



Full wwPDB EM Validation Report ⓘ

Jun 4, 2026 – 04:30 PM JST

PDB ID : 8ZMP / pdb_00008zmp
EMDB ID : EMD-60253
Title : Cryo-EM structure of the spike glycoprotein from Bat SARS-like coronavirus (Bat SL-CoV) WIV1 in locked state
Authors : Liu, C.; Beck, F.; Nagy, I.; Bohn, S.; Plitzko, J.; Baumeister, W.; Zhang, X.; Zinzula, L.
Deposited on : 2024-05-23
Resolution : 3.38 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
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 : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

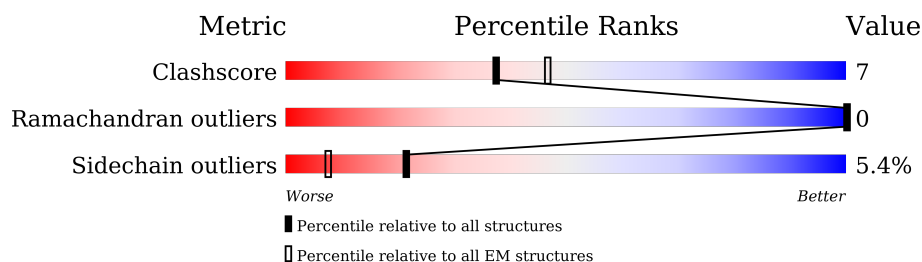
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.38 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.



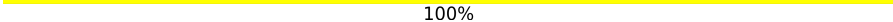
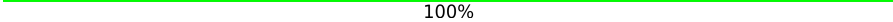
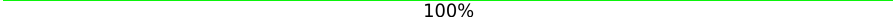
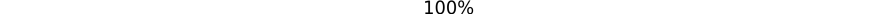
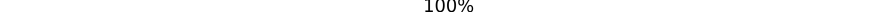
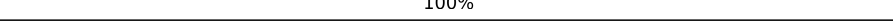
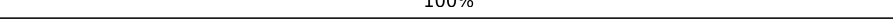
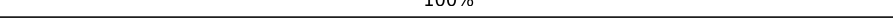
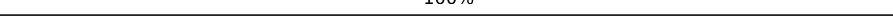
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1213	69% 17% • 12%
1	B	1213	70% 17% • 12%
1	C	1213	70% 16% • 12%
2	D	2	100%
2	F	2	100%
2	H	2	50% 50%
2	I	2	100%
2	J	2	100%
2	K	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	L	2	 100%
2	M	2	 100%
2	O	2	 100%
2	Q	2	 50% 50%
2	R	2	 100%
2	S	2	 100%
2	T	2	 50% 50%
2	U	2	 100%
2	V	2	 100%
2	X	2	 100%
2	Z	2	 50% 50%
2	a	2	 100%
2	b	2	 100%
2	c	2	 50% 50%
2	d	2	 100%
3	E	3	 100%
3	N	3	 100%
3	W	3	 100%
4	G	4	 75% 25%
4	P	4	 75% 25%
4	Y	4	 75% 25%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26175 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1066	Total	C	N	O	S	0	0
			8308	5301	1384	1579	44		
1	B	1066	Total	C	N	O	S	0	0
			8308	5301	1384	1579	44		
1	C	1066	Total	C	N	O	S	0	0
			8308	5301	1384	1579	44		

There are 117 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	initiating methionine	UNP U5WHZ7
A	623	HIS	TYR	conflict	UNP U5WHZ7
A	1167	ASP	ASN	conflict	UNP U5WHZ7
A	1195	GLY	-	expression tag	UNP U5WHZ7
A	1196	GLY	-	expression tag	UNP U5WHZ7
A	1197	SER	-	expression tag	UNP U5WHZ7
A	1198	GLY	-	expression tag	UNP U5WHZ7
A	1199	TYR	-	expression tag	UNP U5WHZ7
A	1200	ILE	-	expression tag	UNP U5WHZ7
A	1201	PRO	-	expression tag	UNP U5WHZ7
A	1202	GLU	-	expression tag	UNP U5WHZ7
A	1203	ALA	-	expression tag	UNP U5WHZ7
A	1204	PRO	-	expression tag	UNP U5WHZ7
A	1205	ARG	-	expression tag	UNP U5WHZ7
A	1206	ASP	-	expression tag	UNP U5WHZ7
A	1207	GLY	-	expression tag	UNP U5WHZ7
A	1208	GLN	-	expression tag	UNP U5WHZ7
A	1209	ALA	-	expression tag	UNP U5WHZ7
A	1210	TYR	-	expression tag	UNP U5WHZ7
A	1211	VAL	-	expression tag	UNP U5WHZ7
A	1212	ARG	-	expression tag	UNP U5WHZ7
A	1213	LYS	-	expression tag	UNP U5WHZ7
A	1214	ASP	-	expression tag	UNP U5WHZ7
A	1215	GLY	-	expression tag	UNP U5WHZ7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1216	GLU	-	expression tag	UNP U5WHZ7
A	1217	TRP	-	expression tag	UNP U5WHZ7
A	1218	VAL	-	expression tag	UNP U5WHZ7
A	1219	LEU	-	expression tag	UNP U5WHZ7
A	1220	LEU	-	expression tag	UNP U5WHZ7
A	1221	SER	-	expression tag	UNP U5WHZ7
A	1222	THR	-	expression tag	UNP U5WHZ7
A	1223	PHE	-	expression tag	UNP U5WHZ7
A	1224	LEU	-	expression tag	UNP U5WHZ7
A	1225	HIS	-	expression tag	UNP U5WHZ7
A	1226	HIS	-	expression tag	UNP U5WHZ7
A	1227	HIS	-	expression tag	UNP U5WHZ7
A	1228	HIS	-	expression tag	UNP U5WHZ7
A	1229	HIS	-	expression tag	UNP U5WHZ7
A	1230	HIS	-	expression tag	UNP U5WHZ7
B	18	MET	-	initiating methionine	UNP U5WHZ7
B	623	HIS	TYR	conflict	UNP U5WHZ7
B	1167	ASP	ASN	conflict	UNP U5WHZ7
B	1195	GLY	-	expression tag	UNP U5WHZ7
B	1196	GLY	-	expression tag	UNP U5WHZ7
B	1197	SER	-	expression tag	UNP U5WHZ7
B	1198	GLY	-	expression tag	UNP U5WHZ7
B	1199	TYR	-	expression tag	UNP U5WHZ7
B	1200	ILE	-	expression tag	UNP U5WHZ7
B	1201	PRO	-	expression tag	UNP U5WHZ7
B	1202	GLU	-	expression tag	UNP U5WHZ7
B	1203	ALA	-	expression tag	UNP U5WHZ7
B	1204	PRO	-	expression tag	UNP U5WHZ7
B	1205	ARG	-	expression tag	UNP U5WHZ7
B	1206	ASP	-	expression tag	UNP U5WHZ7
B	1207	GLY	-	expression tag	UNP U5WHZ7
B	1208	GLN	-	expression tag	UNP U5WHZ7
B	1209	ALA	-	expression tag	UNP U5WHZ7
B	1210	TYR	-	expression tag	UNP U5WHZ7
B	1211	VAL	-	expression tag	UNP U5WHZ7
B	1212	ARG	-	expression tag	UNP U5WHZ7
B	1213	LYS	-	expression tag	UNP U5WHZ7
B	1214	ASP	-	expression tag	UNP U5WHZ7
B	1215	GLY	-	expression tag	UNP U5WHZ7
B	1216	GLU	-	expression tag	UNP U5WHZ7
B	1217	TRP	-	expression tag	UNP U5WHZ7
B	1218	VAL	-	expression tag	UNP U5WHZ7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1219	LEU	-	expression tag	UNP U5WHZ7
B	1220	LEU	-	expression tag	UNP U5WHZ7
B	1221	SER	-	expression tag	UNP U5WHZ7
B	1222	THR	-	expression tag	UNP U5WHZ7
B	1223	PHE	-	expression tag	UNP U5WHZ7
B	1224	LEU	-	expression tag	UNP U5WHZ7
B	1225	HIS	-	expression tag	UNP U5WHZ7
B	1226	HIS	-	expression tag	UNP U5WHZ7
B	1227	HIS	-	expression tag	UNP U5WHZ7
B	1228	HIS	-	expression tag	UNP U5WHZ7
B	1229	HIS	-	expression tag	UNP U5WHZ7
B	1230	HIS	-	expression tag	UNP U5WHZ7
C	18	MET	-	initiating methionine	UNP U5WHZ7
C	623	HIS	TYR	conflict	UNP U5WHZ7
C	1167	ASP	ASN	conflict	UNP U5WHZ7
C	1195	GLY	-	expression tag	UNP U5WHZ7
C	1196	GLY	-	expression tag	UNP U5WHZ7
C	1197	SER	-	expression tag	UNP U5WHZ7
C	1198	GLY	-	expression tag	UNP U5WHZ7
C	1199	TYR	-	expression tag	UNP U5WHZ7
C	1200	ILE	-	expression tag	UNP U5WHZ7
C	1201	PRO	-	expression tag	UNP U5WHZ7
C	1202	GLU	-	expression tag	UNP U5WHZ7
C	1203	ALA	-	expression tag	UNP U5WHZ7
C	1204	PRO	-	expression tag	UNP U5WHZ7
C	1205	ARG	-	expression tag	UNP U5WHZ7
C	1206	ASP	-	expression tag	UNP U5WHZ7
C	1207	GLY	-	expression tag	UNP U5WHZ7
C	1208	GLN	-	expression tag	UNP U5WHZ7
C	1209	ALA	-	expression tag	UNP U5WHZ7
C	1210	TYR	-	expression tag	UNP U5WHZ7
C	1211	VAL	-	expression tag	UNP U5WHZ7
C	1212	ARG	-	expression tag	UNP U5WHZ7
C	1213	LYS	-	expression tag	UNP U5WHZ7
C	1214	ASP	-	expression tag	UNP U5WHZ7
C	1215	GLY	-	expression tag	UNP U5WHZ7
C	1216	GLU	-	expression tag	UNP U5WHZ7
C	1217	TRP	-	expression tag	UNP U5WHZ7
C	1218	VAL	-	expression tag	UNP U5WHZ7
C	1219	LEU	-	expression tag	UNP U5WHZ7
C	1220	LEU	-	expression tag	UNP U5WHZ7
C	1221	SER	-	expression tag	UNP U5WHZ7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1222	THR	-	expression tag	UNP U5WHZ7
C	1223	PHE	-	expression tag	UNP U5WHZ7
C	1224	LEU	-	expression tag	UNP U5WHZ7
C	1225	HIS	-	expression tag	UNP U5WHZ7
C	1226	HIS	-	expression tag	UNP U5WHZ7
C	1227	HIS	-	expression tag	UNP U5WHZ7
C	1228	HIS	-	expression tag	UNP U5WHZ7
C	1229	HIS	-	expression tag	UNP U5WHZ7
C	1230	HIS	-	expression tag	UNP U5WHZ7

- 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	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	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	Q	2	Total	C	N	O	0	0
			28	16	2	10		
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		

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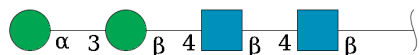
Mol	Chain	Residues	Atoms				AltConf	Trace
2	T	2	Total	C	N	O	0	0
			28	16	2	10		
2	U	2	Total	C	N	O	0	0
			28	16	2	10		
2	V	2	Total	C	N	O	0	0
			28	16	2	10		
2	X	2	Total	C	N	O	0	0
			28	16	2	10		
2	Z	2	Total	C	N	O	0	0
			28	16	2	10		
2	a	2	Total	C	N	O	0	0
			28	16	2	10		
2	b	2	Total	C	N	O	0	0
			28	16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

- 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.



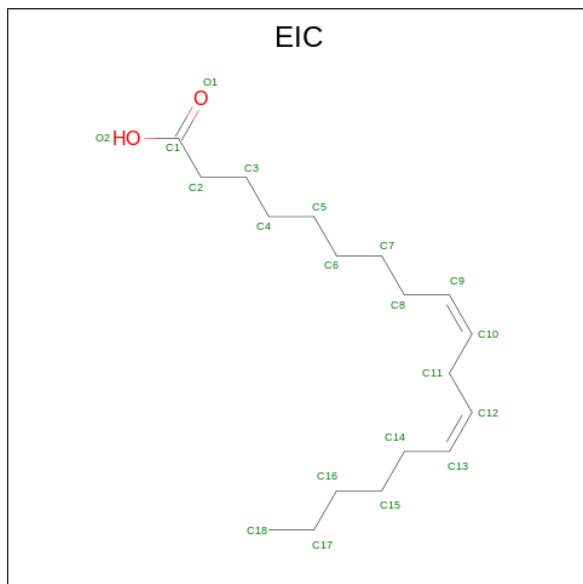
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	N	3	Total	C	N	O	0	0
			39	22	2	15		
3	W	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is an oligosaccharide called 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.



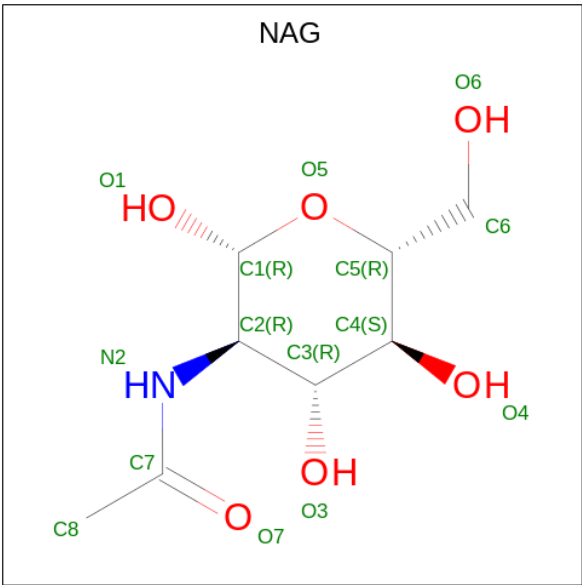
Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	4	Total	C	N	O	0	0
			50	28	2	20		
4	P	4	Total	C	N	O	0	0
			50	28	2	20		
4	Y	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 5 is LINOLEIC ACID (CCD ID: EIC) (formula: $C_{18}H_{32}O_2$).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			20	18	2	
5	B	1	Total	C	O	0
			20	18	2	
5	C	1	Total	C	O	0
			20	18	2	

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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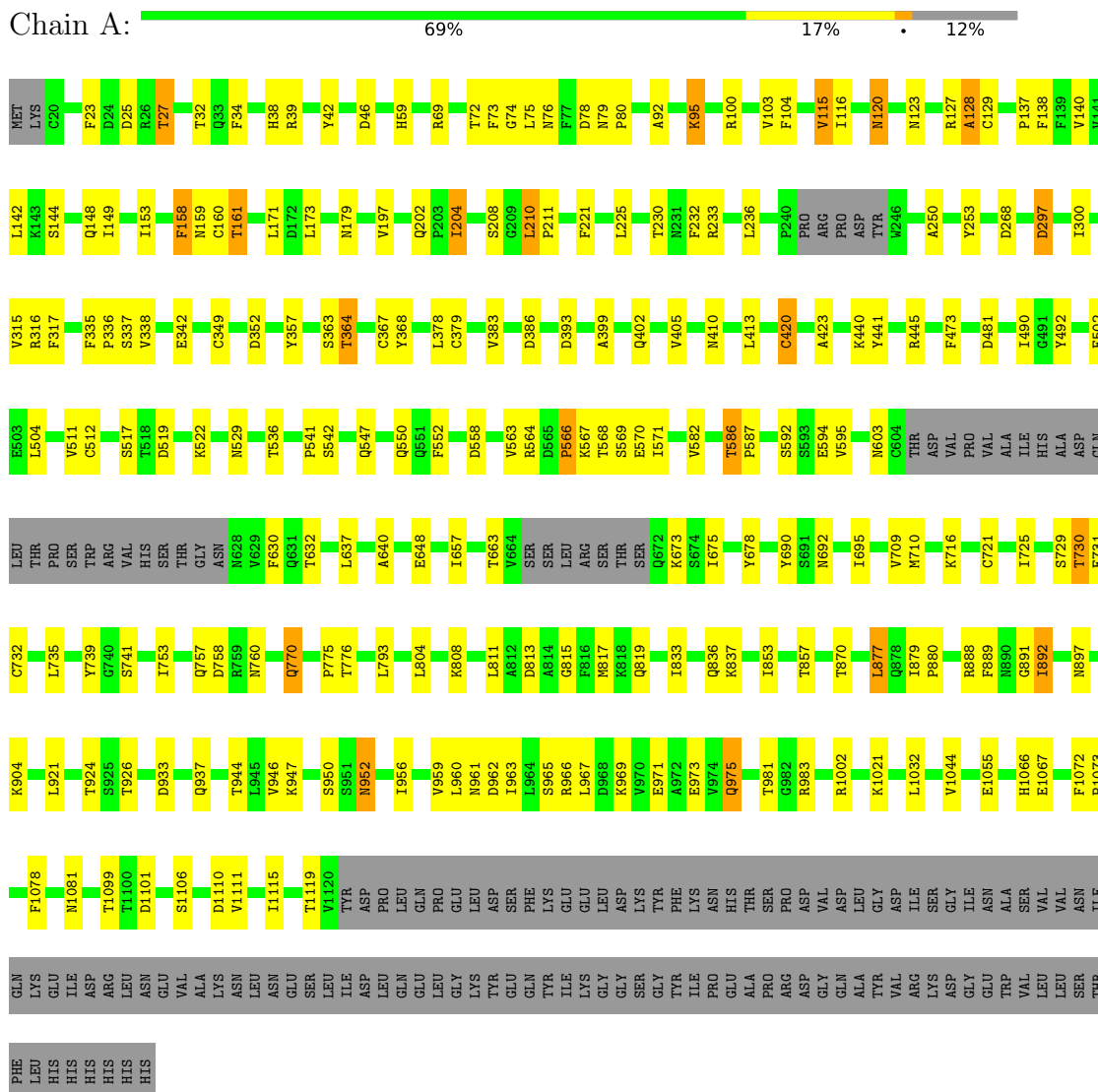
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Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C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

3 Residue-property plots

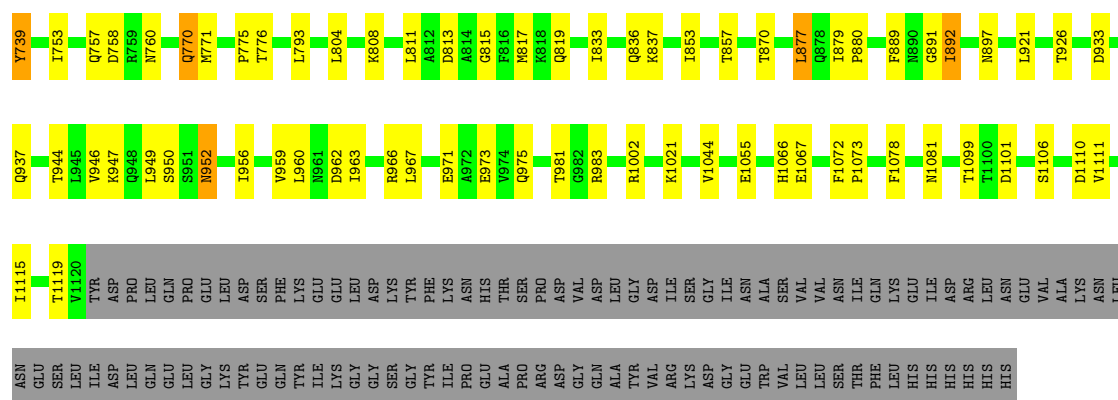
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

- Molecule 1: Spike glycoprotein



- Molecule 1: Spike glycoprotein





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

Chain D: 100%



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

Chain F: 100%



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

Chain H: 50% 50%



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

Chain I: 100%



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

Chain J: 100%

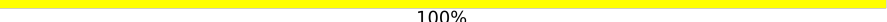


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%

NAG1
NAG2

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

Chain L:  100%

NAG1
NAG2

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

Chain M:  100%

NAG1
NAG2

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

Chain O:  100%

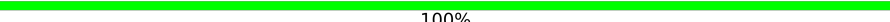
NAG1
NAG2

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

Chain Q:  50% 50%

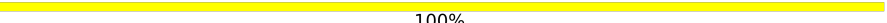
NAG1
NAG2

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

Chain R:  100%

NAG1
NAG2

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

Chain S:  100%

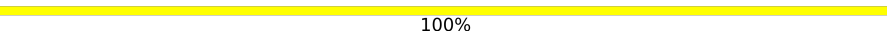
MAG1
MAG2

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

Chain T:  50% 50%

MAG1
MAG2

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

Chain U:  100%

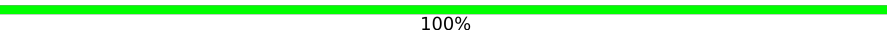
MAG1
MAG2

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

Chain V:  100%

MAG1
MAG2

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

Chain X:  100%

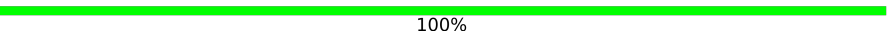
MAG1
MAG2

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

Chain Z:  50% 50%

MAG1
MAG2

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

Chain a:  100%

MAG1
MAG2

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

Chain b:  100%

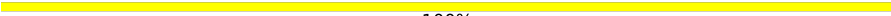
MAG1
MAG2

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

Chain c:  50% 50%

MAG1
MAG2

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

Chain d:  100%

MAG1
MAG2

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

Chain E:  100%

MAG1
MAG2
BMA3

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

Chain N:  100%

MAG1
MAG2
BMA3

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

Chain W:  100%

MAG1
MAG2
BMA3

- Molecule 4: 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

Chain G:  75% 25%

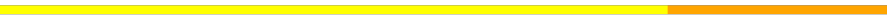


- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  75% 25%



- Molecule 4: 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

Chain Y:  75% 25%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90000	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	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, MAN, NAG, EIC

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	0.34	6/8502 (0.1%)	0.38	5/11565 (0.0%)
1	B	0.34	6/8502 (0.1%)	0.38	5/11565 (0.0%)
1	C	0.34	6/8502 (0.1%)	0.38	5/11565 (0.0%)
All	All	0.34	18/25506 (0.1%)	0.38	15/34695 (0.0%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	210	LEU	CA-C	-7.09	1.45	1.52
1	A	128	ALA	CA-C	-7.09	1.44	1.52
1	A	210	LEU	CA-C	-7.09	1.45	1.52
1	B	210	LEU	CA-C	-7.08	1.45	1.52
1	B	128	ALA	CA-C	-7.08	1.44	1.52
1	C	128	ALA	CA-C	-7.04	1.44	1.52
1	C	127	ARG	CA-C	-6.55	1.44	1.52
1	B	127	ARG	CA-C	-6.53	1.44	1.52
1	A	127	ARG	CA-C	-6.48	1.44	1.52
1	C	566	PRO	CA-C	-5.86	1.44	1.52
1	A	566	PRO	CA-C	-5.85	1.44	1.52
1	B	566	PRO	CA-C	-5.80	1.44	1.52
1	B	128	ALA	C-O	-5.77	1.17	1.23
1	C	128	ALA	C-O	-5.77	1.17	1.23
1	A	128	ALA	C-O	-5.76	1.17	1.23
1	C	161	THR	N-CA	-5.35	1.41	1.46
1	B	161	THR	N-CA	-5.30	1.41	1.46
1	A	161	THR	N-CA	-5.29	1.41	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	ASN	N-CA-C	6.17	119.21	109.96
1	C	159	ASN	N-CA-C	6.15	119.19	109.96
1	B	159	ASN	N-CA-C	6.14	119.17	109.96
1	B	153	ILE	N-CA-C	-6.04	106.92	112.96
1	A	153	ILE	N-CA-C	-6.03	106.93	112.96
1	C	153	ILE	N-CA-C	-6.02	106.94	112.96
1	B	208	SER	N-CA-C	5.90	118.10	108.55
1	A	208	SER	N-CA-C	5.88	118.07	108.55
1	C	208	SER	N-CA-C	5.86	118.04	108.55
1	B	570	GLU	N-CA-C	-5.24	100.55	108.46
1	A	570	GLU	N-CA-C	-5.23	100.56	108.46
1	C	570	GLU	N-CA-C	-5.22	100.58	108.46
1	A	159	ASN	N-CA-CB	-5.20	102.10	109.85
1	B	159	ASN	N-CA-CB	-5.19	102.12	109.85
1	C	159	ASN	N-CA-CB	-5.18	102.14	109.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	8308	0	8072	136	0
1	B	8308	0	8072	139	0
1	C	8308	0	8072	132	0
2	D	28	0	25	0	0
2	F	28	0	25	0	0
2	H	28	0	25	2	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	1	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	O	28	0	25	0	0
2	Q	28	0	25	2	0
2	R	28	0	25	0	0
2	S	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	28	0	25	1	0
2	U	28	0	25	0	0
2	V	28	0	25	0	0
2	X	28	0	25	0	0
2	Z	28	0	25	2	0
2	a	28	0	25	0	0
2	b	28	0	25	0	0
2	c	28	0	25	1	0
2	d	28	0	25	0	0
3	E	39	0	34	1	0
3	N	39	0	34	1	0
3	W	39	0	34	1	0
4	G	50	0	43	2	0
4	P	50	0	43	2	0
4	Y	50	0	43	2	0
5	A	20	0	31	3	0
5	B	20	0	31	3	0
5	C	20	0	31	3	0
6	A	112	0	104	1	0
6	B	112	0	104	1	0
6	C	112	0	104	1	0
All	All	26175	0	25377	385	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 7.

All (385) 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:C:379:CYS:HA	1:C:512:CYS:HB3	1.57	0.87
1:B:379:CYS:HA	1:B:512:CYS:HB3	1.57	0.87
1:A:379:CYS:HA	1:A:512:CYS:HB3	1.57	0.86
1:B:230:THR:HG21	4:P:1:NAG:H62	1.69	0.75
1:A:230:THR:HG21	4:G:1:NAG:H62	1.69	0.74
1:C:230:THR:HG21	4:Y:1:NAG:H62	1.69	0.73
1:B:158:PHE:CZ	3:N:1:NAG:H62	2.27	0.70
1:A:158:PHE:CZ	3:E:1:NAG:H62	2.27	0.69
1:C:158:PHE:CZ	3:W:1:NAG:H62	2.27	0.69
1:A:349:CYS:HB2	1:A:511:VAL:HG23	1.76	0.68
1:C:349:CYS:HB2	1:C:511:VAL:HG23	1.76	0.68
1:C:39:ARG:NH1	1:C:211:PRO:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ARG:NH1	1:B:211:PRO:O	2.28	0.67
1:B:349:CYS:HB2	1:B:511:VAL:HG23	1.76	0.66
1:A:39:ARG:NH1	1:A:211:PRO:O	2.28	0.66
1:A:760:ASN:OD1	1:A:1002:ARG:NH1	2.29	0.66
1:B:204:ILE:HG13	1:B:211:PRO:HG3	1.79	0.65
1:B:760:ASN:OD1	1:B:1002:ARG:NH1	2.29	0.65
1:C:760:ASN:OD1	1:C:1002:ARG:NH1	2.29	0.65
1:C:317:PHE:O	1:C:567:LYS:HE3	1.96	0.65
1:A:204:ILE:HG13	1:A:211:PRO:HG3	1.79	0.65
1:C:204:ILE:HG13	1:C:211:PRO:HG3	1.79	0.64
1:A:317:PHE:O	1:A:567:LYS:HE3	1.96	0.64
1:B:317:PHE:O	1:B:567:LYS:HE3	1.96	0.64
1:C:933:ASP:O	1:C:937:GLN:HG3	2.00	0.62
1:B:933:ASP:O	1:B:937:GLN:HG3	2.00	0.61
1:A:933:ASP:O	1:A:937:GLN:HG3	2.00	0.61
1:B:367:CYS:HB2	1:B:420:CYS:HA	1.84	0.60
1:B:383:VAL:HG22	1:B:502:PHE:HB3	1.84	0.59
1:C:79:ASN:HB3	1:C:236:LEU:HD12	1.85	0.59
1:B:568:THR:O	1:B:569:SER:C	2.45	0.59
1:A:140:VAL:HG23	1:A:149:ILE:HG13	1.84	0.59
1:B:367:CYS:CB	1:B:420:CYS:HA	2.33	0.59
1:C:140:VAL:HG23	1:C:149:ILE:HG13	1.84	0.59
1:C:103:VAL:HG23	1:C:116:ILE:HG22	1.85	0.59
1:A:383:VAL:HG22	1:A:502:PHE:HB3	1.84	0.58
1:A:695:ILE:HG22	1:B:879:ILE:HG13	1.84	0.58
1:B:204:ILE:HG13	1:B:211:PRO:CG	2.33	0.58
1:C:367:CYS:HB2	1:C:420:CYS:HA	1.84	0.58
1:C:383:VAL:HG22	1:C:502:PHE:HB3	1.84	0.58
1:A:879:ILE:HG13	1:C:695:ILE:HG22	1.84	0.58
1:A:103:VAL:HG23	1:A:116:ILE:HG22	1.85	0.58
1:A:367:CYS:CB	1:A:420:CYS:HA	2.33	0.58
1:C:204:ILE:HG13	1:C:211:PRO:CG	2.33	0.58
1:A:204:ILE:HG13	1:A:211:PRO:CG	2.33	0.58
1:B:695:ILE:HG22	1:C:879:ILE:HG13	1.84	0.58
1:C:336:PRO:HG2	1:C:342:GLU:HG3	1.86	0.58
1:C:367:CYS:CB	1:C:420:CYS:HA	2.33	0.58
1:C:547:GLN:OE1	1:C:550:GLN:NE2	2.37	0.58
1:A:336:PRO:HG2	1:A:342:GLU:HG3	1.86	0.57
1:A:367:CYS:HB2	1:A:420:CYS:HA	1.84	0.57
1:B:103:VAL:HG23	1:B:116:ILE:HG22	1.85	0.57
1:B:140:VAL:HG23	1:B:149:ILE:HG13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:SER:OG	1:B:567:LYS:NZ	2.37	0.57
1:A:547:GLN:OE1	1:A:550:GLN:NE2	2.37	0.57
1:A:79:ASN:HB3	1:A:236:LEU:HD12	1.85	0.57
1:C:568:THR:O	1:C:569:SER:C	2.45	0.57
1:B:547:GLN:OE1	1:B:550:GLN:NE2	2.37	0.57
1:B:79:ASN:HB3	1:B:236:LEU:HD12	1.85	0.57
1:C:74:GLY:O	1:C:76:ASN:ND2	2.38	0.57
1:A:568:THR:O	1:A:569:SER:C	2.45	0.57
1:A:517:SER:OG	1:A:567:LYS:NZ	2.38	0.57
1:B:336:PRO:HG2	1:B:342:GLU:HG3	1.86	0.57
1:B:709:VAL:HG22	1:B:1044:VAL:HG22	1.87	0.57
1:B:550:GLN:O	1:B:564:ARG:NH2	2.38	0.56
1:C:517:SER:OG	1:C:567:LYS:NZ	2.38	0.56
1:B:725:ILE:HG22	1:B:983:ARG:HB3	1.87	0.56
1:C:550:GLN:O	1:C:564:ARG:NH2	2.38	0.56
1:A:74:GLY:O	1:A:76:ASN:ND2	2.38	0.56
1:A:550:GLN:O	1:A:564:ARG:NH2	2.38	0.56
1:C:952:ASN:OD1	1:C:952:ASN:N	2.39	0.56
1:C:316:ARG:HH21	1:C:567:LYS:HB2	1.71	0.56
1:C:709:VAL:HG22	1:C:1044:VAL:HG22	1.87	0.56
1:A:592:SER:OG	1:A:594:GLU:OE1	2.24	0.56
1:C:637:LEU:HD21	1:C:640:ALA:HB3	1.87	0.56
1:B:197:VAL:HB	1:B:221:PHE:HB2	1.88	0.56
1:B:637:LEU:HD21	1:B:640:ALA:HB3	1.87	0.56
1:A:547:GLN:H	1:A:550:GLN:HE21	1.53	0.55
1:B:952:ASN:N	1:B:952:ASN:OD1	2.39	0.55
1:A:725:ILE:HG22	1:A:983:ARG:HB3	1.87	0.55
1:B:74:GLY:O	1:B:76:ASN:ND2	2.38	0.55
1:A:637:LEU:HD21	1:A:640:ALA:HB3	1.87	0.55
1:C:547:GLN:H	1:C:550:GLN:HE21	1.53	0.55
1:C:725:ILE:HG22	1:C:983:ARG:HB3	1.87	0.55
1:A:316:ARG:HH21	1:A:567:LYS:HB2	1.71	0.55
1:B:547:GLN:H	1:B:550:GLN:HE21	1.53	0.55
1:C:592:SER:OG	1:C:594:GLU:OE1	2.24	0.55
1:B:316:ARG:HH21	1:B:567:LYS:HB2	1.71	0.54
1:A:709:VAL:HG22	1:A:1044:VAL:HG22	1.87	0.54
1:C:197:VAL:HB	1:C:221:PHE:HB2	1.88	0.54
1:B:592:SER:OG	1:B:594:GLU:OE1	2.24	0.54
1:A:128:ALA:O	1:A:129:CYS:SG	2.66	0.54
1:B:128:ALA:O	1:B:129:CYS:SG	2.66	0.54
1:A:120:ASN:OD1	2:H:1:NAG:N2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:ASN:OD1	1:A:952:ASN:N	2.39	0.54
1:C:128:ALA:O	1:C:129:CYS:SG	2.66	0.54
1:A:197:VAL:HB	1:A:221:PHE:HB2	1.88	0.53
1:B:120:ASN:OD1	2:Q:1:NAG:N2	2.41	0.53
1:C:120:ASN:OD1	2:Z:1:NAG:N2	2.41	0.53
1:B:542:SER:OG	1:B:571:ILE:O	2.24	0.53
1:B:729:SER:O	1:B:730:THR:HG22	2.09	0.53
1:C:38:HIS:O	1:C:38:HIS:ND1	2.42	0.53
1:C:729:SER:O	1:C:730:THR:HG22	2.09	0.53
1:A:27:THR:OG1	1:A:75:LEU:O	2.27	0.53
1:A:729:SER:O	1:A:730:THR:HG22	2.09	0.53
1:C:128:ALA:C	1:C:129:CYS:SG	2.92	0.53
1:C:1099:THR:HG23	1:C:1101:ASP:H	1.73	0.53
1:B:128:ALA:C	1:B:129:CYS:SG	2.92	0.52
1:C:204:ILE:CD1	1:C:211:PRO:HG3	2.39	0.52
1:B:204:ILE:CD1	1:B:211:PRO:HG3	2.40	0.52
1:B:735:LEU:HD21	1:B:973:GLU:HG2	1.91	0.52
1:B:38:HIS:O	1:B:38:HIS:ND1	2.42	0.52
1:A:38:HIS:O	1:A:38:HIS:ND1	2.42	0.52
1:A:204:ILE:CD1	1:A:211:PRO:HG3	2.39	0.52
1:A:967:LEU:HD23	1:A:971:GLU:HB3	1.92	0.52
1:B:770:GLN:N	1:B:770:GLN:OE1	2.43	0.52
1:A:735:LEU:HD21	1:A:973:GLU:HG2	1.91	0.52
1:A:770:GLN:OE1	1:A:770:GLN:N	2.43	0.52
1:C:542:SER:OG	1:C:571:ILE:O	2.24	0.52
1:C:770:GLN:OE1	1:C:770:GLN:N	2.43	0.52
1:B:967:LEU:HD23	1:B:971:GLU:HB3	1.92	0.52
1:C:967:LEU:HD23	1:C:971:GLU:HB3	1.92	0.51
1:B:1099:THR:HG23	1:B:1101:ASP:H	1.73	0.51
1:A:1099:THR:HG23	1:A:1101:ASP:H	1.73	0.51
1:C:27:THR:OG1	1:C:75:LEU:O	2.27	0.51
1:A:128:ALA:C	1:A:129:CYS:SG	2.93	0.51
1:B:171:LEU:HD23	1:B:171:LEU:H	1.76	0.51
1:C:268:ASP:OD1	1:C:268:ASP:N	2.40	0.51
1:A:171:LEU:H	1:A:171:LEU:HD23	1.76	0.51
1:A:819:GLN:HE22	1:C:603:ASN:HD22	1.59	0.51
1:C:142:LEU:HD11	6:C:1302:NAG:H62	1.93	0.51
1:A:137:PRO:HG2	1:A:233:ARG:HD3	1.93	0.51
1:C:735:LEU:HD21	1:C:973:GLU:HG2	1.91	0.51
1:B:603:ASN:HD22	1:C:819:GLN:HE22	1.59	0.50
1:A:142:LEU:HD11	6:A:1302:NAG:H62	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:TYR:OH	1:C:59:HIS:O	2.24	0.50
1:A:741:SER:O	1:A:741:SER:OG	2.27	0.50
1:B:142:LEU:HD11	6:B:1302:NAG:H62	1.93	0.50
1:C:171:LEU:H	1:C:171:LEU:HD23	1.76	0.50
1:A:630:PHE:CE1	1:A:632:THR:HG22	2.47	0.49
1:C:891:GLY:O	1:C:1021:LYS:NZ	2.45	0.49
1:C:137:PRO:HG2	1:C:233:ARG:HD3	1.93	0.49
1:C:663:THR:HG22	1:C:673:LYS:HG2	1.94	0.49
1:B:891:GLY:O	1:B:1021:LYS:NZ	2.45	0.49
1:B:137:PRO:HG2	1:B:233:ARG:HD3	1.94	0.49
1:C:630:PHE:CE1	1:C:632:THR:HG22	2.47	0.49
1:A:100:ARG:NH2	1:A:148:GLN:OE1	2.46	0.49
1:A:297:ASP:OD1	1:A:297:ASP:N	2.39	0.49
1:B:100:ARG:NH2	1:B:148:GLN:OE1	2.46	0.49
1:B:630:PHE:CE1	1:B:632:THR:HG22	2.47	0.49
1:A:891:GLY:O	1:A:1021:LYS:NZ	2.45	0.49
1:C:100:ARG:NH2	1:C:148:GLN:OE1	2.46	0.49
1:A:603:ASN:HD22	1:B:819:GLN:HE22	1.59	0.49
1:B:558:ASP:H	1:C:950:SER:HB3	1.78	0.49
1:A:399:ALA:HB3	1:A:402:GLN:HG3	1.94	0.49
1:A:950:SER:HB3	1:C:558:ASP:H	1.78	0.49
1:B:552:PHE:HD1	1:B:563:VAL:HG22	1.78	0.49
1:C:399:ALA:HB3	1:C:402:GLN:HG3	1.94	0.49
1:A:966:ARG:HA	1:C:378:LEU:HD11	1.95	0.48
1:B:399:ALA:HB3	1:B:402:GLN:HG3	1.94	0.48
1:B:663:THR:HG22	1:B:673:LYS:HG2	1.94	0.48
1:C:960:LEU:C	1:C:962:ASP:H	2.21	0.48
1:C:552:PHE:HD1	1:C:563:VAL:HG22	1.78	0.48
1:A:663:THR:HG22	1:A:673:LYS:HG2	1.94	0.48
1:B:1110:ASP:OD1	1:B:1110:ASP:N	2.47	0.48
1:B:268:ASP:OD1	1:B:268:ASP:N	2.40	0.48
1:B:960:LEU:C	1:B:962:ASP:H	2.22	0.48
1:A:1110:ASP:N	1:A:1110:ASP:OD1	2.47	0.48
1:C:204:ILE:CG1	1:C:211:PRO:HG3	2.43	0.48
1:B:204:ILE:CG1	1:B:211:PRO:HG3	2.44	0.48
1:B:729:SER:C	1:B:731:GLU:H	2.21	0.48
1:A:558:ASP:H	1:B:950:SER:HB3	1.79	0.47
1:C:34:PHE:HE2	1:C:69:ARG:HD3	1.79	0.47
1:A:378:LEU:HD11	1:B:966:ARG:HA	1.96	0.47
1:A:552:PHE:HD1	1:A:563:VAL:HG22	1.78	0.47
1:B:690:TYR:CE1	1:C:880:PRO:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:721:CYS:O	1:C:725:ILE:HG12	2.15	0.47
1:A:364:THR:HG23	1:A:423:ALA:HB3	1.96	0.47
1:A:729:SER:C	1:A:731:GLU:H	2.21	0.47
1:A:42:TYR:OH	1:A:59:HIS:O	2.24	0.47
1:B:34:PHE:HE2	1:B:69:ARG:HD3	1.80	0.47
2:T:1:NAG:H4	2:T:2:NAG:H2	1.71	0.47
1:A:34:PHE:HE2	1:A:69:ARG:HD3	1.79	0.47
1:A:739:TYR:OH	1:A:981:THR:OG1	2.31	0.47
1:B:27:THR:OG1	1:B:75:LEU:O	2.27	0.47
1:B:364:THR:HG23	1:B:423:ALA:HB3	1.95	0.47
1:A:490:ILE:HD11	1:C:490:ILE:HB	1.96	0.47
1:A:721:CYS:O	1:A:725:ILE:HG12	2.14	0.47
1:B:721:CYS:O	1:B:725:ILE:HG12	2.15	0.47
1:B:741:SER:O	1:B:741:SER:OG	2.27	0.47
1:C:364:THR:HG23	1:C:423:ALA:HB3	1.96	0.47
1:B:586:THR:HB	1:B:595:VAL:HG12	1.97	0.47
1:A:880:PRO:HA	1:C:690:TYR:CE1	2.49	0.47
1:B:753:ILE:O	1:B:757:GLN:HG2	2.15	0.47
1:C:729:SER:C	1:C:731:GLU:H	2.22	0.47
1:A:880:PRO:HA	1:C:690:TYR:HE1	1.81	0.46
1:A:960:LEU:C	1:A:962:ASP:H	2.21	0.46
1:C:1110:ASP:OD1	1:C:1110:ASP:N	2.47	0.46
1:A:690:TYR:CE1	1:B:880:PRO:HA	2.51	0.46
1:B:490:ILE:HB	1:C:490:ILE:HD11	1.97	0.46
1:C:586:THR:HB	1:C:595:VAL:HG12	1.97	0.46
1:B:352:ASP:OD1	1:B:352:ASP:N	2.49	0.46
1:A:490:ILE:HB	1:B:490:ILE:HD11	1.97	0.46
1:A:960:LEU:H	1:A:960:LEU:HD23	1.81	0.46
1:C:1073:PRO:HG3	1:C:1078:PHE:CE2	2.51	0.46
1:B:127:ARG:HE	1:B:127:ARG:HB3	1.53	0.46
1:B:1073:PRO:HG3	1:B:1078:PHE:CE2	2.51	0.46
1:A:204:ILE:CG1	1:A:211:PRO:HG3	2.43	0.46
1:A:692:ASN:HA	1:B:880:PRO:HB3	1.98	0.46
1:A:1106:SER:OG	1:B:897:ASN:ND2	2.49	0.46
1:B:690:TYR:HE1	1:C:880:PRO:HA	1.80	0.46
1:A:542:SER:OG	1:A:571:ILE:O	2.24	0.46
1:B:445:ARG:NH2	4:Y:1:NAG:O7	2.43	0.46
1:B:378:LEU:HD11	1:C:966:ARG:HA	1.96	0.46
1:A:880:PRO:HB3	1:C:692:ASN:HA	1.97	0.46
1:C:445:ARG:NH2	4:G:1:NAG:O7	2.43	0.46
1:A:944:THR:HA	1:A:947:LYS:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:GLY:C	1:A:817:MET:H	2.25	0.45
1:C:142:LEU:HD12	1:C:144:SER:HB2	1.98	0.45
1:A:586:THR:HB	1:A:595:VAL:HG12	1.97	0.45
1:A:753:ILE:O	1:A:757:GLN:HG2	2.16	0.45
1:A:811:LEU:HG	1:A:813:ASP:H	1.81	0.45
1:A:1073:PRO:HG3	1:A:1078:PHE:CE2	2.51	0.45
1:B:142:LEU:HD12	1:B:144:SER:HB2	1.98	0.45
1:B:692:ASN:HA	1:C:880:PRO:HB3	1.97	0.45
1:B:811:LEU:HG	1:B:813:ASP:H	1.81	0.45
1:B:944:THR:HA	1:B:947:LYS:HG2	1.98	0.45
1:B:1106:SER:OG	1:C:897:ASN:ND2	2.50	0.45
1:C:811:LEU:HG	1:C:813:ASP:H	1.81	0.45
1:A:961:ASN:O	1:A:965:SER:OG	2.31	0.45
1:C:815:GLY:C	1:C:817:MET:H	2.25	0.45
1:B:1072:PHE:CE2	1:C:897:ASN:HA	2.51	0.45
1:C:753:ILE:O	1:C:757:GLN:HG2	2.16	0.45
1:A:142:LEU:HD12	1:A:144:SER:HB2	1.98	0.45
1:A:897:ASN:ND2	1:C:1106:SER:OG	2.50	0.45
1:B:297:ASP:OD1	1:B:297:ASP:N	2.39	0.45
1:B:815:GLY:C	1:B:817:MET:H	2.25	0.45
1:B:960:LEU:HD23	1:B:960:LEU:H	1.81	0.45
1:A:690:TYR:HE1	1:B:880:PRO:HA	1.82	0.45
1:B:379:CYS:HA	1:B:512:CYS:CB	2.40	0.45
1:C:95:LYS:NZ	1:C:250:ALA:O	2.50	0.45
1:C:123:ASN:ND2	2:Z:1:NAG:H5	2.32	0.45
1:C:944:THR:HA	1:C:947:LYS:HG2	1.98	0.45
2:c:1:NAG:H4	2:c:2:NAG:H2	1.71	0.45
1:C:567:LYS:O	1:C:568:THR:C	2.60	0.45
1:C:1055:GLU:N	1:C:1055:GLU:OE1	2.50	0.45
1:A:104:PHE:HB2	1:A:115:VAL:HG13	1.99	0.45
1:B:853:ILE:O	1:B:857:THR:HG23	2.17	0.45
1:B:1055:GLU:N	1:B:1055:GLU:OE1	2.50	0.45
1:C:104:PHE:HB2	1:C:115:VAL:HG13	1.99	0.45
1:A:836:GLN:HG2	1:A:946:VAL:HG21	2.00	0.44
1:A:1055:GLU:OE1	1:A:1055:GLU:N	2.50	0.44
1:C:836:GLN:HG2	1:C:946:VAL:HG21	2.00	0.44
1:C:960:LEU:HD23	1:C:960:LEU:H	1.81	0.44
1:A:123:ASN:ND2	2:H:1:NAG:H5	2.32	0.44
1:B:42:TYR:OH	1:B:59:HIS:O	2.24	0.44
1:A:95:LYS:NZ	1:A:250:ALA:O	2.50	0.44
1:A:897:ASN:HA	1:C:1072:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1072:PHE:CE2	1:B:897:ASN:HA	2.52	0.44
1:A:853:ILE:O	1:A:857:THR:HG23	2.17	0.44
1:B:870:THR:HG21	1:B:877:LEU:HB2	2.00	0.44
5:C:1301:EIC:H61	5:C:1301:EIC:H91	1.66	0.44
1:B:123:ASN:ND2	2:Q:1:NAG:H5	2.32	0.44
1:C:522:LYS:HD2	1:C:541:PRO:HD3	2.00	0.44
1:A:710:MET:HE2	1:A:710:MET:HB3	1.77	0.44
1:B:95:LYS:NZ	1:B:250:ALA:O	2.50	0.44
1:B:210:LEU:O	1:B:211:PRO:C	2.61	0.44
1:A:352:ASP:OD1	1:A:352:ASP:N	2.49	0.44
1:B:836:GLN:HG2	1:B:946:VAL:HG21	2.00	0.44
1:B:158:PHE:HD1	1:B:158:PHE:HA	1.70	0.43
1:C:853:ILE:O	1:C:857:THR:HG23	2.17	0.43
1:C:210:LEU:O	1:C:211:PRO:C	2.61	0.43
1:C:379:CYS:HA	1:C:512:CYS:CB	2.40	0.43
1:B:104:PHE:HB2	1:B:115:VAL:HG13	1.99	0.43
1:B:921:LEU:HD23	1:B:921:LEU:HA	1.87	0.43
1:C:870:THR:HG21	1:C:877:LEU:HB2	2.00	0.43
1:A:956:ILE:HD11	1:A:963:ILE:HG23	2.00	0.43
1:C:179:ASN:OD1	1:C:179:ASN:N	2.51	0.43
1:A:160:CYS:C	1:A:161:THR:HG23	2.44	0.43
1:A:210:LEU:O	1:A:211:PRO:C	2.61	0.43
1:B:160:CYS:C	1:B:161:THR:HG23	2.44	0.43
1:B:956:ILE:HD11	1:B:963:ILE:HG23	2.00	0.43
1:C:46:ASP:N	1:C:46:ASP:OD1	2.52	0.43
1:C:440:LYS:NZ	1:C:481:ASP:OD2	2.51	0.43
1:B:522:LYS:HD2	1:B:541:PRO:HD3	2.00	0.43
1:A:566:PRO:HB2	1:A:567:LYS:H	1.69	0.43
5:A:1301:EIC:H61	5:A:1301:EIC:H91	1.66	0.43
1:B:775:PRO:O	1:B:776:THR:HG22	2.19	0.43
1:A:357:TYR:HE1	5:A:1301:EIC:H21	1.84	0.43
1:A:870:THR:HG21	1:A:877:LEU:HB2	2.00	0.43
5:A:1301:EIC:H141	5:A:1301:EIC:H112	1.74	0.43
1:A:179:ASN:OD1	1:A:179:ASN:N	2.51	0.43
1:B:567:LYS:O	1:B:568:THR:C	2.60	0.43
1:C:889:PHE:O	1:C:892:ILE:HG22	2.19	0.43
1:A:440:LYS:NZ	1:A:481:ASP:OD2	2.51	0.42
1:A:522:LYS:HD2	1:A:541:PRO:HD3	2.00	0.42
1:B:440:LYS:NZ	1:B:481:ASP:OD2	2.51	0.42
1:B:710:MET:HE2	1:B:710:MET:HB3	1.77	0.42
1:C:956:ILE:HD11	1:C:963:ILE:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:716:LYS:NZ	1:A:758:ASP:OD2	2.52	0.42
1:B:410:ASN:ND2	1:B:441:TYR:HB2	2.35	0.42
1:C:410:ASN:ND2	1:C:441:TYR:HB2	2.35	0.42
1:A:775:PRO:O	1:A:776:THR:HG22	2.19	0.42
1:B:21:LEU:HD12	1:B:21:LEU:HA	1.84	0.42
1:B:889:PHE:O	1:B:892:ILE:HG22	2.19	0.42
1:C:775:PRO:O	1:C:776:THR:HG22	2.19	0.42
1:C:921:LEU:HD23	1:C:921:LEU:HA	1.87	0.42
1:C:315:VAL:HG22	1:C:529:ASN:HB3	2.02	0.42
1:B:315:VAL:HG22	1:B:529:ASN:HB3	2.02	0.42
1:C:566:PRO:HB2	1:C:567:LYS:H	1.69	0.42
1:A:445:ARG:NH2	4:P:1:NAG:O7	2.43	0.42
1:B:357:TYR:HE1	5:B:1301:EIC:H21	1.84	0.42
1:B:517:SER:CB	1:B:567:LYS:HZ2	2.32	0.42
1:A:410:ASN:ND2	1:A:441:TYR:HB2	2.35	0.42
1:A:889:PHE:O	1:A:892:ILE:HG22	2.19	0.42
1:C:78:ASP:HB3	1:C:80:PRO:HD3	2.02	0.42
2:K:1:NAG:H4	2:K:2:NAG:H2	1.71	0.42
1:A:95:LYS:H	1:A:95:LYS:HG3	1.64	0.42
1:A:904:LYS:HE2	1:A:904:LYS:HB2	1.89	0.42
1:B:78:ASP:HB3	1:B:80:PRO:HD3	2.02	0.42
1:B:335:PHE:HA	1:B:336:PRO:HD3	1.94	0.42
1:B:962:ASP:O	1:B:966:ARG:HG3	2.20	0.42
1:C:739:TYR:HH	1:C:981:THR:HG1	1.63	0.42
1:C:833:ILE:O	1:C:837:LYS:HG3	2.20	0.42
1:A:92:ALA:HA	1:A:253:TYR:HA	2.02	0.42
1:C:92:ALA:HA	1:C:253:TYR:HA	2.02	0.42
1:C:393:ASP:OD1	1:C:393:ASP:N	2.53	0.42
1:C:716:LYS:NZ	1:C:758:ASP:OD2	2.52	0.42
1:B:179:ASN:OD1	1:B:179:ASN:N	2.51	0.41
1:C:357:TYR:HE1	5:C:1301:EIC:H21	1.84	0.41
1:C:962:ASP:O	1:C:966:ARG:HG3	2.20	0.41
1:B:1066:HIS:ND1	1:B:1067:GLU:HG2	2.35	0.41
1:C:160:CYS:C	1:C:161:THR:HG23	2.44	0.41
1:B:92:ALA:HA	1:B:253:TYR:HA	2.02	0.41
1:C:1066:HIS:ND1	1:C:1067:GLU:HG2	2.35	0.41
1:A:379:CYS:HA	1:A:512:CYS:CB	2.40	0.41
1:A:393:ASP:OD1	1:A:393:ASP:N	2.53	0.41
1:A:808:LYS:NZ	1:A:924:THR:O	2.44	0.41
1:A:833:ILE:O	1:A:837:LYS:HG3	2.20	0.41
1:A:956:ILE:HD12	1:A:966:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:969:LYS:HB3	1:A:969:LYS:HE3	1.81	0.41
1:A:975:GLN:H	1:A:975:GLN:HG2	1.58	0.41
1:B:833:ILE:O	1:B:837:LYS:HG3	2.20	0.41
1:C:771:MET:HE3	1:C:771:MET:HB3	1.89	0.41
1:A:78:ASP:HB3	1:A:80:PRO:HD3	2.02	0.41
1:B:516:LEU:HD23	1:B:516:LEU:HA	1.85	0.41
1:B:566:PRO:HB2	1:B:567:LYS:H	1.68	0.41
1:C:568:THR:O	1:C:568:THR:OG1	2.28	0.41
1:C:739:TYR:OH	1:C:981:THR:OG1	2.31	0.41
1:B:46:ASP:OD1	1:B:46:ASP:N	2.52	0.41
1:B:808:LYS:NZ	1:B:924:THR:O	2.44	0.41
1:C:587:PRO:HD3	1:C:675:ILE:HD11	2.02	0.41
1:A:46:ASP:OD1	1:A:46:ASP:N	2.52	0.41
1:A:268:ASP:OD1	1:A:268:ASP:N	2.40	0.41
5:B:1301:EIC:H112	5:B:1301:EIC:H141	1.74	0.41
1:A:962:ASP:O	1:A:966:ARG:HG3	2.20	0.41
1:A:1066:HIS:ND1	1:A:1067:GLU:HG2	2.35	0.41
1:B:204:ILE:HD11	1:B:206:ALA:HB3	2.03	0.41
1:B:393:ASP:OD1	1:B:393:ASP:N	2.53	0.41
1:B:956:ILE:HD12	1:B:966:ARG:NH2	2.36	0.41
1:B:28:PRO:HA	1:B:29:PRO:HD3	1.97	0.41
1:B:568:THR:O	1:B:568:THR:OG1	2.28	0.41
1:C:357:TYR:CE1	5:C:1301:EIC:H21	2.56	0.41
1:A:39:ARG:NH2	1:A:202:GLN:OE1	2.50	0.41
1:A:888:ARG:NH1	1:A:1032:LEU:O	2.46	0.41
1:A:315:VAL:HG22	1:A:529:ASN:HB3	2.02	0.40
1:A:587:PRO:HD3	1:A:675:ILE:HD11	2.02	0.40
1:A:648:GLU:O	1:A:678:TYR:OH	2.28	0.40
1:A:921:LEU:HD23	1:A:921:LEU:HA	1.87	0.40
1:B:587:PRO:HD3	1:B:675:ILE:HD11	2.02	0.40
1:C:804:LEU:O	1:C:808:LYS:HG2	2.21	0.40
1:C:949:LEU:HD12	1:C:949:LEU:HA	1.92	0.40
1:A:804:LEU:O	1:A:808:LYS:HG2	2.21	0.40
1:B:567:LYS:C	1:B:568:THR:HG22	2.47	0.40
1:B:716:LYS:NZ	1:B:758:ASP:OD2	2.52	0.40
1:C:95:LYS:H	1:C:95:LYS:HG3	1.64	0.40
1:B:292:LYS:HE2	1:B:292:LYS:HB3	1.92	0.40
1:B:904:LYS:HB2	1:B:904:LYS:HE2	1.89	0.40
5:B:1301:EIC:H91	5:B:1301:EIC:H61	1.66	0.40
1:C:204:ILE:HD11	1:C:206:ALA:HB3	2.03	0.40
1:C:297:ASP:OD1	1:C:297:ASP:N	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:O	1:A:568:THR:C	2.60	0.40
1:B:804:LEU:O	1:B:808:LYS:HG2	2.21	0.40
1:C:315:VAL:HG11	1:C:515:LYS:HG2	2.03	0.40
1:C:956:ILE:HD12	1:C:966:ARG:NH2	2.36	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	1058/1213 (87%)	1008 (95%)	50 (5%)	0	100	100
1	B	1058/1213 (87%)	1008 (95%)	50 (5%)	0	100	100
1	C	1058/1213 (87%)	1009 (95%)	49 (5%)	0	100	100
All	All	3174/3639 (87%)	3025 (95%)	149 (5%)	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	924/1056 (88%)	875 (95%)	49 (5%)	20	47
1	B	924/1056 (88%)	874 (95%)	50 (5%)	20	47
1	C	924/1056 (88%)	873 (94%)	51 (6%)	19	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2772/3168 (88%)	2622 (95%)	150 (5%)	21	47

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	PHE
1	A	25	ASP
1	A	27	THR
1	A	32	THR
1	A	72	THR
1	A	73	PHE
1	A	95	LYS
1	A	115	VAL
1	A	120	ASN
1	A	138	PHE
1	A	158	PHE
1	A	173	LEU
1	A	204	ILE
1	A	225	LEU
1	A	232	PHE
1	A	297	ASP
1	A	300	ILE
1	A	335	PHE
1	A	337	SER
1	A	338	VAL
1	A	363	SER
1	A	364	THR
1	A	368	TYR
1	A	386	ASP
1	A	405	VAL
1	A	413	LEU
1	A	420	CYS
1	A	473	PHE
1	A	492	TYR
1	A	504	LEU
1	A	519	ASP
1	A	536	THR
1	A	582	VAL
1	A	586	THR
1	A	657	ILE
1	A	730	THR
1	A	732	CYS

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Mol	Chain	Res	Type
1	A	770	GLN
1	A	793	LEU
1	A	877	LEU
1	A	892	ILE
1	A	926	THR
1	A	952	ASN
1	A	959	VAL
1	A	975	GLN
1	A	1081	ASN
1	A	1111	VAL
1	A	1115	ILE
1	A	1119	THR
1	B	23	PHE
1	B	25	ASP
1	B	27	THR
1	B	32	THR
1	B	72	THR
1	B	73	PHE
1	B	95	LYS
1	B	115	VAL
1	B	120	ASN
1	B	138	PHE
1	B	158	PHE
1	B	173	LEU
1	B	204	ILE
1	B	225	LEU
1	B	232	PHE
1	B	297	ASP
1	B	300	ILE
1	B	335	PHE
1	B	337	SER
1	B	338	VAL
1	B	363	SER
1	B	364	THR
1	B	368	TYR
1	B	386	ASP
1	B	387	SER
1	B	405	VAL
1	B	413	LEU
1	B	420	CYS
1	B	473	PHE
1	B	492	TYR

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Mol	Chain	Res	Type
1	B	504	LEU
1	B	519	ASP
1	B	536	THR
1	B	582	VAL
1	B	586	THR
1	B	657	ILE
1	B	730	THR
1	B	732	CYS
1	B	770	GLN
1	B	793	LEU
1	B	877	LEU
1	B	892	ILE
1	B	926	THR
1	B	952	ASN
1	B	959	VAL
1	B	975	GLN
1	B	1081	ASN
1	B	1111	VAL
1	B	1115	ILE
1	B	1119	THR
1	C	23	PHE
1	C	25	ASP
1	C	27	THR
1	C	32	THR
1	C	72	THR
1	C	73	PHE
1	C	95	LYS
1	C	115	VAL
1	C	120	ASN
1	C	138	PHE
1	C	158	PHE
1	C	173	LEU
1	C	204	ILE
1	C	225	LEU
1	C	232	PHE
1	C	297	ASP
1	C	300	ILE
1	C	335	PHE
1	C	337	SER
1	C	338	VAL
1	C	363	SER
1	C	364	THR

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Mol	Chain	Res	Type
1	C	368	TYR
1	C	386	ASP
1	C	387	SER
1	C	405	VAL
1	C	413	LEU
1	C	420	CYS
1	C	473	PHE
1	C	492	TYR
1	C	504	LEU
1	C	519	ASP
1	C	536	THR
1	C	582	VAL
1	C	586	THR
1	C	657	ILE
1	C	730	THR
1	C	732	CYS
1	C	739	TYR
1	C	770	GLN
1	C	793	LEU
1	C	877	LEU
1	C	892	ILE
1	C	926	THR
1	C	952	ASN
1	C	959	VAL
1	C	975	GLN
1	C	1081	ASN
1	C	1111	VAL
1	C	1115	ILE
1	C	1119	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	HIS
1	A	550	GLN
1	A	628	ASN
1	A	633	GLN
1	A	787	GLN
1	A	819	GLN
1	A	896	GLN
1	A	897	ASN
1	A	937	GLN

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Mol	Chain	Res	Type
1	A	961	ASN
1	A	1037	GLN
1	B	348	ASN
1	B	550	GLN
1	B	633	GLN
1	B	819	GLN
1	B	896	GLN
1	B	897	ASN
1	B	937	GLN
1	B	961	ASN
1	B	1037	GLN
1	C	348	ASN
1	C	550	GLN
1	C	628	ASN
1	C	633	GLN
1	C	787	GLN
1	C	819	GLN
1	C	896	GLN
1	C	897	ASN
1	C	937	GLN
1	C	961	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

63 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	D	1	2,1	14,14,15	0.72	0	17,19,21	0.89	0
2	NAG	D	2	2	14,14,15	0.73	0	17,19,21	0.83	0
3	NAG	E	1	3,1	14,14,15	0.72	0	17,19,21	0.82	0
3	NAG	E	2	3	14,14,15	0.69	0	17,19,21	1.16	1 (5%)
3	BMA	E	3	3	11,11,12	0.86	0	15,15,17	2.09	3 (20%)
2	NAG	F	1	2,1	14,14,15	0.72	0	17,19,21	0.95	0
2	NAG	F	2	2	14,14,15	0.73	0	17,19,21	0.88	0
4	NAG	G	1	1,4	14,14,15	0.84	0	17,19,21	1.73	3 (17%)
4	NAG	G	2	4	14,14,15	0.71	0	17,19,21	2.38	7 (41%)
4	BMA	G	3	4	11,11,12	0.87	0	15,15,17	1.89	4 (26%)
4	MAN	G	4	4	11,11,12	0.81	1 (9%)	15,15,17	1.21	1 (6%)
2	NAG	H	1	2,1	14,14,15	0.74	0	17,19,21	1.16	1 (5%)
2	NAG	H	2	2	14,14,15	0.71	0	17,19,21	0.87	0
2	NAG	I	1	2,1	14,14,15	0.72	0	17,19,21	0.83	0
2	NAG	I	2	2	14,14,15	0.71	0	17,19,21	0.81	0
2	NAG	J	1	2,1	14,14,15	0.79	0	17,19,21	1.33	2 (11%)
2	NAG	J	2	2	14,14,15	0.72	0	17,19,21	0.91	1 (5%)
2	NAG	K	1	2,1	14,14,15	0.75	0	17,19,21	1.31	2 (11%)
2	NAG	K	2	2	14,14,15	0.79	0	17,19,21	0.91	0
2	NAG	L	1	2,1	14,14,15	0.74	0	17,19,21	1.55	3 (17%)
2	NAG	L	2	2	14,14,15	0.80	0	17,19,21	1.15	2 (11%)
2	NAG	M	1	2,1	14,14,15	0.73	0	17,19,21	0.90	0
2	NAG	M	2	2	14,14,15	0.73	0	17,19,21	0.84	0
3	NAG	N	1	3,1	14,14,15	0.73	0	17,19,21	0.83	0
3	NAG	N	2	3	14,14,15	0.70	0	17,19,21	1.15	1 (5%)
3	BMA	N	3	3	11,11,12	0.85	0	15,15,17	2.09	3 (20%)
2	NAG	O	1	2,1	14,14,15	0.71	0	17,19,21	0.96	0
2	NAG	O	2	2	14,14,15	0.72	0	17,19,21	0.88	0
4	NAG	P	1	1,4	14,14,15	0.84	0	17,19,21	1.74	3 (17%)
4	NAG	P	2	4	14,14,15	0.73	0	17,19,21	2.38	7 (41%)
4	BMA	P	3	4	11,11,12	0.86	0	15,15,17	1.89	4 (26%)
4	MAN	P	4	4	11,11,12	0.80	1 (9%)	15,15,17	1.22	1 (6%)
2	NAG	Q	1	2,1	14,14,15	0.74	0	17,19,21	1.16	1 (5%)
2	NAG	Q	2	2	14,14,15	0.71	0	17,19,21	0.88	0
2	NAG	R	1	2,1	14,14,15	0.71	0	17,19,21	0.84	0
2	NAG	R	2	2	14,14,15	0.71	0	17,19,21	0.81	0
2	NAG	S	1	2,1	14,14,15	0.79	0	17,19,21	1.33	2 (11%)
2	NAG	S	2	2	14,14,15	0.73	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
2	NAG	T	1	2,1	14,14,15	0.74	0	17,19,21	1.31	2 (11%)
2	NAG	T	2	2	14,14,15	0.79	0	17,19,21	0.91	0
2	NAG	U	1	2,1	14,14,15	0.74	0	17,19,21	1.54	3 (17%)
2	NAG	U	2	2	14,14,15	0.80	0	17,19,21	1.15	2 (11%)
2	NAG	V	1	2,1	14,14,15	0.72	0	17,19,21	0.89	0
2	NAG	V	2	2	14,14,15	0.73	0	17,19,21	0.83	0
3	NAG	W	1	3,1	14,14,15	0.72	0	17,19,21	0.82	0
3	NAG	W	2	3	14,14,15	0.69	0	17,19,21	1.16	1 (5%)
3	BMA	W	3	3	11,11,12	0.87	0	15,15,17	2.09	3 (20%)
2	NAG	X	1	2,1	14,14,15	0.72	0	17,19,21	0.96	0
2	NAG	X	2	2	14,14,15	0.74	0	17,19,21	0.88	0
4	NAG	Y	1	1,4	14,14,15	0.83	0	17,19,21	1.73	3 (17%)
4	NAG	Y	2	4	14,14,15	0.72	0	17,19,21	2.38	7 (41%)
4	BMA	Y	3	4	11,11,12	0.87	0	15,15,17	1.89	4 (26%)
4	MAN	Y	4	4	11,11,12	0.81	1 (9%)	15,15,17	1.20	1 (6%)
2	NAG	Z	1	2,1	14,14,15	0.73	0	17,19,21	1.16	1 (5%)
2	NAG	Z	2	2	14,14,15	0.71	0	17,19,21	0.87	0
2	NAG	a	1	2,1	14,14,15	0.72	0	17,19,21	0.83	0
2	NAG	a	2	2	14,14,15	0.72	0	17,19,21	0.81	0
2	NAG	b	1	2,1	14,14,15	0.78	0	17,19,21	1.33	2 (11%)
2	NAG	b	2	2	14,14,15	0.73	0	17,19,21	0.91	1 (5%)
2	NAG	c	1	2,1	14,14,15	0.76	0	17,19,21	1.31	2 (11%)
2	NAG	c	2	2	14,14,15	0.80	0	17,19,21	0.91	0
2	NAG	d	1	2,1	14,14,15	0.73	0	17,19,21	1.55	3 (17%)
2	NAG	d	2	2	14,14,15	0.79	0	17,19,21	1.15	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Y	4	MAN	O5-C1	-2.06	1.40	1.43
4	G	4	MAN	O5-C1	-2.05	1.40	1.43
4	P	4	MAN	O5-C1	-2.03	1.40	1.43

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	3	BMA	C1-O5-C5	6.25	120.66	112.19
3	W	3	BMA	C1-O5-C5	6.24	120.65	112.19
3	E	3	BMA	C1-O5-C5	6.24	120.65	112.19
4	P	1	NAG	C4-C3-C2	5.15	118.57	111.02
4	G	1	NAG	C4-C3-C2	5.15	118.57	111.02
4	Y	1	NAG	C4-C3-C2	5.15	118.56	111.02
4	Y	2	NAG	C4-C3-C2	4.90	118.20	111.02
4	P	2	NAG	C4-C3-C2	4.88	118.17	111.02
4	G	2	NAG	C4-C3-C2	4.88	118.17	111.02
4	G	3	BMA	C1-O5-C5	4.56	118.37	112.19
4	P	3	BMA	C1-O5-C5	4.56	118.37	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	3	BMA	C1-O5-C5	4.55	118.35	112.19
4	Y	2	NAG	O5-C1-C2	-4.46	104.24	111.29
4	G	2	NAG	O5-C1-C2	-4.45	104.26	111.29
4	P	2	NAG	O5-C1-C2	-4.45	104.27	111.29
4	P	2	NAG	C2-N2-C7	4.23	128.92	122.90
4	Y	2	NAG	C2-N2-C7	4.22	128.91	122.90
4	G	2	NAG	C2-N2-C7	4.22	128.91	122.90
2	c	1	NAG	O4-C4-C3	-3.28	102.77	110.35
2	K	1	NAG	O4-C4-C3	-3.28	102.78	110.35
2	T	1	NAG	O4-C4-C3	-3.26	102.80	110.35
4	P	4	MAN	C1-O5-C5	3.19	116.51	112.19
4	G	4	MAN	C1-O5-C5	3.17	116.49	112.19
4	Y	4	MAN	C1-O5-C5	3.13	116.44	112.19
2	J	1	NAG	O5-C1-C2	-3.13	106.35	111.29
2	S	1	NAG	O5-C1-C2	-3.12	106.36	111.29
2	b	1	NAG	O5-C1-C2	-3.12	106.36	111.29
2	d	1	NAG	C2-N2-C7	3.05	127.25	122.90
2	L	1	NAG	C2-N2-C7	3.04	127.24	122.90
2	U	1	NAG	C2-N2-C7	3.04	127.24	122.90
3	W	2	NAG	C2-N2-C7	3.02	127.21	122.90
3	E	2	NAG	C2-N2-C7	3.01	127.19	122.90
3	N	2	NAG	C2-N2-C7	2.99	127.17	122.90
4	P	2	NAG	O4-C4-C3	-2.97	103.48	110.35
2	Q	1	NAG	O5-C1-C2	-2.97	106.60	111.29
2	Z	1	NAG	O5-C1-C2	-2.97	106.60	111.29
4	P	2	NAG	C3-C4-C5	2.96	115.52	110.24
4	G	2	NAG	O4-C4-C3	-2.96	103.52	110.35
2	H	1	NAG	O5-C1-C2	-2.96	106.62	111.29
4	G	2	NAG	C3-C4-C5	2.95	115.50	110.24
4	Y	2	NAG	O4-C4-C3	-2.94	103.55	110.35
4	Y	2	NAG	C3-C4-C5	2.94	115.48	110.24
4	P	1	NAG	C2-N2-C7	2.93	127.07	122.90
4	G	1	NAG	C2-N2-C7	2.92	127.06	122.90
4	Y	1	NAG	C2-N2-C7	2.92	127.06	122.90
4	Y	3	BMA	O3-C3-C2	-2.90	104.44	109.99
4	G	3	BMA	O3-C3-C2	-2.89	104.46	109.99
4	P	3	BMA	O3-C3-C2	-2.88	104.48	109.99
2	U	1	NAG	O4-C4-C3	-2.87	103.72	110.35
2	L	1	NAG	O4-C4-C3	-2.87	103.72	110.35
2	d	1	NAG	O4-C4-C3	-2.86	103.73	110.35
4	G	1	NAG	O4-C4-C3	-2.79	103.90	110.35
4	Y	1	NAG	O4-C4-C3	-2.79	103.90	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	1	NAG	O4-C4-C3	-2.78	103.91	110.35
2	L	2	NAG	C2-N2-C7	2.71	126.77	122.90
2	U	2	NAG	C2-N2-C7	2.71	126.77	122.90
2	d	2	NAG	C2-N2-C7	2.71	126.75	122.90
4	G	2	NAG	C1-O5-C5	-2.69	108.55	112.19
4	Y	2	NAG	C1-O5-C5	-2.67	108.58	112.19
4	P	2	NAG	C1-O5-C5	-2.66	108.58	112.19
2	S	1	NAG	O4-C4-C3	-2.63	104.26	110.35
2	b	1	NAG	O4-C4-C3	-2.63	104.27	110.35
2	T	1	NAG	O5-C1-C2	-2.63	107.14	111.29
2	K	1	NAG	O5-C1-C2	-2.62	107.15	111.29
2	J	1	NAG	O4-C4-C3	-2.61	104.30	110.35
2	c	1	NAG	O5-C1-C2	-2.60	107.18	111.29
4	P	3	BMA	C2-C3-C4	2.58	115.36	110.89
4	G	3	BMA	C2-C3-C4	2.57	115.35	110.89
4	Y	3	BMA	C2-C3-C4	2.56	115.32	110.89
2	d	1	NAG	O5-C1-C2	-2.52	107.31	111.29
2	L	1	NAG	O5-C1-C2	-2.49	107.35	111.29
2	U	1	NAG	O5-C1-C2	-2.48	107.38	111.29
2	L	2	NAG	O5-C1-C2	-2.45	107.41	111.29
2	U	2	NAG	O5-C1-C2	-2.45	107.42	111.29
2	d	2	NAG	O5-C1-C2	-2.44	107.44	111.29
2	S	2	NAG	O5-C1-C2	-2.37	107.55	111.29
2	J	2	NAG	O5-C1-C2	-2.35	107.58	111.29
2	b	2	NAG	O5-C1-C2	-2.35	107.58	111.29
3	N	3	BMA	C3-C4-C5	2.24	114.24	110.24
3	W	3	BMA	C2-C3-C4	2.24	114.78	110.89
3	E	3	BMA	C2-C3-C4	2.24	114.77	110.89
3	N	3	BMA	C2-C3-C4	2.24	114.77	110.89
3	E	3	BMA	C3-C4-C5	2.23	114.22	110.24
3	W	3	BMA	C3-C4-C5	2.22	114.19	110.24
4	P	3	BMA	C3-C4-C5	2.18	114.13	110.24
4	G	3	BMA	C3-C4-C5	2.17	114.11	110.24
4	Y	3	BMA	C3-C4-C5	2.17	114.11	110.24
4	P	2	NAG	O7-C7-N2	2.03	125.69	121.95
4	G	2	NAG	O7-C7-N2	2.02	125.66	121.95
4	Y	2	NAG	O7-C7-N2	2.01	125.64	121.95

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	J	1	NAG	C8-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	K	1	NAG	C8-C7-N2-C2
2	K	1	NAG	O7-C7-N2-C2
2	L	2	NAG	C8-C7-N2-C2
2	L	2	NAG	O7-C7-N2-C2
2	M	1	NAG	C8-C7-N2-C2
2	M	1	NAG	O7-C7-N2-C2
2	O	1	NAG	C8-C7-N2-C2
2	O	1	NAG	O7-C7-N2-C2
2	Q	1	NAG	C8-C7-N2-C2
2	Q	1	NAG	O7-C7-N2-C2
2	Q	2	NAG	C8-C7-N2-C2
2	Q	2	NAG	O7-C7-N2-C2
2	S	1	NAG	C8-C7-N2-C2
2	S	1	NAG	O7-C7-N2-C2
2	T	1	NAG	C8-C7-N2-C2
2	T	1	NAG	O7-C7-N2-C2
2	U	2	NAG	C8-C7-N2-C2
2	U	2	NAG	O7-C7-N2-C2
2	V	1	NAG	C8-C7-N2-C2
2	V	1	NAG	O7-C7-N2-C2
2	X	1	NAG	C8-C7-N2-C2
2	X	1	NAG	O7-C7-N2-C2
2	Z	1	NAG	C8-C7-N2-C2
2	Z	1	NAG	O7-C7-N2-C2
2	Z	2	NAG	C8-C7-N2-C2
2	Z	2	NAG	O7-C7-N2-C2
2	b	1	NAG	C8-C7-N2-C2
2	b	1	NAG	O7-C7-N2-C2
2	c	1	NAG	C8-C7-N2-C2
2	c	1	NAG	O7-C7-N2-C2
2	d	2	NAG	C8-C7-N2-C2
2	d	2	NAG	O7-C7-N2-C2
2	J	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	S	1	NAG	O5-C5-C6-O6
2	b	1	NAG	O5-C5-C6-O6
4	G	4	MAN	C4-C5-C6-O6
4	P	4	MAN	C4-C5-C6-O6
4	Y	4	MAN	C4-C5-C6-O6
4	G	2	NAG	C1-C2-N2-C7
4	P	2	NAG	C1-C2-N2-C7
4	Y	2	NAG	C1-C2-N2-C7
2	H	2	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	Z	2	NAG	O5-C5-C6-O6
2	a	1	NAG	O5-C5-C6-O6
4	G	2	NAG	C3-C2-N2-C7
4	P	2	NAG	C3-C2-N2-C7
4	Y	2	NAG	C3-C2-N2-C7
2	L	1	NAG	C3-C2-N2-C7
2	U	1	NAG	C3-C2-N2-C7
2	d	1	NAG	C3-C2-N2-C7
4	G	4	MAN	O5-C5-C6-O6
4	P	4	MAN	O5-C5-C6-O6
4	Y	4	MAN	O5-C5-C6-O6
3	E	2	NAG	C3-C2-N2-C7
3	N	2	NAG	C3-C2-N2-C7
3	W	2	NAG	C3-C2-N2-C7

There are no ring outliers.

15 monomers are involved in 18 short contacts:

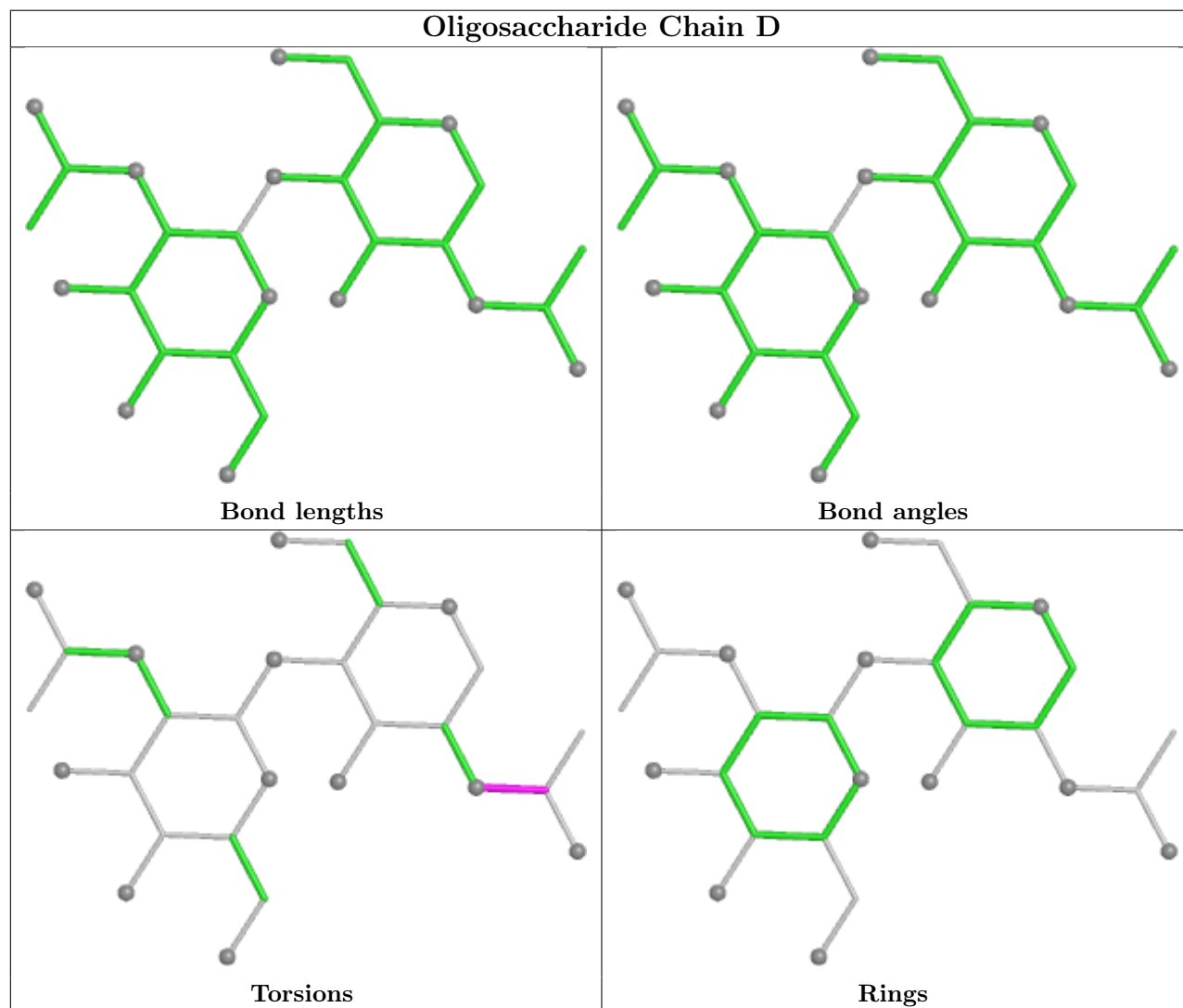
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	2	0
2	T	2	NAG	1	0
2	c	2	NAG	1	0
2	K	1	NAG	1	0
4	P	1	NAG	2	0
2	Q	1	NAG	2	0
2	c	1	NAG	1	0
2	T	1	NAG	1	0
2	K	2	NAG	1	0
2	H	1	NAG	2	0
3	N	1	NAG	1	0

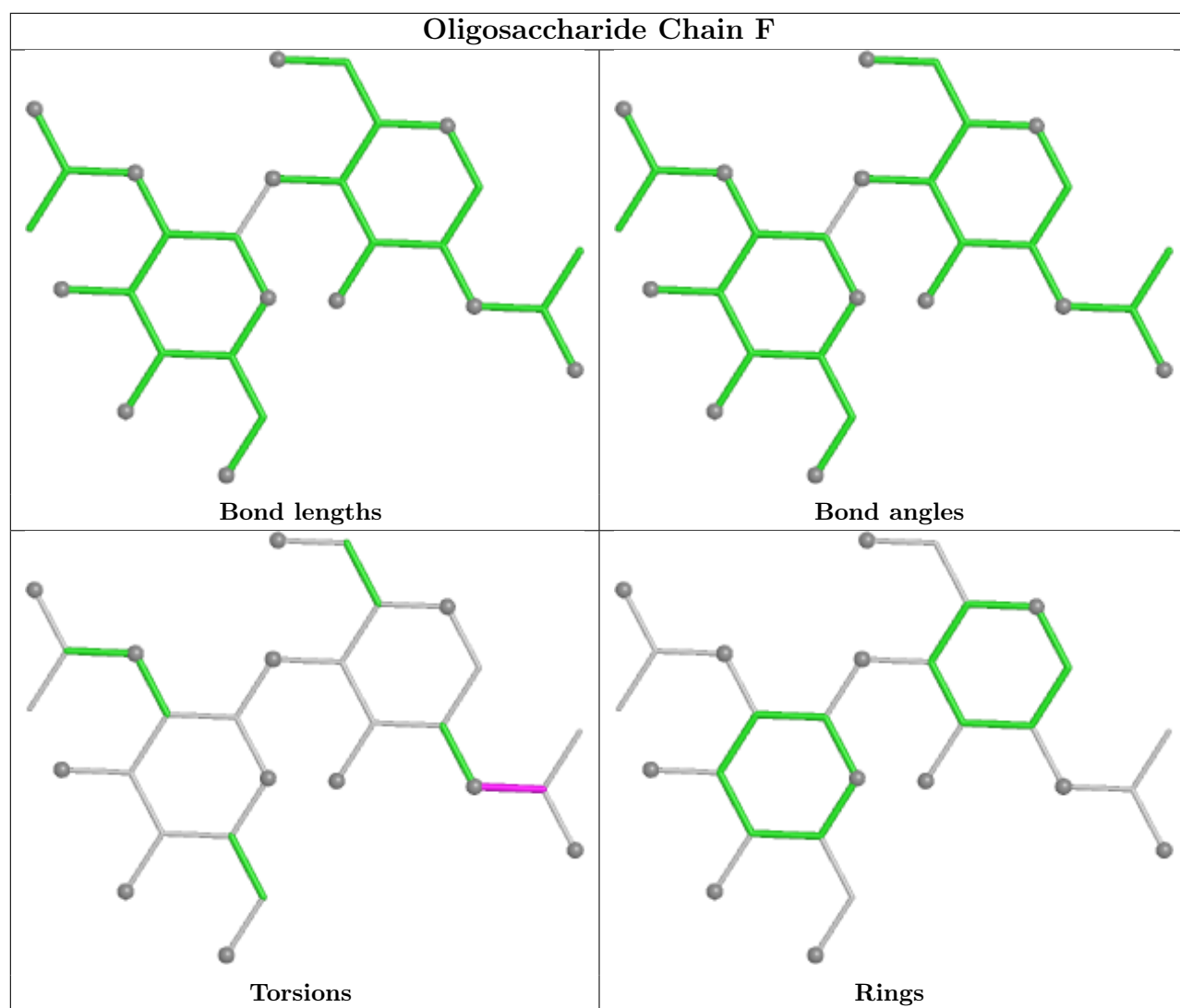
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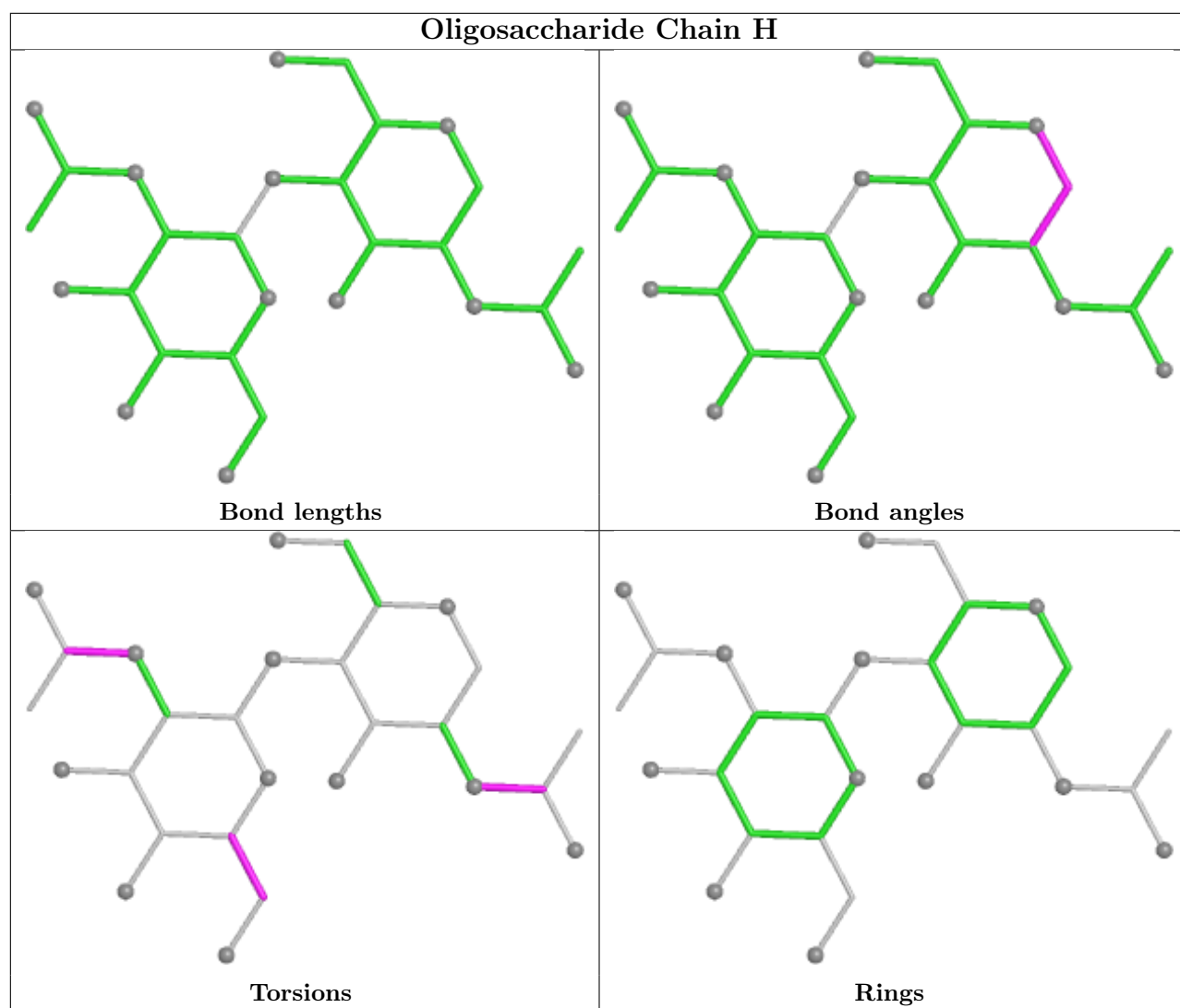
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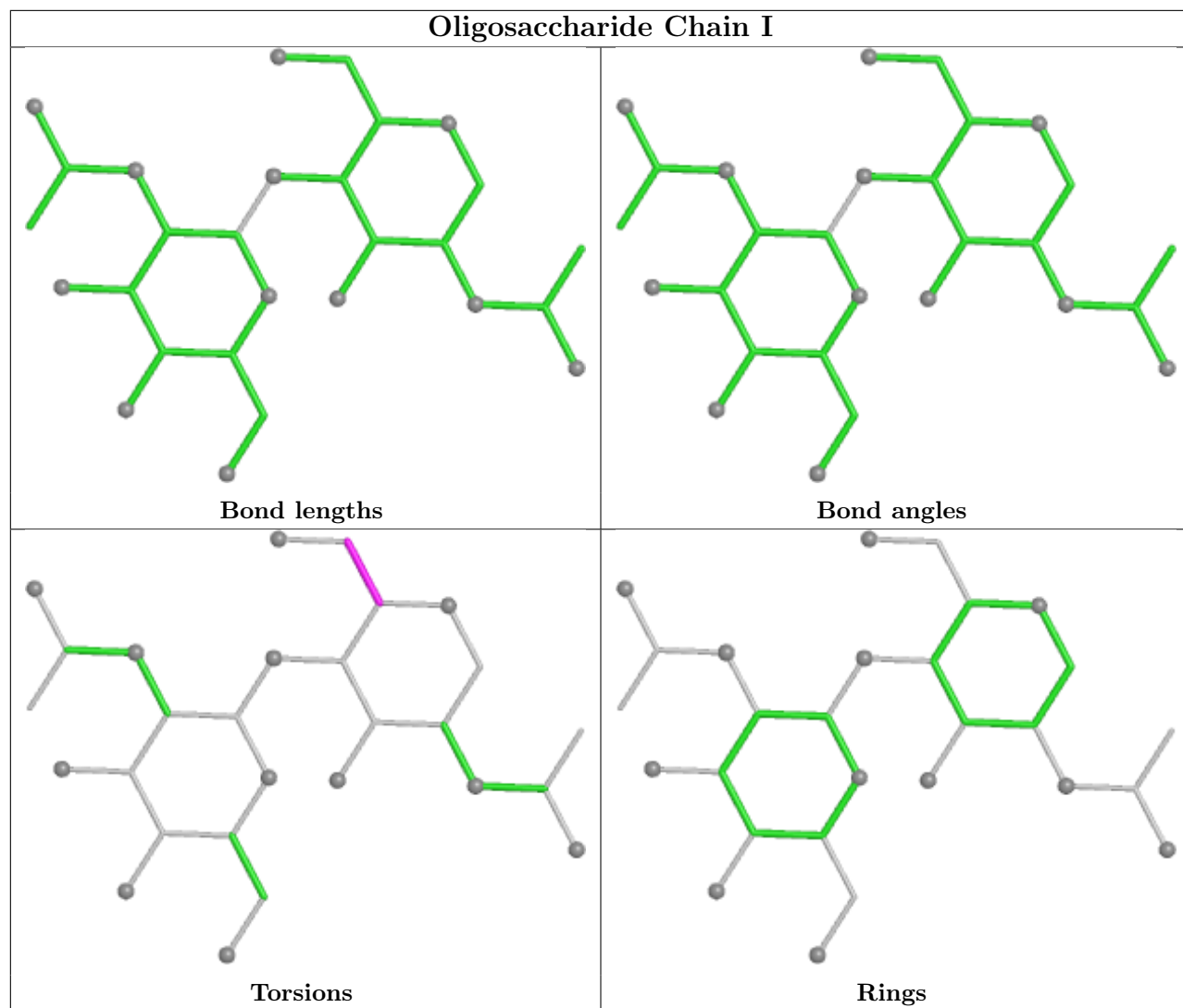
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1	NAG	1	0
4	Y	1	NAG	2	0
3	W	1	NAG	1	0
2	Z	1	NAG	2	0

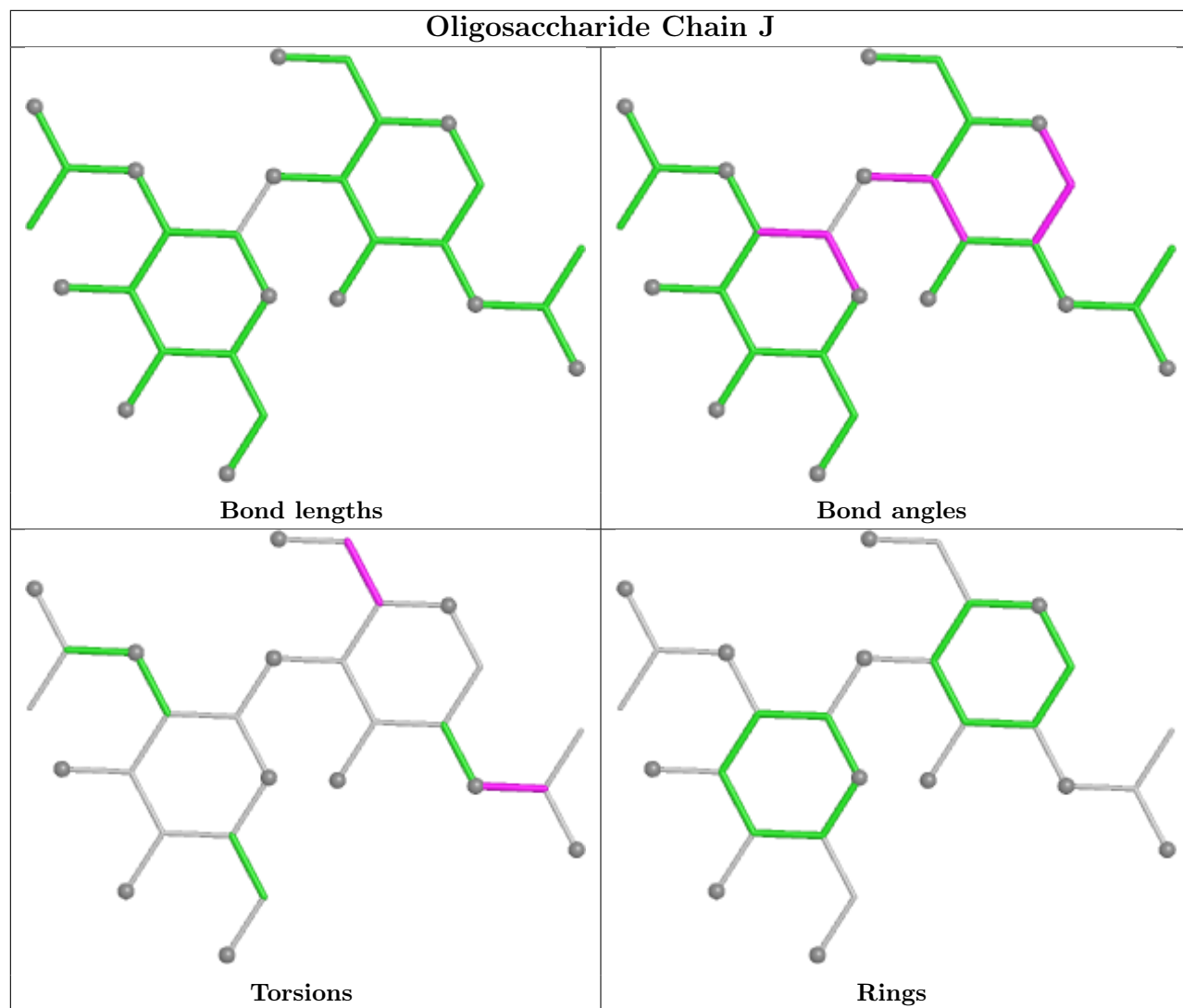
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

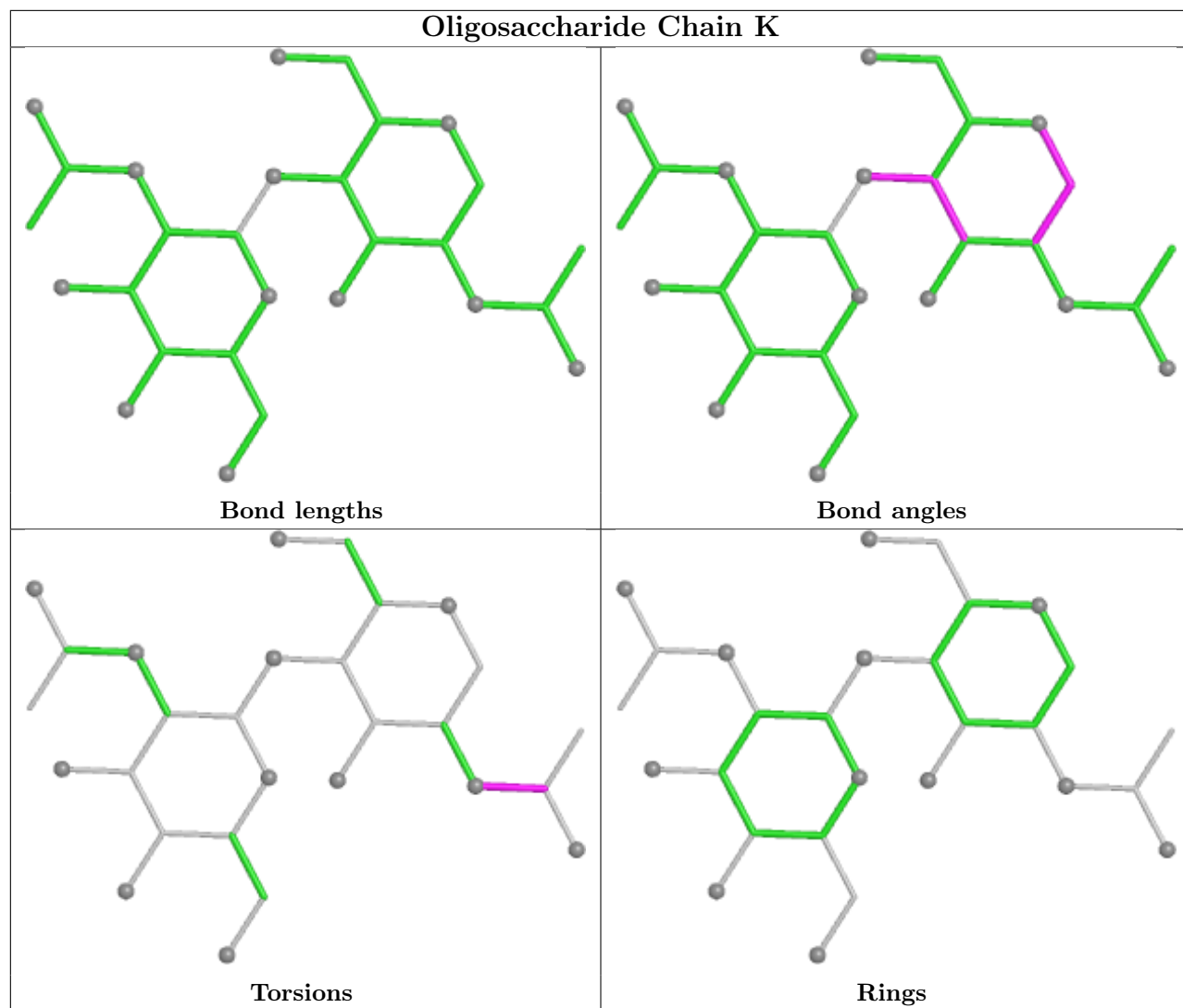


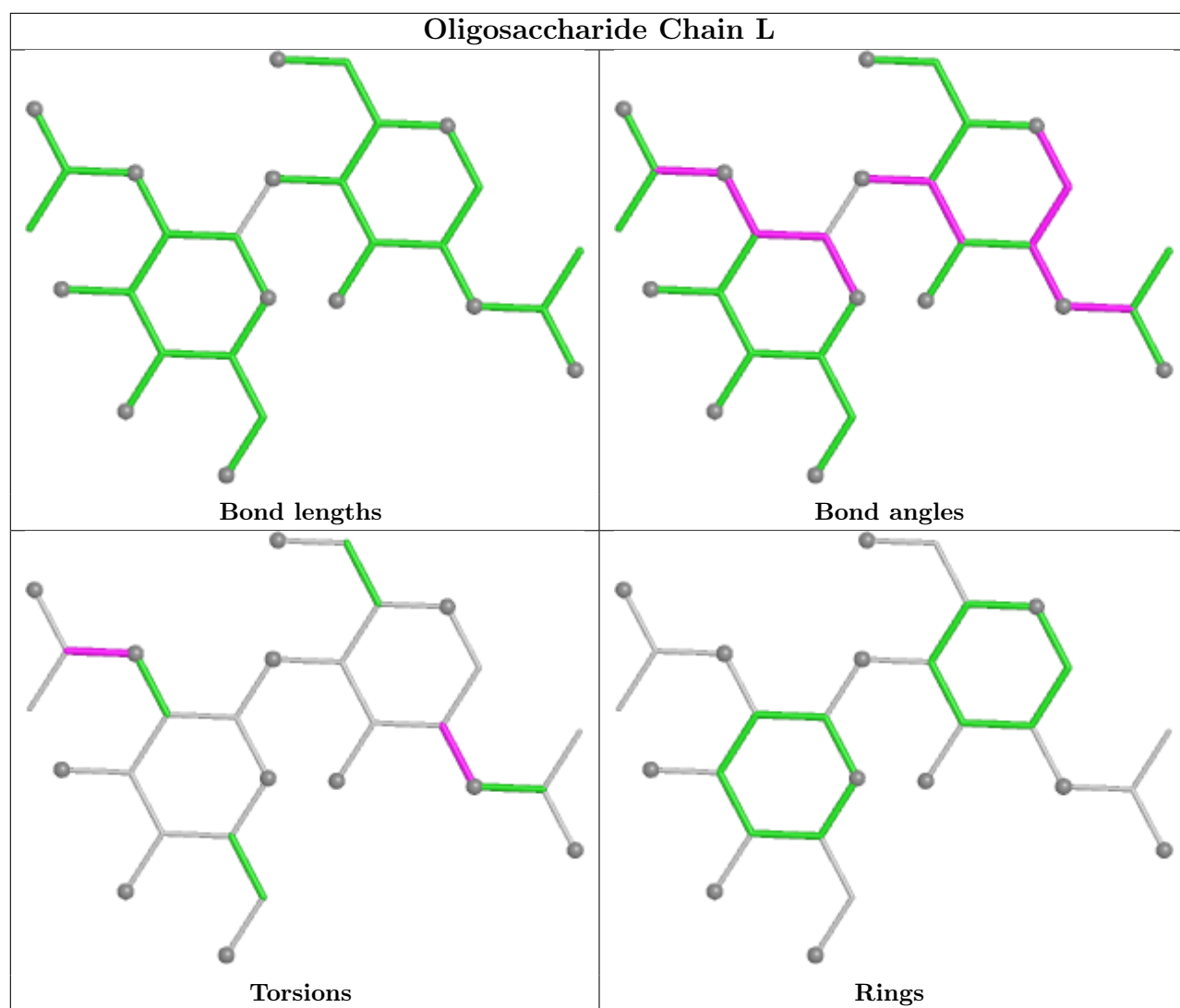


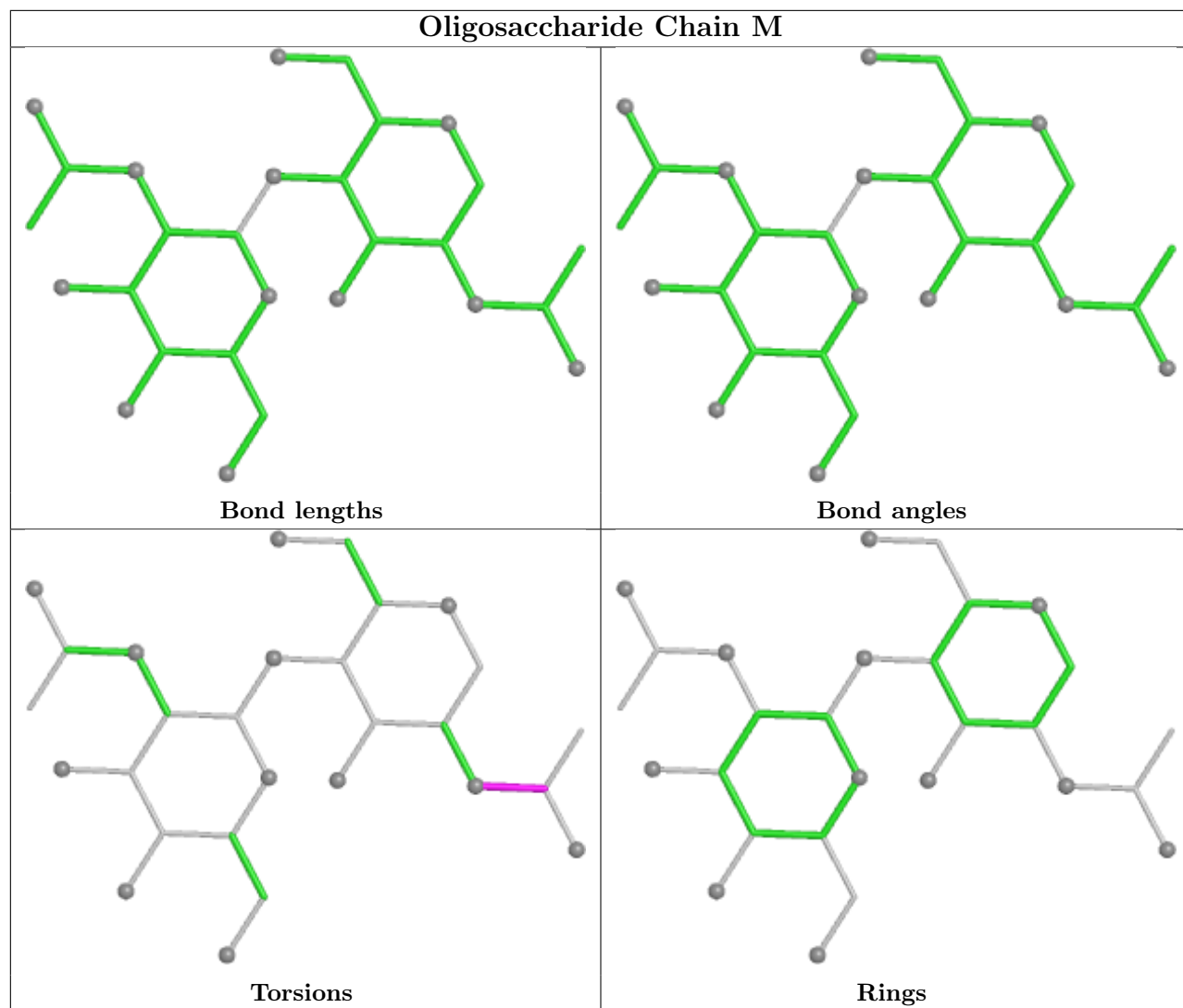


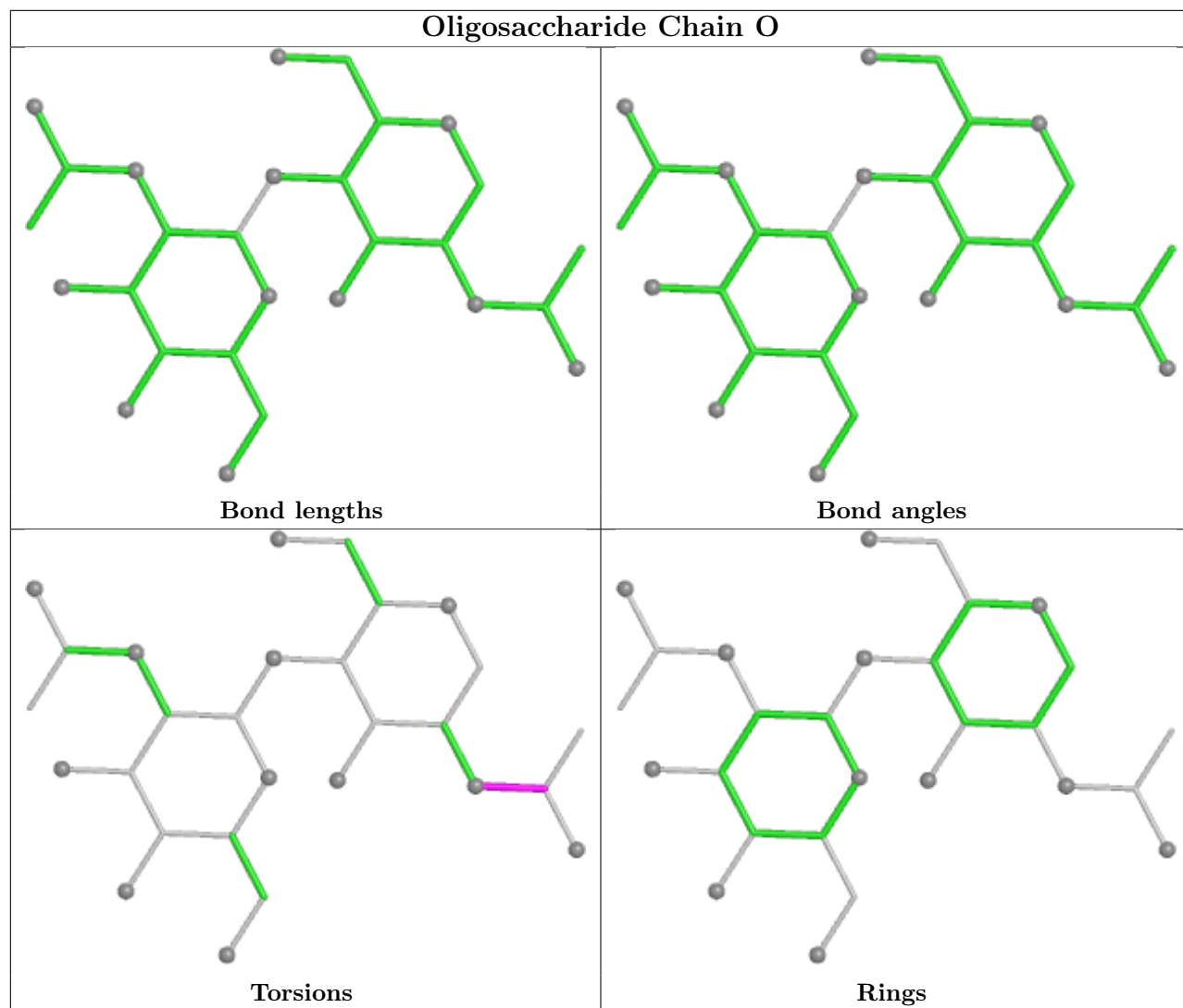


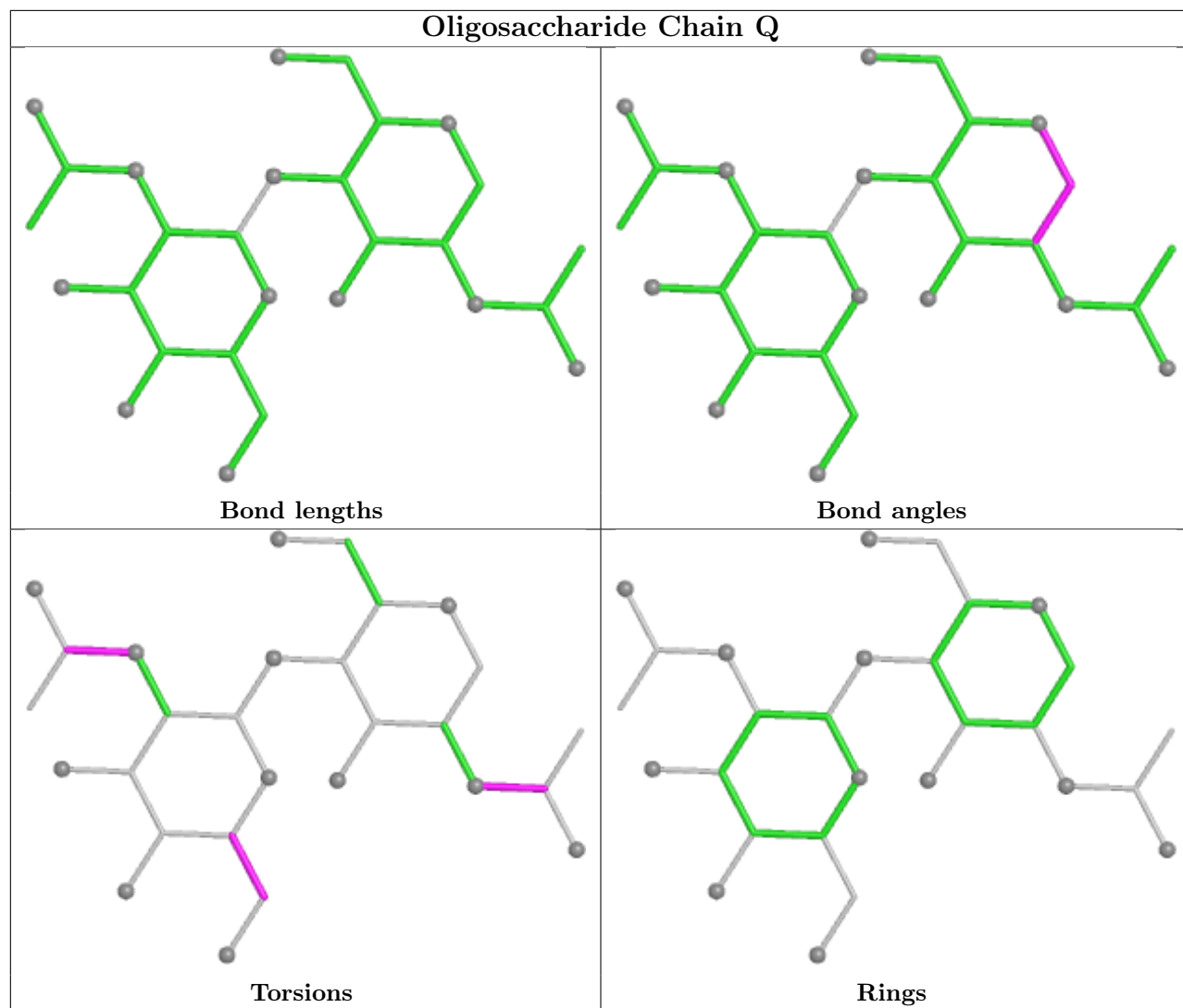


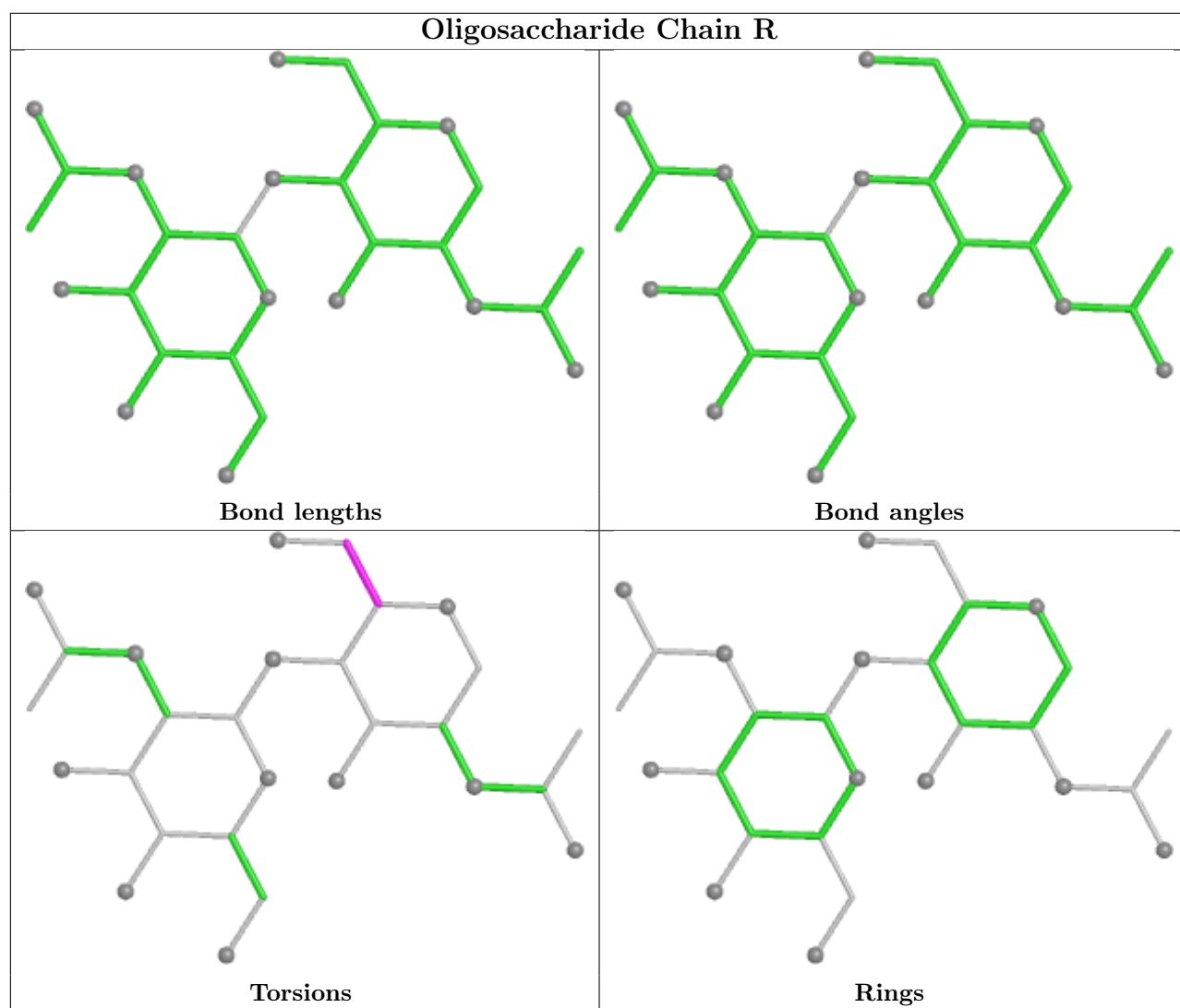


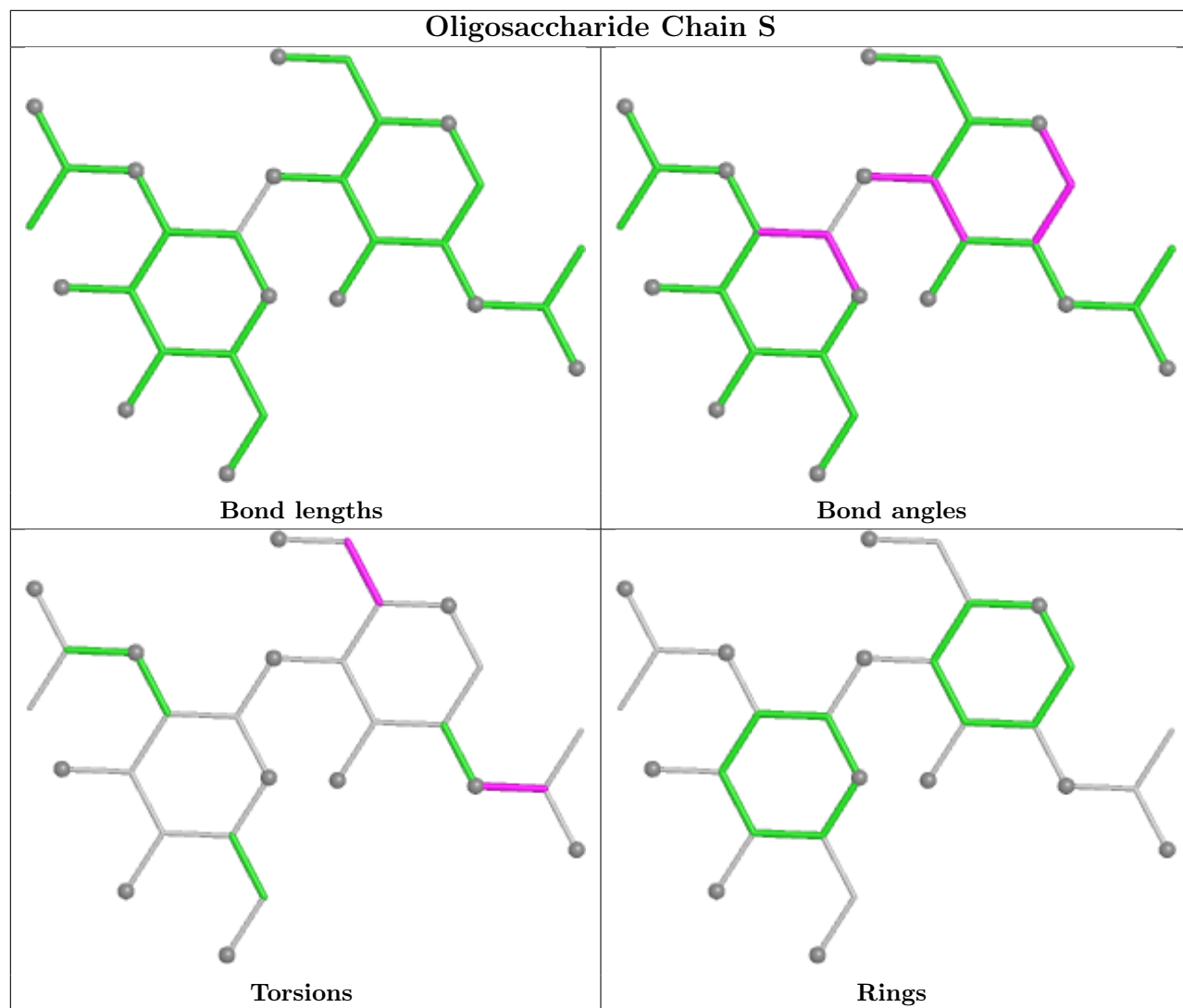


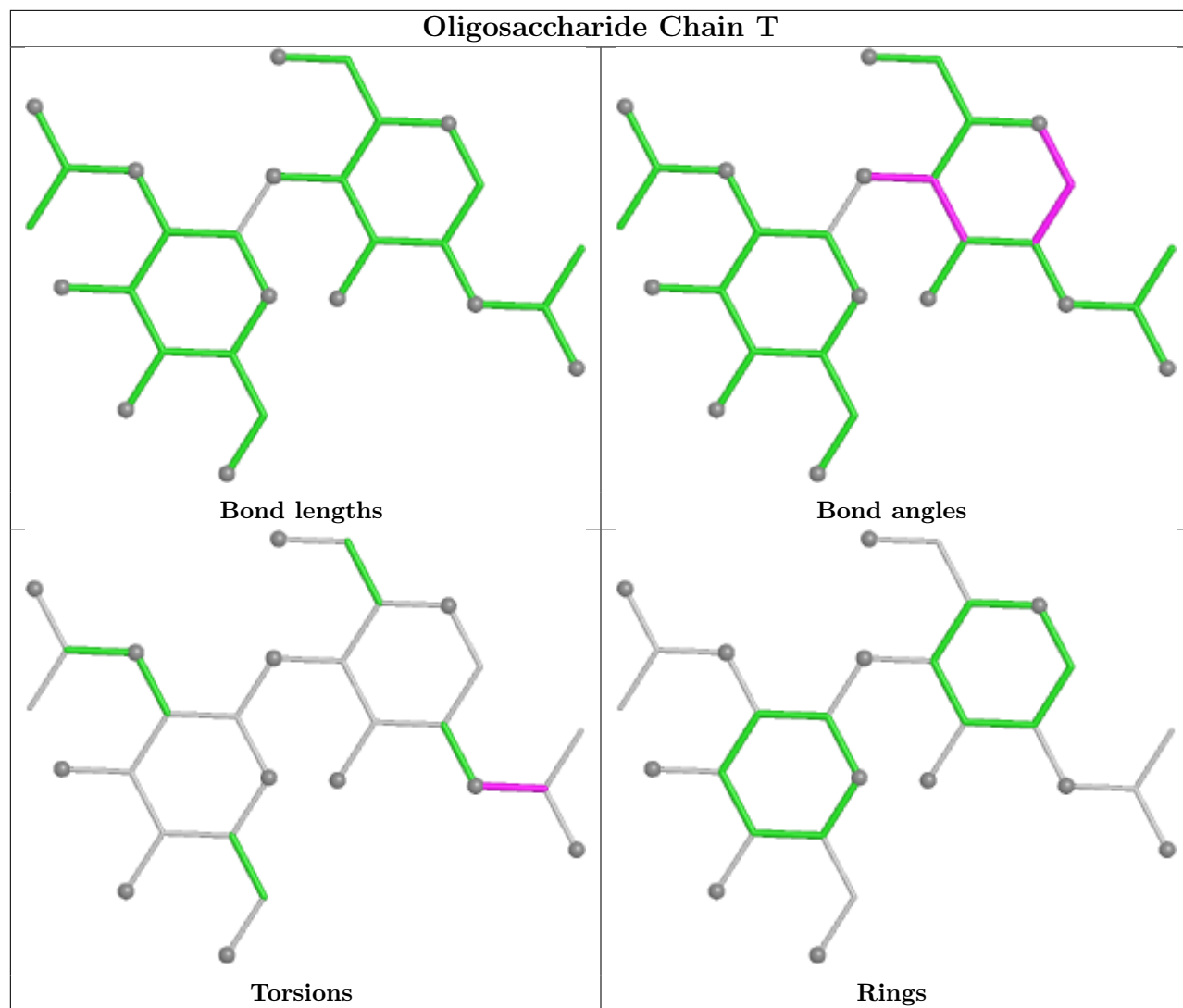


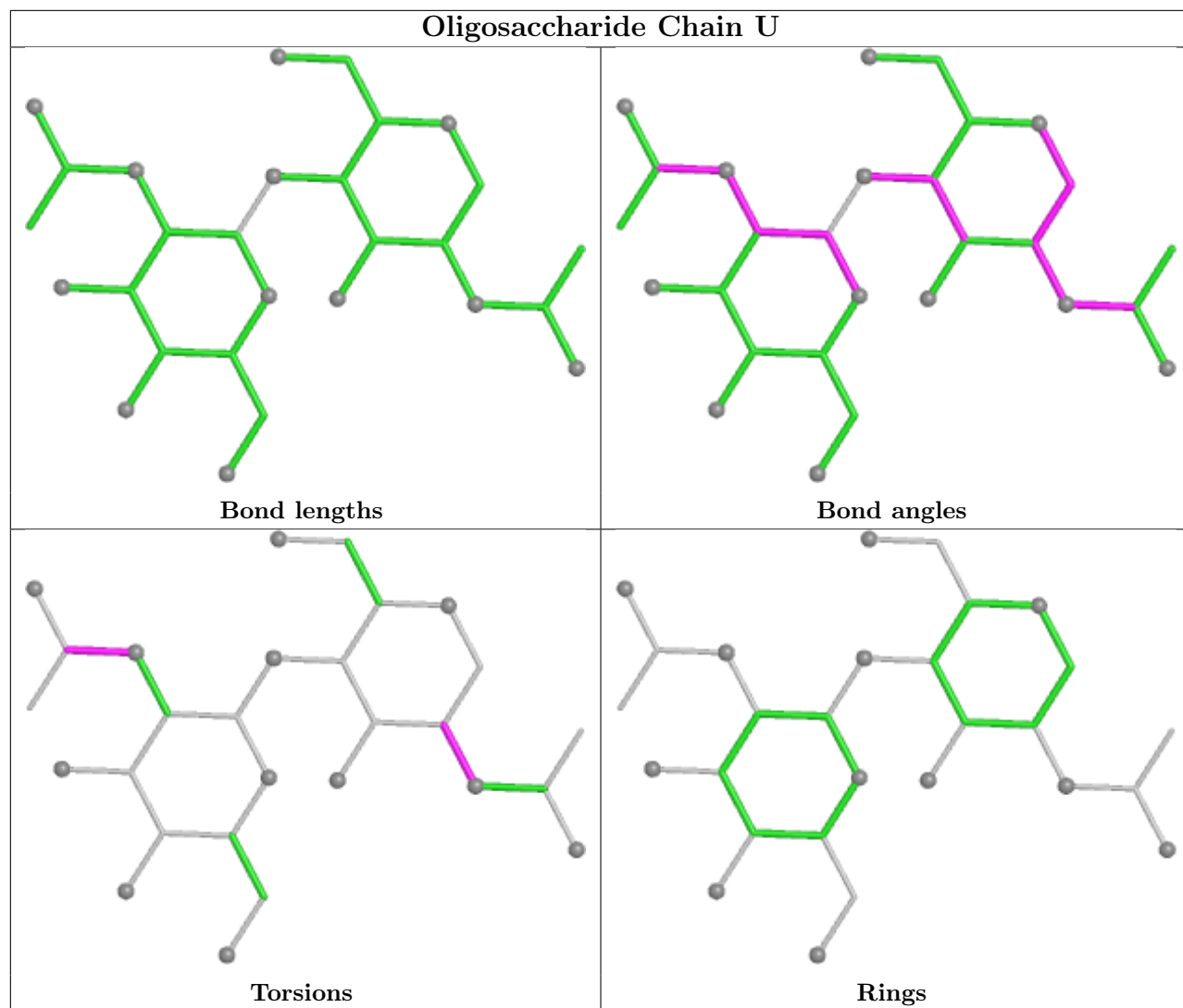


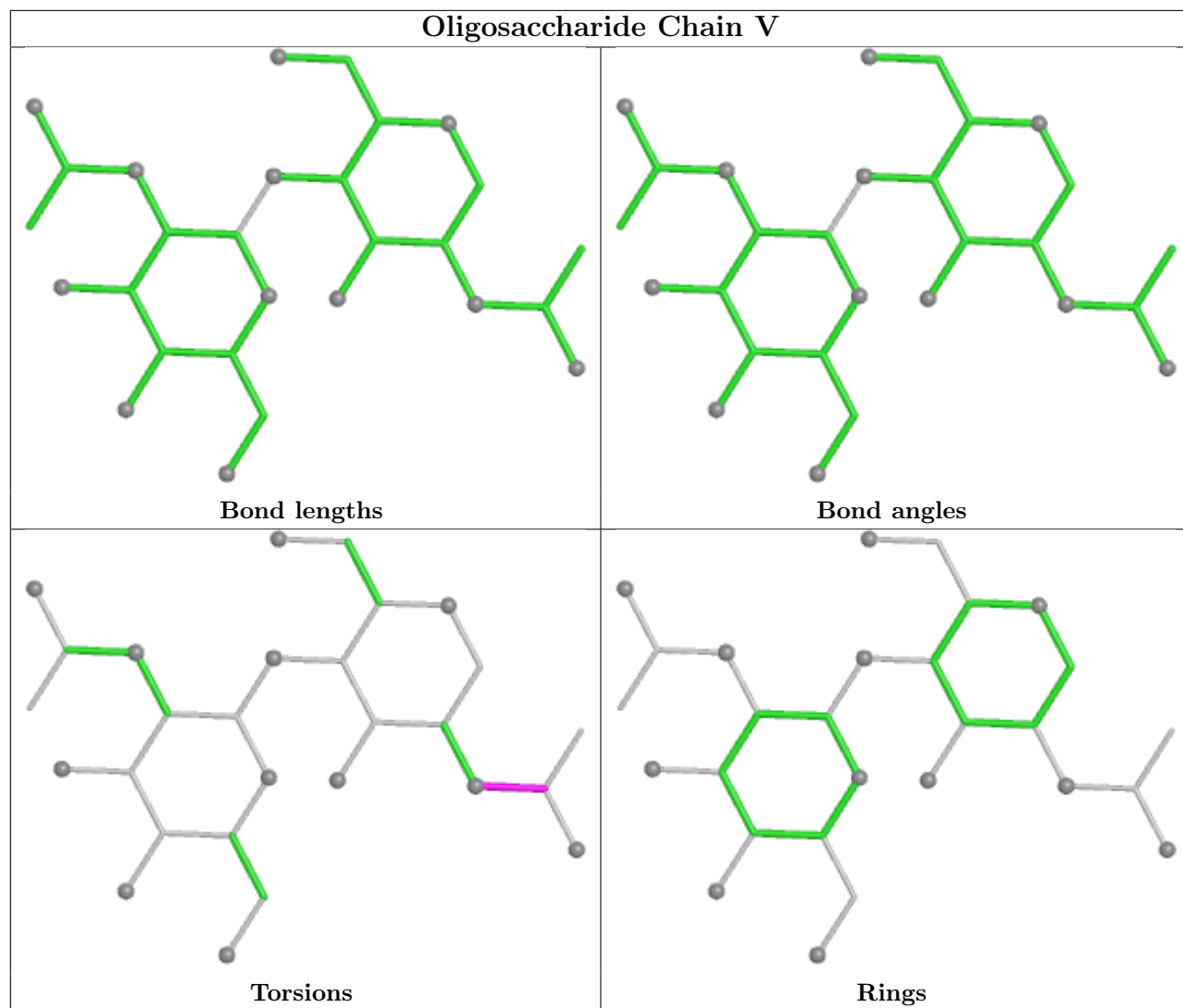


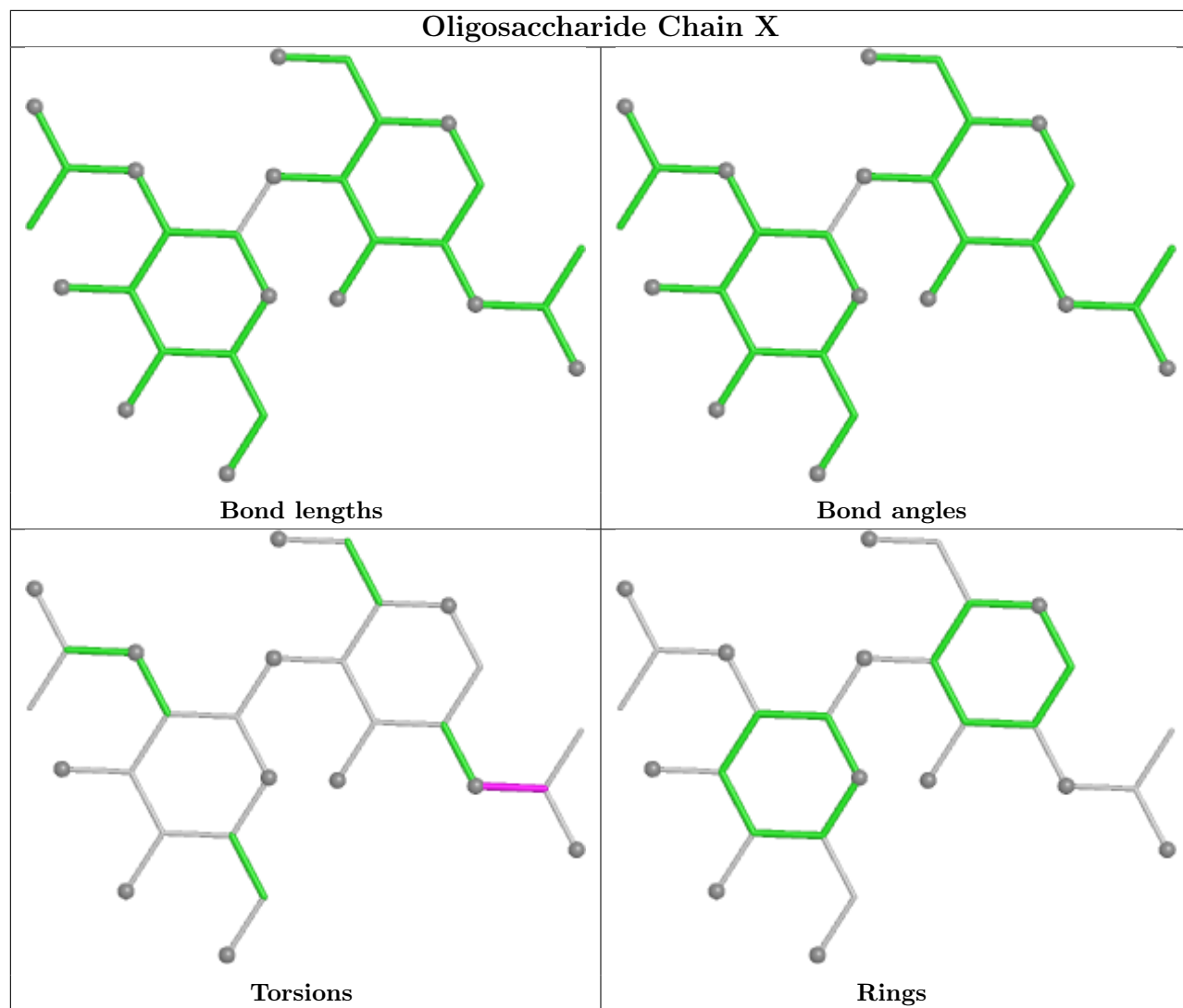


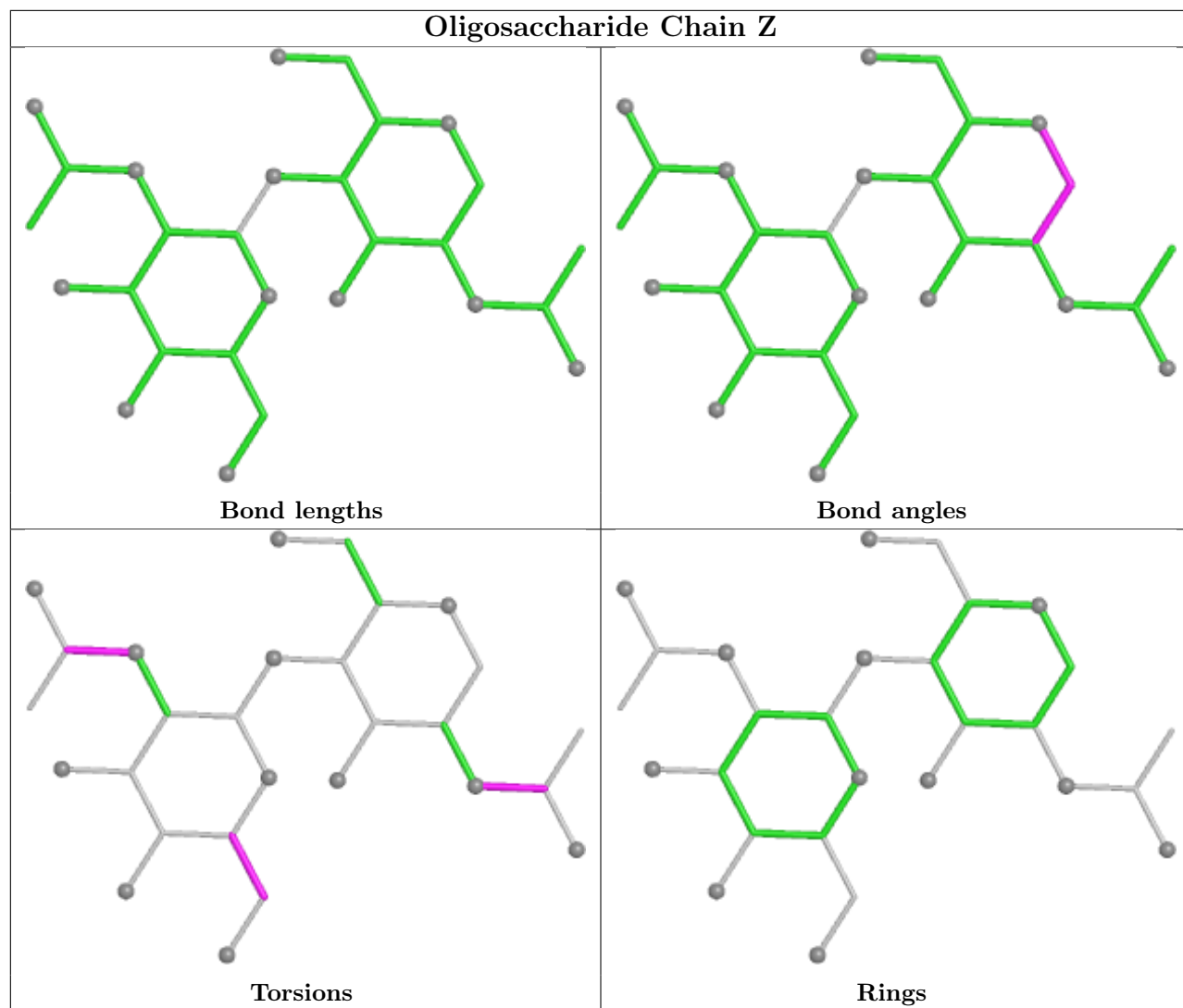


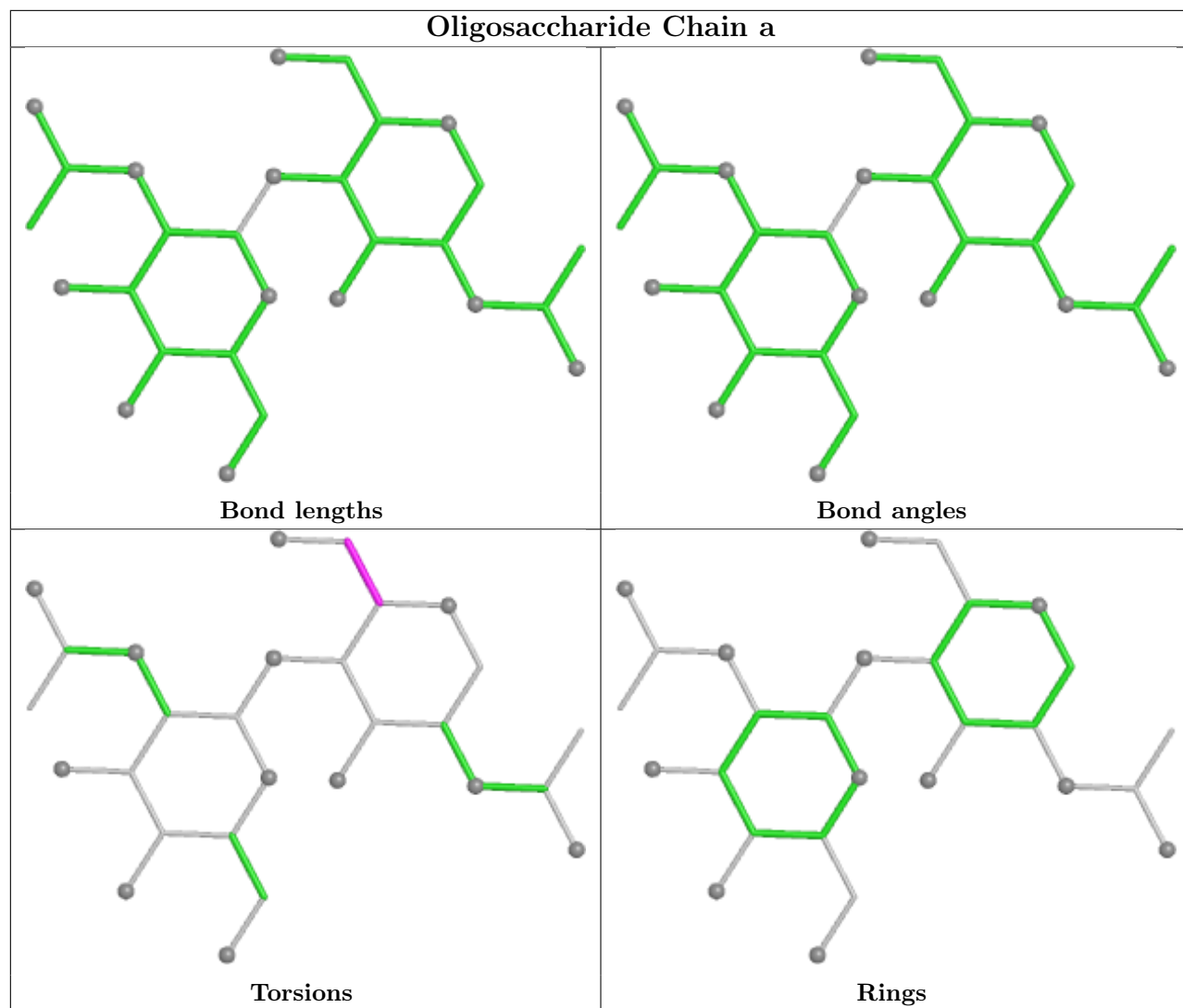


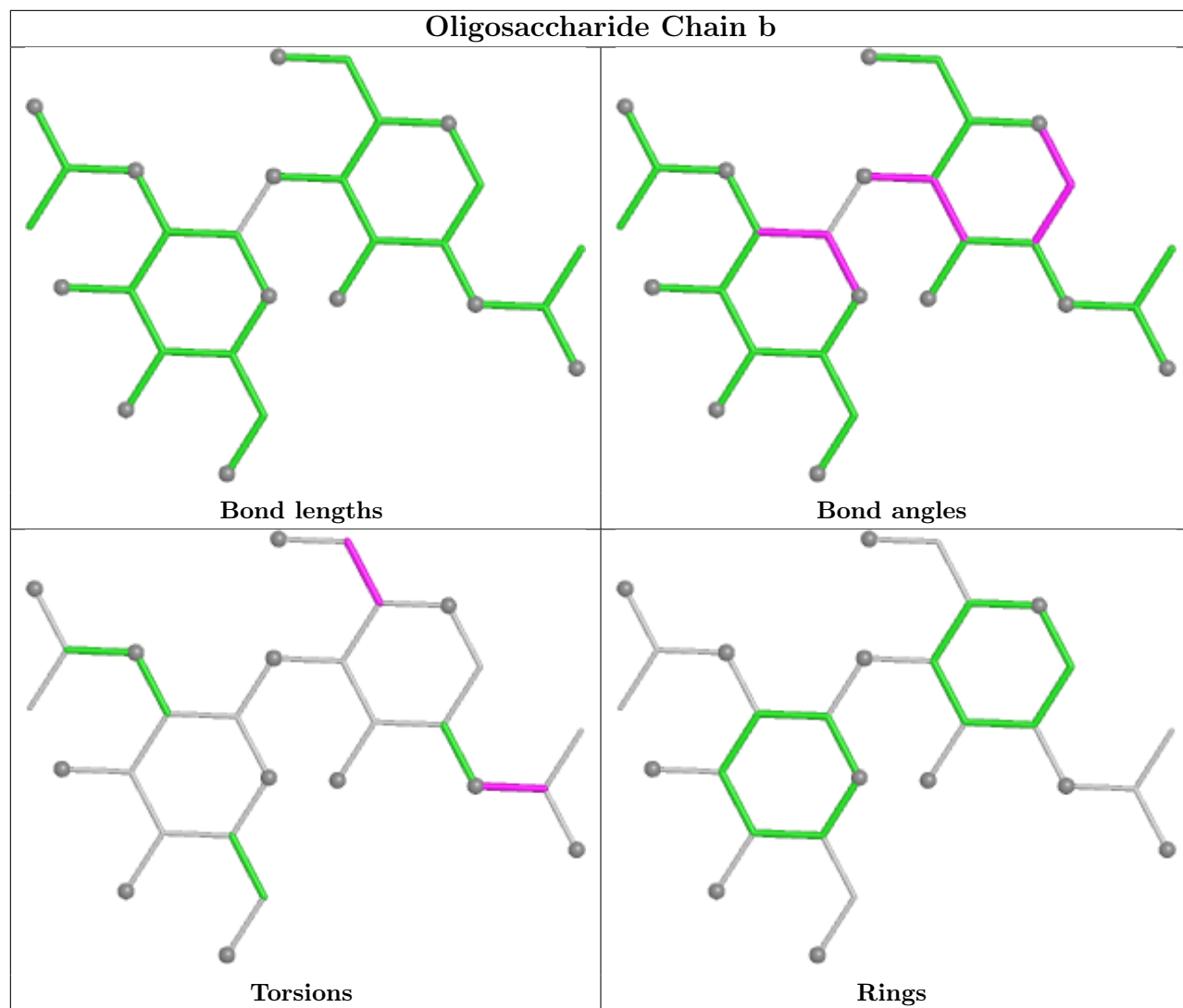


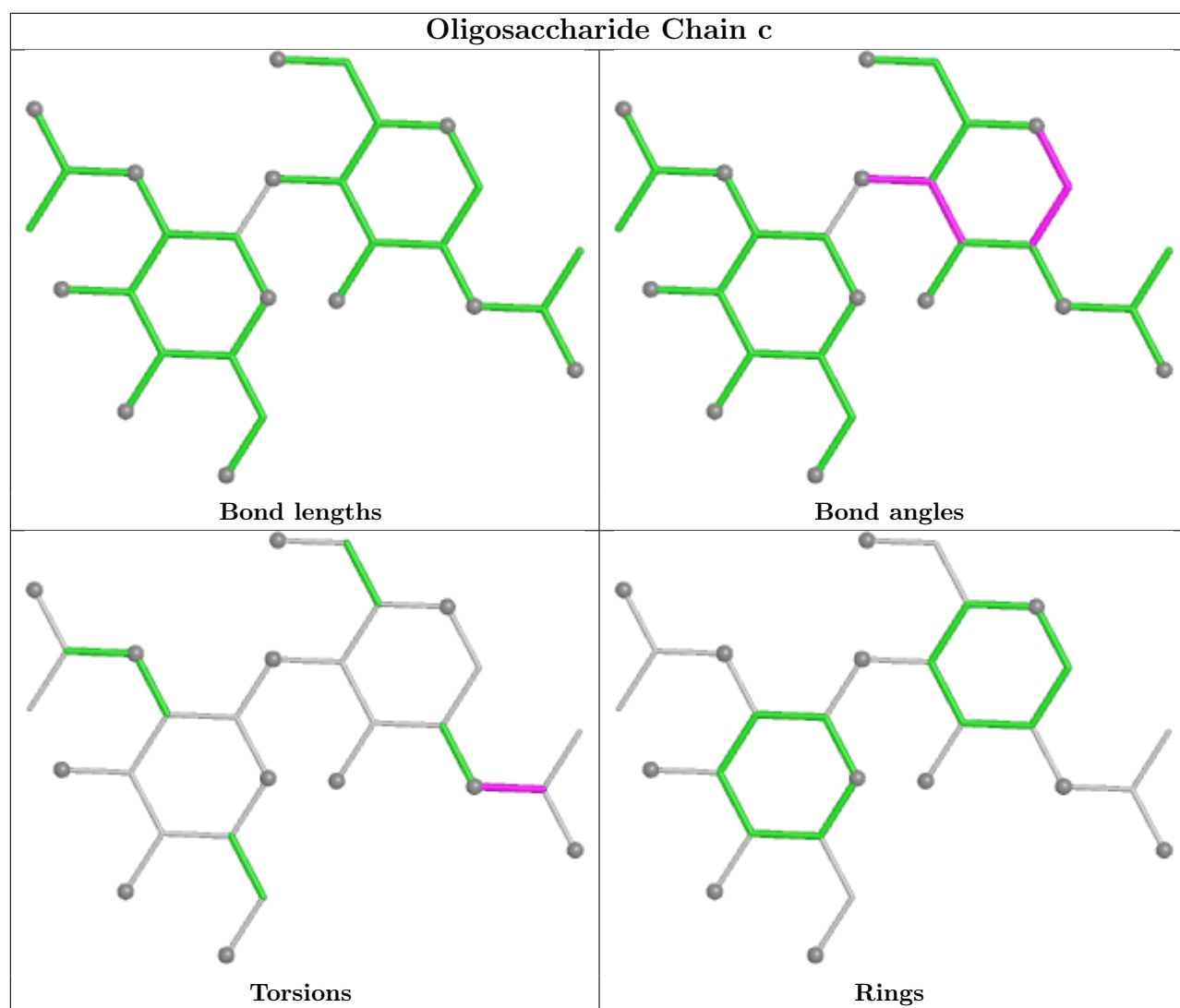


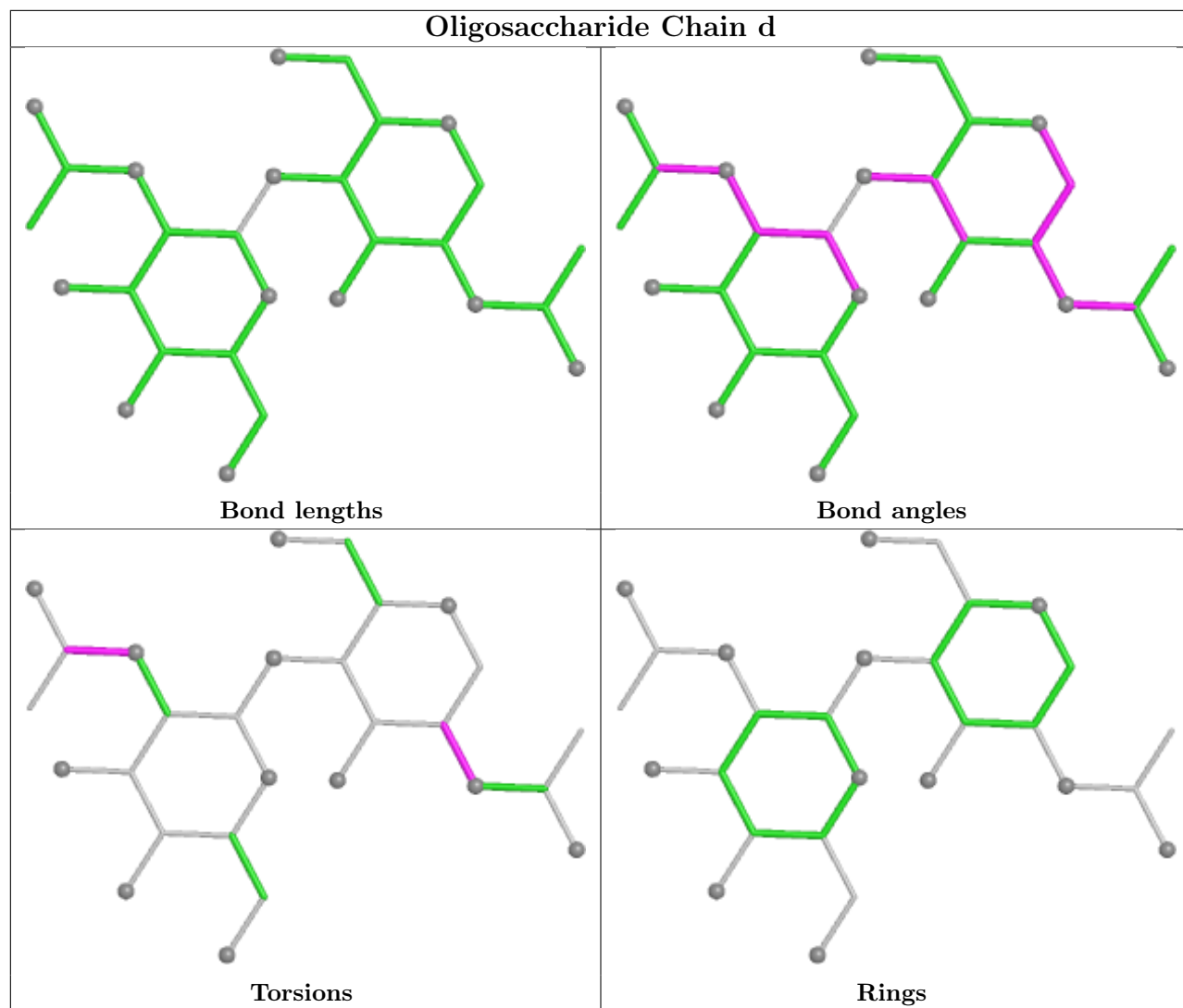


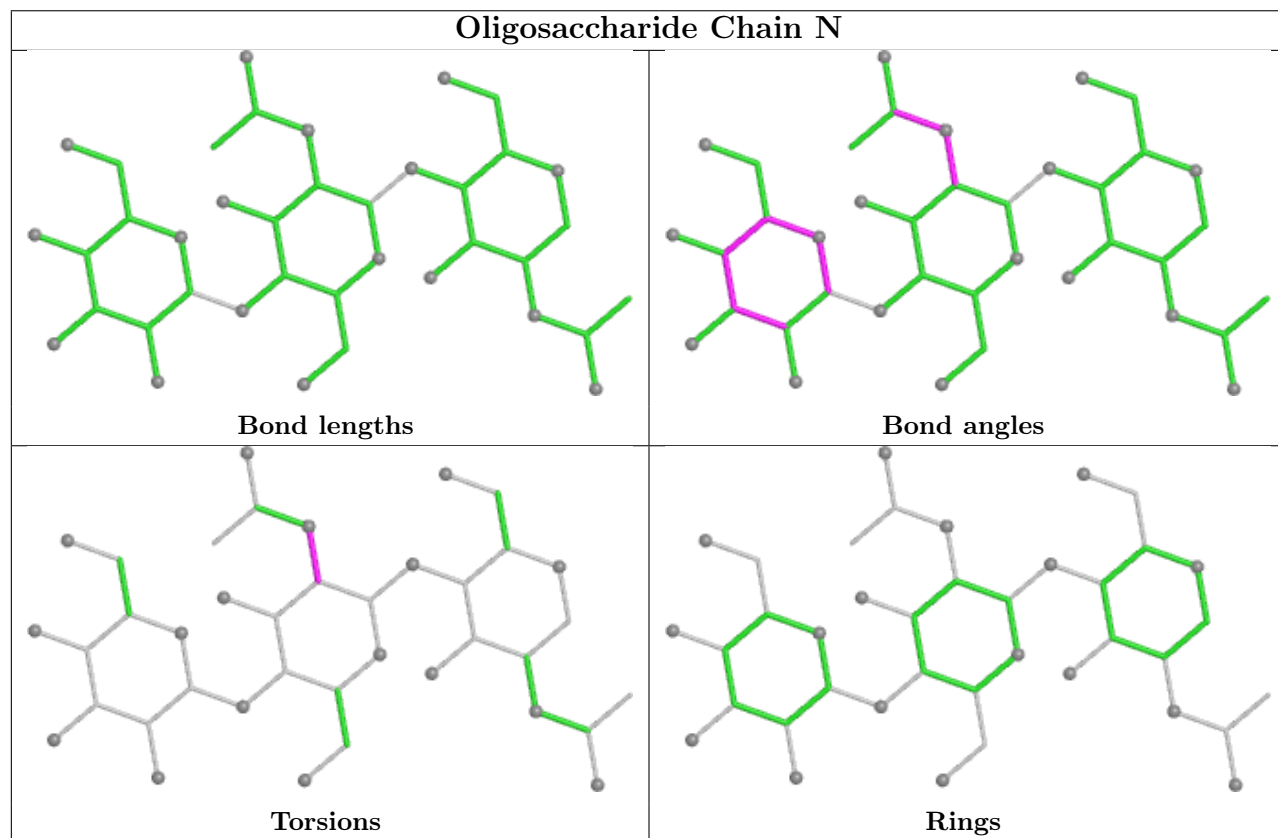
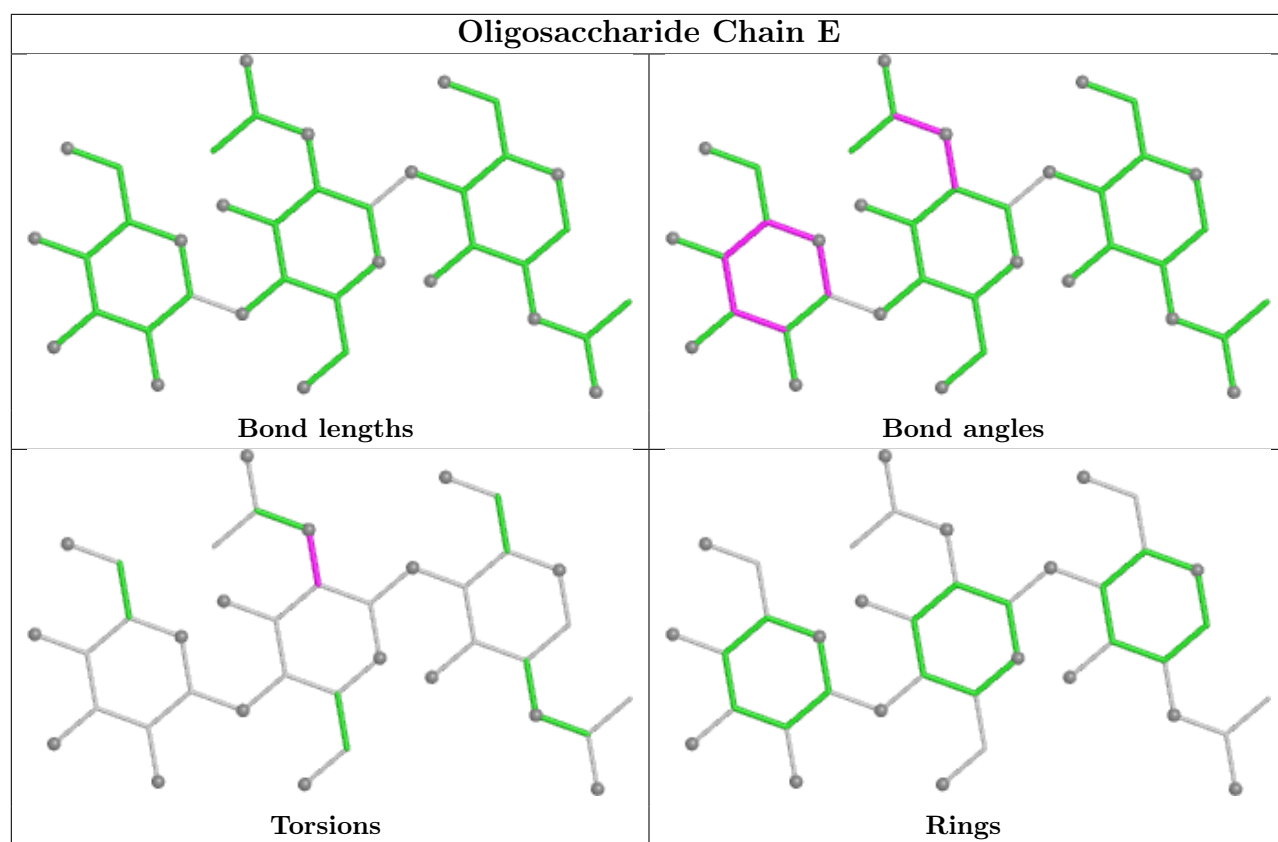


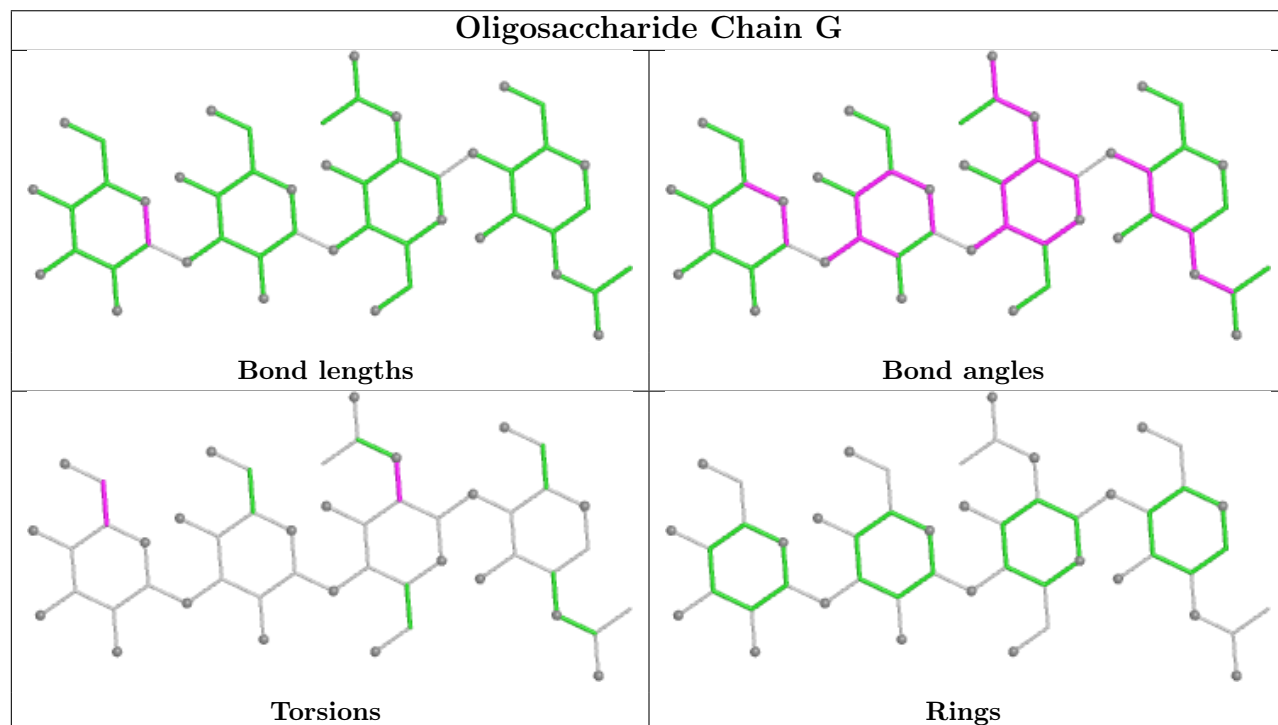
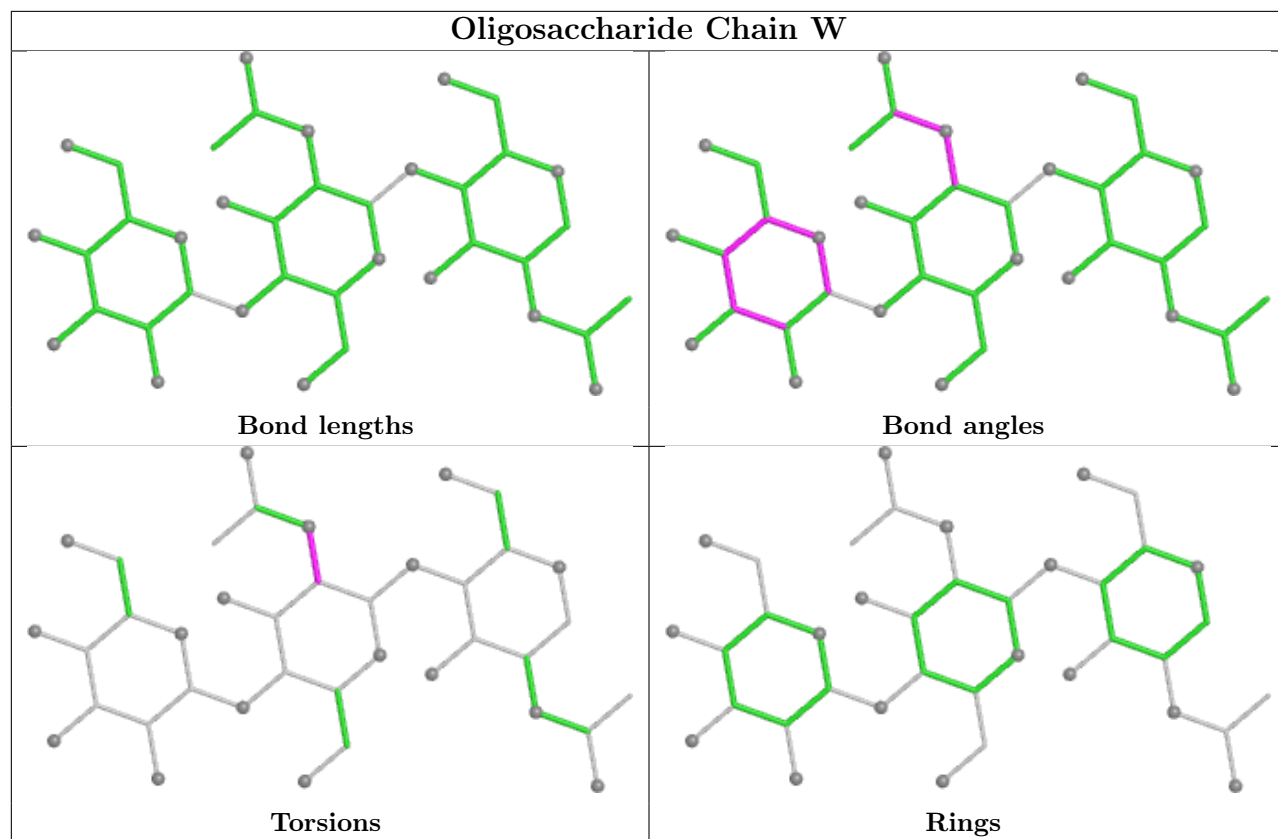


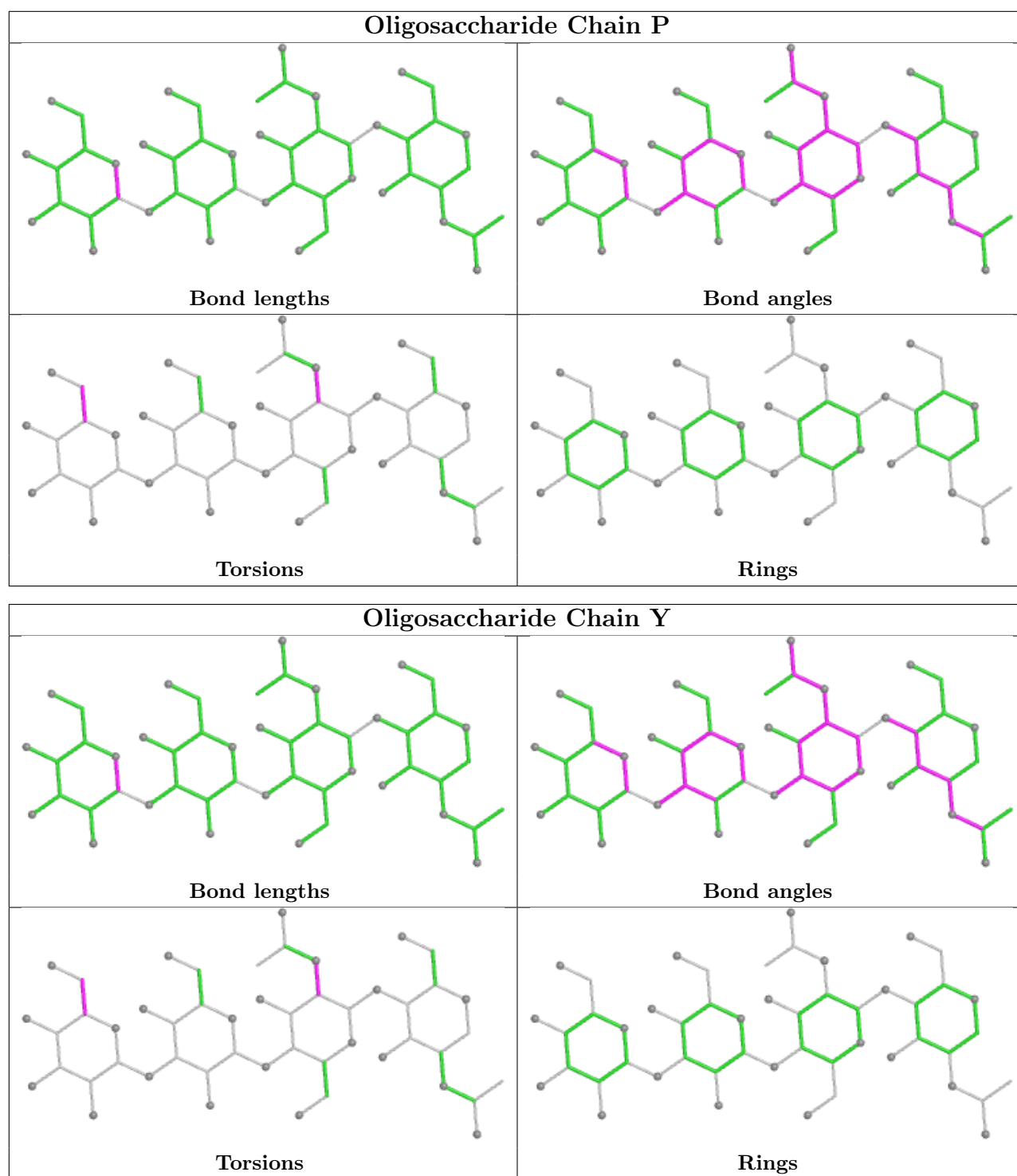












5.6 Ligand geometry [i](#)

27 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
6	NAG	B	1303	1	14,14,15	0.78	0	17,19,21	0.97	0
5	EIC	B	1301	-	19,19,19	0.45	0	19,19,19	0.87	1 (5%)
6	NAG	B	1304	1	14,14,15	0.70	0	17,19,21	0.80	0
6	NAG	C	1304	1	14,14,15	0.70	0	17,19,21	0.80	0
6	NAG	A	1305	1	14,14,15	0.73	0	17,19,21	0.95	1 (5%)
6	NAG	A	1307	1	14,14,15	0.70	0	17,19,21	1.16	1 (5%)
6	NAG	A	1308	1	14,14,15	0.71	0	17,19,21	0.80	0
6	NAG	C	1302	1	14,14,15	0.70	0	17,19,21	1.23	2 (11%)
6	NAG	C	1303	1	14,14,15	0.78	0	17,19,21	0.97	0
6	NAG	A	1302	1	14,14,15	0.70	0	17,19,21	1.23	2 (11%)
6	NAG	A	1304	1	14,14,15	0.71	0	17,19,21	0.80	0
5	EIC	A	1301	-	19,19,19	0.45	0	19,19,19	0.87	1 (5%)
5	EIC	C	1301	-	19,19,19	0.45	0	19,19,19	0.87	1 (5%)
6	NAG	A	1303	1	14,14,15	0.78	0	17,19,21	0.97	0
6	NAG	A	1306	1	14,14,15	0.78	0	17,19,21	0.93	0
6	NAG	C	1306	1	14,14,15	0.79	0	17,19,21	0.93	0
6	NAG	C	1307	1	14,14,15	0.69	0	17,19,21	1.16	1 (5%)
6	NAG	C	1309	1	14,14,15	0.73	0	17,19,21	0.83	0
6	NAG	A	1309	1	14,14,15	0.73	0	17,19,21	0.83	0
6	NAG	B	1308	1	14,14,15	0.71	0	17,19,21	0.80	0
6	NAG	C	1308	1	14,14,15	0.71	0	17,19,21	0.80	0
6	NAG	B	1306	1	14,14,15	0.78	0	17,19,21	0.92	0
6	NAG	C	1305	1	14,14,15	0.74	0	17,19,21	0.96	1 (5%)
6	NAG	B	1302	1	14,14,15	0.70	0	17,19,21	1.23	2 (11%)
6	NAG	B	1305	1	14,14,15	0.74	0	17,19,21	0.95	1 (5%)
6	NAG	B	1307	1	14,14,15	0.71	0	17,19,21	1.16	1 (5%)
6	NAG	B	1309	1	14,14,15	0.74	0	17,19,21	0.83	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1303	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EIC	B	1301	-	-	4/17/17/17	-
6	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1307	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
5	EIC	A	1301	-	-	4/17/17/17	-
5	EIC	C	1301	-	-	4/17/17/17	-
6	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1306	1	-	3/6/23/26	0/1/1/1
6	NAG	C	1306	1	-	3/6/23/26	0/1/1/1
6	NAG	C	1307	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1306	1	-	3/6/23/26	0/1/1/1
6	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1302	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1307	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1309	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1307	NAG	C2-N2-C7	3.12	127.35	122.90
6	B	1307	NAG	C2-N2-C7	3.12	127.35	122.90
6	C	1307	NAG	C2-N2-C7	3.10	127.32	122.90
6	B	1302	NAG	C2-N2-C7	3.09	127.31	122.90
6	A	1302	NAG	C2-N2-C7	3.09	127.30	122.90
6	C	1302	NAG	C2-N2-C7	3.05	127.25	122.90
6	C	1302	NAG	O5-C1-C2	-2.24	107.75	111.29
5	B	1301	EIC	C3-C2-C1	-2.23	108.85	114.47
6	A	1302	NAG	O5-C1-C2	-2.23	107.77	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1302	NAG	O5-C1-C2	-2.22	107.78	111.29
5	A	1301	EIC	C3-C2-C1	-2.22	108.88	114.47
5	C	1301	EIC	C3-C2-C1	-2.20	108.93	114.47
6	C	1305	NAG	C2-N2-C7	2.05	125.82	122.90
6	A	1305	NAG	C2-N2-C7	2.03	125.79	122.90
6	B	1305	NAG	C2-N2-C7	2.02	125.77	122.90

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1305	NAG	C8-C7-N2-C2
6	A	1305	NAG	O7-C7-N2-C2
6	A	1306	NAG	C8-C7-N2-C2
6	A	1306	NAG	O7-C7-N2-C2
6	B	1305	NAG	C8-C7-N2-C2
6	B	1305	NAG	O7-C7-N2-C2
6	B	1306	NAG	C8-C7-N2-C2
6	B	1306	NAG	O7-C7-N2-C2
6	C	1305	NAG	C8-C7-N2-C2
6	C	1305	NAG	O7-C7-N2-C2
6	C	1306	NAG	C8-C7-N2-C2
6	C	1306	NAG	O7-C7-N2-C2
5	A	1301	EIC	C4-C5-C6-C7
5	C	1301	EIC	C4-C5-C6-C7
5	B	1301	EIC	C4-C5-C6-C7
6	A	1306	NAG	O5-C5-C6-O6
6	B	1306	NAG	O5-C5-C6-O6
6	C	1306	NAG	O5-C5-C6-O6
6	A	1302	NAG	C3-C2-N2-C7
6	B	1302	NAG	C3-C2-N2-C7
6	C	1302	NAG	C3-C2-N2-C7
5	A	1301	EIC	C9-C10-C11-C12
5	A	1301	EIC	C10-C11-C12-C13
5	B	1301	EIC	C9-C10-C11-C12
5	B	1301	EIC	C10-C11-C12-C13
5	C	1301	EIC	C9-C10-C11-C12
5	C	1301	EIC	C10-C11-C12-C13
5	A	1301	EIC	C7-C8-C9-C10
5	B	1301	EIC	C7-C8-C9-C10
5	C	1301	EIC	C7-C8-C9-C10
6	A	1307	NAG	C3-C2-N2-C7

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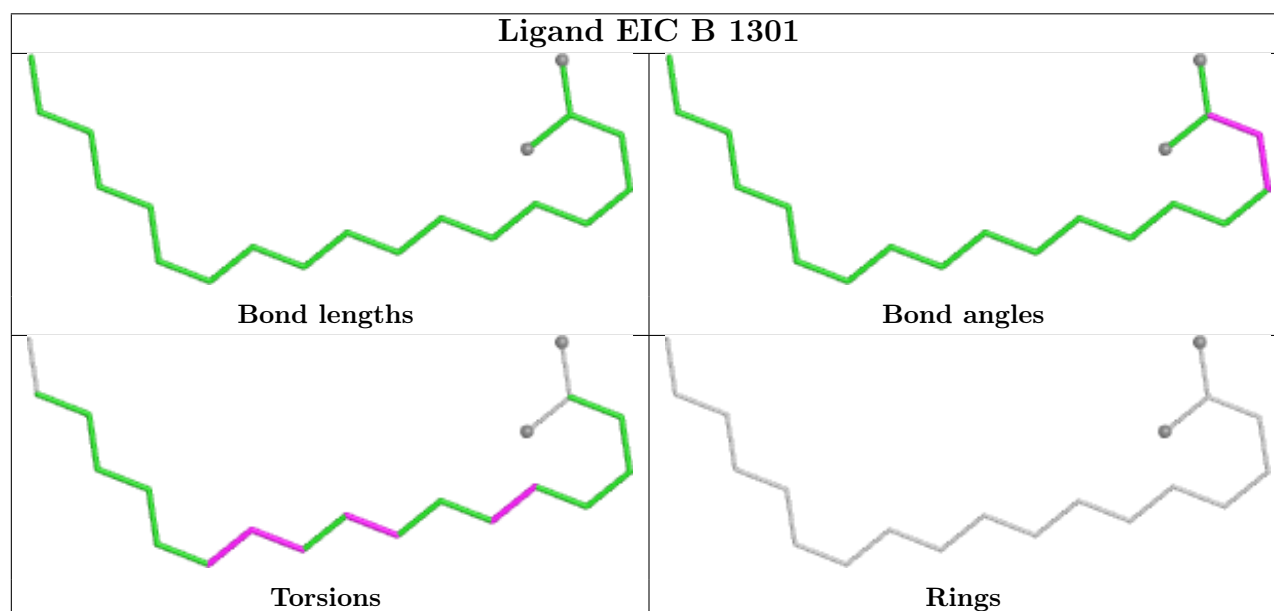
Mol	Chain	Res	Type	Atoms
6	B	1307	NAG	C3-C2-N2-C7
6	C	1307	NAG	C3-C2-N2-C7

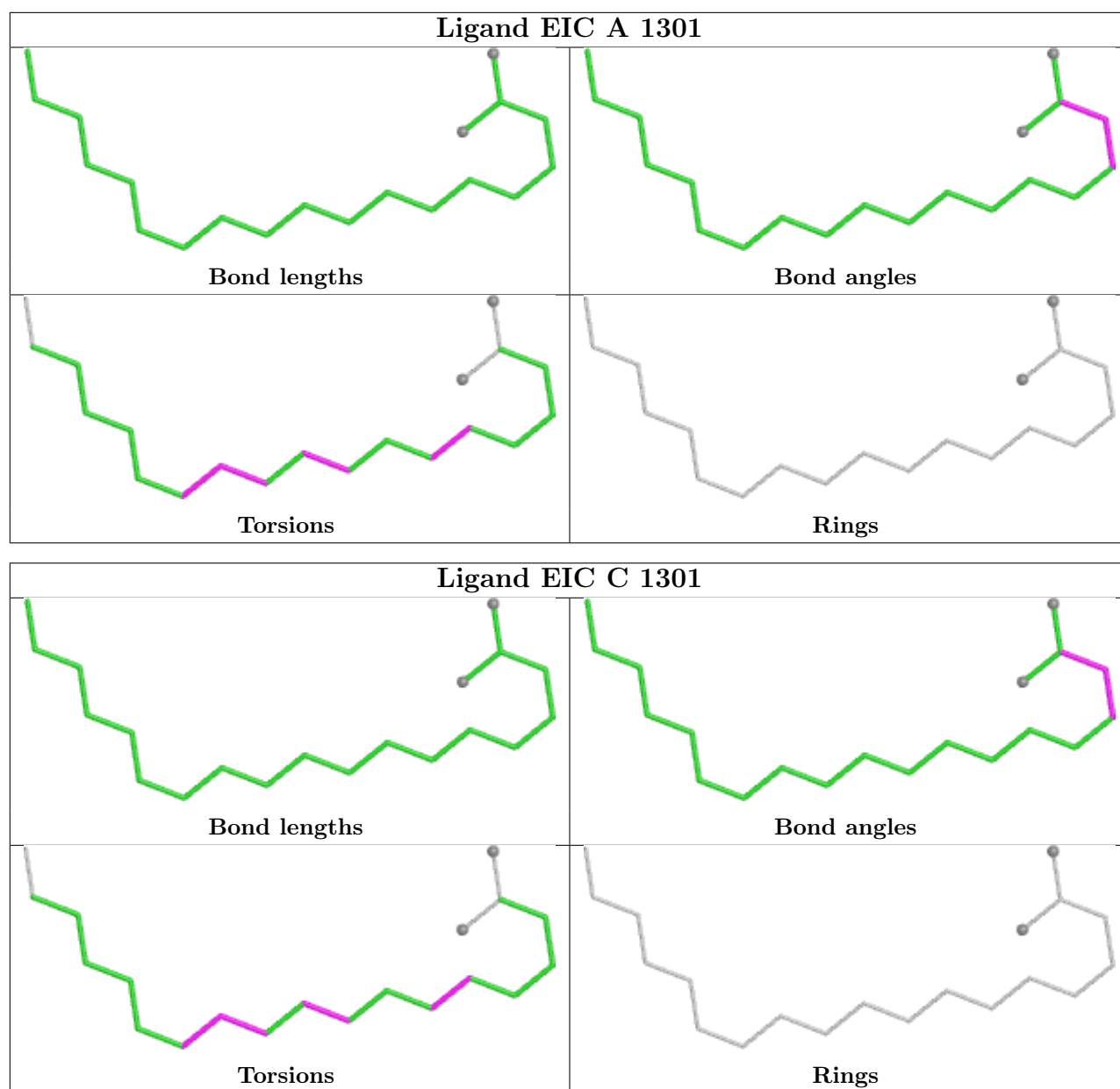
There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1301	EIC	3	0
6	C	1302	NAG	1	0
6	A	1302	NAG	1	0
5	A	1301	EIC	3	0
5	C	1301	EIC	3	0
6	B	1302	NAG	1	0

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





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.