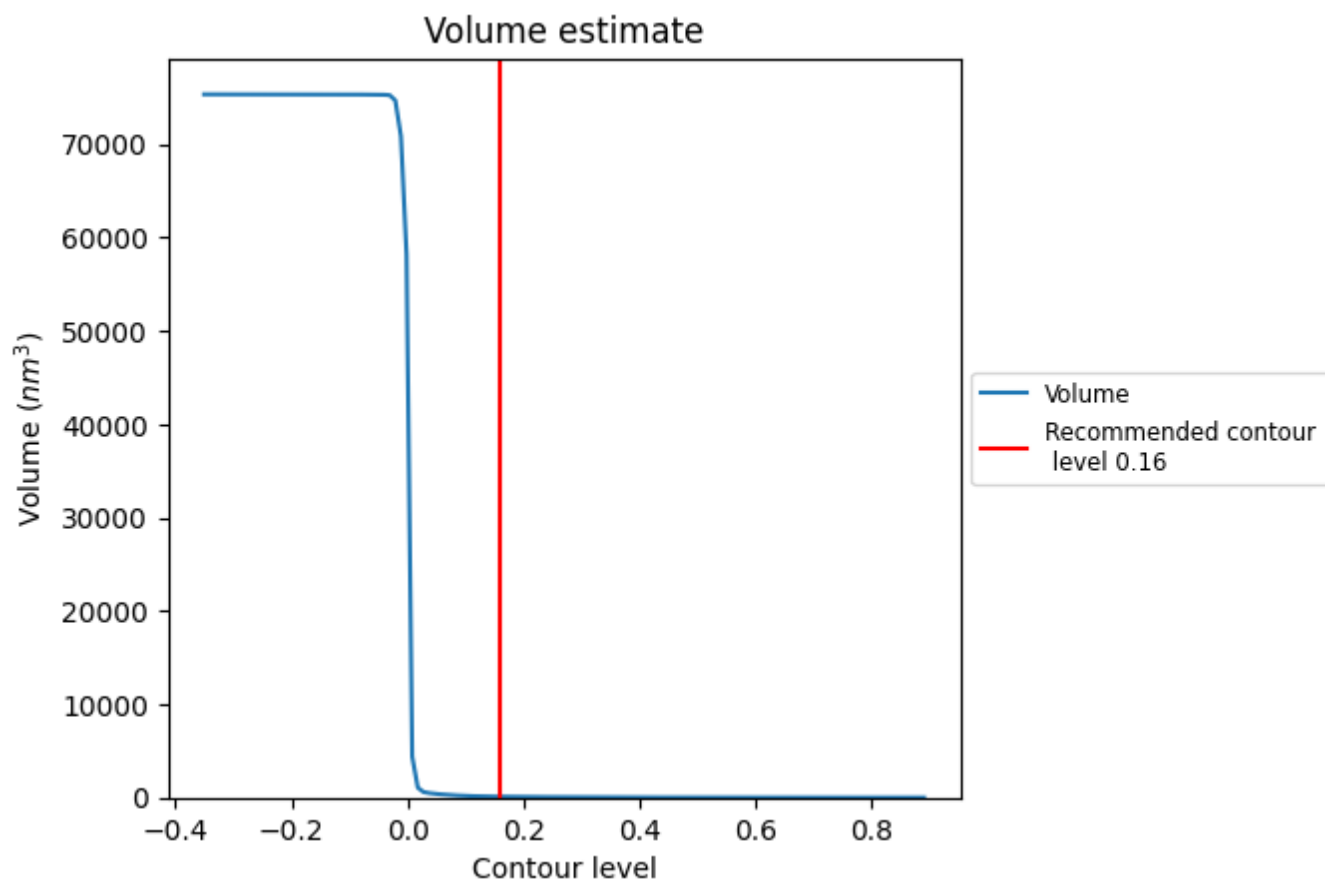
This section contains the results of statistical analysis of the map.

### 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.

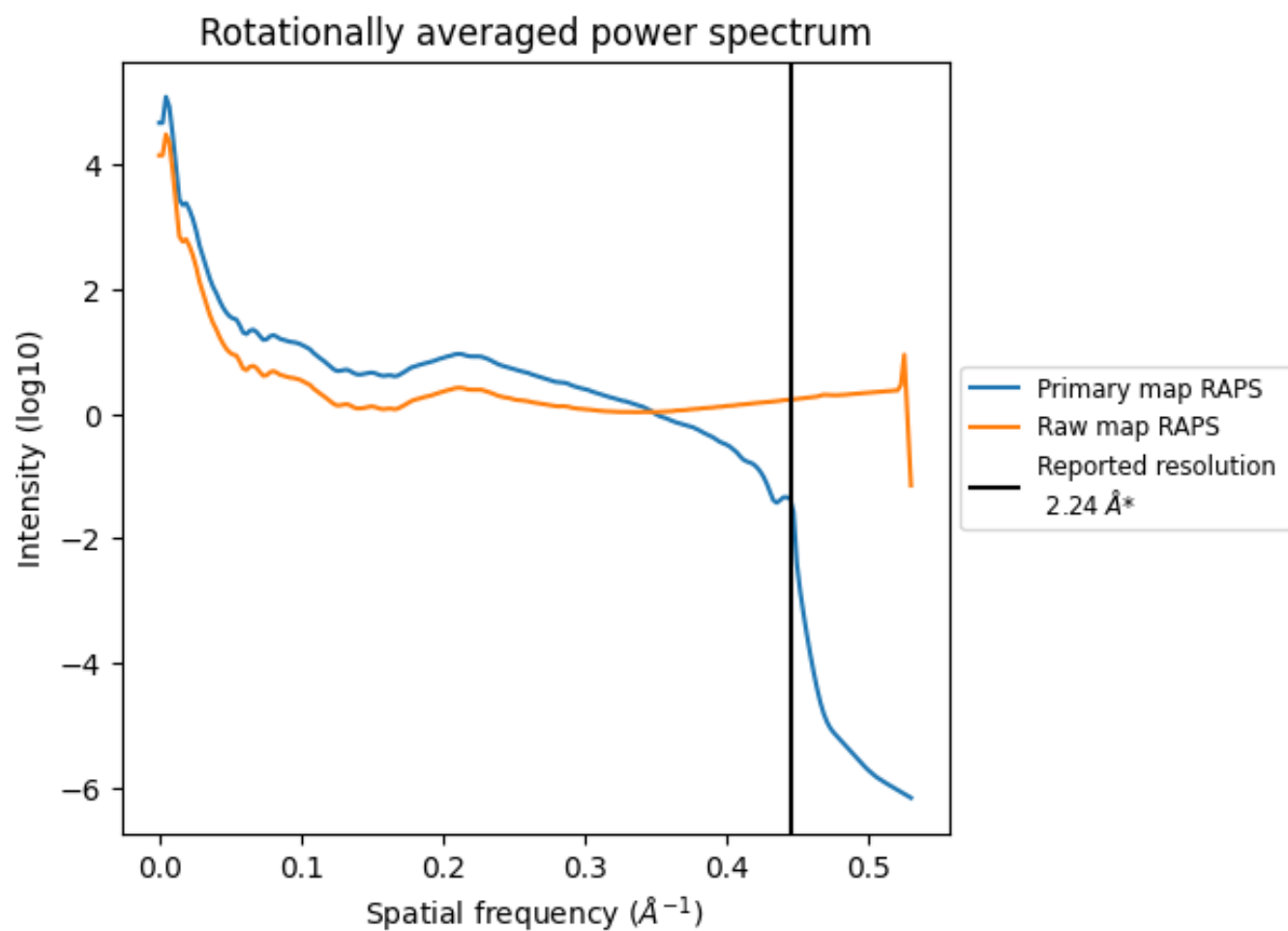
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 94  $\text{nm}^3$ ; this corresponds to an approximate mass of 85 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 ⓘ

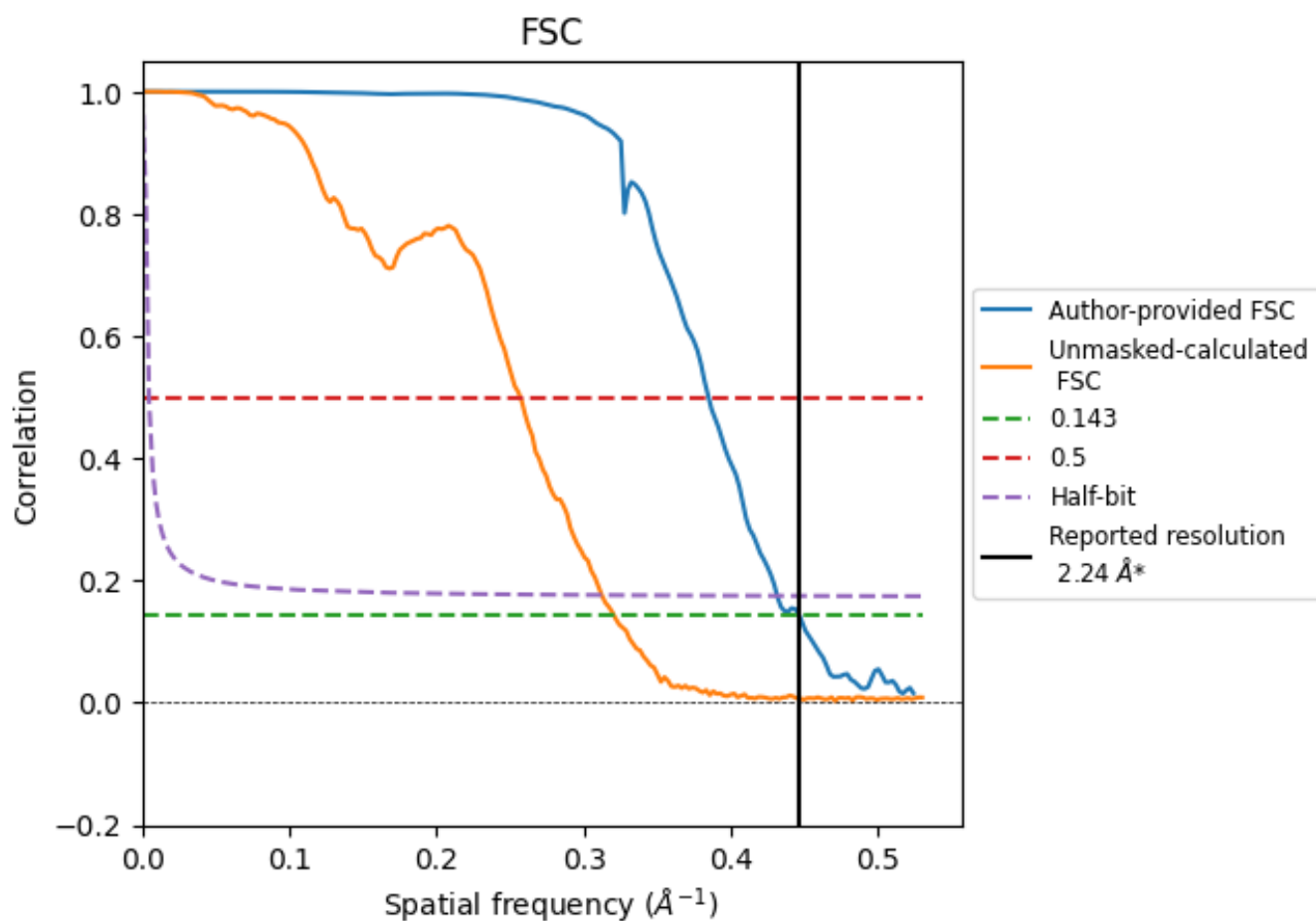


\*Reported resolution corresponds to spatial frequency of 0.446 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

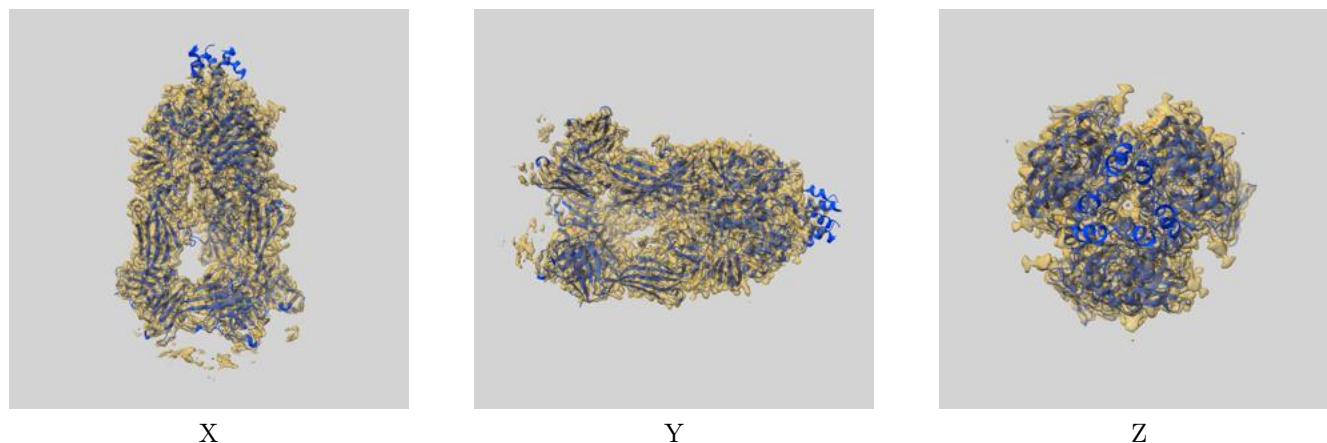
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.24	-	-
Author-provided FSC curve	2.24	2.60	2.32
Unmasked-calculated*	3.12	3.89	3.20

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.12 differs from the reported value 2.24 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-48351 and PDB model 9MLA. Per-residue inclusion information can be found in section [3](#) on page [14](#).

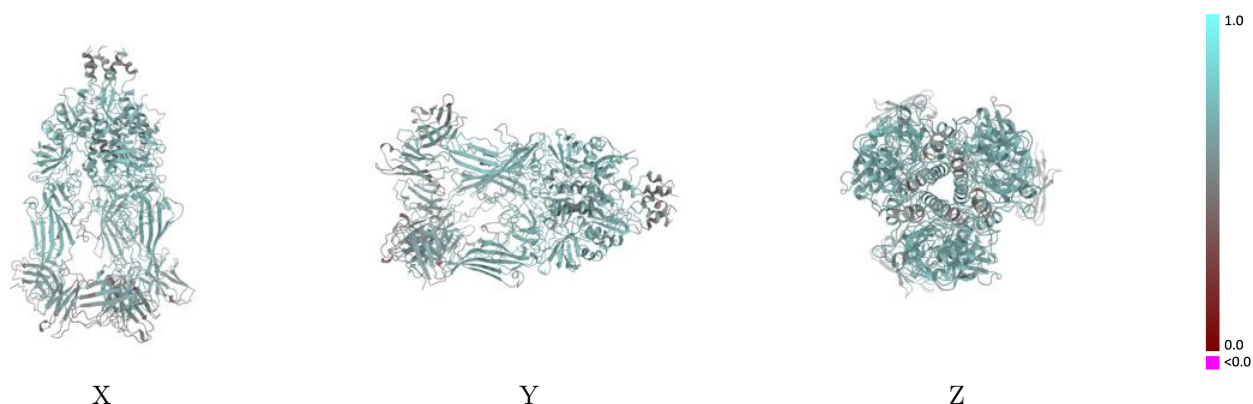
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.16 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.

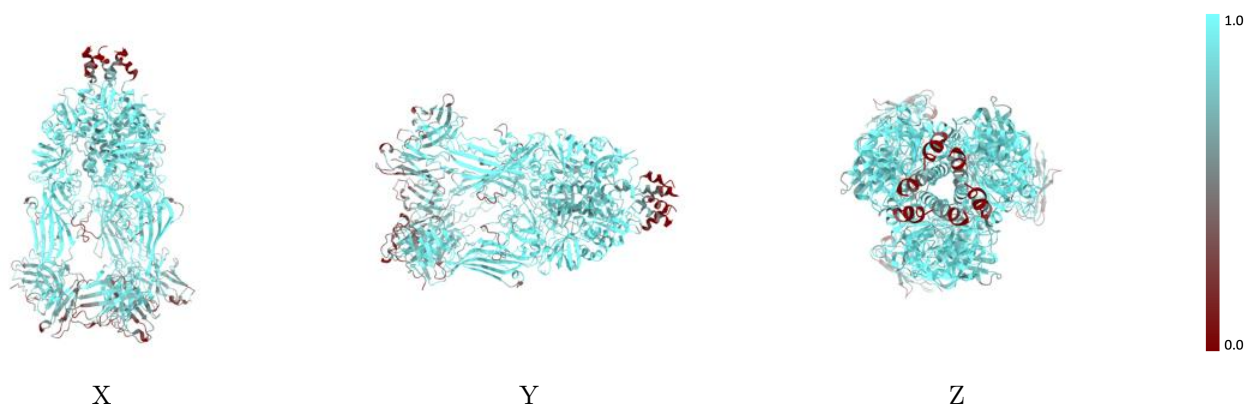


## 9.2 Q-score mapped to coordinate model [i](#)



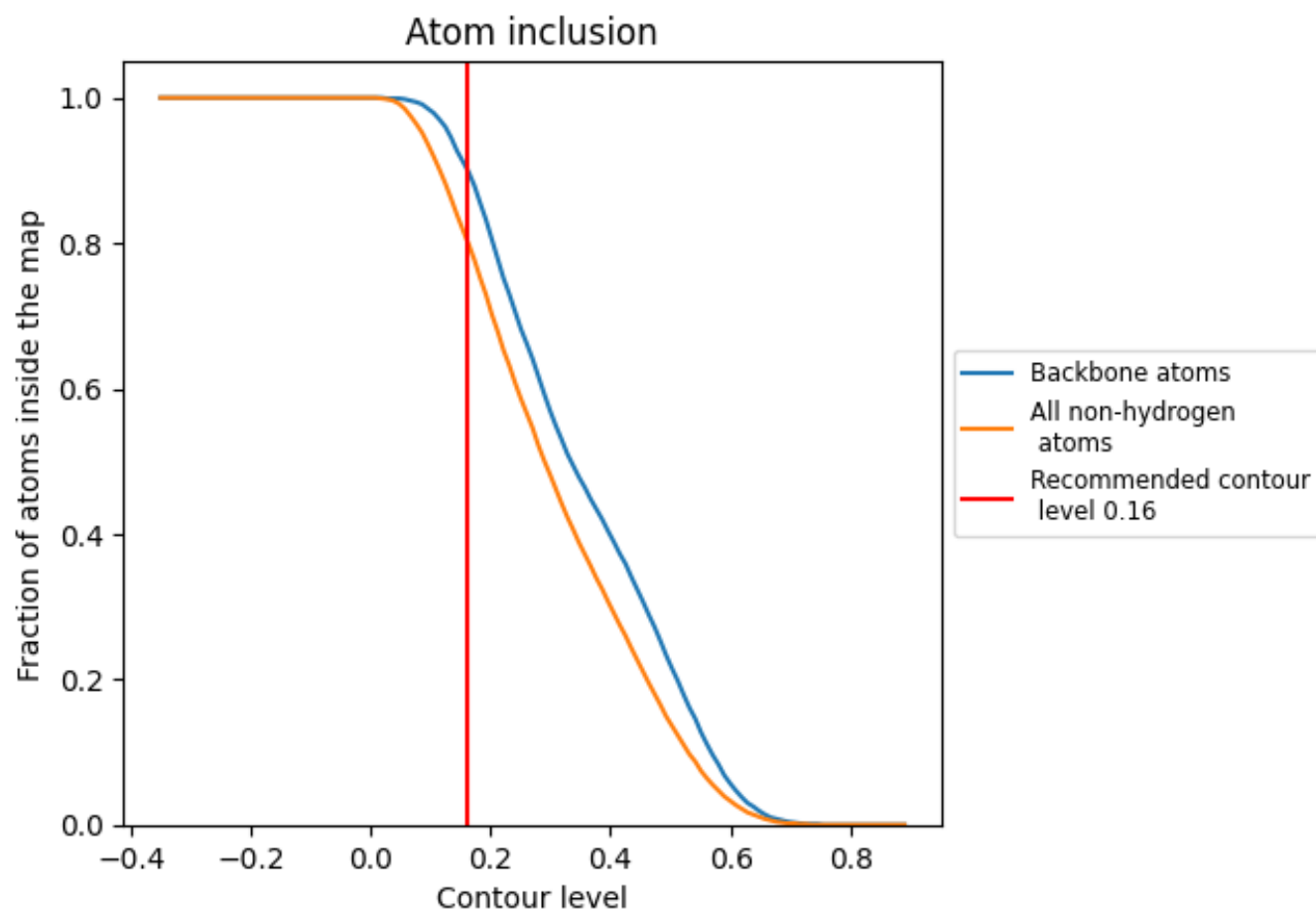
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 80% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8050	 0.6050
A	 0.8820	 0.6380
B	 0.8830	 0.6380
C	 0.8850	 0.6370
D	 0.8570	 0.6330
E	 0.8580	 0.6330
F	 0.8610	 0.6350
G	 0.7030	 0.5430
H	 0.7030	 0.5440
I	 0.7040	 0.5440
J	 0.6940	 0.5440
K	 0.6950	 0.5520
L	 0.6920	 0.5510
M	 0.4920	 0.5040
N	 0.2500	 0.4250
O	 0.5710	 0.5650
P	 0.6070	 0.5480
Q	 0.3570	 0.5260
R	 0.5410	 0.5340
S	 0.2500	 0.4070
T	 0.5000	 0.5560
U	 0.6070	 0.5340
V	 0.3210	 0.5270
W	 0.4750	 0.5120
X	 0.2500	 0.4290
Y	 0.5360	 0.5540
Z	 0.6070	 0.5510
a	 0.3210	 0.5150
b	 0.4870	 0.5210
c	 0.4620	 0.5000
d	 0.4290	 0.5220
e	 0.4870	 0.5180
f	 0.4620	 0.5160
g	 0.4290	 0.5280
h	 0.5130	 0.5260



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Chain	Atom inclusion	Q-score
i	 0.4870	 0.4970
j	 0.4290	 0.5240