



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2022 – 06:31 pm GMT

PDB ID : 7OGU  
Title : Plant peptide hormone receptor complex H1C9S1  
Authors : Roman, A.O.; Jimenez-Sandoval, P.; Santiago, J.  
Deposited on : 2021-05-07  
Resolution : 2.87 Å(reported)

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.26  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.26

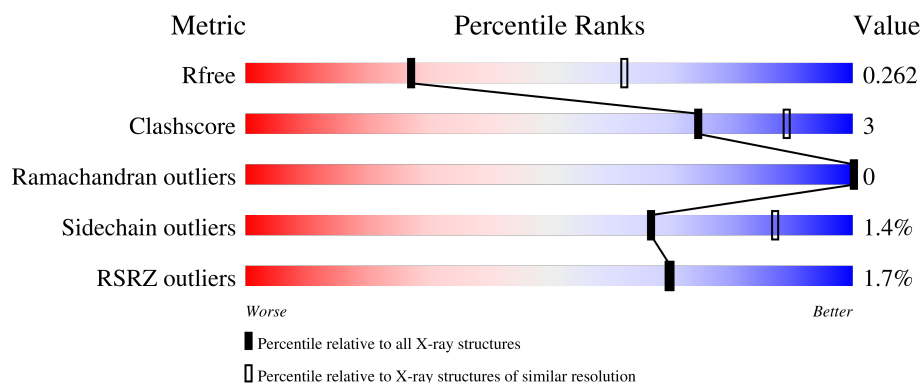
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.87 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))
$R_{free}$	130704	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	617	<div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	DDD	617	<div> <div>88%</div> <div>8%</div> <div>..</div> </div>
1	GGG	617	<div> <div>88%</div> <div>8%</div> <div>.</div> </div>
1	JJJ	617	<div> <div>88%</div> <div>8%</div> <div>.</div> </div>
2	BBB	203	<div> <div>83%</div> <div>8%</div> <div>9%</div> </div>


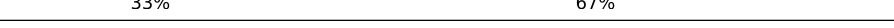
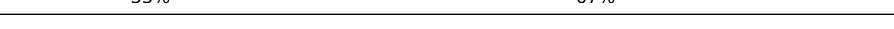
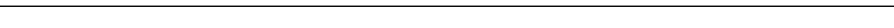
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Mol	Chain	Length	Quality of chain
2	EEE	203	
2	HHH	203	
2	KKK	203	
3	CCC	12	
3	FFF	12	
3	III	12	
3	LLL	12	
4	AaA	2	
4	AlA	2	
4	AqA	2	
4	AsA	2	
4	DeD	2	
4	DgD	2	
4	DmD	2	
4	EdE	2	
4	GgG	2	
4	GlG	2	
4	GnG	2	
4	HaH	2	
4	JaJ	2	
4	JcJ	2	
4	JeJ	2	
4	JgJ	2	
4	JkJ	2	
4	KaK	2	

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Mol	Chain	Length	Quality of chain
5	AcA	4	 100%
5	AhA	4	 25% 75%
5	DiD	4	 50% 50%
6	AnA	3	 33% 67%
7	BaB	3	 100%
7	DaD	3	 33% 67%
7	EaE	3	 33% 67%
7	GaG	3	 33% 67%
7	GdG	3	 67% 33%
8	DpD	4	 50% 50%
9	GjG	2	 50% 50%

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
4	NAG	AqA	2	X	-	-	-
4	NAG	AsA	2	X	-	-	-
4	NAG	DeD	2	X	-	-	-
4	NAG	DgD	2	X	-	-	-
4	NAG	GgG	2	X	-	-	-
4	NAG	GlG	2	X	-	-	-
4	NAG	GnG	2	X	-	-	-
4	NAG	HaH	2	X	-	-	-
4	NAG	JaJ	2	X	-	-	-
4	NAG	JcJ	2	X	-	-	-
4	NAG	JgJ	2	X	-	-	-
4	NAG	JkJ	2	X	-	-	-
4	NAG	KaK	2	X	-	-	-
5	BMA	AcA	3	X	-	-	-
5	MAN	AcA	4	-	-	-	X
5	BMA	AhA	3	X	-	-	-
5	MAN	AhA	4	X	-	-	-
5	BMA	DiD	3	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	BaB	2	X	-	-	-
7	BMA	DaD	3	X	-	-	-
7	NAG	EaE	2	X	-	-	-
7	BMA	EaE	3	X	-	-	-
7	BMA	GaG	3	X	-	-	-
7	BMA	GdG	3	X	-	-	-
8	BMA	DpD	3	X	-	-	-
9	FUC	GjG	2	-	-	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 24430 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 Receptor-like protein kinase HSL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	594	Total	C	N	O	S	0	1	0
			4386	2779	721	871	15			
1	DDD	594	Total	C	N	O	S	0	1	0
			4361	2767	718	860	16			
1	GGG	594	Total	C	N	O	S	0	0	0
			4347	2760	716	855	16			
1	JJJ	593	Total	C	N	O	S	0	1	0
			4325	2748	712	850	15			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	12	GLY	-	expression tag	UNP Q9SGP2
AAA	13	SER	-	expression tag	UNP Q9SGP2
AAA	14	SER	-	expression tag	UNP Q9SGP2
AAA	15	MET	-	expression tag	UNP Q9SGP2
AAA	16	ASP	-	expression tag	UNP Q9SGP2
AAA	619	LEU	-	expression tag	UNP Q9SGP2
AAA	620	GLU	-	expression tag	UNP Q9SGP2
AAA	621	GLY	-	expression tag	UNP Q9SGP2
AAA	622	SER	-	expression tag	UNP Q9SGP2
AAA	623	GLU	-	expression tag	UNP Q9SGP2
AAA	624	ASN	-	expression tag	UNP Q9SGP2
AAA	625	LEU	-	expression tag	UNP Q9SGP2
AAA	626	TYR	-	expression tag	UNP Q9SGP2
AAA	627	PHE	-	expression tag	UNP Q9SGP2
AAA	628	GLN	-	expression tag	UNP Q9SGP2
DDD	12	GLY	-	expression tag	UNP Q9SGP2
DDD	13	SER	-	expression tag	UNP Q9SGP2
DDD	14	SER	-	expression tag	UNP Q9SGP2
DDD	15	MET	-	expression tag	UNP Q9SGP2
DDD	16	ASP	-	expression tag	UNP Q9SGP2
DDD	619	LEU	-	expression tag	UNP Q9SGP2

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	620	GLU	-	expression tag	UNP Q9SGP2
DDD	621	GLY	-	expression tag	UNP Q9SGP2
DDD	622	SER	-	expression tag	UNP Q9SGP2
DDD	623	GLU	-	expression tag	UNP Q9SGP2
DDD	624	ASN	-	expression tag	UNP Q9SGP2
DDD	625	LEU	-	expression tag	UNP Q9SGP2
DDD	626	TYR	-	expression tag	UNP Q9SGP2
DDD	627	PHE	-	expression tag	UNP Q9SGP2
DDD	628	GLN	-	expression tag	UNP Q9SGP2
GGG	12	GLY	-	expression tag	UNP Q9SGP2
GGG	13	SER	-	expression tag	UNP Q9SGP2
GGG	14	SER	-	expression tag	UNP Q9SGP2
GGG	15	MET	-	expression tag	UNP Q9SGP2
GGG	16	ASP	-	expression tag	UNP Q9SGP2
GGG	619	LEU	-	expression tag	UNP Q9SGP2
GGG	620	GLU	-	expression tag	UNP Q9SGP2
GGG	621	GLY	-	expression tag	UNP Q9SGP2
GGG	622	SER	-	expression tag	UNP Q9SGP2
GGG	623	GLU	-	expression tag	UNP Q9SGP2
GGG	624	ASN	-	expression tag	UNP Q9SGP2
GGG	625	LEU	-	expression tag	UNP Q9SGP2
GGG	626	TYR	-	expression tag	UNP Q9SGP2
GGG	627	PHE	-	expression tag	UNP Q9SGP2
GGG	628	GLN	-	expression tag	UNP Q9SGP2
JJJ	12	GLY	-	expression tag	UNP Q9SGP2
JJJ	13	SER	-	expression tag	UNP Q9SGP2
JJJ	14	SER	-	expression tag	UNP Q9SGP2
JJJ	15	MET	-	expression tag	UNP Q9SGP2
JJJ	16	ASP	-	expression tag	UNP Q9SGP2
JJJ	619	LEU	-	expression tag	UNP Q9SGP2
JJJ	620	GLU	-	expression tag	UNP Q9SGP2
JJJ	621	GLY	-	expression tag	UNP Q9SGP2
JJJ	622	SER	-	expression tag	UNP Q9SGP2
JJJ	623	GLU	-	expression tag	UNP Q9SGP2
JJJ	624	ASN	-	expression tag	UNP Q9SGP2
JJJ	625	LEU	-	expression tag	UNP Q9SGP2
JJJ	626	TYR	-	expression tag	UNP Q9SGP2
JJJ	627	PHE	-	expression tag	UNP Q9SGP2
JJJ	628	GLN	-	expression tag	UNP Q9SGP2

- Molecule 2 is a protein called Somatic embryogenesis receptor kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	185	Total	C	N	O	S	0	1	0
			1371	867	230	270	4			
2	EEE	185	Total	C	N	O	S	0	2	0
			1369	864	233	267	5			
2	HHH	185	Total	C	N	O	S	0	2	0
			1377	871	233	268	5			
2	KKK	185	Total	C	N	O	S	0	2	0
			1373	871	232	266	4			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	20	GLY	-	expression tag	UNP Q94AG2
BBB	21	SER	-	expression tag	UNP Q94AG2
BBB	22	SER	-	expression tag	UNP Q94AG2
BBB	23	MET	-	expression tag	UNP Q94AG2
BBB	212	LEU	-	expression tag	UNP Q94AG2
BBB	213	GLU	-	expression tag	UNP Q94AG2
BBB	214	GLY	-	expression tag	UNP Q94AG2
BBB	215	SER	-	expression tag	UNP Q94AG2
BBB	216	LEU	-	expression tag	UNP Q94AG2
BBB	217	GLU	-	expression tag	UNP Q94AG2
BBB	218	ASN	-	expression tag	UNP Q94AG2
BBB	219	LEU	-	expression tag	UNP Q94AG2
BBB	220	TYR	-	expression tag	UNP Q94AG2
BBB	221	PHE	-	expression tag	UNP Q94AG2
BBB	222	GLN	-	expression tag	UNP Q94AG2
EEE	20	GLY	-	expression tag	UNP Q94AG2
EEE	21	SER	-	expression tag	UNP Q94AG2
EEE	22	SER	-	expression tag	UNP Q94AG2
EEE	23	MET	-	expression tag	UNP Q94AG2
EEE	212	LEU	-	expression tag	UNP Q94AG2
EEE	213	GLU	-	expression tag	UNP Q94AG2
EEE	214	GLY	-	expression tag	UNP Q94AG2
EEE	215	SER	-	expression tag	UNP Q94AG2
EEE	216	LEU	-	expression tag	UNP Q94AG2
EEE	217	GLU	-	expression tag	UNP Q94AG2
EEE	218	ASN	-	expression tag	UNP Q94AG2
EEE	219	LEU	-	expression tag	UNP Q94AG2
EEE	220	TYR	-	expression tag	UNP Q94AG2
EEE	221	PHE	-	expression tag	UNP Q94AG2
EEE	222	GLN	-	expression tag	UNP Q94AG2
HHH	20	GLY	-	expression tag	UNP Q94AG2

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Chain	Residue	Modelled	Actual	Comment	Reference
HHH	21	SER	-	expression tag	UNP Q94AG2
HHH	22	SER	-	expression tag	UNP Q94AG2
HHH	23	MET	-	expression tag	UNP Q94AG2
HHH	212	LEU	-	expression tag	UNP Q94AG2
HHH	213	GLU	-	expression tag	UNP Q94AG2
HHH	214	GLY	-	expression tag	UNP Q94AG2
HHH	215	SER	-	expression tag	UNP Q94AG2
HHH	216	LEU	-	expression tag	UNP Q94AG2
HHH	217	GLU	-	expression tag	UNP Q94AG2
HHH	218	ASN	-	expression tag	UNP Q94AG2
HHH	219	LEU	-	expression tag	UNP Q94AG2
HHH	220	TYR	-	expression tag	UNP Q94AG2
HHH	221	PHE	-	expression tag	UNP Q94AG2
HHH	222	GLN	-	expression tag	UNP Q94AG2
KKK	20	GLY	-	expression tag	UNP Q94AG2
KKK	21	SER	-	expression tag	UNP Q94AG2
KKK	22	SER	-	expression tag	UNP Q94AG2
KKK	23	MET	-	expression tag	UNP Q94AG2
KKK	212	LEU	-	expression tag	UNP Q94AG2
KKK	213	GLU	-	expression tag	UNP Q94AG2
KKK	214	GLY	-	expression tag	UNP Q94AG2
KKK	215	SER	-	expression tag	UNP Q94AG2
KKK	216	LEU	-	expression tag	UNP Q94AG2
KKK	217	GLU	-	expression tag	UNP Q94AG2
KKK	218	ASN	-	expression tag	UNP Q94AG2
KKK	219	LEU	-	expression tag	UNP Q94AG2
KKK	220	TYR	-	expression tag	UNP Q94AG2
KKK	221	PHE	-	expression tag	UNP Q94AG2
KKK	222	GLN	-	expression tag	UNP Q94AG2

- Molecule 3 is a protein called CLAVATA3/ESR (CLE)-related protein 9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	CCC	12	Total	C	N	O	0	0	0
			88	54	16	18			
3	FFF	12	Total	C	N	O	0	0	0
			83	49	16	18			
3	III	11	Total	C	N	O	0	0	0
			78	46	15	17			
3	LLL	11	Total	C	N	O	0	0	0
			78	46	15	17			

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

cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	AaA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	AlA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	AqA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	AsA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	DeD	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	DgD	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	DmD	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	EdE	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	GgG	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	GlG	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	GnG	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	HaH	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	JaJ	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	JcJ	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	JeJ	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	JgJ	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	JkJ	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	KaK	2	Total	C	N	O	0	0	0
			28	16	2	10			

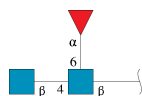
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos

e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



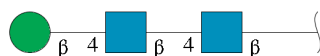
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	AcA	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	AhA	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	DiD	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



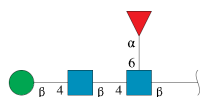
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	AnA	3	Total	C	N	O	0	0	0
			38	22	2	14			

- 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	BaB	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	DaD	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	EaE	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	GaG	3	Total	C	N	O	0	0	0
			39	22	2	15			
7	GdG	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



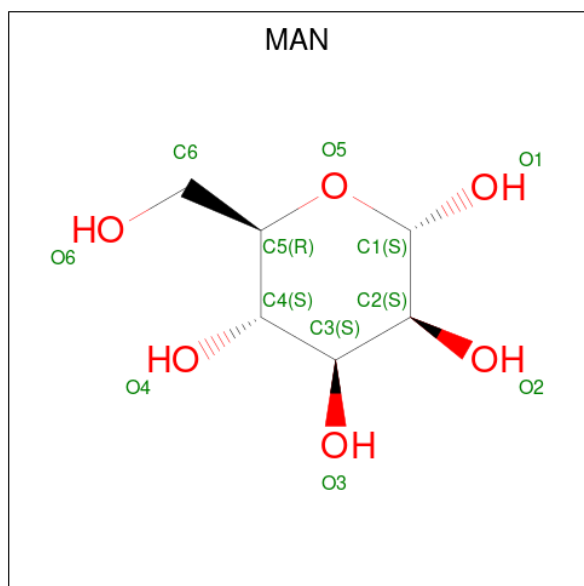
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	DpD	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 9 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	GjG	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 10 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	AAA	1	Total	C	O	0	0
			11	6	5		



- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
11	BBB	1	Total	C	N	O	0	0
			14	8	1	5		
11	BBB	1	Total	C	N	O	0	0
			14	8	1	5		
11	DDD	1	Total	C	N	O	0	0
			14	8	1	5		
11	DDD	1	Total	C	N	O	0	0
			14	8	1	5		
11	EEE	1	Total	C	N	O	0	0
			14	8	1	5		
11	GGG	1	Total	C	N	O	0	0
			14	8	1	5		
11	HHH	1	Total	C	N	O	0	0
			14	8	1	5		
11	JJJ	1	Total	C	N	O	0	0
			14	8	1	5		
11	JJJ	1	Total	C	N	O	0	0
			14	8	1	5		
11	JJJ	1	Total	C	N	O	0	0
			14	8	1	5		
11	JJJ	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 12 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	AAA	2	Total 2	Na 2	0	0
12	BBB	1	Total 1	Na 1	0	0
12	DDD	1	Total 1	Na 1	0	0
12	EEE	1	Total 1	Na 1	0	0
12	GGG	1	Total 1	Na 1	0	0
12	HHH	1	Total 1	Na 1	0	0
12	KKK	1	Total 1	Na 1	0	0

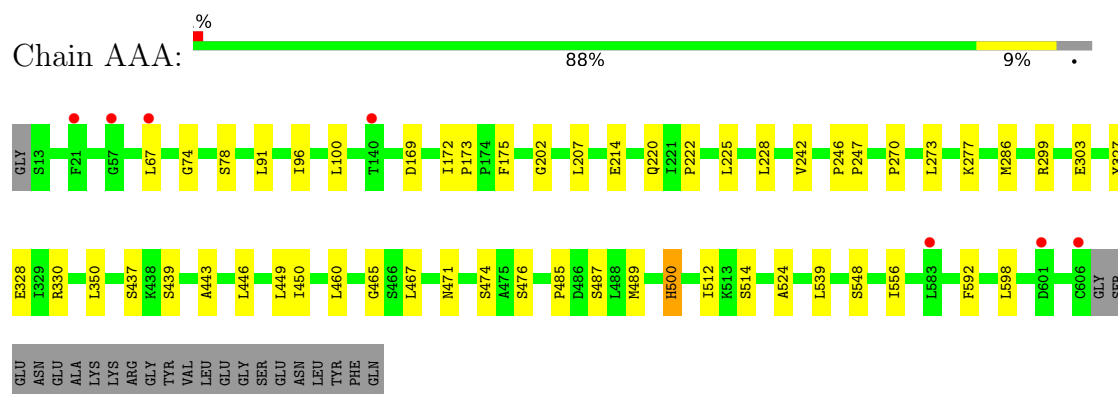
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	AAA	11	Total 11	O 11	0	0
13	BBB	3	Total 3	O 3	0	0
13	DDD	11	Total 11	O 11	0	0
13	EEE	1	Total 1	O 1	0	0
13	GGG	15	Total 15	O 15	0	0
13	JJJ	6	Total 6	O 6	0	0

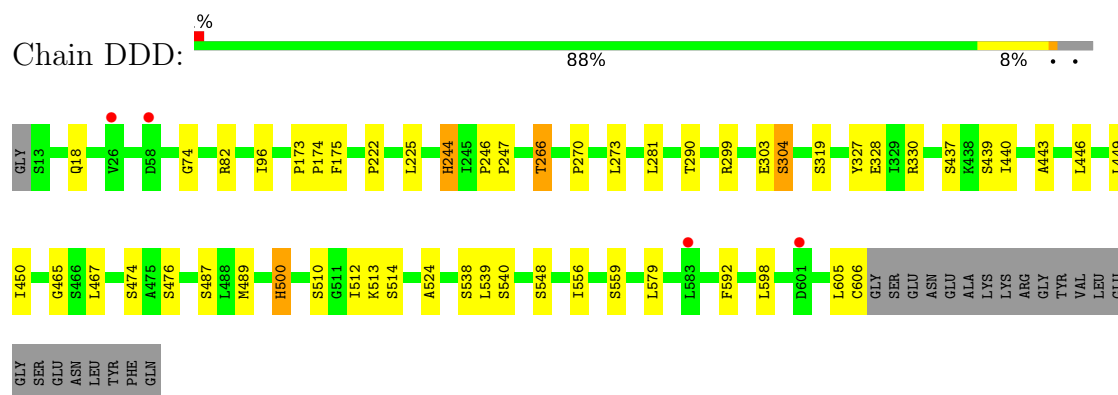
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

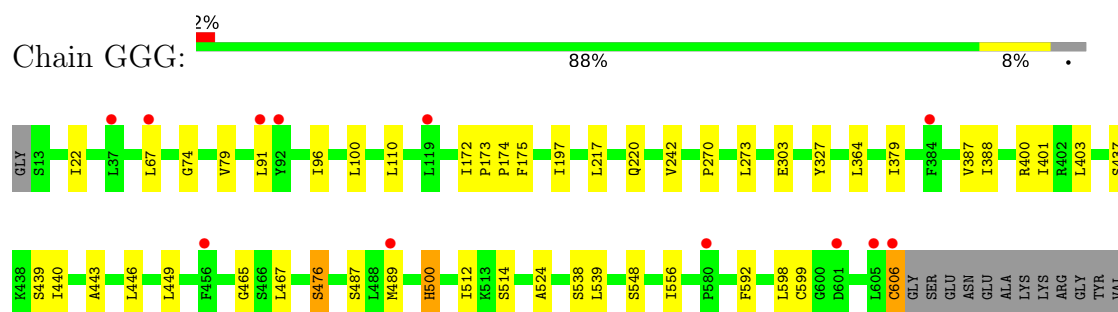
#### • Molecule 1: Receptor-like protein kinase HSL1



#### • Molecule 1: Receptor-like protein kinase HSL1

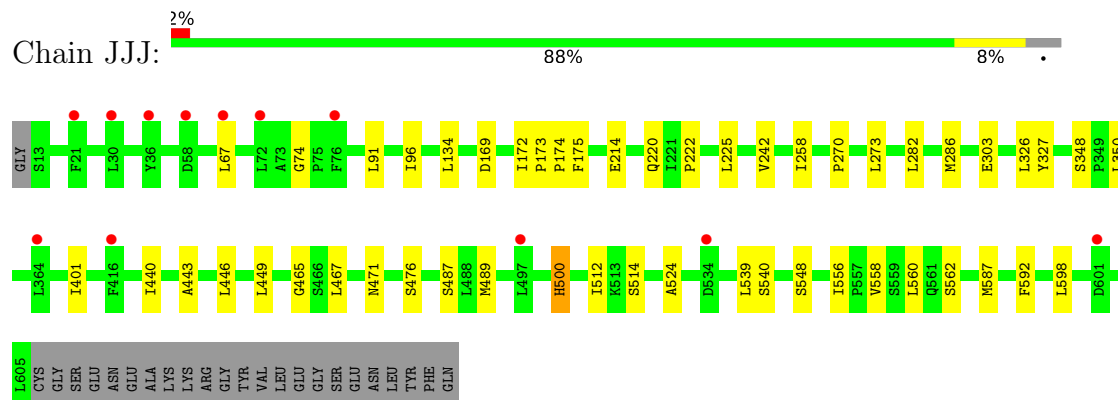


#### • Molecule 1: Receptor-like protein kinase HSL1

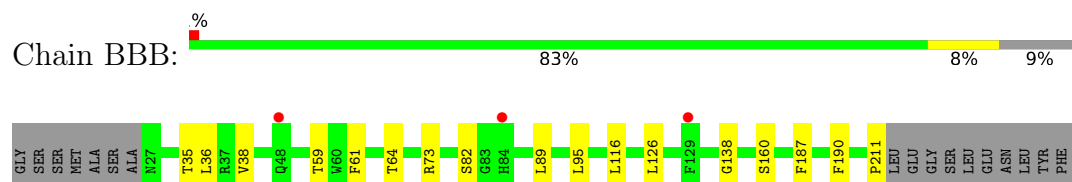


LEU  
GLY  
GLY  
SER  
GLU  
LEU  
TYR  
PHE  
GLN

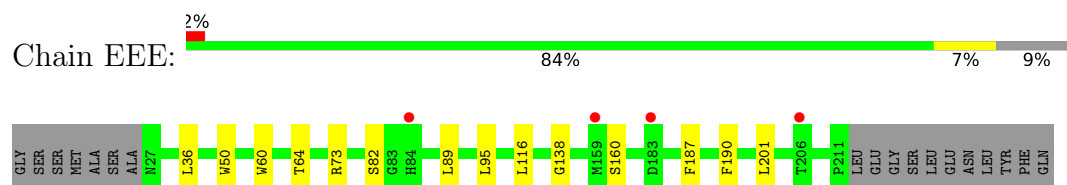
- Molecule 1: Receptor-like protein kinase HSL1



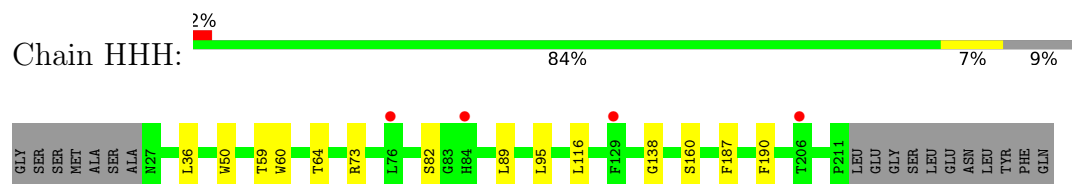
- Molecule 2: Somatic embryogenesis receptor kinase 1



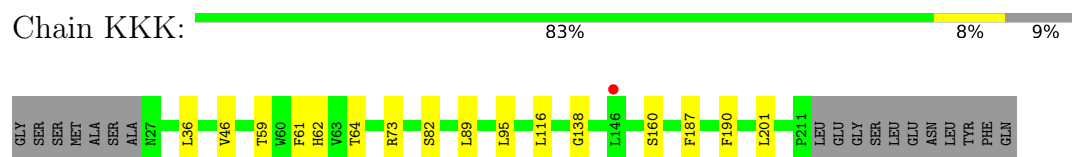
- Molecule 2: Somatic embryogenesis receptor kinase 1



- Molecule 2: Somatic embryogenesis receptor kinase 1

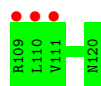


- Molecule 2: Somatic embryogenesis receptor kinase 1

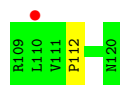


- Molecule 3: CLAVATA3/ESR (CLE)-related protein 9





- Molecule 3: CLAVATA3/ESR (CLE)-related protein 9



- Molecule 3: CLAVATA3/ESR (CLE)-related protein 9



- Molecule 3: CLAVATA3/ESR (CLE)-related protein 9



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



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



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



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

Chain AsA:  100%

MAG1  
MAG2

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

Chain DeD:  50% 50%

MAG1  
MAG2

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

Chain DgD:  50% 50%

MAG1  
MAG2

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

Chain DmD:  100%

MAG1  
MAG2

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

Chain EdE:  100%

MAG1  
MAG2

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

Chain GgG:  50% 50%

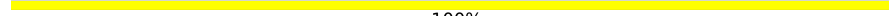
MAG1  
MAG2

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

Chain GlG:  50% 50%

MAG1  
MAG2

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

Chain GnG:  100%

MAG1  
MAG2

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

Chain HaH:  50% 50%

MAG1  
MAG2

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

Chain JaJ:  50% 50%

MAG1  
MAG2

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

Chain JcJ:  100%

MAG1  
MAG2

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

Chain JeJ:  100%

MAG1  
MAG2

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

Chain JgJ:  50% 50%

MAG1  
MAG2

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

Chain JkJ:  50% 50%

NAG1  
NAG2

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

Chain KaK:  100%


NAG1  
NAG2

- Molecule 5: 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 AcA:  100%

NAG1  
NAG2  
BMA3  
MAN4

- Molecule 5: 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 AhA:  25% 75%

NAG1  
NAG2  
BMA3  
MAN4

- Molecule 5: 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 DiD:  50% 50%

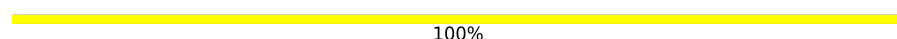
NAG1  
NAG2  
BMA3  
MAN4

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AnA:  33% 67%

NAG1  
NAG2  
FUC3

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

Chain BaB:  100%





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



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



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



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



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.96Å 169.89Å 143.55Å 90.00° 96.74° 90.00°	Depositor
Resolution (Å)	49.09 – 2.87 49.09 – 2.87	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.09-2.87) 99.3 (49.09-2.87)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.238 , 0.262 0.238 , 0.262	Depositor DCC
$R_{free}$ test set	5172 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.3	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	24430	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7121e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FUC, MAN, HYP, NA, BMA, 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	AAA	0.65	0/4471	0.71	0/6110
1	DDD	0.65	0/4446	0.71	0/6079
1	GGG	0.64	0/4432	0.71	0/6059
1	JJJ	0.65	0/4409	0.72	0/6032
2	BBB	0.63	0/1403	0.72	1/1932 (0.1%)
2	EEE	0.62	0/1404	0.71	0/1932
2	HHH	0.63	0/1412	0.71	0/1943
2	KKK	0.63	0/1409	0.70	0/1940
3	CCC	0.61	0/71	0.67	0/92
3	FFF	0.63	0/66	0.72	0/85
3	III	0.60	0/61	0.66	0/78
3	LLL	0.62	0/61	0.68	0/78
All	All	0.64	0/23645	0.71	1/32360 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	JJJ	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	211	PRO	CA-C-O	-5.64	106.66	120.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	JJJ	562	SER	Mainchain

## 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	AAA	4386	0	4189	30	0
1	DDD	4361	0	4142	28	0
1	GGG	4347	0	4111	28	0
1	JJJ	4325	0	4068	28	0
2	BBB	1371	0	1302	11	0
2	EEE	1369	0	1299	9	0
2	HHH	1377	0	1326	8	0
2	KKK	1373	0	1311	11	0
3	CCC	88	0	80	0	0
3	FFF	83	0	64	0	0
3	III	78	0	62	0	0
3	LLL	78	0	62	0	0
4	AaA	28	0	24	0	0
4	AlA	28	0	24	0	0
4	AqA	28	0	25	0	0
4	AsA	28	0	25	0	0
4	DeD	28	0	24	0	0
4	DgD	28	0	25	0	0
4	DmD	28	0	25	0	0
4	EdE	28	0	25	0	0
4	GgG	28	0	25	0	0
4	GlG	28	0	25	0	0
4	GnG	28	0	25	0	0
4	HaH	28	0	25	0	0
4	JaJ	28	0	25	0	0
4	JcJ	28	0	25	0	0
4	JeJ	28	0	25	0	0
4	JgJ	28	0	25	0	0
4	JkJ	28	0	25	0	0
4	KaK	28	0	25	0	0
5	AcA	50	0	43	0	0
5	AhA	50	0	43	0	0
5	DiD	50	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	AnA	38	0	34	0	0
7	BaB	39	0	34	0	0
7	DaD	39	0	34	0	0
7	EaE	39	0	34	0	0
7	GaG	39	0	34	0	0
7	GdG	39	0	33	0	0
8	DpD	49	0	43	0	0
9	GjG	24	0	22	0	0
10	AAA	11	0	10	0	0
11	AAA	14	0	13	0	0
11	BBB	28	0	26	1	0
11	DDD	28	0	26	0	0
11	EEE	14	0	13	0	0
11	GGG	14	0	13	0	0
11	HHH	14	0	13	0	0
11	JJJ	56	0	52	0	0
12	AAA	2	0	0	0	0
12	BBB	1	0	0	0	0
12	DDD	1	0	0	0	0
12	EEE	1	0	0	0	0
12	GGG	1	0	0	0	0
12	HHH	1	0	0	0	0
12	KKK	1	0	0	0	0
13	AAA	11	0	0	0	0
13	BBB	3	0	0	0	0
13	DDD	11	0	0	0	0
13	EEE	1	0	0	0	0
13	GGG	15	0	0	0	0
13	JJJ	6	0	0	0	0
All	All	24430	0	23026	149	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 3.

All (149) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JJJ:465:GLY:HA3	1:JJJ:487:SER:HB2	1.86	0.57
1:AAA:465:GLY:HA3	1:AAA:487:SER:HB2	1.85	0.57
1:AAA:556:ILE:HD11	1:AAA:598:LEU:HD21	1.86	0.57
1:GGG:465:GLY:HA3	1:GGG:487:SER:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JJJ:556:ILE:HD11	1:JJJ:598:LEU:HD21	1.87	0.56
1:DDD:465:GLY:HA3	1:DDD:487:SER:HB2	1.87	0.56
1:AAA:202:GLY:HA2	1:AAA:228:LEU:HD11	1.89	0.54
2:BBB:35:THR:O	2:BBB:38:VAL:HG12	2.07	0.53
1:GGG:446:LEU:HD21	1:GGG:449:LEU:HD13	1.91	0.53
1:DDD:446:LEU:HD21	1:DDD:449:LEU:HD13	1.91	0.52
1:JJJ:446:LEU:HD21	1:JJJ:449:LEU:HD13	1.91	0.52
1:JJJ:592:PHE:HB3	1:JJJ:598:LEU:HD23	1.91	0.52
2:KKK:36:LEU:HD22	2:KKK:89:LEU:HD21	1.91	0.52
1:DDD:450:ILE:HG23	1:DDD:474:SER:HB2	1.92	0.52
2:EEE:36:LEU:HD22	2:EEE:89:LEU:HD21	1.92	0.51
2:HHH:187:PHE:HA	2:HHH:190:PHE:HD2	1.76	0.51
2:EEE:187:PHE:HA	2:EEE:190:PHE:HD2	1.76	0.51
1:JJJ:270:PRO:HG2	1:JJJ:273:LEU:HG	1.93	0.51
2:KKK:187:PHE:HA	2:KKK:190:PHE:HD2	1.76	0.51
1:AAA:270:PRO:HG2	1:AAA:273:LEU:HG	1.93	0.50
1:AAA:446:LEU:HD21	1:AAA:449:LEU:HD13	1.92	0.50
2:HHH:36:LEU:HD22	2:HHH:89:LEU:HD21	1.93	0.50
1:GGG:592:PHE:HB3	1:GGG:598:LEU:HD23	1.94	0.50
1:AAA:592:PHE:HB3	1:AAA:598:LEU:HD23	1.94	0.50
1:DDD:270:PRO:HG2	1:DDD:273:LEU:HG	1.94	0.50
2:BBB:187:PHE:HA	2:BBB:190:PHE:HD2	1.77	0.49
2:EEE:187:PHE:HA	2:EEE:190:PHE:CD2	2.47	0.49
2:HHH:187:PHE:HA	2:HHH:190:PHE:CD2	2.47	0.49
1:AAA:476:SER:HA	1:AAA:500:HIS:O	2.12	0.49
1:AAA:471:ASN:HB3	2:BBB:61:PHE:CE2	2.47	0.49
1:JJJ:303:GLU:HB3	1:JJJ:327:TYR:CE2	2.47	0.49
1:DDD:476:SER:HA	1:DDD:500:HIS:O	2.12	0.49
1:DDD:244:HIS:CE1	1:DDD:247:PRO:HD3	2.47	0.49
1:DDD:303:GLU:HB3	1:DDD:327:TYR:CE2	2.47	0.49
1:JJJ:476:SER:HA	1:JJJ:500:HIS:O	2.12	0.49
1:AAA:303:GLU:HB3	1:AAA:327:TYR:CE2	2.48	0.49
2:KKK:187:PHE:HA	2:KKK:190:PHE:CD2	2.48	0.49
2:BBB:187:PHE:HA	2:BBB:190:PHE:CD2	2.48	0.49
1:GGG:476:SER:HA	1:GGG:500:HIS:O	2.13	0.49
1:GGG:303:GLU:HB3	1:GGG:327:TYR:CE2	2.47	0.48
1:AAA:222:PRO:HG2	1:AAA:225:LEU:HG	1.95	0.48
1:GGG:270:PRO:HG2	1:GGG:273:LEU:HG	1.95	0.48
1:DDD:592:PHE:HB3	1:DDD:598:LEU:HD23	1.95	0.47
1:JJJ:512:ILE:O	1:JJJ:539:LEU:HD21	2.14	0.47
1:AAA:512:ILE:O	1:AAA:539:LEU:HD21	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:JJJ:222:PRO:HG2	1:JJJ:225:LEU:HG	1.96	0.47
2:BBB:36:LEU:HD22	2:BBB:89:LEU:HD21	1.96	0.47
1:DDD:605:LEU:O	1:DDD:606:CYS:SG	2.73	0.47
1:GGG:556:ILE:HD11	1:GGG:598:LEU:HD21	1.97	0.46
2:KKK:46:VAL:HG13	2:KKK:62:HIS:NE2	2.29	0.46
1:GGG:512:ILE:O	1:GGG:539:LEU:HD21	2.16	0.46
1:AAA:286:MET:HB2	1:AAA:286:MET:HE2	1.80	0.46
1:DDD:512:ILE:O	1:DDD:539:LEU:HD21	2.16	0.46
1:JJJ:560:LEU:HA	1:JJJ:560:LEU:HD12	1.84	0.46
1:AAA:74:GLY:O	1:AAA:96:ILE:HA	2.15	0.46
1:JJJ:489:MET:O	1:JJJ:514:SER:HB2	2.16	0.46
1:DDD:222:PRO:HG2	1:DDD:225:LEU:HG	1.98	0.46
1:DDD:328:GLU:OE1	1:DDD:330:ARG:NH1	2.46	0.46
1:JJJ:74:GLY:O	1:JJJ:96:ILE:HA	2.16	0.46
1:AAA:524:ALA:HA	1:AAA:548:SER:O	2.16	0.45
1:GGG:524:ALA:HA	1:GGG:548:SER:O	2.16	0.45
1:DDD:74:GLY:O	1:DDD:96:ILE:HA	2.15	0.45
2:HHH:64:THR:HB	2:HHH:73:ARG:HB2	1.98	0.45
2:EEE:138:GLY:HA3	2:EEE:160:SER:HB2	1.98	0.45
1:JJJ:286:MET:HB2	1:JJJ:286:MET:HE2	1.79	0.45
1:DDD:524:ALA:HA	1:DDD:548:SER:O	2.16	0.45
1:GGG:74:GLY:O	1:GGG:96:ILE:HA	2.16	0.45
1:AAA:173:PRO:HB3	1:AAA:175:PHE:CE2	2.52	0.45
1:DDD:510:SER:O	1:DDD:513:LYS:HG2	2.16	0.45
2:KKK:64:THR:HB	2:KKK:73:ARG:HB2	1.99	0.45
1:GGG:489:MET:O	1:GGG:514:SER:HB2	2.17	0.45
2:EEE:64:THR:HB	2:EEE:73:ARG:HB2	1.99	0.44
1:JJJ:524:ALA:HA	1:JJJ:548:SER:O	2.16	0.44
2:BBB:95:LEU:HD23	2:BBB:116:LEU:HD13	2.00	0.44
2:HHH:138:GLY:HA3	2:HHH:160:SER:HB2	1.98	0.44
1:DDD:489:MET:O	1:DDD:514:SER:HB2	2.18	0.44
2:KKK:138:GLY:HA3	2:KKK:160:SER:HB2	1.99	0.44
2:HHH:95:LEU:HD23	2:HHH:116:LEU:HD13	1.99	0.44
1:GGG:173:PRO:HB3	1:GGG:175:PHE:CE2	2.53	0.44
1:DDD:244:HIS:HA	1:DDD:266:THR:O	2.18	0.43
1:DDD:556:ILE:HD12	1:DDD:579:LEU:HD23	2.00	0.43
1:AAA:489:MET:O	1:AAA:514:SER:HB2	2.18	0.43
2:HHH:89:LEU:O	2:HHH:116:LEU:HD21	2.19	0.43
1:JJJ:258:ILE:HB	1:JJJ:282:LEU:HD12	2.01	0.43
2:BBB:126:LEU:HD21	11:BBB:301:NAG:O7	2.18	0.43
2:BBB:64:THR:HB	2:BBB:73:ARG:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:138:GLY:HA3	2:BBB:160:SER:HB2	2.00	0.43
2:EEE:95:LEU:HD23	2:EEE:116:LEU:HD13	2.01	0.43
1:JJJ:134:LEU:HD12	1:JJJ:134:LEU:HA	1.90	0.43
2:KKK:95:LEU:HD23	2:KKK:116:LEU:HD13	2.00	0.43
1:AAA:450:ILE:HG23	1:AAA:474:SER:HB2	2.00	0.43
2:EEE:89:LEU:O	2:EEE:116:LEU:HD21	2.19	0.43
1:GGG:172:ILE:HA	1:GGG:173:PRO:HD3	1.92	0.43
1:DDD:18:GLN:HE22	1:DDD:82:ARG:HH11	1.67	0.43
1:GGG:110:LEU:HD23	1:GGG:110:LEU:HA	1.91	0.43
1:DDD:173:PRO:HB3	1:DDD:175:PHE:CE2	2.54	0.43
1:JJJ:173:PRO:HB3	1:JJJ:175:PHE:CE2	2.52	0.43
1:JJJ:173:PRO:HA	1:JJJ:174:PRO:HD3	1.95	0.43
1:JJJ:598:LEU:HD12	1:JJJ:598:LEU:HA	1.92	0.43
1:AAA:328:GLU:OE1	1:AAA:330:ARG:NH1	2.45	0.42
1:DDD:281:LEU:HD23	1:DDD:304:SER:HB3	2.01	0.42
2:KKK:201:LEU:HD23	2:KKK:201:LEU:HA	1.88	0.42
2:KKK:89:LEU:O	2:KKK:116:LEU:HD21	2.19	0.42
1:DDD:443:ALA:O	1:DDD:467:LEU:HD22	2.19	0.42
1:JJJ:471:ASN:HB3	2:KKK:61:PHE:CE2	2.54	0.42
1:GGG:437:SER:HB3	1:GGG:439:SER:OG	2.20	0.42
1:JJJ:326:LEU:O	1:JJJ:348:SER:HB2	2.19	0.42
1:AAA:437:SER:HB3	1:AAA:439:SER:OG	2.20	0.42
1:DDD:440:ILE:HG13	1:DDD:467:LEU:HD11	2.02	0.42
1:AAA:207:LEU:HB3	1:AAA:228:LEU:HD23	2.02	0.41
1:AAA:471:ASN:HB3	2:BBB:61:PHE:CZ	2.55	0.41
2:BBB:89:LEU:O	2:BBB:116:LEU:HD21	2.19	0.41
1:GGG:22:ILE:HG23	1:GGG:79:VAL:HG22	2.02	0.41
1:JJJ:471:ASN:HB3	2:KKK:61:PHE:CZ	2.54	0.41
1:JJJ:443:ALA:O	1:JJJ:467:LEU:HD22	2.20	0.41
1:AAA:67:LEU:HB2	1:AAA:91:LEU:HD23	2.02	0.41
1:AAA:100:LEU:HD12	1:AAA:100:LEU:HA	1.90	0.41
1:AAA:350:LEU:HD12	1:AAA:350:LEU:HA	1.89	0.41
1:AAA:246:PRO:HA	1:AAA:247:PRO:HD3	1.96	0.41
1:JJJ:350:LEU:HD12	1:JJJ:350:LEU:HA	1.89	0.41
1:AAA:460:LEU:O	1:AAA:485:PRO:HG3	2.19	0.41
1:GGG:364:LEU:HD23	1:GGG:364:LEU:HA	1.86	0.41
1:JJJ:67:LEU:HB2	1:JJJ:91:LEU:HD23	2.03	0.41
1:JJJ:220:GLN:HA	1:JJJ:242:VAL:O	2.21	0.41
1:DDD:246:PRO:HA	1:DDD:247:PRO:HD3	1.95	0.41
1:GGG:440:ILE:HG13	1:GGG:467:LEU:HD11	2.02	0.41
1:GGG:443:ALA:O	1:GGG:467:LEU:HD22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:172:ILE:HA	1:AAA:173:PRO:HD3	1.92	0.41
1:DDD:173:PRO:HA	1:DDD:174:PRO:HD3	1.95	0.41
1:DDD:437:SER:HB3	1:DDD:439:SER:OG	2.20	0.41
1:DDD:556:ILE:HD11	1:DDD:598:LEU:HD21	2.03	0.41
1:GGG:387:VAL:HG12	1:GGG:388:ILE:O	2.21	0.41
1:AAA:598:LEU:HD12	1:AAA:598:LEU:HA	1.95	0.41
1:GGG:379:ILE:HG12	1:GGG:403:LEU:HA	2.03	0.41
1:AAA:443:ALA:O	1:AAA:467:LEU:HD22	2.22	0.40
1:DDD:500:HIS:HA	1:DDD:524:ALA:O	2.21	0.40
2:EEE:50:TRP:HA	2:EEE:60:TRP:CD2	2.56	0.40
2:EEE:201:LEU:HD23	2:EEE:201:LEU:HA	1.88	0.40
1:GGG:67:LEU:HB2	1:GGG:91:LEU:HD23	2.02	0.40
1:GGG:197:ILE:HG12	1:GGG:217:LEU:HD13	2.04	0.40
2:HHH:50:TRP:HA	2:HHH:60:TRP:CD2	2.57	0.40
1:JJJ:172:ILE:HA	1:JJJ:173:PRO:HD3	1.91	0.40
1:GGG:599:CYS:HA	1:GGG:606:CYS:CB	2.51	0.40
1:GGG:100:LEU:HD12	1:GGG:100:LEU:HA	1.90	0.40
1:GGG:500:HIS:HA	1:GGG:524:ALA:O	2.22	0.40
1:JJJ:440:ILE:HG13	1:JJJ:467:LEU:HD11	2.02	0.40
1:AAA:220:GLN:HA	1:AAA:242:VAL:O	2.22	0.40
1:GGG:173:PRO:HA	1:GGG:174:PRO:HD3	1.96	0.40
1:GGG:220:GLN:HA	1:GGG:242:VAL:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	AAA	593/617 (96%)	585 (99%)	8 (1%)	0	100	100
1	DDD	593/617 (96%)	584 (98%)	9 (2%)	0	100	100
1	GGG	592/617 (96%)	584 (99%)	8 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	JJJ	592/617 (96%)	583 (98%)	9 (2%)	0	100	100
2	BBB	184/203 (91%)	183 (100%)	1 (0%)	0	100	100
2	EEE	185/203 (91%)	184 (100%)	1 (0%)	0	100	100
2	HHH	185/203 (91%)	184 (100%)	1 (0%)	0	100	100
2	KKK	185/203 (91%)	184 (100%)	1 (0%)	0	100	100
3	CCC	8/12 (67%)	7 (88%)	1 (12%)	0	100	100
3	FFF	8/12 (67%)	7 (88%)	1 (12%)	0	100	100
3	III	7/12 (58%)	6 (86%)	1 (14%)	0	100	100
3	LLL	7/12 (58%)	6 (86%)	1 (14%)	0	100	100
All	All	3139/3328 (94%)	3097 (99%)	42 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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 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	AAA	476/540 (88%)	470 (99%)	6 (1%)	69	88
1	DDD	465/540 (86%)	455 (98%)	10 (2%)	52	80
1	GGG	460/540 (85%)	454 (99%)	6 (1%)	69	88
1	JJJ	451/540 (84%)	444 (98%)	7 (2%)	62	85
2	BBB	155/184 (84%)	153 (99%)	2 (1%)	69	88
2	EEE	154/184 (84%)	153 (99%)	1 (1%)	86	95
2	HHH	157/184 (85%)	155 (99%)	2 (1%)	69	88
2	KKK	154/184 (84%)	152 (99%)	2 (1%)	69	88
3	CCC	8/9 (89%)	8 (100%)	0	100	100
3	FFF	6/9 (67%)	6 (100%)	0	100	100
3	III	6/9 (67%)	6 (100%)	0	100	100
3	LLL	6/9 (67%)	6 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2498/2932 (85%)	2462 (99%)	36 (1%)	67 87

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	78	SER
1	AAA	169	ASP
1	AAA	214	GLU
1	AAA	277	LYS
1	AAA	299	ARG
1	AAA	500	HIS
2	BBB	59	THR
2	BBB	82	SER
1	DDD	244	HIS
1	DDD	266	THR
1	DDD	290	THR
1	DDD	299	ARG
1	DDD	304	SER
1	DDD	319	SER
1	DDD	500	HIS
1	DDD	538	SER
1	DDD	540	SER
1	DDD	559	SER
2	EEE	82	SER
1	GGG	400	ARG
1	GGG	401	ILE
1	GGG	476	SER
1	GGG	500	HIS
1	GGG	538	SER
1	GGG	606	CYS
2	HHH	59	THR
2	HHH	82	SER
1	JJJ	169	ASP
1	JJJ	214	GLU
1	JJJ	401	ILE
1	JJJ	500	HIS
1	JJJ	540	SER
1	JJJ	558	VAL
1	JJJ	587	MET
2	KKK	59	THR
2	KKK	82	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	HYP	LLL	112	3	6,8,9	0.63	0	5,10,12	0.84	0
3	HYP	III	112	3	6,8,9	0.57	0	5,10,12	0.93	0
3	HYP	FFF	115	3	6,8,9	0.51	0	5,10,12	0.87	0
3	HYP	FFF	112	3	6,8,9	0.64	0	5,10,12	1.39	1 (20%)
3	HYP	CCC	115	3	6,8,9	0.54	0	5,10,12	0.89	0
3	HYP	LLL	115	3	6,8,9	0.52	0	5,10,12	0.76	0
3	HYP	III	115	3	6,8,9	0.52	0	5,10,12	0.79	0
3	HYP	CCC	112	3	6,8,9	0.65	0	5,10,12	1.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HYP	LLL	112	3	-	0/0/11/13	0/1/1/1
3	HYP	III	112	3	-	0/0/11/13	0/1/1/1
3	HYP	FFF	115	3	-	0/0/11/13	0/1/1/1
3	HYP	FFF	112	3	-	0/0/11/13	0/1/1/1
3	HYP	CCC	115	3	-	0/0/11/13	0/1/1/1
3	HYP	LLL	115	3	-	0/0/11/13	0/1/1/1
3	HYP	III	115	3	-	0/0/11/13	0/1/1/1
3	HYP	CCC	112	3	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	FFF	112	HYP	CB-CG-CD	2.09	105.82	103.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

72 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	AaA	1	12,1,4	14,14,15	0.38	0	17,19,21	1.06	1 (5%)
4	NAG	AaA	2	4	14,14,15	0.38	0	17,19,21	1.18	2 (11%)
5	NAG	AcA	1	5,1	14,14,15	0.42	0	17,19,21	1.30	2 (11%)
5	NAG	AcA	2	5	14,14,15	0.25	0	17,19,21	1.02	1 (5%)
5	BMA	AcA	3	5	11,11,12	0.52	0	15,15,17	1.15	1 (6%)
5	MAN	AcA	4	5	11,11,12	0.41	0	15,15,17	1.03	2 (13%)
5	NAG	AhA	1	5,1	14,14,15	0.37	0	17,19,21	0.93	1 (5%)
5	NAG	AhA	2	5	14,14,15	0.43	0	17,19,21	1.17	1 (5%)
5	BMA	AhA	3	5	11,11,12	0.61	0	15,15,17	1.22	1 (6%)
5	MAN	AhA	4	5	11,11,12	0.40	0	15,15,17	0.72	0
4	NAG	AlA	1	12,1,4	14,14,15	0.51	0	17,19,21	0.87	0
4	NAG	AlA	2	4	14,14,15	0.30	0	17,19,21	0.90	1 (5%)
6	NAG	AnA	1	6,1	14,14,15	0.48	0	17,19,21	1.34	3 (17%)
6	NAG	AnA	2	6	14,14,15	0.39	0	17,19,21	0.99	1 (5%)
6	FUC	AnA	3	6	10,10,11	0.40	0	14,14,16	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	AqA	1	1,4	14,14,15	0.45	0	17,19,21	1.29	2 (11%)
4	NAG	AqA	2	4	14,14,15	0.39	0	17,19,21	1.07	2 (11%)
4	NAG	AsA	1	1,4	14,14,15	0.48	0	17,19,21	1.20	2 (11%)
4	NAG	AsA	2	4	14,14,15	0.36	0	17,19,21	0.87	1 (5%)
7	NAG	BaB	1	7,2	14,14,15	0.47	0	17,19,21	1.83	4 (23%)
7	NAG	BaB	2	7	14,14,15	0.51	0	17,19,21	1.22	2 (11%)
7	BMA	BaB	3	7	11,11,12	0.46	0	15,15,17	1.15	2 (13%)
7	NAG	DaD	1	7,1	14,14,15	0.43	0	17,19,21	1.45	4 (23%)
7	NAG	DaD	2	7	14,14,15	0.33	0	17,19,21	1.18	1 (5%)
7	BMA	DaD	3	7	11,11,12	0.43	0	15,15,17	0.98	0
4	NAG	DeD	1	12,1,4	14,14,15	0.47	0	17,19,21	0.82	0
4	NAG	DeD	2	4	14,14,15	0.49	0	17,19,21	0.93	1 (5%)
4	NAG	DgD	1	1,4	14,14,15	0.35	0	17,19,21	1.44	3 (17%)
4	NAG	DgD	2	4	14,14,15	0.42	0	17,19,21	0.87	0
5	NAG	DiD	1	5,1	14,14,15	0.33	0	17,19,21	0.69	0
5	NAG	DiD	2	5	14,14,15	0.38	0	17,19,21	1.03	1 (5%)
5	BMA	DiD	3	5	11,11,12	0.44	0	15,15,17	0.75	0
5	MAN	DiD	4	5	11,11,12	0.49	0	15,15,17	0.93	1 (6%)
4	NAG	DmD	1	1,4	14,14,15	0.43	0	17,19,21	1.01	1 (5%)
4	NAG	DmD	2	4	14,14,15	0.38	0	17,19,21	0.91	1 (5%)
8	NAG	DpD	1	1,8	14,14,15	0.42	0	17,19,21	0.83	0
8	NAG	DpD	2	8	14,14,15	0.49	0	17,19,21	1.34	1 (5%)
8	BMA	DpD	3	8	11,11,12	0.45	0	15,15,17	0.94	1 (6%)
8	FUC	DpD	4	8	10,10,11	0.40	0	14,14,16	0.95	0
7	NAG	EaE	1	7,2	14,14,15	0.39	0	17,19,21	1.23	2 (11%)
7	NAG	EaE	2	7	14,14,15	0.48	0	17,19,21	1.19	3 (17%)
7	BMA	EaE	3	7	11,11,12	0.41	0	15,15,17	0.83	0
4	NAG	EdE	1	2,4	14,14,15	0.45	0	17,19,21	0.97	1 (5%)
4	NAG	EdE	2	4	14,14,15	0.29	0	17,19,21	1.03	2 (11%)
7	NAG	GaG	1	7,1	14,14,15	0.58	0	17,19,21	1.53	3 (17%)
7	NAG	GaG	2	7	14,14,15	0.31	0	17,19,21	1.07	0
7	BMA	GaG	3	7	11,11,12	0.48	0	15,15,17	0.97	1 (6%)
7	NAG	GdG	1	7,1,12	14,14,15	0.37	0	17,19,21	1.06	1 (5%)
7	NAG	GdG	2	7	14,14,15	0.47	0	17,19,21	1.09	0
7	BMA	GdG	3	7	11,11,12	0.54	0	15,15,17	1.02	0
4	NAG	GgG	1	1,4	14,14,15	0.38	0	17,19,21	0.68	0
4	NAG	GgG	2	4	14,14,15	0.42	0	17,19,21	1.25	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	GjG	1	1,9	14,14,15	0.57	0	17,19,21	1.23	2 (11%)
9	FUC	GjG	2	9	10,10,11	0.46	0	14,14,16	0.80	0
4	NAG	GlG	1	1,4	14,14,15	0.32	0	17,19,21	0.98	2 (11%)
4	NAG	GlG	2	4	14,14,15	0.33	0	17,19,21	0.62	0
4	NAG	GnG	1	1,4	14,14,15	0.45	0	17,19,21	1.66	2 (11%)
4	NAG	GnG	2	4	14,14,15	0.57	0	17,19,21	1.44	2 (11%)
4	NAG	HaH	1	2,4	14,14,15	0.47	0	17,19,21	1.41	2 (11%)
4	NAG	HaH	2	4	14,14,15	0.49	0	17,19,21	0.92	0
4	NAG	JaJ	1	1,4	14,14,15	0.43	0	17,19,21	1.21	3 (17%)
4	NAG	JaJ	2	4	14,14,15	0.30	0	17,19,21	0.86	0
4	NAG	JcJ	1	1,4	14,14,15	0.44	0	17,19,21	1.37	2 (11%)
4	NAG	JcJ	2	4	14,14,15	0.35	0	17,19,21	1.18	1 (5%)
4	NAG	JeJ	1	1,4	14,14,15	0.59	0	17,19,21	1.42	2 (11%)
4	NAG	JeJ	2	4	14,14,15	0.43	0	17,19,21	0.82	1 (5%)
4	NAG	JgJ	1	1,4	14,14,15	0.29	0	17,19,21	0.90	0
4	NAG	JgJ	2	4	14,14,15	0.47	0	17,19,21	0.90	1 (5%)
4	NAG	JkJ	1	1,4	14,14,15	0.56	0	17,19,21	1.39	3 (17%)
4	NAG	JkJ	2	4	14,14,15	0.41	0	17,19,21	0.72	0
4	NAG	KaK	1	2,4	14,14,15	0.41	0	17,19,21	1.71	5 (29%)
4	NAG	KaK	2	4	14,14,15	0.33	0	17,19,21	0.98	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	AaA	1	12,1,4	-	1/6/23/26	0/1/1/1
4	NAG	AaA	2	4	-	2/6/23/26	0/1/1/1
5	NAG	AcA	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	AcA	2	5	-	0/6/23/26	0/1/1/1
5	BMA	AcA	3	5	1/1/4/5	2/2/19/22	0/1/1/1
5	MAN	AcA	4	5	-	0/2/19/22	0/1/1/1
5	NAG	AhA	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	AhA	2	5	-	2/6/23/26	0/1/1/1
5	BMA	AhA	3	5	1/1/4/5	2/2/19/22	0/1/1/1
5	MAN	AhA	4	5	1/1/4/5	1/2/19/22	0/1/1/1
4	NAG	AlA	1	12,1,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	AlA	2	4	-	1/6/23/26	0/1/1/1
6	NAG	AnA	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	AnA	2	6	-	0/6/23/26	0/1/1/1
6	FUC	AnA	3	6	-	-	0/1/1/1
4	NAG	AqA	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	AqA	2	4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	AsA	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	AsA	2	4	1/1/5/7	2/6/23/26	0/1/1/1
7	NAG	BaB	1	7,2	-	3/6/23/26	0/1/1/1
7	NAG	BaB	2	7	1/1/5/7	2/6/23/26	0/1/1/1
7	BMA	BaB	3	7	-	0/2/19/22	0/1/1/1
7	NAG	DaD	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	DaD	2	7	-	2/6/23/26	0/1/1/1
7	BMA	DaD	3	7	1/1/4/5	2/2/19/22	0/1/1/1
4	NAG	DeD	1	12,1,4	-	2/6/23/26	0/1/1/1
4	NAG	DeD	2	4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	DgD	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	DgD	2	4	1/1/5/7	1/6/23/26	0/1/1/1
5	NAG	DiD	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	DiD	2	5	-	2/6/23/26	0/1/1/1
5	BMA	DiD	3	5	1/1/4/5	0/2/19/22	0/1/1/1
5	MAN	DiD	4	5	-	1/2/19/22	0/1/1/1
4	NAG	DmD	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	DmD	2	4	-	2/6/23/26	0/1/1/1
8	NAG	DpD	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	DpD	2	8	-	2/6/23/26	0/1/1/1
8	BMA	DpD	3	8	1/1/4/5	0/2/19/22	0/1/1/1
8	FUC	DpD	4	8	-	-	0/1/1/1
7	NAG	EaE	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	EaE	2	7	1/1/5/7	4/6/23/26	0/1/1/1
7	BMA	EaE	3	7	1/1/4/5	0/2/19/22	0/1/1/1
4	NAG	EdE	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	EdE	2	4	-	0/6/23/26	0/1/1/1
7	NAG	GaG	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	GaG	2	7	-	0/6/23/26	0/1/1/1
7	BMA	GaG	3	7	1/1/4/5	2/2/19/22	0/1/1/1
7	NAG	GdG	1	7,1,12	-	2/6/23/26	0/1/1/1
7	NAG	GdG	2	7	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	GdG	3	7	1/1/4/5	2/2/19/22	0/1/1/1
4	NAG	GgG	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	GgG	2	4	1/1/5/7	4/6/23/26	0/1/1/1
9	NAG	GjG	1	1,9	-	0/6/23/26	0/1/1/1
9	FUC	GjG	2	9	-	-	0/1/1/1
4	NAG	GlG	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	GlG	2	4	1/1/5/7	1/6/23/26	0/1/1/1
4	NAG	GnG	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	GnG	2	4	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	HaH	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	HaH	2	4	1/1/5/7	4/6/23/26	0/1/1/1
4	NAG	JaJ	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	JaJ	2	4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	JcJ	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	JcJ	2	4	1/1/5/7	3/6/23/26	0/1/1/1
4	NAG	JeJ	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	JeJ	2	4	-	2/6/23/26	0/1/1/1
4	NAG	JgJ	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	JgJ	2	4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	JkJ	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	JkJ	2	4	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	KaK	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	KaK	2	4	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	GnG	1	NAG	C1-O5-C5	5.44	119.57	112.19
4	JcJ	1	NAG	C1-O5-C5	4.66	118.51	112.19
4	HaH	1	NAG	C1-O5-C5	4.01	117.63	112.19
8	DpD	2	NAG	C1-O5-C5	3.96	117.56	112.19
7	BaB	1	NAG	C8-C7-N2	3.93	122.75	116.10
4	KaK	1	NAG	C8-C7-N2	3.91	122.73	116.10
7	BaB	1	NAG	C2-N2-C7	3.85	128.38	122.90
7	GaG	1	NAG	C1-O5-C5	3.67	117.16	112.19
4	JeJ	1	NAG	O5-C1-C2	3.60	116.97	111.29
7	EaE	1	NAG	C1-O5-C5	3.60	117.07	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	GnG	2	NAG	C1-O5-C5	3.50	116.93	112.19
4	JkJ	1	NAG	C1-O5-C5	3.46	116.88	112.19
4	JcJ	2	NAG	O5-C5-C6	3.37	112.49	107.20
4	DgD	1	NAG	C1-O5-C5	3.35	116.73	112.19
7	BaB	2	NAG	C1-O5-C5	3.25	116.59	112.19
5	AhA	2	NAG	C1-O5-C5	3.16	116.48	112.19
5	AhA	3	BMA	O5-C5-C6	3.15	112.14	107.20
9	GjG	1	NAG	O5-C5-C6	3.00	111.91	107.20
4	AqA	1	NAG	C1-O5-C5	2.94	116.18	112.19
7	DaD	1	NAG	C1-O5-C5	2.93	116.17	112.19
7	GaG	1	NAG	O5-C1-C2	-2.93	106.66	111.29
6	AnA	1	NAG	C1-O5-C5	2.91	116.13	112.19
4	AsA	1	NAG	C4-C3-C2	-2.90	106.77	111.02
7	GaG	1	NAG	C1-C2-N2	2.88	115.41	110.49
4	KaK	1	NAG	C2-N2-C7	2.84	126.94	122.90
4	DgD	1	NAG	C4-C3-C2	-2.72	107.03	111.02
4	KaK	2	NAG	O5-C5-C6	2.71	111.45	107.20
4	AaA	2	NAG	O5-C5-C6	2.69	111.42	107.20
7	EaE	2	NAG	C8-C7-N2	2.69	120.65	116.10
5	AcA	1	NAG	C1-O5-C5	2.67	115.81	112.19
7	GdG	1	NAG	C1-O5-C5	2.66	115.80	112.19
4	AsA	1	NAG	C1-O5-C5	2.63	115.75	112.19
4	AqA	1	NAG	C4-C3-C2	-2.62	107.18	111.02
4	KaK	1	NAG	C1-C2-N2	-2.60	106.05	110.49
4	JaJ	1	NAG	C1-C2-N2	2.59	114.92	110.49
4	JeJ	1	NAG	O4-C4-C5	2.59	115.73	109.30
4	AaA	1	NAG	O5-C5-C6	2.58	111.25	107.20
7	EaE	1	NAG	O5-C1-C2	-2.58	107.21	111.29
4	GgG	2	NAG	O5-C5-C6	2.57	111.23	107.20
4	KaK	1	NAG	O5-C5-C6	2.56	111.22	107.20
4	EdE	2	NAG	C4-C3-C2	-2.56	107.27	111.02
4	GlG	1	NAG	C4-C3-C2	-2.53	107.31	111.02
6	AnA	1	NAG	C1-C2-N2	-2.47	106.27	110.49
7	DaD	1	NAG	O5-C1-C2	-2.45	107.41	111.29
4	KaK	1	NAG	O7-C7-N2	-2.45	117.45	121.95
5	AcA	1	NAG	O5-C1-C2	-2.45	107.43	111.29
5	AcA	4	MAN	O5-C1-C2	-2.44	107.01	110.77
5	DiD	2	NAG	O4-C4-C3	-2.43	104.73	110.35
4	GnG	2	NAG	O5-C1-C2	-2.39	107.51	111.29
4	HaH	1	NAG	O5-C1-C2	-2.37	107.55	111.29
4	JaJ	1	NAG	O5-C1-C2	-2.33	107.60	111.29
8	DpD	3	BMA	O5-C5-C6	2.33	110.86	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AcA	2	NAG	O5-C5-C6	2.33	110.86	107.20
7	BaB	1	NAG	O5-C5-C6	2.33	110.85	107.20
4	AqA	2	NAG	C8-C7-N2	2.31	120.01	116.10
7	DaD	1	NAG	O3-C3-C4	-2.29	105.05	110.35
5	DiD	4	MAN	O5-C5-C6	2.29	110.80	107.20
7	DaD	2	NAG	C1-O5-C5	2.28	115.28	112.19
6	AnA	2	NAG	O5-C5-C6	2.26	110.75	107.20
4	AlA	2	NAG	C1-O5-C5	2.26	115.25	112.19
5	AcA	4	MAN	O5-C5-C6	2.23	110.70	107.20
7	BaB	1	NAG	O7-C7-N2	-2.22	117.86	121.95
4	DgD	1	NAG	O5-C1-C2	-2.21	107.79	111.29
4	JkJ	1	NAG	C2-N2-C7	2.20	126.03	122.90
7	DaD	1	NAG	C6-C5-C4	-2.19	107.86	113.00
7	BaB	2	NAG	O5-C1-C2	-2.19	107.83	111.29
7	EaE	2	NAG	C2-N2-C7	2.17	125.99	122.90
7	BaB	3	BMA	O5-C5-C6	2.17	110.60	107.20
4	EdE	1	NAG	C1-C2-N2	-2.16	106.79	110.49
4	AsA	2	NAG	O5-C5-C6	2.16	110.59	107.20
4	JaJ	1	NAG	C1-O5-C5	2.16	115.11	112.19
7	BaB	3	BMA	C1-C2-C3	2.15	112.31	109.67
5	AcA	3	BMA	C1-C2-C3	2.15	112.31	109.67
4	AqA	2	NAG	C2-N2-C7	2.11	125.91	122.90
4	GnG	1	NAG	O4-C4-C5	2.11	114.53	109.30
4	GgG	2	NAG	C2-N2-C7	2.10	125.89	122.90
4	JeJ	2	NAG	C2-N2-C7	2.09	125.88	122.90
4	DeD	2	NAG	O5-C5-C6	2.06	110.43	107.20
4	JkJ	1	NAG	O7-C7-N2	2.06	125.73	121.95
4	DmD	1	NAG	O4-C4-C5	2.04	114.37	109.30
4	GlG	1	NAG	C1-O5-C5	2.04	114.96	112.19
4	JcJ	1	NAG	O5-C5-C4	-2.04	105.86	110.83
5	AhA	1	NAG	C4-C3-C2	-2.03	108.04	111.02
7	GaG	3	BMA	O5-C5-C6	2.03	110.38	107.20
9	GjG	1	NAG	C3-C4-C5	-2.03	106.62	110.24
7	EaE	2	NAG	C1-C2-N2	-2.01	107.05	110.49
6	AnA	1	NAG	O5-C5-C6	2.01	110.36	107.20
4	AaA	2	NAG	O5-C5-C4	-2.01	105.94	110.83
4	JgJ	2	NAG	O5-C5-C6	2.01	110.35	107.20
4	EdE	2	NAG	O5-C1-C2	-2.00	108.12	111.29
4	DmD	2	NAG	C1-O5-C5	2.00	114.90	112.19

All (24) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	AqA	2	NAG	C1
4	AsA	2	NAG	C1
4	DeD	2	NAG	C1
4	DgD	2	NAG	C1
4	GgG	2	NAG	C1
4	GlG	2	NAG	C1
4	GnG	2	NAG	C1
4	HaH	2	NAG	C1
4	JaJ	2	NAG	C1
4	JcJ	2	NAG	C1
4	JgJ	2	NAG	C1
4	JkJ	2	NAG	C1
4	KaK	2	NAG	C1
5	AcA	3	BMA	C1
5	AhA	3	BMA	C1
5	AhA	4	MAN	C1
5	DiD	3	BMA	C1
7	BaB	2	NAG	C1
7	DaD	3	BMA	C1
7	EaE	2	NAG	C1
7	EaE	3	BMA	C1
7	GaG	3	BMA	C1
7	GdG	3	BMA	C1
8	DpD	3	BMA	C1

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	DgD	2	NAG	C3-C2-N2-C7
4	GgG	2	NAG	C1-C2-N2-C7
4	HaH	2	NAG	C3-C2-N2-C7
4	JkJ	1	NAG	C3-C2-N2-C7
4	GgG	1	NAG	O5-C5-C6-O6
5	AhA	1	NAG	C4-C5-C6-O6
4	DeD	1	NAG	O5-C5-C6-O6
4	HaH	2	NAG	O5-C5-C6-O6
5	DiD	2	NAG	O5-C5-C6-O6
4	JkJ	2	NAG	O5-C5-C6-O6
8	DpD	2	NAG	O5-C5-C6-O6
5	AhA	3	BMA	C4-C5-C6-O6
4	GgG	2	NAG	O5-C5-C6-O6
4	JcJ	1	NAG	O5-C5-C6-O6
4	GgG	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	AhA	1	NAG	O5-C5-C6-O6
7	BaB	2	NAG	C4-C5-C6-O6
4	DmD	2	NAG	O5-C5-C6-O6
4	JgJ	2	NAG	O5-C5-C6-O6
4	JeJ	2	NAG	C4-C5-C6-O6
4	JcJ	1	NAG	C4-C5-C6-O6
4	KaK	1	NAG	C4-C5-C6-O6
7	GdG	3	BMA	C4-C5-C6-O6
4	HaH	2	NAG	C4-C5-C6-O6
4	GgG	2	NAG	C4-C5-C6-O6
4	JeJ	1	NAG	C4-C5-C6-O6
4	JgJ	2	NAG	C4-C5-C6-O6
4	GnG	2	NAG	O5-C5-C6-O6
4	JeJ	1	NAG	O5-C5-C6-O6
4	DeD	1	NAG	C4-C5-C6-O6
5	DiD	2	NAG	C4-C5-C6-O6
4	AqA	2	NAG	C8-C7-N2-C2
4	AqA	2	NAG	O7-C7-N2-C2
4	GnG	2	NAG	C8-C7-N2-C2
4	GnG	2	NAG	O7-C7-N2-C2
4	KaK	1	NAG	C8-C7-N2-C2
4	KaK	1	NAG	O7-C7-N2-C2
7	BaB	1	NAG	C8-C7-N2-C2
7	BaB	1	NAG	O7-C7-N2-C2
7	EaE	2	NAG	C8-C7-N2-C2
7	EaE	2	NAG	O7-C7-N2-C2
7	BaB	2	NAG	O5-C5-C6-O6
4	JgJ	1	NAG	O5-C5-C6-O6
4	DmD	2	NAG	C4-C5-C6-O6
4	AsA	2	NAG	O5-C5-C6-O6
7	GdG	2	NAG	O5-C5-C6-O6
7	GdG	1	NAG	O5-C5-C6-O6
4	AsA	2	NAG	C4-C5-C6-O6
7	GdG	3	BMA	O5-C5-C6-O6
5	AcA	1	NAG	O5-C5-C6-O6
4	JeJ	2	NAG	O5-C5-C6-O6
7	DaD	3	BMA	C4-C5-C6-O6
7	GdG	2	NAG	C4-C5-C6-O6
4	HaH	1	NAG	O5-C5-C6-O6
5	AhA	3	BMA	O5-C5-C6-O6
7	GaG	3	BMA	O5-C5-C6-O6
5	AcA	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	GaG	3	BMA	C4-C5-C6-O6
4	JkJ	2	NAG	C4-C5-C6-O6
4	AlA	1	NAG	O5-C5-C6-O6
7	EaE	2	NAG	O5-C5-C6-O6
7	EaE	2	NAG	C4-C5-C6-O6
4	GlG	2	NAG	O5-C5-C6-O6
4	KaK	1	NAG	O5-C5-C6-O6
7	DaD	3	BMA	O5-C5-C6-O6
4	JgJ	1	NAG	C4-C5-C6-O6
4	AqA	1	NAG	C4-C5-C6-O6
7	GdG	1	NAG	C4-C5-C6-O6
4	JaJ	2	NAG	O5-C5-C6-O6
5	AhA	2	NAG	O5-C5-C6-O6
4	AqA	1	NAG	O5-C5-C6-O6
5	AhA	4	MAN	O5-C5-C6-O6
4	GnG	1	NAG	O5-C5-C6-O6
4	DgD	1	NAG	C3-C2-N2-C7
4	JaJ	2	NAG	C3-C2-N2-C7
5	AhA	2	NAG	C4-C5-C6-O6
4	HaH	1	NAG	C4-C5-C6-O6
7	DaD	2	NAG	O5-C5-C6-O6
5	AcA	3	BMA	C4-C5-C6-O6
4	GlG	1	NAG	O5-C5-C6-O6
7	DaD	2	NAG	C4-C5-C6-O6
4	GlG	1	NAG	C4-C5-C6-O6
5	AcA	3	BMA	O5-C5-C6-O6
8	DpD	2	NAG	C4-C5-C6-O6
4	AaA	2	NAG	C4-C5-C6-O6
4	GnG	2	NAG	C4-C5-C6-O6
4	GgG	2	NAG	C3-C2-N2-C7
4	EdE	1	NAG	O5-C5-C6-O6
4	AaA	2	NAG	O5-C5-C6-O6
4	AaA	1	NAG	O5-C5-C6-O6
7	BaB	1	NAG	C1-C2-N2-C7
4	JcJ	2	NAG	C4-C5-C6-O6
6	AnA	1	NAG	C4-C5-C6-O6
5	DiD	4	MAN	C4-C5-C6-O6
4	AlA	1	NAG	C4-C5-C6-O6
4	HaH	2	NAG	C1-C2-N2-C7
4	AlA	2	NAG	O5-C5-C6-O6
4	EdE	1	NAG	C4-C5-C6-O6
4	JcJ	2	NAG	C3-C2-N2-C7

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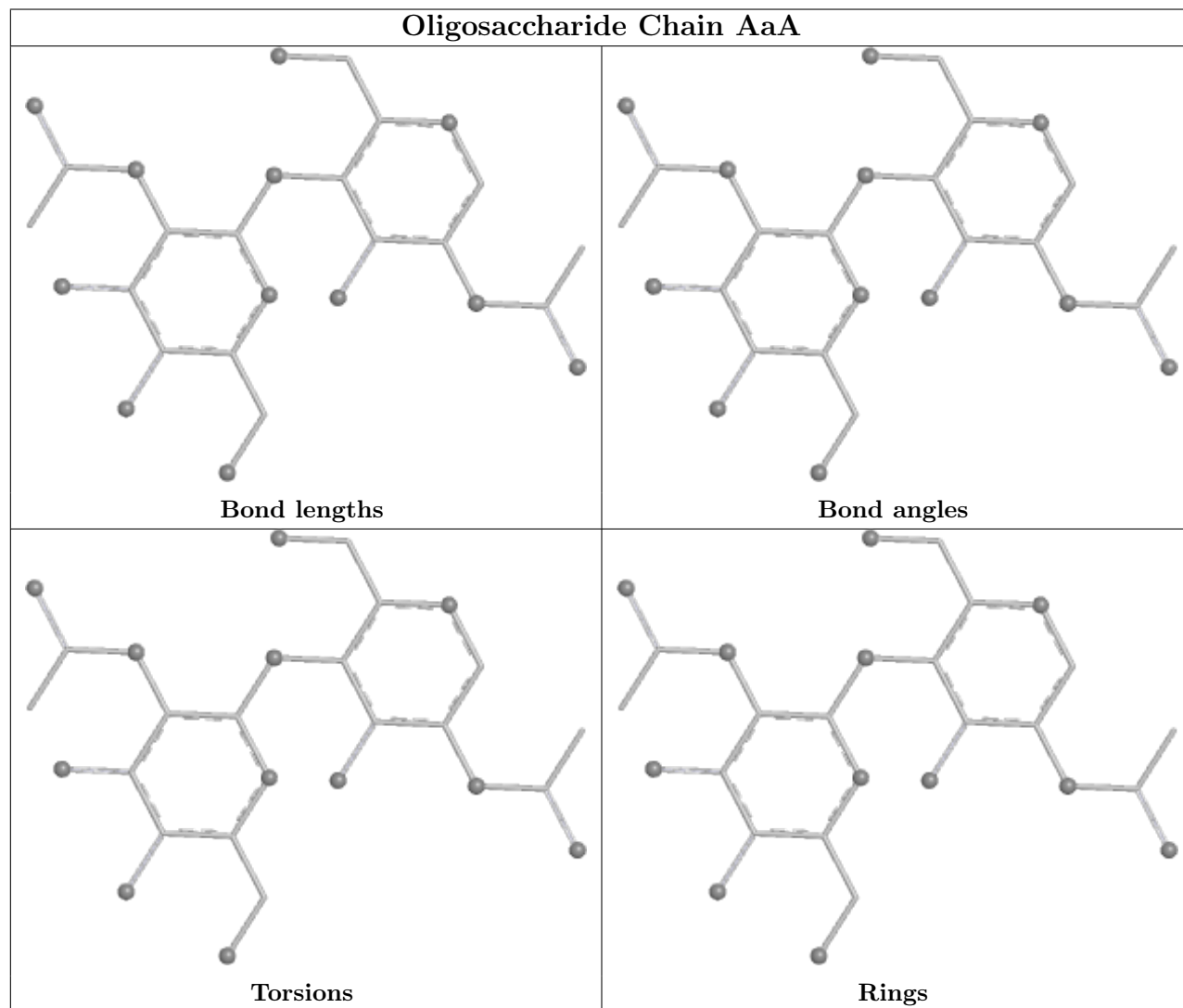
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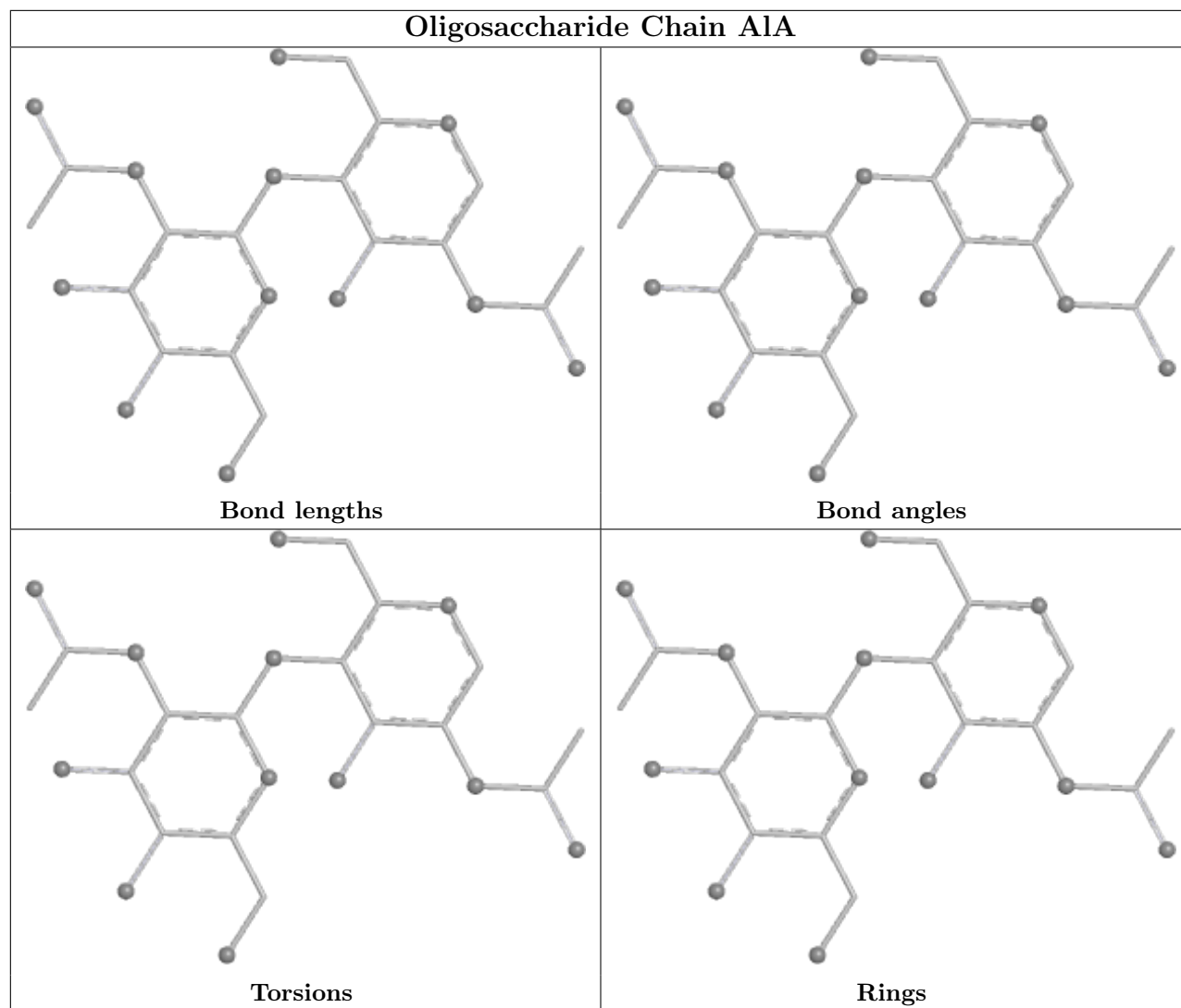
Mol	Chain	Res	Type	Atoms
4	JcJ	2	NAG	O5-C5-C6-O6

There are no ring outliers.

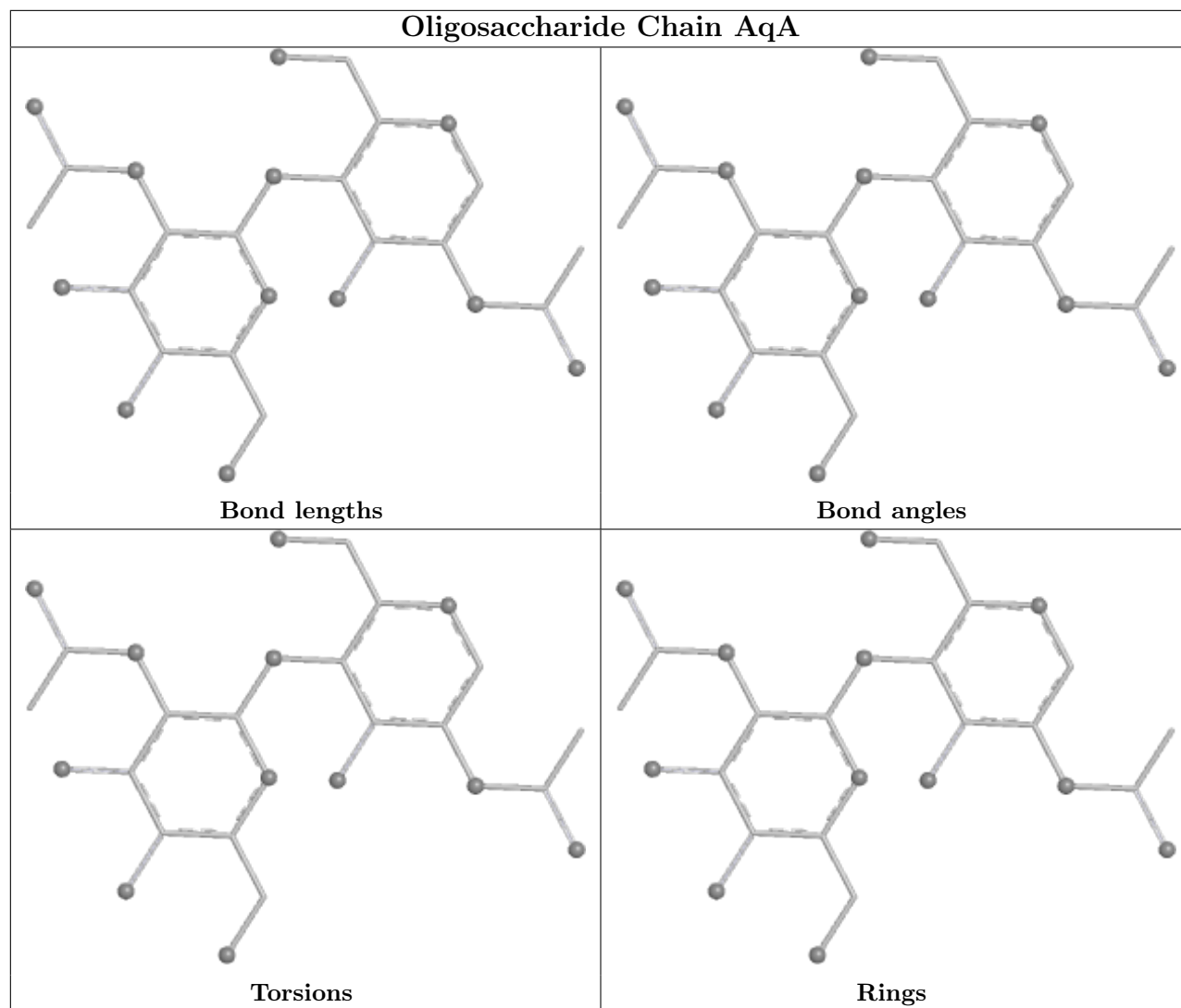
No monomer is involved in short contacts.

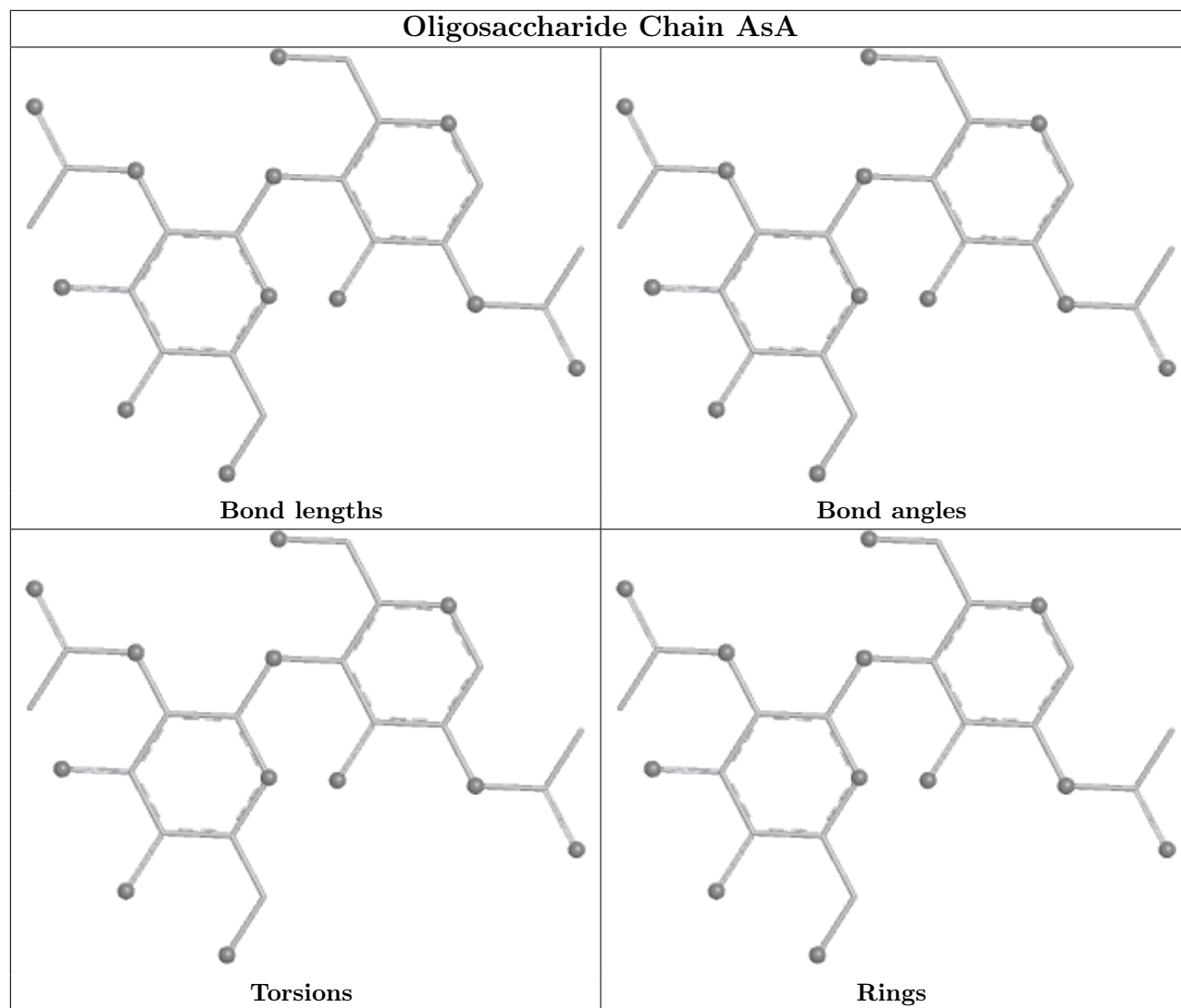
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

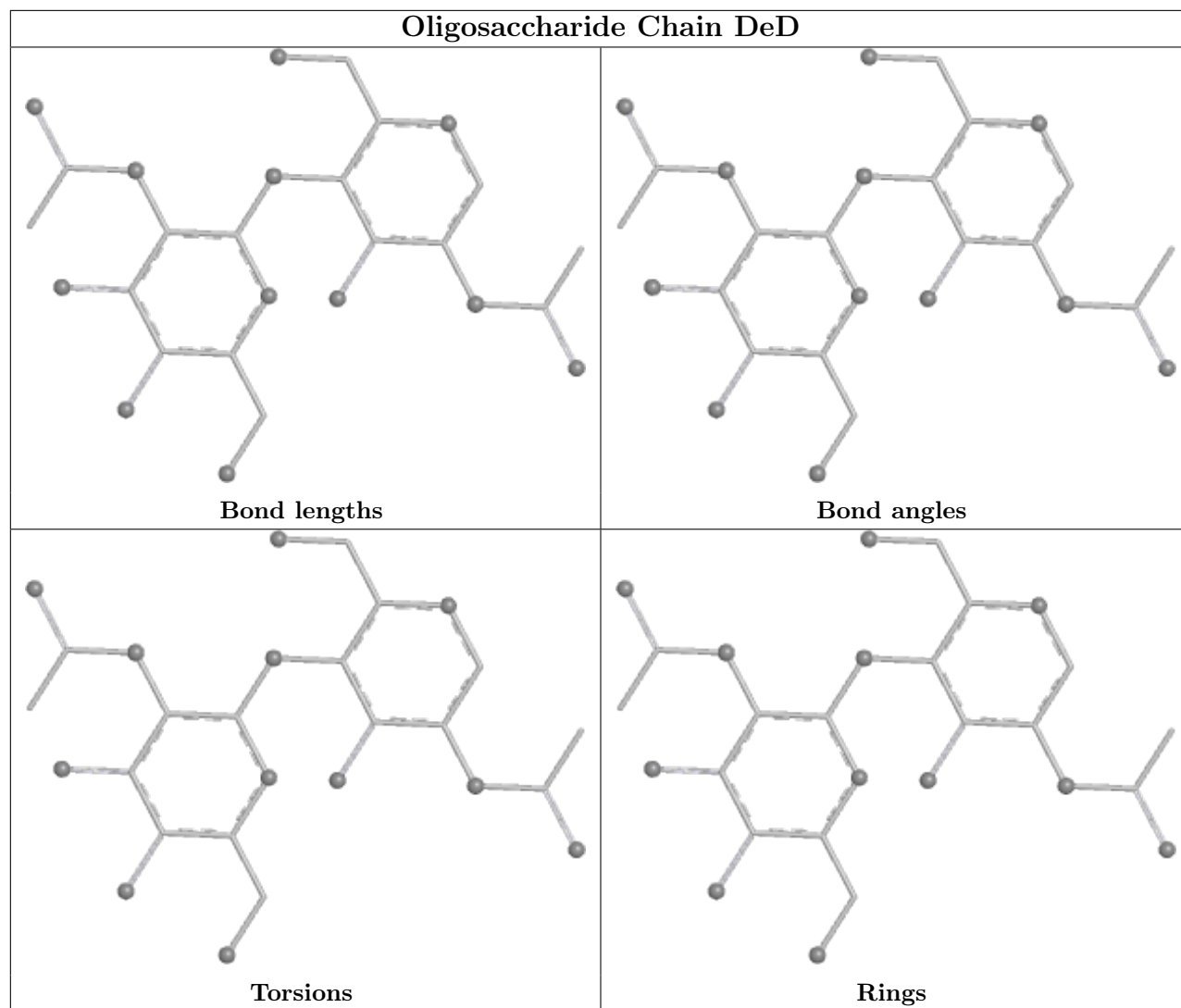


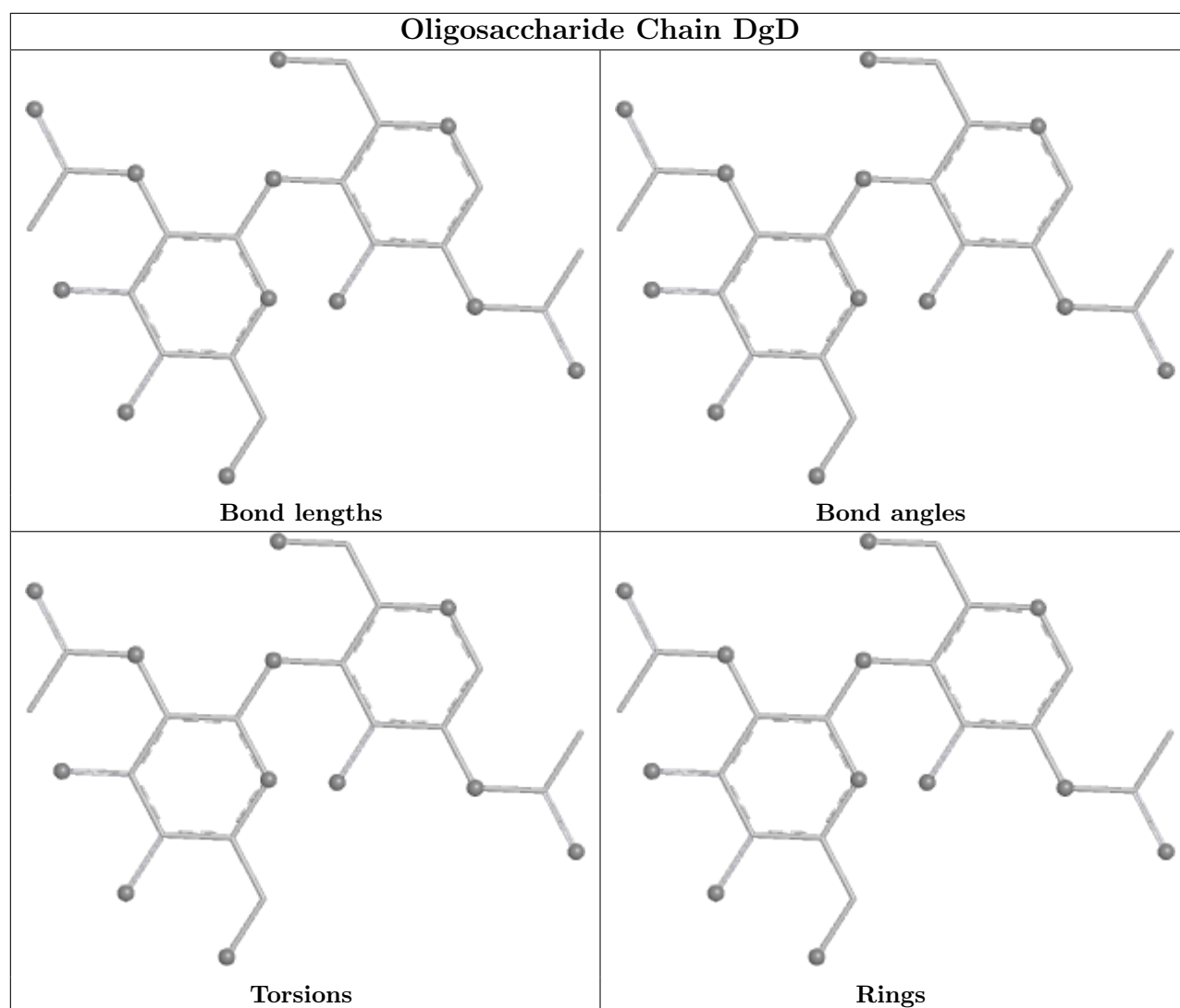


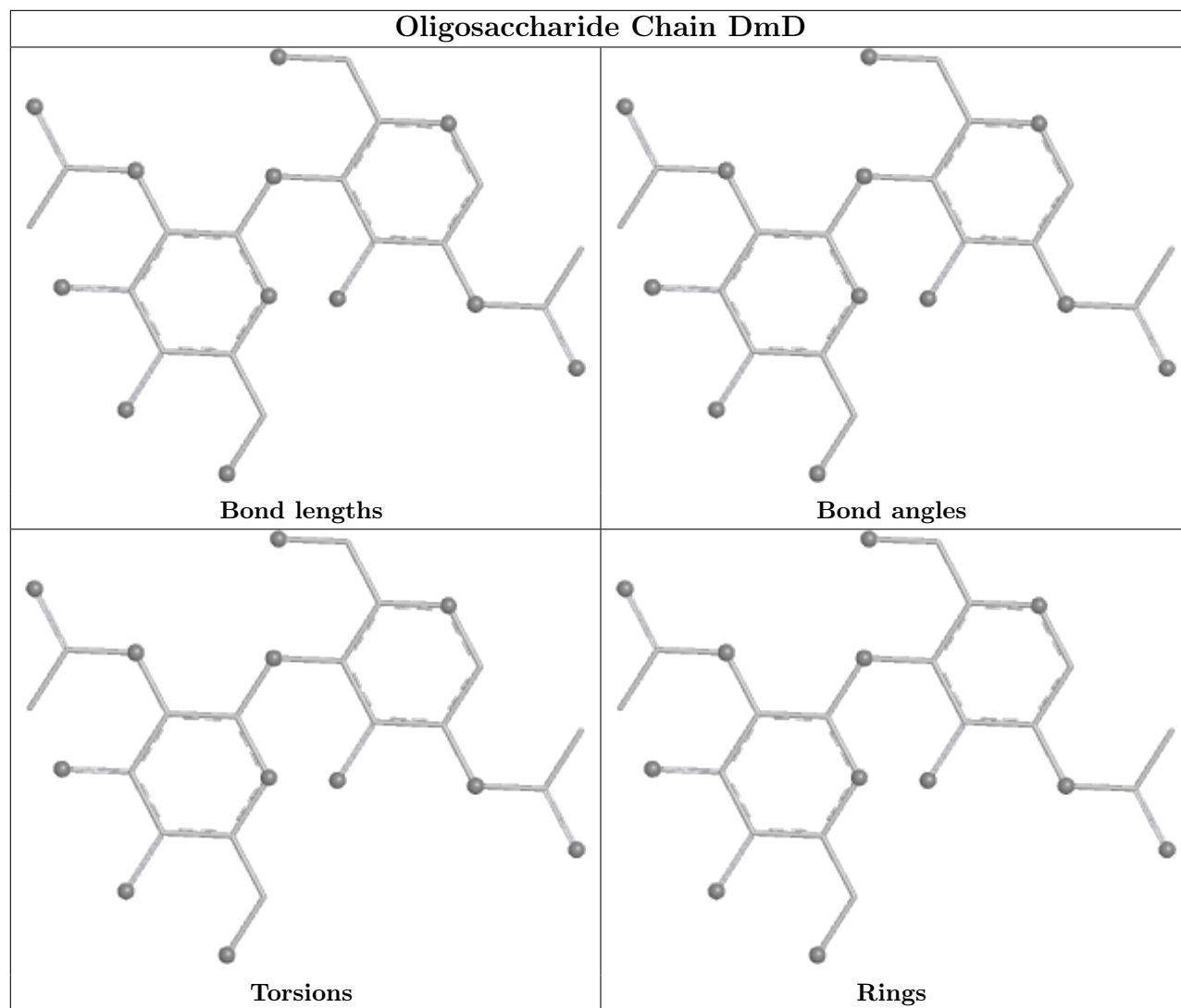


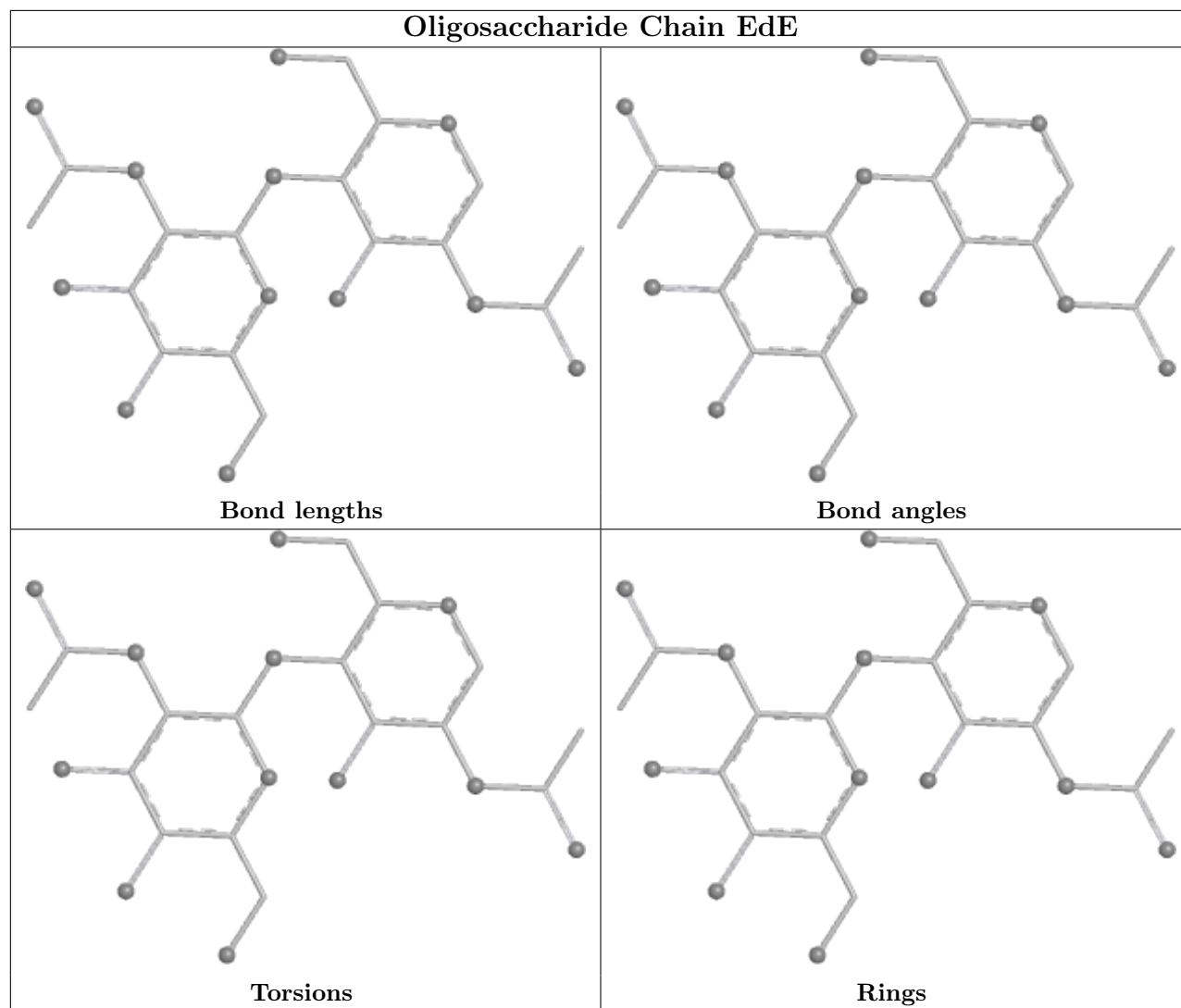


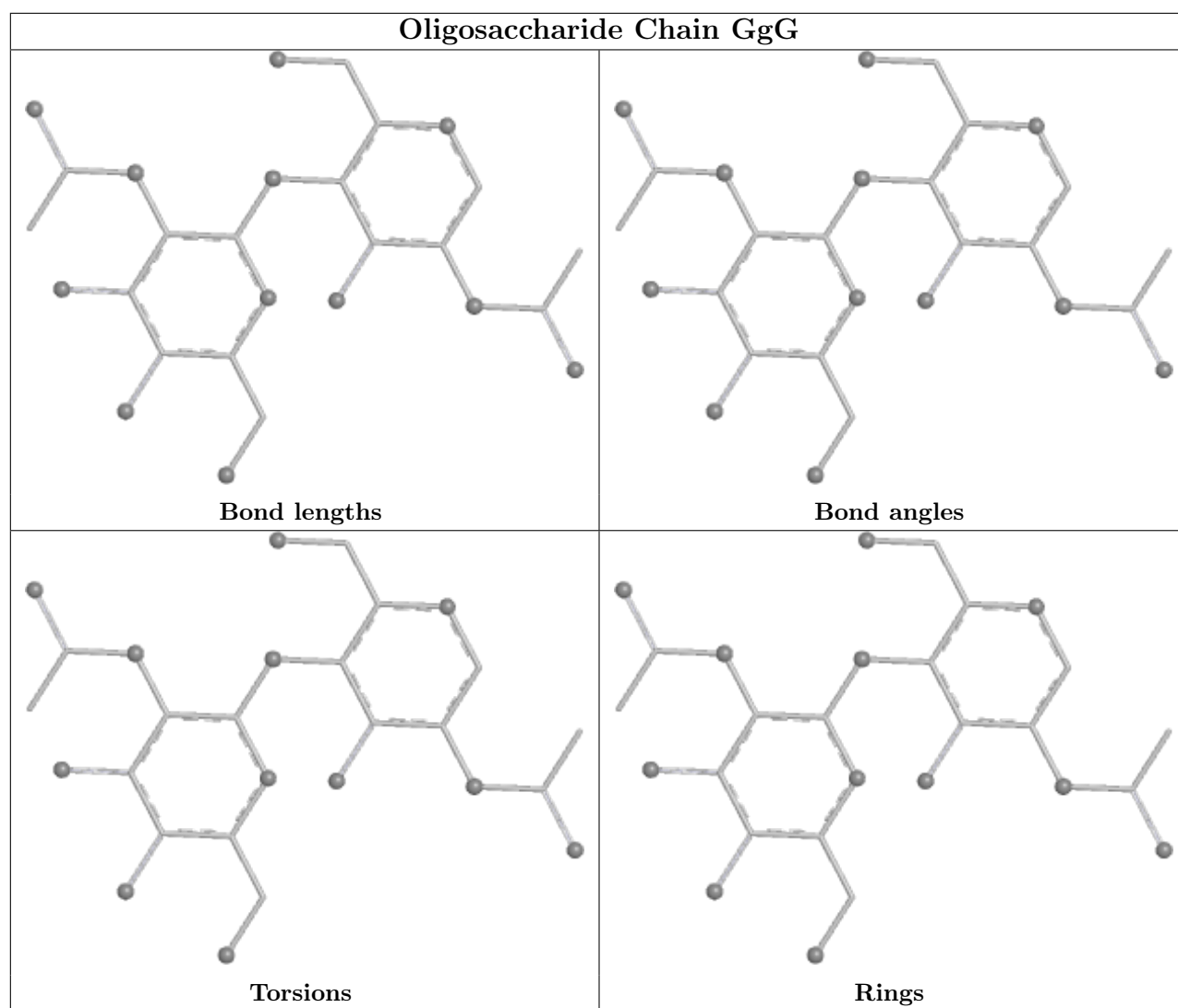


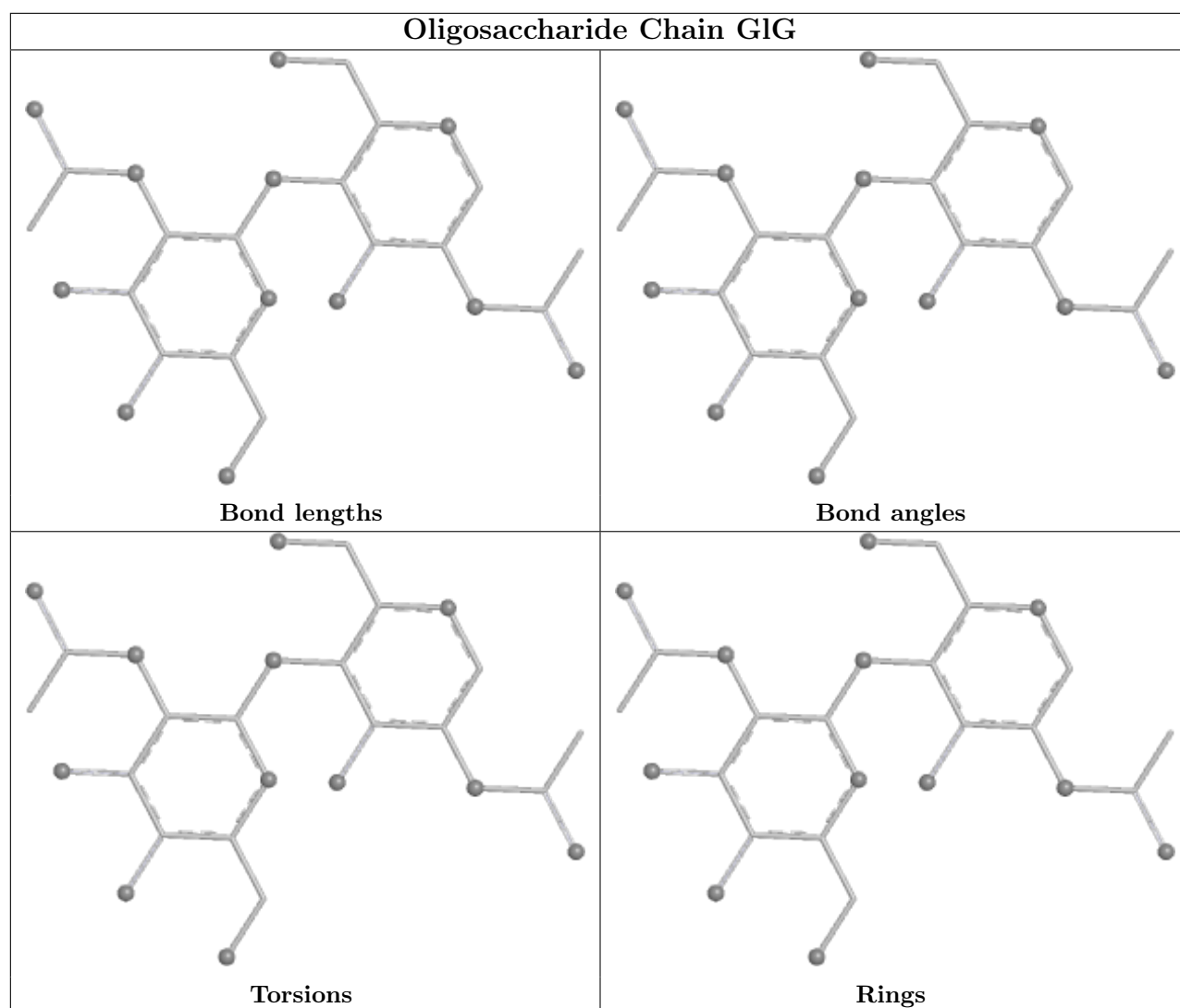




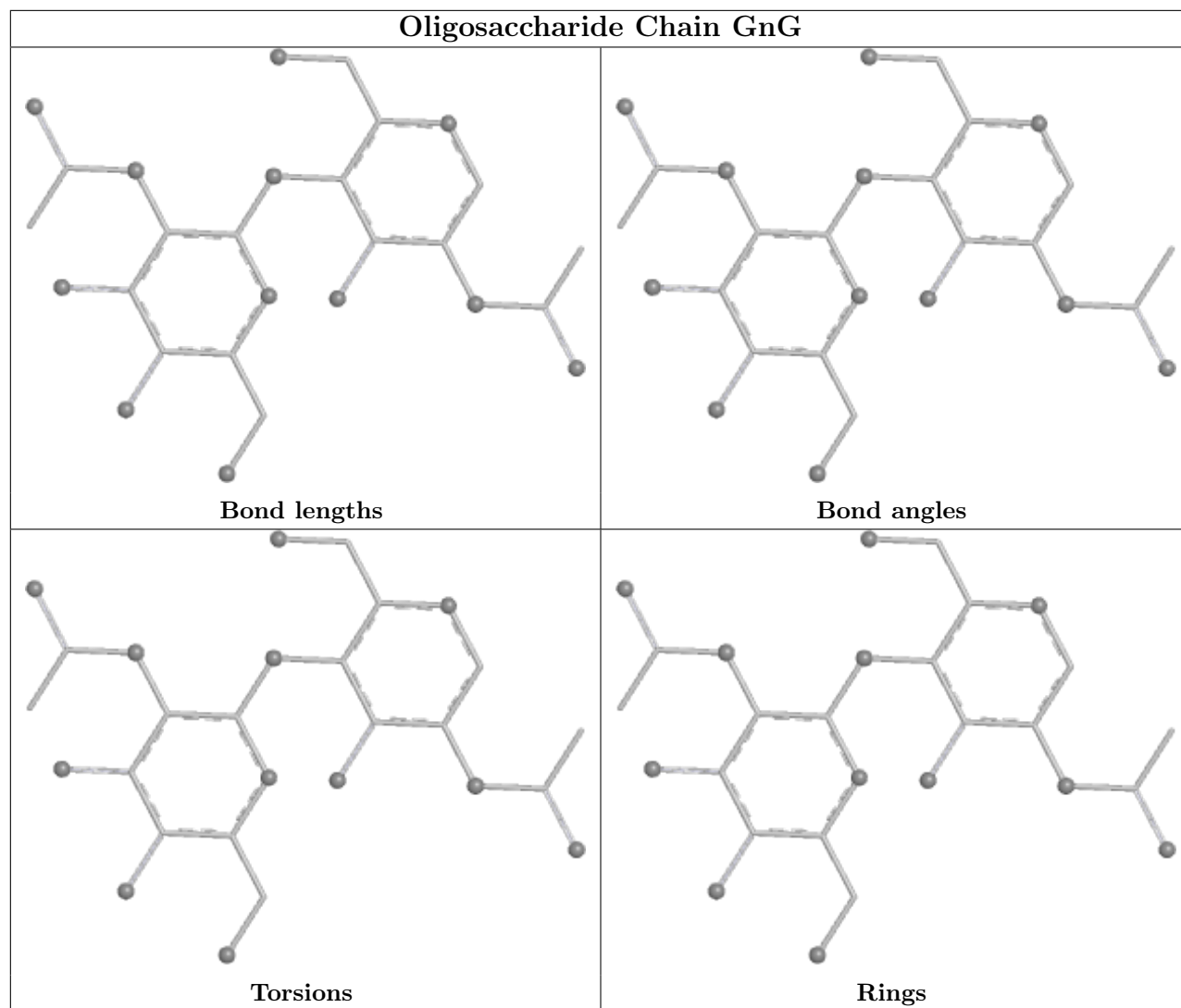


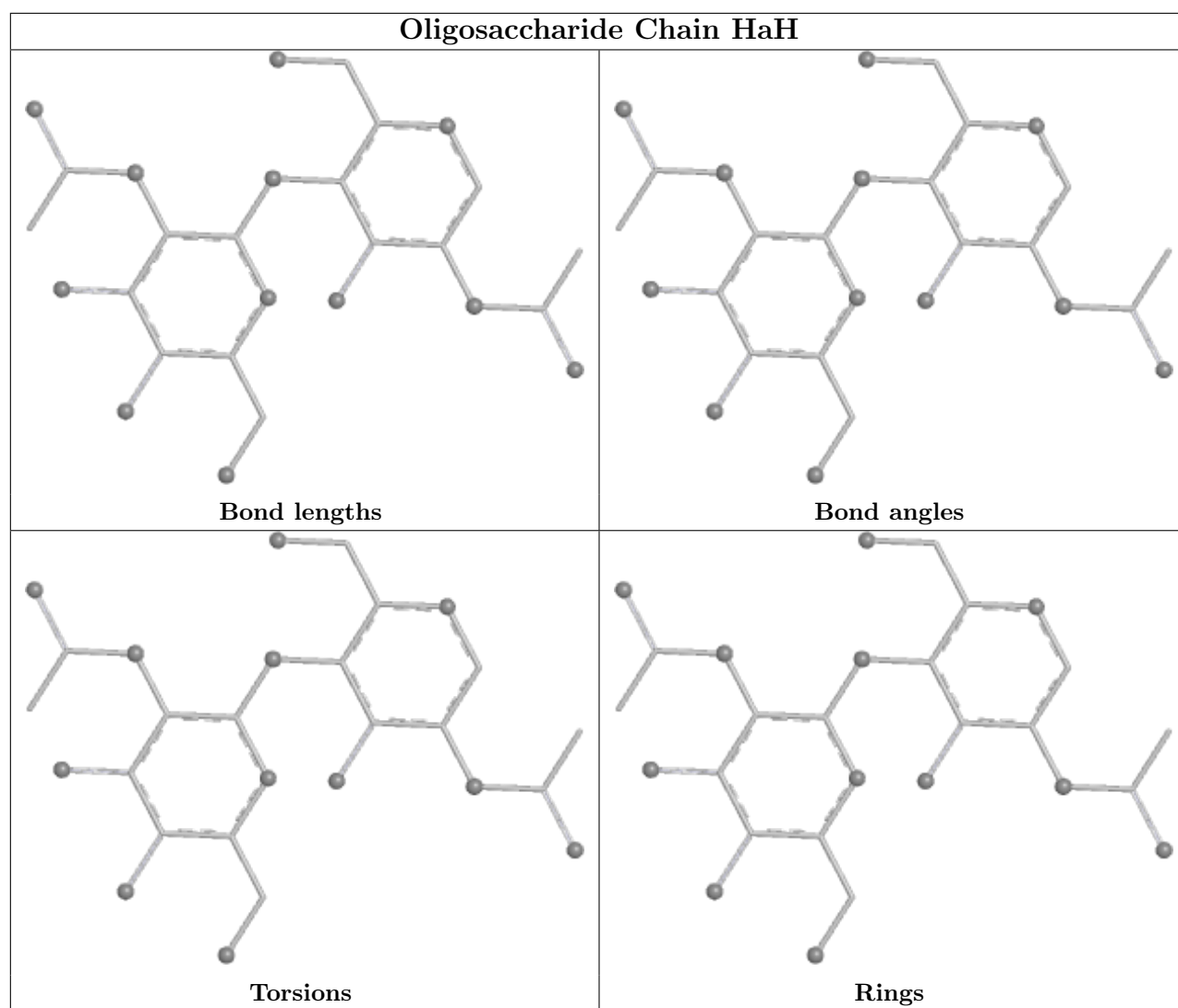




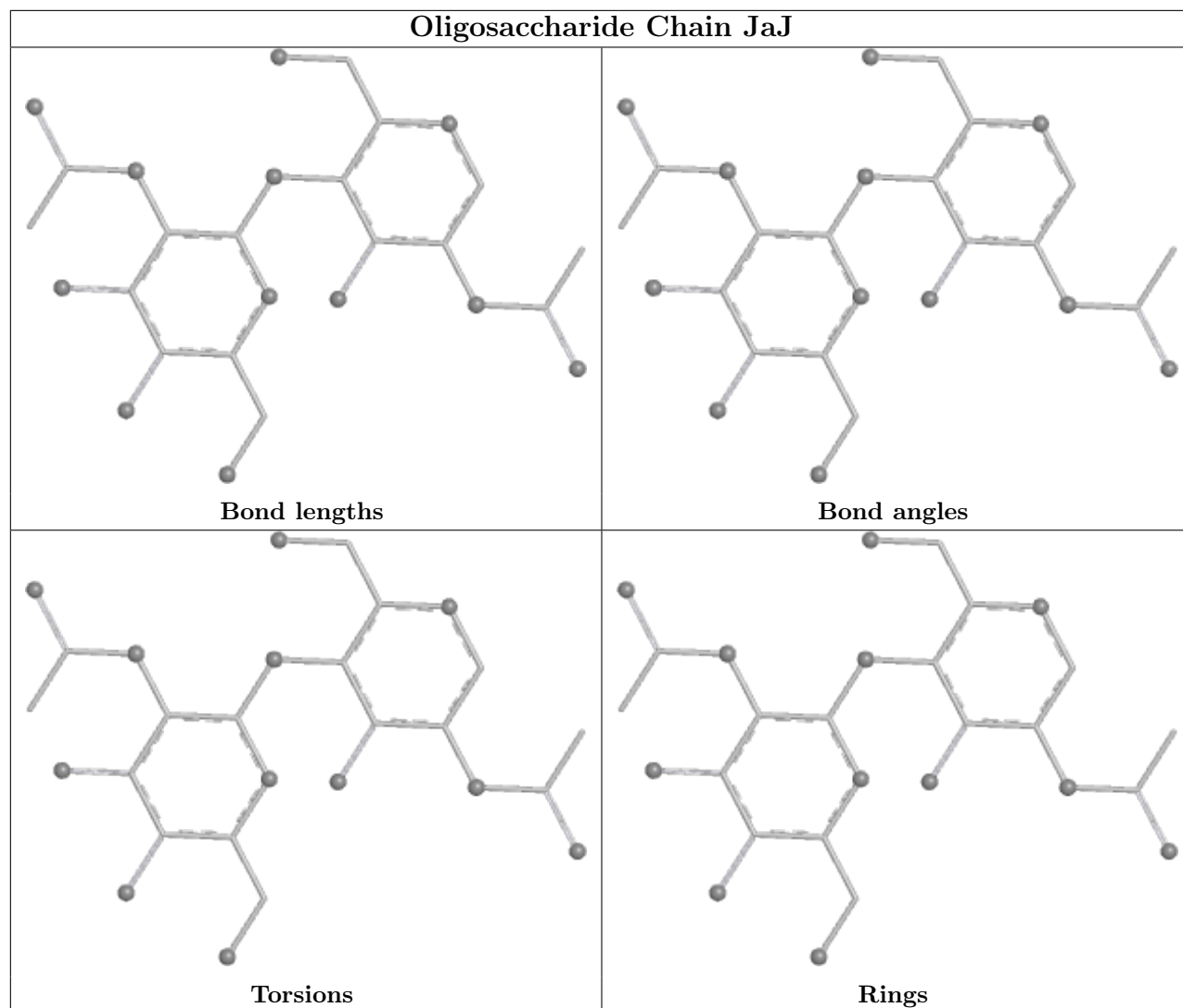


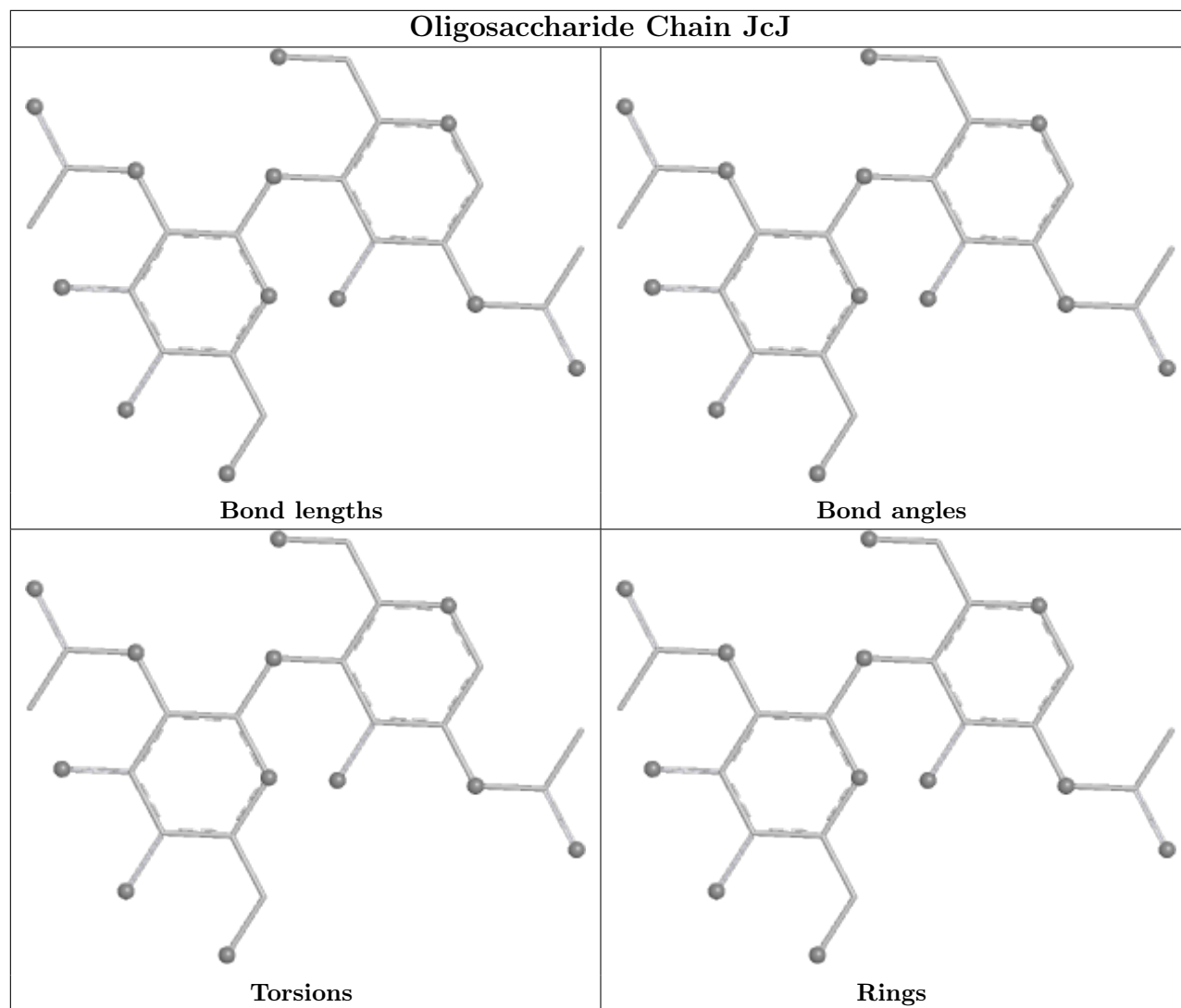




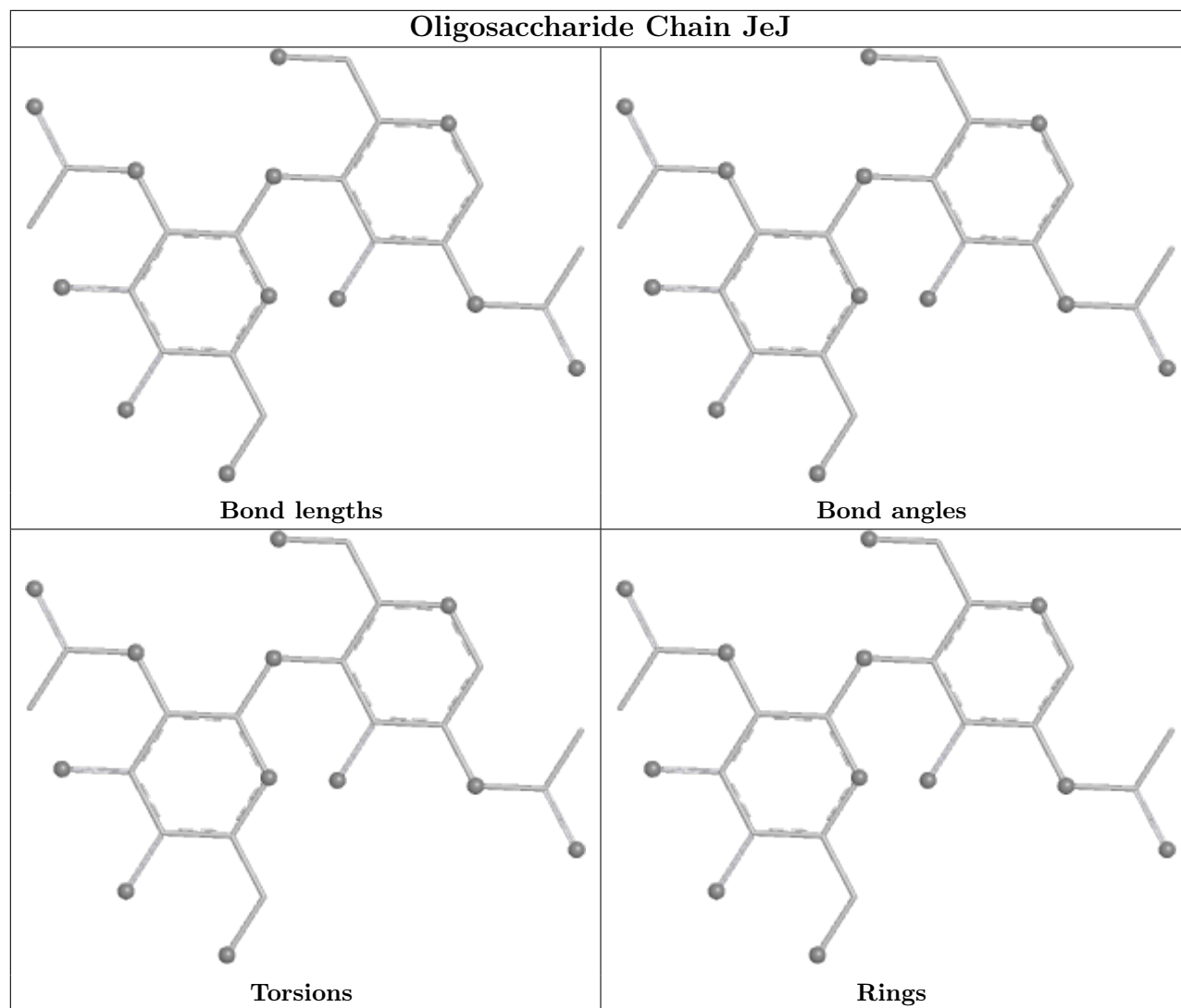


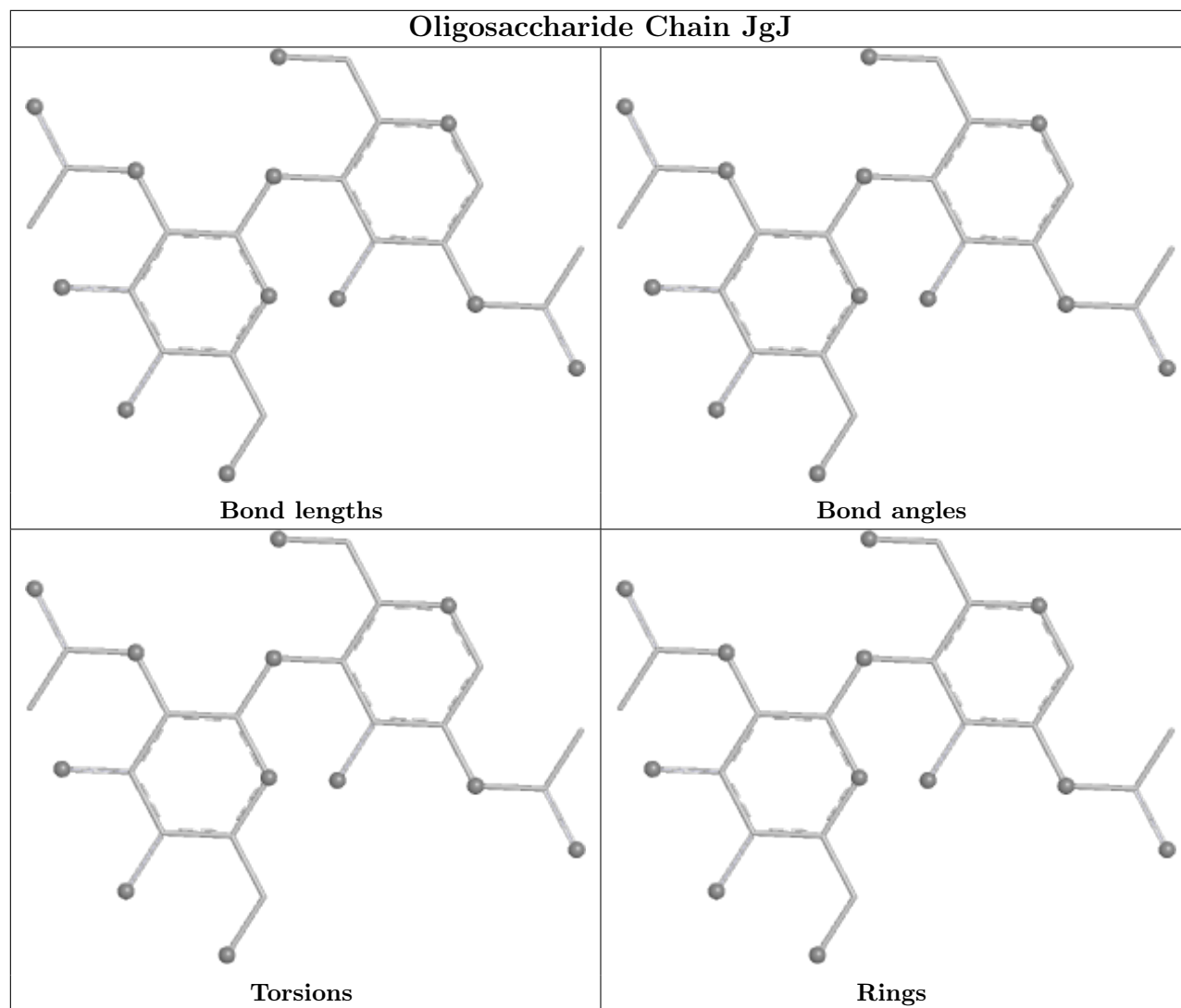
## Oligosaccharide Chain JaJ



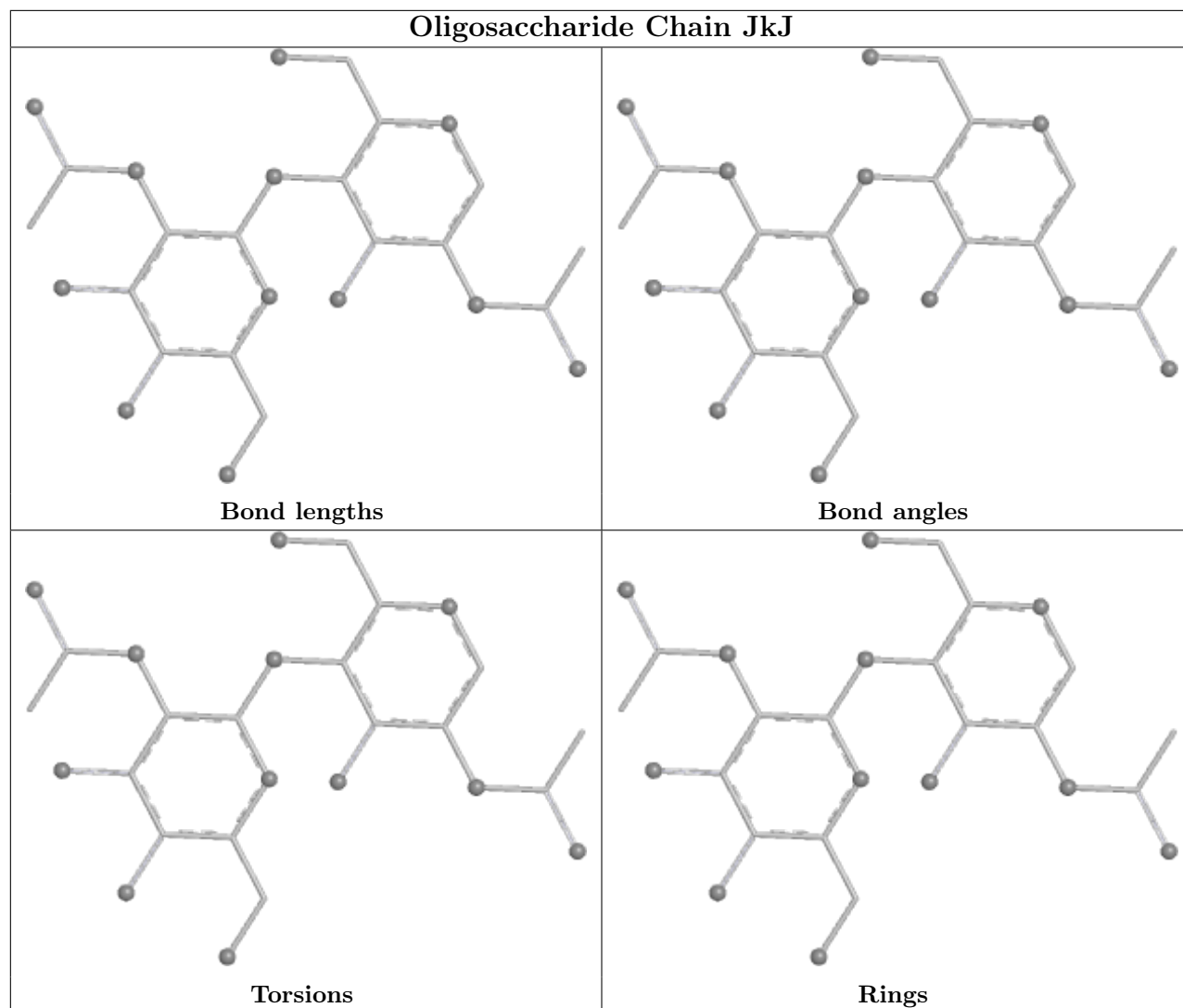


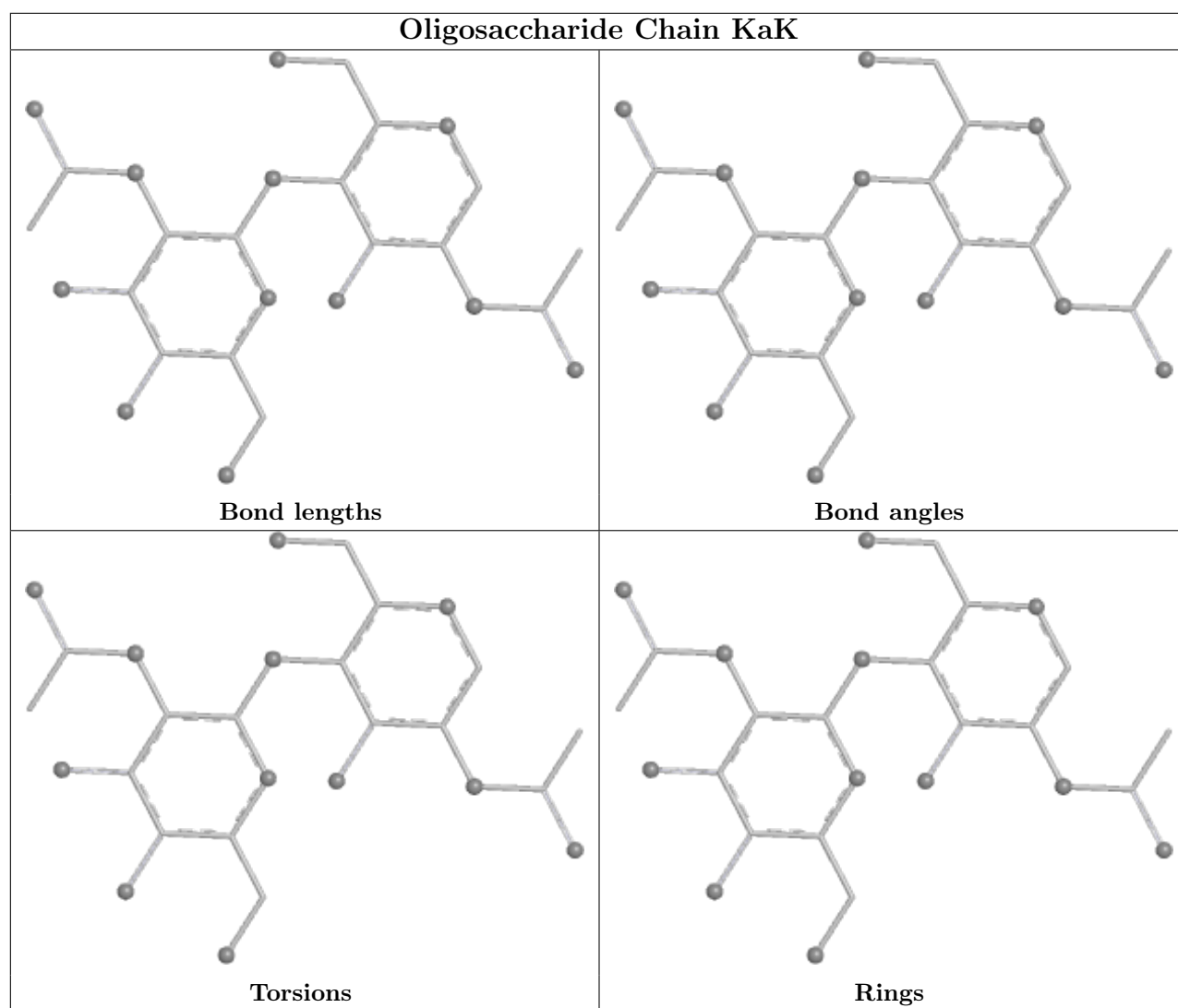
## Oligosaccharide Chain JeJ



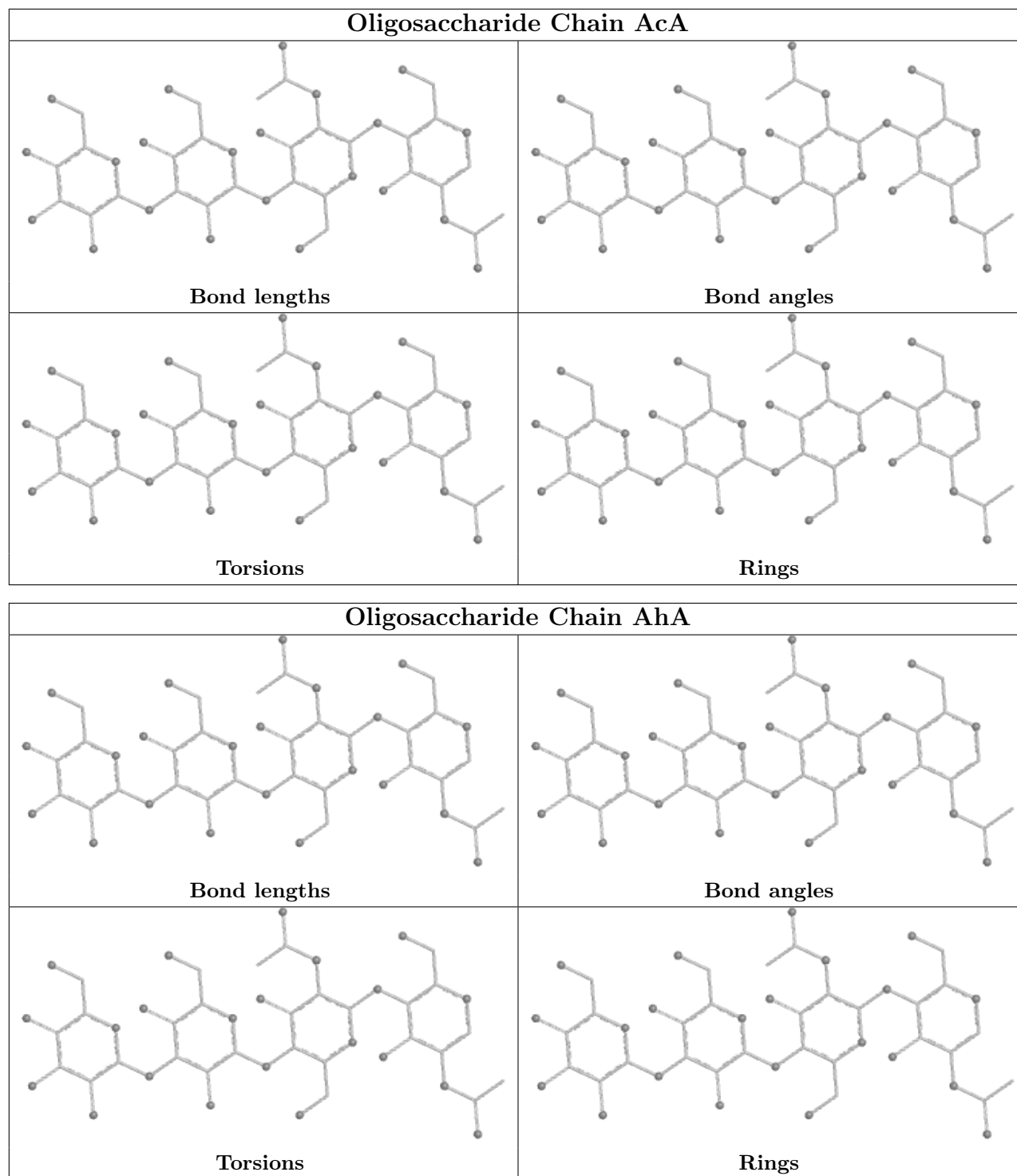


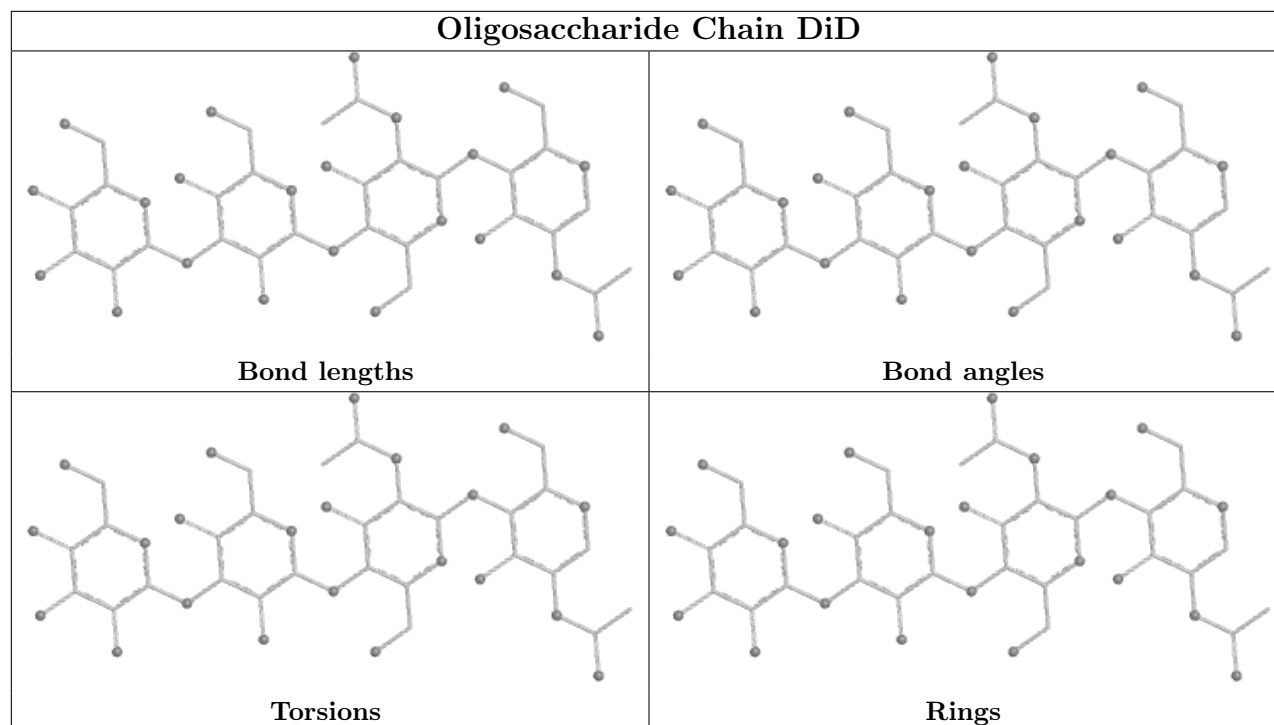
## Oligosaccharide Chain JkJ

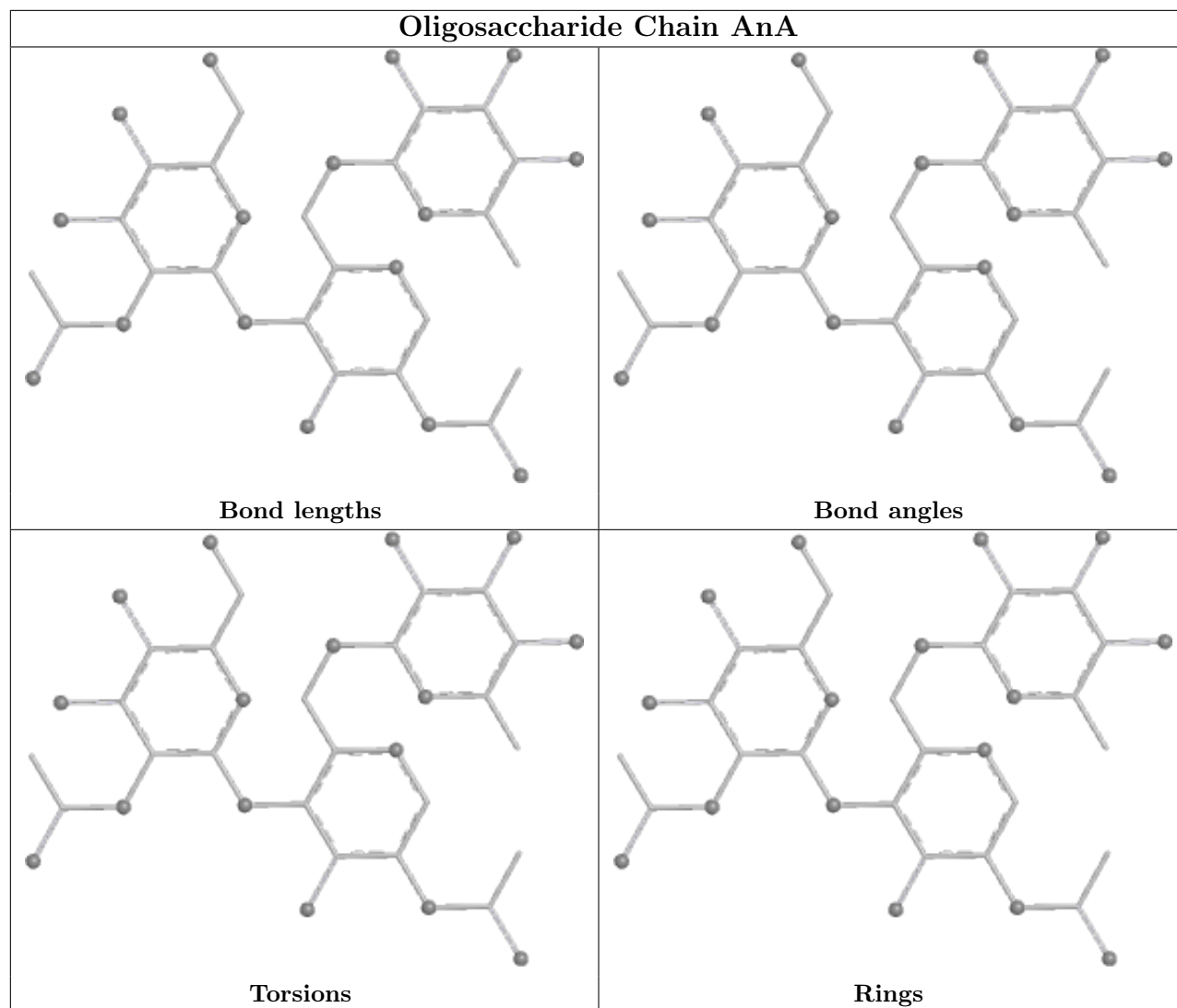


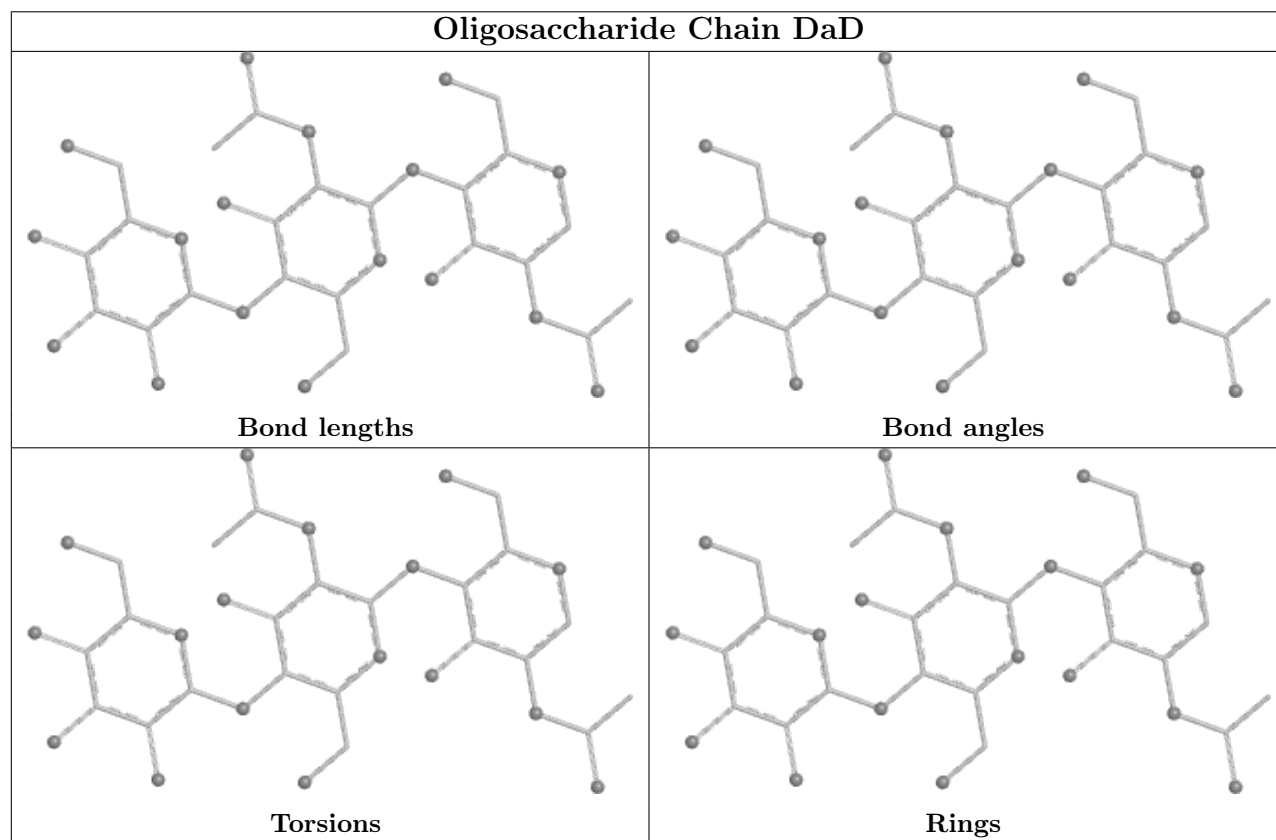
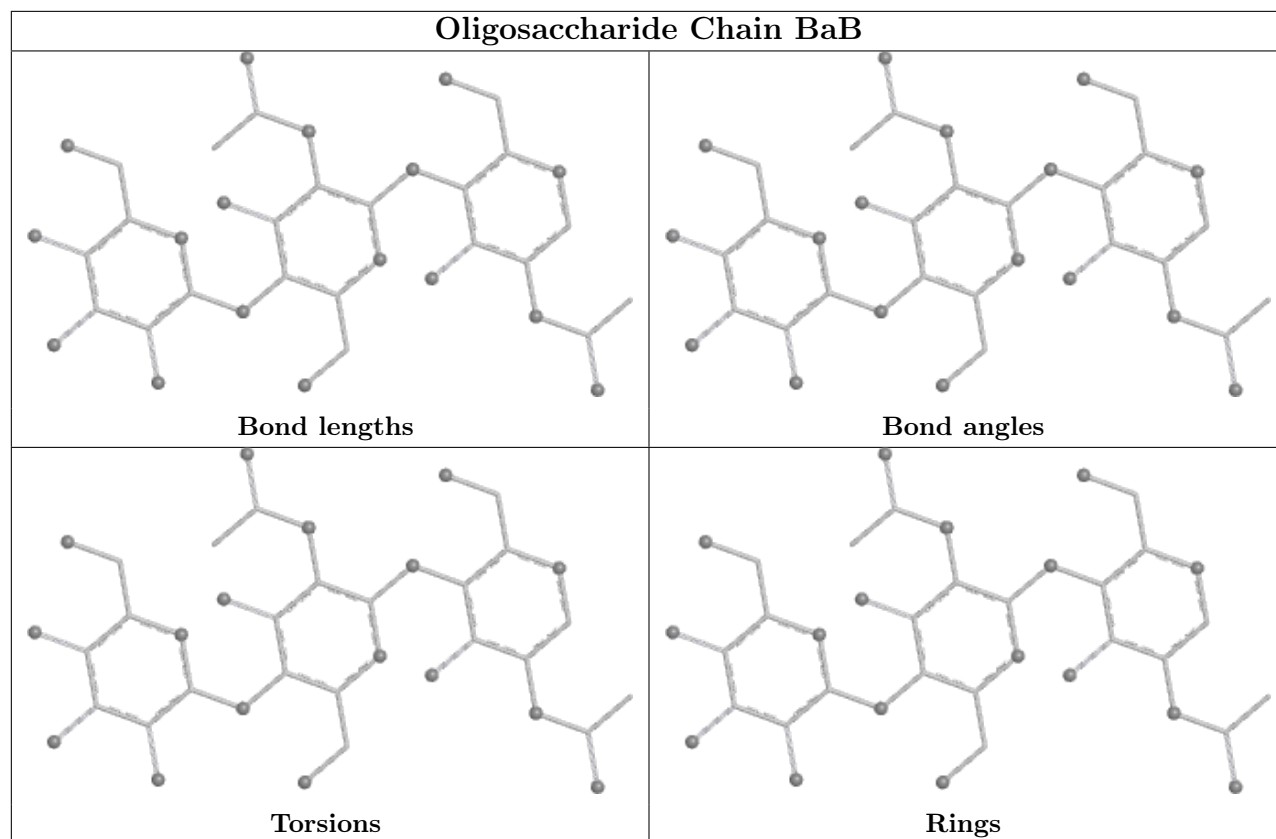




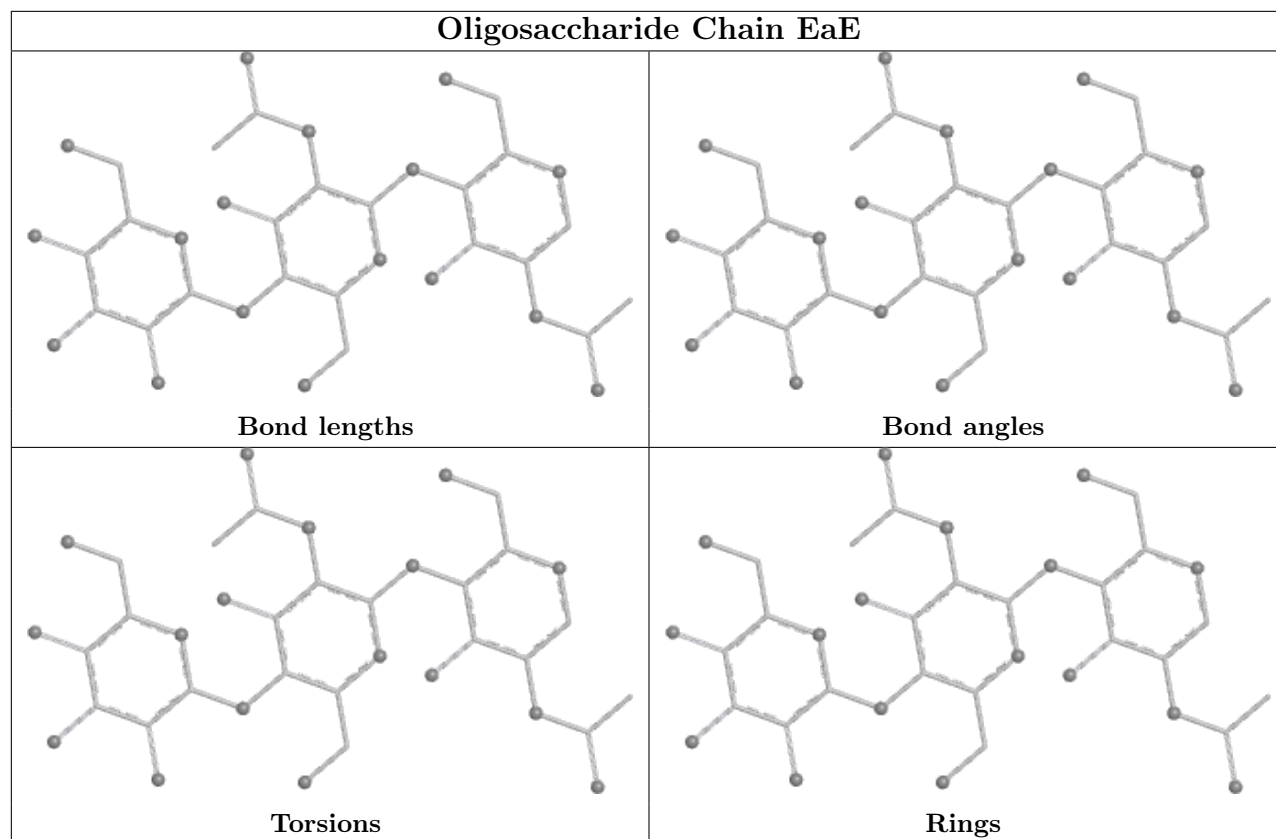




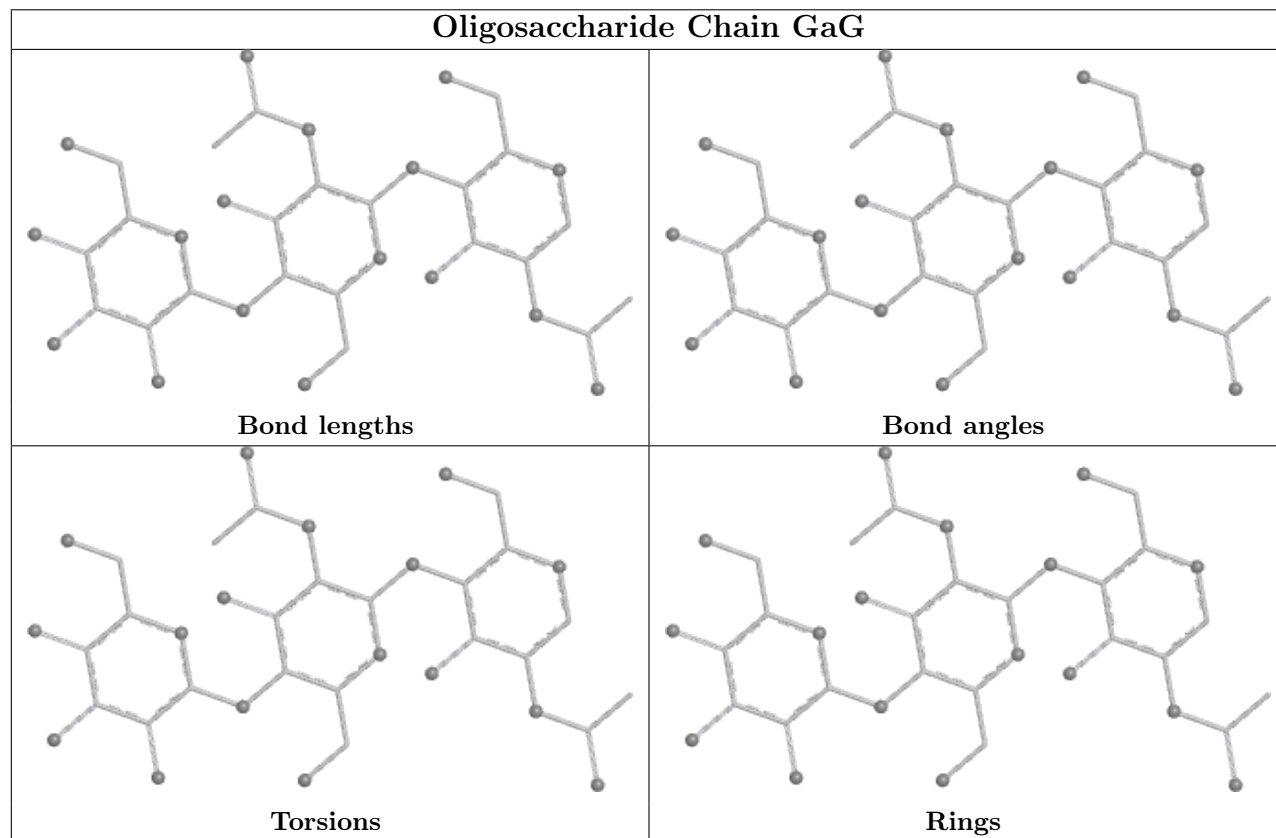


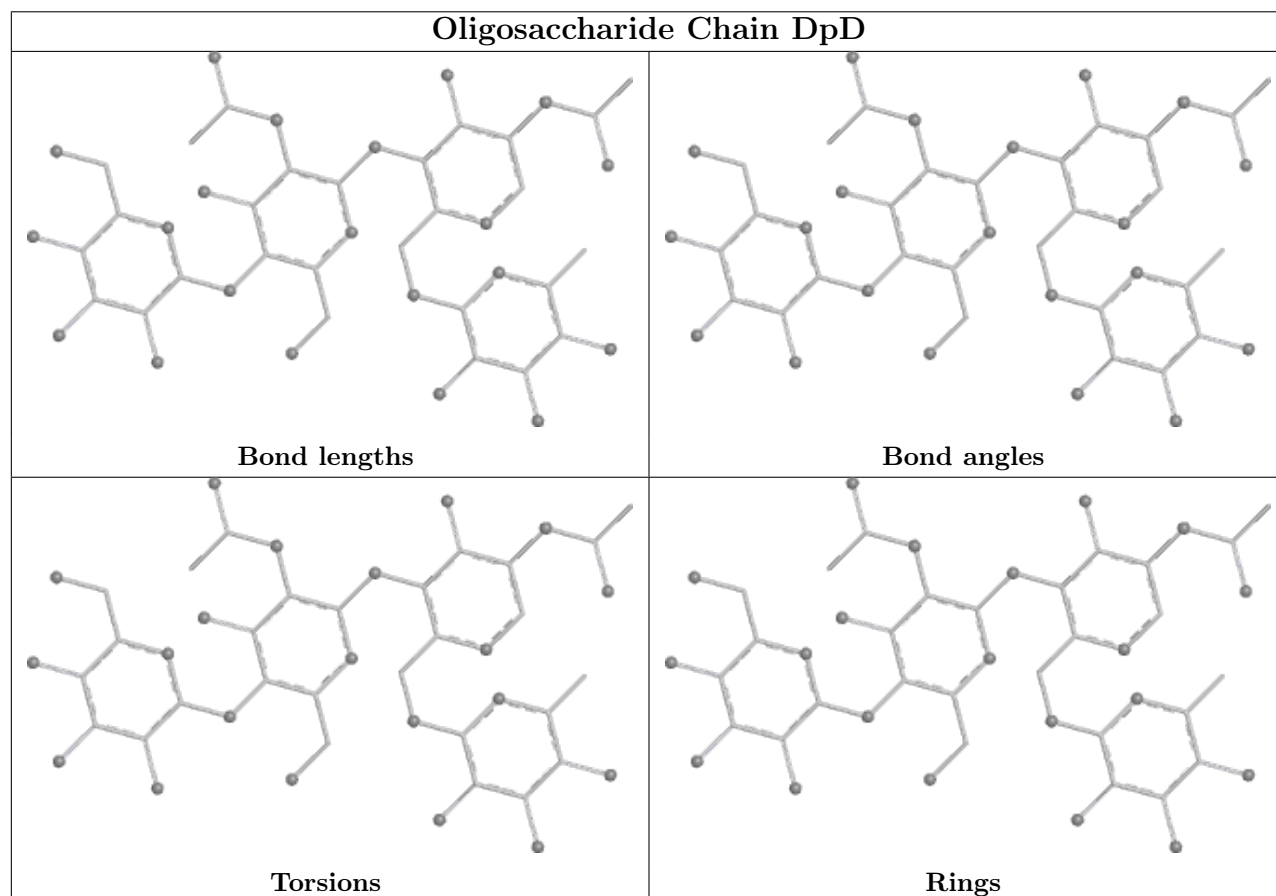
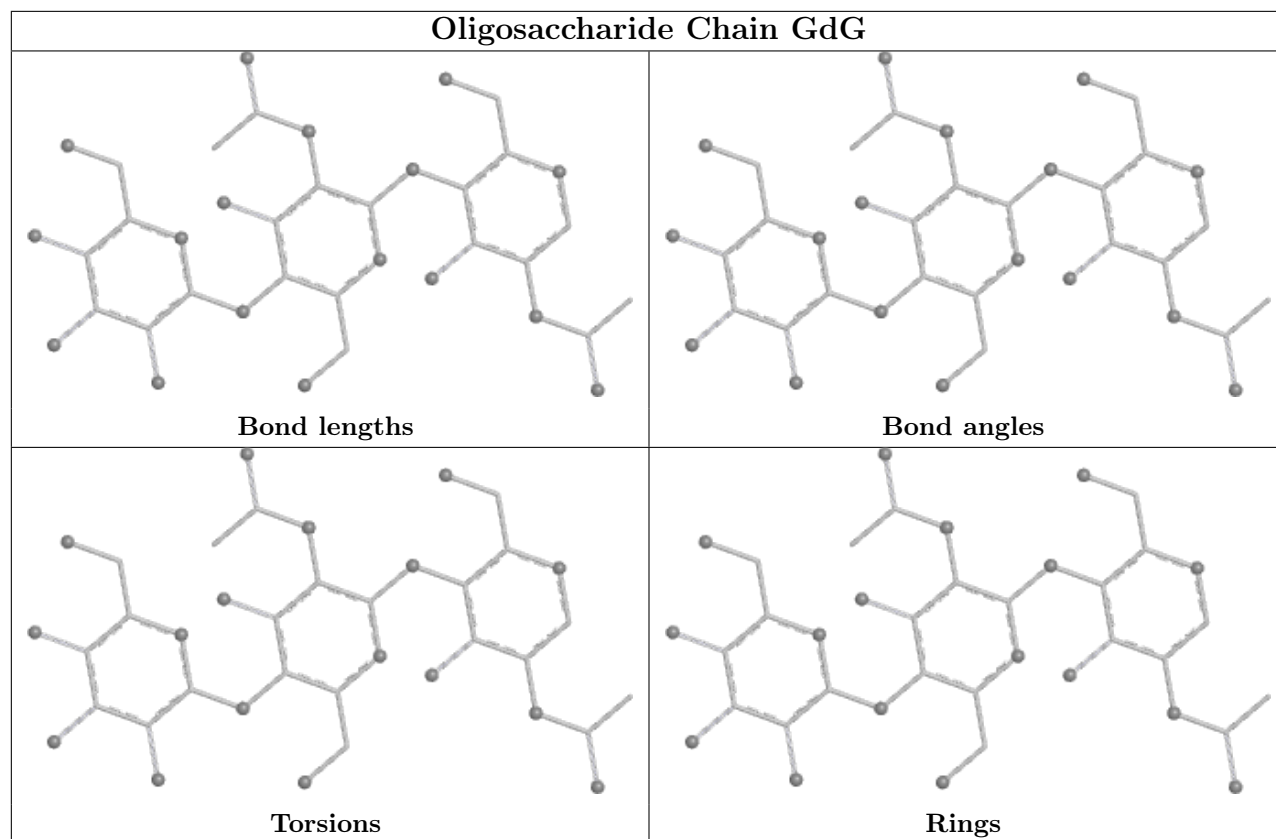


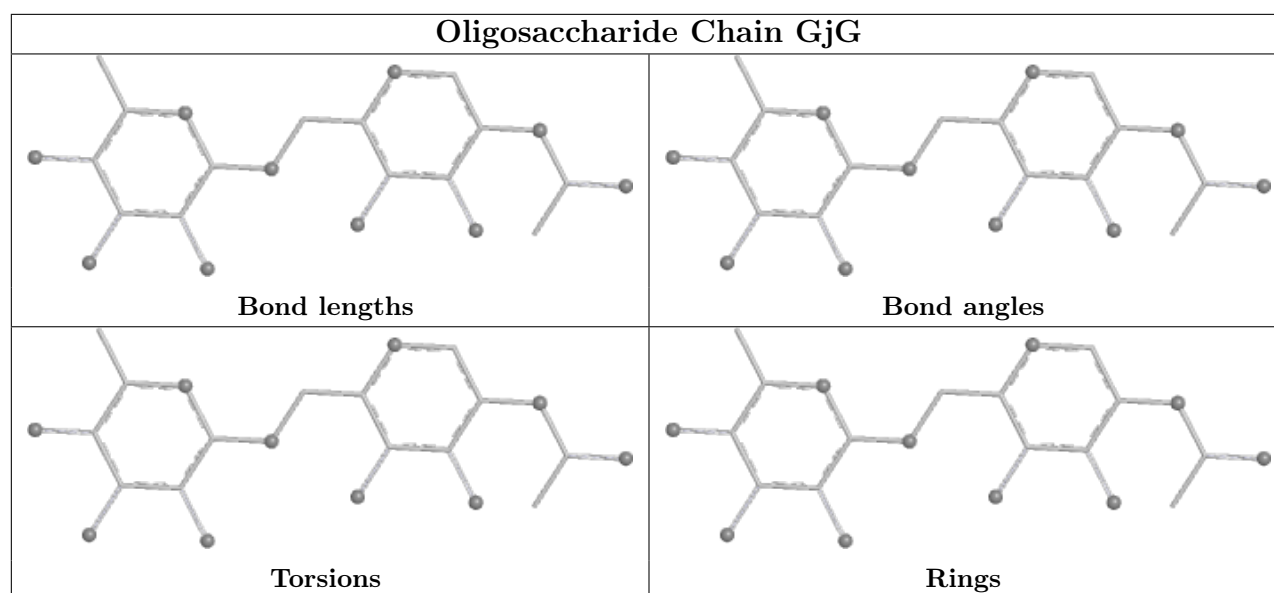
## Oligosaccharide Chain EaE



## Oligosaccharide Chain GaG







## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 for Mogul analysis.

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
11	NAG	DDD	702	1	14,14,15	0.53	0	17,19,21	1.15	1 (5%)
11	NAG	EEE	301	2	14,14,15	0.53	0	17,19,21	1.04	1 (5%)
11	NAG	DDD	701	1	14,14,15	0.46	0	17,19,21	0.99	0
11	NAG	BBB	301	2	14,14,15	0.44	0	17,19,21	1.39	2 (11%)
11	NAG	JJJ	702	1	14,14,15	0.40	0	17,19,21	1.29	2 (11%)
11	NAG	JJJ	701	1	14,14,15	0.49	0	17,19,21	1.05	1 (5%)
11	NAG	HHH	301	2	14,14,15	0.39	0	17,19,21	1.39	2 (11%)
11	NAG	GGG	701	1	14,14,15	0.63	0	17,19,21	1.34	2 (11%)
11	NAG	JJJ	703	1	14,14,15	0.61	0	17,19,21	1.29	3 (17%)
11	NAG	JJJ	704	1	14,14,15	0.46	0	17,19,21	0.98	1 (5%)
11	NAG	BBB	302	2	14,14,15	0.73	0	17,19,21	2.19	6 (35%)
11	NAG	AAA	702	1	14,14,15	0.47	0	17,19,21	1.07	1 (5%)
10	MAN	AAA	701	-	11,11,12	0.54	0	15,15,17	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
11	NAG	DDD	702	1	-	2/6/23/26	0/1/1/1
11	NAG	EEE	301	2	-	0/6/23/26	0/1/1/1
11	NAG	DDD	701	1	-	2/6/23/26	0/1/1/1
11	NAG	BBB	301	2	-	1/6/23/26	0/1/1/1
11	NAG	JJJ	702	1	-	2/6/23/26	0/1/1/1
11	NAG	JJJ	701	1	-	1/6/23/26	0/1/1/1
11	NAG	HHH	301	2	-	2/6/23/26	0/1/1/1
11	NAG	GGG	701	1	-	2/6/23/26	0/1/1/1
11	NAG	JJJ	703	1	-	2/6/23/26	0/1/1/1
11	NAG	JJJ	704	1	-	1/6/23/26	0/1/1/1
11	NAG	BBB	302	2	-	4/6/23/26	0/1/1/1
11	NAG	AAA	702	1	-	2/6/23/26	0/1/1/1
10	MAN	AAA	701	-	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	BBB	302	NAG	O5-C1-C2	-4.91	103.53	111.29
11	BBB	302	NAG	C1-O5-C5	4.47	118.25	112.19
11	BBB	301	NAG	C1-C2-N2	-3.67	104.22	110.49
11	HHH	301	NAG	C1-C2-N2	-3.64	104.27	110.49
11	JJJ	702	NAG	C1-O5-C5	3.46	116.88	112.19
11	HHH	301	NAG	C1-O5-C5	3.42	116.82	112.19
11	BBB	302	NAG	C1-C2-N2	3.26	116.06	110.49
11	BBB	301	NAG	C1-O5-C5	2.98	116.23	112.19
11	JJJ	703	NAG	C1-O5-C5	2.97	116.21	112.19
11	JJJ	703	NAG	O5-C1-C2	-2.90	106.71	111.29
11	GGG	701	NAG	C1-O5-C5	2.85	116.06	112.19
11	GGG	701	NAG	O5-C1-C2	-2.84	106.81	111.29
11	DDD	702	NAG	C1-O5-C5	2.79	115.98	112.19
11	EEE	301	NAG	O5-C5-C6	2.56	111.22	107.20
11	BBB	302	NAG	C4-C3-C2	-2.49	107.37	111.02
11	JJJ	702	NAG	O5-C1-C2	-2.45	107.41	111.29
11	BBB	302	NAG	C6-C5-C4	-2.45	107.27	113.00
11	BBB	302	NAG	C8-C7-N2	2.43	120.21	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	JJJ	703	NAG	O5-C5-C6	2.37	110.92	107.20
11	JJJ	701	NAG	O5-C5-C6	2.30	110.81	107.20
11	JJJ	704	NAG	C1-C2-N2	2.27	114.37	110.49
11	AAA	702	NAG	C1-O5-C5	2.09	115.02	112.19

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	DDD	701	NAG	O5-C5-C6-O6
11	DDD	702	NAG	O5-C5-C6-O6
11	AAA	702	NAG	O5-C5-C6-O6
11	BBB	302	NAG	C4-C5-C6-O6
11	BBB	302	NAG	O5-C5-C6-O6
11	JJJ	703	NAG	O5-C5-C6-O6
11	AAA	702	NAG	C4-C5-C6-O6
11	JJJ	703	NAG	C4-C5-C6-O6
11	BBB	302	NAG	C8-C7-N2-C2
11	BBB	302	NAG	O7-C7-N2-C2
11	JJJ	702	NAG	O5-C5-C6-O6
11	HHH	301	NAG	O5-C5-C6-O6
11	DDD	702	NAG	C4-C5-C6-O6
11	GGG	701	NAG	O5-C5-C6-O6
11	DDD	701	NAG	C4-C5-C6-O6
11	GGG	701	NAG	C4-C5-C6-O6
11	HHH	301	NAG	C4-C5-C6-O6
11	JJJ	702	NAG	C4-C5-C6-O6
11	JJJ	704	NAG	O5-C5-C6-O6
10	AAA	701	MAN	C4-C5-C6-O6
11	JJJ	701	NAG	O5-C5-C6-O6
10	AAA	701	MAN	O5-C5-C6-O6
11	BBB	301	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	BBB	301	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AAA	594/617 (96%)	0.27	7 (1%) 79 78	35, 52, 79, 136	0
1	DDD	594/617 (96%)	0.21	4 (0%) 87 87	33, 51, 73, 125	0
1	GGG	594/617 (96%)	0.32	12 (2%) 65 63	40, 58, 83, 132	0
1	JJJ	593/617 (96%)	0.40	12 (2%) 65 63	42, 60, 87, 112	0
2	BBB	185/203 (91%)	0.37	3 (1%) 72 71	40, 52, 73, 98	0
2	EEE	185/203 (91%)	0.39	4 (2%) 62 60	39, 55, 75, 94	0
2	HHH	185/203 (91%)	0.47	4 (2%) 62 60	44, 57, 80, 93	0
2	KKK	185/203 (91%)	0.41	1 (0%) 91 90	44, 57, 77, 91	0
3	CCC	10/12 (83%)	1.18	3 (30%) 0 0	44, 57, 95, 97	0
3	FFF	10/12 (83%)	0.70	1 (10%) 7 5	46, 55, 99, 101	0
3	III	9/12 (75%)	0.51	1 (11%) 5 4	51, 55, 74, 82	0
3	LLL	9/12 (75%)	0.83	1 (11%) 5 4	50, 59, 74, 88	0
All	All	3153/3328 (94%)	0.33	53 (1%) 70 70	33, 56, 82, 136	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	GGG	601	ASP	4.4
3	CCC	110	LEU	4.3
1	DDD	601	ASP	4.1
1	AAA	601	ASP	4.0
1	JJJ	58	ASP	4.0
1	JJJ	21	PHE	3.7
1	GGG	119	LEU	3.7
1	AAA	67	LEU	3.7
1	JJJ	67	LEU	3.3
2	EEE	206	THR	3.2
1	GGG	580	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
3	FFF	110	LEU	3.2
1	GGG	91	LEU	2.9
3	III	110	LEU	2.9
1	AAA	57	GLY	2.9
3	LLL	110	LEU	2.9
2	HHH	84	HIS	2.8
1	JJJ	36	TYR	2.8
2	HHH	206	THR	2.7
1	GGG	489	MET	2.7
2	EEE	159	MET	2.7
1	GGG	67	LEU	2.7
1	GGG	37	LEU	2.6
2	EEE	183	ASP	2.6
1	AAA	583	LEU	2.6
1	GGG	605	LEU	2.5
1	GGG	384	PHE	2.5
1	JJJ	364	LEU	2.4
1	AAA	140	THR	2.3
1	JJJ	72	LEU	2.3
1	AAA	606	CYS	2.3
1	DDD	26	VAL	2.3
1	JJJ	76	PHE	2.3
3	CCC	109	ARG	2.2
1	JJJ	30	LEU	2.2
1	GGG	606	CYS	2.2
1	JJJ	497	LEU	2.2
1	DDD	58	ASP	2.2
2	KKK	146	LEU	2.2
1	DDD	583	LEU	2.2
1	GGG	456	PHE	2.2
2	BBB	129	PHE	2.2
1	JJJ	534	ASP	2.2
2	BBB	84	HIS	2.2
1	JJJ	416	PHE	2.1
2	EEE	84	HIS	2.1
1	JJJ	601	ASP	2.1
1	GGG	92	TYR	2.1
2	BBB	48	GLN	2.1
1	AAA	21	PHE	2.1
3	CCC	111	VAL	2.1
2	HHH	129	PHE	2.1
2	HHH	76	LEU	2.0

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	HYP	FFF	112	8/9	0.89	0.20	65,69,72,73	0
3	HYP	FFF	115	8/9	0.91	0.16	53,54,55,56	0
3	HYP	III	115	8/9	0.91	0.12	63,65,67,69	0
3	HYP	LLL	112	8/9	0.92	0.23	67,69,71,73	0
3	HYP	III	112	8/9	0.93	0.17	72,73,76,79	0
3	HYP	LLL	115	8/9	0.93	0.17	56,63,64,65	0
3	HYP	CCC	112	8/9	0.94	0.19	63,67,69,70	0
3	HYP	CCC	115	8/9	0.94	0.15	55,58,59,59	0

## 6.3 Carbohydrates ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	MAN	AcA	4	11/12	0.58	0.47	123,142,149,152	0
7	BMA	GaG	3	11/12	0.61	0.23	107,110,117,117	0
7	BMA	GdG	3	11/12	0.62	0.27	102,112,117,121	0
5	MAN	DiD	4	11/12	0.66	0.32	119,132,139,139	0
9	FUC	GjG	2	10/11	0.66	0.51	105,112,116,120	0
7	BMA	EaE	3	11/12	0.69	0.30	104,119,124,128	0
5	MAN	AhA	4	11/12	0.69	0.37	102,110,117,117	0
5	BMA	DiD	3	11/12	0.70	0.33	106,117,123,131	0
4	NAG	JeJ	2	14/15	0.71	0.32	89,104,109,112	0
4	NAG	GgG	2	14/15	0.72	0.22	90,97,105,109	0
7	BMA	BaB	3	11/12	0.72	0.33	101,104,108,108	0
4	NAG	HaH	2	14/15	0.73	0.35	112,116,117,118	0
5	BMA	AhA	3	11/12	0.73	0.25	93,101,105,112	0
4	NAG	EdE	2	14/15	0.75	0.32	92,108,115,115	0
8	BMA	DpD	3	11/12	0.75	0.17	108,118,124,131	0
4	NAG	AlA	2	14/15	0.75	0.21	101,107,109,110	0
4	NAG	JkJ	2	14/15	0.76	0.36	116,126,132,135	0
8	FUC	DpD	4	10/11	0.77	0.26	92,95,98,98	0
4	NAG	AqA	2	14/15	0.77	0.18	90,99,103,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	GnG	2	14/15	0.78	0.36	99,112,119,132	0
4	NAG	GlG	2	14/15	0.79	0.28	103,106,108,109	0
4	NAG	JeJ	1	14/15	0.80	0.15	71,80,90,92	0
4	NAG	AaA	2	14/15	0.80	0.30	82,93,99,101	0
8	NAG	DpD	2	14/15	0.80	0.18	85,91,102,113	0
4	NAG	DgD	2	14/15	0.81	0.19	96,103,113,120	0
4	NAG	JgJ	2	14/15	0.81	0.28	83,96,104,104	0
7	BMA	DaD	3	11/12	0.82	0.22	95,102,105,106	0
4	NAG	HaH	1	14/15	0.82	0.26	80,90,96,97	0
4	NAG	AqA	1	14/15	0.83	0.13	59,67,75,86	0
6	FUC	AnA	3	10/11	0.83	0.35	84,86,91,93	0
7	NAG	BaB	2	14/15	0.83	0.33	88,97,102,103	0
5	BMA	AcA	3	11/12	0.83	0.28	105,113,117,124	0
7	NAG	BaB	1	14/15	0.84	0.31	82,85,89,92	0
7	NAG	EaE	2	14/15	0.84	0.23	90,100,105,107	0
4	NAG	KaK	1	14/15	0.84	0.26	86,91,94,94	0
4	NAG	JaJ	2	14/15	0.84	0.18	73,77,82,85	0
9	NAG	GjG	1	14/15	0.84	0.19	75,79,88,95	0
7	NAG	GdG	2	14/15	0.84	0.20	80,95,101,110	0
4	NAG	DeD	2	14/15	0.86	0.20	79,91,98,102	0
7	NAG	EaE	1	14/15	0.86	0.20	73,77,85,85	0
6	NAG	AnA	2	14/15	0.86	0.18	75,88,94,99	0
4	NAG	KaK	2	14/15	0.87	0.26	83,91,95,95	0
4	NAG	GgG	1	14/15	0.87	0.17	68,80,83,86	0
4	NAG	AsA	2	14/15	0.88	0.18	77,95,99,102	0
5	NAG	DiD	1	14/15	0.88	0.20	63,68,75,79	0
4	NAG	GlG	1	14/15	0.88	0.19	66,70,75,83	0
7	NAG	GaG	2	14/15	0.88	0.19	62,81,85,92	0
5	NAG	AhA	2	14/15	0.88	0.21	59,66,71,83	0
4	NAG	JkJ	1	14/15	0.88	0.18	80,89,96,103	0
5	NAG	AcA	2	14/15	0.89	0.18	72,85,92,94	0
7	NAG	DaD	2	14/15	0.89	0.16	52,65,72,80	0
5	NAG	DiD	2	14/15	0.89	0.14	76,78,84,95	0
4	NAG	AlA	1	14/15	0.89	0.16	58,69,73,81	0
4	NAG	DmD	2	14/15	0.89	0.23	77,84,87,92	0
4	NAG	JgJ	1	14/15	0.90	0.21	74,81,84,86	0
4	NAG	DeD	1	14/15	0.90	0.15	53,61,65,72	0
4	NAG	GnG	1	14/15	0.90	0.22	72,80,82,89	0
4	NAG	AsA	1	14/15	0.90	0.15	58,64,70,77	0
4	NAG	DgD	1	14/15	0.90	0.15	65,72,82,84	0
4	NAG	JcJ	1	14/15	0.91	0.13	52,69,76,78	0
4	NAG	AaA	1	14/15	0.91	0.16	53,64,68,76	0

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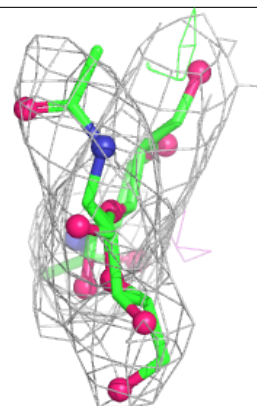
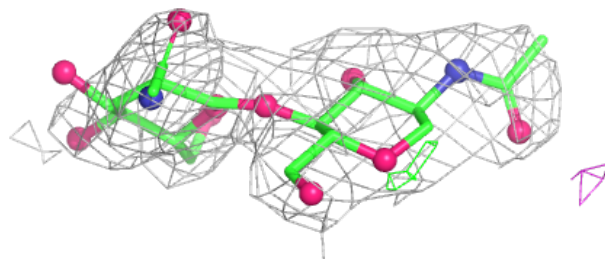
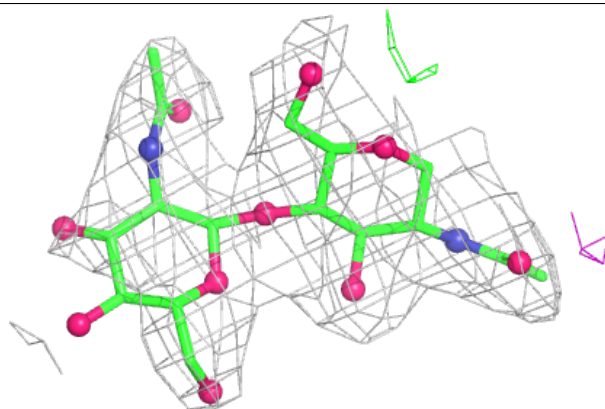
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	NAG	DpD	1	14/15	0.92	0.15	60,63,74,77	0
4	NAG	DmD	1	14/15	0.92	0.19	68,73,82,83	0
6	NAG	AnA	1	14/15	0.92	0.13	58,65,75,84	0
7	NAG	GdG	1	14/15	0.92	0.15	58,69,79,81	0
4	NAG	JcJ	2	14/15	0.92	0.21	75,83,88,90	0
5	NAG	AcA	1	14/15	0.92	0.22	54,59,62,71	0
4	NAG	EdE	1	14/15	0.93	0.23	67,71,76,90	0
7	NAG	DaD	1	14/15	0.93	0.19	35,42,44,52	0
7	NAG	GaG	1	14/15	0.94	0.18	45,47,52,61	0
4	NAG	JaJ	1	14/15	0.94	0.19	49,54,57,60	0
5	NAG	AhA	1	14/15	0.95	0.17	48,50,57,59	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

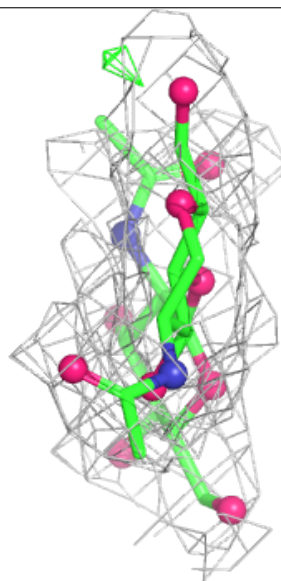
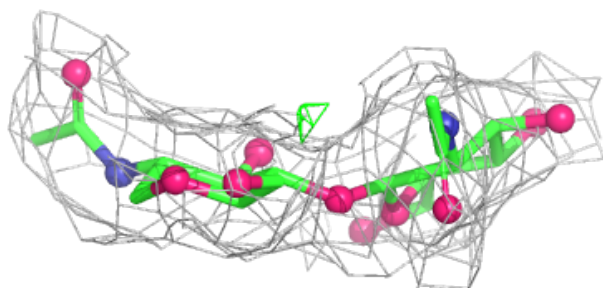
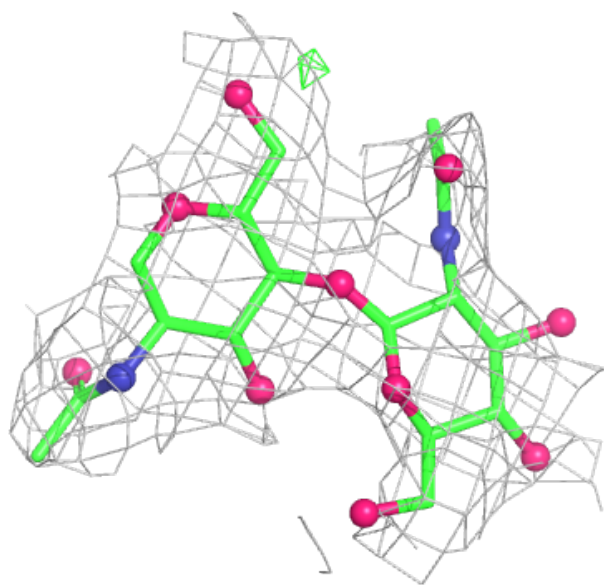
#### Electron density around Chain AaA:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain A1A:**

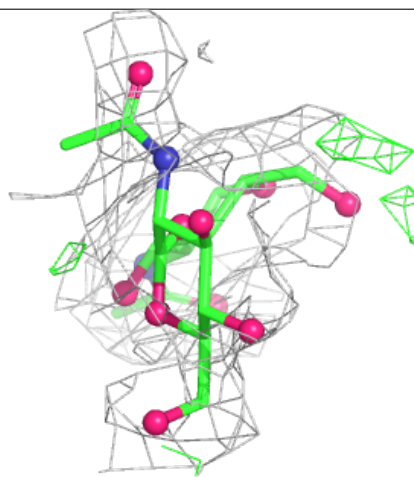
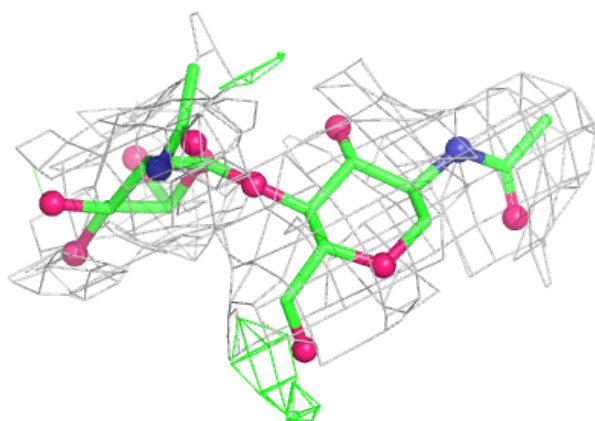
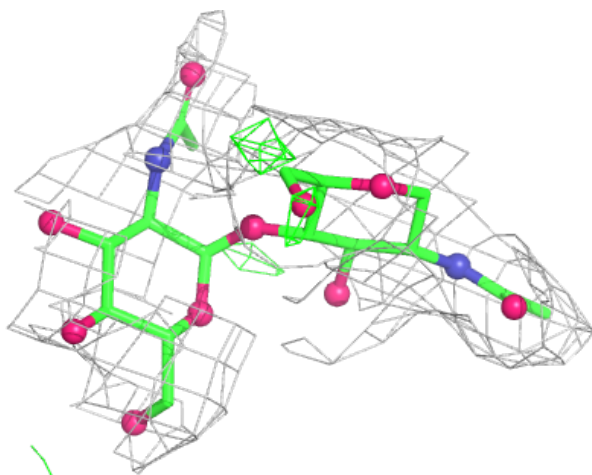
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





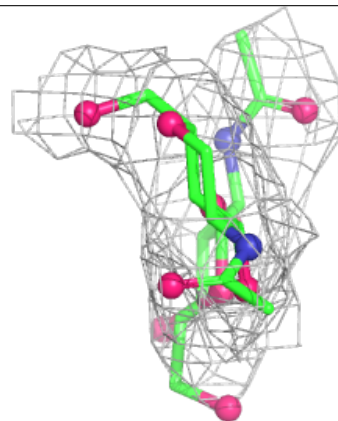
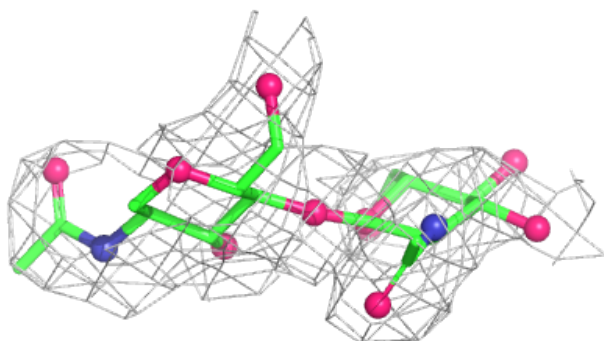
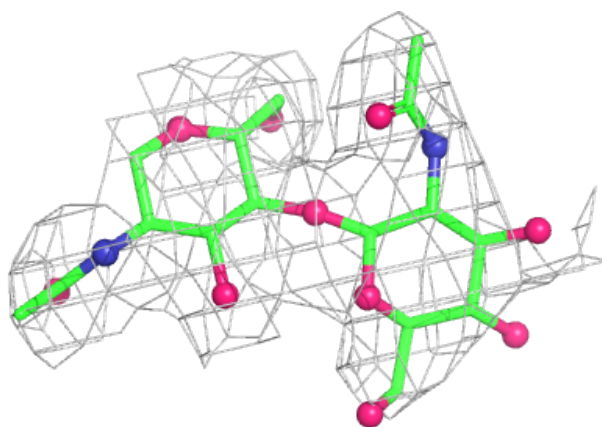
**Electron density around Chain AqA:**

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and green (positive)



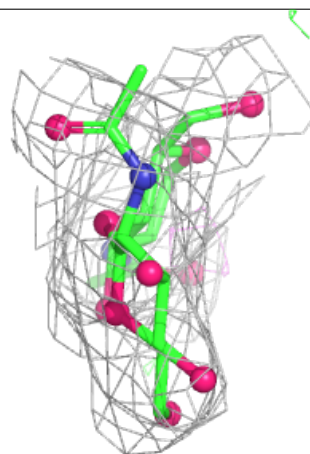
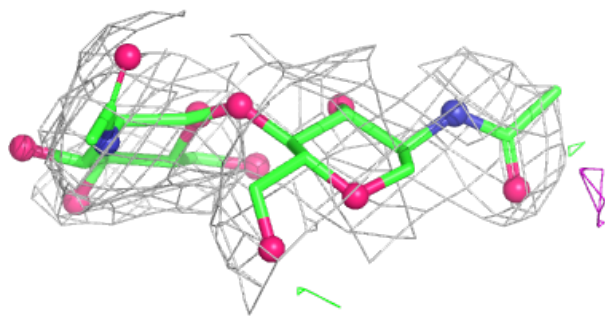
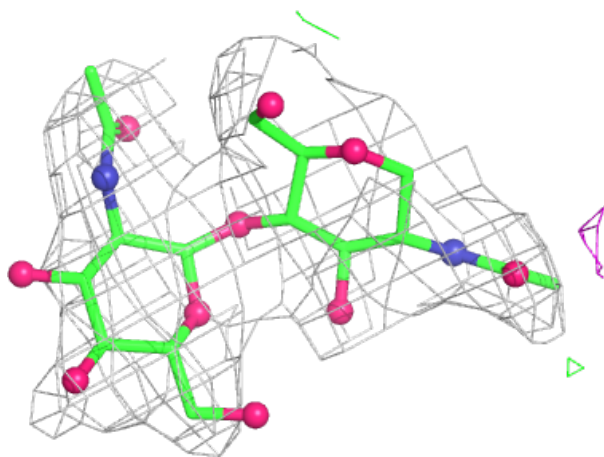
**Electron density around Chain AsA:**

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and green (positive)



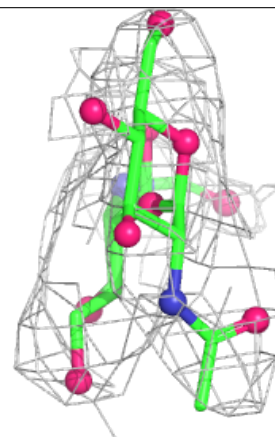
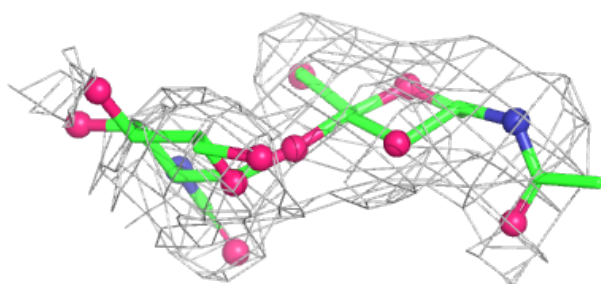
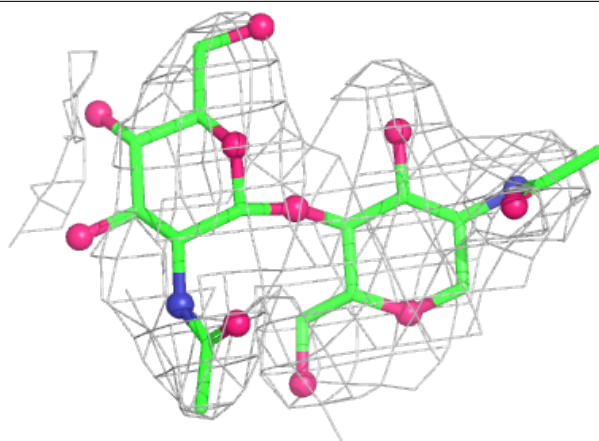
**Electron density around Chain DeD:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



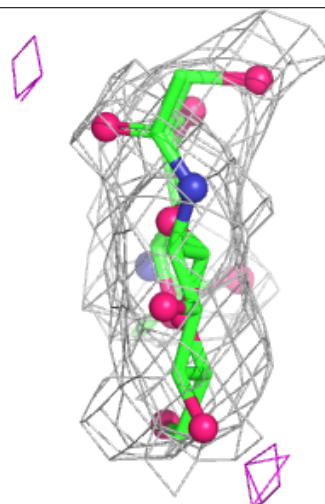
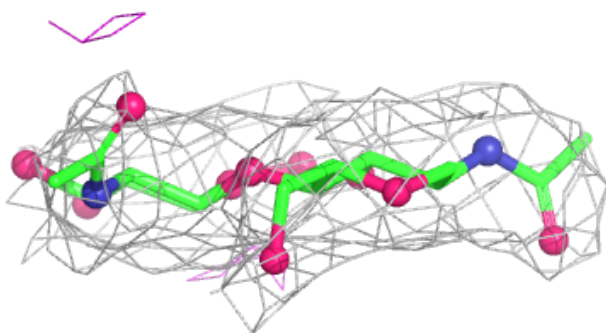
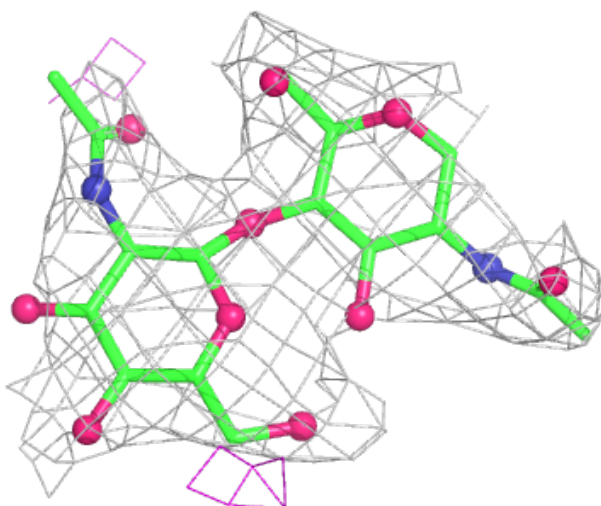
**Electron density around Chain DgD:**

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 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



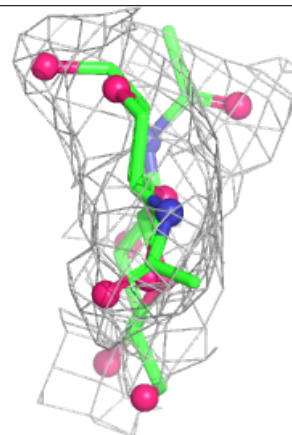
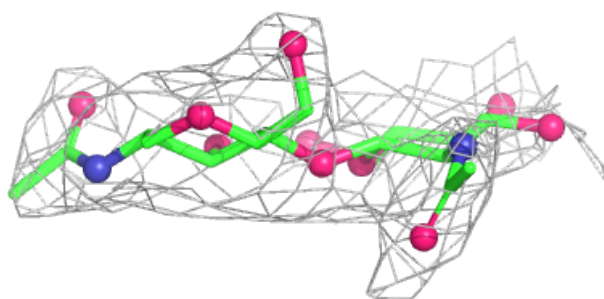
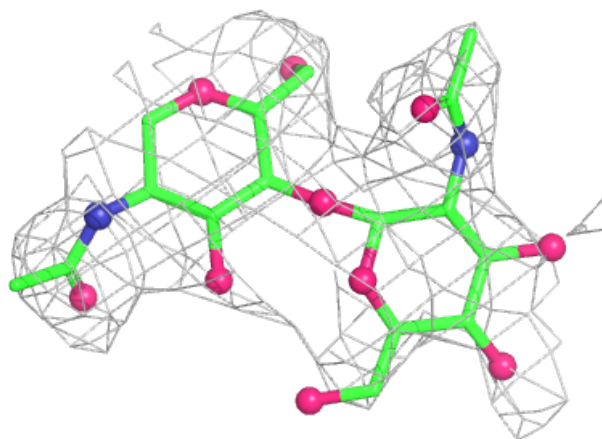
**Electron density around Chain DmD:**

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and green (positive)



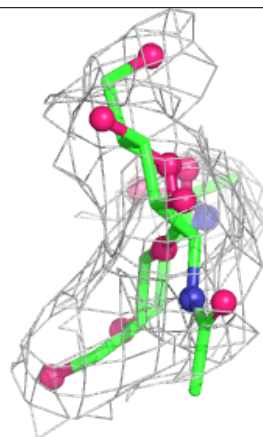
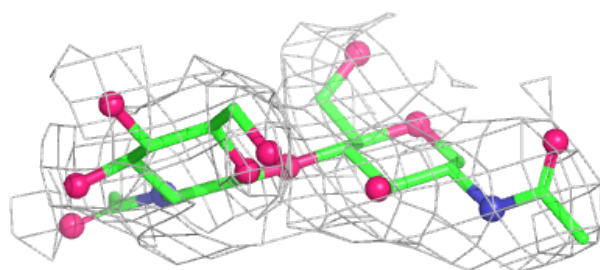
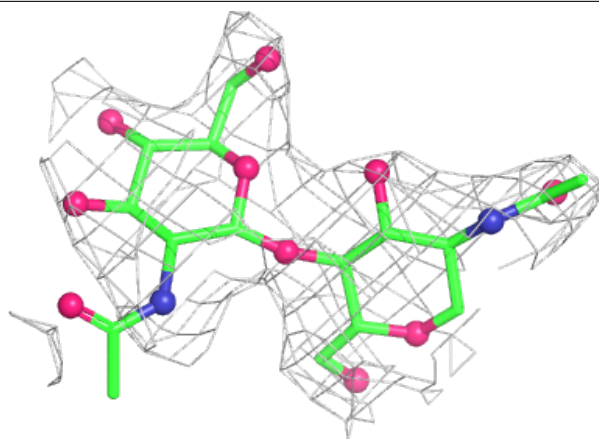
**Electron density around Chain EdE:**

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and green (positive)



**Electron density around Chain GgG:**

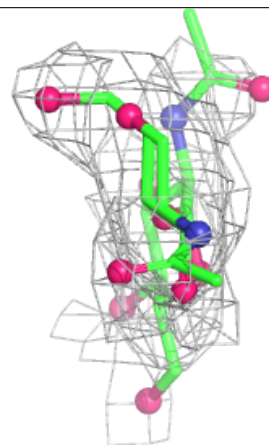
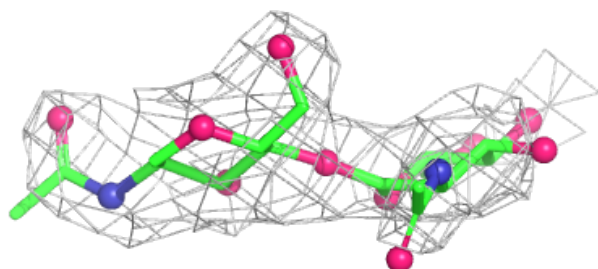
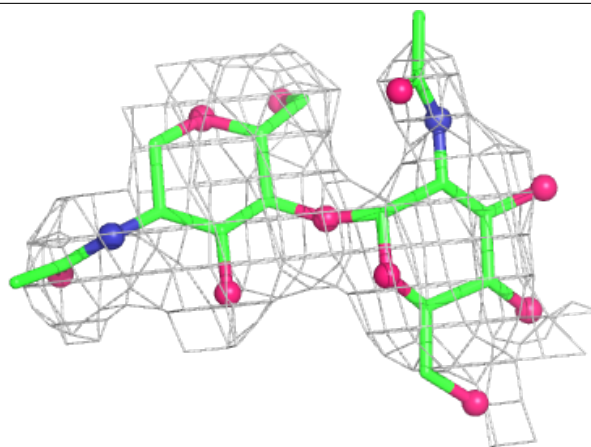
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
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and green (positive)



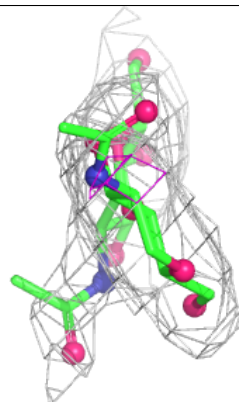
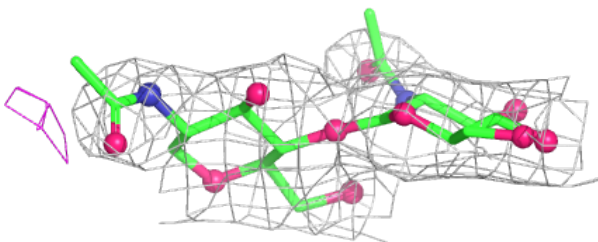
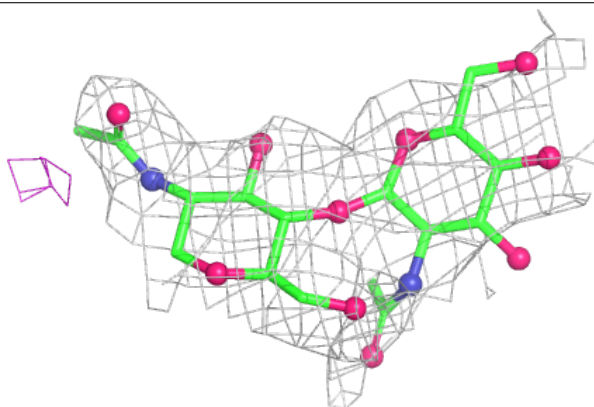


**Electron density around Chain GIG:**

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and green (positive)

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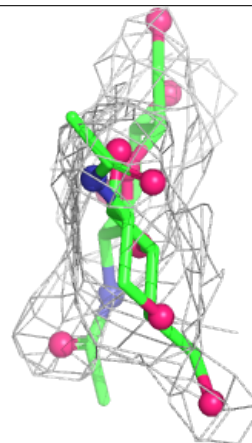
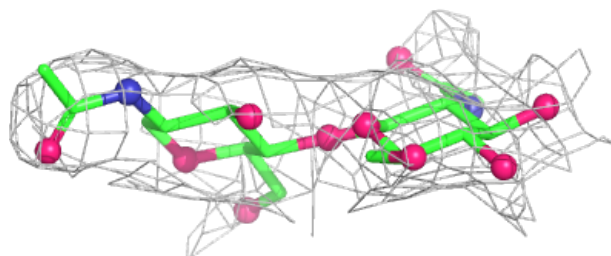
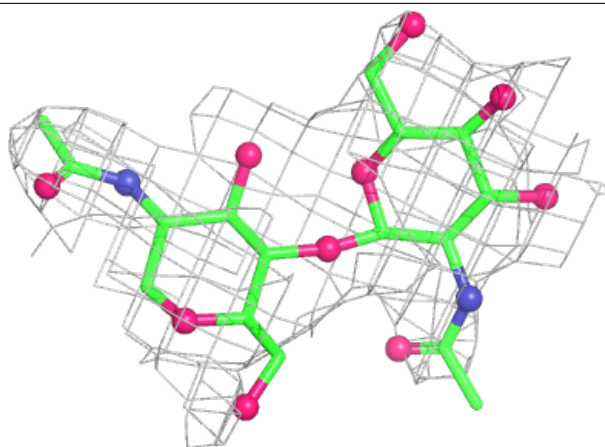
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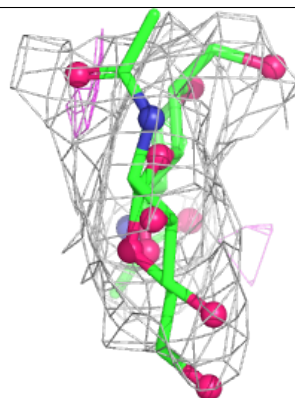
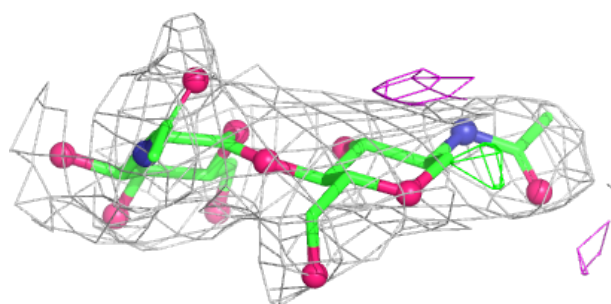
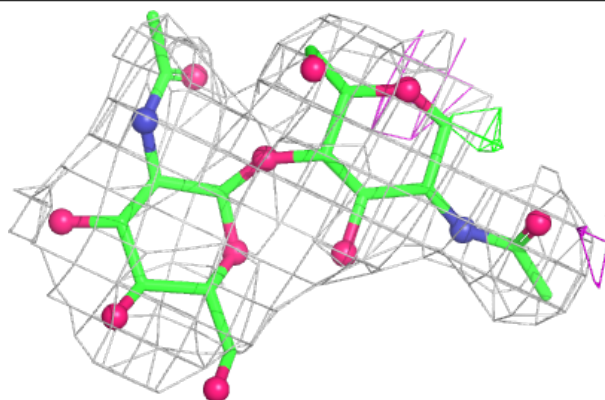


**Electron density around Chain HaH:**

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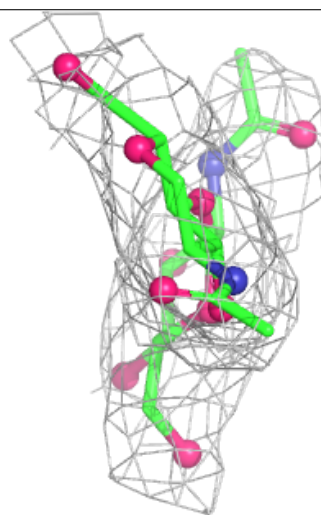
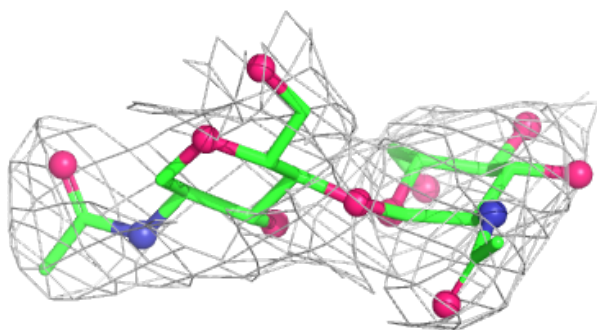
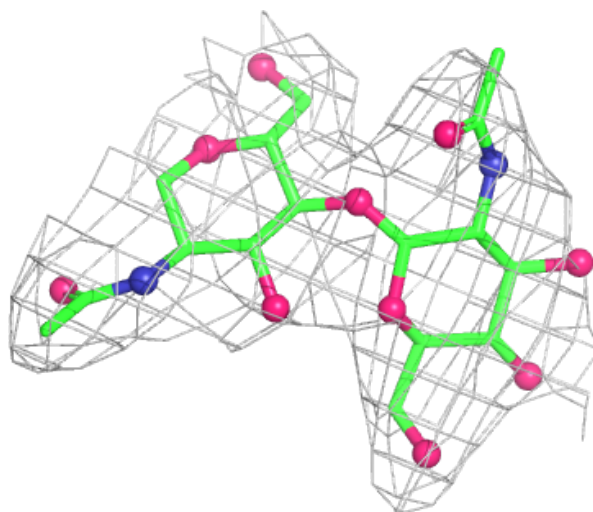
**Electron density around Chain JaJ:**

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and green (positive)



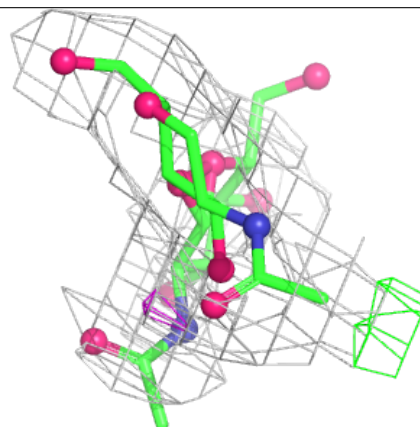
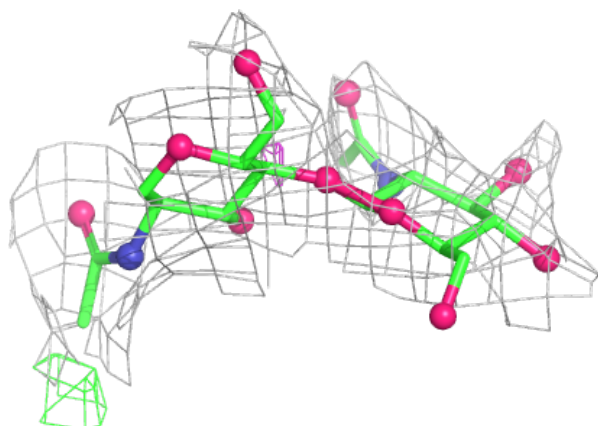
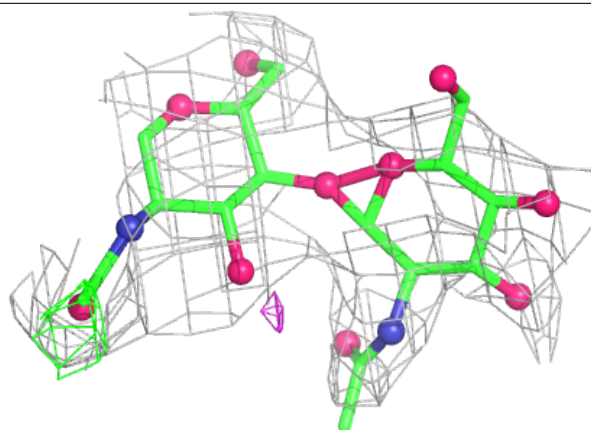
**Electron density around Chain JcJ:**

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and green (positive)



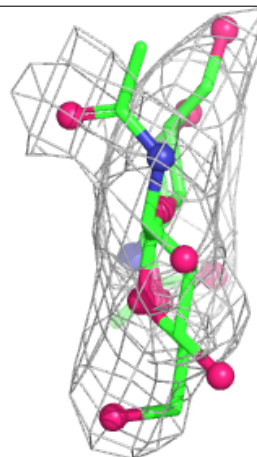
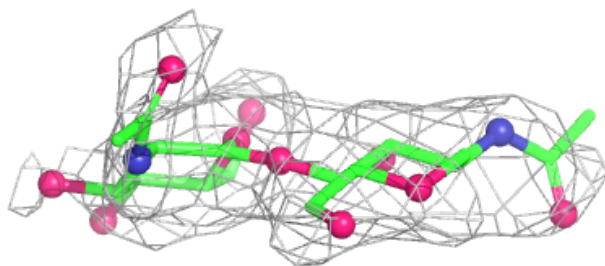
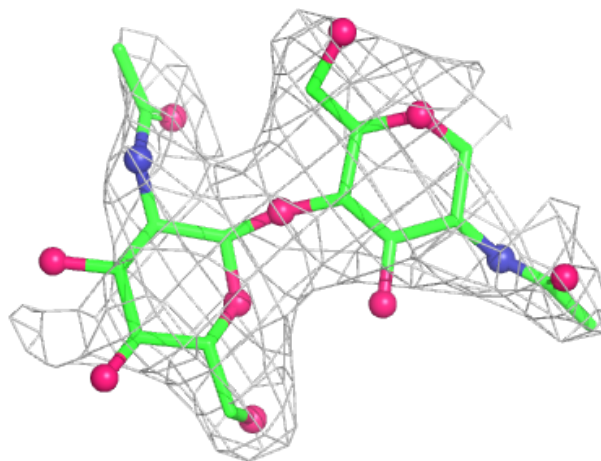
**Electron density around Chain JeJ:**

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 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



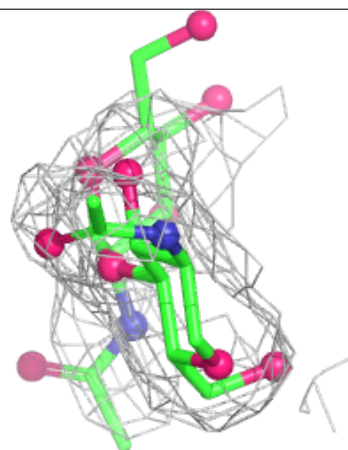
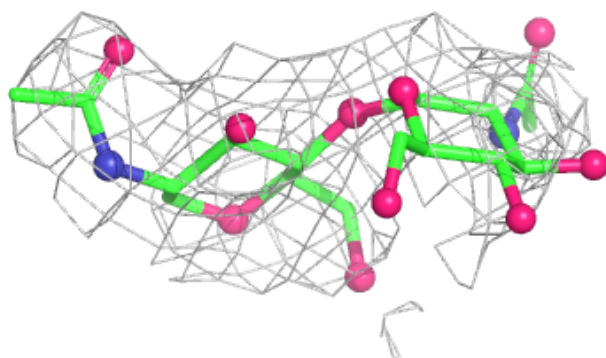
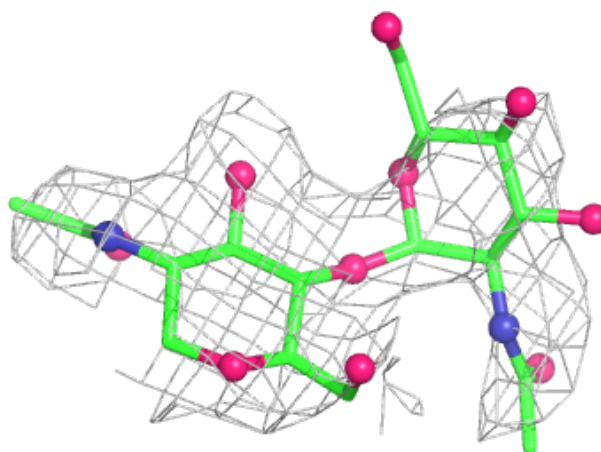
**Electron density around Chain JgJ:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



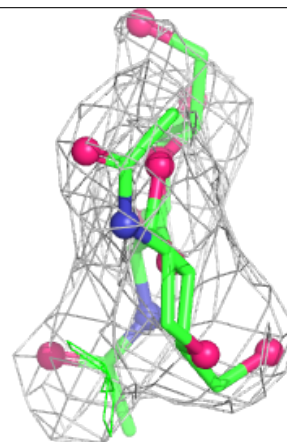
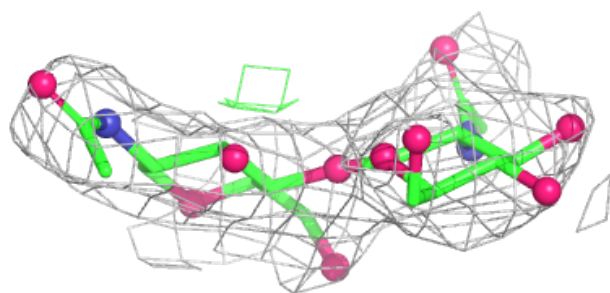
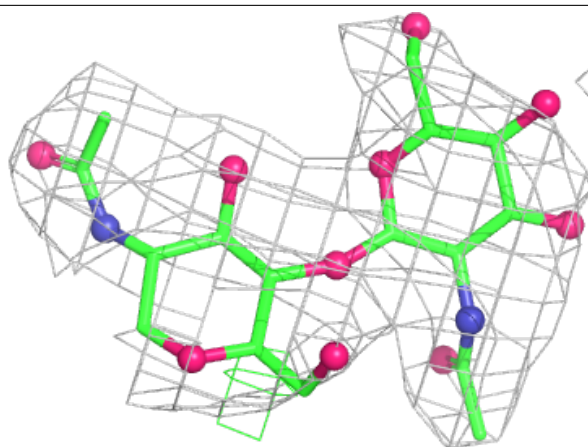
**Electron density around Chain JkJ:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

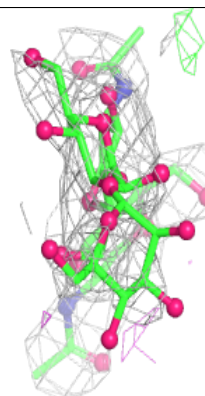
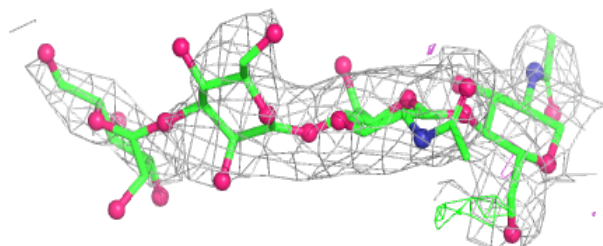
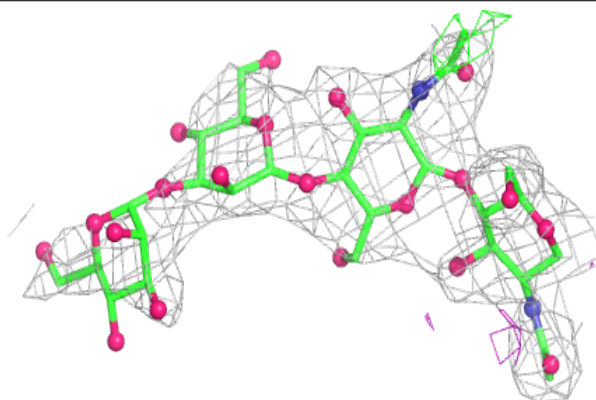


**Electron density around Chain KaK:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain AcA:**

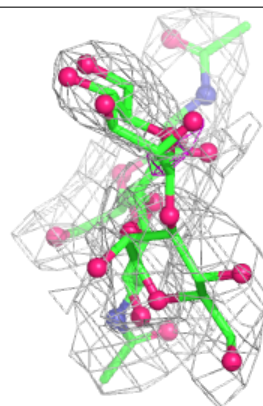
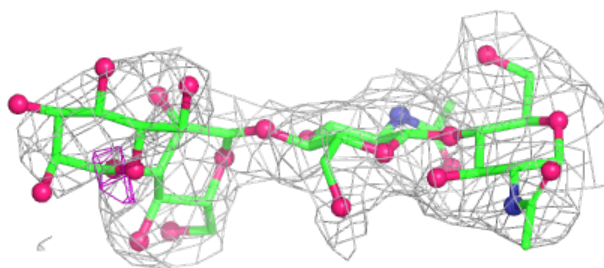
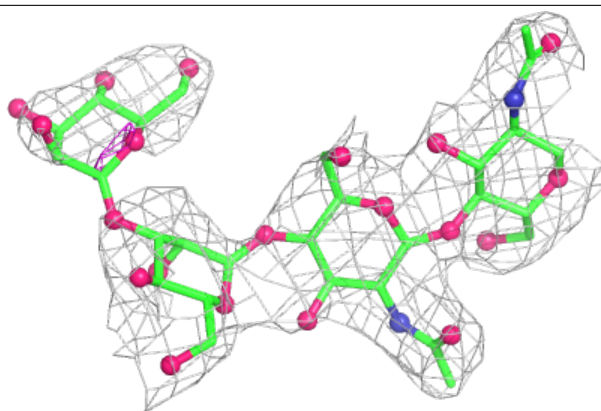
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



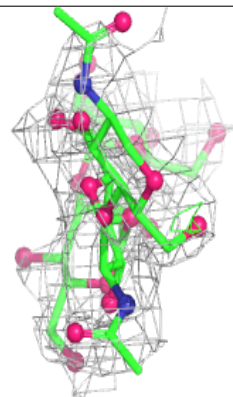
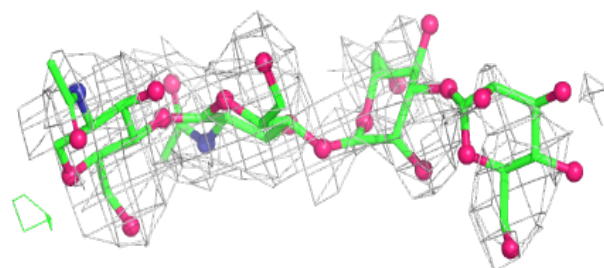
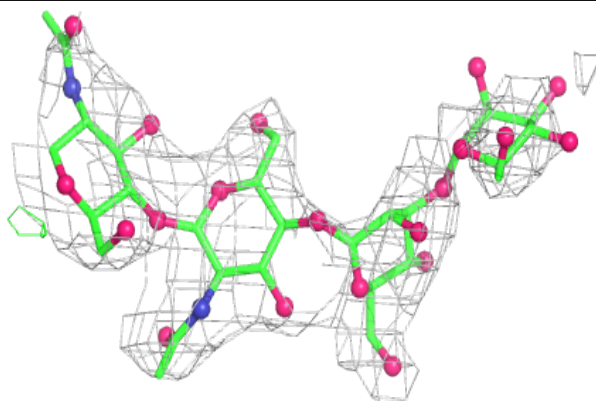


**Electron density around Chain AhA:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

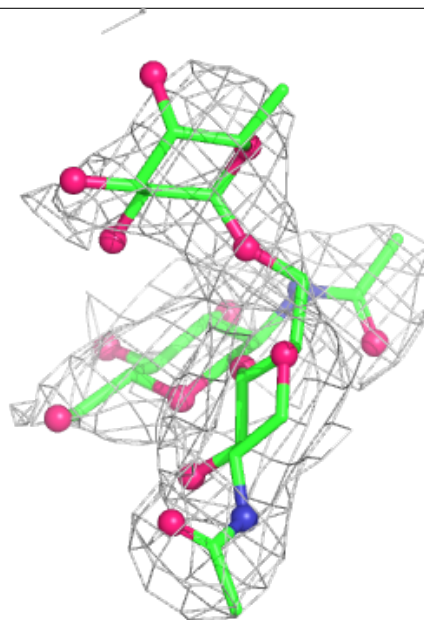
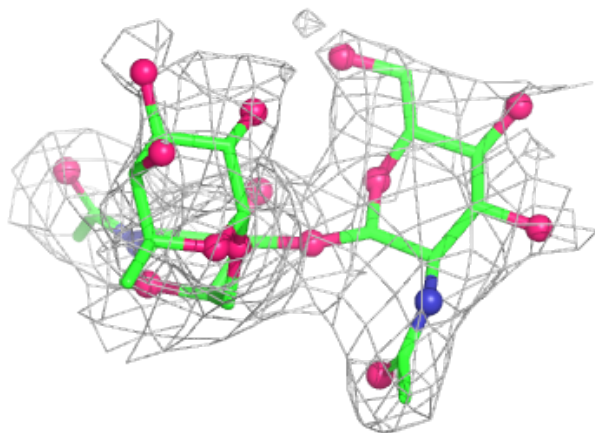
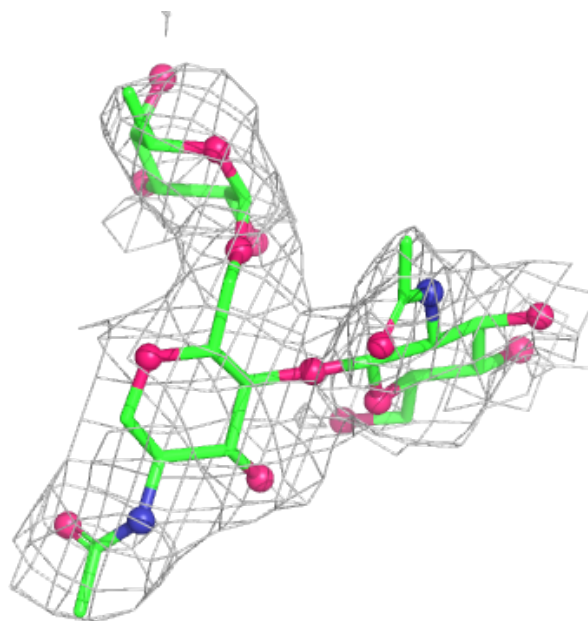
**Electron density around Chain DiD:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain AnA:**

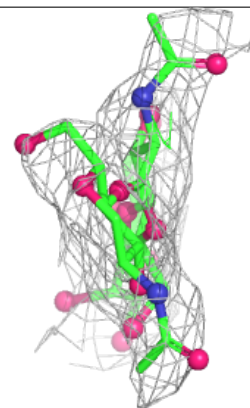
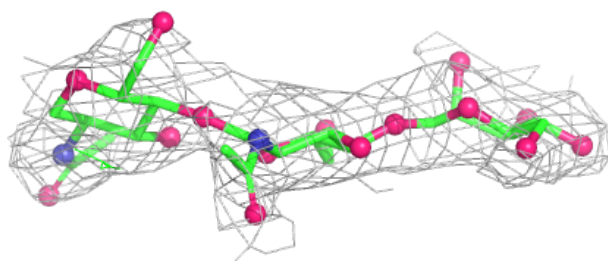
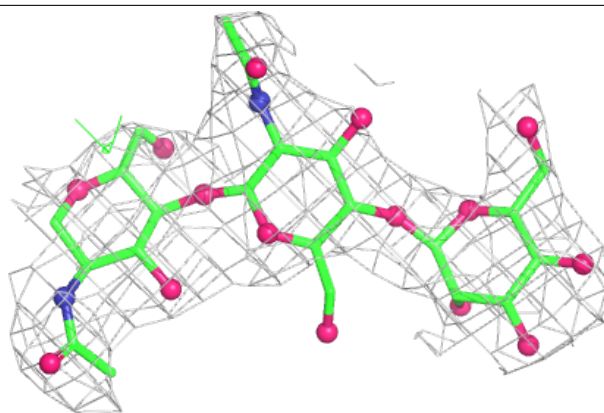
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



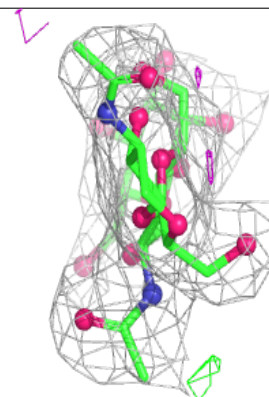
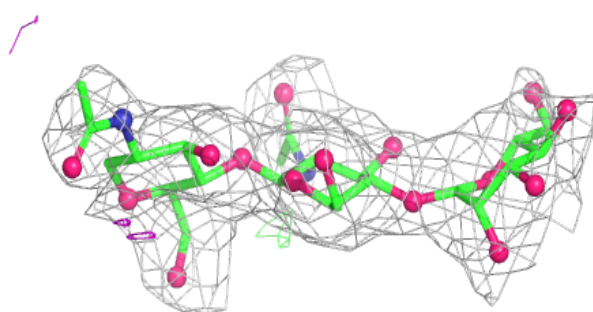
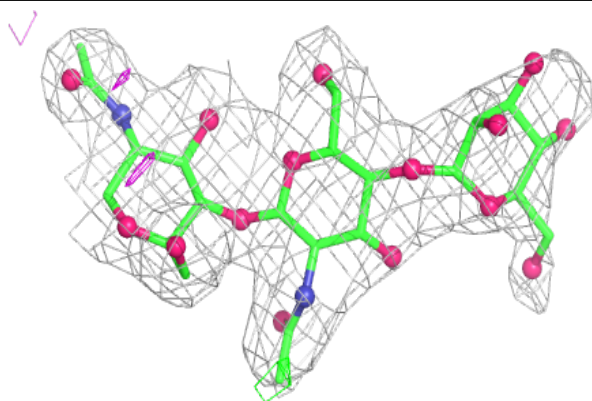


**Electron density around Chain BaB:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

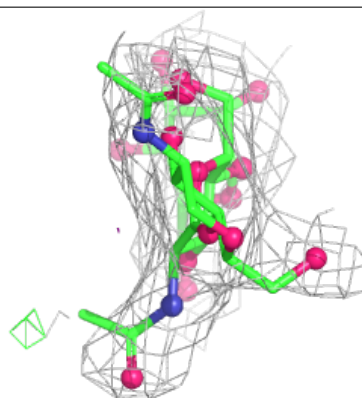
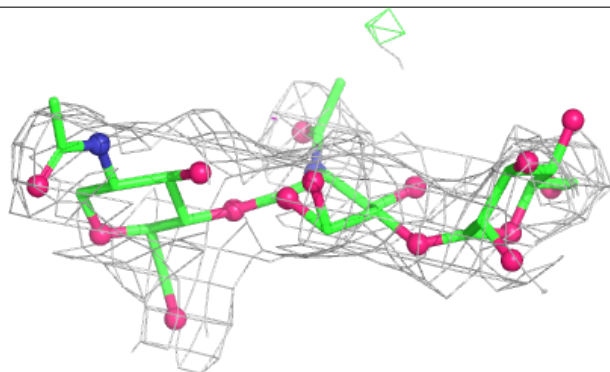
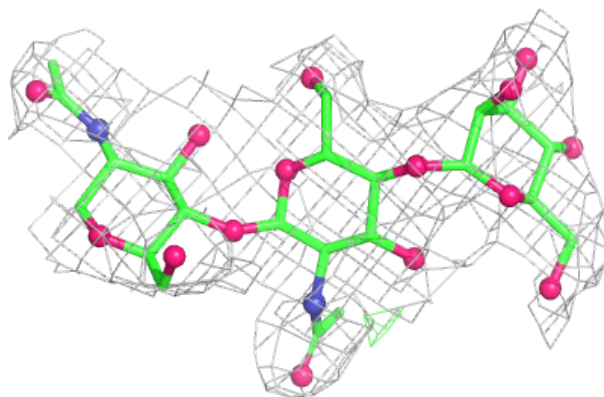
**Electron density around Chain DaD:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

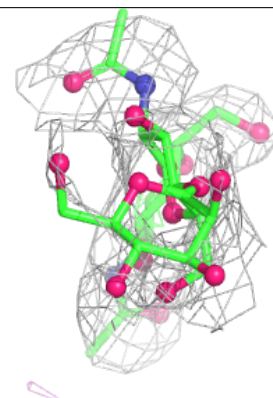
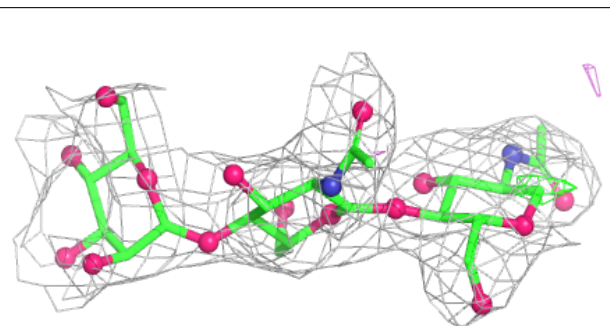
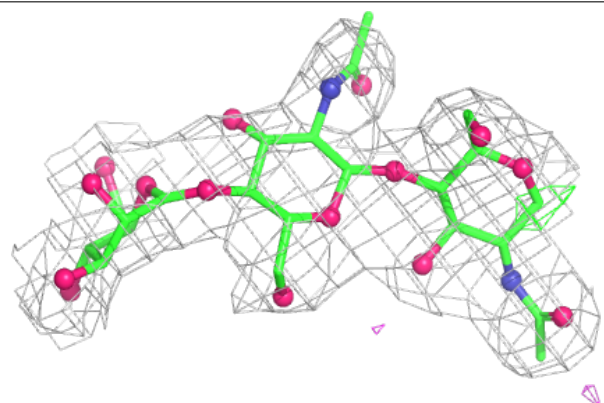


**Electron density around Chain EaE:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

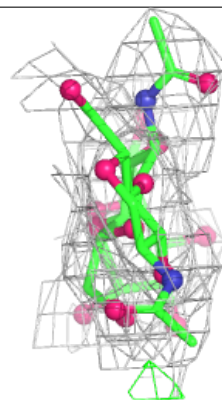
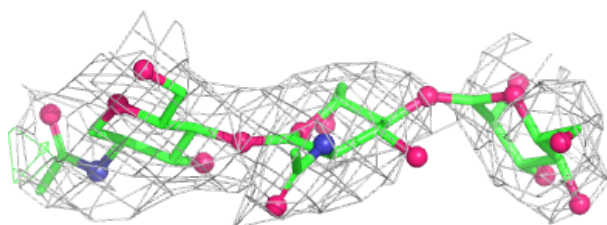
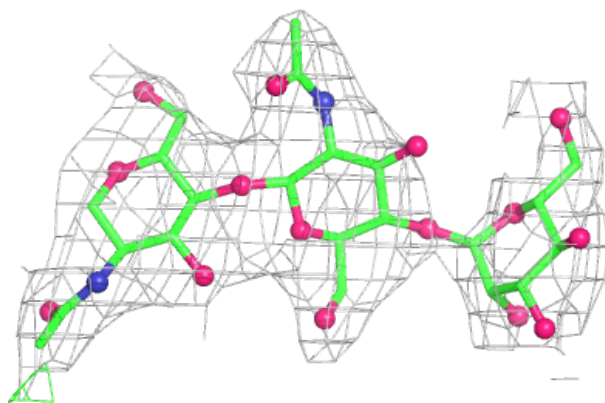
**Electron density around Chain GaG:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

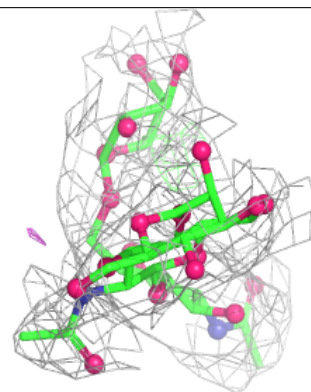
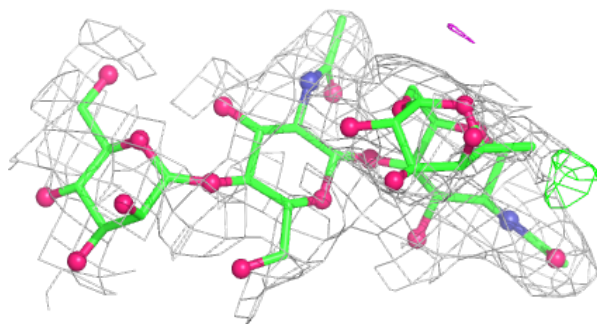
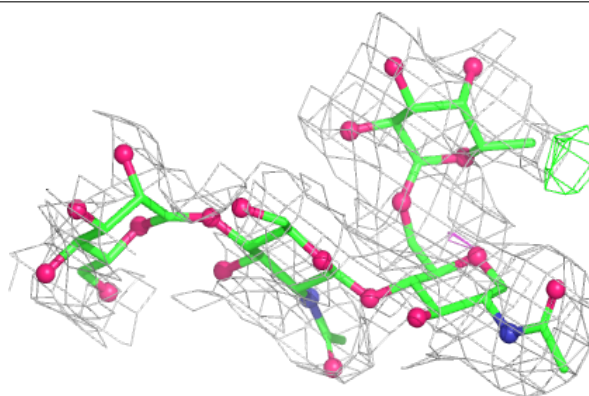


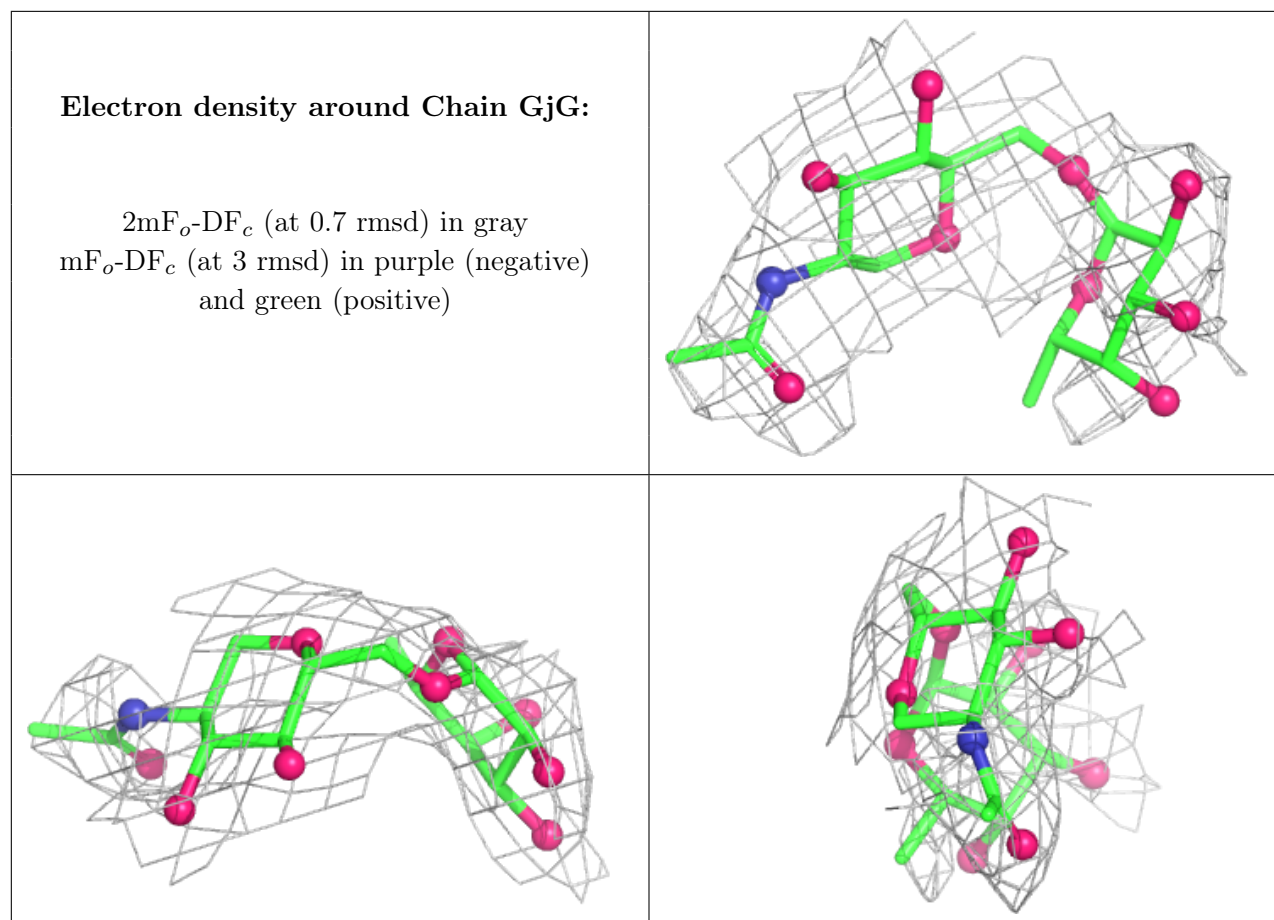
**Electron density around Chain GdG:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain DpD:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
10	MAN	AAA	701	11/12	0.48	0.34	106,118,121,122	0
12	NA	AAA	703	1/1	0.50	0.20	37,37,37,37	0
11	NAG	EEE	301	14/15	0.52	0.25	96,104,111,113	0
11	NAG	BBB	302	14/15	0.73	0.18	80,96,99,100	0
11	NAG	BBB	301	14/15	0.79	0.24	68,74,77,79	0
11	NAG	AAA	702	14/15	0.79	0.28	76,80,85,86	0
12	NA	GGG	702	1/1	0.79	0.12	52,52,52,52	0
11	NAG	JJJ	702	14/15	0.80	0.19	73,79,84,88	0
12	NA	AAA	704	1/1	0.81	0.18	44,44,44,44	0
11	NAG	JJJ	701	14/15	0.81	0.20	72,80,87,88	0
11	NAG	GGG	701	14/15	0.82	0.28	70,76,83,86	0
12	NA	DDD	703	1/1	0.82	0.17	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
11	NAG	DDD	701	14/15	0.82	0.31	64,77,84,85	0
11	NAG	HHH	301	14/15	0.83	0.32	71,75,82,84	0
11	NAG	DDD	702	14/15	0.84	0.26	62,74,80,81	0
11	NAG	JJJ	703	14/15	0.84	0.16	73,75,80,80	0
11	NAG	JJJ	704	14/15	0.86	0.22	72,77,81,87	0
12	NA	KKK	301	1/1	0.89	0.15	28,28,28,28	0
12	NA	BBB	303	1/1	0.95	0.28	21,21,21,21	0
12	NA	HHH	302	1/1	0.96	0.15	27,27,27,27	0
12	NA	EEE	302	1/1	0.96	0.17	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.