



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:11 PM UTC

PDB ID : 6ORN / pdb_00006orn
EMDB ID : EMD-20175
Title : Modified BG505 SOSIP-based immunogen RC1 in complex with the elicited V3-glycan patch bNAb 10-1074
Authors : Abernathy, M.E.; Gristick, H.B.; Bjorkman, P.J.
Deposited on : 2019-04-30
Resolution : 4.05 Å(reported)
Based on initial model : 5T3Z

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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

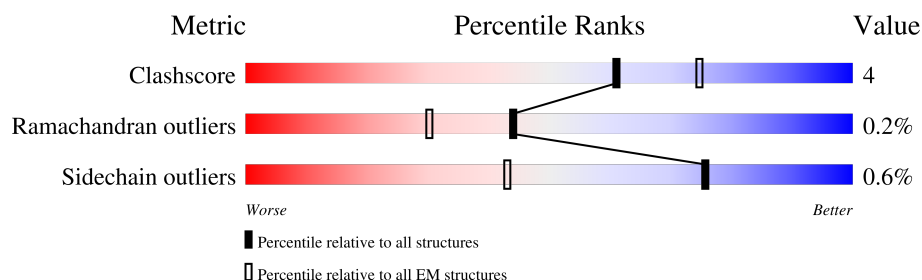
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.05 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.



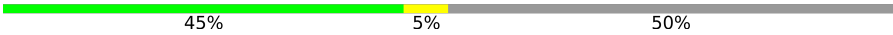
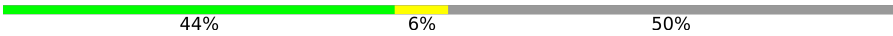
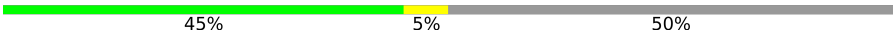
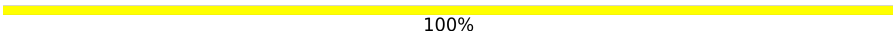
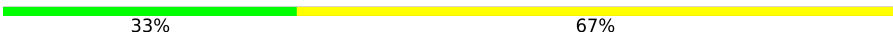
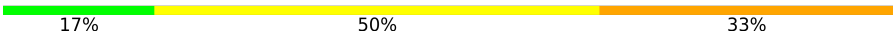
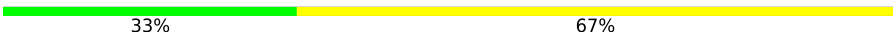
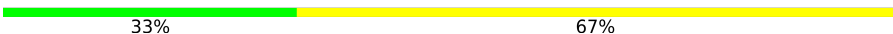
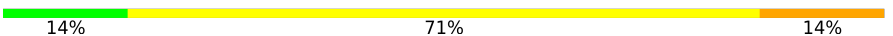
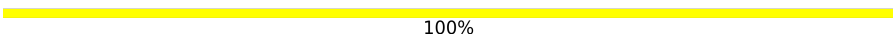
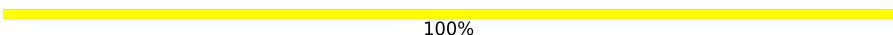
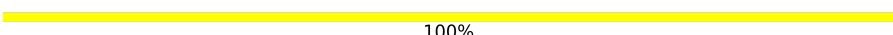
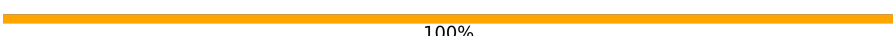
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	C	153	
1	J	153	
1	Q	153	
2	G	481	
2	K	481	
2	R	481	
3	A	238	
3	F	238	
3	O	238	

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Mol	Chain	Length	Quality of chain
4	B	214	
4	I	214	
4	P	214	
5	D	6	
5	W	6	
5	b	6	
6	E	3	
6	L	3	
6	V	3	
7	H	7	
7	U	7	
8	M	2	
8	N	2	
8	S	2	
8	T	2	
8	X	2	
8	Y	2	
8	Z	2	
8	a	2	
8	c	2	
8	d	2	
8	f	2	
8	g	2	
9	e	6	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 20338 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 RC1 variant of HIV-1 Env glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	124	Total	C	N	O	S	0	0
			987	622	171	188	6		
1	J	124	Total	C	N	O	S	0	0
			987	622	171	188	6		
1	Q	124	Total	C	N	O	S	0	0
			987	622	171	188	6		

- Molecule 2 is a protein called RC1 variant of HIV-1 Env glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	442	Total	C	N	O	S	0	0
			3485	2199	612	646	28		
2	K	442	Total	C	N	O	S	0	0
			3485	2199	612	646	28		
2	R	442	Total	C	N	O	S	0	0
			3485	2199	612	646	28		

- Molecule 3 is a protein called 10-1074 antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		
3	F	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		
3	O	133	Total	C	N	O	S	0	0
			1041	657	175	205	4		

- Molecule 4 is a protein called 10-1074 antibody Fab light chain.

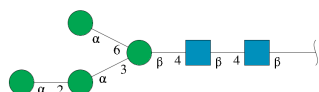
Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	107	Total	C	N	O	S	0	0
			824	515	152	154	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	107	Total	C	N	O	S	0	0
			824	515	152	154	3		
4	P	107	Total	C	N	O	S	0	0
			824	515	152	154	3		

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



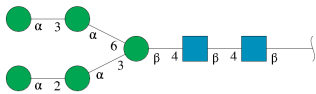
Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	6	Total	C	N	O		0	0
			72	40	2	30			
5	W	6	Total	C	N	O		0	0
			72	40	2	30			
5	b	6	Total	C	N	O		0	0
			72	40	2	30			

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



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

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	7	Total	C	N	O	0	0
			83	46	2	35		
7	U	7	Total	C	N	O	0	0
			83	46	2	35		

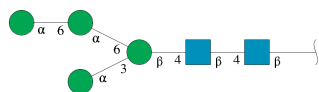
- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	M	2	Total	C	N	O	0	0
			28	16	2	10		
8	N	2	Total	C	N	O	0	0
			28	16	2	10		
8	S	2	Total	C	N	O	0	0
			28	16	2	10		
8	T	2	Total	C	N	O	0	0
			28	16	2	10		
8	X	2	Total	C	N	O	0	0
			28	16	2	10		
8	Y	2	Total	C	N	O	0	0
			28	16	2	10		
8	Z	2	Total	C	N	O	0	0
			28	16	2	10		
8	a	2	Total	C	N	O	0	0
			28	16	2	10		
8	c	2	Total	C	N	O	0	0
			28	16	2	10		
8	d	2	Total	C	N	O	0	0
			28	16	2	10		
8	f	2	Total	C	N	O	0	0
			28	16	2	10		
8	g	2	Total	C	N	O	0	0
			28	16	2	10		

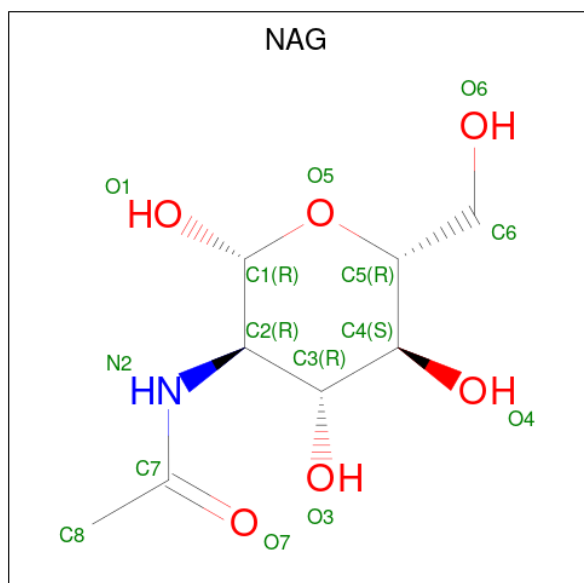
- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyran

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



Mol	Chain	Residues	Atoms				AltConf	Trace
9	e	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				AltConf
10	G	1	Total 14	C 8	N 1	O 5	0
10	G	1	Total 14	C 8	N 1	O 5	0
10	G	1	Total 14	C 8	N 1	O 5	0
10	G	1	Total 14	C 8	N 1	O 5	0
10	G	1	Total 14	C 8	N 1	O 5	0
10	J	1	Total 14	C 8	N 1	O 5	0
10	J	1	Total 14	C 8	N 1	O 5	0
10	J	1	Total 14	C 8	N 1	O 5	0
10	K	1	Total 14	C 8	N 1	O 5	0
10	K	1	Total 14	C 8	N 1	O 5	0
10	K	1	Total 14	C 8	N 1	O 5	0
10	K	1	Total 14	C 8	N 1	O 5	0
10	K	1	Total 14	C 8	N 1	O 5	0
10	K	1	Total 14	C 8	N 1	O 5	0
10	K	1	Total 14	C 8	N 1	O 5	0
10	K	1	Total 14	C 8	N 1	O 5	0
10	Q	1	Total 14	C 8	N 1	O 5	0
10	Q	1	Total 14	C 8	N 1	O 5	0
10	Q	1	Total 14	C 8	N 1	O 5	0
10	R	1	Total 14	C 8	N 1	O 5	0
10	R	1	Total 14	C 8	N 1	O 5	0
10	R	1	Total 14	C 8	N 1	O 5	0

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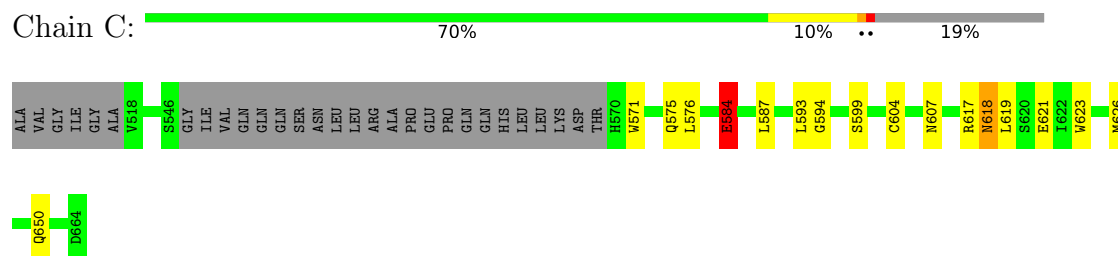
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Mol	Chain	Residues	Atoms				AltConf
10	R	1	Total	C	N	O	0
			14	8	1	5	
10	R	1	Total	C	N	O	0
			14	8	1	5	

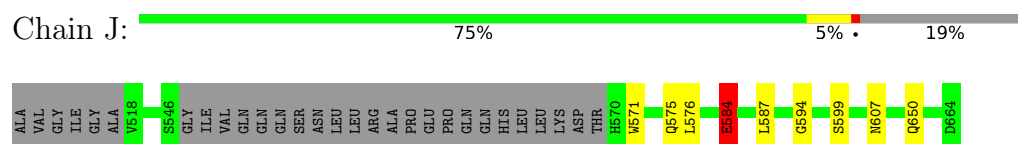
3 Residue-property plots [i](#)

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.

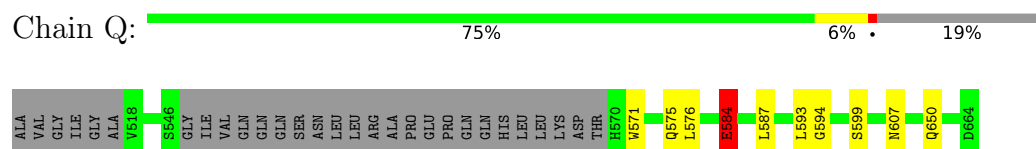
- Molecule 1: RC1 variant of HIV-1 Env glycoprotein gp41



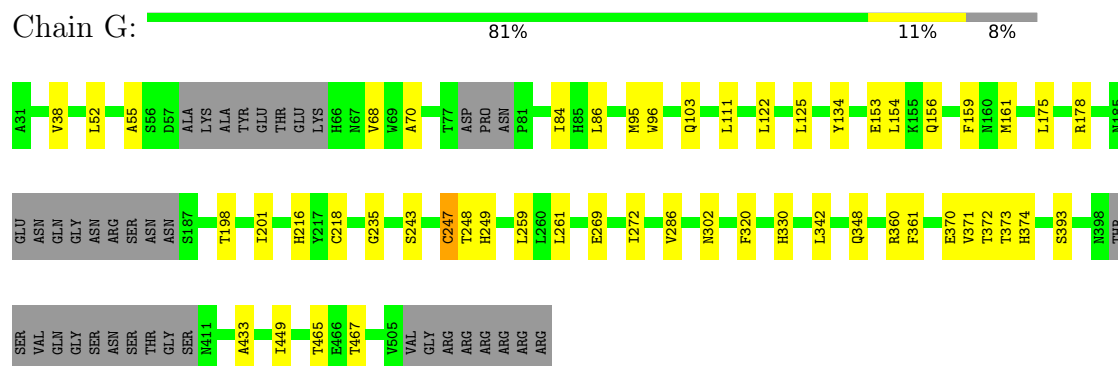
- Molecule 1: RC1 variant of HIV-1 Env glycoprotein gp41



- Molecule 1: RC1 variant of HIV-1 Env glycoprotein gp41

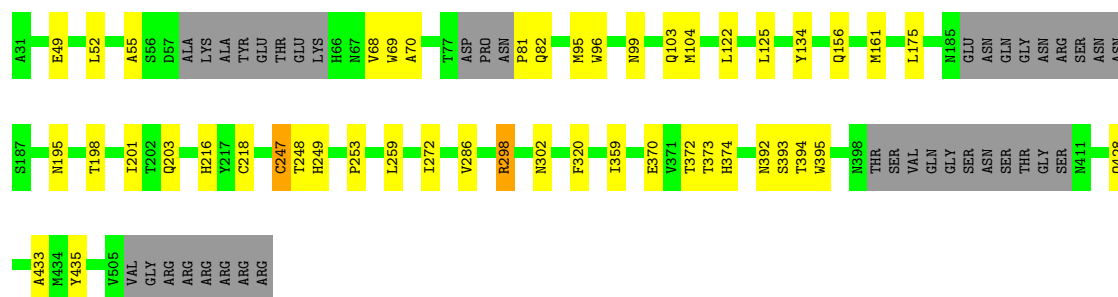


- Molecule 2: RC1 variant of HIV-1 Env glycoprotein gp120



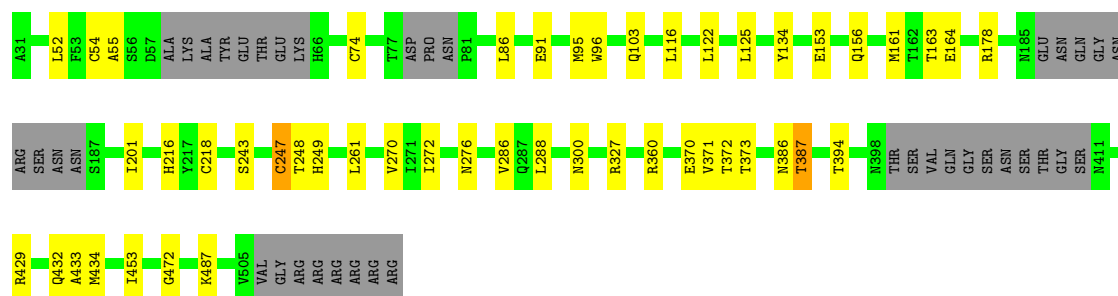
- Molecule 2: RC1 variant of HIV-1 Env glycoprotein gp120

Chain K: 

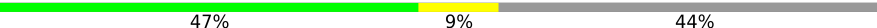


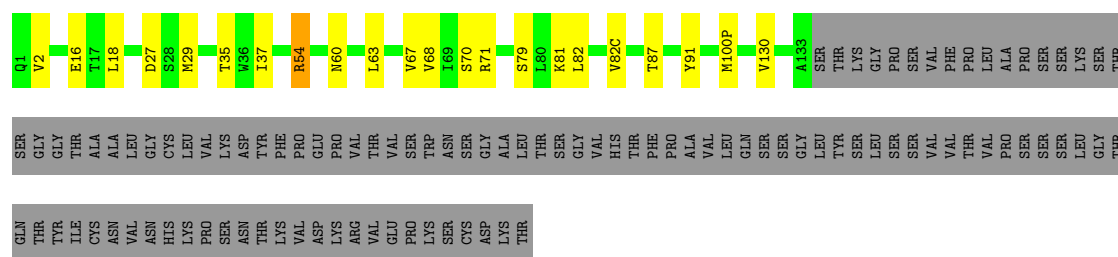
- Molecule 2: RC1 variant of HIV-1 Env glycoprotein gp120

Chain R: 

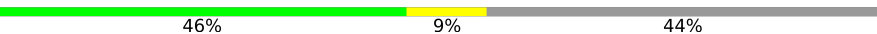


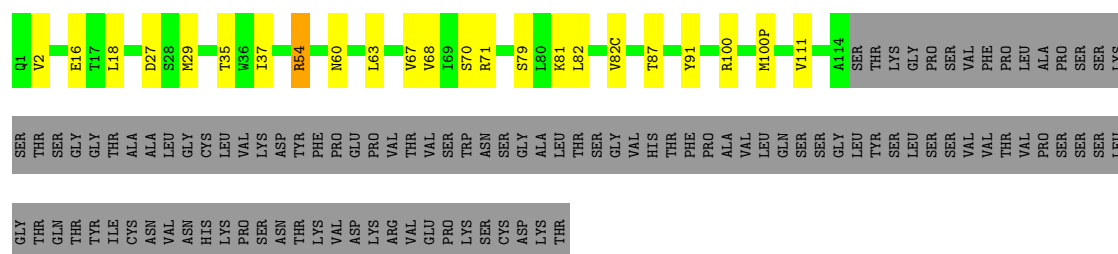
- Molecule 3: 10-1074 antibody Fab heavy chain

Chain A: 

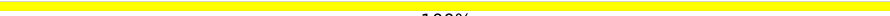


- Molecule 3: 10-1074 antibody Fab heavy chain

Chain F: 



- Molecule 3: 10-1074 antibody Fab heavy chain

Chain D:  100%

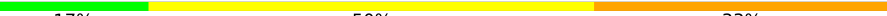
NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  33% 67%

NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  17% 50% 33%

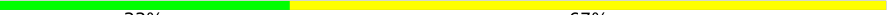
NAG1
NAG2
BMA3
MAN4
MAN5
MAN6

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

Chain E:  67% 33%

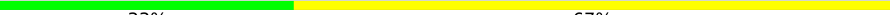
NAG1
NAG2
BMA3

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

Chain L:  33% 67%

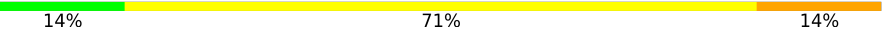
NAG1
NAG2
BMA3

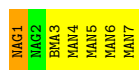
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  33% 67%

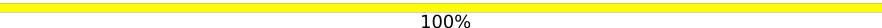
NAG1
NAG2
BMA3

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

Chain H:  14% 71% 14%

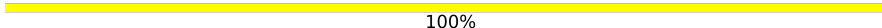


- Molecule 7: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-3)- α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain U:  100%



- Molecule 8: 2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain M:  100%



- Molecule 8: 2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain N:  50% 50%



- Molecule 8: 2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain S:  50% 50%



- Molecule 8: 2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain T:  50% 50%



- Molecule 8: 2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain X:  50% 50%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  50% 50%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  50% 50%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:  50% 50%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:  100%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:  50% 50%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  50% 50%

 MAG1
MAG2

- Molecule 9: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:  17% 50% 33%

 MAG1
MAG2
MAN3
MAN4
MAN5
MAN6

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	122013	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3400	Depositor
Magnification	73000	Depositor
Image detector	FEI FALCON III (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, BMA, MAN

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	C	0.33	0/1006	0.73	3/1365 (0.2%)
1	J	0.31	0/1006	0.59	2/1365 (0.1%)
1	Q	0.31	0/1006	0.59	2/1365 (0.1%)
2	G	0.33	0/3558	0.65	1/4827 (0.0%)
2	K	0.32	0/3558	0.62	0/4827
2	R	0.32	0/3558	0.60	0/4827
3	A	0.26	0/1066	0.53	1/1451 (0.1%)
3	F	0.26	0/1066	0.53	1/1451 (0.1%)
3	O	0.26	0/1066	0.53	1/1451 (0.1%)
4	B	0.26	0/845	0.53	0/1148
4	I	0.26	0/845	0.53	0/1148
4	P	0.26	0/845	0.53	0/1148
All	All	0.30	0/19425	0.60	11/26373 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	1
2	K	0	2
2	R	0	3
All	All	0	6

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	618	ASN	CB-CA-C	-11.22	88.82	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	302	ASN	N-CA-C	5.87	117.78	110.91
1	C	584	GLU	CA-CB-CG	5.62	125.34	114.10
1	Q	584	GLU	CA-CB-CG	5.61	125.31	114.10
1	J	584	GLU	CA-CB-CG	5.60	125.31	114.10
1	J	584	GLU	CB-CG-CD	5.53	122.00	112.60
1	C	584	GLU	CB-CG-CD	5.53	122.00	112.60
1	Q	584	GLU	CB-CG-CD	5.52	121.99	112.60
3	A	54	ARG	CG-CD-NE	5.39	123.85	112.00
3	F	54	ARG	CG-CD-NE	5.37	123.81	112.00
3	O	54	ARG	CG-CD-NE	5.36	123.79	112.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	261	LEU	Peptide
2	K	298	ARG	Peptide
2	K	392	ASN	Peptide
2	R	261	LEU	Peptide
2	R	386	ASN	Peptide
2	R	387	THR	Peptide

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	C	987	0	953	20	0
1	J	987	0	953	6	0
1	Q	987	0	953	7	0
2	G	3485	0	3435	30	0
2	K	3485	0	3435	25	0
2	R	3485	0	3434	26	0
3	A	1041	0	1005	11	0
3	F	1041	0	1005	13	0
3	O	1041	0	1005	12	0
4	B	824	0	788	7	0
4	I	824	0	788	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	824	0	788	7	0
5	D	72	0	61	0	0
5	W	72	0	61	0	0
5	b	72	0	61	1	0
6	E	39	0	34	0	0
6	L	39	0	34	0	0
6	V	39	0	34	0	0
7	H	83	0	70	1	0
7	U	83	0	70	0	0
8	M	28	0	25	0	0
8	N	28	0	25	0	0
8	S	28	0	25	0	0
8	T	28	0	25	0	0
8	X	28	0	25	0	0
8	Y	28	0	25	0	0
8	Z	28	0	25	0	0
8	a	28	0	25	0	0
8	c	28	0	25	1	0
8	d	28	0	25	1	0
8	f	28	0	25	0	0
8	g	28	0	25	0	0
9	e	72	0	61	1	0
10	C	42	0	39	4	0
10	G	126	0	117	1	0
10	J	42	0	39	0	0
10	K	98	0	91	0	0
10	Q	42	0	39	0	0
10	R	70	0	65	0	0
All	All	20338	0	19718	175	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 (175) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:618:ASN:HB2	1:C:621:GLU:HG2	1.32	1.09
10:C:702:NAG:H82	10:C:702:NAG:H3	1.39	1.02
1:C:617:ARG:NH1	1:C:626:MET:HE1	1.89	0.88
1:C:618:ASN:CB	1:C:621:GLU:HG2	2.17	0.72
1:C:618:ASN:HB2	1:C:621:GLU:CG	2.19	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:55:ALA:HB3	2:R:216:HIS:HB2	1.75	0.69
2:K:55:ALA:HB3	2:K:216:HIS:HB2	1.76	0.68
2:G:55:ALA:HB3	2:G:216:HIS:HB2	1.76	0.67
2:R:52:LEU:H	2:R:103:GLN:HE22	1.43	0.66
10:C:702:NAG:H82	10:C:702:NAG:C3	2.21	0.66
2:K:52:LEU:H	2:K:103:GLN:HE22	1.44	0.66
2:R:300:ASN:HD21	2:R:327:ARG:H	1.45	0.65
2:R:453:ILE:HD12	2:R:472:GLY:HA3	1.76	0.65
2:R:370:GLU:HG3	2:R:371:VAL:HG23	1.79	0.65
1:C:571:TRP:O	1:C:575:GLN:NE2	2.30	0.64
2:G:370:GLU:HG3	2:G:371:VAL:HG23	1.79	0.64
1:J:571:TRP:O	1:J:575:GLN:NE2	2.30	0.64
1:Q:571:TRP:O	1:Q:575:GLN:NE2	2.30	0.64
1:C:617:ARG:CZ	1:C:626:MET:HE1	2.28	0.63
1:C:617:ARG:NH1	1:C:626:MET:CE	2.61	0.63
2:R:116:LEU:HD11	2:R:434:MET:HE2	1.80	0.62
2:G:52:LEU:H	2:G:103:GLN:HE22	1.46	0.62
1:C:618:ASN:HB2	1:C:621:GLU:H	1.64	0.61
3:A:37:ILE:HB	3:A:91:TYR:HB2	1.83	0.61
3:F:37:ILE:HB	3:F:91:TYR:HB2	1.83	0.61
3:O:87:THR:HG22	3:O:111:VAL:H	1.66	0.61
3:O:37:ILE:HB	3:O:91:TYR:HB2	1.83	0.61
3:A:87:THR:HG22	3:A:130:VAL:H	1.66	0.60
1:J:607:ASN:OD1	1:J:650:GLN:NE2	2.34	0.60
3:F:87:THR:HG22	3:F:111:VAL:H	1.66	0.60
1:C:607:ASN:OD1	1:C:650:GLN:NE2	2.34	0.59
1:Q:607:ASN:OD1	1:Q:650:GLN:NE2	2.35	0.59
2:R:360:ARG:HG3	2:R:394:THR:HG22	1.85	0.58
3:A:67:VAL:HG12	3:A:82:LEU:HG	1.85	0.58
3:F:67:VAL:HG12	3:F:82:LEU:HG	1.85	0.57
2:G:125:LEU:HA	2:G:161:MET:HE1	1.87	0.57
3:F:68:VAL:HB	3:F:81:LYS:HB2	1.86	0.57
3:O:67:VAL:HG12	3:O:82:LEU:HG	1.85	0.57
2:G:330:HIS:NE2	7:H:1:NAG:O7	2.34	0.57
3:A:68:VAL:HB	3:A:81:LYS:HB2	1.86	0.56
3:O:68:VAL:HB	3:O:81:LYS:HB2	1.86	0.56
1:J:584:GLU:HA	1:J:587:LEU:HB2	1.88	0.56
2:R:95:MET:HG3	2:R:96:TRP:HD1	1.70	0.56
2:R:201:ILE:HG22	2:R:433:ALA:HB3	1.88	0.55
1:C:584:GLU:N	1:C:584:GLU:OE1	2.39	0.55
2:G:95:MET:HG3	2:G:96:TRP:HD1	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:20:ARG:HG2	4:B:74:THR:HG22	1.89	0.54
1:C:584:GLU:HA	1:C:587:LEU:HB2	1.88	0.54
1:Q:584:GLU:HA	1:Q:587:LEU:HB2	1.88	0.54
2:K:201:ILE:HG22	2:K:433:ALA:HB3	1.88	0.54
2:R:272:ILE:HG22	2:R:286:VAL:HG12	1.90	0.53
4:I:20:ARG:HG2	4:I:74:THR:HG22	1.89	0.53
4:P:20:ARG:HG2	4:P:74:THR:HG22	1.89	0.53
1:J:584:GLU:OE1	1:J:584:GLU:N	2.39	0.52
2:G:68:VAL:HG23	2:G:70:ALA:H	1.74	0.52
2:G:134:TYR:HB2	2:G:156:GLN:HB2	1.92	0.52
2:G:218:CYS:HA	2:G:247:CYS:HB3	1.91	0.52
2:G:70:ALA:HA	2:G:111:LEU:HD21	1.91	0.52
2:G:272:ILE:HG22	2:G:286:VAL:HG12	1.90	0.52
10:C:702:NAG:H3	10:C:702:NAG:C8	2.16	0.51
1:C:618:ASN:OD1	1:C:621:GLU:CD	2.52	0.51
2:K:134:TYR:HB2	2:K:156:GLN:HB2	1.92	0.51
1:Q:584:GLU:N	1:Q:584:GLU:OE1	2.39	0.51
2:R:218:CYS:HA	2:R:247:CYS:HB3	1.91	0.51
2:K:298:ARG:HH12	2:K:302:ASN:ND2	2.09	0.51
2:R:125:LEU:HA	2:R:161:MET:HE1	1.93	0.51
2:R:122:LEU:HD21	2:R:125:LEU:HD13	1.92	0.51
2:G:248:THR:OG1	2:G:249:HIS:N	2.44	0.51
3:F:100:ARG:NH1	4:I:31:ARG:O	2.44	0.51
1:C:618:ASN:CB	1:C:621:GLU:H	2.22	0.50
2:K:298:ARG:HH12	2:K:302:ASN:HD21	1.59	0.50
2:G:159:PHE:HA	10:G:602:NAG:H82	1.92	0.50
2:K:248:THR:OG1	2:K:249:HIS:N	2.44	0.50
3:F:35:THR:HG21	3:F:100(P):MET:HE2	1.94	0.50
2:R:248:THR:OG1	2:R:249:HIS:N	2.45	0.50
2:G:122:LEU:HD21	2:G:125:LEU:HD13	1.94	0.49
2:K:218:CYS:HA	2:K:247:CYS:HB3	1.93	0.49
1:C:594:GLY:HA2	1:C:599:SER:HB3	1.95	0.49
3:O:35:THR:HG21	3:O:100(P):MET:HE2	1.94	0.49
2:G:201:ILE:HG22	2:G:433:ALA:HB3	1.93	0.49
2:K:272:ILE:HG22	2:K:286:VAL:HG12	1.95	0.49
2:K:370:GLU:OE1	2:K:428:GLN:NE2	2.46	0.49
1:J:594:GLY:HA2	1:J:599:SER:HB3	1.95	0.49
1:Q:594:GLY:HA2	1:Q:599:SER:HB3	1.95	0.48
4:P:27:ALA:HA	4:P:90:MET:HE3	1.96	0.48
2:R:95:MET:HG3	2:R:96:TRP:CD1	2.48	0.48
3:A:35:THR:HG21	3:A:100(P):MET:HE2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:27:ALA:HA	4:B:90:MET:HE3	1.96	0.48
4:I:27:ALA:HA	4:I:90:MET:HE3	1.96	0.47
2:K:69:TRP:HZ2	2:K:253:PRO:HG2	1.78	0.47
3:O:18:LEU:HD13	3:O:82(C):VAL:HG11	1.97	0.47
2:R:372:THR:HG23	2:R:373:THR:HG23	1.97	0.47
2:K:49:GLU:HG2	2:K:99:ASN:HB2	1.97	0.47
2:K:125:LEU:HA	2:K:161:MET:HE1	1.97	0.47
3:O:29:MET:HE2	3:O:71:ARG:HH21	1.79	0.47
3:F:29:MET:HE2	3:F:71:ARG:HH21	1.79	0.46
3:A:29:MET:HE2	3:A:71:ARG:HH21	1.79	0.46
2:K:122:LEU:HD21	2:K:125:LEU:HD13	1.98	0.46
3:A:18:LEU:HD13	3:A:82(C):VAL:HG11	1.97	0.46
3:F:18:LEU:HD13	3:F:82(C):VAL:HG11	1.97	0.46
1:C:618:ASN:H	1:C:621:GLU:HG2	1.80	0.46
1:J:607:ASN:H	1:J:650:GLN:HE22	1.65	0.45
10:C:702:NAG:C3	10:C:702:NAG:C8	2.85	0.45
1:Q:607:ASN:H	1:Q:650:GLN:HE22	1.65	0.45
2:R:134:TYR:HB2	2:R:156:GLN:HB2	1.99	0.45
1:C:607:ASN:H	1:C:650:GLN:HE22	1.65	0.45
2:G:153:GLU:HA	2:G:178:ARG:HB2	1.98	0.45
2:K:68:VAL:HG23	2:K:70:ALA:H	1.81	0.45
2:R:429:ARG:NH2	2:R:432:GLN:OE1	2.50	0.45
3:O:100:ARG:NH1	4:P:31:ARG:O	2.50	0.45
5:b:4:MAN:H2	5:b:5:MAN:H2	1.70	0.45
4:P:26:GLN:HA	4:P:70:ARG:HH22	1.82	0.44
4:P:32:ALA:HA	4:P:51:ASN:HD21	1.83	0.44
4:I:26:GLN:HA	4:I:70:ARG:HH22	1.82	0.44
2:G:360:ARG:HB3	2:G:467:THR:HG22	2.00	0.44
2:R:91:GLU:OE2	2:R:487:LYS:NZ	2.40	0.44
4:B:26:GLN:HA	4:B:70:ARG:HH22	1.82	0.44
4:I:32:ALA:HA	4:I:51:ASN:HD21	1.83	0.44
2:G:95:MET:HE2	2:G:235:GLY:HA3	1.98	0.44
2:K:203:GLN:HA	2:K:435:TYR:HB3	1.99	0.44
4:I:97:SER:OG	4:I:98:PHE:N	2.51	0.44
4:P:97:SER:OG	4:P:98:PHE:N	2.51	0.44
2:G:134:TYR:HD2	2:G:154:LEU:HD13	1.83	0.44
2:K:81:PRO:HB2	2:K:82:GLN:H	1.61	0.44
9:e:3:BMA:H3	9:e:6:MAN:H2	1.74	0.44
4:B:97:SER:OG	4:B:98:PHE:N	2.51	0.43
2:G:175:LEU:HB2	2:G:320:PHE:HD2	1.82	0.43
3:F:2:VAL:HG22	3:F:27:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:54:CYS:HB2	2:R:74:CYS:HB2	1.90	0.43
4:B:32:ALA:HA	4:B:51:ASN:HD21	1.83	0.43
3:F:60:ASN:HB3	3:F:63:LEU:HD23	2.01	0.43
4:I:27:ALA:H	4:I:70:ARG:HH22	1.67	0.43
4:P:27:ALA:H	4:P:70:ARG:HH22	1.67	0.43
3:O:60:ASN:HB3	3:O:63:LEU:HD23	2.01	0.42
3:O:70:SER:HB2	3:O:79:SER:HB2	2.01	0.42
2:G:95:MET:HE3	2:G:96:TRP:HE1	1.84	0.42
2:G:269:GLU:OE2	2:G:348:GLN:NE2	2.53	0.42
2:R:153:GLU:HA	2:R:178:ARG:HB2	2.01	0.42
3:O:2:VAL:HG22	3:O:27:ASP:HB2	2.00	0.42
2:K:195:ASN:OD1	2:K:198:THR:OG1	2.38	0.42
2:R:163:THR:OG1	2:R:164:GLU:N	2.51	0.42
2:G:259:LEU:HD22	2:G:449:ILE:HD11	2.01	0.42
2:K:95:MET:HG3	2:K:96:TRP:CE3	2.55	0.42
2:K:259:LEU:HB2	2:K:374:HIS:CE1	2.55	0.42
4:B:27:ALA:H	4:B:70:ARG:HH22	1.67	0.42
1:C:604:CYS:HB3	2:G:38:VAL:HG22	2.01	0.42
3:F:100:ARG:CZ	4:I:30:SER:HB3	2.50	0.42
4:B:66(A):ASP:OD1	4:B:66(A):ASP:N	2.52	0.42
2:K:372:THR:HG23	2:K:373:THR:HG23	2.02	0.42
3:F:70:SER:HB2	3:F:79:SER:HB2	2.01	0.42
2:G:84:ILE:O	2:G:243:SER:OG	2.34	0.41
1:Q:593:LEU:HD23	1:Q:599:SER:HA	2.02	0.41
3:A:2:VAL:HG22	3:A:27:ASP:HB2	2.00	0.41
3:A:70:SER:HB2	3:A:79:SER:HB2	2.01	0.41
8:d:1:NAG:H4	8:d:2:NAG:H2	1.93	0.41
2:K:175:LEU:HB2	2:K:320:PHE:HD2	1.85	0.41
3:A:60:ASN:HB3	3:A:63:LEU:HD23	2.01	0.41
1:C:593:LEU:HD23	1:C:599:SER:HA	2.03	0.41
2:G:95:MET:HG3	2:G:96:TRP:CD1	2.52	0.41
2:G:342:LEU:HD22	2:G:361:PHE:HE2	1.86	0.41
2:R:86:LEU:HD13	2:R:243:SER:HA	2.02	0.41
1:C:619:LEU:HD12	1:C:623:TRP:CD1	2.56	0.41
2:G:86:LEU:HD13	2:G:243:SER:HA	2.03	0.41
2:G:372:THR:HG23	2:G:373:THR:HG23	2.03	0.41
2:R:270:VAL:HG12	2:R:288:LEU:HA	2.02	0.41
2:K:359:ILE:O	2:K:394:THR:OG1	2.37	0.41
3:A:16:GLU:H	3:A:82(C):VAL:HG22	1.86	0.41
1:C:619:LEU:HD12	1:C:623:TRP:HD1	1.86	0.41
2:G:259:LEU:HB2	2:G:374:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:394:THR:OG1	2:K:395:TRP:N	2.54	0.40
3:F:16:GLU:H	3:F:82(C):VAL:HG22	1.86	0.40
3:O:16:GLU:H	3:O:82(C):VAL:HG22	1.86	0.40
2:R:216:HIS:ND1	2:R:248:THR:O	2.54	0.40
2:K:104:MET:HE2	2:K:104:MET:HB2	1.96	0.40
2:R:276:ASN:HB3	8:c:1:NAG:C7	2.51	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	C	120/153 (78%)	113 (94%)	7 (6%)	0	100	100
1	J	120/153 (78%)	113 (94%)	7 (6%)	0	100	100
1	Q	120/153 (78%)	113 (94%)	7 (6%)	0	100	100
2	G	432/481 (90%)	390 (90%)	40 (9%)	2 (0%)	24	61
2	K	432/481 (90%)	401 (93%)	30 (7%)	1 (0%)	43	75
2	R	432/481 (90%)	391 (90%)	40 (9%)	1 (0%)	43	75
3	A	131/238 (55%)	125 (95%)	6 (5%)	0	100	100
3	F	131/238 (55%)	125 (95%)	6 (5%)	0	100	100
3	O	131/238 (55%)	125 (95%)	6 (5%)	0	100	100
4	B	105/214 (49%)	96 (91%)	9 (9%)	0	100	100
4	I	105/214 (49%)	96 (91%)	9 (9%)	0	100	100
4	P	105/214 (49%)	96 (91%)	9 (9%)	0	100	100
All	All	2364/3258 (73%)	2184 (92%)	176 (7%)	4 (0%)	44	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	R	387	THR
2	G	393	SER
2	G	465	THR
2	K	393	SER

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	C	107/130 (82%)	105 (98%)	2 (2%)	50	67
1	J	107/130 (82%)	105 (98%)	2 (2%)	50	67
1	Q	107/130 (82%)	105 (98%)	2 (2%)	50	67
2	G	395/428 (92%)	393 (100%)	2 (0%)	81	82
2	K	395/428 (92%)	394 (100%)	1 (0%)	86	85
2	R	395/428 (92%)	394 (100%)	1 (0%)	86	85
3	A	116/208 (56%)	115 (99%)	1 (1%)	70	77
3	F	116/208 (56%)	115 (99%)	1 (1%)	70	77
3	O	116/208 (56%)	115 (99%)	1 (1%)	70	77
4	B	85/178 (48%)	85 (100%)	0	100	100
4	I	85/178 (48%)	85 (100%)	0	100	100
4	P	85/178 (48%)	85 (100%)	0	100	100
All	All	2109/2832 (74%)	2096 (99%)	13 (1%)	76	81

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	576	LEU
1	C	584	GLU
2	G	198	THR
2	G	247	CYS
1	J	576	LEU
1	J	584	GLU
2	K	247	CYS

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Mol	Chain	Res	Type
1	Q	576	LEU
1	Q	584	GLU
2	R	247	CYS
3	A	54	ARG
3	F	54	ARG
3	O	54	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	585	HIS
1	C	650	GLN
1	C	651	ASN
1	C	652	GLN
2	G	103	GLN
2	G	203	GLN
2	G	315	GLN
2	G	348	GLN
2	G	377	ASN
1	J	650	GLN
1	J	651	ASN
1	J	652	GLN
2	K	103	GLN
2	K	302	ASN
2	K	348	GLN
2	K	377	ASN
1	Q	585	HIS
1	Q	650	GLN
1	Q	651	ASN
1	Q	652	GLN
2	R	82	GLN
2	R	103	GLN
2	R	188	ASN
2	R	300	ASN
2	R	352	HIS
3	A	3	GLN
3	A	39	GLN
3	F	3	GLN
3	O	3	GLN
4	B	34	GLN
4	B	89	HIS
4	I	34	GLN

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Mol	Chain	Res	Type
4	P	34	GLN
4	P	89	HIS

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 ⓘ

71 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	$\# Z > 2$
5	NAG	D	1	5,2	14,14,15	0.82	1 (7%)	17,19,21	0.87	0
5	NAG	D	2	5	14,14,15	0.59	0	17,19,21	1.00	1 (5%)
5	BMA	D	3	5	11,11,12	0.67	0	15,15,17	1.43	2 (13%)
5	MAN	D	4	5	11,11,12	0.79	0	15,15,17	1.19	2 (13%)
5	MAN	D	5	5	11,11,12	1.03	1 (9%)	15,15,17	0.89	1 (6%)
5	MAN	D	6	5	11,11,12	0.71	0	15,15,17	1.07	2 (13%)
6	NAG	E	1	2,6	14,14,15	0.56	0	17,19,21	0.70	0
6	NAG	E	2	6	14,14,15	0.31	0	17,19,21	0.52	0
6	BMA	E	3	6	11,11,12	0.64	0	15,15,17	1.00	2 (13%)
7	NAG	H	1	2,7	14,14,15	0.39	0	17,19,21	1.25	1 (5%)
7	NAG	H	2	7	14,14,15	0.30	0	17,19,21	0.81	0
7	BMA	H	3	7	11,11,12	1.33	1 (9%)	15,15,17	1.38	3 (20%)
7	MAN	H	4	7	11,11,12	0.68	0	15,15,17	1.49	2 (13%)
7	MAN	H	5	7	11,11,12	1.12	1 (9%)	15,15,17	1.89	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	H	6	7	11,11,12	0.72	0	15,15,17	1.05	2 (13%)
7	MAN	H	7	7	11,11,12	0.82	0	15,15,17	0.96	2 (13%)
6	NAG	L	1	2,6	14,14,15	0.47	0	17,19,21	1.11	1 (5%)
6	NAG	L	2	6	14,14,15	1.15	1 (7%)	17,19,21	1.02	2 (11%)
6	BMA	L	3	6	11,11,12	0.85	0	15,15,17	0.77	0
8	NAG	M	1	2,8	14,14,15	0.41	0	17,19,21	1.06	1 (5%)
8	NAG	M	2	8	14,14,15	0.16	0	17,19,21	0.72	1 (5%)
8	NAG	N	1	2,8	14,14,15	0.63	0	17,19,21	1.07	1 (5%)
8	NAG	N	2	8	14,14,15	0.35	0	17,19,21	0.53	0
8	NAG	S	1	2,8	14,14,15	1.66	1 (7%)	17,19,21	1.76	3 (17%)
8	NAG	S	2	8	14,14,15	0.24	0	17,19,21	0.57	0
8	NAG	T	1	2,8	14,14,15	0.35	0	17,19,21	0.70	1 (5%)
8	NAG	T	2	8	14,14,15	0.48	0	17,19,21	0.52	0
7	NAG	U	1	2,7	14,14,15	0.38	0	17,19,21	0.80	1 (5%)
7	NAG	U	2	7	14,14,15	0.33	0	17,19,21	1.07	1 (5%)
7	BMA	U	3	7	11,11,12	0.63	0	15,15,17	1.25	2 (13%)
7	MAN	U	4	7	11,11,12	0.77	0	15,15,17	1.65	4 (26%)
7	MAN	U	5	7	11,11,12	0.91	0	15,15,17	0.92	1 (6%)
7	MAN	U	6	7	11,11,12	0.73	0	15,15,17	1.03	2 (13%)
7	MAN	U	7	7	11,11,12	0.80	0	15,15,17	0.94	2 (13%)
6	NAG	V	1	2,6	14,14,15	1.72	3 (21%)	17,19,21	2.53	6 (35%)
6	NAG	V	2	6	14,14,15	0.23	0	17,19,21	0.49	0
6	BMA	V	3	6	11,11,12	0.69	0	15,15,17	1.07	1 (6%)
5	NAG	W	1	5,2	14,14,15	0.48	0	17,19,21	0.59	0
5	NAG	W	2	5	14,14,15	0.26	0	17,19,21	0.80	0
5	BMA	W	3	5	11,11,12	1.27	1 (9%)	15,15,17	1.16	2 (13%)
5	MAN	W	4	5	11,11,12	0.73	0	15,15,17	1.39	3 (20%)
5	MAN	W	5	5	11,11,12	1.31	2 (18%)	15,15,17	1.96	3 (20%)
5	MAN	W	6	5	11,11,12	1.65	3 (27%)	15,15,17	2.42	2 (13%)
8	NAG	X	1	2,8	14,14,15	0.41	0	17,19,21	1.12	1 (5%)
8	NAG	X	2	8	14,14,15	0.32	0	17,19,21	0.55	0
8	NAG	Y	1	2,8	14,14,15	0.70	0	17,19,21	1.32	3 (17%)
8	NAG	Y	2	8	14,14,15	0.28	0	17,19,21	0.50	0
8	NAG	Z	1	2,8	14,14,15	0.22	0	17,19,21	1.48	2 (11%)
8	NAG	Z	2	8	14,14,15	0.63	1 (7%)	17,19,21	0.72	1 (5%)
8	NAG	a	1	2,8	14,14,15	0.47	0	17,19,21	1.09	2 (11%)
8	NAG	a	2	8	14,14,15	0.47	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	b	1	5,2	14,14,15	0.31	0	17,19,21	0.58	0
5	NAG	b	2	5	14,14,15	0.73	1 (7%)	17,19,21	2.38	3 (17%)
5	BMA	b	3	5	11,11,12	0.60	0	15,15,17	1.17	2 (13%)
5	MAN	b	4	5	11,11,12	0.87	1 (9%)	15,15,17	1.26	2 (13%)
5	MAN	b	5	5	11,11,12	1.11	1 (9%)	15,15,17	1.08	1 (6%)
5	MAN	b	6	5	11,11,12	0.73	0	15,15,17	0.98	2 (13%)
8	NAG	c	1	2,8	14,14,15	0.48	0	17,19,21	0.98	1 (5%)
8	NAG	c	2	8	14,14,15	0.54	0	17,19,21	0.53	0
8	NAG	d	1	2,8	14,14,15	0.43	0	17,19,21	0.79	1 (5%)
8	NAG	d	2	8	14,14,15	0.75	1 (7%)	17,19,21	0.70	1 (5%)
9	NAG	e	1	2,9	14,14,15	0.44	0	17,19,21	0.57	0
9	NAG	e	2	9	14,14,15	0.81	1 (7%)	17,19,21	1.19	2 (11%)
9	BMA	e	3	9	11,11,12	1.32	1 (9%)	15,15,17	2.04	4 (26%)
9	MAN	e	4	9	11,11,12	1.05	1 (9%)	15,15,17	0.88	1 (6%)
9	MAN	e	5	9	11,11,12	1.19	1 (9%)	15,15,17	1.66	3 (20%)
9	MAN	e	6	9	11,11,12	1.24	1 (9%)	15,15,17	1.48	2 (13%)
8	NAG	f	1	2,8	14,14,15	0.42	0	17,19,21	1.07	1 (5%)
8	NAG	f	2	8	14,14,15	0.27	0	17,19,21	0.59	0
8	NAG	g	1	2,8	14,14,15	0.71	1 (7%)	17,19,21	1.35	2 (11%)
8	NAG	g	2	8	14,14,15	0.24	0	17,19,21	0.55	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
5	NAG	D	1	5,2	-	4/6/23/26	0/1/1/1
5	NAG	D	2	5	-	4/6/23/26	0/1/1/1
5	BMA	D	3	5	-	0/2/19/22	0/1/1/1
5	MAN	D	4	5	-	0/2/19/22	0/1/1/1
5	MAN	D	5	5	-	2/2/19/22	0/1/1/1
5	MAN	D	6	5	-	2/2/19/22	0/1/1/1
6	NAG	E	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	E	2	6	-	2/6/23/26	0/1/1/1
6	BMA	E	3	6	-	0/2/19/22	0/1/1/1
7	NAG	H	1	2,7	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	H	2	7	-	2/6/23/26	0/1/1/1
7	BMA	H	3	7	-	1/2/19/22	0/1/1/1
7	MAN	H	4	7	-	0/2/19/22	0/1/1/1
7	MAN	H	5	7	-	1/2/19/22	1/1/1/1
7	MAN	H	6	7	-	0/2/19/22	0/1/1/1
7	MAN	H	7	7	-	0/2/19/22	0/1/1/1
6	NAG	L	1	2,6	-	4/6/23/26	0/1/1/1
6	NAG	L	2	6	-	1/6/23/26	0/1/1/1
6	BMA	L	3	6	-	2/2/19/22	0/1/1/1
8	NAG	M	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	M	2	8	-	2/6/23/26	0/1/1/1
8	NAG	N	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	N	2	8	-	3/6/23/26	0/1/1/1
8	NAG	S	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	S	2	8	-	2/6/23/26	0/1/1/1
8	NAG	T	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	T	2	8	-	3/6/23/26	0/1/1/1
7	NAG	U	1	2,7	-	3/6/23/26	0/1/1/1
7	NAG	U	2	7	-	3/6/23/26	0/1/1/1
7	BMA	U	3	7	-	0/2/19/22	0/1/1/1
7	MAN	U	4	7	-	0/2/19/22	0/1/1/1
7	MAN	U	5	7	-	1/2/19/22	0/1/1/1
7	MAN	U	6	7	-	1/2/19/22	0/1/1/1
7	MAN	U	7	7	-	2/2/19/22	0/1/1/1
6	NAG	V	1	2,6	-	6/6/23/26	0/1/1/1
6	NAG	V	2	6	-	2/6/23/26	0/1/1/1
6	BMA	V	3	6	-	0/2/19/22	0/1/1/1
5	NAG	W	1	5,2	-	3/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
5	BMA	W	3	5	-	2/2/19/22	0/1/1/1
5	MAN	W	4	5	-	2/2/19/22	0/1/1/1
5	MAN	W	5	5	-	2/2/19/22	0/1/1/1
5	MAN	W	6	5	-	1/2/19/22	0/1/1/1
8	NAG	X	1	2,8	-	4/6/23/26	0/1/1/1
8	NAG	X	2	8	-	1/6/23/26	0/1/1/1
8	NAG	Y	1	2,8	-	4/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	Z	1	2,8	-	3/6/23/26	0/1/1/1
8	NAG	Z	2	8	-	0/6/23/26	0/1/1/1
8	NAG	a	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	a	2	8	-	4/6/23/26	0/1/1/1
5	NAG	b	1	5,2	-	1/6/23/26	0/1/1/1
5	NAG	b	2	5	-	5/6/23/26	0/1/1/1
5	BMA	b	3	5	-	0/2/19/22	0/1/1/1
5	MAN	b	4	5	-	2/2/19/22	0/1/1/1
5	MAN	b	5	5	-	2/2/19/22	0/1/1/1
5	MAN	b	6	5	-	0/2/19/22	0/1/1/1
8	NAG	c	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	c	2	8	-	0/6/23/26	0/1/1/1
8	NAG	d	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	d	2	8	-	2/6/23/26	0/1/1/1
9	NAG	e	1	2,9	-	2/6/23/26	0/1/1/1
9	NAG	e	2	9	-	1/6/23/26	0/1/1/1
9	BMA	e	3	9	-	1/2/19/22	0/1/1/1
9	MAN	e	4	9	-	1/2/19/22	0/1/1/1
9	MAN	e	5	9	-	2/2/19/22	0/1/1/1
9	MAN	e	6	9	-	2/2/19/22	0/1/1/1
8	NAG	f	1	2,8	-	4/6/23/26	0/1/1/1
8	NAG	f	2	8	-	2/6/23/26	0/1/1/1
8	NAG	g	1	2,8	-	4/6/23/26	0/1/1/1
8	NAG	g	2	8	-	0/6/23/26	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	S	1	NAG	O5-C1	-6.04	1.33	1.43
6	V	1	NAG	O5-C1	-4.95	1.35	1.43
6	L	2	NAG	O5-C1	-3.90	1.37	1.43
9	e	6	MAN	C1-C2	3.54	1.60	1.52
5	W	6	MAN	O5-C5	3.42	1.50	1.43
7	H	3	BMA	O5-C1	-3.38	1.38	1.43
6	V	1	NAG	C1-C2	3.22	1.56	1.52
5	W	6	MAN	O5-C1	3.13	1.48	1.43
5	W	3	BMA	O5-C1	-2.97	1.38	1.43
9	e	4	MAN	O5-C1	-2.96	1.38	1.43
5	b	5	MAN	C1-C2	2.95	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1	NAG	O5-C1	-2.85	1.38	1.43
7	H	5	MAN	O5-C5	2.71	1.48	1.43
5	W	5	MAN	O5-C5	2.69	1.48	1.43
9	e	3	BMA	C4-C5	2.53	1.58	1.53
5	D	5	MAN	O5-C1	-2.52	1.39	1.43
9	e	2	NAG	O5-C1	-2.39	1.39	1.43
8	g	1	NAG	C1-C2	2.38	1.55	1.52
5	W	5	MAN	C1-C2	2.38	1.57	1.52
5	W	6	MAN	C1-C2	2.22	1.57	1.52
9	e	5	MAN	C4-C3	2.19	1.58	1.52
8	d	2	NAG	C1-C2	2.18	1.55	1.52
8	Z	2	NAG	C1-C2	2.17	1.55	1.52
5	b	4	MAN	O5-C1	-2.08	1.40	1.43
5	b	2	NAG	C1-C2	2.03	1.55	1.52
6	V	1	NAG	C3-C2	2.02	1.56	1.52

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	W	6	MAN	C1-O5-C5	8.59	123.70	112.19
5	b	2	NAG	C2-N2-C7	8.37	134.12	122.90
6	V	1	NAG	C2-N2-C7	7.81	133.37	122.90
5	W	5	MAN	C1-O5-C5	5.94	120.15	112.19
7	H	5	MAN	C1-O5-C5	5.87	120.05	112.19
9	e	3	BMA	C1-C2-C3	-5.80	101.20	109.64
9	e	5	MAN	C1-O5-C5	5.15	119.09	112.19
8	Z	1	NAG	C1-O5-C5	4.95	118.82	112.19
9	e	6	MAN	C1-O5-C5	4.40	118.08	112.19
7	H	4	MAN	C1-O5-C5	4.39	118.07	112.19
8	S	1	NAG	C4-C3-C2	4.19	117.16	111.02
7	U	4	MAN	C1-O5-C5	4.17	117.77	112.19
5	D	3	BMA	C1-O5-C5	4.05	117.61	112.19
5	b	2	NAG	C1-C2-N2	4.01	116.76	110.43
8	S	1	NAG	O4-C4-C3	-3.99	100.96	110.38
7	H	3	BMA	C1-O5-C5	3.83	117.32	112.19
5	W	4	MAN	C1-O5-C5	3.66	117.09	112.19
6	V	1	NAG	C4-C3-C2	3.58	116.27	111.02
8	g	1	NAG	C1-O5-C5	3.57	116.97	112.19
5	b	4	MAN	O2-C2-C3	-3.56	102.79	110.15
7	H	1	NAG	C2-N2-C7	3.39	127.44	122.90
6	V	1	NAG	C1-C2-N2	3.35	115.71	110.43
5	D	2	NAG	C2-N2-C7	3.24	127.24	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	4	MAN	O2-C2-C3	-3.23	103.47	110.15
7	U	2	NAG	C2-N2-C7	3.22	127.21	122.90
5	D	4	MAN	O2-C2-C3	-3.19	103.54	110.15
5	b	3	BMA	C1-O5-C5	3.17	116.44	112.19
8	X	1	NAG	C2-N2-C7	3.15	127.12	122.90
6	L	1	NAG	C2-N2-C7	3.13	127.10	122.90
8	M	1	NAG	C2-N2-C7	3.13	127.09	122.90
7	U	3	BMA	C1-O5-C5	3.12	116.37	112.19
8	c	1	NAG	C1-O5-C5	3.07	116.30	112.19
8	a	1	NAG	C2-N2-C7	3.04	126.98	122.90
8	Y	1	NAG	C2-N2-C7	3.00	126.91	122.90
8	N	1	NAG	O3-C3-C2	-2.99	103.19	109.40
8	g	1	NAG	C2-N2-C7	2.91	126.80	122.90
6	V	3	BMA	C1-O5-C5	2.91	116.08	112.19
7	H	6	MAN	C1-O5-C5	2.91	116.08	112.19
8	Z	1	NAG	O4-C4-C5	2.86	116.36	109.32
7	H	5	MAN	O2-C2-C3	-2.85	104.25	110.15
8	f	1	NAG	C2-N2-C7	2.79	126.64	122.90
6	V	1	NAG	C1-O5-C5	-2.76	108.49	112.19
5	D	6	MAN	C1-O5-C5	2.73	115.84	112.19
5	W	5	MAN	C1-C2-C3	2.71	113.59	109.64
5	W	5	MAN	O2-C2-C3	-2.70	104.56	110.15
6	L	2	NAG	C4-C3-C2	2.68	114.95	111.02
9	e	2	NAG	C3-C4-C5	2.68	115.08	110.23
6	E	3	BMA	C1-O5-C5	2.67	115.76	112.19
5	D	4	MAN	C1-O5-C5	2.64	115.72	112.19
9	e	6	MAN	O2-C2-C3	-2.64	104.69	110.15
8	S	1	NAG	C3-C4-C5	2.60	114.95	110.23
8	Z	2	NAG	C1-O5-C5	2.54	115.59	112.19
9	e	3	BMA	O3-C3-C2	2.54	115.23	110.05
5	W	4	MAN	O2-C2-C3	-2.51	104.96	110.15
6	V	1	NAG	C3-C4-C5	2.49	114.75	110.23
7	H	4	MAN	O2-C2-C3	-2.47	105.04	110.15
7	H	7	MAN	O2-C2-C3	-2.46	105.05	110.15
7	U	5	MAN	O2-C2-C3	-2.45	105.07	110.15
5	D	6	MAN	O2-C2-C3	-2.45	105.08	110.15
7	U	6	MAN	O2-C2-C3	-2.43	105.11	110.15
6	L	2	NAG	O3-C3-C2	-2.43	104.35	109.40
8	Y	1	NAG	O3-C3-C2	-2.42	104.37	109.40
5	b	4	MAN	C1-O5-C5	2.40	115.41	112.19
5	b	6	MAN	O2-C2-C3	-2.40	105.19	110.15
7	U	7	MAN	O2-C2-C3	-2.39	105.19	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	d	2	NAG	C1-O5-C5	2.38	115.38	112.19
5	W	6	MAN	O2-C2-C3	-2.38	105.21	110.15
9	e	4	MAN	O2-C2-C3	-2.38	105.22	110.15
8	M	2	NAG	C1-O5-C5	2.36	115.35	112.19
9	e	3	BMA	O2-C2-C3	-2.35	105.29	110.15
5	b	5	MAN	O2-C2-C3	-2.34	105.30	110.15
7	H	6	MAN	O2-C2-C3	-2.34	105.31	110.15
5	b	6	MAN	C1-O5-C5	2.31	115.28	112.19
5	D	5	MAN	O2-C2-C3	-2.30	105.39	110.15
5	W	4	MAN	C1-C2-C3	-2.29	106.31	109.64
5	W	3	BMA	C1-O5-C5	2.28	115.24	112.19
7	U	6	MAN	C1-O5-C5	2.27	115.23	112.19
9	e	5	MAN	O2-C2-C3	-2.25	105.49	110.15
7	U	3	BMA	O2-C2-C3	-2.25	105.49	110.15
5	b	3	BMA	O2-C2-C3	-2.17	105.66	110.15
8	Y	1	NAG	O4-C4-C3	2.16	115.47	110.38
5	b	2	NAG	C8-C7-N2	2.16	119.69	116.12
5	D	3	BMA	O2-C2-C3	-2.15	105.70	110.15
6	V	1	NAG	C8-C7-N2	2.14	119.67	116.12
7	H	3	BMA	O2-C2-C3	-2.14	105.73	110.15
7	H	7	MAN	C1-O5-C5	2.12	115.03	112.19
7	U	4	MAN	C1-C2-C3	-2.11	106.57	109.64
7	U	4	MAN	O2-C2-C1	2.11	114.05	109.22
9	e	2	NAG	O4-C4-C3	-2.10	105.43	110.38
9	e	5	MAN	C2-C3-C4	2.09	114.54	110.86
8	d	1	NAG	C1-O5-C5	2.09	114.99	112.19
7	H	5	MAN	C1-C2-C3	2.09	112.68	109.64
5	W	3	BMA	O2-C2-C3	-2.08	105.85	110.15
8	a	1	NAG	C1-O5-C5	2.07	114.95	112.19
9	e	3	BMA	O5-C1-C2	-2.03	105.95	110.79
7	U	1	NAG	C1-O5-C5	2.03	114.90	112.19
7	U	7	MAN	C1-O5-C5	2.02	114.90	112.19
7	H	3	BMA	O5-C5-C6	-2.01	103.75	107.66
6	E	3	BMA	O2-C2-C3	-2.01	105.99	110.15
8	T	1	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	f	2	NAG	C4-C5-C6-O6
8	S	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	D	5	MAN	C4-C5-C6-O6
8	Z	1	NAG	C4-C5-C6-O6
8	f	2	NAG	O5-C5-C6-O6
8	g	1	NAG	C4-C5-C6-O6
6	E	2	NAG	O5-C5-C6-O6
8	S	1	NAG	O5-C5-C6-O6
8	Y	1	NAG	O5-C5-C6-O6
7	H	1	NAG	C4-C5-C6-O6
6	L	3	BMA	O5-C5-C6-O6
9	e	5	MAN	C4-C5-C6-O6
8	d	2	NAG	C4-C5-C6-O6
9	e	5	MAN	O5-C5-C6-O6
5	D	5	MAN	O5-C5-C6-O6
9	e	1	NAG	C4-C5-C6-O6
5	D	1	NAG	O5-C5-C6-O6
7	U	7	MAN	O5-C5-C6-O6
8	Z	1	NAG	O5-C5-C6-O6
6	E	2	NAG	C4-C5-C6-O6
6	L	3	BMA	C4-C5-C6-O6
5	D	2	NAG	O5-C5-C6-O6
5	W	3	BMA	O5-C5-C6-O6
8	g	1	NAG	O5-C5-C6-O6
6	L	1	NAG	C4-C5-C6-O6
6	V	2	NAG	O5-C5-C6-O6
8	a	2	NAG	O5-C5-C6-O6
8	X	1	NAG	C4-C5-C6-O6
8	f	1	NAG	C4-C5-C6-O6
7	H	1	NAG	O5-C5-C6-O6
8	Y	1	NAG	C4-C5-C6-O6
6	V	1	NAG	C4-C5-C6-O6
6	V	2	NAG	C4-C5-C6-O6
5	D	2	NAG	C4-C5-C6-O6
7	H	3	BMA	O5-C5-C6-O6
7	H	2	NAG	C4-C5-C6-O6
5	D	1	NAG	C8-C7-N2-C2
5	D	1	NAG	O7-C7-N2-C2
5	b	2	NAG	C8-C7-N2-C2
5	b	2	NAG	O7-C7-N2-C2
6	V	1	NAG	C8-C7-N2-C2
6	V	1	NAG	O7-C7-N2-C2
7	U	1	NAG	C8-C7-N2-C2
7	U	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
8	M	2	NAG	C8-C7-N2-C2
8	M	2	NAG	O7-C7-N2-C2
8	N	2	NAG	C8-C7-N2-C2
8	N	2	NAG	O7-C7-N2-C2
8	T	1	NAG	C8-C7-N2-C2
8	T	1	NAG	O7-C7-N2-C2
8	T	2	NAG	C8-C7-N2-C2
8	T	2	NAG	O7-C7-N2-C2
8	a	2	NAG	C8-C7-N2-C2
8	a	2	NAG	O7-C7-N2-C2
8	c	1	NAG	C8-C7-N2-C2
8	c	1	NAG	O7-C7-N2-C2
5	b	4	MAN	O5-C5-C6-O6
9	e	4	MAN	O5-C5-C6-O6
9	e	6	MAN	O5-C5-C6-O6
6	E	1	NAG	O5-C5-C6-O6
8	d	2	NAG	O5-C5-C6-O6
5	W	5	MAN	O5-C5-C6-O6
8	d	1	NAG	O5-C5-C6-O6
9	e	2	NAG	O5-C5-C6-O6
9	e	1	NAG	O5-C5-C6-O6
9	e	3	BMA	O5-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
5	W	1	NAG	O5-C5-C6-O6
8	f	1	NAG	O5-C5-C6-O6
5	W	6	MAN	O5-C5-C6-O6
7	U	2	NAG	O5-C5-C6-O6
8	X	1	NAG	O5-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6
7	H	2	NAG	O5-C5-C6-O6
7	U	7	MAN	C4-C5-C6-O6
7	U	6	MAN	O5-C5-C6-O6
5	D	1	NAG	C4-C5-C6-O6
8	X	2	NAG	O5-C5-C6-O6
7	U	1	NAG	O5-C5-C6-O6
6	L	2	NAG	O5-C5-C6-O6
7	U	5	MAN	O5-C5-C6-O6
8	N	1	NAG	O5-C5-C6-O6
8	T	2	NAG	O5-C5-C6-O6
5	b	2	NAG	O5-C5-C6-O6
7	H	5	MAN	O5-C5-C6-O6
8	N	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	b	5	MAN	C4-C5-C6-O6
5	W	2	NAG	C4-C5-C6-O6
5	W	3	BMA	C4-C5-C6-O6
8	a	2	NAG	C4-C5-C6-O6
5	D	6	MAN	C4-C5-C6-O6
8	S	2	NAG	C4-C5-C6-O6
5	D	6	MAN	O5-C5-C6-O6
5	W	5	MAN	C4-C5-C6-O6
5	D	2	NAG	C3-C2-N2-C7
6	L	1	NAG	C3-C2-N2-C7
8	M	1	NAG	C3-C2-N2-C7
8	X	1	NAG	C3-C2-N2-C7
8	Y	1	NAG	C3-C2-N2-C7
8	f	1	NAG	C3-C2-N2-C7
5	W	2	NAG	O5-C5-C6-O6
8	S	2	NAG	O5-C5-C6-O6
6	E	1	NAG	C4-C5-C6-O6
5	W	4	MAN	O5-C5-C6-O6
5	W	4	MAN	C4-C5-C6-O6
5	b	1	NAG	C4-C5-C6-O6
8	N	2	NAG	C4-C5-C6-O6
8	d	1	NAG	C4-C5-C6-O6
5	D	2	NAG	C1-C2-N2-C7
5	W	1	NAG	C1-C2-N2-C7
5	b	2	NAG	C1-C2-N2-C7
6	L	1	NAG	C1-C2-N2-C7
6	V	1	NAG	C1-C2-N2-C7
7	H	1	NAG	C1-C2-N2-C7
7	U	2	NAG	C1-C2-N2-C7
8	M	1	NAG	C1-C2-N2-C7
8	X	1	NAG	C1-C2-N2-C7
8	Y	1	NAG	C1-C2-N2-C7
8	Z	1	NAG	C1-C2-N2-C7
8	a	1	NAG	C1-C2-N2-C7
8	f	1	NAG	C1-C2-N2-C7
8	g	1	NAG	C1-C2-N2-C7
5	b	2	NAG	C3-C2-N2-C7
6	V	1	NAG	C3-C2-N2-C7
7	H	1	NAG	C3-C2-N2-C7
7	U	2	NAG	C3-C2-N2-C7
8	a	1	NAG	C3-C2-N2-C7
8	g	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	W	1	NAG	C4-C5-C6-O6
9	e	6	MAN	C4-C5-C6-O6
5	b	5	MAN	O5-C5-C6-O6
5	b	4	MAN	C4-C5-C6-O6

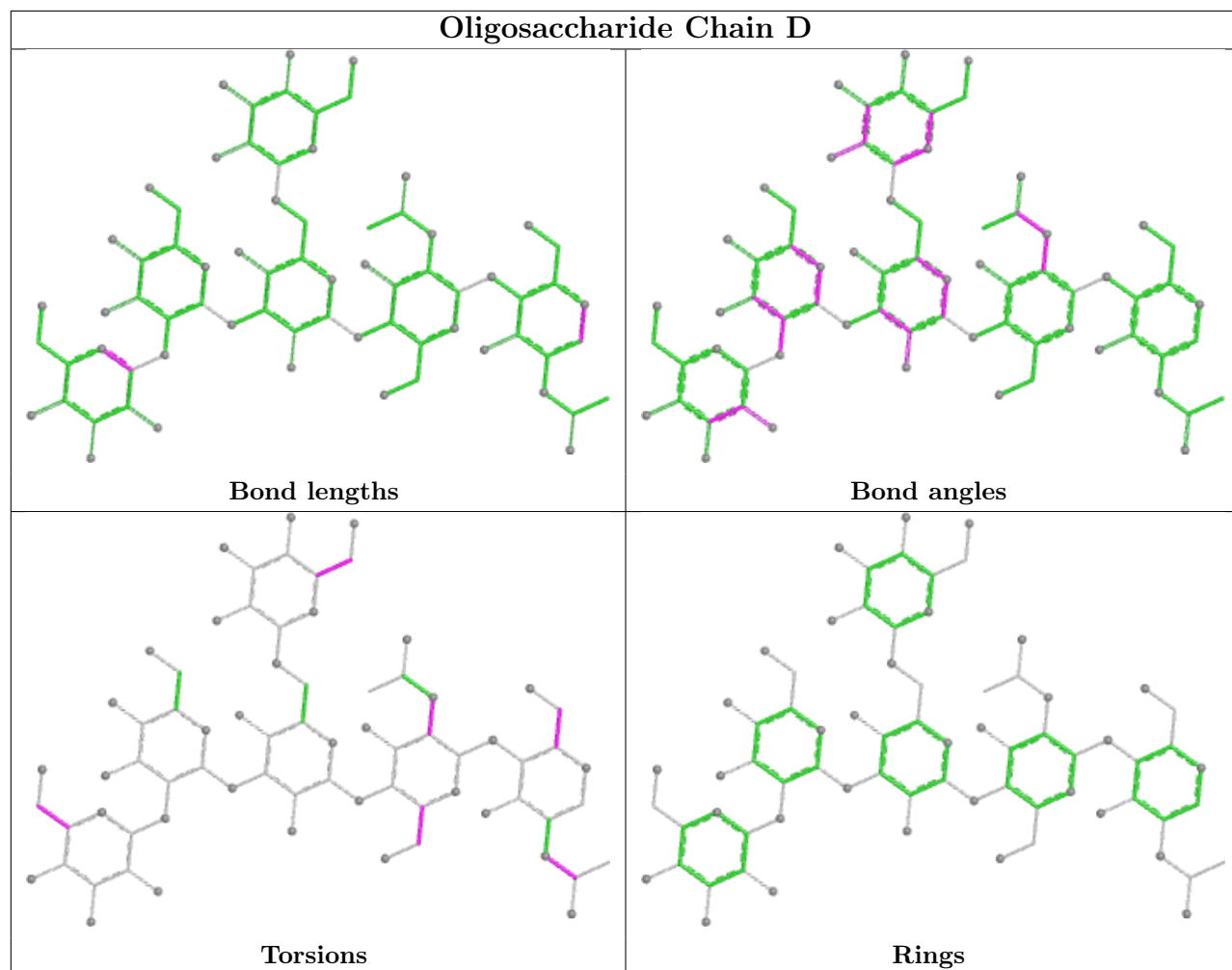
All (1) ring outliers are listed below:

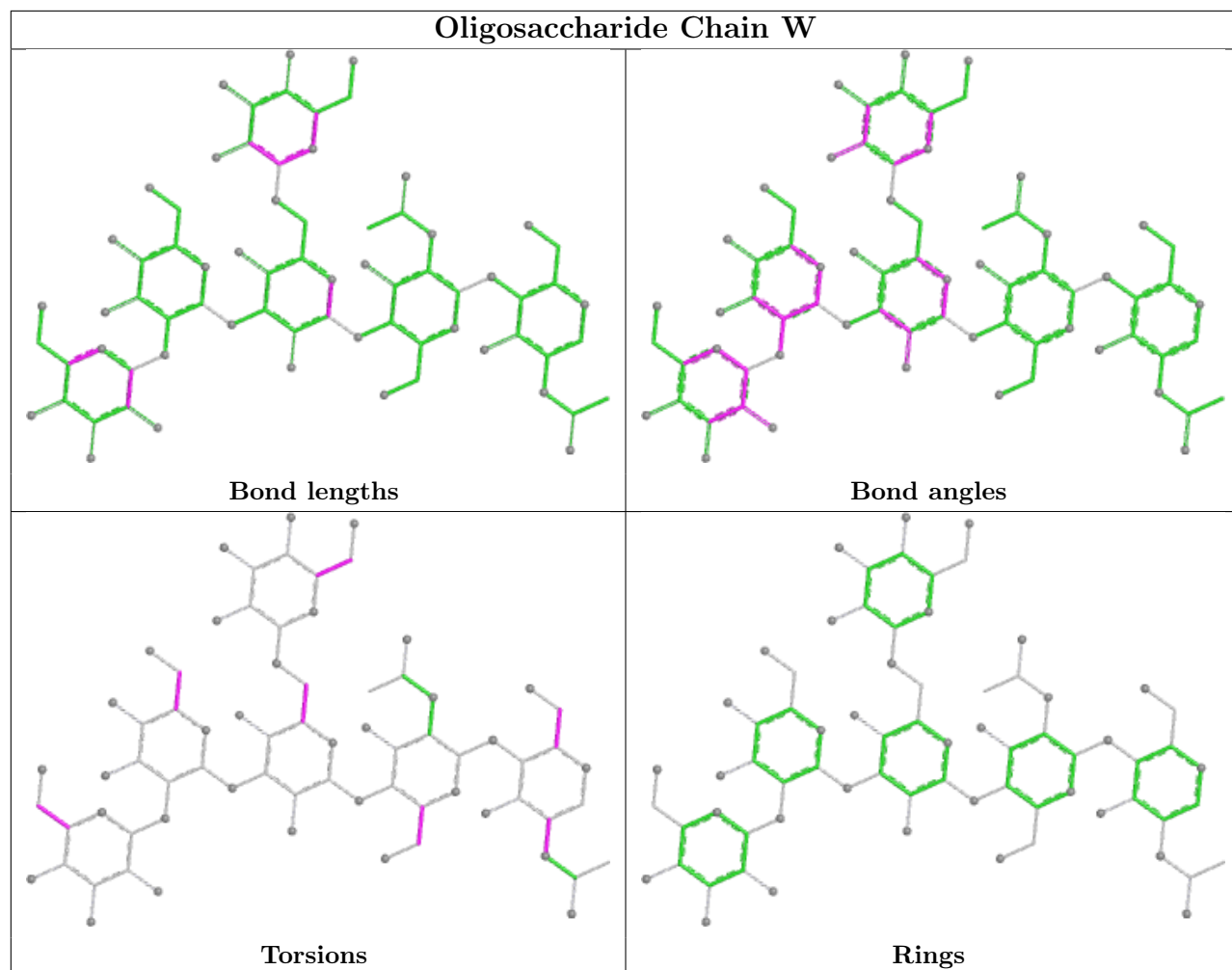
Mol	Chain	Res	Type	Atoms
7	H	5	MAN	C1-C2-C3-C4-C5-O5

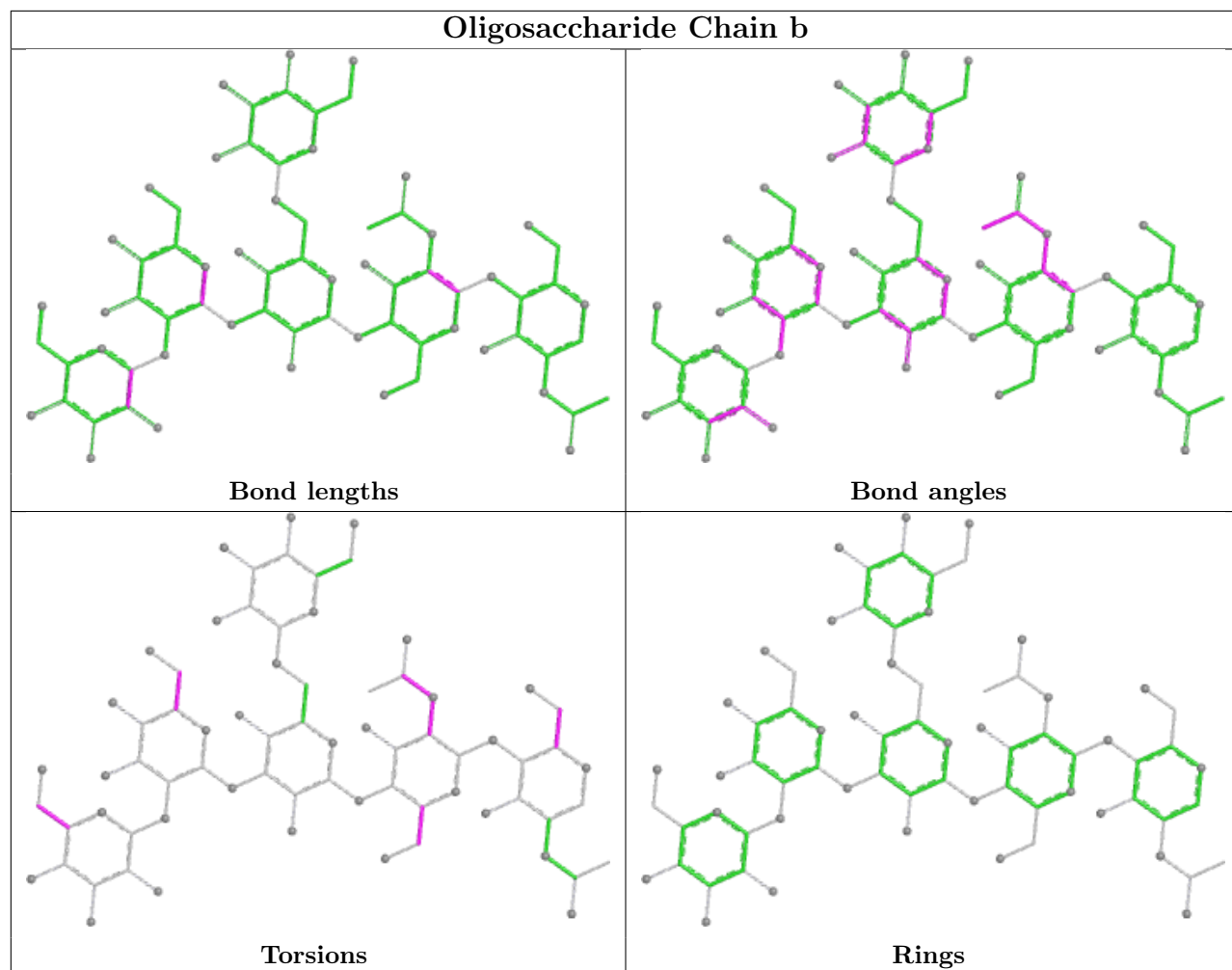
8 monomers are involved in 5 short contacts:

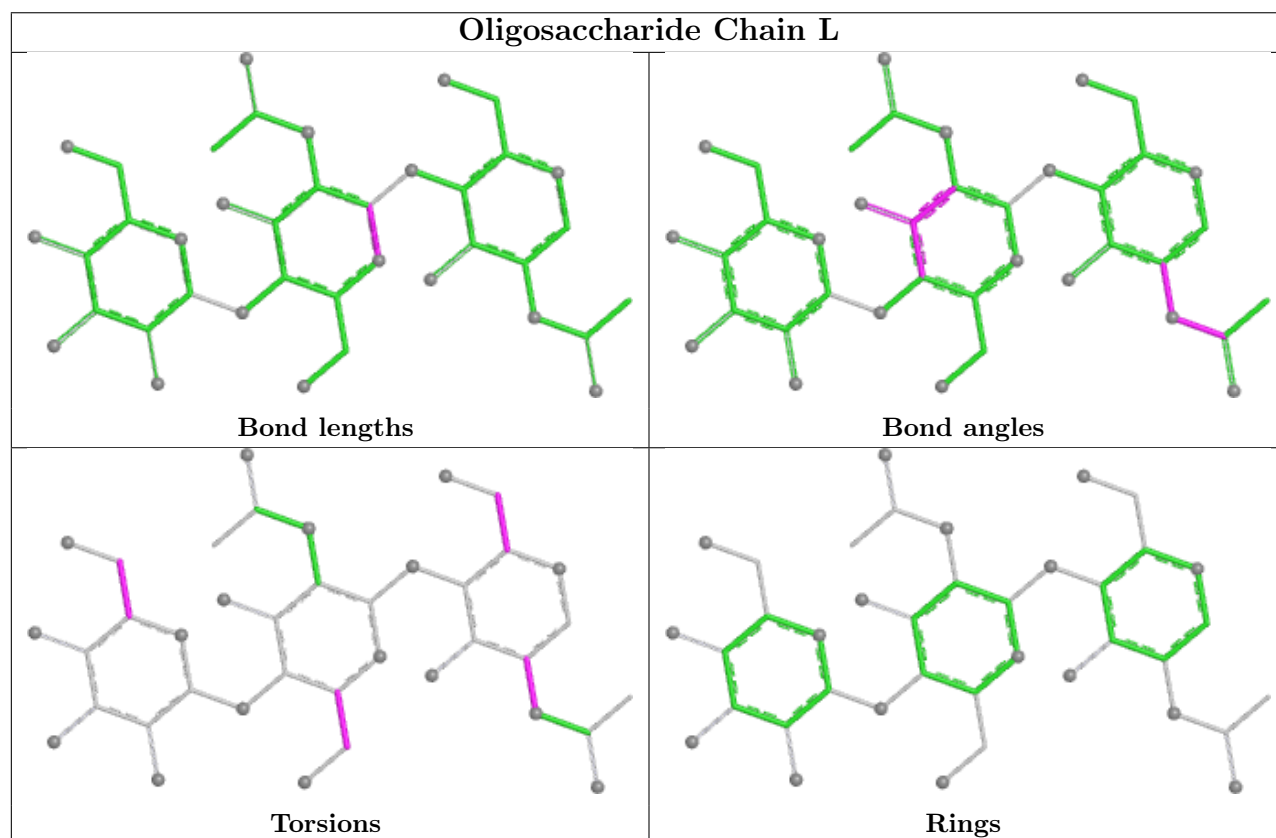
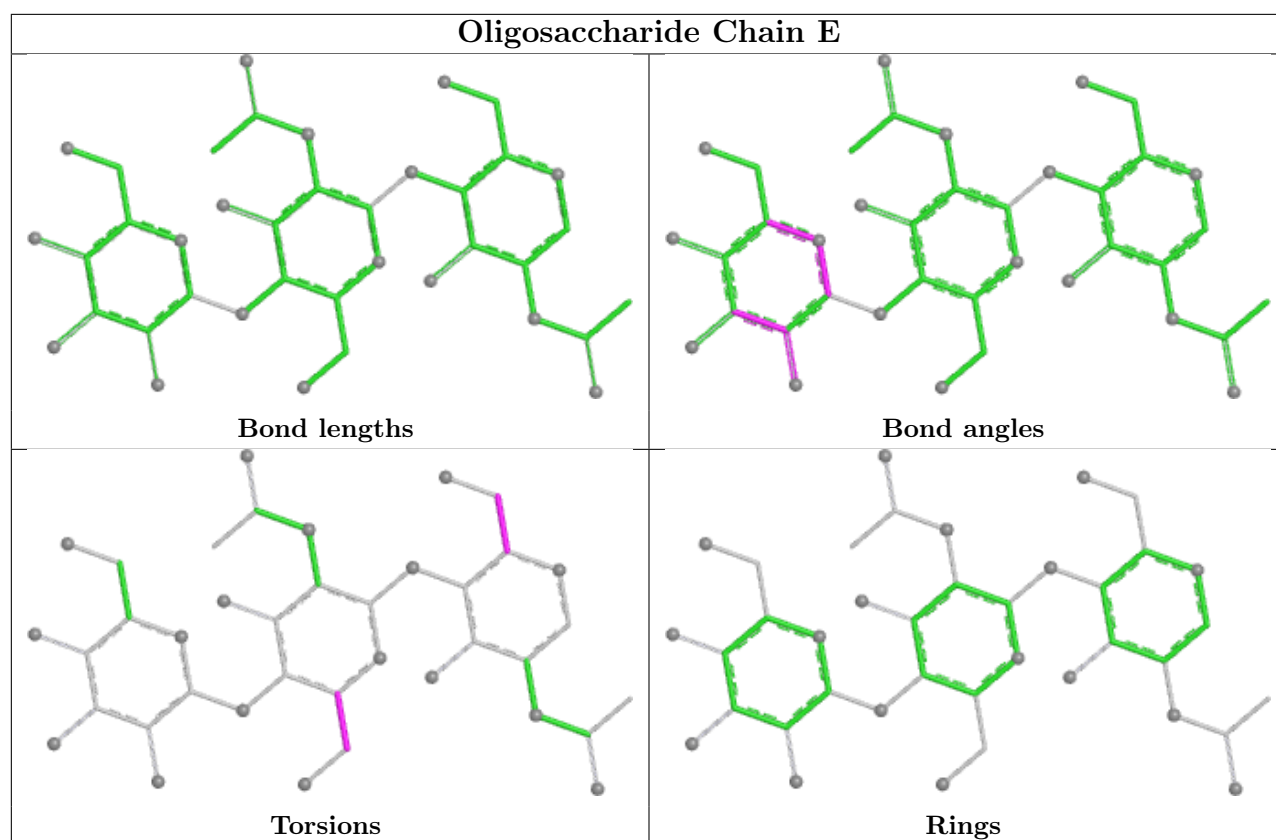
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	d	2	NAG	1	0
7	H	1	NAG	1	0
9	e	3	BMA	1	0
8	c	1	NAG	1	0
8	d	1	NAG	1	0
5	b	5	MAN	1	0
5	b	4	MAN	1	0
9	e	6	MAN	1	0

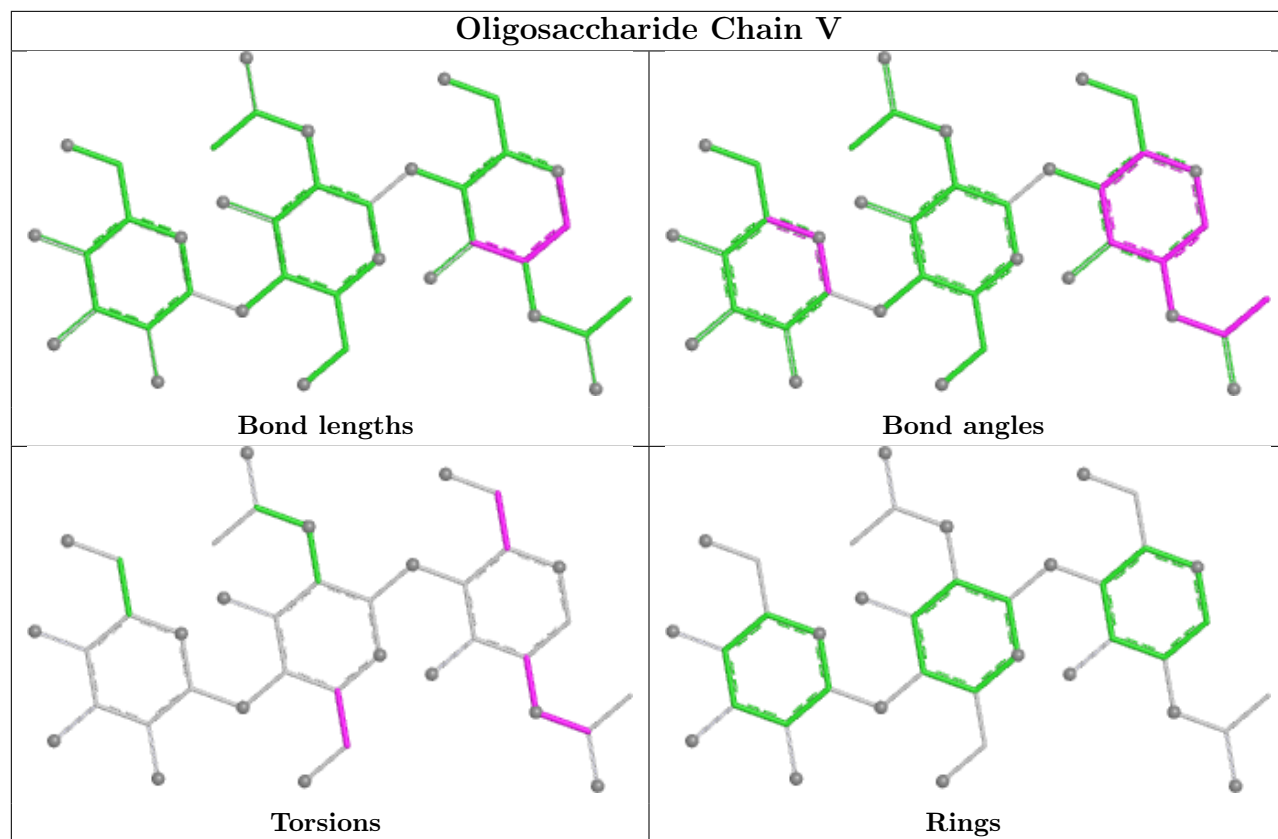
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

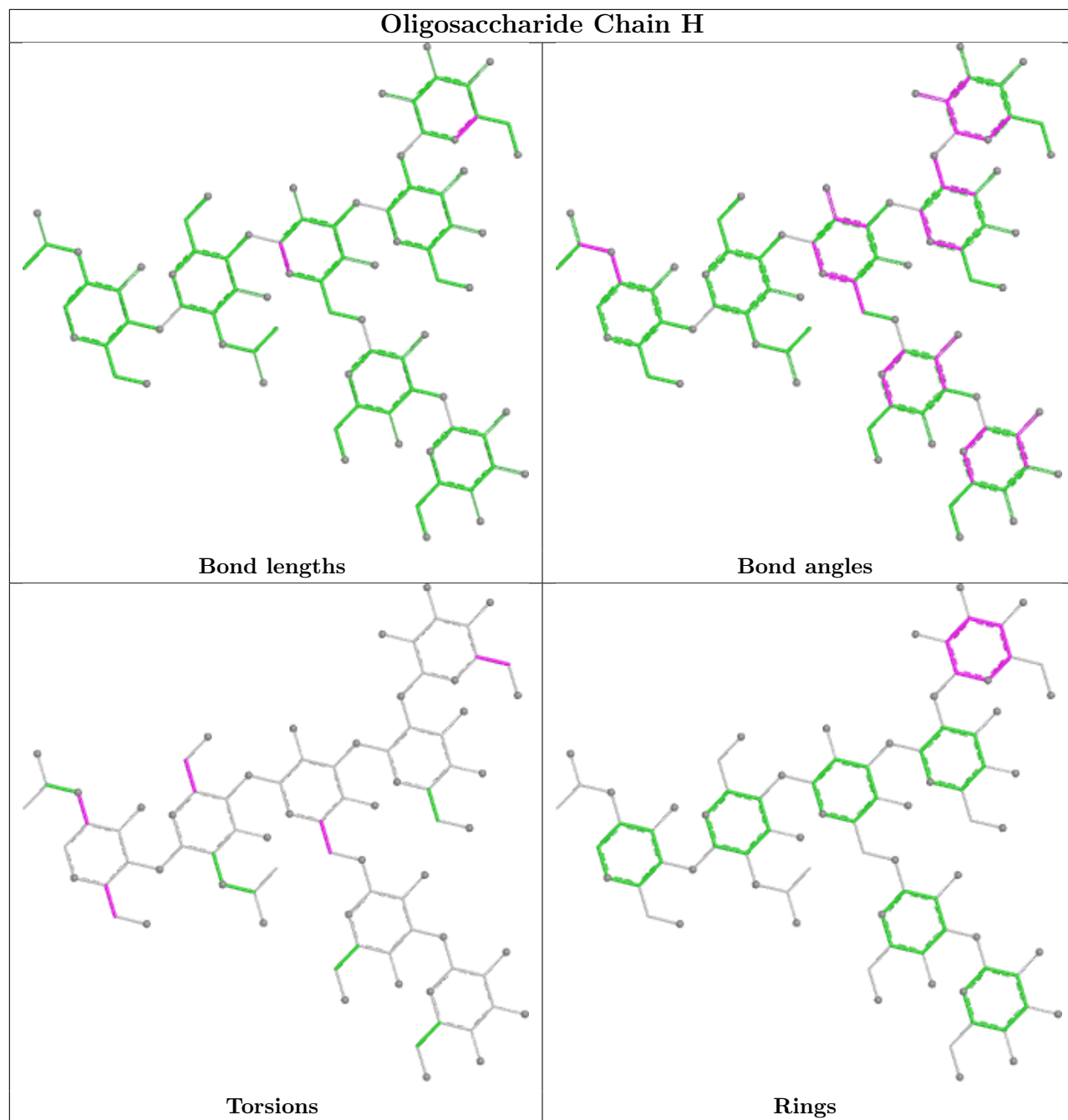


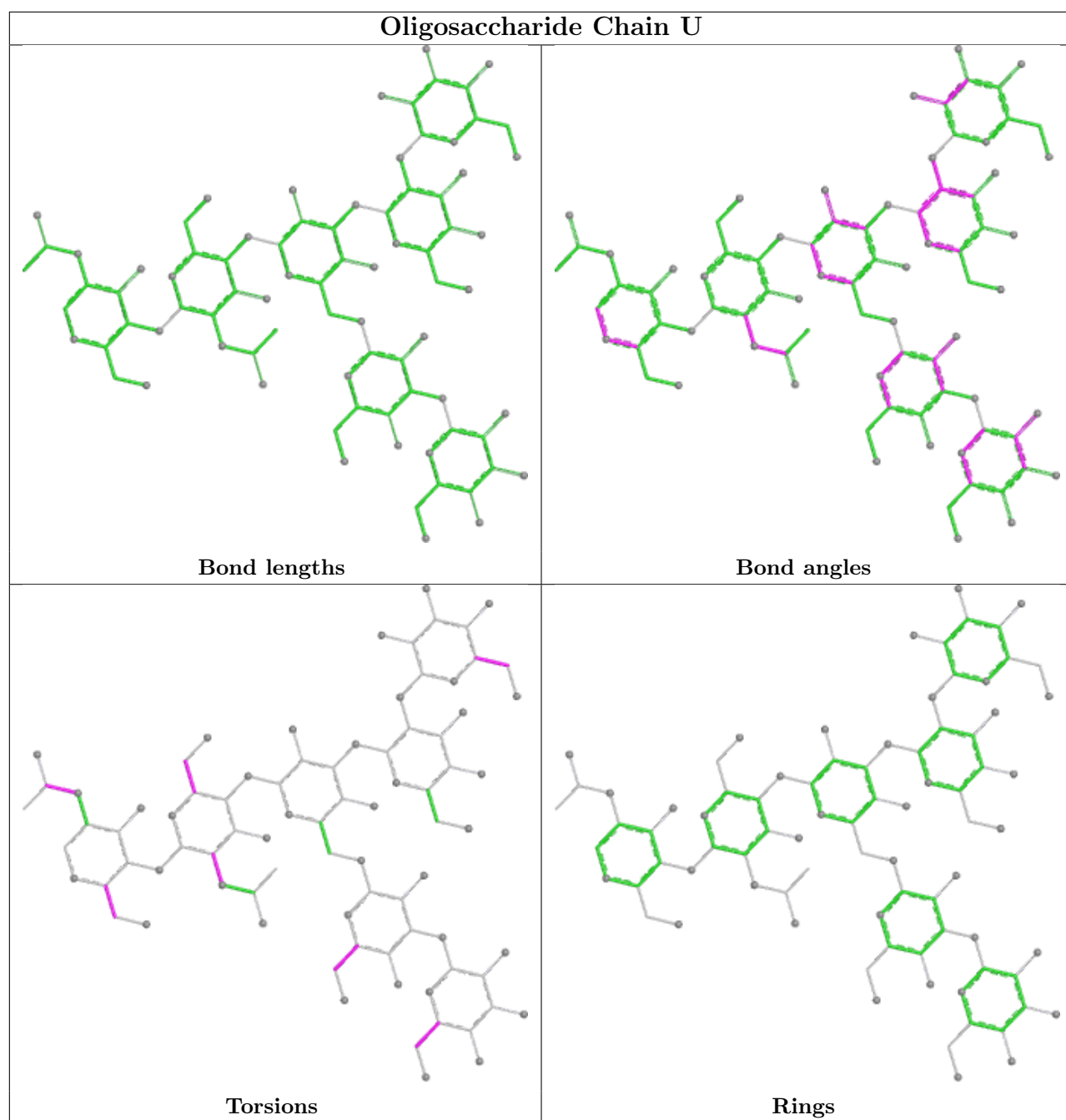


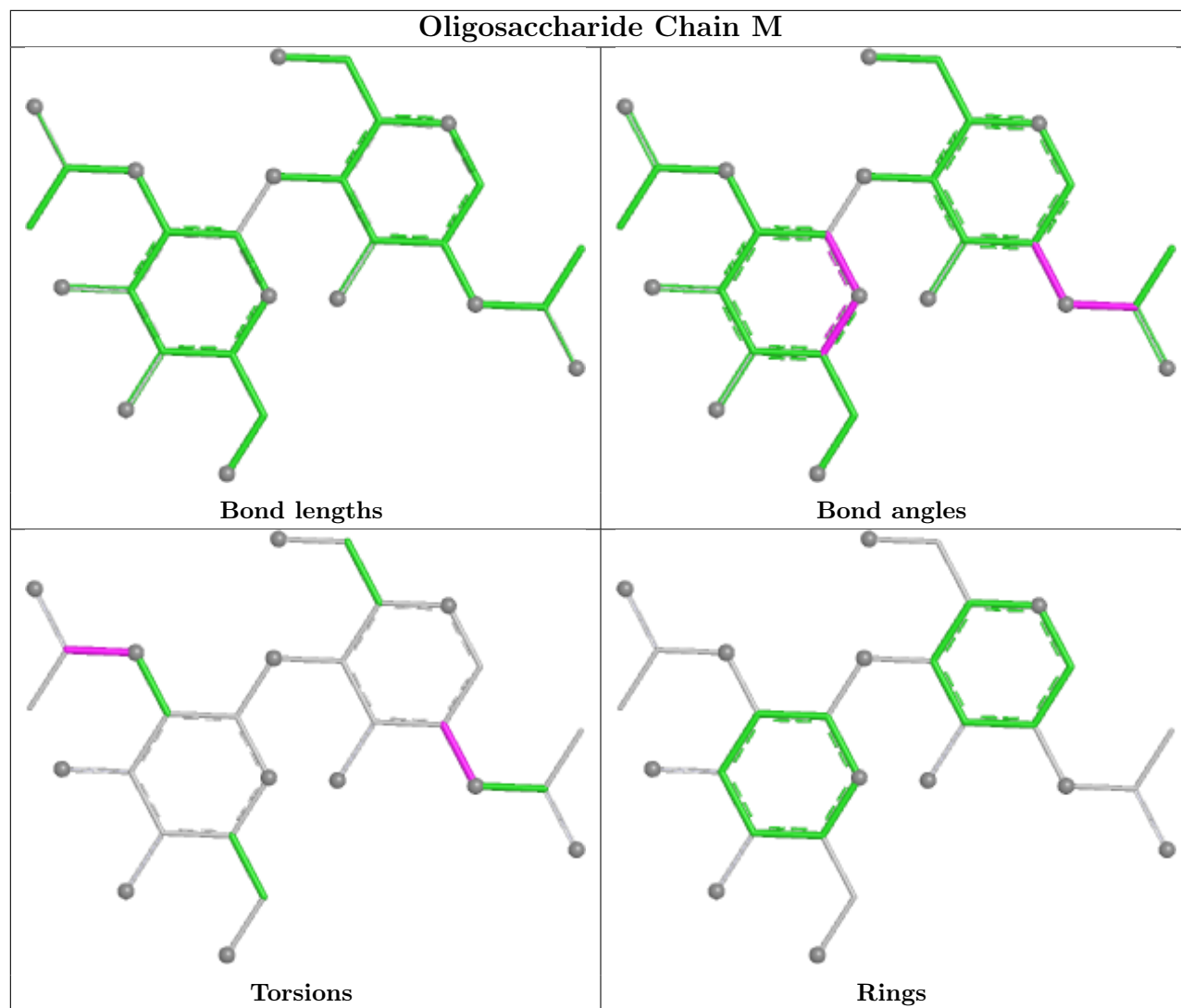


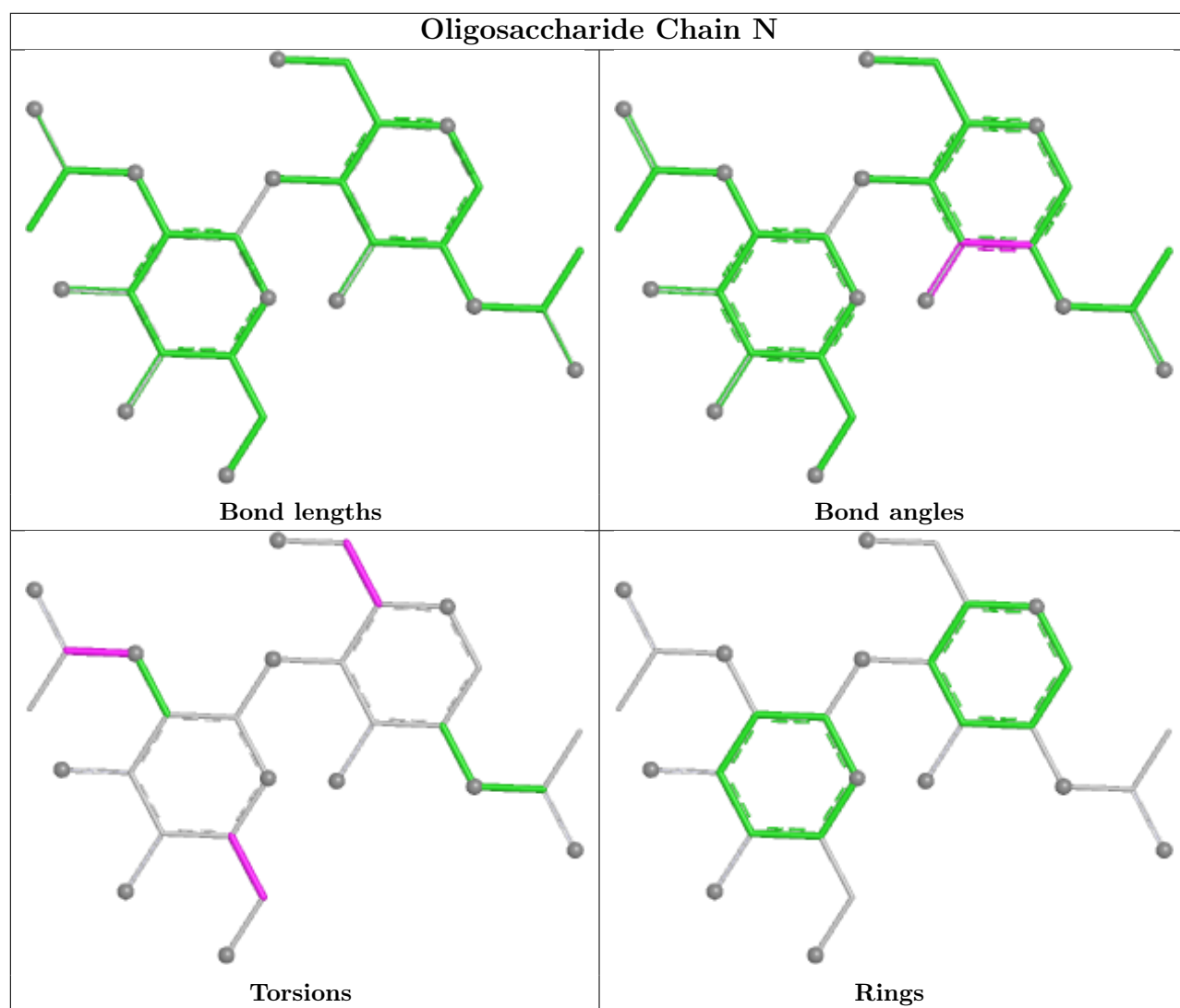


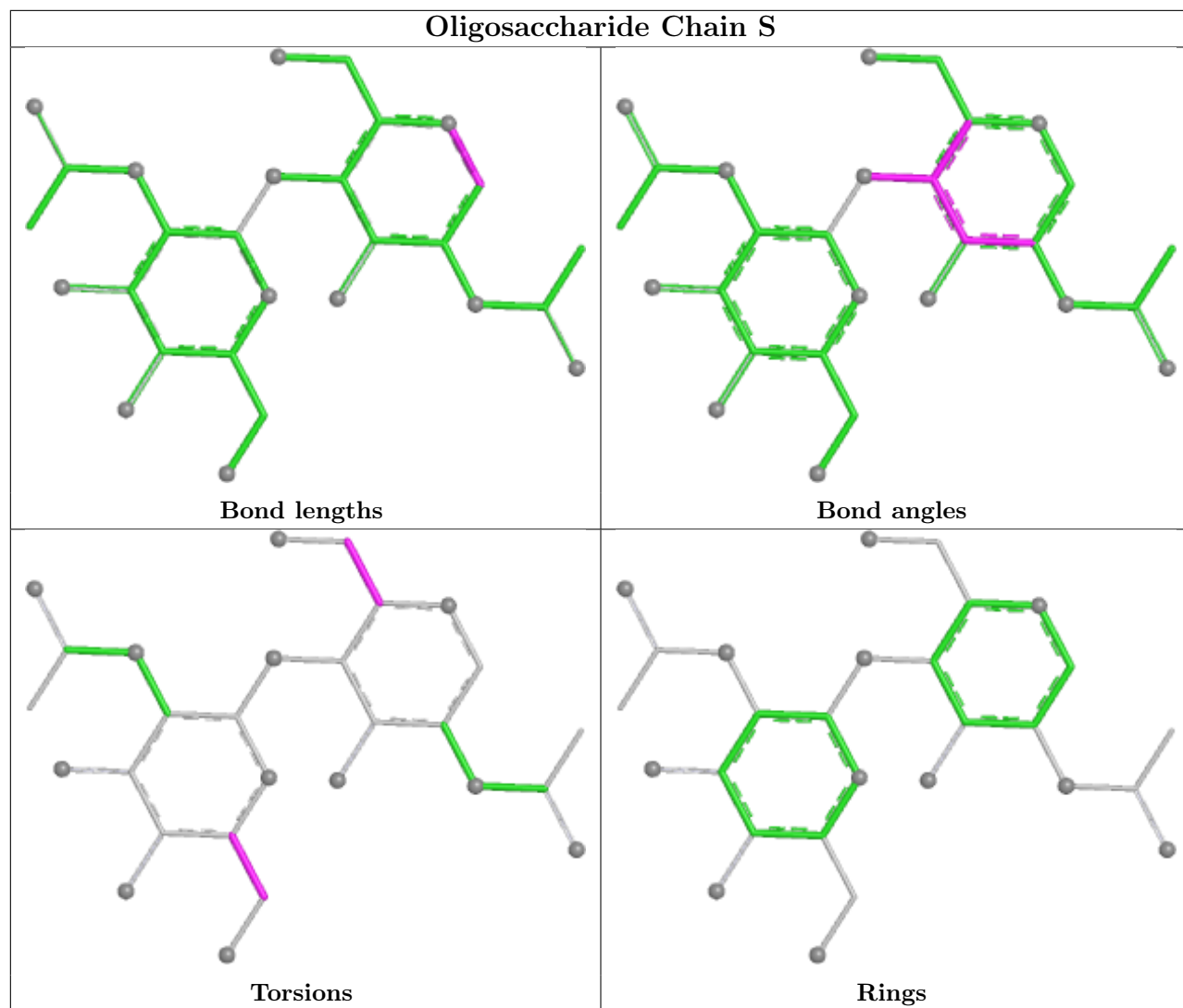


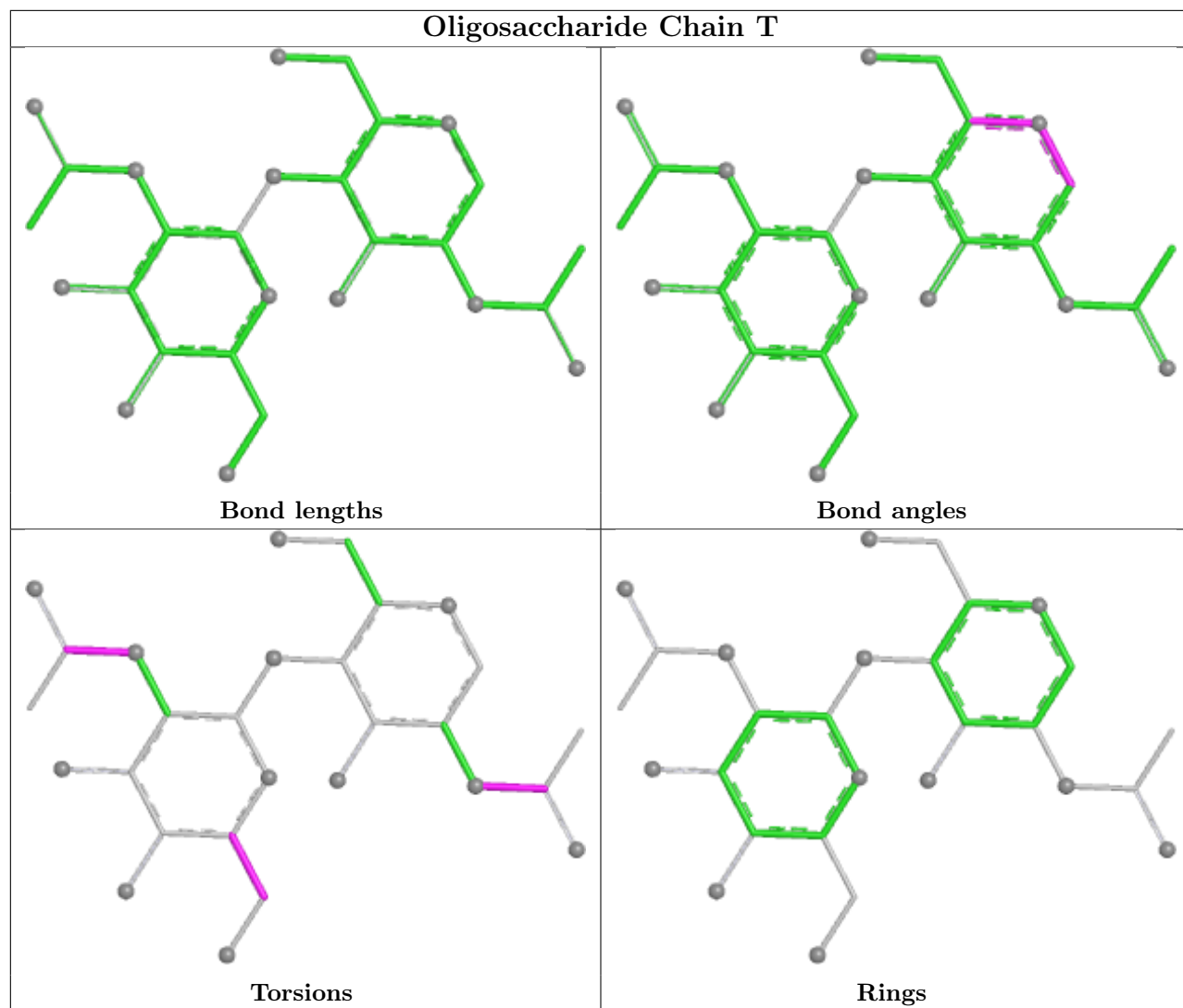


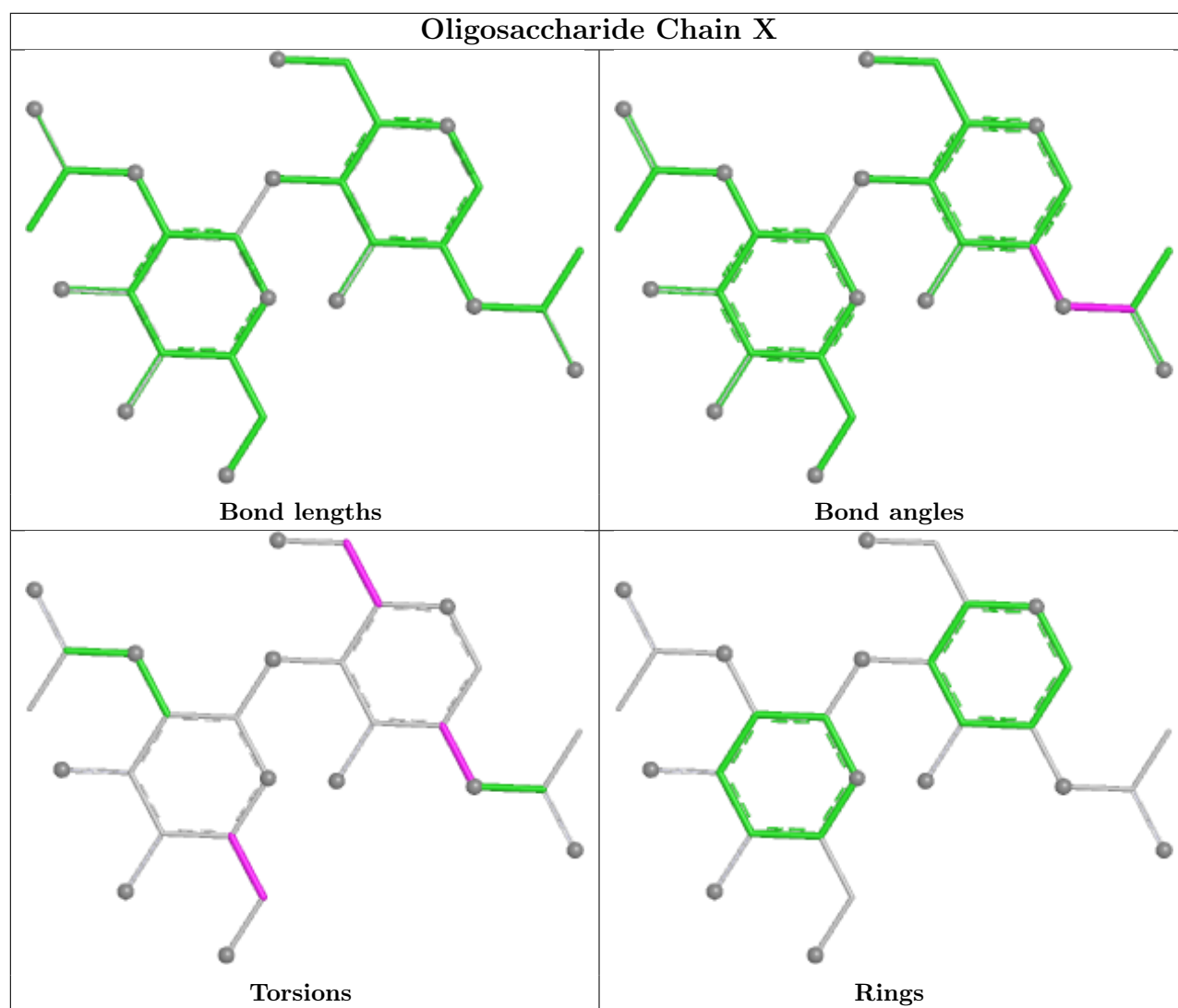


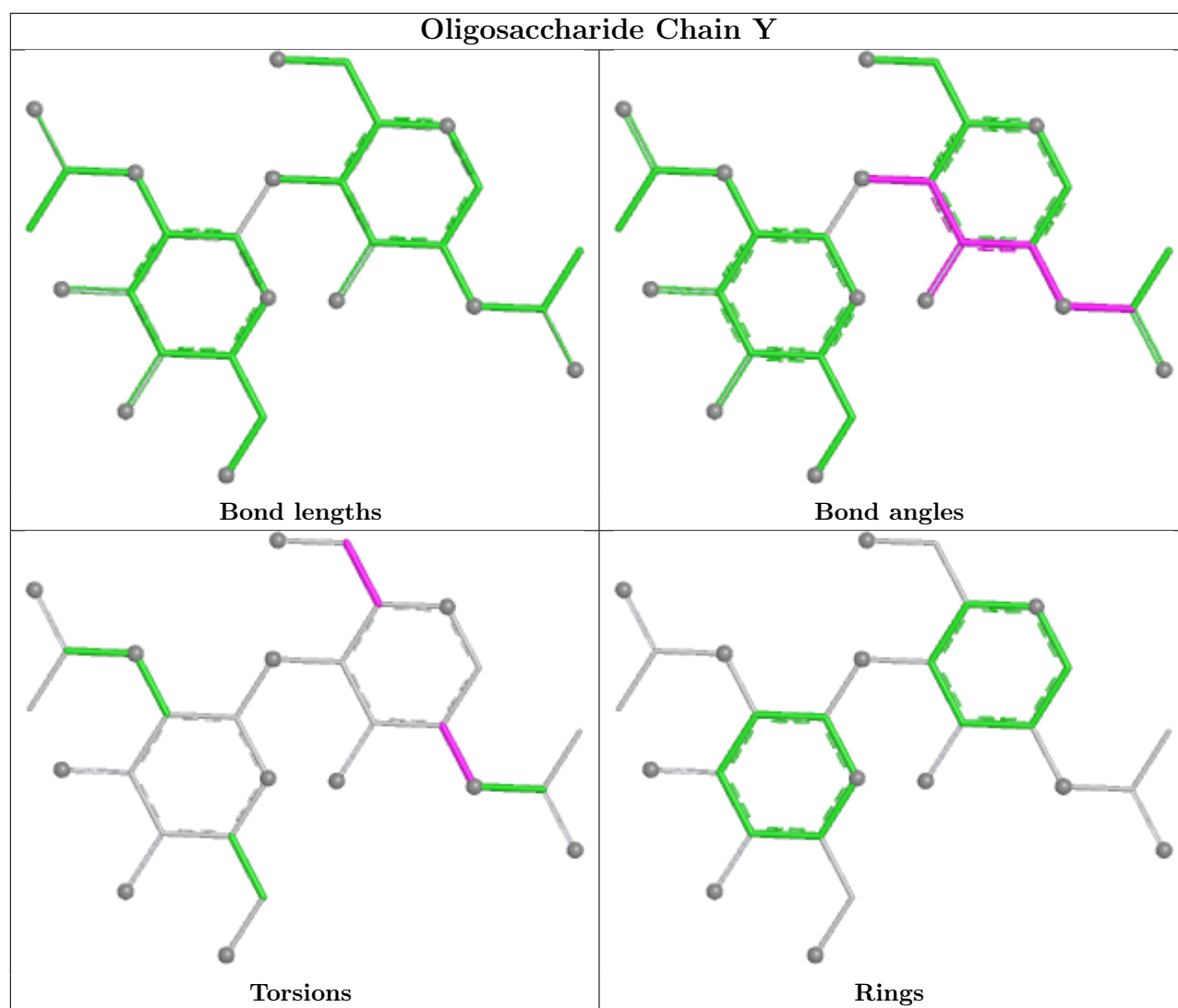


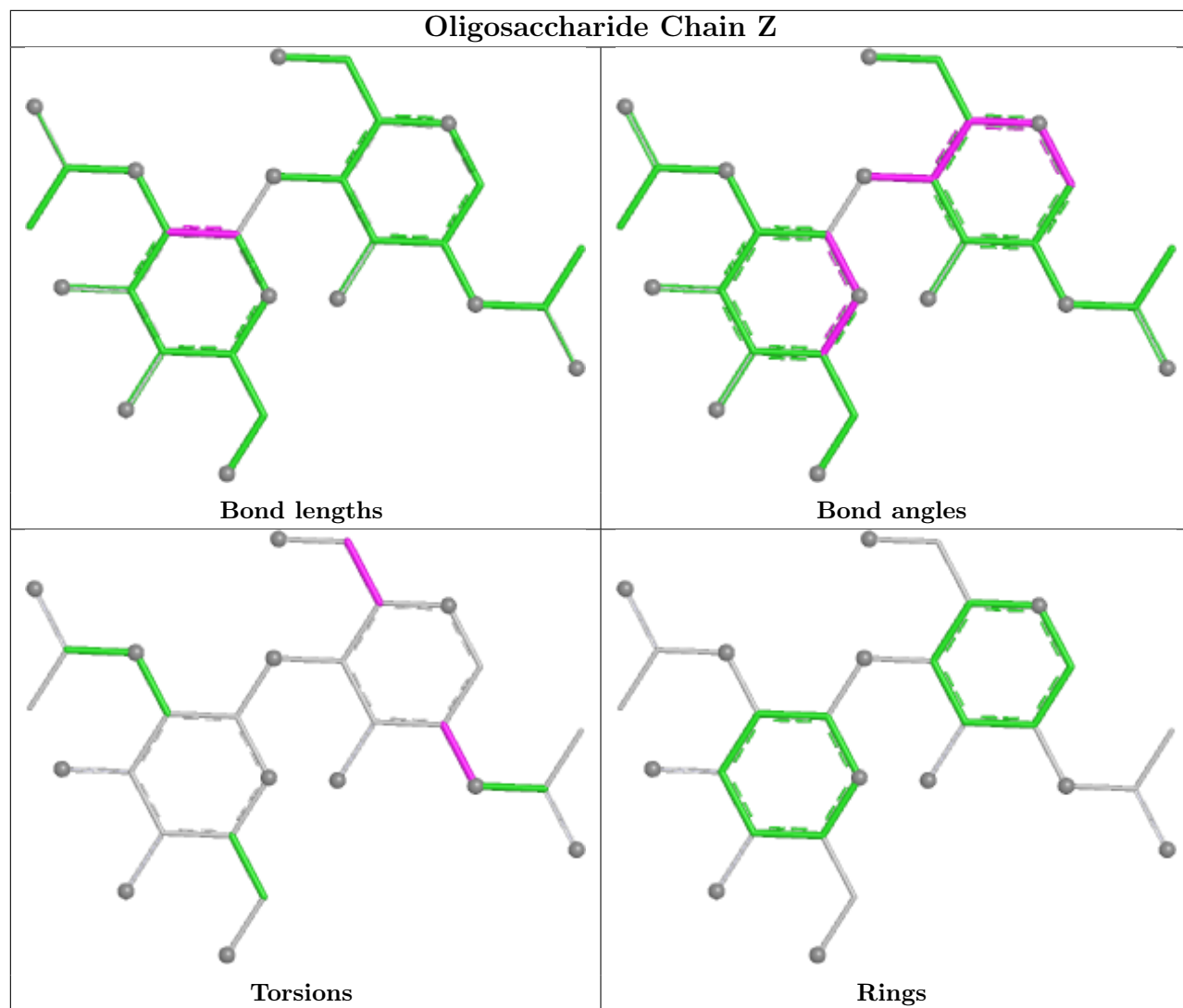


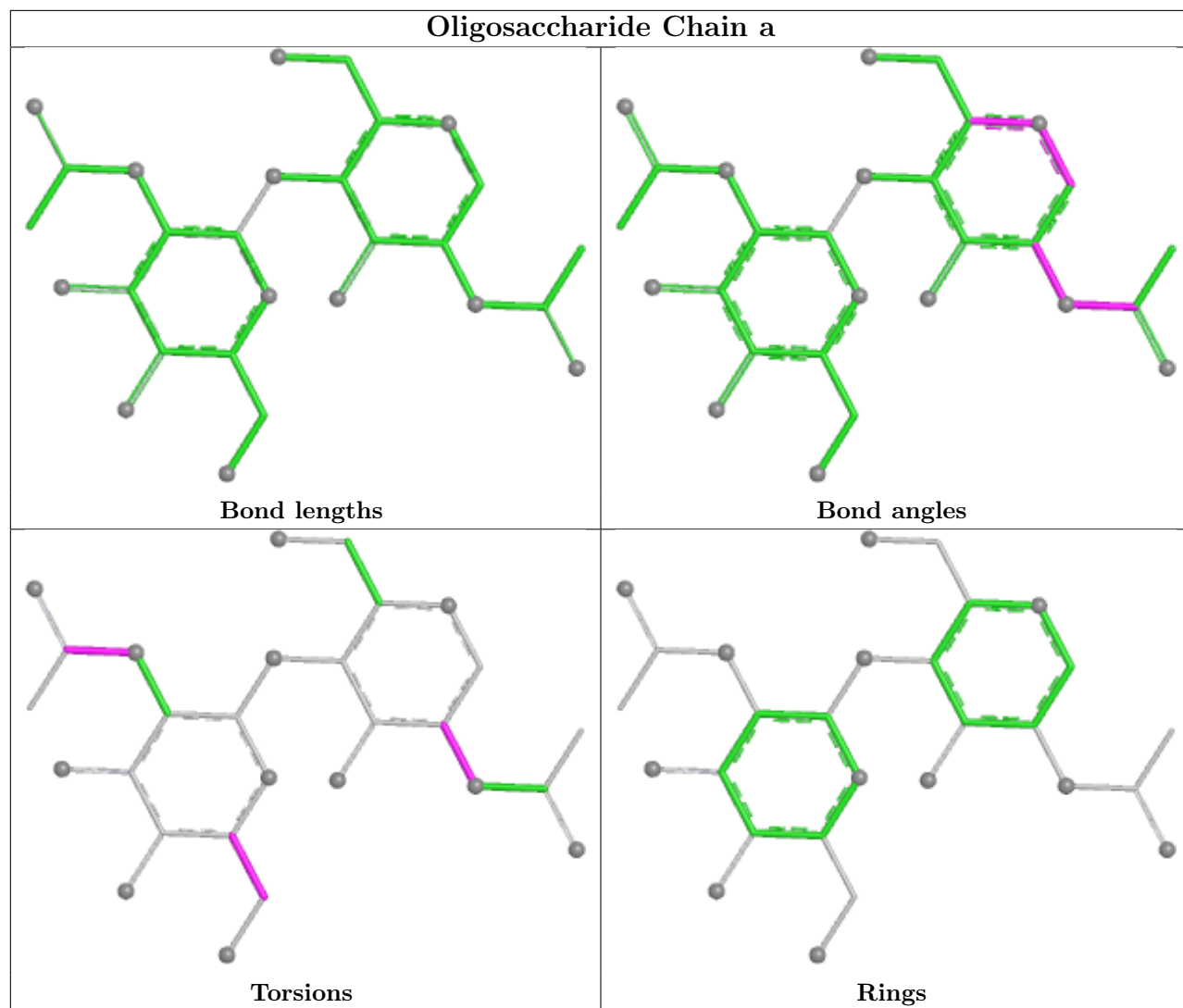


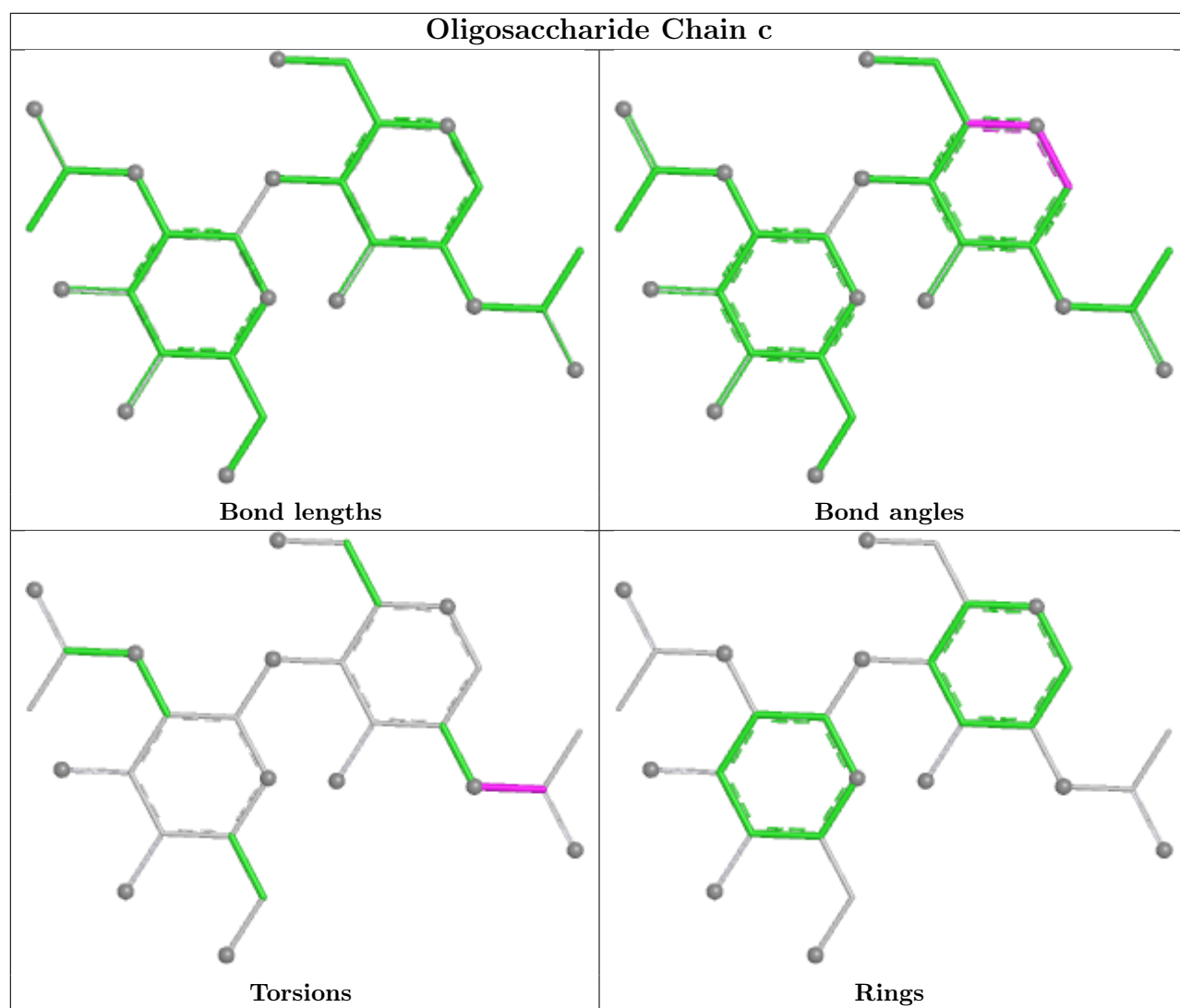


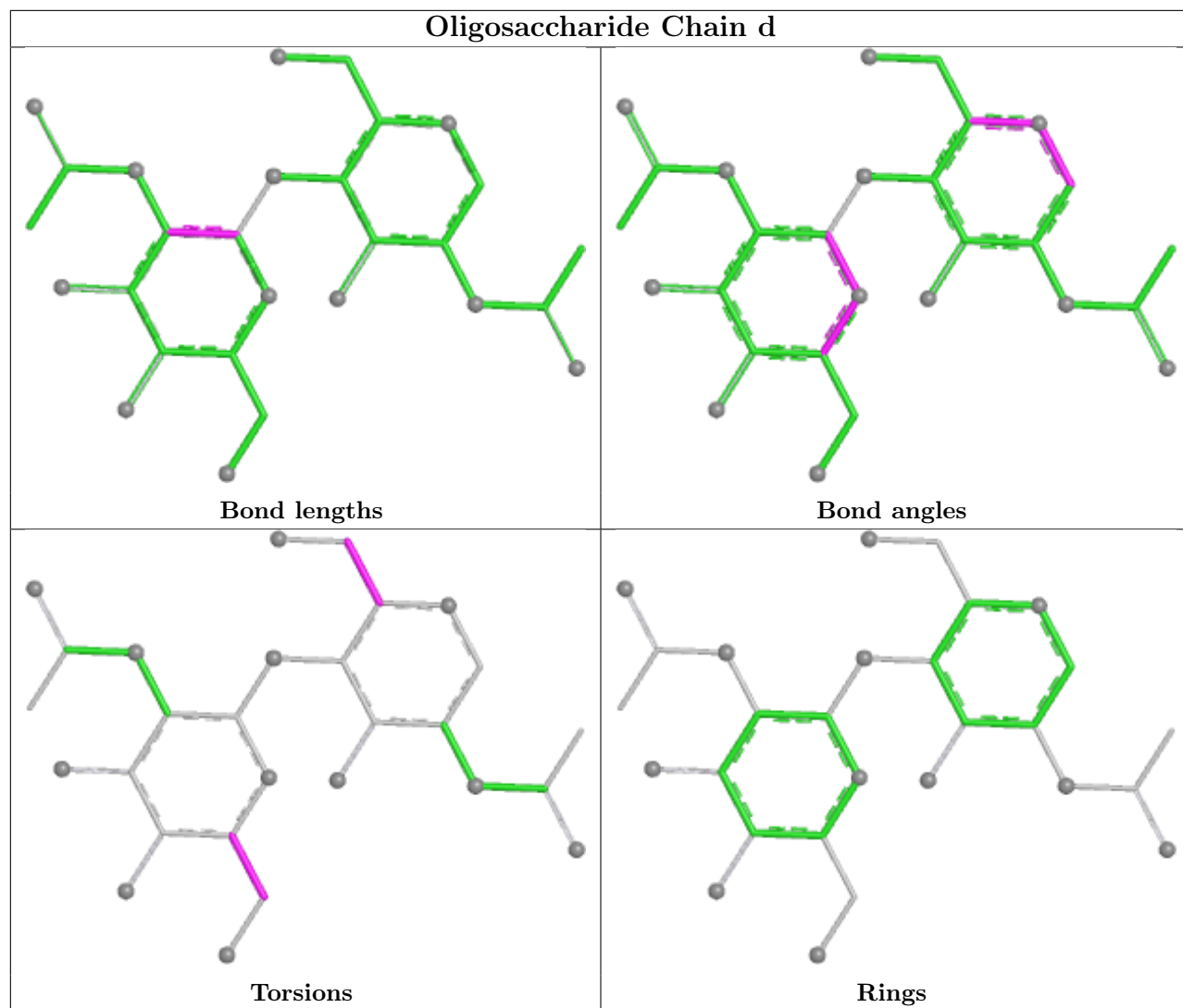


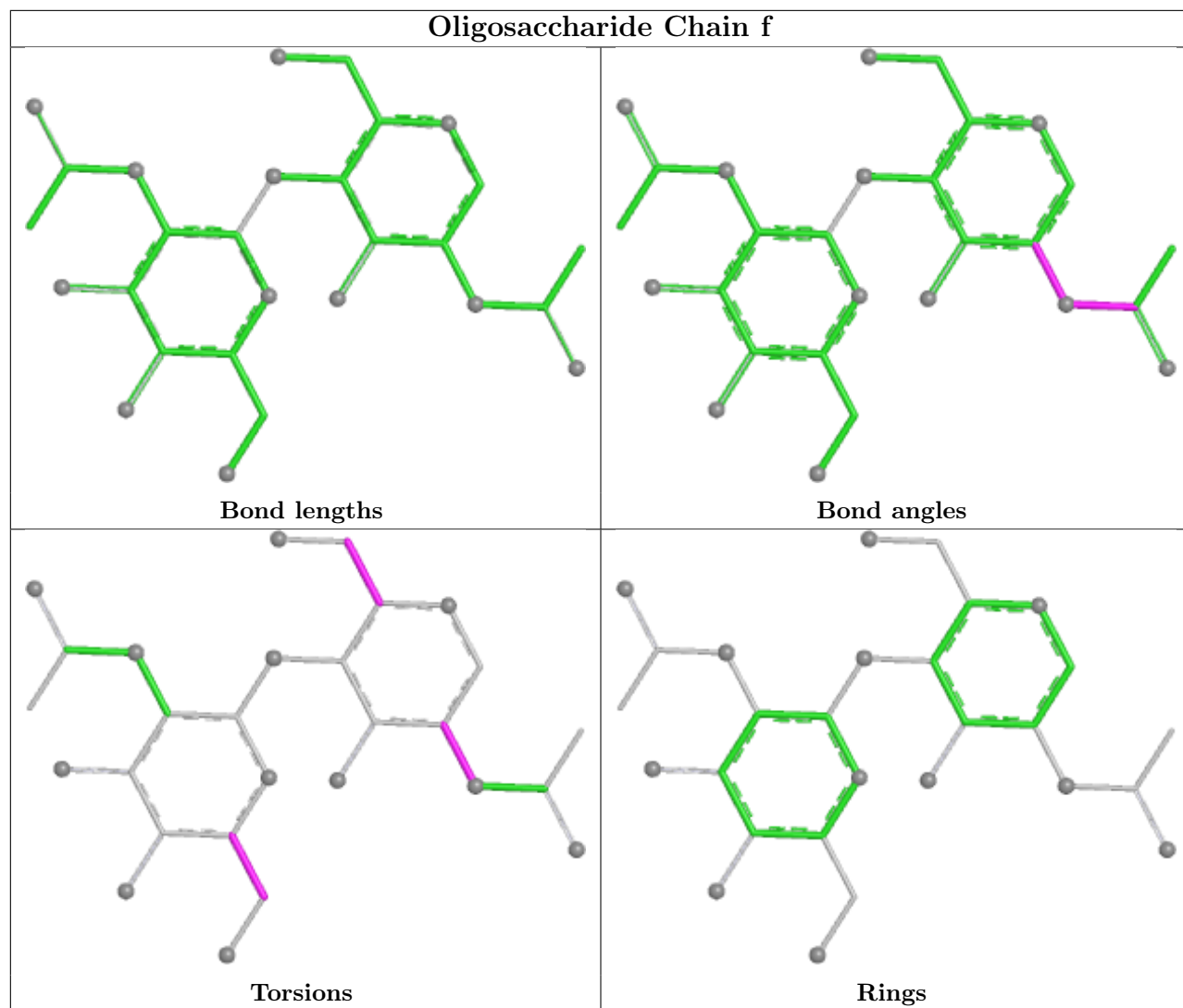


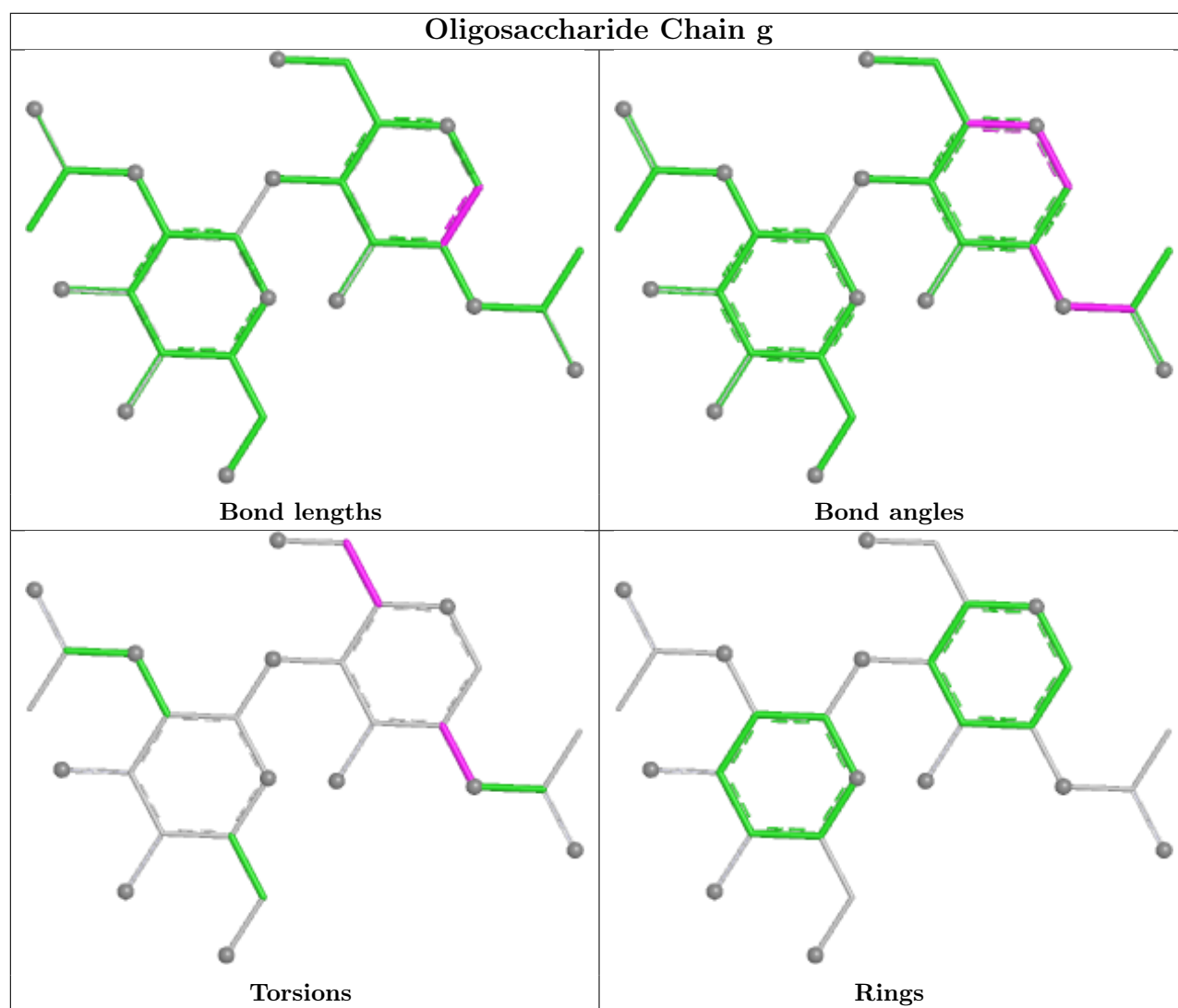


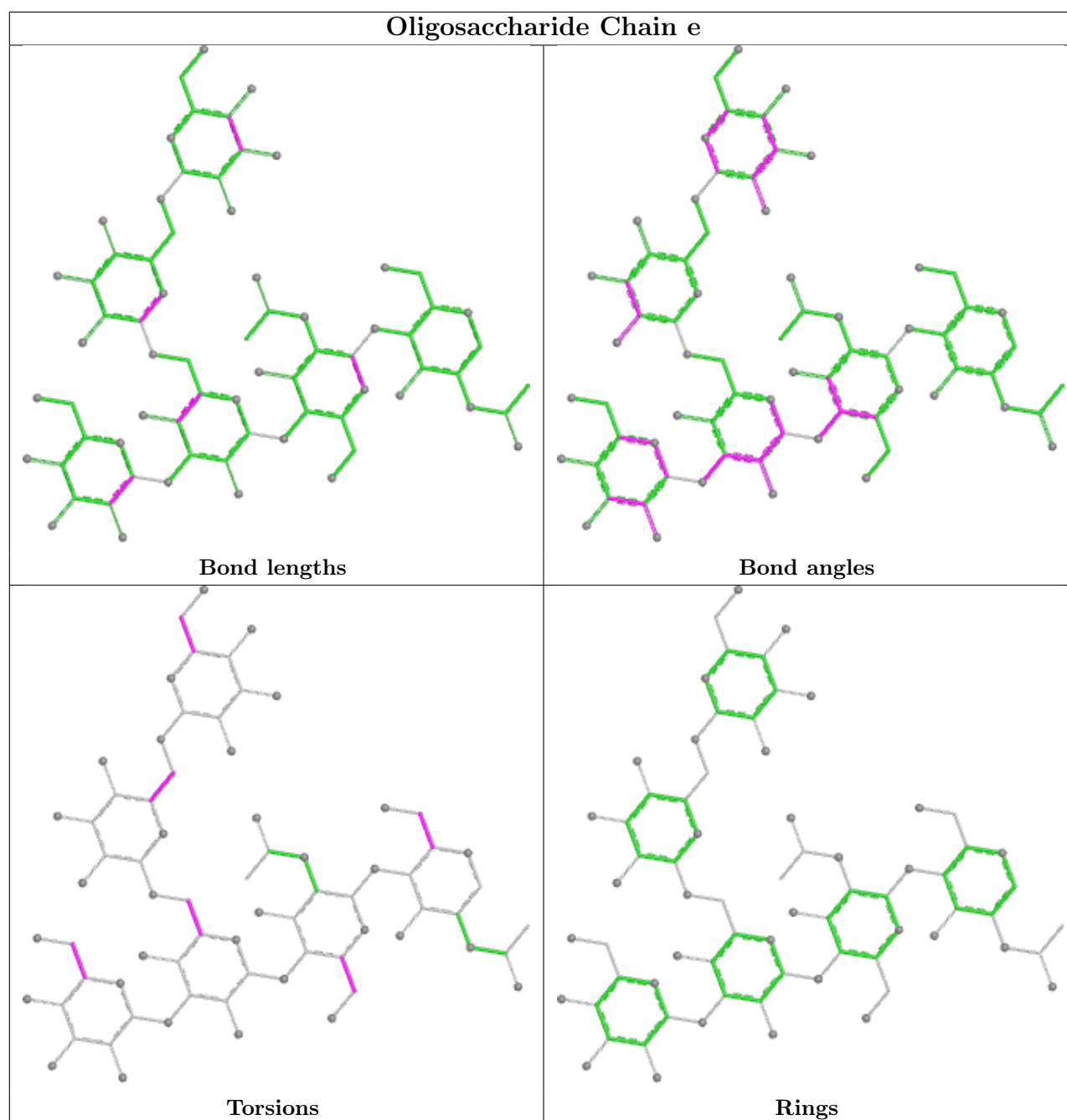












5.6 Ligand geometry [i](#)

30 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	NAG	K	628	2	14,14,15	0.76	1 (7%)	17,19,21	0.66	0
10	NAG	K	619	2	14,14,15	0.39	0	17,19,21	1.01	1 (5%)
10	NAG	R	629	2	14,14,15	0.77	1 (7%)	17,19,21	0.59	0
10	NAG	K	601	2	14,14,15	0.32	0	17,19,21	0.66	0
10	NAG	G	604	2	14,14,15	0.25	0	17,19,21	0.52	0
10	NAG	C	702	1	14,14,15	1.09	1 (7%)	17,19,21	1.74	2 (11%)
10	NAG	C	703	1	14,14,15	0.40	0	17,19,21	0.75	0
10	NAG	Q	702	1	14,14,15	1.01	1 (7%)	17,19,21	2.35	3 (17%)
10	NAG	J	701	1	14,14,15	0.47	0	17,19,21	0.96	1 (5%)
10	NAG	K	631	2	14,14,15	0.66	1 (7%)	17,19,21	0.51	0
10	NAG	Q	701	1	14,14,15	0.48	0	17,19,21	0.96	1 (5%)
10	NAG	K	608	2	14,14,15	0.24	0	17,19,21	0.52	0
10	NAG	G	628	2	14,14,15	0.67	1 (7%)	17,19,21	0.51	0
10	NAG	G	601	2	14,14,15	0.47	0	17,19,21	1.12	2 (11%)
10	NAG	G	603	2	14,14,15	0.37	0	17,19,21	0.43	0
10	NAG	R	607	2	14,14,15	0.23	0	17,19,21	0.63	1 (5%)
10	NAG	R	616	2	14,14,15	0.30	0	17,19,21	0.60	0
10	NAG	G	602	2	14,14,15	0.37	0	17,19,21	0.66	0
10	NAG	R	626	2	14,14,15	0.67	0	17,19,21	0.70	1 (5%)
10	NAG	G	623	2	14,14,15	0.46	0	17,19,21	1.26	2 (11%)
10	NAG	R	625	2	14,14,15	0.46	0	17,19,21	1.19	2 (11%)
10	NAG	C	701	1	14,14,15	0.41	0	17,19,21	0.55	0
10	NAG	G	614	2	14,14,15	0.42	0	17,19,21	1.01	1 (5%)
10	NAG	J	703	1	14,14,15	0.42	0	17,19,21	0.55	0
10	NAG	G	624	2	14,14,15	0.31	0	17,19,21	0.52	0
10	NAG	K	627	2	14,14,15	0.44	0	17,19,21	1.26	2 (11%)
10	NAG	Q	703	1	14,14,15	0.42	0	17,19,21	0.54	0
10	NAG	J	702	1	14,14,15	1.00	1 (7%)	17,19,21	2.35	3 (17%)
10	NAG	G	615	2	14,14,15	0.40	0	17,19,21	1.01	1 (5%)
10	NAG	K	620	2	14,14,15	0.37	0	17,19,21	1.00	1 (5%)

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
10	NAG	K	628	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	K	619	2	-	3/6/23/26	0/1/1/1
10	NAG	R	629	2	-	1/6/23/26	0/1/1/1
10	NAG	K	601	2	-	4/6/23/26	0/1/1/1
10	NAG	G	604	2	-	1/6/23/26	0/1/1/1
10	NAG	C	702	1	-	4/6/23/26	0/1/1/1
10	NAG	C	703	1	-	1/6/23/26	0/1/1/1
10	NAG	Q	702	1	-	4/6/23/26	0/1/1/1
10	NAG	J	701	1	-	4/6/23/26	0/1/1/1
10	NAG	K	631	2	-	1/6/23/26	0/1/1/1
10	NAG	Q	701	1	-	4/6/23/26	0/1/1/1
10	NAG	K	608	2	-	0/6/23/26	0/1/1/1
10	NAG	G	628	2	-	2/6/23/26	0/1/1/1
10	NAG	G	601	2	-	3/6/23/26	0/1/1/1
10	NAG	G	603	2	-	2/6/23/26	0/1/1/1
10	NAG	R	607	2	-	0/6/23/26	0/1/1/1
10	NAG	R	616	2	-	4/6/23/26	0/1/1/1
10	NAG	G	602	2	-	2/6/23/26	0/1/1/1
10	NAG	R	626	2	-	2/6/23/26	0/1/1/1
10	NAG	G	623	2	-	4/6/23/26	0/1/1/1
10	NAG	R	625	2	-	4/6/23/26	0/1/1/1
10	NAG	C	701	1	-	2/6/23/26	0/1/1/1
10	NAG	G	614	2	-	3/6/23/26	0/1/1/1
10	NAG	J	703	1	-	2/6/23/26	0/1/1/1
10	NAG	G	624	2	-	2/6/23/26	0/1/1/1
10	NAG	K	627	2	-	4/6/23/26	0/1/1/1
10	NAG	Q	703	1	-	2/6/23/26	0/1/1/1
10	NAG	J	702	1	-	4/6/23/26	0/1/1/1
10	NAG	G	615	2	-	4/6/23/26	0/1/1/1
10	NAG	K	620	2	-	4/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Q	702	NAG	C1-C2	2.93	1.56	1.52
10	J	702	NAG	C1-C2	2.86	1.56	1.52
10	R	629	NAG	C1-C2	2.70	1.56	1.52
10	K	628	NAG	C1-C2	2.64	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	628	NAG	C1-C2	2.35	1.55	1.52
10	K	631	NAG	C1-C2	2.32	1.55	1.52
10	C	702	NAG	C2-N2	-2.01	1.42	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	702	NAG	C2-N2-C7	8.40	134.16	122.90
10	J	702	NAG	C2-N2-C7	8.37	134.12	122.90
10	C	702	NAG	C2-N2-C7	-5.86	115.05	122.90
10	J	702	NAG	C1-C2-N2	3.67	116.22	110.43
10	Q	702	NAG	C1-C2-N2	3.63	116.16	110.43
10	K	627	NAG	C2-N2-C7	3.53	127.64	122.90
10	G	623	NAG	C2-N2-C7	3.48	127.56	122.90
10	R	625	NAG	C2-N2-C7	3.40	127.46	122.90
10	Q	701	NAG	C2-N2-C7	3.24	127.25	122.90
10	J	701	NAG	C2-N2-C7	3.21	127.21	122.90
10	G	601	NAG	C2-N2-C7	3.21	127.20	122.90
10	G	614	NAG	C2-N2-C7	3.18	127.16	122.90
10	K	619	NAG	C2-N2-C7	3.16	127.13	122.90
10	G	623	NAG	C1-O5-C5	3.11	116.35	112.19
10	G	615	NAG	C2-N2-C7	3.06	127.00	122.90
10	K	627	NAG	C1-O5-C5	3.04	116.26	112.19
10	C	702	NAG	C1-C2-N2	-2.97	105.75	110.43
10	K	620	NAG	C2-N2-C7	2.95	126.86	122.90
10	R	625	NAG	C1-O5-C5	2.68	115.77	112.19
10	R	626	NAG	C1-O5-C5	2.43	115.44	112.19
10	G	601	NAG	C1-O5-C5	2.35	115.33	112.19
10	J	702	NAG	C8-C7-N2	2.17	119.72	116.12
10	Q	702	NAG	C8-C7-N2	2.15	119.68	116.12
10	R	607	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	C	702	NAG	C1-C2-N2-C7
10	C	702	NAG	C8-C7-N2-C2
10	C	702	NAG	O7-C7-N2-C2
10	R	626	NAG	C4-C5-C6-O6
10	K	601	NAG	C4-C5-C6-O6
10	G	624	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	K	627	NAG	O5-C5-C6-O6
10	G	623	NAG	O5-C5-C6-O6
10	K	601	NAG	O5-C5-C6-O6
10	R	626	NAG	O5-C5-C6-O6
10	C	701	NAG	C4-C5-C6-O6
10	J	703	NAG	C4-C5-C6-O6
10	Q	703	NAG	C4-C5-C6-O6
10	J	701	NAG	O5-C5-C6-O6
10	Q	701	NAG	O5-C5-C6-O6
10	G	623	NAG	C4-C5-C6-O6
10	K	620	NAG	O5-C5-C6-O6
10	G	615	NAG	O5-C5-C6-O6
10	R	625	NAG	O5-C5-C6-O6
10	K	627	NAG	C4-C5-C6-O6
10	R	616	NAG	O5-C5-C6-O6
10	R	625	NAG	C4-C5-C6-O6
10	C	701	NAG	O5-C5-C6-O6
10	J	703	NAG	O5-C5-C6-O6
10	Q	703	NAG	O5-C5-C6-O6
10	G	624	NAG	O5-C5-C6-O6
10	J	701	NAG	C4-C5-C6-O6
10	Q	701	NAG	C4-C5-C6-O6
10	J	702	NAG	C8-C7-N2-C2
10	J	702	NAG	O7-C7-N2-C2
10	K	601	NAG	C8-C7-N2-C2
10	K	601	NAG	O7-C7-N2-C2
10	Q	702	NAG	C8-C7-N2-C2
10	Q	702	NAG	O7-C7-N2-C2
10	R	616	NAG	C8-C7-N2-C2
10	R	616	NAG	O7-C7-N2-C2
10	G	602	NAG	C4-C5-C6-O6
10	G	601	NAG	O5-C5-C6-O6
10	G	603	NAG	O5-C5-C6-O6
10	K	620	NAG	C4-C5-C6-O6
10	R	629	NAG	O5-C5-C6-O6
10	G	615	NAG	C4-C5-C6-O6
10	K	628	NAG	O5-C5-C6-O6
10	G	602	NAG	O5-C5-C6-O6
10	G	628	NAG	O5-C5-C6-O6
10	K	619	NAG	O5-C5-C6-O6
10	K	631	NAG	O5-C5-C6-O6
10	R	616	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	G	614	NAG	O5-C5-C6-O6
10	J	701	NAG	C1-C2-N2-C7
10	Q	701	NAG	C1-C2-N2-C7
10	G	601	NAG	C3-C2-N2-C7
10	G	614	NAG	C3-C2-N2-C7
10	G	615	NAG	C3-C2-N2-C7
10	K	619	NAG	C3-C2-N2-C7
10	K	628	NAG	C4-C5-C6-O6
10	C	703	NAG	C1-C2-N2-C7
10	G	601	NAG	C1-C2-N2-C7
10	G	604	NAG	C1-C2-N2-C7
10	G	614	NAG	C1-C2-N2-C7
10	G	615	NAG	C1-C2-N2-C7
10	G	623	NAG	C1-C2-N2-C7
10	G	628	NAG	C1-C2-N2-C7
10	J	702	NAG	C1-C2-N2-C7
10	K	619	NAG	C1-C2-N2-C7
10	K	620	NAG	C1-C2-N2-C7
10	K	627	NAG	C1-C2-N2-C7
10	Q	702	NAG	C1-C2-N2-C7
10	R	625	NAG	C1-C2-N2-C7
10	C	702	NAG	C3-C2-N2-C7
10	G	623	NAG	C3-C2-N2-C7
10	J	701	NAG	C3-C2-N2-C7
10	J	702	NAG	C3-C2-N2-C7
10	K	620	NAG	C3-C2-N2-C7
10	K	627	NAG	C3-C2-N2-C7
10	Q	701	NAG	C3-C2-N2-C7
10	Q	702	NAG	C3-C2-N2-C7
10	R	625	NAG	C3-C2-N2-C7
10	G	603	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	702	NAG	4	0
10	G	602	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20175. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.