



Full wwPDB EM Validation Report ⓘ

Jul 29, 2024 – 08:03 pm BST

PDB ID : 8OZQ
EMDB ID : EMD-17318
Title : In situ subtomogram average of Prototype Foamy Virus Env hexamer of trimers
Authors : Calcraft, T.; Nans, A.; Rosenthal, P.B.
Deposited on : 2023-05-09
Resolution : 10.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

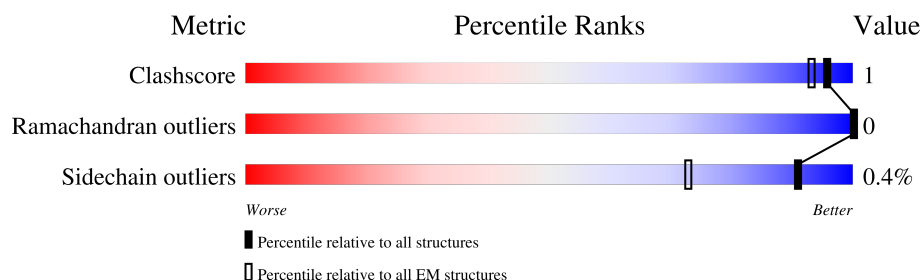
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.00 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.



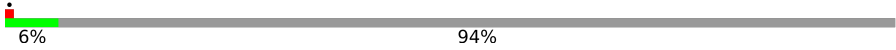







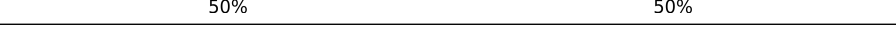
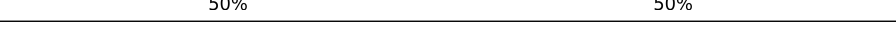



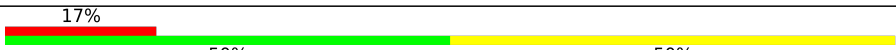
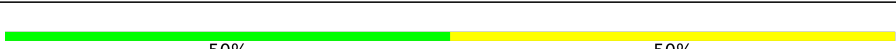





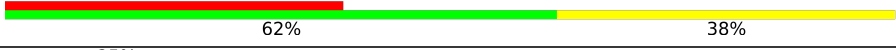
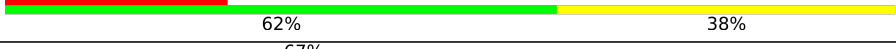



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	988	 6% 94%
1	B	988	 40% 58%
1	C	988	 40% 58%
1	D	988	 40% 59%
1	E	988	 6% 94%
1	F	988	 99%
1	G	988	 40% 59%
1	H	988	 40% 59%

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Mol	Chain	Length	Quality of chain
1	I	988	
1	L	988	
2	M	2	
2	N	2	
2	O	2	
2	Y	2	
2	Z	2	
2	a	2	
2	b	2	
2	c	2	
2	d	2	
3	S	3	
3	T	3	
3	U	3	
4	V	6	
4	W	6	
4	X	6	
5	P	4	
5	Q	4	
5	R	4	
6	e	8	
6	f	8	
6	g	8	
7	h	6	
7	i	6	

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Mol	Chain	Length	Quality of chain
7	j	6	<div><div></div><div>67%</div><div></div><div>50%</div><div>50%</div></div>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 22752 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	58	Total	C	N	O	S	0	0
			466	309	76	77	4		
1	B	411	Total	C	N	O	S	0	0
			3380	2164	561	636	19		
1	D	405	Total	C	N	O	S	0	0
			3190	2054	536	586	14		
1	F	11	Total	C	N	O	S	0	0
			94	61	18	14	1		
1	H	405	Total	C	N	O	S	0	0
			3190	2054	536	586	14		
1	L	405	Total	C	N	O	S	0	0
			3190	2054	536	586	14		
1	E	58	Total	C	N	O	S	0	0
			466	309	76	77	4		
1	I	58	Total	C	N	O	S	0	0
			466	309	76	77	4		
1	C	411	Total	C	N	O	S	0	0
			3380	2164	561	636	19		
1	G	405	Total	C	N	O	S	0	0
			3328	2133	549	628	18		

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



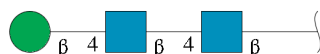
Mol	Chain	Residues	Atoms				AltConf	Trace
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	a	2	Total	C	N	O	0	0
			28	16	2	10		

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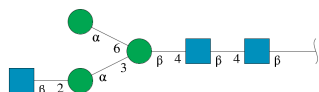
Mol	Chain	Residues	Atoms				AltConf	Trace
2	b	2	Total	C	N	O	0	0
			28	16	2	10		
2	c	2	Total	C	N	O	0	0
			28	16	2	10		
2	d	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16	2	10		
2	Y	2	Total	C	N	O	0	0
			28	16	2	10		
2	Z	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 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
3	U	3	Total	C	N	O	0	0
			39	22	2	15		
3	S	3	Total	C	N	O	0	0
			39	22	2	15		
3	T	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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
4	X	6	Total	C	N	O	0	0
			75	42	3	30		

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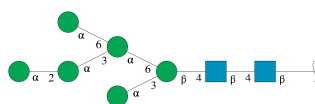
Mol	Chain	Residues	Atoms				AltConf	Trace
4	V	6	Total	C	N	O	0	0
			75	42	3	30		
4	W	6	Total	C	N	O	0	0
			75	42	3	30		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



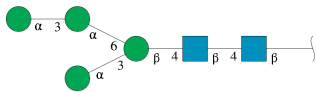
Mol	Chain	Residues	Atoms				AltConf	Trace
5	R	4	Total	C	N	O	0	0
			50	28	2	20		
5	P	4	Total	C	N	O	0	0
			50	28	2	20		
5	Q	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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.



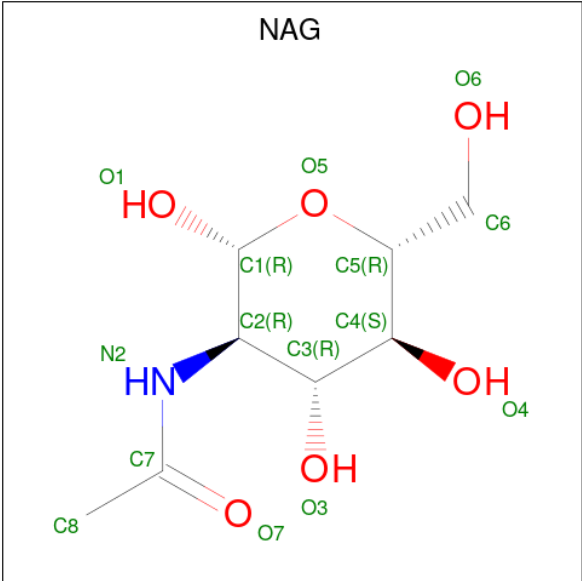
Mol	Chain	Residues	Atoms				AltConf	Trace
6	e	8	Total	C	N	O	0	0
			94	52	2	40		
6	f	8	Total	C	N	O	0	0
			94	52	2	40		
6	g	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
7	h	6	Total	C	N	O	0	0
			72	40	2	30		
7	i	6	Total	C	N	O	0	0
			72	40	2	30		
7	j	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



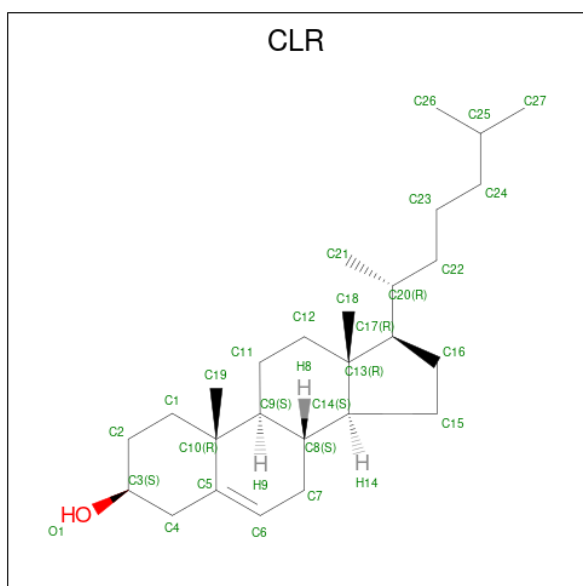
Mol	Chain	Residues	Atoms				AltConf
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	

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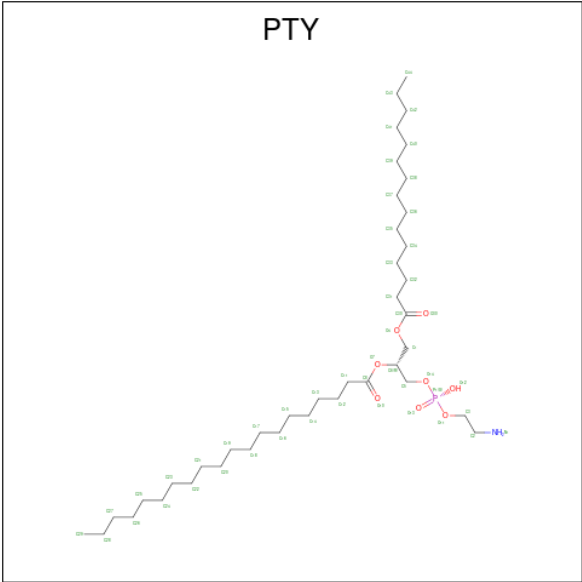
Mol	Chain	Residues	Atoms				AltConf
8	G	1	Total	C	N	O	0
			14	8	1	5	
8	G	1	Total	C	N	O	0
			14	8	1	5	
8	G	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 9 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
9	D	1	Total	C	O		0
			28	27	1		
9	H	1	Total	C	O		0
			28	27	1		
9	L	1	Total	C	O		0
			28	27	1		

- Molecule 10 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	D	1	Total	C	N	O	P	0
			50	40	1	8	1	
10	H	1	Total	C	N	O	P	0
			50	40	1	8	1	
10	L	1	Total	C	N	O	P	0
			50	40	1	8	1	

LEU SER GLY THR ALN GLY PHE THR GLY THR ALA PHE SER LEU LEU TYR LEU LYS PRO LEU LEU LEU GLY VAL GLY VAL LEU LEU LEU LEU PHE LYS LEU VAL SER TRP THR PRO THR LYS LYS ASN CUN

- Molecule 1: Envelope glycoprotein

Chain B:



MET	ALA	PRO	PRO	MET	THR	LEU	GLN	GLN	TRP	TRP	ILE	ILE	TRP	LYS	ASN	ALA	HIS	GLU	LEU	GLN	ASN	THR	THR	THR	THR	THR	GLU	GLN	GLN	LYS	GLU	GLN	ILE	ILE	LEU	LEU	ASP	ASP	ILE	ILE	GLN	ASN	GLU	GLU	GLU	VAL	VAL	GLN	PRO	THR	THR	ARG	ARG	ASP	LYS	PHE	ARG	TYR	LEU	LEU	LEU	TYR	THR
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CYS	CYS	ALA	THR	SER	SER	ARG	VAL	LEU	LEU	TRP	ILE	PHE	LEU	VAL	CYS	ILE	LEU	LEU	ILE	ILE	VAL	VAL	SER	CYS	PHE	VAL	VAL	THR	THR	ILE	ILE	SER	ARG	SER	ILE	GLN	LEU	TRP	ASN	LYS	ASP	ILE	ILE	GLN	GLN	VAL	LEU	GLY	PRO	VAL	VAL	ILE	ILE	THR	THR	GLN	GLN	ARG	ALA	VAL	VAL	Tyr	GLN	PRO	PRO	LEU	TYR
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K408	D409	M410	I411	S412	GLN	LEU	VAL	PRO	GLU	CYS	ASP	GLY	PHE	ASN	ASN	SER	LYS	TRP	MET	HIS	MET	HIS	P432	E443	K444	C449	R450	D451	G452	E453	T454	K455	S468	K491	R540	V543	G544	L545	I546	D547	P548	K549	S553	V554	P555	N556	V557	T558	R559	F560																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											

YES	YES	CYS	ASN	ASN	ASN	ARG	LYS	ARG	ARG	ARG	SER	VAL	ASP	ASN	ARG	LEU	LEU	ARG	SER	NET	GLY	TYR	TYR	ALA	ALA	LEU	GLY	GLY	THR	GLN	THR	LEU	SER	GLN	ILE	SER	ASP	ILE	ASN	GLN	GLY	GLY	THR	TYR	ILE	THR	LEU	ASP	HIS	VAL	THR	THR	LEU	NET	NET	GLU	ALA
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THR	LEU	HIS	ASP	ILE	SER	VAL	MET	GLY	GLU	MET	PHE	ALA	VAL	GLN	HIS	LEU	HIS	THR	HIS	LEU	ASN	HIS	LEU	LYS	THR	MET	LEU	LEU	GLU	ARG	ARG	ILE	ASP	TRP	THR	THR	TYR	MET	SER	SER	SER	THR	THR	TRP	LEU	GLN	GLN	GLN	LEU	GLN	LYS	ASP	SER	ASP	GLU	MET	LYS	VAL	LYS	ILE	LYS	ARG	ILE
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ALA ARG SER LEU VAL TYR THR HIS SER SER PRO THR ALA ALA THR TRP TRP LEU LEU VAL ILE PRO LYS HIS ILE TYR LEU ASN ASN TRP TRP VAL VAL ASN ASN ILE GLY GLY HIS HIS LEU VAL LYS SER ALA SER GLY GLN GLN LEU THR HIS VAL ILE ILE

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

LYS ASP VAL
SER ASP
PRO TRP
THR PRO
ALA ALA
ALA ALA
ALA ALA
SER SER
ALA SER
LEU LEU
GLN GLN
GLY GLY
ILE ILE
GLY GLY
PHE PHE
LEU LEU
SER SER
GLY GLY
THR THR
ALA ALA
GLN GLN
ILE ILE
PHE PHE
GLY GLY
TYR TYR
LEU LEU
LYS LYS
PRO PRO
ILE ILE
ILE ILE
ILE ILE
ILE ILE
PHE PHE
PHE PHE
LYS LYS
ILE ILE
VAL VAL
SER SER
TRP TRP
ILE ILE
PRO PRO

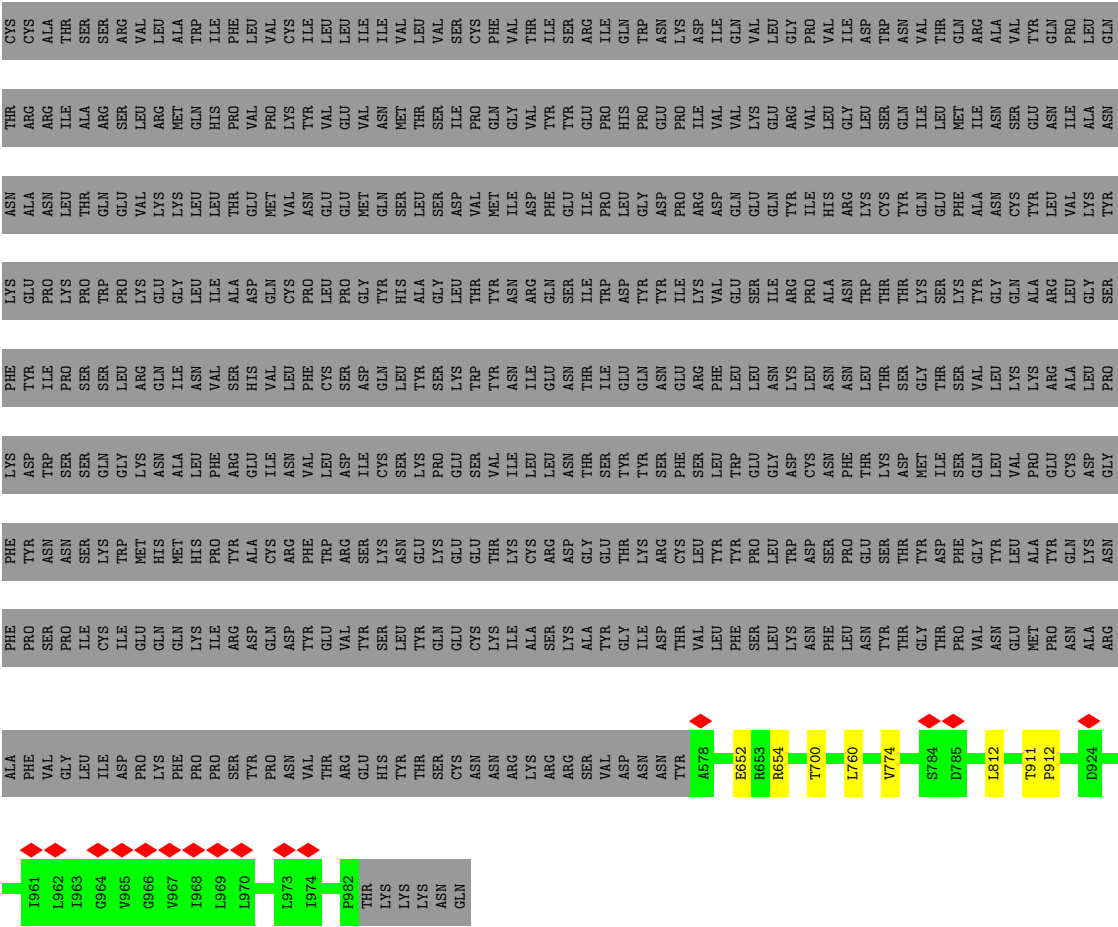
THR
LYS
LYS
LYS
ASN
GLN

- Molecule 1: Envelope glycoprotein

Chain D:



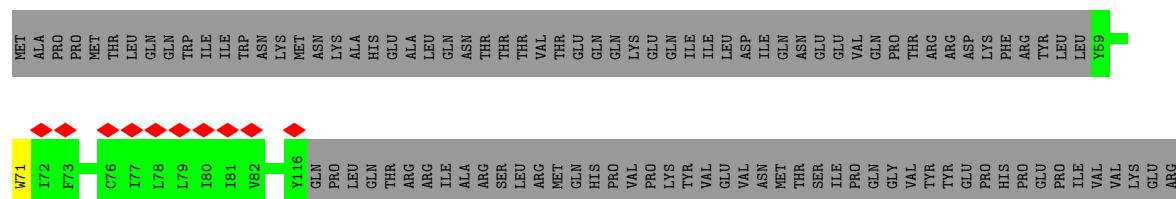
MET	ALA	PRO	PRO	MET	THR	LEU	GLN	GLN	TRP	ILE	ILE	TRP	LYS	MET	ASN	LYS	ALA	ALA	LEU	GLN	ASN	THR	THR	THR	VAL	THR	GLU	GLN	GLN	LYS	GLU	GLN	ILE	ILE	LEU	LEU	ASP	ASP	LYS	THR	GLN	ASN	GLU	GLU	VAL	VAL	GLN	PRO	THR	ARG	ARG	ARG	ASP	ASP	PHE	ARG	TYR	TYR	LEU	LEU	LEU	TYR	THR
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● Molecule 1: Envelope glycoprotein

Chain F: 99%





[illegible]

- Molecule 1: Envelope glycoprotein

Chain I: 6% 94%

[illegible]

TRP	ALA	PRO	PHE	THR	LYS	MET
ILE	ALA	ASN	VAL	ILE	ARG	MET
PRO	THR	LEU	GLN	ALA	ALA	ALA
THR	LYS	GLN	VAL	HIS	ALA	THR
LYS	ASP	LEU	ASN	PRO	ARG	THR
LYS	VAL	ARG	PRO	TVR	SER	HIS
ASN	TRP	LEU	LEU	GLU	LEU	ASP
GLN	PRO	PRO	LYS	ILE	VAL	ILE
	ALA	HIS	ASN	ILE	SER	
	ALA	LEU	GLY	ASN	TVR	VAL
	ALA	VAL	SER	LYS	VAL	MET
	SER	GLY	TVR	GLU	LYS	GLU
	ALA	ILE	LEU	CYS	GLN	GLY
	LEU	ILE	VAL	VAL	THR	MET
	GLN	ALA	LEU	GLU	HIS	PHE
	GLY	ILE	ALA	THR	SER	ALA
	ILE	ILE	SER	ILE	VAL	VAL
	GLY	LYS	SER	TVR	PRO	GLN
	ASN	GLY	THR	LEU	THR	HIS
	PHE	ILE	ASP	HIS	ALA	LEU
	LEU	LYS	CYS	LEU	THR	HIS
	SER	ILE	GLN	GLU	ALA	THR
	GLY	GLU	ILE	ASP	TRP	HIS
	THR	VAL	PRO	CYS	GLU	LEU
	ALA	THR	PRO	THR	ILE	ASN
	GLN	SER	TYR	ARG	ILE	ASN
	ILE	GLY	PRO	ASP	TVR	LYS
	ILE	GLY	PRO	ASP	TYR	THR
	PHE	GLU	SER	TVR	GLU	MET
	GLY	SER	ILE	VAL	LEU	LEU
	THR	ILE	VAL	ILE	VAL	LEU
	ALA	LYS	THR	CYS	VAL	LEU
	PHE	GLU	VAL	GLU	ILE	GLU
	SER	GLN	ASN	VAL	PRO	ARG
	LEU	ILE	GLU	VAL	LYS	ARG
	LEU	GLU	THR	LYS	HIS	ILE
	GLY	ARG	THR	ILE	ASP	ILE
	TYR	ALA	SER	VAL	TYR	THR
	LEU	LYS	CYS	GLN	LEU	THR
	LYS	ALA	PHE	PRO	ASN	TYR
	PRO	GLU	GLY	CYS	ASN	MET
	ILE	LEU	LEU	GLY	TRP	SER
	ILE	LEU	ASP	GLY	ASN	SER
	ILE	ARG	PHE	SER	VAL	SER
	GLY	LEU	LYS	SER	VAL	TRP
	VAL	ASP	ARG	ASN	LEU	GLN
	GLY	ILE	PRO	THR	ILE	GLN
	VAL	HIS	LEU	SER	GLY	GLN
	ILE	GLU	VAL	ASP	HIS	GLN
	LEU	GLY	ALA	CYS	LEU	GLN
	LEU	ASP	GLU	PRO	VAL	GLN
	VAL	THR	GLU	VAL	LYS	LYS
	ILE	PRO	ARG	TRP	SER	SER
	LEU	ALA	LEU	ALA	ALA	ASP
	ILE	TRP	SER	GLU	GLY	ASP
	PHE	ILE	PHE	ALA	GLN	GLU
	LYS	GLN	GLU	VAL	LEU	MET
	ILE	GLN	PRO	LYS	THR	LYS
	VAL	LEU	ARG	PRO	HIS	VAL
	STR	ALA	THR	GLU	VAL	THR

- Molecule 1: Envelope glycoprotein

Chain G:  40% 59%

[illegible]

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



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



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



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



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



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



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

Chain O:  50% 50%



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

Chain Y:  50% 50% 50%



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

Chain Z:  50% 100% 50%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  33% 67% 67%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  33% 67% 67%



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  33% 67% 67%



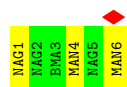
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 



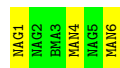
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V: 

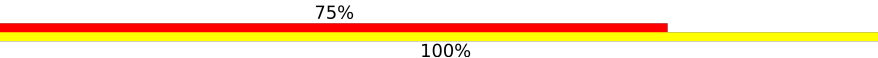


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: 



- Molecule 5: 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: 

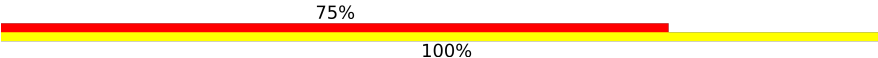


- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 

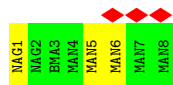


- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

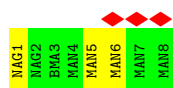
Chain Q: 



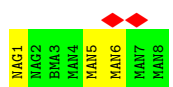
- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



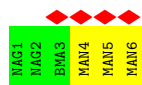
- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



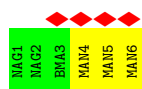
- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



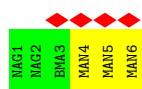
- Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of subtomograms used	5697	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 ($e^-/\text{\AA}^2$)	107.42	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.198	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.0702	Depositor
Map size (Å)	441.6, 441.6, 441.6	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.76, 2.76, 2.76	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, PTY, CLR, MAN, 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	0.72	0/476	0.71	0/653
1	B	0.68	0/3469	0.76	0/4705
1	C	0.68	0/3469	0.75	0/4705
1	D	0.69	0/3260	0.77	0/4441
1	E	0.72	0/476	0.71	0/653
1	F	0.66	0/97	0.78	0/130
1	G	0.68	0/3416	0.75	0/4634
1	H	0.69	0/3260	0.77	0/4441
1	I	0.72	0/476	0.71	0/653
1	L	0.69	0/3260	0.77	0/4441
All	All	0.69	0/21659	0.76	0/29456

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	466	0	488	0	0
1	B	3380	0	3293	9	0
1	C	3380	0	3293	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3190	0	3242	7	0
1	E	466	0	488	1	0
1	F	94	0	97	3	0
1	G	3328	0	3241	11	0
1	H	3190	0	3242	7	0
1	I	466	0	488	0	0
1	L	3190	0	3242	4	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	O	28	0	25	0	0
2	Y	28	0	25	0	0
2	Z	28	0	25	0	0
2	a	28	0	25	0	0
2	b	28	0	25	0	0
2	c	28	0	25	0	0
2	d	28	0	25	0	0
3	S	39	0	34	0	0
3	T	39	0	34	0	0
3	U	39	0	34	0	0
4	V	75	0	64	0	0
4	W	75	0	64	0	0
4	X	75	0	64	0	0
5	P	50	0	43	0	0
5	Q	50	0	43	0	0
5	R	50	0	43	0	0
6	e	94	0	79	0	0
6	f	94	0	79	0	0
6	g	94	0	79	0	0
7	h	72	0	61	0	0
7	i	72	0	61	0	0
7	j	72	0	61	0	0
8	B	42	0	39	0	0
8	C	42	0	39	0	0
8	G	42	0	39	0	0
9	D	28	0	46	0	0
9	H	28	0	46	0	0
9	L	28	0	46	0	0
10	D	50	0	79	0	0
10	H	50	0	79	0	0
10	L	50	0	79	0	0
All	All	22752	0	22674	39	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 1.

All (39) 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:D:700:THR:HG21	1:C:197:ASN:OD1	1.96	0.64
1:B:134:VAL:HG21	1:C:138:VAL:HG23	1.80	0.64
1:H:700:THR:HG21	1:G:197:ASN:OD1	1.98	0.62
1:B:138:VAL:HG23	1:C:134:VAL:HG21	1.80	0.62
1:D:700:THR:HG23	1:C:193:THR:HG23	1.83	0.60
1:F:137:TYR:HE1	1:G:133:PRO:HG3	1.67	0.59
1:G:136:LYS:HG2	1:G:137:TYR:H	1.71	0.56
1:C:136:LYS:HG2	1:C:137:TYR:H	1.71	0.56
1:H:700:THR:HG23	1:G:193:THR:HG23	1.88	0.55
1:G:277:ILE:HG21	1:G:298:LEU:HD12	1.89	0.55
1:B:136:LYS:HG2	1:B:137:TYR:H	1.71	0.54
1:B:277:ILE:HG21	1:B:298:LEU:HD12	1.89	0.53
1:C:277:ILE:HG21	1:C:298:LEU:HD12	1.88	0.53
1:F:137:TYR:CE1	1:G:133:PRO:HG3	2.48	0.49
1:D:652:GLU:OE2	1:L:654:ARG:NH1	2.47	0.48
1:B:358:ALA:HA	1:B:370:ALA:HB3	1.97	0.46
1:G:358:ALA:HA	1:G:370:ALA:HB3	1.97	0.46
1:C:358:ALA:HA	1:C:370:ALA:HB3	1.97	0.45
1:L:760:LEU:HD22	1:L:774:VAL:HG22	1.99	0.45
1:B:134:VAL:HG21	1:C:138:VAL:CG2	2.47	0.44
1:C:277:ILE:HD11	1:C:302:TYR:HB2	2.00	0.44
1:D:760:LEU:HD22	1:D:774:VAL:HG22	1.99	0.44
1:G:277:ILE:HD11	1:G:302:TYR:HB2	2.00	0.44
1:B:277:ILE:HD11	1:B:302:TYR:HB2	2.00	0.43
1:F:131:GLN:HB3	1:G:137:TYR:CD1	2.53	0.43
1:H:760:LEU:HD22	1:H:774:VAL:HG22	1.99	0.43
1:D:654:ARG:NH1	1:H:652:GLU:OE2	2.52	0.43
1:C:337:GLU:O	1:C:341:LEU:HG	2.20	0.42
1:G:136:LYS:HG2	1:G:137:TYR:N	2.34	0.42
1:D:911:THR:HB	1:D:912:PRO:HD3	2.02	0.42
1:D:774:VAL:HG21	1:C:160:VAL:HG22	2.02	0.42
1:G:337:GLU:O	1:G:341:LEU:HG	2.20	0.42
1:H:975:PHE:CE2	1:E:71:TRP:CH2	3.08	0.41
1:H:911:THR:HB	1:H:912:PRO:HD3	2.02	0.41
1:L:911:THR:HB	1:L:912:PRO:HD3	2.02	0.41
1:B:337:GLU:O	1:B:341:LEU:HG	2.20	0.41
1:B:138:VAL:CG2	1:C:134:VAL:HG21	2.47	0.41
1:H:654:ARG:NH1	1:L:652:GLU:OE2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:LYS:HG2	1:C:137:TYR:N	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	56/988 (6%)	55 (98%)	1 (2%)	0	100	100
1	B	405/988 (41%)	379 (94%)	26 (6%)	0	100	100
1	C	405/988 (41%)	379 (94%)	26 (6%)	0	100	100
1	D	403/988 (41%)	377 (94%)	26 (6%)	0	100	100
1	E	56/988 (6%)	55 (98%)	1 (2%)	0	100	100
1	F	9/988 (1%)	7 (78%)	2 (22%)	0	100	100
1	G	399/988 (40%)	374 (94%)	25 (6%)	0	100	100
1	H	403/988 (41%)	377 (94%)	26 (6%)	0	100	100
1	I	56/988 (6%)	55 (98%)	1 (2%)	0	100	100
1	L	403/988 (41%)	377 (94%)	26 (6%)	0	100	100
All	All	2595/9880 (26%)	2435 (94%)	160 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	54/899 (6%)	54 (100%)	0	100	100
1	B	382/899 (42%)	380 (100%)	2 (0%)	88	93
1	C	382/899 (42%)	380 (100%)	2 (0%)	88	93
1	D	356/899 (40%)	355 (100%)	1 (0%)	92	95
1	E	54/899 (6%)	54 (100%)	0	100	100
1	F	11/899 (1%)	11 (100%)	0	100	100
1	G	376/899 (42%)	374 (100%)	2 (0%)	88	93
1	H	356/899 (40%)	355 (100%)	1 (0%)	92	95
1	I	54/899 (6%)	54 (100%)	0	100	100
1	L	356/899 (40%)	355 (100%)	1 (0%)	92	95
All	All	2381/8990 (26%)	2372 (100%)	9 (0%)	91	94

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	151	TYR
1	B	405	ASN
1	D	812	LEU
1	H	812	LEU
1	L	812	LEU
1	C	151	TYR
1	C	405	ASN
1	G	151	TYR
1	G	405	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

99 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$
2	NAG	M	1	2,1	14,14,15	0.32	0	17,19,21	1.35	2 (11%)
2	NAG	M	2	2	14,14,15	0.33	0	17,19,21	0.75	0
2	NAG	N	1	2,1	14,14,15	0.32	0	17,19,21	1.34	2 (11%)
2	NAG	N	2	2	14,14,15	0.34	0	17,19,21	0.75	0
2	NAG	O	1	2,1	14,14,15	0.32	0	17,19,21	1.34	2 (11%)
2	NAG	O	2	2	14,14,15	0.34	0	17,19,21	0.75	0
5	NAG	P	1	5,1	14,14,15	0.35	0	17,19,21	1.00	1 (5%)
5	NAG	P	2	5	14,14,15	0.36	0	17,19,21	0.96	1 (5%)
5	BMA	P	3	5	11,11,12	0.41	0	15,15,17	0.86	1 (6%)
5	MAN	P	4	5	11,11,12	0.44	0	15,15,17	0.86	1 (6%)
5	NAG	Q	1	5,1	14,14,15	0.35	0	17,19,21	1.00	1 (5%)
5	NAG	Q	2	5	14,14,15	0.35	0	17,19,21	0.96	1 (5%)
5	BMA	Q	3	5	11,11,12	0.40	0	15,15,17	0.86	1 (6%)
5	MAN	Q	4	5	11,11,12	0.45	0	15,15,17	0.85	1 (6%)
5	NAG	R	1	5,1	14,14,15	0.35	0	17,19,21	1.00	1 (5%)
5	NAG	R	2	5	14,14,15	0.37	0	17,19,21	0.95	1 (5%)
5	BMA	R	3	5	11,11,12	0.40	0	15,15,17	0.86	1 (6%)
5	MAN	R	4	5	11,11,12	0.44	0	15,15,17	0.86	1 (6%)
3	NAG	S	1	3,1	14,14,15	0.42	0	17,19,21	1.41	2 (11%)
3	NAG	S	2	3	14,14,15	0.41	0	17,19,21	1.55	3 (17%)
3	BMA	S	3	3	11,11,12	0.33	0	15,15,17	0.64	0
3	NAG	T	1	3,1	14,14,15	0.44	0	17,19,21	1.41	2 (11%)
3	NAG	T	2	3	14,14,15	0.41	0	17,19,21	1.55	3 (17%)
3	BMA	T	3	3	11,11,12	0.34	0	15,15,17	0.65	0
3	NAG	U	1	3,1	14,14,15	0.43	0	17,19,21	1.40	2 (11%)
3	NAG	U	2	3	14,14,15	0.41	0	17,19,21	1.55	3 (17%)
3	BMA	U	3	3	11,11,12	0.34	0	15,15,17	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	V	1	4,1	14,14,15	0.49	0	17,19,21	1.10	1 (5%)
4	NAG	V	2	4	14,14,15	0.31	0	17,19,21	0.78	0
4	BMA	V	3	4	11,11,12	0.36	0	15,15,17	0.78	0
4	MAN	V	4	4	11,11,12	0.65	0	15,15,17	1.38	2 (13%)
4	NAG	V	5	4	14,14,15	0.26	0	17,19,21	0.88	0
4	MAN	V	6	4	11,11,12	0.36	0	15,15,17	0.87	1 (6%)
4	NAG	W	1	4,1	14,14,15	0.48	0	17,19,21	1.08	1 (5%)
4	NAG	W	2	4	14,14,15	0.30	0	17,19,21	0.80	0
4	BMA	W	3	4	11,11,12	0.36	0	15,15,17	0.76	0
4	MAN	W	4	4	11,11,12	0.66	0	15,15,17	1.38	2 (13%)
4	NAG	W	5	4	14,14,15	0.28	0	17,19,21	0.88	0
4	MAN	W	6	4	11,11,12	0.35	0	15,15,17	0.86	1 (6%)
4	NAG	X	1	4,1	14,14,15	0.48	0	17,19,21	1.10	1 (5%)
4	NAG	X	2	4	14,14,15	0.28	0	17,19,21	0.78	0
4	BMA	X	3	4	11,11,12	0.36	0	15,15,17	0.78	0
4	MAN	X	4	4	11,11,12	0.63	0	15,15,17	1.38	2 (13%)
4	NAG	X	5	4	14,14,15	0.25	0	17,19,21	0.88	1 (5%)
4	MAN	X	6	4	11,11,12	0.35	0	15,15,17	0.87	1 (6%)
2	NAG	Y	1	2,1	14,14,15	0.40	0	17,19,21	0.75	0
2	NAG	Y	2	2	14,14,15	0.31	0	17,19,21	1.00	2 (11%)
2	NAG	Z	1	2,1	14,14,15	0.41	0	17,19,21	0.75	0
2	NAG	Z	2	2	14,14,15	0.32	0	17,19,21	0.99	1 (5%)
2	NAG	a	1	2,1	14,14,15	0.41	0	17,19,21	0.76	0
2	NAG	a	2	2	14,14,15	0.30	0	17,19,21	1.00	2 (11%)
2	NAG	b	1	2,1	14,14,15	0.38	0	17,19,21	0.79	0
2	NAG	b	2	2	14,14,15	0.31	0	17,19,21	1.15	2 (11%)
2	NAG	c	1	2,1	14,14,15	0.37	0	17,19,21	0.79	0
2	NAG	c	2	2	14,14,15	0.30	0	17,19,21	1.16	2 (11%)
2	NAG	d	1	2,1	14,14,15	0.37	0	17,19,21	0.79	0
2	NAG	d	2	2	14,14,15	0.30	0	17,19,21	1.15	2 (11%)
6	NAG	e	1	6,1	14,14,15	0.38	0	17,19,21	1.17	1 (5%)
6	NAG	e	2	6	14,14,15	0.43	0	17,19,21	0.85	0
6	BMA	e	3	6	11,11,12	0.37	0	15,15,17	0.64	0
6	MAN	e	4	6	11,11,12	0.35	0	15,15,17	0.79	0
6	MAN	e	5	6	11,11,12	0.33	0	15,15,17	0.94	1 (6%)
6	MAN	e	6	6	11,11,12	0.35	0	15,15,17	0.88	1 (6%)
6	MAN	e	7	6	11,11,12	0.40	0	15,15,17	0.69	0
6	MAN	e	8	6	11,11,12	0.33	0	15,15,17	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	f	1	6,1	14,14,15	0.37	0	17,19,21	1.17	1 (5%)
6	NAG	f	2	6	14,14,15	0.45	0	17,19,21	0.84	0
6	BMA	f	3	6	11,11,12	0.38	0	15,15,17	0.64	0
6	MAN	f	4	6	11,11,12	0.36	0	15,15,17	0.80	0
6	MAN	f	5	6	11,11,12	0.34	0	15,15,17	0.94	1 (6%)
6	MAN	f	6	6	11,11,12	0.35	0	15,15,17	0.87	1 (6%)
6	MAN	f	7	6	11,11,12	0.40	0	15,15,17	0.67	0
6	MAN	f	8	6	11,11,12	0.34	0	15,15,17	0.69	0
6	NAG	g	1	6,1	14,14,15	0.37	0	17,19,21	1.18	1 (5%)
6	NAG	g	2	6	14,14,15	0.44	0	17,19,21	0.83	0
6	BMA	g	3	6	11,11,12	0.37	0	15,15,17	0.64	0
6	MAN	g	4	6	11,11,12	0.36	0	15,15,17	0.80	0
6	MAN	g	5	6	11,11,12	0.34	0	15,15,17	0.94	1 (6%)
6	MAN	g	6	6	11,11,12	0.36	0	15,15,17	0.88	1 (6%)
6	MAN	g	7	6	11,11,12	0.40	0	15,15,17	0.68	0
6	MAN	g	8	6	11,11,12	0.33	0	15,15,17	0.70	0
7	NAG	h	1	7,1	14,14,15	0.54	0	17,19,21	1.05	0
7	NAG	h	2	7	14,14,15	0.48	0	17,19,21	0.81	0
7	BMA	h	3	7	11,11,12	0.40	0	15,15,17	0.66	0
7	MAN	h	4	7	11,11,12	0.38	0	15,15,17	0.86	1 (6%)
7	MAN	h	5	7	11,11,12	0.33	0	15,15,17	0.85	1 (6%)
7	MAN	h	6	7	11,11,12	0.36	0	15,15,17	0.76	1 (6%)
7	NAG	i	1	7,1	14,14,15	0.52	0	17,19,21	1.07	0
7	NAG	i	2	7	14,14,15	0.49	0	17,19,21	0.81	0
7	BMA	i	3	7	11,11,12	0.39	0	15,15,17	0.66	0
7	MAN	i	4	7	11,11,12	0.38	0	15,15,17	0.86	1 (6%)
7	MAN	i	5	7	11,11,12	0.32	0	15,15,17	0.86	1 (6%)
7	MAN	i	6	7	11,11,12	0.37	0	15,15,17	0.76	1 (6%)
7	NAG	j	1	7,1	14,14,15	0.52	0	17,19,21	1.06	0
7	NAG	j	2	7	14,14,15	0.49	0	17,19,21	0.82	0
7	BMA	j	3	7	11,11,12	0.40	0	15,15,17	0.66	0
7	MAN	j	4	7	11,11,12	0.38	0	15,15,17	0.87	1 (6%)
7	MAN	j	5	7	11,11,12	0.33	0	15,15,17	0.86	1 (6%)
7	MAN	j	6	7	11,11,12	0.36	0	15,15,17	0.77	1 (6%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	X	3	4	-	0/2/19/22	0/1/1/1
4	MAN	X	4	4	-	1/2/19/22	0/1/1/1
4	NAG	X	5	4	-	1/6/23/26	0/1/1/1
4	MAN	X	6	4	-	0/2/19/22	0/1/1/1
2	NAG	Y	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Y	2	2	-	1/6/23/26	0/1/1/1
2	NAG	Z	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	1/6/23/26	0/1/1/1
2	NAG	a	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	a	2	2	-	1/6/23/26	0/1/1/1
2	NAG	b	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	b	2	2	-	4/6/23/26	0/1/1/1
2	NAG	c	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	c	2	2	-	4/6/23/26	0/1/1/1
2	NAG	d	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	d	2	2	-	4/6/23/26	0/1/1/1
6	NAG	e	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	e	2	6	-	2/6/23/26	0/1/1/1
6	BMA	e	3	6	-	0/2/19/22	0/1/1/1
6	MAN	e	4	6	-	0/2/19/22	0/1/1/1
6	MAN	e	5	6	-	0/2/19/22	0/1/1/1
6	MAN	e	6	6	-	0/2/19/22	0/1/1/1
6	MAN	e	7	6	-	0/2/19/22	0/1/1/1
6	MAN	e	8	6	-	0/2/19/22	0/1/1/1
6	NAG	f	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	f	2	6	-	2/6/23/26	0/1/1/1
6	BMA	f	3	6	-	0/2/19/22	0/1/1/1
6	MAN	f	4	6	-	0/2/19/22	0/1/1/1
6	MAN	f	5	6	-	0/2/19/22	0/1/1/1
6	MAN	f	6	6	-	0/2/19/22	0/1/1/1
6	MAN	f	7	6	-	0/2/19/22	0/1/1/1
6	MAN	f	8	6	-	0/2/19/22	0/1/1/1
6	NAG	g	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	g	2	6	-	2/6/23/26	0/1/1/1
6	BMA	g	3	6	-	0/2/19/22	0/1/1/1
6	MAN	g	4	6	-	0/2/19/22	0/1/1/1
6	MAN	g	5	6	-	0/2/19/22	0/1/1/1
6	MAN	g	6	6	-	0/2/19/22	0/1/1/1
6	MAN	g	7	6	-	0/2/19/22	0/1/1/1
6	MAN	g	8	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	h	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	h	2	7	-	0/6/23/26	0/1/1/1
7	BMA	h	3	7	-	0/2/19/22	0/1/1/1
7	MAN	h	4	7	-	1/2/19/22	0/1/1/1
7	MAN	h	5	7	-	0/2/19/22	0/1/1/1
7	MAN	h	6	7	-	0/2/19/22	0/1/1/1
7	NAG	i	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	i	2	7	-	0/6/23/26	0/1/1/1
7	BMA	i	3	7	-	0/2/19/22	0/1/1/1
7	MAN	i	4	7	-	1/2/19/22	0/1/1/1
7	MAN	i	5	7	-	0/2/19/22	0/1/1/1
7	MAN	i	6	7	-	0/2/19/22	0/1/1/1
7	NAG	j	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	j	2	7	-	0/6/23/26	0/1/1/1
7	BMA	j	3	7	-	0/2/19/22	0/1/1/1
7	MAN	j	4	7	-	1/2/19/22	0/1/1/1
7	MAN	j	5	7	-	0/2/19/22	0/1/1/1
7	MAN	j	6	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	4	MAN	O2-C2-C1	4.05	117.43	109.15
4	W	4	MAN	O2-C2-C1	4.04	117.41	109.15
4	X	4	MAN	O2-C2-C1	4.03	117.39	109.15
3	U	2	NAG	C2-N2-C7	3.85	128.38	122.90
3	T	2	NAG	C2-N2-C7	3.83	128.35	122.90
3	S	2	NAG	C2-N2-C7	3.79	128.30	122.90
4	V	1	NAG	C1-O5-C5	3.40	116.80	112.19
4	X	1	NAG	C1-O5-C5	3.39	116.79	112.19
4	W	1	NAG	C1-O5-C5	3.35	116.73	112.19
2	M	1	NAG	C1-O5-C5	3.34	116.72	112.19
2	O	1	NAG	C1-O5-C5	3.32	116.69	112.19
2	N	1	NAG	C1-O5-C5	3.30	116.66	112.19
3	S	1	NAG	C2-N2-C7	3.26	127.55	122.90
3	U	1	NAG	C2-N2-C7	3.25	127.53	122.90
3	T	1	NAG	C2-N2-C7	3.25	127.53	122.90
6	f	1	NAG	C1-O5-C5	3.00	116.26	112.19
6	g	1	NAG	C1-O5-C5	2.97	116.22	112.19
6	e	1	NAG	C1-O5-C5	2.95	116.19	112.19
5	Q	1	NAG	C1-C2-N2	-2.85	105.62	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	1	NAG	C1-C2-N2	-2.84	105.63	110.49
5	R	1	NAG	C1-C2-N2	-2.82	105.67	110.49
3	T	1	NAG	C8-C7-N2	2.82	120.87	116.10
4	X	4	MAN	C1-O5-C5	2.81	116.00	112.19
4	V	4	MAN	C1-O5-C5	2.81	116.00	112.19
3	S	1	NAG	C8-C7-N2	2.80	120.84	116.10
4	W	4	MAN	C1-O5-C5	2.80	115.98	112.19
3	U	1	NAG	C8-C7-N2	2.78	120.81	116.10
2	b	2	NAG	C2-N2-C7	2.76	126.83	122.90
2	d	2	NAG	C2-N2-C7	2.75	126.81	122.90
2	c	2	NAG	C2-N2-C7	2.73	126.79	122.90
3	S	2	NAG	C4-C3-C2	2.67	114.93	111.02
3	U	2	NAG	C4-C3-C2	2.65	114.90	111.02
6	g	5	MAN	C1-O5-C5	2.63	115.76	112.19
3	T	2	NAG	C4-C3-C2	2.63	114.87	111.02
2	M	1	NAG	O5-C1-C2	-2.63	107.14	111.29
6	f	5	MAN	C1-O5-C5	2.62	115.75	112.19
6	e	5	MAN	C1-O5-C5	2.61	115.73	112.19
2	O	1	NAG	O5-C1-C2	-2.57	107.23	111.29
2	N	1	NAG	O5-C1-C2	-2.56	107.24	111.29
7	j	4	MAN	C1-O5-C5	2.54	115.64	112.19
6	e	6	MAN	C1-O5-C5	2.50	115.58	112.19
7	i	4	MAN	C1-O5-C5	2.50	115.58	112.19
7	h	4	MAN	C1-O5-C5	2.49	115.57	112.19
5	P	2	NAG	C1-O5-C5	2.49	115.56	112.19
5	Q	2	NAG	C1-O5-C5	2.47	115.55	112.19
6	g	6	MAN	C1-O5-C5	2.46	115.52	112.19
6	f	6	MAN	C1-O5-C5	2.46	115.52	112.19
5	R	2	NAG	C1-O5-C5	2.44	115.50	112.19
3	S	2	NAG	C1-C2-N2	-2.44	106.33	110.49
3	T	2	NAG	C1-C2-N2	-2.42	106.35	110.49
2	c	2	NAG	C8-C7-N2	2.41	120.17	116.10
2	b	2	NAG	C8-C7-N2	2.40	120.15	116.10
3	U	2	NAG	C1-C2-N2	-2.39	106.40	110.49
2	d	2	NAG	C8-C7-N2	2.39	120.15	116.10
4	V	6	MAN	C1-O5-C5	2.36	115.39	112.19
7	i	5	MAN	C1-O5-C5	2.36	115.38	112.19
4	X	6	MAN	C1-O5-C5	2.35	115.38	112.19
4	W	6	MAN	C1-O5-C5	2.34	115.36	112.19
7	h	5	MAN	C1-O5-C5	2.33	115.35	112.19
7	j	5	MAN	C1-O5-C5	2.32	115.34	112.19
7	j	6	MAN	C1-O5-C5	2.28	115.28	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	h	6	MAN	C1-O5-C5	2.24	115.22	112.19
7	i	6	MAN	C1-O5-C5	2.23	115.22	112.19
5	Q	3	BMA	C1-O5-C5	2.14	115.09	112.19
5	R	3	BMA	C1-O5-C5	2.13	115.08	112.19
5	P	3	BMA	C1-O5-C5	2.13	115.08	112.19
5	P	4	MAN	C1-C2-C3	2.13	112.28	109.67
2	Y	2	NAG	O5-C1-C2	-2.11	107.96	111.29
2	Z	2	NAG	O5-C1-C2	-2.11	107.96	111.29
5	R	4	MAN	C1-C2-C3	2.09	112.24	109.67
2	a	2	NAG	O5-C1-C2	-2.09	107.98	111.29
5	Q	4	MAN	C1-C2-C3	2.07	112.22	109.67
2	a	2	NAG	C1-O5-C5	2.04	114.96	112.19
2	Y	2	NAG	C1-O5-C5	2.01	114.92	112.19
4	X	5	NAG	O5-C1-C2	-2.00	108.12	111.29

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	U	2	NAG	C3-C2-N2-C7
3	S	2	NAG	C3-C2-N2-C7
3	T	2	NAG	C3-C2-N2-C7
2	b	1	NAG	O5-C5-C6-O6
2	c	1	NAG	O5-C5-C6-O6
2	d	1	NAG	O5-C5-C6-O6
2	b	1	NAG	C4-C5-C6-O6
2	c	1	NAG	C4-C5-C6-O6
2	d	1	NAG	C4-C5-C6-O6
2	b	2	NAG	C8-C7-N2-C2
2	b	2	NAG	O7-C7-N2-C2
2	c	2	NAG	C8-C7-N2-C2
2	c	2	NAG	O7-C7-N2-C2
2	d	2	NAG	C8-C7-N2-C2
2	d	2	NAG	O7-C7-N2-C2
3	U	1	NAG	C8-C7-N2-C2
3	U	1	NAG	O7-C7-N2-C2
3	S	1	NAG	C8-C7-N2-C2
3	S	1	NAG	O7-C7-N2-C2
3	T	1	NAG	C8-C7-N2-C2
3	T	1	NAG	O7-C7-N2-C2
6	g	2	NAG	C4-C5-C6-O6
6	e	2	NAG	C4-C5-C6-O6

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

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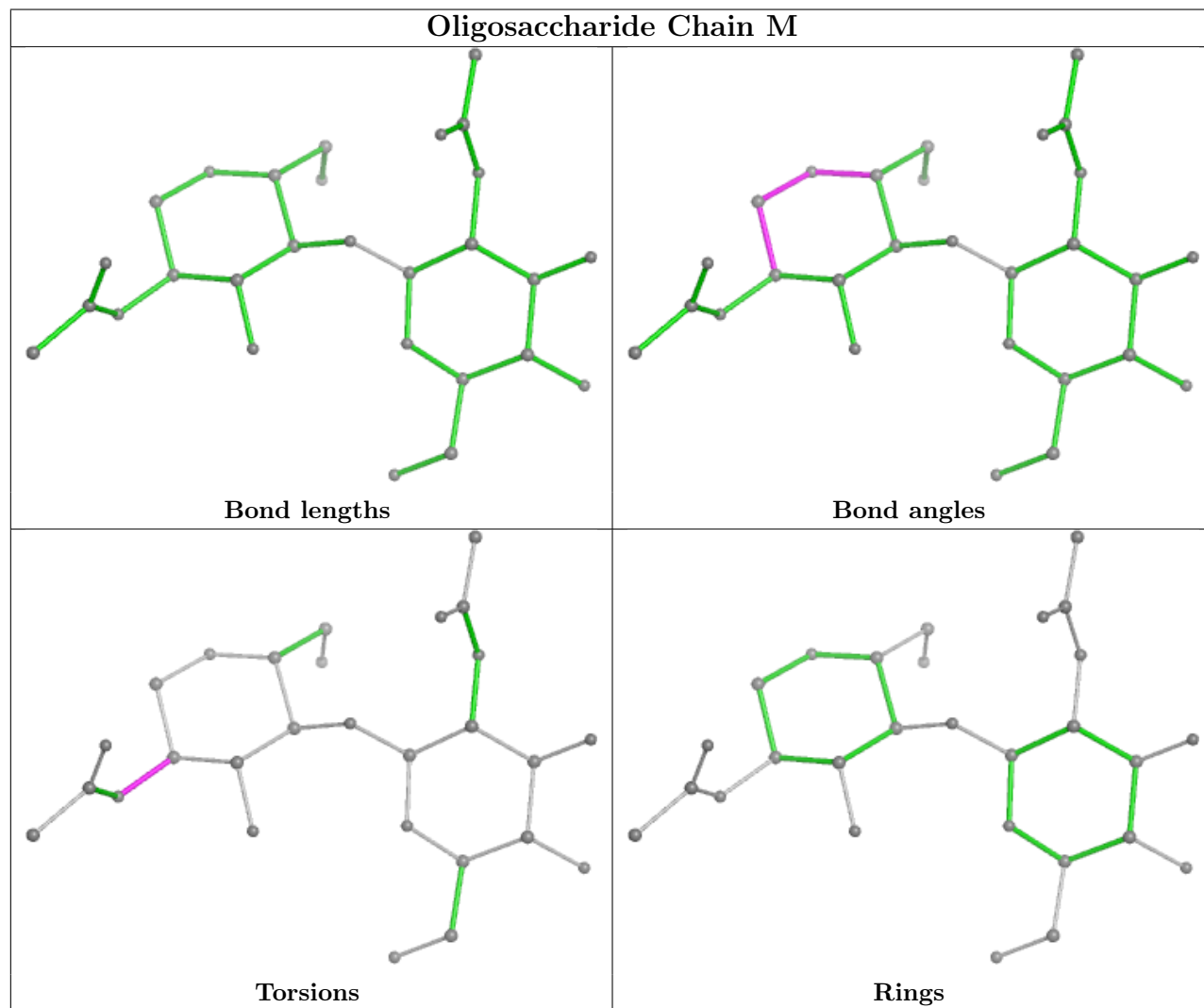
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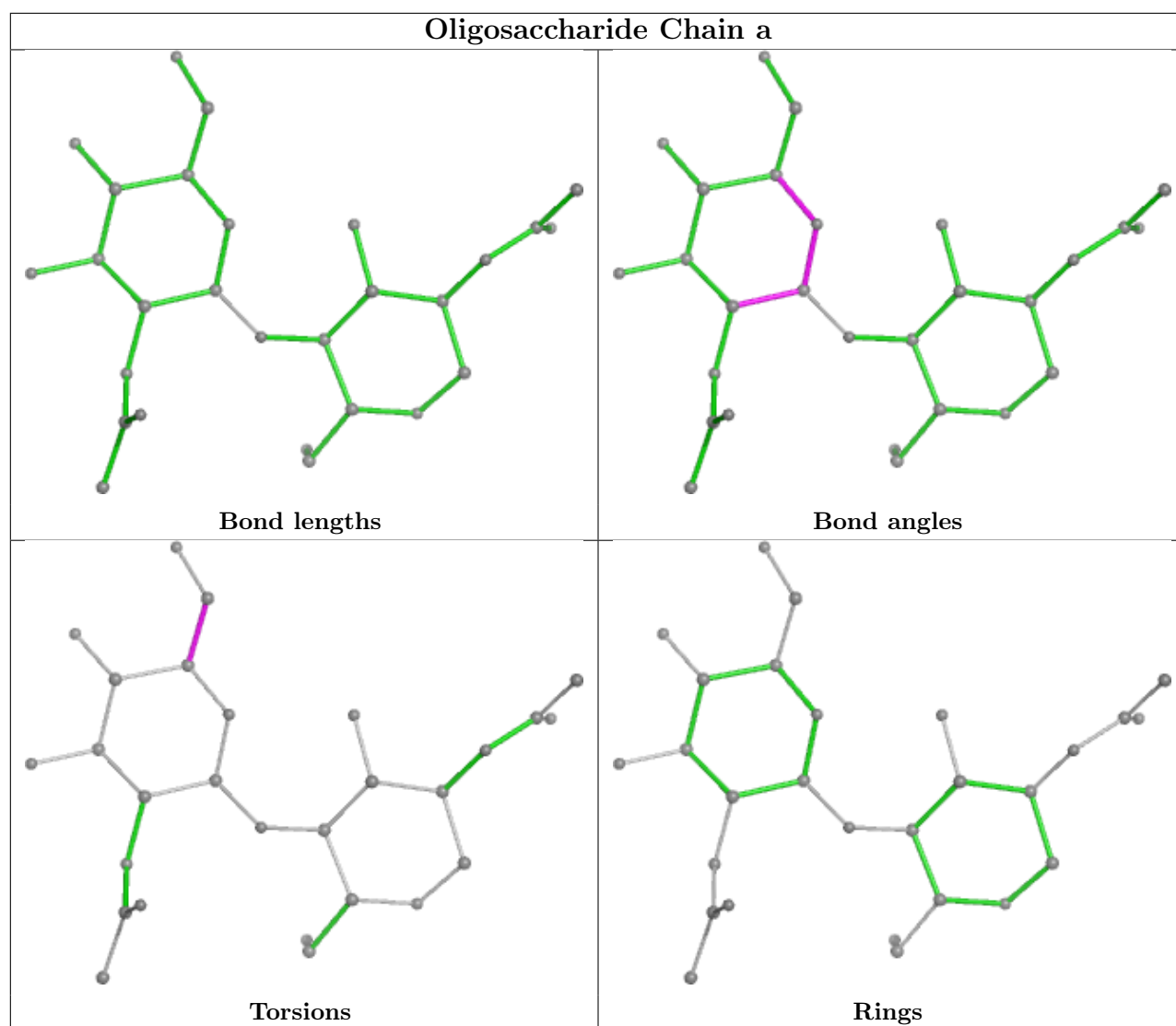
Mol	Chain	Res	Type	Atoms
3	T	2	NAG	C1-C2-N2-C7

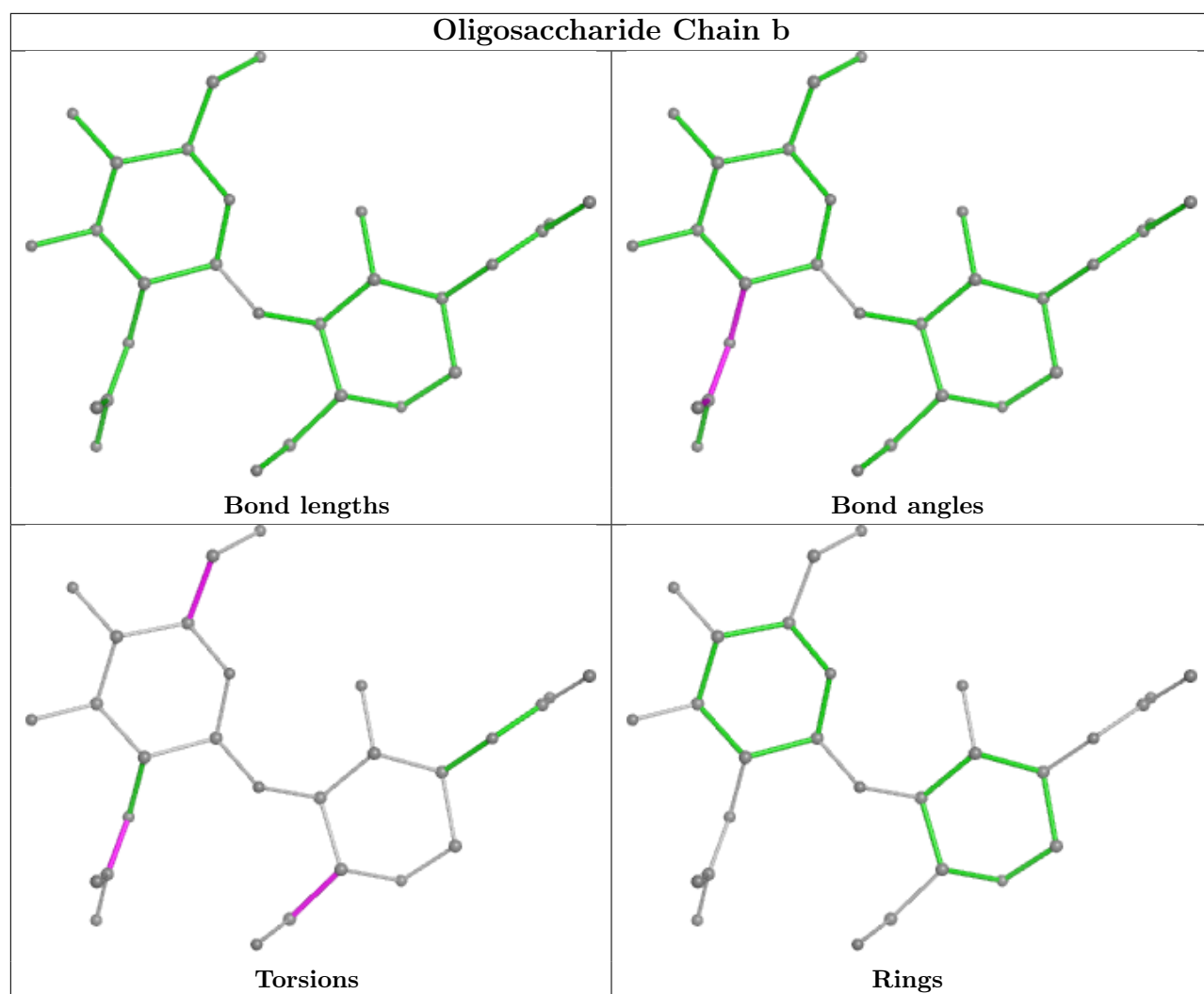
There are no ring outliers.

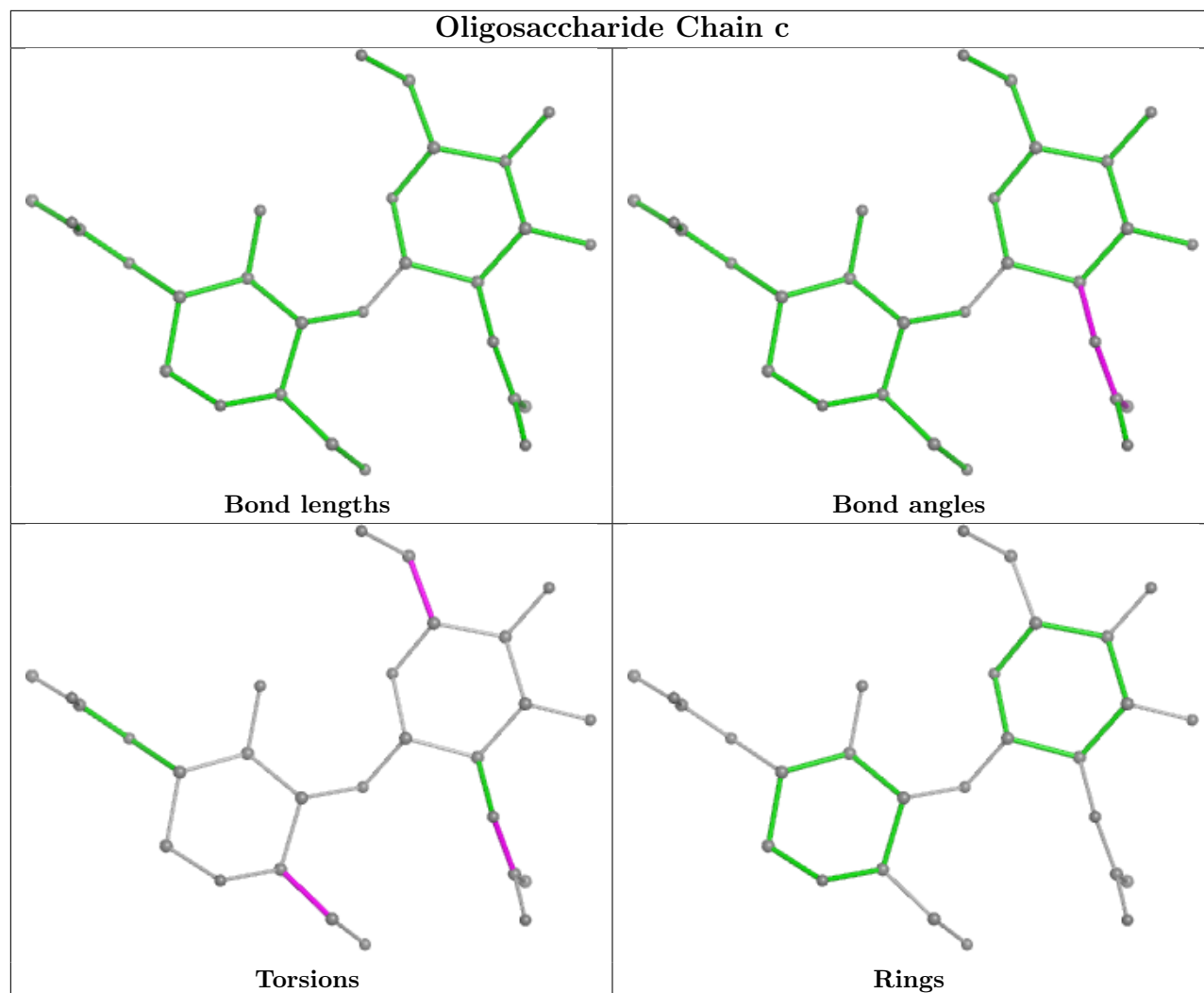
No monomer is involved in short contacts.

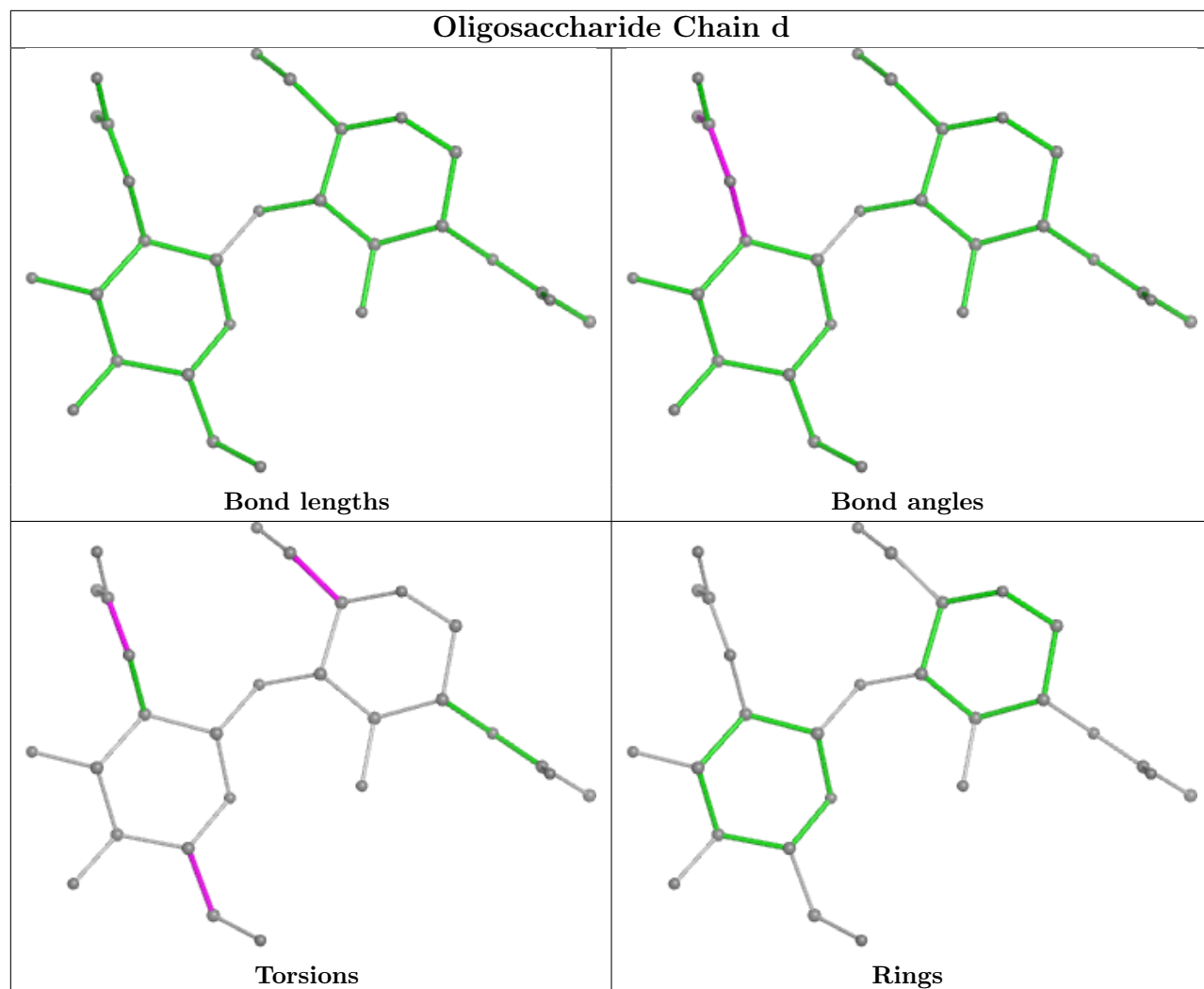
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

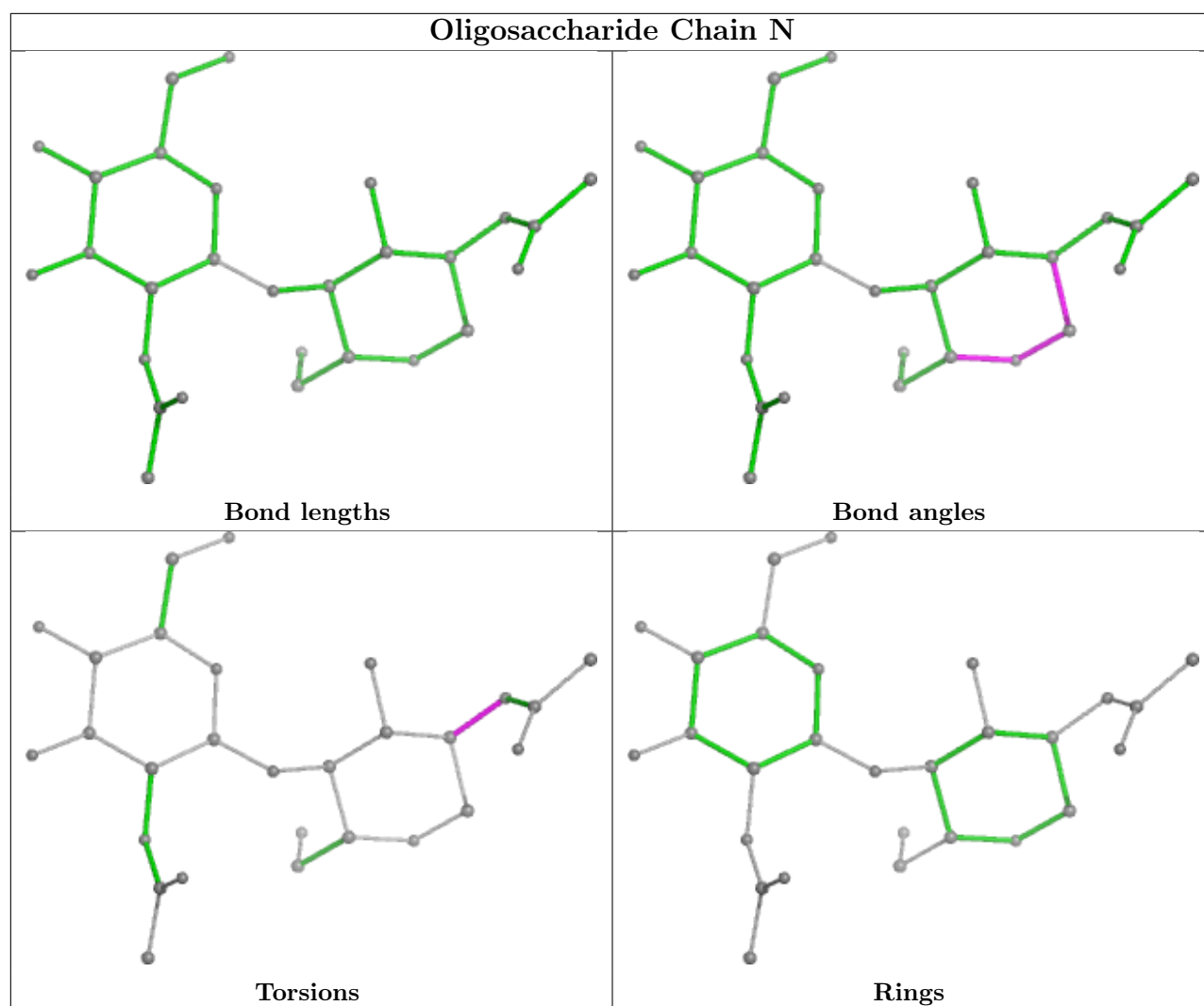


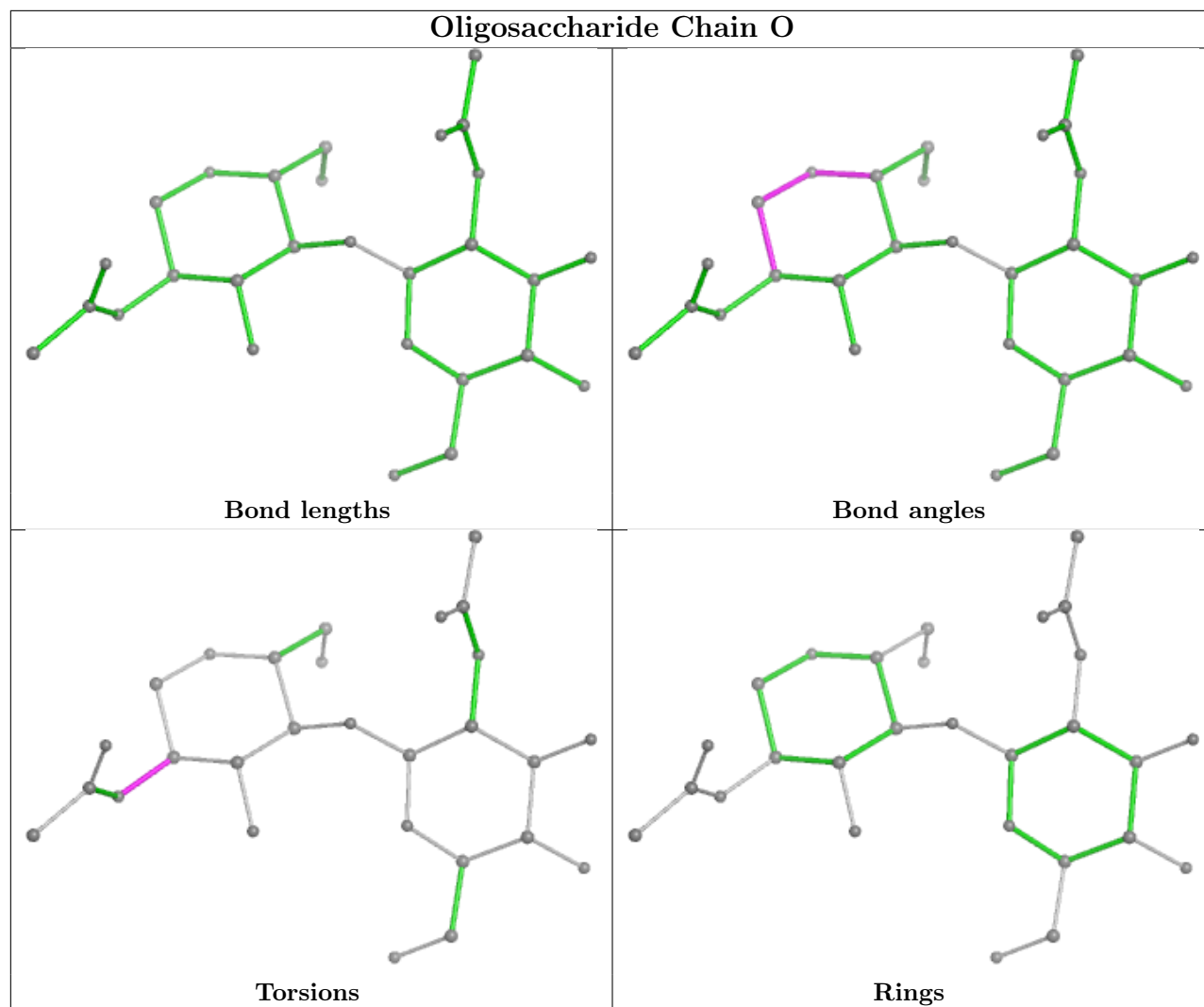


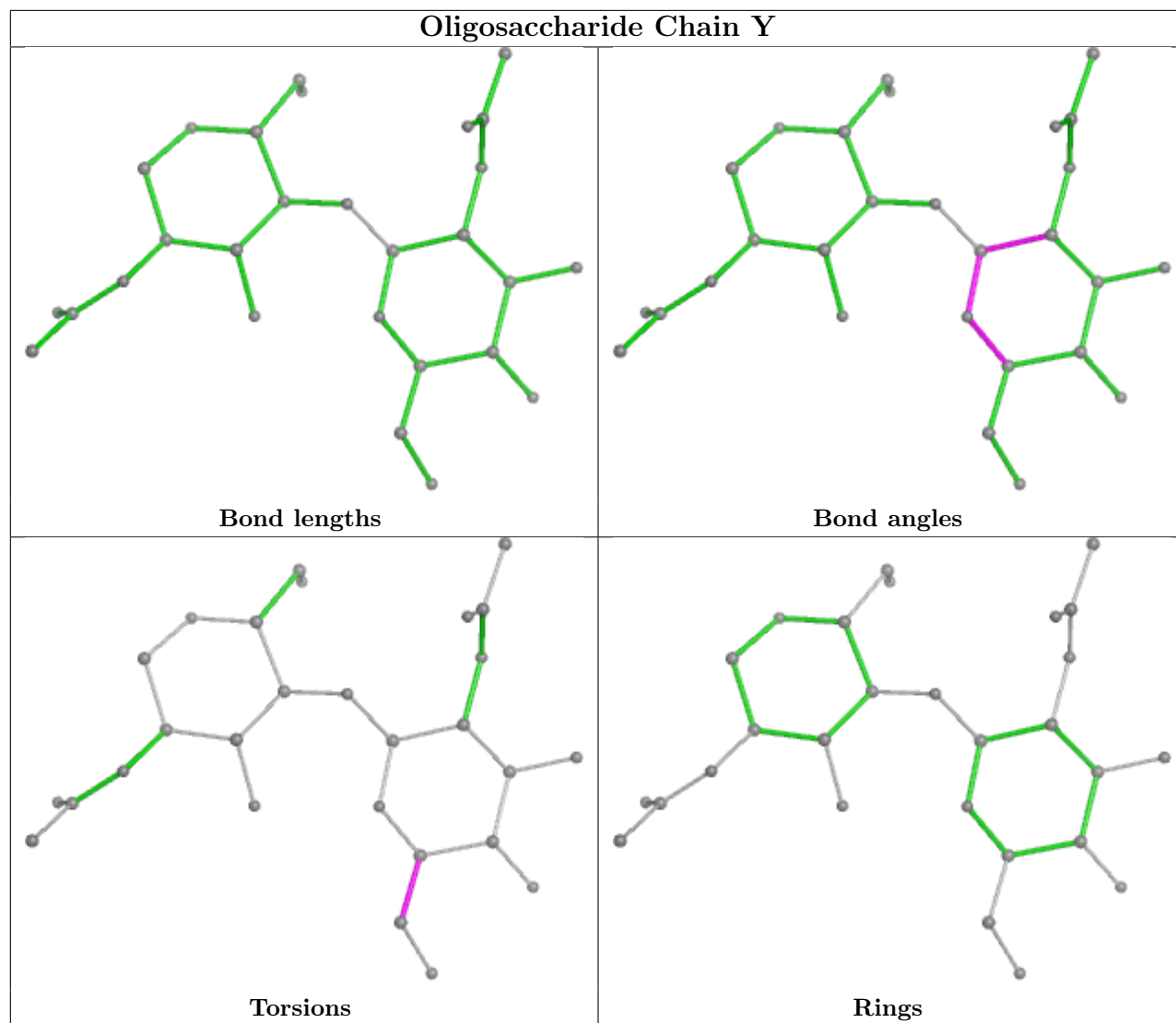


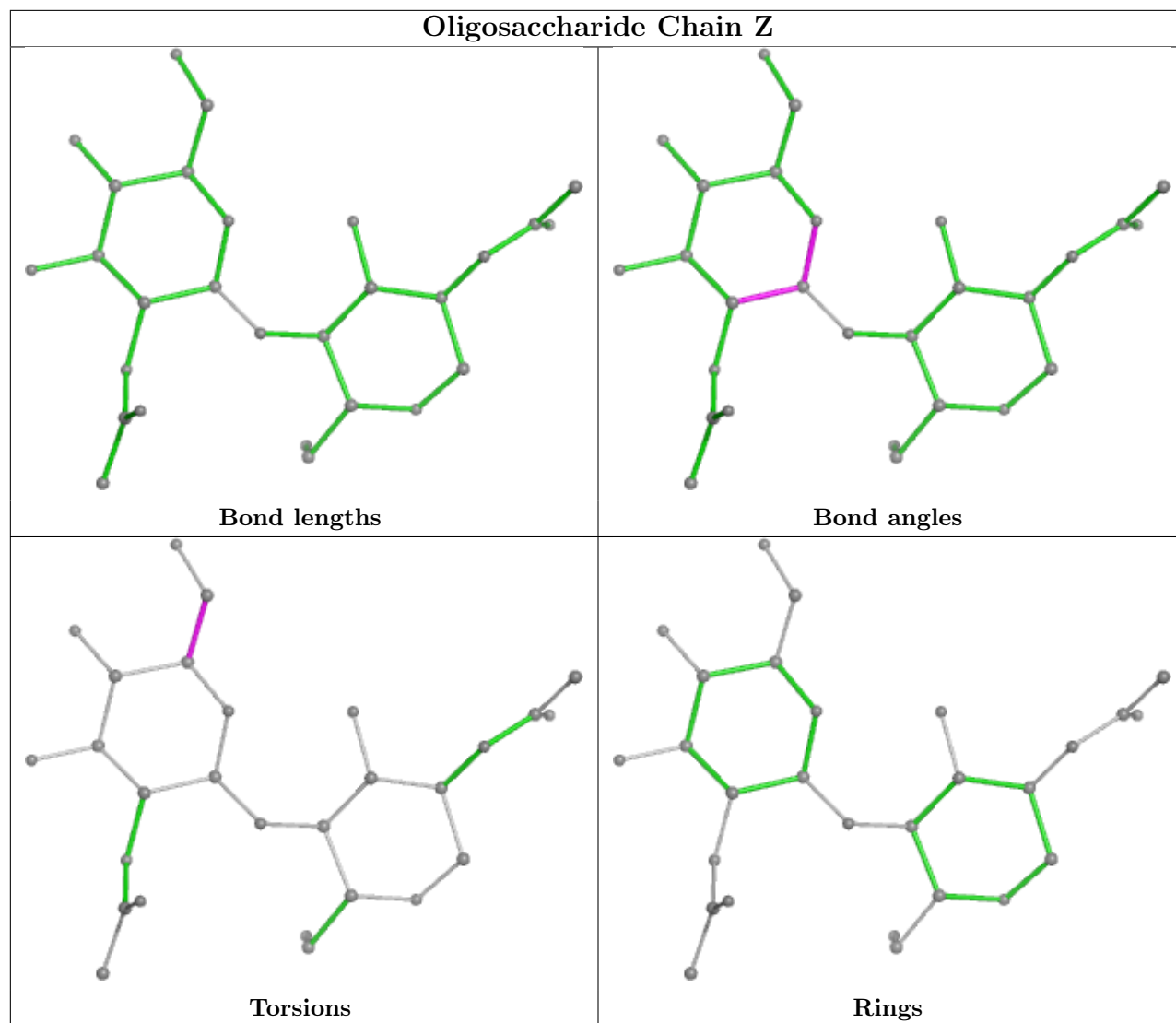


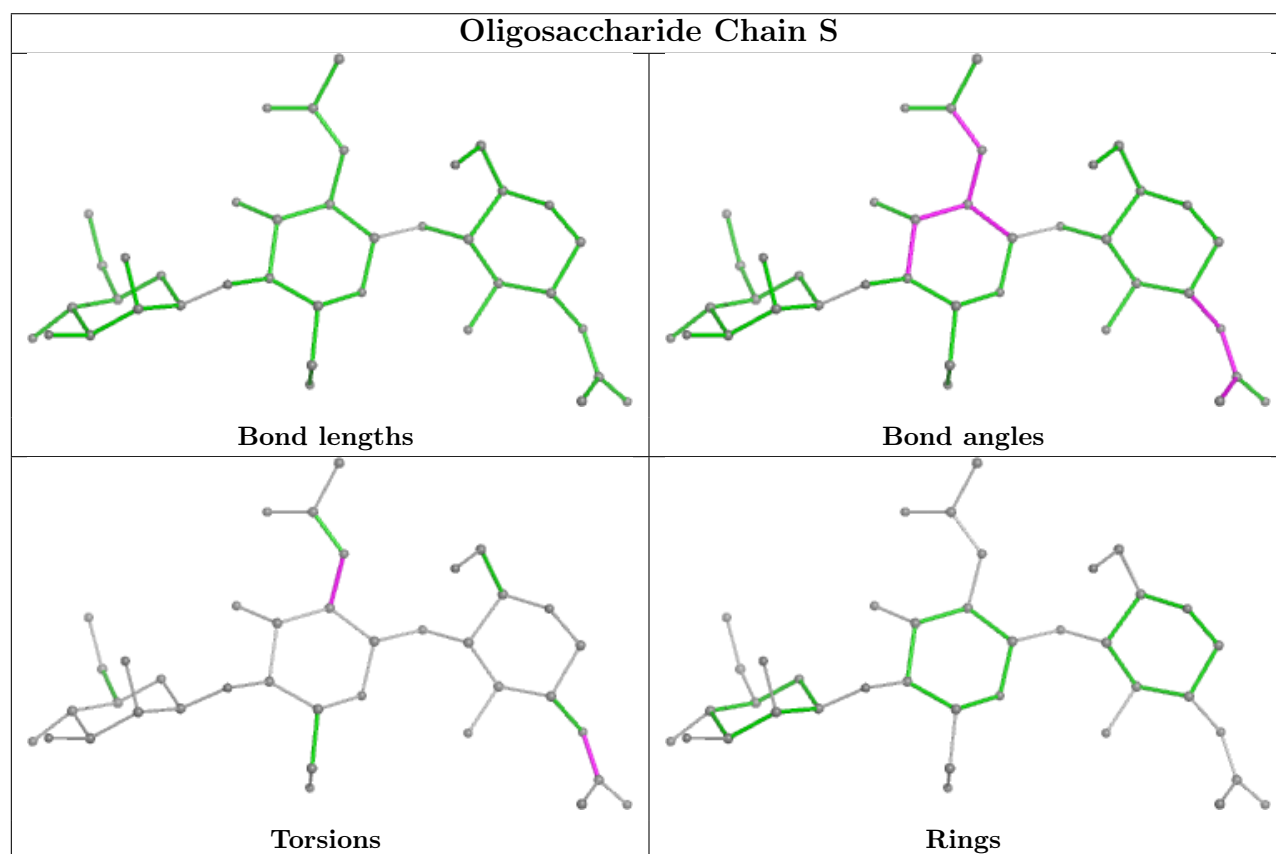
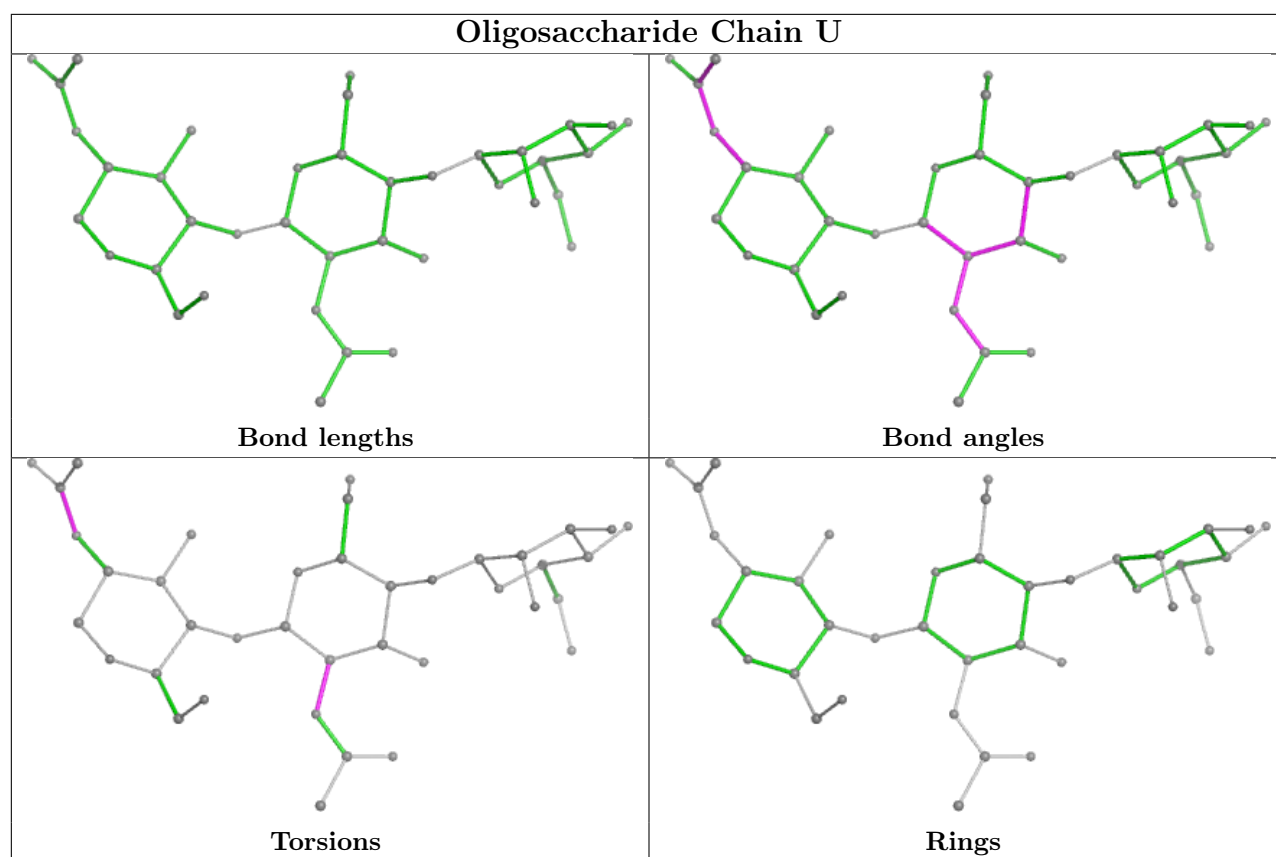


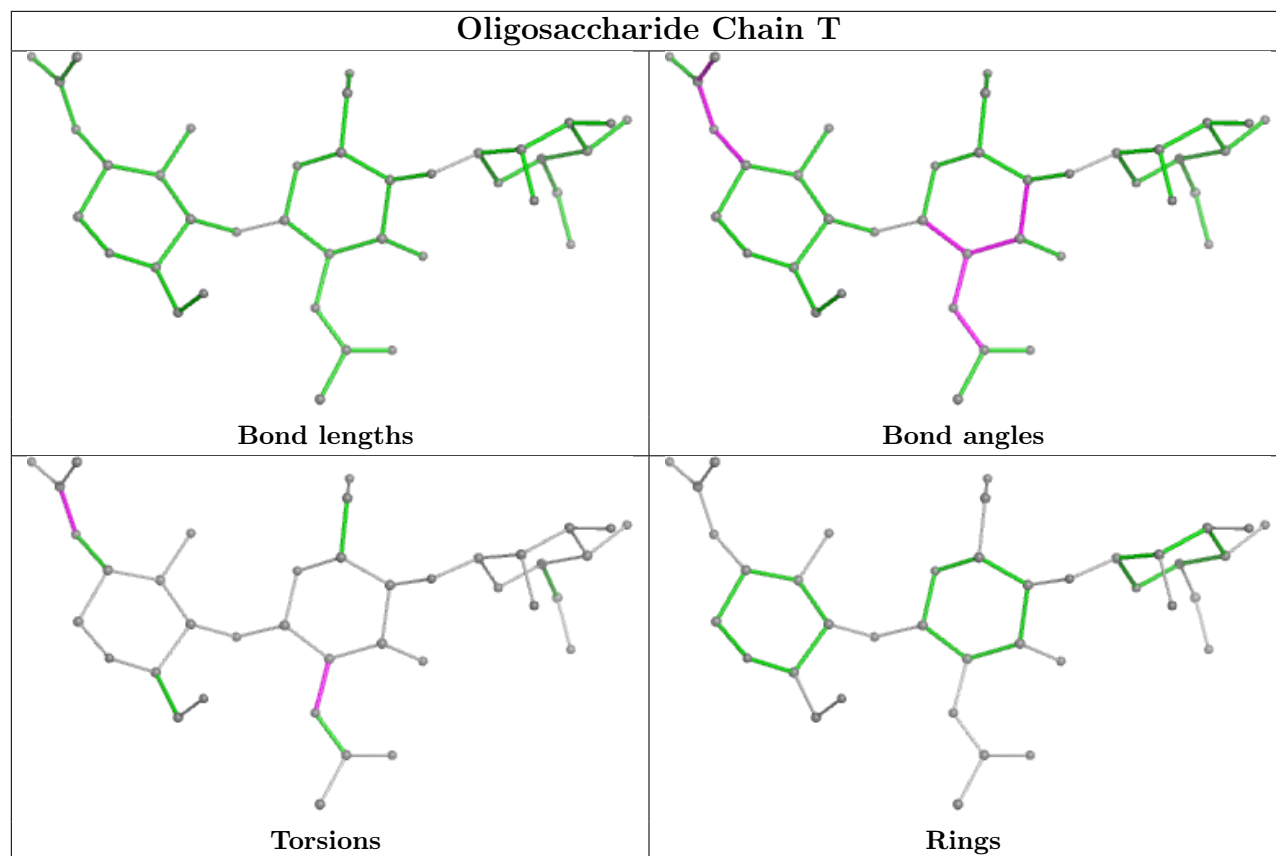


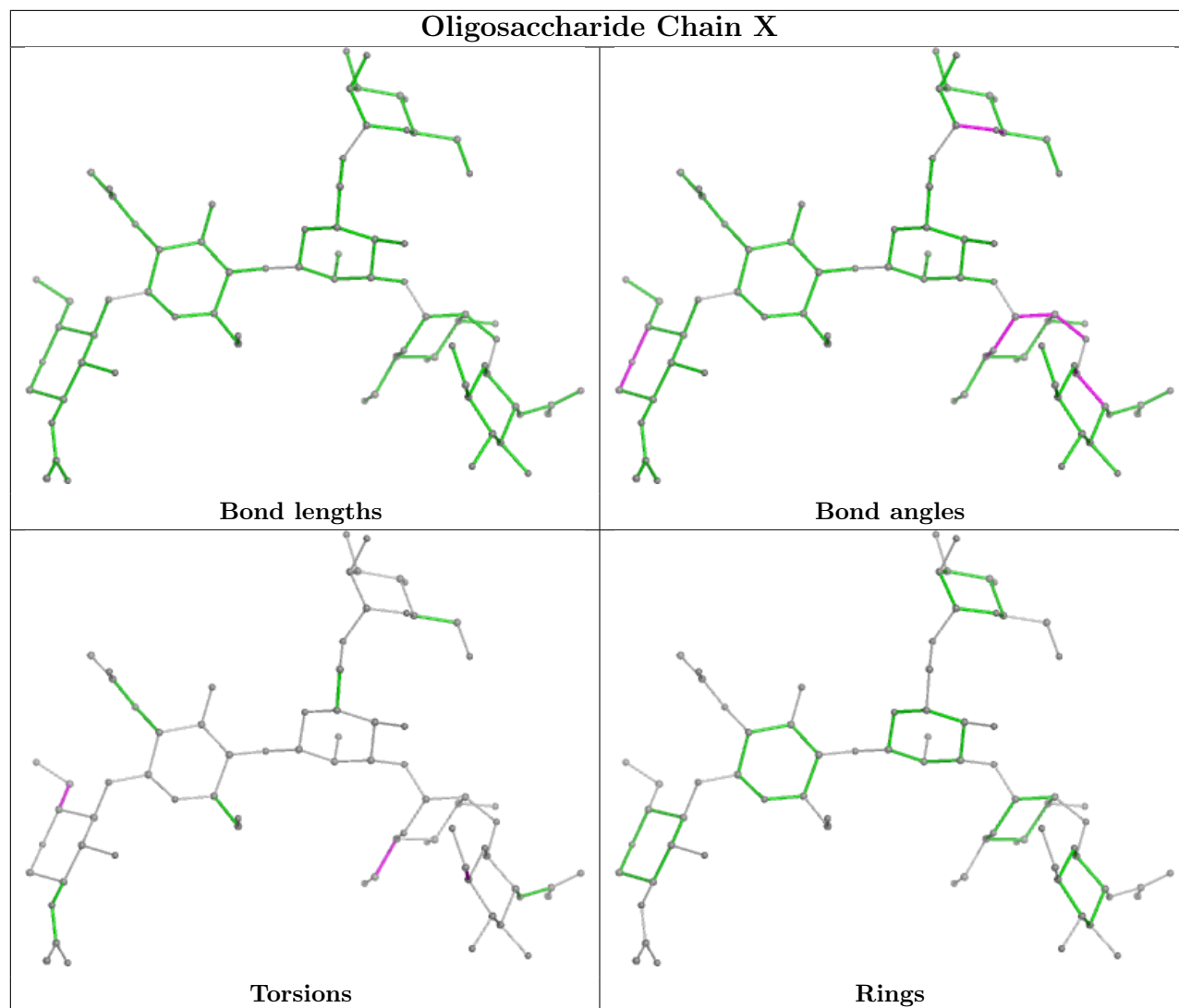


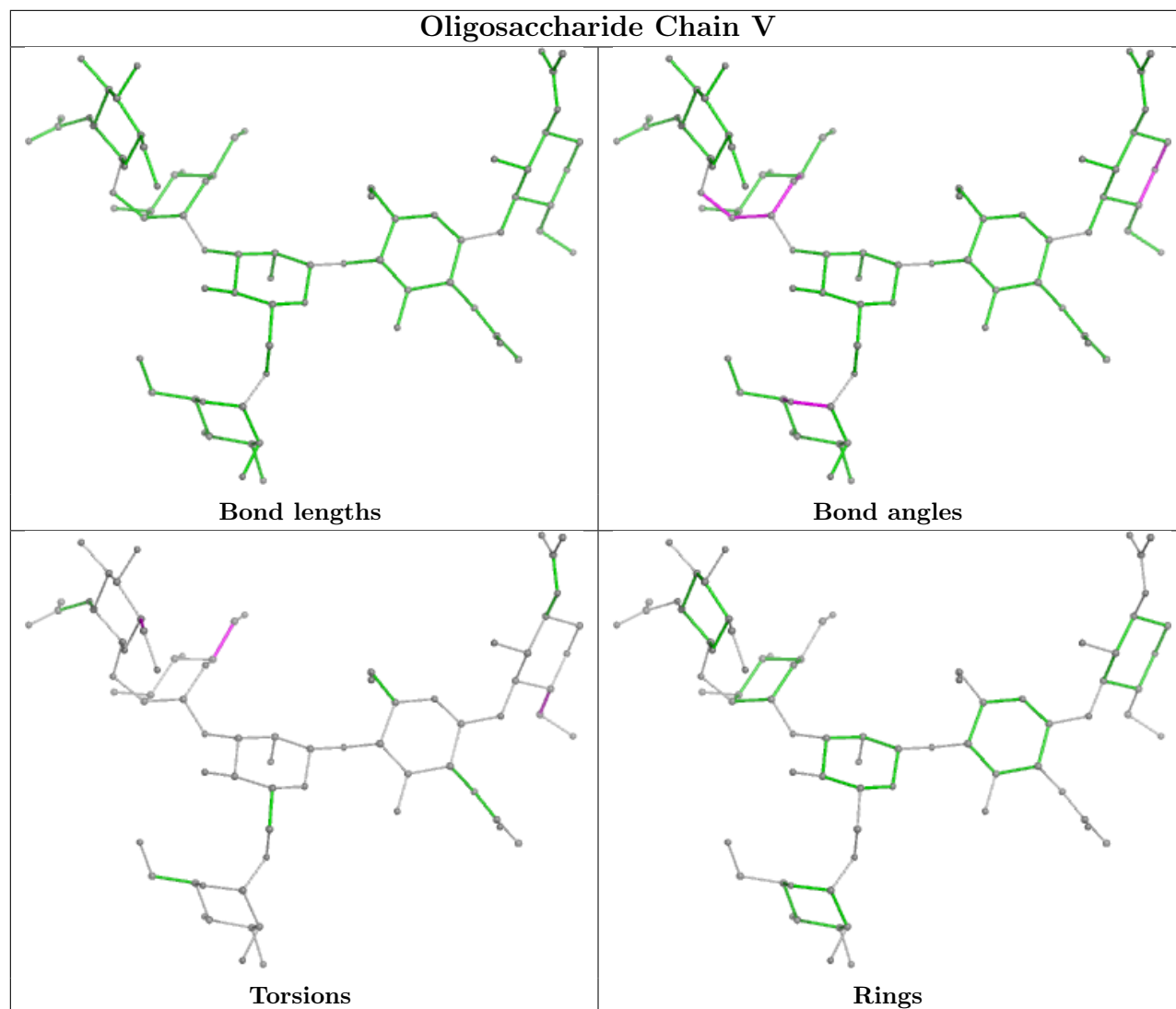


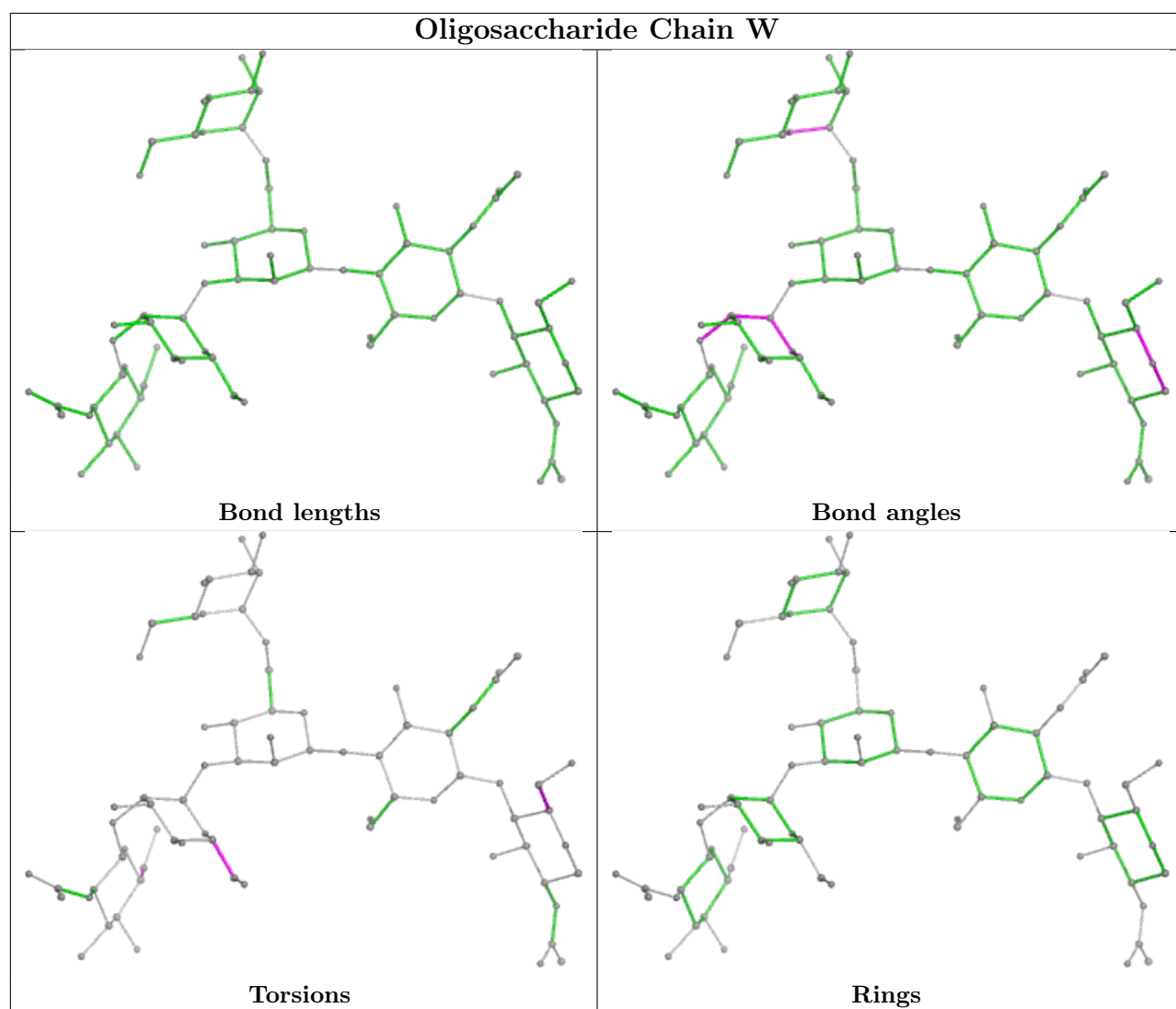


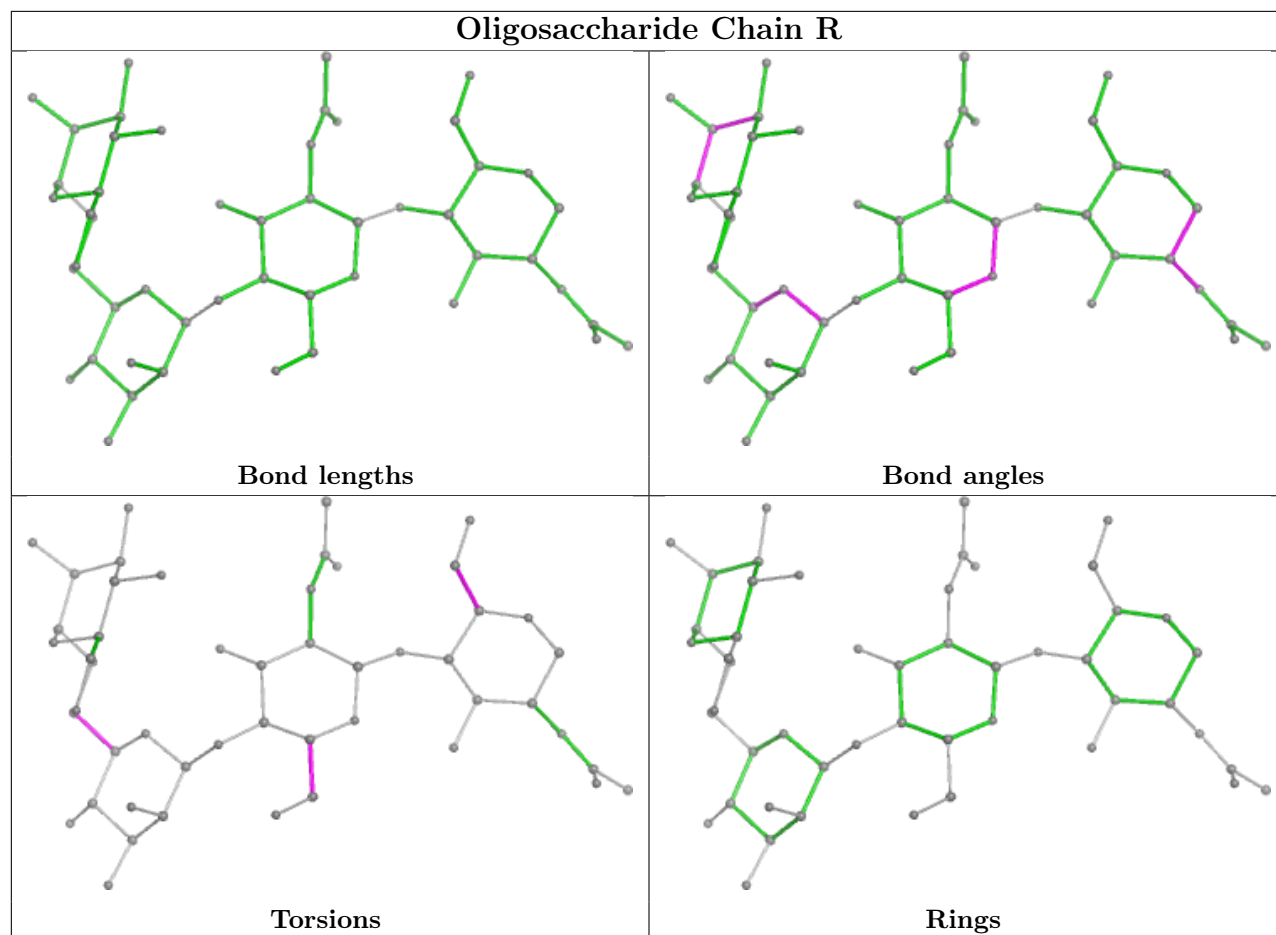


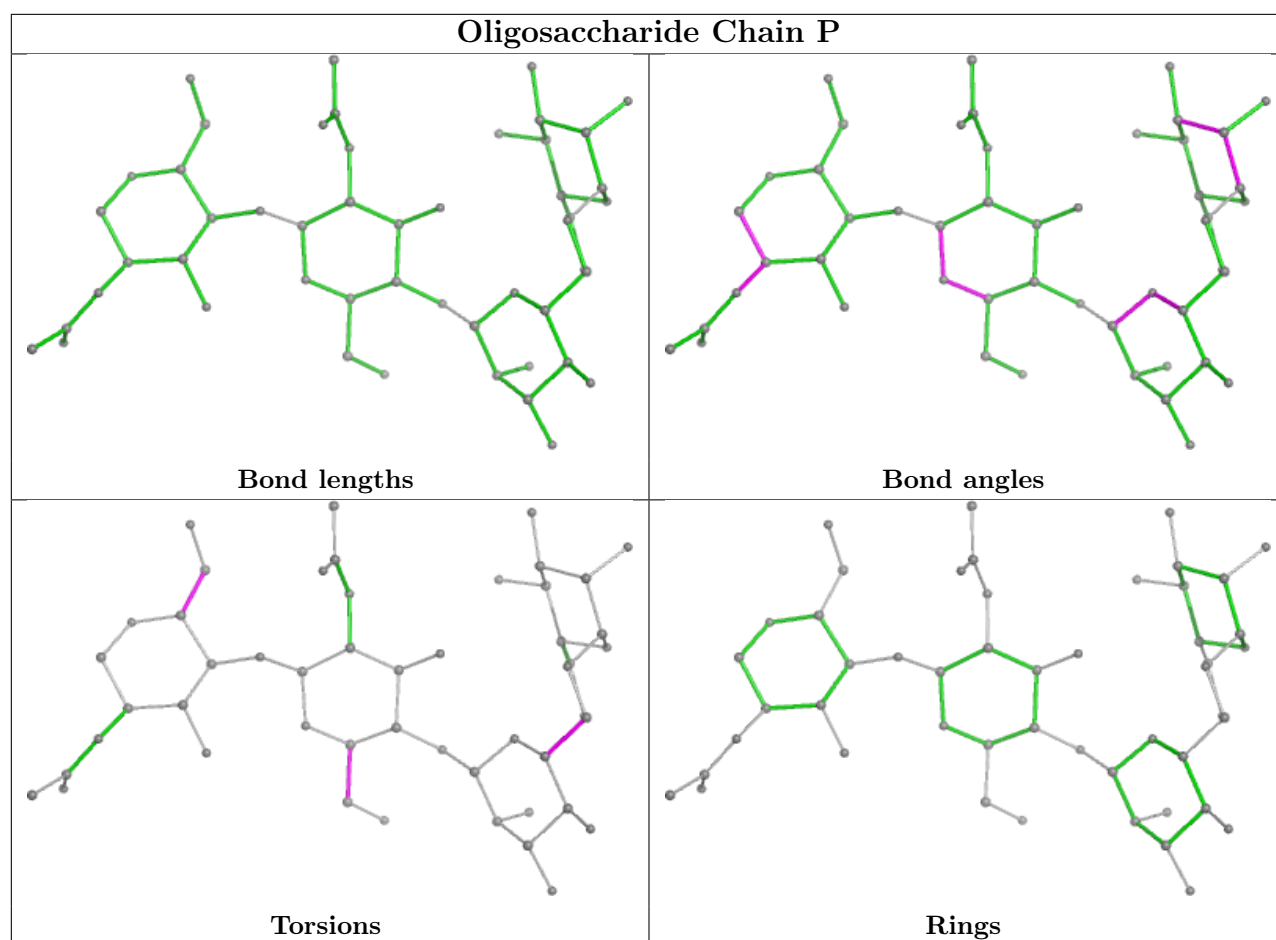


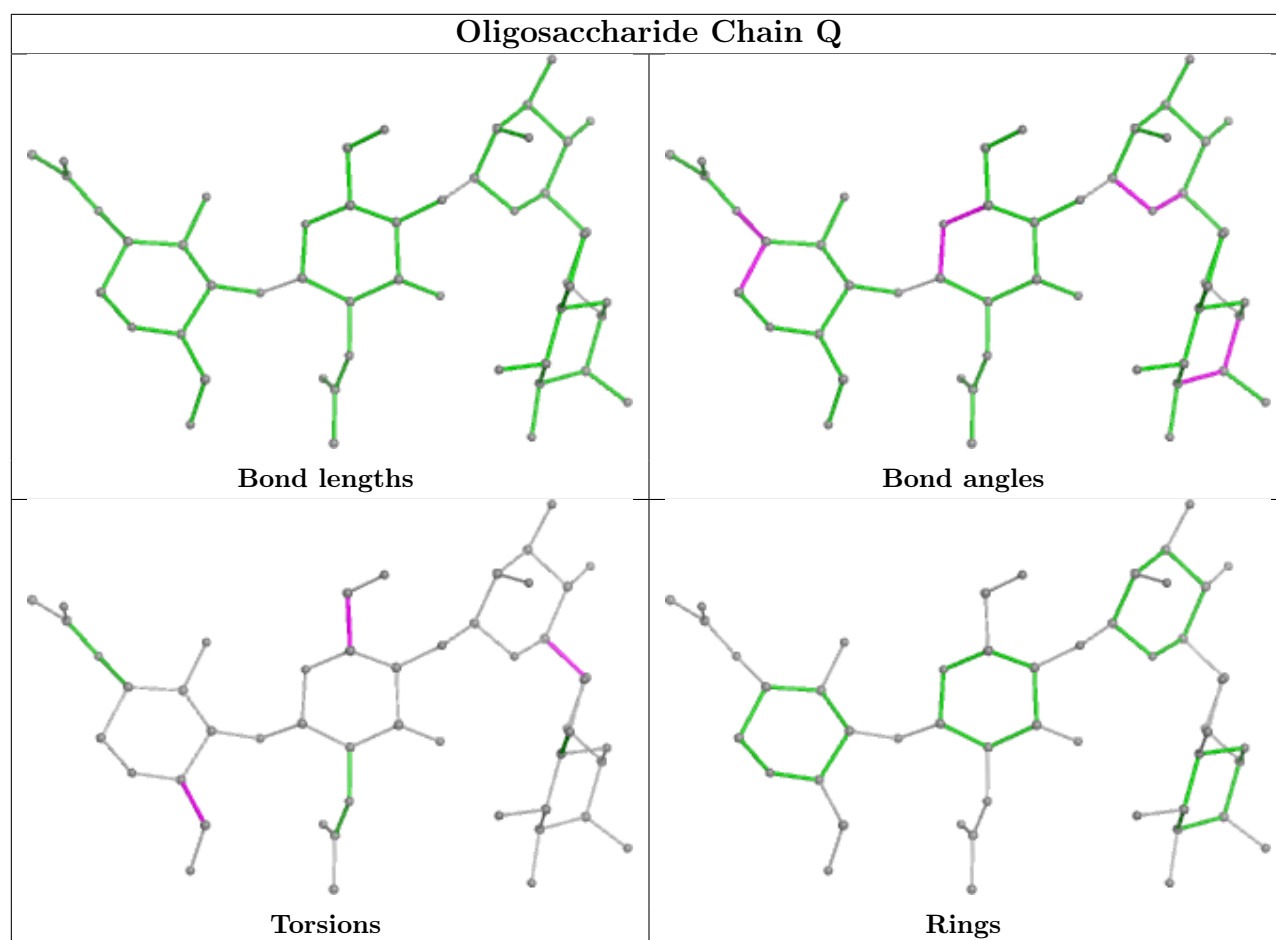


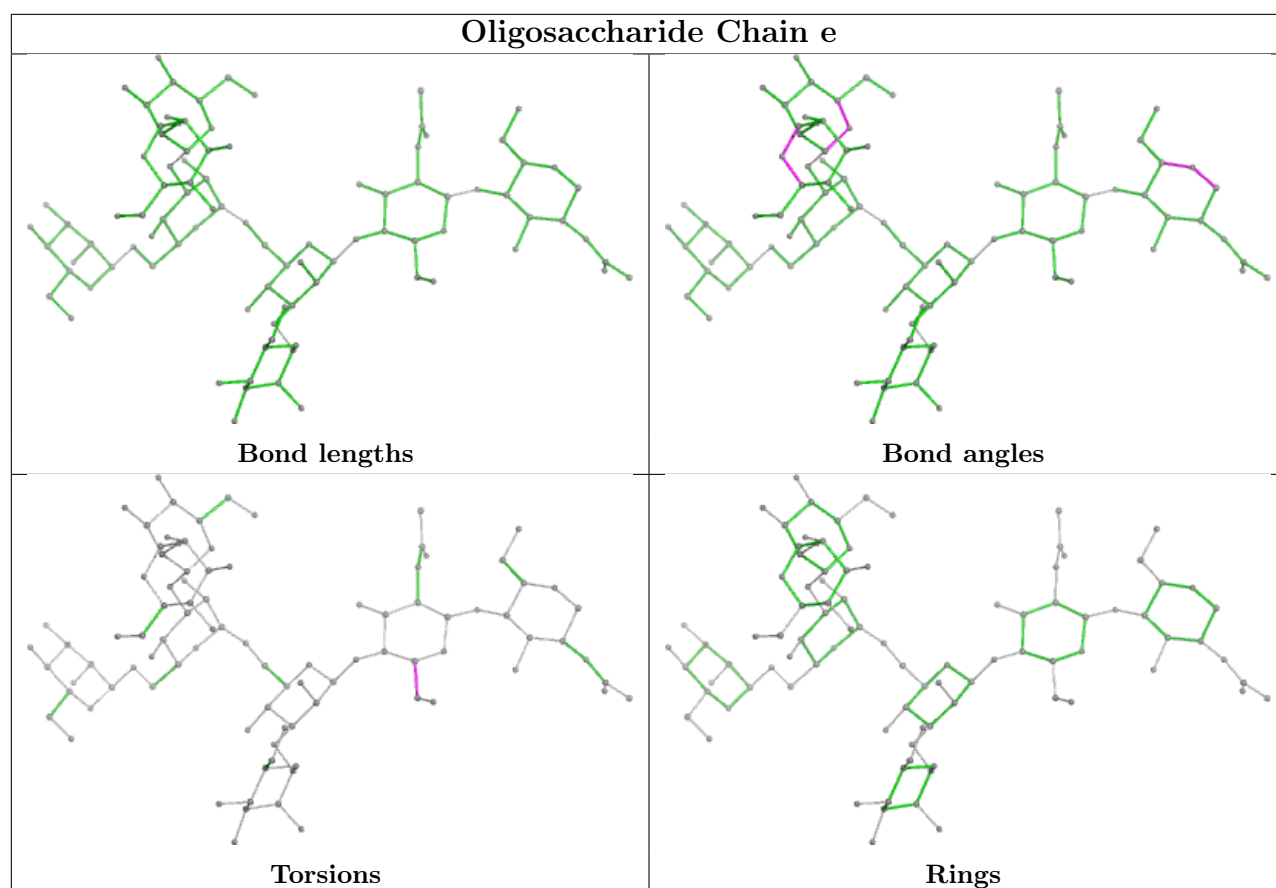


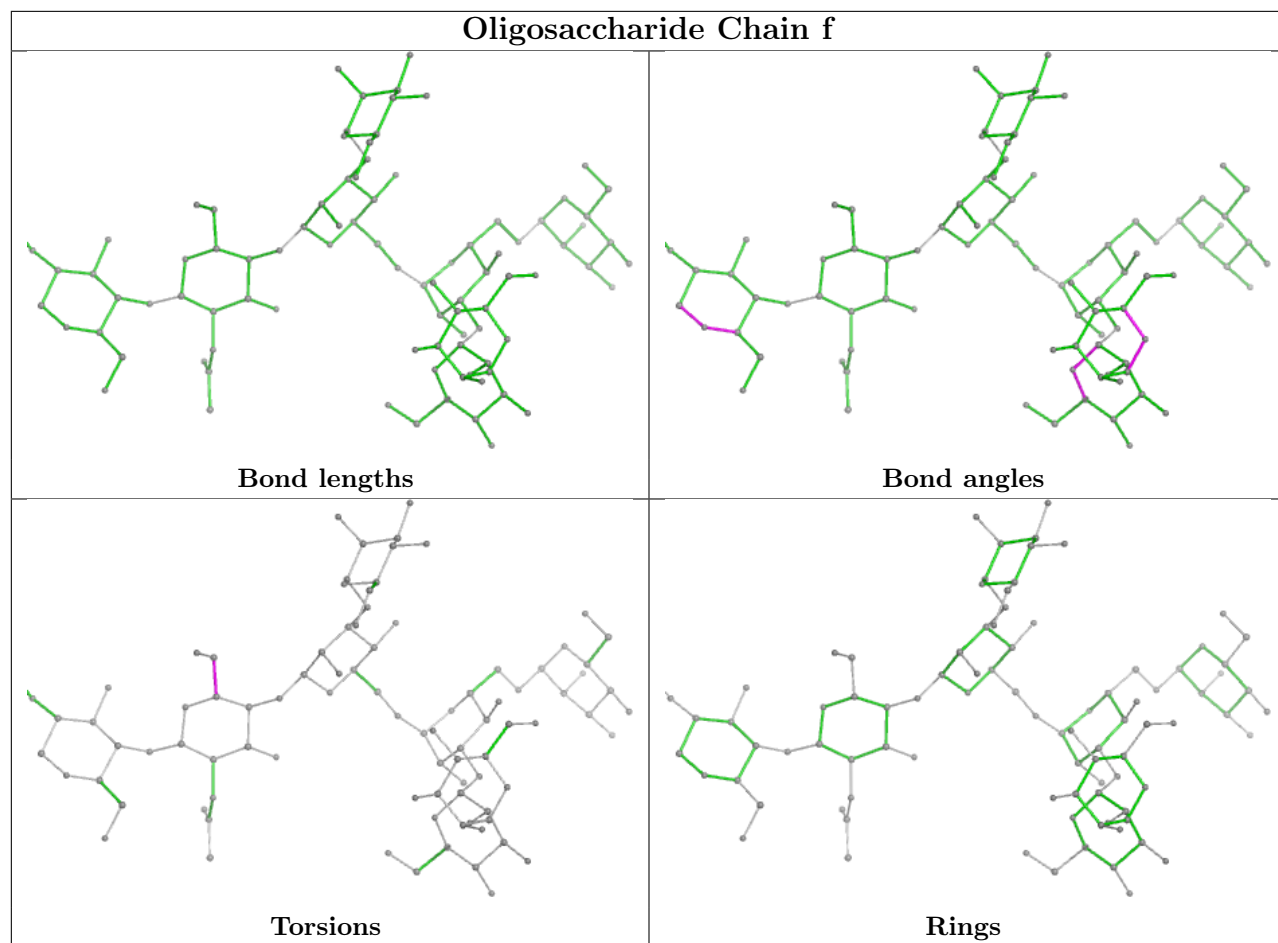


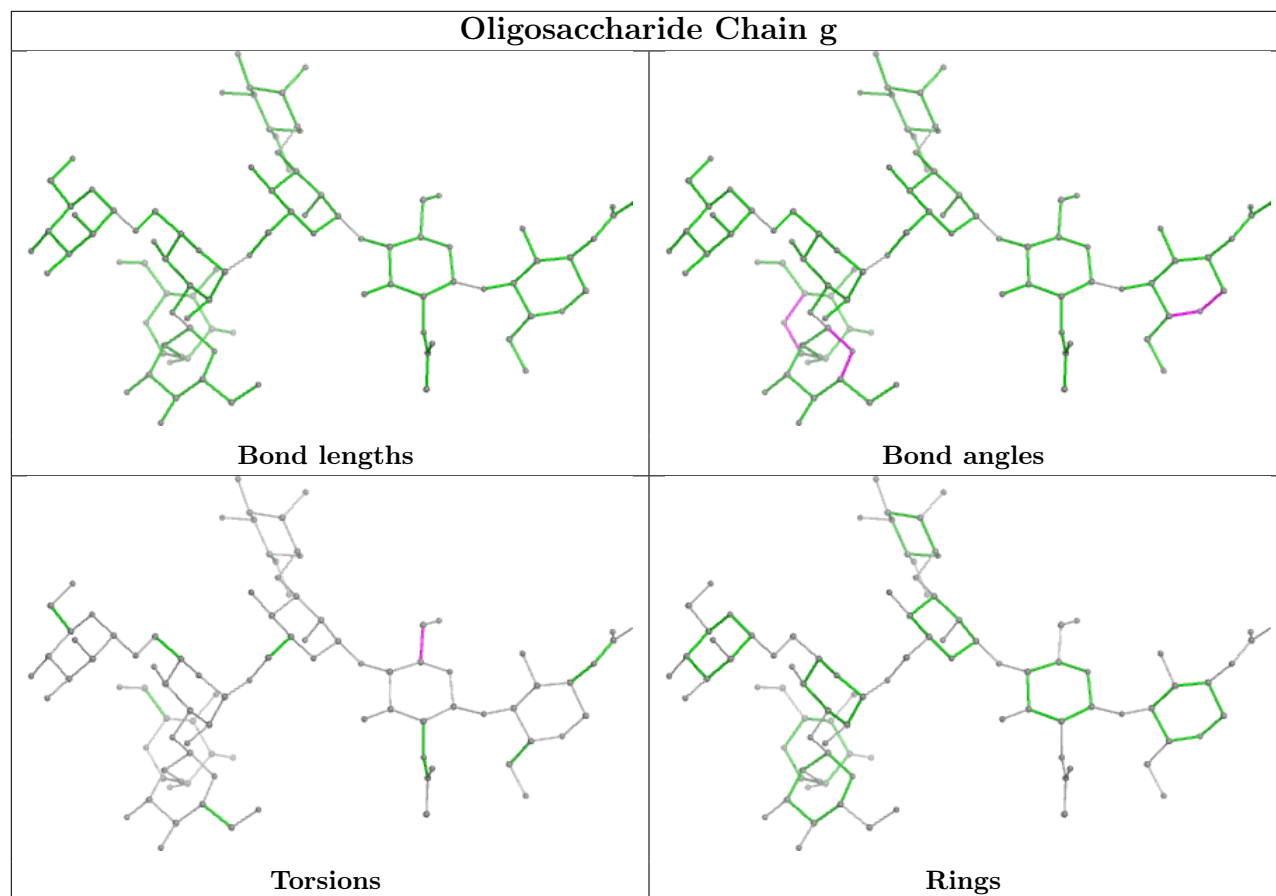


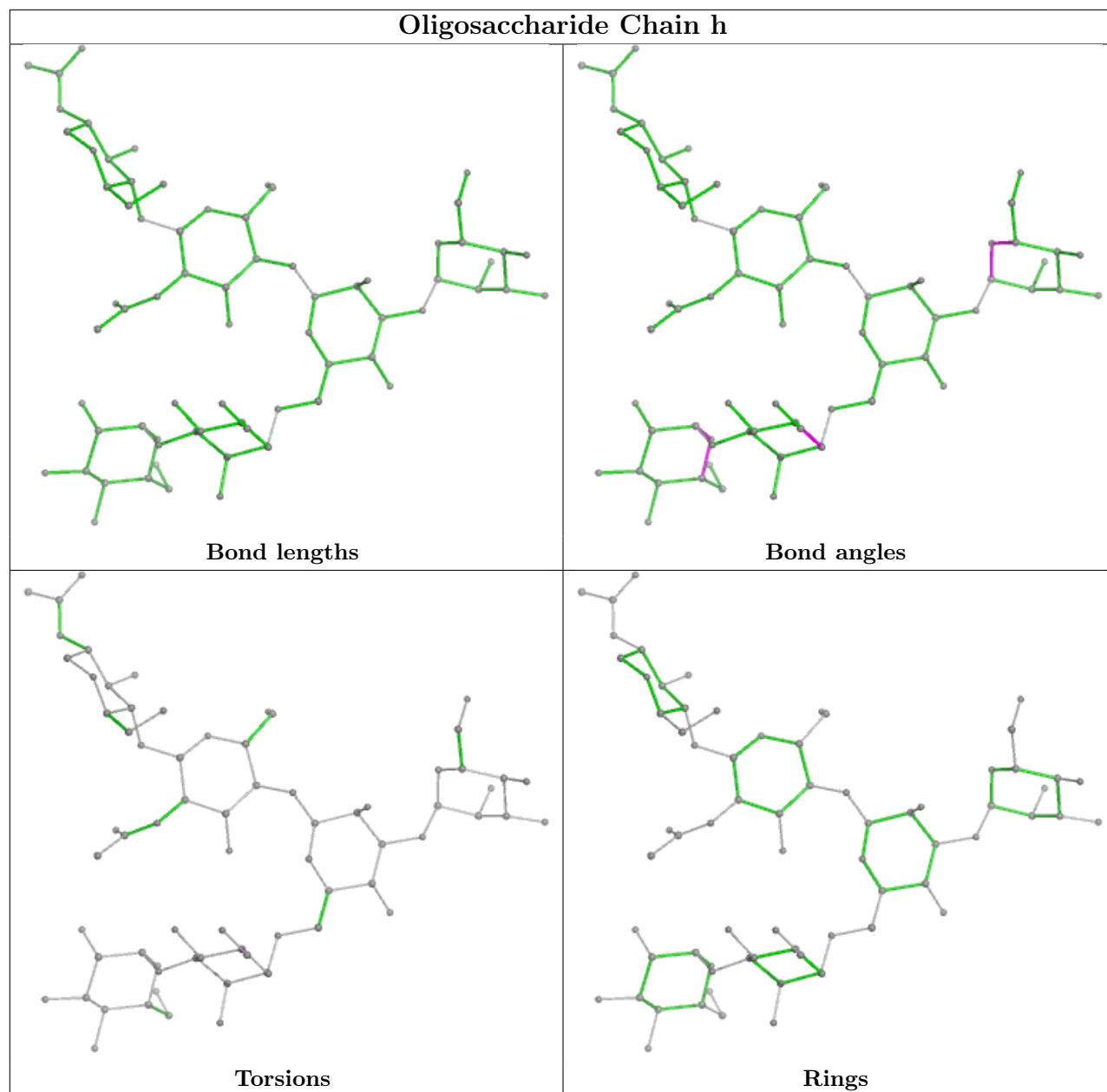


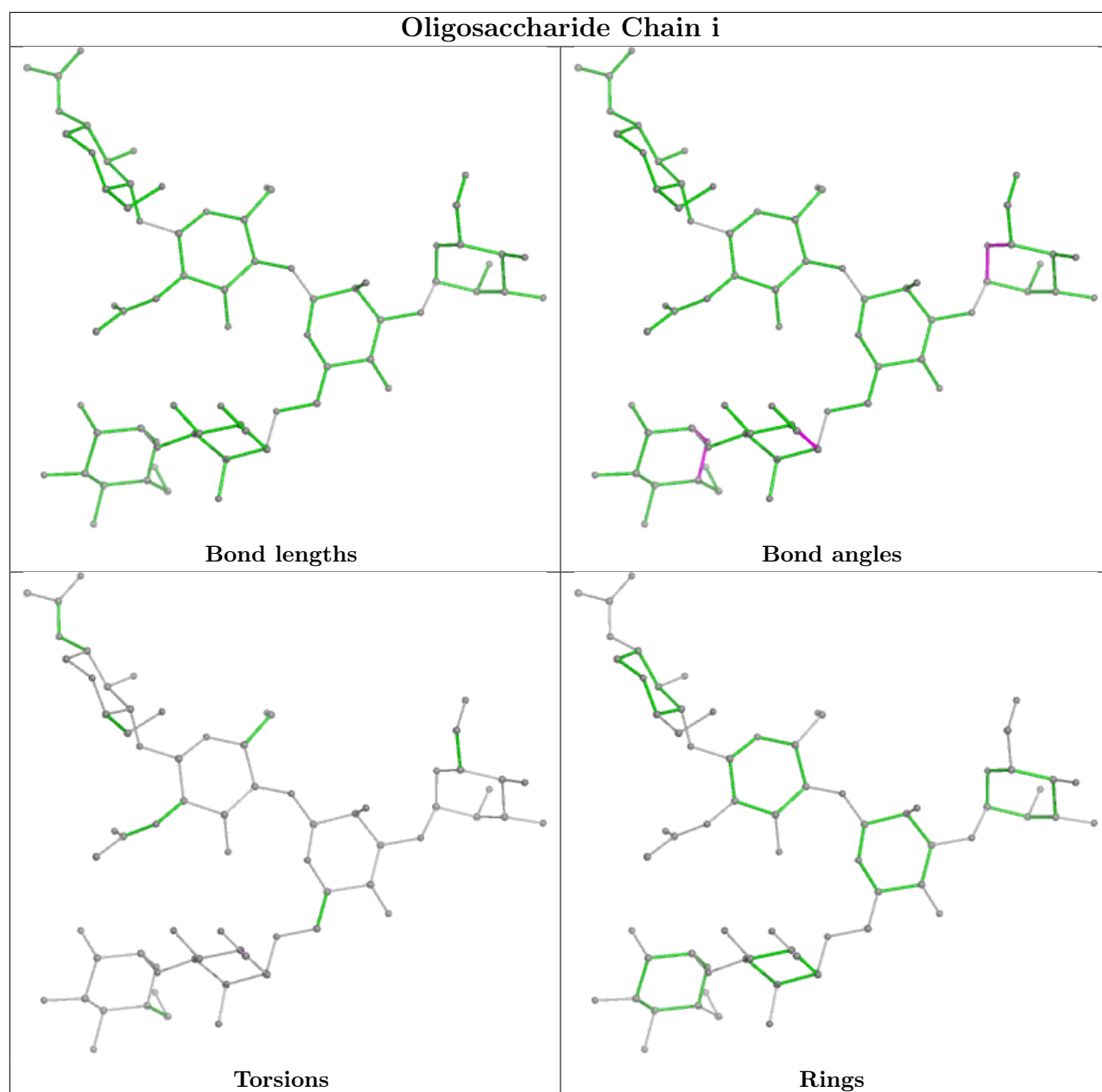


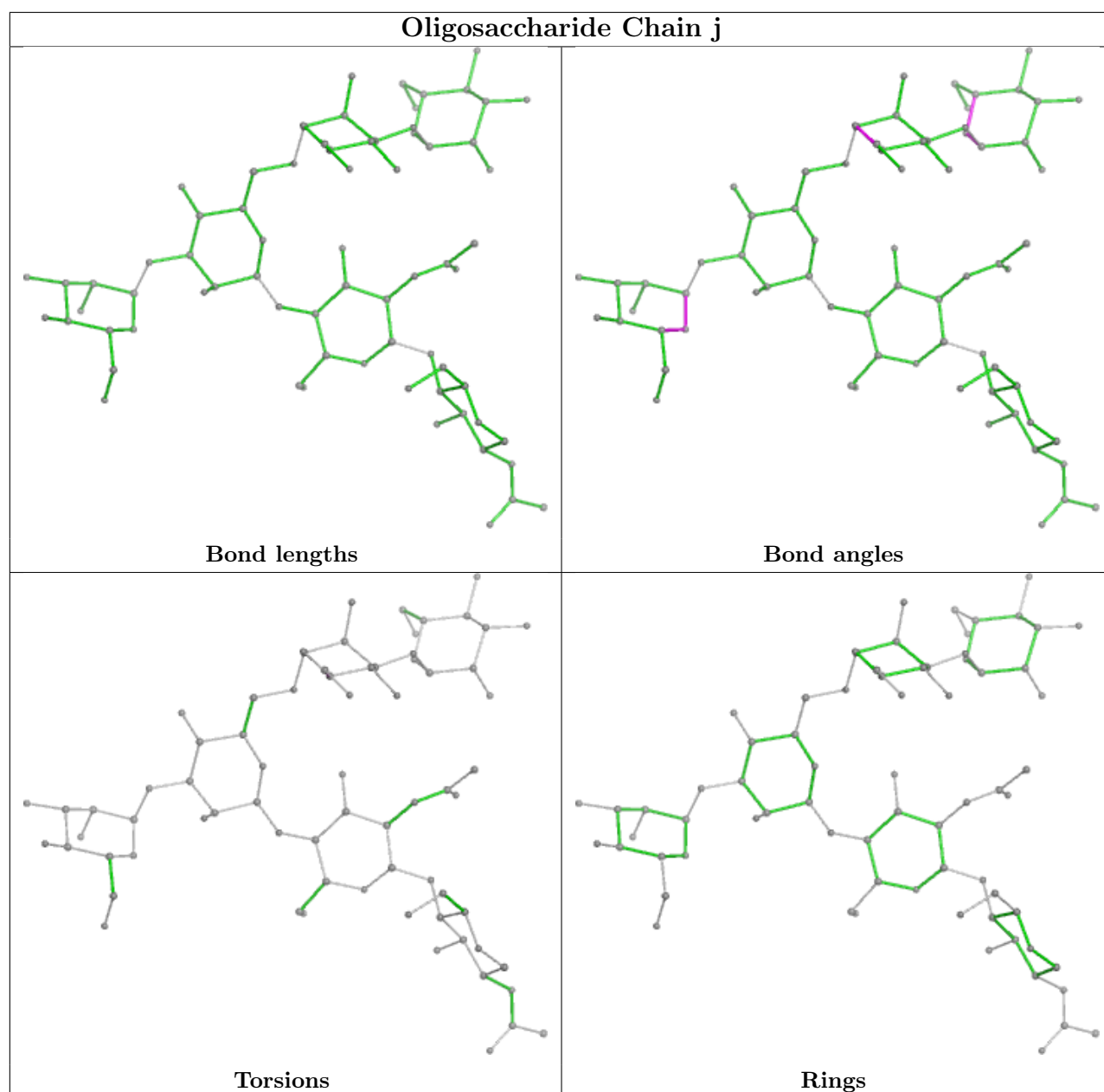












5.6 Ligand geometry [i](#)

15 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
8	NAG	B	1003	1	14,14,15	0.32	0	17,19,21	1.27	3 (17%)
9	CLR	L	1100	-	31,31,31	0.35	0	48,48,48	0.57	0
8	NAG	G	1002	1	14,14,15	0.38	0	17,19,21	0.87	1 (5%)
9	CLR	D	1100	-	31,31,31	0.35	0	48,48,48	0.57	0
8	NAG	G	1001	1	14,14,15	0.30	0	17,19,21	0.59	0
8	NAG	B	1002	1	14,14,15	0.39	0	17,19,21	0.88	1 (5%)
8	NAG	C	1002	1	14,14,15	0.39	0	17,19,21	0.88	1 (5%)
8	NAG	G	1003	1	14,14,15	0.32	0	17,19,21	1.26	3 (17%)
10	PTY	D	1101	-	49,49,49	0.26	0	52,54,54	0.30	0
10	PTY	H	1101	-	49,49,49	0.26	0	52,54,54	0.30	0
8	NAG	B	1001	1	14,14,15	0.31	0	17,19,21	0.59	0
8	NAG	C	1001	1	14,14,15	0.32	0	17,19,21	0.59	0
9	CLR	H	1100	-	31,31,31	0.35	0	48,48,48	0.57	0
10	PTY	L	1101	-	49,49,49	0.26	0	52,54,54	0.30	0
8	NAG	C	1003	1	14,14,15	0.33	0	17,19,21	1.26	3 (17%)

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
8	NAG	B	1003	1	-	2/6/23/26	0/1/1/1
9	CLR	L	1100	-	-	6/10/68/68	0/4/4/4
8	NAG	G	1002	1	-	1/6/23/26	0/1/1/1
9	CLR	D	1100	-	-	6/10/68/68	0/4/4/4
8	NAG	G	1001	1	-	1/6/23/26	0/1/1/1
8	NAG	B	1002	1	-	1/6/23/26	0/1/1/1
8	NAG	C	1002	1	-	1/6/23/26	0/1/1/1
8	NAG	G	1003	1	-	2/6/23/26	0/1/1/1
10	PTY	D	1101	-	-	16/53/53/53	-
10	PTY	H	1101	-	-	16/53/53/53	-
8	NAG	B	1001	1	-	1/6/23/26	0/1/1/1
8	NAG	C	1001	1	-	1/6/23/26	0/1/1/1
9	CLR	H	1100	-	-	6/10/68/68	0/4/4/4
10	PTY	L	1101	-	-	16/53/53/53	-
8	NAG	C	1003	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1003	NAG	C2-N2-C7	2.67	126.70	122.90
8	C	1003	NAG	C2-N2-C7	2.64	126.66	122.90
8	G	1003	NAG	C2-N2-C7	2.63	126.65	122.90
8	B	1003	NAG	C8-C7-N2	2.58	120.47	116.10
8	C	1003	NAG	C8-C7-N2	2.58	120.46	116.10
8	G	1003	NAG	C8-C7-N2	2.55	120.42	116.10
8	B	1003	NAG	C1-O5-C5	2.49	115.57	112.19
8	G	1003	NAG	C1-O5-C5	2.49	115.57	112.19
8	C	1003	NAG	C1-O5-C5	2.46	115.53	112.19
8	C	1002	NAG	C2-N2-C7	2.23	126.07	122.90
8	B	1002	NAG	C2-N2-C7	2.18	126.00	122.90
8	G	1002	NAG	C2-N2-C7	2.16	125.98	122.90

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	1003	NAG	C8-C7-N2-C2
8	B	1003	NAG	O7-C7-N2-C2
8	C	1003	NAG	C8-C7-N2-C2
8	C	1003	NAG	O7-C7-N2-C2
8	G	1003	NAG	C8-C7-N2-C2
8	G	1003	NAG	O7-C7-N2-C2
9	D	1100	CLR	C20-C22-C23-C24
9	H	1100	CLR	C20-C22-C23-C24
9	L	1100	CLR	C20-C22-C23-C24
10	D	1101	PTY	C11-C8-O7-C6
10	H	1101	PTY	C11-C8-O7-C6
10	L	1101	PTY	C11-C8-O7-C6
10	D	1101	PTY	O10-C8-O7-C6
10	H	1101	PTY	O10-C8-O7-C6
10	L	1101	PTY	O10-C8-O7-C6
10	D	1101	PTY	C18-C19-C20-C21
10	L	1101	PTY	C18-C19-C20-C21
10	H	1101	PTY	C18-C19-C20-C21
10	D	1101	PTY	C25-C26-C27-C28
10	H	1101	PTY	C25-C26-C27-C28
10	L	1101	PTY	C25-C26-C27-C28
10	D	1101	PTY	C15-C16-C17-C18
10	H	1101	PTY	C15-C16-C17-C18
10	L	1101	PTY	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
10	D	1101	PTY	C40-C41-C42-C43
10	H	1101	PTY	C40-C41-C42-C43
10	L	1101	PTY	C40-C41-C42-C43
10	H	1101	PTY	C12-C13-C14-C15
10	D	1101	PTY	C12-C13-C14-C15
10	L	1101	PTY	C12-C13-C14-C15
8	B	1001	NAG	O5-C5-C6-O6
8	C	1001	NAG	O5-C5-C6-O6
8	G	1001	NAG	O5-C5-C6-O6
10	D	1101	PTY	C35-C36-C37-C38
10	H	1101	PTY	C35-C36-C37-C38
10	L	1101	PTY	C35-C36-C37-C38
9	D	1100	CLR	C21-C20-C22-C23
9	H	1100	CLR	C21-C20-C22-C23
9	L	1100	CLR	C21-C20-C22-C23
10	D	1101	PTY	O4-C1-C6-O7
10	H	1101	PTY	O4-C1-C6-O7
10	L	1101	PTY	O4-C1-C6-O7
10	D	1101	PTY	C6-C5-O14-P1
10	H	1101	PTY	C6-C5-O14-P1
10	L	1101	PTY	C6-C5-O14-P1
9	D	1100	CLR	C16-C17-C20-C22
9	H	1100	CLR	C16-C17-C20-C22
9	L	1100	CLR	C16-C17-C20-C22
9	D	1100	CLR	C13-C17-C20-C22
9	H	1100	CLR	C13-C17-C20-C22
9	L	1100	CLR	C13-C17-C20-C22
10	D	1101	PTY	C33-C34-C35-C36
10	H	1101	PTY	C33-C34-C35-C36
10	L	1101	PTY	C33-C34-C35-C36
10	D	1101	PTY	O14-C5-C6-O7
10	H	1101	PTY	O14-C5-C6-O7
10	L	1101	PTY	O14-C5-C6-O7
9	D	1100	CLR	C13-C17-C20-C21
9	H	1100	CLR	C13-C17-C20-C21
9	L	1100	CLR	C13-C17-C20-C21
10	H	1101	PTY	C26-C27-C28-C29
10	D	1101	PTY	C26-C27-C28-C29
10	L	1101	PTY	C26-C27-C28-C29
10	L	1101	PTY	C20-C21-C22-C23
10	D	1101	PTY	C20-C21-C22-C23
10	H	1101	PTY	C20-C21-C22-C23

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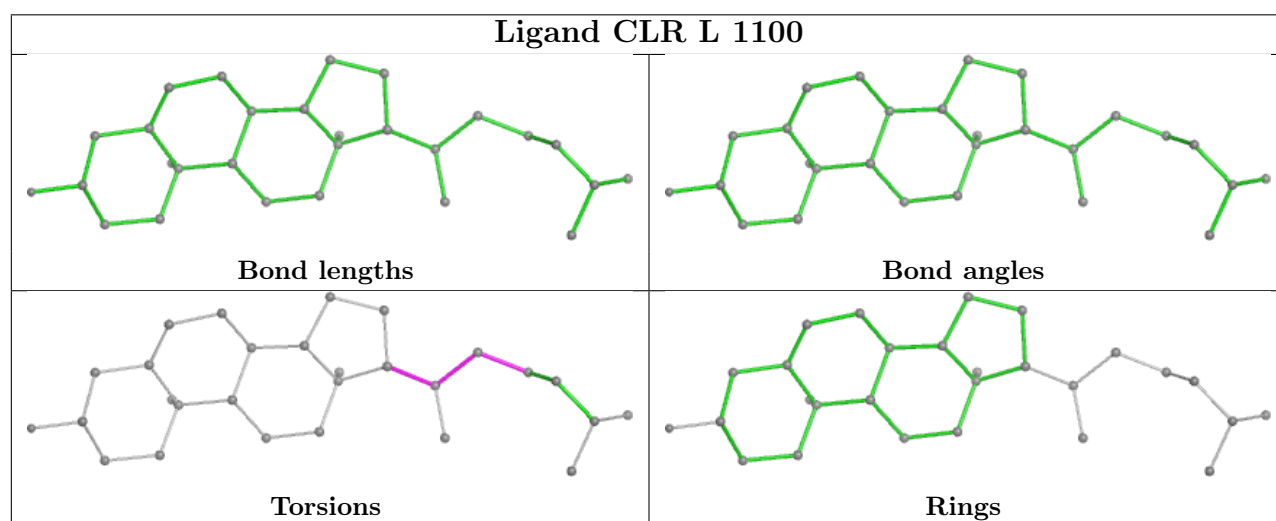
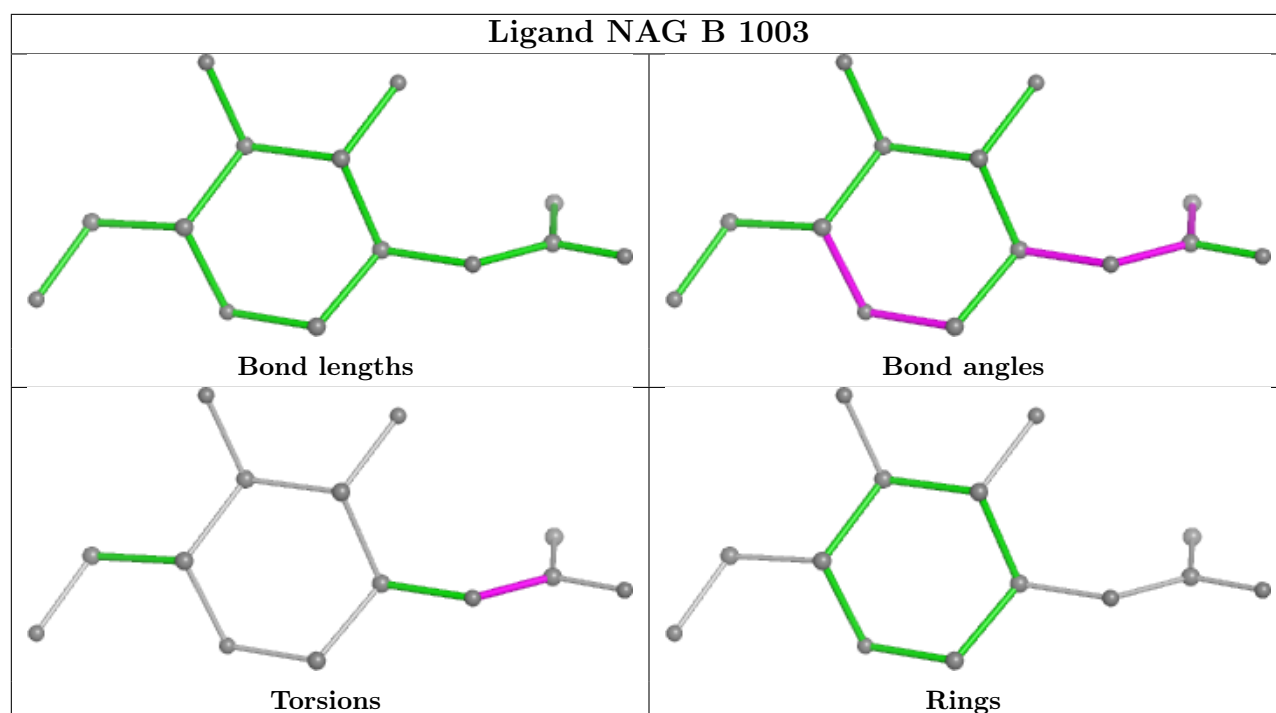
Continued from previous page...

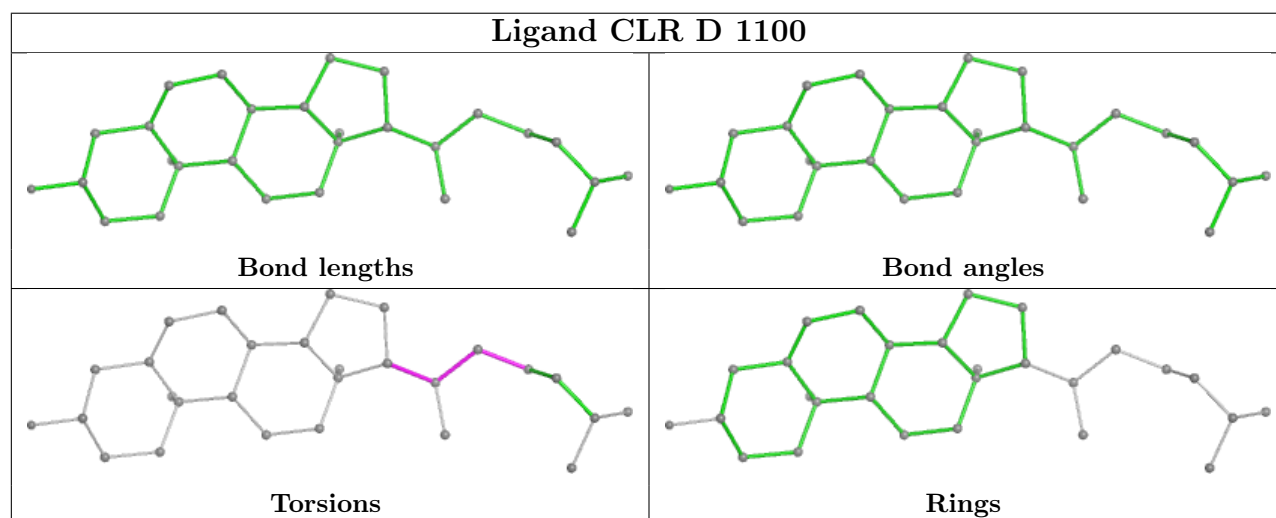
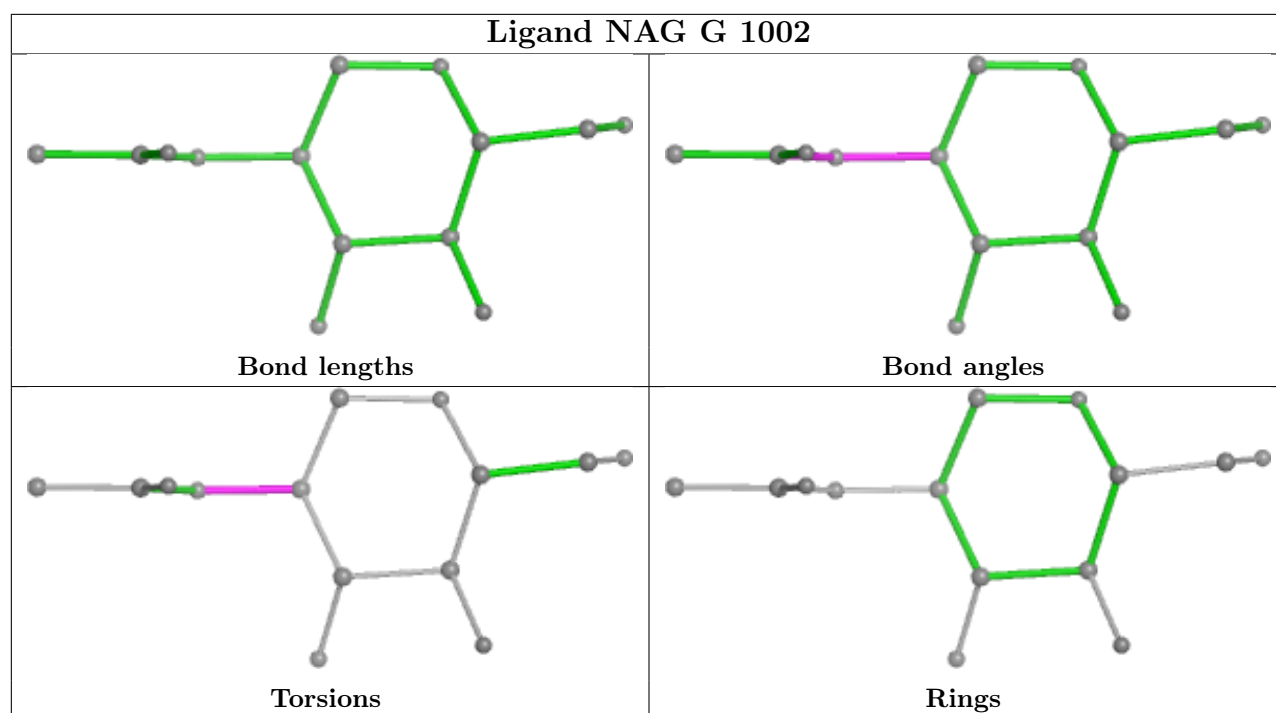
Mol	Chain	Res	Type	Atoms
9	D	1100	CLR	C16-C17-C20-C21
9	L	1100	CLR	C16-C17-C20-C21
9	H	1100	CLR	C16-C17-C20-C21
8	B	1002	NAG	C3-C2-N2-C7
8	C	1002	NAG	C3-C2-N2-C7
8	G	1002	NAG	C3-C2-N2-C7
10	D	1101	PTY	O4-C1-C6-C5
10	H	1101	PTY	O4-C1-C6-C5
10	L	1101	PTY	O4-C1-C6-C5
10	D	1101	PTY	C38-C39-C40-C41
10	H	1101	PTY	C38-C39-C40-C41
10	L	1101	PTY	C38-C39-C40-C41

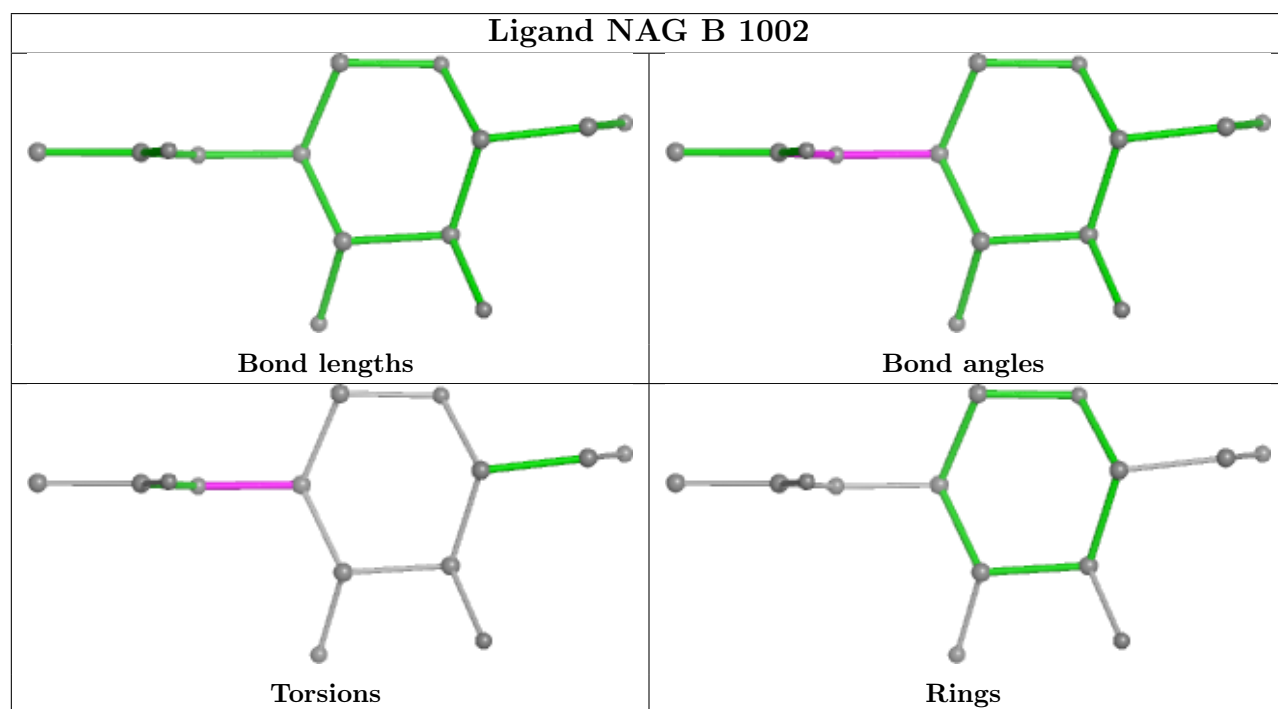
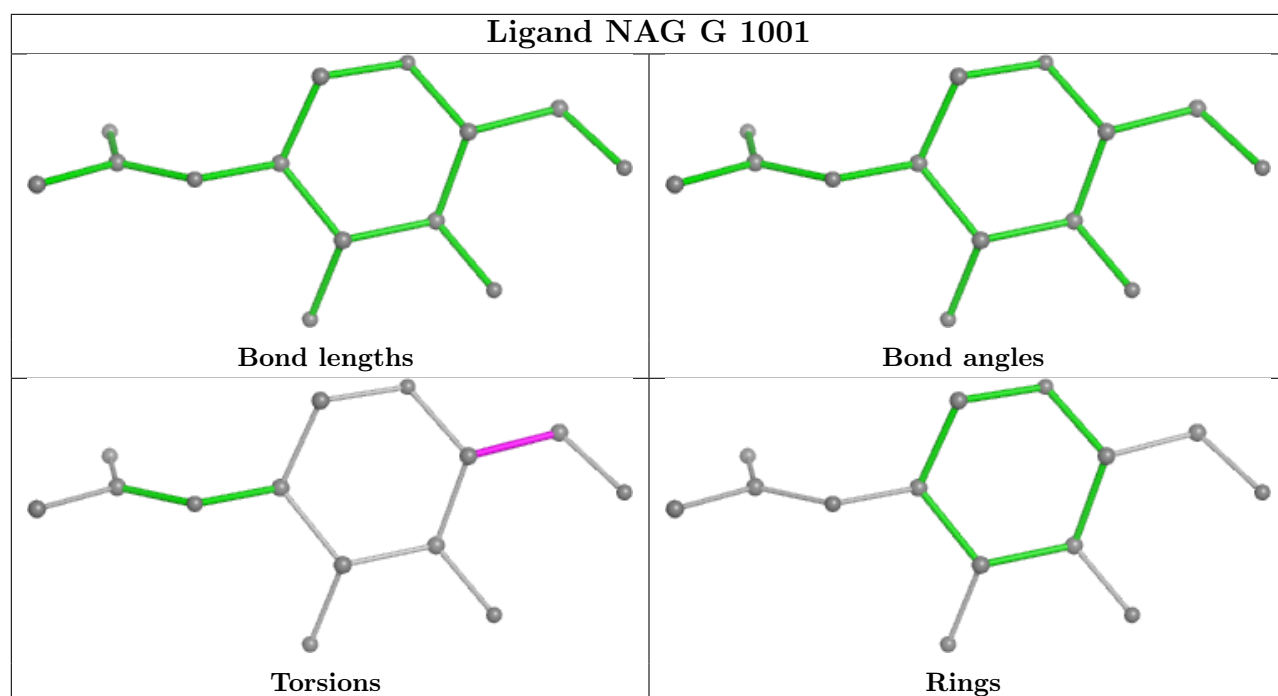
There are no ring outliers.

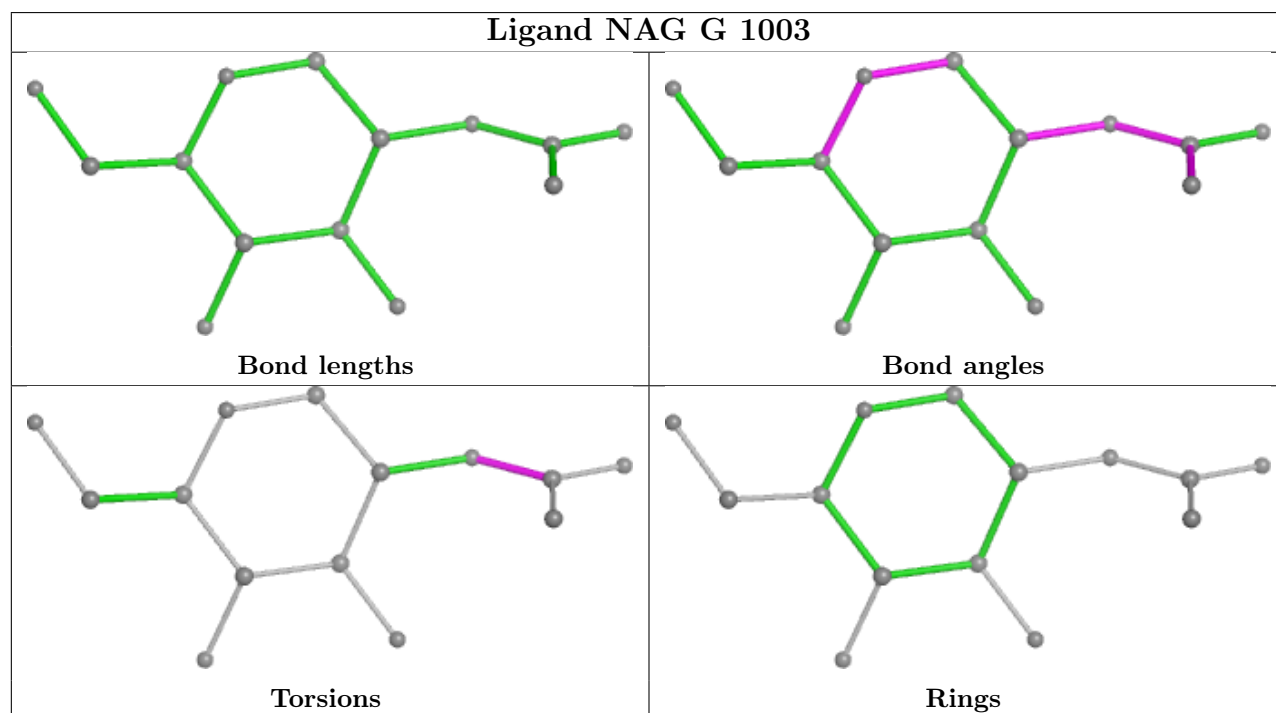
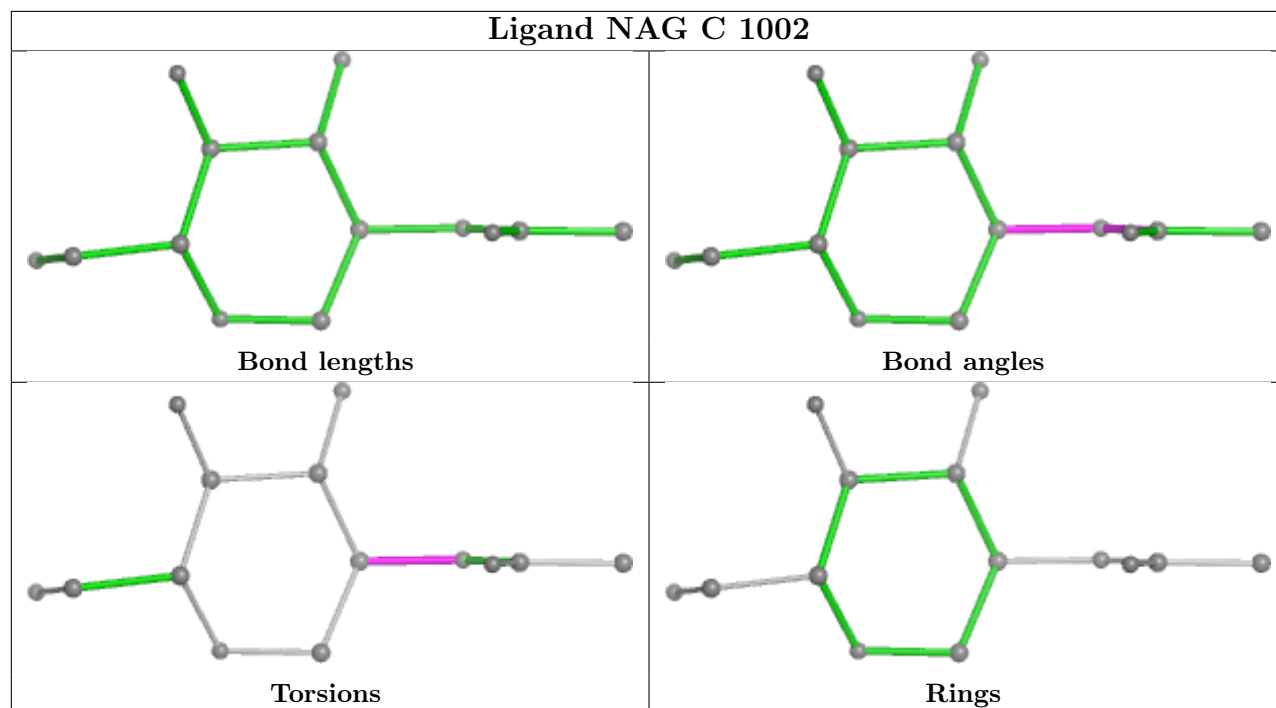
No monomer is involved in short contacts.

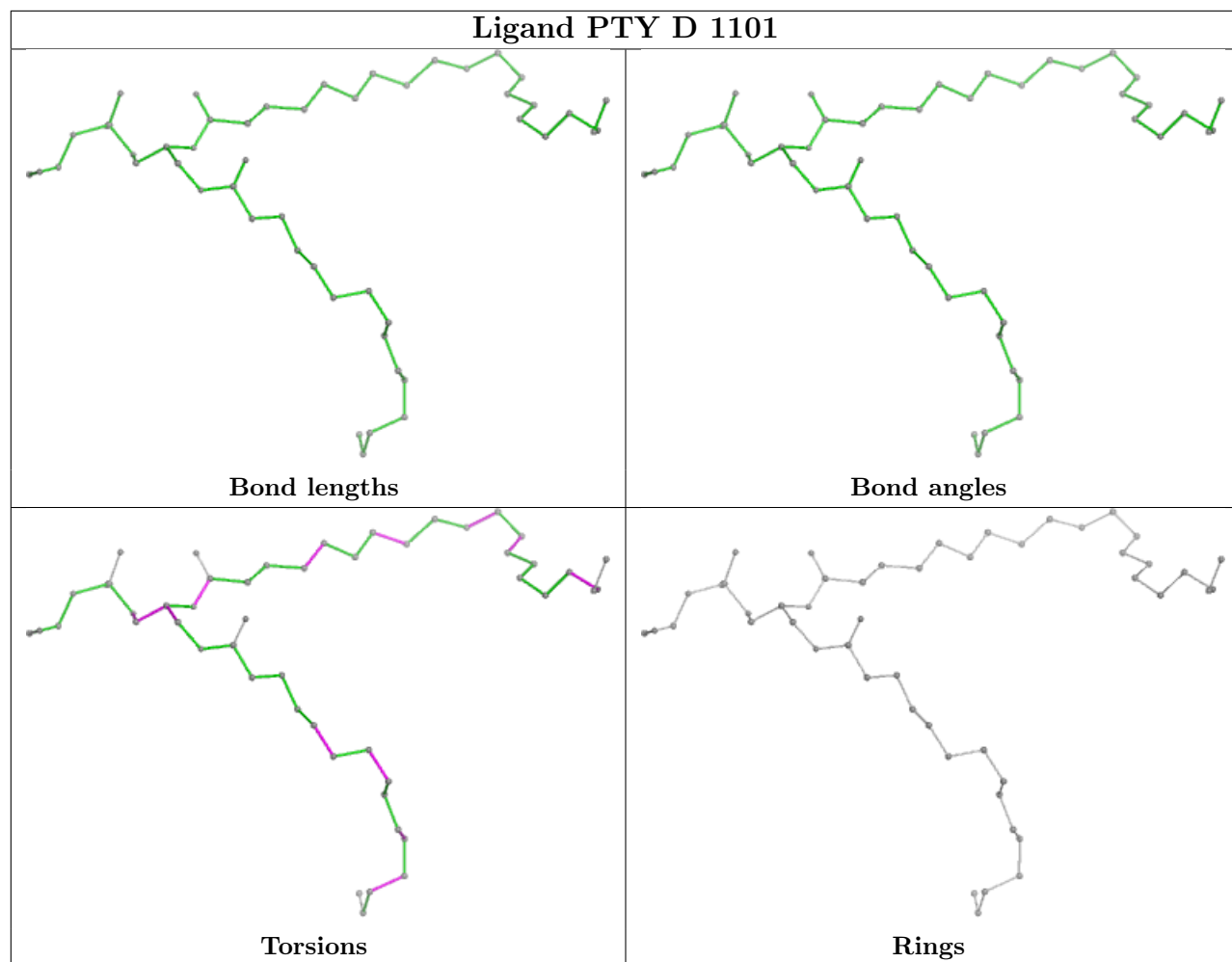
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

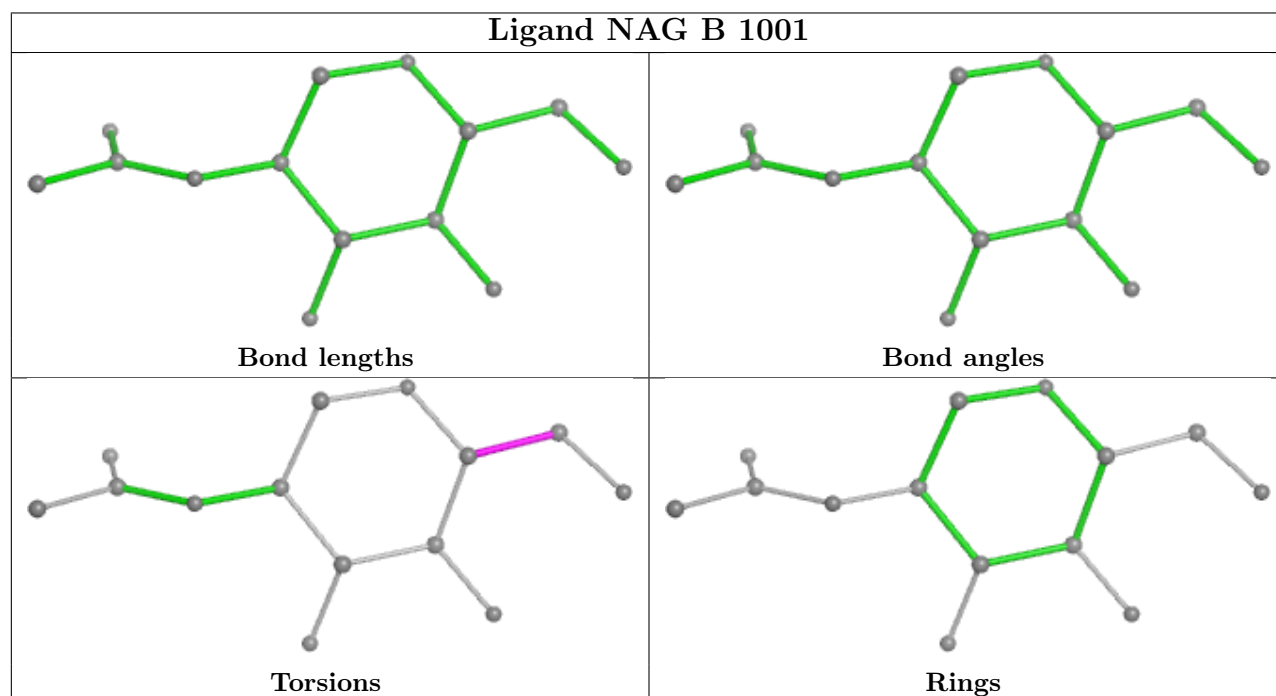
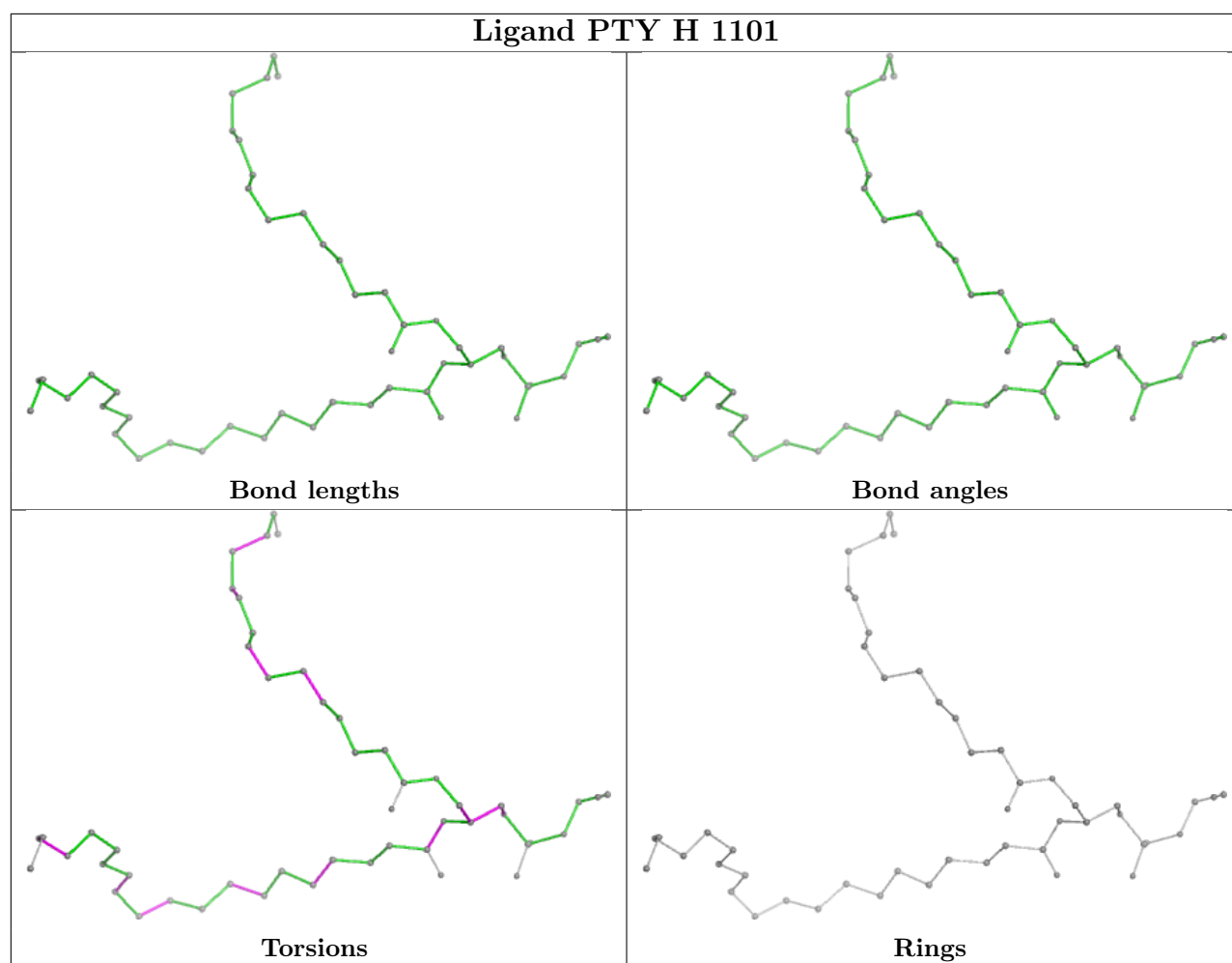




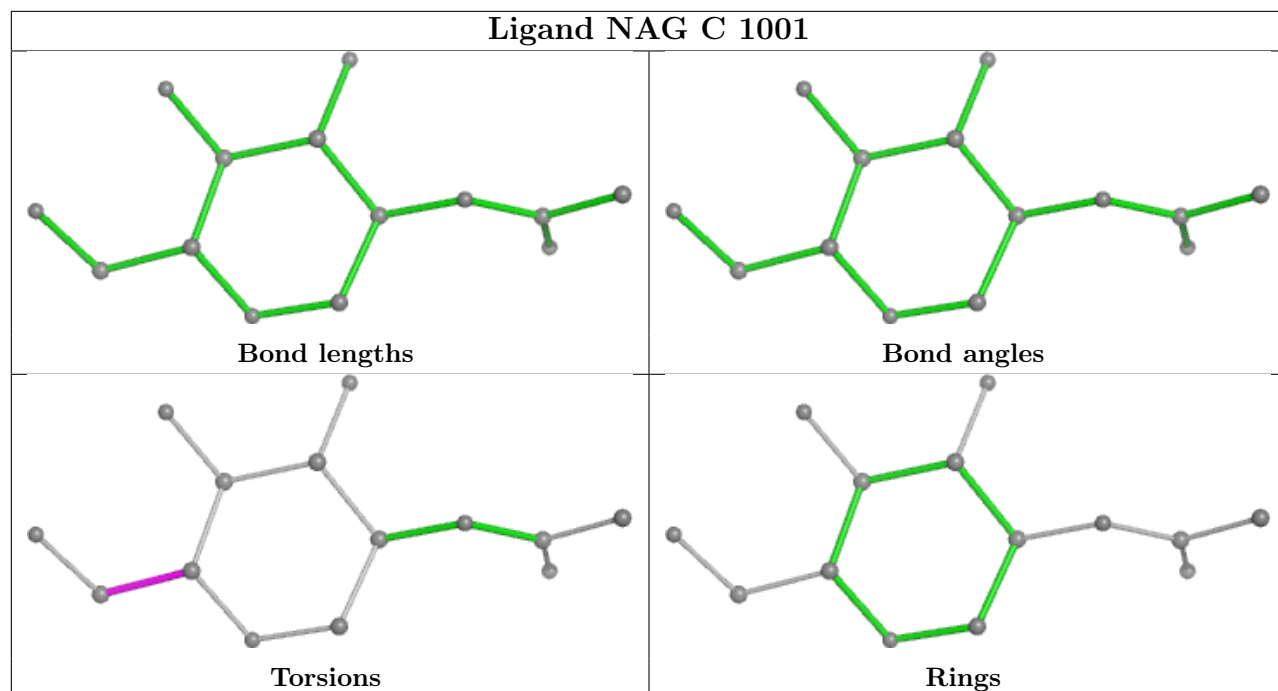




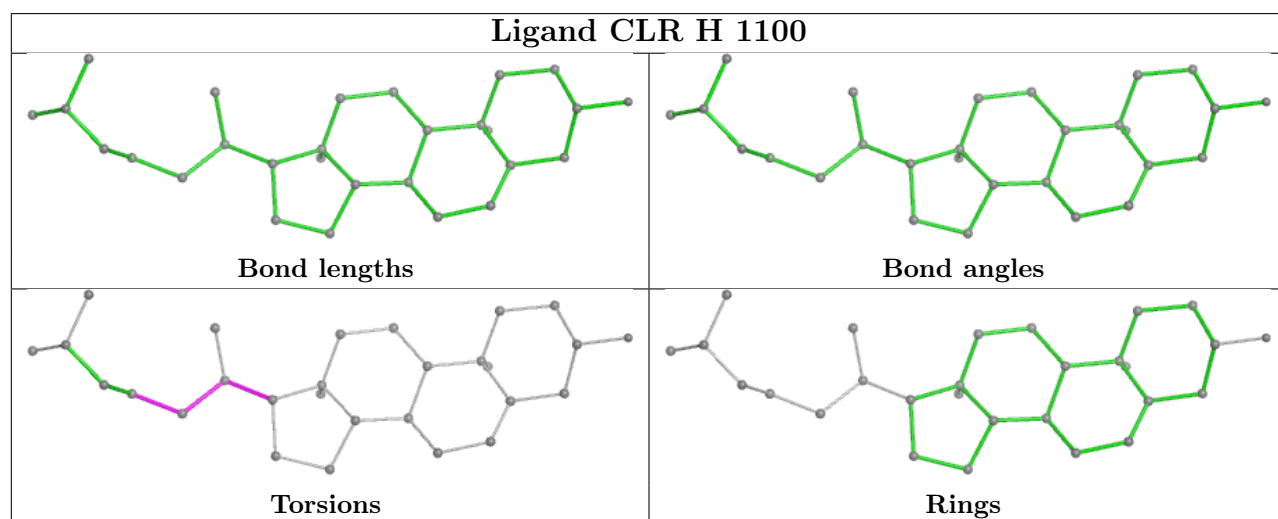


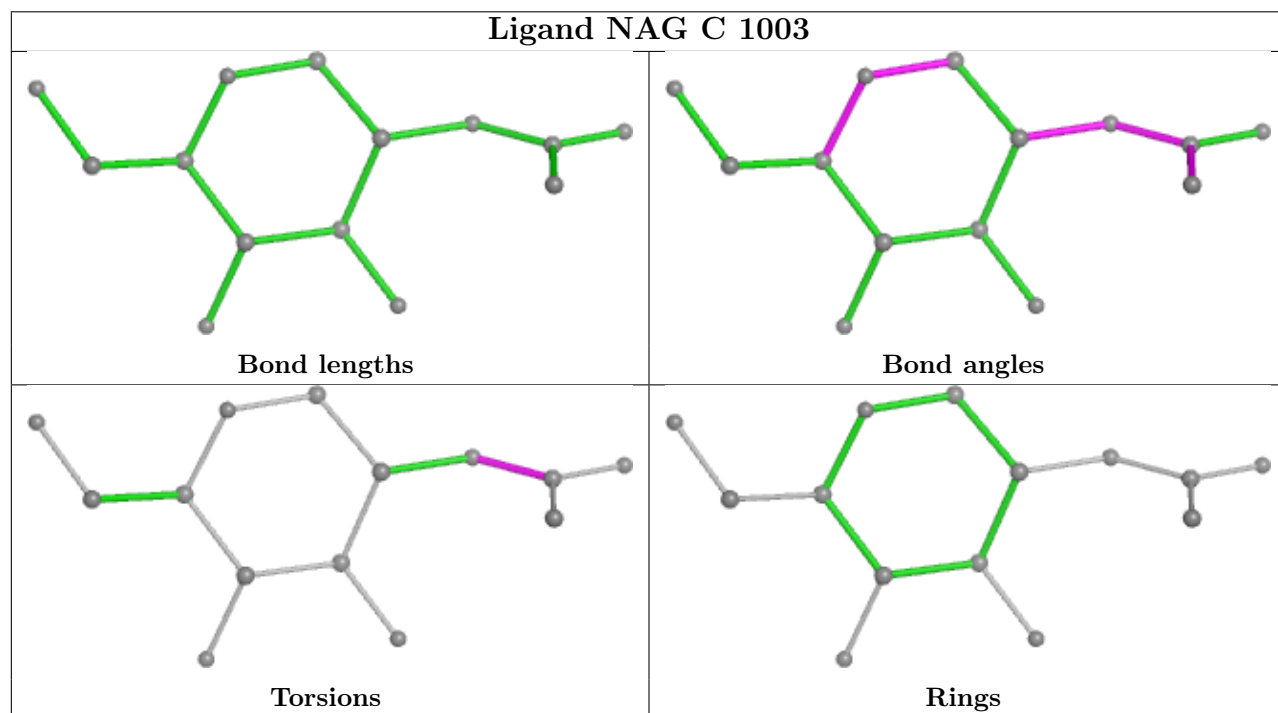
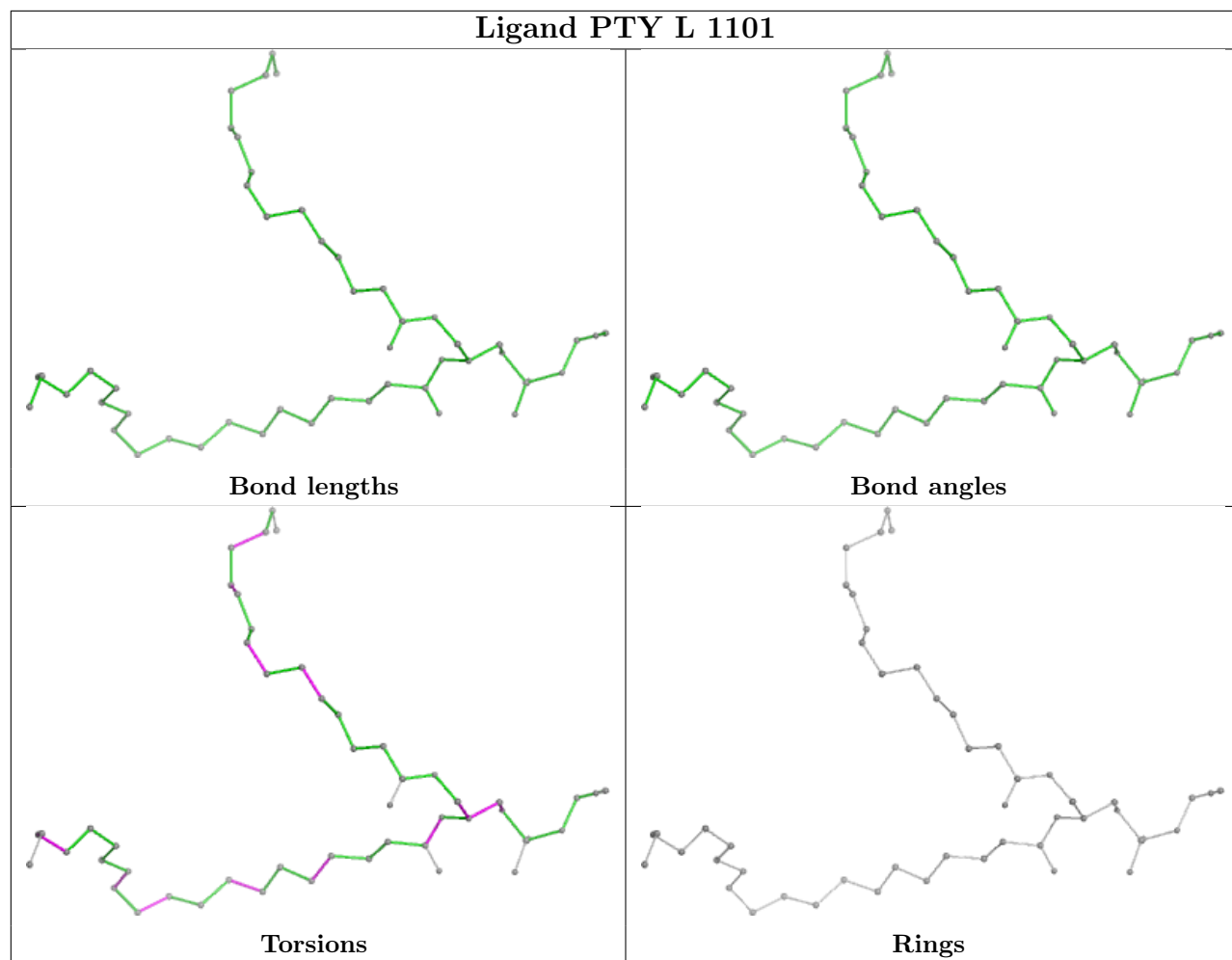


Ligand NAG C 1001



Ligand CLR H 1100





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-17318. These allow visual inspection of the internal detail of the map and identification of artifacts.

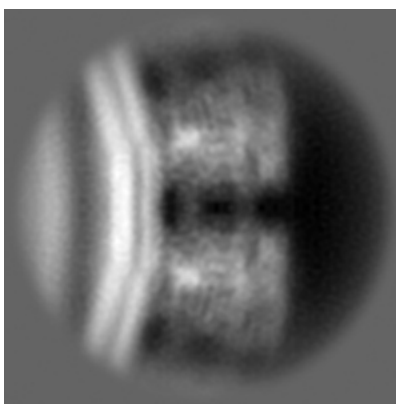
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

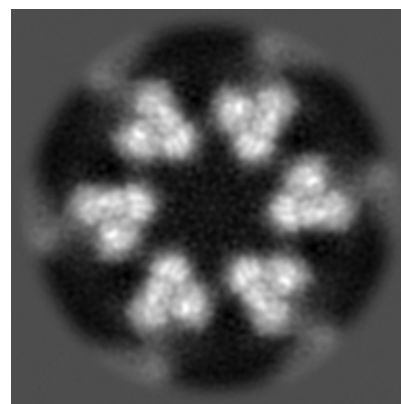
6.1.1 Primary map



X

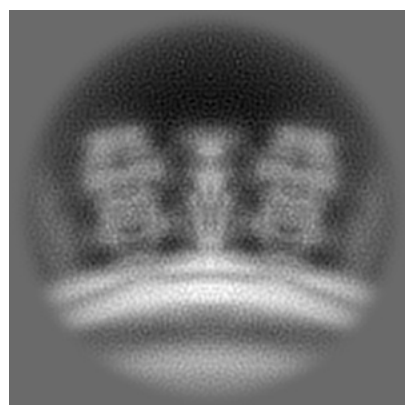


Y

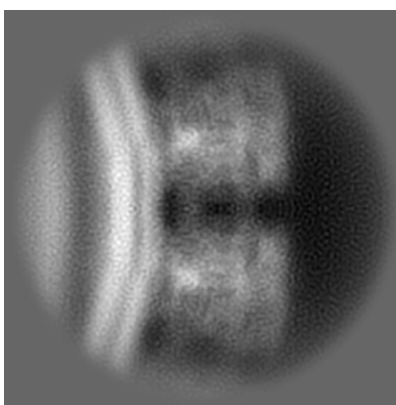


Z

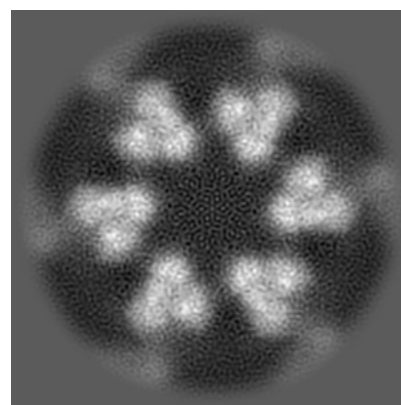
6.1.2 Raw map



X



Y



Z

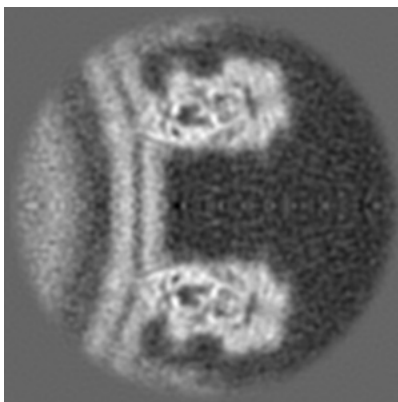
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

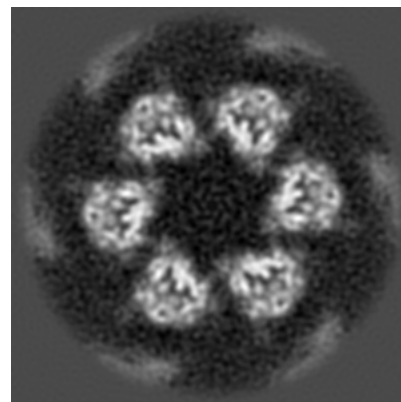
6.2.1 Primary map



X Index: 80



Y Index: 80

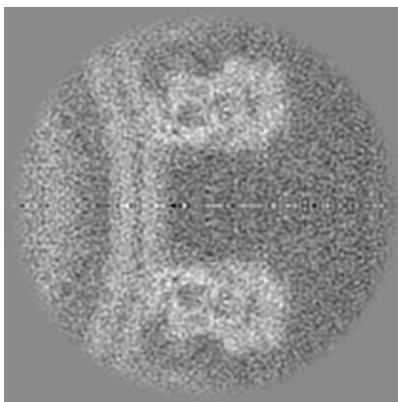


Z Index: 80

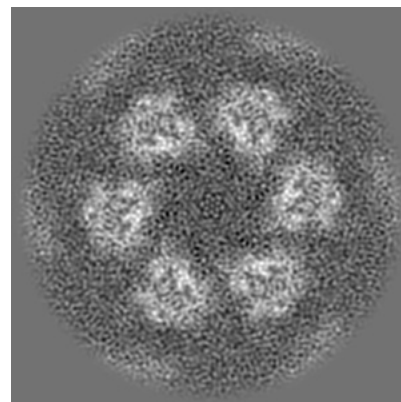
6.2.2 Raw map



X Index: 80



Y Index: 80

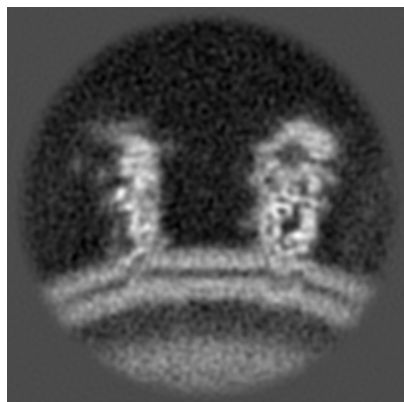


Z Index: 80

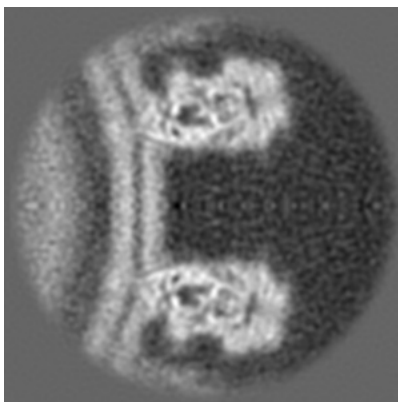
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

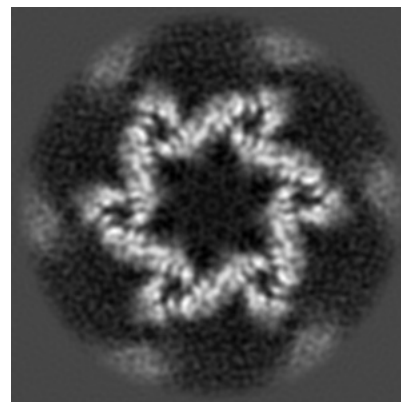
6.3.1 Primary map



X Index: 92

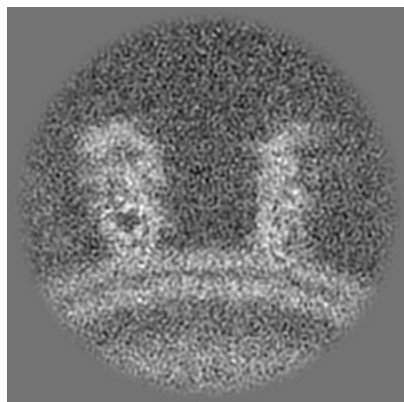


Y Index: 80

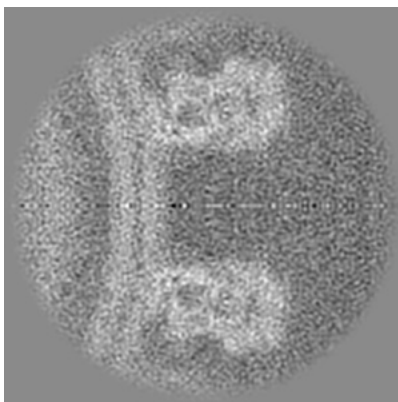


Z Index: 75

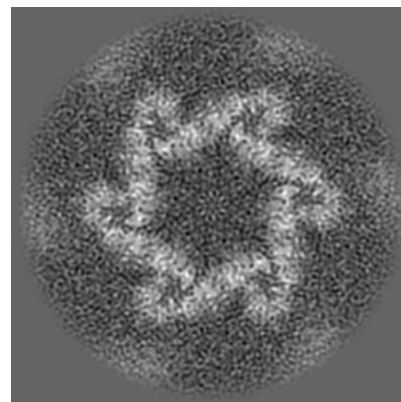
6.3.2 Raw map



X Index: 67



Y Index: 80

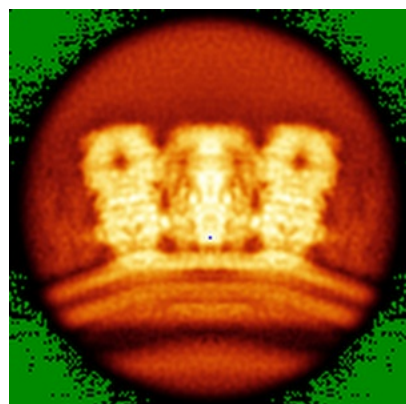


Z Index: 76

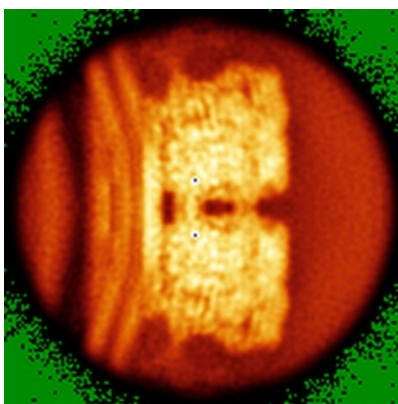
The images above show the largest variance slices of the map in three orthogonal directions.

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

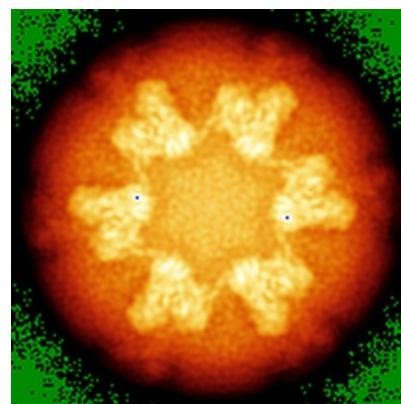
6.4.1 Primary map



X

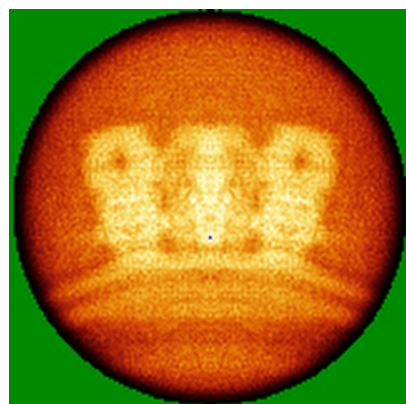


Y

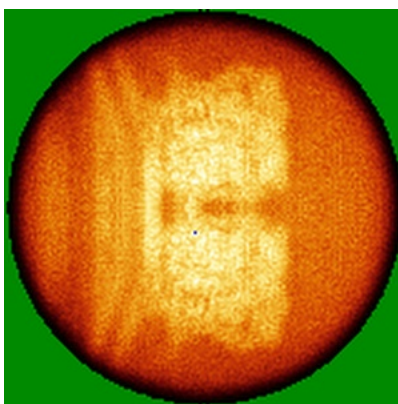


Z

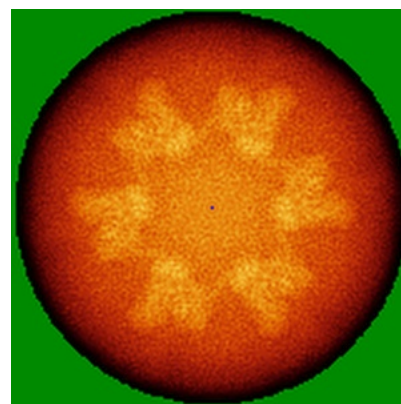
6.4.2 Raw map



X



Y

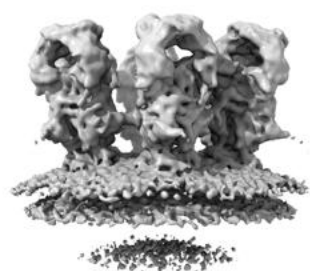


Z

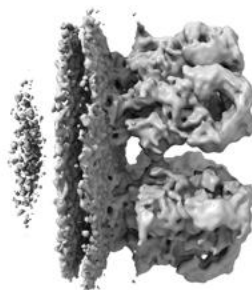
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

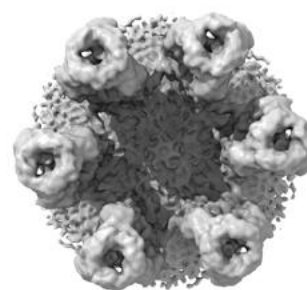
6.5.1 Primary map



X



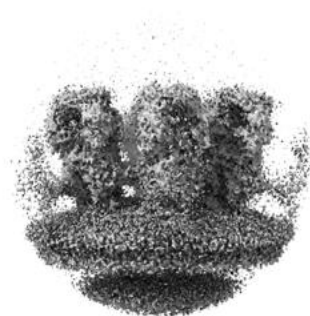
Y



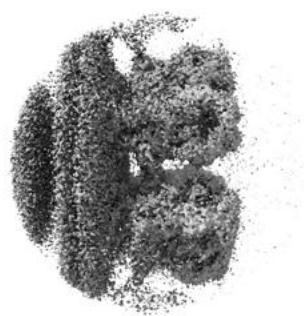
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0702. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

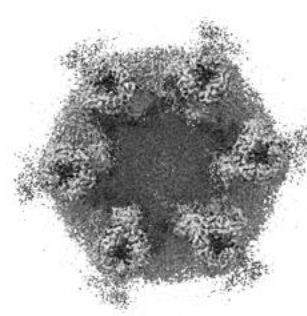
6.5.2 Raw map



X



Y



Z

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

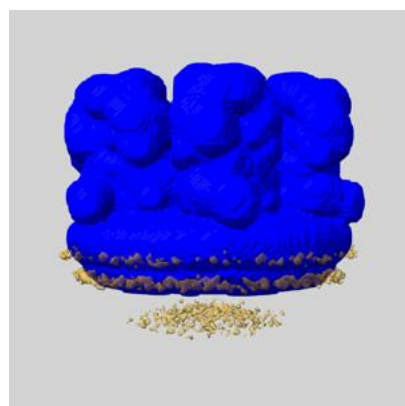
6.6 Mask visualisation [i](#)

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

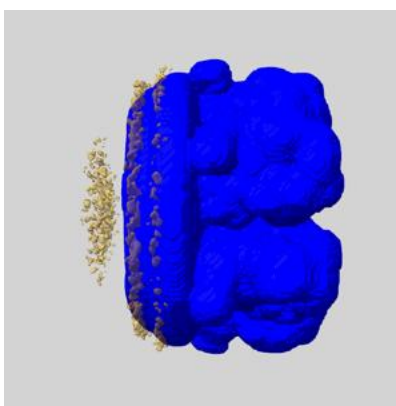
A mask typically either:

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

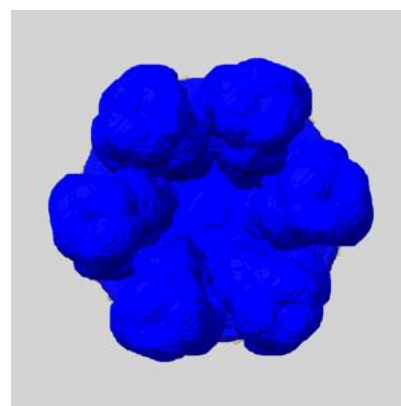
6.6.1 emd_17318_msk_1.map [i](#)



X



Y

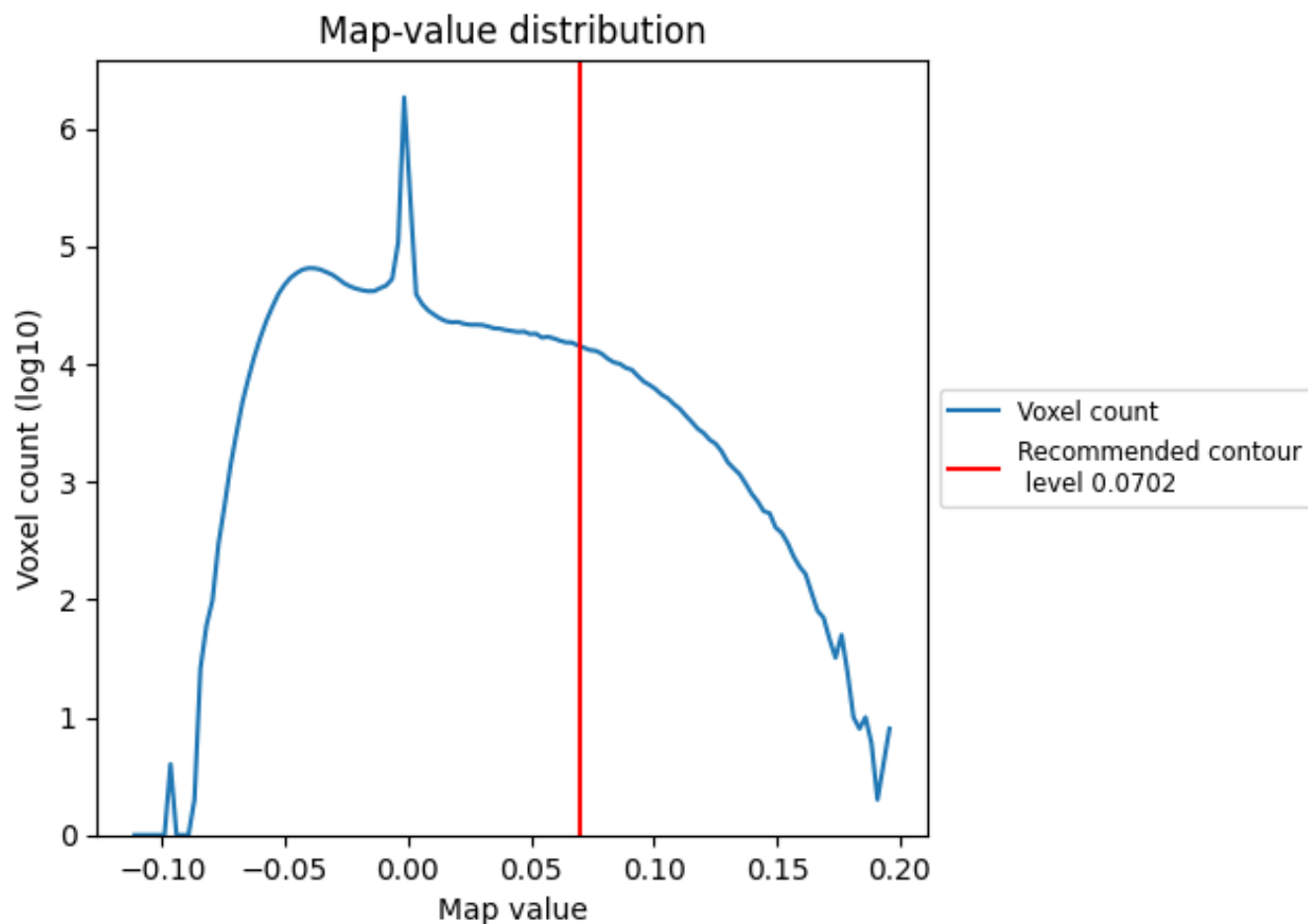


Z

7 Map analysis [i](#)

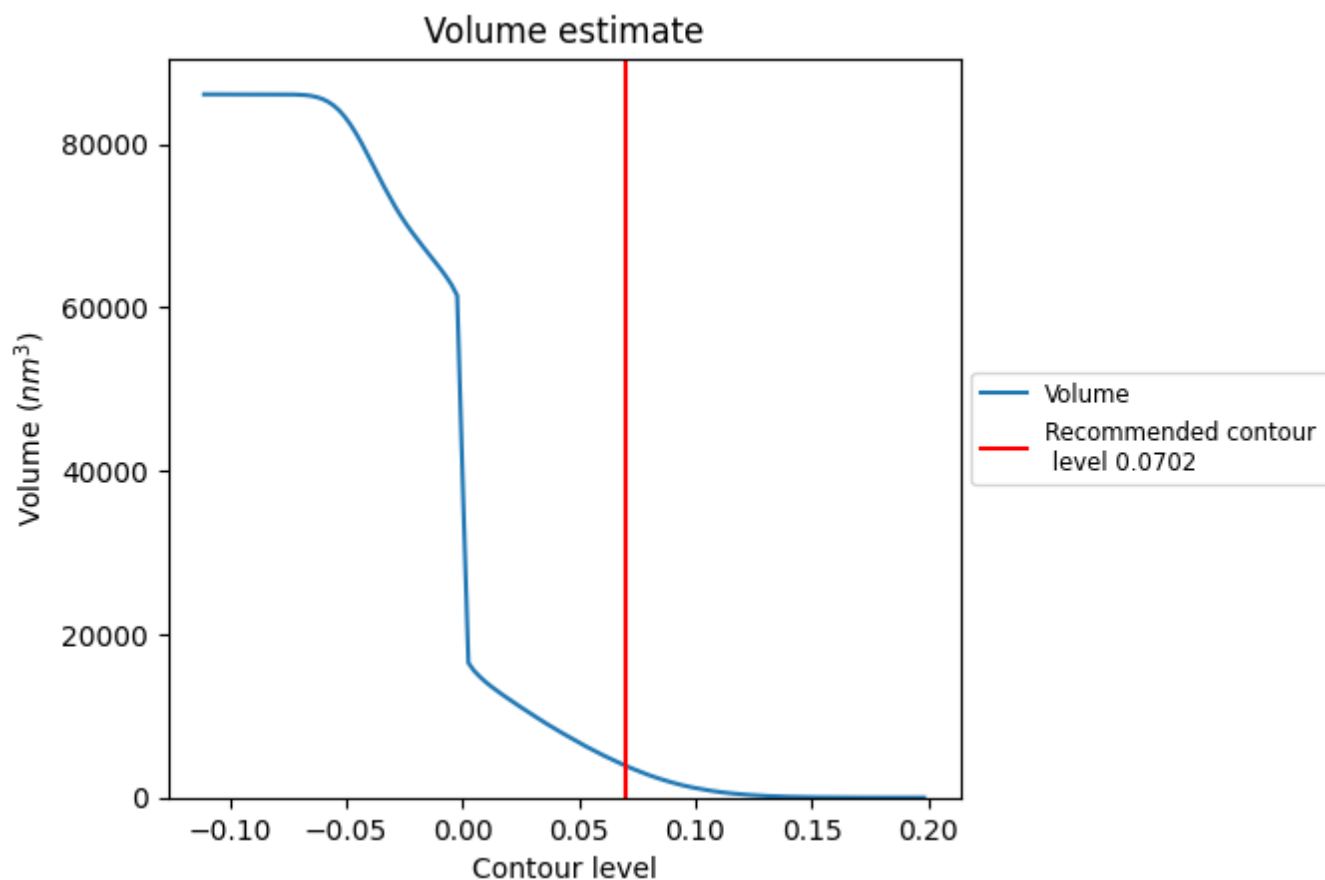
This section contains the results of statistical analysis of the map.

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.

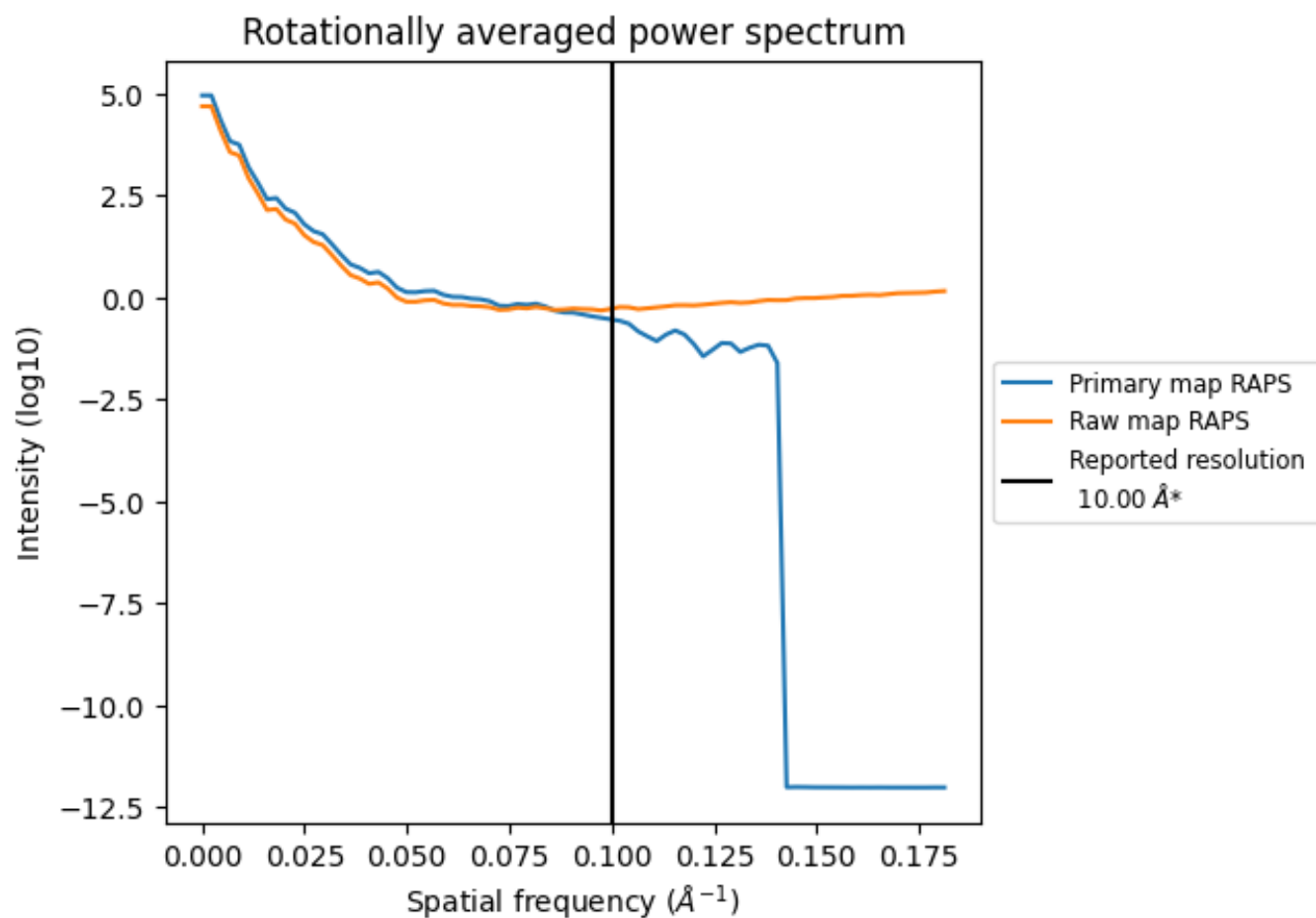
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3872 nm³; this corresponds to an approximate mass of 3497 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 ⓘ

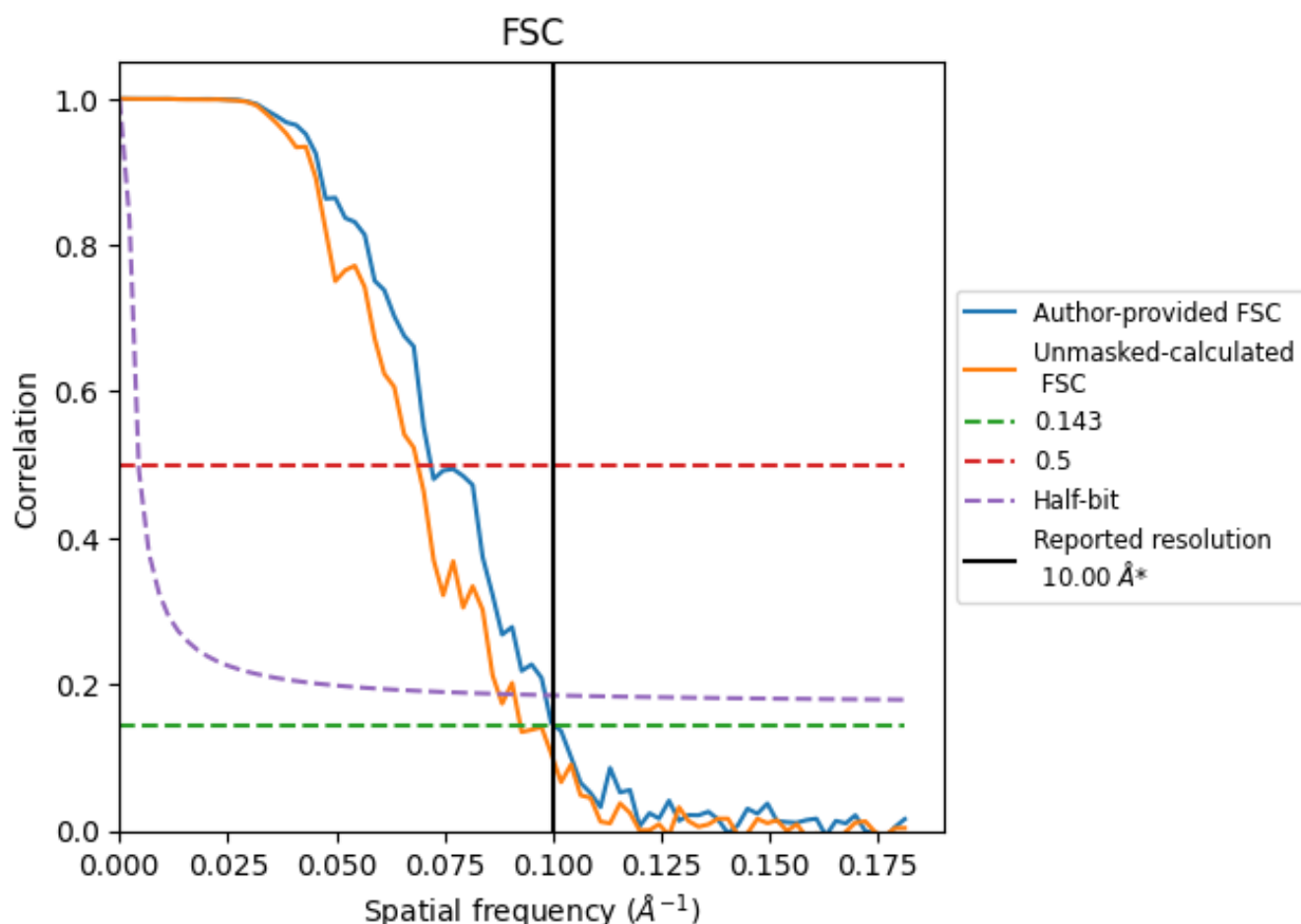


*Reported resolution corresponds to spatial frequency of 0.100 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.100 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.00	-	-
Author-provided FSC curve	9.95	13.93	10.17
Unmasked-calculated*	10.80	14.53	11.43

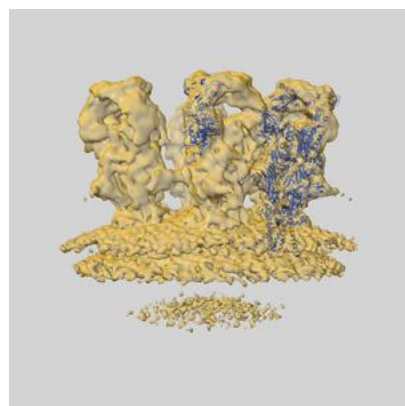
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

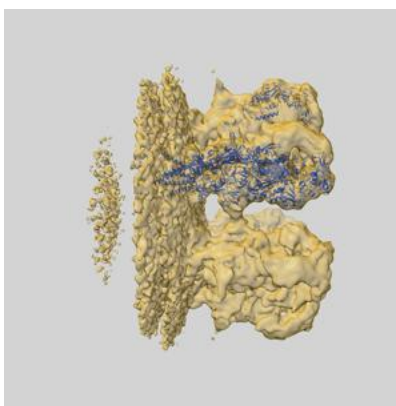
This section contains information regarding the fit between EMDB map EMD-17318 and PDB model 8OZQ. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlays

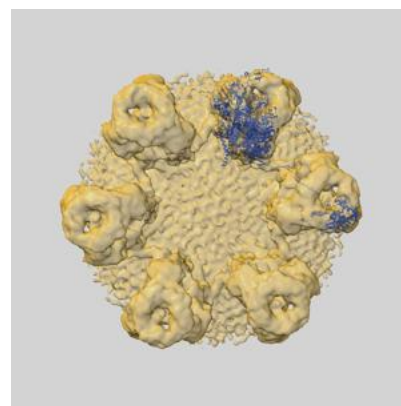
9.1.1 Map-model overlay [i](#)



X

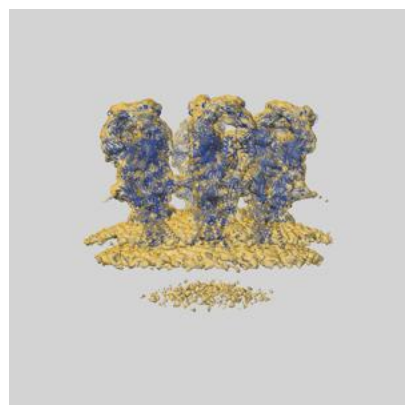


Y

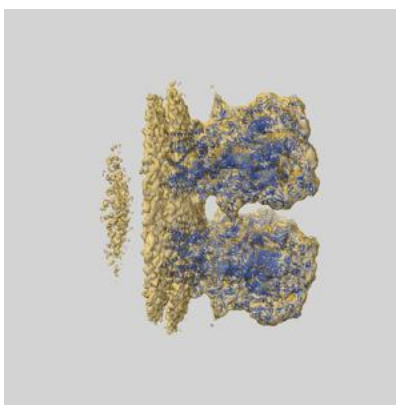


Z

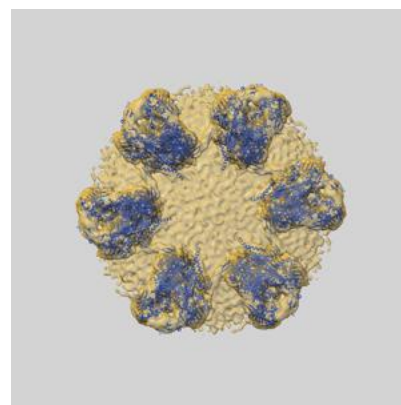
9.1.2 Map-model assembly overlay [i](#)



X



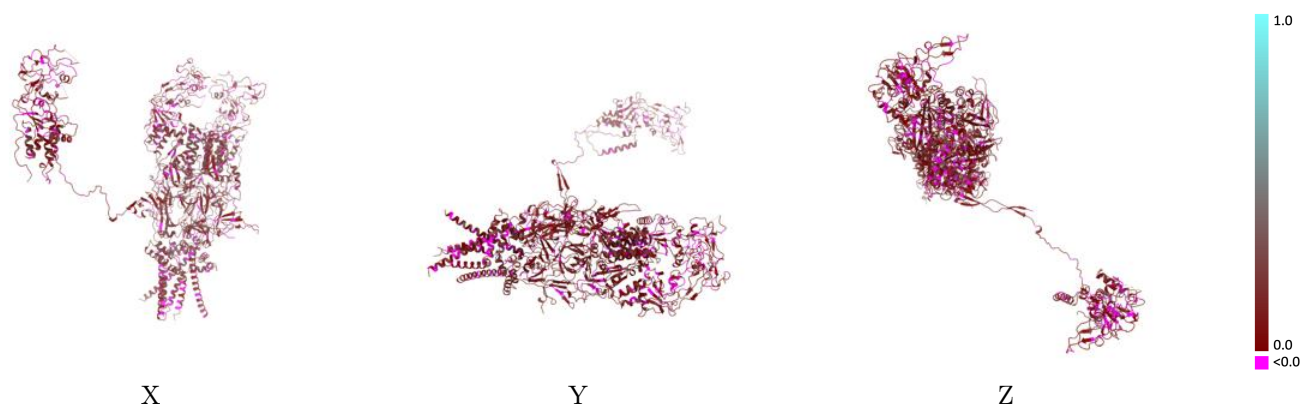
Y



Z

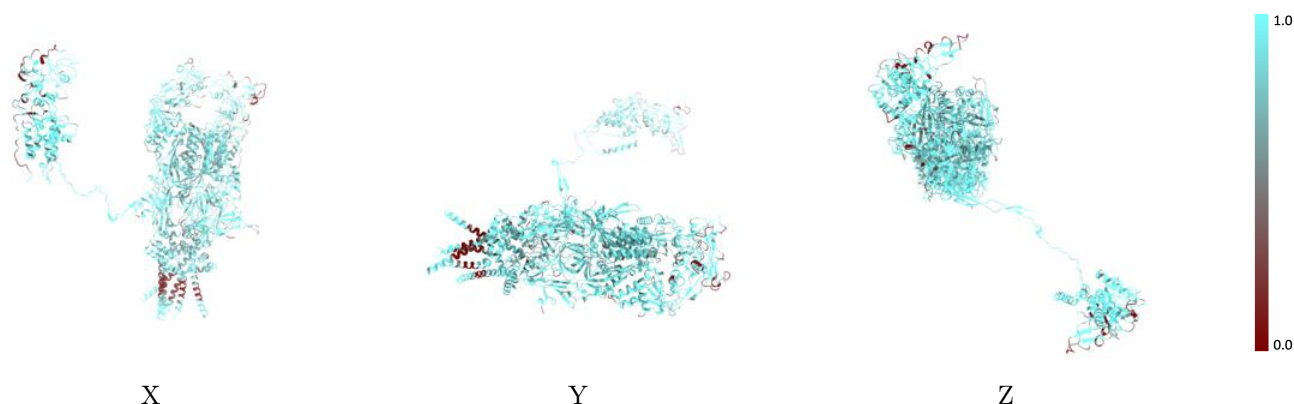
The images above show the 3D surface view of the map at the recommended contour level 0.0702 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



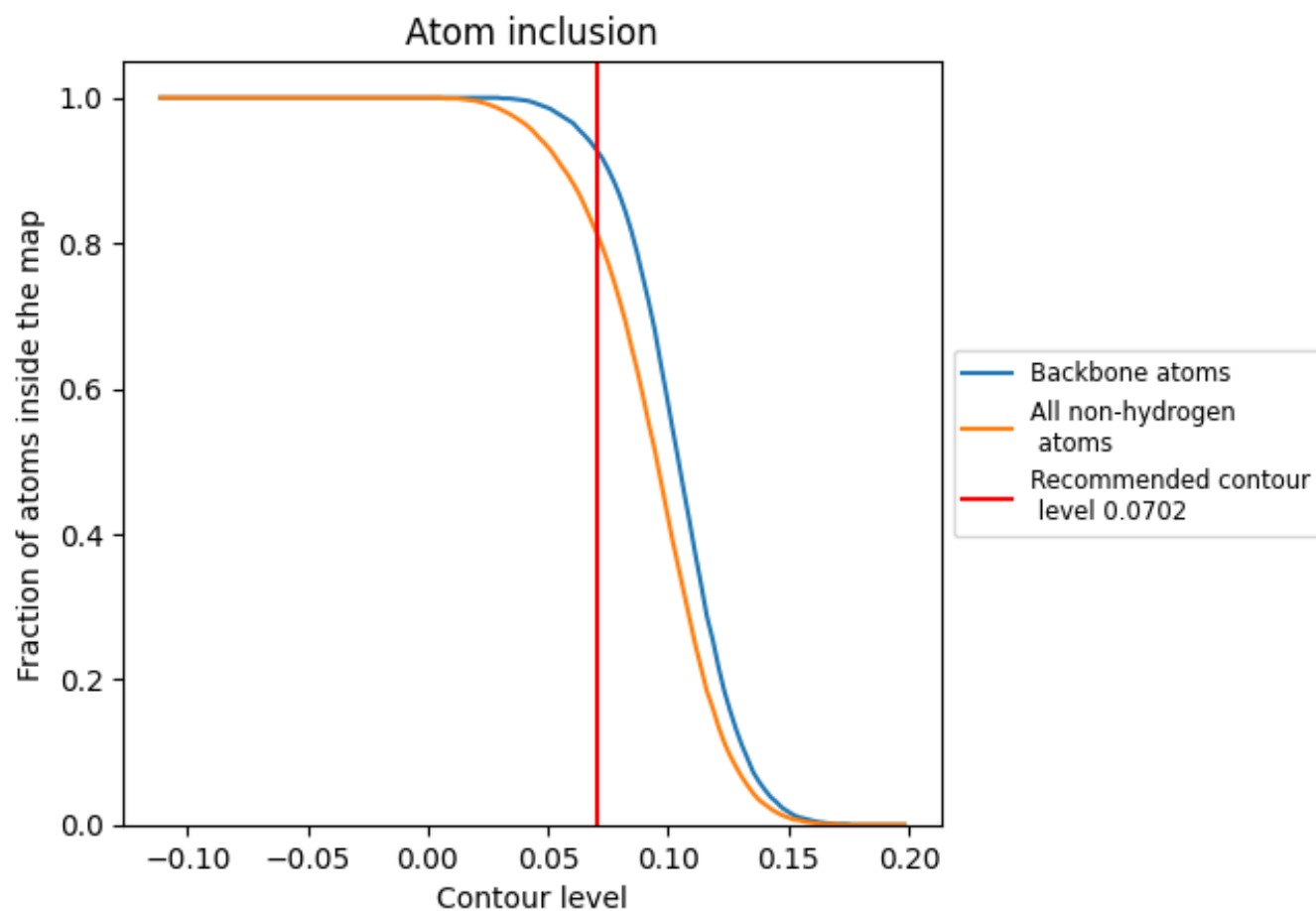
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0702).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0702) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8140	 0.1090
A	 0.7080	 0.0820
B	 0.8330	 0.1050
C	 0.8390	 0.1000
D	 0.8520	 0.1230
E	 0.7580	 0.1370
F	 0.7470	 0.1090
G	 0.8500	 0.0930
H	 0.8260	 0.1100
I	 0.7340	 0.1200
L	 0.8460	 0.1220
M	 0.2500	 0.0710
N	 0.5710	 0.0720
O	 0.8210	 0.2900
P	 0.4400	 0.1060
Q	 0.2600	 0.1390
R	 0.3600	 0.1600
S	 0.3080	 0.0800
T	 0.1540	 -0.0260
U	 0.1540	 -0.0450
V	 0.7470	 0.0530
W	 0.7870	 0.0400
X	 0.5470	 -0.0220
Y	 0.4290	 0.2140
Z	 0.0710	 0.1620
a	 0.4640	 0.2650
b	 0.5710	 0.0720
c	 0.5360	 0.1090
d	 0.7500	 0.1390
e	 0.6380	 0.1470
f	 0.5850	 0.1050
g	 0.7230	 0.1300
h	 0.3470	 0.1330
i	 0.2500	 0.0940
j	 0.2920	 0.2000

