



## wwPDB EM Validation Summary Report ⓘ

Jul 15, 2025 – 11:18 AM JST

PDB ID : 8ZI4 / pdb\_00008zi4  
EMDB ID : EMD-60121  
Title : Cryo-EM structure of wtEP-trypsinogen  
Authors : Song, Q.Y.; Ding, Z.Y.; Huang, H.J.  
Deposited on : 2024-05-13  
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis	: <b>FAILED</b>
Mogul	: 1.8.5 (274361), CSD as541be (2020)
MolProbity	: 4-5-2 with Phenix2.0rc1
Percentile statistics	: 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	: <b>FAILED</b>
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.44

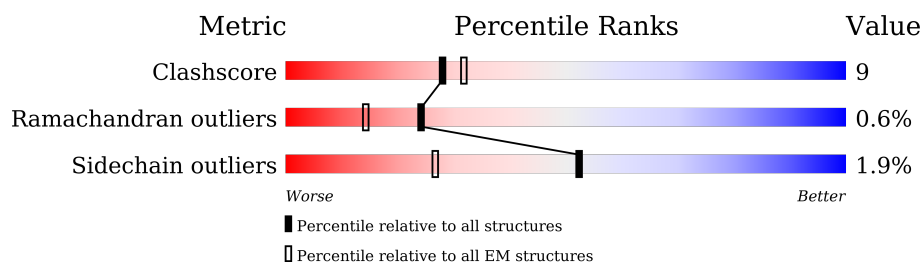
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.95 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	C	232	
2	D	235	
3	A	603	
4	B	3	
4	E	3	
4	L	3	
4	M	3	
4	N	3	
4	O	3	

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Mol	Chain	Length	Quality of chain
5	F	2	 100%
5	G	2	 100%
6	H	4	 75% 25%
6	K	4	 25% 25% 50%
7	I	3	 100%
8	J	4	 50% 25% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	NAG	A	802	-	-	X	-
9	NAG	A	803	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 8818 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 Serine protease 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	232	Total	C	N	O	S	0	0
			1755	1095	304	344	12		

- Molecule 2 is a protein called Enteropeptidase catalytic light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	235	Total	C	N	O	S	0	0
			1835	1161	319	340	15		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	825	ALA	HIS	engineered mutation	UNP P98073
D	876	ALA	ASP	engineered mutation	UNP P98073
D	971	ALA	SER	engineered mutation	UNP P98073

- Molecule 3 is a protein called Enteropeptidase non-catalytic heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	603	Total	C	N	O	S	0	0
			4693	2960	775	929	29		

- Molecule 4 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
4	B	3	Total	C	N	O		0	0
			39	22	2	15			

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

- Molecule 5 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
5	F	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	4	Total	C	N	O	0	0
			50	28	2	20		
6	K	4	Total	C	N	O	0	0
			50	28	2	20		

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



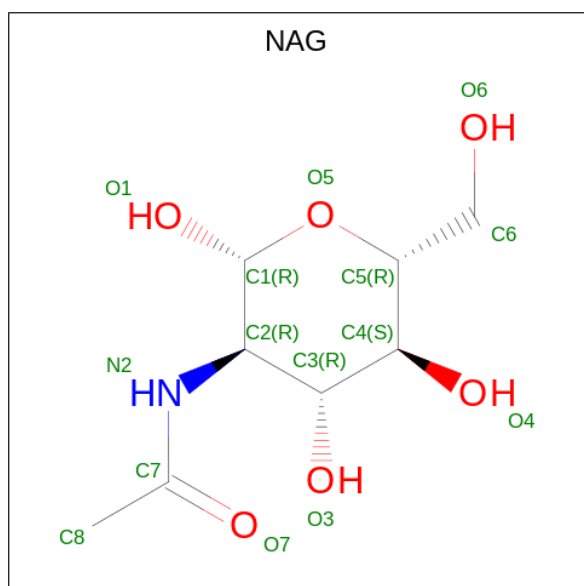
Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	J	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf
9	D	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	

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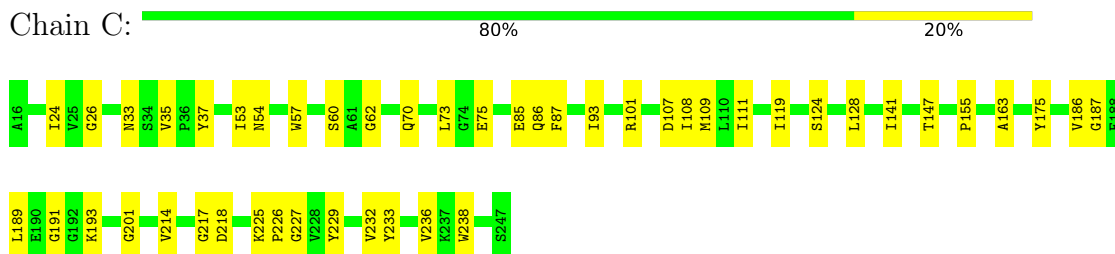
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Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	

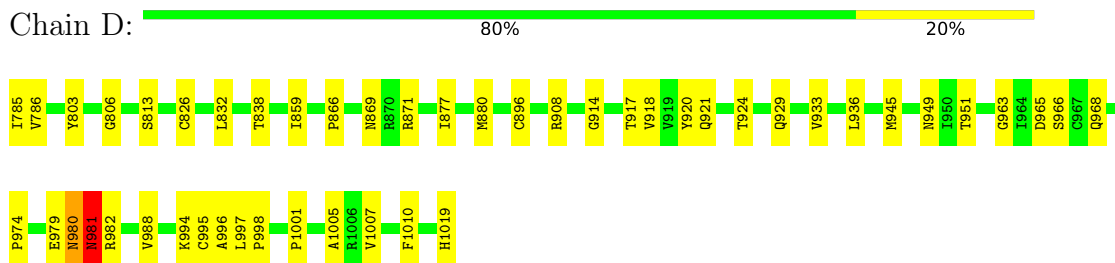
### 3 Residue-property plots

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

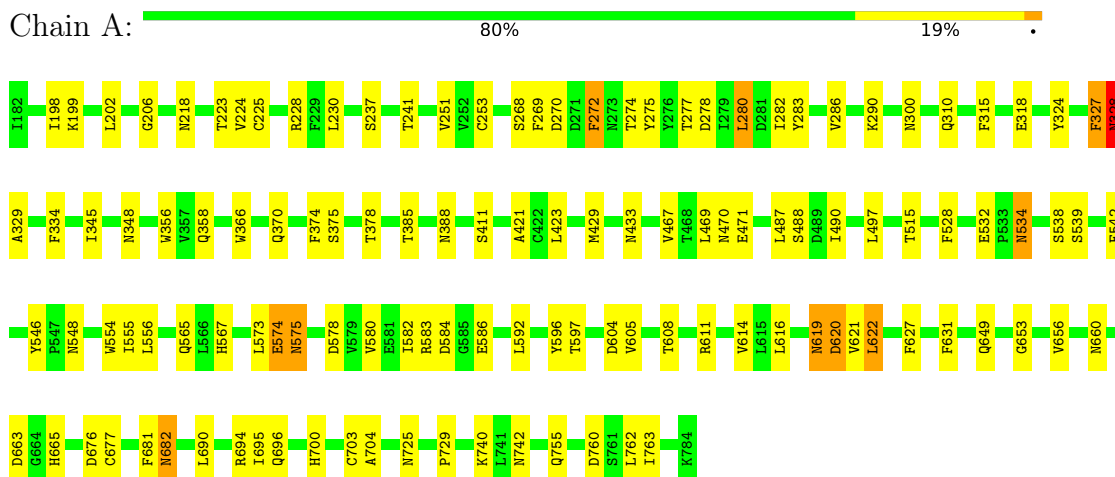
- Molecule 1: Serine protease 1



- Molecule 2: Enteropeptidase catalytic light chain



- Molecule 3: Enteropeptidase non-catalytic heavy chain



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



Chain B:  100%

NA01  
NA02  
BM03

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

Chain E:  100%


NA01  
NA02  
BM03

- Molecule 4: 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%

NA01  
NA02  
BM03

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

Chain M:  67% 33%

NA01  
NA02  
BM03

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

Chain N:  100%

NA01  
NA02  
BM03

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

Chain O:  100%

NA01  
NA02  
BM03

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

Chain F:  100%

NA01  
NA02

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

Chain G:  100%


NAG1  
NAG2

- Molecule 6: 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:  75% 25%

NAG1  
NAG2  
BMA3  
MAN4

- Molecule 6: 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 K:  25% 25% 50%

NAG1  
NAG2  
BMA3  
MAN4

- Molecule 7: beta-D-mannopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

NAG1  
NAG2  
BMA3

- Molecule 8: 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 J:  50% 25% 25%

NAG1  
NAG2  
BMA3  
MAN4

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	311357	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	46	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.07	0/1792	0.24	0/2431
2	D	0.13	0/1883	0.28	0/2563
3	A	0.14	0/4813	0.36	6/6558 (0.1%)
All	All	0.13	0/8488	0.32	6/11552 (0.1%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	682	ASN	CA-CB-CG	9.15	121.75	112.60
3	A	327	PHE	O-C-N	6.95	131.75	123.27
3	A	328	ASN	CA-C-N	-6.60	111.24	122.33
3	A	328	ASN	C-N-CA	-6.60	111.24	122.33
3	A	682	ASN	CA-C-N	-5.37	116.77	122.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1755	0	1695	30	0
2	D	1835	0	1763	30	0
3	A	4693	0	4411	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	39	0	34	0	0
4	E	39	0	34	0	0
4	L	39	0	34	1	0
4	M	39	0	34	1	0
4	N	39	0	34	0	0
4	O	39	0	34	0	0
5	F	28	0	25	0	0
5	G	28	0	25	5	0
6	H	50	0	43	0	0
6	K	50	0	43	2	0
7	I	39	0	34	0	0
8	J	50	0	43	1	0
9	A	42	0	39	18	0
9	D	14	0	13	0	0
All	All	8818	0	8338	162	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 9.

The worst 5 of 162 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)
3:A:315:PHE:HE1	3:A:327:PHE:CE2	1.63	1.17
3:A:690:LEU:CB	9:A:802:NAG:H82	1.86	1.05
3:A:690:LEU:HB2	9:A:802:NAG:H82	1.44	0.96
3:A:315:PHE:CE1	3:A:327:PHE:CE2	2.55	0.94
3:A:315:PHE:HE1	3:A:327:PHE:CD2	1.88	0.91

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	230/232 (99%)	221 (96%)	9 (4%)	0	100	100
2	D	233/235 (99%)	218 (94%)	12 (5%)	3 (1%)	10	27
3	A	601/603 (100%)	551 (92%)	47 (8%)	3 (0%)	25	50
All	All	1064/1070 (99%)	990 (93%)	68 (6%)	6 (1%)	24	46

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	224	VAL
3	A	575	ASN
2	D	786	VAL
2	D	980	ASN
2	D	981	ASN

### 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	192/192 (100%)	191 (100%)	1 (0%)	86	93
2	D	196/196 (100%)	190 (97%)	6 (3%)	35	59
3	A	529/529 (100%)	519 (98%)	10 (2%)	52	73
All	All	917/917 (100%)	900 (98%)	17 (2%)	52	73

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	620	ASP
3	A	682	ASN
3	A	272	PHE
3	A	280	LEU
3	A	328	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	480	ASN
3	A	748	HIS
3	A	700	HIS
3	A	310	GLN
3	A	466	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

37 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	$\# Z  > 2$
4	NAG	B	1	4,2	14,14,15	0.21	0	17,19,21	0.44	0
4	NAG	B	2	4	14,14,15	0.27	0	17,19,21	0.53	0
4	BMA	B	3	4	11,11,12	0.58	0	15,15,17	0.75	0
4	NAG	E	1	4,2	14,14,15	0.25	0	17,19,21	0.46	0
4	NAG	E	2	4	14,14,15	0.22	0	17,19,21	0.41	0
4	BMA	E	3	4	11,11,12	0.58	0	15,15,17	0.82	0
5	NAG	F	1	2,5	14,14,15	0.23	0	17,19,21	0.44	0
5	NAG	F	2	5	14,14,15	0.30	0	17,19,21	0.45	0
5	NAG	G	1	2,5	14,14,15	0.70	0	17,19,21	1.96	3 (17%)
5	NAG	G	2	5	14,14,15	0.52	0	17,19,21	1.30	3 (17%)
6	NAG	H	1	3,6	14,14,15	0.26	0	17,19,21	0.38	0
6	NAG	H	2	6	14,14,15	0.30	0	17,19,21	0.60	0
6	BMA	H	3	6	11,11,12	0.67	0	15,15,17	0.76	0
6	MAN	H	4	6	11,11,12	0.68	0	15,15,17	1.00	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	I	1	3,7	14,14,15	0.29	0	17,19,21	0.53	0
7	NAG	I	2	7	14,14,15	0.32	0	17,19,21	0.46	0
7	BMA	I	3	7	11,11,12	0.62	0	15,15,17	0.74	0
8	NAG	J	1	3,8	14,14,15	0.39	0	17,19,21	1.25	1 (5%)
8	NAG	J	2	8	14,14,15	0.22	0	17,19,21	0.47	0
8	BMA	J	3	8	11,11,12	0.58	0	15,15,17	0.70	0
8	MAN	J	4	8	11,11,12	0.75	0	15,15,17	1.23	2 (13%)
6	NAG	K	1	3,6	14,14,15	0.74	1 (7%)	17,19,21	0.74	1 (5%)
6	NAG	K	2	6	14,14,15	0.79	1 (7%)	17,19,21	0.68	0
6	BMA	K	3	6	11,11,12	0.58	0	15,15,17	0.83	0
6	MAN	K	4	6	11,11,12	0.64	0	15,15,17	0.94	2 (13%)
4	NAG	L	1	3,4	14,14,15	0.24	0	17,19,21	1.20	2 (11%)
4	NAG	L	2	4	14,14,15	0.35	0	17,19,21	0.69	1 (5%)
4	BMA	L	3	4	11,11,12	0.59	0	15,15,17	0.78	0
4	NAG	M	1	3,4	14,14,15	0.17	0	17,19,21	0.40	0
4	NAG	M	2	4	14,14,15	0.23	0	17,19,21	0.47	0
4	BMA	M	3	4	11,11,12	0.60	0	15,15,17	0.73	0
4	NAG	N	1	3,4	14,14,15	0.42	0	17,19,21	0.49	0
4	NAG	N	2	4	14,14,15	0.32	0	17,19,21	0.48	0
4	BMA	N	3	4	11,11,12	0.62	0	15,15,17	0.80	0
4	NAG	O	1	3,4	14,14,15	0.22	0	17,19,21	0.40	0
4	NAG	O	2	4	14,14,15	0.26	0	17,19,21	0.53	0
4	BMA	O	3	4	11,11,12	0.57	0	15,15,17	0.77	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
4	NAG	B	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	B	2	4	-	1/6/23/26	0/1/1/1
4	BMA	B	3	4	-	0/2/19/22	0/1/1/1
4	NAG	E	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	1/2/19/22	0/1/1/1
5	NAG	F	1	2,5	-	1/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	NAG	G	1	2,5	-	6/6/23/26	0/1/1/1
5	NAG	G	2	5	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	H	1	3,6	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	1/6/23/26	0/1/1/1
6	BMA	H	3	6	-	1/2/19/22	0/1/1/1
6	MAN	H	4	6	-	1/2/19/22	0/1/1/1
7	NAG	I	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	I	2	7	-	2/6/23/26	0/1/1/1
7	BMA	I	3	7	-	0/2/19/22	0/1/1/1
8	NAG	J	1	3,8	-	3/6/23/26	0/1/1/1
8	NAG	J	2	8	-	4/6/23/26	0/1/1/1
8	BMA	J	3	8	-	2/2/19/22	0/1/1/1
8	MAN	J	4	8	-	0/2/19/22	1/1/1/1
6	NAG	K	1	3,6	-	4/6/23/26	0/1/1/1
6	NAG	K	2	6	-	3/6/23/26	0/1/1/1
6	BMA	K	3	6	-	1/2/19/22	0/1/1/1
6	MAN	K	4	6	-	0/2/19/22	0/1/1/1
4	NAG	L	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	L	2	4	-	1/6/23/26	0/1/1/1
4	BMA	L	3	4	-	0/2/19/22	0/1/1/1
4	NAG	M	1	3,4	-	4/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	BMA	M	3	4	-	0/2/19/22	0/1/1/1
4	NAG	N	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	BMA	N	3	4	-	0/2/19/22	0/1/1/1
4	NAG	O	1	3,4	-	4/6/23/26	0/1/1/1
4	NAG	O	2	4	-	3/6/23/26	0/1/1/1
4	BMA	O	3	4	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	1	NAG	O5-C1	-2.60	1.39	1.43
6	K	2	NAG	C1-C2	2.10	1.55	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	1	NAG	C1-O5-C5	4.60	118.43	112.19
8	J	1	NAG	C2-N2-C7	4.31	129.04	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	1	NAG	O4-C4-C5	4.21	119.76	109.30
5	G	1	NAG	O5-C1-C2	-4.11	104.80	111.29
8	J	4	MAN	C1-O5-C5	3.66	117.15	112.19

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
8	J	2	NAG	O5-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
7	I	2	NAG	O5-C5-C6-O6

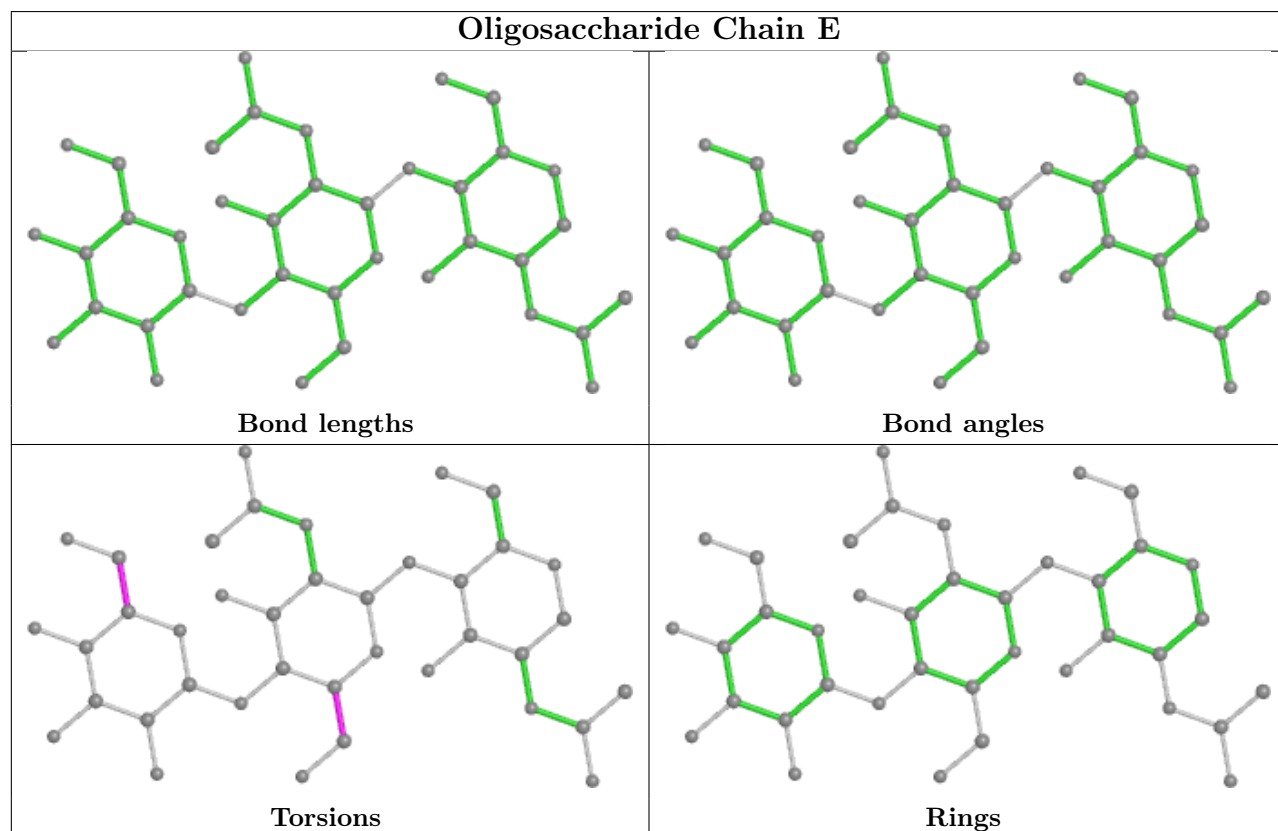
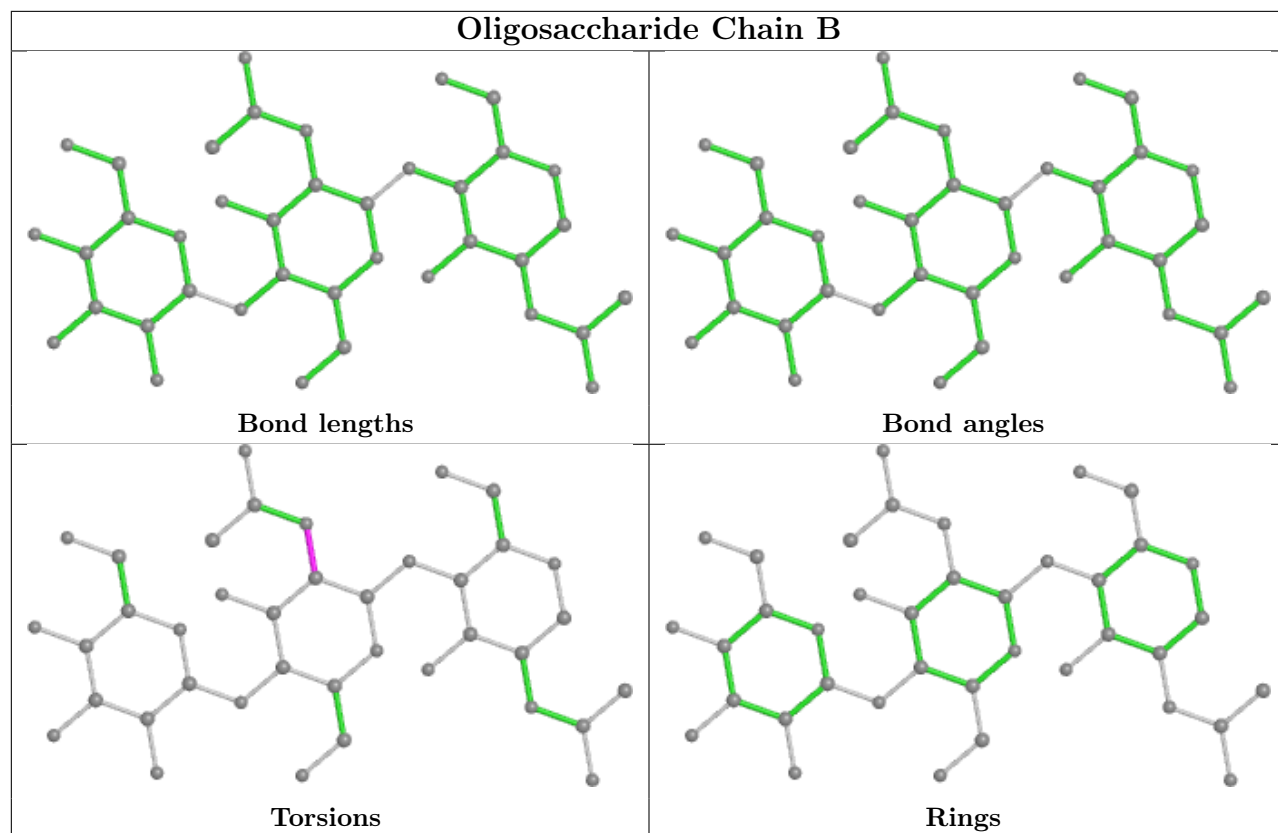
All (1) ring outliers are listed below:

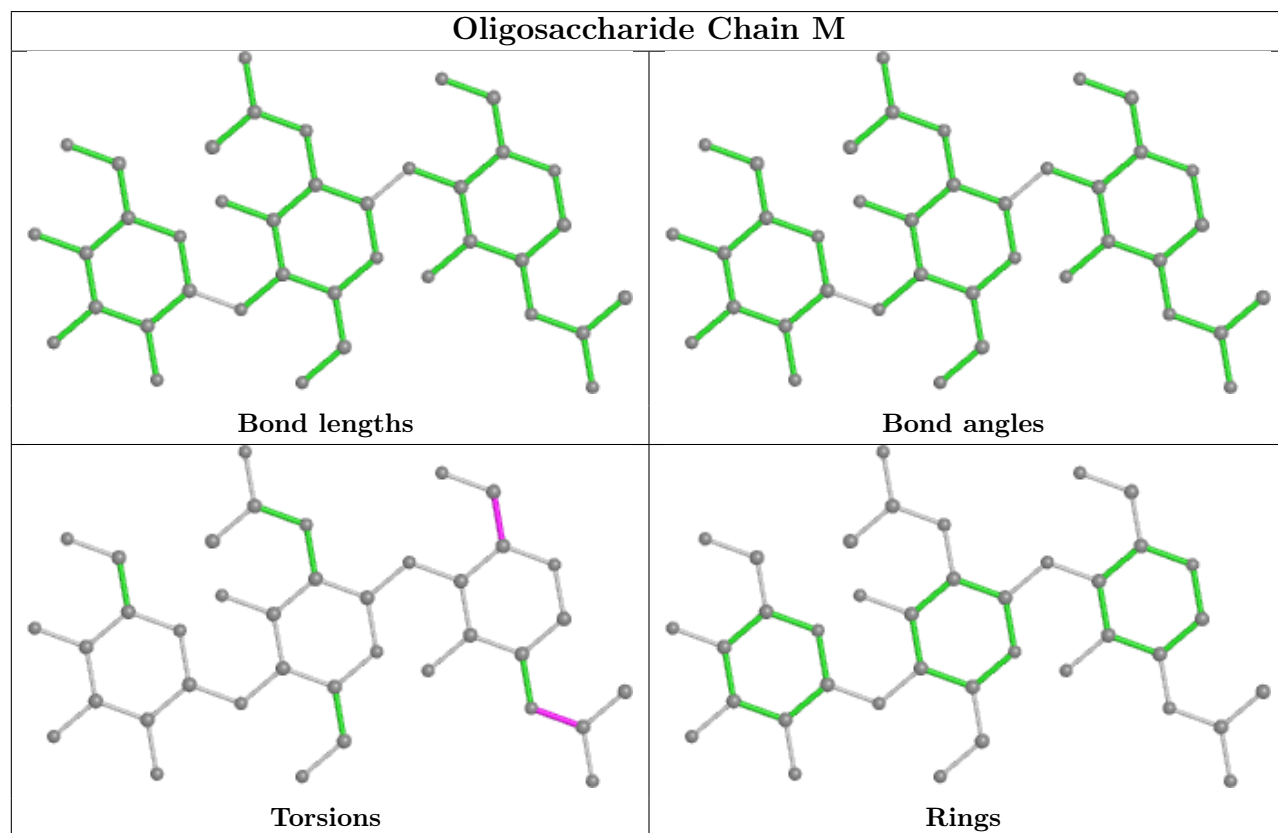
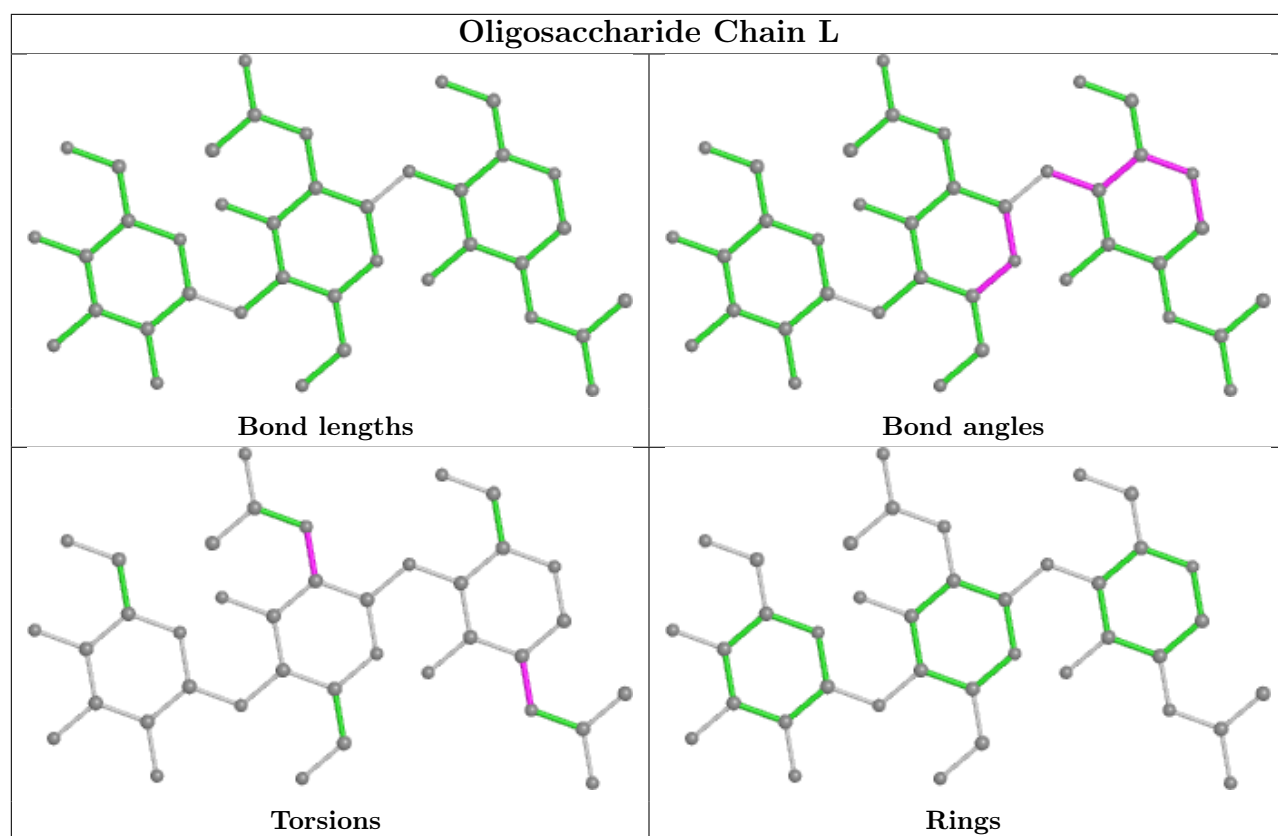
Mol	Chain	Res	Type	Atoms
8	J	4	MAN	C1-C2-C3-C4-C5-O5

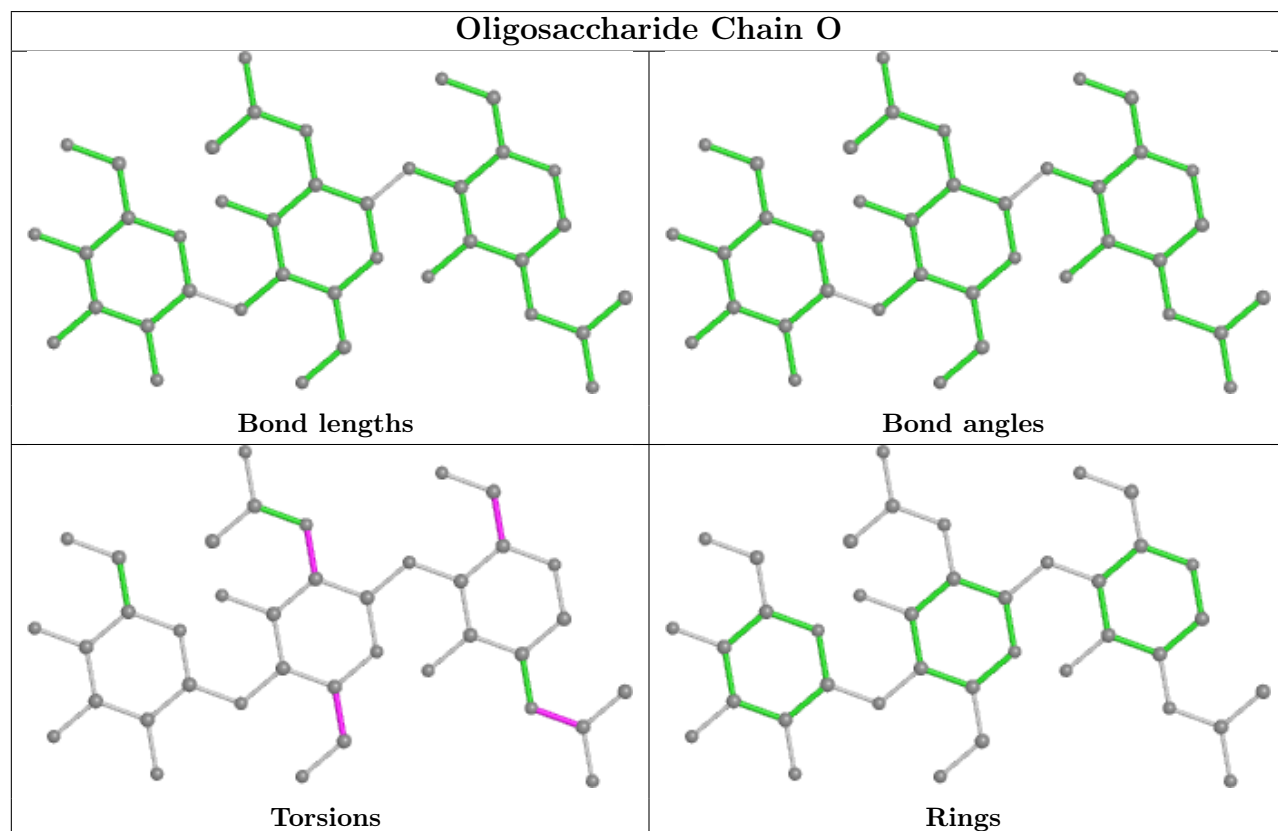
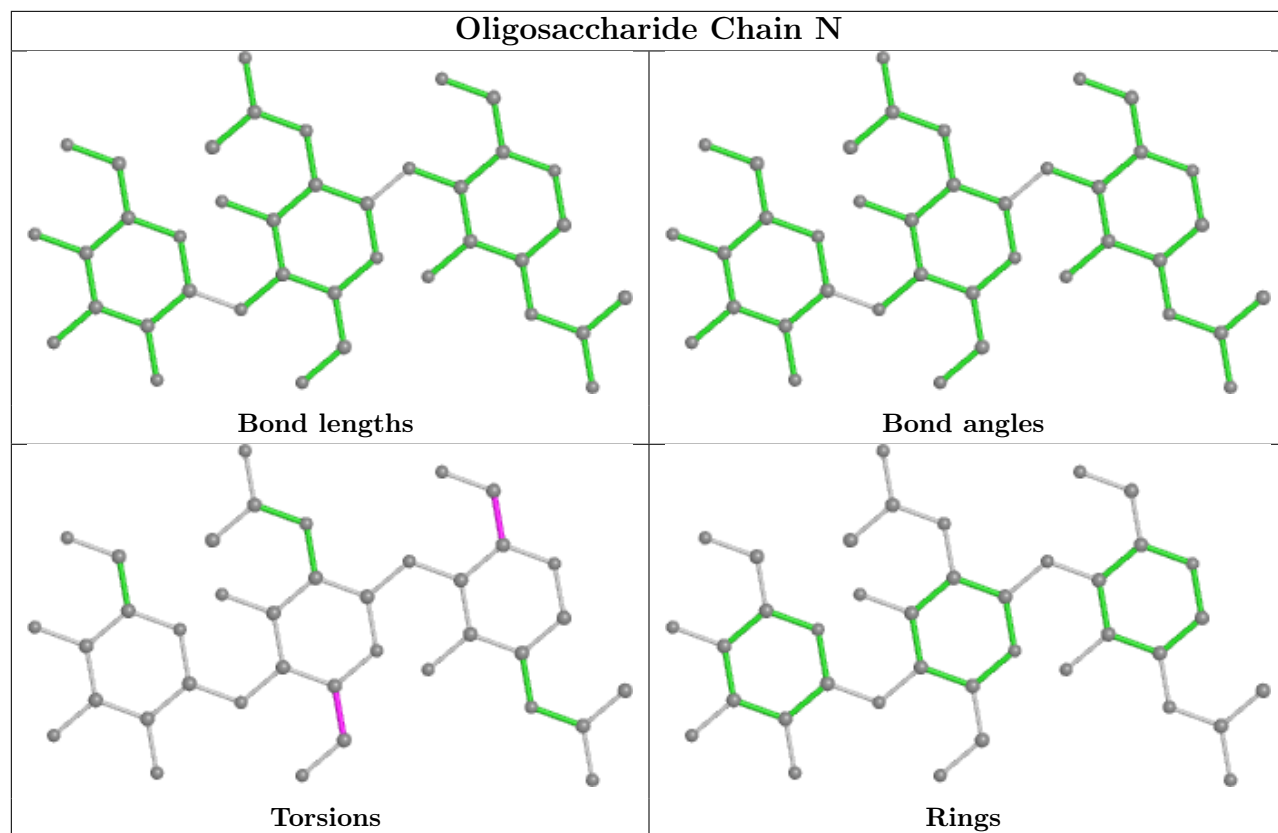
8 monomers are involved in 10 short contacts:

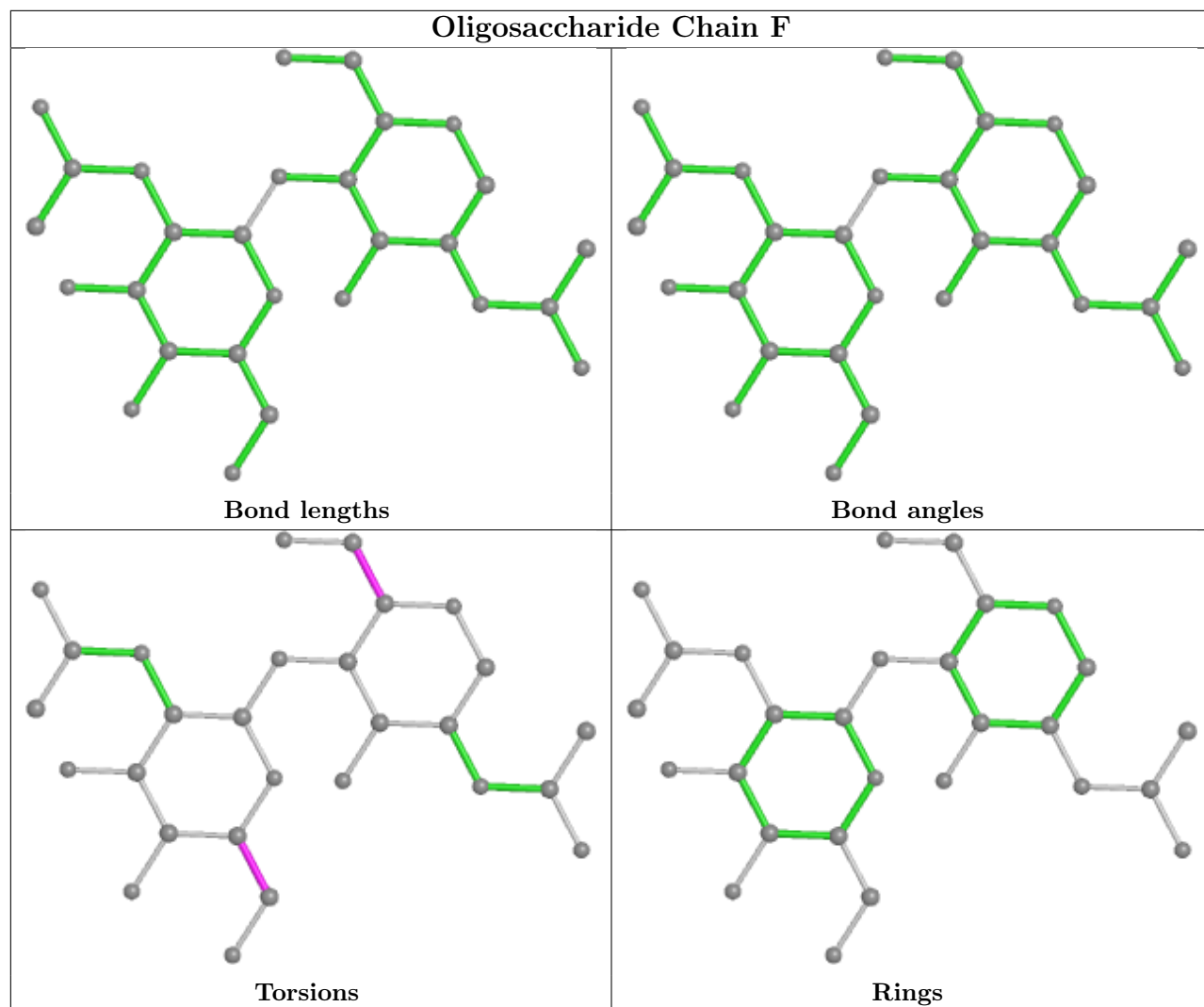
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	2	NAG	1	0
4	L	2	NAG	1	0
5	G	2	NAG	1	0
5	G	1	NAG	4	0
4	M	1	NAG	1	0
4	L	1	NAG	1	0
8	J	1	NAG	1	0
6	K	1	NAG	2	0

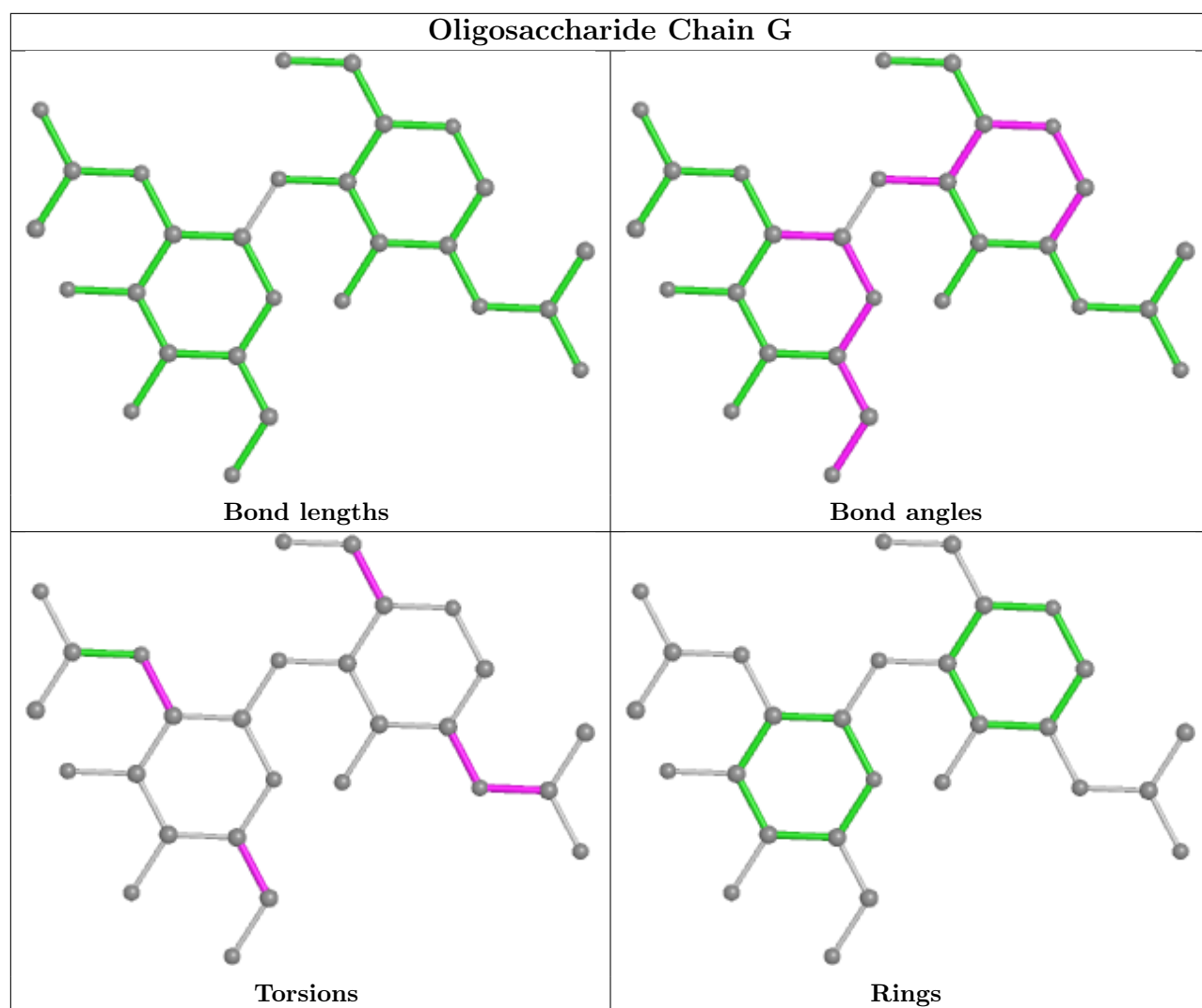
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

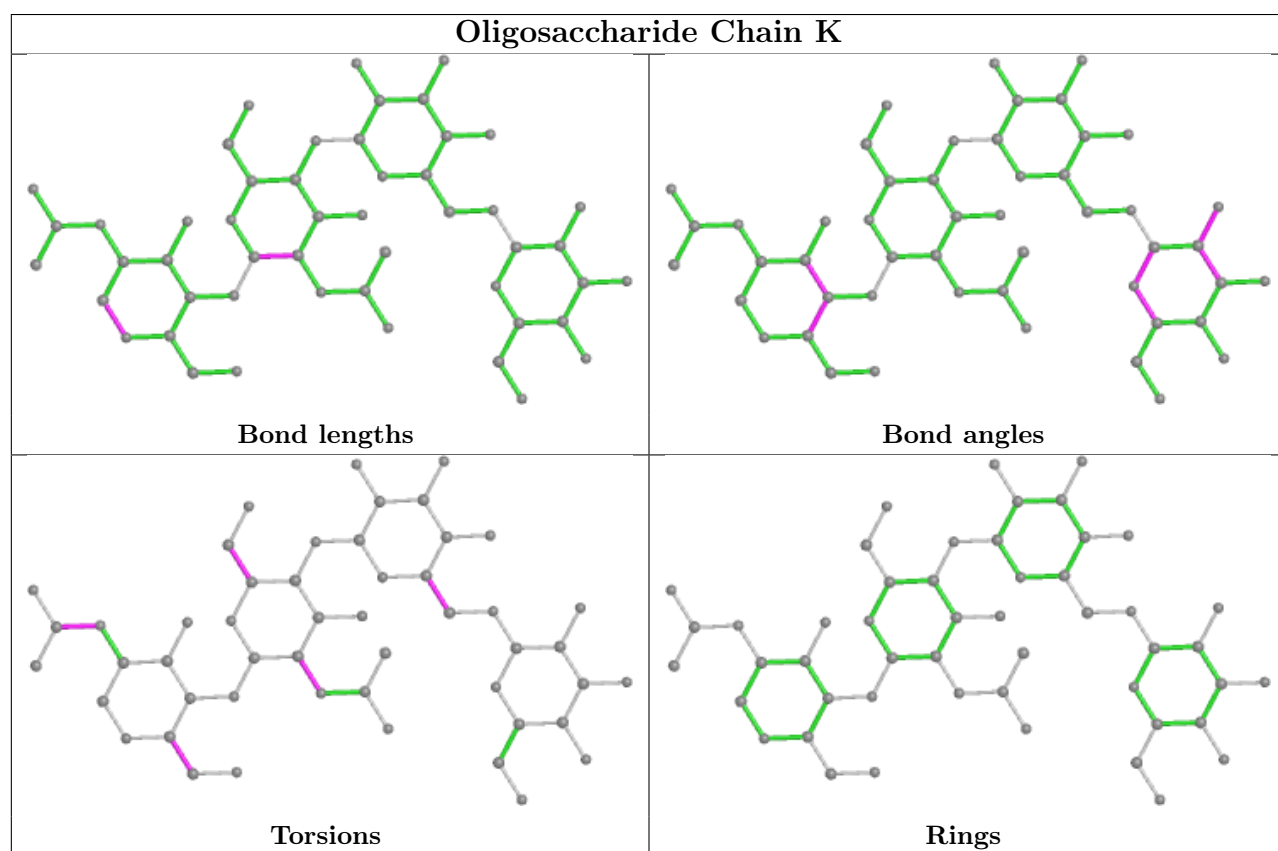
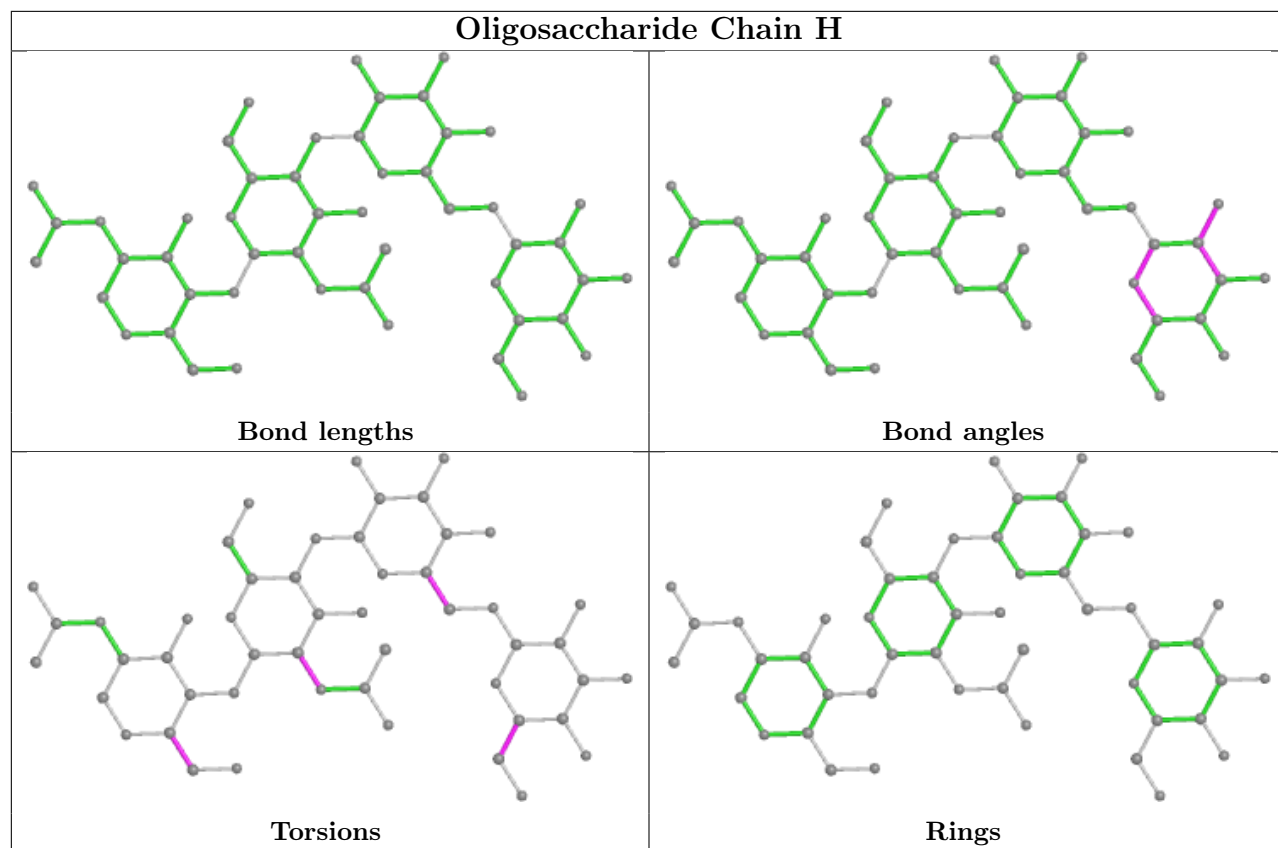




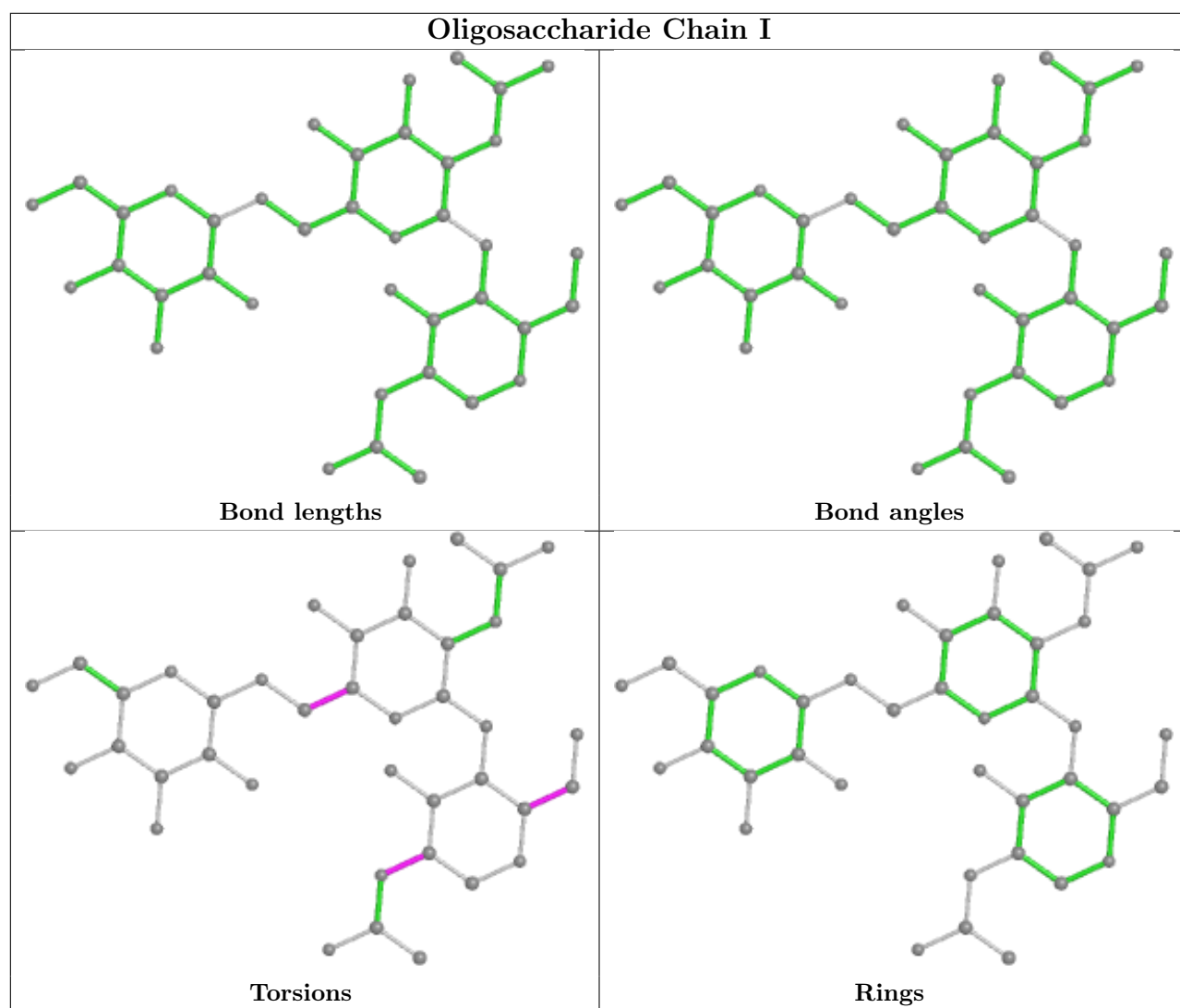


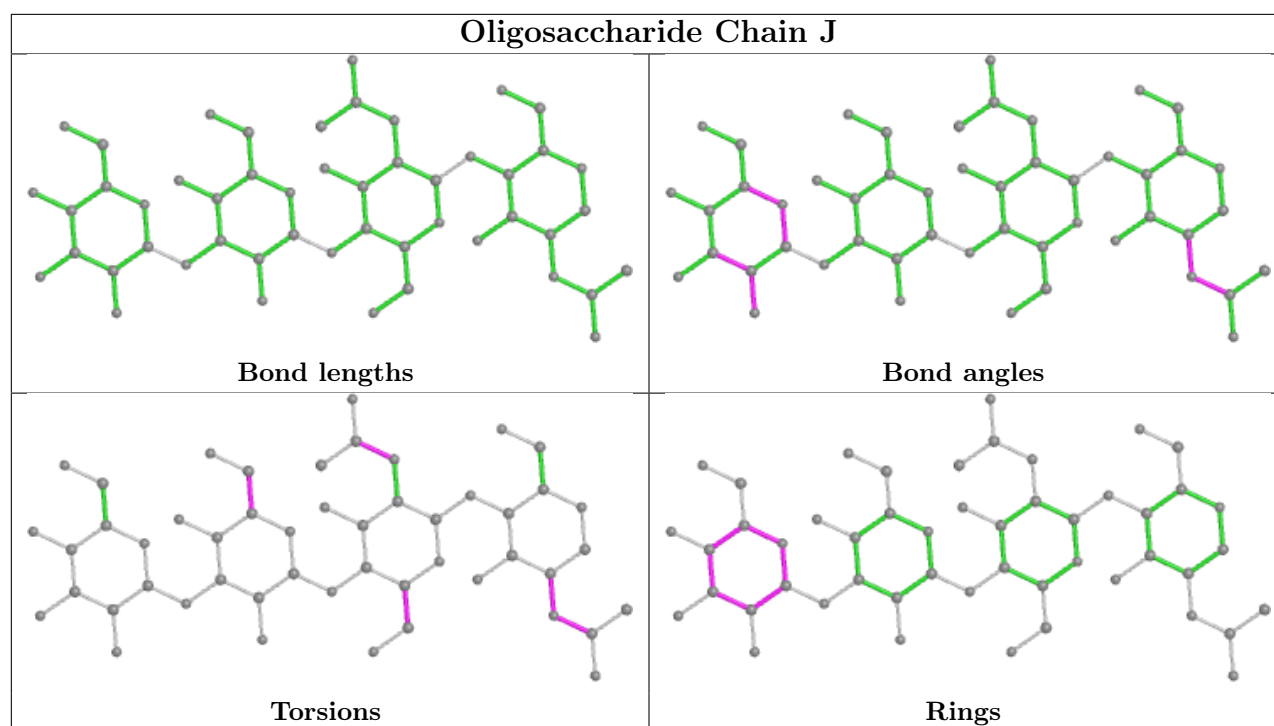












## 5.6 Ligand geometry [i](#)

4 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	$\# Z  > 2$
9	NAG	A	803	3	14,14,15	1.32	2 (14%)	17,19,21	1.82	3 (17%)
9	NAG	A	801	3	14,14,15	0.27	0	17,19,21	0.44	0
9	NAG	A	802	3	14,14,15	0.79	0	17,19,21	2.65	7 (41%)
9	NAG	D	1101	2	14,14,15	0.20	0	17,19,21	0.41	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
9	NAG	A	803	3	-	4/6/23/26	0/1/1/1
9	NAG	A	801	3	-	4/6/23/26	0/1/1/1
9	NAG	A	802	3	-	4/6/23/26	0/1/1/1
9	NAG	D	1101	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	803	NAG	O7-C7	-3.19	1.16	1.23
9	A	803	NAG	C3-C2	-2.56	1.47	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	802	NAG	O5-C1-C2	-5.54	102.54	111.29
9	A	802	NAG	O5-C5-C6	4.60	114.42	107.20
9	A	803	NAG	O3-C3-C2	-4.27	100.63	109.47
9	A	802	NAG	C2-N2-C7	4.00	128.60	122.90
9	A	802	NAG	O4-C4-C3	3.97	119.53	110.35

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	802	NAG	C3-C2-N2-C7
9	A	803	NAG	C3-C2-N2-C7
9	A	801	NAG	C4-C5-C6-O6
9	A	802	NAG	O5-C5-C6-O6
9	A	803	NAG	C8-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	803	NAG	8	0
9	A	801	NAG	1	0
9	A	802	NAG	9	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.