



Full wwPDB EM Validation Report ⓘ

Apr 13, 2026 – 09:50 PM JST

PDB ID : 9VVJ / pdb_00009vvj
EMDB ID : EMD-65382
Title : Cryo-EM structure of the erlin1/2 complex purified using DDM and GDN
Authors : Yan, L.; Gao, N.
Deposited on : 2025-07-15
Resolution : 2.60 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
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

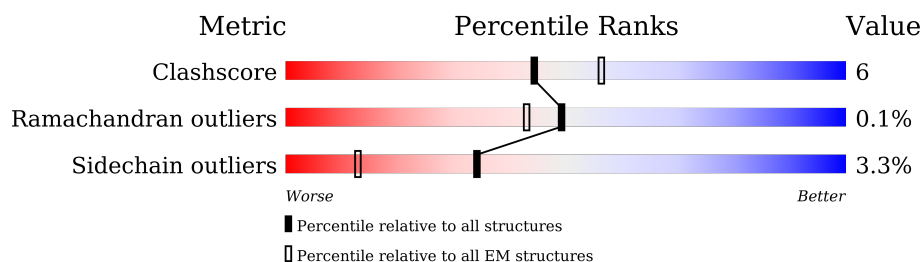
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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	304	81% 18% .
1	B	304	87% 12% .
1	C	304	80% 20% .
1	D	304	81% 18% .
1	E	304	81% 18% .
1	F	304	83% 16%
1	G	304	81% 18% .
1	H	304	81% 18% .
1	I	304	84% 16% .



















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Mol	Chain	Length	Quality of chain
1	J	304	
1	K	304	
1	L	304	
1	M	304	
2	a	304	
2	b	304	
2	c	304	
2	d	304	
2	e	304	
2	f	304	
2	g	304	
2	h	304	
2	i	304	
2	j	304	
2	k	304	
2	l	304	
2	m	304	
3	N	2	
3	O	2	
3	P	2	
3	Q	2	
3	R	2	
3	S	2	
3	T	2	
3	U	2	

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Mol	Chain	Length	Quality of chain
3	V	2	 50% 50%
3	W	2	 50% 50%
3	X	2	 50% 50%
3	Y	2	 50% 50%
3	Z	2	 50% 50%
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	 50% 50%
3	u	2	 50% 50%
3	v	2	 50% 50%
3	w	2	 50% 50%
3	x	2	 50% 50%
3	y	2	 50% 50%
3	z	2	 50% 50%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 63388 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	304	Total	C	N	O	S	0	0
			2423	1555	410	449	9		
1	M	304	Total	C	N	O	S	0	0
			2423	1555	410	449	9		
1	L	304	Total	C	N	O	S	0	0
			2423	1555	410	449	9		
1	K	304	Total	C	N	O	S	0	0
			2423	1555	410	449	9		
1	F	304	Total	C	N	O	S	0	0
			2423	1555	410	449	9		
1	E	304	Total	C	N	O	S	0	0
			2423	1555	410	449	9		
1	D	304	Total	C	N	O	S	0	0
			2423	1555	410	449	9		
1	C	304	Total	C	N	O	S	0	0
			2423	1555	410	449	9		
1	B	304	Total	C	N	O	S	0	0
			2423	1555	410	449	9		
1	J	304	Total	C	N	O	S	0	0
			2423	1555	410	449	9		
1	I	304	Total	C	N	O	S	0	0
			2423	1555	410	449	9		
1	H	304	Total	C	N	O	S	0	0
			2423	1555	410	449	9		
1	G	304	Total	C	N	O	S	0	0
			2423	1555	410	449	9		

- Molecule 2 is a protein called Erlin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	304	Total	C	N	O	S	0	0
			2397	1537	391	455	14		
2	m	304	Total	C	N	O	S	0	0
			2397	1537	391	455	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	k	304	Total	C	N	O	S	0	0
			2397	1537	391	455	14		
2	l	304	Total	C	N	O	S	0	0
			2397	1537	391	455	14		
2	f	304	Total	C	N	O	S	0	0
			2397	1537	391	455	14		
2	d	304	Total	C	N	O	S	0	0
			2397	1537	391	455	14		
2	b	304	Total	C	N	O	S	0	0
			2397	1537	391	455	14		
2	c	304	Total	C	N	O	S	0	0
			2397	1537	391	455	14		
2	e	304	Total	C	N	O	S	0	0
			2397	1537	391	455	14		
2	i	304	Total	C	N	O	S	0	0
			2397	1537	391	455	14		
2	g	304	Total	C	N	O	S	0	0
			2397	1537	391	455	14		
2	h	304	Total	C	N	O	S	0	0
			2397	1537	391	455	14		
2	j	304	Total	C	N	O	S	0	0
			2397	1537	391	455	14		

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
f	295	MET	ILE	conflict	UNP O94905
d	295	MET	ILE	conflict	UNP O94905
b	295	MET	ILE	conflict	UNP O94905
c	295	MET	ILE	conflict	UNP O94905
e	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

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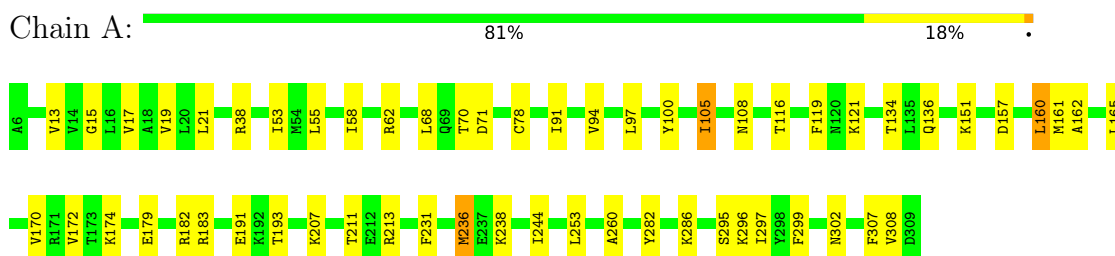
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Mol	Chain	Residues	Atoms				AltConf	Trace
3	t	2	Total	C	N	O	0	0
			28	16	2	10		
3	u	2	Total	C	N	O	0	0
			28	16	2	10		
3	v	2	Total	C	N	O	0	0
			28	16	2	10		
3	w	2	Total	C	N	O	0	0
			28	16	2	10		
3	x	2	Total	C	N	O	0	0
			28	16	2	10		
3	y	2	Total	C	N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

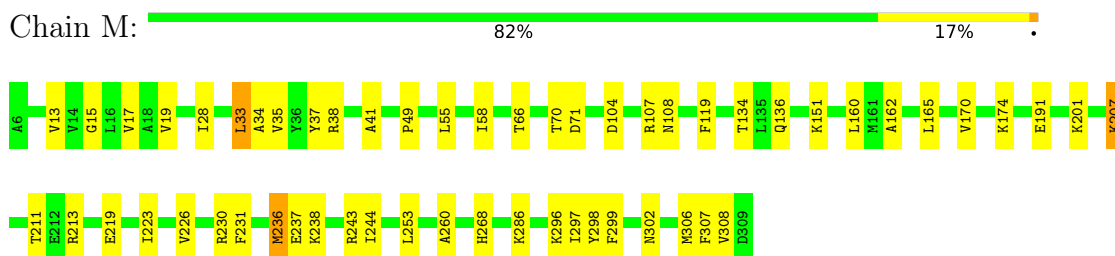
3 Residue-property plots

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.

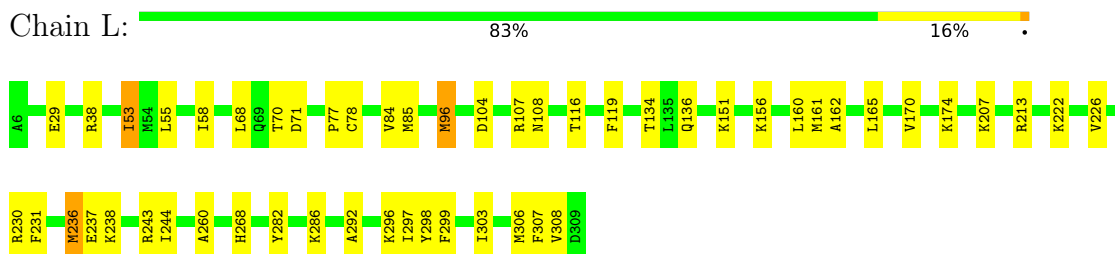
- Molecule 1: Erlin-1



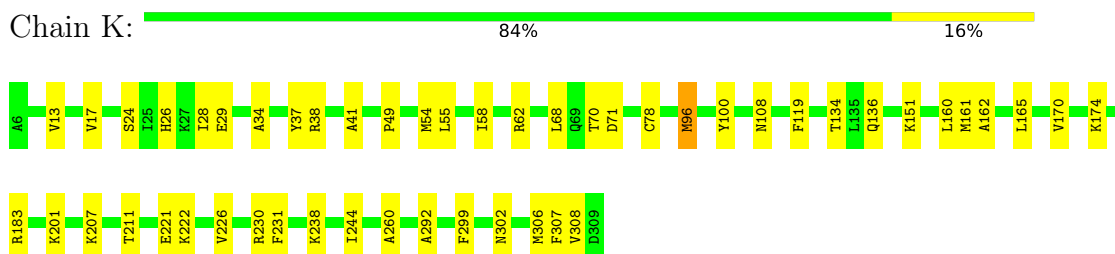
- Molecule 1: Erlin-1



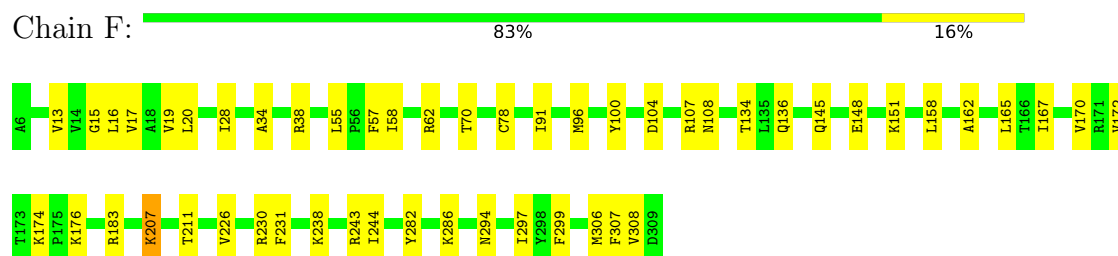
- Molecule 1: Erlin-1



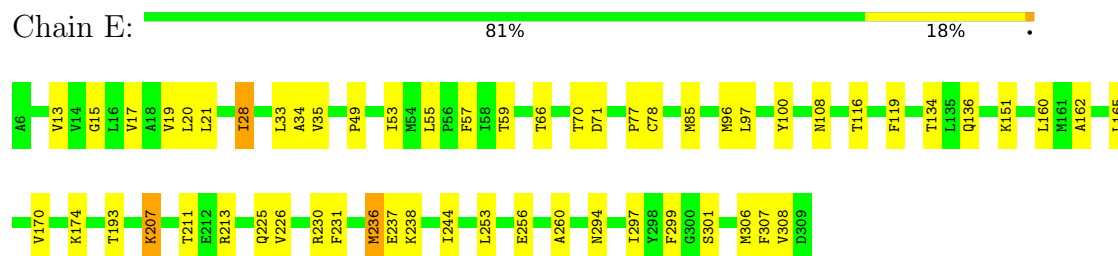
- Molecule 1: Erlin-1



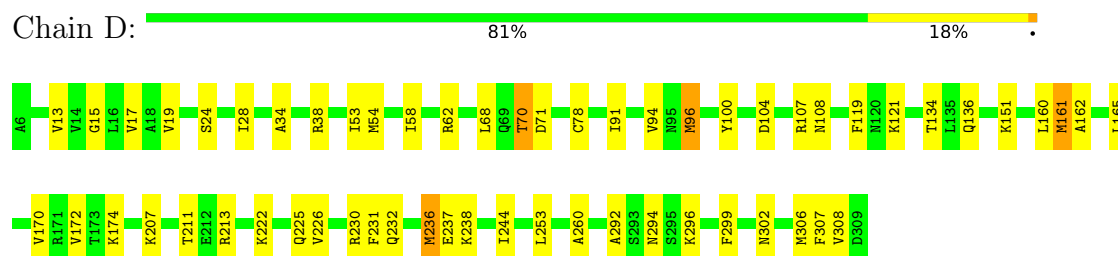
• Molecule 1: Erlin-1



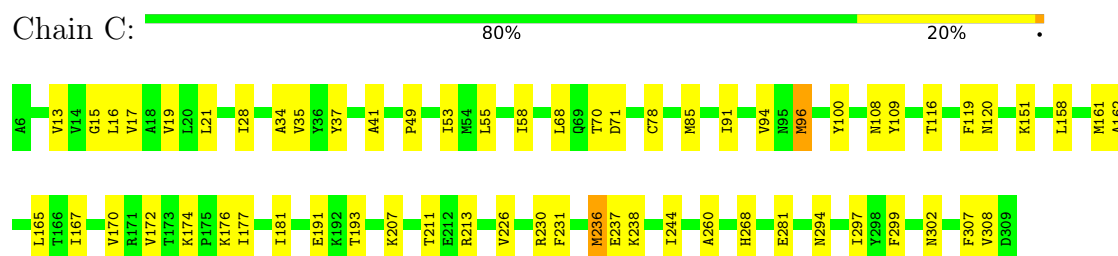
• Molecule 1: Erlin-1



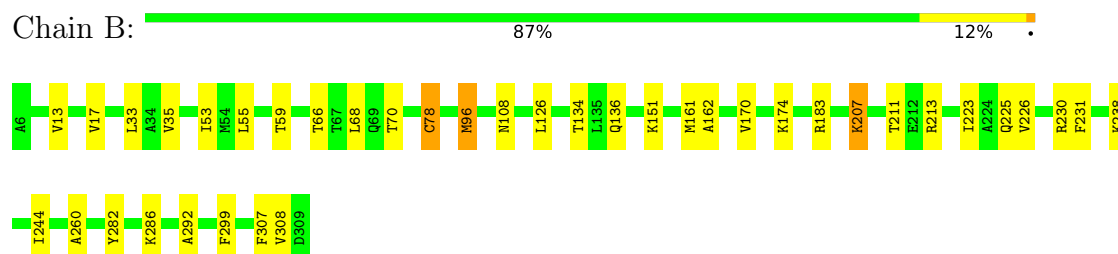
• Molecule 1: Erlin-1



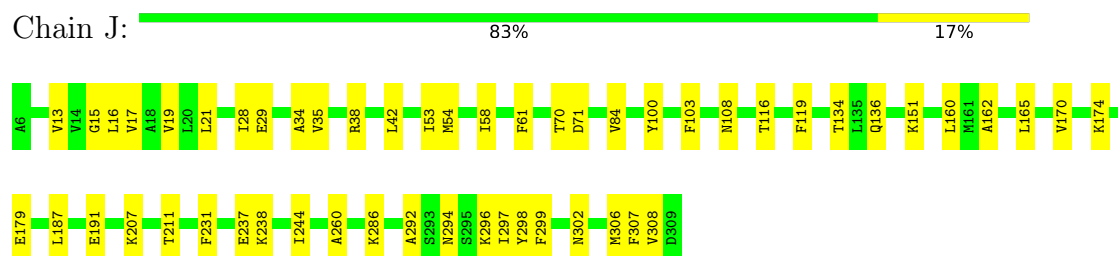
• Molecule 1: Erlin-1



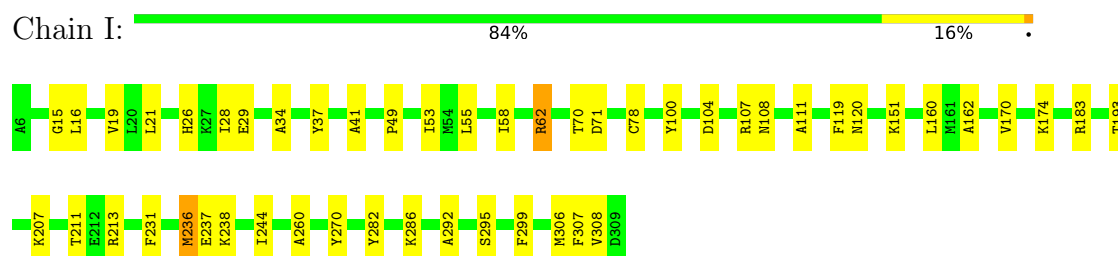
• Molecule 1: Erlin-1



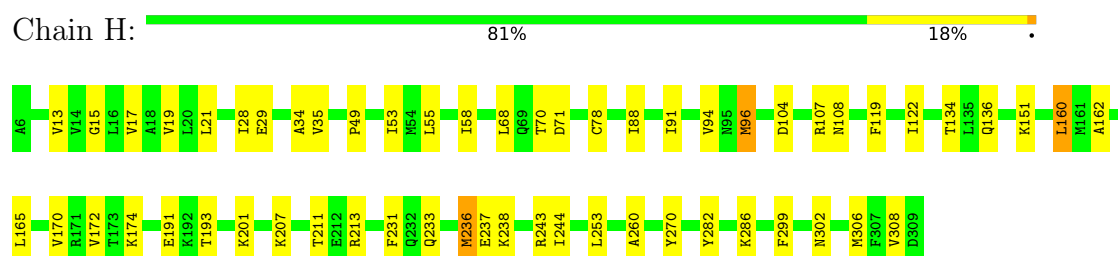
- Molecule 1: Erlin-1



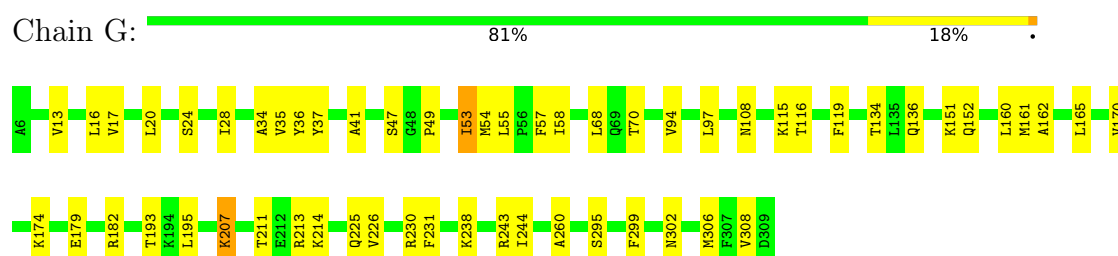
- Molecule 1: Erlin-1



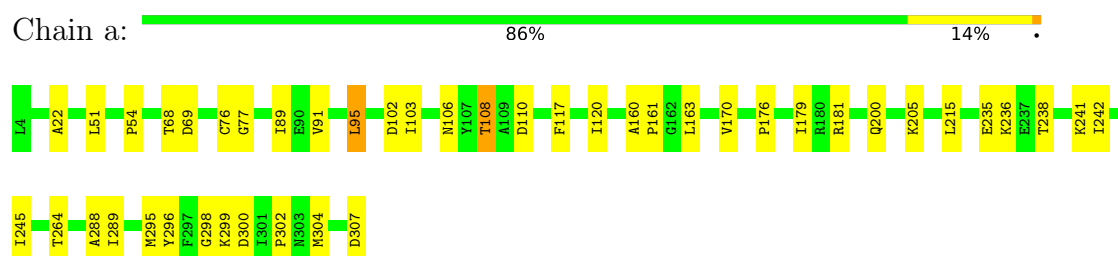
- Molecule 1: Erlin-1




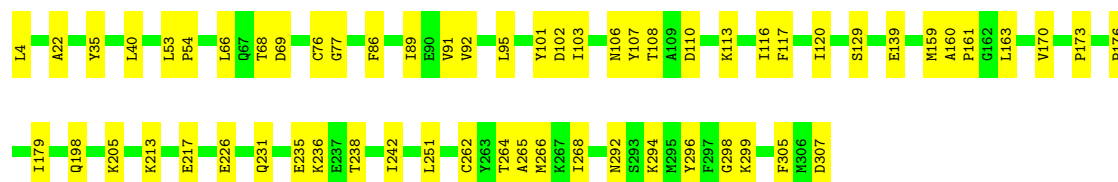
- Molecule 1: Erlin-1




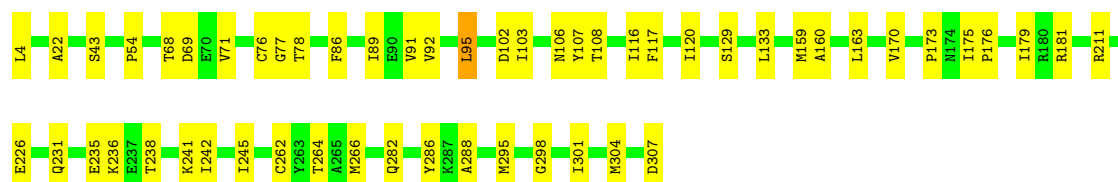
- Molecule 2: Erlin-2




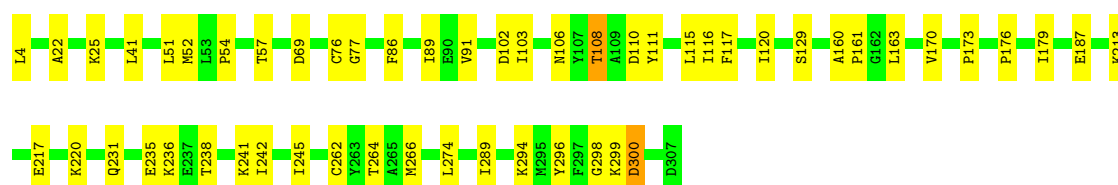
• Molecule 2: Erlin-2

Chain m:  80% 20%


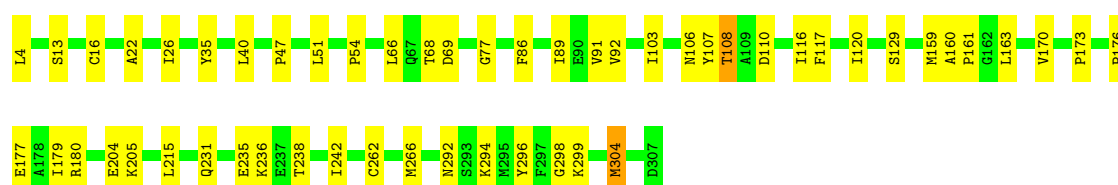
• Molecule 2: Erlin-2

Chain k:  82% 17%


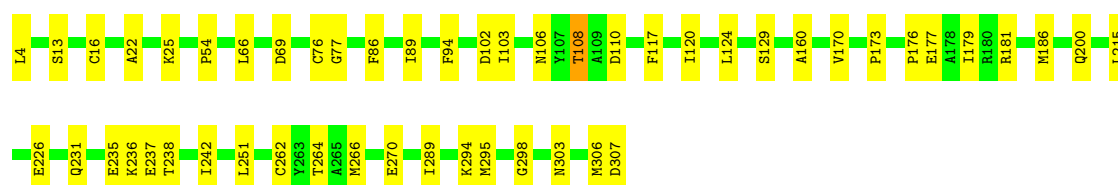
• Molecule 2: Erlin-2

Chain l:  83% 17%


• Molecule 2: Erlin-2

Chain f:  83% 17%


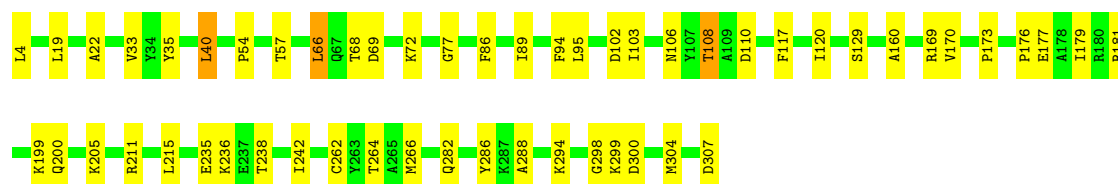
• Molecule 2: Erlin-2

Chain d:  83% 16%


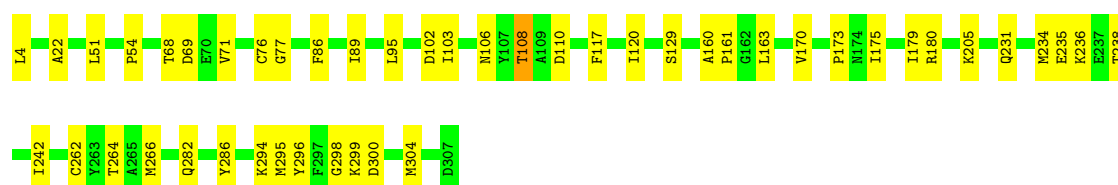
• Molecule 2: Erlin-2

Chain b:  86% 14%


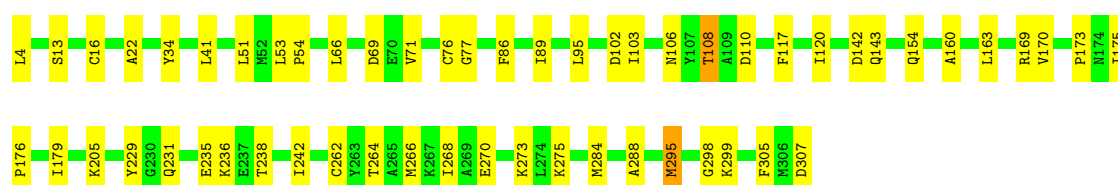
• Molecule 2: Erlin-2

Chain c:  82% 17%


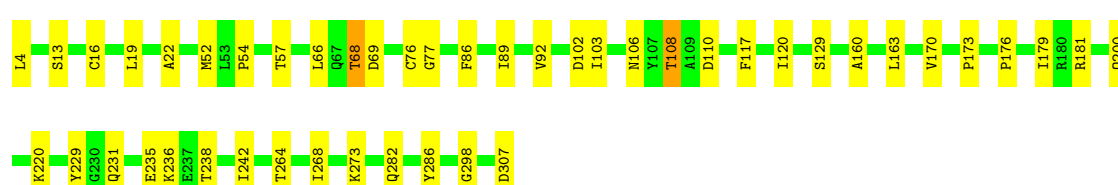
• Molecule 2: Erlin-2

Chain e:  85% 15%

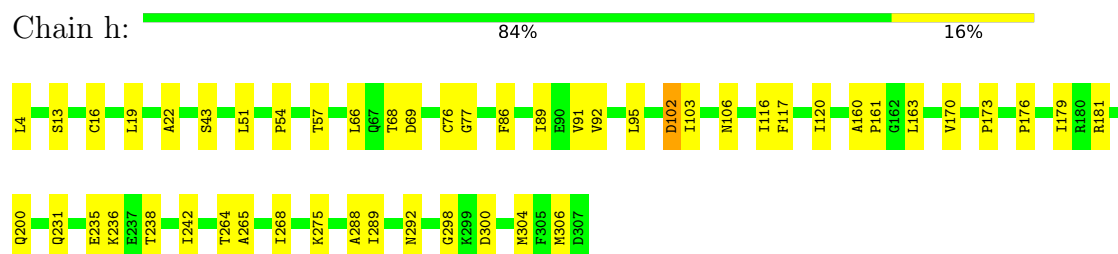
• Molecule 2: Erlin-2

Chain i:  82% 18%

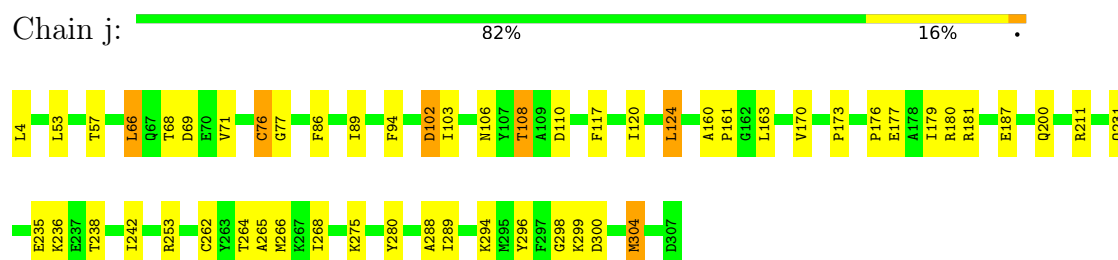
• Molecule 2: Erlin-2

Chain g:  85% 14%

• Molecule 2: Erlin-2



• Molecule 2: Erlin-2



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



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



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



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



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

Chain R:  50% 50%



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

Chain S:  50% 50%



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

Chain T:  50% 50%



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

Chain U:  50% 50%



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

Chain V:  50% 50%



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

Chain W:  50% 50%



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

Chain X:  50% 50%



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

Chain Y:



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

Chain Z:



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

Chain n:



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

Chain o:



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

Chain p:



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

Chain q:



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

Chain r:  50% 50%



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

Chain s:  50% 50%



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

Chain t:  50% 50%



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

Chain u:  50% 50%



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

Chain v:  50% 50%



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

Chain w:  50% 50%



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

Chain x:  50% 50%



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

Chain y:  50% 50%



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

Chain z:  50% 50%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25074	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 ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (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	0.15	0/2466	0.36	0/3331
1	B	0.15	0/2466	0.35	0/3331
1	C	0.14	0/2466	0.36	0/3331
1	D	0.15	0/2466	0.35	0/3331
1	E	0.14	0/2466	0.35	0/3331
1	F	0.15	0/2466	0.36	0/3331
1	G	0.15	0/2466	0.36	0/3331
1	H	0.15	0/2466	0.34	0/3331
1	I	0.15	0/2466	0.36	0/3331
1	J	0.14	0/2466	0.34	0/3331
1	K	0.15	0/2466	0.35	0/3331
1	L	0.15	0/2466	0.35	0/3331
1	M	0.14	0/2466	0.35	0/3331
2	a	0.15	0/2438	0.34	0/3289
2	b	0.15	0/2438	0.35	0/3289
2	c	0.15	0/2438	0.34	0/3289
2	d	0.15	0/2438	0.34	0/3289
2	e	0.15	0/2438	0.34	0/3289
2	f	0.15	0/2438	0.34	0/3289
2	g	0.16	0/2438	0.34	0/3289
2	h	0.15	0/2438	0.33	0/3289
2	i	0.15	0/2438	0.36	0/3289
2	j	0.15	0/2438	0.34	0/3289
2	k	0.16	0/2438	0.35	0/3289
2	l	0.15	0/2438	0.34	0/3289
2	m	0.15	0/2438	0.35	0/3289
All	All	0.15	0/63752	0.35	0/86060

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2423	0	2482	42	0
1	B	2423	0	2482	29	0
1	C	2423	0	2482	46	0
1	D	2423	0	2482	46	0
1	E	2423	0	2482	42	0
1	F	2423	0	2482	43	0
1	G	2423	0	2482	42	0
1	H	2423	0	2482	44	0
1	I	2423	0	2482	37	0
1	J	2423	0	2482	37	0
1	K	2423	0	2482	38	0
1	L	2423	0	2482	40	0
1	M	2423	0	2482	42	0
2	a	2397	0	2435	36	0
2	b	2397	0	2435	31	0
2	c	2397	0	2435	40	0
2	d	2397	0	2435	37	0
2	e	2397	0	2435	37	0
2	f	2397	0	2435	39	0
2	g	2397	0	2435	33	0
2	h	2397	0	2435	35	0
2	i	2397	0	2435	41	0
2	j	2397	0	2435	44	0
2	k	2397	0	2435	40	0
2	l	2397	0	2435	39	0
2	m	2397	0	2435	42	0
3	N	28	0	25	3	0
3	O	28	0	25	6	0
3	P	28	0	25	3	0
3	Q	28	0	25	5	0
3	R	28	0	25	3	0
3	S	28	0	25	3	0
3	T	28	0	25	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	U	28	0	25	5	0
3	V	28	0	25	3	0
3	W	28	0	25	5	0
3	X	28	0	25	3	0
3	Y	28	0	25	3	0
3	Z	28	0	25	5	0
3	n	28	0	25	3	0
3	o	28	0	25	3	0
3	p	28	0	25	5	0
3	q	28	0	25	5	0
3	r	28	0	25	5	0
3	s	28	0	25	3	0
3	t	28	0	25	3	0
3	u	28	0	25	5	0
3	v	28	0	25	3	0
3	w	28	0	25	3	0
3	x	28	0	25	5	0
3	y	28	0	25	6	0
3	z	28	0	25	6	0
All	All	63388	0	64571	816	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 6.

All (816) 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:L:308:VAL:HB	1:K:308:VAL:HG13	1.66	0.76
2:i:22:ALA:HB2	2:i:54:PRO:HG3	1.68	0.75
2:a:176:PRO:HG2	2:a:179:ILE:HD13	1.69	0.74
2:f:108:THR:HG23	2:f:110:ASP:H	1.53	0.73
2:c:22:ALA:HB2	2:c:54:PRO:HG3	1.69	0.73
1:K:308:VAL:HB	1:J:308:VAL:HG13	1.71	0.73
1:F:308:VAL:HB	1:E:308:VAL:HG13	1.70	0.73
1:G:213:ARG:HG3	2:g:220:LYS:HB2	1.70	0.73
1:E:308:VAL:HB	1:D:308:VAL:HG13	1.69	0.73
1:D:260:ALA:HB2	2:d:264:THR:HG22	1.71	0.72
2:k:22:ALA:HB2	2:k:54:PRO:HG3	1.71	0.72
1:M:308:VAL:HB	1:L:308:VAL:HG13	1.70	0.71
1:H:308:VAL:HB	1:G:308:VAL:HG13	1.72	0.71
1:A:308:VAL:HB	1:M:308:VAL:HG13	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:260:ALA:HB2	2:l:264:THR:HG22	1.73	0.71
2:b:22:ALA:HB2	2:b:54:PRO:HG3	1.73	0.71
1:J:308:VAL:HB	1:I:308:VAL:HG13	1.73	0.71
1:D:308:VAL:HB	1:C:308:VAL:HG13	1.72	0.71
2:g:22:ALA:HB2	2:g:54:PRO:HG3	1.72	0.70
1:I:55:LEU:HD22	1:I:58:ILE:HD11	1.72	0.70
2:a:22:ALA:HB2	2:a:54:PRO:HG3	1.72	0.70
2:m:22:ALA:HB2	2:m:54:PRO:HG3	1.72	0.70
2:j:176:PRO:HG2	2:j:179:ILE:HD13	1.72	0.70
1:G:260:ALA:HB2	2:g:264:THR:HG22	1.74	0.70
1:I:260:ALA:HB2	2:i:264:THR:HG22	1.74	0.69
2:d:106:ASN:HD22	3:Z:1:NAG:H83	1.58	0.69
1:F:308:VAL:HG13	1:G:308:VAL:HB	1.73	0.69
1:M:260:ALA:HB2	2:m:264:THR:HG22	1.75	0.69
2:h:22:ALA:HB2	2:h:54:PRO:HG3	1.72	0.69
2:d:22:ALA:HB2	2:d:54:PRO:HG3	1.73	0.69
1:E:28:ILE:HG12	1:E:34:ALA:HB2	1.76	0.68
1:B:213:ARG:HG3	2:b:220:LYS:HB2	1.76	0.67
1:I:28:ILE:HG22	1:I:49:PRO:HA	1.77	0.67
1:A:308:VAL:HG13	1:B:308:VAL:HB	1.75	0.67
2:a:108:THR:HG23	2:a:110:ASP:H	1.58	0.67
2:j:106:ASN:HD22	3:z:1:NAG:H83	1.58	0.67
2:h:106:ASN:HD22	3:y:1:NAG:H83	1.58	0.67
2:m:108:THR:HG23	2:m:110:ASP:H	1.58	0.67
1:I:308:VAL:HB	1:H:308:VAL:HG13	1.75	0.67
1:H:260:ALA:HB2	2:h:264:THR:HG22	1.77	0.67
1:I:108:ASN:HD22	3:t:1:NAG:H83	1.58	0.67
1:J:260:ALA:HB2	2:j:264:THR:HG22	1.77	0.66
1:E:306:MET:HE1	1:D:306:MET:HE3	1.77	0.66
1:G:108:ASN:HD22	3:w:1:NAG:H83	1.60	0.66
1:B:260:ALA:HB2	2:b:264:THR:HG22	1.75	0.66
2:a:236:LYS:HG3	1:B:244:ILE:HG23	1.76	0.66
2:f:22:ALA:HB2	2:f:54:PRO:HG3	1.76	0.66
2:a:106:ASN:HD22	3:O:1:NAG:H83	1.61	0.66
1:L:231:PHE:HB3	2:l:238:THR:HG21	1.78	0.66
2:g:106:ASN:HD22	3:x:1:NAG:H83	1.61	0.66
1:A:97:LEU:HD11	1:A:105:ILE:HD12	1.78	0.65
2:k:106:ASN:HD22	3:T:1:NAG:H83	1.61	0.65
2:m:106:ASN:HD22	3:Q:1:NAG:H83	1.62	0.65
1:F:108:ASN:HD22	3:V:1:NAG:H83	1.62	0.65
1:D:244:ILE:HG23	2:c:236:LYS:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:106:ASN:HD22	3:p:1:NAG:H83	1.61	0.65
1:L:108:ASN:HD22	3:R:1:NAG:H83	1.62	0.65
1:C:260:ALA:HB2	2:c:264:THR:HG22	1.77	0.65
2:i:108:THR:HG23	2:i:110:ASP:H	1.62	0.65
2:l:176:PRO:HG2	2:l:179:ILE:HD13	1.77	0.65
2:e:106:ASN:HD22	3:r:1:NAG:H83	1.62	0.65
1:A:260:ALA:HB2	2:a:264:THR:HG22	1.78	0.65
1:A:297:ILE:HG12	2:a:304:MET:HE1	1.79	0.65
1:M:55:LEU:HD22	1:M:58:ILE:HD11	1.79	0.65
1:K:108:ASN:HD22	3:S:1:NAG:H83	1.62	0.65
2:c:262:CYS:O	2:c:266:MET:HG2	1.97	0.65
2:f:106:ASN:HD22	3:W:1:NAG:H83	1.62	0.65
1:C:308:VAL:HB	1:B:308:VAL:HG13	1.79	0.65
1:D:108:ASN:HD22	3:Y:1:NAG:H83	1.62	0.65
1:C:226:VAL:HG12	1:C:230:ARG:HH12	1.62	0.65
2:i:106:ASN:HD22	3:u:1:NAG:H83	1.61	0.65
1:K:260:ALA:HB2	2:k:264:THR:HG22	1.79	0.64
2:e:22:ALA:HB2	2:e:54:PRO:HG3	1.77	0.64
1:C:244:ILE:HG23	2:b:236:LYS:HG3	1.79	0.64
1:B:108:ASN:HD22	3:o:1:NAG:H83	1.60	0.64
1:I:231:PHE:HB3	2:i:238:THR:HG21	1.80	0.64
1:K:28:ILE:HG12	1:K:34:ALA:HB2	1.80	0.63
2:l:106:ASN:HD22	3:U:1:NAG:H83	1.63	0.63
1:M:231:PHE:HB3	2:m:238:THR:HG21	1.79	0.63
1:E:244:ILE:HG23	2:d:236:LYS:HG3	1.81	0.63
1:I:244:ILE:HG23	2:h:236:LYS:HG3	1.79	0.63
1:A:231:PHE:HB3	2:a:238:THR:HG21	1.81	0.63
1:L:213:ARG:HG3	2:l:220:LYS:HB2	1.79	0.63
2:c:106:ASN:HD22	3:q:1:NAG:H83	1.64	0.63
1:H:244:ILE:HG23	2:g:236:LYS:HG3	1.81	0.63
2:b:68:THR:HG22	2:b:92:VAL:HG22	1.81	0.63
1:M:306:MET:HE1	1:L:306:MET:HE3	1.81	0.63
1:C:231:PHE:HB3	2:c:238:THR:HG21	1.81	0.63
2:g:108:THR:HG23	2:g:110:ASP:H	1.64	0.62
1:H:108:ASN:HD22	3:v:1:NAG:H83	1.64	0.62
1:D:226:VAL:HG12	1:D:230:ARG:HH12	1.65	0.62
1:M:33:LEU:HD12	1:M:66:THR:HG21	1.81	0.62
1:M:302:ASN:HD21	2:l:299:LYS:HG3	1.64	0.62
1:E:260:ALA:HB2	2:e:264:THR:HG22	1.81	0.62
1:M:244:ILE:HG23	2:l:236:LYS:HG3	1.81	0.62
2:f:236:LYS:HG3	1:G:244:ILE:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:108:THR:HG23	2:c:110:ASP:H	1.63	0.62
1:K:244:ILE:HG23	2:j:236:LYS:HG3	1.82	0.61
1:M:28:ILE:HG12	1:M:34:ALA:HB2	1.82	0.61
1:F:244:ILE:HG23	2:e:236:LYS:HG3	1.83	0.61
1:D:231:PHE:HB3	2:d:238:THR:HG21	1.82	0.61
1:A:244:ILE:HG23	2:m:236:LYS:HG3	1.82	0.61
1:L:244:ILE:HG23	2:k:236:LYS:HG3	1.81	0.61
1:K:55:LEU:HD22	1:K:58:ILE:HD11	1.81	0.61
1:H:55:LEU:HD22	1:H:58:ILE:HD11	1.83	0.61
2:j:262:CYS:O	2:j:266:MET:HG2	2.01	0.61
2:m:305:PHE:HZ	2:l:289:ILE:HD11	1.64	0.61
2:h:176:PRO:HG2	2:h:179:ILE:HD13	1.82	0.60
1:J:231:PHE:HB3	2:j:238:THR:HG21	1.83	0.60
1:A:108:ASN:HD22	3:N:1:NAG:H83	1.64	0.60
2:f:179:ILE:HG23	1:G:193:THR:HG21	1.81	0.60
1:C:28:ILE:HG12	1:C:34:ALA:HB2	1.82	0.60
2:j:108:THR:HG23	2:j:110:ASP:H	1.66	0.60
2:j:66:LEU:HD23	2:j:94:PHE:HB3	1.82	0.60
1:I:28:ILE:HG12	1:I:34:ALA:HB2	1.84	0.60
1:F:231:PHE:HB3	2:f:238:THR:HG21	1.82	0.60
2:l:22:ALA:HB2	2:l:54:PRO:HG3	1.83	0.60
2:m:68:THR:HG22	2:m:92:VAL:HG22	1.84	0.60
1:K:231:PHE:HB3	2:k:238:THR:HG21	1.83	0.60
1:L:174:LYS:HE2	2:k:77:GLY:HA3	1.84	0.60
2:m:262:CYS:O	2:m:266:MET:HG2	2.02	0.60
1:J:108:ASN:HD22	3:s:1:NAG:H83	1.67	0.60
2:i:175:ILE:HD12	2:i:179:ILE:HB	1.84	0.60
2:d:108:THR:HG23	2:d:110:ASP:H	1.65	0.59
1:G:151:LYS:HG3	1:G:170:VAL:HG23	1.84	0.59
1:E:193:THR:HG21	2:d:179:ILE:HG23	1.83	0.59
2:d:66:LEU:HD12	2:d:94:PHE:HB3	1.83	0.59
2:c:176:PRO:HG2	2:c:179:ILE:HD13	1.85	0.59
2:k:262:CYS:O	2:k:266:MET:HG2	2.02	0.59
2:c:117:PHE:HA	2:c:120:ILE:HD12	1.85	0.59
1:M:28:ILE:HG22	1:M:49:PRO:HA	1.84	0.59
2:e:108:THR:HG23	2:e:110:ASP:H	1.67	0.59
1:H:151:LYS:HG3	1:H:170:VAL:HG23	1.85	0.59
1:H:231:PHE:HB3	2:h:238:THR:HG21	1.84	0.59
1:K:28:ILE:HG22	1:K:49:PRO:HA	1.83	0.58
1:B:231:PHE:HB3	2:b:238:THR:HG21	1.83	0.58
1:J:244:ILE:HG23	2:i:236:LYS:HG3	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:231:PHE:HB3	2:g:238:THR:HG21	1.84	0.58
1:L:151:LYS:HG3	1:L:170:VAL:HG23	1.85	0.58
1:F:55:LEU:HD22	1:F:58:ILE:HD11	1.84	0.58
1:C:108:ASN:HD22	3:n:1:NAG:H83	1.68	0.58
2:e:262:CYS:O	2:e:266:MET:HG2	2.03	0.58
2:l:108:THR:HG23	2:l:110:ASP:H	1.68	0.58
1:G:55:LEU:HD22	1:G:58:ILE:HD11	1.86	0.58
2:g:176:PRO:HG2	2:g:179:ILE:HD13	1.84	0.58
1:M:108:ASN:HD22	3:P:1:NAG:H83	1.69	0.57
1:E:108:ASN:HD22	3:X:1:NAG:H83	1.68	0.57
1:E:151:LYS:HG3	1:E:170:VAL:HG23	1.86	0.57
1:C:91:ILE:HG12	1:C:172:VAL:HG12	1.86	0.57
1:M:151:LYS:HG3	1:M:170:VAL:HG23	1.86	0.57
2:l:117:PHE:HA	2:l:120:ILE:HD12	1.86	0.57
1:E:231:PHE:HB3	2:e:238:THR:HG21	1.85	0.57
1:F:151:LYS:HG3	1:F:170:VAL:HG23	1.87	0.57
2:i:89:ILE:HG12	2:i:170:VAL:HG12	1.86	0.57
1:C:158:LEU:HD12	1:C:167:ILE:HD11	1.86	0.57
1:A:91:ILE:HG12	1:A:172:VAL:HG12	1.86	0.56
1:E:28:ILE:HG22	1:E:49:PRO:HA	1.86	0.56
2:j:89:ILE:HG12	2:j:170:VAL:HG12	1.87	0.56
2:f:304:MET:HG3	1:G:299:PHE:HE2	1.69	0.56
2:f:89:ILE:HG12	2:f:170:VAL:HG12	1.87	0.56
1:K:238:LYS:HG3	2:k:242:ILE:HG12	1.87	0.56
1:C:28:ILE:HG22	1:C:49:PRO:HA	1.85	0.56
1:B:162:ALA:HA	3:o:1:NAG:H82	1.88	0.56
1:H:162:ALA:HA	3:v:1:NAG:H82	1.88	0.56
2:m:89:ILE:HG12	2:m:170:VAL:HG12	1.88	0.56
2:d:117:PHE:HA	2:d:120:ILE:HD12	1.88	0.56
2:e:231:GLN:O	2:e:234:MET:HG3	2.05	0.56
2:a:77:GLY:HA3	1:B:174:LYS:HE2	1.88	0.56
2:j:117:PHE:HA	2:j:120:ILE:HD12	1.88	0.56
1:E:213:ARG:HH11	1:E:213:ARG:HG2	1.70	0.55
1:C:55:LEU:HD22	1:C:58:ILE:HD11	1.87	0.55
2:c:35:TYR:HE2	2:c:40:LEU:HG	1.70	0.55
1:D:207:LYS:O	1:D:211:THR:HG23	2.07	0.55
1:B:207:LYS:O	1:B:211:THR:HG23	2.06	0.55
1:B:238:LYS:HG3	2:b:242:ILE:HG12	1.88	0.55
1:G:28:ILE:HG12	1:G:34:ALA:HB2	1.88	0.55
1:E:207:LYS:O	1:E:211:THR:HG23	2.07	0.55
1:K:151:LYS:HG3	1:K:170:VAL:HG23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:306:MET:SD	1:D:306:MET:HG2	2.46	0.55
1:H:28:ILE:HG22	1:H:49:PRO:HA	1.88	0.55
1:F:238:LYS:HG3	2:f:242:ILE:HG12	1.89	0.55
1:D:230:ARG:NH1	1:D:230:ARG:HB2	2.22	0.55
1:M:104:ASP:HA	1:M:107:ARG:HG2	1.90	0.54
1:K:13:VAL:O	1:K:17:VAL:HG23	2.07	0.54
2:l:289:ILE:HG22	2:l:294:LYS:HD3	1.89	0.54
1:B:151:LYS:HG3	1:B:170:VAL:HG23	1.88	0.54
1:D:91:ILE:HG12	1:D:172:VAL:HG12	1.88	0.54
1:D:174:LYS:HE2	2:c:77:GLY:HA3	1.89	0.54
2:k:117:PHE:HA	2:k:120:ILE:HD12	1.88	0.54
1:C:13:VAL:O	1:C:17:VAL:HG23	2.08	0.54
1:G:13:VAL:O	1:G:17:VAL:HG23	2.08	0.54
1:D:104:ASP:HA	1:D:107:ARG:HG2	1.89	0.54
1:C:207:LYS:O	1:C:211:THR:HG23	2.08	0.54
1:I:151:LYS:HG3	1:I:170:VAL:HG23	1.89	0.54
2:i:117:PHE:HA	2:i:120:ILE:HD12	1.90	0.54
1:D:151:LYS:HG3	1:D:170:VAL:HG23	1.90	0.54
1:F:158:LEU:HD12	1:F:167:ILE:HD11	1.89	0.54
1:C:174:LYS:HE2	2:b:77:GLY:HA3	1.90	0.54
1:A:13:VAL:O	1:A:17:VAL:HG23	2.08	0.54
1:D:238:LYS:HG3	2:d:242:ILE:HG12	1.89	0.54
1:H:13:VAL:O	1:H:17:VAL:HG23	2.08	0.54
1:G:28:ILE:HG22	1:G:49:PRO:HA	1.89	0.54
1:M:13:VAL:O	1:M:17:VAL:HG23	2.08	0.54
2:k:95:LEU:HD21	2:k:103:ILE:HG13	1.89	0.54
1:C:230:ARG:HB2	1:C:230:ARG:NH1	2.23	0.54
2:a:117:PHE:HA	2:a:120:ILE:HD12	1.89	0.54
1:K:207:LYS:O	1:K:211:THR:HG23	2.07	0.54
1:M:174:LYS:HE2	2:l:77:GLY:HA3	1.89	0.54
2:m:176:PRO:HG2	2:m:179:ILE:HD13	1.90	0.54
2:e:89:ILE:HG12	2:e:170:VAL:HG12	1.88	0.54
1:H:174:LYS:HE2	2:g:77:GLY:HA3	1.90	0.54
1:E:77:PRO:HB3	1:E:85:MET:HE1	1.89	0.53
1:E:162:ALA:HA	3:X:1:NAG:H82	1.90	0.53
1:F:207:LYS:O	1:F:211:THR:HG23	2.08	0.53
1:I:174:LYS:HE2	2:h:77:GLY:HA3	1.90	0.53
2:l:89:ILE:HG12	2:l:170:VAL:HG12	1.90	0.53
1:B:13:VAL:O	1:B:17:VAL:HG23	2.08	0.53
2:h:103:ILE:HD13	3:y:1:NAG:H81	1.90	0.53
1:F:176:LYS:NZ	1:F:176:LYS:HB3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:13:VAL:O	1:J:17:VAL:HG23	2.09	0.53
1:F:13:VAL:O	1:F:17:VAL:HG23	2.09	0.53
1:J:207:LYS:O	1:J:211:THR:HG23	2.08	0.53
1:I:207:LYS:O	1:I:211:THR:HG23	2.07	0.53
2:g:89:ILE:HG12	2:g:170:VAL:HG12	1.89	0.53
2:k:68:THR:HG22	2:k:92:VAL:HG22	1.90	0.53
1:D:13:VAL:O	1:D:17:VAL:HG23	2.08	0.53
1:C:238:LYS:HG3	2:c:242:ILE:HG12	1.91	0.53
2:c:89:ILE:HG12	2:c:170:VAL:HG12	1.91	0.53
1:H:207:LYS:O	1:H:211:THR:HG23	2.08	0.53
1:A:183:ARG:NH1	1:A:183:ARG:HB2	2.24	0.53
1:A:207:LYS:O	1:A:211:THR:HG23	2.08	0.53
1:K:302:ASN:HD21	2:j:299:LYS:HG2	1.74	0.52
1:E:174:LYS:HE2	2:d:77:GLY:HA3	1.91	0.52
1:J:42:LEU:HD23	1:J:103:PHE:CE1	2.43	0.52
1:A:162:ALA:HA	3:N:1:NAG:H82	1.90	0.52
1:M:207:LYS:O	1:M:211:THR:HG23	2.08	0.52
2:j:103:ILE:HD13	3:z:1:NAG:H81	1.91	0.52
2:e:175:ILE:HD12	2:e:179:ILE:HB	1.92	0.52
1:C:151:LYS:HG3	1:C:170:VAL:HG23	1.91	0.52
2:h:117:PHE:HA	2:h:120:ILE:HD12	1.92	0.52
2:a:95:LEU:HD21	2:a:103:ILE:HG13	1.92	0.52
2:i:264:THR:O	2:i:268:ILE:HG22	2.09	0.52
1:K:174:LYS:HE2	2:j:77:GLY:HA3	1.92	0.52
1:A:151:LYS:HG3	1:A:170:VAL:HG23	1.90	0.52
2:m:213:LYS:O	2:m:217:GLU:HG3	2.10	0.52
1:E:33:LEU:HD13	1:E:66:THR:HG21	1.91	0.52
2:b:117:PHE:HA	2:b:120:ILE:HD12	1.90	0.52
1:L:299:PHE:HE2	2:k:304:MET:HG3	1.75	0.52
1:D:162:ALA:HA	3:Y:1:NAG:H82	1.91	0.52
1:I:162:ALA:HA	3:t:1:NAG:H82	1.91	0.52
1:G:207:LYS:O	1:G:211:THR:HG23	2.09	0.52
1:E:134:THR:HG22	1:E:136:GLN:H	1.75	0.52
2:d:102:ASP:HB3	3:Z:1:NAG:O7	2.10	0.52
2:e:299:LYS:HB3	2:e:299:LYS:NZ	2.25	0.52
1:J:151:LYS:HG3	1:J:170:VAL:HG23	1.91	0.52
1:K:68:LEU:HD23	1:K:96:MET:HB2	1.92	0.51
2:k:91:VAL:HG11	2:k:116:ILE:HG21	1.93	0.51
1:I:306:MET:SD	1:H:306:MET:HG2	2.50	0.51
2:i:95:LEU:HD11	2:i:103:ILE:HG13	1.92	0.51
2:i:102:ASP:HB3	3:u:1:NAG:O7	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:f:117:PHE:HA	2:f:120:ILE:HD12	1.91	0.51
1:C:231:PHE:CZ	2:c:235:GLU:HG2	2.46	0.51
1:M:134:THR:HG22	1:M:136:GLN:H	1.76	0.51
2:i:266:MET:O	2:i:270:GLU:HG2	2.11	0.51
2:j:53:LEU:HD12	2:j:53:LEU:H	1.76	0.51
1:K:306:MET:HG3	1:J:306:MET:HB3	1.92	0.51
2:k:102:ASP:HB3	3:T:1:NAG:O7	2.11	0.51
2:f:77:GLY:HA3	1:G:174:LYS:HE2	1.93	0.51
2:e:117:PHE:HA	2:e:120:ILE:HD12	1.92	0.51
1:G:243:ARG:HG3	1:G:243:ARG:HH11	1.76	0.51
2:c:33:VAL:HB	2:c:40:LEU:HD21	1.93	0.51
1:I:238:LYS:HG3	2:i:242:ILE:HG12	1.92	0.51
2:l:213:LYS:O	2:l:217:GLU:HG3	2.11	0.51
1:E:213:ARG:HG2	1:E:213:ARG:NH1	2.26	0.51
2:m:117:PHE:HA	2:m:120:ILE:HD12	1.92	0.50
2:a:288:ALA:HB1	1:B:292:ALA:HB3	1.93	0.50
1:E:15:GLY:O	1:E:19:VAL:HG23	2.11	0.50
1:H:28:ILE:HG12	1:H:34:ALA:HB2	1.93	0.50
2:h:95:LEU:HD13	2:h:163:LEU:HD13	1.94	0.50
1:A:15:GLY:O	1:A:19:VAL:HG23	2.12	0.50
1:A:236:MET:HE1	2:m:226:GLU:HA	1.94	0.50
2:a:181:ARG:HG3	2:a:181:ARG:HH11	1.77	0.50
2:c:282:GLN:HG2	2:c:286:TYR:CE1	2.47	0.50
1:I:15:GLY:O	1:I:19:VAL:HG23	2.10	0.50
2:a:89:ILE:HG12	2:a:170:VAL:HG12	1.93	0.50
1:J:298:TYR:CE2	2:i:295:MET:HE2	2.46	0.50
2:a:103:ILE:HD13	3:O:1:NAG:H81	1.93	0.50
1:E:238:LYS:HG3	2:e:242:ILE:HG12	1.94	0.50
2:b:102:ASP:HB3	3:p:1:NAG:O7	2.12	0.50
1:M:243:ARG:HG3	1:M:243:ARG:HH11	1.76	0.50
1:K:162:ALA:HA	3:S:1:NAG:H82	1.94	0.50
2:f:177:GLU:HG3	2:f:180:ARG:HH21	1.76	0.50
1:D:134:THR:HG22	1:D:136:GLN:H	1.77	0.50
1:M:15:GLY:O	1:M:19:VAL:HG23	2.12	0.50
1:K:226:VAL:HG12	1:K:230:ARG:HH12	1.76	0.50
1:H:68:LEU:HD23	1:H:96:MET:HB2	1.94	0.50
1:C:294:ASN:H	2:c:294:LYS:NZ	2.10	0.49
1:I:282:TYR:O	1:I:286:LYS:HG2	2.11	0.49
2:k:103:ILE:HD13	3:T:1:NAG:H81	1.94	0.49
2:b:103:ILE:HD13	3:p:1:NAG:H81	1.94	0.49
1:G:179:GLU:HG2	1:G:182:ARG:HH21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:282:TYR:O	1:F:286:LYS:HG2	2.12	0.49
1:C:15:GLY:O	1:C:19:VAL:HG23	2.12	0.49
1:I:213:ARG:HG2	1:I:213:ARG:HH11	1.76	0.49
1:H:238:LYS:HG3	2:h:242:ILE:HG23	1.93	0.49
1:D:15:GLY:O	1:D:19:VAL:HG23	2.12	0.49
2:c:102:ASP:HB3	3:q:1:NAG:O7	2.12	0.49
1:J:15:GLY:O	1:J:19:VAL:HG23	2.12	0.49
1:J:299:PHE:HA	2:j:298:GLY:O	2.12	0.49
1:J:302:ASN:HD21	2:i:299:LYS:HG2	1.78	0.49
1:F:15:GLY:O	1:F:19:VAL:HG23	2.12	0.49
2:d:89:ILE:HG12	2:d:170:VAL:HG12	1.94	0.49
1:H:15:GLY:O	1:H:19:VAL:HG23	2.12	0.49
1:H:91:ILE:HG12	1:H:172:VAL:HG12	1.93	0.49
1:J:174:LYS:HE2	2:i:77:GLY:HA3	1.94	0.49
2:i:284:MET:HE3	2:i:284:MET:HA	1.95	0.49
1:G:306:MET:HE2	1:G:306:MET:HB3	1.72	0.49
1:M:38:ARG:HG2	1:M:38:ARG:HH11	1.78	0.49
1:L:55:LEU:HD22	1:L:58:ILE:HD11	1.94	0.49
1:H:270:TYR:HD2	2:h:275:LYS:HD2	1.77	0.49
2:j:76:CYS:HB2	2:j:124:LEU:HD13	1.94	0.49
2:k:175:ILE:HD12	2:k:179:ILE:HB	1.95	0.49
2:c:103:ILE:HD13	3:q:1:NAG:H81	1.95	0.49
2:g:264:THR:O	2:g:268:ILE:HG22	2.12	0.49
2:h:89:ILE:HG12	2:h:170:VAL:HG12	1.94	0.49
2:j:181:ARG:HG3	2:j:181:ARG:HH11	1.78	0.49
1:A:296:LYS:HB3	2:a:295:MET:HG2	1.94	0.48
1:K:38:ARG:HD3	1:K:58:ILE:HD13	1.94	0.48
1:H:243:ARG:HG3	1:H:243:ARG:HH11	1.78	0.48
2:j:253:ARG:HG3	2:j:253:ARG:HH11	1.78	0.48
1:A:193:THR:HG21	2:m:179:ILE:HG23	1.94	0.48
1:L:162:ALA:HA	3:R:1:NAG:H82	1.93	0.48
2:d:103:ILE:HD13	3:Z:1:NAG:H81	1.94	0.48
2:h:68:THR:HG22	2:h:92:VAL:HG22	1.95	0.48
1:F:162:ALA:HA	3:V:1:NAG:H82	1.95	0.48
2:g:68:THR:HG22	2:g:92:VAL:HG22	1.95	0.48
2:f:176:PRO:HG2	2:f:179:ILE:HD12	1.95	0.48
2:k:160:ALA:HA	3:T:1:NAG:H82	1.95	0.48
1:C:176:LYS:NZ	1:C:176:LYS:HB3	2.29	0.48
1:J:162:ALA:HA	3:s:1:NAG:H82	1.95	0.48
1:H:299:PHE:HA	2:h:298:GLY:O	2.14	0.48
2:g:117:PHE:HA	2:g:120:ILE:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:265:ALA:HA	2:m:268:ILE:HG22	1.95	0.48
1:L:85:MET:HE3	1:L:85:MET:HB3	1.70	0.48
1:F:297:ILE:HG23	2:f:296:TYR:HD2	1.77	0.48
2:b:69:ASP:HB3	2:b:117:PHE:CZ	2.48	0.48
2:e:231:GLN:O	2:e:235:GLU:HG3	2.13	0.48
1:I:26:HIS:HD2	1:I:28:ILE:HD13	1.77	0.48
1:I:193:THR:HG21	2:h:179:ILE:HG23	1.95	0.48
1:G:20:LEU:HD23	1:G:57:PHE:HE2	1.78	0.48
2:f:299:LYS:HG3	1:G:302:ASN:HD21	1.78	0.48
1:D:299:PHE:HA	2:d:298:GLY:O	2.14	0.48
2:j:262:CYS:SG	2:j:266:MET:HE2	2.53	0.48
1:F:134:THR:HG22	1:F:136:GLN:H	1.79	0.48
1:D:213:ARG:HG2	1:D:213:ARG:HH11	1.78	0.48
1:G:162:ALA:HA	3:w:1:NAG:H82	1.95	0.48
1:K:62:ARG:HG2	1:K:62:ARG:HH11	1.79	0.48
2:l:102:ASP:HB3	3:U:1:NAG:O7	2.14	0.48
1:F:243:ARG:HH11	1:F:243:ARG:HG3	1.78	0.48
2:d:160:ALA:HA	3:Z:1:NAG:H82	1.96	0.48
1:A:121:LYS:NZ	1:A:161:MET:HE1	2.29	0.48
2:f:68:THR:HG22	2:f:92:VAL:HG22	1.96	0.48
2:f:69:ASP:HB3	2:f:117:PHE:CZ	2.49	0.48
2:g:102:ASP:HB3	3:x:1:NAG:O7	2.13	0.48
1:A:302:ASN:HD21	2:m:299:LYS:HG2	1.79	0.47
2:m:305:PHE:CZ	2:l:289:ILE:HD11	2.47	0.47
1:L:297:ILE:HG23	2:l:296:TYR:HD2	1.80	0.47
1:F:38:ARG:HG2	1:F:38:ARG:HH11	1.78	0.47
1:B:33:LEU:HD13	1:B:66:THR:HG21	1.96	0.47
1:A:213:ARG:HG2	1:A:213:ARG:HH11	1.80	0.47
1:L:238:LYS:HG3	2:l:242:ILE:HG12	1.96	0.47
1:L:282:TYR:O	1:L:286:LYS:HG2	2.14	0.47
1:C:299:PHE:HA	2:c:298:GLY:O	2.14	0.47
2:c:69:ASP:HB3	2:c:117:PHE:CZ	2.49	0.47
2:h:13:SER:HA	2:h:16:CYS:SG	2.54	0.47
1:A:238:LYS:HG3	2:a:242:ILE:HG12	1.95	0.47
2:f:13:SER:HA	2:f:16:CYS:SG	2.54	0.47
1:J:296:LYS:HD3	1:J:298:TYR:CE1	2.49	0.47
2:g:103:ILE:HD13	3:x:1:NAG:H81	1.95	0.47
2:b:89:ILE:HG12	2:b:170:VAL:HG12	1.96	0.47
1:H:193:THR:HG21	2:g:179:ILE:HG23	1.96	0.47
1:L:134:THR:HG22	1:L:136:GLN:H	1.79	0.47
2:l:161:PRO:HD2	3:U:1:NAG:H82	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:253:ARG:HG3	2:j:253:ARG:NH1	2.29	0.47
1:D:302:ASN:HD21	2:c:299:LYS:HG3	1.79	0.47
1:J:294:ASN:H	2:j:294:LYS:NZ	2.13	0.47
2:g:13:SER:HA	2:g:16:CYS:SG	2.55	0.47
2:h:265:ALA:HA	2:h:268:ILE:HG22	1.96	0.47
1:L:296:LYS:HD3	1:L:298:TYR:CE1	2.49	0.47
2:l:103:ILE:HD13	3:U:1:NAG:H81	1.95	0.47
1:F:104:ASP:O	1:F:107:ARG:HG3	2.15	0.47
1:E:299:PHE:HA	2:e:298:GLY:O	2.15	0.47
1:J:297:ILE:HG23	2:j:296:TYR:HD2	1.80	0.47
1:G:299:PHE:HA	2:g:298:GLY:O	2.14	0.47
2:a:299:LYS:NZ	2:a:299:LYS:HB3	2.30	0.47
1:K:134:THR:HG22	1:K:136:GLN:H	1.80	0.47
2:k:176:PRO:HG2	2:k:179:ILE:HG13	1.97	0.47
2:f:161:PRO:HD2	3:W:1:NAG:H82	1.96	0.47
2:i:13:SER:HA	2:i:16:CYS:SG	2.54	0.47
1:K:201:LYS:HE3	1:K:201:LYS:HB2	1.68	0.47
1:F:174:LYS:HE2	2:e:77:GLY:HA3	1.96	0.47
2:f:103:ILE:HD13	3:W:1:NAG:H81	1.96	0.47
2:d:262:CYS:O	2:d:266:MET:HG2	2.15	0.47
1:C:68:LEU:HD23	1:C:96:MET:HB2	1.97	0.47
1:B:299:PHE:HA	2:b:298:GLY:O	2.15	0.47
2:b:266:MET:O	2:b:270:GLU:HG2	2.15	0.47
2:h:160:ALA:HA	3:y:1:NAG:H82	1.97	0.47
2:a:102:ASP:HB3	3:O:1:NAG:O7	2.15	0.46
2:m:95:LEU:HD11	2:m:103:ILE:HG13	1.97	0.46
1:F:226:VAL:HG12	1:F:230:ARG:HH22	1.80	0.46
1:E:226:VAL:HG12	1:E:230:ARG:HH22	1.80	0.46
1:C:236:MET:HE1	2:b:226:GLU:HA	1.97	0.46
1:J:286:LYS:HD2	1:J:286:LYS:HA	1.69	0.46
1:A:299:PHE:HA	2:a:298:GLY:O	2.15	0.46
2:k:89:ILE:HG12	2:k:170:VAL:HG12	1.97	0.46
2:h:69:ASP:HB3	2:h:117:PHE:CZ	2.50	0.46
2:h:231:GLN:O	2:h:235:GLU:HG3	2.15	0.46
2:k:282:GLN:HG2	2:k:286:TYR:CE1	2.50	0.46
2:d:13:SER:HA	2:d:16:CYS:SG	2.56	0.46
1:H:213:ARG:NH1	1:H:213:ARG:HG2	2.30	0.46
1:A:299:PHE:HE1	2:m:294:LYS:HB3	1.80	0.46
1:M:296:LYS:HD3	1:M:298:TYR:CE1	2.50	0.46
1:F:230:ARG:HB2	1:F:230:ARG:NH1	2.30	0.46
1:F:294:ASN:H	2:f:294:LYS:NZ	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:LEU:HD22	1:C:94:VAL:HG12	1.98	0.46
2:a:200:GLN:HB2	1:B:211:THR:HG22	1.98	0.46
2:m:231:GLN:O	2:m:235:GLU:HG3	2.15	0.46
1:K:222:LYS:HD3	2:j:211:ARG:HA	1.97	0.46
1:A:38:ARG:HG2	1:A:38:ARG:HH11	1.80	0.46
1:E:230:ARG:NH1	1:E:230:ARG:HB2	2.31	0.46
2:m:103:ILE:HD13	3:Q:1:NAG:H81	1.98	0.46
2:k:69:ASP:HB3	2:k:117:PHE:CZ	2.51	0.46
1:A:174:LYS:NZ	2:m:129:SER:HB3	2.31	0.46
1:L:38:ARG:HD3	1:L:58:ILE:HD13	1.98	0.46
1:L:230:ARG:NH1	1:L:230:ARG:HB2	2.31	0.46
1:E:85:MET:HE3	1:E:85:MET:HB3	1.70	0.46
2:g:69:ASP:HB3	2:g:117:PHE:CZ	2.51	0.46
2:a:161:PRO:HD2	3:O:1:NAG:H82	1.96	0.46
1:E:294:ASN:H	2:e:294:LYS:NZ	2.14	0.46
1:C:162:ALA:HA	3:n:1:NAG:H82	1.98	0.46
2:e:102:ASP:HB3	3:r:1:NAG:O7	2.16	0.46
2:e:161:PRO:HD2	3:r:1:NAG:H82	1.98	0.46
1:H:134:THR:HG22	1:H:136:GLN:H	1.81	0.46
1:A:134:THR:HG22	1:A:136:GLN:H	1.82	0.45
2:k:160:ALA:HA	3:T:1:NAG:C8	2.46	0.45
2:k:307:ASP:HA	2:l:300:ASP:OD2	2.16	0.45
1:C:297:ILE:HG12	2:c:304:MET:HE1	1.98	0.45
2:e:234:MET:HE2	2:e:234:MET:HB2	1.80	0.45
1:I:104:ASP:O	1:I:107:ARG:HG3	2.16	0.45
2:i:103:ILE:HD13	3:u:1:NAG:H81	1.97	0.45
2:m:40:LEU:HD23	2:m:101:TYR:CE1	2.51	0.45
1:B:282:TYR:O	1:B:286:LYS:HG2	2.16	0.45
2:b:160:ALA:HA	3:p:1:NAG:C8	2.46	0.45
1:I:62:ARG:HH11	1:I:111:ALA:HB3	1.82	0.45
1:I:292:ALA:HB3	2:h:288:ALA:HB1	1.98	0.45
2:i:262:CYS:SG	2:i:266:MET:HE2	2.56	0.45
2:j:160:ALA:HA	3:z:1:NAG:C8	2.46	0.45
1:A:213:ARG:HG2	1:A:213:ARG:NH1	2.32	0.45
2:a:300:ASP:OD1	2:m:307:ASP:HA	2.16	0.45
1:M:238:LYS:HG3	2:m:242:ILE:HG12	1.97	0.45
2:d:160:ALA:HA	3:Z:1:NAG:C8	2.46	0.45
2:b:160:ALA:HA	3:p:1:NAG:H82	1.98	0.45
1:I:120:ASN:HB3	2:i:169:ARG:NH1	2.32	0.45
2:m:69:ASP:HB3	2:m:117:PHE:CZ	2.52	0.45
1:L:299:PHE:HA	2:l:298:GLY:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:262:CYS:O	2:i:266:MET:HG2	2.17	0.45
1:G:230:ARG:NH1	1:G:230:ARG:HB2	2.31	0.45
2:j:69:ASP:HB3	2:j:117:PHE:CZ	2.52	0.45
1:F:299:PHE:HA	2:f:298:GLY:O	2.16	0.45
2:f:129:SER:HB3	1:G:174:LYS:NZ	2.31	0.45
1:E:297:ILE:HG23	2:e:296:TYR:HD2	1.81	0.45
2:i:160:ALA:HA	3:u:1:NAG:C8	2.47	0.45
1:H:213:ARG:HG2	1:H:213:ARG:HH11	1.80	0.45
1:G:238:LYS:HG3	2:g:242:ILE:HG12	1.99	0.45
2:j:231:GLN:O	2:j:235:GLU:HG3	2.16	0.45
1:L:299:PHE:CE2	2:k:304:MET:HG3	2.51	0.45
1:K:292:ALA:HB3	2:j:288:ALA:HB1	1.99	0.45
1:K:299:PHE:HA	2:k:298:GLY:O	2.17	0.45
1:E:21:LEU:HD23	1:E:21:LEU:HA	1.80	0.45
1:C:120:ASN:HB3	2:c:169:ARG:NH2	2.32	0.45
1:F:183:ARG:HG3	1:F:183:ARG:HH11	1.81	0.45
2:j:160:ALA:HA	3:z:1:NAG:H82	1.99	0.45
1:M:174:LYS:NZ	2:l:129:SER:HB3	2.32	0.45
2:k:86:PHE:CZ	2:k:173:PRO:HG3	2.52	0.45
1:C:236:MET:HG3	1:C:237:GLU:N	2.32	0.45
1:L:174:LYS:NZ	2:k:129:SER:HB3	2.32	0.45
1:F:299:PHE:HE2	2:e:304:MET:HG3	1.82	0.45
2:f:160:ALA:HA	3:W:1:NAG:C8	2.47	0.45
1:G:134:THR:HG22	1:G:136:GLN:H	1.82	0.45
2:h:160:ALA:HA	3:y:1:NAG:C8	2.47	0.45
2:l:299:LYS:NZ	2:l:299:LYS:HB3	2.32	0.44
2:c:307:ASP:OD1	2:c:307:ASP:C	2.60	0.44
2:i:86:PHE:CZ	2:i:173:PRO:HG3	2.52	0.44
1:H:237:GLU:HG2	2:g:229:TYR:CE1	2.52	0.44
1:A:295:SER:HB3	2:m:292:ASN:ND2	2.32	0.44
1:E:13:VAL:O	1:E:17:VAL:HG23	2.17	0.44
1:E:55:LEU:HB2	1:E:59:THR:OG1	2.17	0.44
1:E:236:MET:HE1	2:d:226:GLU:HA	1.98	0.44
2:e:95:LEU:HD11	2:e:103:ILE:HG13	1.98	0.44
1:A:68:LEU:HD22	1:A:94:VAL:HG12	1.97	0.44
2:m:107:TYR:O	2:m:108:THR:HG22	2.17	0.44
2:l:262:CYS:O	2:l:266:MET:HG2	2.17	0.44
2:f:262:CYS:O	2:f:266:MET:HG2	2.18	0.44
1:J:237:GLU:HG2	2:i:229:TYR:CE1	2.52	0.44
1:I:183:ARG:HB2	1:I:183:ARG:NH1	2.32	0.44
2:a:160:ALA:HA	3:O:1:NAG:C8	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:213:ARG:HG2	1:I:213:ARG:NH1	2.32	0.44
1:H:104:ASP:HA	1:H:107:ARG:HG2	2.00	0.44
2:g:282:GLN:HG2	2:g:286:TYR:CE1	2.53	0.44
2:j:71:VAL:HG23	2:j:89:ILE:HB	1.99	0.44
2:m:161:PRO:HD2	3:Q:1:NAG:H82	1.98	0.44
1:K:71:ASP:HB3	1:K:119:PHE:CZ	2.53	0.44
2:k:236:LYS:HD3	2:k:236:LYS:HA	1.81	0.44
2:f:176:PRO:HG2	2:f:179:ILE:CD1	2.48	0.44
1:B:55:LEU:HB2	1:B:59:THR:OG1	2.17	0.44
2:c:160:ALA:HA	3:q:1:NAG:C8	2.48	0.44
1:J:238:LYS:HG3	2:j:242:ILE:HG23	2.00	0.44
2:g:160:ALA:HA	3:x:1:NAG:C8	2.47	0.44
1:A:21:LEU:HD12	1:A:21:LEU:HA	1.83	0.44
1:M:71:ASP:HB3	1:M:119:PHE:CZ	2.53	0.44
1:M:162:ALA:HA	3:P:1:NAG:H82	1.99	0.44
2:l:160:ALA:HA	3:U:1:NAG:C8	2.48	0.44
1:C:71:ASP:HB3	1:C:119:PHE:CZ	2.52	0.44
2:a:304:MET:HG3	1:B:299:PHE:HE2	1.82	0.44
2:l:52:MET:HG3	2:l:57:THR:HB	1.99	0.44
2:f:91:VAL:HG11	2:f:116:ILE:HG21	1.99	0.44
2:d:86:PHE:CZ	2:d:173:PRO:HG3	2.53	0.44
2:i:34:TYR:HB2	2:i:41:LEU:HD12	1.99	0.44
2:i:69:ASP:HB3	2:i:117:PHE:CZ	2.53	0.44
1:M:213:ARG:HG2	1:M:213:ARG:HH11	1.83	0.44
1:L:296:LYS:HD3	1:L:298:TYR:HE1	1.83	0.44
2:f:231:GLN:O	2:f:235:GLU:HG3	2.18	0.44
1:D:121:LYS:NZ	1:D:161:MET:HE1	2.33	0.44
2:d:231:GLN:O	2:d:235:GLU:HG3	2.18	0.44
2:e:160:ALA:HA	3:r:1:NAG:C8	2.48	0.44
1:J:54:MET:HE1	1:J:61:PHE:HB3	1.99	0.44
2:g:181:ARG:NH1	2:g:181:ARG:HB2	2.33	0.44
1:L:236:MET:HE1	2:k:226:GLU:HA	1.99	0.43
1:D:162:ALA:HA	3:Y:1:NAG:C8	2.48	0.43
1:C:37:TYR:HA	1:C:41:ALA:O	2.18	0.43
1:J:28:ILE:HG13	1:J:34:ALA:HB2	2.00	0.43
2:j:102:ASP:HB3	3:z:1:NAG:O7	2.17	0.43
2:a:69:ASP:HB3	2:a:117:PHE:CZ	2.53	0.43
1:L:53:ILE:HD12	1:L:53:ILE:O	2.18	0.43
1:L:162:ALA:HA	3:R:1:NAG:C8	2.48	0.43
1:K:37:TYR:HA	1:K:41:ALA:O	2.19	0.43
1:D:211:THR:HG22	2:c:200:GLN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:THR:HG22	1:B:136:GLN:H	1.84	0.43
2:c:66:LEU:HD12	2:c:94:PHE:HB3	2.00	0.43
1:J:134:THR:HG22	1:J:136:GLN:H	1.83	0.43
2:i:160:ALA:HA	3:u:1:NAG:H82	2.00	0.43
1:A:253:LEU:HD23	1:A:253:LEU:HA	1.90	0.43
2:a:241:LYS:O	2:a:245:ILE:HG12	2.18	0.43
1:L:104:ASP:HA	1:L:107:ARG:HG2	1.98	0.43
2:k:231:GLN:O	2:k:235:GLU:HG3	2.17	0.43
1:D:62:ARG:HG2	1:D:62:ARG:HH11	1.84	0.43
2:d:176:PRO:HG2	2:d:179:ILE:CD1	2.49	0.43
1:H:243:ARG:HG3	1:H:243:ARG:NH1	2.32	0.43
1:A:179:GLU:HG2	1:A:182:ARG:NH1	2.33	0.43
2:a:160:ALA:HA	3:O:1:NAG:H82	2.00	0.43
1:M:162:ALA:HA	3:P:1:NAG:C8	2.49	0.43
2:m:160:ALA:HA	3:Q:1:NAG:C8	2.47	0.43
2:m:251:LEU:HD23	2:m:251:LEU:HA	1.88	0.43
2:k:71:VAL:HG23	2:k:89:ILE:HB	2.01	0.43
1:D:71:ASP:HB3	1:D:119:PHE:CZ	2.52	0.43
1:D:294:ASN:H	2:d:294:LYS:NZ	2.17	0.43
2:e:103:ILE:HD13	3:r:1:NAG:H81	2.00	0.43
2:i:71:VAL:HG23	2:i:89:ILE:HB	1.99	0.43
1:G:162:ALA:HA	3:w:1:NAG:C8	2.48	0.43
1:G:238:LYS:HG3	2:g:242:ILE:HG23	2.00	0.43
1:D:213:ARG:HG2	1:D:213:ARG:NH1	2.34	0.43
1:D:296:LYS:HB3	2:d:295:MET:HG2	2.00	0.43
2:d:303:ASN:HA	2:d:306:MET:HG3	2.01	0.43
2:d:307:ASP:HA	2:e:300:ASP:OD1	2.19	0.43
1:B:183:ARG:HG3	1:B:183:ARG:HH11	1.83	0.43
1:I:71:ASP:HB3	1:I:119:PHE:CZ	2.54	0.43
2:h:91:VAL:HG11	2:h:116:ILE:HG21	2.00	0.43
1:M:238:LYS:HG3	2:m:242:ILE:HG23	1.99	0.43
1:L:156:LYS:NZ	1:L:156:LYS:HB3	2.33	0.43
2:l:241:LYS:O	2:l:245:ILE:HG12	2.17	0.43
2:f:236:LYS:HG3	1:G:244:ILE:HG12	2.01	0.43
1:C:231:PHE:CE2	2:c:235:GLU:HG2	2.52	0.43
2:j:161:PRO:HD2	3:z:1:NAG:H82	1.99	0.43
1:A:55:LEU:HD22	1:A:58:ILE:HD11	2.00	0.43
1:A:231:PHE:CE2	2:a:235:GLU:HG2	2.54	0.43
1:A:282:TYR:CZ	1:A:286:LYS:HD2	2.53	0.43
1:K:183:ARG:HG3	1:K:183:ARG:HH11	1.83	0.43
1:F:174:LYS:NZ	2:e:129:SER:HB3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:TYR:CD1	1:D:100:TYR:C	2.97	0.43
2:d:266:MET:O	2:d:270:GLU:HG2	2.18	0.43
1:B:78:CYS:HB2	1:B:126:LEU:HD21	2.00	0.43
1:I:299:PHE:HA	2:i:298:GLY:O	2.19	0.43
2:g:160:ALA:HA	3:x:1:NAG:H82	2.01	0.43
1:M:299:PHE:HA	2:m:298:GLY:O	2.19	0.43
2:f:86:PHE:CZ	2:f:173:PRO:HG3	2.54	0.43
2:f:292:ASN:ND2	1:G:295:SER:HB3	2.33	0.43
1:C:85:MET:HE3	1:C:85:MET:HB3	1.96	0.43
2:g:231:GLN:O	2:g:235:GLU:HG3	2.17	0.43
2:h:19:LEU:HD23	2:h:19:LEU:HA	1.84	0.43
1:K:38:ARG:HD3	1:K:58:ILE:CD1	2.49	0.43
1:F:16:LEU:HD23	1:F:16:LEU:HA	1.91	0.43
1:F:306:MET:SD	1:E:306:MET:HG2	2.59	0.43
2:h:102:ASP:HB3	3:y:1:NAG:O7	2.19	0.43
2:a:300:ASP:OD2	2:a:302:PRO:HD2	2.19	0.43
2:f:107:TYR:O	2:f:108:THR:HG22	2.18	0.43
2:d:69:ASP:HB3	2:d:117:PHE:CZ	2.54	0.43
1:C:177:ILE:HD12	1:C:181:ILE:HB	2.00	0.43
2:b:236:LYS:HD3	2:b:236:LYS:HA	1.83	0.43
2:i:231:GLN:O	2:i:235:GLU:HG3	2.19	0.43
1:M:243:ARG:HG3	1:M:243:ARG:NH1	2.34	0.42
1:L:226:VAL:HG12	1:L:230:ARG:HH22	1.84	0.42
1:L:236:MET:HG3	1:L:237:GLU:N	2.34	0.42
1:D:68:LEU:HD23	1:D:96:MET:HB3	2.00	0.42
1:D:222:LYS:HD3	2:c:211:ARG:HA	2.00	0.42
2:c:19:LEU:HD23	2:c:19:LEU:HA	1.82	0.42
2:a:307:ASP:HA	2:b:300:ASP:OD1	2.20	0.42
1:M:226:VAL:HG12	1:M:230:ARG:HH22	1.84	0.42
1:M:297:ILE:HG23	2:m:296:TYR:HD2	1.83	0.42
1:F:162:ALA:HA	3:V:1:NAG:C8	2.48	0.42
2:h:181:ARG:HB2	2:h:181:ARG:CZ	2.49	0.42
2:c:236:LYS:HD3	2:c:236:LYS:HA	1.82	0.42
1:G:226:VAL:HG12	1:G:230:ARG:HH22	1.83	0.42
2:j:177:GLU:HG3	2:j:180:ARG:HH12	1.84	0.42
1:M:219:GLU:O	1:M:223:ILE:HG12	2.19	0.42
2:k:179:ILE:H	2:k:179:ILE:HG12	1.65	0.42
2:l:236:LYS:HA	2:l:236:LYS:HD3	1.79	0.42
1:F:20:LEU:HD23	1:F:57:PHE:HE1	1.84	0.42
1:E:211:THR:HG22	2:d:200:GLN:HB2	2.00	0.42
1:J:16:LEU:HD23	1:J:16:LEU:HA	1.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:21:LEU:HD12	1:J:21:LEU:HA	1.84	0.42
2:i:142:ASP:OD1	2:i:143:GLN:HG2	2.19	0.42
1:H:201:LYS:HE2	1:H:201:LYS:HB2	1.62	0.42
1:A:100:TYR:CD1	1:A:100:TYR:C	2.97	0.42
2:m:102:ASP:HB3	3:Q:1:NAG:O7	2.20	0.42
1:K:238:LYS:HG3	2:k:242:ILE:HG23	2.01	0.42
2:l:69:ASP:HB3	2:l:117:PHE:CZ	2.55	0.42
2:l:262:CYS:SG	2:l:266:MET:HE2	2.59	0.42
1:E:71:ASP:HB3	1:E:119:PHE:CZ	2.54	0.42
1:D:238:LYS:HG3	2:d:242:ILE:HG23	2.01	0.42
1:I:270:TYR:HD2	2:i:275:LYS:HD2	1.84	0.42
1:H:21:LEU:HD12	1:H:21:LEU:HA	1.86	0.42
1:G:24:SER:HA	1:G:54:MET:HG3	2.02	0.42
2:g:19:LEU:HD23	2:g:19:LEU:HA	1.89	0.42
2:g:307:ASP:HA	2:h:300:ASP:OD1	2.20	0.42
2:j:265:ALA:HA	2:j:268:ILE:HG22	2.00	0.42
1:K:26:HIS:HD2	1:K:28:ILE:HD13	1.85	0.42
2:k:107:TYR:OH	2:k:159:MET:HG2	2.19	0.42
2:l:91:VAL:HG11	2:l:116:ILE:HG21	2.02	0.42
1:F:62:ARG:NH1	1:F:62:ARG:HG2	2.34	0.42
1:D:62:ARG:HG2	1:D:62:ARG:NH1	2.35	0.42
1:G:36:TYR:HE2	1:G:47:SER:HB3	1.85	0.42
2:a:91:VAL:HG21	2:a:120:ILE:HD11	2.01	0.42
1:F:306:MET:HB2	1:F:306:MET:HE2	1.84	0.42
1:E:100:TYR:CD1	1:E:100:TYR:C	2.97	0.42
1:D:236:MET:HG3	1:D:237:GLU:N	2.34	0.42
1:C:191:GLU:OE2	2:c:199:LYS:HE2	2.20	0.42
1:H:68:LEU:HD22	1:H:94:VAL:HG12	2.01	0.42
1:H:282:TYR:O	1:H:286:LYS:HG2	2.19	0.42
1:A:160:LEU:H	1:A:160:LEU:HG	1.76	0.42
1:F:148:GLU:H	1:F:148:GLU:CD	2.27	0.42
1:F:244:ILE:HG12	2:e:236:LYS:HG3	2.02	0.42
2:f:51:LEU:H	2:f:51:LEU:HD23	1.85	0.42
1:D:292:ALA:HB3	2:c:288:ALA:HB1	2.01	0.42
2:b:205:LYS:HD3	2:b:205:LYS:HA	1.81	0.42
1:I:21:LEU:HD12	1:I:21:LEU:HA	1.86	0.42
1:H:160:LEU:H	1:H:160:LEU:HG	1.76	0.42
2:g:86:PHE:CZ	2:g:173:PRO:HG3	2.54	0.42
1:A:162:ALA:HA	3:N:1:NAG:C8	2.49	0.42
1:K:299:PHE:HE2	2:j:304:MET:HG3	1.85	0.42
2:b:86:PHE:CZ	2:b:173:PRO:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:307:ASP:HA	2:c:300:ASP:OD1	2.20	0.42
1:J:187:LEU:O	1:J:191:GLU:HG2	2.19	0.42
1:I:16:LEU:HD23	1:I:16:LEU:HA	1.91	0.42
1:I:162:ALA:HA	3:t:1:NAG:C8	2.49	0.42
2:i:176:PRO:HG2	2:i:179:ILE:HG13	2.02	0.42
1:H:233:GLN:O	1:H:237:GLU:HG3	2.20	0.42
1:M:107:ARG:HE	1:M:107:ARG:HB2	1.67	0.42
2:m:86:PHE:CZ	2:m:173:PRO:HG3	2.55	0.42
1:K:211:THR:HG22	2:j:200:GLN:HB2	2.02	0.42
2:l:86:PHE:CZ	2:l:173:PRO:HG3	2.55	0.42
2:d:177:GLU:HG3	2:d:181:ARG:HH12	1.85	0.42
1:C:109:TYR:OH	1:C:161:MET:HG2	2.20	0.42
1:B:226:VAL:HG12	1:B:230:ARG:HH12	1.84	0.42
2:e:180:ARG:HH11	2:e:180:ARG:HG2	1.85	0.42
1:I:211:THR:HG22	2:h:200:GLN:HB2	2.02	0.42
1:G:16:LEU:HD23	1:G:16:LEU:HA	1.91	0.42
1:L:77:PRO:HB3	1:L:85:MET:HE1	2.00	0.41
1:K:162:ALA:HA	3:S:1:NAG:C8	2.49	0.41
1:J:71:ASP:HB3	1:J:119:PHE:CZ	2.55	0.41
2:i:307:ASP:HA	2:j:300:ASP:OD1	2.20	0.41
1:H:236:MET:HG3	1:H:237:GLU:N	2.34	0.41
1:A:174:LYS:HE2	2:m:77:GLY:HA3	2.01	0.41
1:L:84:VAL:HG21	2:l:187:GLU:HG3	2.02	0.41
1:L:292:ALA:HB3	2:k:288:ALA:HB1	2.02	0.41
1:F:91:ILE:HG12	1:F:172:VAL:HG12	2.01	0.41
1:E:253:LEU:HD23	1:E:253:LEU:HA	1.91	0.41
1:B:238:LYS:HG3	2:b:242:ILE:HG23	2.02	0.41
2:e:69:ASP:HB3	2:e:117:PHE:CZ	2.55	0.41
2:e:180:ARG:HG2	2:e:180:ARG:NH1	2.34	0.41
1:H:253:LEU:HD23	1:H:253:LEU:HA	1.90	0.41
1:G:243:ARG:HG3	1:G:243:ARG:NH1	2.34	0.41
2:h:161:PRO:HD2	3:y:1:NAG:H82	2.01	0.41
1:M:213:ARG:HG2	1:M:213:ARG:NH1	2.34	0.41
1:L:286:LYS:HB3	1:L:286:LYS:HE2	1.97	0.41
2:k:301:ILE:HD13	2:j:289:ILE:HG21	2.03	0.41
2:f:160:ALA:HA	3:W:1:NAG:H82	2.02	0.41
1:D:38:ARG:HD3	1:D:58:ILE:HD13	2.02	0.41
1:D:70:THR:HB	1:D:94:VAL:HG22	2.01	0.41
1:B:286:LYS:HB3	1:B:286:LYS:HE2	1.96	0.41
2:c:160:ALA:HA	3:q:1:NAG:H82	2.02	0.41
1:J:100:TYR:CD1	1:J:100:TYR:C	2.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:174:LYS:NZ	2:g:129:SER:HB3	2.35	0.41
2:g:52:MET:HG3	2:g:57:THR:HB	2.02	0.41
1:K:24:SER:HA	1:K:54:MET:HG3	2.01	0.41
2:f:35:TYR:HE1	2:f:40:LEU:HD13	1.86	0.41
1:E:236:MET:HG3	1:E:237:GLU:N	2.35	0.41
1:C:162:ALA:HA	3:n:1:NAG:C8	2.50	0.41
1:C:193:THR:HG21	2:b:179:ILE:HG23	2.03	0.41
2:e:86:PHE:CZ	2:e:173:PRO:HG3	2.54	0.41
1:A:71:ASP:HB3	1:A:119:PHE:CZ	2.55	0.41
1:L:71:ASP:HB3	1:L:119:PHE:CZ	2.55	0.41
1:F:243:ARG:HG3	1:F:243:ARG:NH1	2.34	0.41
1:E:20:LEU:HD23	1:E:57:PHE:HE2	1.84	0.41
2:d:251:LEU:HD23	2:d:251:LEU:HA	1.90	0.41
2:e:236:LYS:HA	2:e:236:LYS:HD3	1.84	0.41
2:i:305:PHE:HZ	2:h:289:ILE:HD11	1.86	0.41
1:H:71:ASP:HB3	1:H:119:PHE:CZ	2.56	0.41
1:M:37:TYR:HA	1:M:41:ALA:O	2.21	0.41
1:M:236:MET:HG3	1:M:237:GLU:N	2.35	0.41
2:m:35:TYR:HE1	2:m:40:LEU:HD12	1.85	0.41
2:m:91:VAL:HG11	2:m:116:ILE:HG21	2.03	0.41
2:l:111:TYR:HB2	2:l:115:LEU:HD12	2.03	0.41
1:D:174:LYS:NZ	2:c:129:SER:HB3	2.36	0.41
1:J:244:ILE:HG12	2:i:236:LYS:HG3	2.02	0.41
2:a:215:LEU:HD11	1:B:225:GLN:OE1	2.21	0.41
1:D:24:SER:HA	1:D:54:MET:HG2	2.02	0.41
1:D:28:ILE:HG13	1:D:34:ALA:HB2	2.01	0.41
2:e:295:MET:HE3	2:e:295:MET:HB3	1.84	0.41
1:J:162:ALA:HA	3:s:1:NAG:C8	2.50	0.41
1:I:100:TYR:CD1	1:I:100:TYR:C	2.98	0.41
1:G:53:ILE:HD12	1:G:53:ILE:O	2.21	0.41
1:G:68:LEU:HD22	1:G:94:VAL:HG12	2.03	0.41
2:h:306:MET:HE2	2:h:306:MET:HB3	1.87	0.41
1:L:222:LYS:HD3	2:k:211:ARG:HA	2.01	0.41
1:C:281:GLU:H	1:C:281:GLU:CD	2.28	0.41
2:b:55:PHE:CD1	2:b:55:PHE:N	2.87	0.41
1:J:84:VAL:HG21	2:j:187:GLU:HG3	2.03	0.41
1:M:253:LEU:HD23	1:M:253:LEU:HA	1.90	0.41
1:K:100:TYR:CD1	1:K:100:TYR:C	2.99	0.41
2:k:78:THR:HG21	2:k:133:LEU:HA	2.03	0.41
2:k:181:ARG:CZ	2:k:181:ARG:HB2	2.50	0.41
2:k:241:LYS:O	2:k:245:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:231:GLN:O	2:l:235:GLU:HG3	2.19	0.41
1:F:145:GLN:HA	1:F:148:GLU:OE2	2.21	0.41
2:f:204:GLU:OE2	1:G:214:LYS:HD3	2.21	0.41
1:D:253:LEU:HD23	1:D:253:LEU:HA	1.90	0.41
2:d:176:PRO:HG2	2:d:179:ILE:HD12	2.03	0.41
1:C:230:ARG:HB2	1:C:230:ARG:HH11	1.86	0.41
2:b:172:LYS:HA	2:b:173:PRO:HD3	1.97	0.41
2:c:177:GLU:HG2	2:c:181:ARG:HH12	1.85	0.41
2:e:71:VAL:HG23	2:e:89:ILE:HB	2.03	0.41
1:J:238:LYS:HG3	2:j:242:ILE:HG12	2.01	0.41
1:I:37:TYR:HA	1:I:41:ALA:O	2.21	0.41
1:I:236:MET:HG3	1:I:237:GLU:N	2.36	0.41
2:i:205:LYS:HA	2:i:205:LYS:HD3	1.87	0.41
1:H:162:ALA:HA	3:v:1:NAG:C8	2.50	0.41
1:G:37:TYR:HA	1:G:41:ALA:O	2.21	0.41
2:j:181:ARG:HG3	2:j:181:ARG:NH1	2.35	0.41
2:m:53:LEU:HA	2:m:54:PRO:HD3	1.93	0.41
1:F:62:ARG:HG2	1:F:62:ARG:HH11	1.86	0.41
1:E:225:GLN:OE1	2:d:215:LEU:HD11	2.21	0.41
1:D:68:LEU:HD22	1:D:94:VAL:HG12	2.03	0.41
1:C:213:ARG:NH1	1:C:213:ARG:HG2	2.36	0.41
1:C:302:ASN:N	1:C:302:ASN:HD22	2.16	0.41
2:e:282:GLN:HG2	2:e:286:TYR:CE1	2.56	0.41
2:i:53:LEU:HA	2:i:54:PRO:HD3	1.96	0.41
2:h:51:LEU:H	2:h:51:LEU:HD23	1.86	0.41
2:a:205:LYS:HA	2:a:205:LYS:HD3	1.80	0.40
1:M:201:LYS:HE2	1:M:201:LYS:HB2	1.84	0.40
1:L:238:LYS:HG3	2:l:242:ILE:HG23	2.02	0.40
1:F:100:TYR:CD1	1:F:100:TYR:C	2.99	0.40
1:F:294:ASN:H	2:f:294:LYS:HZ1	1.68	0.40
1:B:68:LEU:HD23	1:B:96:MET:HB2	2.03	0.40
1:J:38:ARG:HD3	1:J:58:ILE:CD1	2.51	0.40
1:H:107:ARG:HG3	1:H:108:ASN:N	2.37	0.40
2:h:86:PHE:CZ	2:h:173:PRO:HG3	2.56	0.40
2:b:111:TYR:HD2	2:b:115:LEU:HD12	1.86	0.40
2:j:86:PHE:CZ	2:j:173:PRO:HG3	2.56	0.40
2:j:275:LYS:HD3	2:j:280:TYR:CZ	2.56	0.40
1:A:238:LYS:HG3	2:a:242:ILE:HG23	2.03	0.40
2:a:296:TYR:CZ	2:a:298:GLY:HA3	2.57	0.40
1:F:28:ILE:HG13	1:F:34:ALA:HB2	2.03	0.40
1:E:174:LYS:NZ	2:d:129:SER:HB3	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:236:LYS:HD3	2:d:236:LYS:HA	1.81	0.40
1:C:100:TYR:CD2	1:C:100:TYR:C	2.99	0.40
2:b:142:ASP:OD1	2:b:143:GLN:HG2	2.22	0.40
2:e:179:ILE:H	2:e:179:ILE:HG12	1.62	0.40
1:M:191:GLU:HB3	2:m:198:GLN:HB3	2.02	0.40
1:M:299:PHE:HE1	2:l:294:LYS:HB3	1.85	0.40
1:L:68:LEU:HD23	1:L:96:MET:HB2	2.02	0.40
1:K:244:ILE:HG12	2:j:236:LYS:HG3	2.02	0.40
1:C:21:LEU:HD23	1:C:21:LEU:HA	1.82	0.40
1:B:162:ALA:HA	3:o:1:NAG:C8	2.50	0.40
2:b:282:GLN:HG2	2:b:286:TYR:CE2	2.56	0.40
1:H:119:PHE:HA	1:H:122:ILE:HD12	2.03	0.40
1:H:211:THR:HG22	2:g:200:GLN:HB2	2.03	0.40
1:H:302:ASN:N	1:H:302:ASN:HD22	2.20	0.40
1:G:115:LYS:HA	1:G:119:PHE:HB2	2.04	0.40
2:f:26:ILE:HB	2:f:47:PRO:HA	2.03	0.40
2:f:215:LEU:HD11	1:G:225:GLN:OE1	2.22	0.40
1:E:162:ALA:HA	3:X:1:NAG:C8	2.51	0.40
1:D:225:GLN:OE1	2:c:215:LEU:HD11	2.21	0.40
1:C:16:LEU:HD23	1:C:16:LEU:HA	1.90	0.40
2:c:86:PHE:CZ	2:c:173:PRO:HG3	2.56	0.40
1:J:292:ALA:HB3	2:i:288:ALA:HB1	2.02	0.40
1:I:295:SER:HB3	2:h:292:ASN:ND2	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	302/304 (99%)	295 (98%)	7 (2%)	0	100	100
1	B	302/304 (99%)	295 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	302/304 (99%)	295 (98%)	7 (2%)	0	100	100
1	D	302/304 (99%)	295 (98%)	7 (2%)	0	100	100
1	E	302/304 (99%)	295 (98%)	7 (2%)	0	100	100
1	F	302/304 (99%)	295 (98%)	7 (2%)	0	100	100
1	G	302/304 (99%)	295 (98%)	7 (2%)	0	100	100
1	H	302/304 (99%)	294 (97%)	8 (3%)	0	100	100
1	I	302/304 (99%)	296 (98%)	6 (2%)	0	100	100
1	J	302/304 (99%)	294 (97%)	8 (3%)	0	100	100
1	K	302/304 (99%)	294 (97%)	8 (3%)	0	100	100
1	L	302/304 (99%)	295 (98%)	7 (2%)	0	100	100
1	M	302/304 (99%)	295 (98%)	7 (2%)	0	100	100
2	a	302/304 (99%)	297 (98%)	4 (1%)	1 (0%)	36	58
2	b	302/304 (99%)	297 (98%)	5 (2%)	0	100	100
2	c	302/304 (99%)	297 (98%)	4 (1%)	1 (0%)	36	58
2	d	302/304 (99%)	297 (98%)	4 (1%)	1 (0%)	36	58
2	e	302/304 (99%)	297 (98%)	4 (1%)	1 (0%)	36	58
2	f	302/304 (99%)	297 (98%)	4 (1%)	1 (0%)	36	58
2	g	302/304 (99%)	297 (98%)	4 (1%)	1 (0%)	36	58
2	h	302/304 (99%)	297 (98%)	5 (2%)	0	100	100
2	i	302/304 (99%)	297 (98%)	4 (1%)	1 (0%)	36	58
2	j	302/304 (99%)	297 (98%)	4 (1%)	1 (0%)	36	58
2	k	302/304 (99%)	297 (98%)	4 (1%)	1 (0%)	36	58
2	l	302/304 (99%)	297 (98%)	4 (1%)	1 (0%)	36	58
2	m	302/304 (99%)	297 (98%)	5 (2%)	0	100	100
All	All	7852/7904 (99%)	7694 (98%)	148 (2%)	10 (0%)	49	70

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	k	108	THR
2	a	108	THR
2	l	108	THR
2	d	108	THR
2	c	108	THR

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Mol	Chain	Res	Type
2	e	108	THR
2	i	108	THR
2	g	108	THR
2	j	108	THR
2	f	108	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	259/259 (100%)	247 (95%)	12 (5%)	24	49
1	B	259/259 (100%)	250 (96%)	9 (4%)	32	59
1	C	259/259 (100%)	249 (96%)	10 (4%)	28	55
1	D	259/259 (100%)	249 (96%)	10 (4%)	28	55
1	E	259/259 (100%)	244 (94%)	15 (6%)	18	39
1	F	259/259 (100%)	253 (98%)	6 (2%)	44	71
1	G	259/259 (100%)	248 (96%)	11 (4%)	26	52
1	H	259/259 (100%)	248 (96%)	11 (4%)	26	52
1	I	259/259 (100%)	251 (97%)	8 (3%)	35	63
1	J	259/259 (100%)	250 (96%)	9 (4%)	32	59
1	K	259/259 (100%)	250 (96%)	9 (4%)	32	59
1	L	259/259 (100%)	244 (94%)	15 (6%)	18	39
1	M	259/259 (100%)	249 (96%)	10 (4%)	28	55
2	a	260/260 (100%)	254 (98%)	6 (2%)	44	71
2	b	260/260 (100%)	255 (98%)	5 (2%)	50	75
2	c	260/260 (100%)	252 (97%)	8 (3%)	35	63
2	d	260/260 (100%)	253 (97%)	7 (3%)	39	67
2	e	260/260 (100%)	254 (98%)	6 (2%)	44	71
2	f	260/260 (100%)	254 (98%)	6 (2%)	44	71
2	g	260/260 (100%)	254 (98%)	6 (2%)	44	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	h	260/260 (100%)	253 (97%)	7 (3%)	39	67
2	i	260/260 (100%)	252 (97%)	8 (3%)	35	63
2	j	260/260 (100%)	251 (96%)	9 (4%)	32	59
2	k	260/260 (100%)	254 (98%)	6 (2%)	44	71
2	l	260/260 (100%)	252 (97%)	8 (3%)	35	63
2	m	260/260 (100%)	252 (97%)	8 (3%)	35	63
All	All	6747/6747 (100%)	6522 (97%)	225 (3%)	34	61

All (225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ILE
1	A	62	ARG
1	A	70	THR
1	A	78	CYS
1	A	105	ILE
1	A	116	THR
1	A	157	ASP
1	A	160	LEU
1	A	165	LEU
1	A	191	GLU
1	A	236	MET
1	A	307	PHE
2	a	51	LEU
2	a	68	THR
2	a	76	CYS
2	a	95	LEU
2	a	163	LEU
2	a	289	ILE
1	M	33	LEU
1	M	35	VAL
1	M	70	THR
1	M	160	LEU
1	M	165	LEU
1	M	207	LYS
1	M	236	MET
1	M	268	HIS
1	M	286	LYS
1	M	307	PHE
2	m	4	LEU

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Mol	Chain	Res	Type
2	m	66	LEU
2	m	76	CYS
2	m	113	LYS
2	m	139	GLU
2	m	159	MET
2	m	163	LEU
2	m	205	LYS
1	L	29	GLU
1	L	53	ILE
1	L	70	THR
1	L	78	CYS
1	L	96	MET
1	L	116	THR
1	L	160	LEU
1	L	161	MET
1	L	165	LEU
1	L	207	LYS
1	L	236	MET
1	L	243	ARG
1	L	268	HIS
1	L	303	ILE
1	L	307	PHE
1	K	29	GLU
1	K	70	THR
1	K	78	CYS
1	K	96	MET
1	K	160	LEU
1	K	161	MET
1	K	165	LEU
1	K	221	GLU
1	K	307	PHE
2	k	4	LEU
2	k	43	SER
2	k	76	CYS
2	k	95	LEU
2	k	163	LEU
2	k	295	MET
2	l	4	LEU
2	l	25	LYS
2	l	41	LEU
2	l	51	LEU
2	l	76	CYS

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Mol	Chain	Res	Type
2	l	163	LEU
2	l	274	LEU
2	l	300	ASP
1	F	70	THR
1	F	78	CYS
1	F	96	MET
1	F	165	LEU
1	F	207	LYS
1	F	307	PHE
2	f	4	LEU
2	f	66	LEU
2	f	159	MET
2	f	163	LEU
2	f	205	LYS
2	f	304	MET
1	E	28	ILE
1	E	35	VAL
1	E	53	ILE
1	E	70	THR
1	E	78	CYS
1	E	96	MET
1	E	97	LEU
1	E	116	THR
1	E	160	LEU
1	E	165	LEU
1	E	207	LYS
1	E	236	MET
1	E	256	GLU
1	E	301	SER
1	E	307	PHE
1	D	53	ILE
1	D	70	THR
1	D	78	CYS
1	D	96	MET
1	D	160	LEU
1	D	161	MET
1	D	165	LEU
1	D	232	GLN
1	D	236	MET
1	D	307	PHE
2	d	4	LEU
2	d	25	LYS

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Mol	Chain	Res	Type
2	d	76	CYS
2	d	124	LEU
2	d	186	MET
2	d	237	GLU
2	d	289	ILE
1	C	35	VAL
1	C	53	ILE
1	C	70	THR
1	C	78	CYS
1	C	96	MET
1	C	116	THR
1	C	165	LEU
1	C	236	MET
1	C	268	HIS
1	C	307	PHE
1	B	35	VAL
1	B	53	ILE
1	B	70	THR
1	B	78	CYS
1	B	96	MET
1	B	161	MET
1	B	207	LYS
1	B	223	ILE
1	B	307	PHE
2	b	4	LEU
2	b	43	SER
2	b	76	CYS
2	b	159	MET
2	b	275	LYS
2	c	4	LEU
2	c	40	LEU
2	c	57	THR
2	c	66	LEU
2	c	68	THR
2	c	72	LYS
2	c	95	LEU
2	c	205	LYS
2	e	4	LEU
2	e	51	LEU
2	e	68	THR
2	e	76	CYS
2	e	163	LEU

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Mol	Chain	Res	Type
2	e	205	LYS
1	J	29	GLU
1	J	35	VAL
1	J	53	ILE
1	J	70	THR
1	J	116	THR
1	J	160	LEU
1	J	165	LEU
1	J	179	GLU
1	J	307	PHE
1	I	29	GLU
1	I	53	ILE
1	I	62	ARG
1	I	70	THR
1	I	78	CYS
1	I	160	LEU
1	I	236	MET
1	I	307	PHE
2	i	4	LEU
2	i	51	LEU
2	i	66	LEU
2	i	76	CYS
2	i	154	GLN
2	i	163	LEU
2	i	273	LYS
2	i	295	MET
1	H	29	GLU
1	H	35	VAL
1	H	53	ILE
1	H	70	THR
1	H	78	CYS
1	H	88	ILE
1	H	96	MET
1	H	160	LEU
1	H	165	LEU
1	H	191	GLU
1	H	236	MET
1	G	35	VAL
1	G	53	ILE
1	G	70	THR
1	G	97	LEU
1	G	116	THR

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Mol	Chain	Res	Type
1	G	152	GLN
1	G	160	LEU
1	G	161	MET
1	G	165	LEU
1	G	195	LEU
1	G	207	LYS
2	g	4	LEU
2	g	66	LEU
2	g	68	THR
2	g	76	CYS
2	g	163	LEU
2	g	273	LYS
2	h	4	LEU
2	h	43	SER
2	h	57	THR
2	h	66	LEU
2	h	76	CYS
2	h	102	ASP
2	h	304	MET
2	j	4	LEU
2	j	57	THR
2	j	66	LEU
2	j	68	THR
2	j	76	CYS
2	j	102	ASP
2	j	124	LEU
2	j	163	LEU
2	j	304	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	123	HIS
1	A	202	GLN
2	a	147	ASN
1	M	65	GLN
1	M	124	HIS
1	M	202	GLN
1	M	302	ASN
2	m	147	ASN
2	m	174	ASN

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Mol	Chain	Res	Type
1	L	52	HIS
1	L	124	HIS
1	L	202	GLN
1	K	202	GLN
1	K	302	ASN
2	k	122	HIS
2	k	126	GLN
2	k	147	ASN
2	k	174	ASN
2	k	200	GLN
2	k	223	GLN
2	l	122	HIS
2	l	147	ASN
2	l	174	ASN
1	F	65	GLN
1	F	123	HIS
1	F	124	HIS
1	F	202	GLN
2	f	122	HIS
2	f	126	GLN
2	f	174	ASN
2	f	223	GLN
1	E	65	GLN
1	E	123	HIS
1	E	124	HIS
1	E	202	GLN
1	D	75	ASN
1	D	123	HIS
1	D	124	HIS
1	D	202	GLN
1	D	302	ASN
2	d	126	GLN
2	d	143	GLN
2	d	147	ASN
2	d	174	ASN
1	C	124	HIS
1	C	202	GLN
1	B	65	GLN
1	B	123	HIS
1	B	202	GLN
2	b	126	GLN
2	b	147	ASN

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Mol	Chain	Res	Type
2	b	282	GLN
2	c	122	HIS
2	c	147	ASN
2	c	174	ASN
2	c	198	GLN
2	e	147	ASN
1	J	123	HIS
1	J	202	GLN
1	J	268	HIS
1	I	52	HIS
1	I	123	HIS
1	I	124	HIS
1	I	128	GLN
1	I	202	GLN
2	i	122	HIS
2	i	126	GLN
2	i	147	ASN
2	i	174	ASN
1	H	65	GLN
1	H	124	HIS
1	H	133	HIS
1	H	202	GLN
1	G	124	HIS
1	G	202	GLN
1	G	268	HIS
1	G	302	ASN
2	g	126	GLN
2	g	143	GLN
2	g	147	ASN
2	g	174	ASN
2	h	126	GLN
2	h	143	GLN
2	h	147	ASN
2	h	174	ASN
2	j	126	GLN
2	j	147	ASN

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	0.75	0	17,19,21	1.25	2 (11%)
3	NAG	N	2	3	14,14,15	0.72	0	17,19,21	0.87	0
3	NAG	O	1	3,2	14,14,15	0.72	0	17,19,21	1.14	1 (5%)
3	NAG	O	2	3	14,14,15	0.71	0	17,19,21	0.89	0
3	NAG	P	1	1,3	14,14,15	0.72	0	17,19,21	1.20	2 (11%)
3	NAG	P	2	3	14,14,15	0.73	0	17,19,21	0.90	0
3	NAG	Q	1	3,2	14,14,15	0.68	0	17,19,21	1.20	1 (5%)
3	NAG	Q	2	3	14,14,15	0.73	0	17,19,21	0.91	0
3	NAG	R	1	1,3	14,14,15	0.74	0	17,19,21	1.26	2 (11%)
3	NAG	R	2	3	14,14,15	0.73	0	17,19,21	0.91	1 (5%)
3	NAG	S	1	1,3	14,14,15	0.72	0	17,19,21	1.25	2 (11%)
3	NAG	S	2	3	14,14,15	0.71	0	17,19,21	0.89	0
3	NAG	T	1	3,2	14,14,15	0.71	0	17,19,21	1.19	2 (11%)
3	NAG	T	2	3	14,14,15	0.73	0	17,19,21	0.90	1 (5%)
3	NAG	U	1	3,2	14,14,15	0.71	0	17,19,21	1.21	1 (5%)
3	NAG	U	2	3	14,14,15	0.72	0	17,19,21	0.91	0
3	NAG	V	1	1,3	14,14,15	0.74	0	17,19,21	1.23	2 (11%)
3	NAG	V	2	3	14,14,15	0.73	0	17,19,21	0.91	1 (5%)
3	NAG	W	1	3,2	14,14,15	0.70	0	17,19,21	1.18	1 (5%)
3	NAG	W	2	3	14,14,15	0.73	0	17,19,21	0.90	0
3	NAG	X	1	1,3	14,14,15	0.74	0	17,19,21	1.28	2 (11%)
3	NAG	X	2	3	14,14,15	0.73	0	17,19,21	0.91	0
3	NAG	Y	1	1,3	14,14,15	0.75	0	17,19,21	1.25	2 (11%)
3	NAG	Y	2	3	14,14,15	0.71	0	17,19,21	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	Z	1	3,2	14,14,15	0.69	0	17,19,21	1.24	2 (11%)
3	NAG	Z	2	3	14,14,15	0.71	0	17,19,21	0.90	0
3	NAG	n	1	1,3	14,14,15	0.73	0	17,19,21	1.21	2 (11%)
3	NAG	n	2	3	14,14,15	0.72	0	17,19,21	0.89	1 (5%)
3	NAG	o	1	1,3	14,14,15	0.74	0	17,19,21	1.28	2 (11%)
3	NAG	o	2	3	14,14,15	0.72	0	17,19,21	0.90	0
3	NAG	p	1	3,2	14,14,15	0.71	0	17,19,21	1.20	1 (5%)
3	NAG	p	2	3	14,14,15	0.73	0	17,19,21	0.93	1 (5%)
3	NAG	q	1	3,2	14,14,15	0.71	0	17,19,21	1.18	1 (5%)
3	NAG	q	2	3	14,14,15	0.72	0	17,19,21	0.90	0
3	NAG	r	1	3,2	14,14,15	0.70	0	17,19,21	1.20	1 (5%)
3	NAG	r	2	3	14,14,15	0.74	0	17,19,21	0.91	0
3	NAG	s	1	1,3	14,14,15	0.74	0	17,19,21	1.24	2 (11%)
3	NAG	s	2	3	14,14,15	0.72	0	17,19,21	0.90	0
3	NAG	t	1	1,3	14,14,15	0.74	0	17,19,21	1.26	1 (5%)
3	NAG	t	2	3	14,14,15	0.73	0	17,19,21	0.89	1 (5%)
3	NAG	u	1	3,2	14,14,15	0.72	0	17,19,21	1.24	1 (5%)
3	NAG	u	2	3	14,14,15	0.73	0	17,19,21	0.90	0
3	NAG	v	1	1,3	14,14,15	0.74	0	17,19,21	1.22	2 (11%)
3	NAG	v	2	3	14,14,15	0.73	0	17,19,21	0.90	1 (5%)
3	NAG	w	1	1,3	14,14,15	0.74	0	17,19,21	1.25	2 (11%)
3	NAG	w	2	3	14,14,15	0.72	0	17,19,21	0.88	0
3	NAG	x	1	3,2	14,14,15	0.71	0	17,19,21	1.21	1 (5%)
3	NAG	x	2	3	14,14,15	0.72	0	17,19,21	0.92	0
3	NAG	y	1	3,2	14,14,15	0.70	0	17,19,21	1.15	1 (5%)
3	NAG	y	2	3	14,14,15	0.72	0	17,19,21	0.90	0
3	NAG	z	1	3,2	14,14,15	0.72	0	17,19,21	1.16	1 (5%)
3	NAG	z	2	3	14,14,15	0.72	0	17,19,21	0.90	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	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	NAG	O	1	3,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	0/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	0/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	0/6/23/26	0/1/1/1
3	NAG	T	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	T	2	3	-	0/6/23/26	0/1/1/1
3	NAG	U	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	0/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	V	2	3	-	0/6/23/26	0/1/1/1
3	NAG	W	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	W	2	3	-	0/6/23/26	0/1/1/1
3	NAG	X	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Y	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Z	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	0/6/23/26	0/1/1/1
3	NAG	n	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	n	2	3	-	0/6/23/26	0/1/1/1
3	NAG	o	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	o	2	3	-	0/6/23/26	0/1/1/1
3	NAG	p	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	p	2	3	-	0/6/23/26	0/1/1/1
3	NAG	q	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	q	2	3	-	0/6/23/26	0/1/1/1
3	NAG	r	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	r	2	3	-	0/6/23/26	0/1/1/1
3	NAG	s	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	s	2	3	-	0/6/23/26	0/1/1/1
3	NAG	t	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	t	2	3	-	0/6/23/26	0/1/1/1
3	NAG	u	1	3,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	u	2	3	-	0/6/23/26	0/1/1/1
3	NAG	v	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	v	2	3	-	0/6/23/26	0/1/1/1
3	NAG	w	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	w	2	3	-	0/6/23/26	0/1/1/1
3	NAG	x	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	x	2	3	-	0/6/23/26	0/1/1/1
3	NAG	y	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	y	2	3	-	0/6/23/26	0/1/1/1
3	NAG	z	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	z	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	t	1	NAG	C2-N2-C7	3.02	127.20	122.90
3	o	1	NAG	C2-N2-C7	2.92	127.06	122.90
3	X	1	NAG	C2-N2-C7	2.86	126.97	122.90
3	S	1	NAG	C2-N2-C7	2.64	126.67	122.90
3	N	1	NAG	C2-N2-C7	2.64	126.66	122.90
3	v	1	NAG	C2-N2-C7	2.64	126.66	122.90
3	R	1	NAG	C2-N2-C7	2.62	126.64	122.90
3	w	1	NAG	C2-N2-C7	2.62	126.63	122.90
3	s	1	NAG	C2-N2-C7	2.61	126.62	122.90
3	Y	1	NAG	C2-N2-C7	2.59	126.59	122.90
3	V	1	NAG	C2-N2-C7	2.55	126.53	122.90
3	n	1	NAG	C2-N2-C7	2.50	126.46	122.90
3	Z	1	NAG	C1-O5-C5	2.47	115.54	112.19
3	Q	1	NAG	C1-O5-C5	2.36	115.39	112.19
3	U	1	NAG	C1-O5-C5	2.34	115.37	112.19
3	S	1	NAG	C1-O5-C5	2.33	115.35	112.19
3	Y	1	NAG	C1-O5-C5	2.32	115.34	112.19
3	x	1	NAG	C1-O5-C5	2.32	115.34	112.19
3	N	1	NAG	C1-O5-C5	2.31	115.32	112.19
3	u	1	NAG	C1-O5-C5	2.29	115.29	112.19
3	T	1	NAG	C1-O5-C5	2.28	115.28	112.19
3	o	1	NAG	C1-O5-C5	2.27	115.27	112.19
3	r	1	NAG	C1-O5-C5	2.25	115.25	112.19
3	W	1	NAG	C1-O5-C5	2.25	115.24	112.19
3	P	1	NAG	C1-O5-C5	2.23	115.22	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	2	NAG	O5-C1-C2	-2.22	107.78	111.29
3	X	1	NAG	C1-O5-C5	2.21	115.18	112.19
3	n	1	NAG	C1-O5-C5	2.20	115.17	112.19
3	R	1	NAG	C1-O5-C5	2.19	115.16	112.19
3	s	1	NAG	C1-O5-C5	2.17	115.14	112.19
3	w	1	NAG	C1-O5-C5	2.16	115.11	112.19
3	z	1	NAG	C1-O5-C5	2.13	115.08	112.19
3	O	1	NAG	C1-O5-C5	2.13	115.07	112.19
3	q	1	NAG	C1-O5-C5	2.13	115.07	112.19
3	y	1	NAG	C2-N2-C7	2.12	125.92	122.90
3	p	1	NAG	C1-O5-C5	2.12	115.07	112.19
3	v	1	NAG	C1-O5-C5	2.12	115.06	112.19
3	V	1	NAG	C1-O5-C5	2.12	115.06	112.19
3	v	2	NAG	O5-C1-C2	-2.12	107.95	111.29
3	P	1	NAG	C2-N2-C7	2.10	125.89	122.90
3	Z	1	NAG	C2-N2-C7	2.08	125.87	122.90
3	n	2	NAG	O5-C1-C2	-2.06	108.04	111.29
3	R	2	NAG	O5-C1-C2	-2.04	108.07	111.29
3	t	2	NAG	O5-C1-C2	-2.02	108.10	111.29
3	p	2	NAG	C1-O5-C5	2.02	114.93	112.19
3	T	1	NAG	C2-N2-C7	2.01	125.76	122.90
3	T	2	NAG	C1-O5-C5	2.00	114.91	112.19

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	N	1	NAG	C8-C7-N2-C2
3	N	1	NAG	O7-C7-N2-C2
3	O	1	NAG	C8-C7-N2-C2
3	O	1	NAG	O7-C7-N2-C2
3	P	1	NAG	C8-C7-N2-C2
3	P	1	NAG	O7-C7-N2-C2
3	Q	1	NAG	C8-C7-N2-C2
3	Q	1	NAG	O7-C7-N2-C2
3	R	1	NAG	C8-C7-N2-C2
3	R	1	NAG	O7-C7-N2-C2
3	S	1	NAG	C8-C7-N2-C2
3	S	1	NAG	O7-C7-N2-C2
3	T	1	NAG	C8-C7-N2-C2
3	T	1	NAG	O7-C7-N2-C2
3	U	1	NAG	C8-C7-N2-C2

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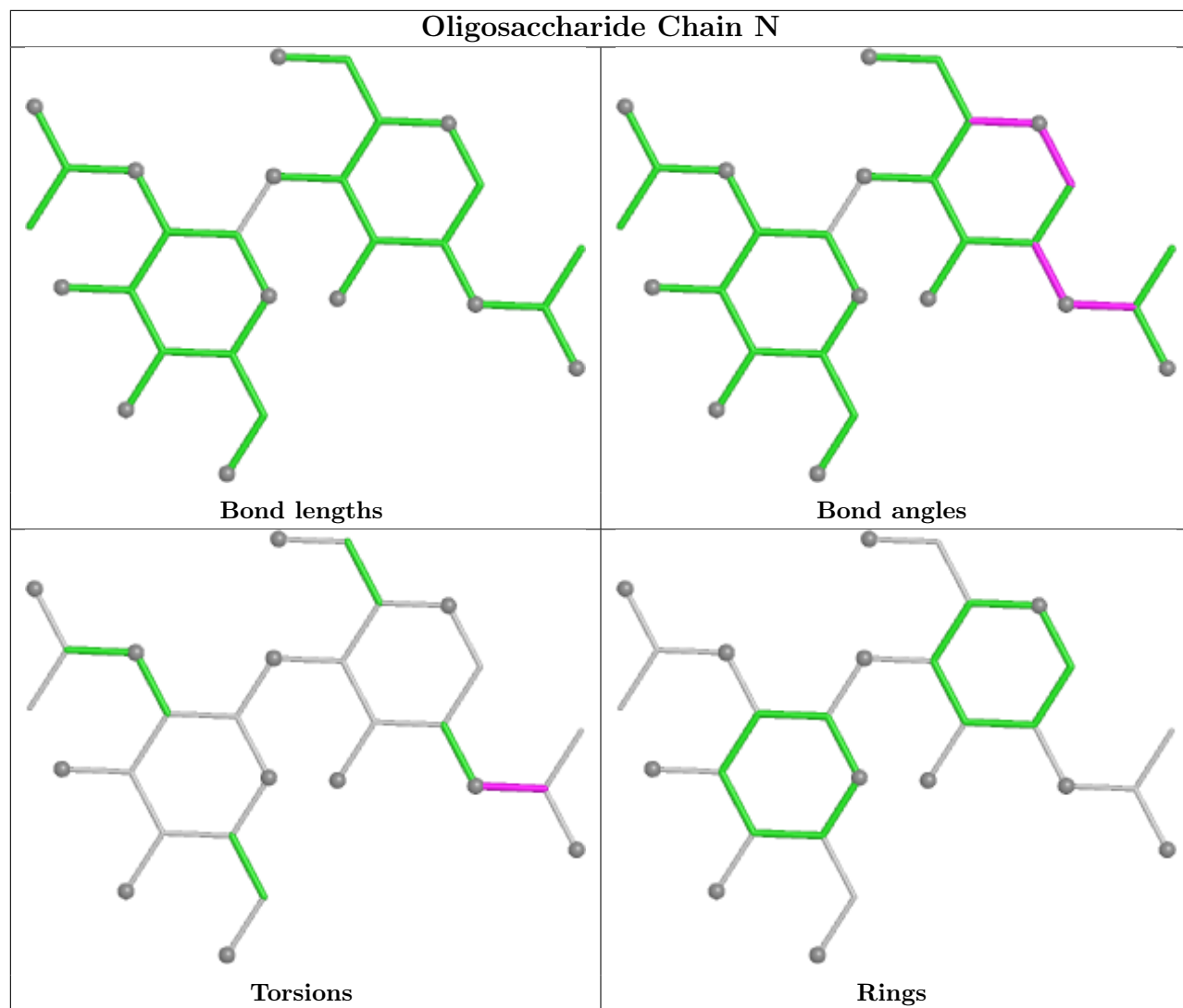
Mol	Chain	Res	Type	Atoms
3	U	1	NAG	O7-C7-N2-C2
3	V	1	NAG	C8-C7-N2-C2
3	V	1	NAG	O7-C7-N2-C2
3	W	1	NAG	C8-C7-N2-C2
3	W	1	NAG	O7-C7-N2-C2
3	X	1	NAG	C8-C7-N2-C2
3	X	1	NAG	O7-C7-N2-C2
3	Y	1	NAG	C8-C7-N2-C2
3	Y	1	NAG	O7-C7-N2-C2
3	Z	1	NAG	C8-C7-N2-C2
3	Z	1	NAG	O7-C7-N2-C2
3	n	1	NAG	C8-C7-N2-C2
3	n	1	NAG	O7-C7-N2-C2
3	o	1	NAG	C8-C7-N2-C2
3	o	1	NAG	O7-C7-N2-C2
3	p	1	NAG	C8-C7-N2-C2
3	p	1	NAG	O7-C7-N2-C2
3	q	1	NAG	C8-C7-N2-C2
3	q	1	NAG	O7-C7-N2-C2
3	r	1	NAG	C8-C7-N2-C2
3	r	1	NAG	O7-C7-N2-C2
3	s	1	NAG	C8-C7-N2-C2
3	s	1	NAG	O7-C7-N2-C2
3	t	1	NAG	C8-C7-N2-C2
3	t	1	NAG	O7-C7-N2-C2
3	u	1	NAG	C8-C7-N2-C2
3	u	1	NAG	O7-C7-N2-C2
3	v	1	NAG	C8-C7-N2-C2
3	v	1	NAG	O7-C7-N2-C2
3	w	1	NAG	C8-C7-N2-C2
3	w	1	NAG	O7-C7-N2-C2
3	x	1	NAG	C8-C7-N2-C2
3	x	1	NAG	O7-C7-N2-C2
3	y	1	NAG	C8-C7-N2-C2
3	y	1	NAG	O7-C7-N2-C2
3	z	1	NAG	C8-C7-N2-C2
3	z	1	NAG	O7-C7-N2-C2

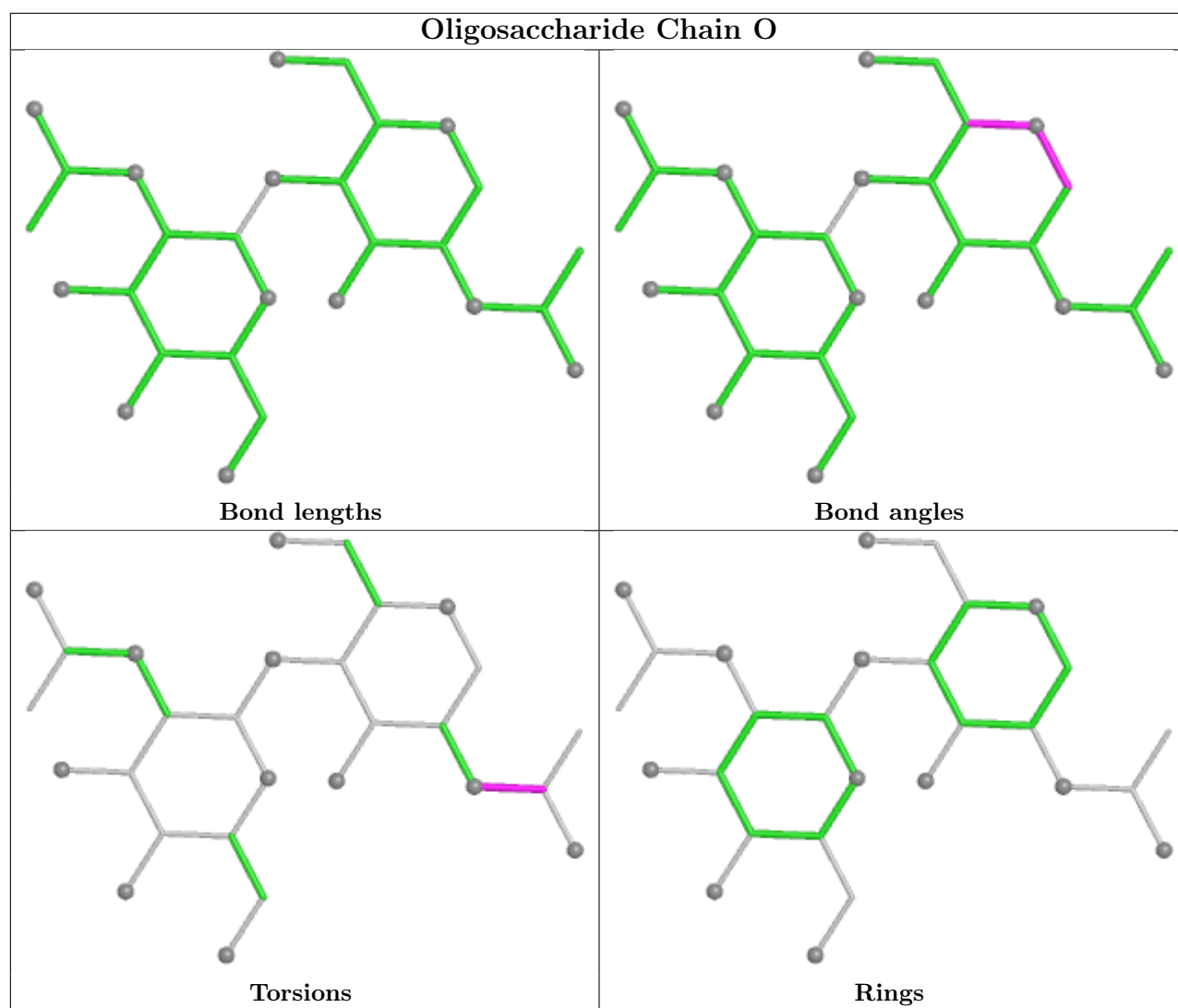
There are no ring outliers.

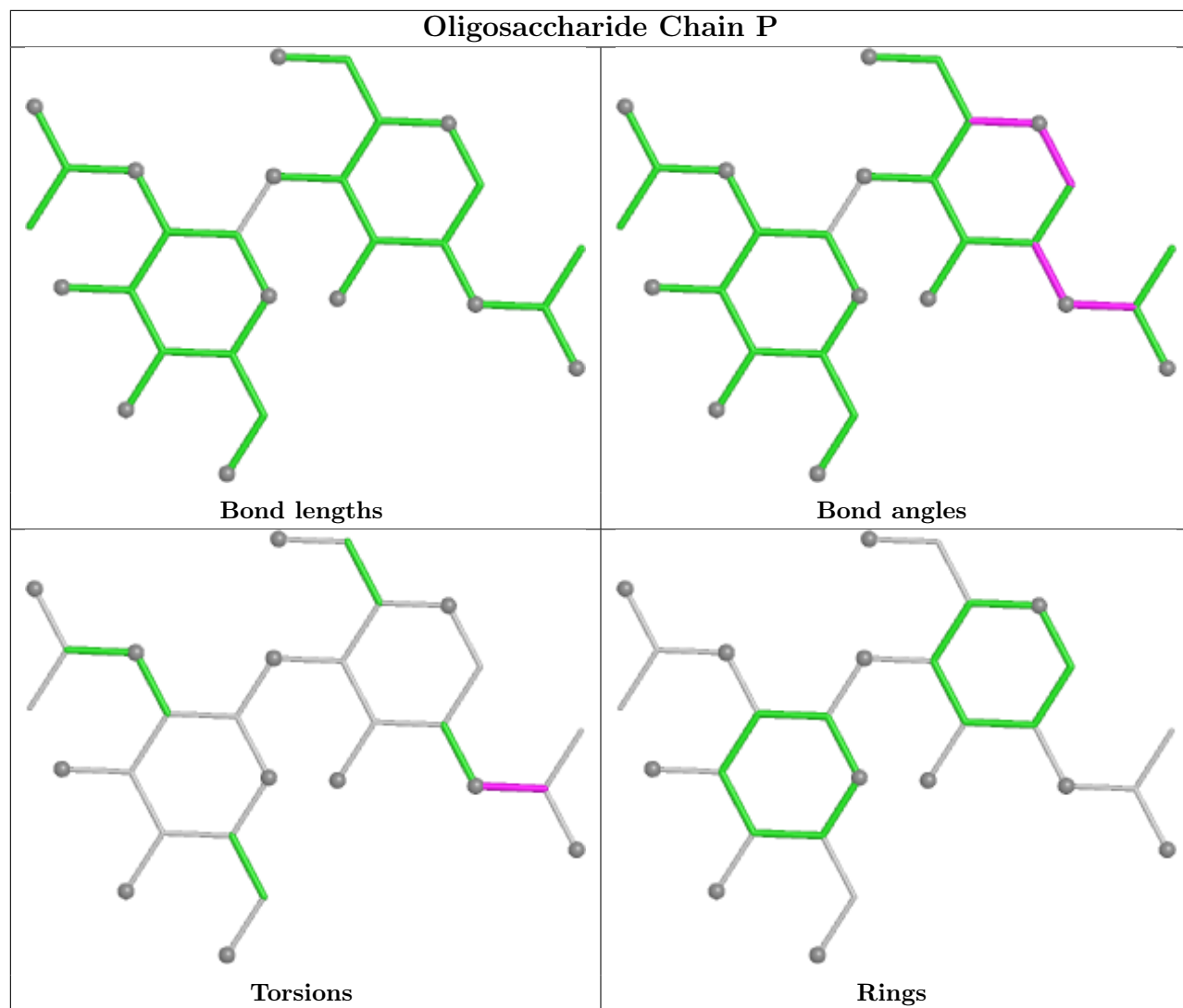
26 monomers are involved in 107 short contacts:

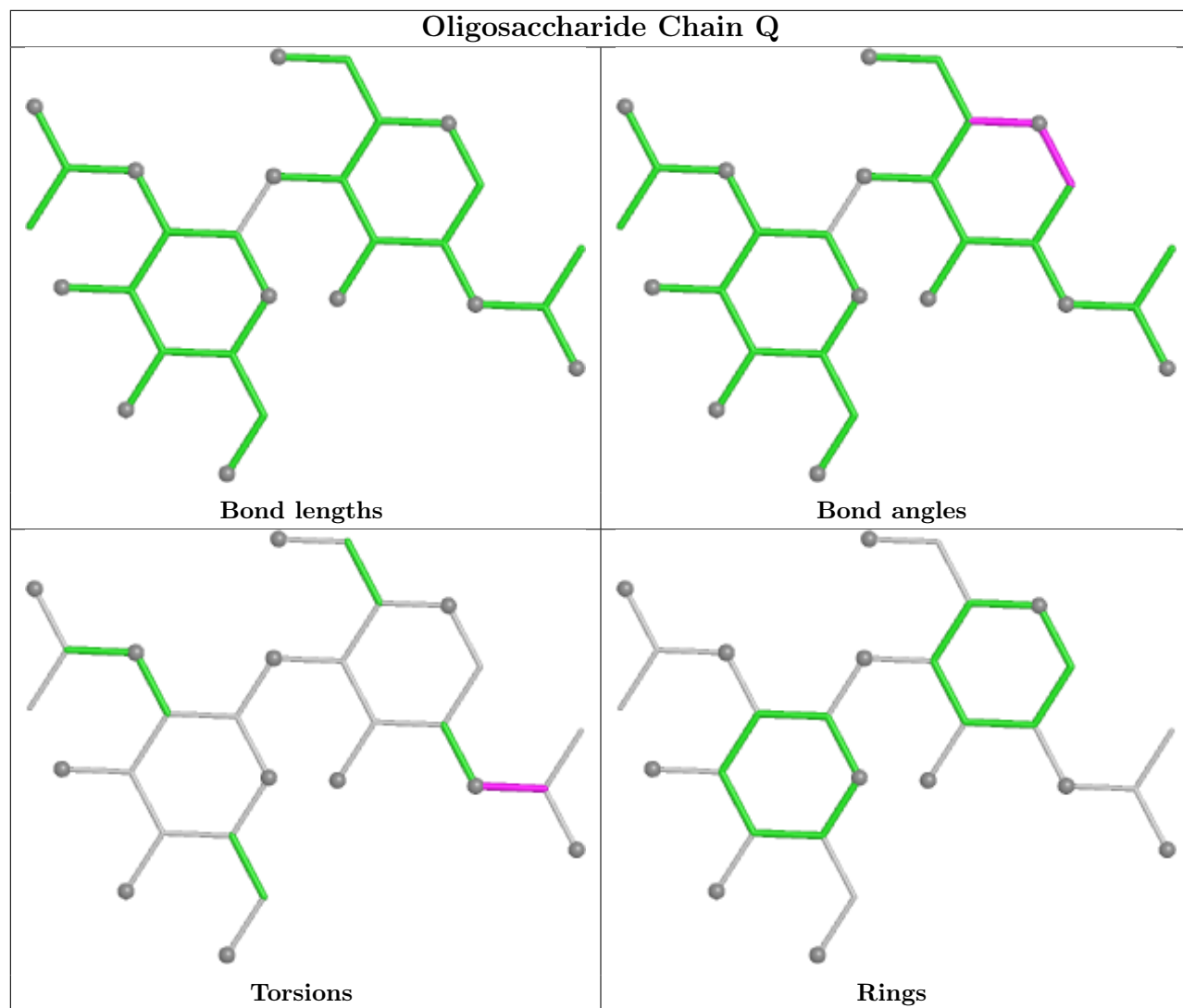
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	p	1	NAG	5	0
3	N	1	NAG	3	0
3	P	1	NAG	3	0
3	t	1	NAG	3	0
3	R	1	NAG	3	0
3	z	1	NAG	6	0
3	Z	1	NAG	5	0
3	Y	1	NAG	3	0
3	S	1	NAG	3	0
3	o	1	NAG	3	0
3	y	1	NAG	6	0
3	W	1	NAG	5	0
3	V	1	NAG	3	0
3	X	1	NAG	3	0
3	q	1	NAG	5	0
3	w	1	NAG	3	0
3	O	1	NAG	6	0
3	s	1	NAG	3	0
3	u	1	NAG	5	0
3	U	1	NAG	5	0
3	v	1	NAG	3	0
3	T	1	NAG	5	0
3	x	1	NAG	5	0
3	r	1	NAG	5	0
3	Q	1	NAG	5	0
3	n	1	NAG	3	0

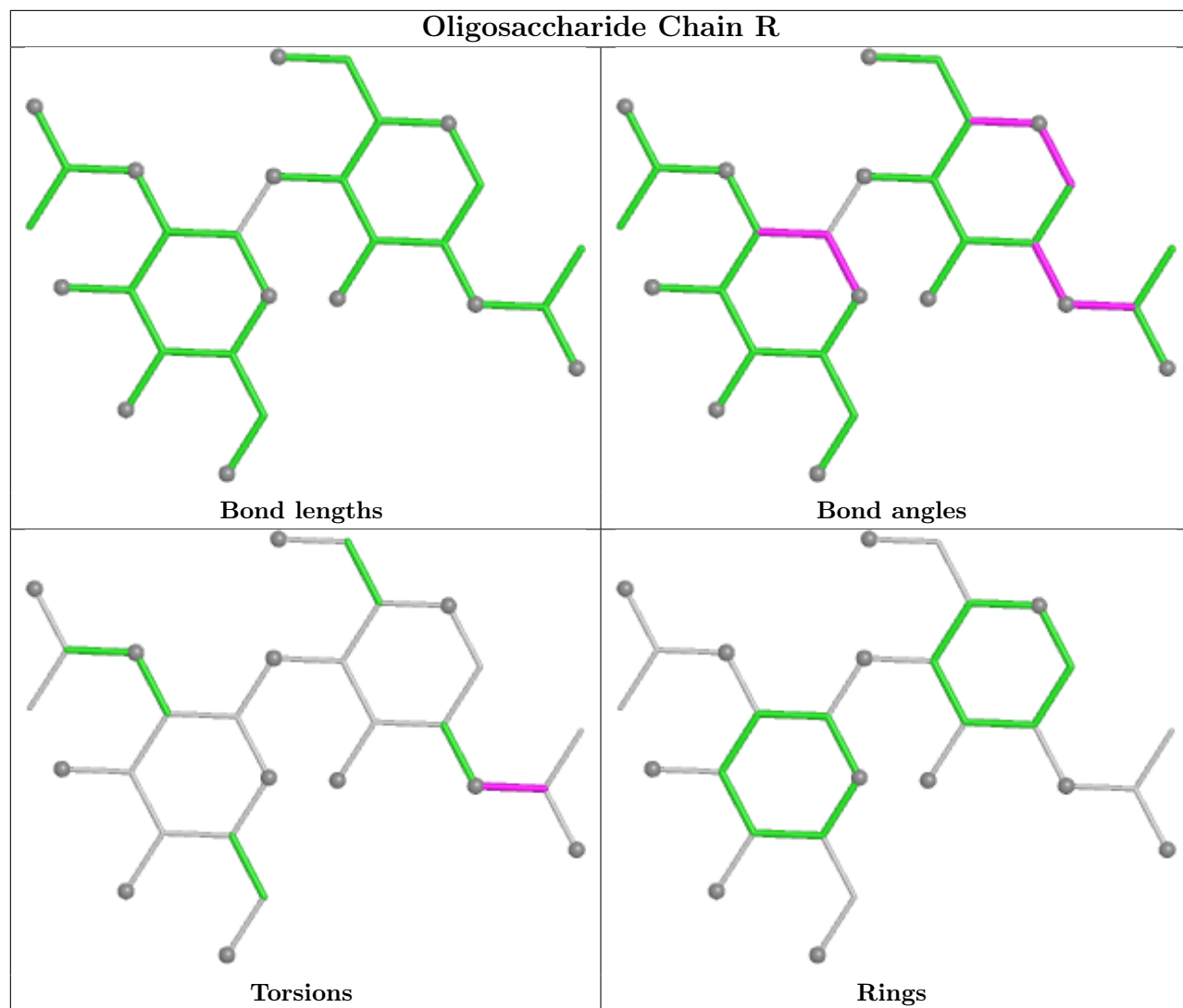
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

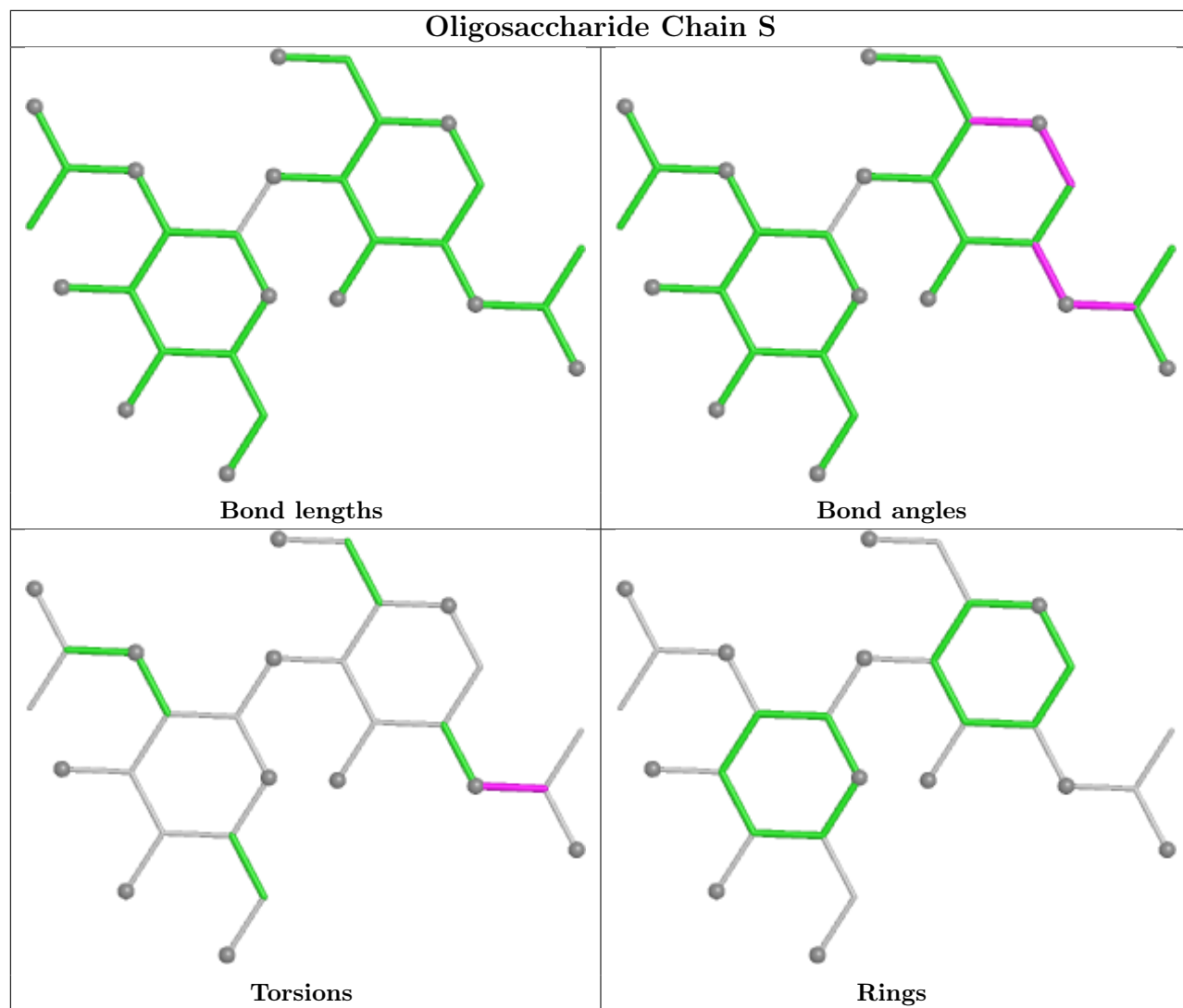


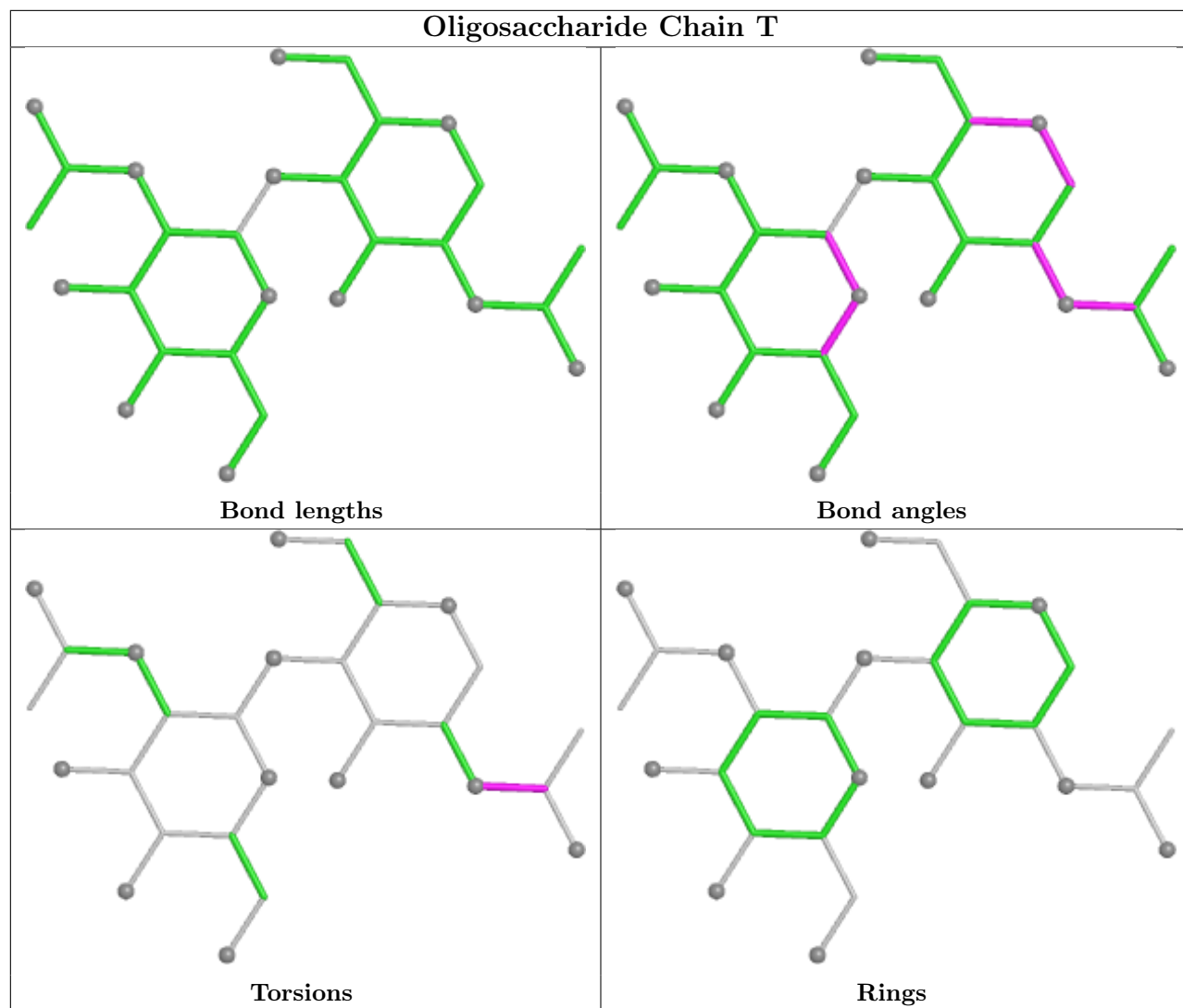


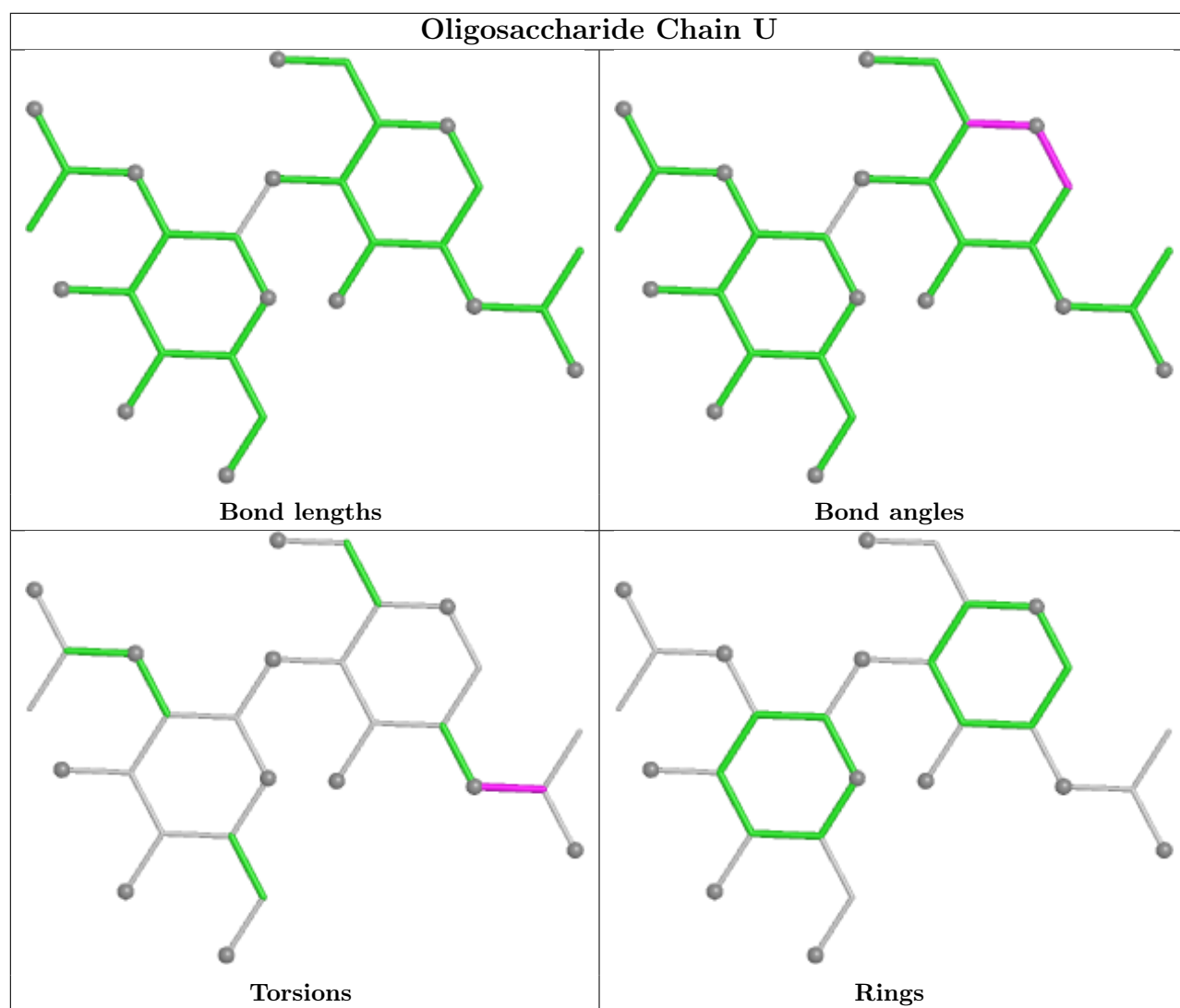


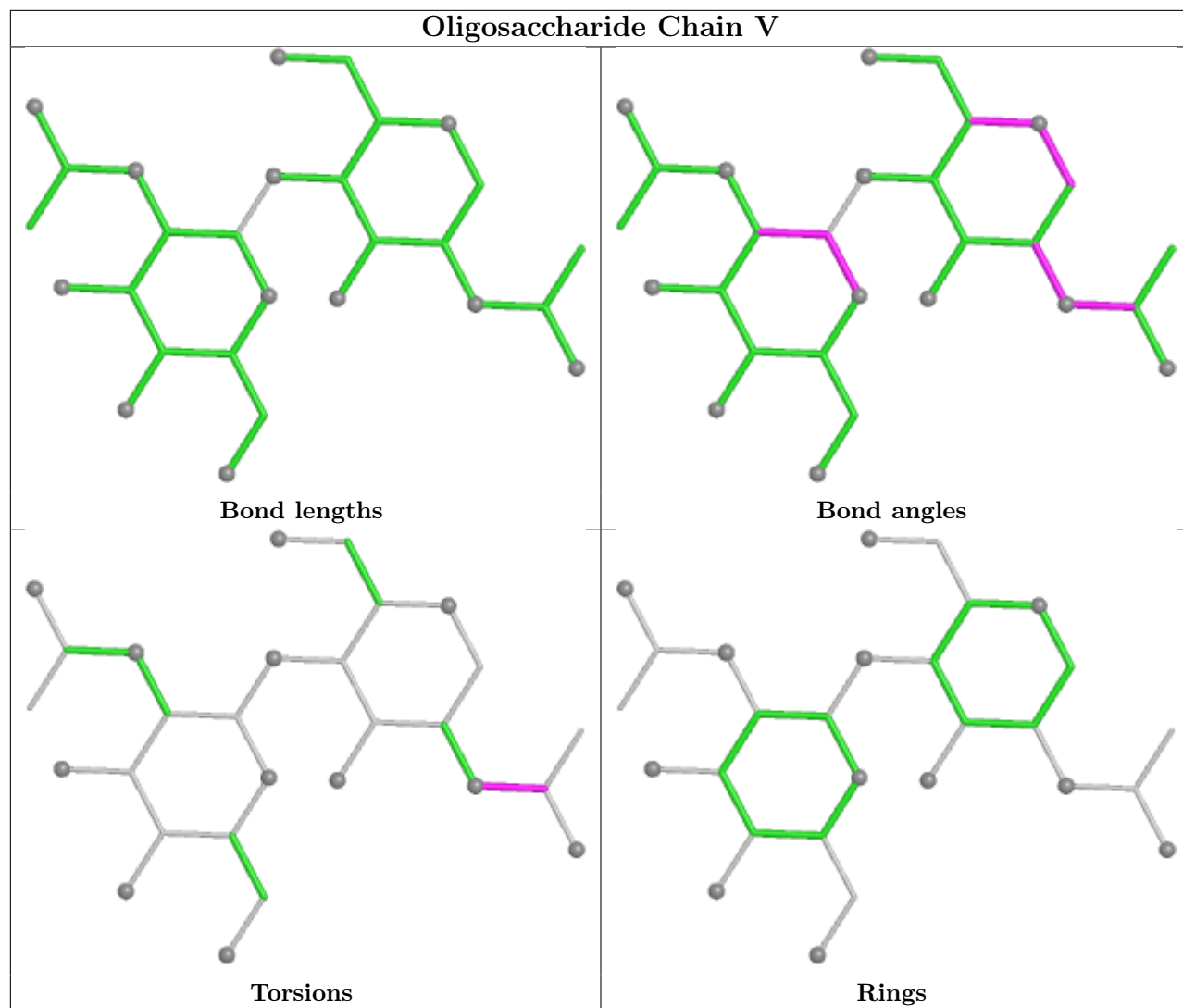


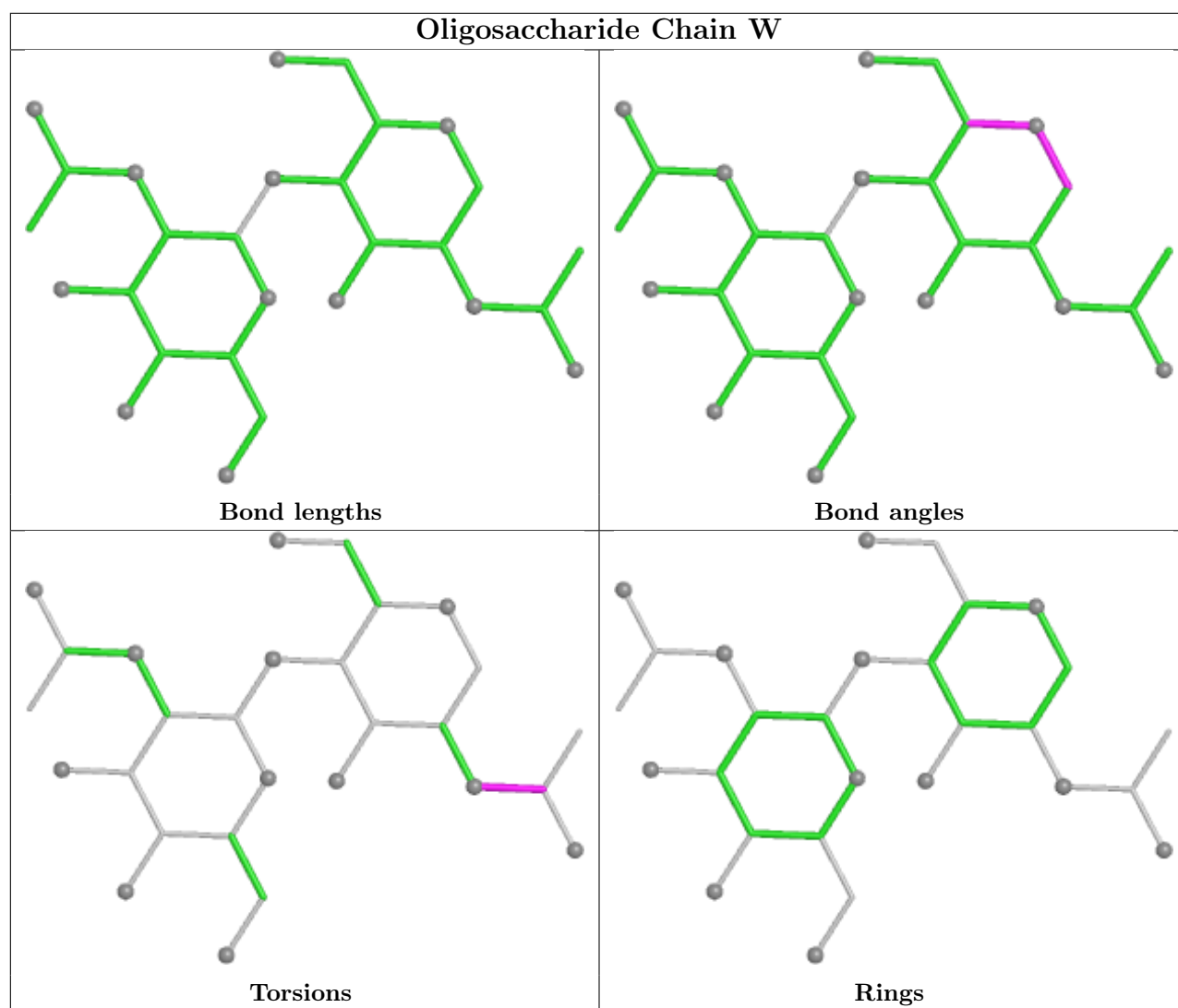


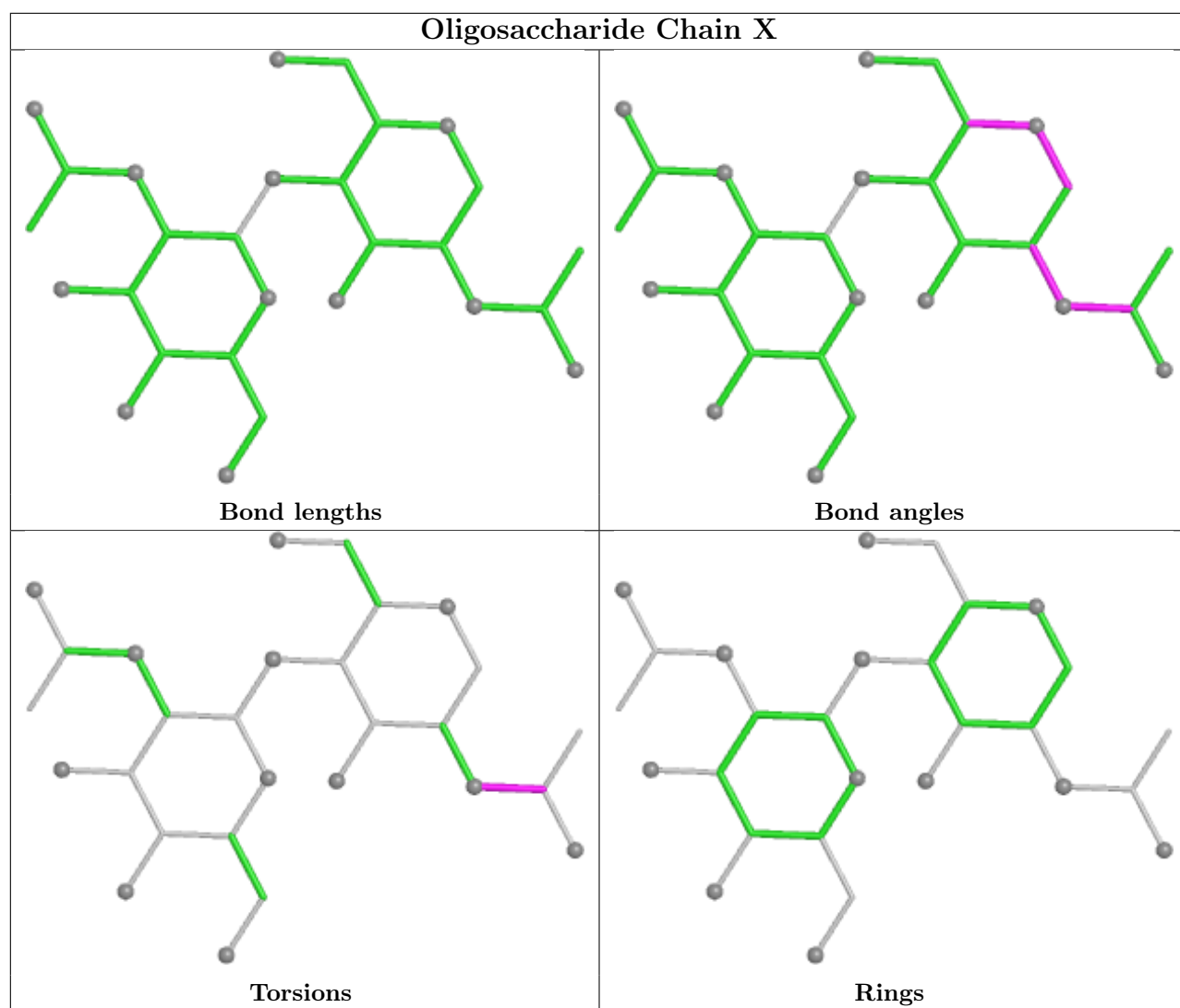


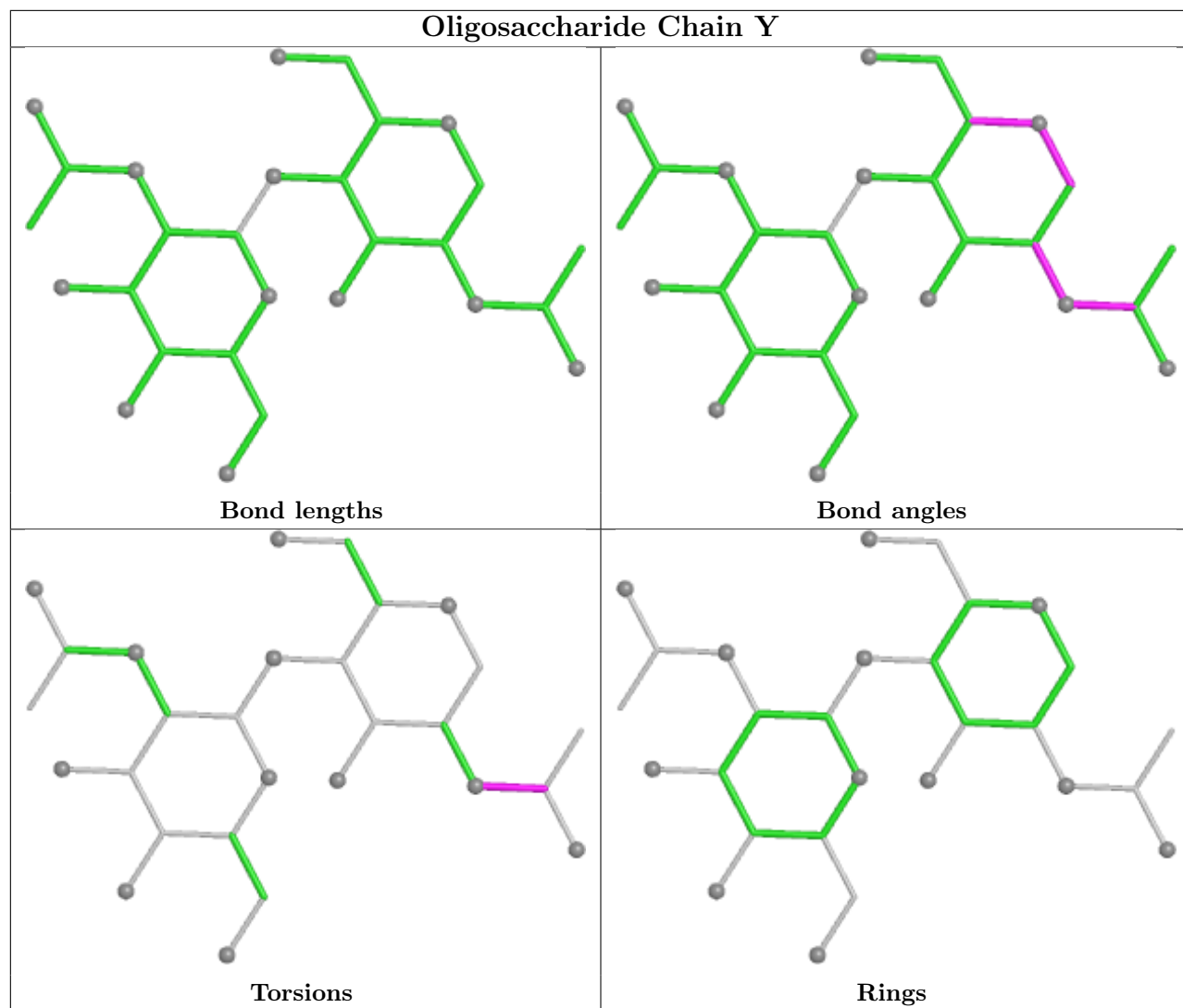


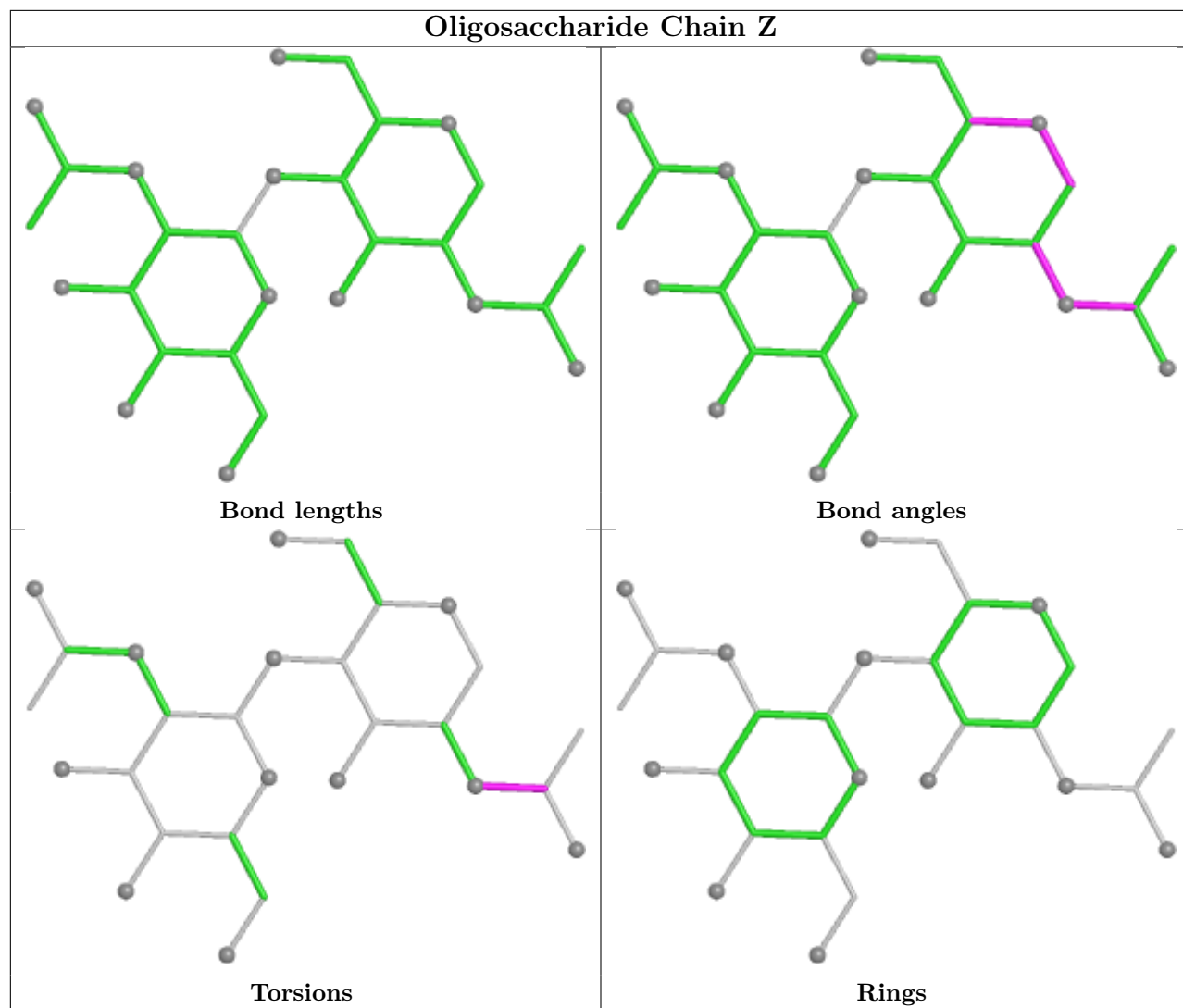


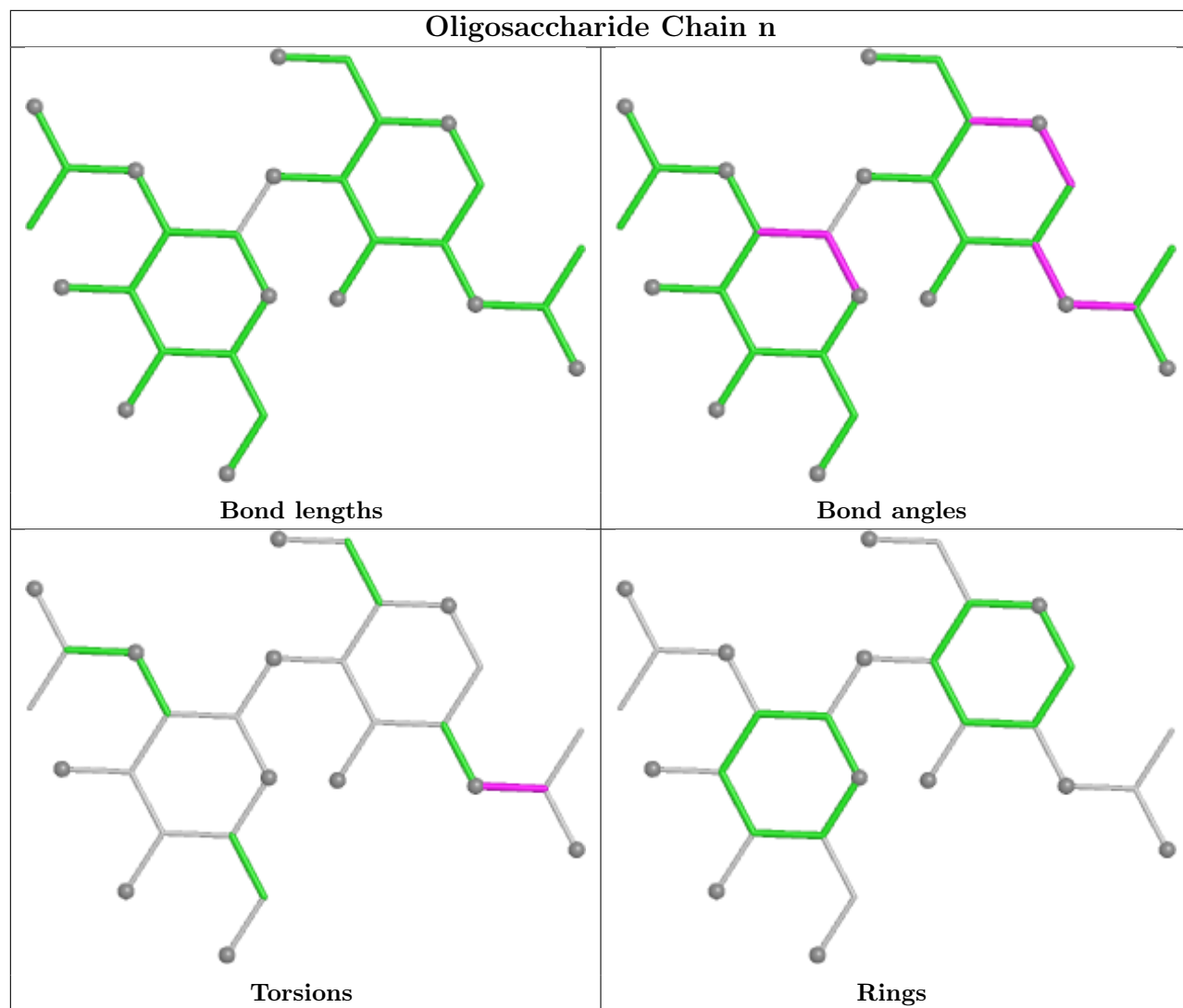


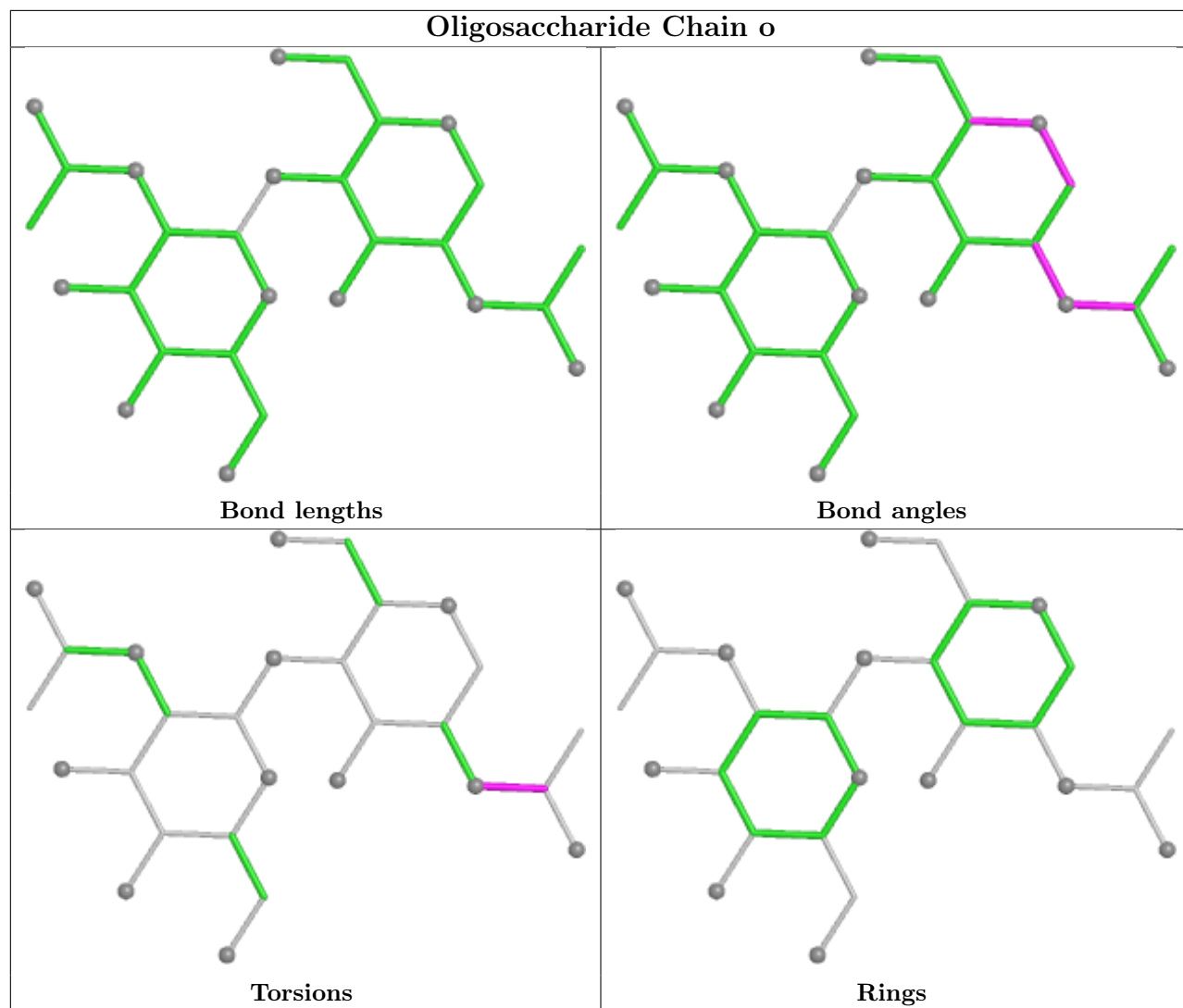


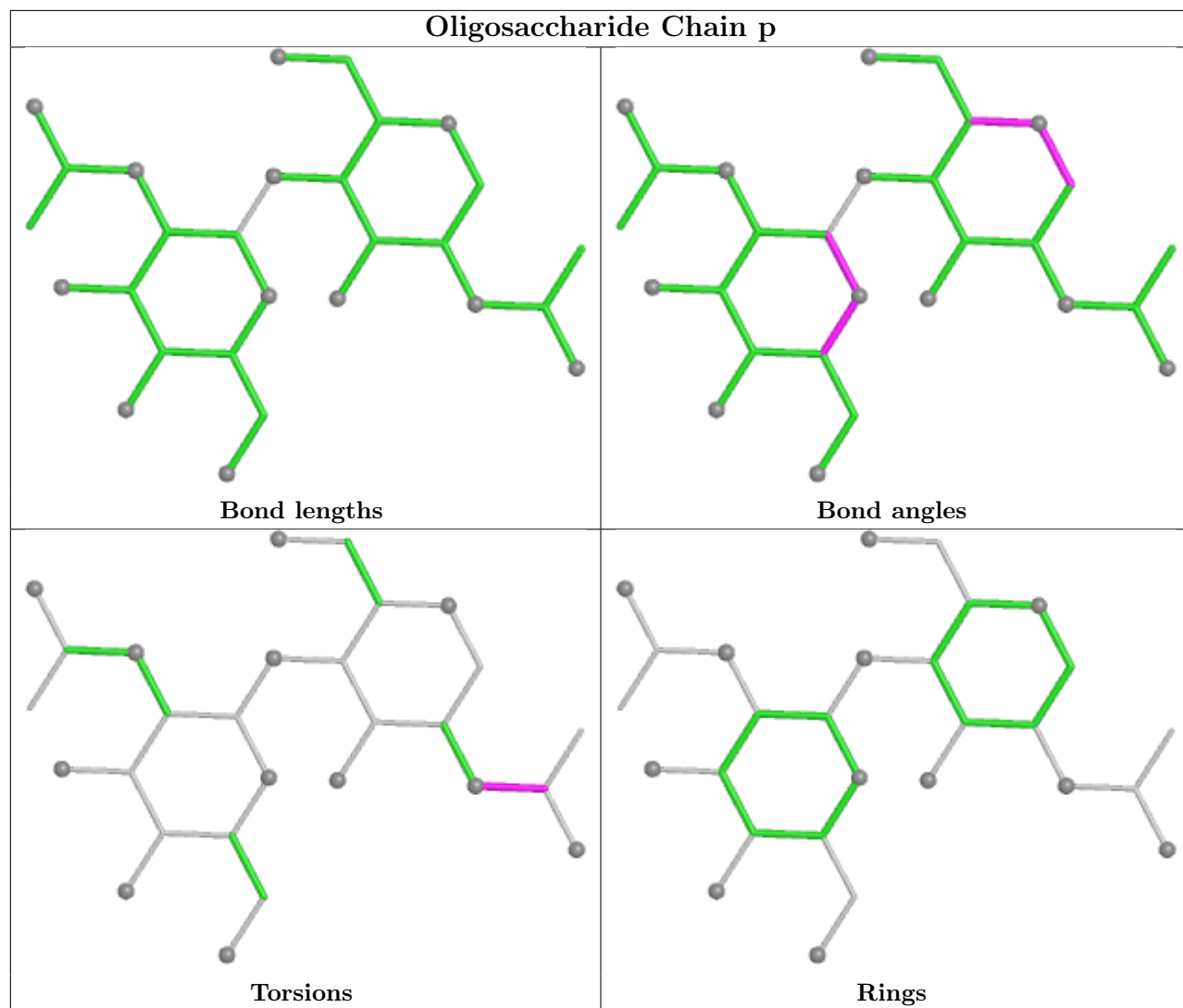


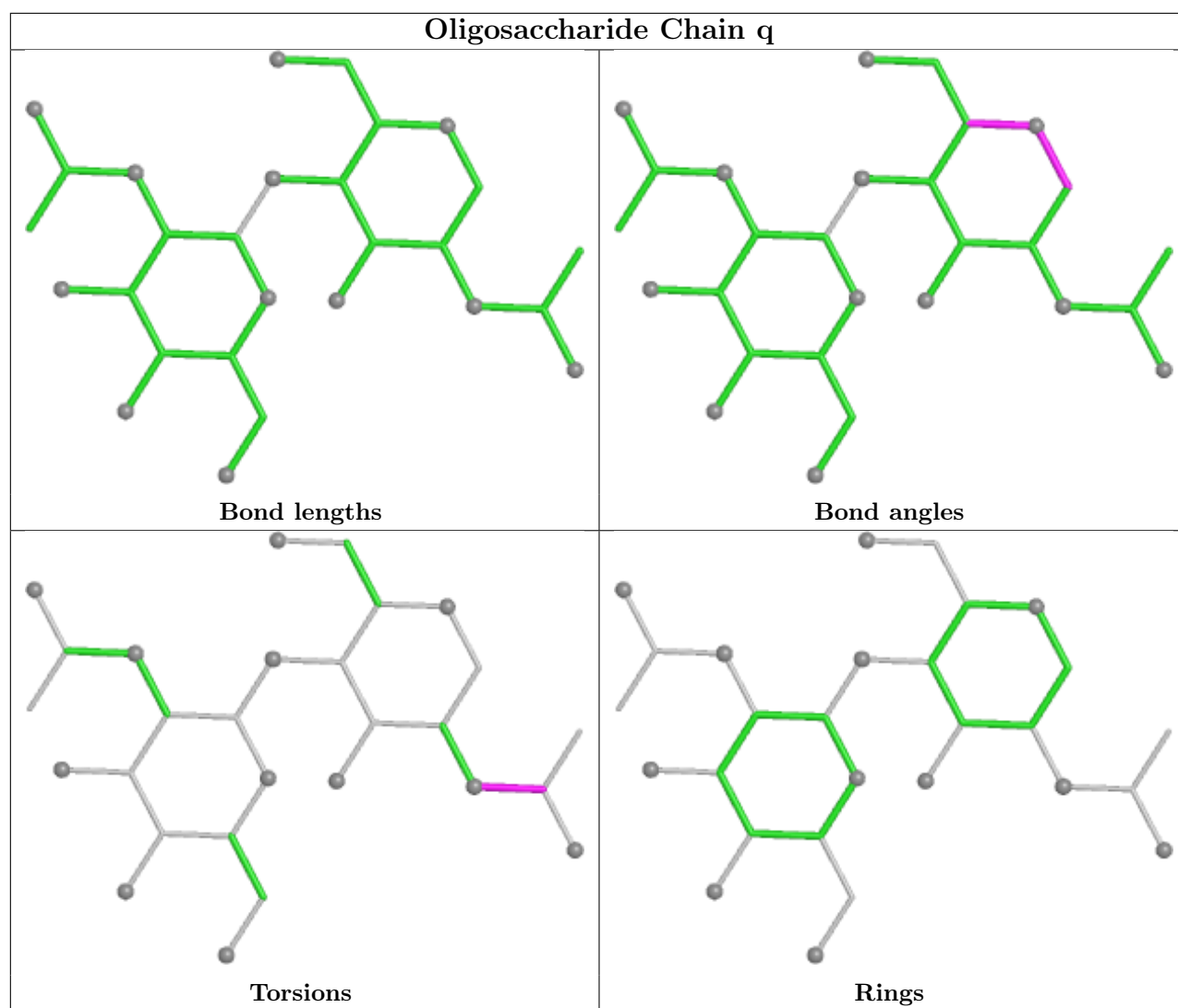


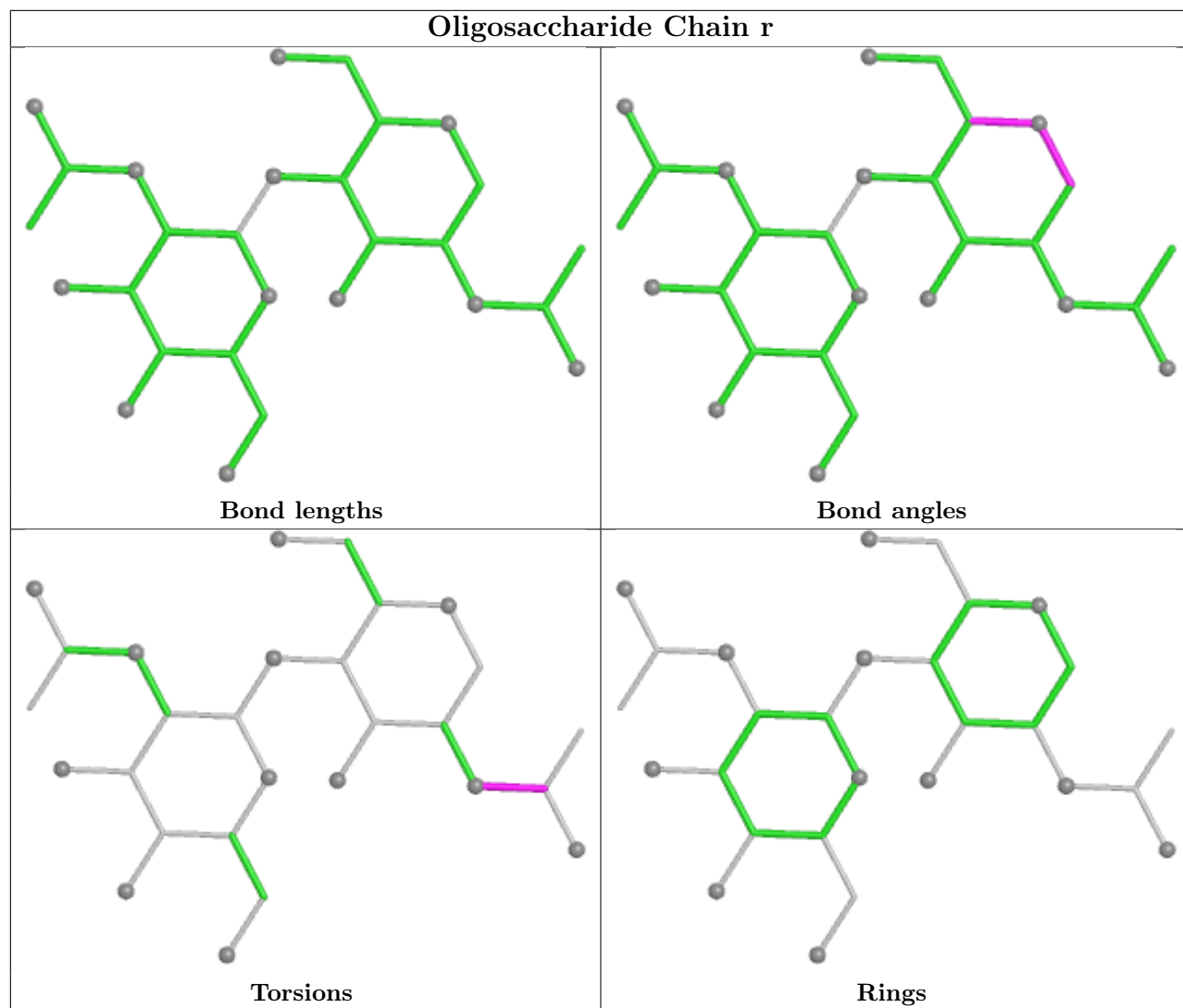


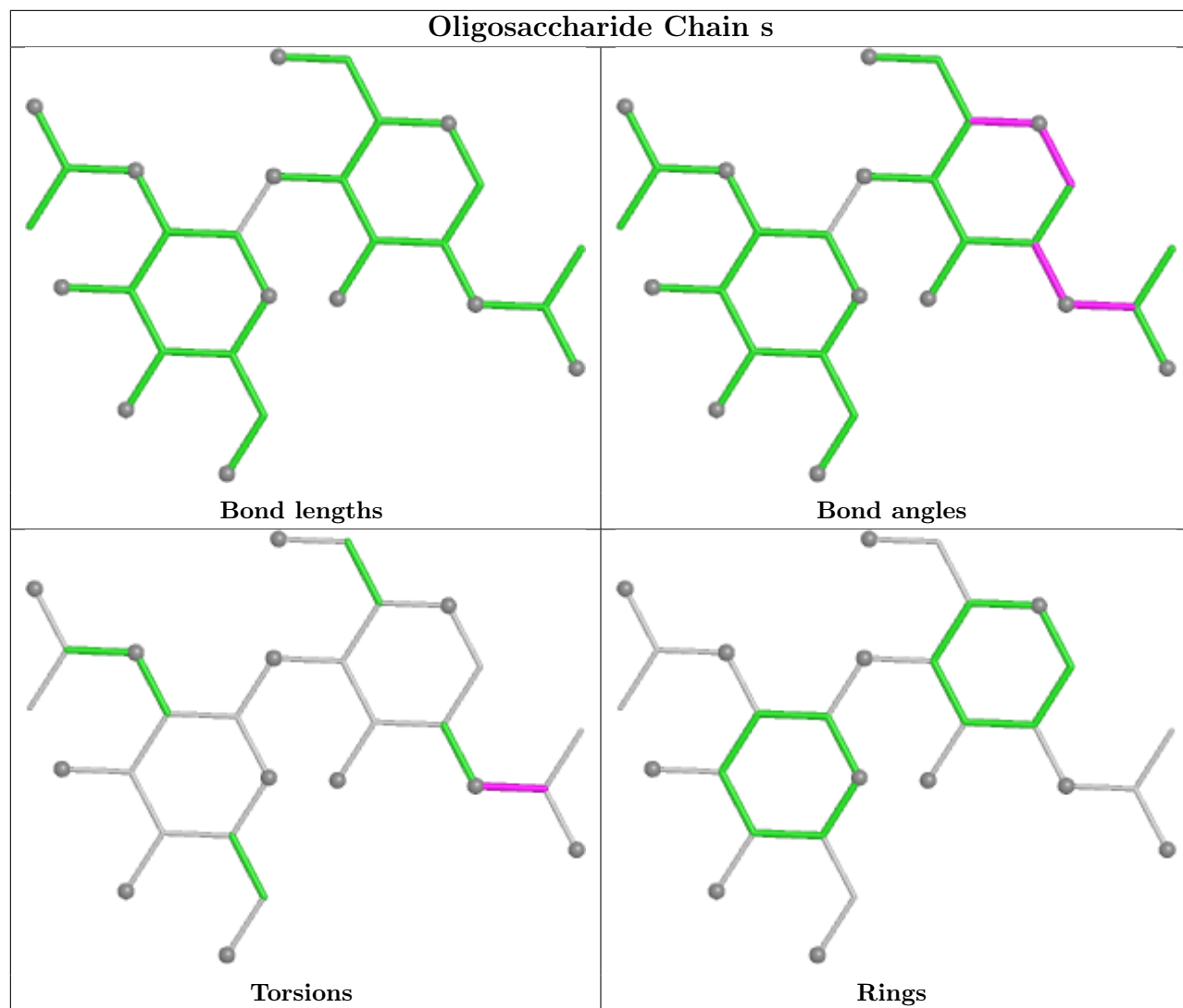


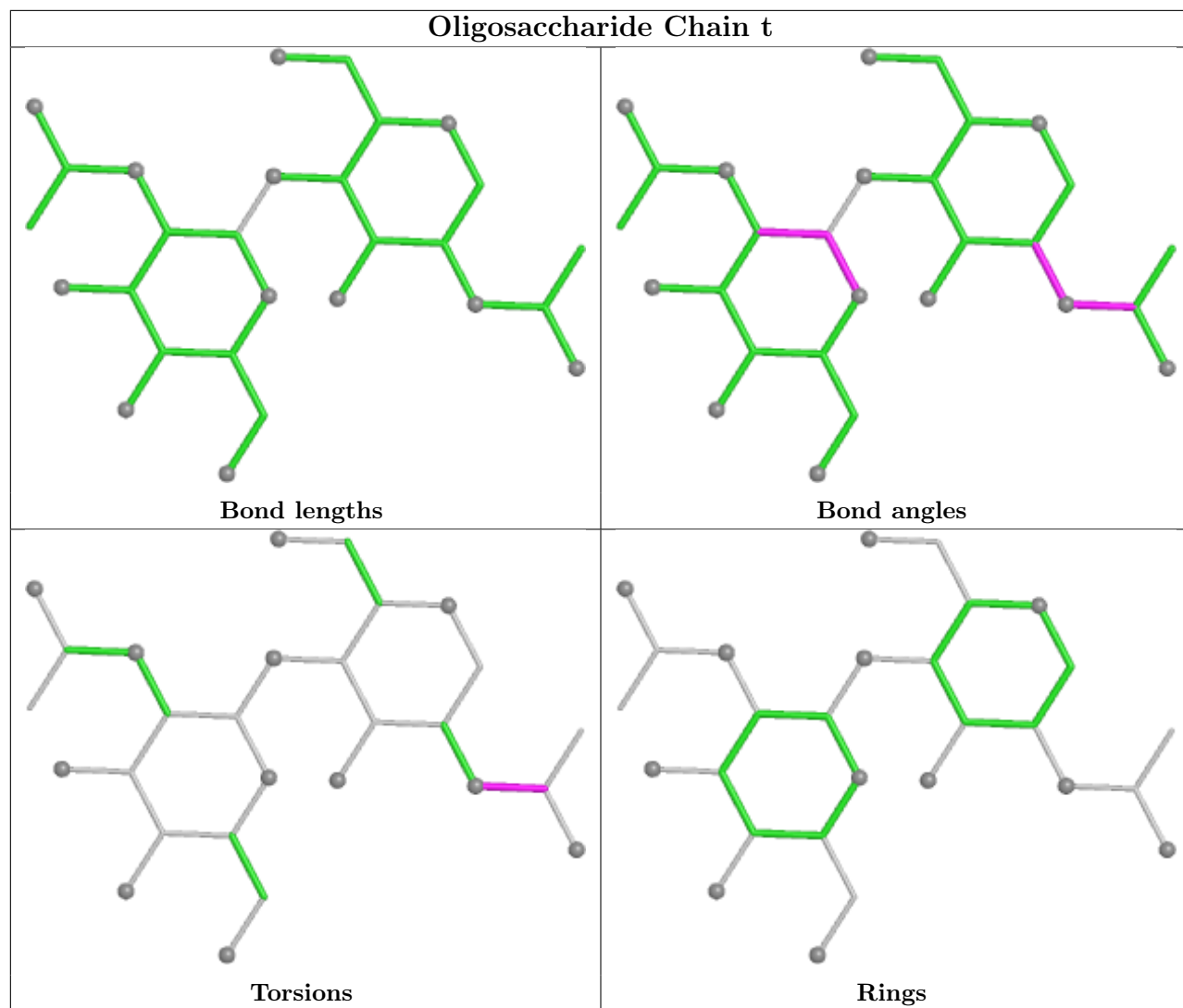


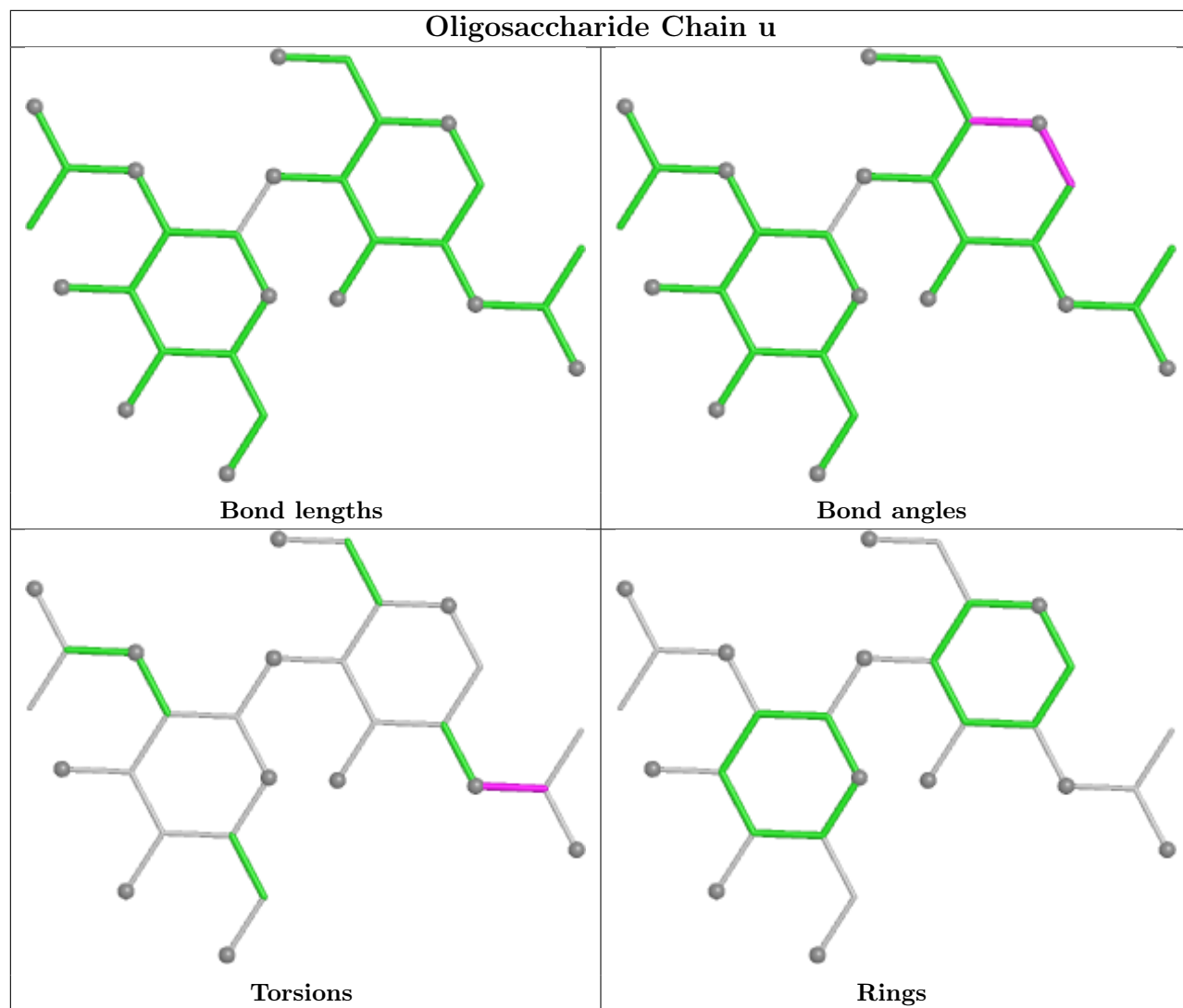


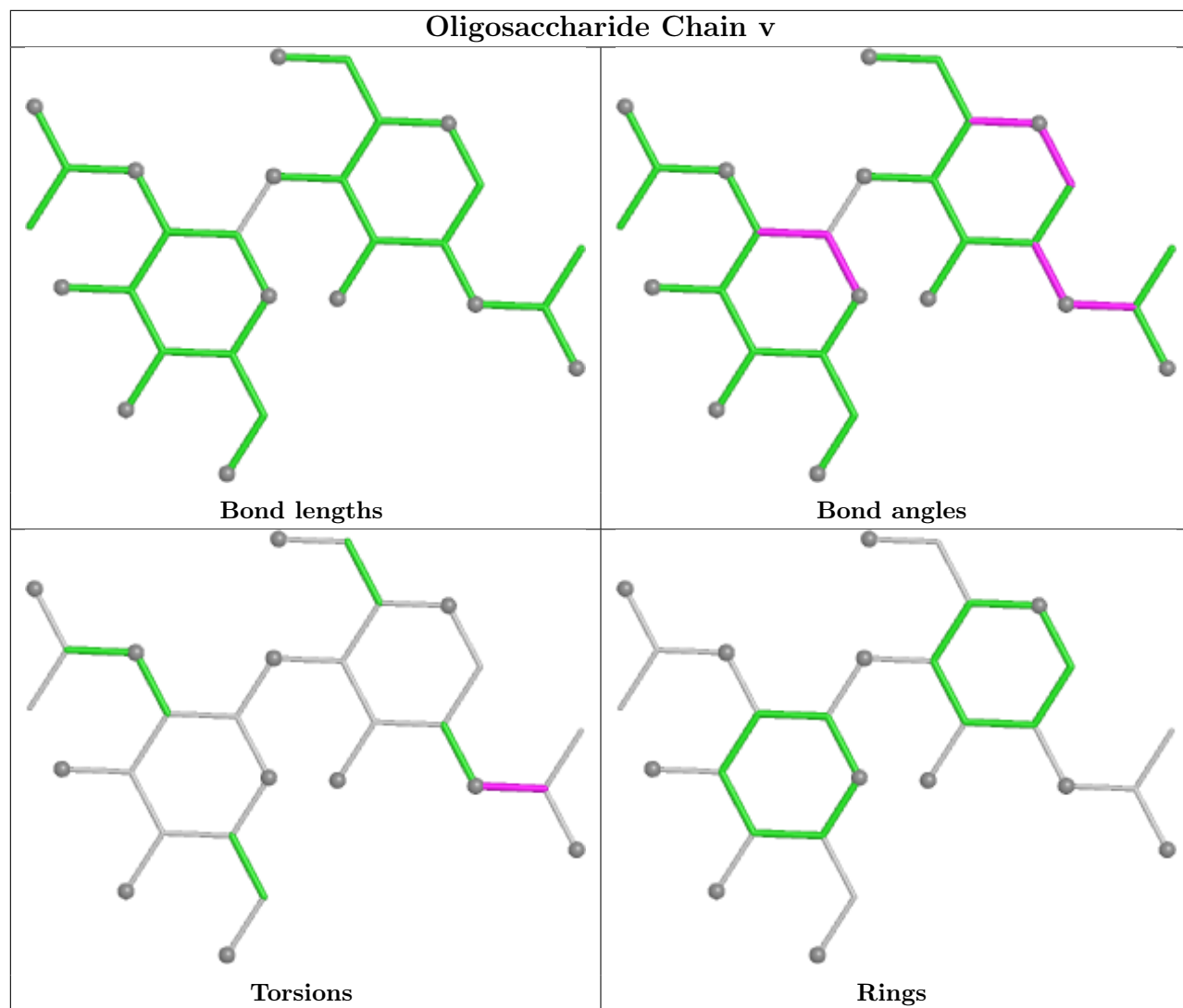


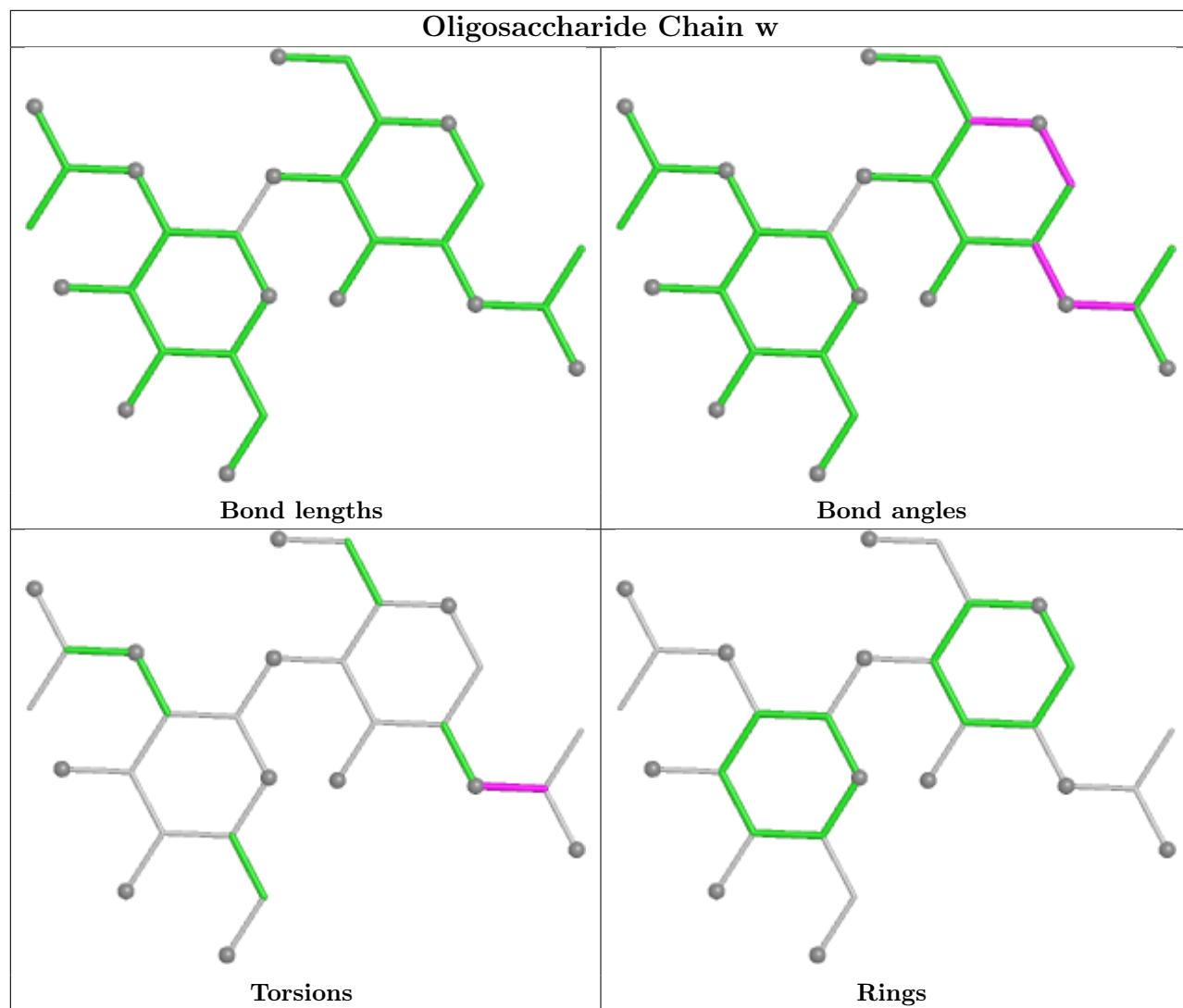


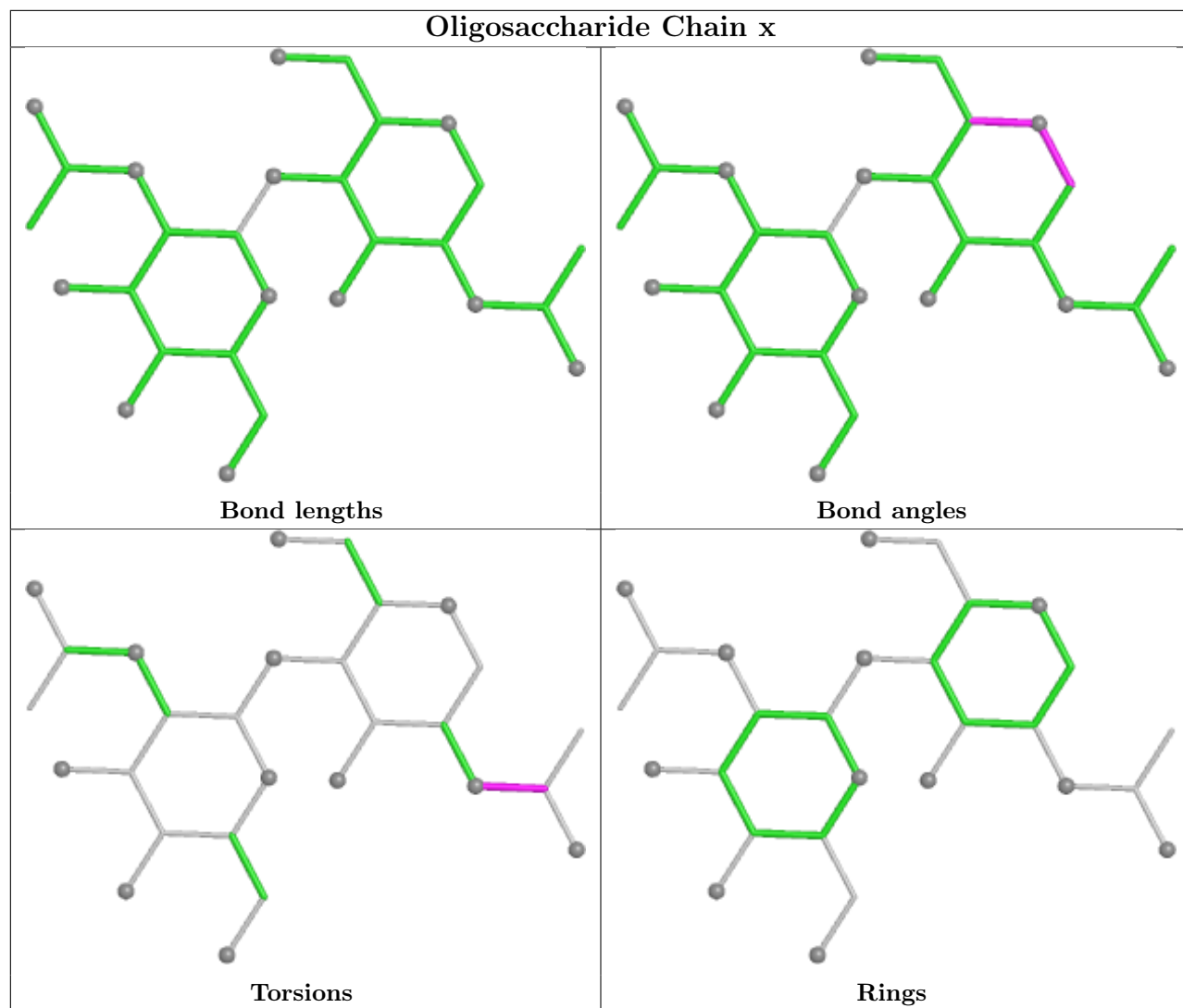


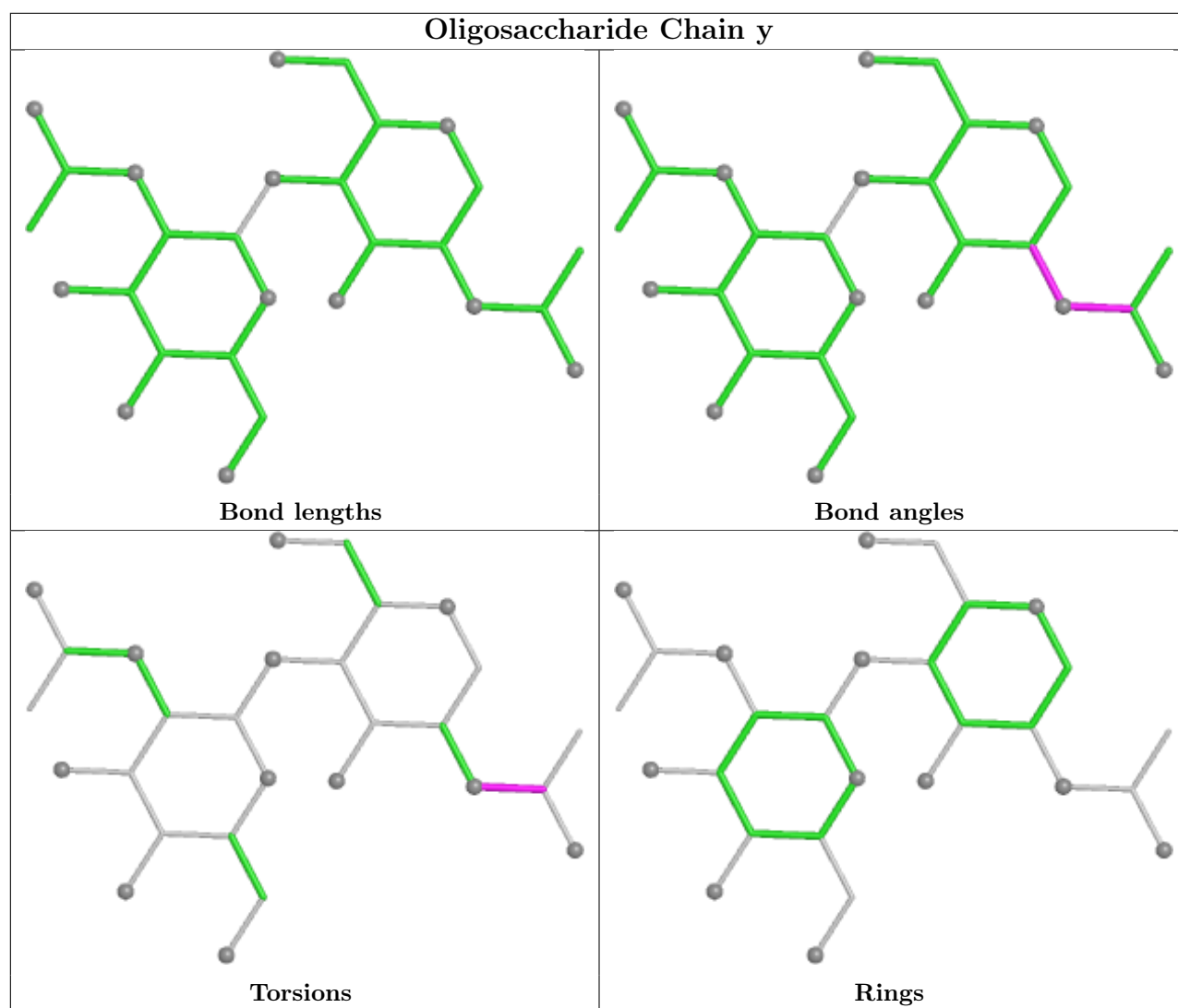


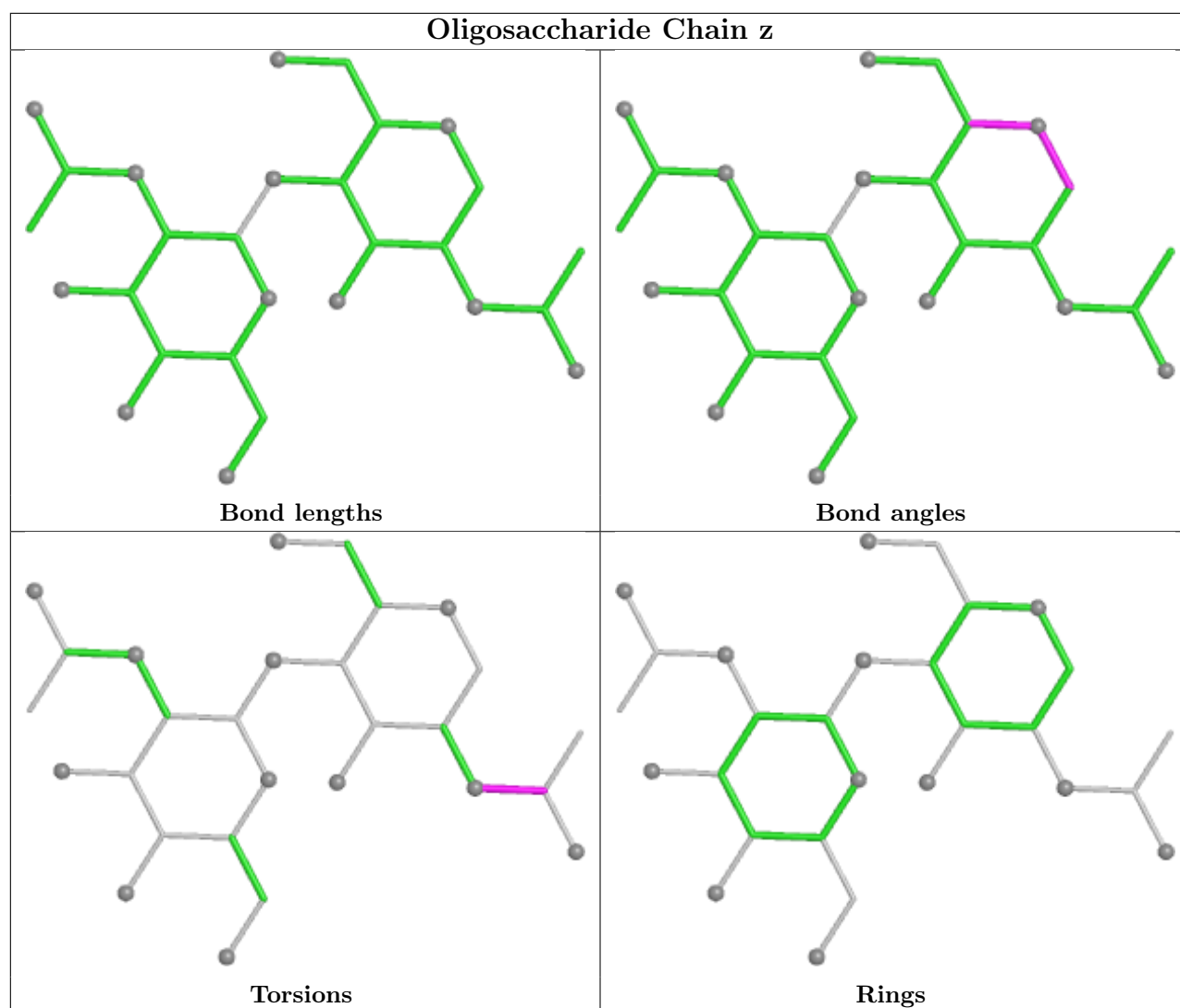












5.6 Ligand geometry [i](#)

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.