



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 16, 2024 – 05:29 AM EST

PDB ID : 6CH8
Title : Crystal structure of a natively-glycosylated BG505 SOSIP.664 HIV-1 Envelope Trimer in complex with the broadly-neutralizing antibodies BG18 and 35O22
Authors : Barnes, C.O.; Bjorkman, P.J.
Deposited on : 2018-02-22
Resolution : 4.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

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:

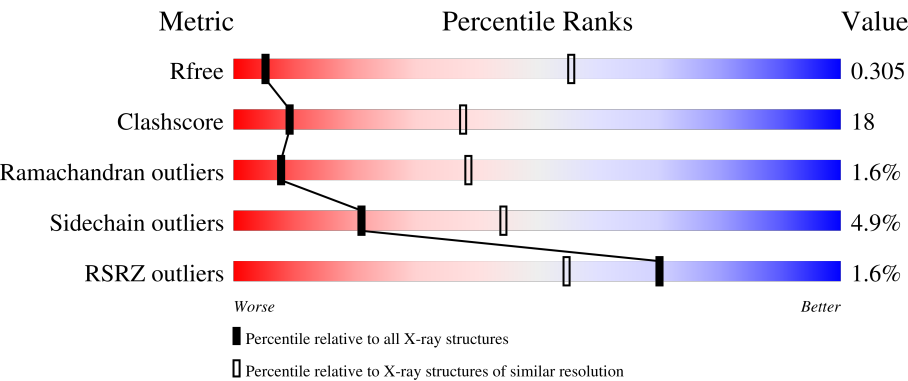
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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.



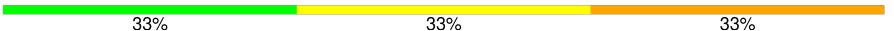


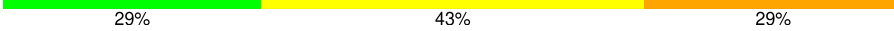





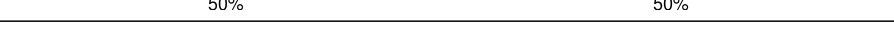
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	164625	1145 (4.40-3.80)
Clashscore	180529	1211 (4.40-3.80)
Ramachandran outliers	177936	1140 (4.40-3.80)
Sidechain outliers	177891	1127 (4.40-3.80)
RSRZ outliers	164620	1143 (4.40-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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	B	153	<div><div>3%</div><div>63%</div><div>25%</div><div>•</div><div>9%</div></div>
2	D	243	<div><div>%</div><div>69%</div><div>25%</div><div>•</div><div>•</div></div>
3	E	216	<div><div>%</div><div>74%</div><div>23%</div><div>•</div></div>
4	G	479	<div><div>2%</div><div>58%</div><div>33%</div><div>•</div><div>6%</div></div>
5	Q	241	<div><div></div><div>65%</div><div>25%</div><div>•</div><div>5%</div></div>
6	R	215	<div><div>%</div><div>60%</div><div>33%</div><div>5%</div><div>•</div></div>

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Mol	Chain	Length	Quality of chain
7	A	3	
7	O	3	
8	C	5	
8	J	5	
9	F	7	
10	H	5	
10	U	5	
11	I	7	
12	K	4	
12	T	4	
13	L	4	
14	M	7	
15	N	8	
16	P	6	
17	S	8	
18	V	9	

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
17	NAG	S	1	-	-	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 12325 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	139	Total	C	N	O	S	0	0	0
			1109	700	195	208	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	CYS	THR	engineered mutation	UNP Q2N0S7

- Molecule 2 is a protein called 35O22 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	235	Total	C	N	O	S	0	0	0
			1753	1110	295	340	8			

- Molecule 3 is a protein called 35O22 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	210	Total	C	N	O	S	0	0	0
			1592	998	264	322	8			

- Molecule 4 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	451	Total	C	N	O	S	0	0	0
			3537	2220	625	665	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6

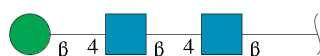
- Molecule 5 is a protein called BG18 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Q	228	Total	C	N	O	S	0	0	0
			1678	1055	286	329	8			

- Molecule 6 is a protein called BG18 Light Chain.

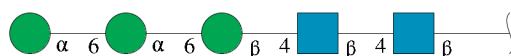
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	R	211	Total	C	N	O	S	0	0	0
			1514	947	253	308	6			

- Molecule 7 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.



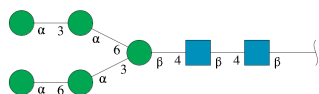
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	A	3	Total	C	N	O		0	0	0
			39	22	2	15				
7	O	3	Total	C	N	O		0	0	0
			39	22	2	15				

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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.



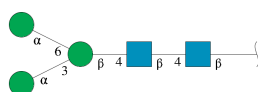
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	C	5	Total	C	N	O		0	0	0
			61	34	2	25				
8	J	5	Total	C	N	O		0	0	0
			61	34	2	25				

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



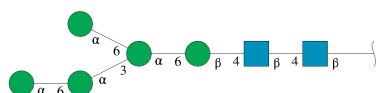
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	F	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 10 is an oligosaccharide called 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				ZeroOcc	AltConf	Trace
10	H	5	Total	C	N	O	0	0	0
			61	34	2	25			
10	U	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 12 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.



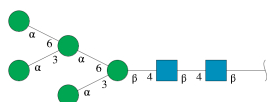
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
12	T	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 13 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.



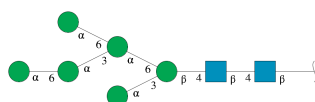
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[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.



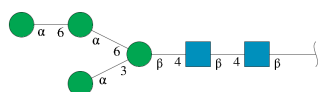
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 15 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[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.



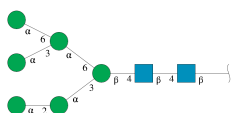
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	N	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 16 is an oligosaccharide called 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.



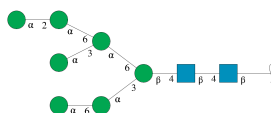
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	P	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 17 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	S	8	Total	C	N	O	0	0	0
			94	52	2	40			

- Molecule 18 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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.

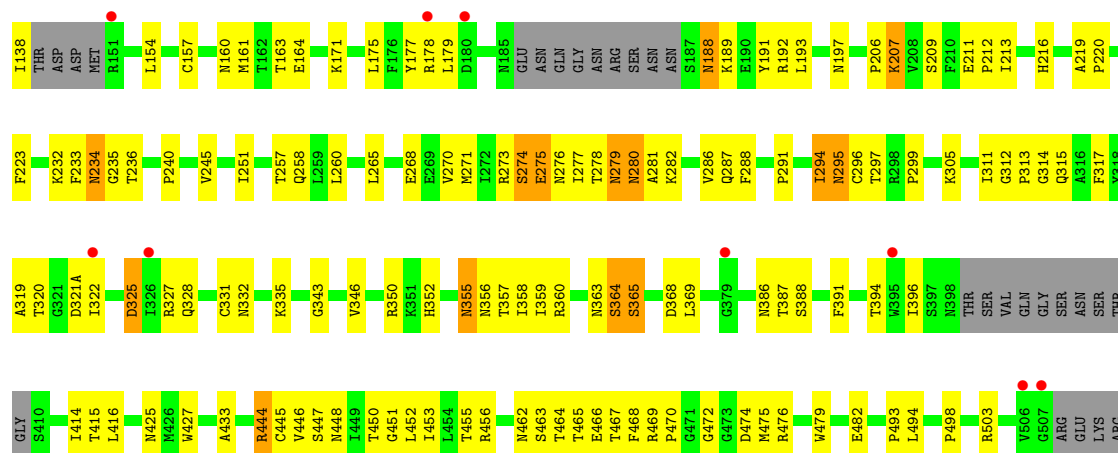


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	V	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 19 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

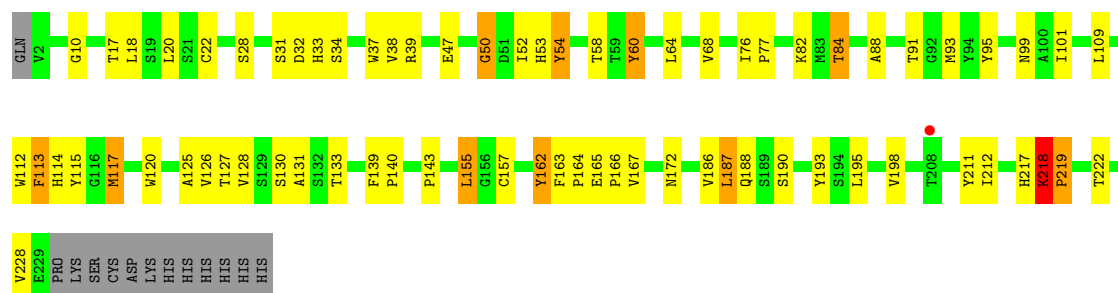


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	B	1	Total	C	N	O	0	0
			14	8	1	5		
19	G	1	Total	C	N	O	0	0
			14	8	1	5		
19	G	1	Total	C	N	O	0	0
			14	8	1	5		
19	G	1	Total	C	N	O	0	0
			14	8	1	5		



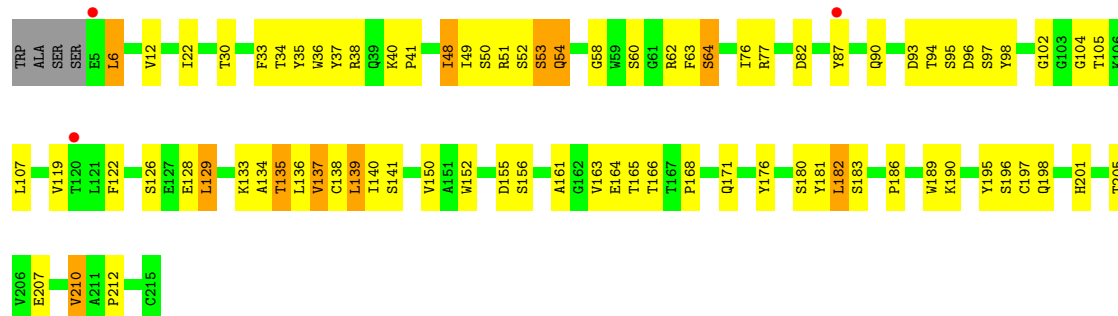
• Molecule 5: BG18 Heavy Chain

Chain Q: 65% 25% 5%



• Molecule 6: BG18 Light Chain

Chain R: 60% 33% 5%



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

Chain A: 67% 33%



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

Chain O: 



- Molecule 8: alpha-D-mannopyranose-(1-6)-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 C: 



- Molecule 8: alpha-D-mannopyranose-(1-6)-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 J: 



- Molecule 9: alpha-D-mannopyranose-(1-6)-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 F: 



- Molecule 10: 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: 



- Molecule 10: 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 U: 




- Molecule 11: α -D-mannopyranose-(1-6)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] 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 I: 



- Molecule 12: α -D-mannopyranose-(1-3)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain K: 



- Molecule 12: α -D-mannopyranose-(1-3)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain T: 




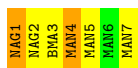
- Molecule 13: α -D-mannopyranose-(1-6)- β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain L: 



- Molecule 14: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain M: 



- Molecule 15: α -D-mannopyranose-(1-6)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain N: 



- Molecule 16: α -D-mannopyranose-(1-6)- α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain P: 

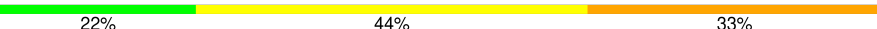
NAG1	NAG2	BMA3	MAN4	MAN5	MAN6
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- Molecule 17: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain S: 

NAG1	NAG2	BMA3	MAN4	MAN5	MAN6	MAN7	MAN8
------	------	------	------	------	------	------	------

- Molecule 18: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-6)- α -D-mannopyranose-(1-3)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain V: 

NAG1	NAG2	BMA3	MAN4	MAN5	MAN6	MAN7	MAN8	MAN9
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4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	239.22Å 239.22Å 355.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.51 – 4.10 39.51 – 4.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.51-4.10) 99.7 (39.51-4.10)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 4.13Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.229 , 0.274 0.261 , 0.305	Depositor DCC
R_{free} test set	1554 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	163.4	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 189.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12325	wwPDB-VP
Average B, all atoms (Å ²)	226.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	B	0.28	0/1127	0.60	2/1527 (0.1%)
2	D	0.27	0/1798	0.52	1/2450 (0.0%)
3	E	0.25	0/1635	0.48	0/2235
4	G	0.28	0/3610	0.54	3/4901 (0.1%)
5	Q	0.27	0/1721	0.51	0/2353
6	R	0.27	0/1552	0.59	2/2129 (0.1%)
All	All	0.27	0/11443	0.54	8/15595 (0.1%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	627	THR	N-CA-C	6.58	128.77	111.00
4	G	464	THR	N-CA-C	6.11	127.51	111.00
4	G	279	ASN	N-CA-C	-5.83	95.27	111.00
1	B	556	LEU	CA-CB-CG	5.75	128.53	115.30
6	R	137	VAL	N-CA-C	-5.70	95.60	111.00

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	B	1109	0	1103	47	1
2	D	1753	0	1713	66	0
3	E	1592	0	1530	35	0
4	G	3537	0	3469	158	0
5	Q	1678	0	1590	55	0
6	R	1514	0	1411	81	0
7	A	39	0	34	2	0
7	O	39	0	34	2	0
8	C	61	0	52	1	0
8	J	61	0	52	1	0
9	F	83	0	70	4	0
10	H	61	0	52	2	0
10	U	61	0	52	3	0
11	I	83	0	70	5	0
12	K	50	0	43	2	0
12	T	50	0	43	0	0
13	L	50	0	43	0	0
14	M	83	0	69	3	0
15	N	94	0	79	3	0
16	P	72	0	61	0	0
17	S	94	0	79	15	0
18	V	105	0	87	4	0
19	B	14	0	13	0	0
19	G	42	0	39	1	0
All	All	12325	0	11788	432	1

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 18.

The worst 5 of 432 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)
4:G:386:ASN:HD21	17:S:1:NAG:C2	1.24	1.48
4:G:386:ASN:ND2	17:S:1:NAG:C1	1.75	1.45
1:B:626:MET:O	1:B:627:THR:CG2	1.79	1.30
1:B:624:ASP:O	2:D:98:ARG:HG3	1.35	1.22
4:G:386:ASN:ND2	17:S:1:NAG:N2	1.86	1.21

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:MET:O	1:B:652:GLN:NE2[2_545]	2.11	0.09

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 X-ray entries followed by that with respect to entries of similar resolution.

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	B	135/153 (88%)	124 (92%)	10 (7%)	1 (1%)	19	56
2	D	233/243 (96%)	205 (88%)	25 (11%)	3 (1%)	10	42
3	E	208/216 (96%)	185 (89%)	23 (11%)	0	100	100
4	G	443/479 (92%)	386 (87%)	54 (12%)	3 (1%)	19	56
5	Q	226/241 (94%)	184 (81%)	35 (16%)	7 (3%)	3	26
6	R	209/215 (97%)	143 (68%)	57 (27%)	9 (4%)	2	21
All	All	1454/1547 (94%)	1227 (84%)	204 (14%)	23 (2%)	8	39

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	554	ASN
2	D	201	LYS
5	Q	50	GLY
6	R	62	ARG
6	R	212	PRO

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 X-ray entries followed by that with respect to entries of similar resolution.

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	B	121/129 (94%)	115 (95%)	6 (5%)	20	44
2	D	194/206 (94%)	183 (94%)	11 (6%)	17	41
3	E	183/189 (97%)	182 (100%)	1 (0%)	86	90
4	G	400/426 (94%)	376 (94%)	24 (6%)	16	39
5	Q	181/208 (87%)	171 (94%)	10 (6%)	18	42
6	R	161/182 (88%)	152 (94%)	9 (6%)	17	41
All	All	1240/1340 (92%)	1179 (95%)	61 (5%)	21	44

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	G	275	GLU
6	R	60	SER
4	G	350	ARG
6	R	54	GLN
6	R	150	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	96	ASN
3	E	174	ASN
4	G	386	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

90 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$
7	NAG	A	1	1,7	14,14,15	0.27	0	17,19,21	1.38	1 (5%)
7	NAG	A	2	7	14,14,15	0.35	0	17,19,21	0.68	0
7	BMA	A	3	7	11,11,12	0.24	0	15,15,17	0.79	0
8	NAG	C	1	1,8	14,14,15	0.29	0	17,19,21	0.83	0
8	NAG	C	2	8	14,14,15	0.32	0	17,19,21	1.15	2 (11%)
8	BMA	C	3	8	11,11,12	0.44	0	15,15,17	0.94	0
8	MAN	C	4	8	11,11,12	0.35	0	15,15,17	0.99	0
8	MAN	C	5	8	11,11,12	0.22	0	15,15,17	0.61	0
9	NAG	F	1	9,4	14,14,15	0.29	0	17,19,21	1.92	6 (35%)
9	NAG	F	2	9	14,14,15	0.26	0	17,19,21	1.65	2 (11%)
9	BMA	F	3	9	11,11,12	0.37	0	15,15,17	1.15	0
9	MAN	F	4	9	11,11,12	0.31	0	15,15,17	0.91	1 (6%)
9	MAN	F	5	9	11,11,12	0.25	0	15,15,17	0.71	0
9	MAN	F	6	9	11,11,12	0.45	0	15,15,17	0.88	0
9	MAN	F	7	9	11,11,12	0.26	0	15,15,17	0.73	0
10	NAG	H	1	10,4	14,14,15	0.28	0	17,19,21	0.90	0
10	NAG	H	2	10	14,14,15	0.31	0	17,19,21	0.59	0
10	BMA	H	3	10	11,11,12	0.31	0	15,15,17	0.82	0
10	MAN	H	4	10	11,11,12	0.94	1 (9%)	15,15,17	1.79	3 (20%)
10	MAN	H	5	10	11,11,12	0.25	0	15,15,17	0.62	0
11	NAG	I	1	11,4	14,14,15	0.28	0	17,19,21	0.92	1 (5%)
11	NAG	I	2	11	14,14,15	0.30	0	17,19,21	0.67	0
11	BMA	I	3	11	11,11,12	0.32	0	15,15,17	0.82	1 (6%)
11	MAN	I	4	11	11,11,12	0.79	0	15,15,17	2.12	4 (26%)
11	MAN	I	5	11	11,11,12	0.49	0	15,15,17	1.09	2 (13%)
11	MAN	I	6	11	11,11,12	0.30	0	15,15,17	0.75	0
11	MAN	I	7	11	11,11,12	0.43	0	15,15,17	0.94	0
8	NAG	J	1	8,4	14,14,15	0.69	0	17,19,21	0.86	1 (5%)
8	NAG	J	2	8	14,14,15	0.42	0	17,19,21	1.06	1 (5%)
8	BMA	J	3	8	11,11,12	0.30	0	15,15,17	0.82	0
8	MAN	J	4	8	11,11,12	0.25	0	15,15,17	0.58	0
8	MAN	J	5	8	11,11,12	0.26	0	15,15,17	0.66	0
12	NAG	K	1	12,4	14,14,15	0.47	0	17,19,21	2.25	6 (35%)
12	NAG	K	2	12	14,14,15	0.37	0	17,19,21	0.92	1 (5%)
12	BMA	K	3	12	11,11,12	0.31	0	15,15,17	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MAN	K	4	12	11,11,12	0.26	0	15,15,17	0.82	1 (6%)
13	NAG	L	1	13,4	14,14,15	0.28	0	17,19,21	0.92	0
13	NAG	L	2	13	14,14,15	0.39	0	17,19,21	1.06	1 (5%)
13	BMA	L	3	13	11,11,12	0.30	0	15,15,17	0.71	0
13	MAN	L	4	13	11,11,12	0.26	0	15,15,17	0.56	0
14	NAG	M	1	14,4	14,14,15	0.31	0	17,19,21	0.90	1 (5%)
14	NAG	M	2	14	14,14,15	0.42	0	17,19,21	0.87	1 (5%)
14	BMA	M	3	14	11,11,12	0.73	0	15,15,17	1.28	2 (13%)
14	MAN	M	4	14	11,11,12	0.36	0	15,15,17	1.82	4 (26%)
14	MAN	M	5	14	11,11,12	0.45	0	15,15,17	1.19	2 (13%)
14	MAN	M	6	14	11,11,12	0.26	0	15,15,17	0.66	0
14	MAN	M	7	14	11,11,12	0.56	0	15,15,17	1.07	2 (13%)
15	NAG	N	1	15	14,14,15	0.94	1 (7%)	17,19,21	3.14	5 (29%)
15	NAG	N	2	15	14,14,15	0.28	0	17,19,21	0.81	1 (5%)
15	BMA	N	3	15	11,11,12	0.31	0	15,15,17	1.37	1 (6%)
15	MAN	N	4	15	11,11,12	0.28	0	15,15,17	0.70	0
15	MAN	N	5	15	11,11,12	0.26	0	15,15,17	0.78	0
15	MAN	N	6	15	11,11,12	0.23	0	15,15,17	0.71	0
15	MAN	N	7	15	11,11,12	0.25	0	15,15,17	0.64	0
15	MAN	N	8	15	11,11,12	0.56	0	15,15,17	1.23	2 (13%)
7	NAG	O	1	7,4	14,14,15	0.31	0	17,19,21	2.31	4 (23%)
7	NAG	O	2	7	14,14,15	0.29	0	17,19,21	0.96	1 (5%)
7	BMA	O	3	7	11,11,12	0.22	0	15,15,17	0.65	0
16	NAG	P	1	4,16	14,14,15	0.26	0	17,19,21	1.12	1 (5%)
16	NAG	P	2	16	14,14,15	0.44	0	17,19,21	1.41	2 (11%)
16	BMA	P	3	16	11,11,12	0.50	0	15,15,17	1.07	1 (6%)
16	MAN	P	4	16	11,11,12	0.31	0	15,15,17	0.62	0
16	MAN	P	5	16	11,11,12	0.27	0	15,15,17	0.73	0
16	MAN	P	6	16	11,11,12	0.27	0	15,15,17	0.70	0
17	NAG	S	1	17	14,14,15	0.27	0	17,19,21	1.54	3 (17%)
17	NAG	S	2	17	14,14,15	0.51	0	17,19,21	1.27	1 (5%)
17	BMA	S	3	17	11,11,12	0.51	0	15,15,17	1.07	1 (6%)
17	MAN	S	4	17	11,11,12	0.34	0	15,15,17	0.64	0
17	MAN	S	5	17	11,11,12	0.24	0	15,15,17	0.60	0
17	MAN	S	6	17	11,11,12	0.30	0	15,15,17	0.68	0
17	MAN	S	7	17	11,11,12	0.26	0	15,15,17	0.66	0
17	MAN	S	8	17	11,11,12	0.24	0	15,15,17	0.64	0
12	NAG	T	1	12,4	14,14,15	0.33	0	17,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	NAG	T	2	12	14,14,15	0.35	0	17,19,21	0.93	1 (5%)
12	BMA	T	3	12	11,11,12	0.25	0	15,15,17	0.78	0
12	MAN	T	4	12	11,11,12	0.32	0	15,15,17	0.84	0
10	NAG	U	1	10,4	14,14,15	0.27	0	17,19,21	1.08	2 (11%)
10	NAG	U	2	10	14,14,15	0.42	0	17,19,21	1.92	4 (23%)
10	BMA	U	3	10	11,11,12	0.46	0	15,15,17	1.83	4 (26%)
10	MAN	U	4	10	11,11,12	1.04	1 (9%)	15,15,17	1.74	3 (20%)
10	MAN	U	5	10	11,11,12	0.90	1 (9%)	15,15,17	1.87	3 (20%)
18	NAG	V	1	18,4	14,14,15	0.28	0	17,19,21	0.96	1 (5%)
18	NAG	V	2	18	14,14,15	0.30	0	17,19,21	0.61	0
18	BMA	V	3	18	11,11,12	0.29	0	15,15,17	1.12	1 (6%)
18	MAN	V	4	18	11,11,12	0.25	0	15,15,17	0.93	0
18	MAN	V	5	18	11,11,12	0.23	0	15,15,17	0.87	0
18	MAN	V	6	18	11,11,12	0.23	0	15,15,17	0.84	1 (6%)
18	MAN	V	7	18	11,11,12	0.54	0	15,15,17	1.16	1 (6%)
18	MAN	V	8	18	11,11,12	0.50	0	15,15,17	1.04	1 (6%)
18	MAN	V	9	18	11,11,12	0.57	0	15,15,17	1.17	2 (13%)

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	A	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	A	2	7	-	3/6/23/26	0/1/1/1
7	BMA	A	3	7	-	1/2/19/22	0/1/1/1
8	NAG	C	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	5/6/23/26	0/1/1/1
8	BMA	C	3	8	-	0/2/19/22	0/1/1/1
8	MAN	C	4	8	-	2/2/19/22	0/1/1/1
8	MAN	C	5	8	-	1/2/19/22	0/1/1/1
9	NAG	F	1	9,4	-	3/6/23/26	0/1/1/1
9	NAG	F	2	9	-	4/6/23/26	0/1/1/1
9	BMA	F	3	9	-	1/2/19/22	0/1/1/1
9	MAN	F	4	9	-	2/2/19/22	0/1/1/1
9	MAN	F	5	9	-	0/2/19/22	0/1/1/1
9	MAN	F	6	9	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	F	7	9	-	0/2/19/22	0/1/1/1
10	NAG	H	1	10,4	-	0/6/23/26	0/1/1/1
10	NAG	H	2	10	-	5/6/23/26	0/1/1/1
10	BMA	H	3	10	-	0/2/19/22	0/1/1/1
10	MAN	H	4	10	-	0/2/19/22	0/1/1/1
10	MAN	H	5	10	-	0/2/19/22	0/1/1/1
11	NAG	I	1	11,4	-	4/6/23/26	0/1/1/1
11	NAG	I	2	11	-	3/6/23/26	0/1/1/1
11	BMA	I	3	11	-	0/2/19/22	0/1/1/1
11	MAN	I	4	11	-	2/2/19/22	0/1/1/1
11	MAN	I	5	11	-	1/2/19/22	0/1/1/1
11	MAN	I	6	11	-	0/2/19/22	0/1/1/1
11	MAN	I	7	11	-	1/2/19/22	0/1/1/1
8	NAG	J	1	8,4	-	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	0/1/1/1
8	MAN	J	5	8	-	1/2/19/22	0/1/1/1
12	NAG	K	1	12,4	-	2/6/23/26	0/1/1/1
12	NAG	K	2	12	-	3/6/23/26	0/1/1/1
12	BMA	K	3	12	-	0/2/19/22	0/1/1/1
12	MAN	K	4	12	-	1/2/19/22	0/1/1/1
13	NAG	L	1	13,4	-	2/6/23/26	0/1/1/1
13	NAG	L	2	13	-	3/6/23/26	0/1/1/1
13	BMA	L	3	13	-	2/2/19/22	0/1/1/1
13	MAN	L	4	13	-	0/2/19/22	0/1/1/1
14	NAG	M	1	14,4	-	3/6/23/26	0/1/1/1
14	NAG	M	2	14	-	3/6/23/26	0/1/1/1
14	BMA	M	3	14	-	0/2/19/22	0/1/1/1
14	MAN	M	4	14	-	1/2/19/22	0/1/1/1
14	MAN	M	5	14	-	0/2/19/22	0/1/1/1
14	MAN	M	6	14	-	0/2/19/22	0/1/1/1
14	MAN	M	7	14	-	2/2/19/22	0/1/1/1
15	NAG	N	1	15	-	5/6/23/26	0/1/1/1
15	NAG	N	2	15	-	3/6/23/26	0/1/1/1
15	BMA	N	3	15	-	2/2/19/22	0/1/1/1
15	MAN	N	4	15	-	2/2/19/22	0/1/1/1
15	MAN	N	5	15	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	MAN	N	6	15	-	0/2/19/22	0/1/1/1
15	MAN	N	7	15	-	2/2/19/22	0/1/1/1
15	MAN	N	8	15	-	0/2/19/22	0/1/1/1
7	NAG	O	1	7,4	-	2/6/23/26	0/1/1/1
7	NAG	O	2	7	-	3/6/23/26	0/1/1/1
7	BMA	O	3	7	-	0/2/19/22	0/1/1/1
16	NAG	P	1	4,16	-	2/6/23/26	0/1/1/1
16	NAG	P	2	16	-	1/6/23/26	0/1/1/1
16	BMA	P	3	16	-	1/2/19/22	0/1/1/1
16	MAN	P	4	16	-	2/2/19/22	0/1/1/1
16	MAN	P	5	16	-	0/2/19/22	0/1/1/1
16	MAN	P	6	16	-	0/2/19/22	0/1/1/1
17	NAG	S	1	17	-	5/6/23/26	0/1/1/1
17	NAG	S	2	17	-	4/6/23/26	0/1/1/1
17	BMA	S	3	17	-	2/2/19/22	0/1/1/1
17	MAN	S	4	17	-	1/2/19/22	0/1/1/1
17	MAN	S	5	17	-	1/2/19/22	0/1/1/1
17	MAN	S	6	17	-	2/2/19/22	0/1/1/1
17	MAN	S	7	17	-	1/2/19/22	0/1/1/1
17	MAN	S	8	17	-	1/2/19/22	0/1/1/1
12	NAG	T	1	12,4	-	2/6/23/26	0/1/1/1
12	NAG	T	2	12	-	2/6/23/26	0/1/1/1
12	BMA	T	3	12	-	0/2/19/22	0/1/1/1
12	MAN	T	4	12	-	0/2/19/22	0/1/1/1
10	NAG	U	1	10,4	-	2/6/23/26	0/1/1/1
10	NAG	U	2	10	-	4/6/23/26	0/1/1/1
10	BMA	U	3	10	-	2/2/19/22	0/1/1/1
10	MAN	U	4	10	-	2/2/19/22	0/1/1/1
10	MAN	U	5	10	-	0/2/19/22	0/1/1/1
18	NAG	V	1	18,4	-	4/6/23/26	0/1/1/1
18	NAG	V	2	18	-	0/6/23/26	0/1/1/1
18	BMA	V	3	18	-	0/2/19/22	0/1/1/1
18	MAN	V	4	18	-	2/2/19/22	0/1/1/1
18	MAN	V	5	18	-	0/2/19/22	0/1/1/1
18	MAN	V	6	18	-	0/2/19/22	0/1/1/1
18	MAN	V	7	18	-	0/2/19/22	0/1/1/1
18	MAN	V	8	18	-	2/2/19/22	0/1/1/1
18	MAN	V	9	18	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	1	NAG	O5-C1	-2.87	1.38	1.43
10	U	4	MAN	O5-C1	2.73	1.48	1.43
10	H	4	MAN	O5-C1	2.35	1.47	1.43
10	U	5	MAN	O5-C1	2.15	1.47	1.43

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	1	NAG	C1-O5-C5	-9.69	99.20	112.19
7	O	1	NAG	C1-O5-C5	-6.25	103.82	112.19
10	U	2	NAG	O4-C4-C5	-5.73	95.22	109.32
12	K	1	NAG	C1-O5-C5	-5.49	104.83	112.19
10	U	5	MAN	C1-O5-C5	5.24	119.21	112.19

There are no chirality outliers.

5 of 143 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1	NAG	C8-C7-N2-C2
7	A	1	NAG	O7-C7-N2-C2
7	A	2	NAG	C8-C7-N2-C2
7	A	2	NAG	O7-C7-N2-C2
8	C	2	NAG	C3-C2-N2-C7

There are no ring outliers.

37 monomers are involved in 47 short contacts:

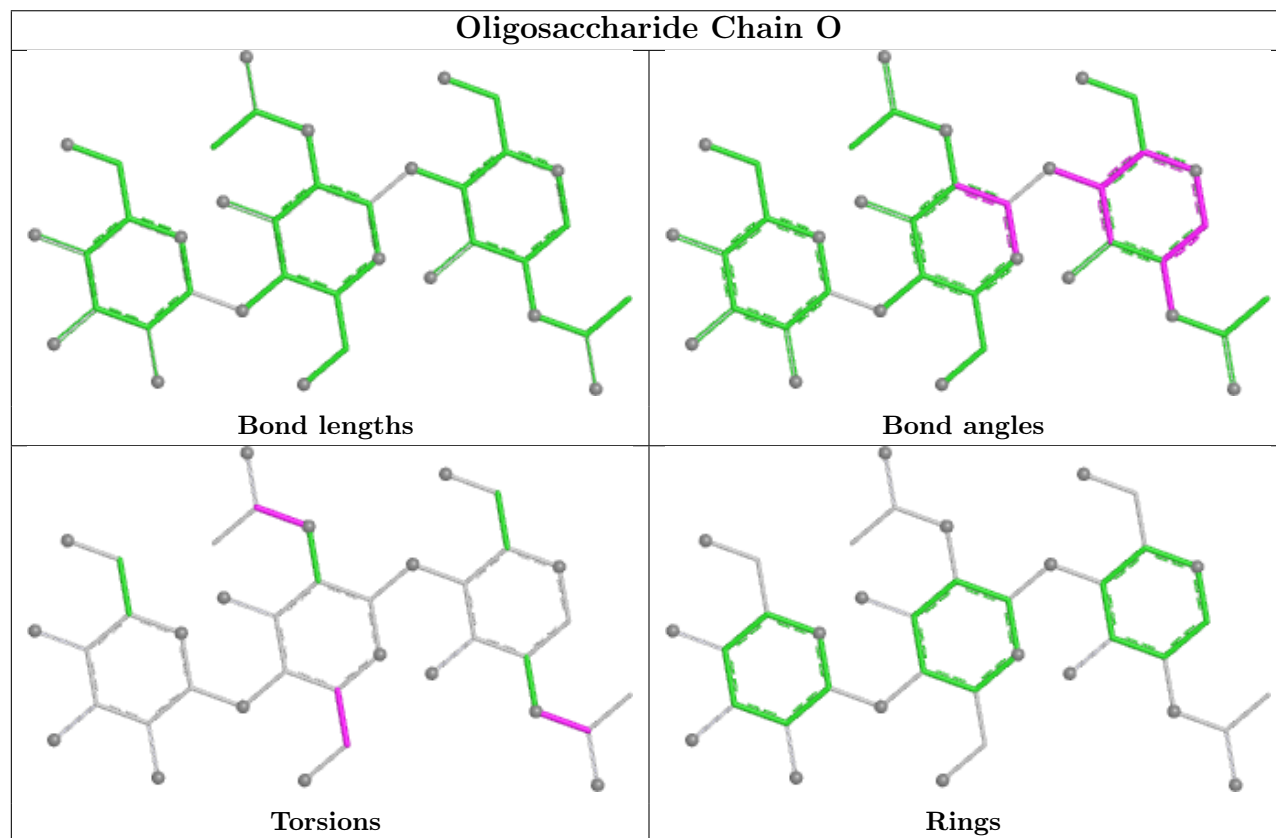
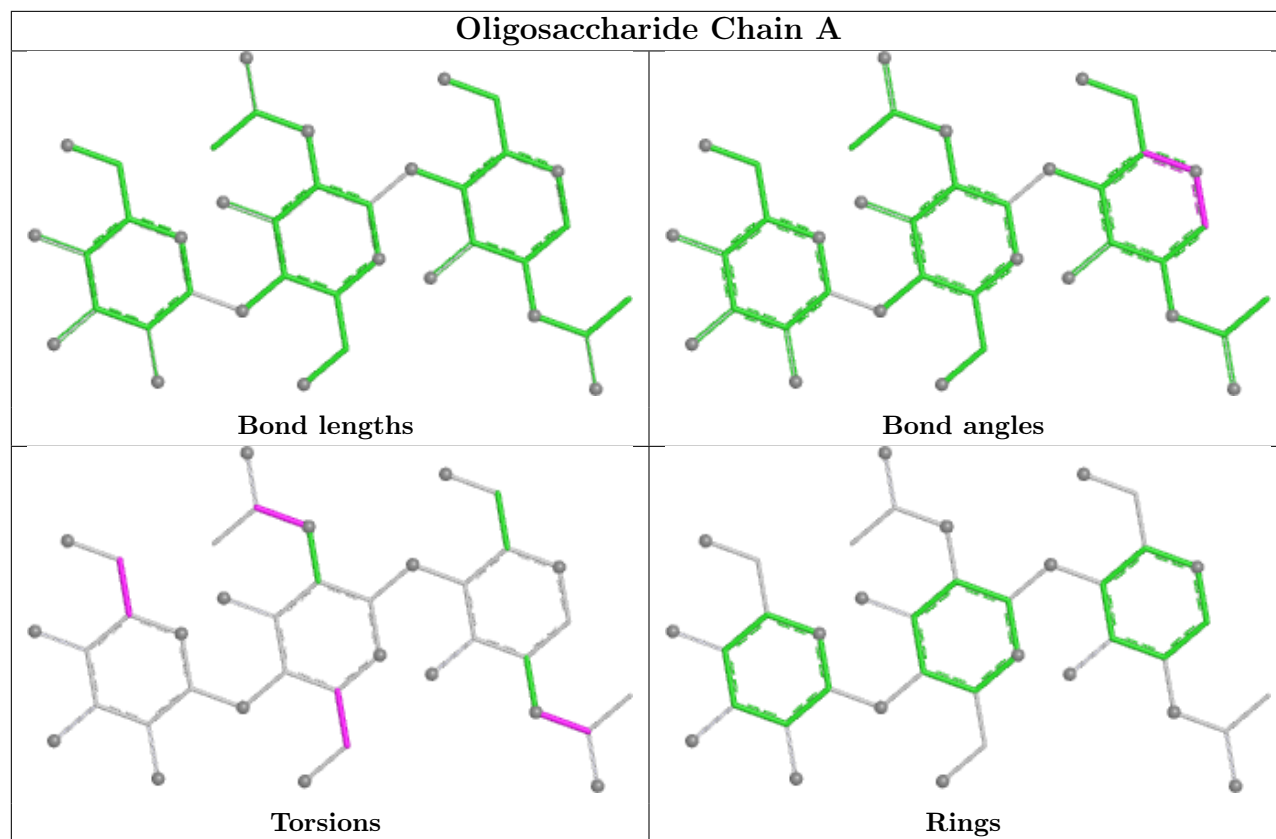
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1	NAG	1	0
9	F	6	MAN	1	0
18	V	6	MAN	1	0
8	C	3	BMA	1	0
8	J	2	NAG	1	0
9	F	1	NAG	1	0
7	A	2	NAG	1	0
11	I	1	NAG	1	0
18	V	2	NAG	1	0
17	S	2	NAG	2	0
14	M	4	MAN	1	0
15	N	1	NAG	1	0

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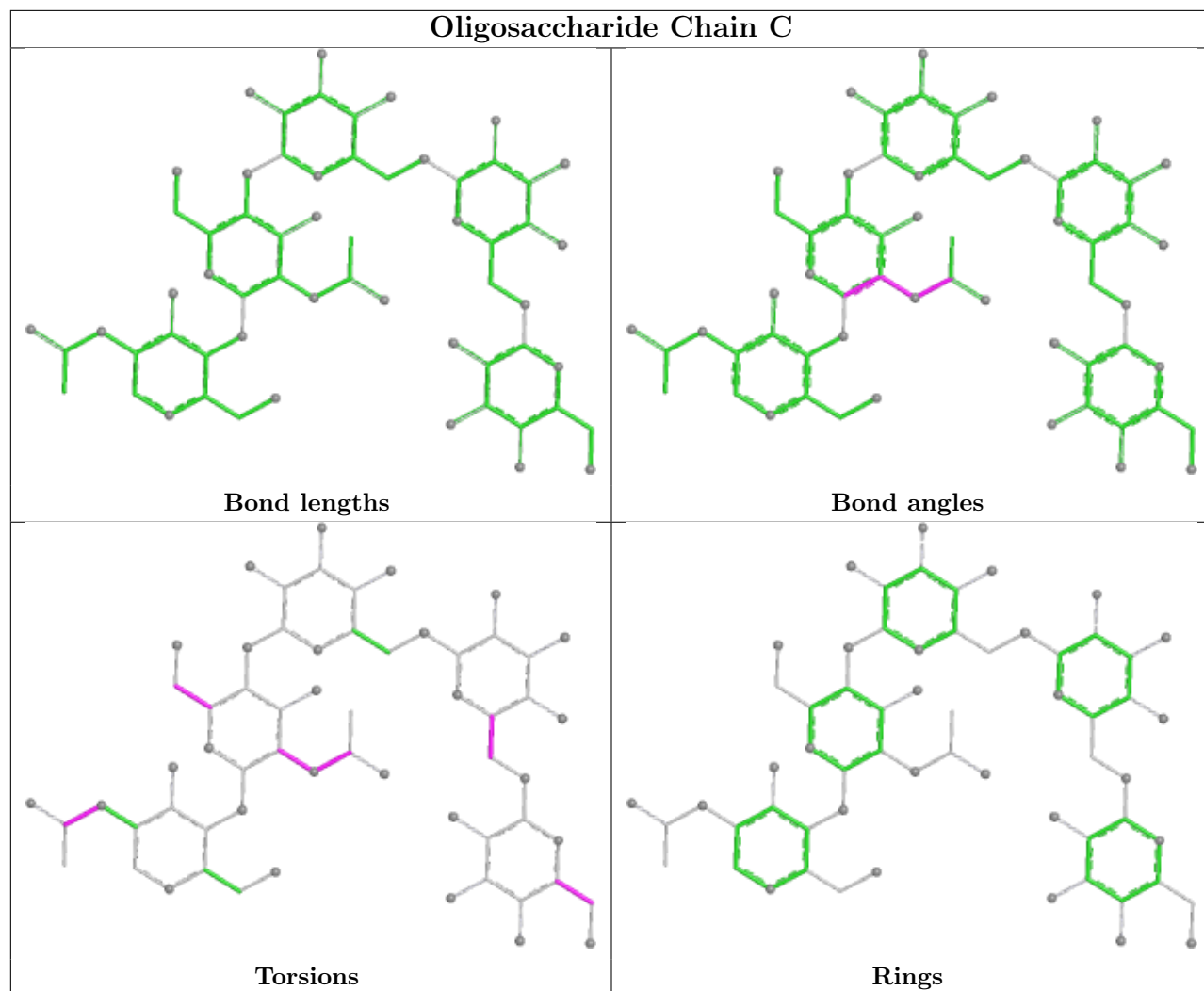
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	3	BMA	1	0
14	M	1	NAG	2	0
11	I	2	NAG	1	0
9	F	3	BMA	2	0
15	N	3	BMA	2	0
10	H	4	MAN	1	0
18	V	9	MAN	1	0
10	U	5	MAN	2	0
15	N	6	MAN	1	0
11	I	5	MAN	3	0
10	H	2	NAG	1	0
10	H	3	BMA	2	0
17	S	3	BMA	1	0
12	K	1	NAG	2	0
11	I	4	MAN	4	0
9	F	2	NAG	1	0
10	U	3	BMA	3	0
11	I	7	MAN	1	0
7	O	1	NAG	2	0
18	V	1	NAG	1	0
8	C	2	NAG	1	0
10	U	4	MAN	1	0
15	N	2	NAG	2	0
17	S	1	NAG	14	0
12	K	2	NAG	1	0

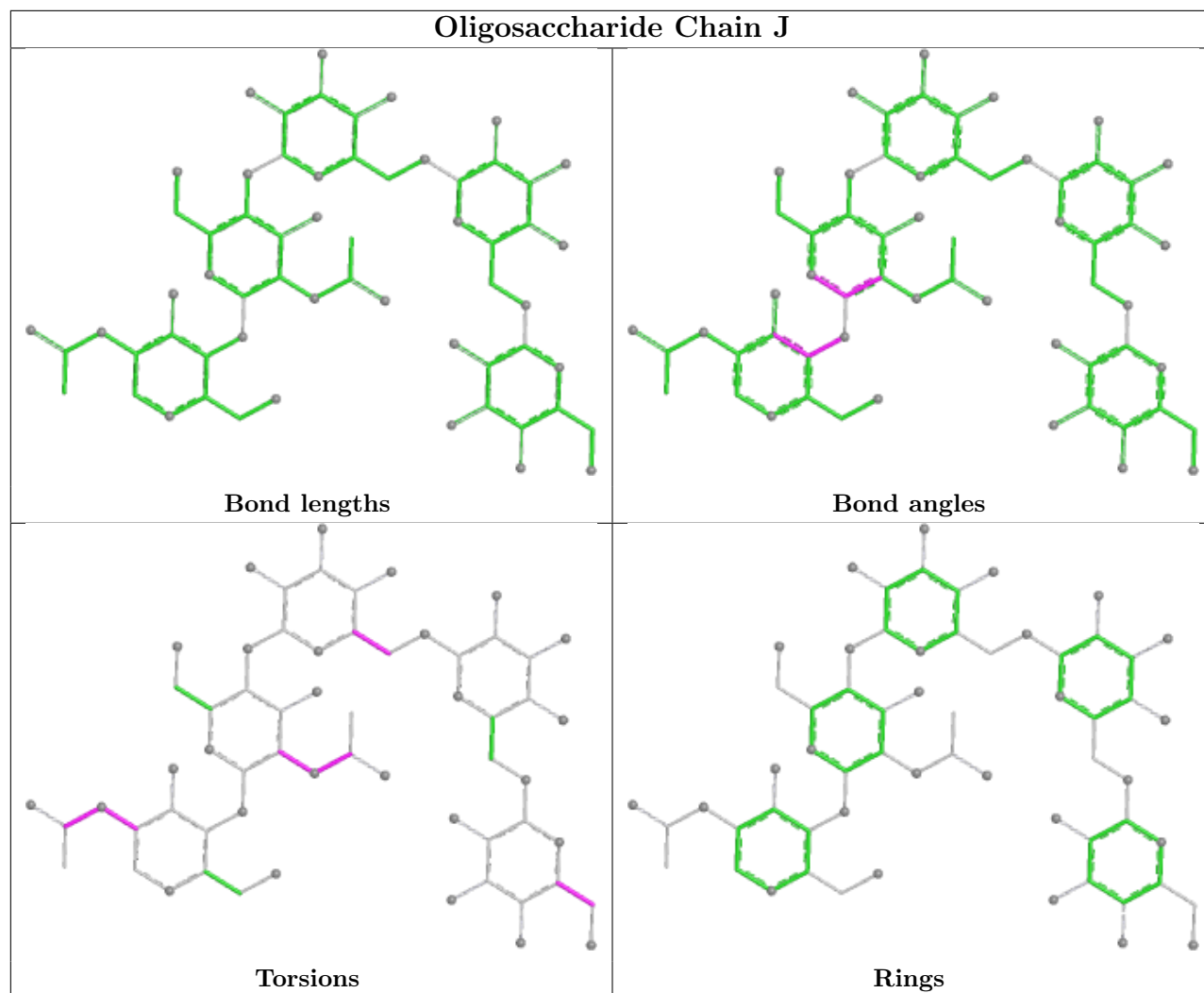
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

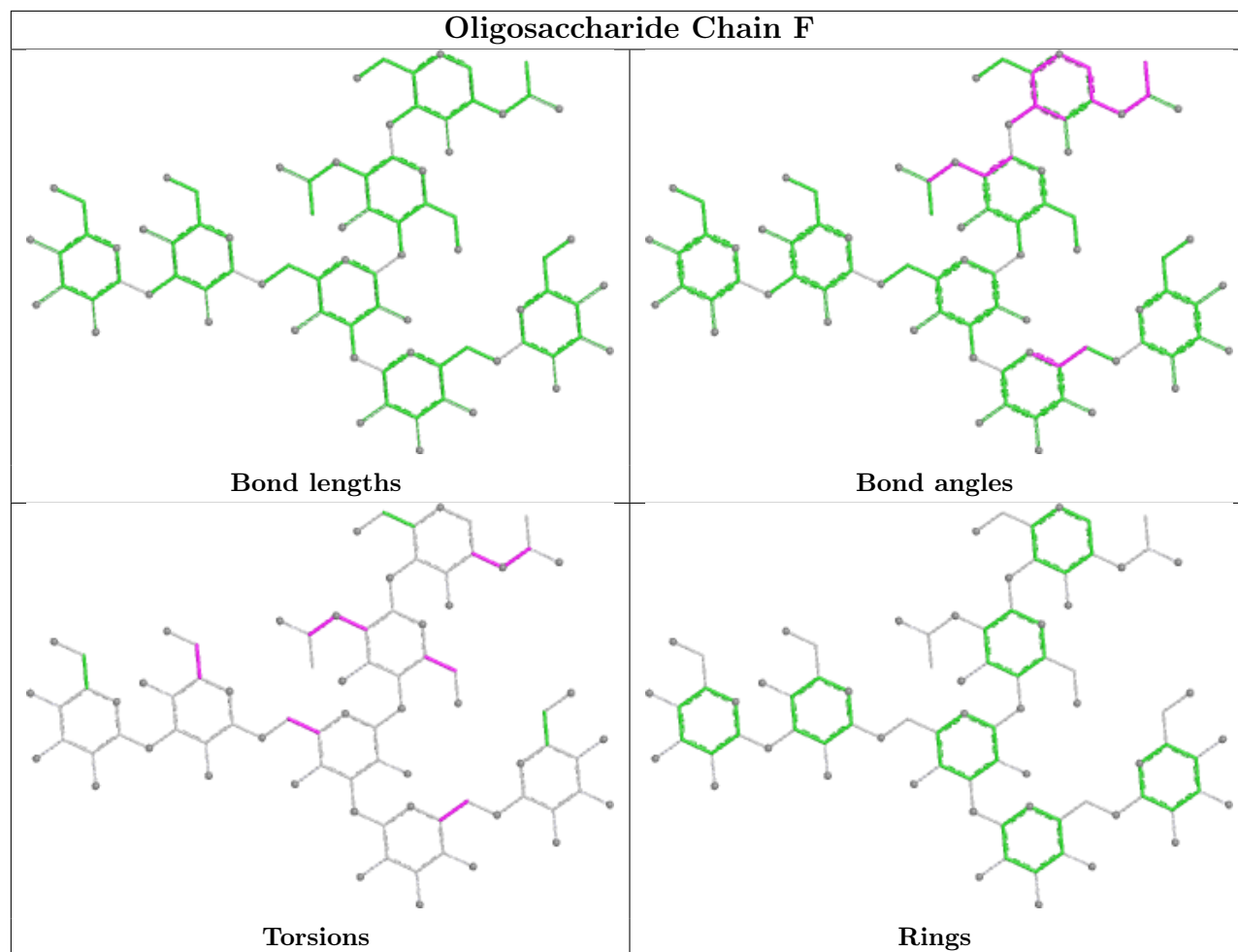


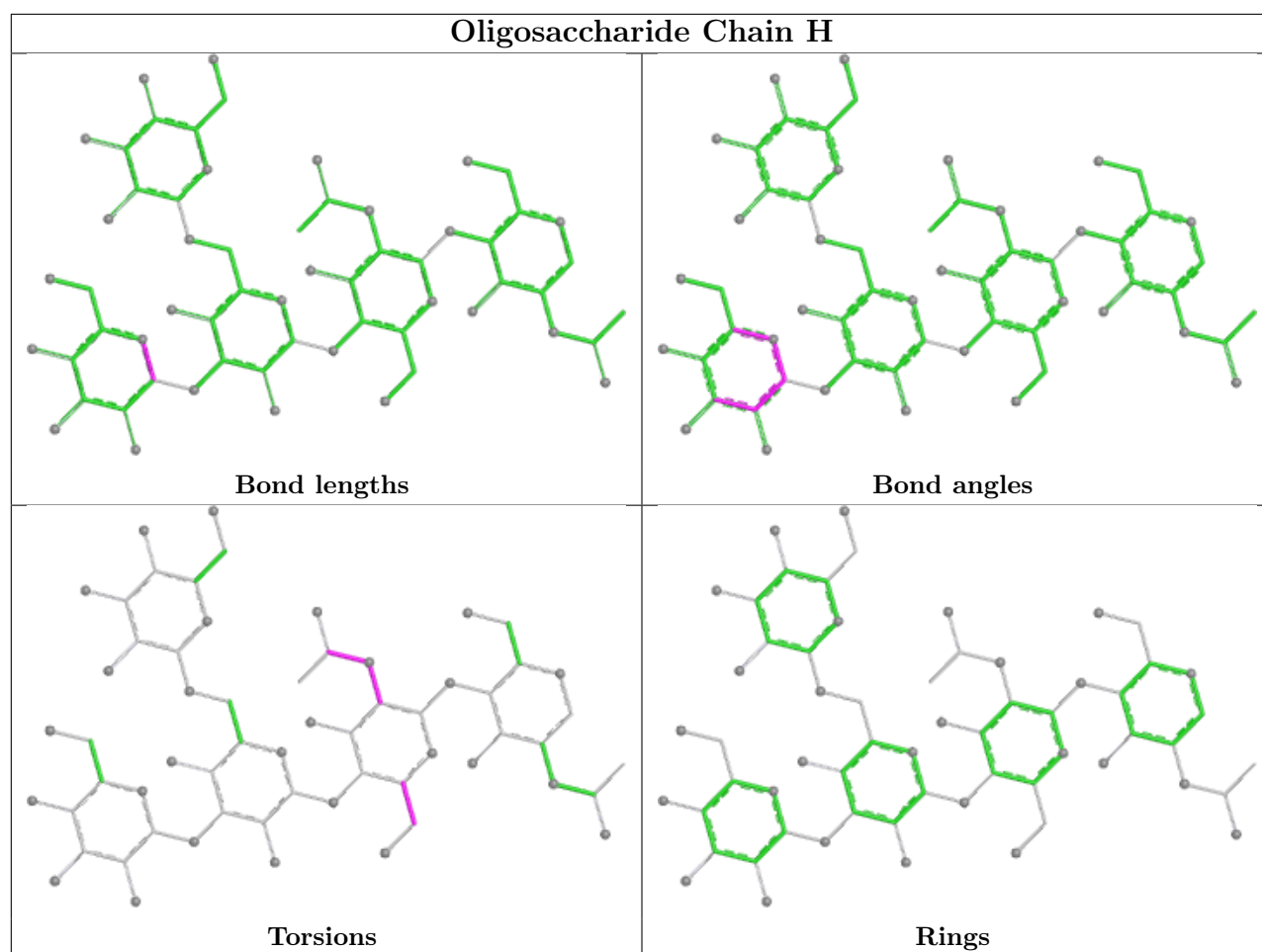
Oligosaccharide Chain C

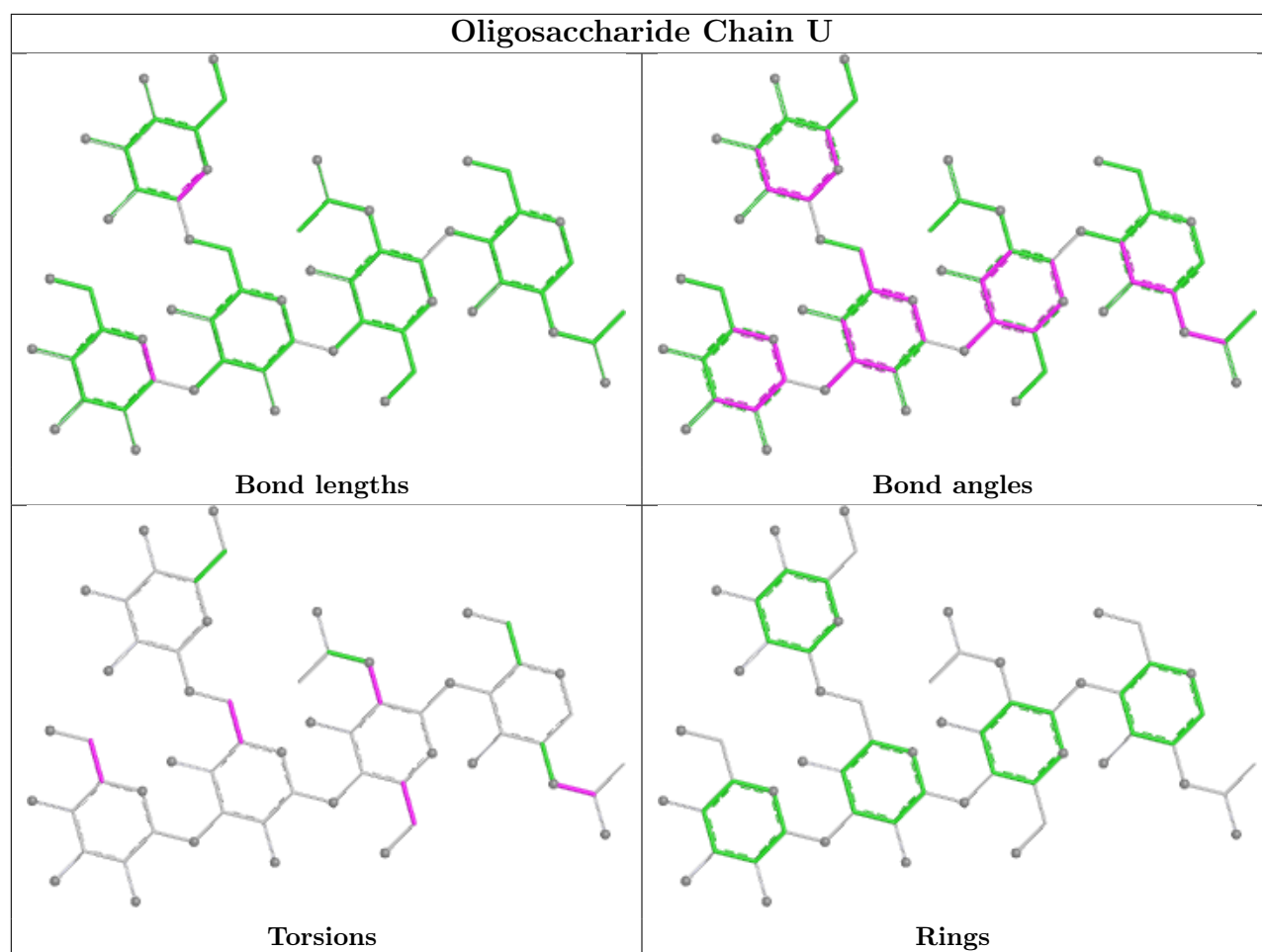


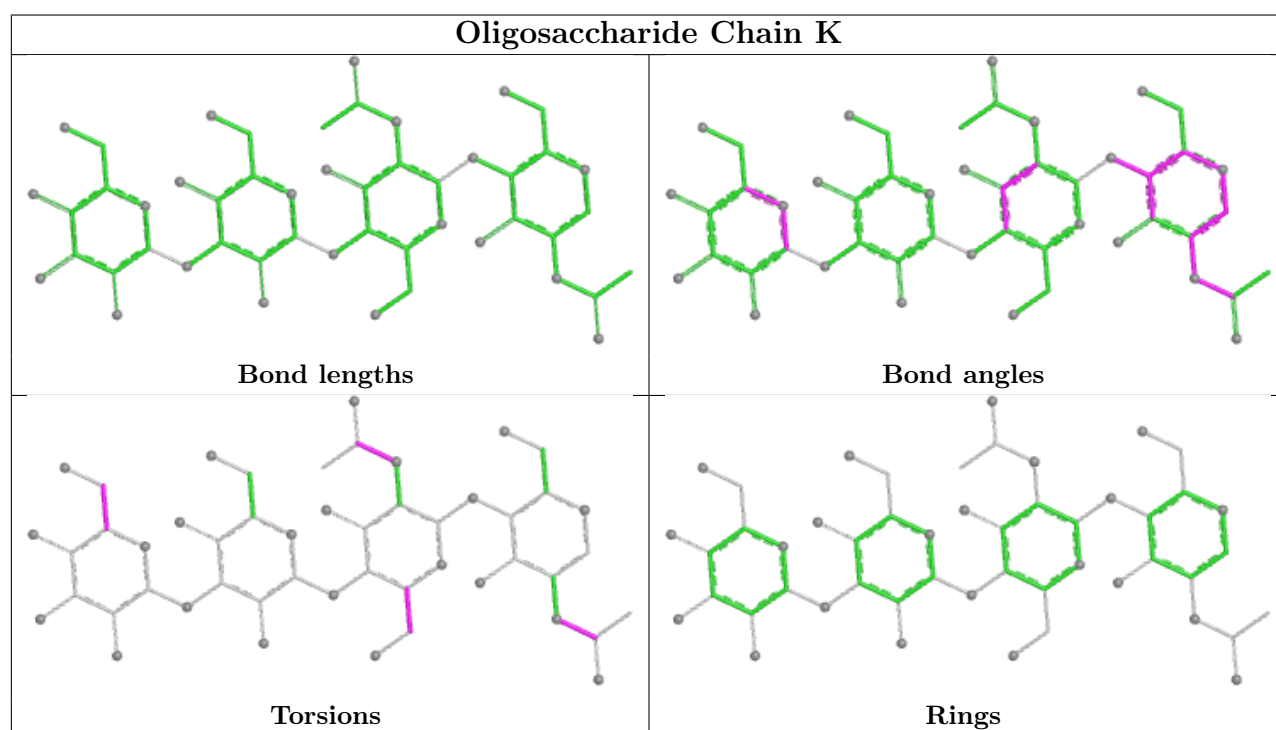
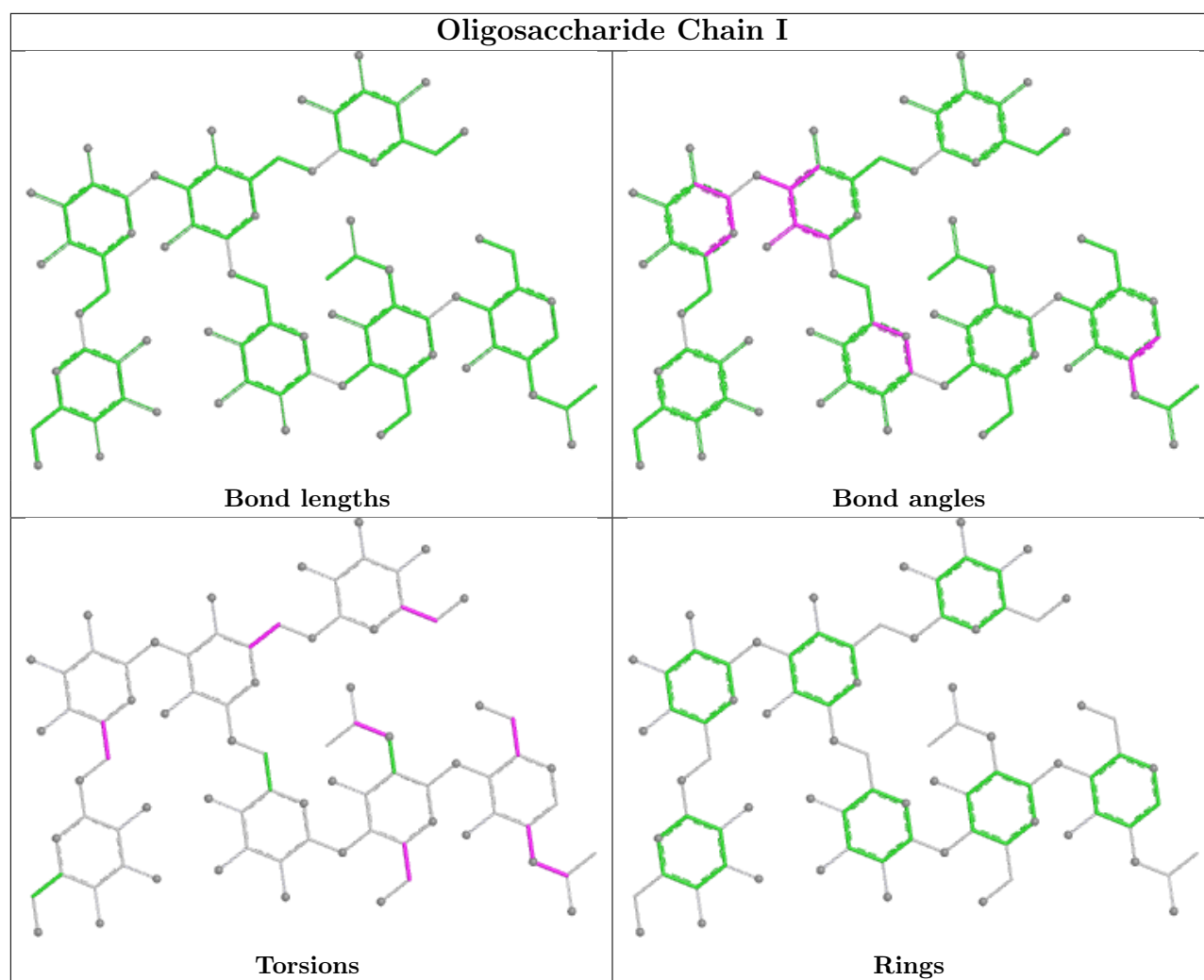
Oligosaccharide Chain J



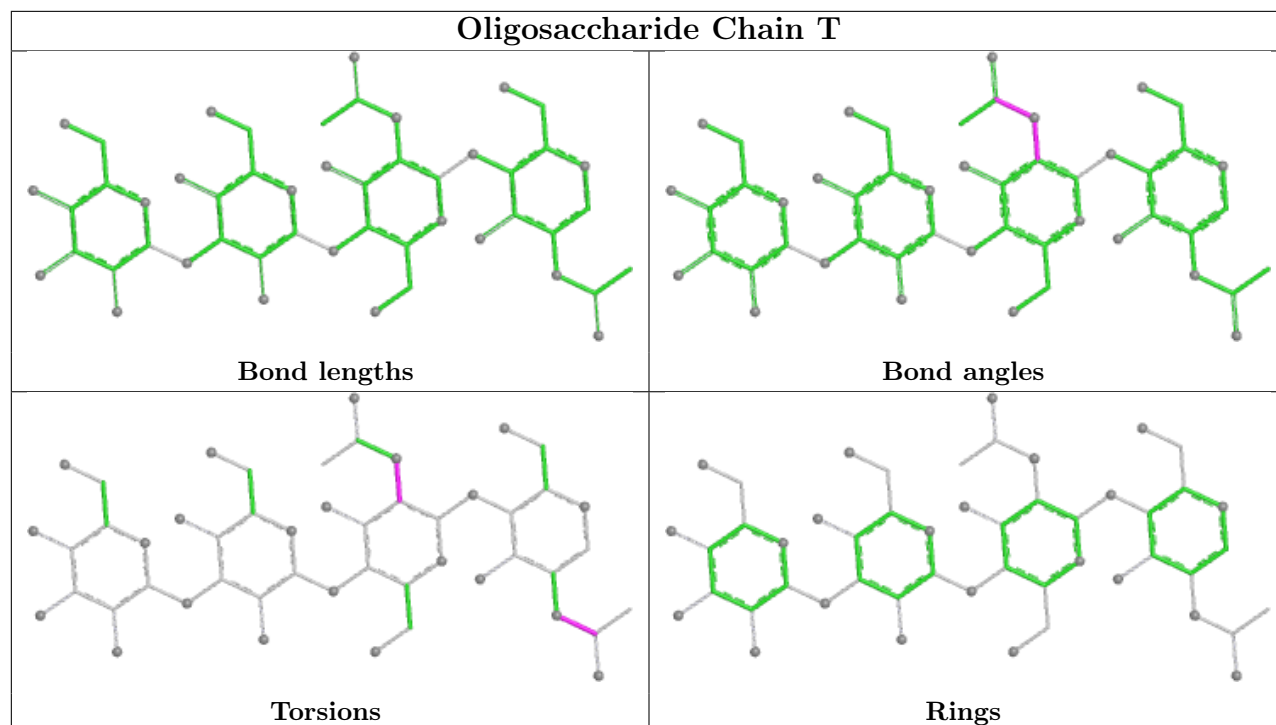




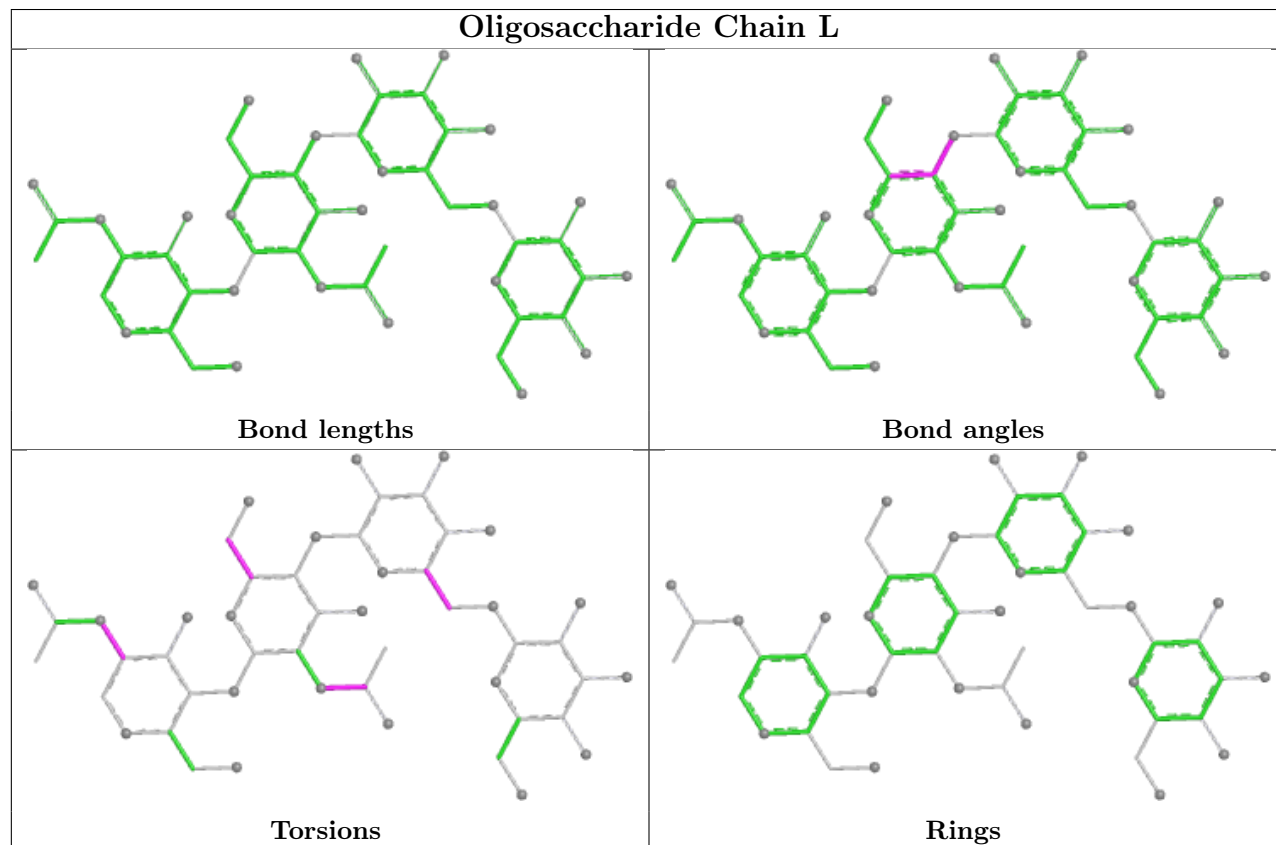


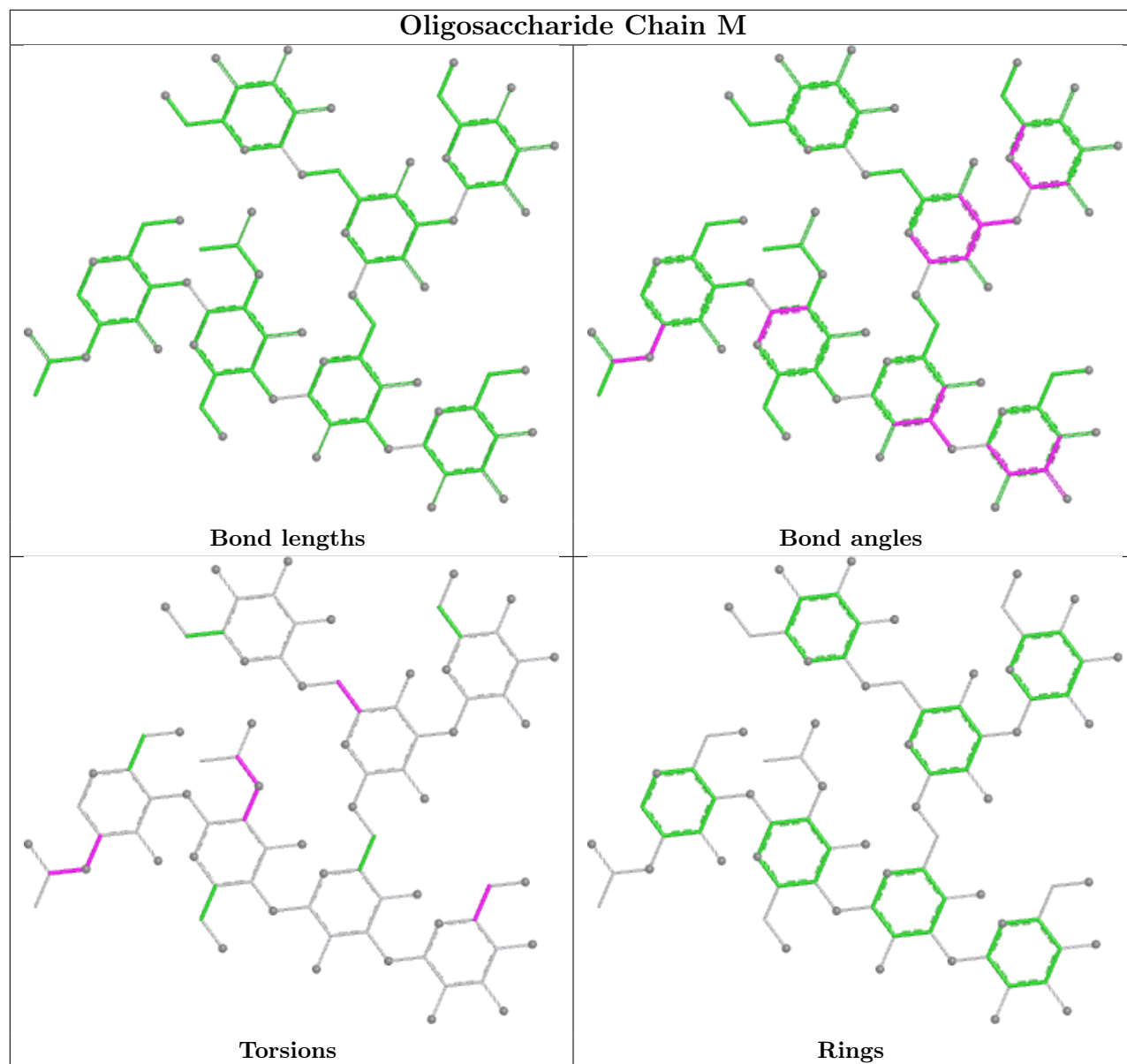


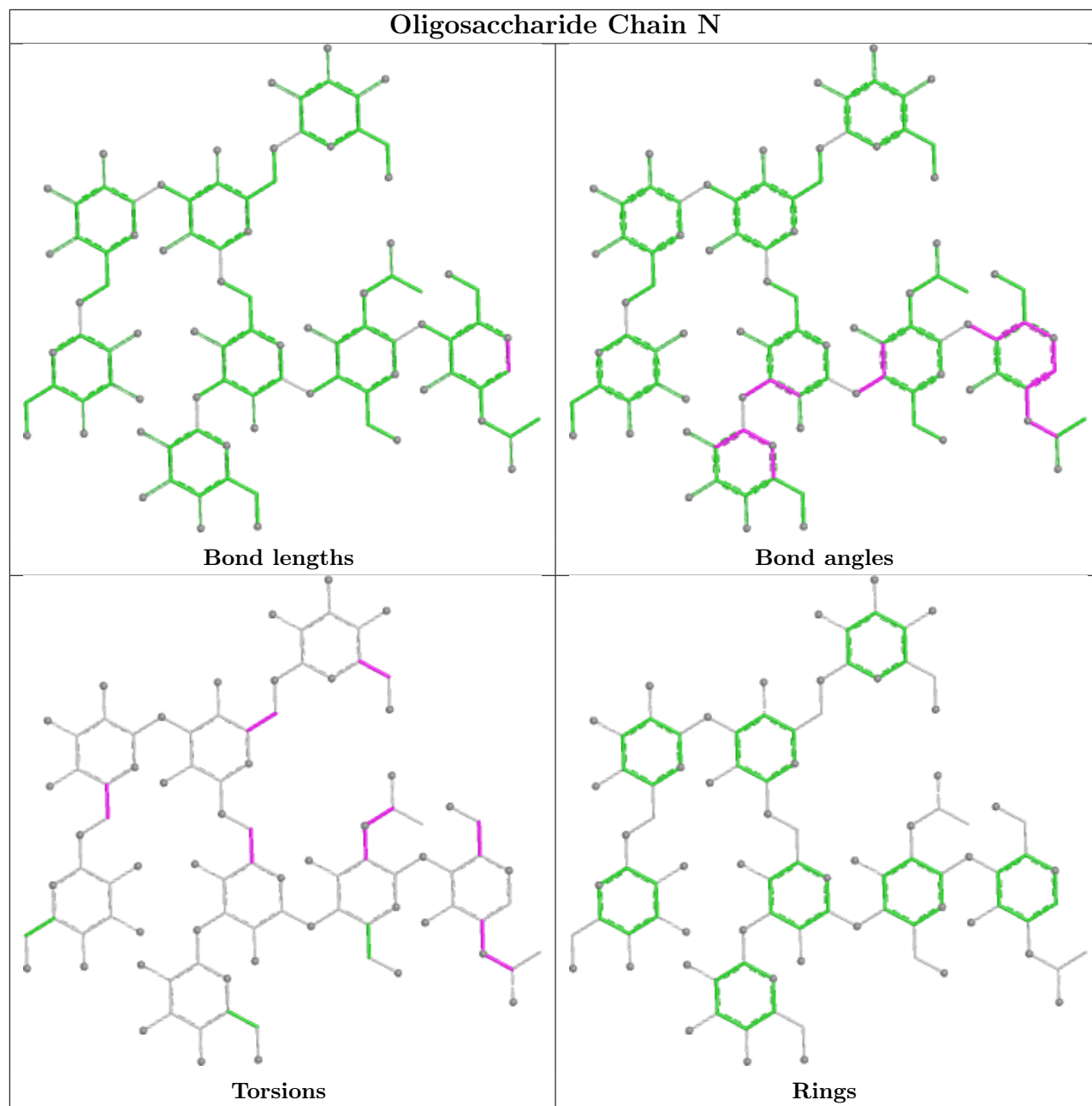
Oligosaccharide Chain T

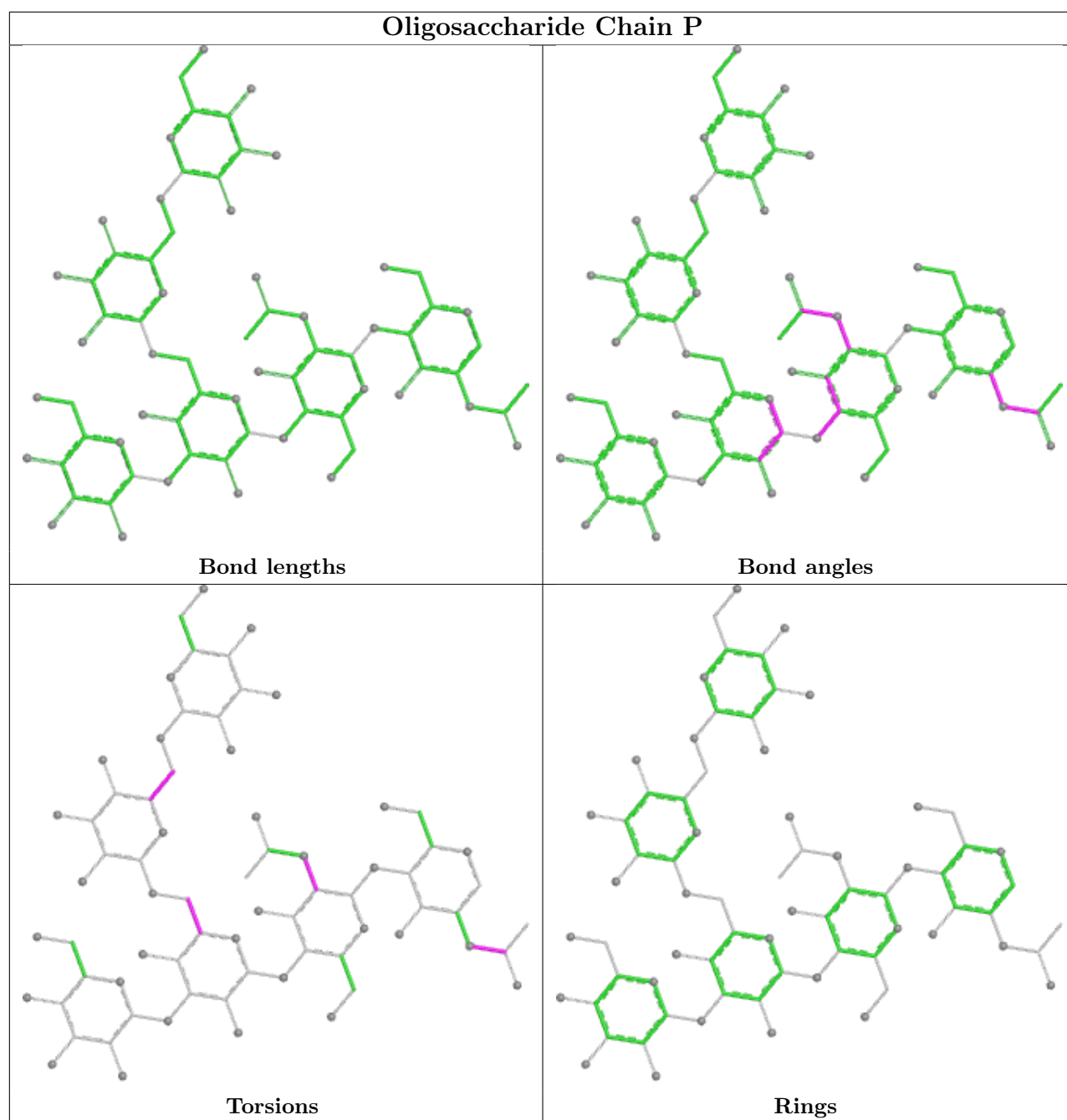


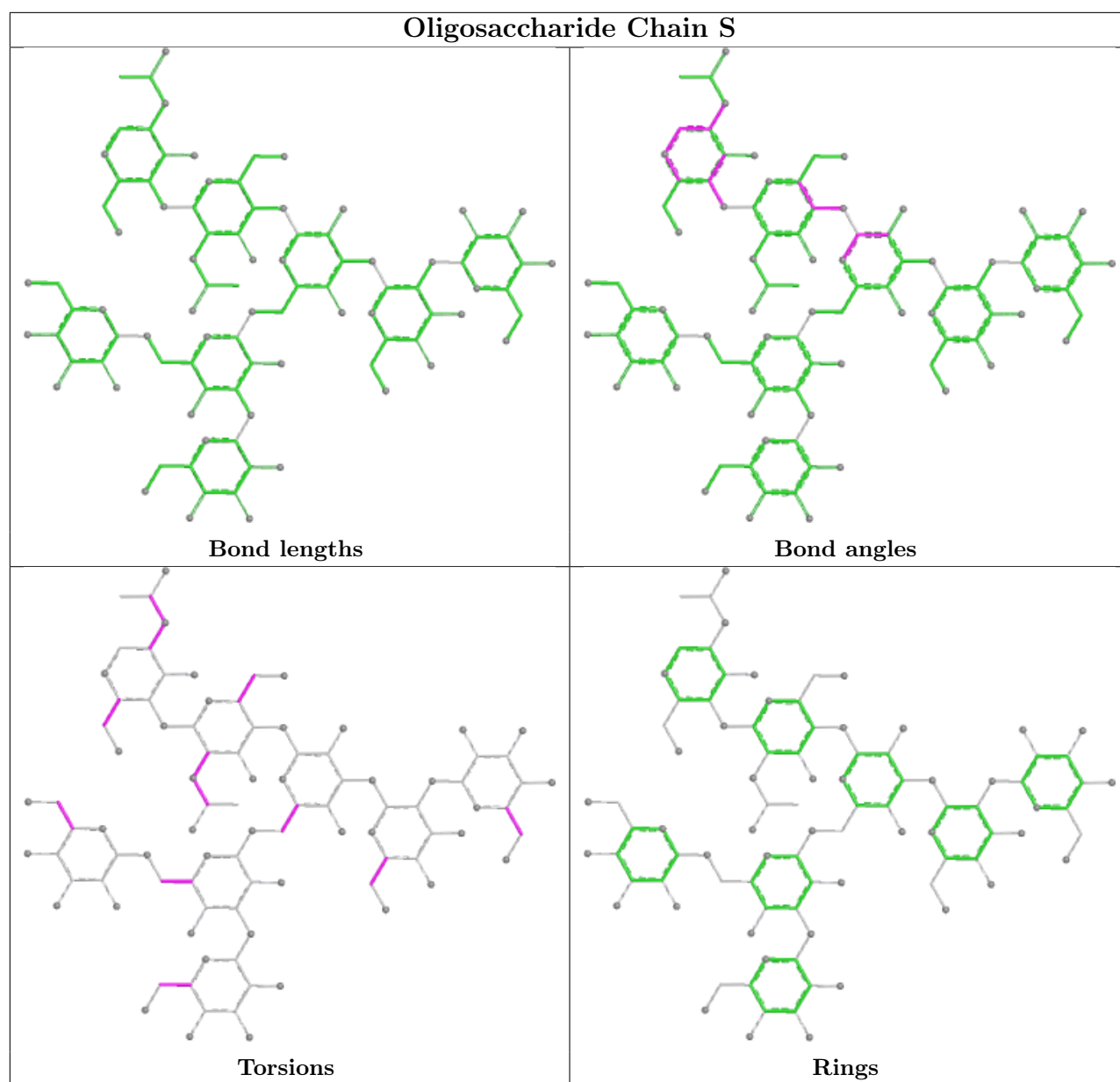
Oligosaccharide Chain L

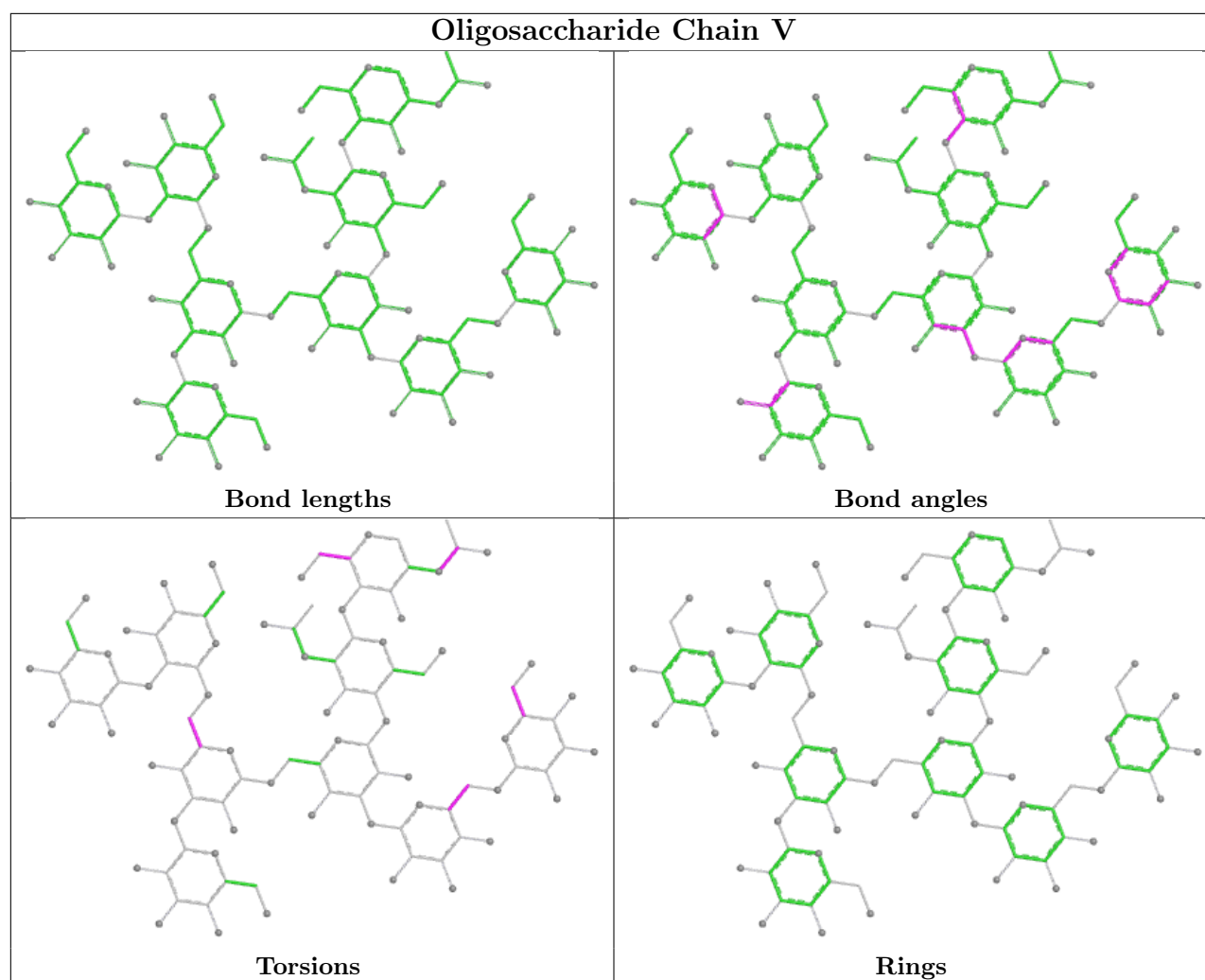












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
19	NAG	G	603	4	14,14,15	0.32	0	17,19,21	0.83	0
19	NAG	G	602	4	14,14,15	0.36	0	17,19,21	0.89	0
19	NAG	G	601	4	14,14,15	0.30	0	17,19,21	0.74	0
19	NAG	B	701	1	14,14,15	0.29	0	17,19,21	0.61	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
19	NAG	G	603	4	-	3/6/23/26	0/1/1/1
19	NAG	G	602	4	-	3/6/23/26	0/1/1/1
19	NAG	G	601	4	-	4/6/23/26	0/1/1/1
19	NAG	B	701	1	-	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 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	B	701	NAG	C8-C7-N2-C2
19	B	701	NAG	O7-C7-N2-C2
19	G	602	NAG	C1-C2-N2-C7
19	G	603	NAG	C3-C2-N2-C7
19	G	603	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	G	603	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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Warning: The R factor obtained from EDS is 0.2969, which does not match the depositor's R factor of 0.229. Please interpret the results in this section carefully.

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	B	139/153 (90%)	0.37	5 (3%)	46 35	110, 185, 251, 286	0
2	D	235/243 (96%)	0.05	2 (0%)	81 67	155, 240, 318, 372	0
3	E	210/216 (97%)	0.22	3 (1%)	73 58	150, 223, 312, 352	0
4	G	451/479 (94%)	0.18	9 (1%)	64 49	129, 186, 258, 335	0
5	Q	228/241 (94%)	0.05	1 (0%)	89 79	170, 227, 285, 309	0
6	R	211/215 (98%)	0.26	3 (1%)	73 58	184, 257, 311, 324	0
All	All	1474/1547 (95%)	0.17	23 (1%)	70 55	110, 214, 303, 372	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	507	GLY	7.4
4	G	379	GLY	3.7
1	B	564	HIS	3.2
4	G	151	ARG	3.1
4	G	326	ILE	3.0

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

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

6.3 Carbohydrates [i](#)

SUGAR-RSR INFOmissingINFO

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
19	NAG	B	701	14/15	0.43	0.16	243,269,290,304	0
19	NAG	G	603	14/15	0.57	0.13	287,309,323,326	0
19	NAG	G	602	14/15	0.63	0.14	213,276,292,301	0
19	NAG	G	601	14/15	0.65	0.11	248,277,292,297	0

6.5 Other polymers [i](#)

There are no such residues in this entry.