



## Full wwPDB EM Validation Report ⓘ

Apr 13, 2026 – 09:23 PM JST

PDB ID : 9VVG / pdb\_00009vvg  
EMDB ID : EMD-65379  
Title : Cryo-EM structure of the erlin1/2 complex purified using GDN and CHS  
Authors : Yan, L.; Xu, Z.; Gao, N.  
Deposited on : 2025-07-15  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
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

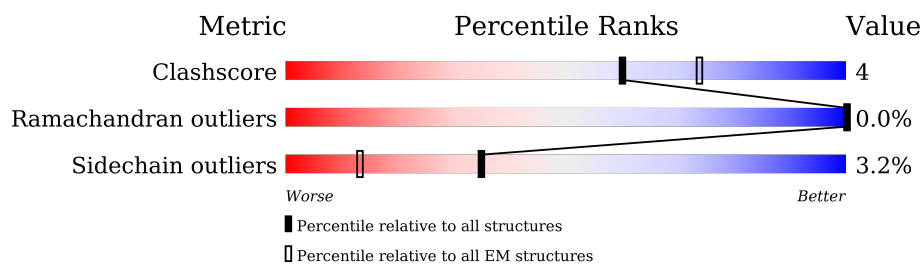
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.70 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.














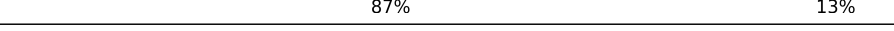







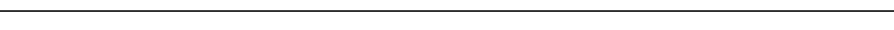

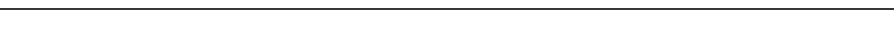
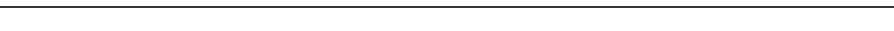


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	297	
1	B	297	
1	C	297	
1	D	297	
1	E	297	
1	F	297	
1	G	297	
1	H	297	
1	I	297	



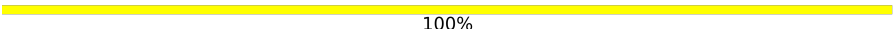


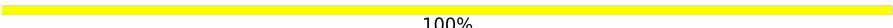
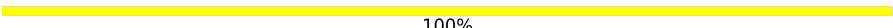
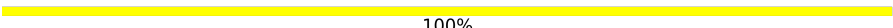


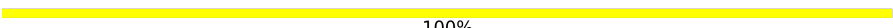


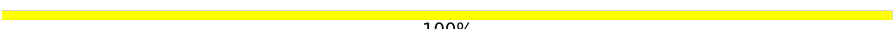


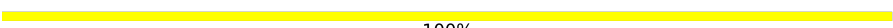

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Mol	Chain	Length	Quality of chain
1	J	297	 85% 13%
1	K	297	 86% 12%
1	L	297	 86% 13%
1	M	297	 87% 13%
2	a	299	 87% 12%
2	b	299	 85% 15%
2	c	299	 88% 12%
2	d	299	 89% 11%
2	e	299	 88% 12%
2	f	299	 87% 13%
2	g	299	 89% 11%
2	h	299	 87% 13%
2	i	299	 89% 11%
2	j	299	 88% 11%
2	k	299	 88% 11%
2	l	299	 86% 13%
2	m	299	 87% 13%
3	N	2	 50% 50%
3	O	2	 50% 50%
3	P	2	 50% 50%
3	Q	2	 50% 50%
3	R	2	 50% 50%
3	S	2	 50% 50%
3	T	2	 100%
3	U	2	 100%

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Mol	Chain	Length	Quality of chain
3	V	2	 50% 50%
3	W	2	 50% 50%
3	X	2	 100%
3	Y	2	 50% 50%
3	Z	2	 50% 50%
3	n	2	 100%
3	o	2	 100%
3	p	2	 100%
3	q	2	 50% 50%
3	r	2	 50% 50%
3	s	2	 100%
3	t	2	 50% 50%
3	u	2	 50% 50%
3	v	2	 100%
3	w	2	 50% 50%
3	x	2	 50% 50%
3	y	2	 100%
3	z	2	 50% 50%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 62374 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 Erlin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	297	Total 2375	C 1524	N 400	O 442	S 9	0	0
1	M	297	Total 2375	C 1524	N 400	O 442	S 9	0	0
1	L	297	Total 2375	C 1524	N 400	O 442	S 9	0	0
1	K	297	Total 2375	C 1524	N 400	O 442	S 9	0	0
1	J	297	Total 2375	C 1524	N 400	O 442	S 9	0	0
1	I	297	Total 2375	C 1524	N 400	O 442	S 9	0	0
1	H	297	Total 2375	C 1524	N 400	O 442	S 9	0	0
1	G	297	Total 2375	C 1524	N 400	O 442	S 9	0	0
1	C	297	Total 2375	C 1524	N 400	O 442	S 9	0	0
1	B	297	Total 2375	C 1524	N 400	O 442	S 9	0	0
1	F	297	Total 2375	C 1524	N 400	O 442	S 9	0	0
1	E	297	Total 2375	C 1524	N 400	O 442	S 9	0	0
1	D	297	Total 2375	C 1524	N 400	O 442	S 9	0	0

- Molecule 2 is a protein called Erlin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	299	Total 2367	C 1516	N 386	O 451	S 14	0	0
2	m	299	Total 2367	C 1516	N 386	O 451	S 14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	k	299	Total 2367	C 1516	N 386	O 451	S 14	0	0
2	l	299	Total 2367	C 1516	N 386	O 451	S 14	0	0
2	i	299	Total 2367	C 1516	N 386	O 451	S 14	0	0
2	g	299	Total 2367	C 1516	N 386	O 451	S 14	0	0
2	h	299	Total 2367	C 1516	N 386	O 451	S 14	0	0
2	j	299	Total 2367	C 1516	N 386	O 451	S 14	0	0
2	b	299	Total 2367	C 1516	N 386	O 451	S 14	0	0
2	c	299	Total 2367	C 1516	N 386	O 451	S 14	0	0
2	f	299	Total 2367	C 1516	N 386	O 451	S 14	0	0
2	d	299	Total 2367	C 1516	N 386	O 451	S 14	0	0
2	e	299	Total 2367	C 1516	N 386	O 451	S 14	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	295	MET	ILE	conflict	UNP O94905
m	295	MET	ILE	conflict	UNP O94905
k	295	MET	ILE	conflict	UNP O94905
l	295	MET	ILE	conflict	UNP O94905
i	295	MET	ILE	conflict	UNP O94905
g	295	MET	ILE	conflict	UNP O94905
h	295	MET	ILE	conflict	UNP O94905
j	295	MET	ILE	conflict	UNP O94905
b	295	MET	ILE	conflict	UNP O94905
c	295	MET	ILE	conflict	UNP O94905
f	295	MET	ILE	conflict	UNP O94905
d	295	MET	ILE	conflict	UNP O94905
e	295	MET	ILE	conflict	UNP O94905

- Molecule 3 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
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	V	2	Total	C	N	O	0	0
			28	16	2	10		
3	W	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	2	Total	C	N	O	0	0
			28	16	2	10		
3	Y	2	Total	C	N	O	0	0
			28	16	2	10		
3	Z	2	Total	C	N	O	0	0
			28	16	2	10		
3	n	2	Total	C	N	O	0	0
			28	16	2	10		
3	o	2	Total	C	N	O	0	0
			28	16	2	10		
3	p	2	Total	C	N	O	0	0
			28	16	2	10		
3	q	2	Total	C	N	O	0	0
			28	16	2	10		
3	r	2	Total	C	N	O	0	0
			28	16	2	10		
3	s	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	t	2	Total	C	N	O	0	0
			28	16	2	10		
3	u	2	Total	C	N	O	0	0
			28	16	2	10		
3	v	2	Total	C	N	O	0	0
			28	16	2	10		
3	w	2	Total	C	N	O	0	0
			28	16	2	10		
3	x	2	Total	C	N	O	0	0
			28	16	2	10		
3	y	2	Total	C	N	O	0	0
			28	16	2	10		
3	z	2	Total	C	N	O	0	0
			28	16	2	10		

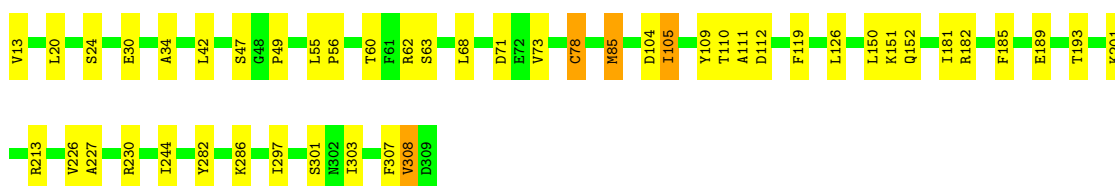


### 3 Residue-property plots


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.

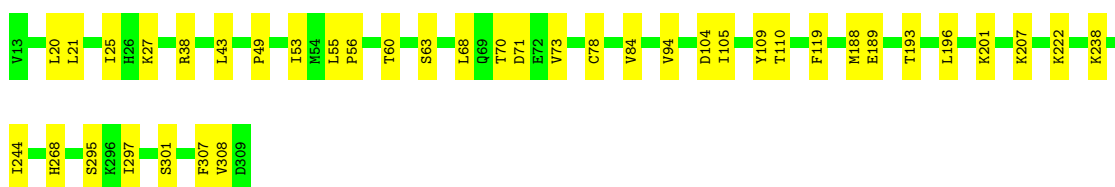
- Molecule 1: Erlin-1

Chain A: 




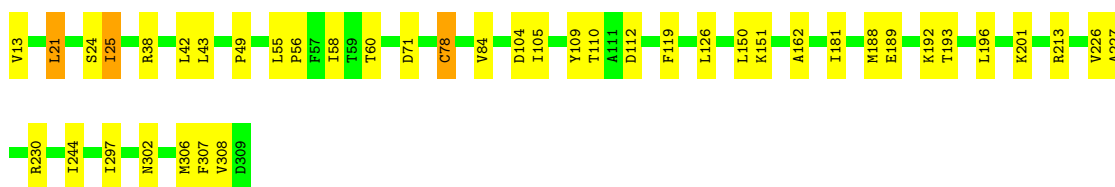
- Molecule 1: Erlin-1

Chain M: 




- Molecule 1: Erlin-1

Chain L: 

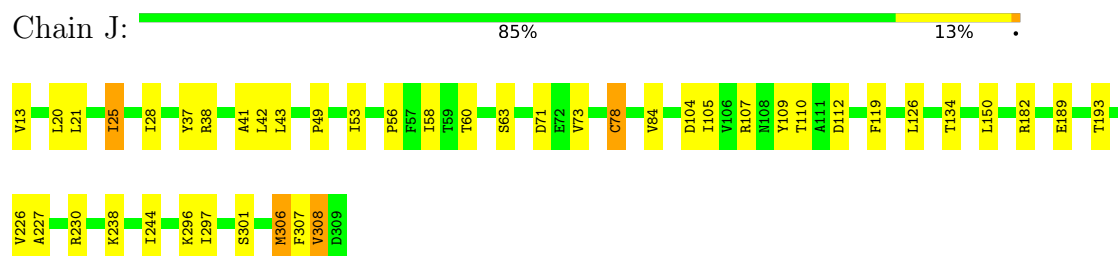


- Molecule 1: Erlin-1

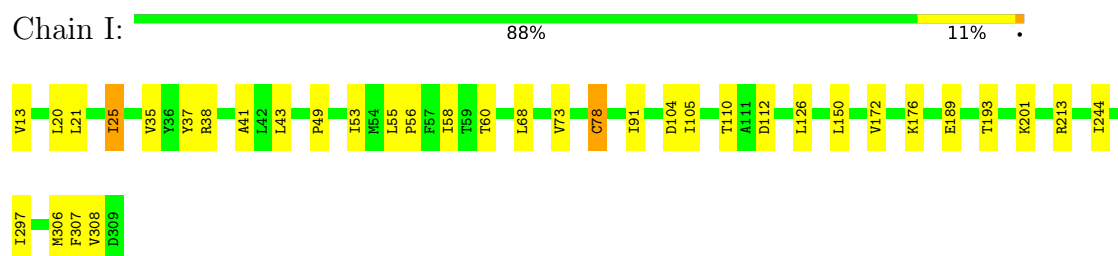
Chain K: 



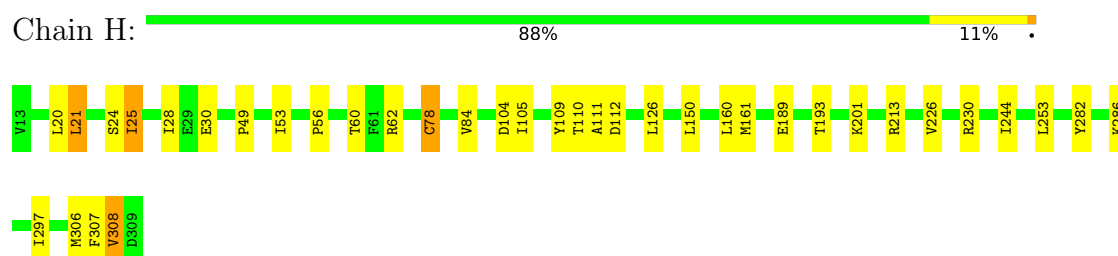
## • Molecule 1: Erlin-1



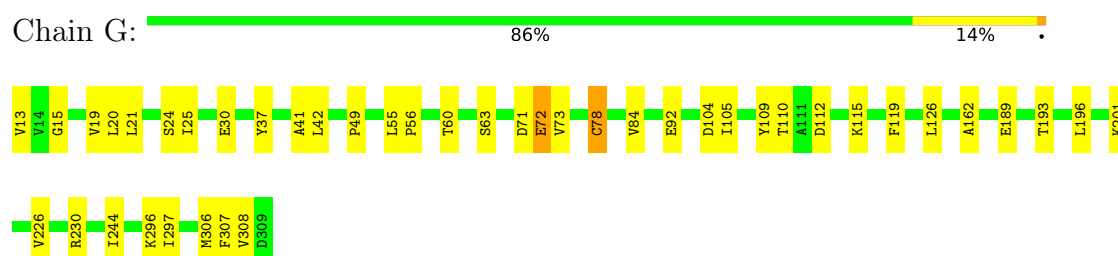
## • Molecule 1: Erlin-1



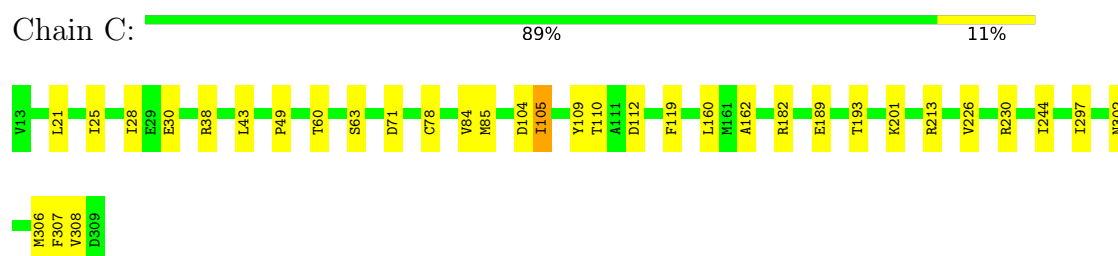
## • Molecule 1: Erlin-1



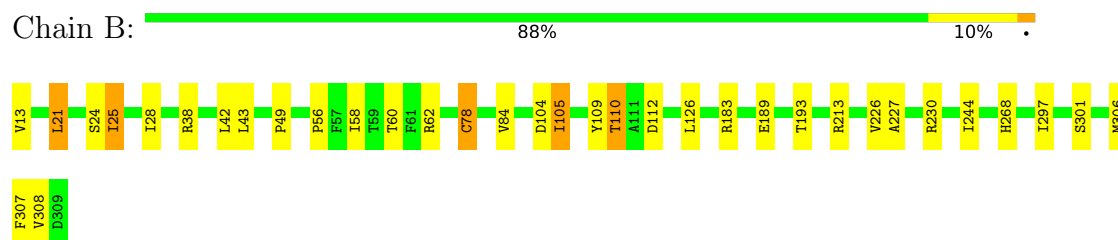
## • Molecule 1: Erlin-1



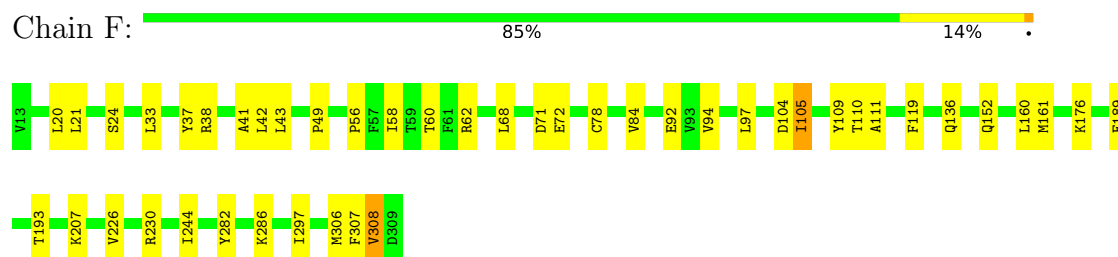
## • Molecule 1: Erlin-1



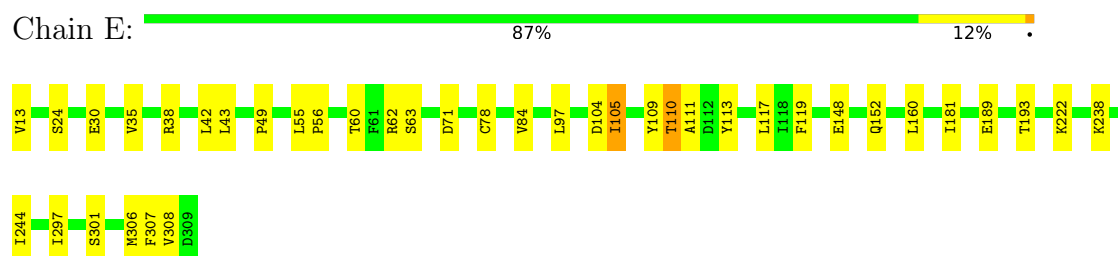
## • Molecule 1: Erlin-1



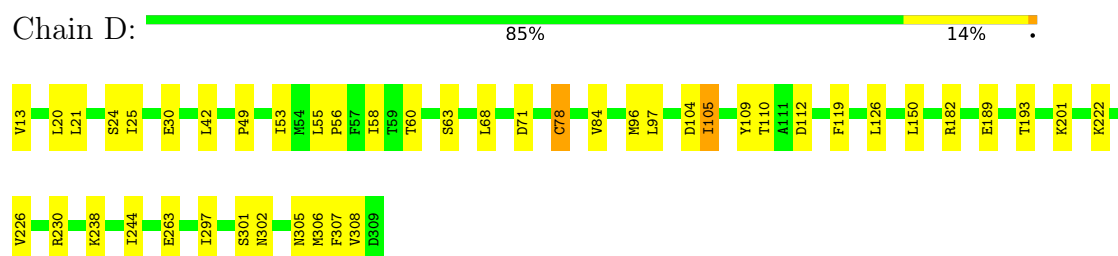
## • Molecule 1: Erlin-1



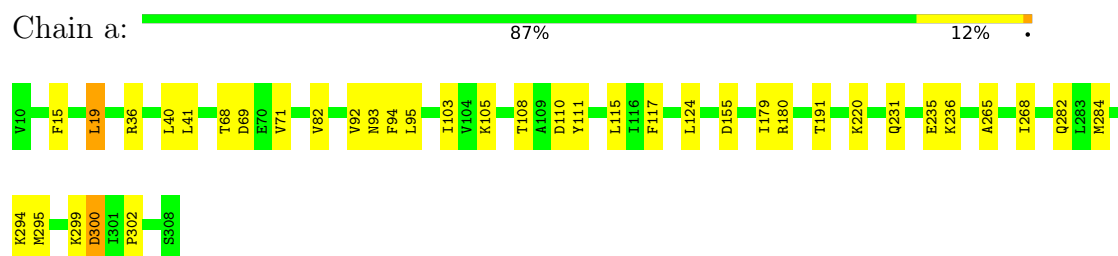
## • Molecule 1: Erlin-1




## • Molecule 1: Erlin-1

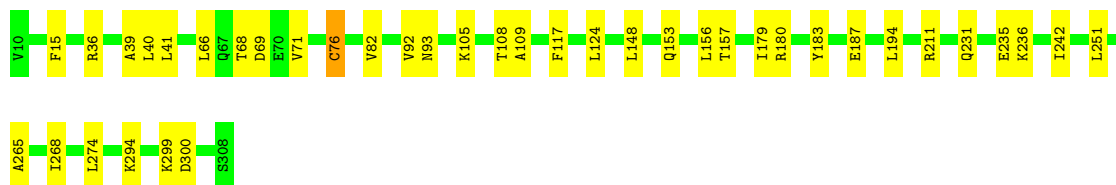


## • Molecule 2: Erlin-2




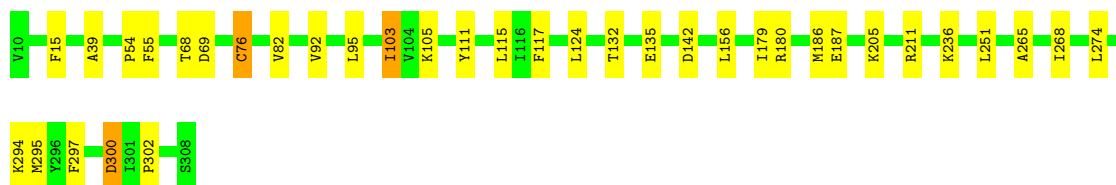
## • Molecule 2: Erlin-2

Chain m:  87% 13%




• Molecule 2: Erlin-2

Chain k:  88% 11%




• Molecule 2: Erlin-2

Chain l:  86% 13%




• Molecule 2: Erlin-2

Chain i:  89% 11%




• Molecule 2: Erlin-2

Chain g:  89% 11%



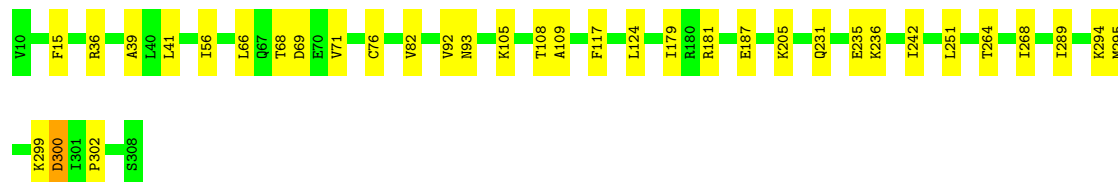
• Molecule 2: Erlin-2

Chain h:  87% 13%



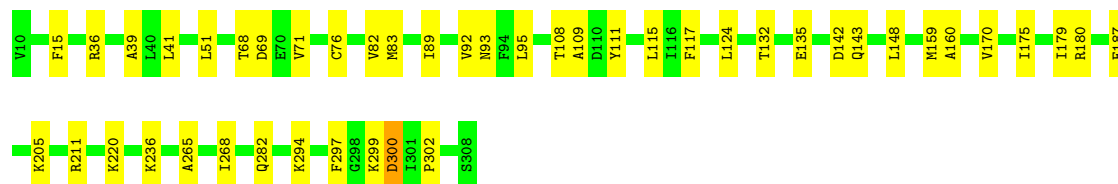
- Molecule 2: Erlin-2

Chain j: 88% 11%



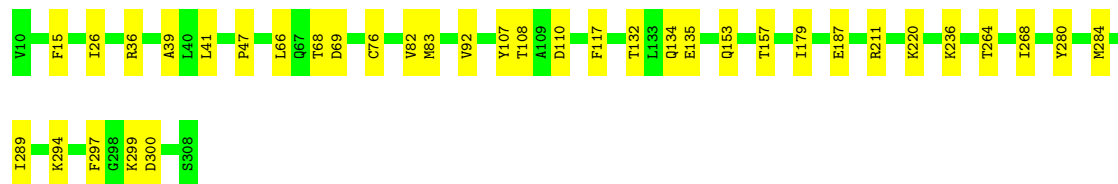
- Molecule 2: Erlin-2

Chain b: 85% 15%



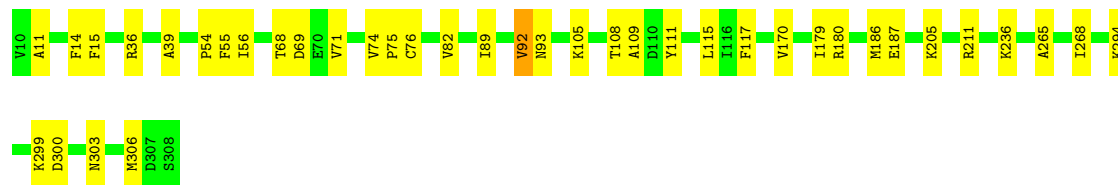
- Molecule 2: Erlin-2

Chain c: 88% 12%



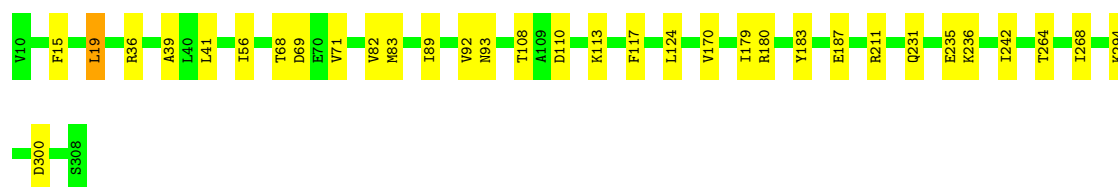
- Molecule 2: Erlin-2

Chain f: 87% 13%



- Molecule 2: Erlin-2

Chain d: 89% 11%



- Molecule 2: Erlin-2

Chain e: 88% 12%



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

Chain N: 50% 50%



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

Chain O: 50% 50%



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

Chain P: 50% 50%



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

Chain Q: 50% 50%



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

Chain R:  50% 50%

NAG1  
NAG2

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

Chain S:  50% 50%

NAG1  
NAG2

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

Chain T:  100%

NAG1  
NAG2

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

Chain U:  100%

NAG1  
NAG2

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

Chain V:  50% 50%

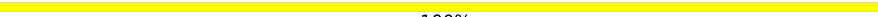
NAG1  
NAG2

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

Chain W:  50% 50%

NAG1  
NAG2

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

Chain X:  100%

NAG1  
NAG2

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

Chain Y:  50% 50%

MAG1  
MAG2

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

Chain Z:  50% 50%

MAG1  
MAG2

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

Chain n:  100%

MAG1  
MAG2

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

Chain o:  100%

MAG1  
MAG2

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

Chain p:  100%

MAG1  
MAG2

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

Chain q:  50% 50%

MAG1  
MAG2


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



Chain r:  50% 50%

MAG1  
MAG2

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

Chain s:  100%

MAG1  
MAG2

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

Chain t:  50% 50%


MAG1  
MAG2

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

Chain u:  50% 50%

MAG1  
MAG2

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

Chain v:  100%

MAG1  
MAG2

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

Chain w:  50% 50%

MAG1  
MAG2

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

Chain x:  50% 50%

MAG1  
MAG2

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

Chain y:  100%

MAG1  
MAG2

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

Chain z:  50% 50%

MAG1  
MAG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36885	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.20	0/2418	0.37	0/3265
1	B	0.20	0/2418	0.38	0/3265
1	C	0.20	0/2418	0.40	0/3265
1	D	0.20	0/2418	0.38	0/3265
1	E	0.20	0/2418	0.40	0/3265
1	F	0.20	0/2418	0.40	0/3265
1	G	0.20	0/2418	0.38	0/3265
1	H	0.20	0/2418	0.38	0/3265
1	I	0.20	0/2418	0.40	0/3265
1	J	0.20	0/2418	0.39	0/3265
1	K	0.20	0/2418	0.39	0/3265
1	L	0.20	0/2418	0.38	0/3265
1	M	0.20	0/2418	0.38	0/3265
2	a	0.19	0/2408	0.40	2/3247 (0.1%)
2	b	0.19	0/2408	0.40	2/3247 (0.1%)
2	c	0.19	0/2408	0.40	2/3247 (0.1%)
2	d	0.19	0/2408	0.41	2/3247 (0.1%)
2	e	0.19	0/2408	0.40	2/3247 (0.1%)
2	f	0.19	0/2408	0.41	2/3247 (0.1%)
2	g	0.19	0/2408	0.41	2/3247 (0.1%)
2	h	0.19	0/2408	0.41	2/3247 (0.1%)
2	i	0.19	0/2408	0.40	2/3247 (0.1%)
2	j	0.19	0/2408	0.40	2/3247 (0.1%)
2	k	0.19	0/2408	0.41	2/3247 (0.1%)
2	l	0.19	0/2408	0.40	2/3247 (0.1%)
2	m	0.19	0/2408	0.41	2/3247 (0.1%)
All	All	0.19	0/62738	0.40	26/84656 (0.0%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	300	ASP	CA-C-N	5.68	123.82	120.24
2	a	300	ASP	C-N-CA	5.68	123.82	120.24
2	c	300	ASP	CA-C-N	5.63	123.79	120.24
2	c	300	ASP	C-N-CA	5.63	123.79	120.24
2	m	300	ASP	CA-C-N	5.63	123.79	120.24
2	m	300	ASP	C-N-CA	5.63	123.79	120.24
2	g	300	ASP	CA-C-N	5.54	123.73	120.24
2	g	300	ASP	C-N-CA	5.54	123.73	120.24
2	k	300	ASP	CA-C-N	5.45	123.67	120.24
2	k	300	ASP	C-N-CA	5.45	123.67	120.24
2	e	300	ASP	CA-C-N	5.41	123.65	120.24
2	e	300	ASP	C-N-CA	5.41	123.65	120.24
2	j	300	ASP	CA-C-N	5.33	123.59	120.24
2	j	300	ASP	C-N-CA	5.33	123.59	120.24
2	h	300	ASP	CA-C-N	5.29	123.57	120.24
2	h	300	ASP	C-N-CA	5.29	123.57	120.24
2	i	300	ASP	CA-C-N	5.28	123.56	120.24
2	i	300	ASP	C-N-CA	5.28	123.56	120.24
2	d	300	ASP	CA-C-N	5.21	123.52	120.24
2	d	300	ASP	C-N-CA	5.21	123.52	120.24
2	l	300	ASP	CA-C-N	5.12	123.47	120.24
2	l	300	ASP	C-N-CA	5.12	123.47	120.24
2	f	300	ASP	CA-C-N	5.11	123.46	120.24
2	f	300	ASP	C-N-CA	5.11	123.46	120.24
2	b	300	ASP	CA-C-N	5.03	123.41	120.24
2	b	300	ASP	C-N-CA	5.03	123.41	120.24

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	2375	0	2425	31	0
1	B	2375	0	2425	23	0
1	C	2375	0	2425	28	0
1	D	2375	0	2425	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2375	0	2425	25	0
1	F	2375	0	2425	27	0
1	G	2375	0	2425	31	0
1	H	2375	0	2425	29	0
1	I	2375	0	2425	26	0
1	J	2375	0	2425	29	0
1	K	2375	0	2425	28	0
1	L	2375	0	2425	31	0
1	M	2375	0	2425	29	0
2	a	2367	0	2398	23	0
2	b	2367	0	2398	28	0
2	c	2367	0	2398	24	0
2	d	2367	0	2398	24	0
2	e	2367	0	2398	24	0
2	f	2367	0	2398	29	0
2	g	2367	0	2398	27	0
2	h	2367	0	2398	22	0
2	i	2367	0	2398	18	0
2	j	2367	0	2398	23	0
2	k	2367	0	2398	28	0
2	l	2367	0	2398	30	0
2	m	2367	0	2398	30	0
3	N	28	0	25	2	0
3	O	28	0	25	1	0
3	P	28	0	25	2	0
3	Q	28	0	25	0	0
3	R	28	0	25	2	0
3	S	28	0	25	2	0
3	T	28	0	25	0	0
3	U	28	0	25	0	0
3	V	28	0	25	2	0
3	W	28	0	25	2	0
3	X	28	0	25	0	0
3	Y	28	0	25	2	0
3	Z	28	0	25	2	0
3	n	28	0	25	1	0
3	o	28	0	25	0	0
3	p	28	0	25	0	0
3	q	28	0	25	2	0
3	r	28	0	25	2	0
3	s	28	0	25	1	0
3	t	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	u	28	0	25	2	0
3	v	28	0	25	0	0
3	w	28	0	25	2	0
3	x	28	0	25	2	0
3	y	28	0	25	0	0
3	z	28	0	25	0	0
All	All	62374	0	63349	559	0

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

All (559) 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:M:68:LEU:HD22	1:M:94:VAL:HG12	1.66	0.77
1:L:227:ALA:HA	1:L:230:ARG:HD3	1.67	0.75
1:E:104:ASP:HB3	3:w:1:NAG:H82	1.69	0.74
1:A:104:ASP:HB3	3:N:1:NAG:H82	1.74	0.70
1:J:226:VAL:HG12	1:J:230:ARG:HD2	1.73	0.70
1:D:104:ASP:HB3	3:x:1:NAG:H82	1.73	0.70
1:A:105:ILE:HG13	3:N:1:NAG:H81	1.74	0.69
1:K:104:ASP:HB3	3:S:1:NAG:H82	1.74	0.69
1:I:306:MET:SD	1:H:306:MET:HE3	2.32	0.69
1:M:297:ILE:HB	2:l:294:LYS:HG3	1.75	0.68
1:B:226:VAL:HG12	1:B:230:ARG:HD2	1.74	0.68
1:H:104:ASP:HB3	3:Y:1:NAG:H82	1.75	0.68
1:G:104:ASP:HB3	3:Z:1:NAG:H82	1.76	0.68
1:L:104:ASP:HB3	3:R:1:NAG:H82	1.75	0.68
1:E:105:ILE:HG13	3:w:1:NAG:H81	1.77	0.67
1:F:104:ASP:HB3	3:u:1:NAG:H82	1.77	0.67
1:M:49:PRO:HB2	2:l:39:ALA:HB2	1.77	0.67
2:c:68:THR:HG22	2:c:92:VAL:HG22	1.75	0.66
2:d:180:ARG:HH11	2:d:180:ARG:HG2	1.59	0.66
2:c:39:ALA:HB2	1:D:49:PRO:HB2	1.78	0.66
1:K:244:ILE:HG23	2:j:236:LYS:HG3	1.79	0.65
2:b:180:ARG:HG2	2:b:180:ARG:HH11	1.61	0.65
1:C:49:PRO:HB2	2:b:39:ALA:HB2	1.79	0.65
1:L:49:PRO:HB2	2:k:39:ALA:HB2	1.79	0.65
2:h:68:THR:HG22	2:h:92:VAL:HG13	1.79	0.65
1:J:227:ALA:HA	1:J:230:ARG:HD3	1.79	0.65
1:M:222:LYS:HB2	2:l:211:ARG:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:211:ARG:HG2	2:f:211:ARG:HH11	1.62	0.64
1:A:244:ILE:HG23	2:m:236:LYS:HG3	1.79	0.64
1:L:226:VAL:HG12	1:L:230:ARG:HD2	1.79	0.64
1:I:193:THR:HG21	2:h:179:ILE:HG23	1.79	0.64
2:l:68:THR:HG22	2:l:92:VAL:HG13	1.79	0.64
1:I:297:ILE:HB	2:h:294:LYS:HG3	1.80	0.64
1:B:227:ALA:HA	1:B:230:ARG:HD3	1.80	0.64
1:L:193:THR:HG21	2:k:179:ILE:HG23	1.80	0.64
1:L:297:ILE:HB	2:k:294:LYS:HG3	1.80	0.64
1:F:49:PRO:HB2	2:e:39:ALA:HB2	1.80	0.64
1:B:104:ASP:HB3	3:r:1:NAG:H82	1.80	0.64
1:D:182:ARG:HG2	1:D:182:ARG:HH11	1.63	0.63
1:L:306:MET:HE2	1:K:306:MET:HE2	1.80	0.63
1:J:20:LEU:HG	1:J:56:PRO:HG3	1.80	0.63
2:i:68:THR:HG22	2:i:92:VAL:HG13	1.80	0.63
1:C:244:ILE:HG23	2:b:236:LYS:HG3	1.79	0.63
2:a:179:ILE:HG23	1:B:193:THR:HG21	1.80	0.63
1:K:15:GLY:O	1:K:19:VAL:HG22	1.98	0.63
2:l:180:ARG:HG2	2:l:180:ARG:HH11	1.62	0.63
1:G:244:ILE:HG23	2:f:236:LYS:HG3	1.80	0.63
2:e:68:THR:HG22	2:e:92:VAL:HG13	1.81	0.63
2:f:180:ARG:HH11	2:f:180:ARG:HG2	1.64	0.63
1:I:104:ASP:HB3	3:W:1:NAG:H82	1.80	0.63
2:j:68:THR:HG22	2:j:92:VAL:HG13	1.82	0.62
2:c:108:THR:HG23	2:c:110:ASP:H	1.63	0.62
1:H:110:THR:HG23	1:H:112:ASP:H	1.64	0.62
1:D:20:LEU:O	1:D:24:SER:HB2	1.99	0.62
1:A:193:THR:HG21	2:m:179:ILE:HG23	1.82	0.62
2:c:236:LYS:HG3	1:D:244:ILE:HG23	1.80	0.62
1:A:213:ARG:HG2	2:a:220:LYS:HB2	1.81	0.62
1:G:297:ILE:HB	2:f:294:LYS:HG3	1.82	0.62
1:F:244:ILE:HG23	2:e:236:LYS:HG3	1.81	0.62
2:k:211:ARG:HG2	2:k:211:ARG:HH11	1.64	0.61
2:g:211:ARG:HH11	2:g:211:ARG:HG2	1.65	0.61
1:C:105:ILE:HG12	3:q:1:NAG:H81	1.82	0.61
1:C:104:ASP:HB3	3:q:1:NAG:H82	1.82	0.61
1:L:181:ILE:HG23	2:l:191:THR:HG21	1.81	0.61
1:E:49:PRO:HB2	2:d:39:ALA:HB2	1.82	0.61
1:L:244:ILE:HG23	2:k:236:LYS:HG3	1.82	0.61
2:d:68:THR:HG22	2:d:92:VAL:HG13	1.83	0.61
1:K:297:ILE:HB	2:j:294:LYS:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:297:ILE:HB	2:d:294:LYS:HG3	1.82	0.60
1:A:297:ILE:HB	2:m:294:LYS:HG3	1.83	0.60
2:m:68:THR:HG22	2:m:92:VAL:HG22	1.84	0.60
2:f:68:THR:HG22	2:f:92:VAL:HG13	1.83	0.60
1:G:226:VAL:HG12	1:G:230:ARG:HH12	1.66	0.60
1:C:297:ILE:HB	2:b:294:LYS:HG3	1.83	0.60
2:a:108:THR:HG22	2:a:110:ASP:H	1.67	0.60
1:C:226:VAL:HG12	1:C:230:ARG:HH12	1.66	0.60
2:c:179:ILE:HG23	1:D:193:THR:HG21	1.82	0.60
1:J:244:ILE:HG23	2:i:236:LYS:HG3	1.84	0.60
2:b:68:THR:HG22	2:b:92:VAL:HG13	1.84	0.60
1:E:244:ILE:HG23	2:d:236:LYS:HG3	1.82	0.59
1:I:38:ARG:HB3	1:I:43:LEU:HD21	1.82	0.59
1:F:297:ILE:HB	2:e:294:LYS:HG3	1.84	0.59
2:e:180:ARG:HG2	2:e:180:ARG:HH11	1.67	0.59
1:G:193:THR:HG21	2:f:179:ILE:HG23	1.83	0.59
1:K:193:THR:HG21	2:j:179:ILE:HG23	1.84	0.59
1:I:105:ILE:HG12	3:W:1:NAG:H81	1.85	0.59
1:C:193:THR:HG21	2:b:179:ILE:HG23	1.85	0.59
1:M:104:ASP:HB3	3:P:1:NAG:H82	1.84	0.59
1:M:244:ILE:HG23	2:l:236:LYS:HG3	1.83	0.59
2:g:68:THR:HG22	2:g:92:VAL:HG13	1.85	0.59
2:a:236:LYS:HG3	1:B:244:ILE:HG23	1.83	0.59
2:m:180:ARG:HG2	2:m:180:ARG:HH11	1.68	0.59
1:G:20:LEU:HG	1:G:56:PRO:HG2	1.84	0.59
1:J:193:THR:HG21	2:i:179:ILE:HG23	1.85	0.58
1:I:20:LEU:HG	1:I:56:PRO:HG3	1.85	0.58
1:L:110:THR:HG23	1:L:112:ASP:H	1.67	0.58
1:J:110:THR:HG23	1:J:112:ASP:H	1.69	0.58
1:E:193:THR:HG21	2:d:179:ILE:HG23	1.85	0.58
1:M:196:LEU:HB3	2:l:186:MET:HE2	1.86	0.58
1:M:193:THR:HG21	2:l:179:ILE:HG23	1.86	0.58
1:B:110:THR:HG23	1:B:112:ASP:H	1.69	0.58
2:c:294:LYS:HG3	1:D:297:ILE:HB	1.85	0.58
1:F:193:THR:HG21	2:e:179:ILE:HG23	1.85	0.58
1:A:226:VAL:HG12	1:A:230:ARG:HD2	1.84	0.57
2:a:68:THR:HG22	2:a:92:VAL:HG13	1.86	0.57
1:A:181:ILE:HG23	2:a:191:THR:HG21	1.86	0.57
1:H:193:THR:HG21	2:g:179:ILE:HG23	1.84	0.57
1:G:84:VAL:HG21	2:g:187:GLU:HG3	1.85	0.57
1:H:297:ILE:HB	2:g:294:LYS:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:ARG:HG2	1:C:182:ARG:HH11	1.69	0.57
1:A:109:TYR:O	1:A:110:THR:HG22	2.05	0.57
1:M:105:ILE:HG12	3:P:1:NAG:H81	1.87	0.57
1:C:213:ARG:HG2	2:c:220:LYS:HB2	1.87	0.57
1:B:213:ARG:HG2	2:b:220:LYS:HB2	1.86	0.57
1:K:110:THR:HG22	1:K:112:ASP:H	1.70	0.56
2:c:132:THR:HG22	2:c:135:GLU:HG3	1.87	0.56
2:a:294:LYS:HG3	1:B:297:ILE:HB	1.87	0.56
1:J:105:ILE:HG12	3:V:1:NAG:H81	1.88	0.56
1:I:213:ARG:HG2	2:i:220:LYS:HB2	1.87	0.56
1:I:110:THR:HG22	1:I:112:ASP:H	1.69	0.56
1:G:109:TYR:O	1:G:110:THR:HG22	2.05	0.56
2:e:132:THR:HG22	2:e:135:GLU:HG3	1.86	0.56
1:G:105:ILE:HG12	3:Z:1:NAG:H81	1.88	0.56
1:F:84:VAL:HG21	2:f:187:GLU:HG3	1.87	0.56
2:k:132:THR:HG22	2:k:135:GLU:HG3	1.87	0.55
1:H:109:TYR:O	1:H:110:THR:HG22	2.06	0.55
1:H:49:PRO:HB2	2:g:39:ALA:HB2	1.88	0.55
1:G:15:GLY:O	1:G:19:VAL:HG22	2.07	0.55
1:K:268:HIS:CE1	2:k:274:LEU:HD12	2.42	0.55
1:D:109:TYR:O	1:D:110:THR:HG22	2.06	0.55
2:l:108:THR:HG23	2:l:110:ASP:H	1.72	0.55
1:J:297:ILE:HB	2:i:294:LYS:HG3	1.88	0.55
1:D:105:ILE:HG13	3:x:1:NAG:H81	1.87	0.55
1:L:109:TYR:O	1:L:110:THR:HG22	2.06	0.55
2:j:36:ARG:HB2	2:j:41:LEU:HD21	1.89	0.55
1:E:181:ILE:HG23	2:e:191:THR:HG21	1.88	0.55
1:L:196:LEU:HB3	2:k:186:MET:HE2	1.90	0.54
1:K:55:LEU:HD23	1:K:56:PRO:HD2	1.89	0.54
2:k:68:THR:HG22	2:k:92:VAL:HG22	1.89	0.54
2:f:180:ARG:HG2	2:f:180:ARG:NH1	2.23	0.54
1:D:182:ARG:HG2	1:D:182:ARG:NH1	2.23	0.54
2:g:211:ARG:HG2	2:g:211:ARG:NH1	2.23	0.54
2:d:108:THR:HG22	2:d:110:ASP:H	1.73	0.54
1:M:268:HIS:HE1	2:m:274:LEU:HD12	1.73	0.54
1:L:38:ARG:HB3	1:L:43:LEU:HD21	1.90	0.54
1:J:109:TYR:O	1:J:110:THR:HG22	2.08	0.54
1:J:306:MET:HE2	1:I:306:MET:SD	2.48	0.54
1:H:226:VAL:HG12	1:H:230:ARG:HD2	1.90	0.54
1:K:84:VAL:HG21	2:k:187:GLU:HG3	1.89	0.54
2:h:299:LYS:NZ	2:h:299:LYS:HB3	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:180:ARG:HG2	2:l:180:ARG:NH1	2.23	0.53
1:H:105:ILE:HG12	3:Y:1:NAG:H81	1.89	0.53
1:C:109:TYR:O	1:C:110:THR:HG22	2.07	0.53
1:C:110:THR:HG23	1:C:112:ASP:H	1.73	0.53
1:B:38:ARG:HB3	1:B:43:LEU:HD21	1.91	0.53
1:F:226:VAL:O	1:F:230:ARG:HG3	2.08	0.53
1:J:21:LEU:O	1:J:25:ILE:HG13	2.09	0.53
1:D:226:VAL:HG12	1:D:230:ARG:HH12	1.74	0.53
2:k:211:ARG:HG2	2:k:211:ARG:NH1	2.22	0.53
1:J:104:ASP:HB3	3:V:1:NAG:H82	1.91	0.53
1:M:84:VAL:HG21	2:m:187:GLU:HG3	1.90	0.53
2:b:299:LYS:NZ	2:b:299:LYS:HB3	2.24	0.53
1:K:105:ILE:HG12	3:S:1:NAG:H81	1.91	0.52
1:G:72:GLU:HG3	1:G:92:GLU:HG2	1.91	0.52
1:J:84:VAL:HG21	2:j:187:GLU:HG3	1.92	0.52
1:H:244:ILE:HG23	2:g:236:LYS:HG3	1.90	0.52
1:C:84:VAL:HG21	2:c:187:GLU:HG3	1.91	0.52
2:b:180:ARG:HG2	2:b:180:ARG:NH1	2.22	0.52
2:f:211:ARG:HG2	2:f:211:ARG:NH1	2.25	0.52
1:J:38:ARG:HB3	1:J:43:LEU:HD21	1.91	0.52
1:B:109:TYR:O	1:B:110:THR:HG22	2.09	0.52
2:b:36:ARG:HB2	2:b:41:LEU:HD21	1.90	0.52
2:c:211:ARG:HG3	1:D:222:LYS:HB2	1.91	0.52
2:f:69:ASP:HB3	2:f:117:PHE:CZ	2.45	0.52
2:i:33:VAL:HB	2:i:40:LEU:HD11	1.90	0.52
2:m:299:LYS:HB3	2:m:299:LYS:NZ	2.23	0.52
1:F:308:VAL:HG22	1:E:308:VAL:HB	1.92	0.52
1:G:21:LEU:O	1:G:25:ILE:HG12	2.09	0.52
2:g:40:LEU:H	2:g:40:LEU:HD23	1.74	0.52
1:C:38:ARG:HB3	1:C:43:LEU:HD21	1.92	0.52
1:M:268:HIS:CE1	2:m:274:LEU:HD12	2.45	0.51
1:E:62:ARG:NH1	1:E:111:ALA:HB3	2.25	0.51
1:M:189:GLU:HG3	2:l:82:VAL:HG21	1.92	0.51
1:J:71:ASP:HB3	1:J:119:PHE:CZ	2.46	0.51
1:I:176:LYS:NZ	1:I:176:LYS:HB3	2.24	0.51
2:l:284:MET:HE2	2:l:284:MET:HA	1.93	0.51
1:E:84:VAL:HG21	2:e:187:GLU:HG3	1.92	0.51
2:l:69:ASP:HB3	2:l:117:PHE:CZ	2.46	0.51
1:K:268:HIS:HE1	2:k:274:LEU:HD12	1.75	0.51
2:c:26:ILE:HB	2:c:47:PRO:HA	1.93	0.51
1:H:213:ARG:HG2	2:h:220:LYS:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:69:ASP:HB3	2:d:117:PHE:CZ	2.45	0.51
2:i:299:LYS:NZ	2:i:299:LYS:HB3	2.26	0.51
2:f:54:PRO:HB2	2:f:55:PHE:HD2	1.76	0.51
1:D:84:VAL:HG21	2:d:187:GLU:HG3	1.92	0.51
2:m:69:ASP:HB3	2:m:117:PHE:CZ	2.45	0.50
1:I:244:ILE:HG23	2:h:236:LYS:HG3	1.93	0.50
2:i:132:THR:HG22	2:i:135:GLU:HG3	1.93	0.50
1:G:110:THR:HG23	1:G:112:ASP:H	1.76	0.50
2:h:36:ARG:HB2	2:h:41:LEU:HD21	1.92	0.50
2:c:299:LYS:NZ	2:c:299:LYS:HB3	2.27	0.50
1:F:71:ASP:HB3	1:F:119:PHE:CZ	2.46	0.50
1:A:110:THR:HG23	1:A:112:ASP:H	1.75	0.50
1:B:21:LEU:O	1:B:25:ILE:HG13	2.11	0.50
1:B:84:VAL:HG21	2:b:187:GLU:HG3	1.93	0.50
2:f:299:LYS:NZ	2:f:299:LYS:HB3	2.25	0.50
1:M:21:LEU:O	1:M:25:ILE:HG12	2.11	0.50
2:g:299:LYS:NZ	2:g:299:LYS:HB3	2.26	0.50
1:A:227:ALA:HA	1:A:230:ARG:HD3	1.92	0.50
1:L:21:LEU:O	1:L:25:ILE:HG13	2.10	0.50
1:F:105:ILE:HG13	3:u:1:NAG:H81	1.93	0.50
2:g:69:ASP:HB3	2:g:117:PHE:CZ	2.47	0.50
2:d:180:ARG:HG2	2:d:180:ARG:NH1	2.26	0.50
1:E:24:SER:OG	1:E:56:PRO:HG3	2.12	0.50
2:a:300:ASP:HB2	2:a:302:PRO:HD2	1.94	0.49
1:J:38:ARG:HG2	1:J:38:ARG:HH11	1.77	0.49
1:G:24:SER:HB2	1:G:56:PRO:HG3	1.94	0.49
1:B:105:ILE:HG12	3:r:1:NAG:H81	1.93	0.49
2:f:108:THR:HG22	2:f:109:ALA:N	2.27	0.49
1:I:21:LEU:O	1:I:25:ILE:HG13	2.12	0.49
2:f:108:THR:HG22	2:f:109:ALA:H	1.75	0.49
2:h:132:THR:HG22	2:h:135:GLU:HG3	1.95	0.49
1:C:21:LEU:O	1:C:25:ILE:HG13	2.12	0.49
1:H:84:VAL:HG21	2:h:187:GLU:HG3	1.93	0.49
2:h:95:LEU:HD13	2:h:163:LEU:HD13	1.95	0.49
2:b:132:THR:HG22	2:b:135:GLU:HG3	1.93	0.49
1:L:213:ARG:HG2	2:l:220:LYS:HB2	1.95	0.49
2:l:107:TYR:O	2:l:108:THR:HG22	2.13	0.49
1:A:49:PRO:HB2	2:m:39:ALA:HB2	1.94	0.49
2:a:299:LYS:NZ	2:a:299:LYS:HB3	2.27	0.49
1:G:71:ASP:HB3	1:G:119:PHE:CZ	2.48	0.49
2:a:180:ARG:HH11	2:a:180:ARG:HG2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:71:ASP:HB3	1:L:119:PHE:CZ	2.48	0.49
1:L:84:VAL:HG21	2:l:187:GLU:HG3	1.95	0.49
1:I:49:PRO:HB2	2:h:39:ALA:HB2	1.94	0.49
1:C:306:MET:HE2	1:B:306:MET:HB2	1.95	0.49
1:F:97:LEU:HD11	1:F:105:ILE:HD12	1.95	0.49
1:E:222:LYS:HB2	2:d:211:ARG:HG3	1.95	0.49
1:C:105:ILE:HD11	1:C:162:ALA:HB1	1.95	0.49
1:G:230:ARG:NH1	1:G:230:ARG:HB2	2.28	0.48
1:F:109:TYR:O	1:F:110:THR:HG22	2.12	0.48
2:j:69:ASP:HB3	2:j:117:PHE:CZ	2.47	0.48
2:b:69:ASP:HB3	2:b:117:PHE:CZ	2.48	0.48
1:E:148:GLU:O	1:E:152:GLN:HG2	2.12	0.48
2:e:299:LYS:HB3	2:e:299:LYS:NZ	2.28	0.48
2:m:153:GLN:HE21	2:m:157:THR:HG23	1.79	0.48
2:g:54:PRO:HB2	2:g:55:PHE:HD1	1.78	0.48
2:c:107:TYR:O	2:c:108:THR:HG22	2.13	0.48
2:e:69:ASP:HB3	2:e:117:PHE:CZ	2.49	0.48
1:G:49:PRO:HB2	2:f:39:ALA:HB2	1.95	0.48
1:B:24:SER:OG	1:B:56:PRO:HG3	2.13	0.48
2:a:82:VAL:HG21	1:B:189:GLU:HG3	1.95	0.48
2:e:153:GLN:HE21	2:e:157:THR:HG23	1.77	0.48
1:C:230:ARG:HB2	1:C:230:ARG:NH1	2.29	0.48
2:c:69:ASP:HB3	2:c:117:PHE:CZ	2.48	0.48
1:H:21:LEU:O	1:H:25:ILE:HG13	2.14	0.48
2:j:264:THR:O	2:j:268:ILE:HG22	2.14	0.48
1:D:55:LEU:HD23	1:D:56:PRO:HD2	1.96	0.48
1:L:188:MET:HE3	1:L:192:LYS:HD2	1.96	0.48
1:G:308:VAL:HG22	1:F:308:VAL:HB	1.95	0.47
2:k:69:ASP:HB3	2:k:117:PHE:CZ	2.48	0.47
2:l:299:LYS:NZ	2:l:299:LYS:HB3	2.29	0.47
2:j:108:THR:HG22	2:j:109:ALA:N	2.29	0.47
2:f:111:TYR:O	2:f:115:LEU:HB2	2.14	0.47
1:D:110:THR:HG23	1:D:112:ASP:H	1.77	0.47
1:L:105:ILE:HG12	3:R:1:NAG:H81	1.96	0.47
2:i:69:ASP:HB3	2:i:117:PHE:CZ	2.49	0.47
2:f:36:ARG:HG3	2:f:56:ILE:HG22	1.96	0.47
1:A:182:ARG:HG2	1:A:182:ARG:HH11	1.79	0.47
2:a:69:ASP:HB3	2:a:117:PHE:CZ	2.48	0.47
2:h:108:THR:HG22	2:h:109:ALA:N	2.29	0.47
1:M:27:LYS:NZ	1:M:27:LYS:HB2	2.28	0.47
2:m:108:THR:HG22	2:m:109:ALA:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:55:LEU:HD23	1:I:56:PRO:HD2	1.95	0.47
2:m:36:ARG:HB2	2:m:41:LEU:HD21	1.97	0.47
1:K:71:ASP:HB3	1:K:119:PHE:CZ	2.50	0.47
1:G:105:ILE:HD11	1:G:162:ALA:HB1	1.96	0.47
2:g:108:THR:HG22	2:g:109:ALA:N	2.30	0.47
2:c:36:ARG:HB2	2:c:41:LEU:HD21	1.95	0.47
1:D:305:ASN:HB2	1:D:306:MET:HE3	1.96	0.47
1:J:28:ILE:HB	1:J:49:PRO:HA	1.95	0.47
2:j:299:LYS:HB2	2:j:299:LYS:NZ	2.28	0.47
1:C:71:ASP:HB3	1:C:119:PHE:CZ	2.50	0.47
2:k:95:LEU:HD11	2:k:103:ILE:HD12	1.97	0.47
1:H:62:ARG:NH1	1:H:111:ALA:HB3	2.30	0.47
2:h:69:ASP:HB3	2:h:117:PHE:CZ	2.50	0.47
1:F:62:ARG:HH21	1:F:111:ALA:HB3	1.80	0.47
1:A:62:ARG:NH2	1:A:111:ALA:HB3	2.29	0.46
2:i:108:THR:HG22	2:i:109:ALA:N	2.30	0.46
2:c:264:THR:O	2:c:268:ILE:HG22	2.15	0.46
2:i:10:VAL:HG22	2:i:12:SER:H	1.80	0.46
1:F:38:ARG:HB3	1:F:43:LEU:HD21	1.98	0.46
1:M:20:LEU:HG	1:M:56:PRO:HG2	1.98	0.46
1:A:20:LEU:O	1:A:24:SER:HB2	2.16	0.46
1:L:24:SER:OG	1:L:56:PRO:HG3	2.15	0.46
1:K:53:ILE:HD12	1:K:53:ILE:HA	1.83	0.46
1:K:34:ALA:HB3	1:K:47:SER:HB3	1.98	0.46
1:C:306:MET:HG2	1:D:306:MET:CG	2.46	0.46
2:d:36:ARG:HB2	2:d:41:LEU:HD21	1.97	0.46
1:I:201:LYS:HE2	1:I:201:LYS:HB2	1.72	0.46
1:H:126:LEU:HD13	1:H:150:LEU:HD11	1.98	0.46
2:c:153:GLN:HE21	2:c:157:THR:HG23	1.80	0.46
1:I:38:ARG:HD3	1:I:58:ILE:HG22	1.97	0.46
1:C:30:GLU:HG2	2:b:39:ALA:HA	1.98	0.46
1:M:109:TYR:O	1:M:110:THR:HG22	2.16	0.45
1:G:189:GLU:HG3	2:f:82:VAL:HG21	1.98	0.45
1:A:308:VAL:HG22	1:M:308:VAL:HB	1.98	0.45
1:M:38:ARG:HB2	1:M:43:LEU:HD21	1.99	0.45
1:C:182:ARG:HG2	1:C:182:ARG:NH1	2.29	0.45
1:E:109:TYR:O	1:E:110:THR:HG22	2.16	0.45
1:A:71:ASP:HB3	1:A:119:PHE:CZ	2.51	0.45
2:h:54:PRO:HB2	2:h:55:PHE:HD1	1.82	0.45
1:F:42:LEU:HD12	1:F:42:LEU:HA	1.85	0.45
1:E:71:ASP:HB3	1:E:119:PHE:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:236:LYS:HA	2:d:236:LYS:HD3	1.84	0.45
1:L:42:LEU:HD12	1:L:42:LEU:HA	1.85	0.45
2:k:54:PRO:HB2	2:k:55:PHE:CD2	2.51	0.45
1:B:28:ILE:HB	1:B:49:PRO:HA	1.98	0.45
1:G:296:LYS:HB3	2:g:295:MET:HG3	1.99	0.45
1:F:24:SER:OG	1:F:56:PRO:HG3	2.17	0.45
1:A:297:ILE:HD12	2:m:294:LYS:HD2	1.99	0.45
2:k:300:ASP:HB2	2:k:302:PRO:HD2	1.99	0.45
2:l:300:ASP:HB2	2:l:302:PRO:HD2	1.99	0.45
2:h:108:THR:HG22	2:h:109:ALA:H	1.80	0.45
1:E:30:GLU:HG2	2:d:39:ALA:HA	1.97	0.45
2:a:105:LYS:HB3	2:a:105:LYS:HE2	1.80	0.45
2:a:111:TYR:O	2:a:115:LEU:HB2	2.17	0.45
1:M:297:ILE:HD12	2:l:294:LYS:HD2	1.99	0.45
2:h:11:ALA:HA	2:h:14:PHE:CD2	2.52	0.45
1:C:308:VAL:HG22	1:B:308:VAL:HB	1.99	0.45
1:F:189:GLU:HG3	2:e:82:VAL:HG21	1.99	0.45
1:D:71:ASP:HB3	1:D:119:PHE:CZ	2.52	0.45
2:m:211:ARG:HG2	2:m:211:ARG:HH11	1.82	0.45
1:J:42:LEU:HD12	1:J:42:LEU:HA	1.88	0.45
1:J:308:VAL:HG22	1:I:308:VAL:HB	1.99	0.45
1:F:176:LYS:NZ	1:F:176:LYS:HB3	2.32	0.45
2:f:303:ASN:HA	2:f:306:MET:HE3	1.99	0.45
1:K:42:LEU:HD12	1:K:42:LEU:HA	1.87	0.44
2:g:105:LYS:HE2	2:g:105:LYS:HB3	1.80	0.44
1:E:42:LEU:HD12	1:E:42:LEU:HA	1.85	0.44
2:e:13:SER:HA	2:e:16:CYS:SG	2.57	0.44
1:M:188:MET:HE2	2:m:194:LEU:HB3	1.98	0.44
1:J:306:MET:HG3	1:I:306:MET:HE2	1.99	0.44
1:H:30:GLU:HG3	2:g:40:LEU:HD23	1.99	0.44
1:G:306:MET:HE2	1:F:306:MET:HG3	1.99	0.44
1:B:306:MET:HE2	1:B:306:MET:HB3	1.68	0.44
2:c:39:ALA:HA	1:D:30:GLU:HG2	2.00	0.44
2:g:300:ASP:HB2	2:g:302:PRO:HD2	1.98	0.44
2:c:82:VAL:HG21	1:D:189:GLU:HG3	2.00	0.44
2:d:83:MET:HE3	2:d:83:MET:HB3	1.70	0.44
2:d:89:ILE:HG12	2:d:170:VAL:HG12	2.00	0.44
1:E:189:GLU:HG3	2:d:82:VAL:HG21	1.99	0.44
2:m:108:THR:HG22	2:m:109:ALA:H	1.83	0.44
2:h:105:LYS:HE2	2:h:105:LYS:HB3	1.82	0.44
2:e:300:ASP:HB2	2:e:302:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:284:MET:HE2	2:a:284:MET:HA	2.00	0.44
1:J:296:LYS:HB3	2:j:295:MET:HG3	1.98	0.44
2:a:295:MET:HE2	2:a:295:MET:HB2	1.85	0.44
1:L:78:CYS:SG	1:L:126:LEU:HG	2.58	0.44
2:k:111:TYR:O	2:k:115:LEU:HB2	2.17	0.44
1:J:182:ARG:HG2	1:J:182:ARG:HH11	1.83	0.44
2:h:295:MET:HE2	2:h:295:MET:HB2	1.83	0.44
2:j:300:ASP:HB2	2:j:302:PRO:HD2	2.00	0.44
1:D:21:LEU:O	1:D:25:ILE:HG13	2.17	0.44
2:e:265:ALA:HA	2:e:268:ILE:HG22	2.00	0.44
1:A:201:LYS:HB2	1:A:201:LYS:HE2	1.73	0.44
1:L:297:ILE:HD12	2:k:294:LYS:HD2	2.00	0.44
1:K:308:VAL:HG22	1:J:308:VAL:HB	2.00	0.44
1:I:308:VAL:HG22	1:H:308:VAL:HB	2.00	0.44
2:i:142:ASP:OD2	2:i:143:GLN:HG2	2.18	0.44
1:D:58:ILE:HD13	1:D:58:ILE:HA	1.86	0.44
2:a:265:ALA:HA	2:a:268:ILE:HG22	1.99	0.44
2:m:251:LEU:HD23	2:m:251:LEU:HA	1.83	0.44
2:b:211:ARG:HH11	2:b:211:ARG:HG2	1.82	0.44
1:D:68:LEU:HD12	1:D:96:MET:HB3	1.98	0.44
2:d:56:ILE:HD13	2:d:56:ILE:HA	1.83	0.44
1:E:238:LYS:HG3	2:e:242:ILE:HG23	1.99	0.43
1:H:308:VAL:HG22	1:G:308:VAL:HB	2.00	0.43
2:j:231:GLN:O	2:j:235:GLU:HG3	2.18	0.43
1:C:28:ILE:HB	1:C:49:PRO:HA	1.98	0.43
2:k:205:LYS:HA	2:k:205:LYS:HD3	1.89	0.43
2:k:251:LEU:HD23	2:k:251:LEU:HA	1.84	0.43
2:l:105:LYS:HE2	2:l:105:LYS:HB3	1.82	0.43
2:j:205:LYS:HA	2:j:205:LYS:HD3	1.89	0.43
2:b:83:MET:HE2	2:b:83:MET:HB2	1.78	0.43
1:A:85:MET:HB3	1:A:85:MET:HE3	1.72	0.43
1:K:58:ILE:HD13	1:K:58:ILE:HA	1.89	0.43
2:i:265:ALA:HA	2:i:268:ILE:HG22	2.00	0.43
2:f:236:LYS:HD3	2:f:236:LYS:HA	1.87	0.43
1:E:97:LEU:HD11	1:E:105:ILE:HD12	2.00	0.43
2:a:36:ARG:HB2	2:a:41:LEU:HD21	1.99	0.43
1:L:105:ILE:HD11	1:L:162:ALA:HB1	1.99	0.43
2:c:83:MET:HE3	2:c:83:MET:HB3	1.79	0.43
1:F:72:GLU:HG2	1:F:92:GLU:HG2	2.00	0.43
1:M:70:THR:HG23	1:M:94:VAL:HG22	2.01	0.43
1:M:71:ASP:HB3	1:M:119:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:297:ILE:HD12	2:g:294:LYS:HD2	2.00	0.43
2:b:265:ALA:HA	2:b:268:ILE:HG22	2.00	0.43
1:J:189:GLU:HG3	2:i:82:VAL:HG21	2.01	0.43
2:b:108:THR:HG22	2:b:109:ALA:N	2.33	0.43
2:b:205:LYS:HA	2:b:205:LYS:HD3	1.90	0.43
2:c:297:PHE:HB3	1:D:302:ASN:O	2.19	0.43
1:E:38:ARG:HH21	1:E:43:LEU:HD13	1.84	0.43
1:A:182:ARG:HG2	1:A:182:ARG:NH1	2.33	0.43
1:G:42:LEU:HD12	1:G:42:LEU:HA	1.86	0.43
2:b:300:ASP:HB2	2:b:302:PRO:HD2	2.00	0.43
2:f:105:LYS:HE2	2:f:105:LYS:HB3	1.79	0.43
2:a:180:ARG:HG2	2:a:180:ARG:NH1	2.34	0.43
1:M:238:LYS:HG3	2:m:242:ILE:HG23	2.01	0.43
2:l:251:LEU:HD23	2:l:251:LEU:HA	1.85	0.43
2:j:105:LYS:HB3	2:j:105:LYS:HE2	1.82	0.43
2:e:236:LYS:HD3	2:e:236:LYS:HA	1.83	0.43
2:g:153:GLN:HE21	2:g:157:THR:HG23	1.84	0.43
2:f:11:ALA:HA	2:f:14:PHE:CD2	2.54	0.43
2:a:236:LYS:HD3	2:a:236:LYS:HA	1.84	0.42
2:l:236:LYS:HD3	2:l:236:LYS:HA	1.89	0.42
1:H:189:GLU:HG3	2:g:82:VAL:HG21	2.00	0.42
2:g:11:ALA:HA	2:g:14:PHE:CD2	2.54	0.42
2:h:83:MET:HE2	2:h:83:MET:HB2	1.83	0.42
1:K:236:MET:HE3	1:K:236:MET:HB3	1.91	0.42
2:k:265:ALA:HA	2:k:268:ILE:HG22	2.01	0.42
1:J:78:CYS:SG	1:J:126:LEU:HG	2.59	0.42
1:H:20:LEU:HD23	1:H:21:LEU:HD22	2.01	0.42
1:F:20:LEU:HG	1:F:56:PRO:HG2	2.00	0.42
2:a:231:GLN:O	2:a:235:GLU:HG3	2.18	0.42
1:L:302:ASN:O	2:k:297:PHE:HB3	2.18	0.42
1:J:238:LYS:HG3	2:j:242:ILE:HG23	2.01	0.42
2:j:108:THR:HG22	2:j:109:ALA:H	1.84	0.42
2:c:280:TYR:OH	2:c:284:MET:HE2	2.19	0.42
1:E:55:LEU:HA	1:E:56:PRO:HD3	1.90	0.42
2:i:105:LYS:HB3	2:i:105:LYS:HE2	1.80	0.42
2:c:236:LYS:HD3	2:c:236:LYS:HA	1.85	0.42
1:E:308:VAL:HG22	1:D:308:VAL:HB	2.00	0.42
1:A:20:LEU:O	1:A:24:SER:CB	2.68	0.42
2:a:103:ILE:HG12	3:O:1:NAG:H81	2.02	0.42
1:M:55:LEU:HD12	1:M:55:LEU:HA	1.85	0.42
2:l:205:LYS:HA	2:l:205:LYS:HD3	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:201:LYS:HE2	1:H:201:LYS:HB2	1.76	0.42
1:E:113:TYR:O	1:E:117:LEU:HB2	2.20	0.42
1:L:55:LEU:HA	1:L:56:PRO:HD3	1.89	0.42
2:h:213:LYS:O	2:h:217:GLU:HG3	2.20	0.42
1:A:34:ALA:HB3	1:A:47:SER:HB3	2.01	0.42
1:M:295:SER:HA	2:m:294:LYS:O	2.20	0.42
2:m:179:ILE:HG22	2:m:183:TYR:CE2	2.54	0.42
1:K:297:ILE:HD12	2:j:294:LYS:HD2	2.02	0.42
1:H:78:CYS:SG	1:H:126:LEU:HG	2.60	0.42
1:L:189:GLU:HG3	2:k:82:VAL:HG21	2.02	0.42
1:K:38:ARG:HH21	1:K:43:LEU:HD13	1.85	0.42
1:J:182:ARG:HG2	1:J:182:ARG:NH1	2.35	0.42
1:I:78:CYS:SG	1:I:126:LEU:HG	2.60	0.42
2:j:289:ILE:HD13	2:j:289:ILE:HA	1.87	0.42
1:B:62:ARG:HE	1:B:62:ARG:HB3	1.65	0.42
2:b:89:ILE:HG12	2:b:170:VAL:HG12	2.01	0.42
2:k:76:CYS:HB2	2:k:124:LEU:HD11	2.01	0.42
1:C:85:MET:HE3	1:C:85:MET:HB3	1.90	0.42
2:f:205:LYS:HA	2:f:205:LYS:HD3	1.95	0.42
2:e:105:LYS:HB3	2:e:105:LYS:HE2	1.82	0.42
2:m:231:GLN:O	2:m:235:GLU:HG3	2.20	0.42
1:J:306:MET:HG3	1:I:306:MET:HB2	2.01	0.42
1:I:21:LEU:HD13	1:I:21:LEU:HA	1.95	0.42
2:b:160:ALA:HA	3:s:1:NAG:O7	2.20	0.42
2:d:113:LYS:HE3	2:d:113:LYS:HB3	1.94	0.42
2:d:264:THR:O	2:d:268:ILE:HG22	2.20	0.42
1:A:189:GLU:HG3	2:m:82:VAL:HG21	2.01	0.41
1:A:308:VAL:HB	1:B:308:VAL:HG22	2.02	0.41
2:m:265:ALA:HA	2:m:268:ILE:HG22	2.01	0.41
1:L:201:LYS:HE2	1:L:201:LYS:HB2	1.73	0.41
1:H:306:MET:SD	1:G:306:MET:SD	3.18	0.41
2:f:89:ILE:HG12	2:f:170:VAL:HG12	2.01	0.41
2:m:105:LYS:HE2	2:m:105:LYS:HB3	1.81	0.41
1:D:42:LEU:HD12	1:D:42:LEU:HA	1.86	0.41
2:e:108:THR:HG22	2:e:110:ASP:H	1.85	0.41
1:A:30:GLU:HG2	2:m:39:ALA:HA	2.02	0.41
1:K:189:GLU:HG3	2:j:82:VAL:HG21	2.02	0.41
2:l:265:ALA:HA	2:l:268:ILE:HG22	2.01	0.41
1:F:207:LYS:HA	1:F:207:LYS:HD3	1.82	0.41
1:D:201:LYS:HB2	1:D:201:LYS:HE2	1.73	0.41
1:I:189:GLU:HG3	2:h:82:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:78:CYS:SG	1:G:126:LEU:HG	2.61	0.41
2:g:265:ALA:HA	2:g:268:ILE:HG22	2.03	0.41
2:e:289:ILE:HD13	2:e:289:ILE:HA	1.89	0.41
2:a:19:LEU:HD13	2:a:19:LEU:HA	1.88	0.41
1:K:78:CYS:SG	1:K:126:LEU:HG	2.60	0.41
1:H:24:SER:OG	1:H:56:PRO:HG3	2.21	0.41
1:G:55:LEU:HA	1:G:56:PRO:HD3	1.88	0.41
2:g:67:GLN:HG3	2:g:93:ASN:OD1	2.21	0.41
1:B:78:CYS:SG	1:B:126:LEU:HG	2.60	0.41
2:b:159:MET:HE2	2:b:159:MET:HB3	1.89	0.41
2:d:179:ILE:HG22	2:d:183:TYR:CE2	2.56	0.41
1:L:188:MET:CE	1:L:192:LYS:HD2	2.51	0.41
1:K:49:PRO:HB2	2:j:39:ALA:HB2	2.01	0.41
2:l:36:ARG:HB2	2:l:41:LEU:HD21	2.01	0.41
2:l:153:GLN:HE22	2:l:165:ILE:H	1.68	0.41
2:j:251:LEU:HD23	2:j:251:LEU:HA	1.83	0.41
2:b:142:ASP:OD1	2:b:143:GLN:HG2	2.21	0.41
2:f:265:ALA:HA	2:f:268:ILE:HG22	2.02	0.41
2:e:83:MET:HE2	2:e:83:MET:HB2	1.81	0.41
1:A:42:LEU:HD12	1:A:42:LEU:HA	1.88	0.41
1:A:282:TYR:CZ	1:A:286:LYS:HD2	2.55	0.41
2:m:236:LYS:HA	2:m:236:LYS:HD3	1.87	0.41
1:K:13:VAL:HG13	1:K:14:VAL:H	1.84	0.41
2:l:83:MET:HE2	2:l:83:MET:HB2	1.79	0.41
2:l:95:LEU:HD11	2:l:103:ILE:HD12	2.02	0.41
2:g:56:ILE:HD13	2:g:56:ILE:HA	1.89	0.41
1:F:282:TYR:CZ	1:F:286:LYS:HD2	2.56	0.41
1:D:97:LEU:HD11	1:D:105:ILE:HD12	2.03	0.41
1:A:181:ILE:HG22	1:A:185:PHE:CE2	2.56	0.41
1:M:308:VAL:HG22	1:L:308:VAL:HB	2.02	0.41
1:L:297:ILE:HG23	2:l:296:TYR:HD2	1.85	0.41
2:k:105:LYS:HB3	2:k:105:LYS:HE2	1.81	0.41
1:H:160:LEU:HD12	1:H:161:MET:N	2.36	0.41
1:H:253:LEU:HD12	1:H:253:LEU:HA	1.95	0.41
1:G:30:GLU:HG2	2:f:39:ALA:HA	2.03	0.41
1:G:196:LEU:HB3	2:f:186:MET:HE2	2.02	0.41
1:G:201:LYS:HE2	1:G:201:LYS:HB2	1.73	0.41
2:g:108:THR:HG22	2:g:109:ALA:H	1.83	0.41
1:A:55:LEU:HD23	1:A:56:PRO:HD2	2.03	0.41
2:m:156:LEU:HD23	2:m:156:LEU:HA	1.87	0.41
1:J:37:TYR:HA	1:J:41:ALA:O	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:153:GLN:HE22	2:i:165:ILE:H	1.69	0.41
1:H:28:ILE:HB	1:H:49:PRO:HA	2.03	0.41
1:H:282:TYR:CZ	1:H:286:LYS:HD2	2.56	0.41
1:G:37:TYR:HA	1:G:41:ALA:O	2.21	0.41
2:h:153:GLN:HE22	2:h:165:ILE:H	1.68	0.41
2:b:111:TYR:O	2:b:115:LEU:HB2	2.21	0.41
1:F:306:MET:HB3	1:E:306:MET:HG3	2.03	0.41
2:f:74:VAL:HA	2:f:75:PRO:HD3	1.96	0.41
2:e:40:LEU:H	2:e:40:LEU:HD23	1.85	0.41
1:K:30:GLU:HG2	2:j:39:ALA:HA	2.02	0.40
2:k:115:LEU:HD23	2:k:115:LEU:HA	1.87	0.40
2:k:156:LEU:HD23	2:k:156:LEU:HA	1.92	0.40
1:A:78:CYS:SG	1:A:126:LEU:HG	2.62	0.40
1:M:20:LEU:HD23	1:M:21:LEU:HD22	2.03	0.40
1:K:96:MET:HE3	1:K:166:THR:HB	2.03	0.40
1:I:37:TYR:HA	1:I:41:ALA:O	2.21	0.40
2:g:83:MET:HE2	2:g:83:MET:HB2	1.81	0.40
1:C:201:LYS:HB2	1:C:201:LYS:HE2	1.75	0.40
2:b:175:ILE:HD12	2:b:179:ILE:HB	2.02	0.40
1:F:37:TYR:HA	1:F:41:ALA:O	2.22	0.40
1:D:238:LYS:HG3	2:d:242:ILE:HG23	2.04	0.40
2:e:36:ARG:HB2	2:e:41:LEU:HD21	2.03	0.40
1:K:201:LYS:HB2	1:K:201:LYS:HE2	1.76	0.40
2:k:180:ARG:HH11	2:k:180:ARG:HG2	1.86	0.40
1:I:91:ILE:HG12	1:I:172:VAL:HG12	2.03	0.40
2:i:36:ARG:HB2	2:i:41:LEU:HD21	2.02	0.40
1:C:189:GLU:HG3	2:b:82:VAL:HG21	2.04	0.40
1:C:308:VAL:HB	1:D:308:VAL:HG22	2.02	0.40
2:c:294:LYS:HD2	1:D:297:ILE:HD12	2.03	0.40
1:F:160:LEU:HD12	1:F:161:MET:N	2.36	0.40
2:f:55:PHE:C	2:f:56:ILE:HD13	2.46	0.40
1:M:201:LYS:HE2	1:M:201:LYS:HB2	1.74	0.40
2:g:103:ILE:HG12	3:n:1:NAG:H81	2.03	0.40
1:C:302:ASN:O	2:b:297:PHE:HB3	2.22	0.40
1:B:42:LEU:HD12	1:B:42:LEU:HA	1.87	0.40
1:D:78:CYS:SG	1:D:126:LEU:HG	2.61	0.40
2:d:19:LEU:HD13	2:d:19:LEU:HA	1.90	0.40
2:d:231:GLN:O	2:d:235:GLU:HG3	2.20	0.40
2:m:76:CYS:HB2	2:m:124:LEU:HD11	2.03	0.40
2:i:108:THR:HG22	2:i:109:ALA:H	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	295/297 (99%)	290 (98%)	5 (2%)	0	100	100
1	B	295/297 (99%)	288 (98%)	7 (2%)	0	100	100
1	C	295/297 (99%)	290 (98%)	5 (2%)	0	100	100
1	D	295/297 (99%)	291 (99%)	4 (1%)	0	100	100
1	E	295/297 (99%)	290 (98%)	4 (1%)	1 (0%)	36	60
1	F	295/297 (99%)	289 (98%)	6 (2%)	0	100	100
1	G	295/297 (99%)	287 (97%)	8 (3%)	0	100	100
1	H	295/297 (99%)	291 (99%)	4 (1%)	0	100	100
1	I	295/297 (99%)	289 (98%)	6 (2%)	0	100	100
1	J	295/297 (99%)	288 (98%)	7 (2%)	0	100	100
1	K	295/297 (99%)	289 (98%)	6 (2%)	0	100	100
1	L	295/297 (99%)	288 (98%)	7 (2%)	0	100	100
1	M	295/297 (99%)	288 (98%)	7 (2%)	0	100	100
2	a	297/299 (99%)	290 (98%)	7 (2%)	0	100	100
2	b	297/299 (99%)	290 (98%)	7 (2%)	0	100	100
2	c	297/299 (99%)	290 (98%)	7 (2%)	0	100	100
2	d	297/299 (99%)	289 (97%)	8 (3%)	0	100	100
2	e	297/299 (99%)	289 (97%)	8 (3%)	0	100	100
2	f	297/299 (99%)	290 (98%)	7 (2%)	0	100	100
2	g	297/299 (99%)	291 (98%)	6 (2%)	0	100	100
2	h	297/299 (99%)	289 (97%)	8 (3%)	0	100	100
2	i	297/299 (99%)	290 (98%)	7 (2%)	0	100	100
2	j	297/299 (99%)	289 (97%)	8 (3%)	0	100	100
2	k	297/299 (99%)	289 (97%)	8 (3%)	0	100	100
2	l	297/299 (99%)	289 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	m	297/299 (99%)	289 (97%)	8 (3%)	0	100	100
All	All	7696/7748 (99%)	7522 (98%)	173 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	110	THR

### 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	255/255 (100%)	240 (94%)	15 (6%)	18	42
1	B	255/255 (100%)	243 (95%)	12 (5%)	23	51
1	C	255/255 (100%)	249 (98%)	6 (2%)	43	72
1	D	255/255 (100%)	245 (96%)	10 (4%)	28	57
1	E	255/255 (100%)	246 (96%)	9 (4%)	32	61
1	F	255/255 (100%)	243 (95%)	12 (5%)	23	51
1	G	255/255 (100%)	247 (97%)	8 (3%)	35	65
1	H	255/255 (100%)	248 (97%)	7 (3%)	39	69
1	I	255/255 (100%)	245 (96%)	10 (4%)	28	57
1	J	255/255 (100%)	240 (94%)	15 (6%)	18	42
1	K	255/255 (100%)	245 (96%)	10 (4%)	28	57
1	L	255/255 (100%)	246 (96%)	9 (4%)	32	61
1	M	255/255 (100%)	247 (97%)	8 (3%)	35	65
2	a	258/258 (100%)	248 (96%)	10 (4%)	28	57
2	b	258/258 (100%)	249 (96%)	9 (4%)	32	61
2	c	258/258 (100%)	253 (98%)	5 (2%)	50	77
2	d	258/258 (100%)	253 (98%)	5 (2%)	50	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	e	258/258 (100%)	253 (98%)	5 (2%)	50	77
2	f	258/258 (100%)	253 (98%)	5 (2%)	50	77
2	g	258/258 (100%)	257 (100%)	1 (0%)	84	93
2	h	258/258 (100%)	251 (97%)	7 (3%)	39	69
2	i	258/258 (100%)	252 (98%)	6 (2%)	44	73
2	j	258/258 (100%)	250 (97%)	8 (3%)	35	65
2	k	258/258 (100%)	253 (98%)	5 (2%)	50	77
2	l	258/258 (100%)	248 (96%)	10 (4%)	28	57
2	m	258/258 (100%)	251 (97%)	7 (3%)	39	69
All	All	6669/6669 (100%)	6455 (97%)	214 (3%)	35	64

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	60	THR
1	A	63	SER
1	A	68	LEU
1	A	73	VAL
1	A	78	CYS
1	A	85	MET
1	A	105	ILE
1	A	150	LEU
1	A	151	LYS
1	A	152	GLN
1	A	301	SER
1	A	303	ILE
1	A	307	PHE
1	A	308	VAL
2	a	15	PHE
2	a	19	LEU
2	a	40	LEU
2	a	71	VAL
2	a	93	ASN
2	a	94	PHE
2	a	95	LEU
2	a	124	LEU
2	a	155	ASP
2	a	282	GLN

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Mol	Chain	Res	Type
1	M	53	ILE
1	M	60	THR
1	M	63	SER
1	M	73	VAL
1	M	78	CYS
1	M	207	LYS
1	M	301	SER
1	M	307	PHE
2	m	15	PHE
2	m	40	LEU
2	m	66	LEU
2	m	71	VAL
2	m	76	CYS
2	m	93	ASN
2	m	148	LEU
1	L	13	VAL
1	L	21	LEU
1	L	25	ILE
1	L	58	ILE
1	L	60	THR
1	L	78	CYS
1	L	150	LEU
1	L	151	LYS
1	L	307	PHE
1	K	13	VAL
1	K	21	LEU
1	K	29	GLU
1	K	60	THR
1	K	73	VAL
1	K	78	CYS
1	K	160	LEU
1	K	306	MET
1	K	307	PHE
1	K	308	VAL
2	k	15	PHE
2	k	76	CYS
2	k	103	ILE
2	k	142	ASP
2	k	295	MET
2	l	15	PHE
2	l	71	VAL
2	l	76	CYS

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Mol	Chain	Res	Type
2	l	92	VAL
2	l	93	ASN
2	l	103	ILE
2	l	124	LEU
2	l	130	VAL
2	l	142	ASP
2	l	159	MET
1	J	13	VAL
1	J	25	ILE
1	J	53	ILE
1	J	58	ILE
1	J	60	THR
1	J	63	SER
1	J	73	VAL
1	J	78	CYS
1	J	107	ARG
1	J	134	THR
1	J	150	LEU
1	J	301	SER
1	J	306	MET
1	J	307	PHE
1	J	308	VAL
1	I	13	VAL
1	I	25	ILE
1	I	35	VAL
1	I	53	ILE
1	I	60	THR
1	I	68	LEU
1	I	73	VAL
1	I	78	CYS
1	I	150	LEU
1	I	307	PHE
2	i	15	PHE
2	i	71	VAL
2	i	76	CYS
2	i	93	ASN
2	i	95	LEU
2	i	124	LEU
1	H	21	LEU
1	H	25	ILE
1	H	53	ILE
1	H	60	THR

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Mol	Chain	Res	Type
1	H	78	CYS
1	H	307	PHE
1	H	308	VAL
1	G	13	VAL
1	G	60	THR
1	G	63	SER
1	G	72	GLU
1	G	73	VAL
1	G	78	CYS
1	G	115	LYS
1	G	307	PHE
2	g	15	PHE
2	h	15	PHE
2	h	27	GLU
2	h	33	VAL
2	h	56	ILE
2	h	93	ASN
2	h	124	LEU
2	h	282	GLN
2	j	15	PHE
2	j	56	ILE
2	j	66	LEU
2	j	71	VAL
2	j	76	CYS
2	j	93	ASN
2	j	124	LEU
2	j	181	ARG
1	C	60	THR
1	C	63	SER
1	C	78	CYS
1	C	105	ILE
1	C	160	LEU
1	C	307	PHE
1	B	13	VAL
1	B	21	LEU
1	B	25	ILE
1	B	58	ILE
1	B	60	THR
1	B	78	CYS
1	B	105	ILE
1	B	110	THR
1	B	183	ARG

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Mol	Chain	Res	Type
1	B	268	HIS
1	B	301	SER
1	B	307	PHE
2	b	15	PHE
2	b	51	LEU
2	b	71	VAL
2	b	76	CYS
2	b	93	ASN
2	b	95	LEU
2	b	124	LEU
2	b	148	LEU
2	b	282	GLN
2	c	15	PHE
2	c	66	LEU
2	c	76	CYS
2	c	134	GLN
2	c	289	ILE
1	F	21	LEU
1	F	33	LEU
1	F	58	ILE
1	F	60	THR
1	F	68	LEU
1	F	78	CYS
1	F	94	VAL
1	F	105	ILE
1	F	136	GLN
1	F	152	GLN
1	F	307	PHE
1	F	308	VAL
2	f	15	PHE
2	f	71	VAL
2	f	76	CYS
2	f	92	VAL
2	f	93	ASN
1	E	13	VAL
1	E	35	VAL
1	E	60	THR
1	E	63	SER
1	E	78	CYS
1	E	105	ILE
1	E	160	LEU
1	E	301	SER

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Mol	Chain	Res	Type
1	E	307	PHE
1	D	13	VAL
1	D	53	ILE
1	D	60	THR
1	D	63	SER
1	D	78	CYS
1	D	105	ILE
1	D	150	LEU
1	D	263	GLU
1	D	301	SER
1	D	307	PHE
2	d	15	PHE
2	d	19	LEU
2	d	71	VAL
2	d	93	ASN
2	d	124	LEU
2	e	15	PHE
2	e	71	VAL
2	e	76	CYS
2	e	93	ASN
2	e	282	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	124	HIS
1	A	149	ASN
1	A	202	GLN
2	a	131	HIS
2	a	147	ASN
2	a	200	GLN
1	M	123	HIS
1	M	149	ASN
1	M	202	GLN
2	m	122	HIS
2	m	153	GLN
2	m	200	GLN
1	L	123	HIS
1	L	128	GLN
1	L	149	ASN
1	L	202	GLN

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Mol	Chain	Res	Type
1	K	149	ASN
1	K	202	GLN
2	k	122	HIS
2	k	200	GLN
2	l	122	HIS
2	l	126	GLN
2	l	153	GLN
2	l	200	GLN
1	J	128	GLN
1	J	149	ASN
1	I	128	GLN
1	I	149	ASN
2	i	147	ASN
2	i	200	GLN
1	H	123	HIS
1	H	124	HIS
1	H	128	GLN
1	H	149	ASN
1	H	200	GLN
1	H	202	GLN
1	G	123	HIS
1	G	149	ASN
1	G	202	GLN
2	g	73	ASN
2	g	122	HIS
2	g	126	GLN
2	g	147	ASN
2	g	153	GLN
2	g	200	GLN
2	h	50	HIS
2	h	93	ASN
2	h	122	HIS
2	h	143	GLN
2	h	147	ASN
2	j	122	HIS
2	j	126	GLN
2	j	147	ASN
2	j	200	GLN
1	C	123	HIS
1	C	149	ASN
1	B	123	HIS
1	B	124	HIS

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Mol	Chain	Res	Type
1	B	149	ASN
1	B	202	GLN
2	b	122	HIS
2	b	126	GLN
2	b	147	ASN
2	c	24	HIS
2	c	122	HIS
2	c	153	GLN
1	F	123	HIS
1	F	149	ASN
2	f	73	ASN
2	f	122	HIS
2	f	126	GLN
2	f	154	GLN
2	f	200	GLN
1	E	123	HIS
1	E	149	ASN
1	E	202	GLN
1	D	123	HIS
1	D	124	HIS
1	D	149	ASN
1	D	202	GLN
2	d	122	HIS
2	d	147	ASN
2	d	200	GLN
2	e	147	ASN
2	e	153	GLN
2	e	200	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 ⓘ

52 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	$\# Z  > 2$
3	NAG	N	1	1,3	14,14,15	0.74	0	17,19,21	0.99	0
3	NAG	N	2	3	14,14,15	0.72	0	17,19,21	0.83	0
3	NAG	O	1	2,3	14,14,15	0.71	0	17,19,21	1.10	1 (5%)
3	NAG	O	2	3	14,14,15	0.73	0	17,19,21	0.93	1 (5%)
3	NAG	P	1	1,3	14,14,15	0.74	0	17,19,21	0.98	0
3	NAG	P	2	3	14,14,15	0.71	0	17,19,21	0.83	0
3	NAG	Q	1	2,3	14,14,15	0.70	0	17,19,21	1.08	1 (5%)
3	NAG	Q	2	3	14,14,15	0.72	0	17,19,21	0.92	0
3	NAG	R	1	1,3	14,14,15	0.74	0	17,19,21	1.00	0
3	NAG	R	2	3	14,14,15	0.71	0	17,19,21	0.84	0
3	NAG	S	1	1,3	14,14,15	0.73	0	17,19,21	1.00	0
3	NAG	S	2	3	14,14,15	0.72	0	17,19,21	0.85	0
3	NAG	T	1	2,3	14,14,15	0.71	0	17,19,21	1.15	1 (5%)
3	NAG	T	2	3	14,14,15	0.72	0	17,19,21	0.93	1 (5%)
3	NAG	U	1	2,3	14,14,15	0.71	0	17,19,21	1.13	1 (5%)
3	NAG	U	2	3	14,14,15	0.73	0	17,19,21	0.93	1 (5%)
3	NAG	V	1	1,3	14,14,15	0.73	0	17,19,21	1.00	0
3	NAG	V	2	3	14,14,15	0.72	0	17,19,21	0.83	0
3	NAG	W	1	1,3	14,14,15	0.74	0	17,19,21	0.99	0
3	NAG	W	2	3	14,14,15	0.72	0	17,19,21	0.83	0
3	NAG	X	1	2,3	14,14,15	0.72	0	17,19,21	1.11	1 (5%)
3	NAG	X	2	3	14,14,15	0.73	0	17,19,21	0.94	1 (5%)
3	NAG	Y	1	1,3	14,14,15	0.74	0	17,19,21	0.98	0
3	NAG	Y	2	3	14,14,15	0.71	0	17,19,21	0.83	0
3	NAG	Z	1	1,3	14,14,15	0.74	0	17,19,21	0.99	1 (5%)
3	NAG	Z	2	3	14,14,15	0.72	0	17,19,21	0.83	0
3	NAG	n	1	2,3	14,14,15	0.71	0	17,19,21	1.06	0
3	NAG	n	2	3	14,14,15	0.73	0	17,19,21	0.94	1 (5%)
3	NAG	o	1	2,3	14,14,15	0.72	0	17,19,21	1.09	1 (5%)
3	NAG	o	2	3	14,14,15	0.72	0	17,19,21	0.93	1 (5%)
3	NAG	p	1	2,3	14,14,15	0.71	0	17,19,21	1.11	1 (5%)
3	NAG	p	2	3	14,14,15	0.72	0	17,19,21	0.95	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	q	1	1,3	14,14,15	0.73	0	17,19,21	1.01	0
3	NAG	q	2	3	14,14,15	0.71	0	17,19,21	0.83	0
3	NAG	r	1	1,3	14,14,15	0.73	0	17,19,21	1.04	0
3	NAG	r	2	3	14,14,15	0.71	0	17,19,21	0.86	0
3	NAG	s	1	2,3	14,14,15	0.71	0	17,19,21	1.04	0
3	NAG	s	2	3	14,14,15	0.71	0	17,19,21	0.94	1 (5%)
3	NAG	t	1	2,3	14,14,15	0.71	0	17,19,21	1.06	1 (5%)
3	NAG	t	2	3	14,14,15	0.70	0	17,19,21	0.92	0
3	NAG	u	1	1,3	14,14,15	0.74	0	17,19,21	1.06	0
3	NAG	u	2	3	14,14,15	0.71	0	17,19,21	0.83	0
3	NAG	v	1	2,3	14,14,15	0.72	0	17,19,21	1.09	1 (5%)
3	NAG	v	2	3	14,14,15	0.72	0	17,19,21	0.94	1 (5%)
3	NAG	w	1	1,3	14,14,15	0.73	0	17,19,21	1.03	0
3	NAG	w	2	3	14,14,15	0.71	0	17,19,21	0.84	0
3	NAG	x	1	1,3	14,14,15	0.73	0	17,19,21	1.06	1 (5%)
3	NAG	x	2	3	14,14,15	0.72	0	17,19,21	0.85	0
3	NAG	y	1	2,3	14,14,15	0.70	0	17,19,21	1.11	1 (5%)
3	NAG	y	2	3	14,14,15	0.73	0	17,19,21	0.94	1 (5%)
3	NAG	z	1	2,3	14,14,15	0.72	0	17,19,21	1.10	1 (5%)
3	NAG	z	2	3	14,14,15	0.72	0	17,19,21	0.92	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	NAG	O	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	1/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	1/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	NAG	T	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	U	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	1/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	NAG	X	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	X	2	3	-	1/6/23/26	0/1/1/1
3	NAG	Y	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Z	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	0/6/23/26	0/1/1/1
3	NAG	n	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	n	2	3	-	1/6/23/26	0/1/1/1
3	NAG	o	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	o	2	3	-	1/6/23/26	0/1/1/1
3	NAG	p	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	p	2	3	-	1/6/23/26	0/1/1/1
3	NAG	q	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	q	2	3	-	0/6/23/26	0/1/1/1
3	NAG	r	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	r	2	3	-	0/6/23/26	0/1/1/1
3	NAG	s	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	s	2	3	-	1/6/23/26	0/1/1/1
3	NAG	t	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	t	2	3	-	1/6/23/26	0/1/1/1
3	NAG	u	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	u	2	3	-	0/6/23/26	0/1/1/1
3	NAG	v	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	v	2	3	-	1/6/23/26	0/1/1/1
3	NAG	w	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	w	2	3	-	0/6/23/26	0/1/1/1
3	NAG	x	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	x	2	3	-	0/6/23/26	0/1/1/1
3	NAG	y	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	y	2	3	-	1/6/23/26	0/1/1/1
3	NAG	z	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	z	2	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	1	NAG	C1-O5-C5	2.25	115.23	112.19
3	U	1	NAG	C1-O5-C5	2.23	115.22	112.19
3	O	1	NAG	C1-O5-C5	2.17	115.14	112.19
3	Q	1	NAG	C1-O5-C5	2.17	115.13	112.19
3	z	1	NAG	C1-O5-C5	2.16	115.12	112.19
3	p	2	NAG	C1-O5-C5	2.16	115.11	112.19
3	o	1	NAG	C1-O5-C5	2.14	115.09	112.19
3	X	1	NAG	C1-O5-C5	2.13	115.08	112.19
3	p	1	NAG	C1-O5-C5	2.13	115.08	112.19
3	n	2	NAG	C1-O5-C5	2.13	115.07	112.19
3	v	1	NAG	C1-O5-C5	2.12	115.07	112.19
3	v	2	NAG	C1-O5-C5	2.12	115.06	112.19
3	X	2	NAG	C1-O5-C5	2.11	115.05	112.19
3	y	2	NAG	C1-O5-C5	2.10	115.03	112.19
3	t	1	NAG	C1-O5-C5	2.08	115.01	112.19
3	T	2	NAG	C1-O5-C5	2.07	115.00	112.19
3	U	2	NAG	C1-O5-C5	2.07	114.99	112.19
3	y	1	NAG	C1-O5-C5	2.06	114.98	112.19
3	s	2	NAG	C1-O5-C5	2.06	114.98	112.19
3	o	2	NAG	C1-O5-C5	2.05	114.97	112.19
3	O	2	NAG	C1-O5-C5	2.04	114.96	112.19
3	x	1	NAG	O5-C1-C2	-2.03	108.09	111.29
3	Z	1	NAG	O5-C1-C2	-2.02	108.10	111.29

There are no chirality outliers.

All (13) torsion outliers are listed below:

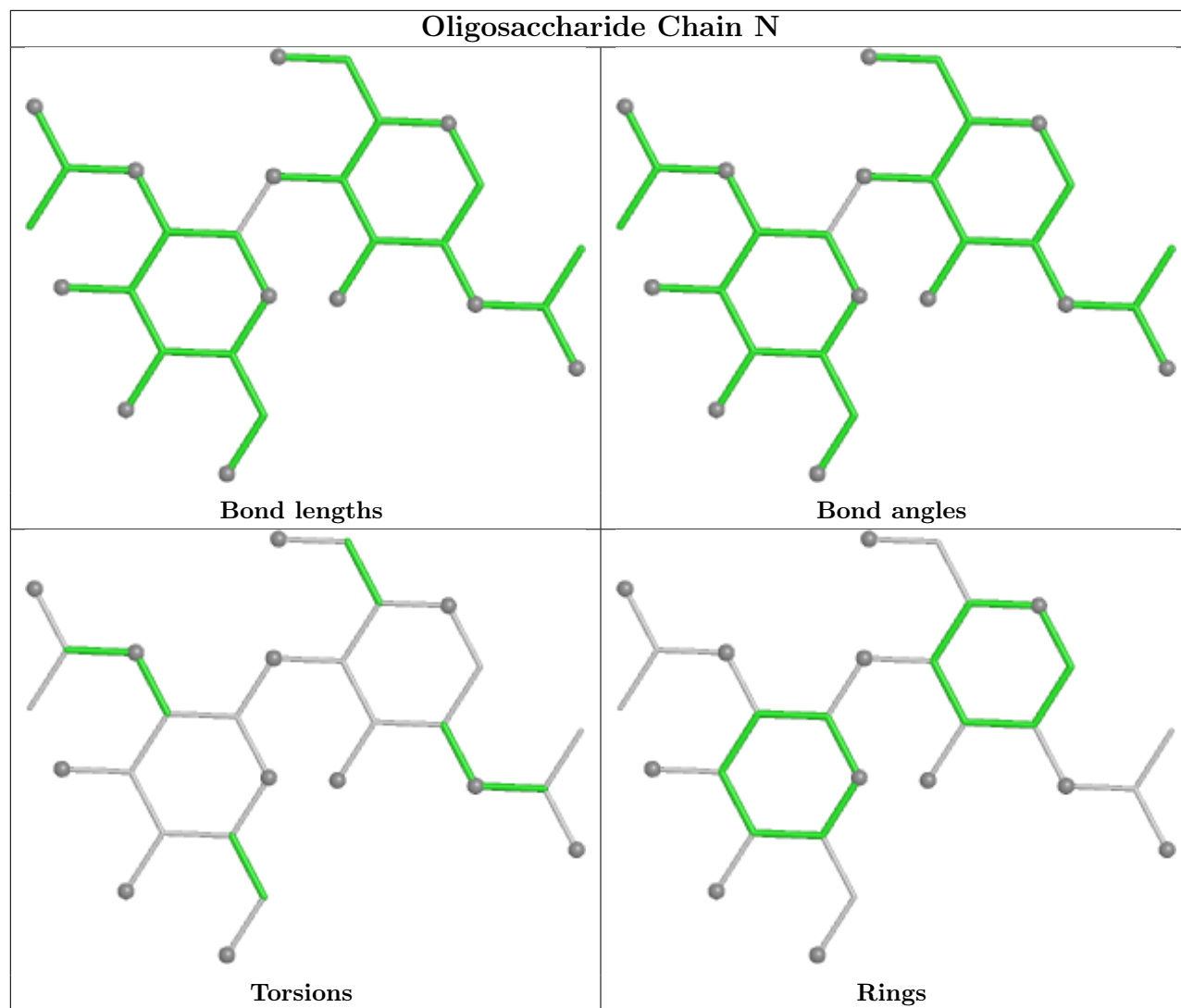
Mol	Chain	Res	Type	Atoms
3	n	2	NAG	O5-C5-C6-O6
3	p	2	NAG	O5-C5-C6-O6
3	s	2	NAG	O5-C5-C6-O6
3	v	2	NAG	O5-C5-C6-O6
3	z	2	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	X	2	NAG	O5-C5-C6-O6
3	o	2	NAG	O5-C5-C6-O6
3	t	2	NAG	O5-C5-C6-O6
3	y	2	NAG	O5-C5-C6-O6

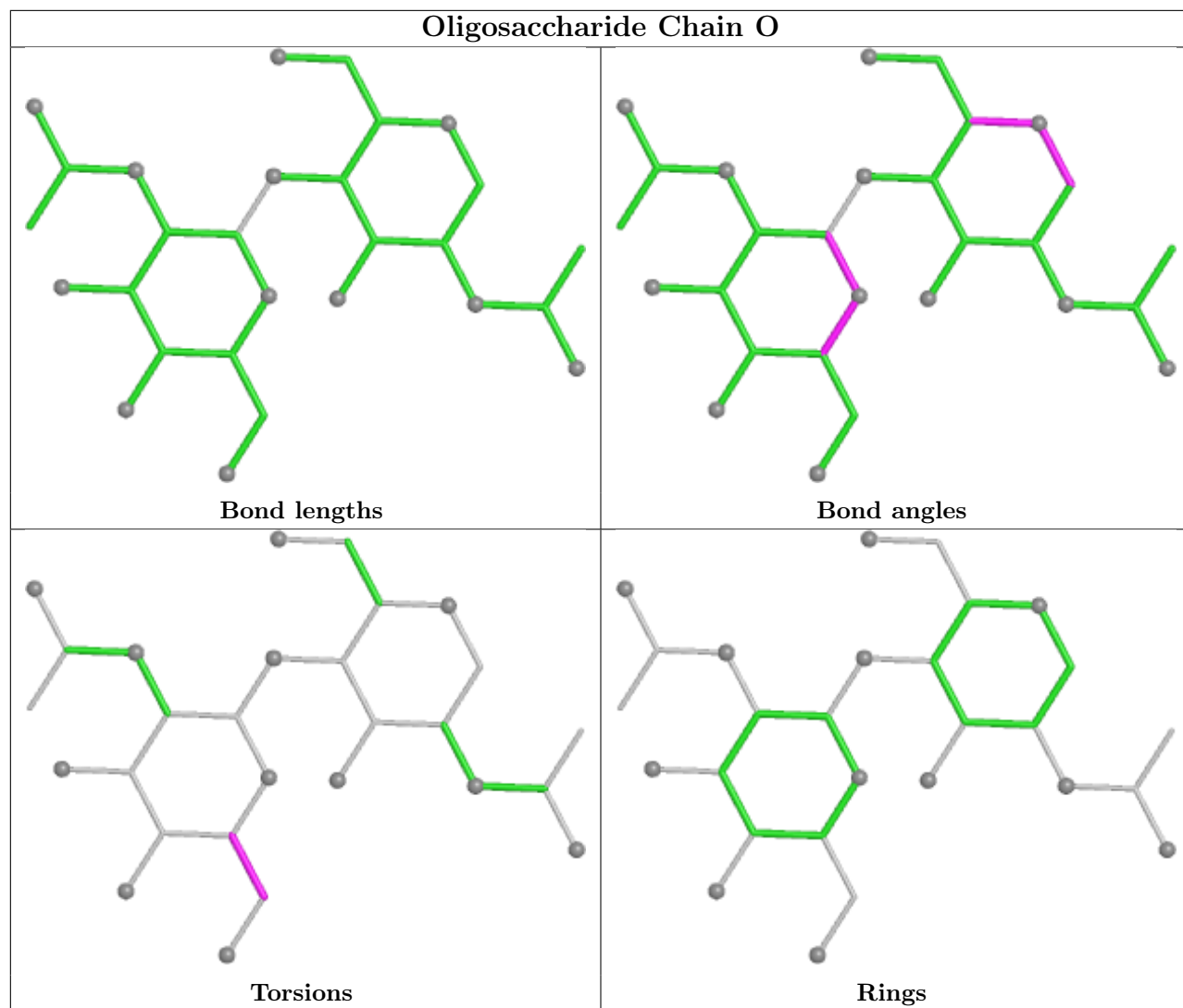
There are no ring outliers.

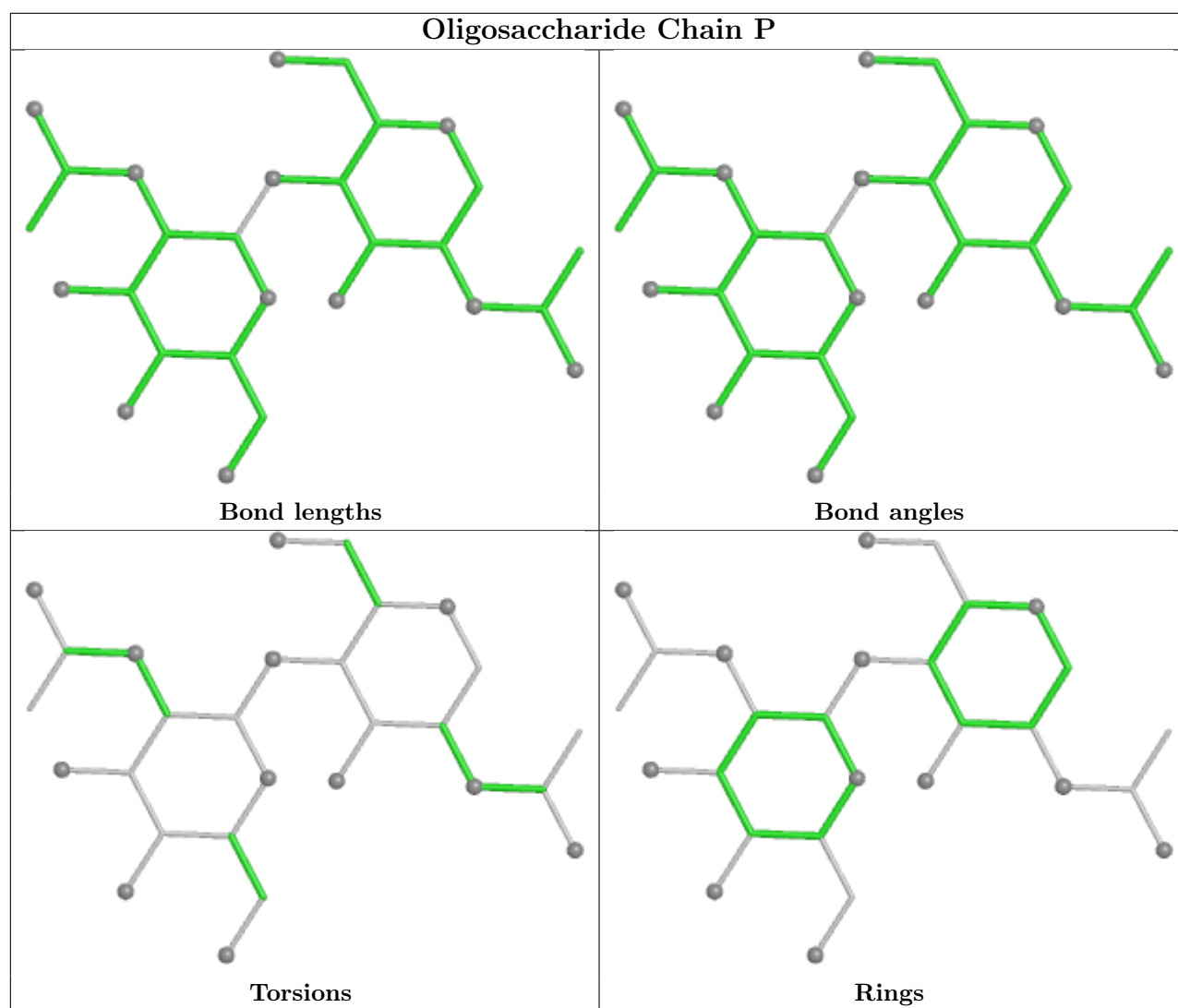
16 monomers are involved in 29 short contacts:

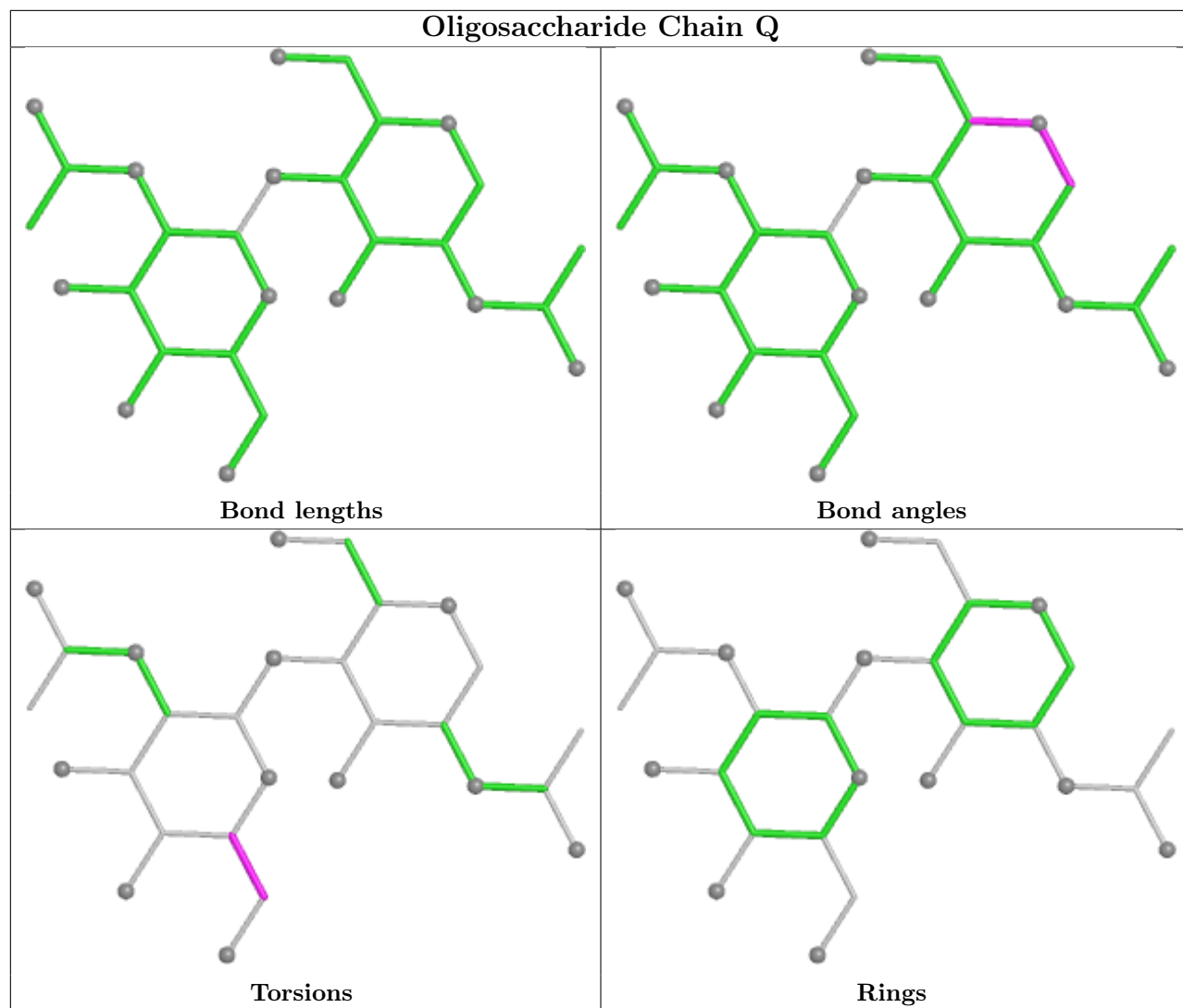
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	1	NAG	1	0
3	n	1	NAG	1	0
3	R	1	NAG	2	0
3	W	1	NAG	2	0
3	s	1	NAG	1	0
3	Z	1	NAG	2	0
3	w	1	NAG	2	0
3	r	1	NAG	2	0
3	V	1	NAG	2	0
3	x	1	NAG	2	0
3	Y	1	NAG	2	0
3	P	1	NAG	2	0
3	N	1	NAG	2	0
3	S	1	NAG	2	0
3	u	1	NAG	2	0
3	q	1	NAG	2	0

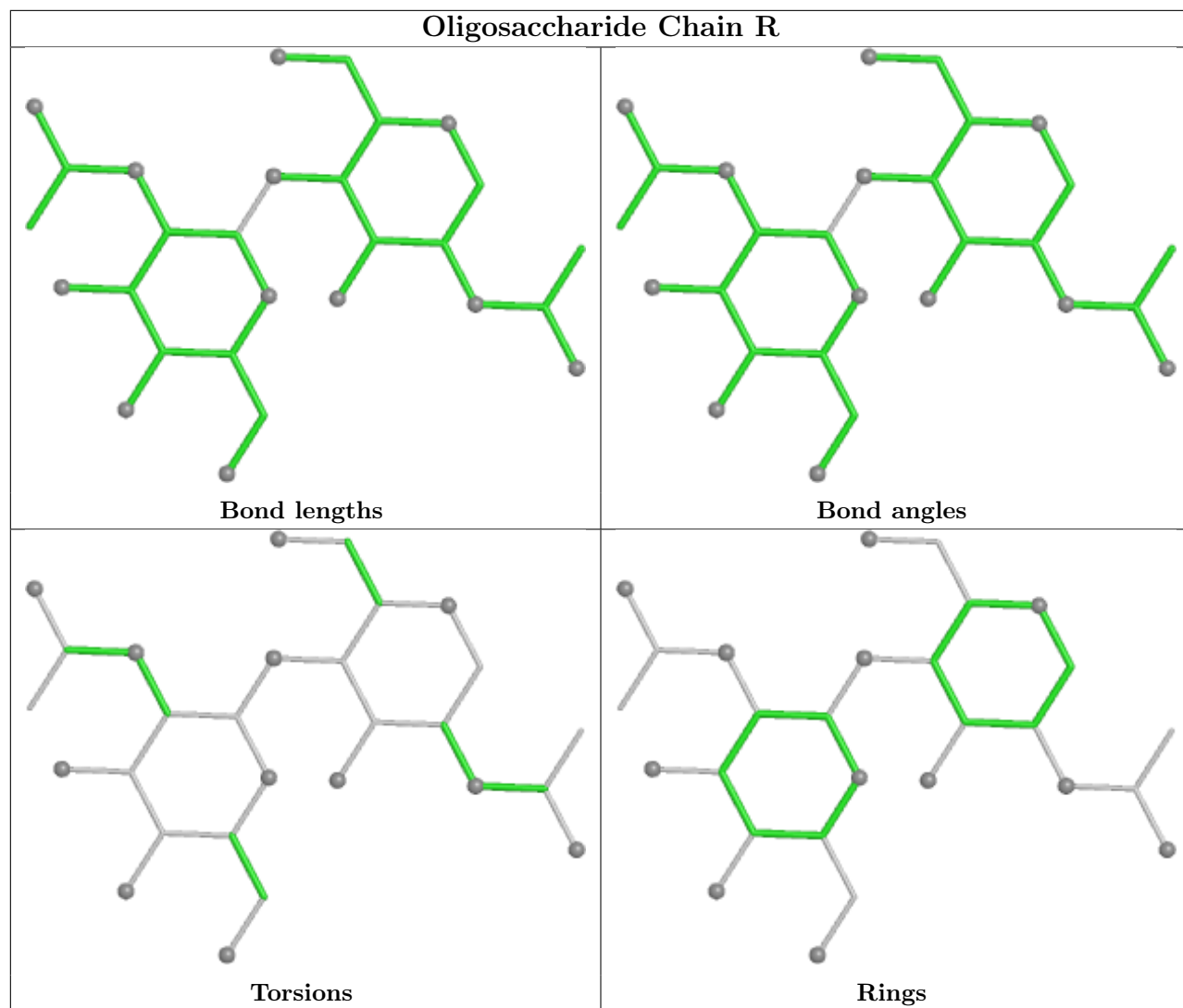
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



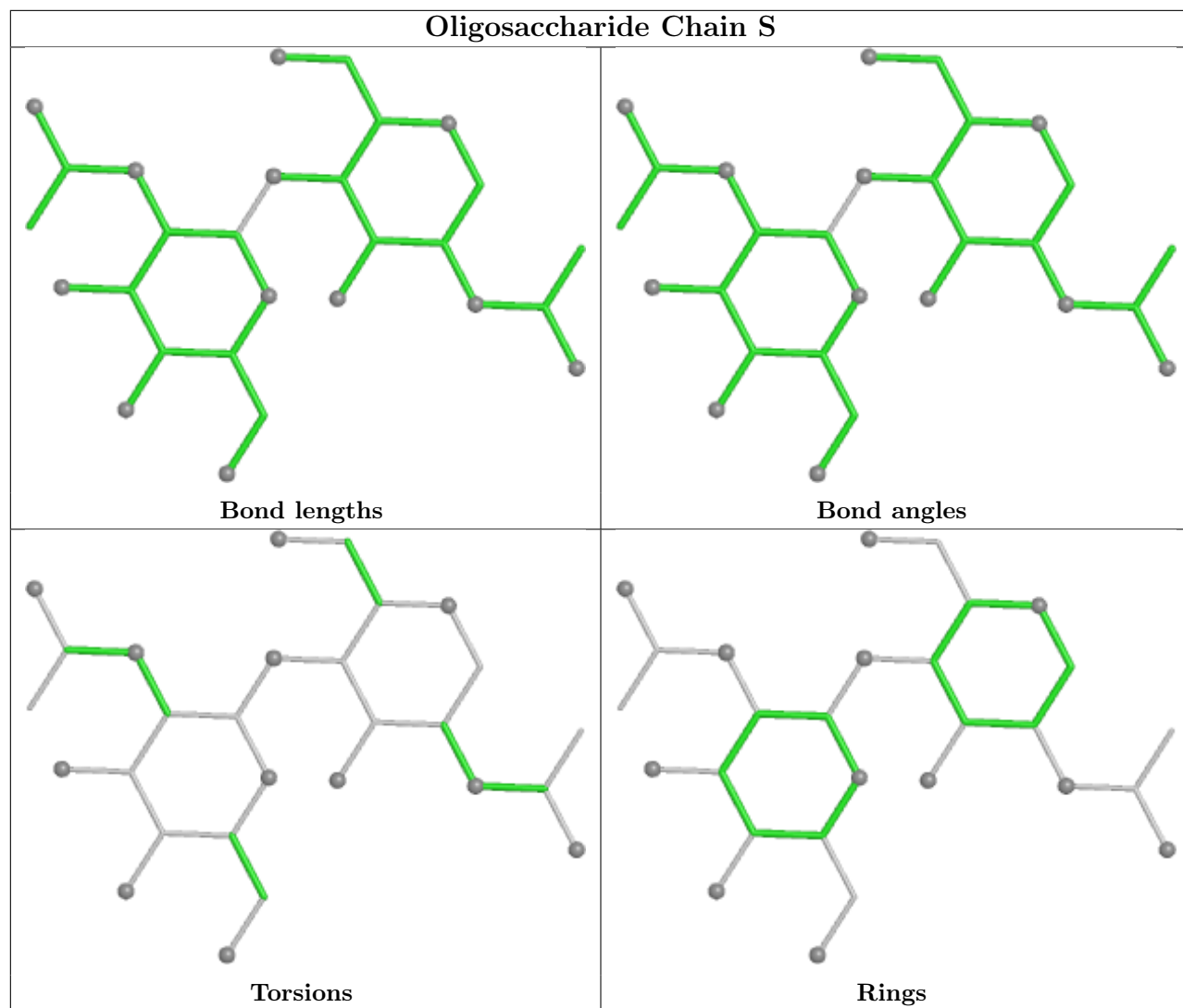


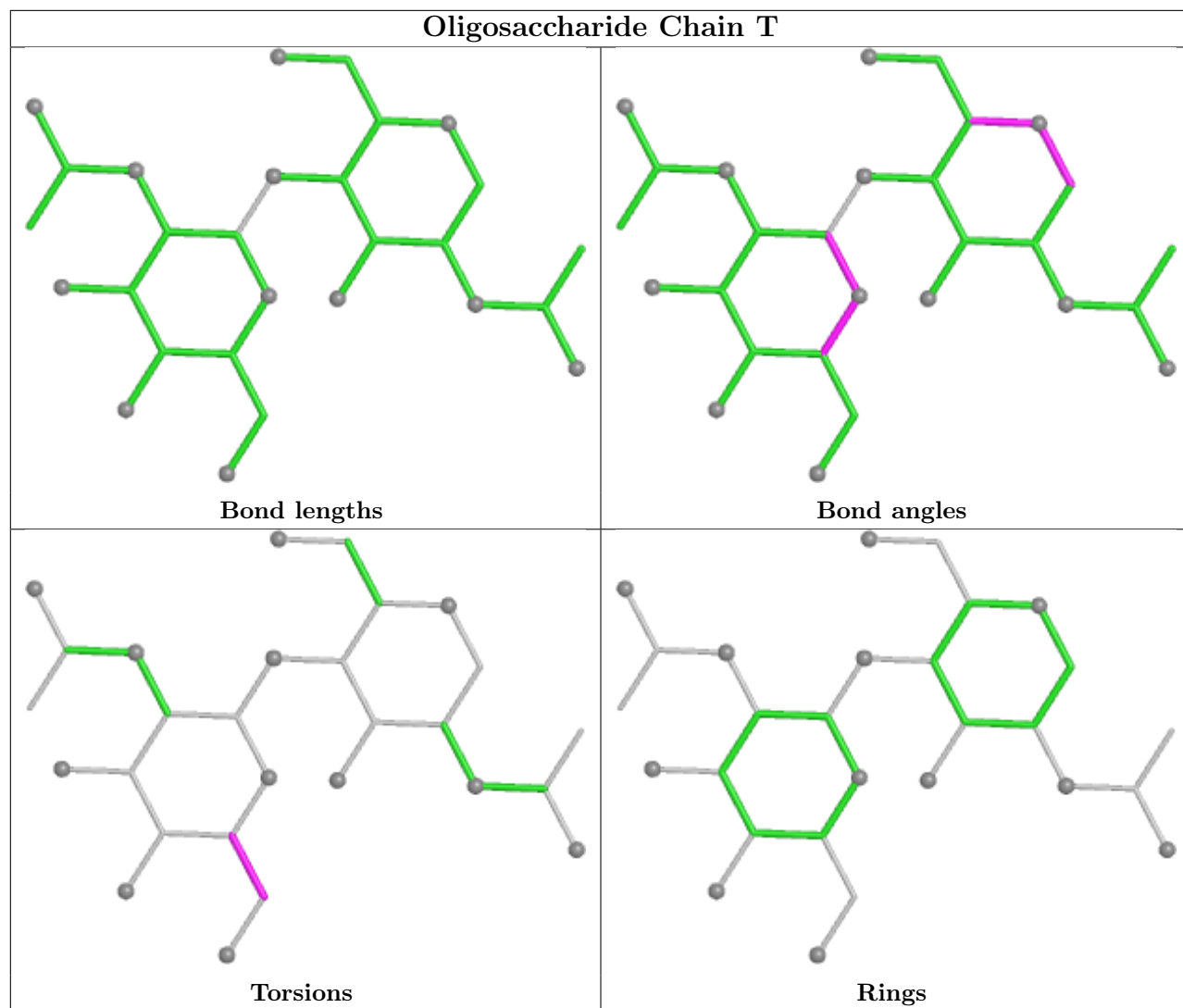


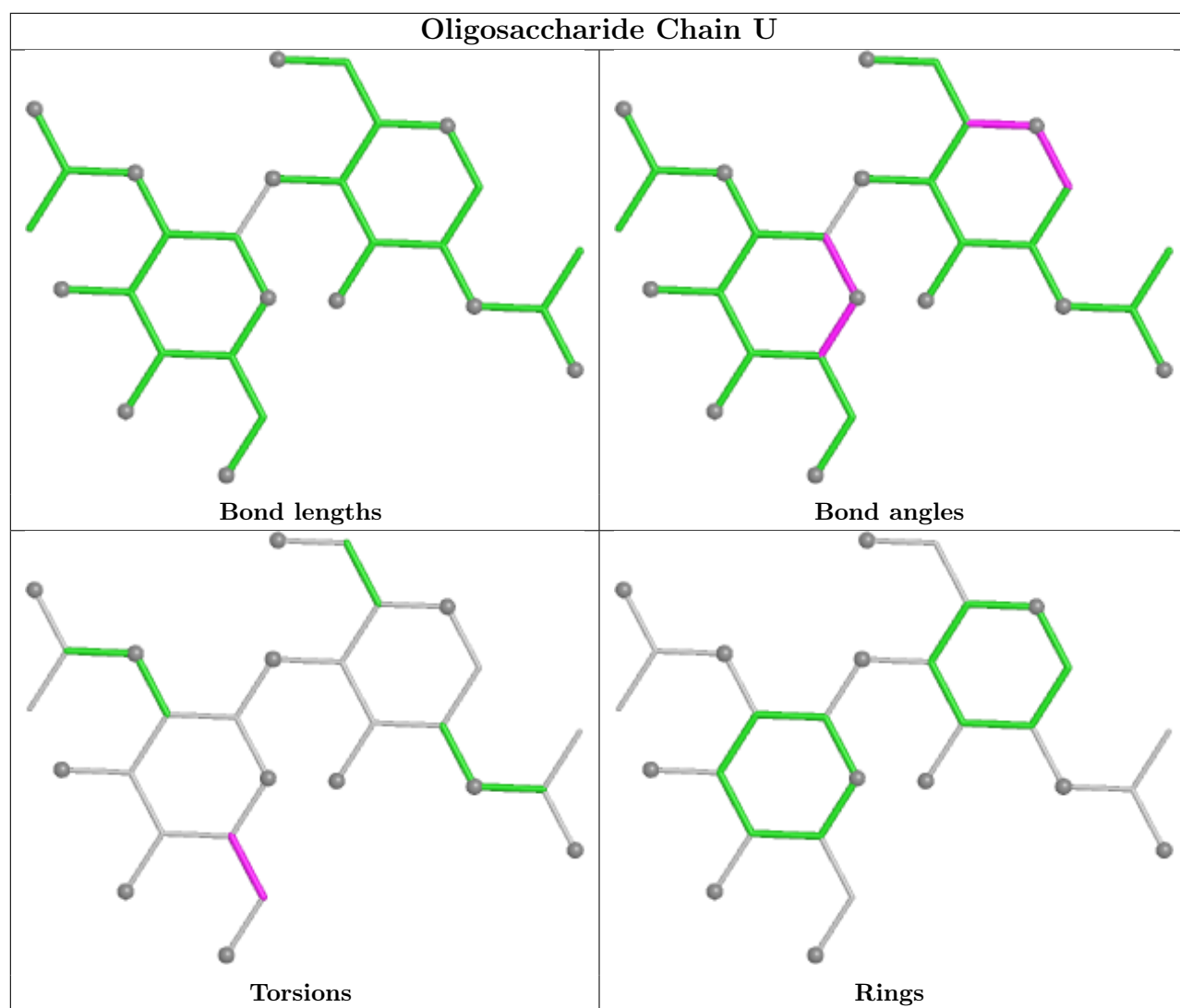


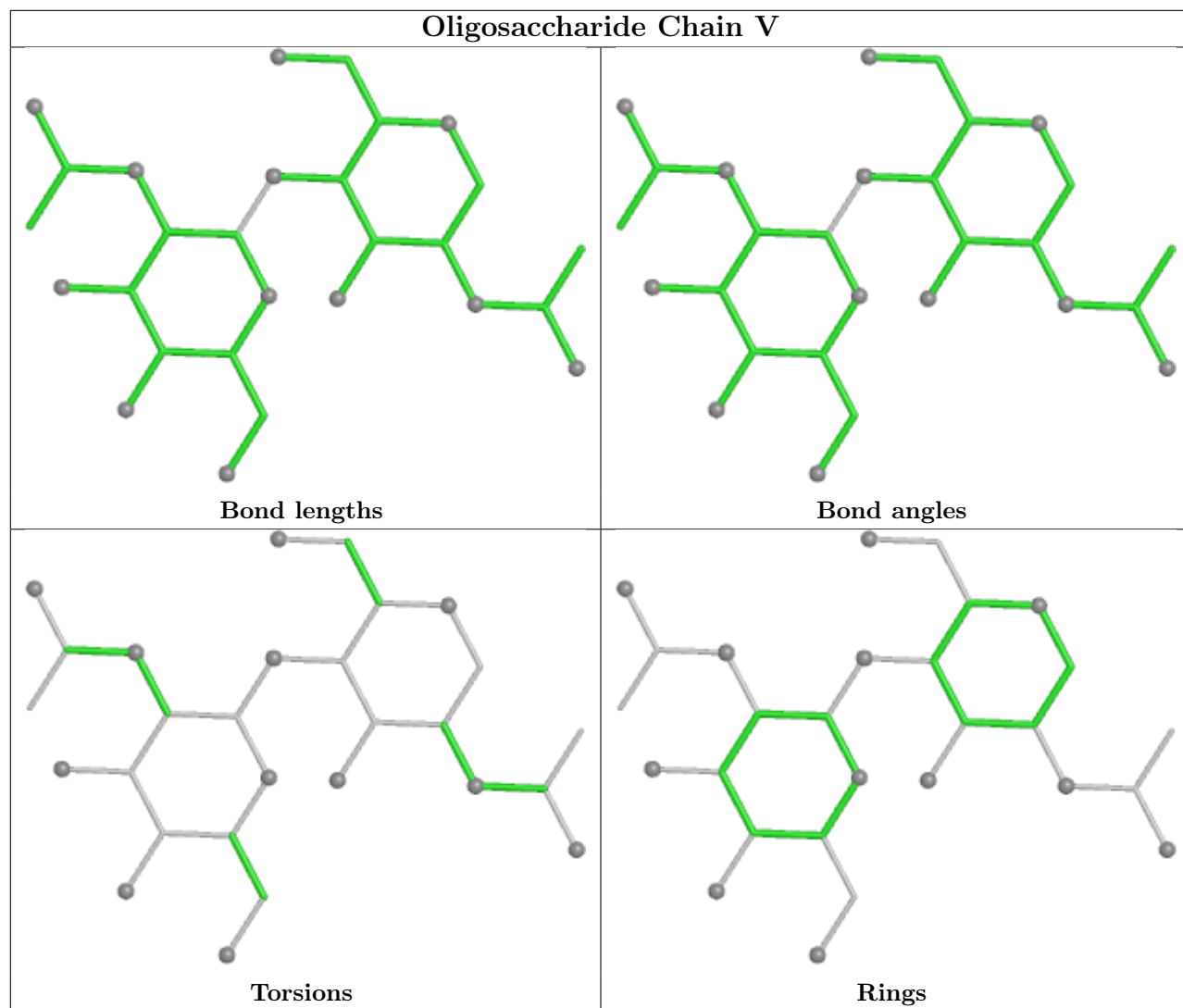


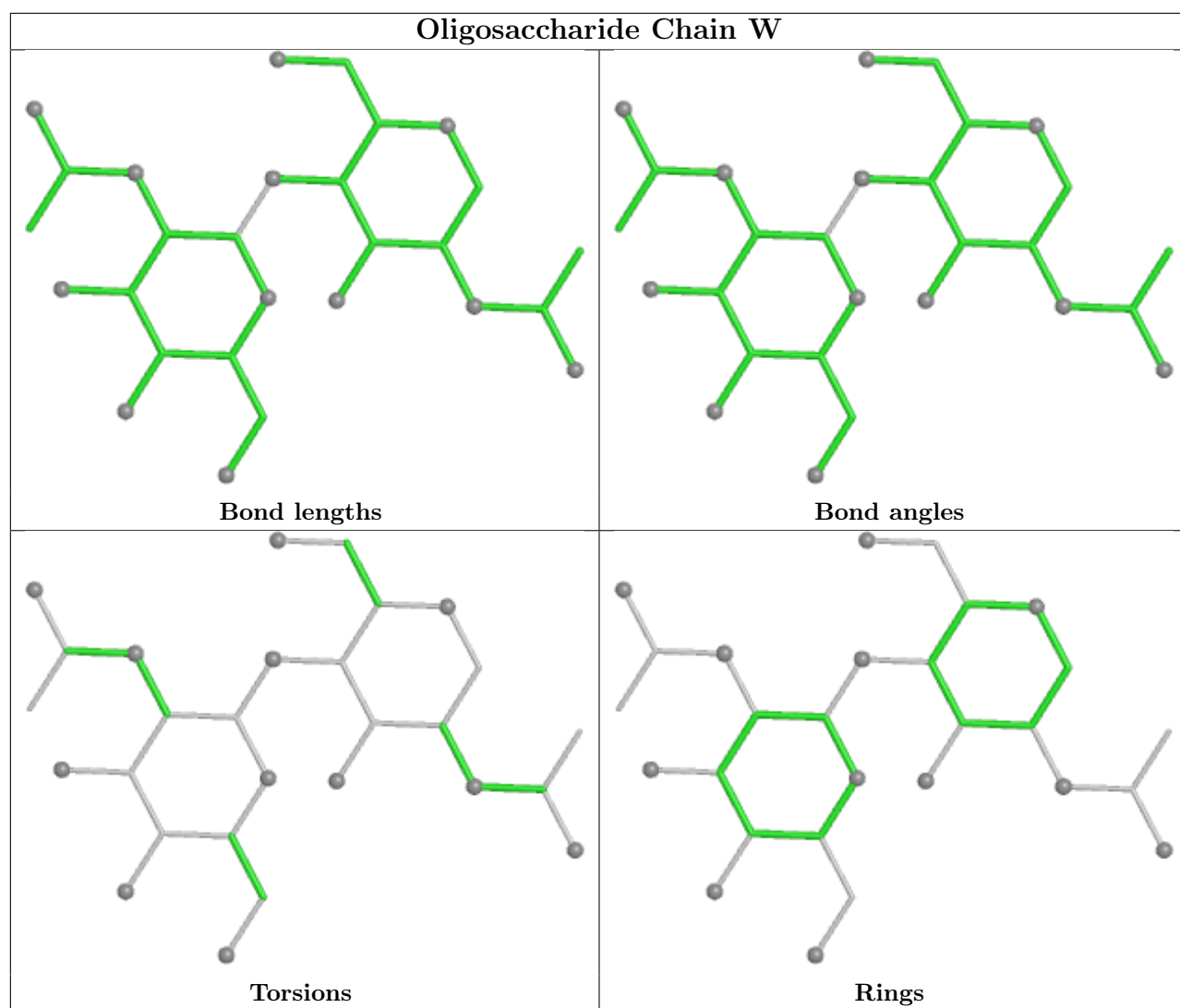


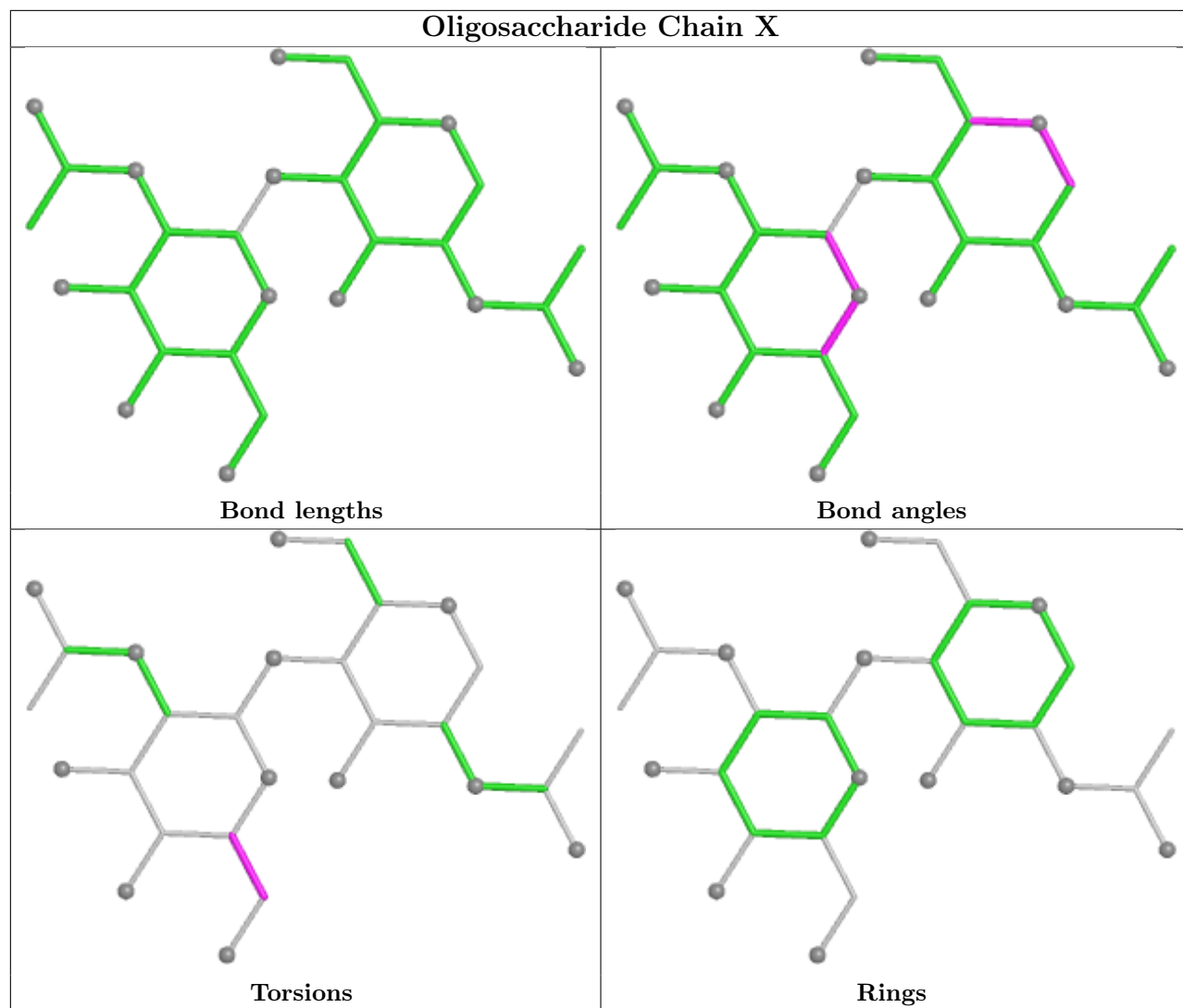


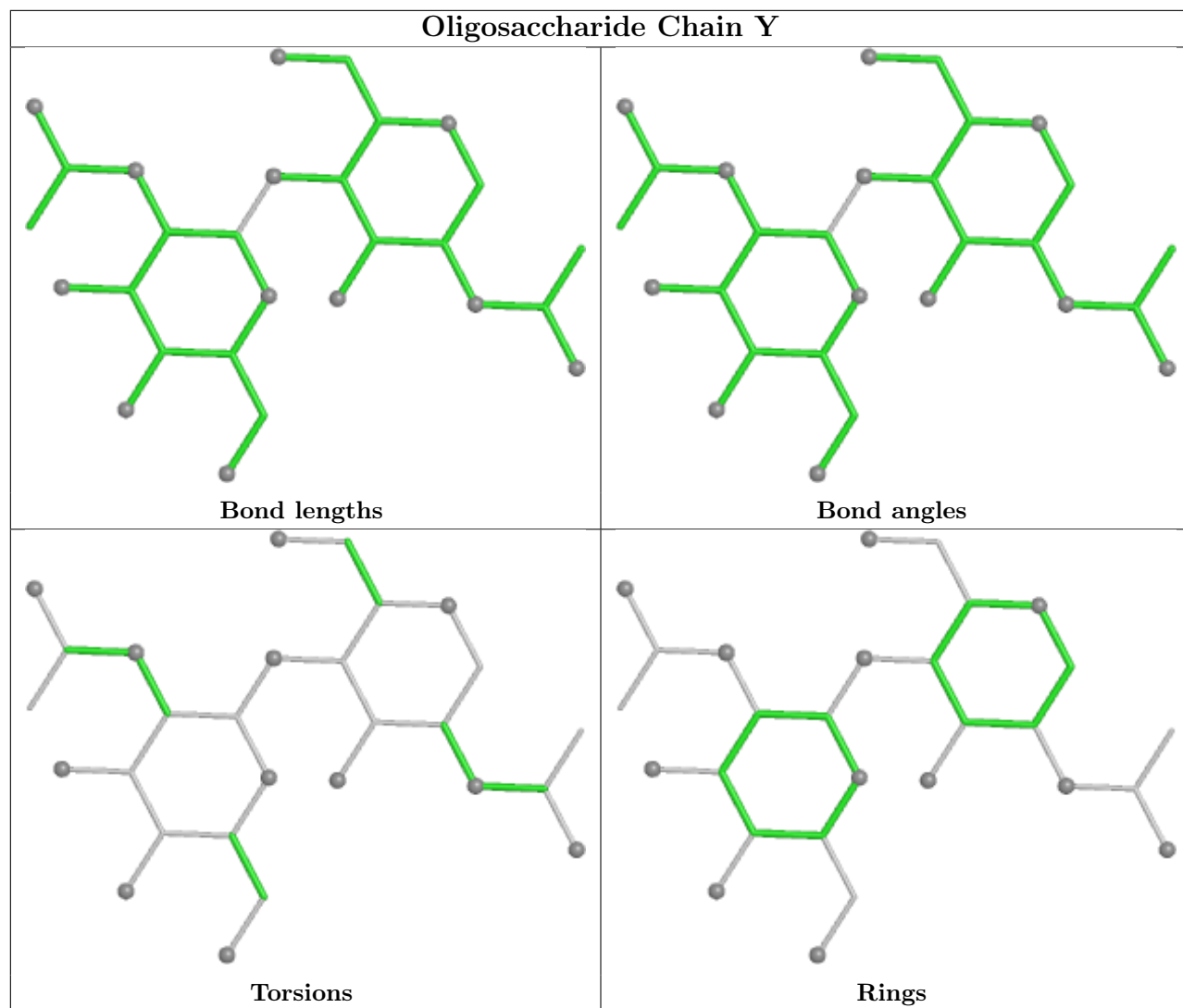


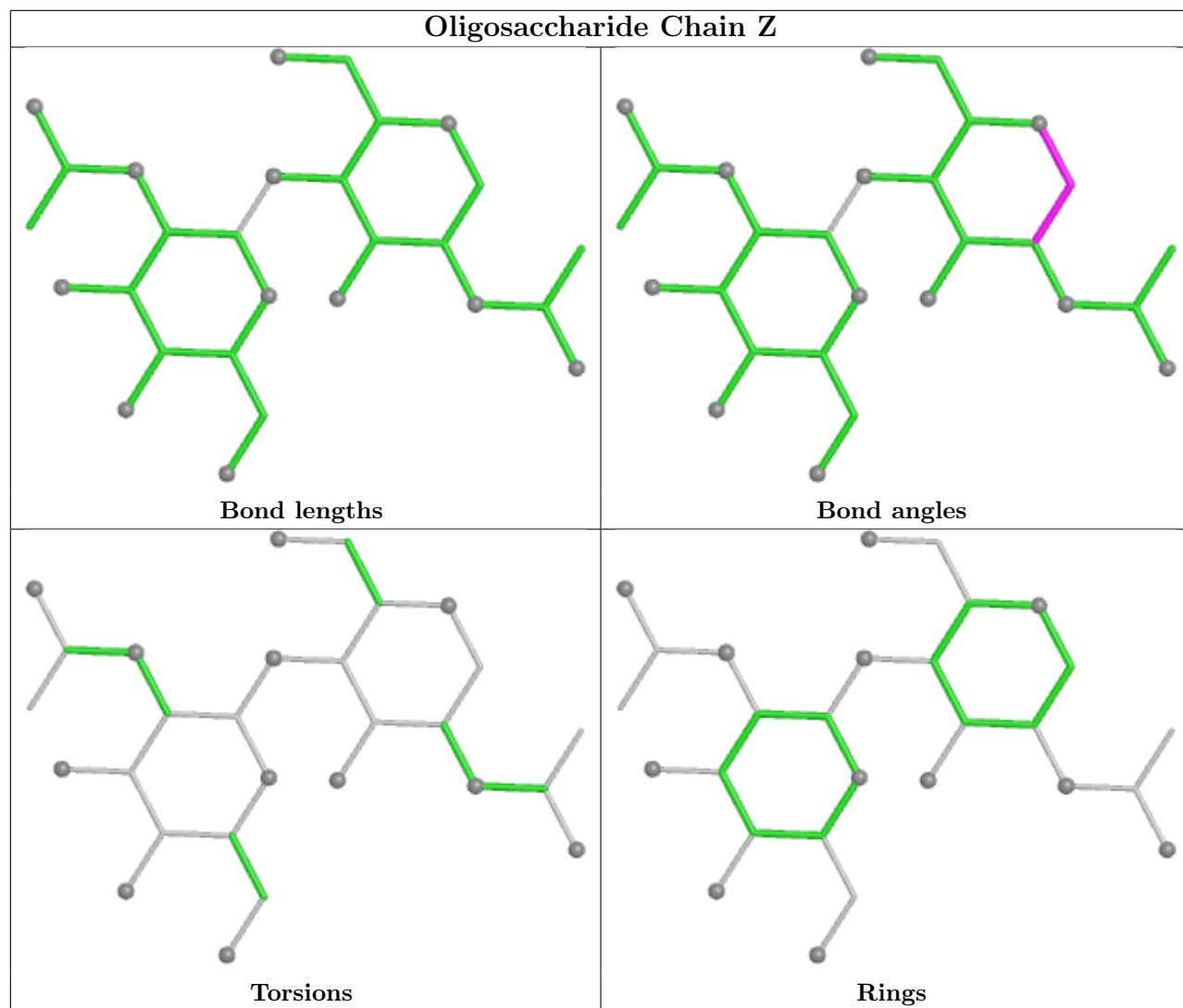




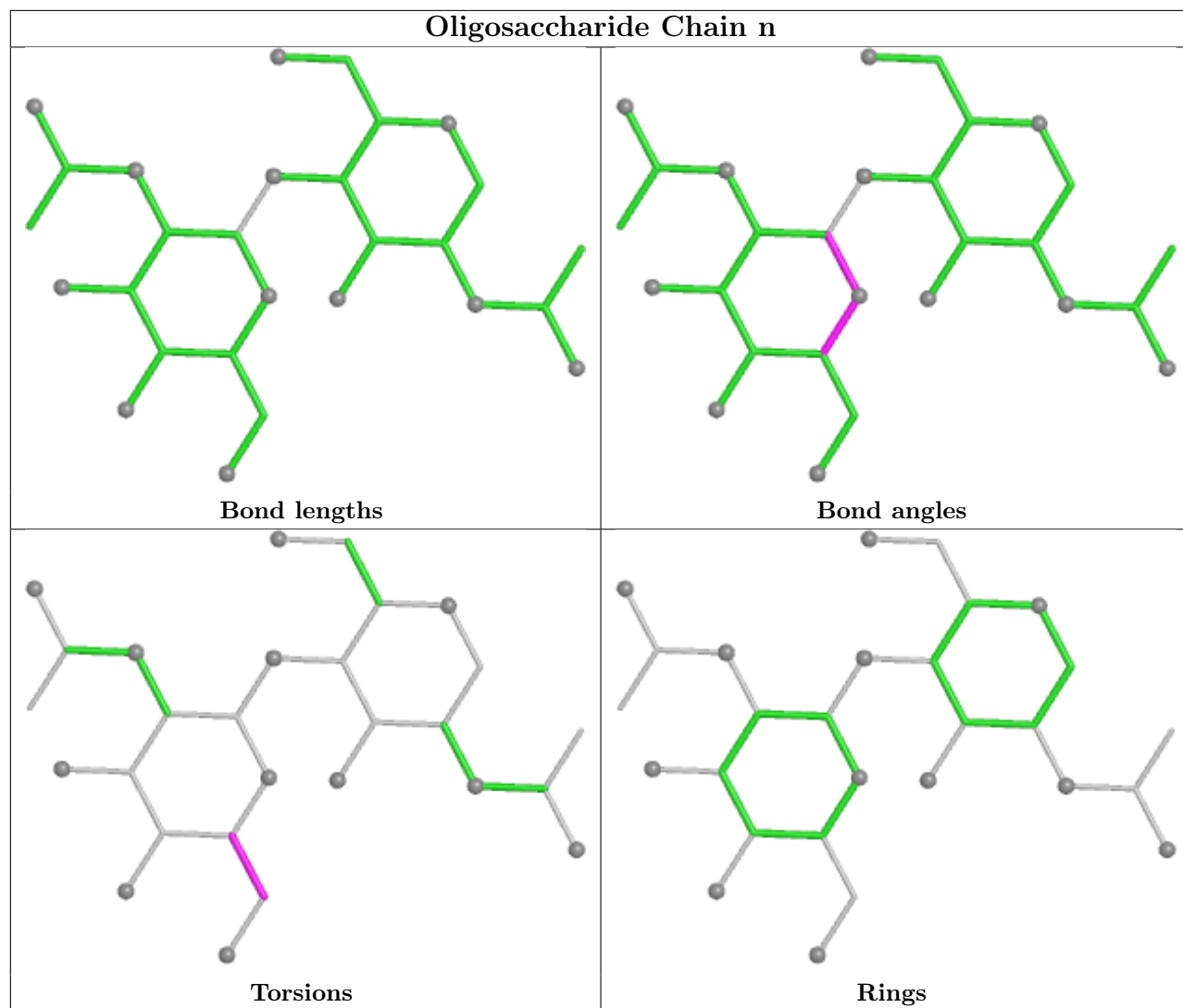


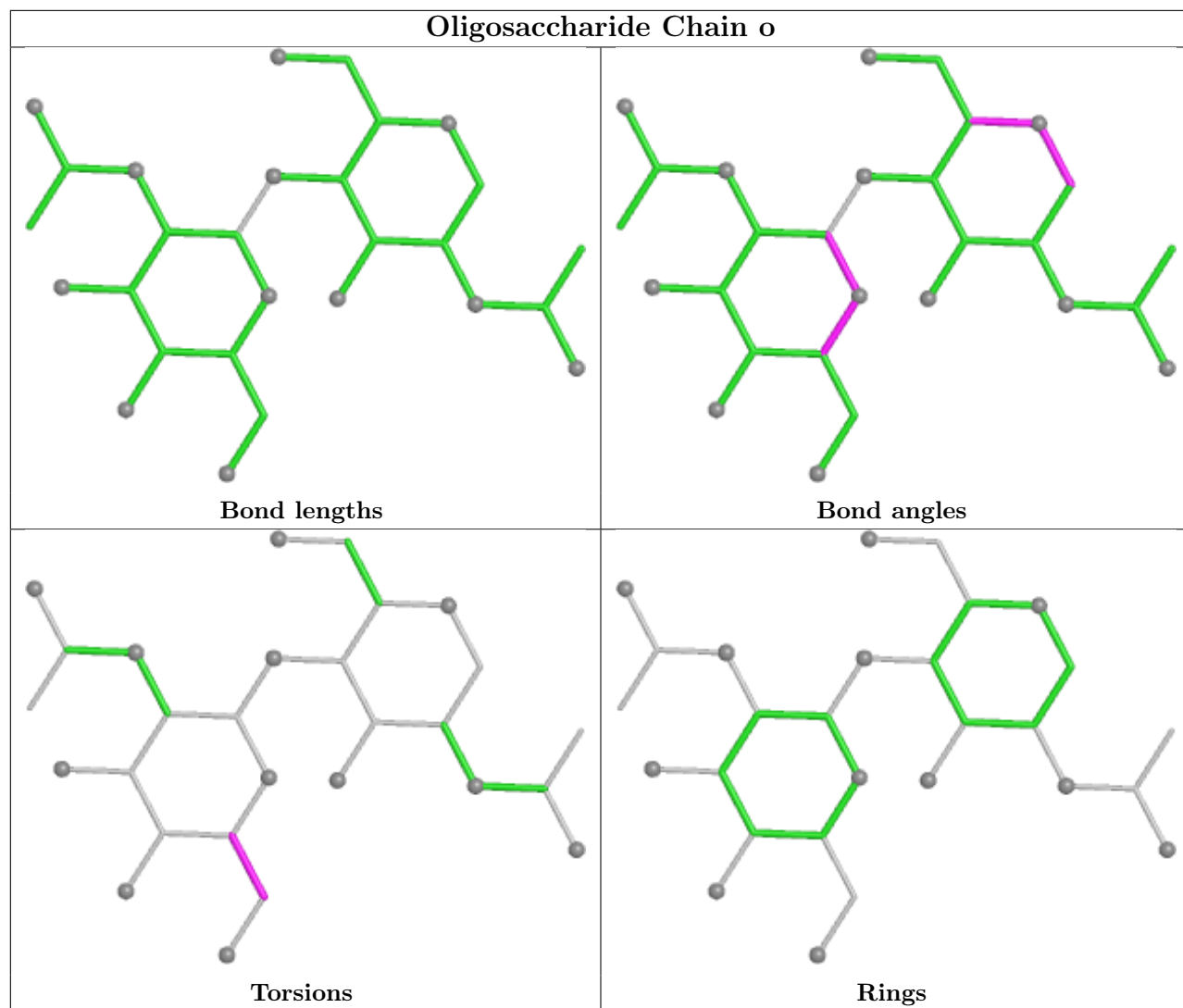


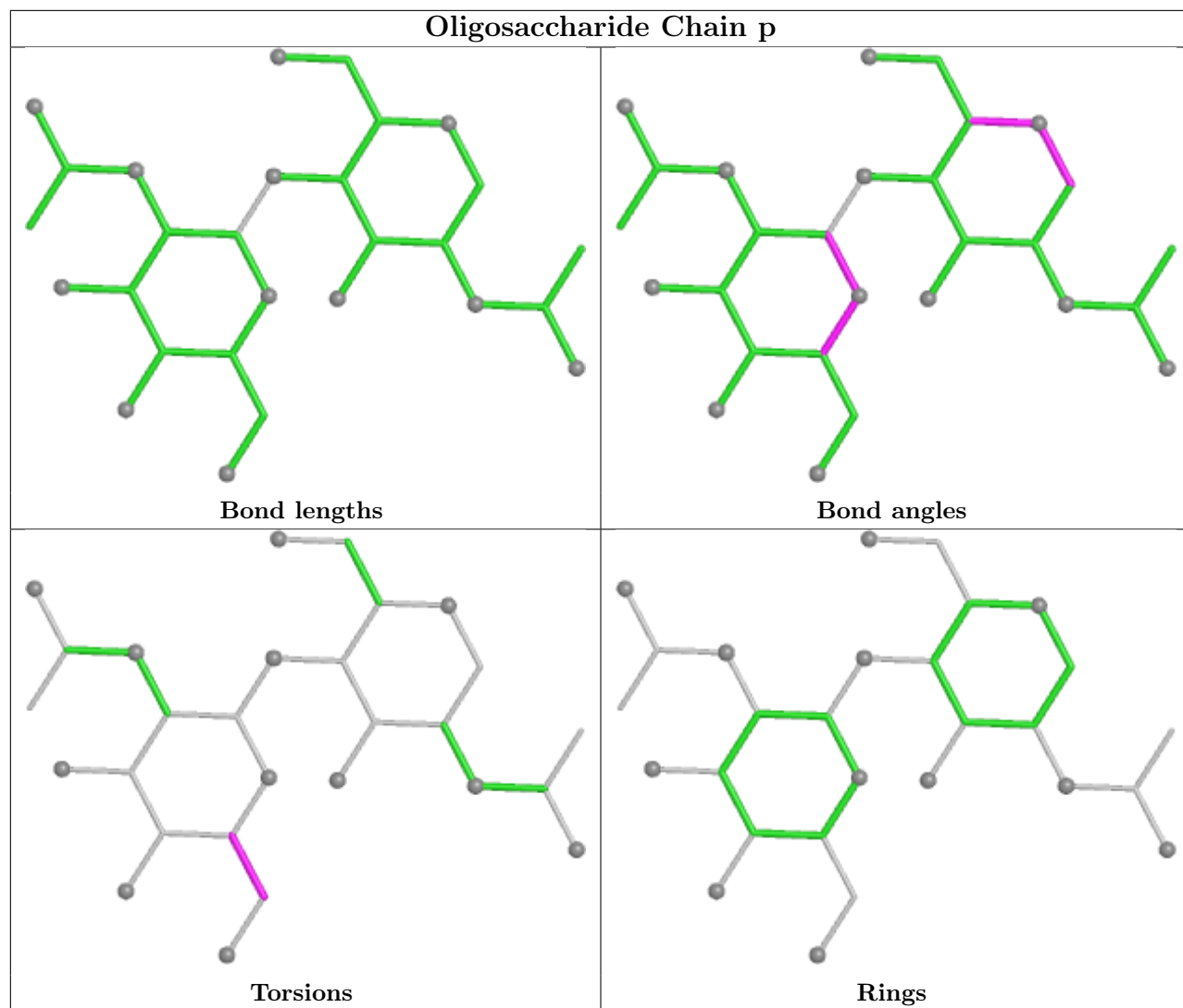


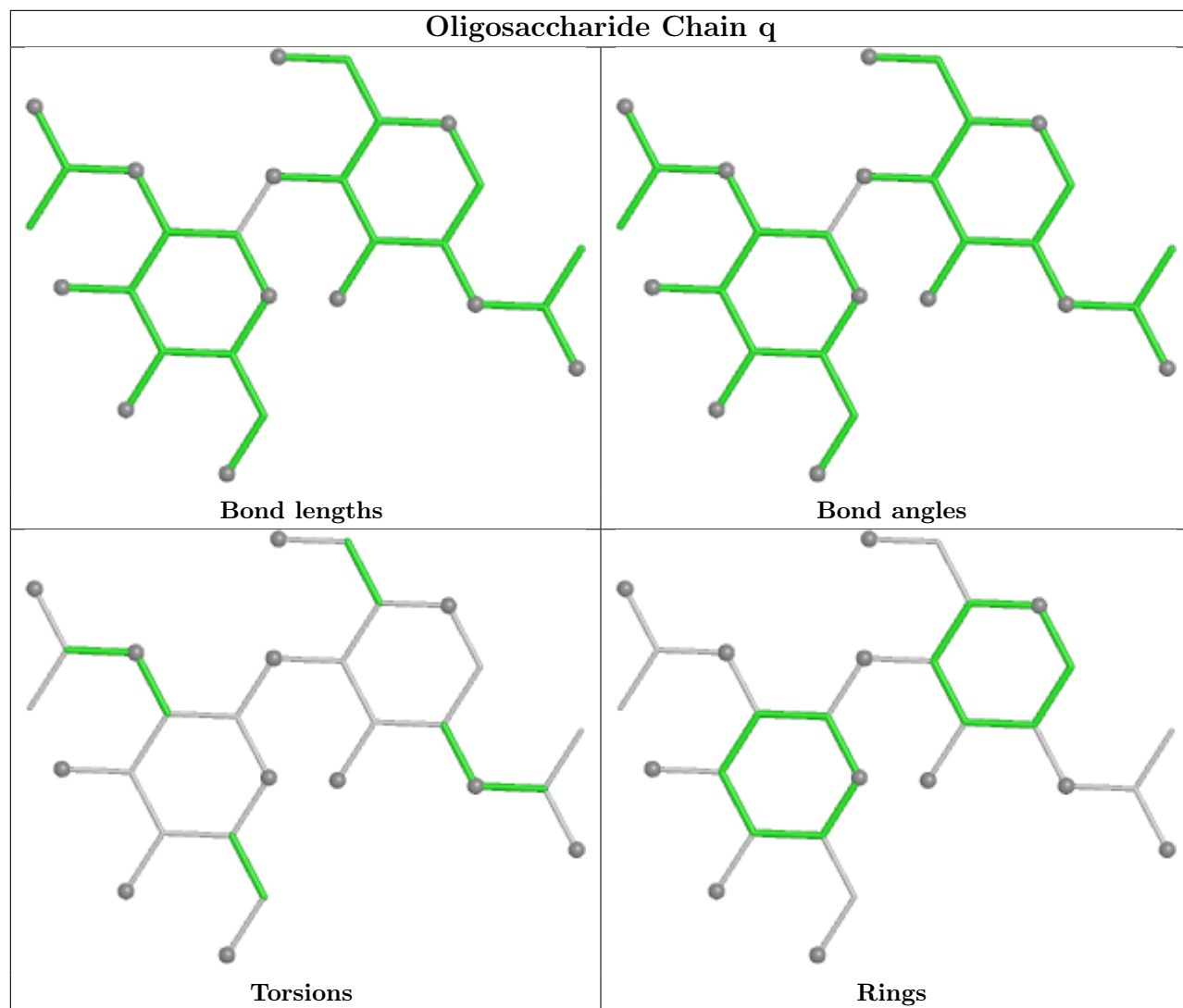


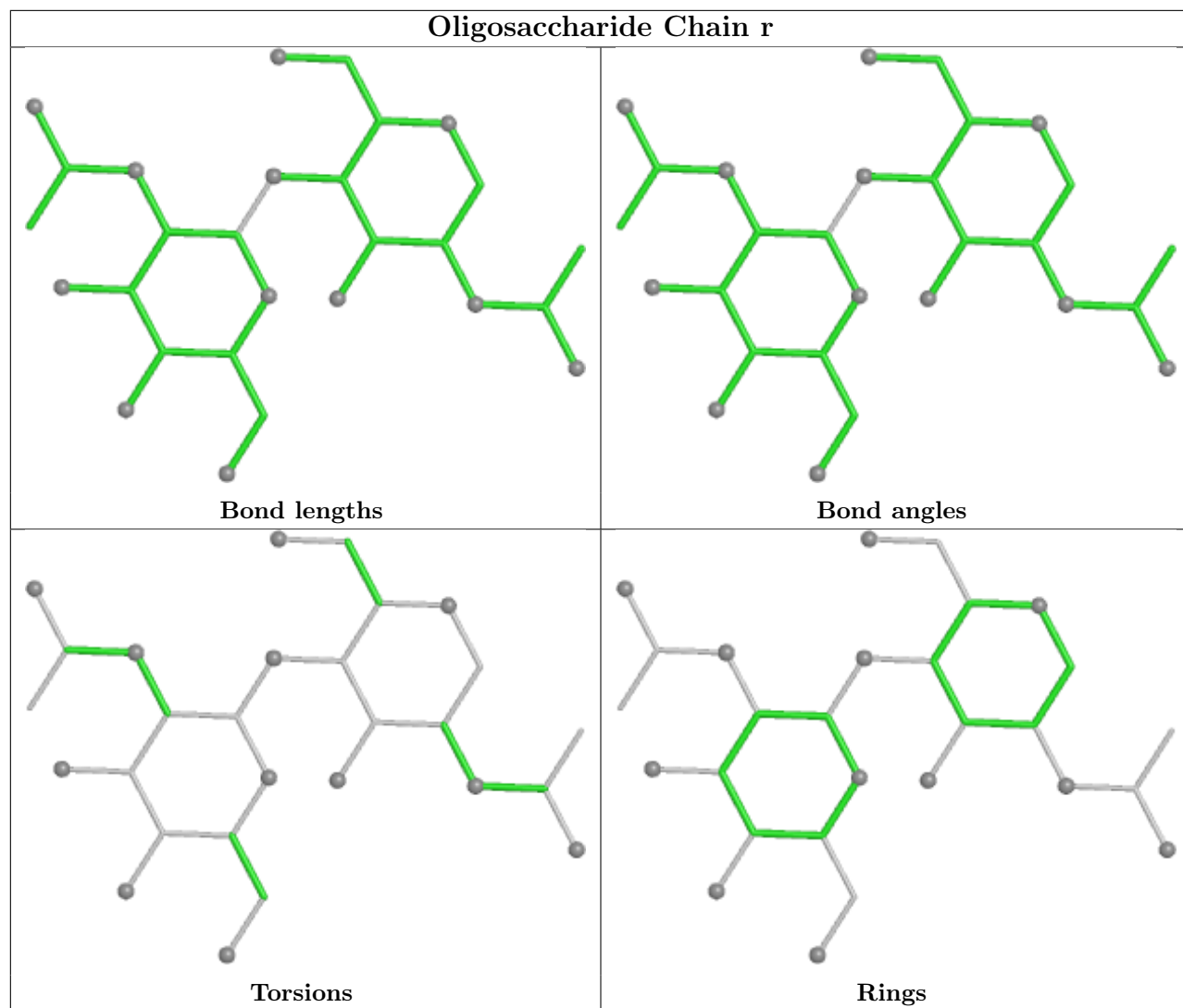


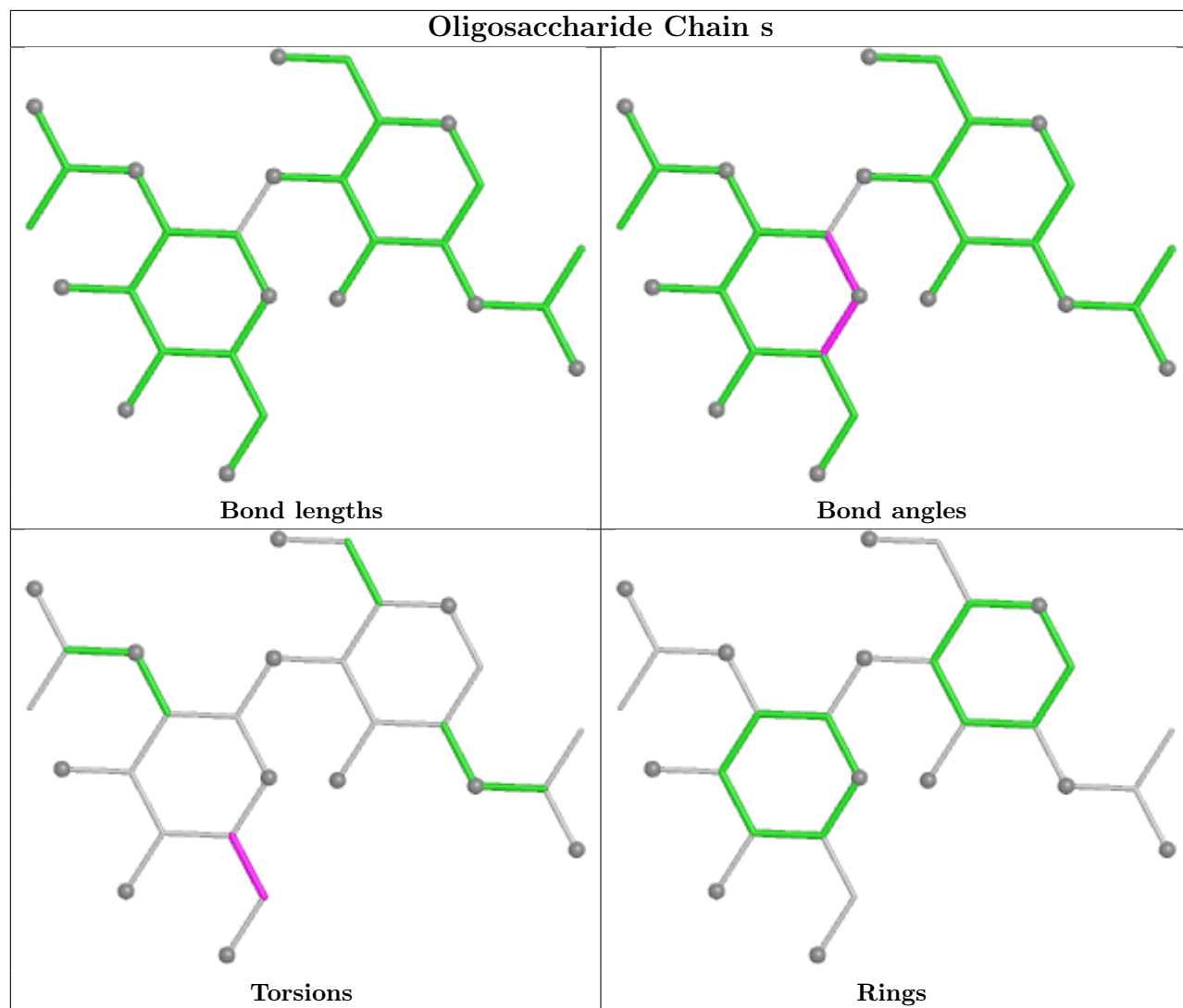


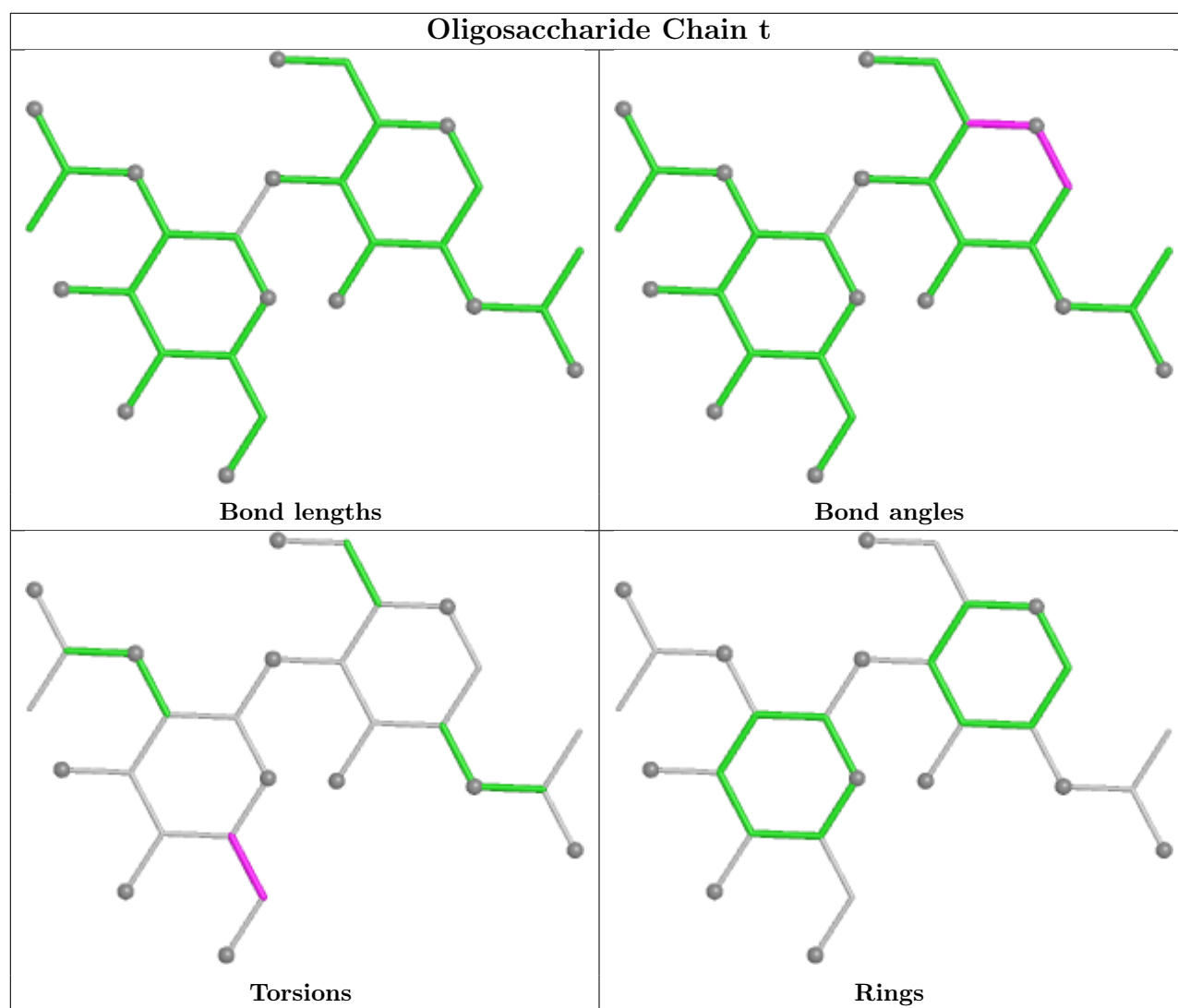


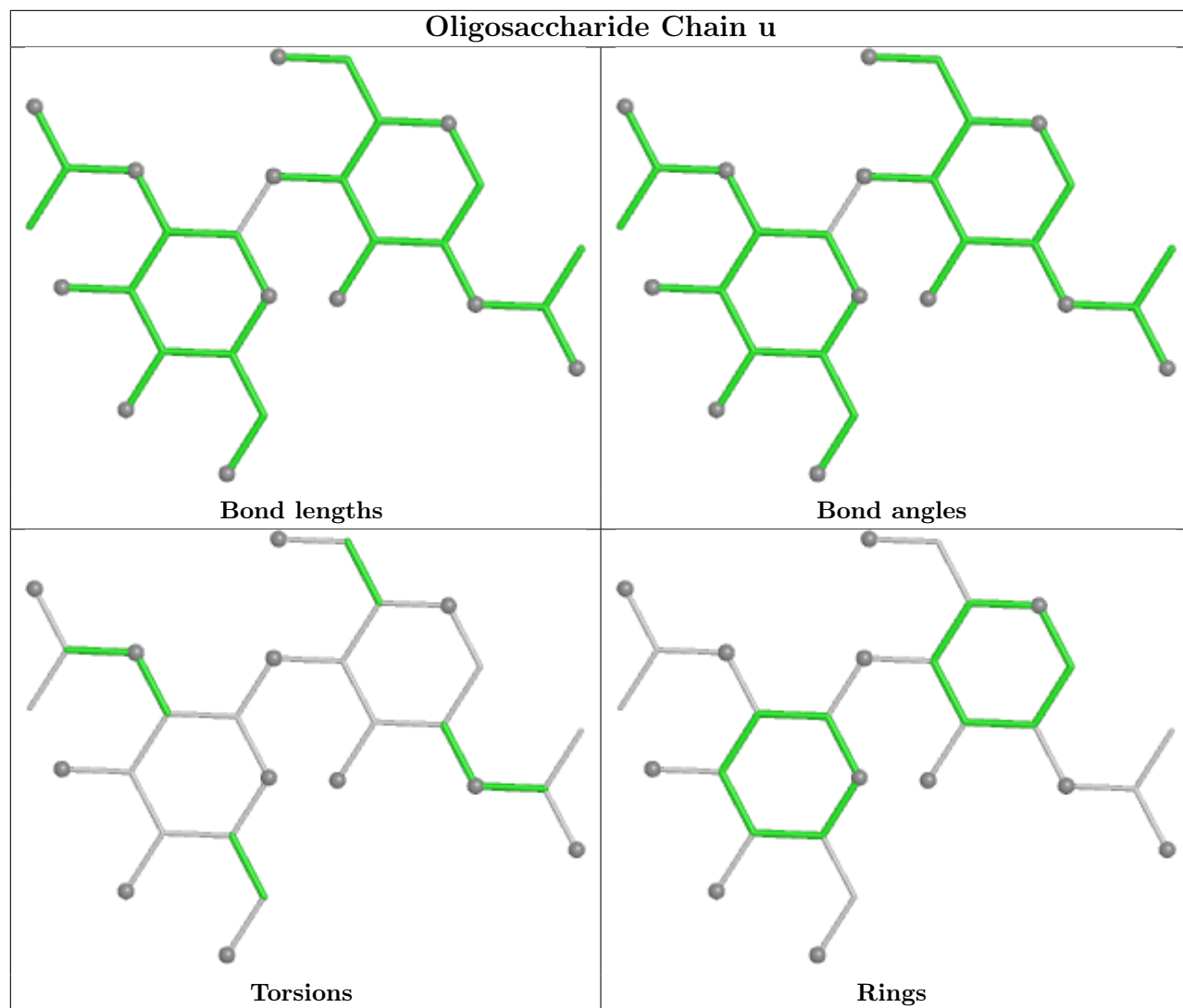




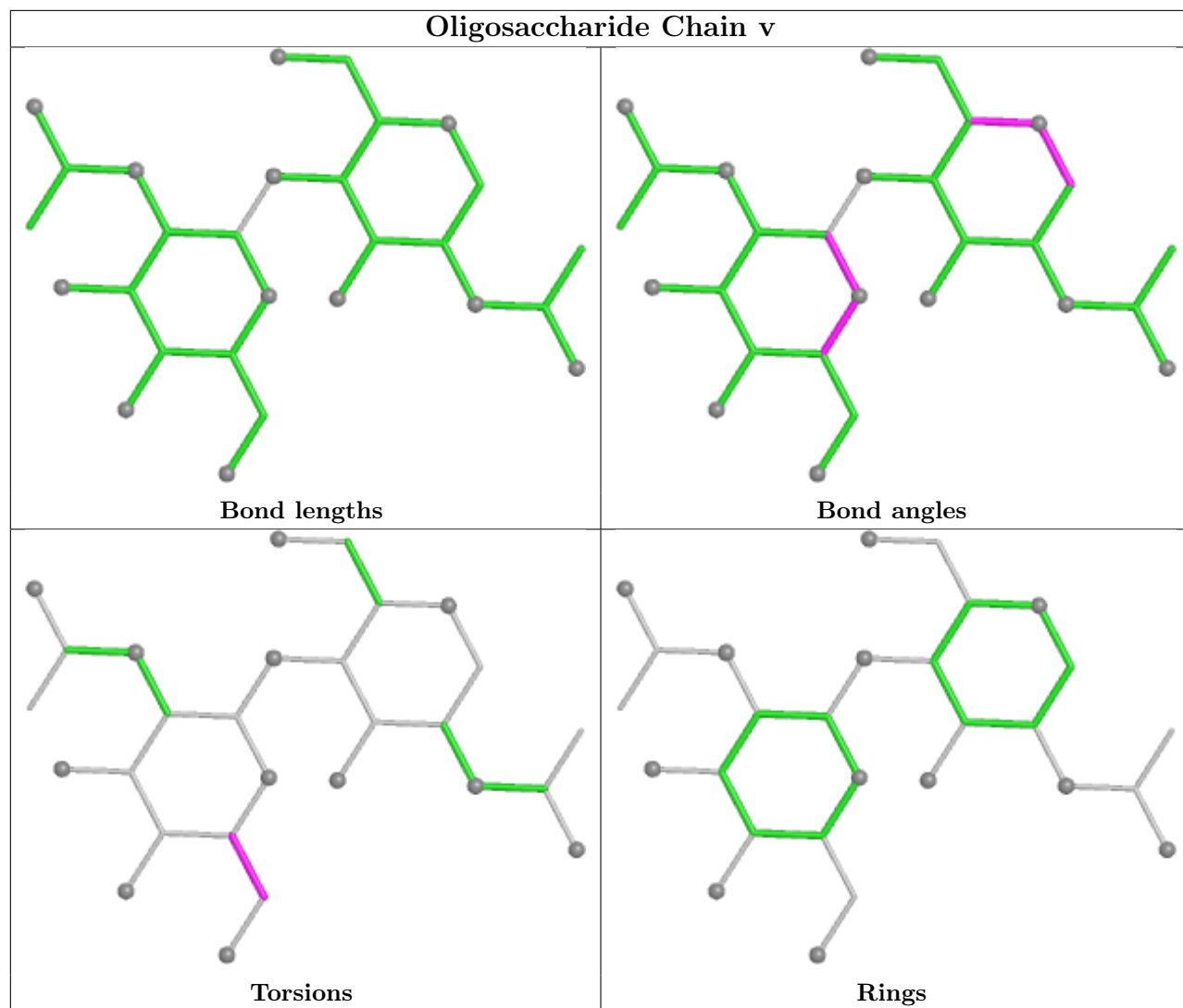


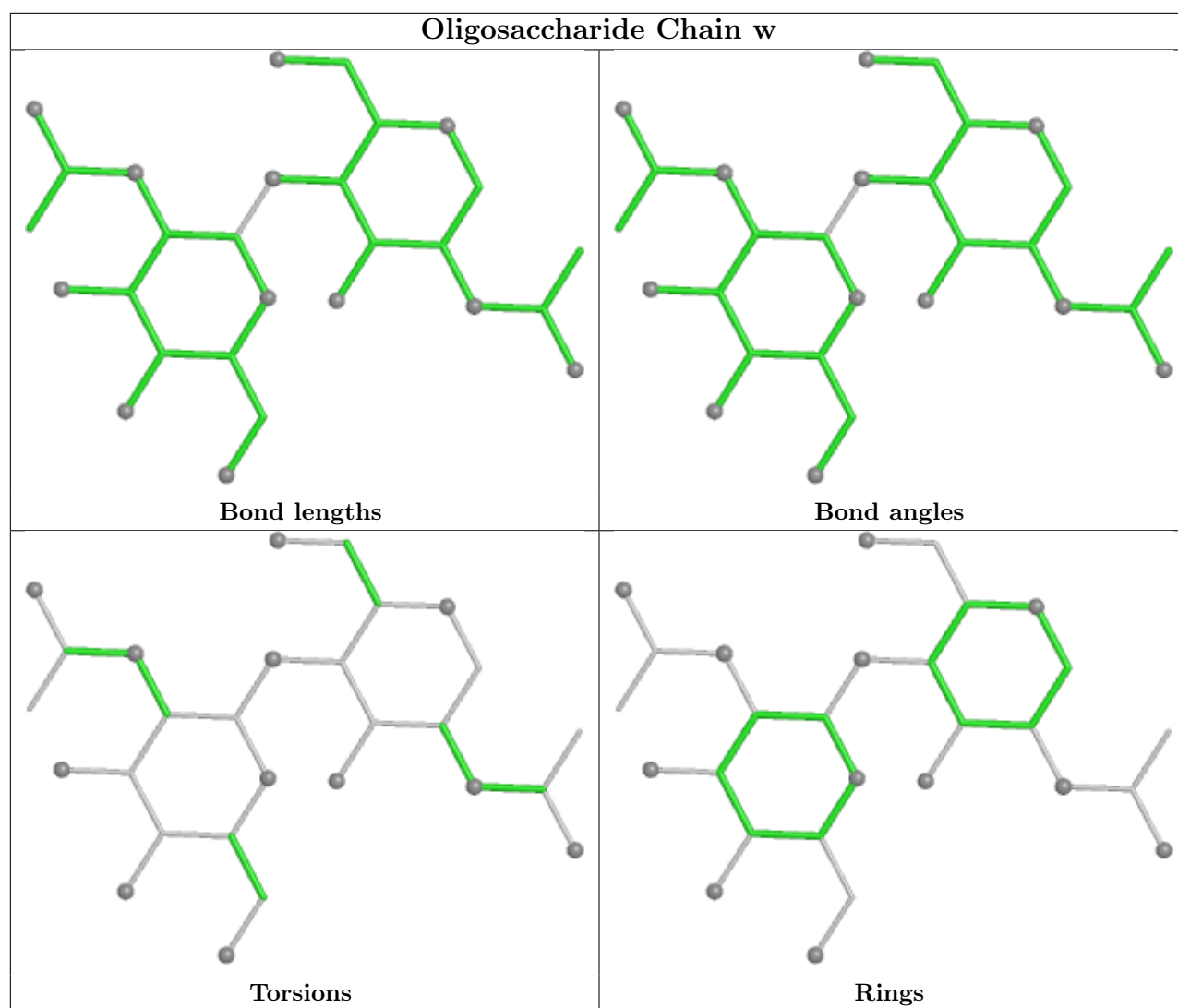


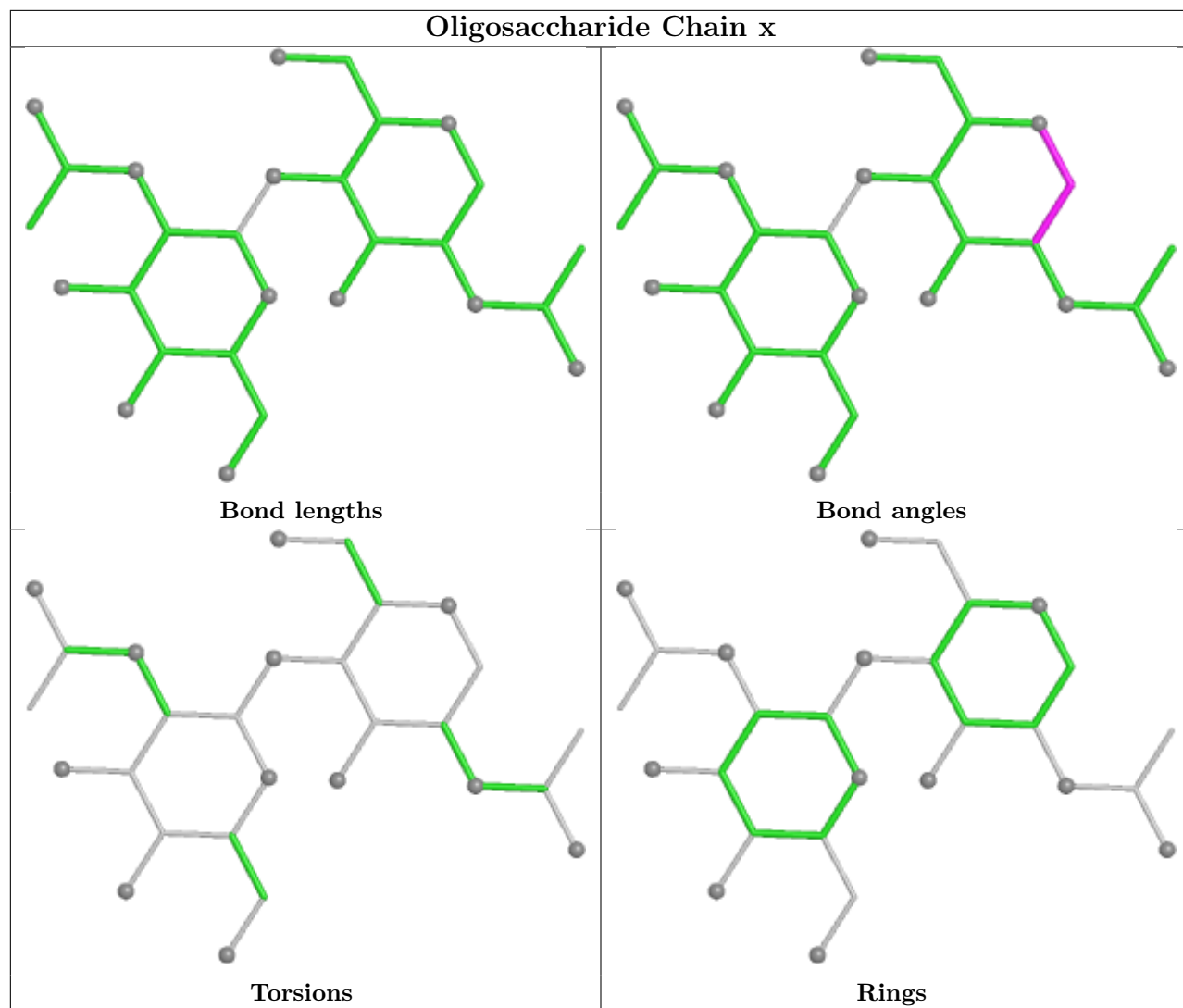


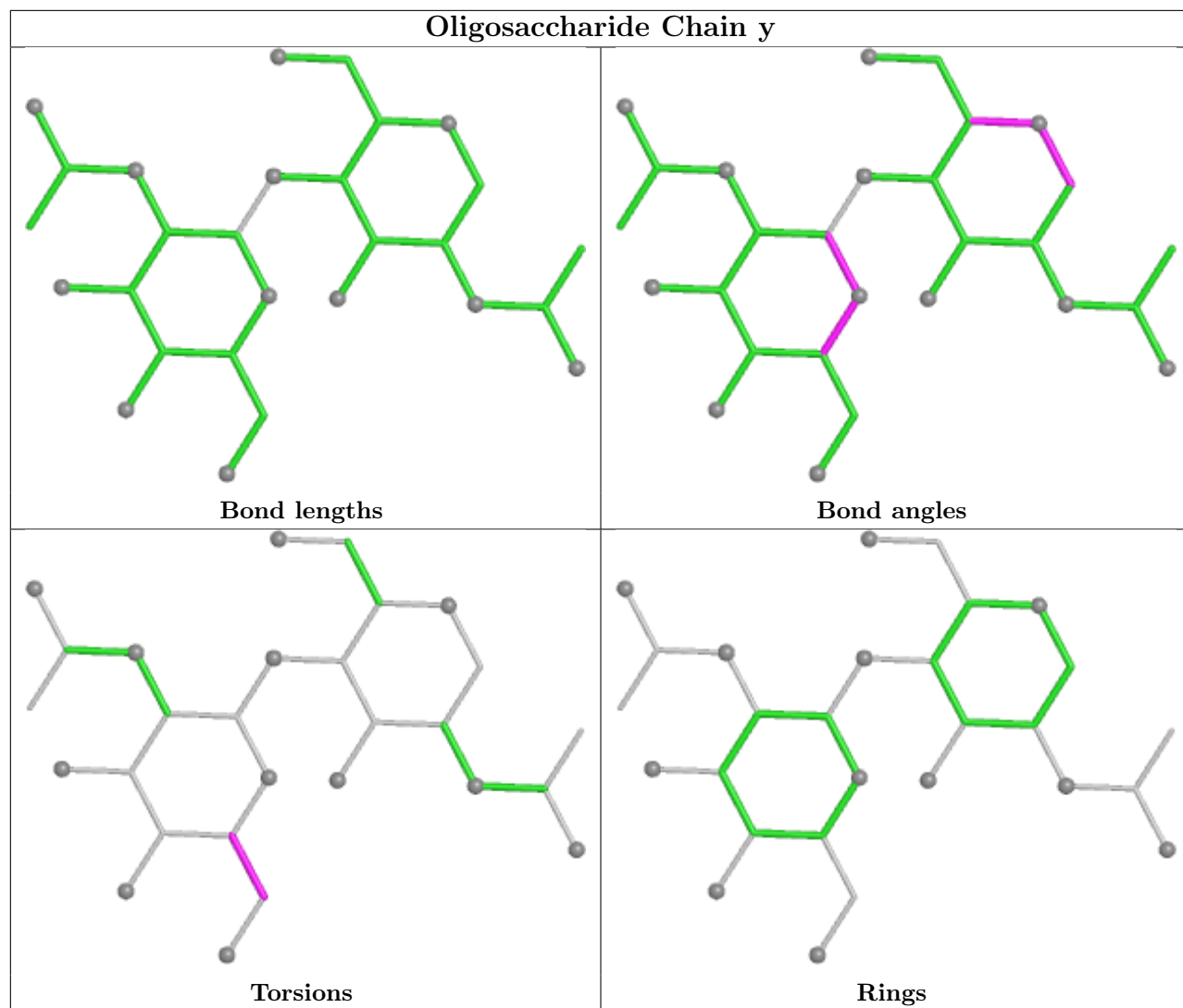


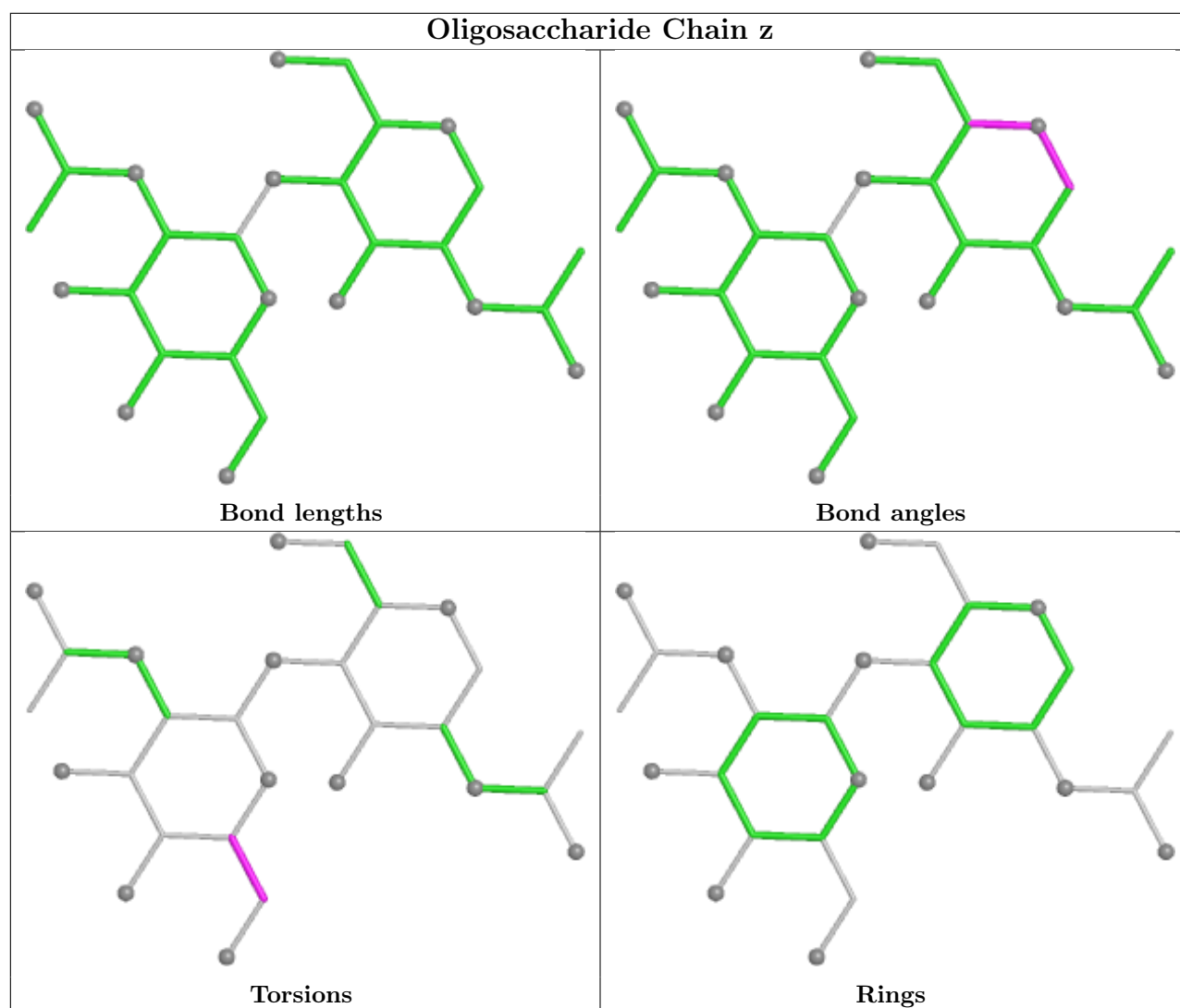












## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.