



## wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 02:35 PM JST

PDB ID : 8ZHN  
EMDB ID : EMD-60109  
Title : SARS-CoV-2 spike trimer (6P) in complex with three H18 and three R1-32 Fabs (one RBD rotated)  
Authors : Yan, Q.; Gao, X.; Liu, B.; Hou, R.; He, P.; Li, Z.; Chen, Q.; Wang, J.; He, J.; Chen, L.; Zhao, J.; Xiong, X.  
Deposited on : 2024-05-11  
Resolution : 4.12 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:

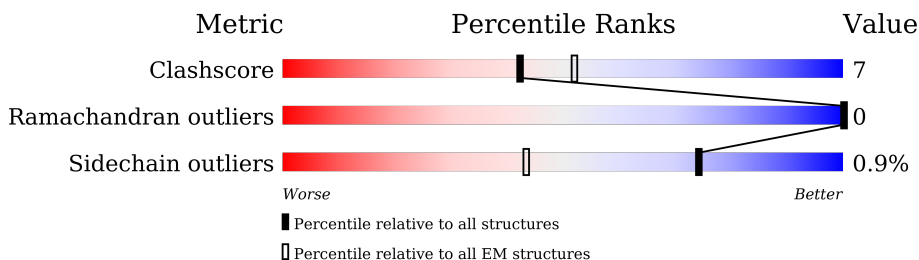
EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.12 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.










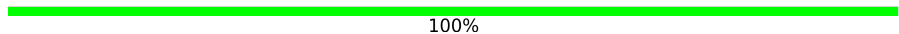

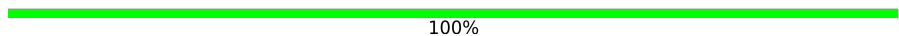
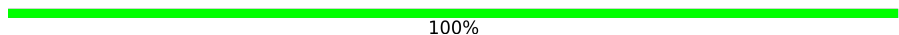
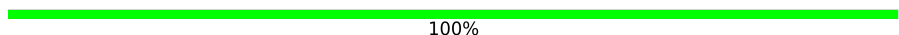
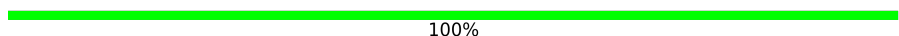
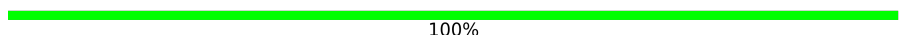

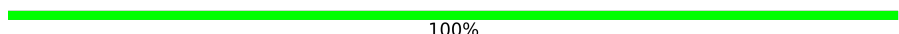

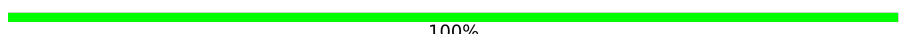
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	1278	68% 15% 17%
1	B	1278	70% 13% 17%
1	C	1278	71% 12% 17%
2	G	228	85% 15%
2	H	228	81% 18%
2	N	228	88% 11%
3	I	214	83% 17%
3	L	214	85% 14%
3	O	214	79% 21%

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Mol	Chain	Length	Quality of chain
4	D	243	 65% 21% 12%
4	F	243	 77% 11% 12%
4	K	243	 76% 12% 12%
5	E	243	 77% 15% 8%
5	J	243	 77% 15% 8%
5	M	243	 77% 15% 8%
6	P	2	 50% 50%
6	Q	2	 100%
6	R	2	 50% 50%
6	S	2	 100%
6	T	2	 100%
6	U	2	 100%
6	V	2	 100%
6	W	2	 100%
6	X	2	 50% 50%
6	Y	2	 100%
6	Z	2	 50% 50%
6	a	2	 100%

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 45273 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein,Fibritin,Expression Tag.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	1066	8344	5324	1394	1588	38	0	0
1	A	1066	8344	5324	1394	1588	38	0	0
1	B	1066	8344	5324	1394	1588	38	0	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1209	GLY	-	linker	UNP P0DTC2
C	1210	SER	-	linker	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1209	GLY	-	linker	UNP P0DTC2
A	1210	SER	-	linker	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	685	SER	ARG	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1209	GLY	-	linker	UNP P0DTC2
B	1210	SER	-	linker	UNP P0DTC2

- Molecule 2 is a protein called Heavy chain of R1-32 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	227	Total	C	N	O	S	0	0
			1661	1045	277	332	7		
2	H	227	Total	C	N	O	S	0	0
			1661	1045	277	332	7		
2	N	227	Total	C	N	O	S	0	0
			1661	1045	277	332	7		

- Molecule 3 is a protein called Light chain of R1-32 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	213	Total	C	N	O	S	0	0
			1557	971	261	321	4		
3	L	213	Total	C	N	O	S	0	0
			1557	971	261	321	4		
3	O	213	Total	C	N	O	S	0	0
			1557	971	261	321	4		

- Molecule 4 is a protein called Light chain of H18 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	213	Total	C	N	O	S	0	0
			1593	989	264	335	5		
4	F	213	Total	C	N	O	S	0	0
			1593	989	264	335	5		
4	K	213	Total	C	N	O	S	0	0
			1593	989	264	335	5		

- Molecule 5 is a protein called Heavy chain of H18 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	224	Total	C	N	O	S	0	0
			1670	1058	276	330	6		
5	J	224	Total	C	N	O	S	0	0
			1670	1058	276	330	6		
5	M	224	Total	C	N	O	S	0	0
			1670	1058	276	330	6		

- Molecule 6 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
6	P	2	Total	C	N	O	0	0
			28	16	2	10		
6	Q	2	Total	C	N	O	0	0
			28	16	2	10		
6	R	2	Total	C	N	O	0	0
			28	16	2	10		
6	S	2	Total	C	N	O	0	0
			28	16	2	10		
6	T	2	Total	C	N	O	0	0
			28	16	2	10		
6	U	2	Total	C	N	O	0	0
			28	16	2	10		
6	V	2	Total	C	N	O	0	0
			28	16	2	10		
6	W	2	Total	C	N	O	0	0
			28	16	2	10		
6	X	2	Total	C	N	O	0	0
			28	16	2	10		
6	Y	2	Total	C	N	O	0	0
			28	16	2	10		
6	Z	2	Total	C	N	O	0	0
			28	16	2	10		
6	a	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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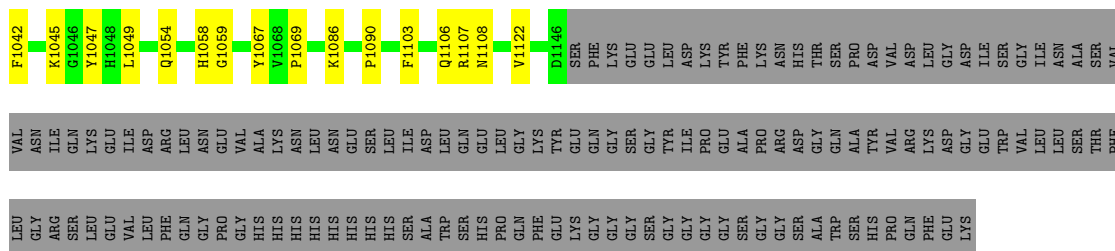
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	A	1	Total 14	8	1	5	0
7	A	1	Total 14	8	1	5	0
7	A	1	Total 14	8	1	5	0
7	A	1	Total 14	8	1	5	0
7	A	1	Total 14	8	1	5	0
7	A	1	Total 14	8	1	5	0
7	A	1	Total 14	8	1	5	0
7	A	1	Total 14	8	1	5	0
7	A	1	Total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



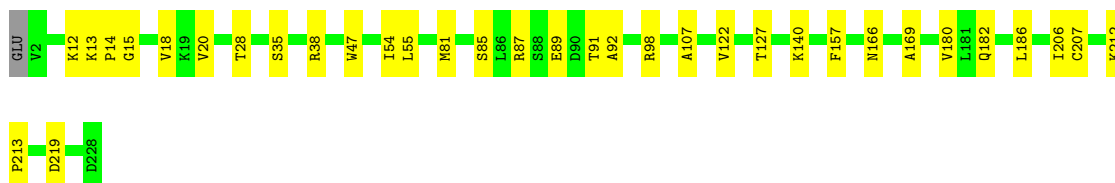






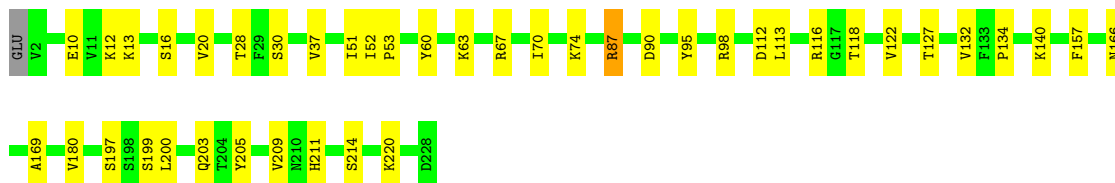
- Molecule 2: Heavy chain of R1-32 Fab

Chain G: 85% 15%



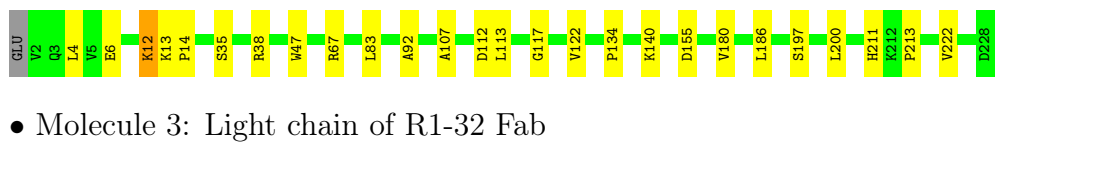
- Molecule 2: Heavy chain of R1-32 Fab

Chain H: 81% 18%



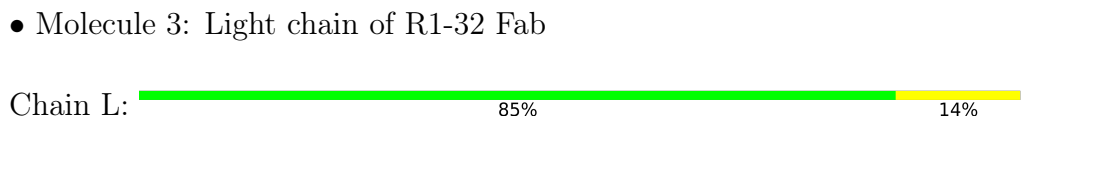
- Molecule 2: Heavy chain of R1-32 Fab

Chain N: 88% 11%



- Molecule 3: Light chain of R1-32 Fab

Chain I: 83% 17%

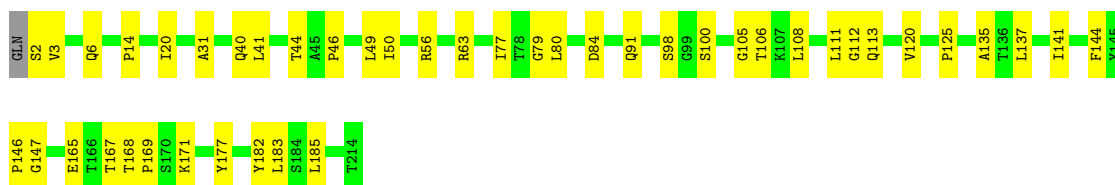
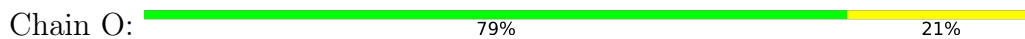


- Molecule 3: Light chain of R1-32 Fab

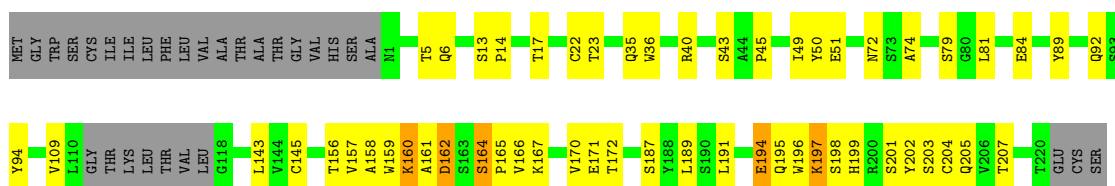
Chain L: 85% 14%



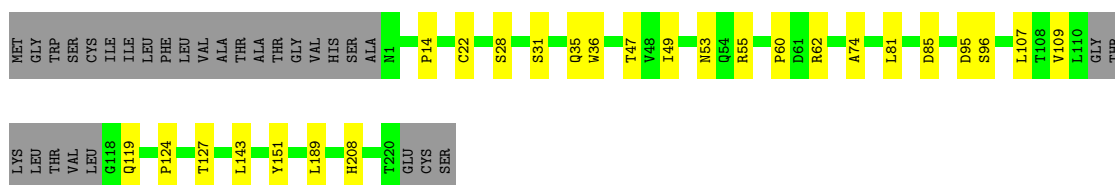
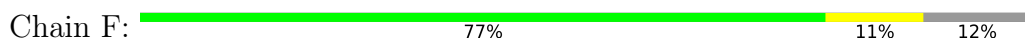
• Molecule 3: Light chain of R1-32 Fab



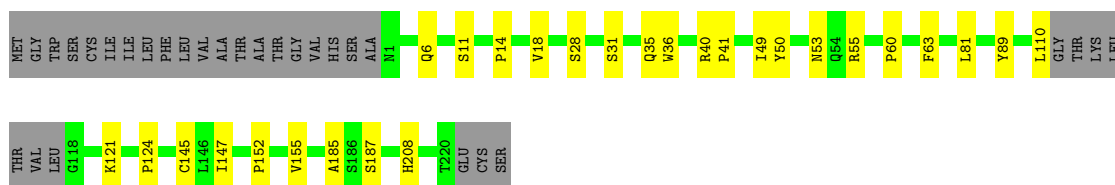
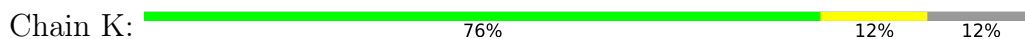
• Molecule 4: Light chain of H18 Fab



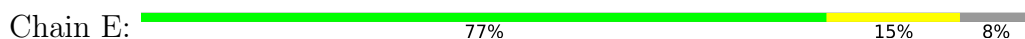
• Molecule 4: Light chain of H18 Fab



• Molecule 4: Light chain of H18 Fab

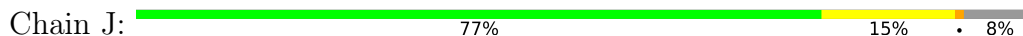


• Molecule 5: Heavy chain of H18 Fab

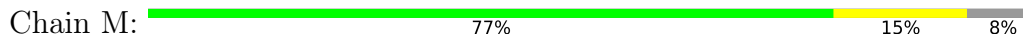




- Molecule 5: Heavy chain of H18 Fab



- Molecule 5: Heavy chain of H18 Fab



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



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



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



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

Chain S:  100%

MAG1  
MAG2

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

Chain T:  100%

MAG1  
MAG2

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

Chain U:  100%

MAG1  
MAG2

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

Chain V:  100%

MAG1  
MAG2

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

Chain W:  100%

MAG1  
MAG2

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

Chain X:  50%

MAG1  
MAG2

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

Chain Y:  100%

MAG1  
MAG2

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

Chain Z:  50% 50%MAG1  
MAG2

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

Chain a:  100%MAG1  
MAG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	13185	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor



## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/8540	0.51	0/11624
1	B	0.26	0/8540	0.50	0/11624
1	C	0.27	0/8540	0.51	0/11624
2	G	0.25	0/1698	0.52	0/2312
2	H	0.25	0/1698	0.51	0/2312
2	N	0.26	0/1698	0.52	0/2312
3	I	0.25	0/1595	0.48	0/2181
3	L	0.26	0/1595	0.49	0/2181
3	O	0.25	0/1595	0.50	0/2181
4	D	0.24	0/1630	0.49	0/2225
4	F	0.25	0/1630	0.50	0/2225
4	K	0.25	0/1630	0.47	0/2225
5	E	0.26	0/1713	0.52	0/2339
5	J	0.25	0/1713	0.50	0/2339
5	M	0.25	0/1713	0.50	0/2339
All	All	0.26	0/45528	0.50	0/62043

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	8344	0	8122	117	0
1	B	8344	0	8123	120	0
1	C	8344	0	8123	100	0
2	G	1661	0	1631	18	0
2	H	1661	0	1631	22	0
2	N	1661	0	1631	18	0
3	I	1557	0	1498	22	0
3	L	1557	0	1498	19	0
3	O	1557	0	1498	28	0
4	D	1593	0	1524	47	0
4	F	1593	0	1524	18	0
4	K	1593	0	1524	20	0
5	E	1670	0	1643	31	0
5	J	1670	0	1643	28	0
5	M	1670	0	1643	29	0
6	P	28	0	25	1	0
6	Q	28	0	25	0	0
6	R	28	0	25	1	0
6	S	28	0	25	0	0
6	T	28	0	25	0	0
6	U	28	0	25	0	0
6	V	28	0	25	0	0
6	W	28	0	25	0	0
6	X	28	0	25	1	0
6	Y	28	0	25	0	0
6	Z	28	0	25	1	0
6	a	28	0	25	0	0
7	A	154	0	143	1	0
7	B	154	0	143	0	0
7	C	154	0	143	2	0
All	All	45273	0	43985	581	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 581 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)
2:N:12:LYS:O	2:N:122:VAL:HG23	1.48	1.11
5:E:99:ARG:HB3	5:E:109:TYR:HB2	1.54	0.89
2:N:13:LYS:HG3	2:N:14:PRO:HD2	1.53	0.89
1:B:335:LEU:HD23	1:B:364:ASP:H	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:35:GLN:HG2	5:M:106:ARG:HB3	1.57	0.86

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	1054/1278 (82%)	1017 (96%)	37 (4%)	0	100	100
1	B	1054/1278 (82%)	1025 (97%)	29 (3%)	0	100	100
1	C	1054/1278 (82%)	1015 (96%)	39 (4%)	0	100	100
2	G	225/228 (99%)	213 (95%)	12 (5%)	0	100	100
2	H	225/228 (99%)	214 (95%)	11 (5%)	0	100	100
2	N	225/228 (99%)	214 (95%)	11 (5%)	0	100	100
3	I	211/214 (99%)	203 (96%)	8 (4%)	0	100	100
3	L	211/214 (99%)	198 (94%)	13 (6%)	0	100	100
3	O	211/214 (99%)	199 (94%)	12 (6%)	0	100	100
4	D	209/243 (86%)	198 (95%)	11 (5%)	0	100	100
4	F	209/243 (86%)	197 (94%)	12 (6%)	0	100	100
4	K	209/243 (86%)	194 (93%)	15 (7%)	0	100	100
5	E	222/243 (91%)	215 (97%)	7 (3%)	0	100	100
5	J	222/243 (91%)	217 (98%)	5 (2%)	0	100	100
5	M	222/243 (91%)	215 (97%)	7 (3%)	0	100	100
All	All	5763/6618 (87%)	5534 (96%)	229 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	934/1106 (84%)	931 (100%)	3 (0%)	91	92
1	B	934/1106 (84%)	928 (99%)	6 (1%)	84	88
1	C	934/1106 (84%)	922 (99%)	12 (1%)	65	77
2	G	184/186 (99%)	181 (98%)	3 (2%)	58	74
2	H	184/186 (99%)	180 (98%)	4 (2%)	47	65
2	N	184/186 (99%)	182 (99%)	2 (1%)	70	80
3	I	174/177 (98%)	173 (99%)	1 (1%)	84	88
3	L	174/177 (98%)	174 (100%)	0	100	100
3	O	174/177 (98%)	174 (100%)	0	100	100
4	D	184/208 (88%)	176 (96%)	8 (4%)	25	48
4	F	184/208 (88%)	184 (100%)	0	100	100
4	K	184/208 (88%)	184 (100%)	0	100	100
5	E	192/209 (92%)	190 (99%)	2 (1%)	73	81
5	J	192/209 (92%)	190 (99%)	2 (1%)	73	81
5	M	192/209 (92%)	191 (100%)	1 (0%)	86	90
All	All	5004/5658 (88%)	4960 (99%)	44 (1%)	74	83

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	328	ARG
2	H	87	ARG
1	B	21	ARG
1	B	336	CYS
2	H	140	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	448	ASN
1	B	532	ASN
5	M	3	GLN
3	O	36	HIS
4	F	119	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

24 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	$\# Z  > 2$
6	NAG	P	1	1,6	14,14,15	0.24	0	17,19,21	0.43	0
6	NAG	P	2	6	14,14,15	0.27	0	17,19,21	0.43	0
6	NAG	Q	1	1,6	14,14,15	0.24	0	17,19,21	0.46	0
6	NAG	Q	2	6	14,14,15	0.24	0	17,19,21	0.41	0
6	NAG	R	1	1,6	14,14,15	0.22	0	17,19,21	0.44	0
6	NAG	R	2	6	14,14,15	0.26	0	17,19,21	0.42	0
6	NAG	S	1	1,6	14,14,15	0.26	0	17,19,21	0.49	0
6	NAG	S	2	6	14,14,15	0.24	0	17,19,21	0.43	0
6	NAG	T	1	1,6	14,14,15	0.23	0	17,19,21	0.43	0
6	NAG	T	2	6	14,14,15	0.26	0	17,19,21	0.42	0
6	NAG	U	1	1,6	14,14,15	0.27	0	17,19,21	0.49	0
6	NAG	U	2	6	14,14,15	0.25	0	17,19,21	0.42	0
6	NAG	V	1	1,6	14,14,15	0.19	0	17,19,21	0.41	0
6	NAG	V	2	6	14,14,15	0.24	0	17,19,21	0.43	0
6	NAG	W	1	1,6	14,14,15	0.24	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	W	2	6	14,14,15	0.26	0	17,19,21	0.44	0
6	NAG	X	1	1,6	14,14,15	0.25	0	17,19,21	0.43	0
6	NAG	X	2	6	14,14,15	0.26	0	17,19,21	0.43	0
6	NAG	Y	1	1,6	14,14,15	0.25	0	17,19,21	0.47	0
6	NAG	Y	2	6	14,14,15	0.27	0	17,19,21	0.41	0
6	NAG	Z	1	1,6	14,14,15	0.25	0	17,19,21	0.43	0
6	NAG	Z	2	6	14,14,15	0.27	0	17,19,21	0.40	0
6	NAG	a	1	1,6	14,14,15	0.28	0	17,19,21	0.50	0
6	NAG	a	2	6	14,14,15	0.24	0	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	P	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	P	2	6	-	2/6/23/26	0/1/1/1
6	NAG	Q	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	2/6/23/26	0/1/1/1
6	NAG	R	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	R	2	6	-	2/6/23/26	0/1/1/1
6	NAG	S	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	S	2	6	-	2/6/23/26	0/1/1/1
6	NAG	T	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	T	2	6	-	2/6/23/26	0/1/1/1
6	NAG	U	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	NAG	V	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	V	2	6	-	2/6/23/26	0/1/1/1
6	NAG	W	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	W	2	6	-	2/6/23/26	0/1/1/1
6	NAG	X	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	X	2	6	-	2/6/23/26	0/1/1/1
6	NAG	Y	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	2/6/23/26	0/1/1/1
6	NAG	Z	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	2/6/23/26	0/1/1/1
6	NAG	a	1	1,6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

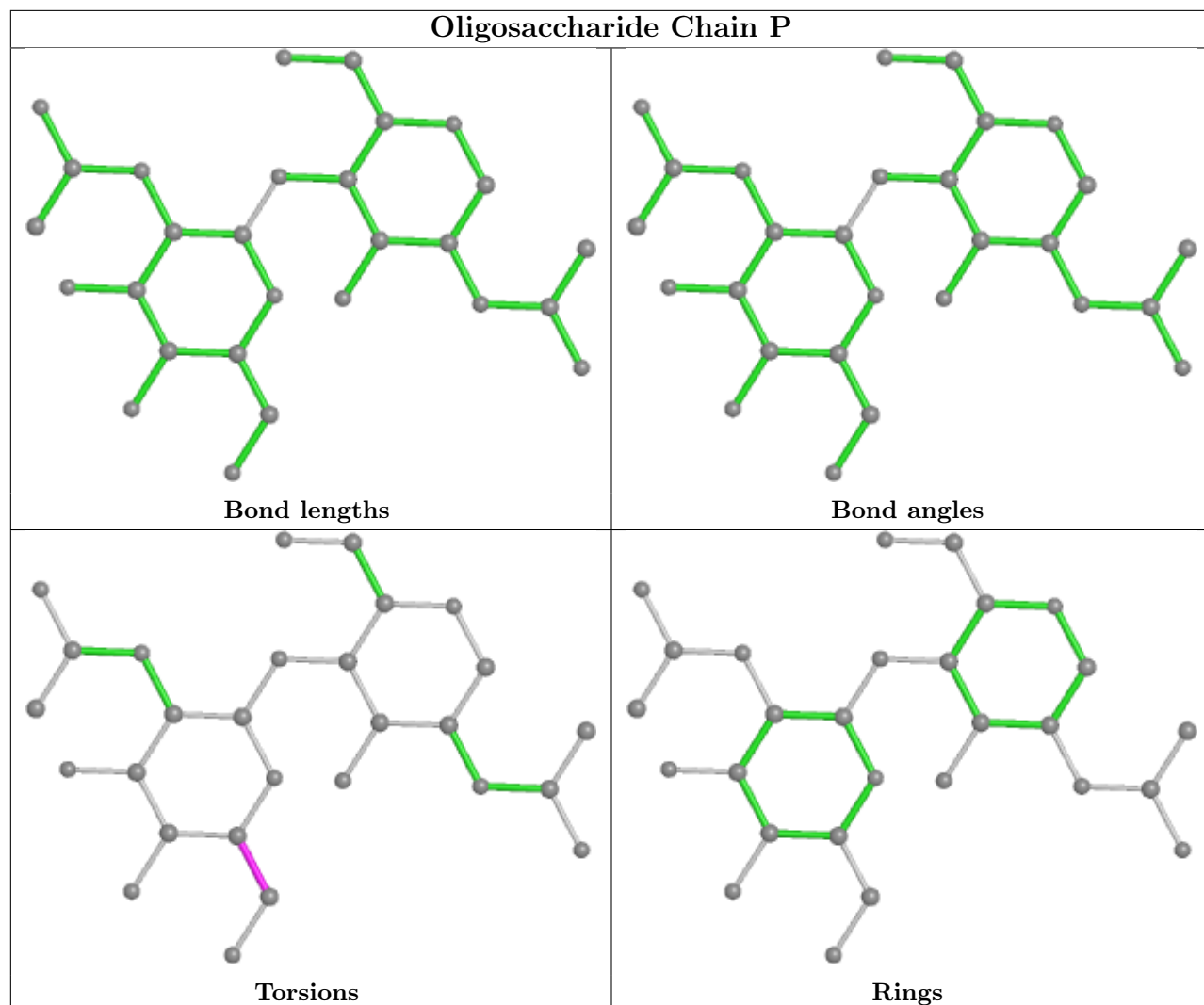
Mol	Chain	Res	Type	Atoms
6	S	2	NAG	O5-C5-C6-O6
6	W	2	NAG	O5-C5-C6-O6
6	a	2	NAG	O5-C5-C6-O6
6	Z	2	NAG	C4-C5-C6-O6
6	R	2	NAG	C4-C5-C6-O6

There are no ring outliers.

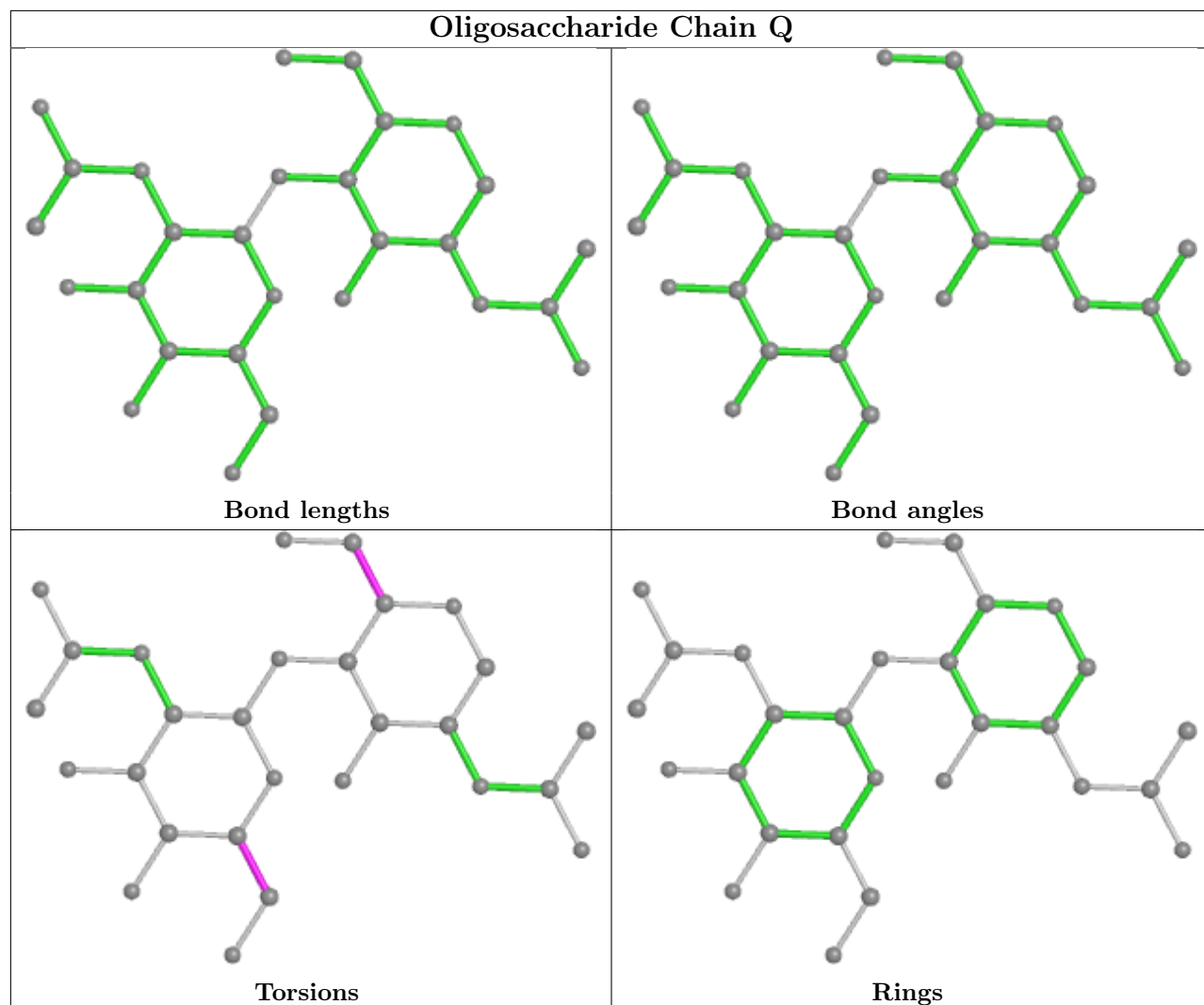
4 monomers are involved in 4 short contacts:

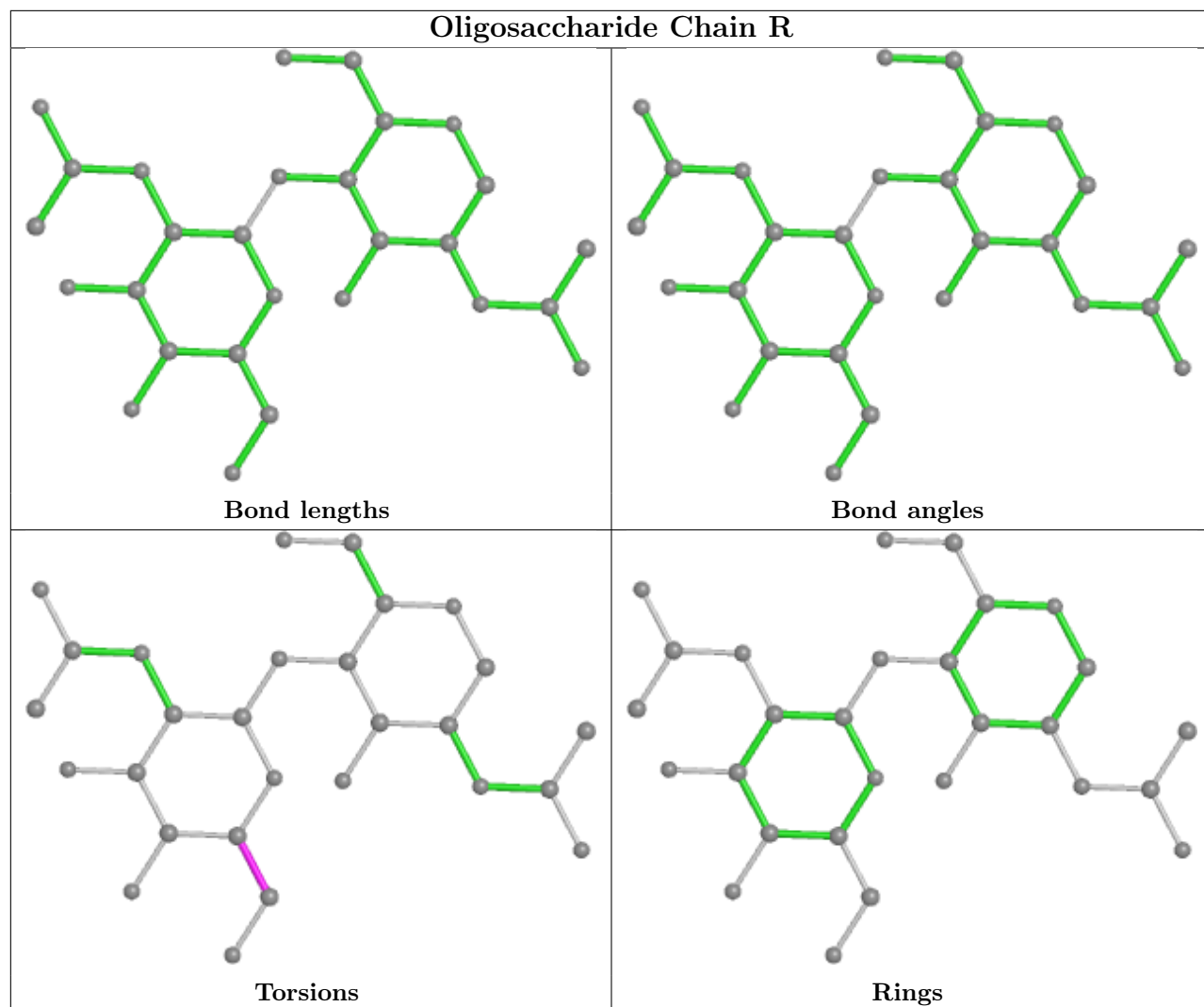
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Z	1	NAG	1	0
6	P	1	NAG	1	0
6	X	1	NAG	1	0
6	R	1	NAG	1	0

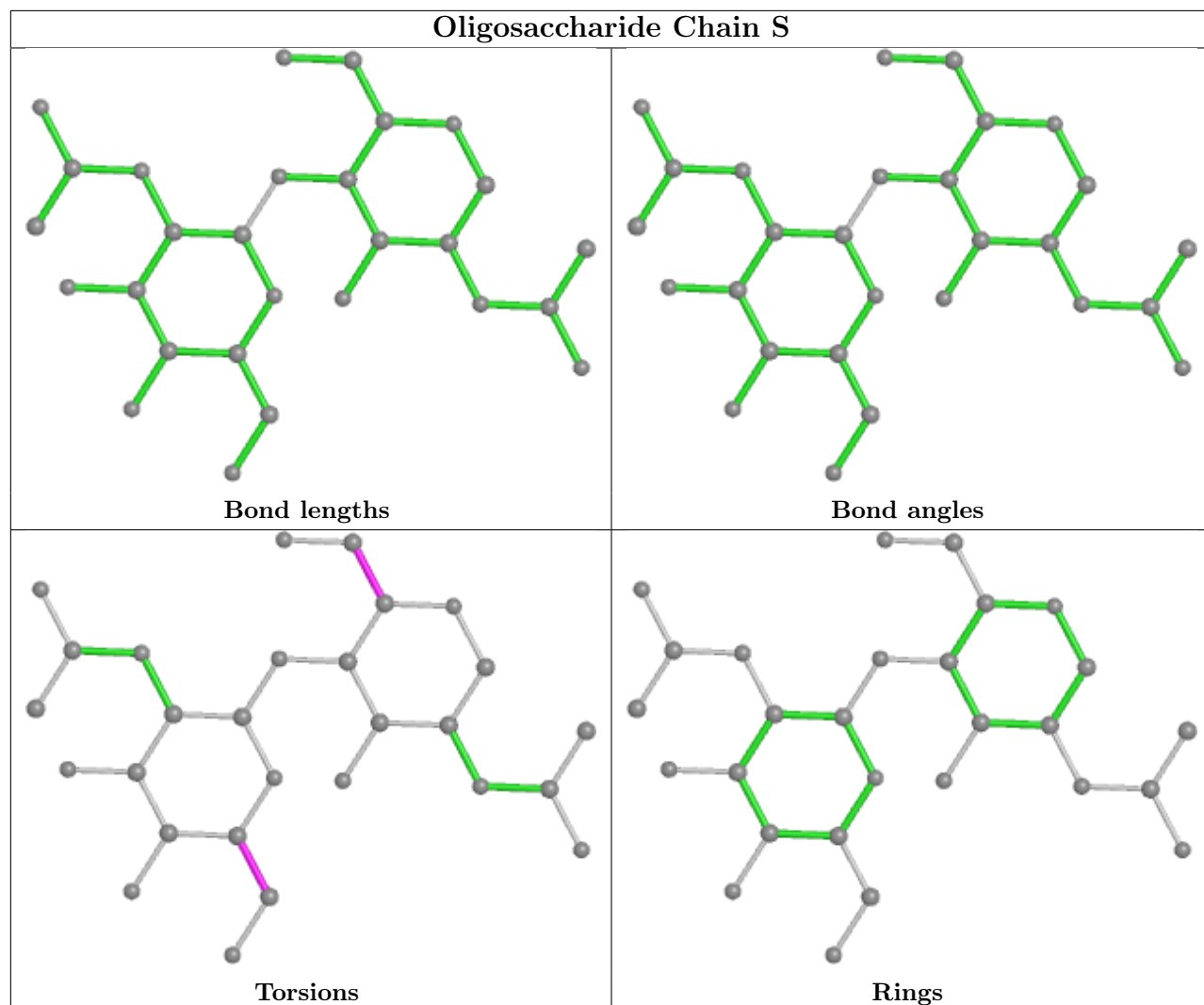
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

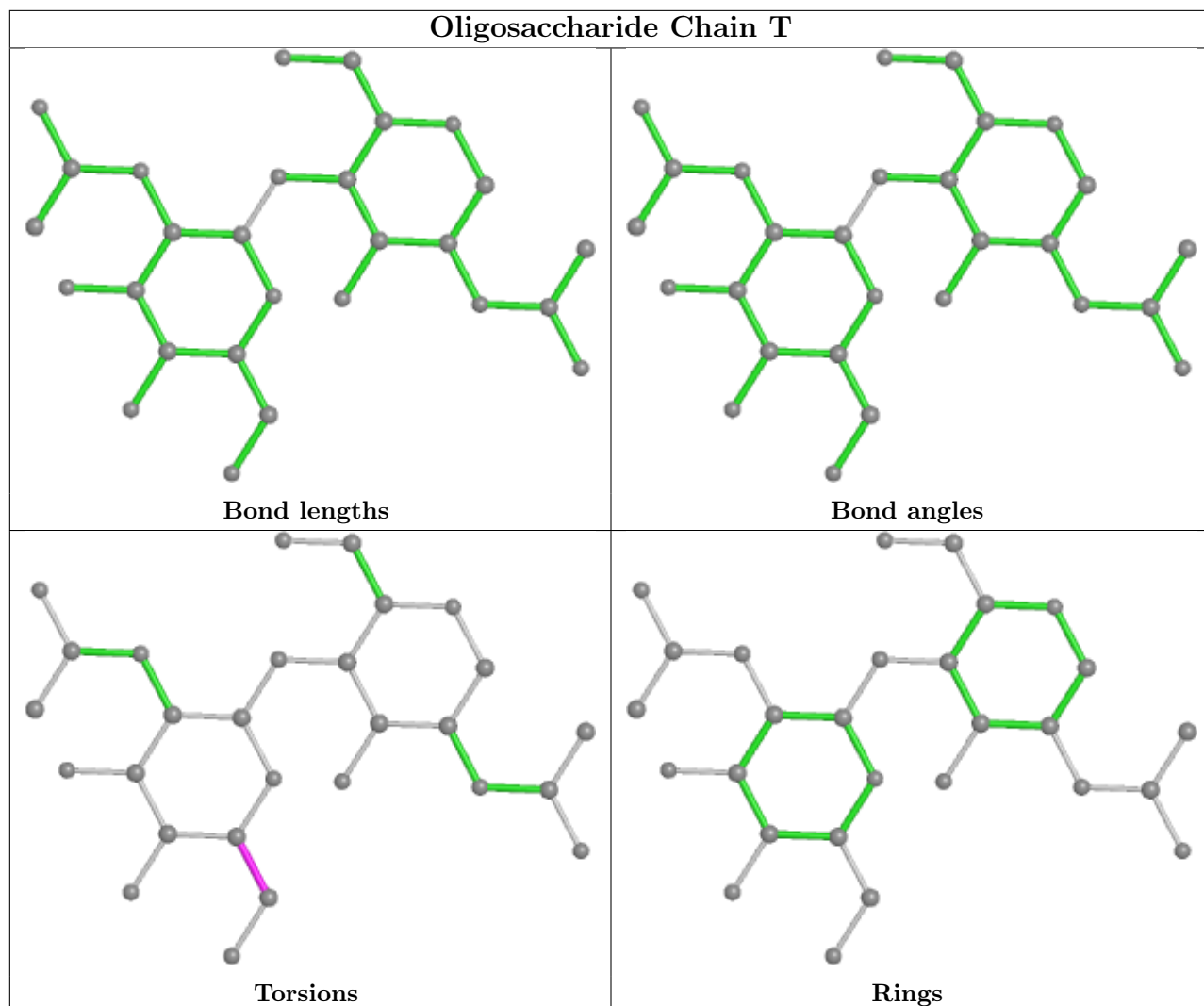


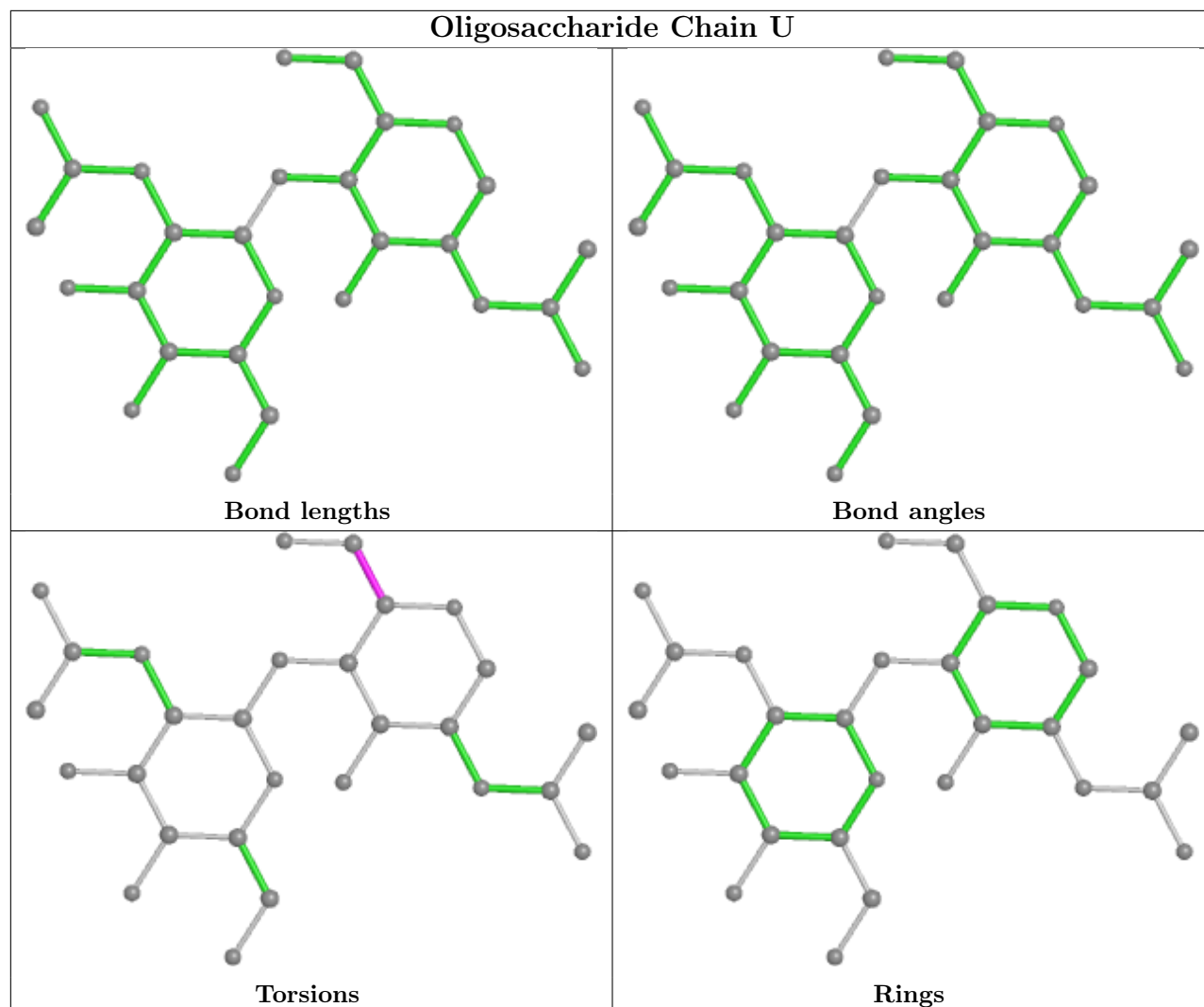


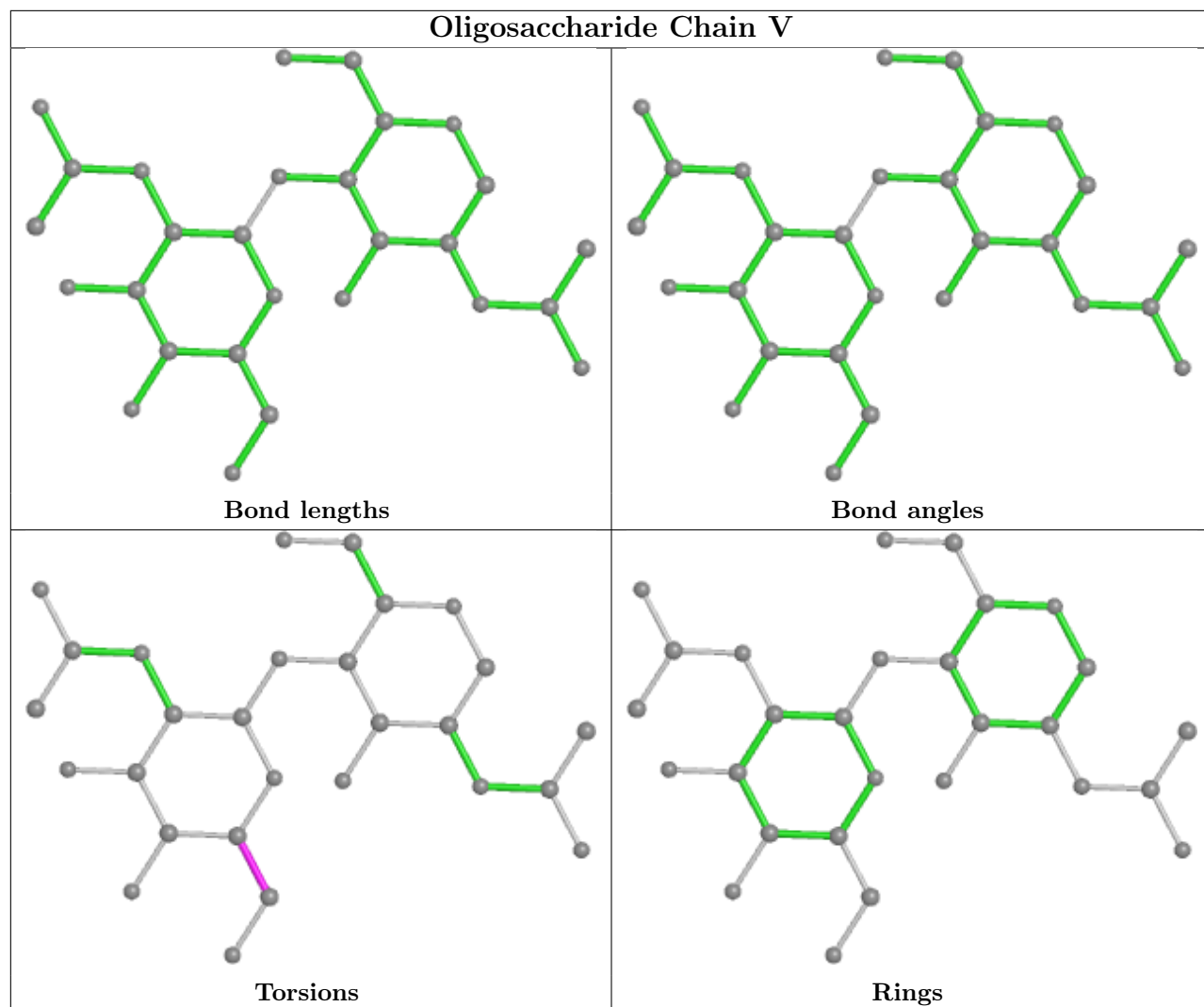


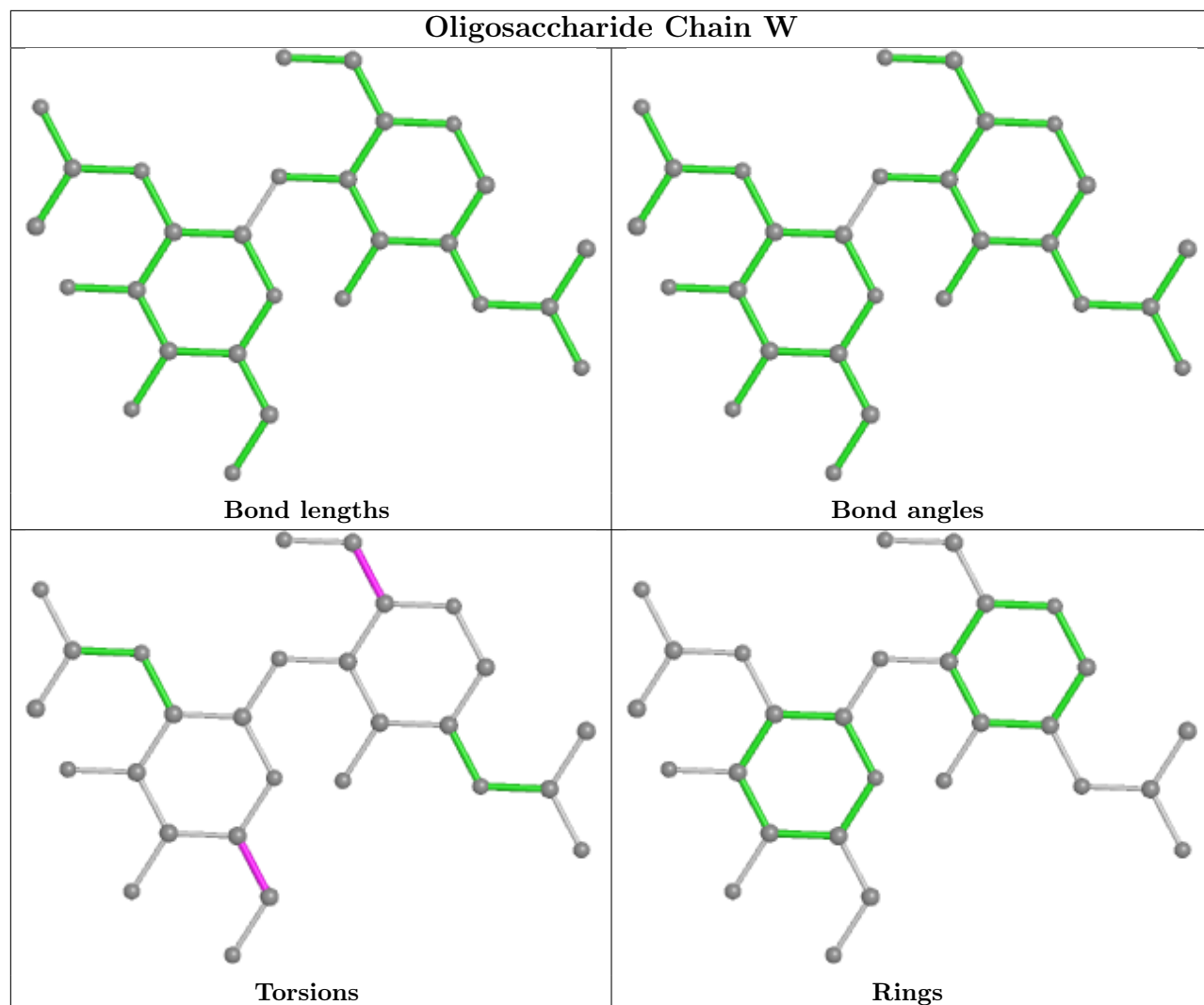


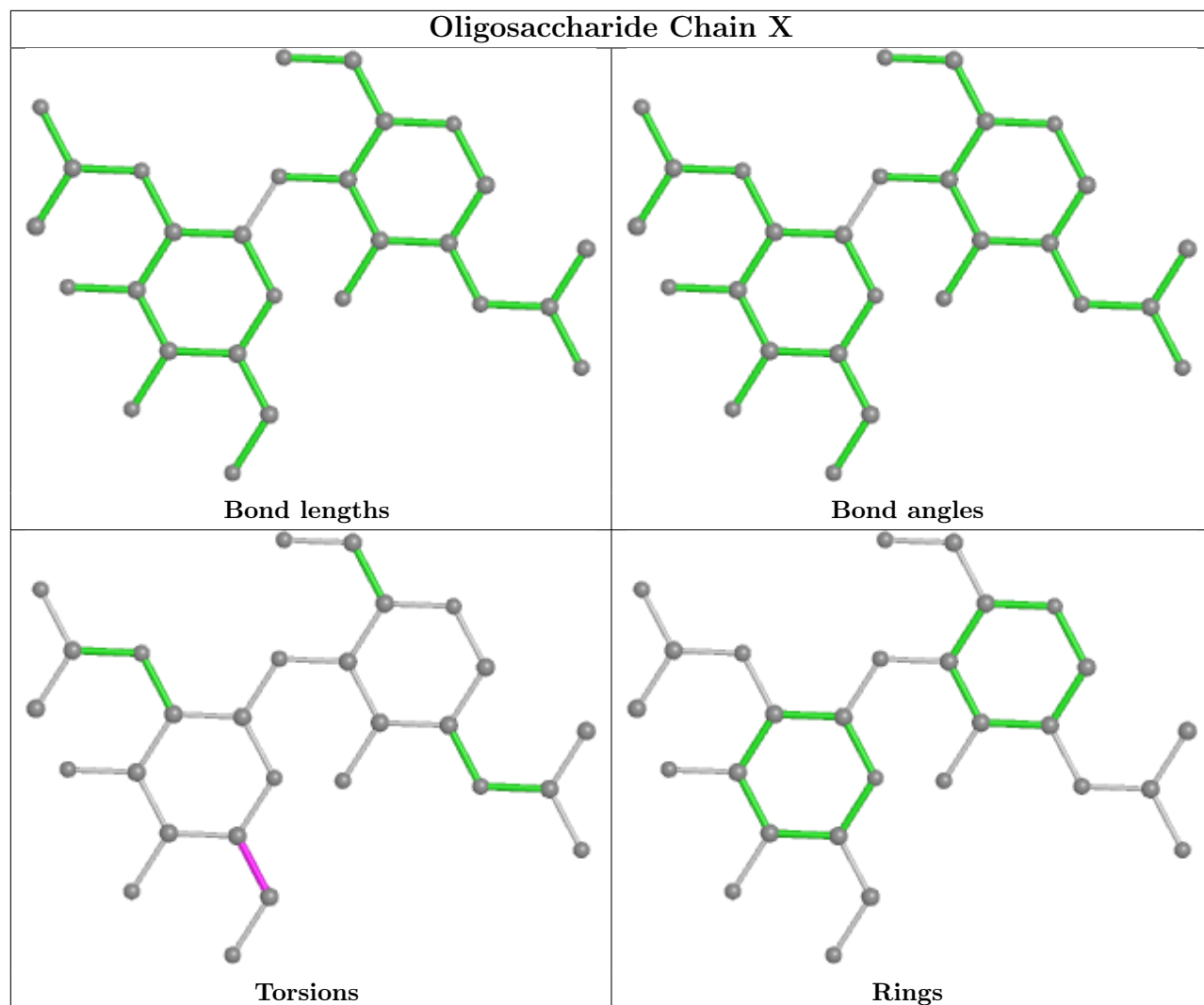




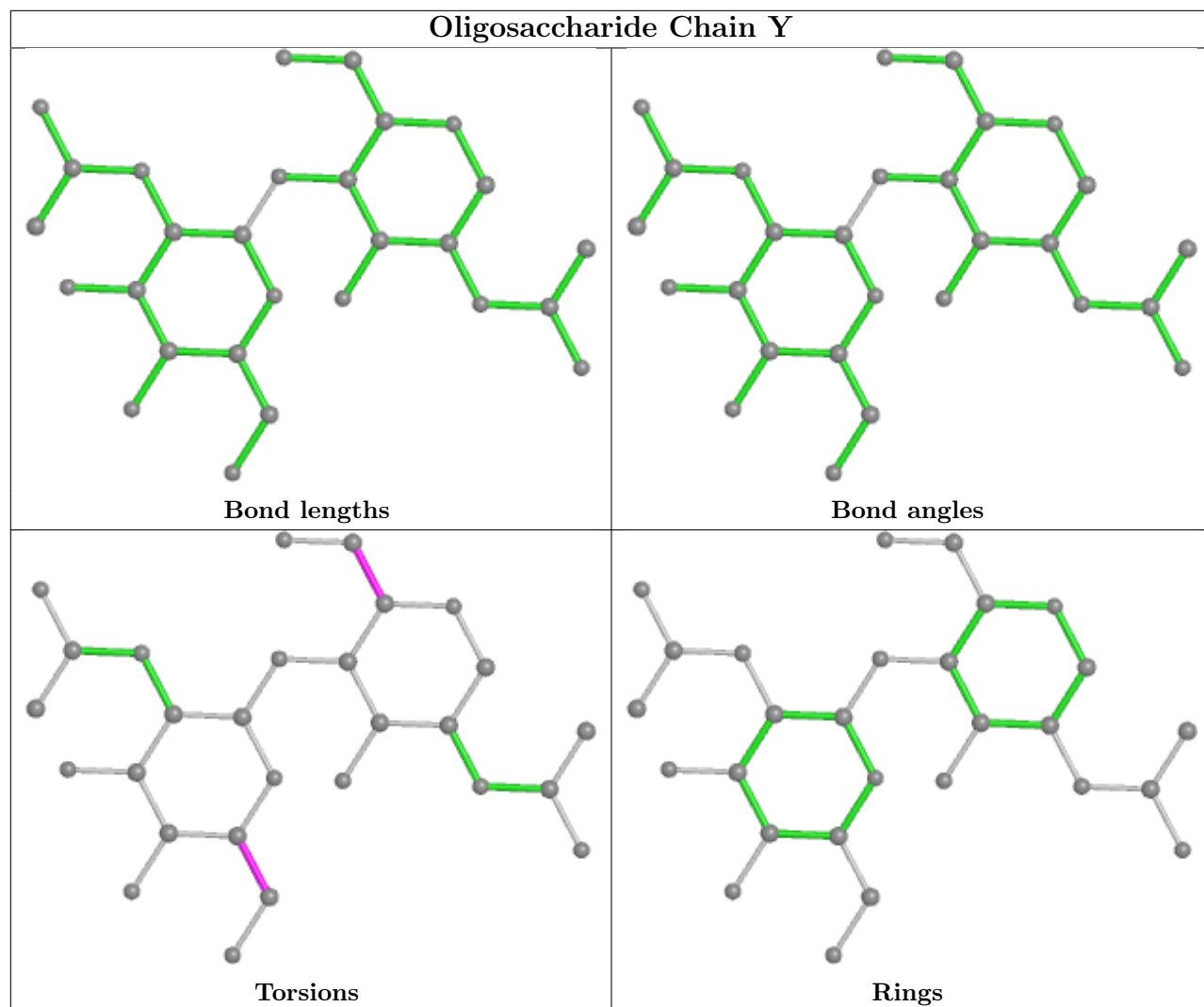


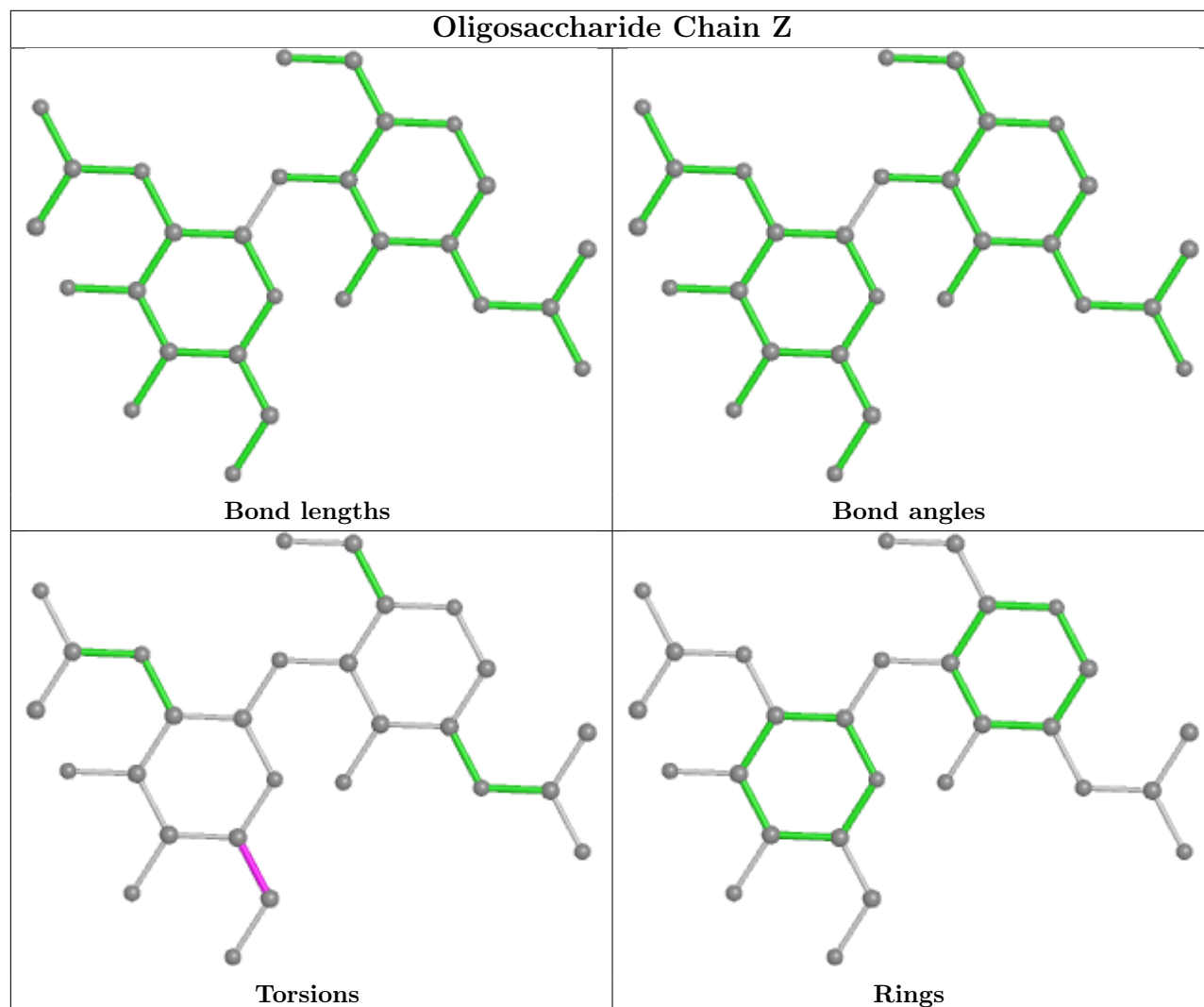


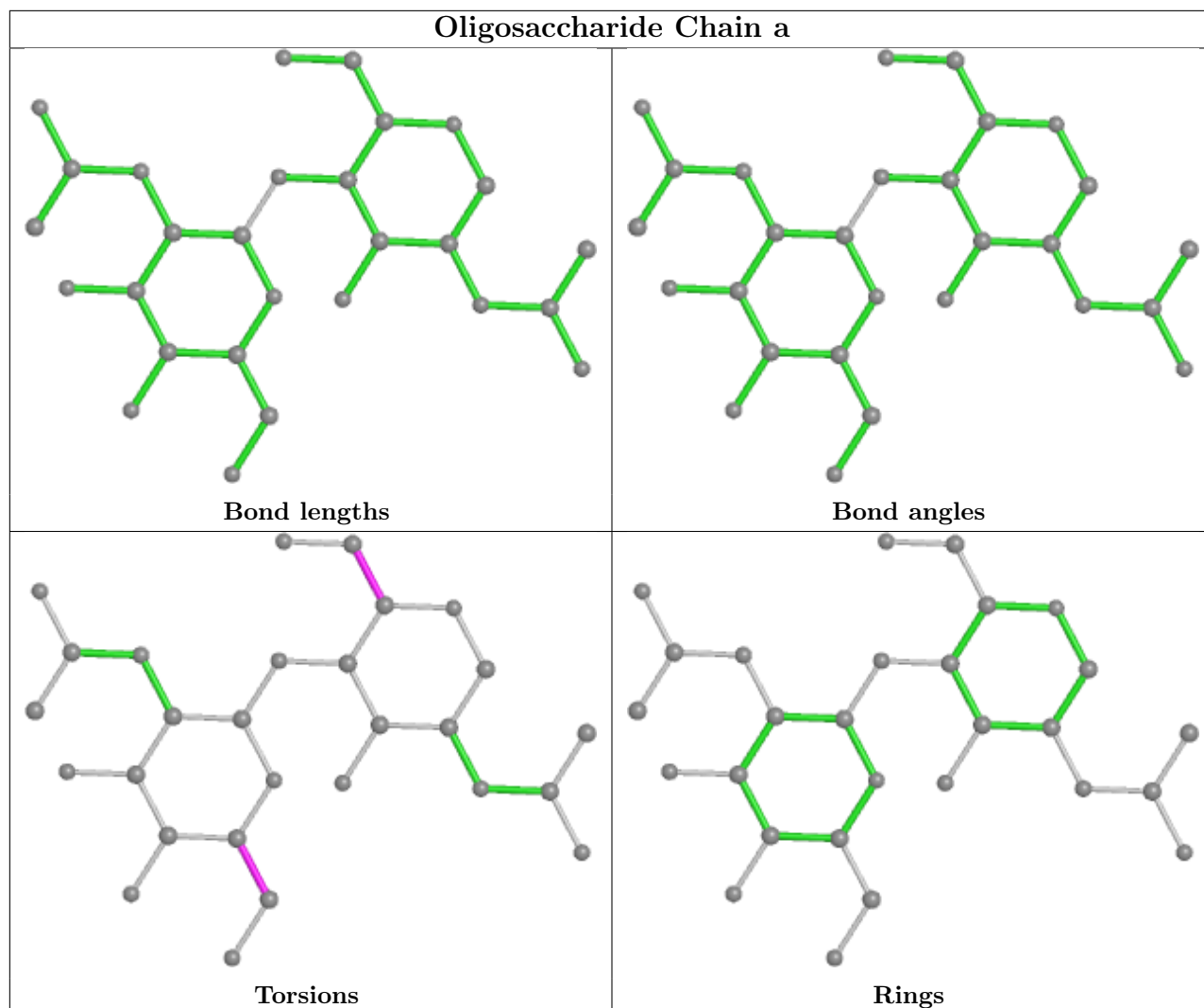












## 5.6 Ligand geometry [i](#)

33 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	$\# Z  > 2$
7	NAG	C	1309	1	14,14,15	0.29	0	17,19,21	0.46	0
7	NAG	B	1302	1	14,14,15	0.20	0	17,19,21	0.44	0
7	NAG	B	1303	1	14,14,15	0.23	0	17,19,21	0.39	0
7	NAG	A	1309	1	14,14,15	0.28	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	B	1301	1	14,14,15	0.41	0	17,19,21	0.38	0
7	NAG	C	1311	1	14,14,15	0.54	0	17,19,21	0.71	1 (5%)
7	NAG	A	1308	1	14,14,15	0.25	0	17,19,21	0.43	0
7	NAG	C	1310	1	14,14,15	0.26	0	17,19,21	0.44	0
7	NAG	C	1305	1	14,14,15	0.29	0	17,19,21	0.44	0
7	NAG	A	1305	1	14,14,15	0.24	0	17,19,21	0.42	0
7	NAG	C	1303	1	14,14,15	0.38	0	17,19,21	0.34	0
7	NAG	C	1302	1	14,14,15	0.40	0	17,19,21	0.32	0
7	NAG	A	1306	1	14,14,15	0.32	0	17,19,21	0.38	0
7	NAG	C	1301	1	14,14,15	0.22	0	17,19,21	0.41	0
7	NAG	C	1306	1	14,14,15	0.22	0	17,19,21	0.42	0
7	NAG	A	1311	1	14,14,15	0.25	0	17,19,21	0.44	0
7	NAG	C	1308	1	14,14,15	0.25	0	17,19,21	0.43	0
7	NAG	A	1303	1	14,14,15	0.50	0	17,19,21	0.53	0
7	NAG	B	1305	1	14,14,15	0.24	0	17,19,21	0.43	0
7	NAG	A	1310	1	14,14,15	0.24	0	17,19,21	0.44	0
7	NAG	A	1304	1	14,14,15	0.26	0	17,19,21	0.45	0
7	NAG	A	1302	1	14,14,15	0.24	0	17,19,21	0.47	0
7	NAG	B	1309	1	14,14,15	0.28	0	17,19,21	0.44	0
7	NAG	B	1310	1	14,14,15	0.27	0	17,19,21	0.45	0
7	NAG	B	1304	1	14,14,15	0.32	0	17,19,21	0.58	1 (5%)
7	NAG	A	1301	1	14,14,15	0.35	0	17,19,21	0.48	0
7	NAG	A	1307	1	14,14,15	0.34	0	17,19,21	0.72	0
7	NAG	B	1311	1	14,14,15	0.30	0	17,19,21	0.49	0
7	NAG	B	1308	1	14,14,15	0.26	0	17,19,21	0.43	0
7	NAG	B	1307	1	14,14,15	0.55	0	17,19,21	0.79	1 (5%)
7	NAG	C	1307	1	14,14,15	0.37	0	17,19,21	0.71	0
7	NAG	C	1304	1	14,14,15	0.34	0	17,19,21	0.47	0
7	NAG	B	1306	1	14,14,15	0.21	0	17,19,21	0.42	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
7	NAG	C	1309	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1301	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1307	1	-	3/6/23/26	0/1/1/1
7	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1307	1	-	3/6/23/26	0/1/1/1
7	NAG	C	1307	1	-	1/6/23/26	0/1/1/1
7	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1306	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1311	NAG	C1-O5-C5	2.56	115.66	112.19
7	B	1307	NAG	C1-O5-C5	2.05	114.97	112.19
7	B	1304	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1302	NAG	C4-C5-C6-O6
7	A	1301	NAG	O5-C5-C6-O6
7	A	1308	NAG	O5-C5-C6-O6
7	A	1301	NAG	C4-C5-C6-O6
7	C	1308	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1306	NAG	1	0
7	C	1306	NAG	2	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.