



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 06:44 AM UTC

PDB ID : 8OZH / pdb_00008ozh
EMDB ID : EMD-17309
Title : In situ cryoEM structure of Prototype Foamy Virus Env trimer
Authors : Calcraft, T.; Nans, A.; Rosenthal, P.B.
Deposited on : 2023-05-09
Resolution : 2.91 Å(reported)

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

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

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:

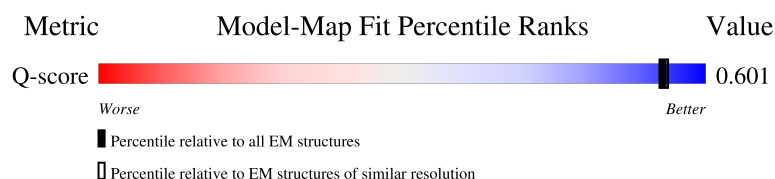
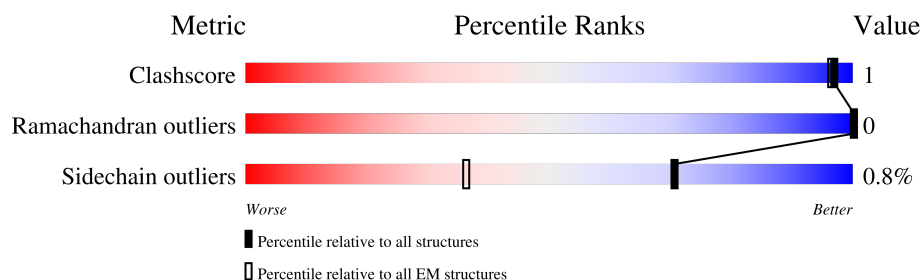
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

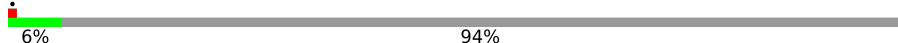
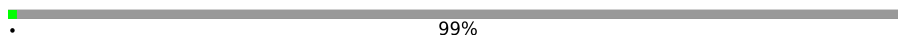
The reported resolution of this entry is 2.91 Å.

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



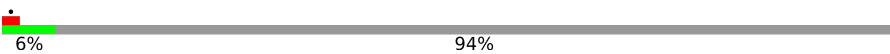
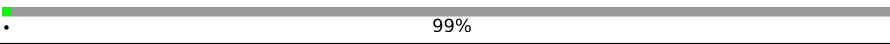
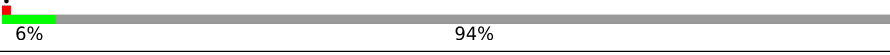
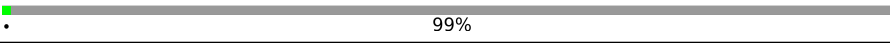
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12972 (2.41 - 3.41)

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	
1	B	988	
1	C	988	
1	D	988	

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Mol	Chain	Length	Quality of chain
1	E	988	 6% 94%
1	F	988	 99%
1	G	988	 40% 59%
1	H	988	 40% 59%
1	I	988	 6% 94%
1	J	988	 99%
1	K	988	 40% 59%
1	L	988	 40% 59%
2	M	2	 50% 50%
2	N	2	 50% 50%
2	O	2	 50% 50%
2	Y	2	 50% 50%
2	Z	2	 50% 50%
2	a	2	 50% 50%
2	b	2	 50% 50%
2	c	2	 50% 50%
2	d	2	 50% 50%
3	S	3	 33% 67% 67%
3	T	3	 33% 67% 67%
3	U	3	 33% 67% 67%
4	V	6	 33% 50% 67%
4	W	6	 33% 50% 67%
4	X	6	 33% 50% 50%
5	P	4	 25% 50% 75%
5	Q	4	 25% 50% 75%

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Mol	Chain	Length	Quality of chain
5	R	4	50% 25% 75%
6	e	8	12% 62% 38%
6	f	8	12% 62% 38%
6	g	8	12% 62% 38%
7	h	6	33% 50% 50%
7	i	6	33% 50% 50%
7	j	6	33% 50% 50%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 22836 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.

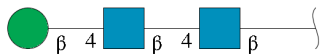
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	58	Total	C	N	O	S	0	0
			466	309	76	77	4		
1	B	11	Total	C	N	O	S	0	0
			94	61	18	14	1		
1	C	405	Total	C	N	O	S	0	0
			3328	2133	549	628	18		
1	D	405	Total	C	N	O	S	0	0
			3190	2054	536	586	14		
1	E	58	Total	C	N	O	S	0	0
			466	309	76	77	4		
1	F	11	Total	C	N	O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

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



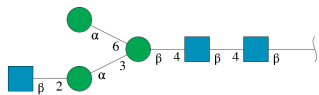
Mol	Chain	Residues	Atoms				AltConf	Trace
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	Y	2	Total	C	N	O	0	0
			28	16	2	10		
2	b	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	Z	2	Total	C	N	O	0	0
			28	16	2	10		
2	c	2	Total	C	N	O	0	0
			28	16	2	10		
2	O	2	Total	C	N	O	0	0
			28	16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



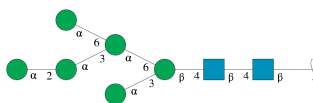
Mol	Chain	Residues	Atoms				AltConf	Trace
4	V	6	Total	C	N	O	0	0
			75	42	3	30		
4	W	6	Total	C	N	O	0	0
			75	42	3	30		
4	X	6	Total	C	N	O	0	0
			75	42	3	30		

- 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.



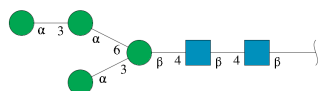
Mol	Chain	Residues	Atoms				AltConf	Trace
5	P	4	Total	C	N	O	0	0
			50	28	2	20		
5	Q	4	Total	C	N	O	0	0
			50	28	2	20		
5	R	4	Total	C	N	O	0	0
			50	28	2	20		

- 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.



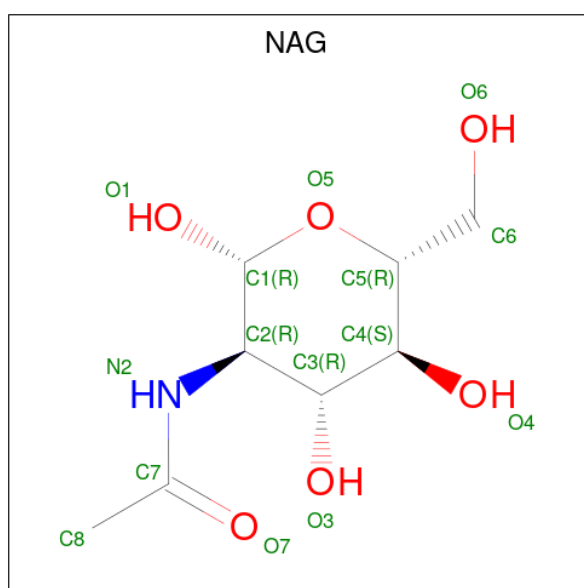
Mol	Chain	Residues	Atoms				AltConf	Trace
6	e	8	Total	C	N	O	0	0
			94	52	2	40		
6	f	8	Total	C	N	O	0	0
			94	52	2	40		
6	g	8	Total	C	N	O	0	0
			94	52	2	40		

- 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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



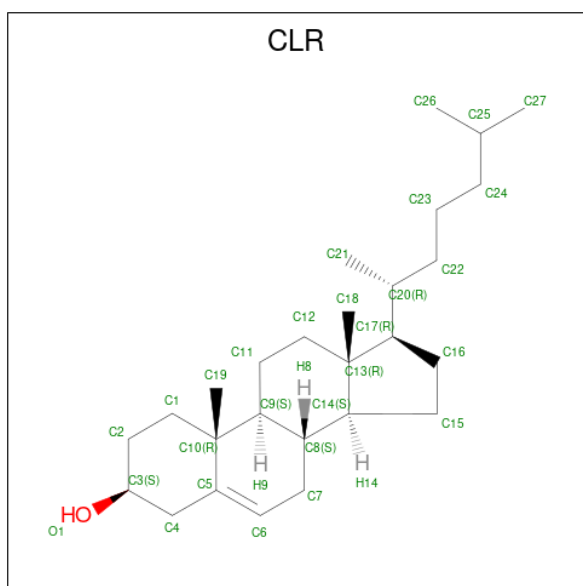
Mol	Chain	Residues	Atoms				AltConf
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	G	1	Total	C	N	O	0
			14	8	1	5	
8	G	1	Total	C	N	O	0
			14	8	1	5	
8	G	1	Total	C	N	O	0
			14	8	1	5	

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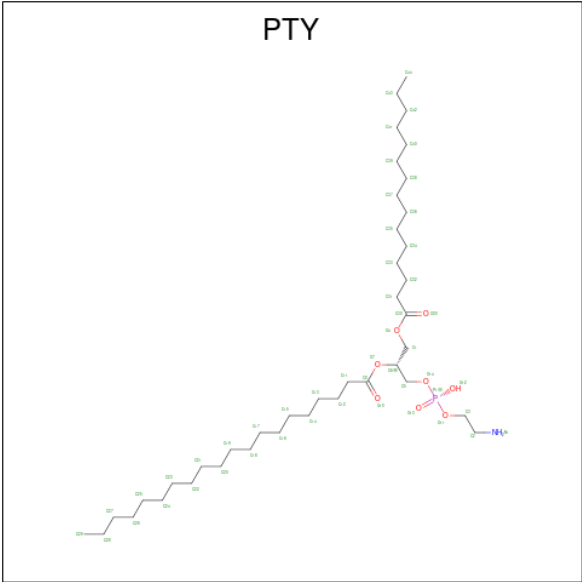
Mol	Chain	Residues	Atoms				AltConf
8	K	1	Total	C	N	O	0
			14	8	1	5	
8	K	1	Total	C	N	O	0
			14	8	1	5	
8	K	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 9 is CHOLESTEROL (CCD ID: 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		

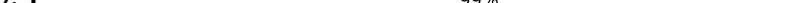
- Molecule 10 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



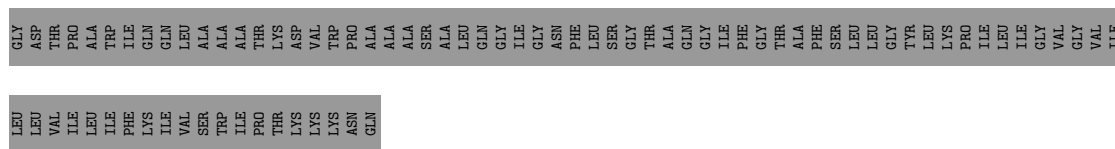
Mol	Chain	Residues	Atoms					AltConf
10	D	1	Total	C	N	O	P	0
			50	40	1	8	1	
10	H	1	Total	C	N	O	P	0
			50	40	1	8	1	
10	L	1	Total	C	N	O	P	0
			50	40	1	8	1	

[illegible]

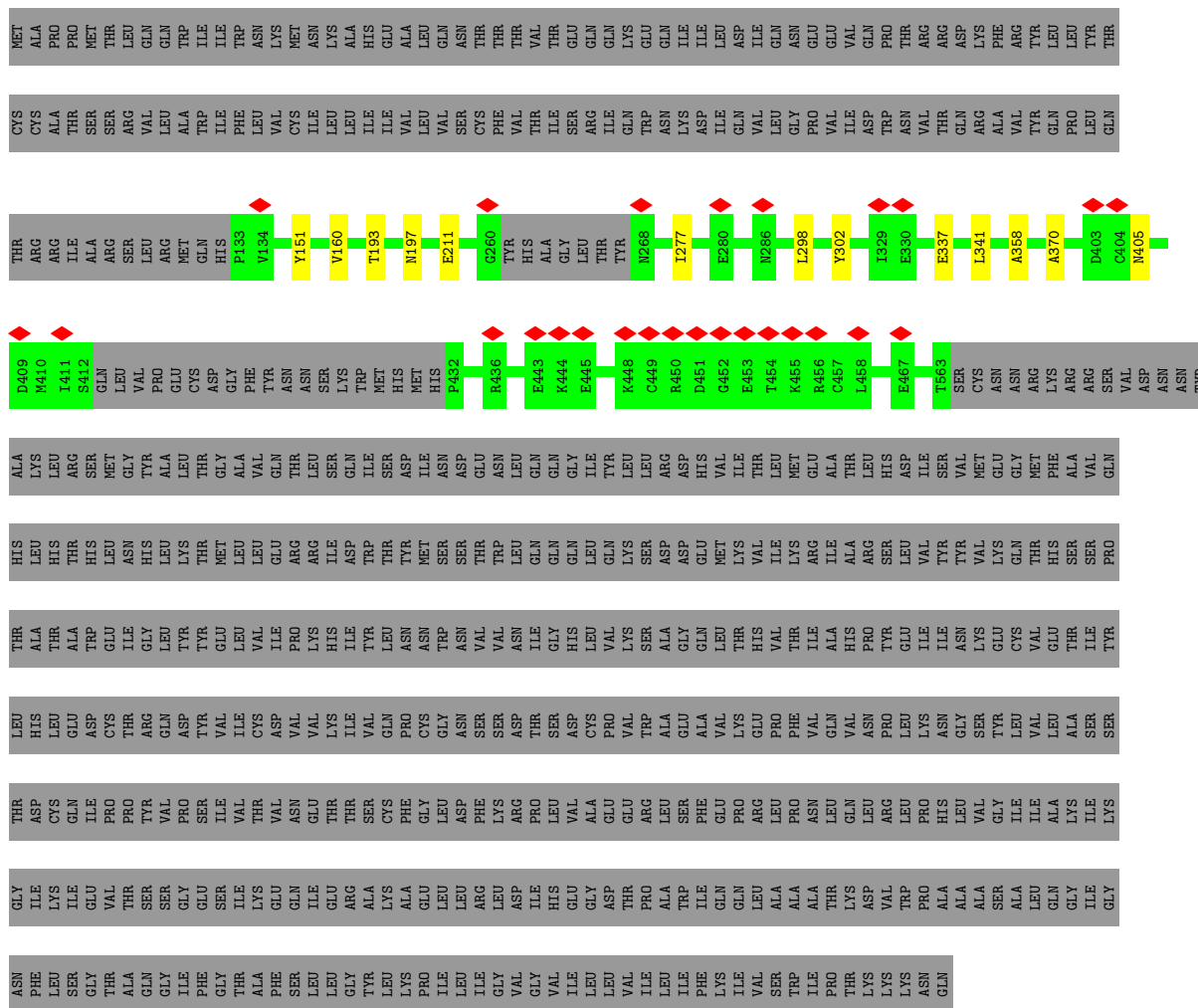
- Molecule 1: Envelope glycoprotein

Chain B:  99%

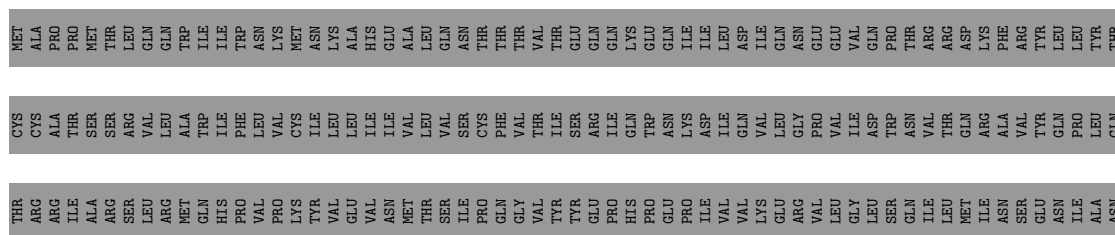
[illegible]

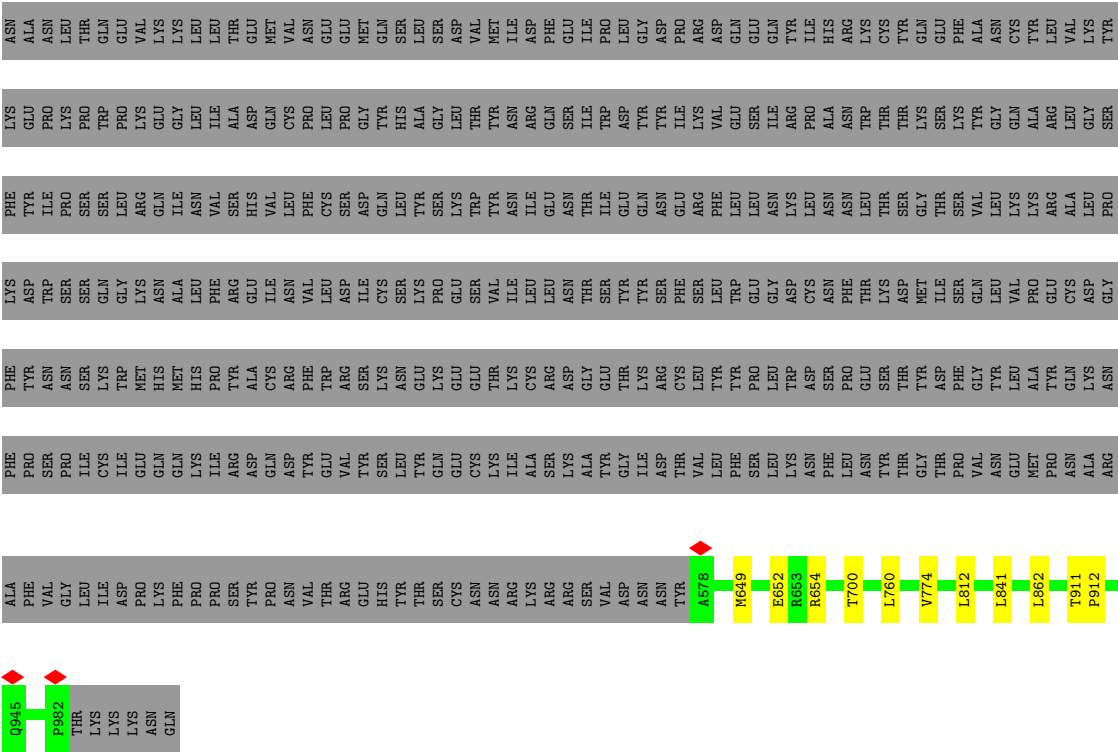


- Molecule 1: Envelope glycoprotein

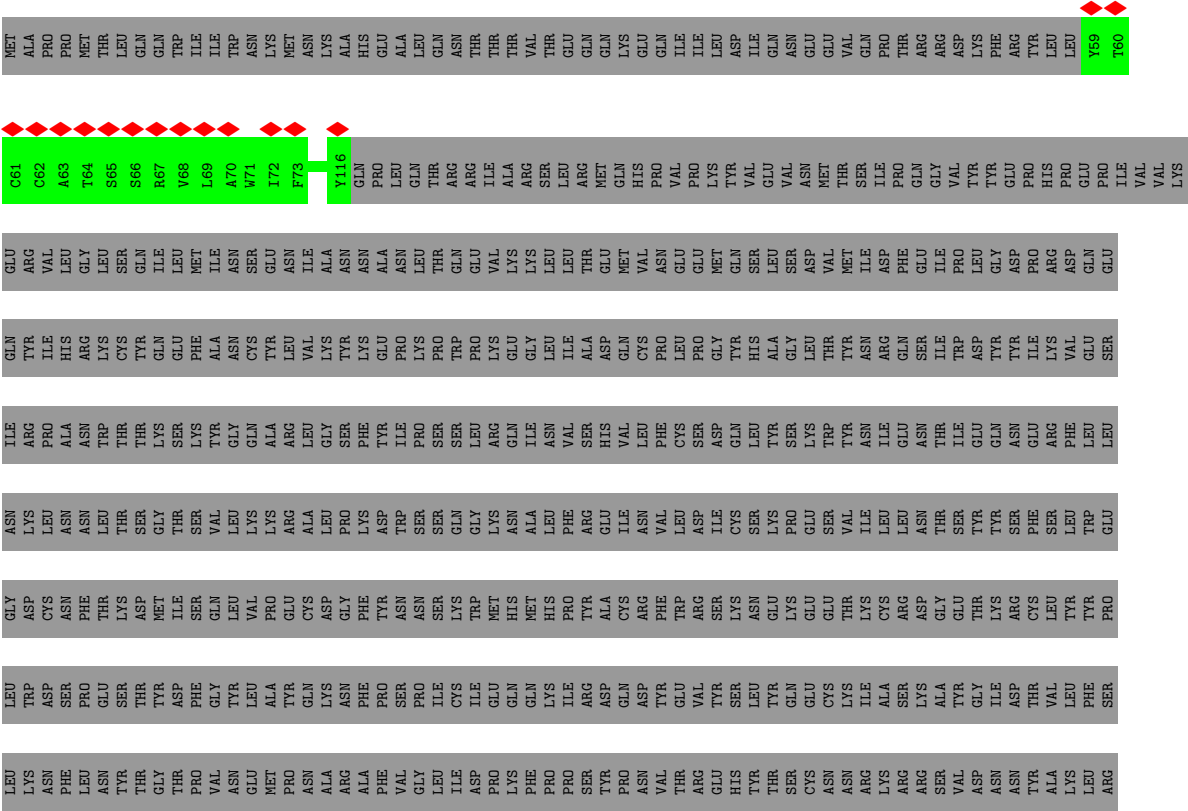


- Molecule 1: Envelope glycoprotein





● Molecule 1: Envelope glycoprotein



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

- Molecule 1: Envelope glycoprotein

Chain F: 99%

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

WORLDWIDE
PDB
PROTEIN DATA BANK

59%

- Molecule 1: Envelope glycoprotein

94%

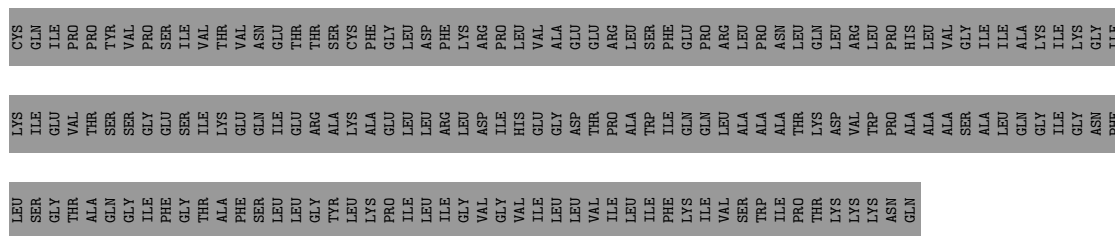


[illegible]

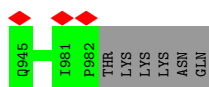
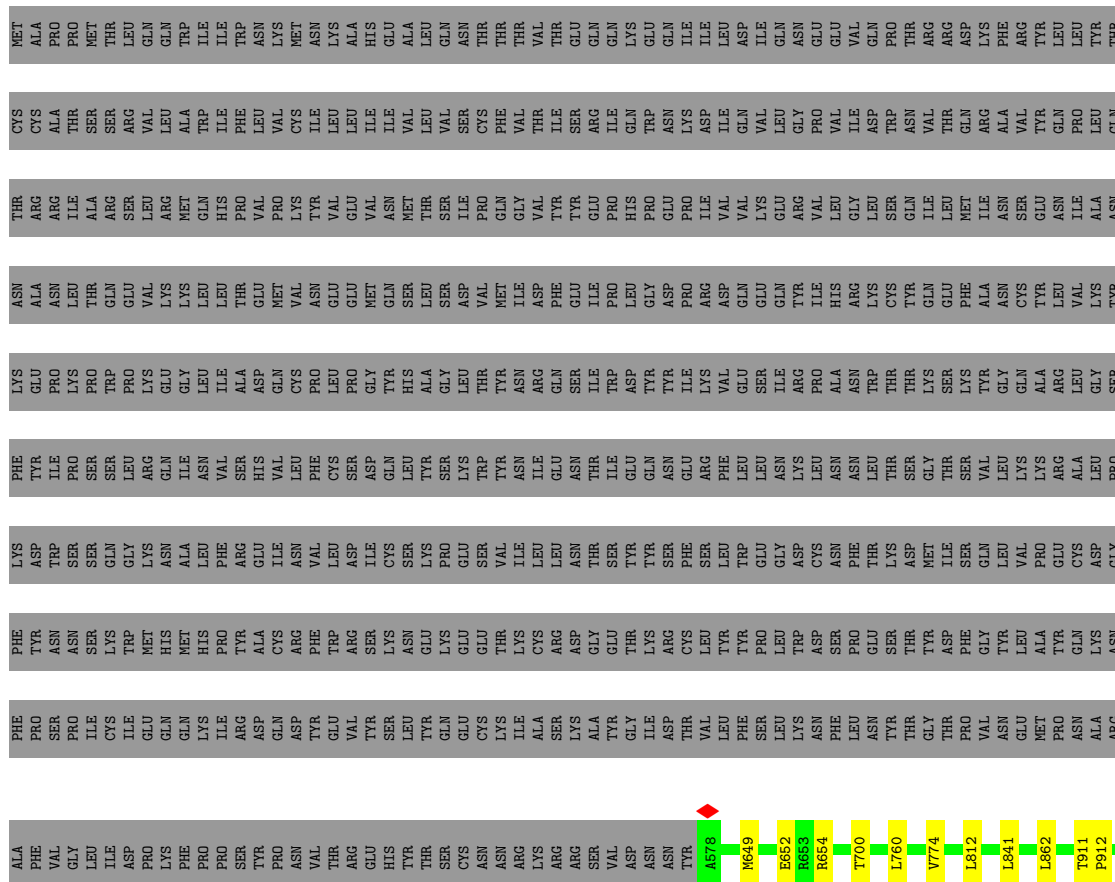
- Molecule 1: Envelope glycoprotein

Chain K:

[illegible]



- Molecule 1: Envelope glycoprotein



- 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



- 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 d:



- 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:



- 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:



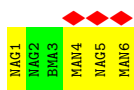
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

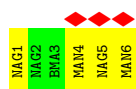


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

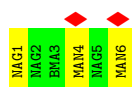
Chain V:



- 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



- 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



- 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



- 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

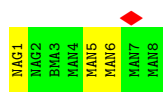


- Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

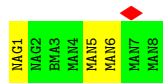


- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

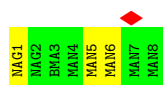




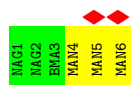
- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



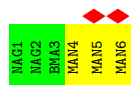
- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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



- 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



- 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



MAN1	
MAN2	
BMA3	
MAN4	
MAN5	
MAN6	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	286827	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 ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.185	Depositor
Minimum map value	-0.119	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	518.4, 518.4, 518.4	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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, PTY, NAG, CLR

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	1.09	0/476	1.62	0/653
1	B	0.92	0/97	1.12	0/130
1	C	1.04	0/3416	1.36	0/4634
1	D	1.07	0/3260	1.40	0/4441
1	E	1.09	0/476	1.62	0/653
1	F	0.92	0/97	1.12	0/130
1	G	1.04	0/3416	1.36	0/4634
1	H	1.08	0/3260	1.40	0/4441
1	I	1.09	0/476	1.62	0/653
1	J	0.92	0/97	1.12	0/130
1	K	1.04	0/3416	1.36	0/4634
1	L	1.08	0/3260	1.40	0/4441
All	All	1.06	0/21747	1.39	0/29574

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	94	0	97	0	0
1	C	3328	0	3241	7	0
1	D	3190	0	3242	8	0
1	E	466	0	488	0	0
1	F	94	0	97	0	0
1	G	3328	0	3241	7	0
1	H	3190	0	3242	7	0
1	I	466	0	488	0	0
1	J	94	0	97	0	0
1	K	3328	0	3241	7	0
1	L	3190	0	3242	8	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	C	42	0	39	0	0
8	G	42	0	39	0	0
8	K	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	H	50	0	79	0	0
10	L	50	0	79	0	0
All	All	22836	0	22764	32	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.

The worst 5 of 32 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:K:197:ASN:OD1	1:L:700:THR:HG21	1.97	0.65
1:C:197:ASN:OD1	1:D:700:THR:HG21	1.97	0.65
1:G:197:ASN:OD1	1:H:700:THR:HG21	1.97	0.64
1:G:277:ILE:HG21	1:G:298:LEU:HD12	1.89	0.55
1:K:277:ILE:HG21	1:K:298:LEU:HD12	1.89	0.54

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	9/988 (1%)	7 (78%)	2 (22%)	0	100	100
1	C	399/988 (40%)	374 (94%)	25 (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%)	376 (93%)	27 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	56/988 (6%)	55 (98%)	1 (2%)	0	100	100
1	J	9/988 (1%)	7 (78%)	2 (22%)	0	100	100
1	K	399/988 (40%)	374 (94%)	25 (6%)	0	100	100
1	L	403/988 (41%)	376 (93%)	27 (7%)	0	100	100
All	All	2601/11856 (22%)	2437 (94%)	164 (6%)	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	54/899 (6%)	54 (100%)	0	100	100
1	B	11/899 (1%)	11 (100%)	0	100	100
1	C	376/899 (42%)	373 (99%)	3 (1%)	73	89
1	D	356/899 (40%)	353 (99%)	3 (1%)	73	89
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%)	373 (99%)	3 (1%)	73	89
1	H	356/899 (40%)	353 (99%)	3 (1%)	73	89
1	I	54/899 (6%)	54 (100%)	0	100	100
1	J	11/899 (1%)	11 (100%)	0	100	100
1	K	376/899 (42%)	373 (99%)	3 (1%)	73	89
1	L	356/899 (40%)	353 (99%)	3 (1%)	73	89
All	All	2391/10788 (22%)	2373 (99%)	18 (1%)	70	89

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	405	ASN

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Mol	Chain	Res	Type
1	L	862	LEU
1	L	841	LEU
1	G	405	ASN
1	K	211	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	893	GLN
1	K	335	GLN
1	K	321	GLN
1	K	478	GLN
1	D	893	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	1,2	14,14,15	0.32	0	17,19,21	1.38	2 (11%)
2	NAG	M	2	2	14,14,15	0.33	0	17,19,21	0.76	0
2	NAG	N	1	1,2	14,14,15	0.32	0	17,19,21	1.37	2 (11%)
2	NAG	N	2	2	14,14,15	0.32	0	17,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	O	1	1,2	14,14,15	0.32	0	17,19,21	1.37	2 (11%)
2	NAG	O	2	2	14,14,15	0.33	0	17,19,21	0.76	0
5	NAG	P	1	1,5	14,14,15	0.36	0	17,19,21	1.04	1 (5%)
5	NAG	P	2	5	14,14,15	0.37	0	17,19,21	0.93	1 (5%)
5	BMA	P	3	5	11,11,12	0.40	0	15,15,17	0.77	1 (6%)
5	MAN	P	4	5	11,11,12	0.42	0	15,15,17	0.76	0
5	NAG	Q	1	1,5	14,14,15	0.35	0	17,19,21	1.04	1 (5%)
5	NAG	Q	2	5	14,14,15	0.37	0	17,19,21	0.92	1 (5%)
5	BMA	Q	3	5	11,11,12	0.39	0	15,15,17	0.77	1 (6%)
5	MAN	Q	4	5	11,11,12	0.43	0	15,15,17	0.76	0
5	NAG	R	1	1,5	14,14,15	0.35	0	17,19,21	1.04	1 (5%)
5	NAG	R	2	5	14,14,15	0.38	0	17,19,21	0.93	1 (5%)
5	BMA	R	3	5	11,11,12	0.39	0	15,15,17	0.77	1 (6%)
5	MAN	R	4	5	11,11,12	0.42	0	15,15,17	0.77	0
3	NAG	S	1	1,3	14,14,15	0.41	0	17,19,21	1.44	2 (11%)
3	NAG	S	2	3	14,14,15	0.43	0	17,19,21	1.58	3 (17%)
3	BMA	S	3	3	11,11,12	0.33	0	15,15,17	0.53	0
3	NAG	T	1	1,3	14,14,15	0.41	0	17,19,21	1.44	2 (11%)
3	NAG	T	2	3	14,14,15	0.43	0	17,19,21	1.58	3 (17%)
3	BMA	T	3	3	11,11,12	0.34	0	15,15,17	0.54	0
3	NAG	U	1	1,3	14,14,15	0.41	0	17,19,21	1.44	2 (11%)
3	NAG	U	2	3	14,14,15	0.43	0	17,19,21	1.58	3 (17%)
3	BMA	U	3	3	11,11,12	0.34	0	15,15,17	0.53	0
4	NAG	V	1	1,4	14,14,15	0.51	0	17,19,21	1.11	1 (5%)
4	NAG	V	2	4	14,14,15	0.30	0	17,19,21	0.80	0
4	BMA	V	3	4	11,11,12	0.35	0	15,15,17	0.70	0
4	MAN	V	4	4	11,11,12	0.65	0	15,15,17	1.26	2 (13%)
4	NAG	V	5	4	14,14,15	0.25	0	17,19,21	0.85	1 (5%)
4	MAN	V	6	4	11,11,12	0.37	0	15,15,17	0.80	1 (6%)
4	NAG	W	1	1,4	14,14,15	0.50	0	17,19,21	1.12	1 (5%)
4	NAG	W	2	4	14,14,15	0.31	0	17,19,21	0.80	0
4	BMA	W	3	4	11,11,12	0.35	0	15,15,17	0.71	0
4	MAN	W	4	4	11,11,12	0.64	0	15,15,17	1.27	2 (13%)
4	NAG	W	5	4	14,14,15	0.25	0	17,19,21	0.84	1 (5%)
4	MAN	W	6	4	11,11,12	0.36	0	15,15,17	0.79	1 (6%)
4	NAG	X	1	1,4	14,14,15	0.50	0	17,19,21	1.12	1 (5%)
4	NAG	X	2	4	14,14,15	0.31	0	17,19,21	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BMA	X	3	4	11,11,12	0.36	0	15,15,17	0.70	0
4	MAN	X	4	4	11,11,12	0.65	0	15,15,17	1.26	2 (13%)
4	NAG	X	5	4	14,14,15	0.25	0	17,19,21	0.84	0
4	MAN	X	6	4	11,11,12	0.37	0	15,15,17	0.79	1 (6%)
2	NAG	Y	1	1,2	14,14,15	0.39	0	17,19,21	0.76	0
2	NAG	Y	2	2	14,14,15	0.32	0	17,19,21	1.00	2 (11%)
2	NAG	Z	1	1,2	14,14,15	0.39	0	17,19,21	0.75	0
2	NAG	Z	2	2	14,14,15	0.33	0	17,19,21	1.00	2 (11%)
2	NAG	a	1	1,2	14,14,15	0.39	0	17,19,21	0.76	0
2	NAG	a	2	2	14,14,15	0.32	0	17,19,21	1.01	2 (11%)
2	NAG	b	1	1,2	14,14,15	0.37	0	17,19,21	0.76	0
2	NAG	b	2	2	14,14,15	0.32	0	17,19,21	1.19	2 (11%)
2	NAG	c	1	1,2	14,14,15	0.38	0	17,19,21	0.76	0
2	NAG	c	2	2	14,14,15	0.32	0	17,19,21	1.19	2 (11%)
2	NAG	d	1	1,2	14,14,15	0.37	0	17,19,21	0.76	0
2	NAG	d	2	2	14,14,15	0.32	0	17,19,21	1.19	2 (11%)
6	NAG	e	1	1,6	14,14,15	0.37	0	17,19,21	1.17	1 (5%)
6	NAG	e	2	6	14,14,15	0.44	0	17,19,21	0.85	0
6	BMA	e	3	6	11,11,12	0.36	0	15,15,17	0.57	0
6	MAN	e	4	6	11,11,12	0.34	0	15,15,17	0.72	0
6	MAN	e	5	6	11,11,12	0.34	0	15,15,17	0.86	1 (6%)
6	MAN	e	6	6	11,11,12	0.35	0	15,15,17	0.81	1 (6%)
6	MAN	e	7	6	11,11,12	0.38	0	15,15,17	0.62	0
6	MAN	e	8	6	11,11,12	0.34	0	15,15,17	0.64	0
6	NAG	f	1	1,6	14,14,15	0.38	0	17,19,21	1.17	1 (5%)
6	NAG	f	2	6	14,14,15	0.44	0	17,19,21	0.85	0
6	BMA	f	3	6	11,11,12	0.37	0	15,15,17	0.57	0
6	MAN	f	4	6	11,11,12	0.34	0	15,15,17	0.72	0
6	MAN	f	5	6	11,11,12	0.34	0	15,15,17	0.86	1 (6%)
6	MAN	f	6	6	11,11,12	0.35	0	15,15,17	0.81	1 (6%)
6	MAN	f	7	6	11,11,12	0.38	0	15,15,17	0.62	0
6	MAN	f	8	6	11,11,12	0.35	0	15,15,17	0.64	0
6	NAG	g	1	1,6	14,14,15	0.37	0	17,19,21	1.17	1 (5%)
6	NAG	g	2	6	14,14,15	0.44	0	17,19,21	0.85	0
6	BMA	g	3	6	11,11,12	0.37	0	15,15,17	0.57	0
6	MAN	g	4	6	11,11,12	0.34	0	15,15,17	0.72	0
6	MAN	g	5	6	11,11,12	0.35	0	15,15,17	0.86	1 (6%)
6	MAN	g	6	6	11,11,12	0.36	0	15,15,17	0.81	1 (6%)
6	MAN	g	7	6	11,11,12	0.38	0	15,15,17	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	g	8	6	11,11,12	0.35	0	15,15,17	0.64	0
7	NAG	h	1	1,7	14,14,15	0.50	0	17,19,21	1.11	0
7	NAG	h	2	7	14,14,15	0.46	0	17,19,21	0.82	0
7	BMA	h	3	7	11,11,12	0.39	0	15,15,17	0.58	0
7	MAN	h	4	7	11,11,12	0.37	0	15,15,17	0.84	1 (6%)
7	MAN	h	5	7	11,11,12	0.33	0	15,15,17	0.80	1 (6%)
7	MAN	h	6	7	11,11,12	0.35	0	15,15,17	0.70	1 (6%)
7	NAG	i	1	1,7	14,14,15	0.50	0	17,19,21	1.11	0
7	NAG	i	2	7	14,14,15	0.46	0	17,19,21	0.82	0
7	BMA	i	3	7	11,11,12	0.40	0	15,15,17	0.58	0
7	MAN	i	4	7	11,11,12	0.36	0	15,15,17	0.83	1 (6%)
7	MAN	i	5	7	11,11,12	0.33	0	15,15,17	0.80	1 (6%)
7	MAN	i	6	7	11,11,12	0.35	0	15,15,17	0.70	1 (6%)
7	NAG	j	1	1,7	14,14,15	0.50	0	17,19,21	1.11	0
7	NAG	j	2	7	14,14,15	0.47	0	17,19,21	0.82	0
7	BMA	j	3	7	11,11,12	0.39	0	15,15,17	0.58	0
7	MAN	j	4	7	11,11,12	0.36	0	15,15,17	0.83	1 (6%)
7	MAN	j	5	7	11,11,12	0.33	0	15,15,17	0.80	1 (6%)
7	MAN	j	6	7	11,11,12	0.35	0	15,15,17	0.70	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	1,2	-	2/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	0/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	0/6/23/26	0/1/1/1
5	NAG	P	1	1,5	-	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	1,5	-	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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	c	1	1,2	-	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	1,2	-	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	1,6	-	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	1,6	-	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	1,6	-	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
7	NAG	h	1	1,7	-	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	1,7	-	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	1,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	2	NAG	C2-N2-C7	4.07	128.35	122.90
3	T	2	NAG	C2-N2-C7	4.06	128.34	122.90
3	S	2	NAG	C2-N2-C7	4.04	128.31	122.90
4	V	4	MAN	O2-C2-C1	3.57	117.39	109.22
4	W	4	MAN	O2-C2-C1	3.57	117.39	109.22

There are no chirality outliers.

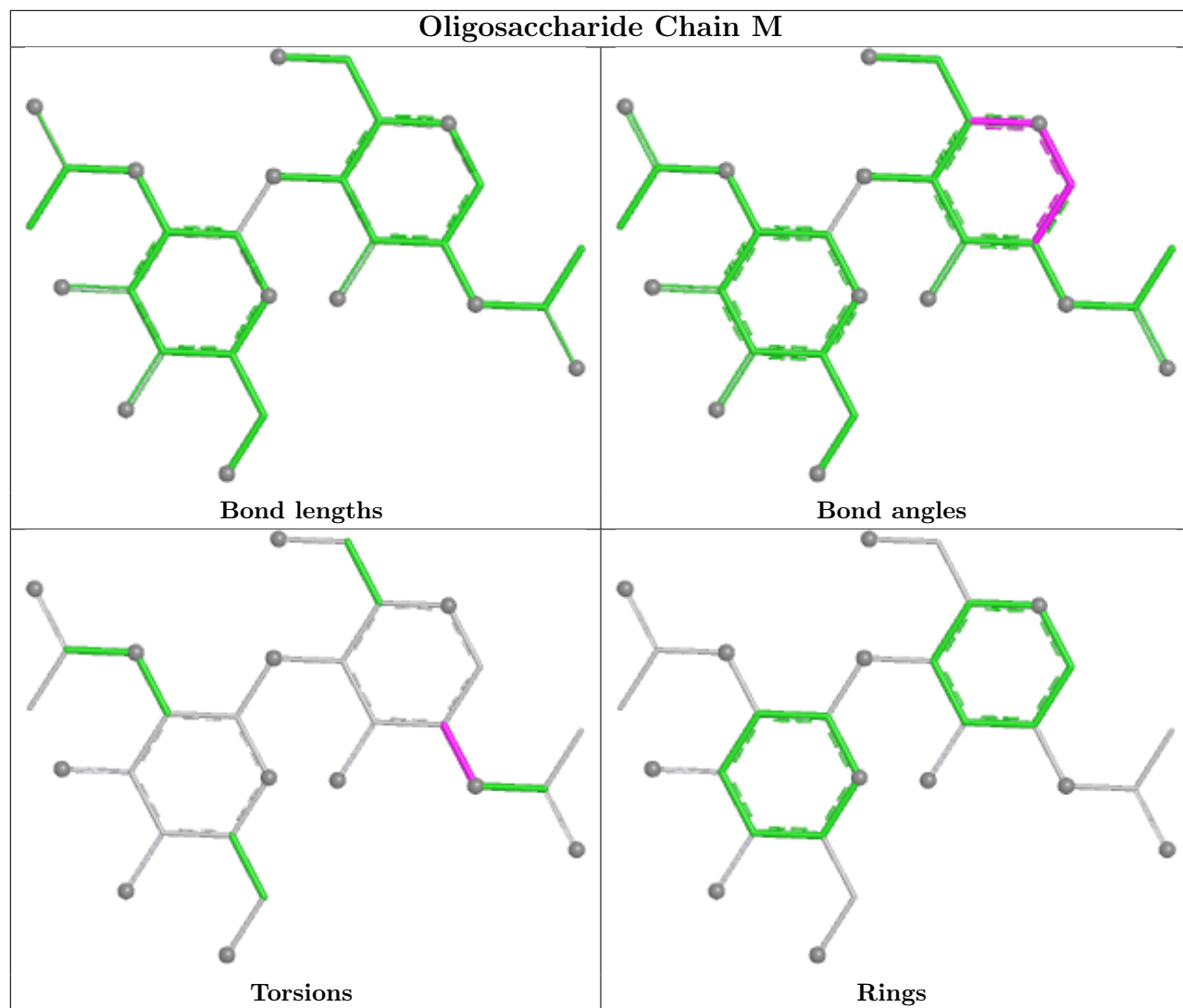
5 of 69 torsion outliers are listed below:

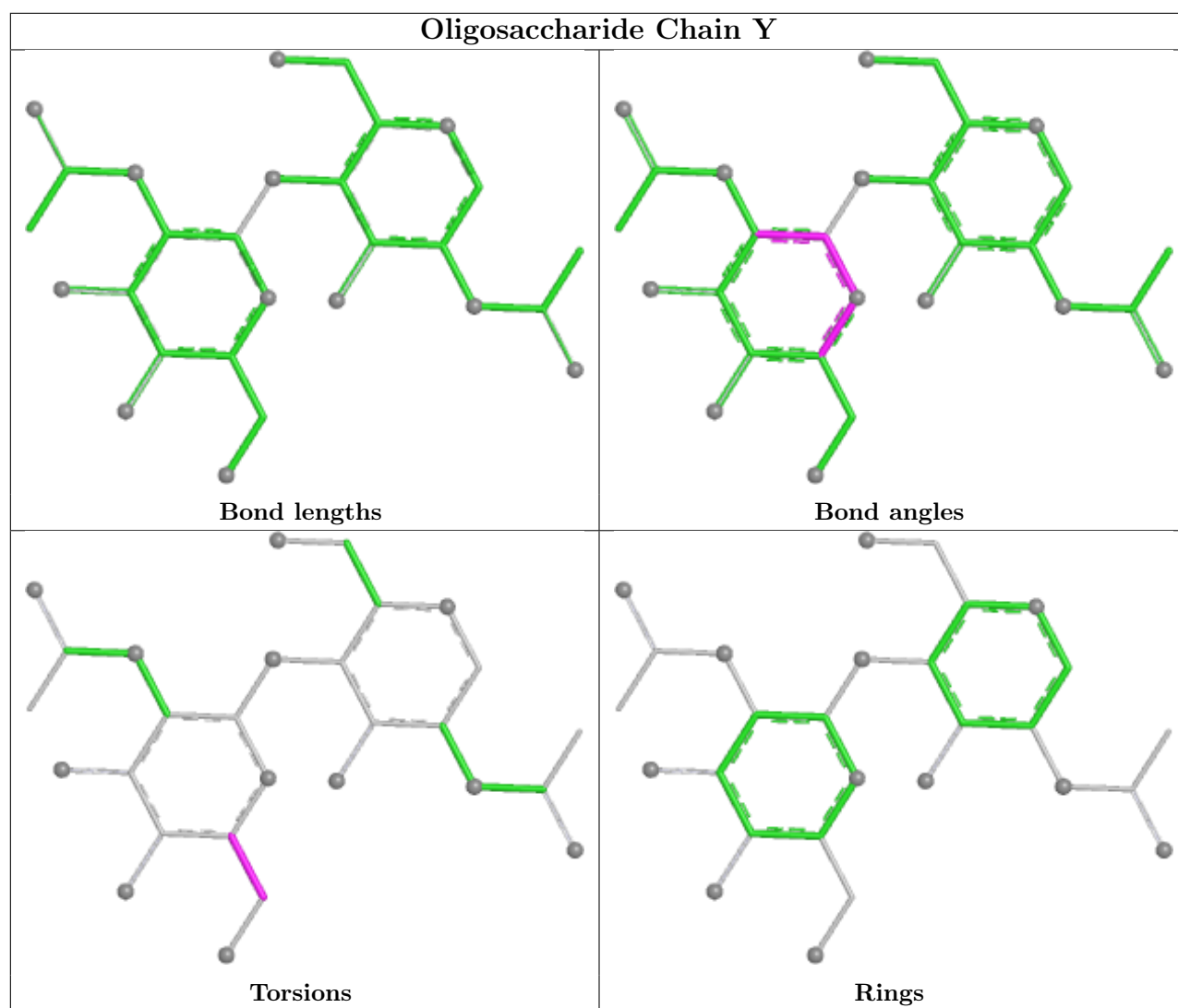
Mol	Chain	Res	Type	Atoms
3	S	2	NAG	C3-C2-N2-C7
3	T	2	NAG	C3-C2-N2-C7
3	U	2	NAG	C3-C2-N2-C7
2	b	1	NAG	O5-C5-C6-O6
2	c	1	NAG	O5-C5-C6-O6

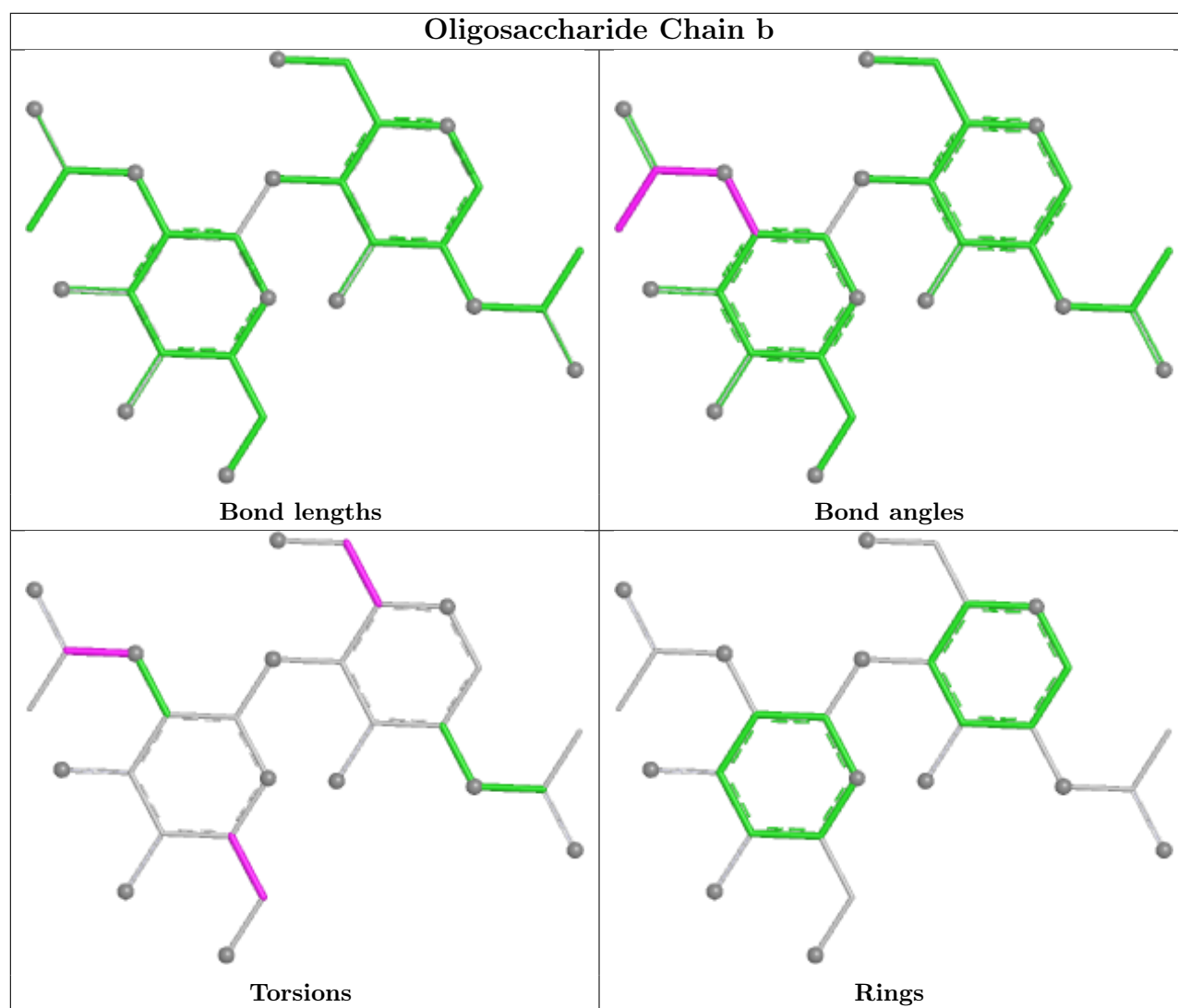
There are no ring outliers.

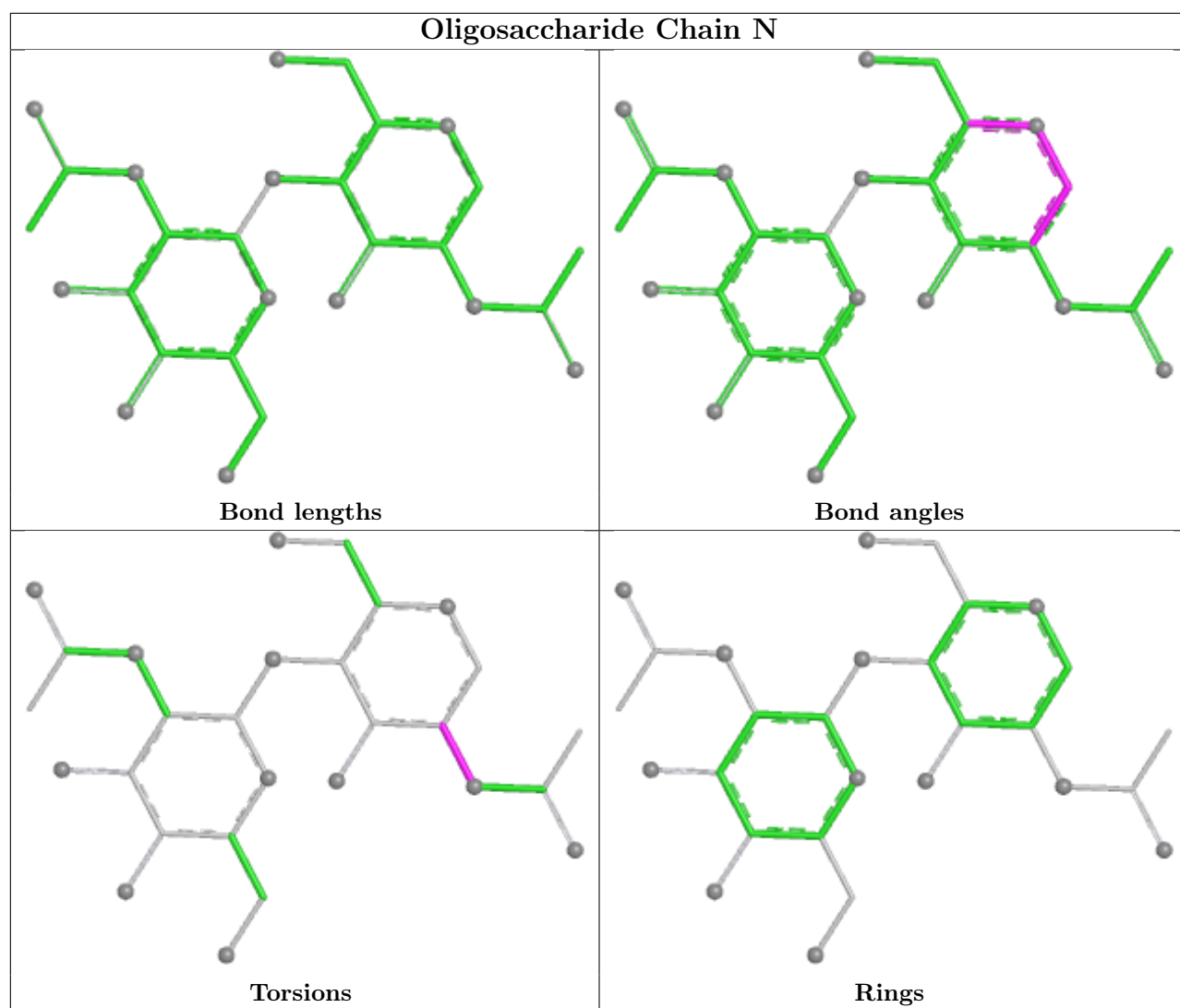
No monomer is involved in short contacts.

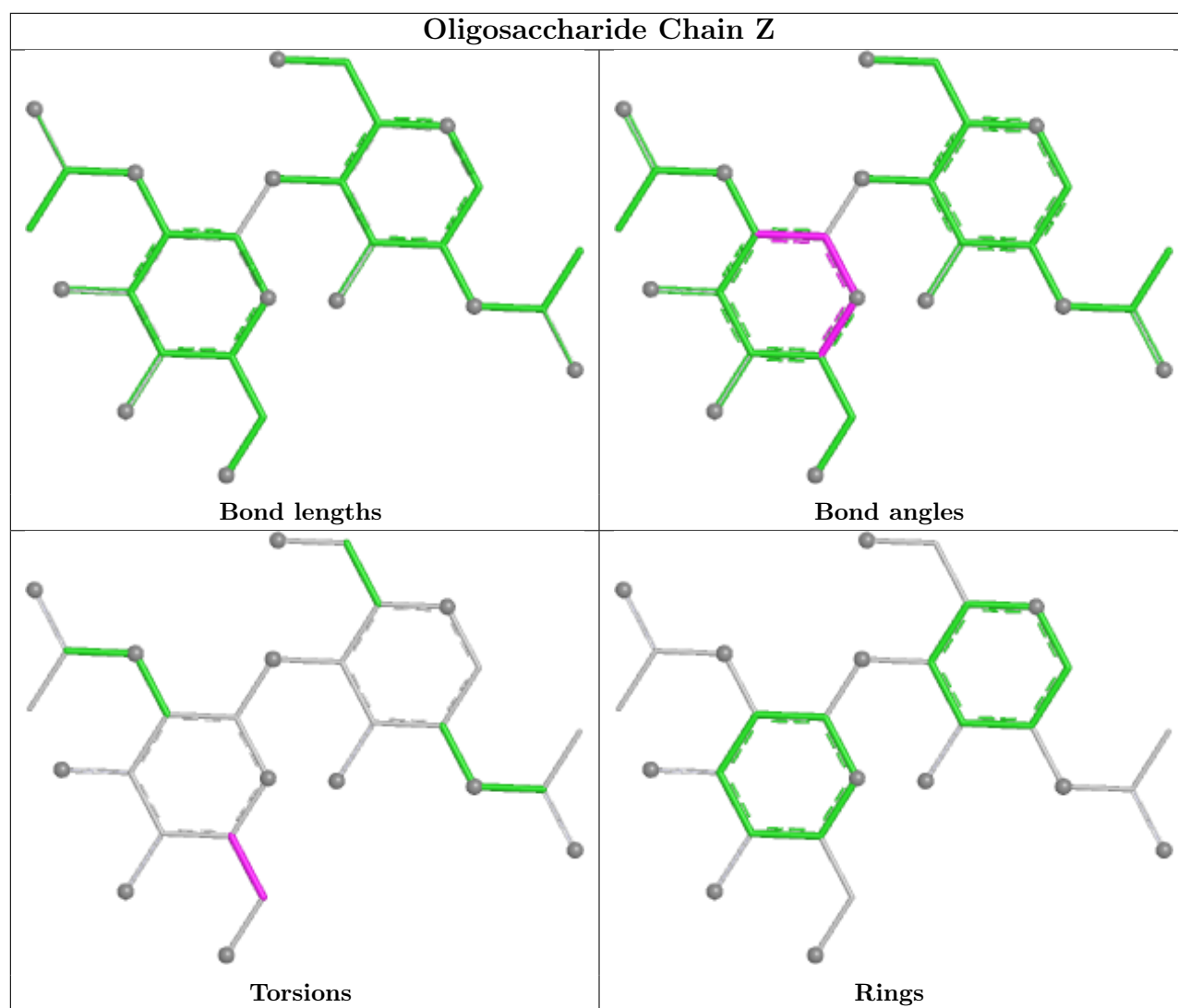
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

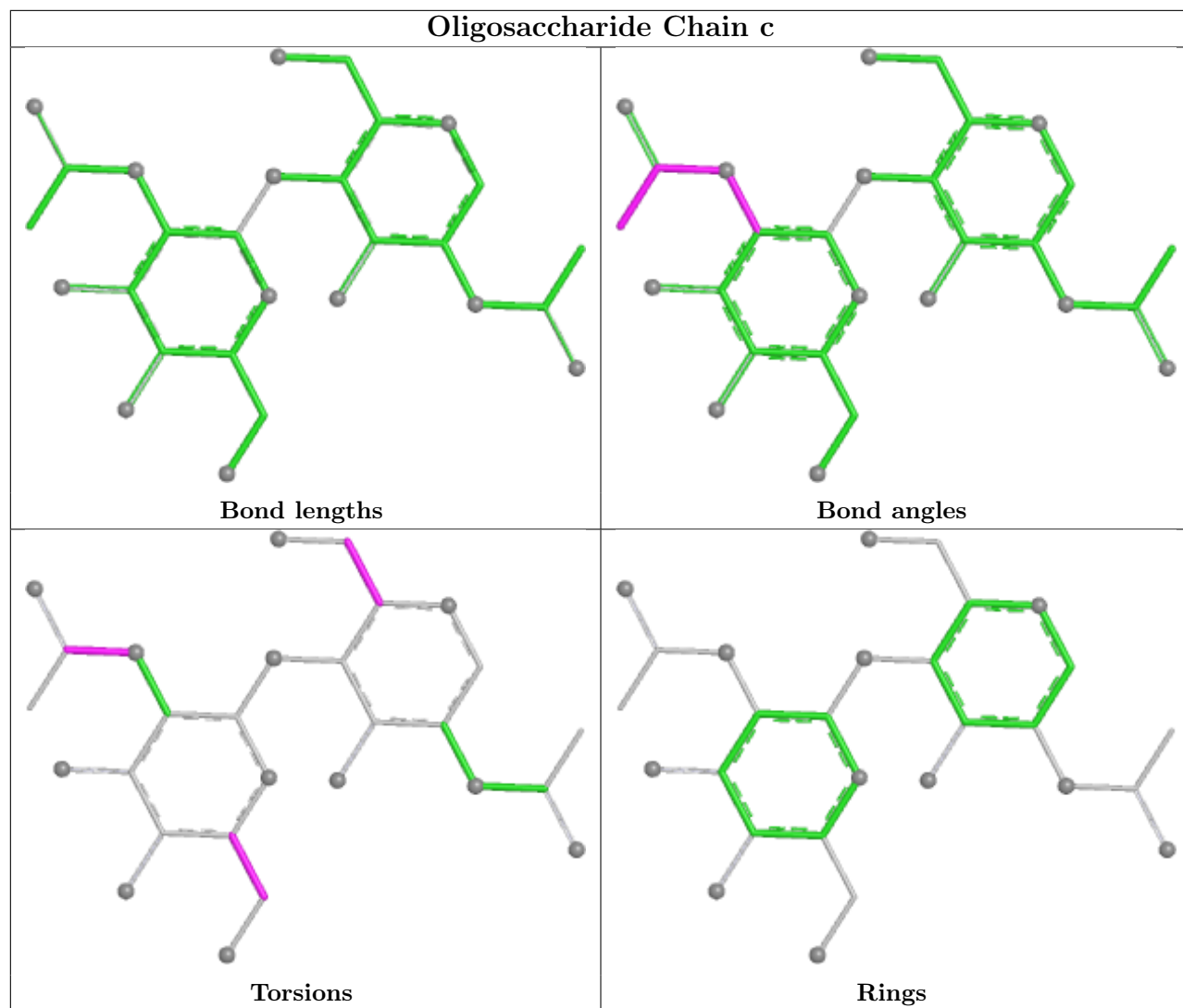


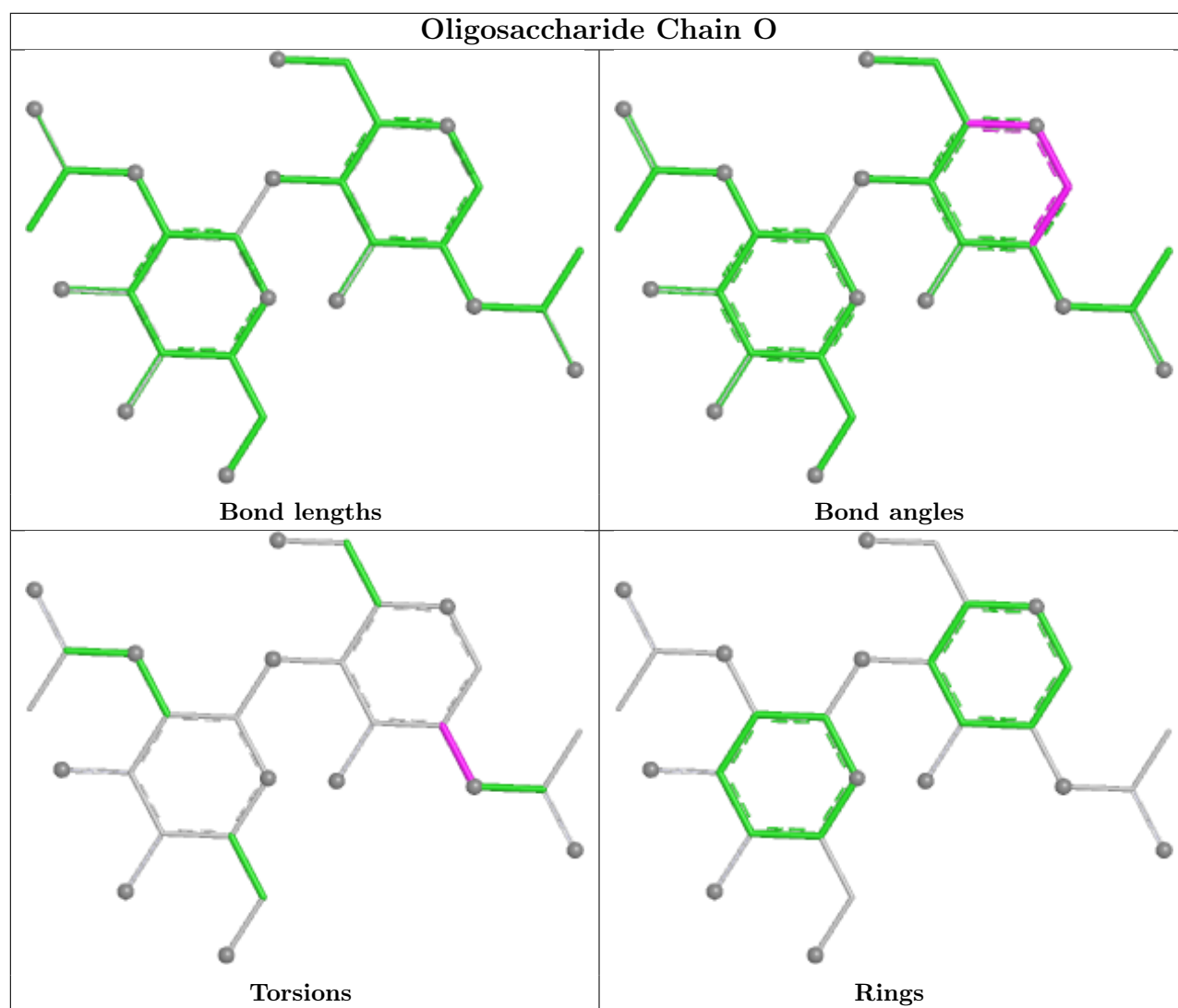


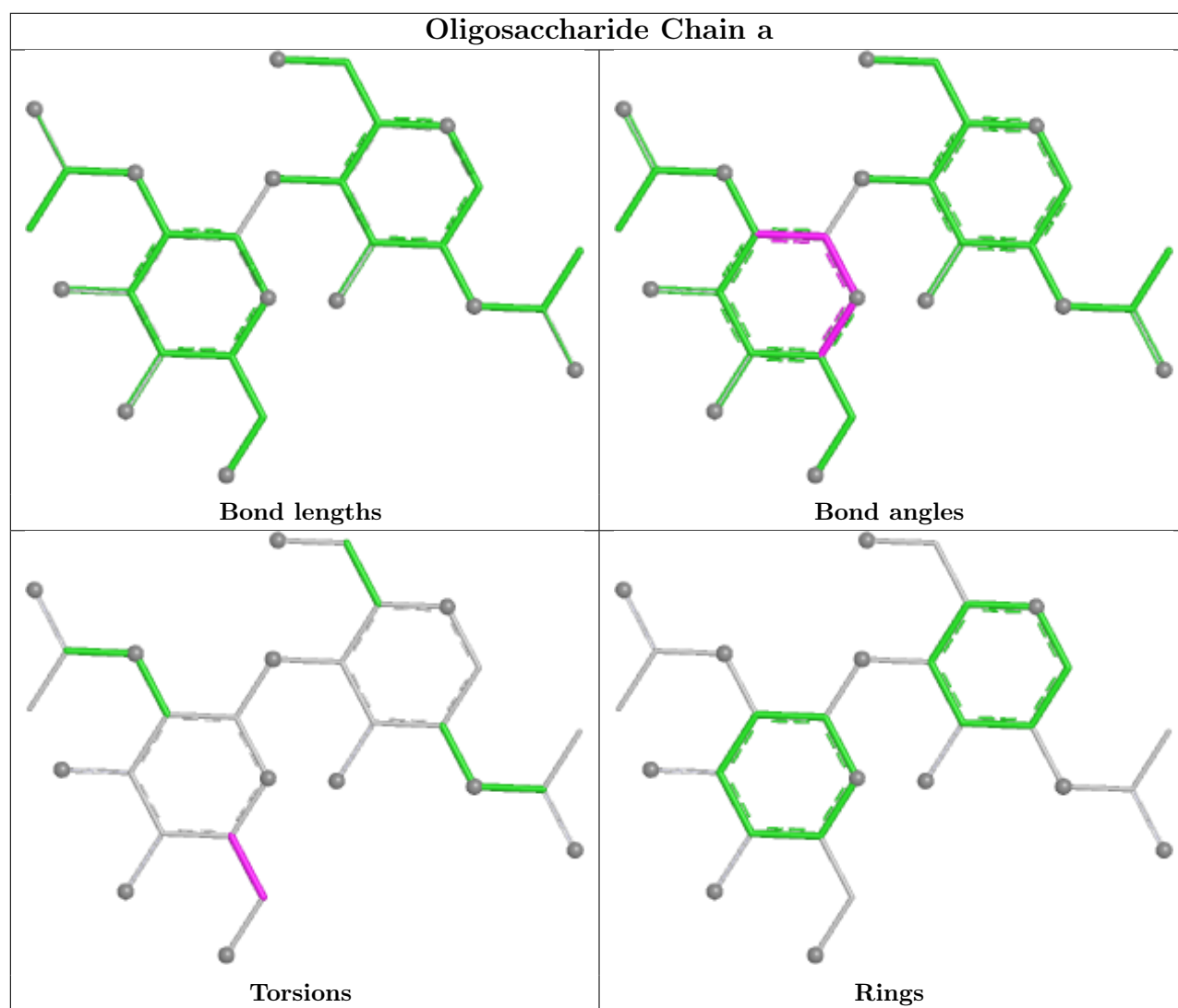


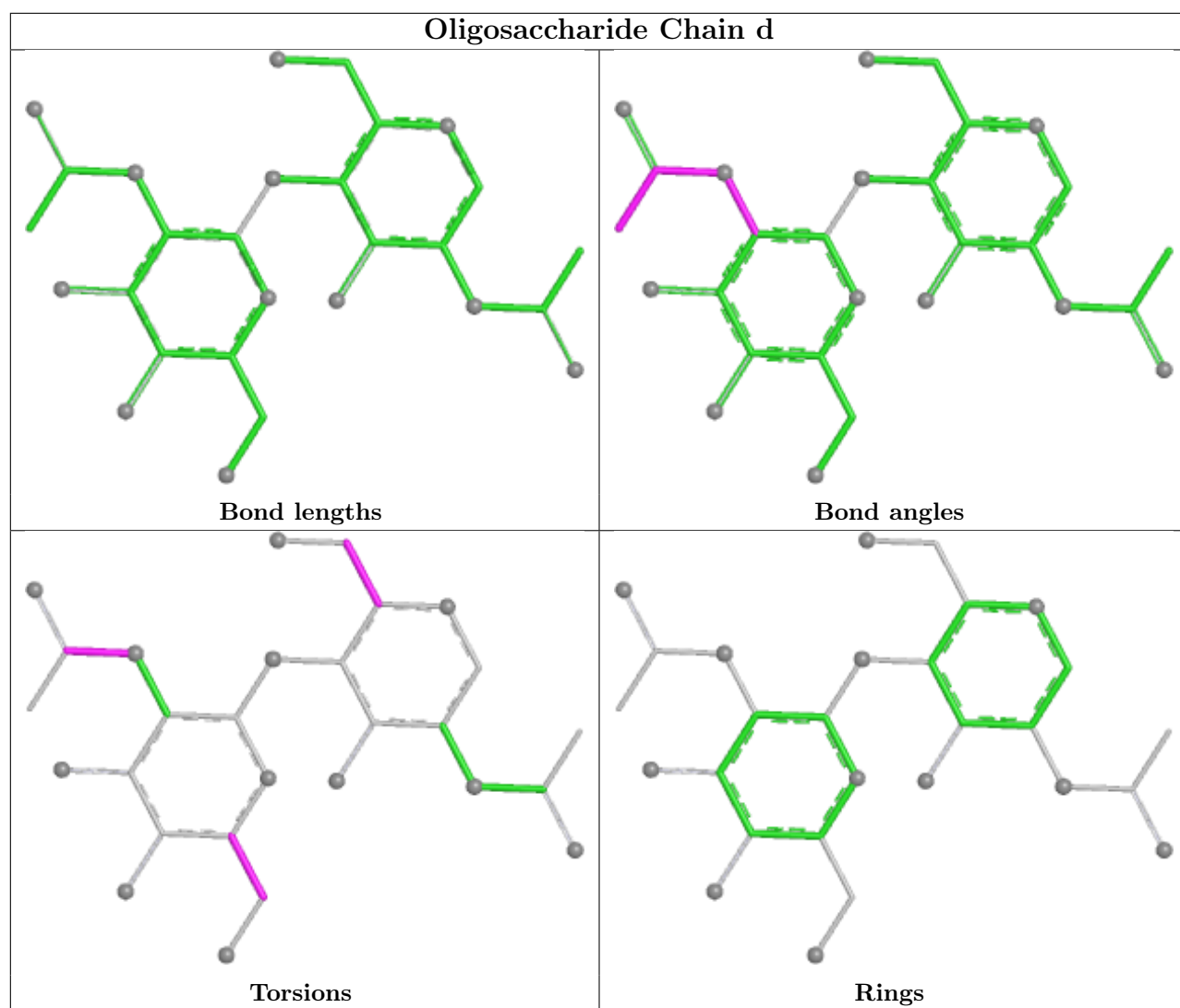


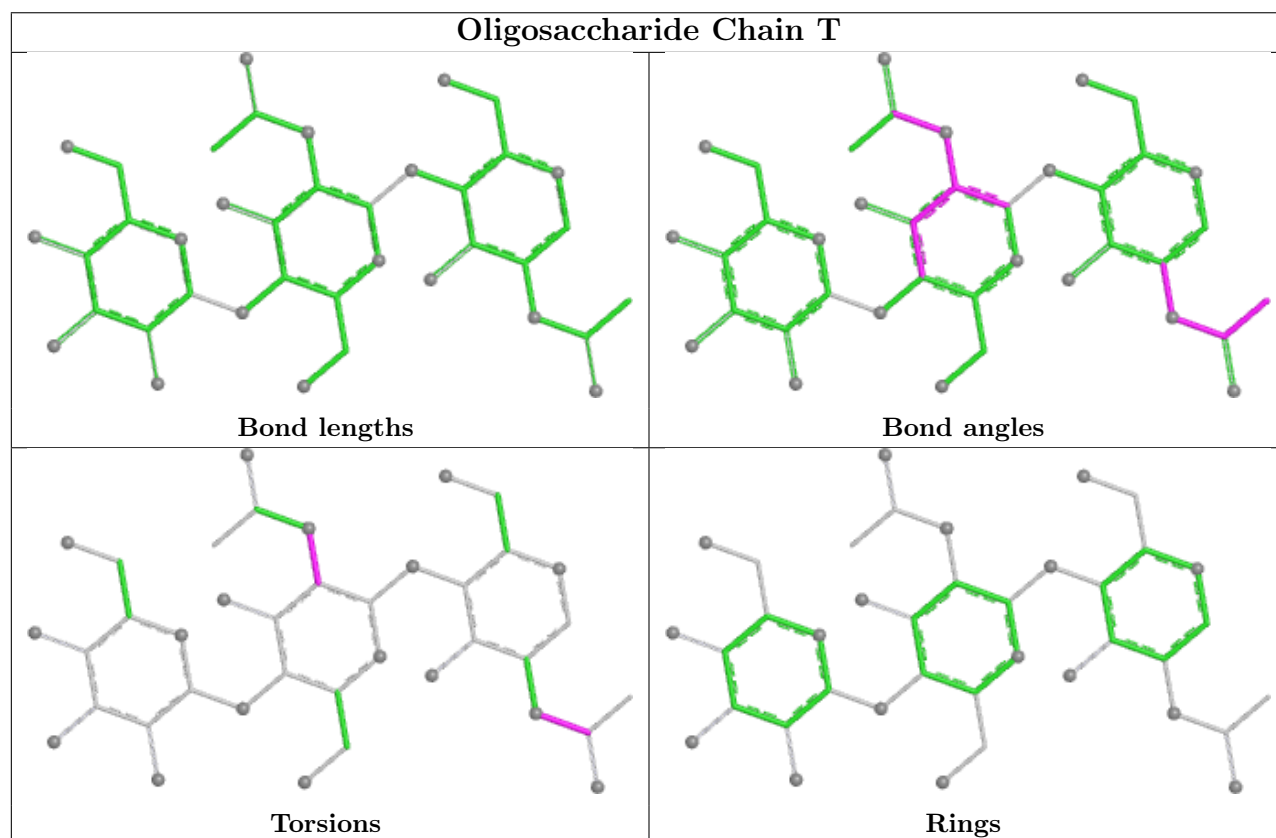
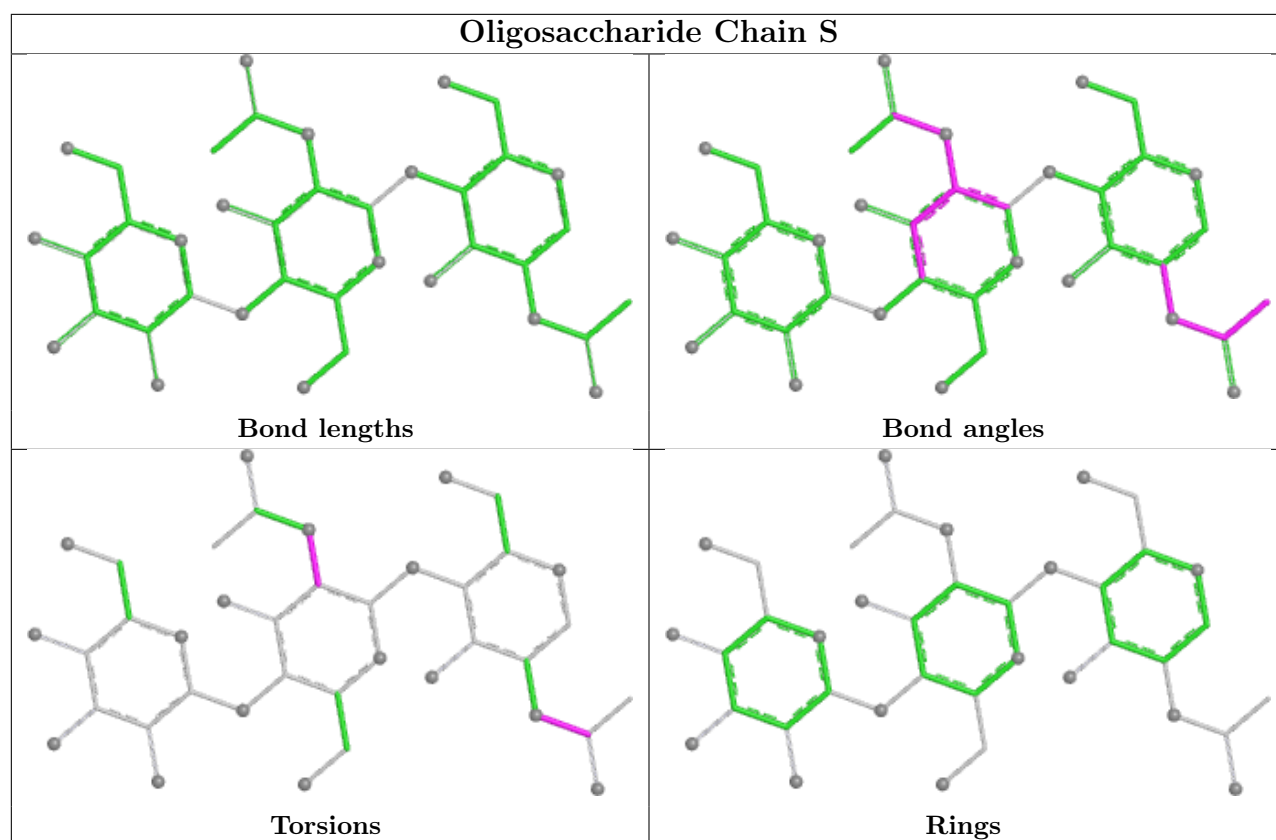


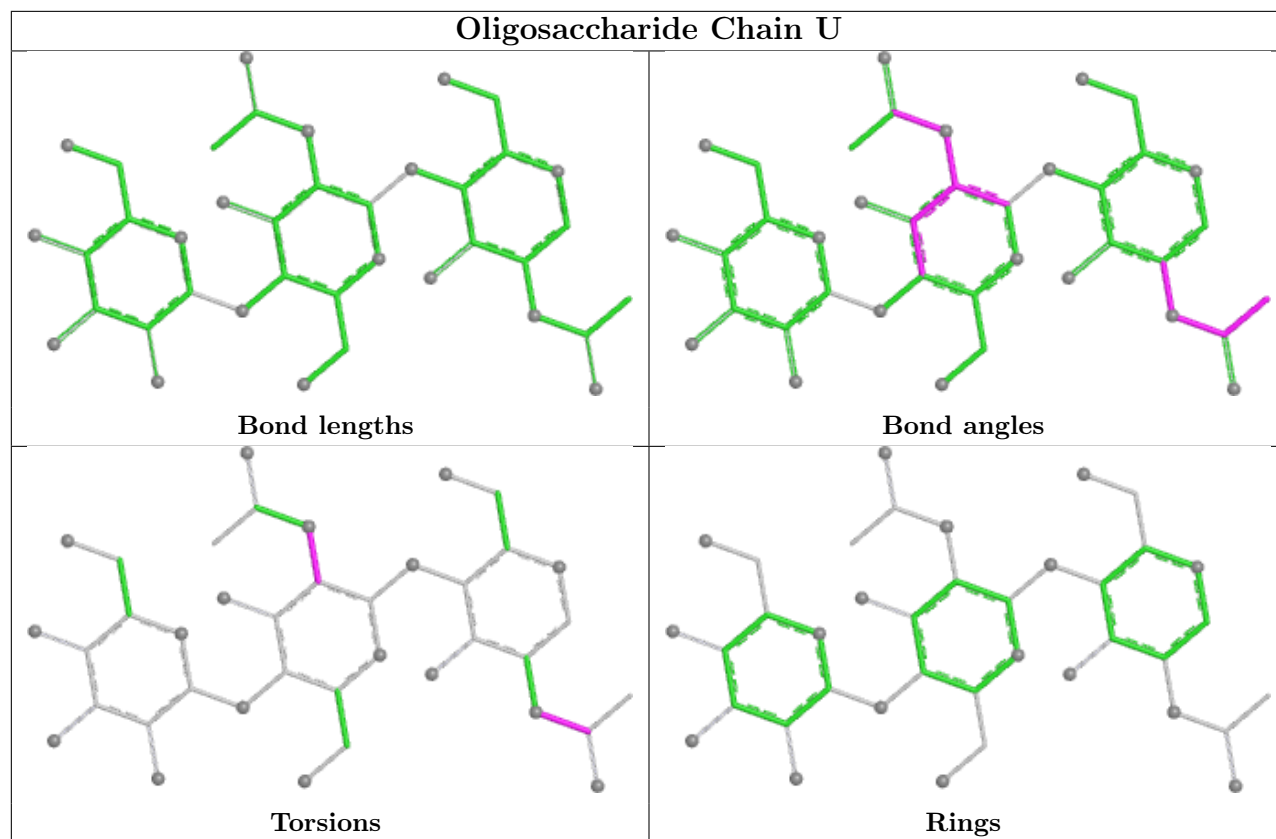


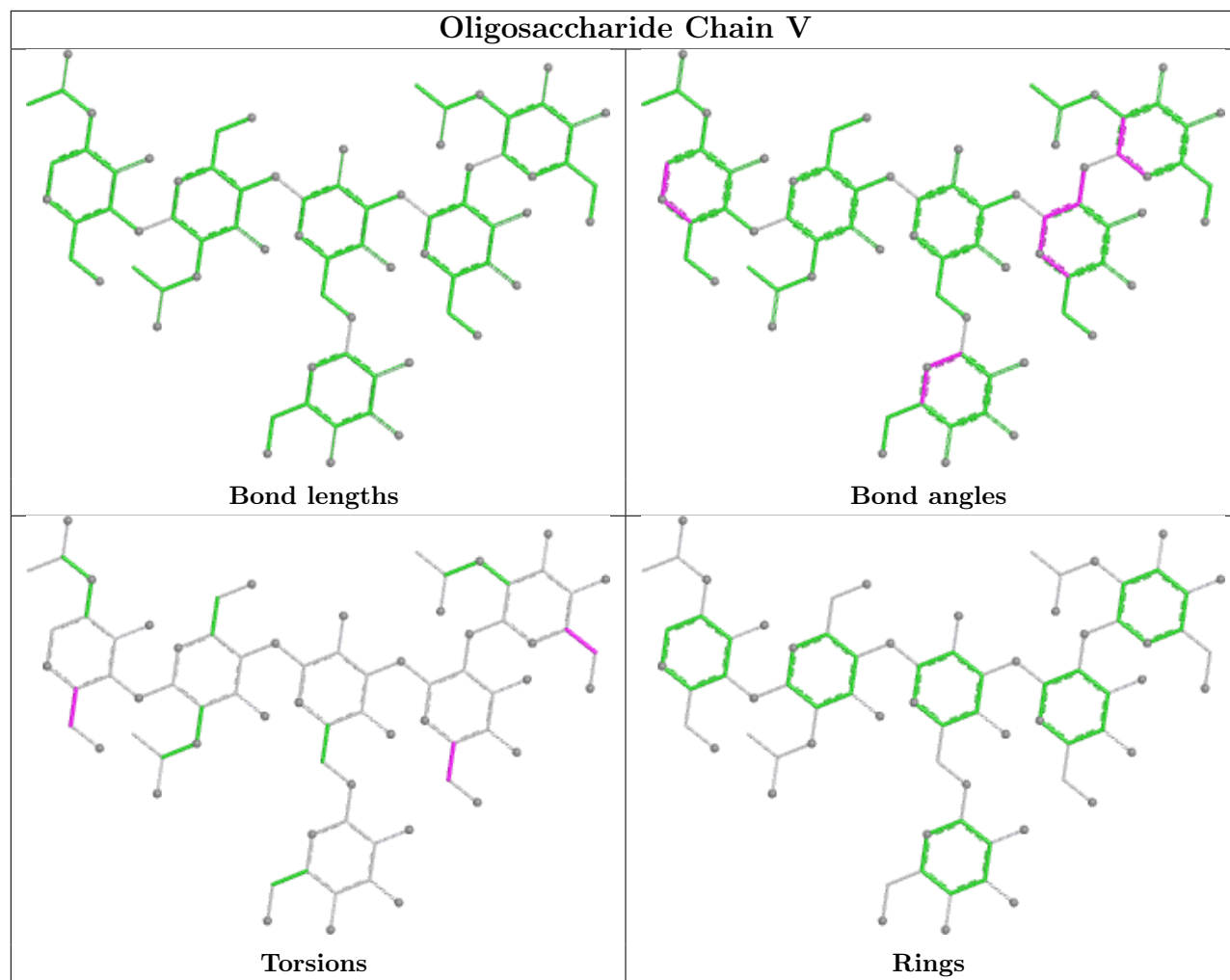


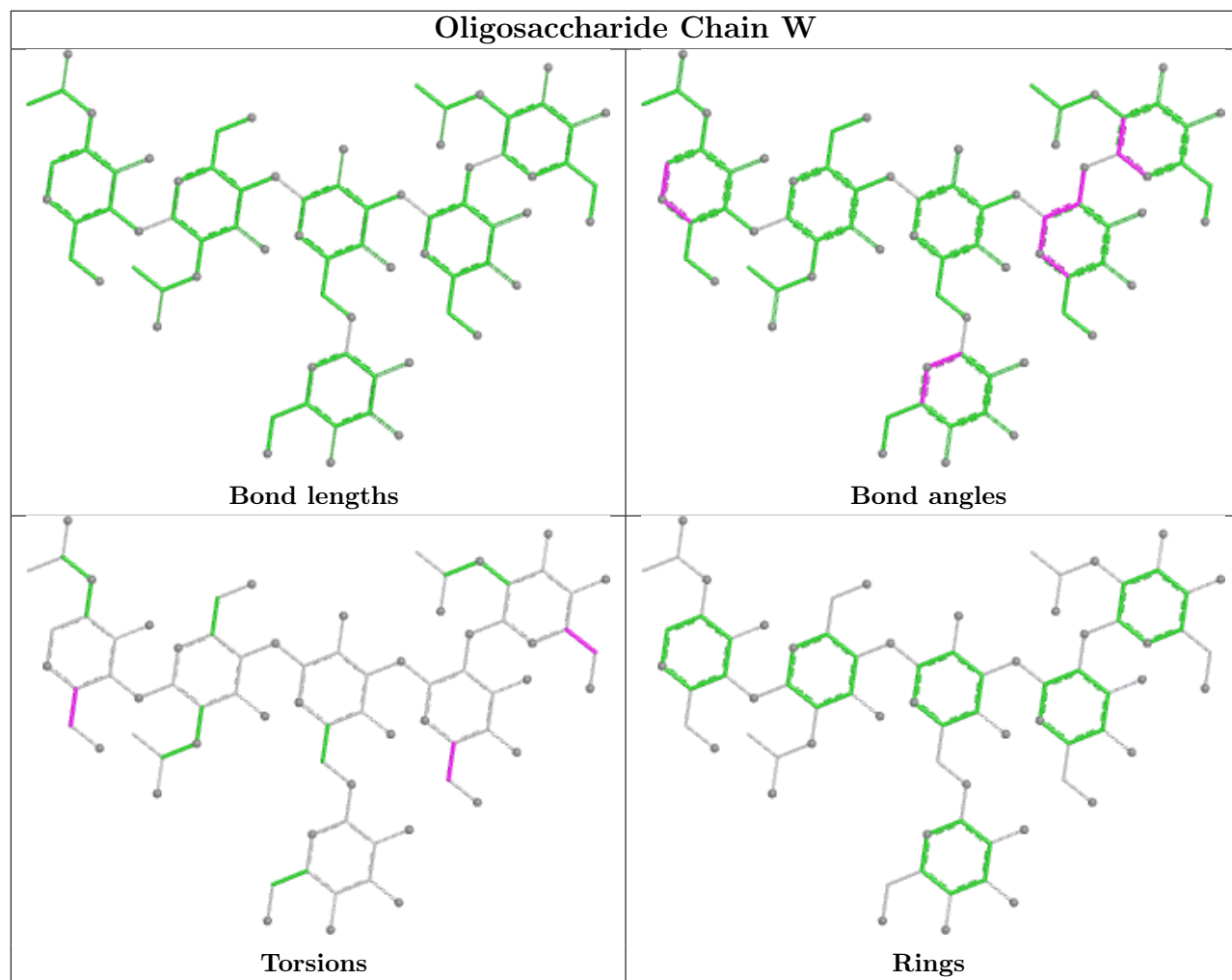


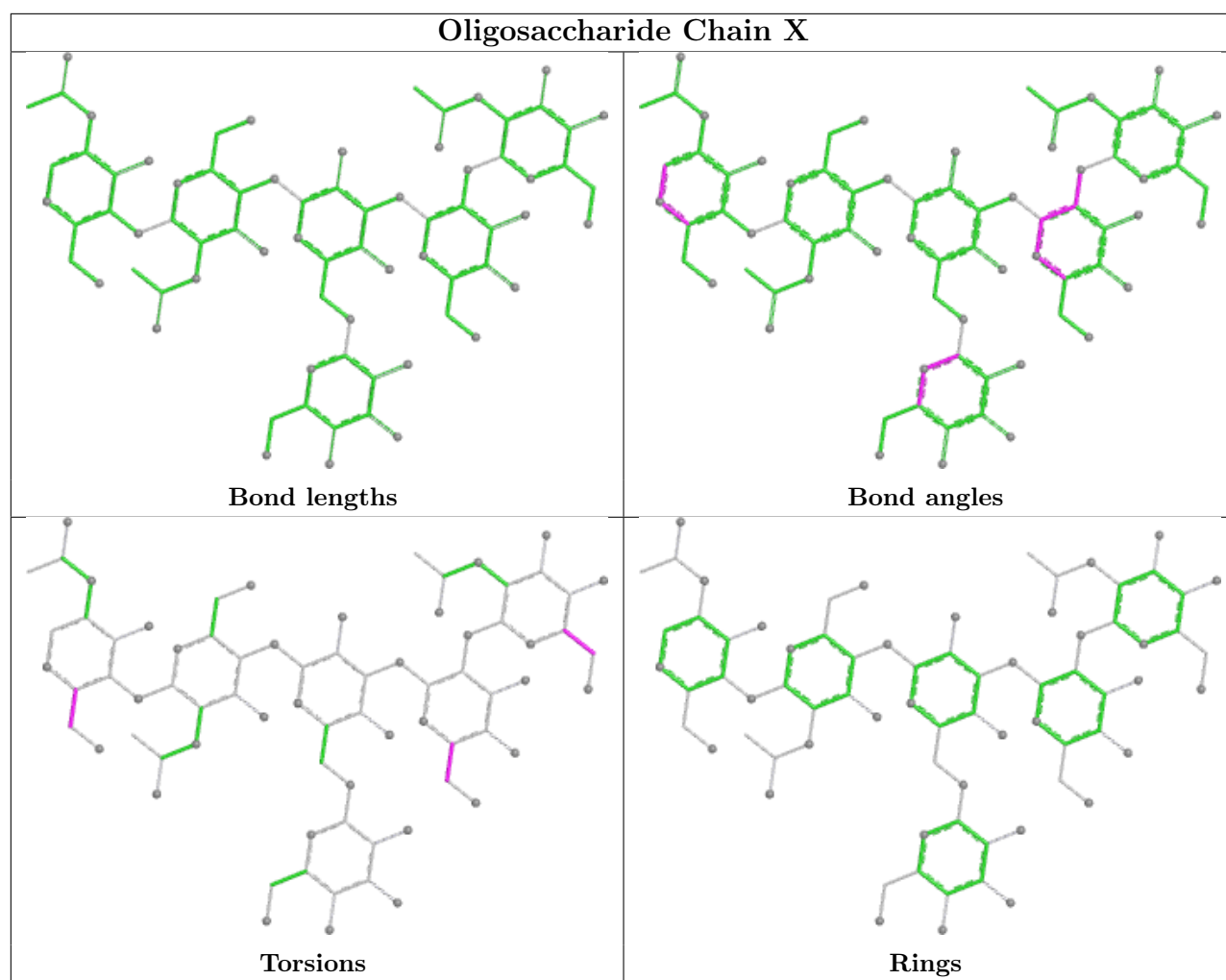


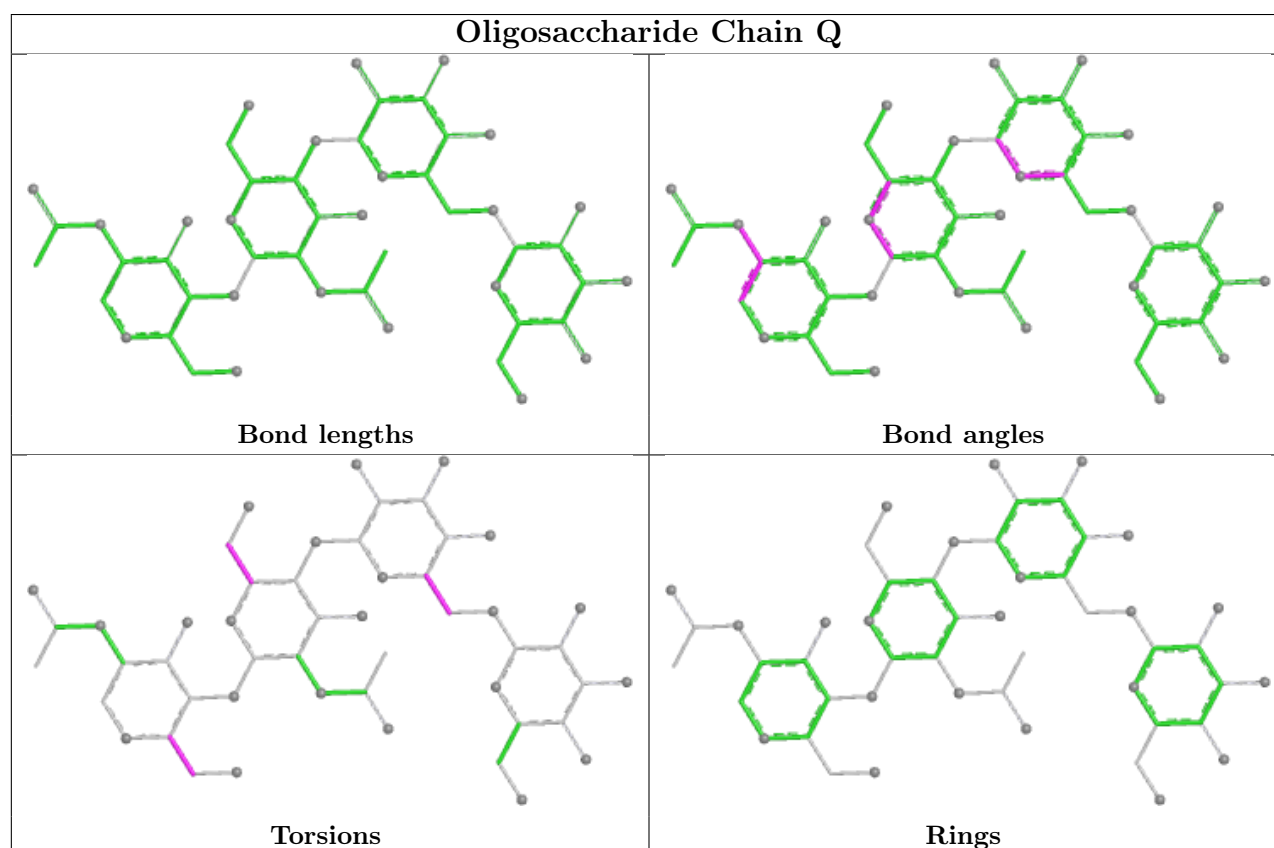
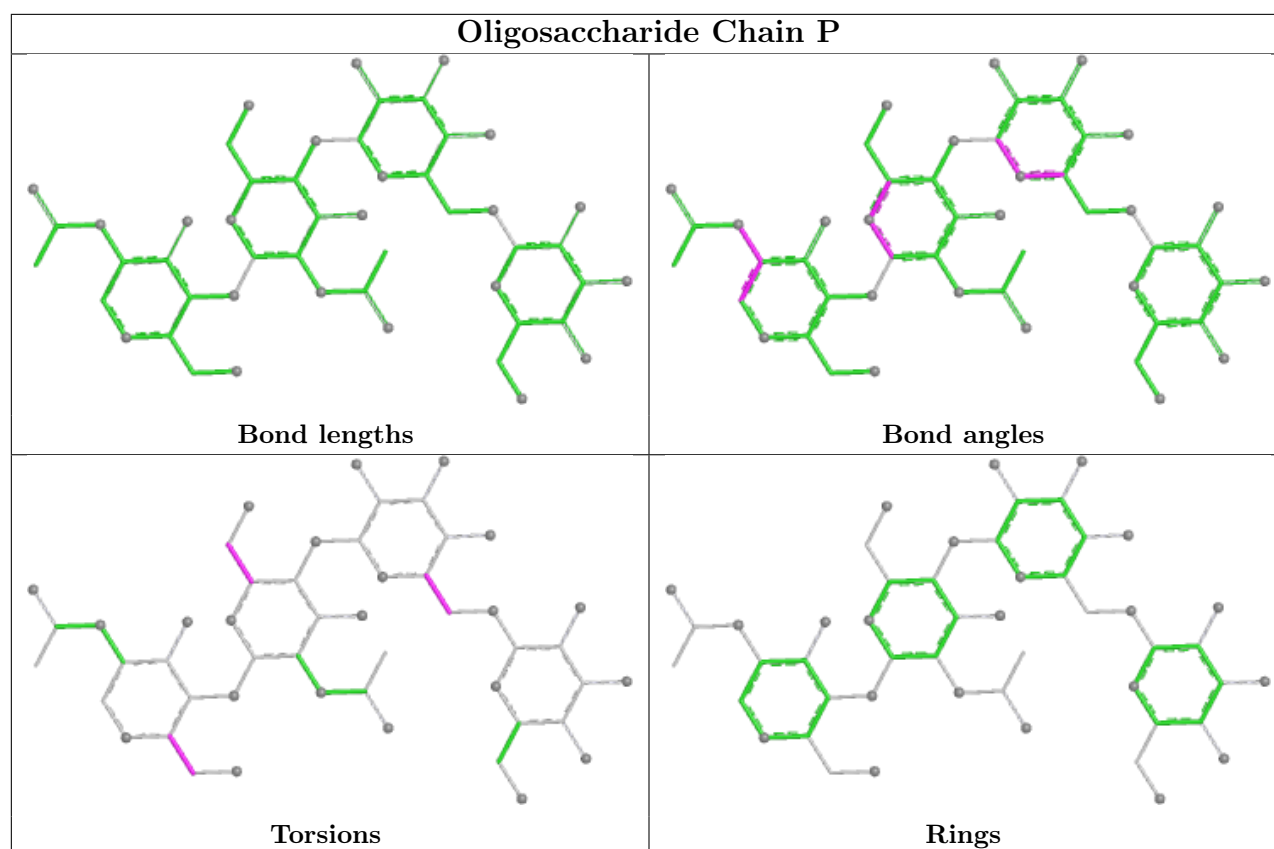


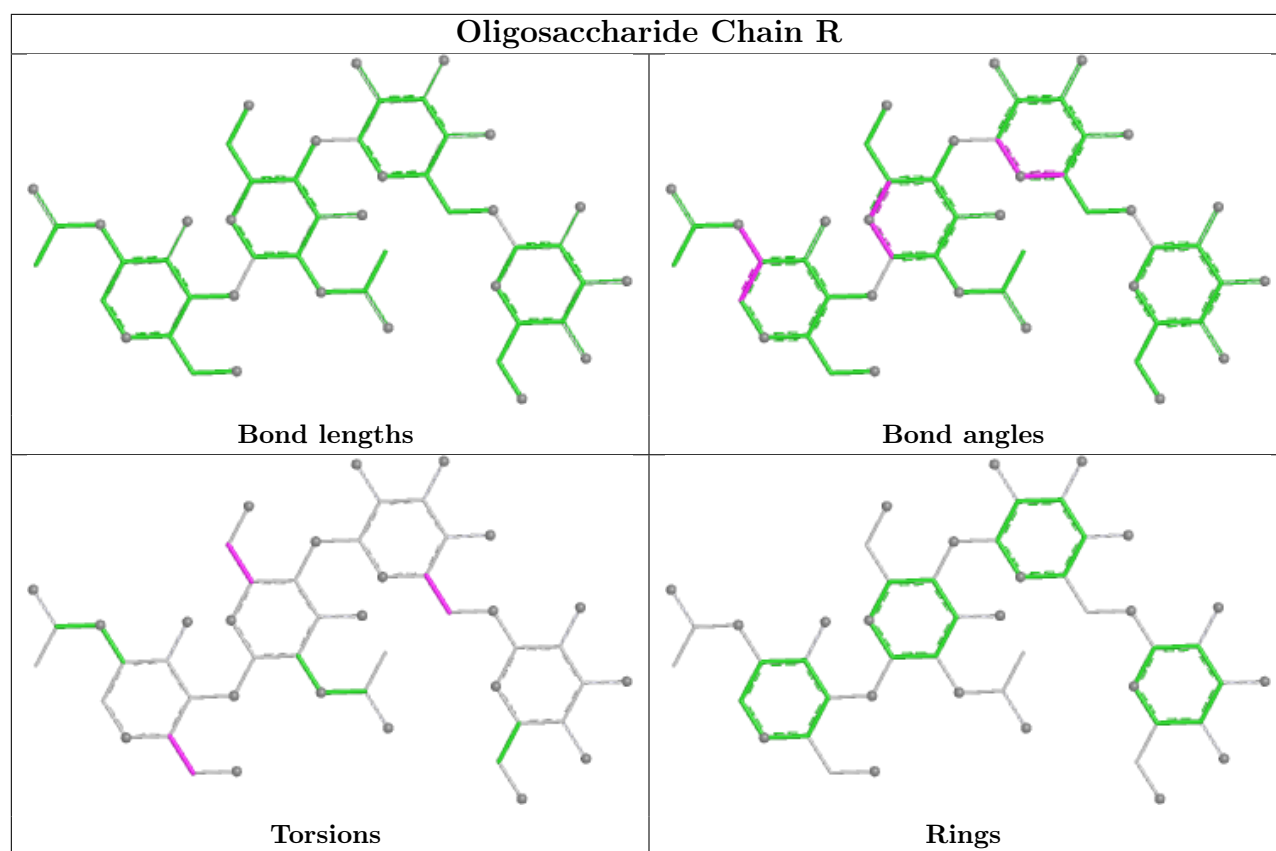


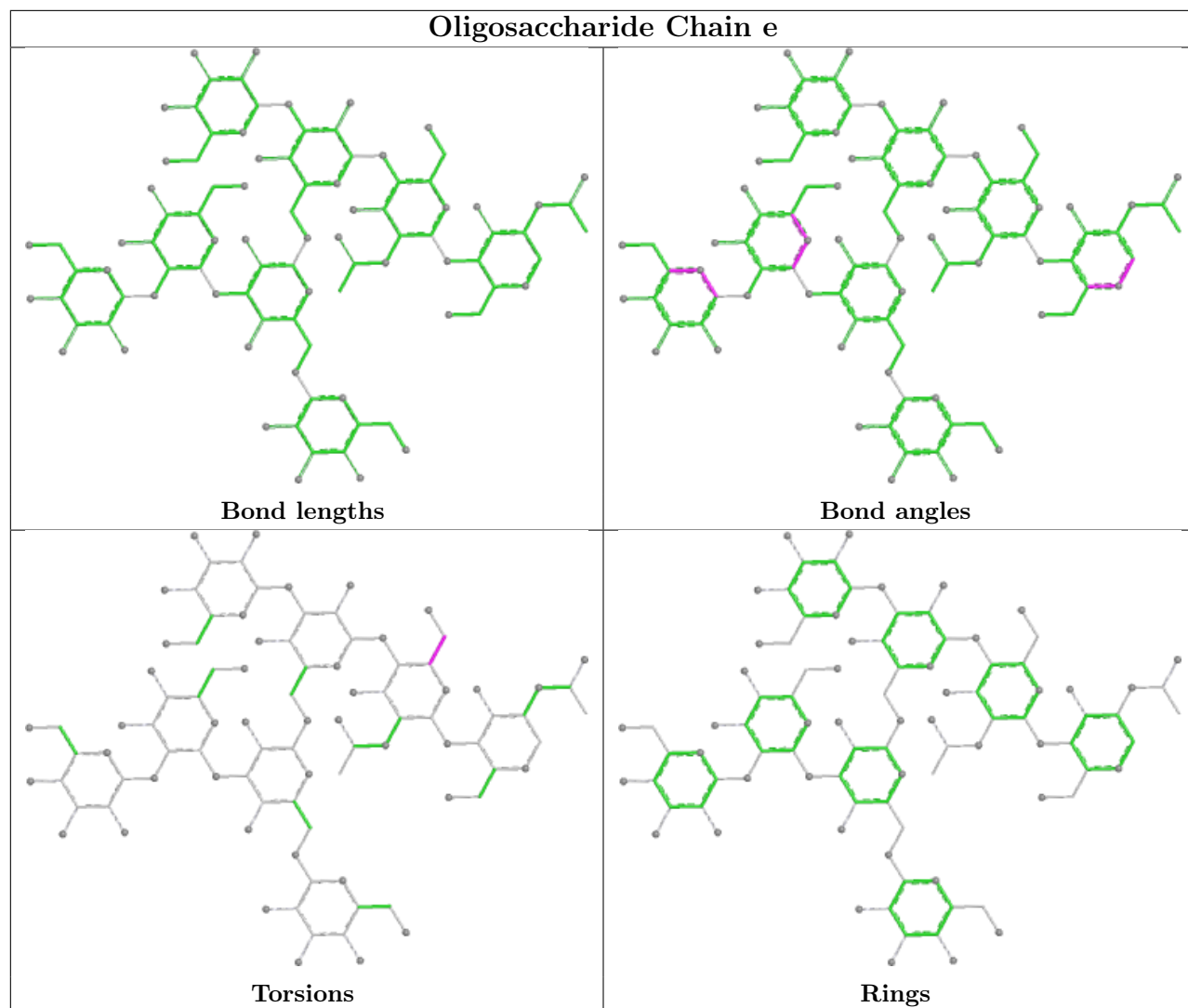


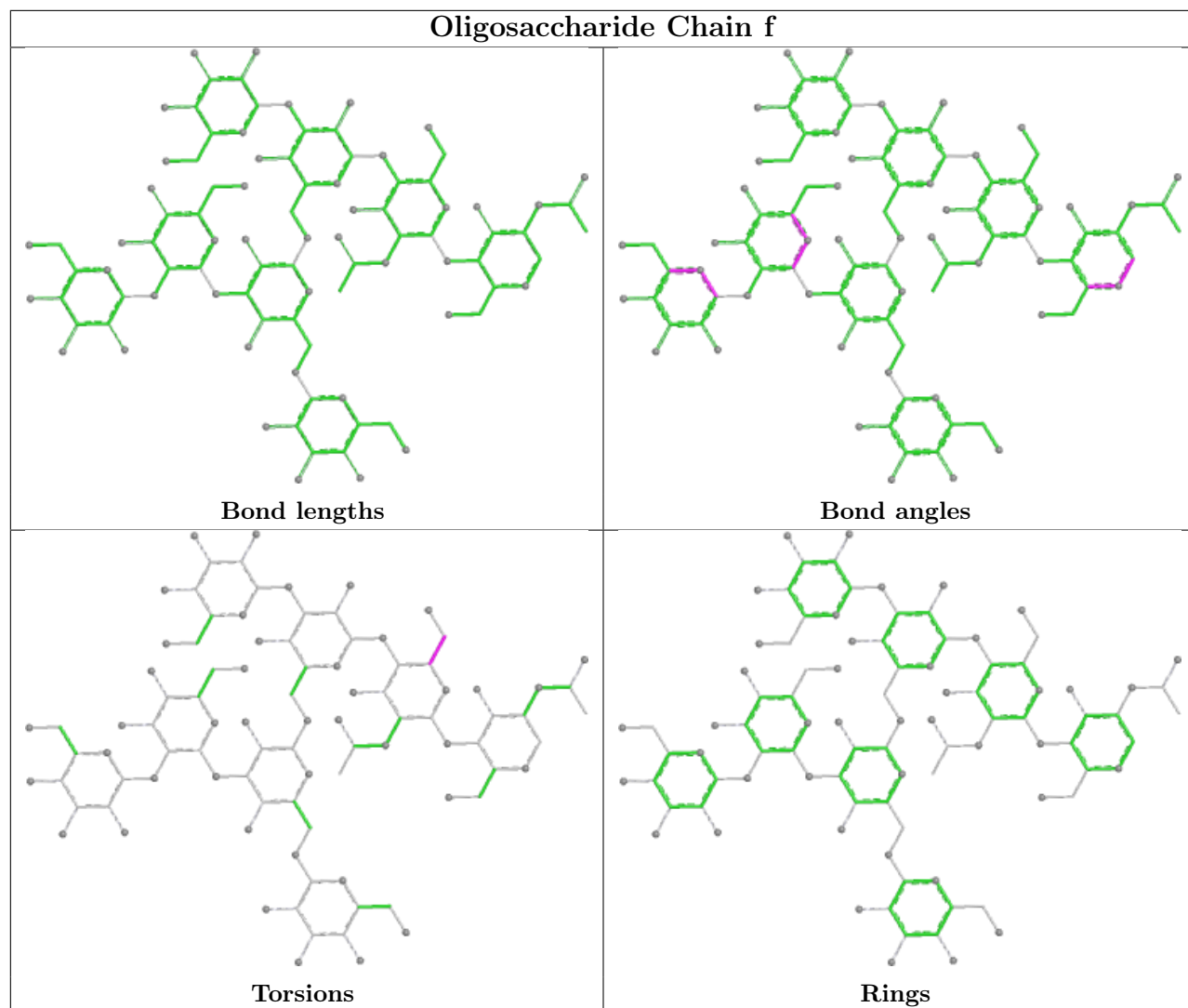


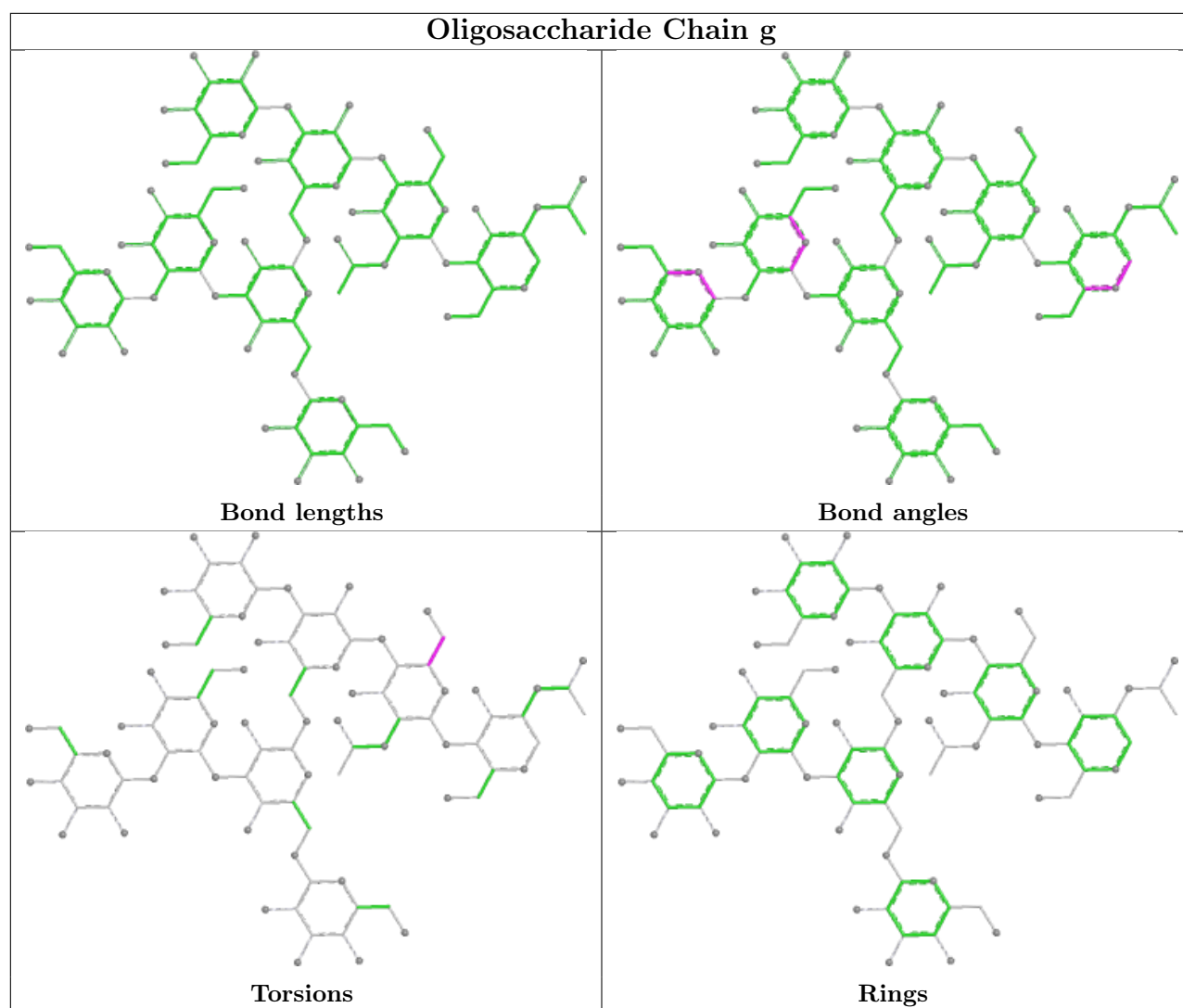


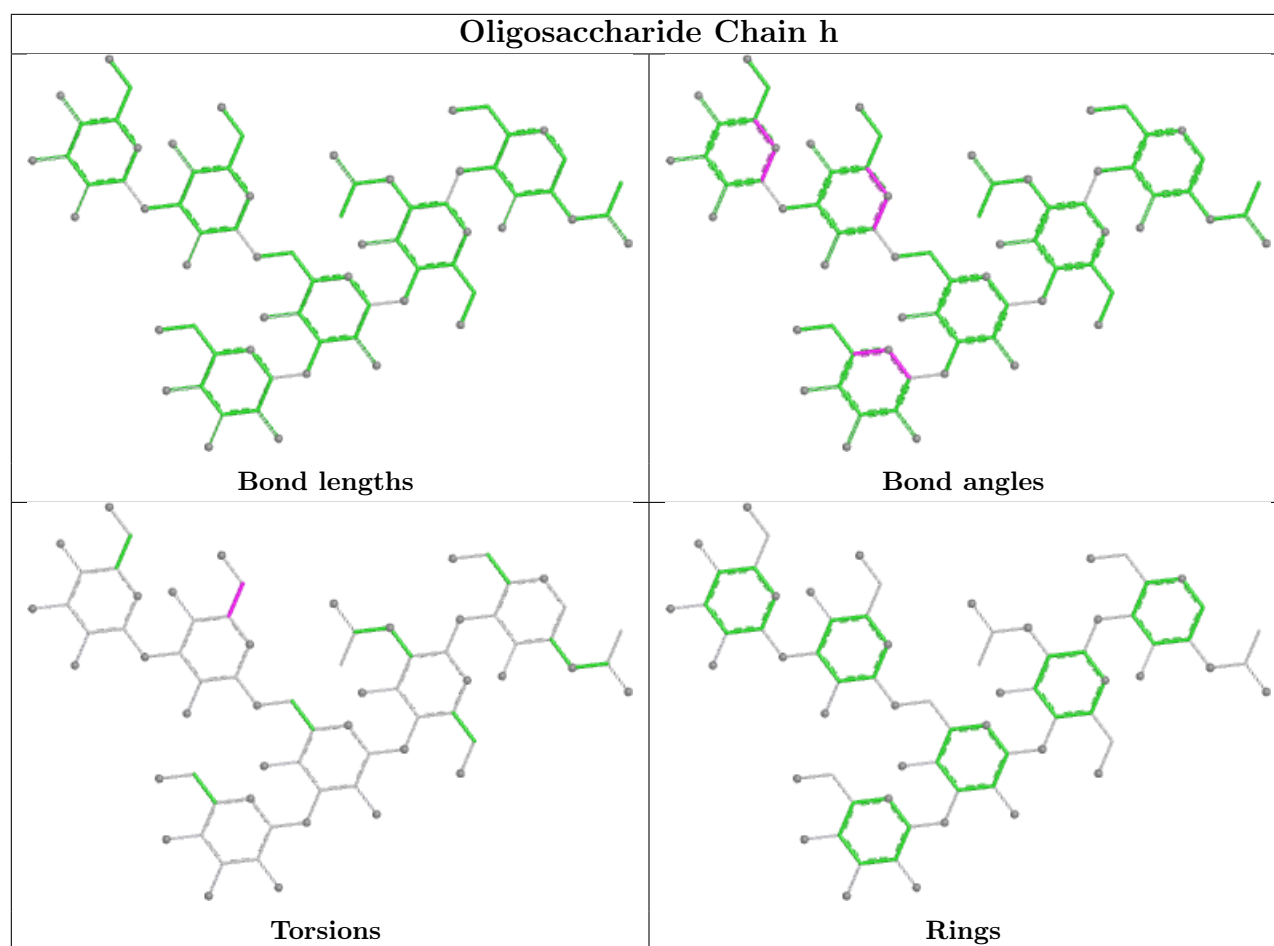


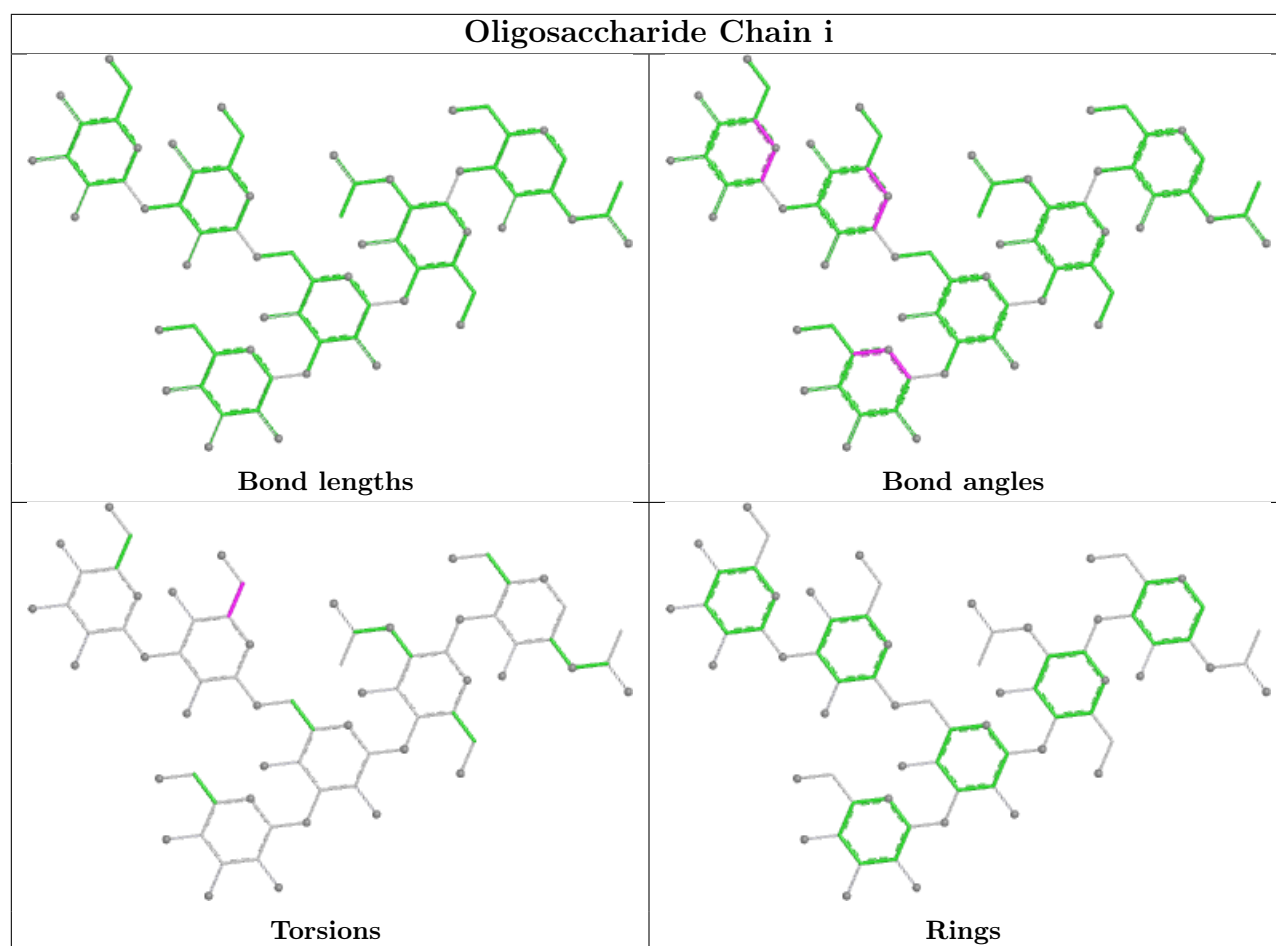


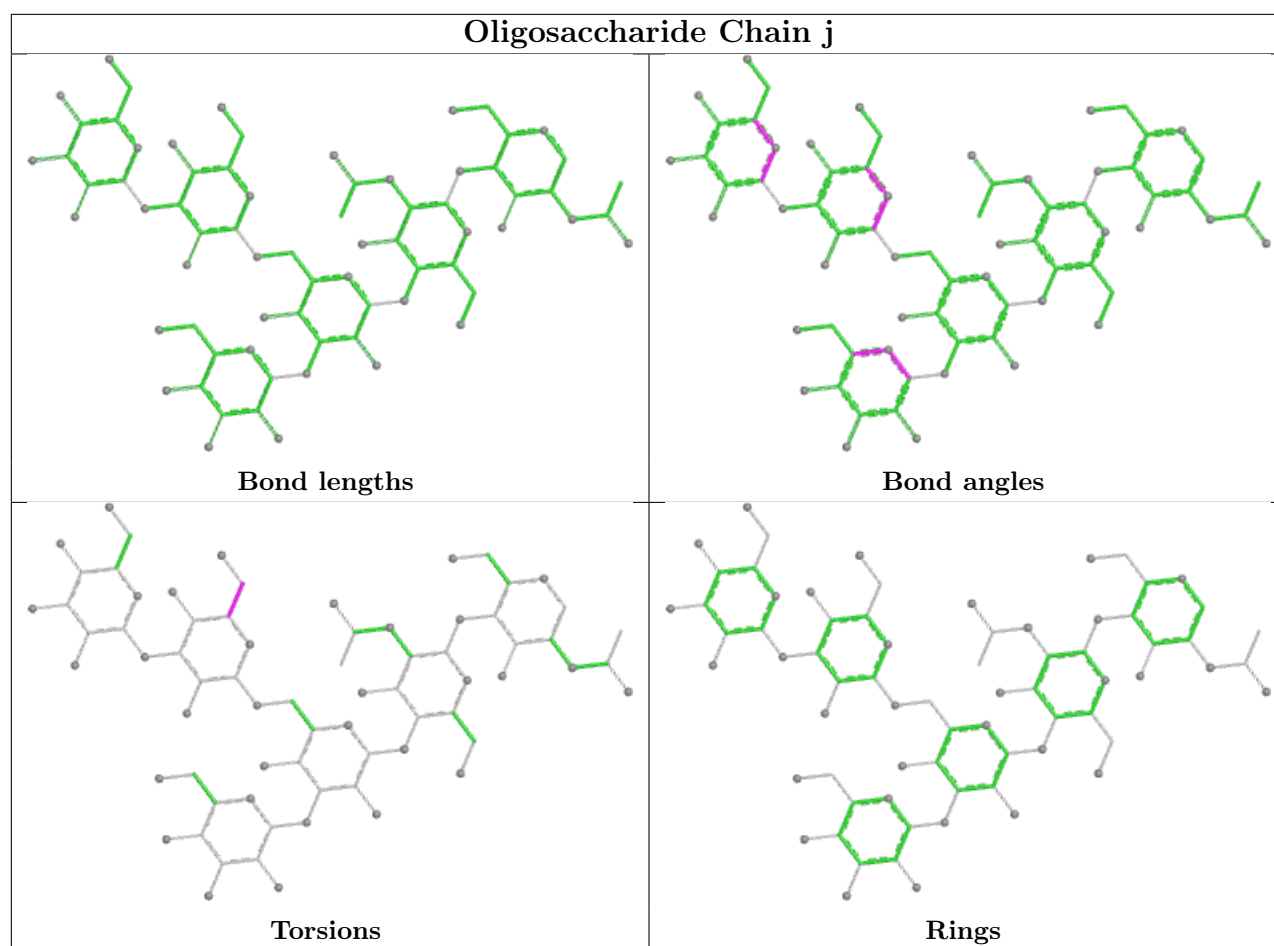












5.6 Ligand geometry [i](#)

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	C	1001	1	14,14,15	0.31	0	17,19,21	0.57	0
8	NAG	K	1003	1	14,14,15	0.33	0	17,19,21	1.29	3 (17%)
8	NAG	C	1003	1	14,14,15	0.33	0	17,19,21	1.29	3 (17%)
9	CLR	H	1100	-	31,31,31	0.36	0	48,48,48	0.58	0
10	PTY	D	1101	-	49,49,49	0.26	0	52,54,54	0.31	0
8	NAG	K	1002	1	14,14,15	0.41	0	17,19,21	0.91	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	PTY	L	1101	-	49,49,49	0.27	0	52,54,54	0.31	0
9	CLR	L	1100	-	31,31,31	0.36	0	48,48,48	0.58	0
10	PTY	H	1101	-	49,49,49	0.26	0	52,54,54	0.31	0
8	NAG	K	1001	1	14,14,15	0.31	0	17,19,21	0.57	0
8	NAG	C	1002	1	14,14,15	0.41	0	17,19,21	0.90	1 (5%)
9	CLR	D	1100	-	31,31,31	0.36	0	48,48,48	0.58	0
8	NAG	G	1003	1	14,14,15	0.33	0	17,19,21	1.29	3 (17%)
8	NAG	G	1002	1	14,14,15	0.40	0	17,19,21	0.91	1 (5%)
8	NAG	G	1001	1	14,14,15	0.31	0	17,19,21	0.57	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
8	NAG	C	1001	1	-	1/6/23/26	0/1/1/1
8	NAG	K	1003	1	-	2/6/23/26	0/1/1/1
8	NAG	C	1003	1	-	2/6/23/26	0/1/1/1
9	CLR	H	1100	-	-	6/10/68/68	0/4/4/4
10	PTY	D	1101	-	-	16/53/53/53	-
8	NAG	K	1002	1	-	2/6/23/26	0/1/1/1
10	PTY	L	1101	-	-	16/53/53/53	-
9	CLR	L	1100	-	-	6/10/68/68	0/4/4/4
10	PTY	H	1101	-	-	16/53/53/53	-
8	NAG	K	1001	1	-	1/6/23/26	0/1/1/1
8	NAG	C	1002	1	-	2/6/23/26	0/1/1/1
9	CLR	D	1100	-	-	6/10/68/68	0/4/4/4
8	NAG	G	1003	1	-	2/6/23/26	0/1/1/1
8	NAG	G	1002	1	-	2/6/23/26	0/1/1/1
8	NAG	G	1001	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1003	NAG	C2-N2-C7	2.83	126.69	122.90
8	K	1003	NAG	C2-N2-C7	2.82	126.68	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	1003	NAG	C2-N2-C7	2.80	126.65	122.90
8	G	1003	NAG	C8-C7-N2	2.61	120.45	116.12
8	C	1003	NAG	C8-C7-N2	2.61	120.44	116.12

There are no chirality outliers.

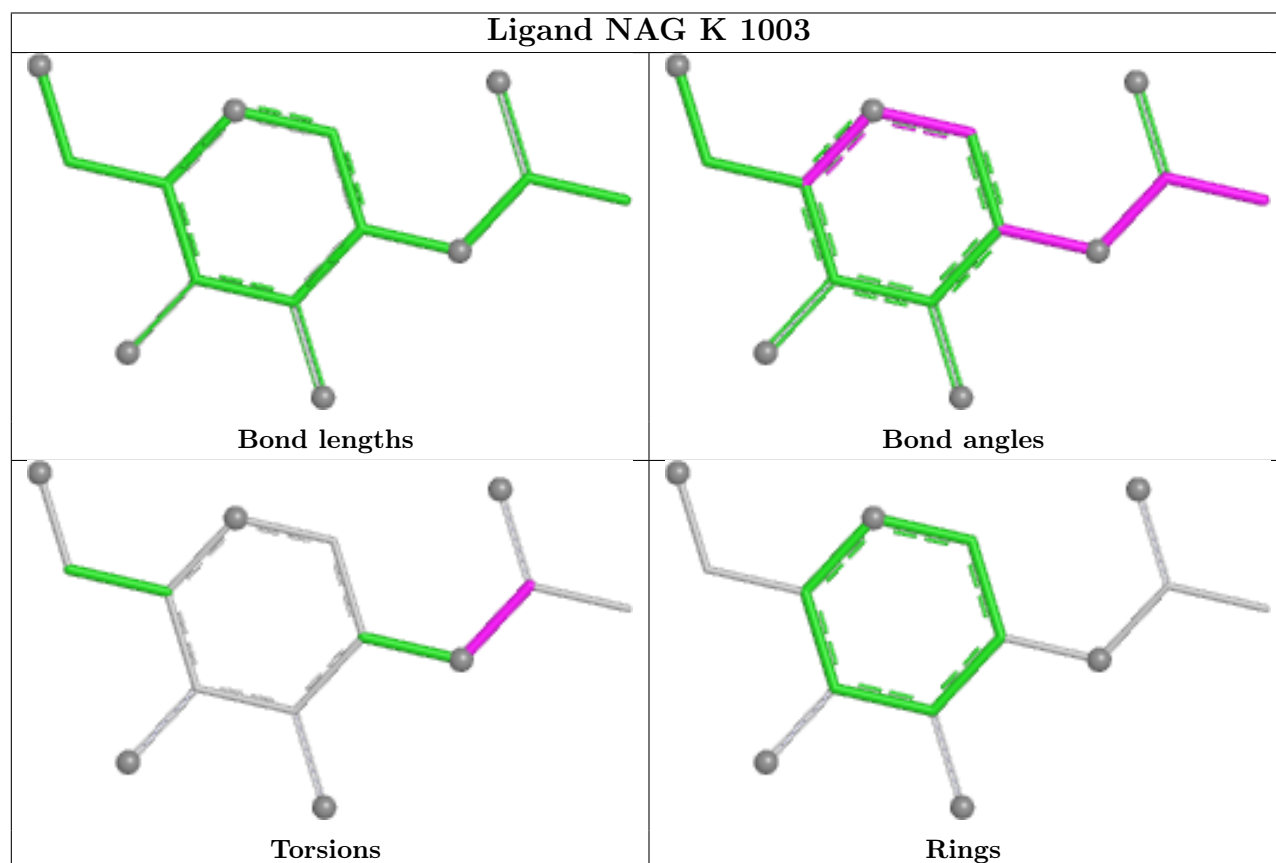
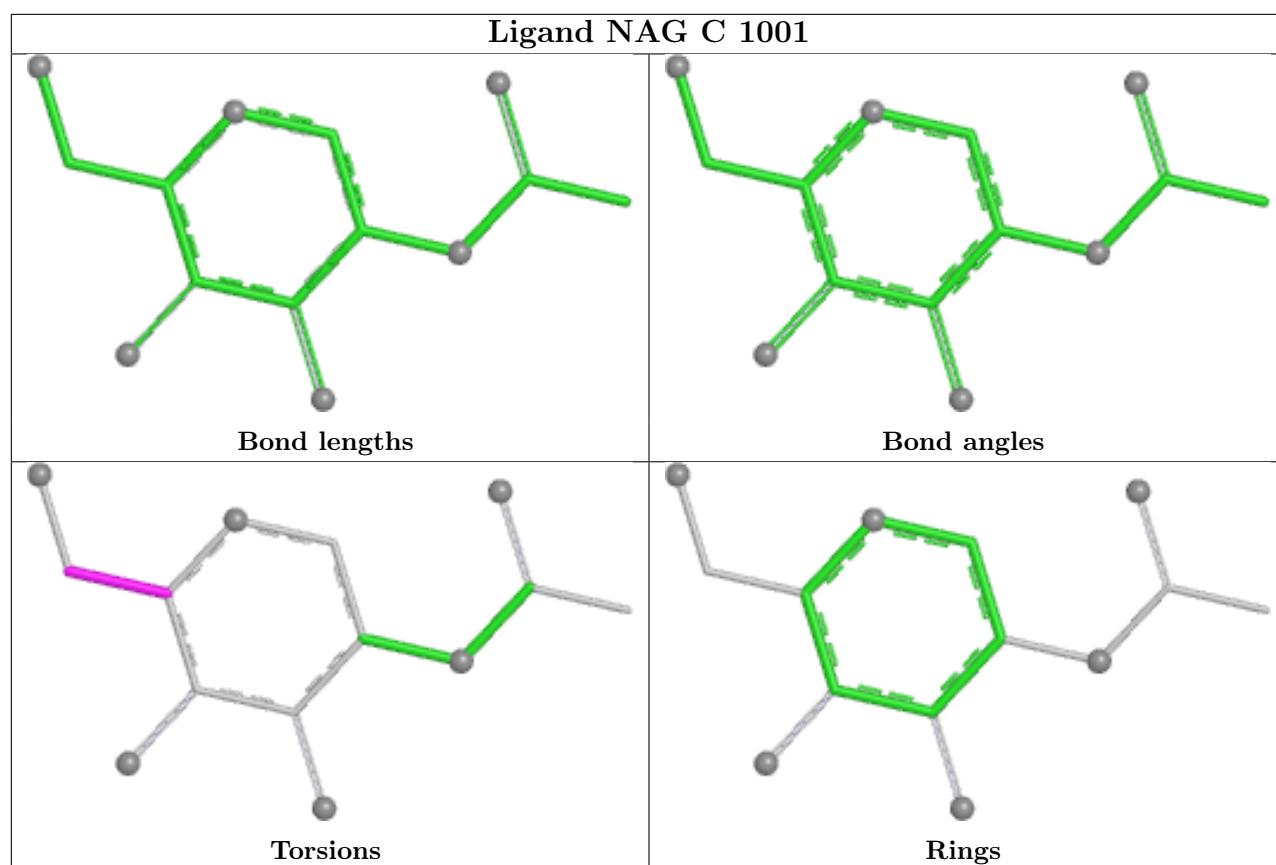
5 of 81 torsion outliers are listed below:

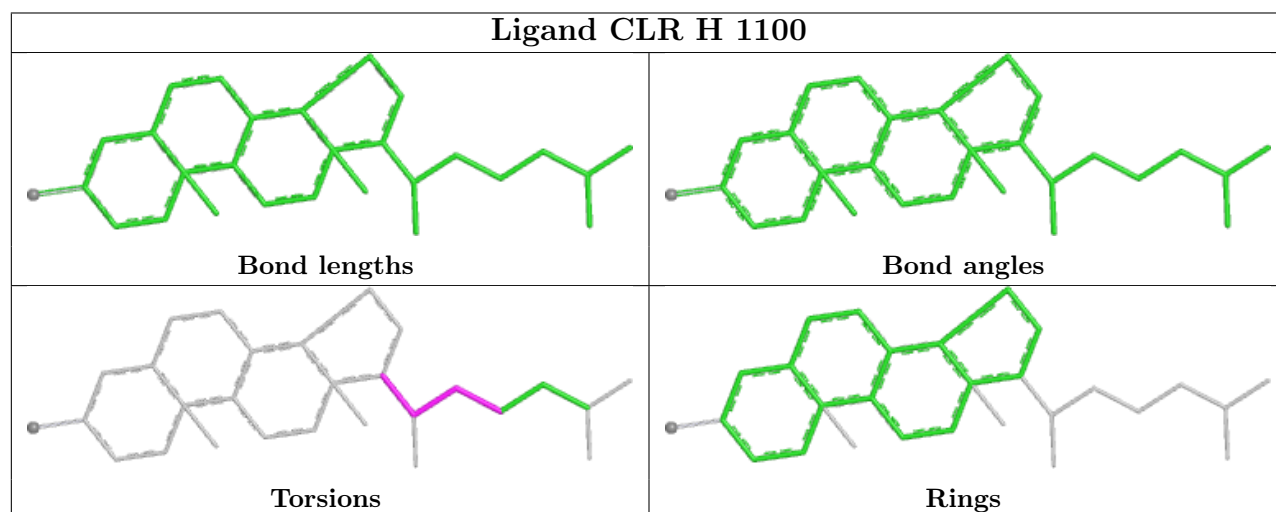
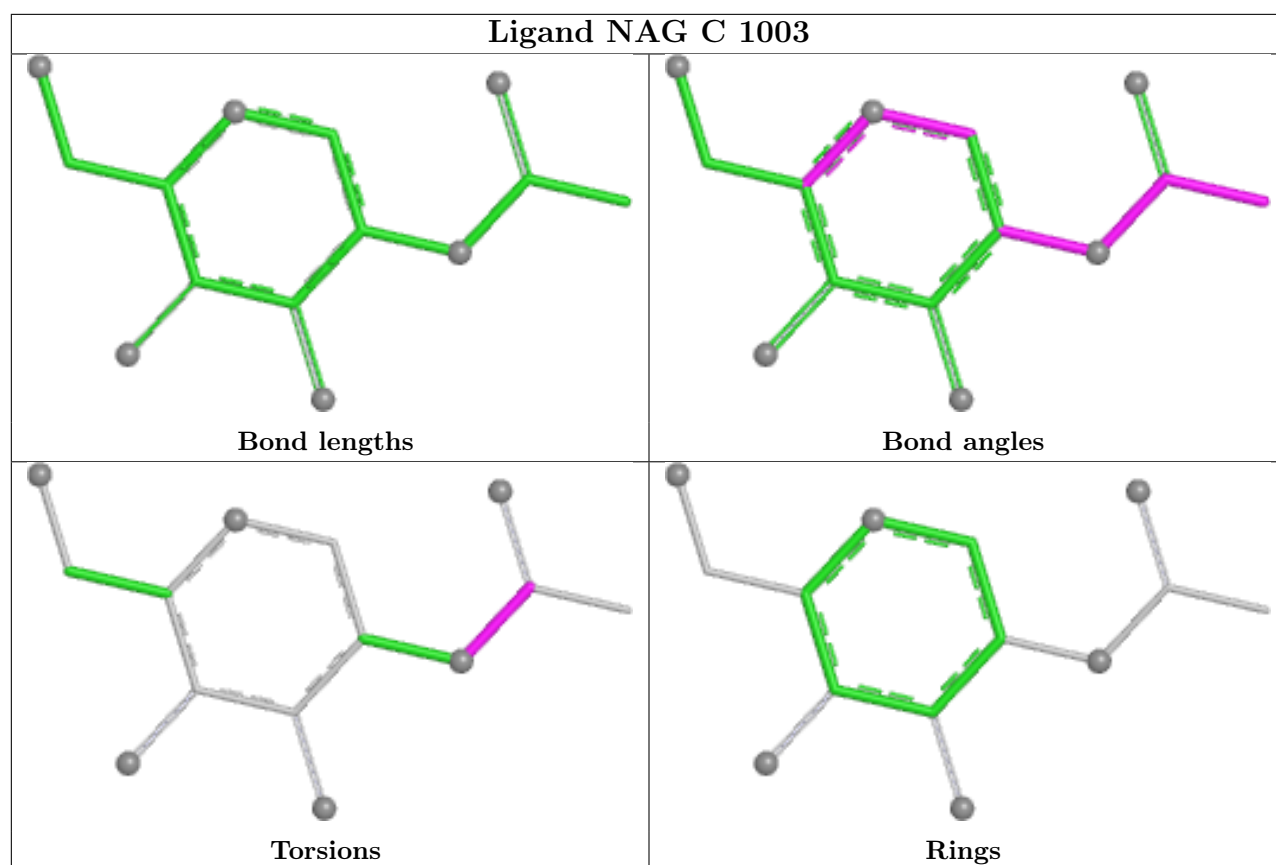
Mol	Chain	Res	Type	Atoms
8	C	1003	NAG	C8-C7-N2-C2
8	C	1003	NAG	O7-C7-N2-C2
8	G	1003	NAG	C8-C7-N2-C2
8	G	1003	NAG	O7-C7-N2-C2
8	K	1003	NAG	C8-C7-N2-C2

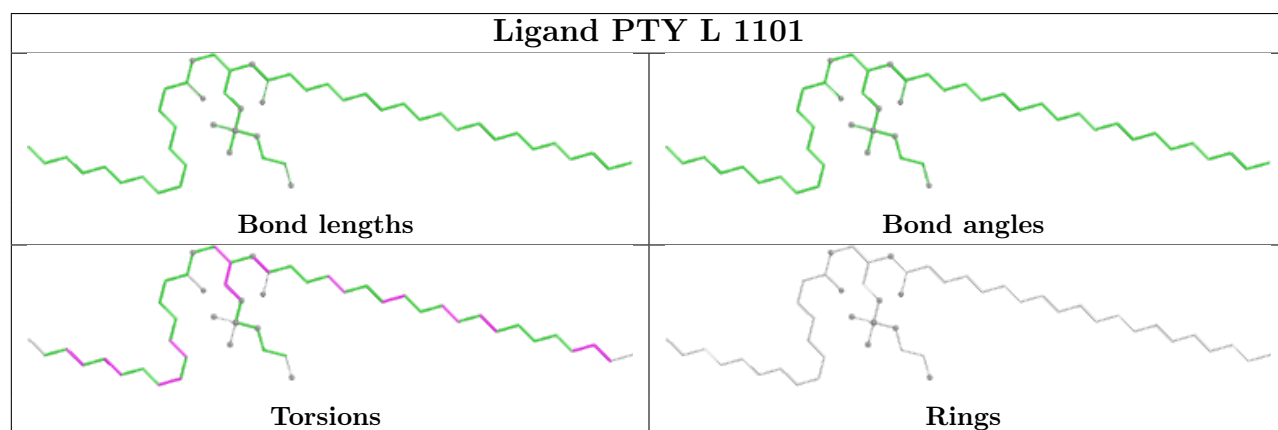
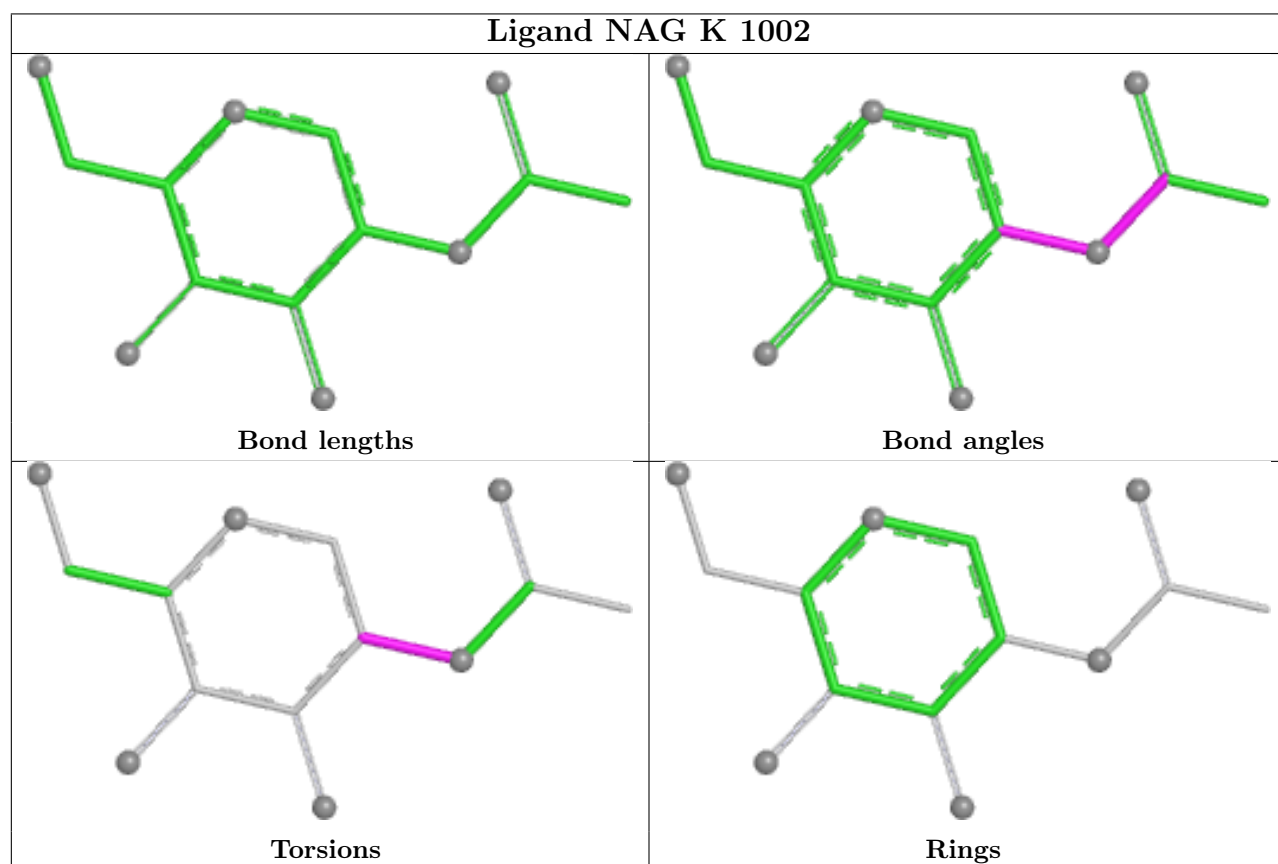
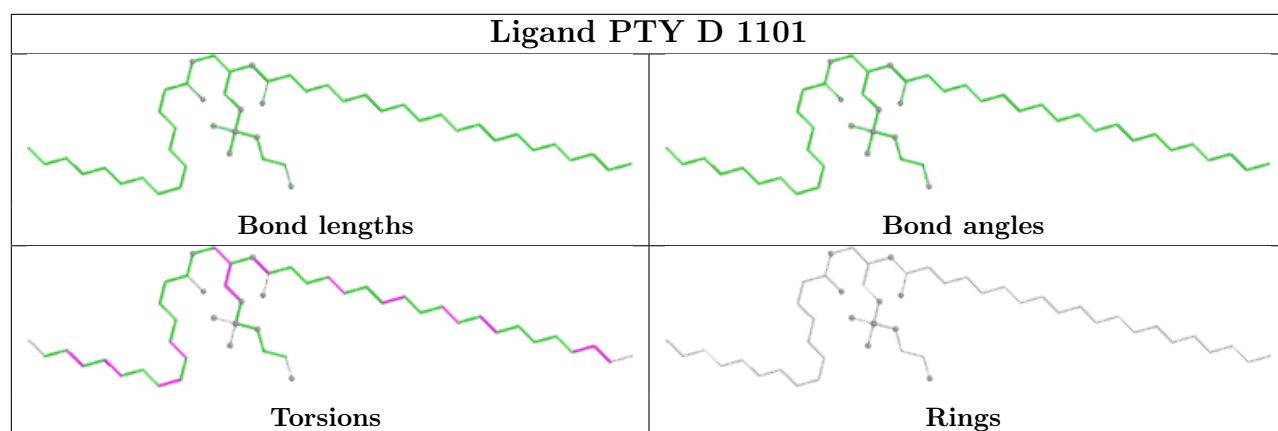
There are no ring outliers.

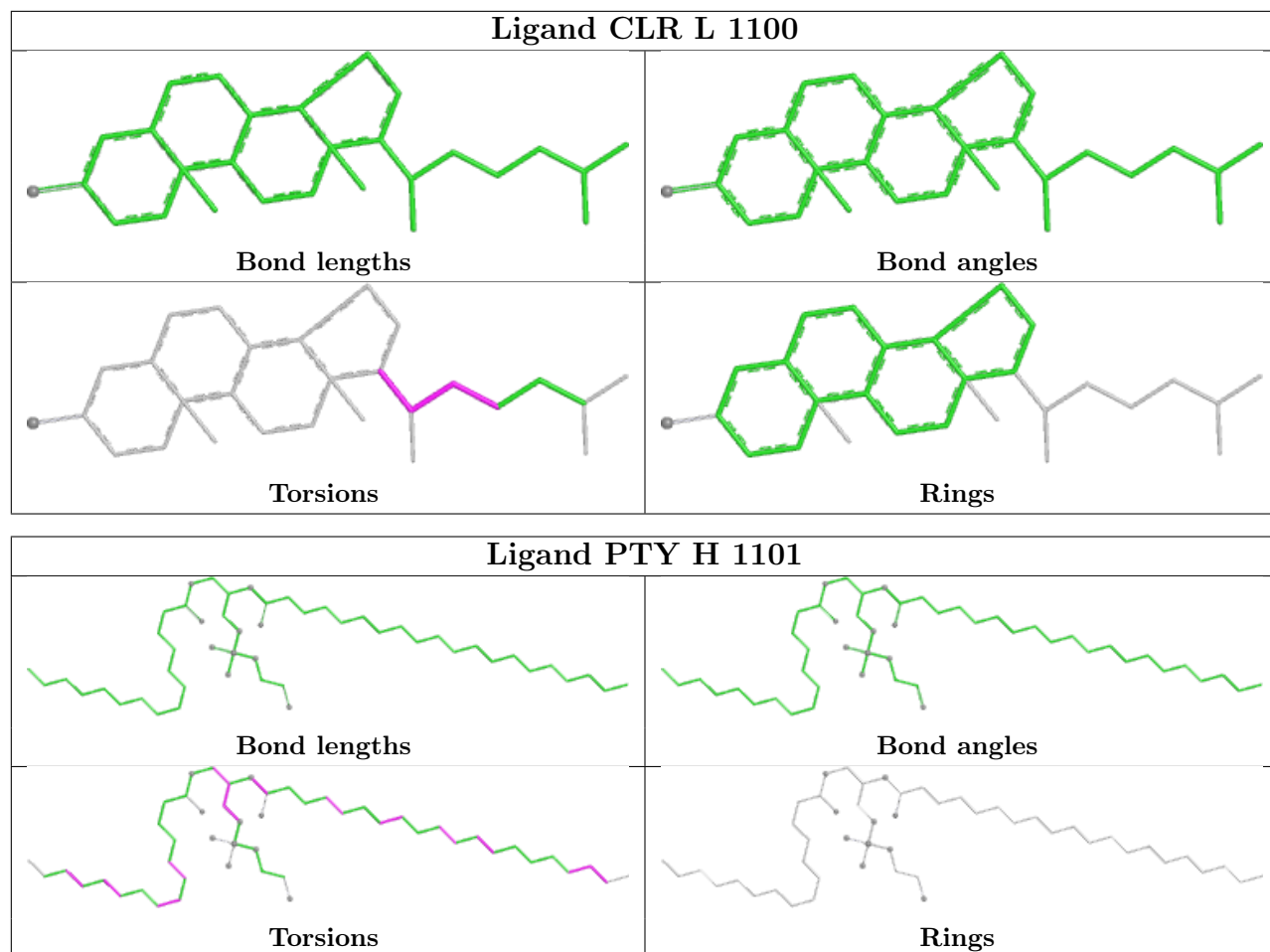
No monomer is involved in short contacts.

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.

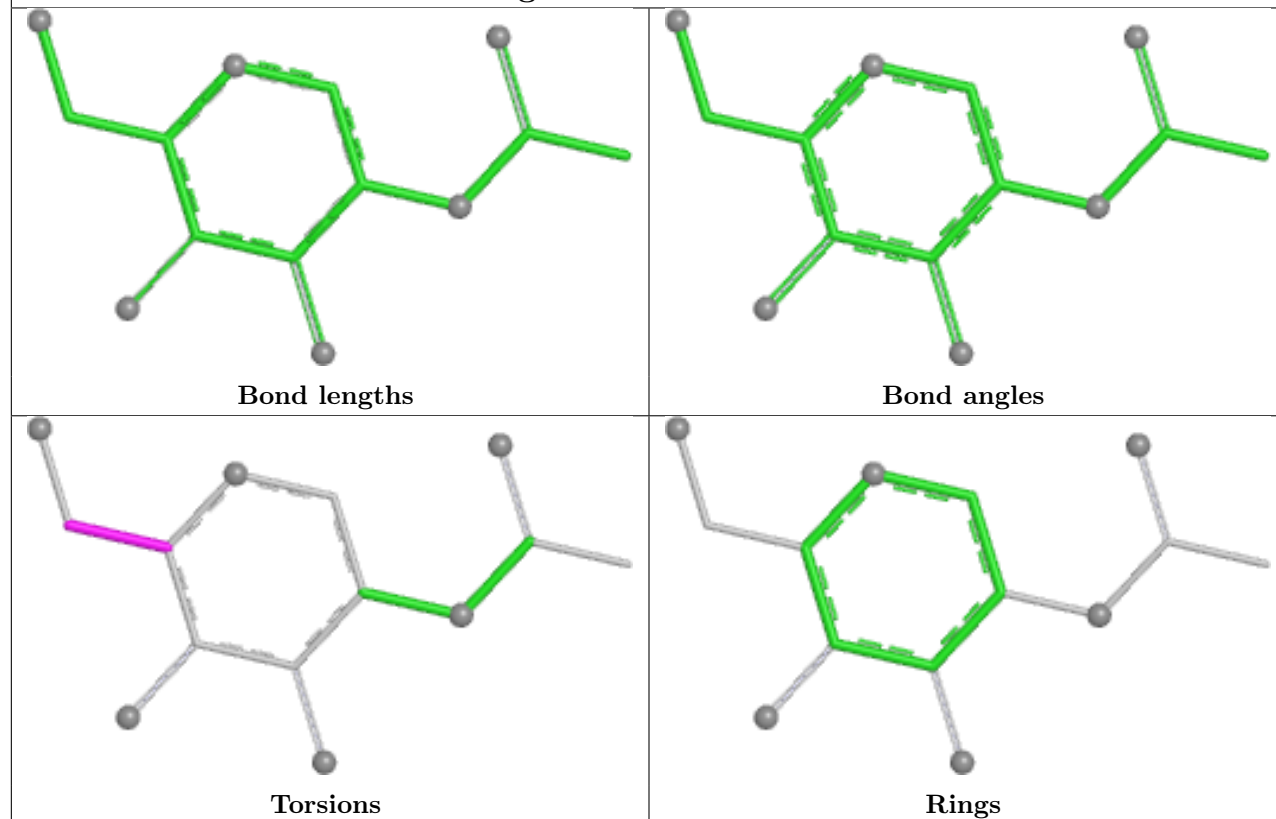




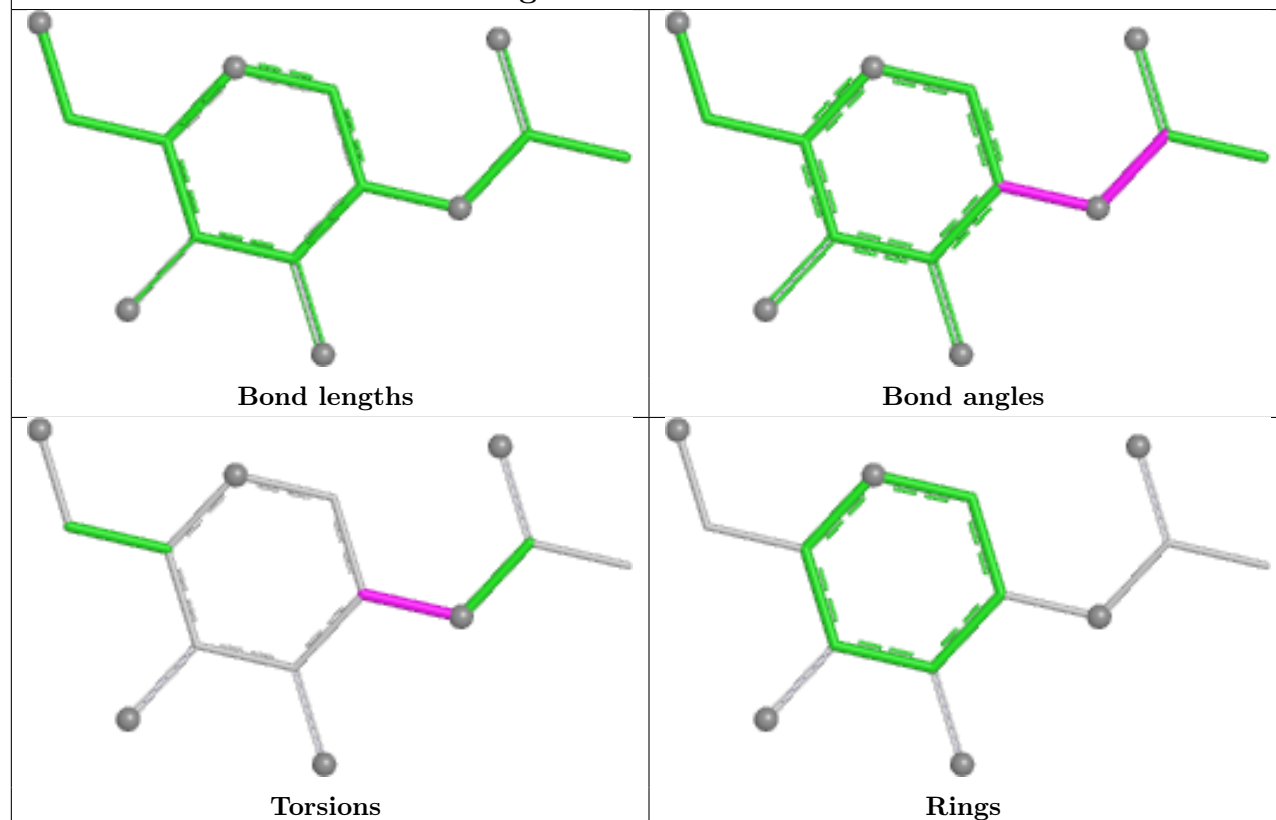


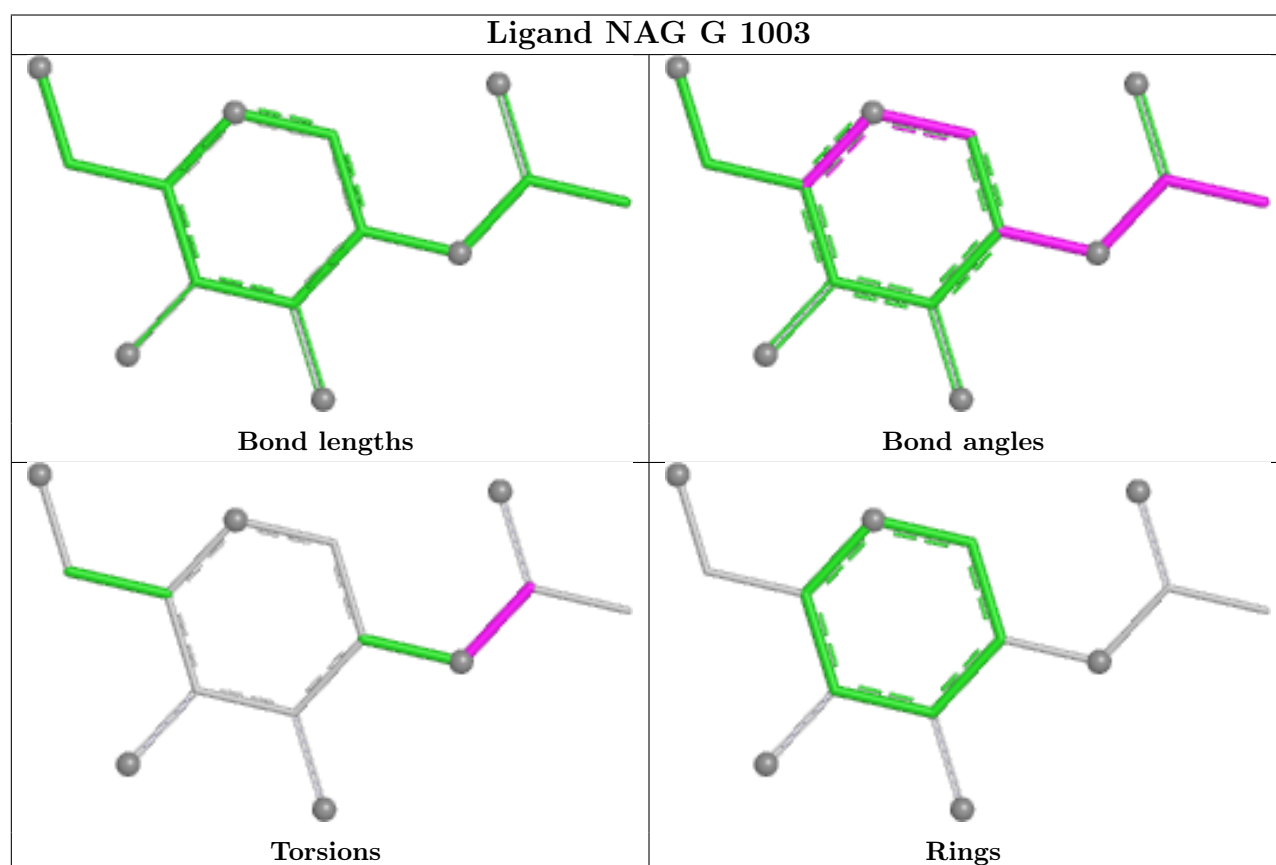
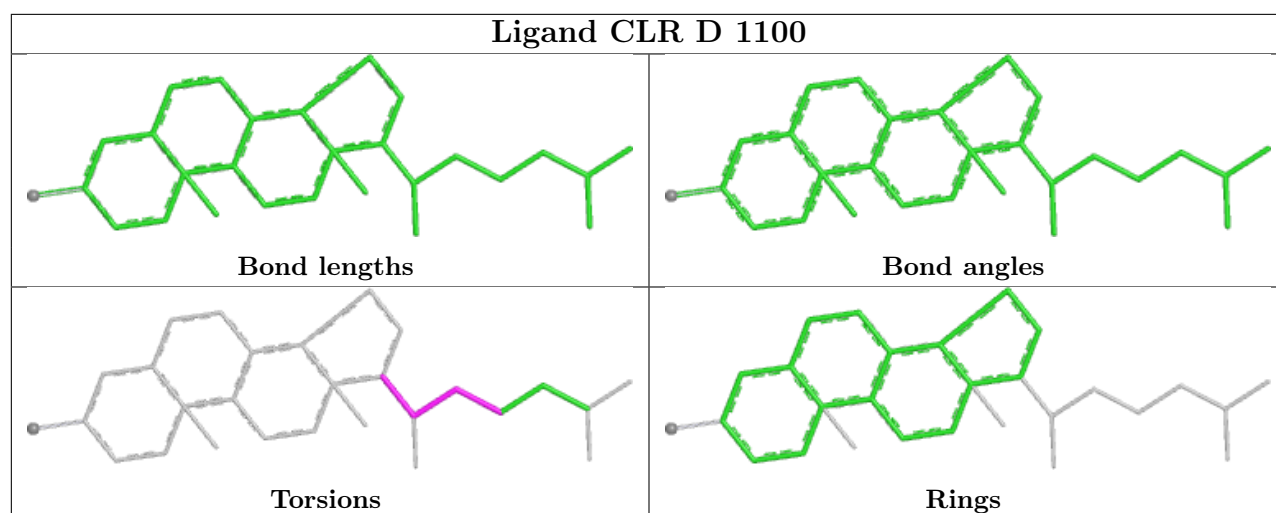


Ligand NAG K 1001

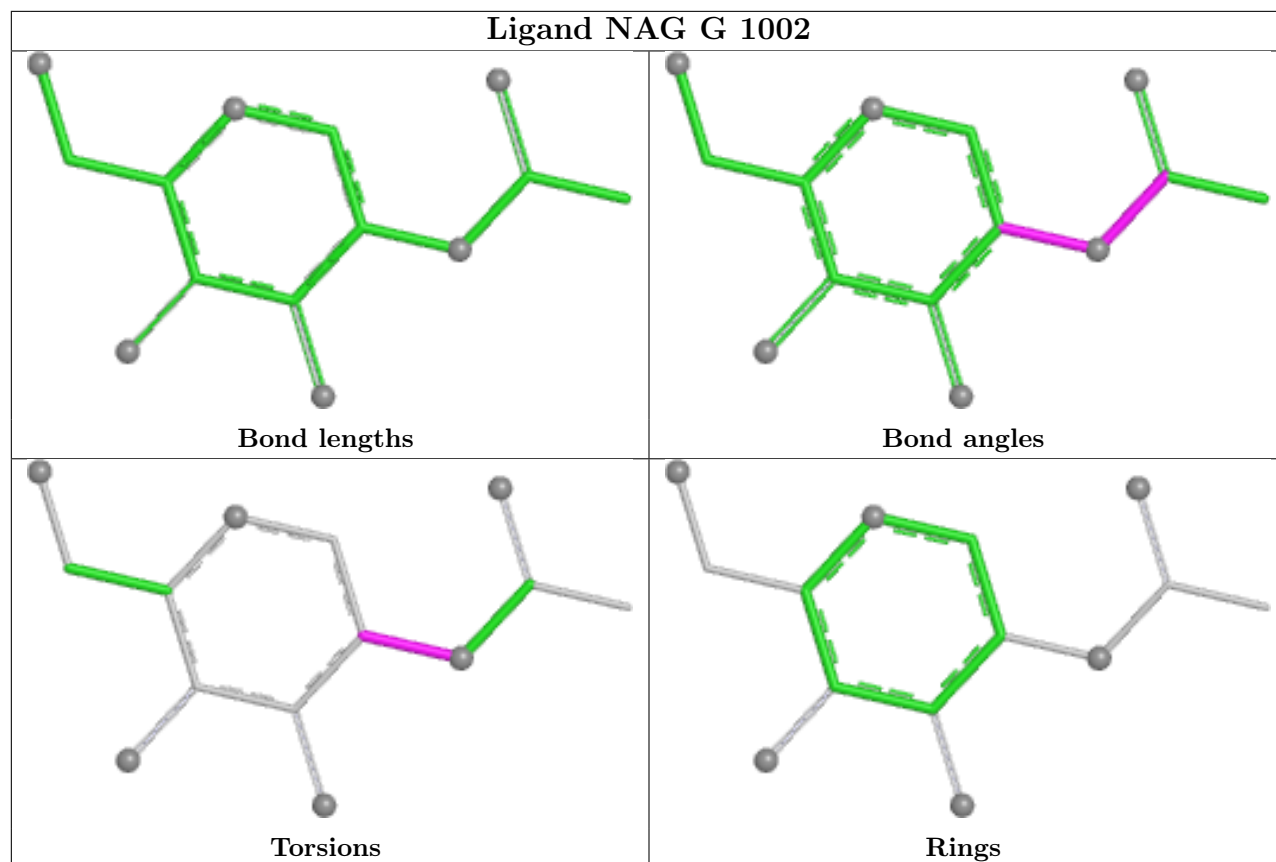


Ligand NAG C 1002

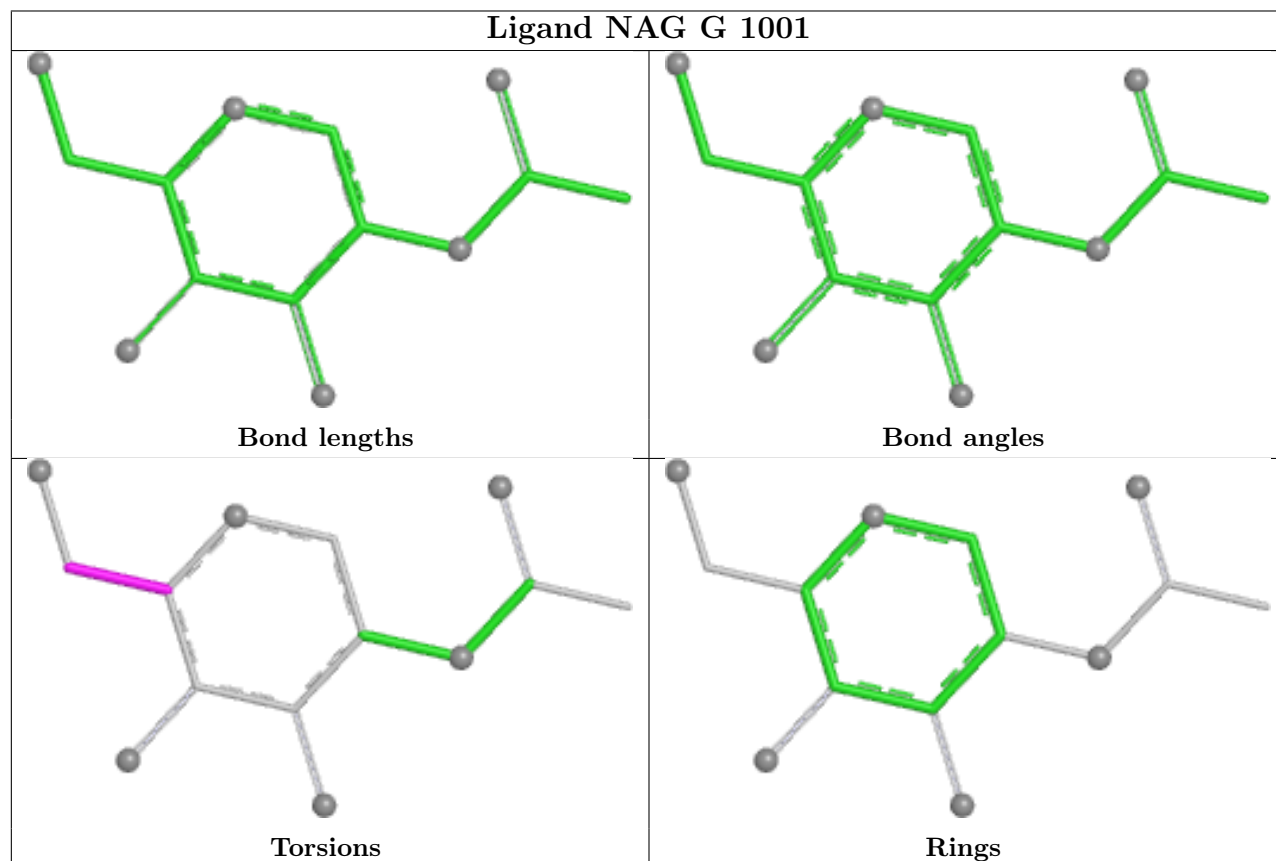




Ligand NAG G 1002



Ligand NAG G 1001



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

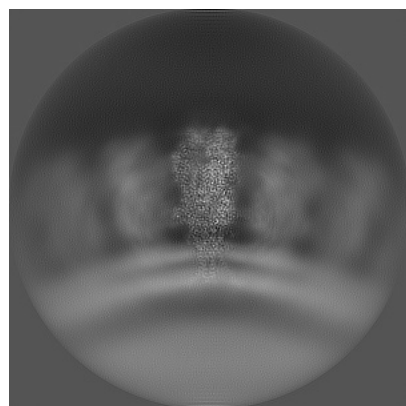
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17309. These allow visual inspection of the internal detail of the map and identification of artifacts.

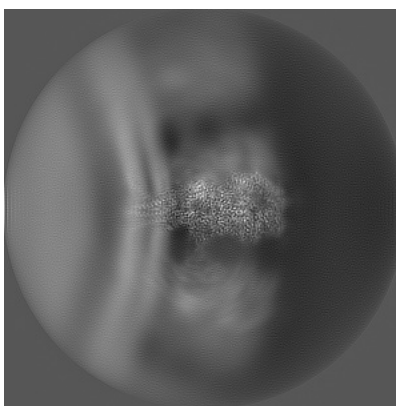
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

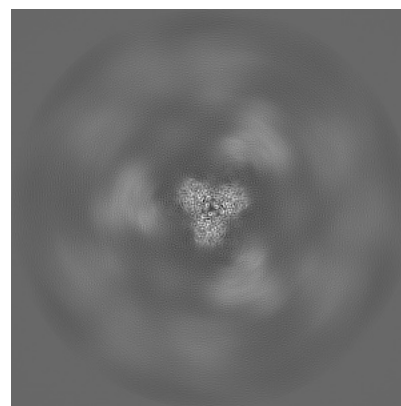
6.1.1 Primary map



X

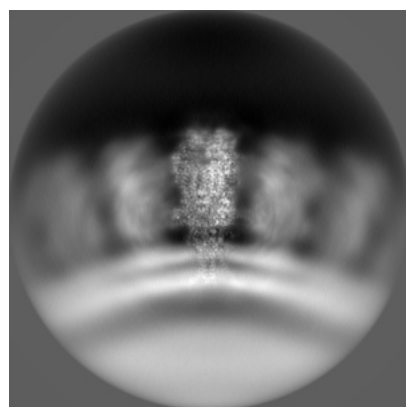


Y

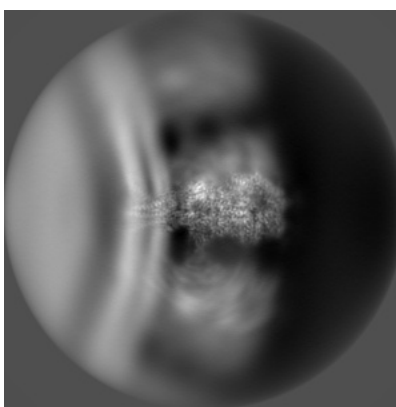


Z

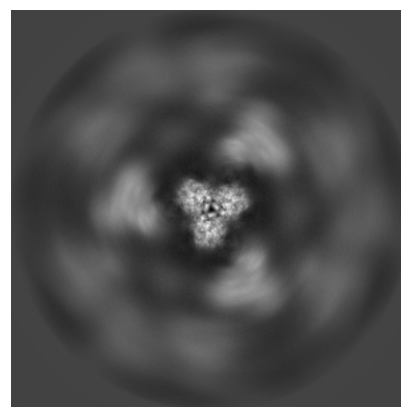
6.1.2 Raw map



X



Y

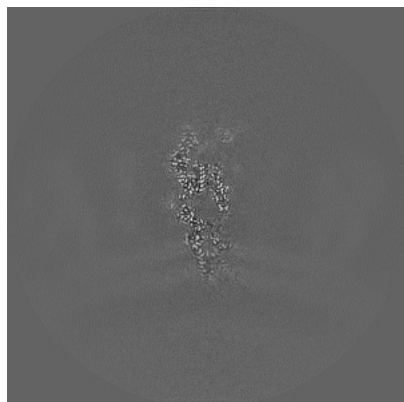


Z

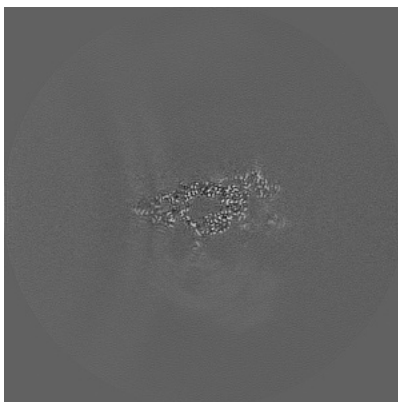
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

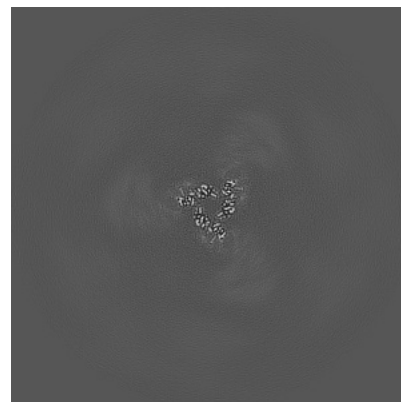
6.2.1 Primary map



X Index: 240

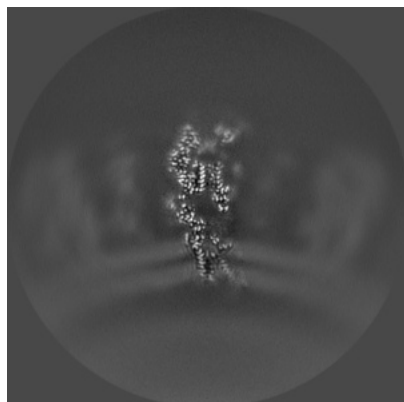


Y Index: 240

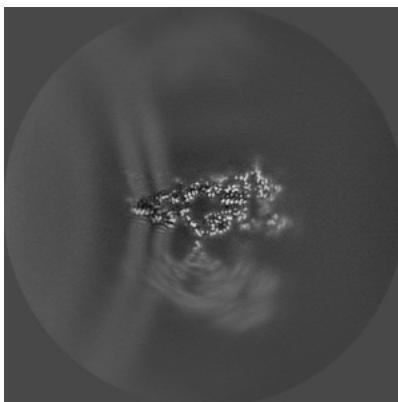


Z Index: 240

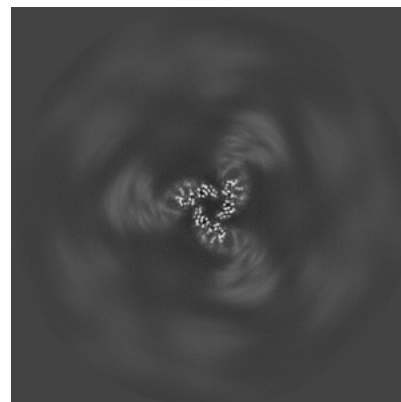
6.2.2 Raw map



X Index: 240



Y Index: 240

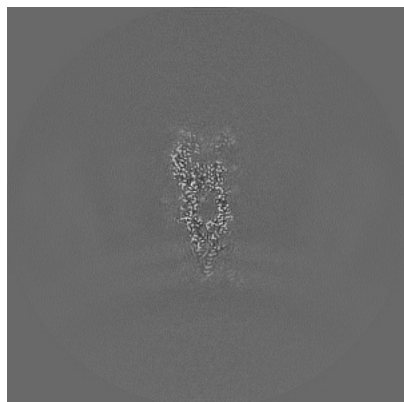


Z Index: 240

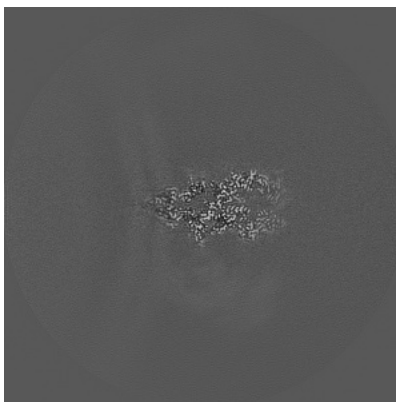
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

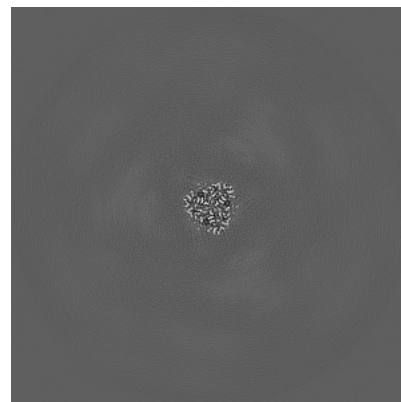
6.3.1 Primary map



X Index: 235

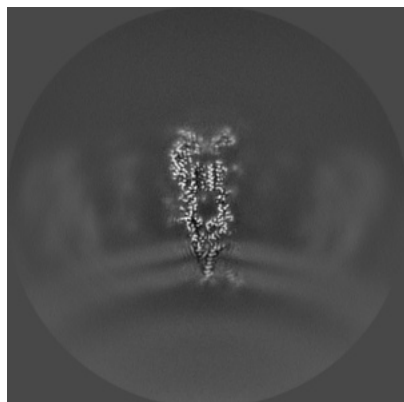


Y Index: 252

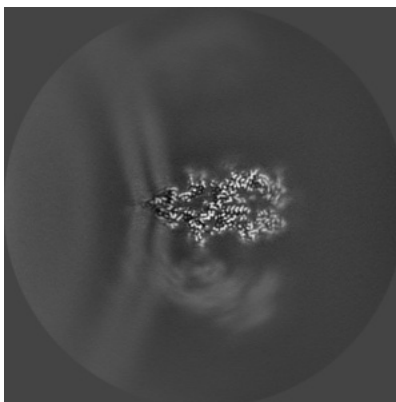


Z Index: 260

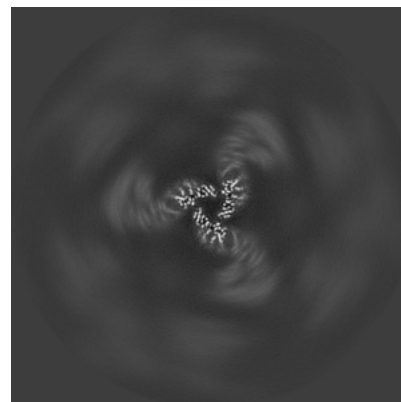
6.3.2 Raw map



X Index: 235



Y Index: 252

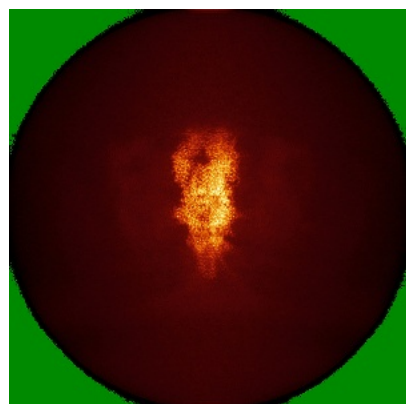


Z Index: 239

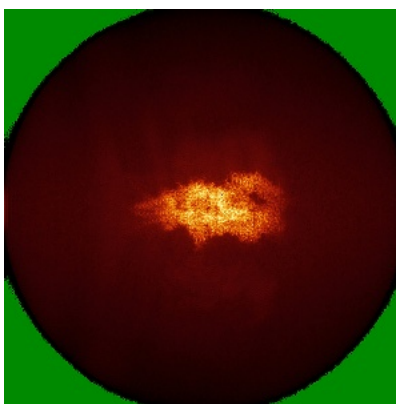
The images above show the largest variance slices of the map in three orthogonal directions.

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

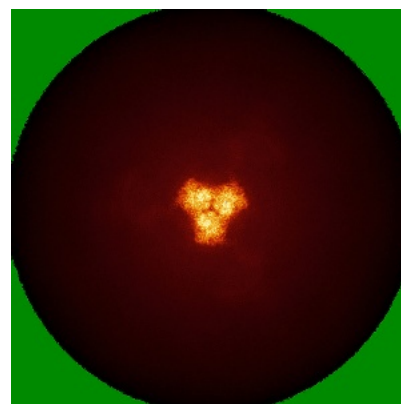
6.4.1 Primary map



X

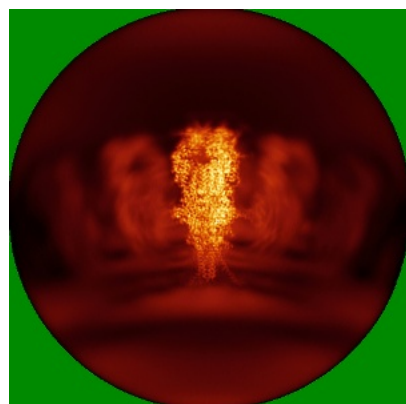


Y

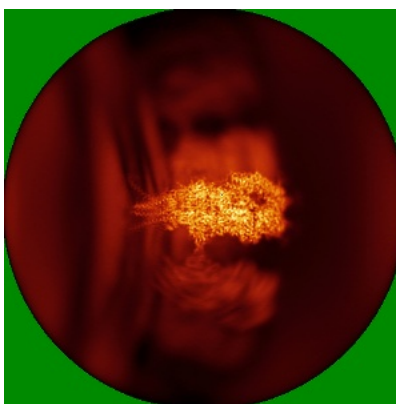


Z

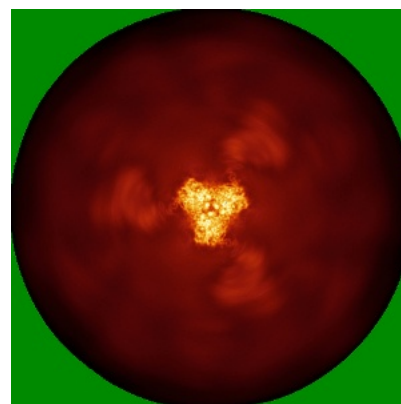
6.4.2 Raw map



X



Y

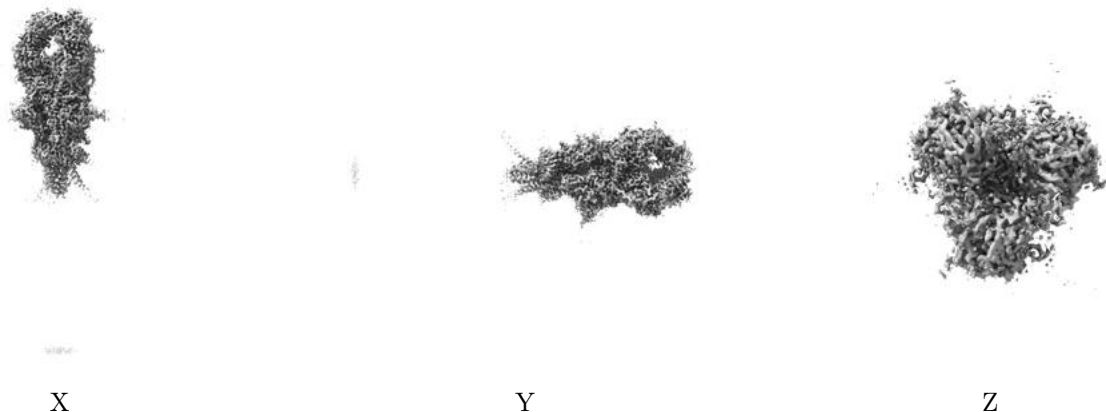


Z

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.

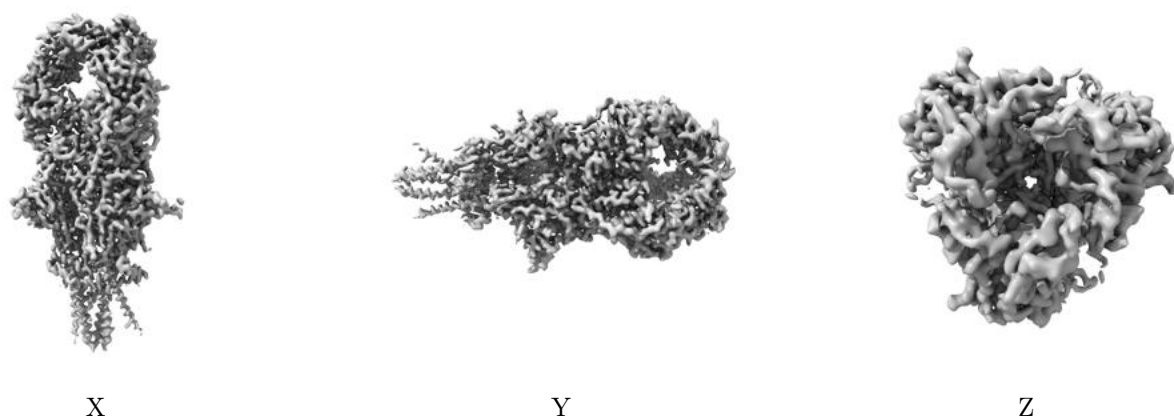
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

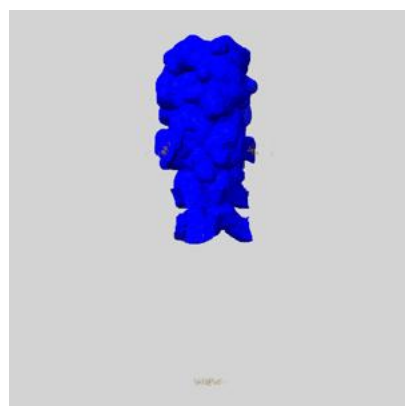
6.6 Mask visualisation [i](#)

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

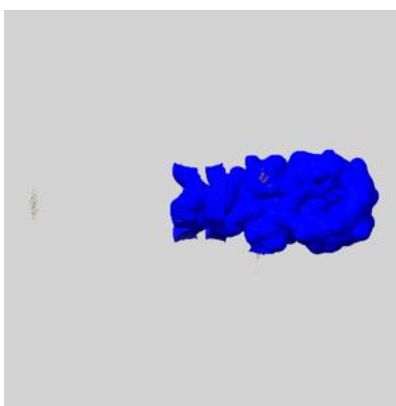
A mask typically either:

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

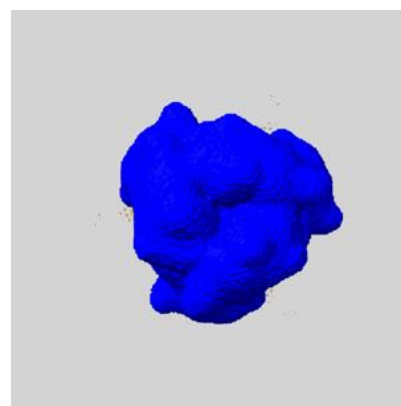
6.6.1 emd_17309_msk_1.map [i](#)



X



Y

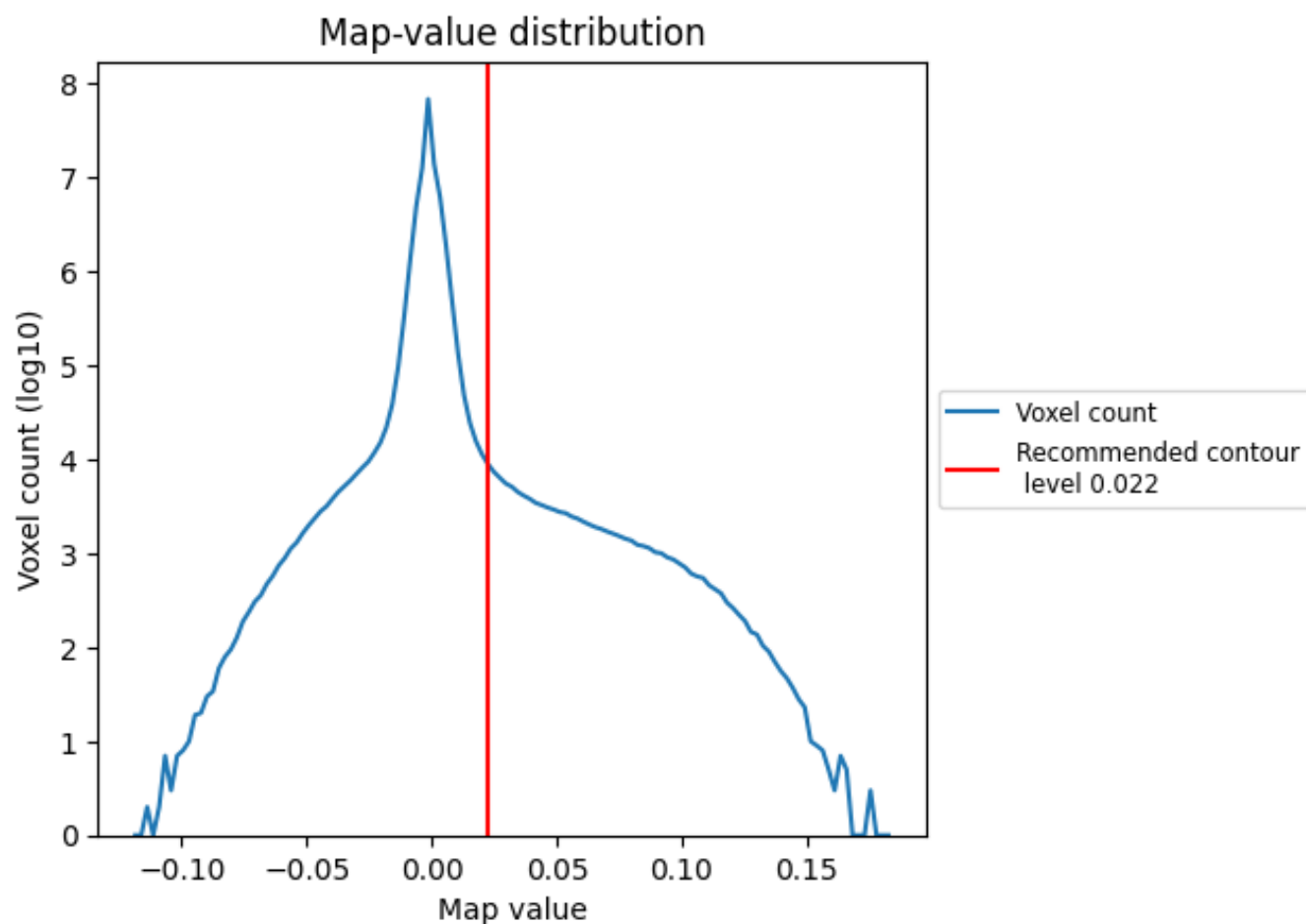


Z

7 Map analysis [i](#)

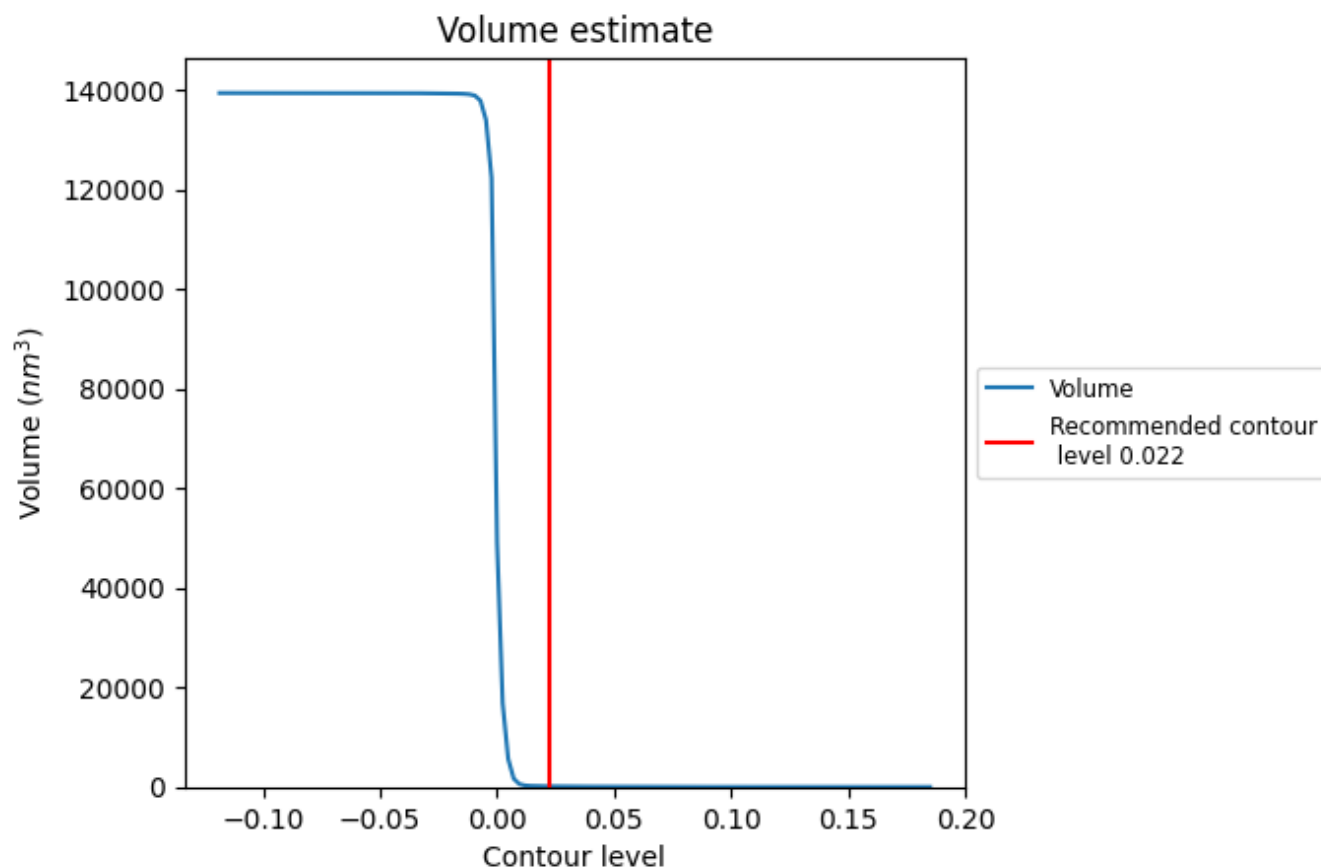
This section contains the results of statistical analysis of the map.

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.

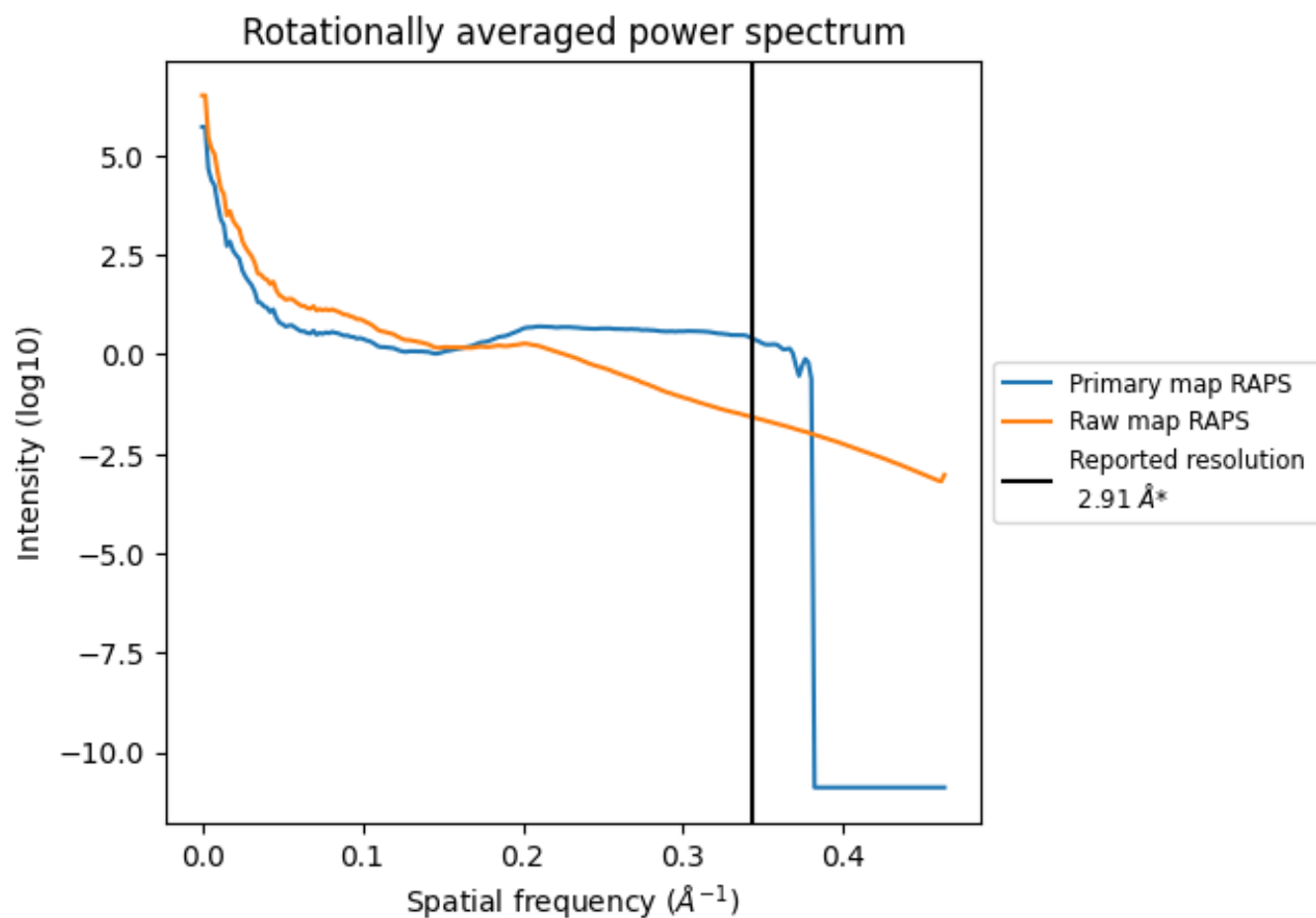
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 126 nm^3 ; this corresponds to an approximate mass of 114 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 ⓘ

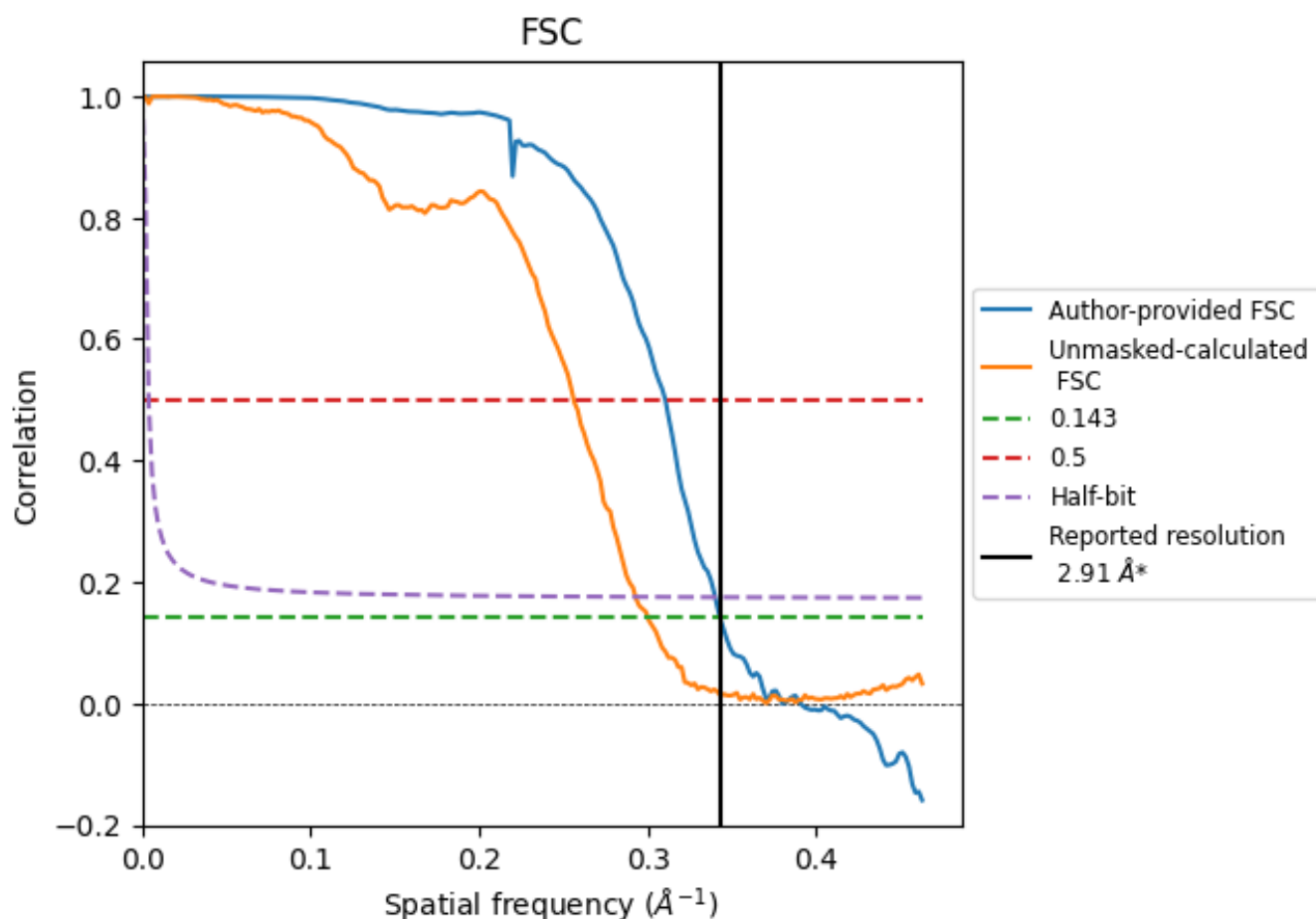


*Reported resolution corresponds to spatial frequency of $0.344 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.344 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	2.92	3.22	2.94
Unmasked-calculated*	3.33	3.90	3.41

*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 3.33 differs from the reported value 2.91 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-17309 and PDB model 8OZH. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)

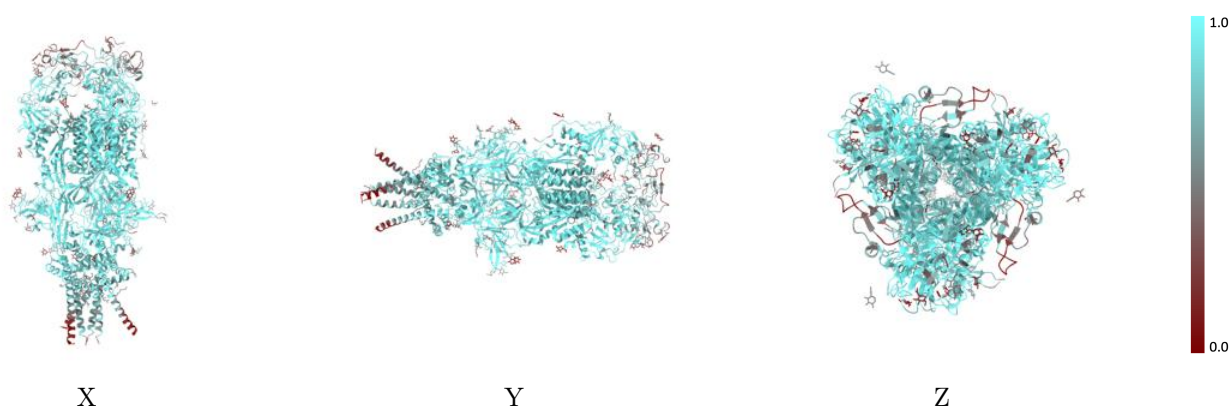
This section was not generated.

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



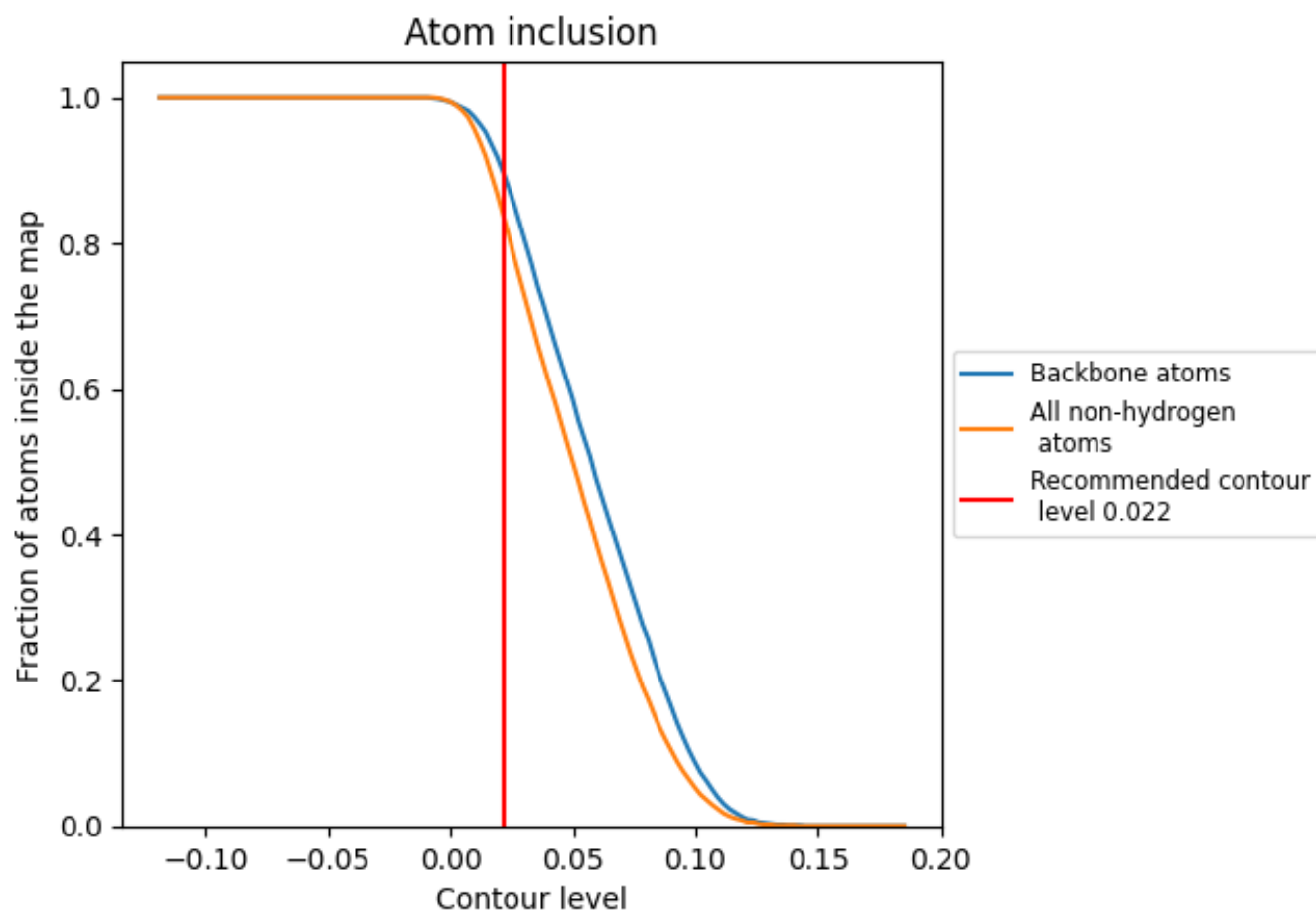
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 83% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8320	 0.6010
A	 0.6880	 0.5530
B	 0.7580	 0.5570
C	 0.8150	 0.5870
D	 0.9020	 0.6310
E	 0.6950	 0.5490
F	 0.7580	 0.5660
G	 0.8160	 0.5850
H	 0.9000	 0.6310
I	 0.6790	 0.5500
J	 0.7800	 0.5670
K	 0.8210	 0.5880
L	 0.8990	 0.6300
M	 0.6430	 0.5310
N	 0.6790	 0.5240
O	 0.6070	 0.5210
P	 0.4600	 0.5210
Q	 0.4400	 0.5140
R	 0.4400	 0.5140
S	 0.2820	 0.4330
T	 0.3080	 0.4360
U	 0.2820	 0.4270
V	 0.6270	 0.5630
W	 0.6270	 0.5680
X	 0.6400	 0.5620
Y	 0.5000	 0.4860
Z	 0.4640	 0.4690
a	 0.5360	 0.4760
b	 0.7140	 0.5440
c	 0.7140	 0.5340
d	 0.6790	 0.5280
e	 0.7450	 0.5720
f	 0.7660	 0.5830
g	 0.7450	 0.5860
h	 0.5970	 0.5750



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Chain	Atom inclusion	Q-score
i	 0.6390	 0.5750
j	 0.6110	 0.5840