



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 06:17 AM EDT

PDB ID : 7OGU / pdb_00007ogu
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

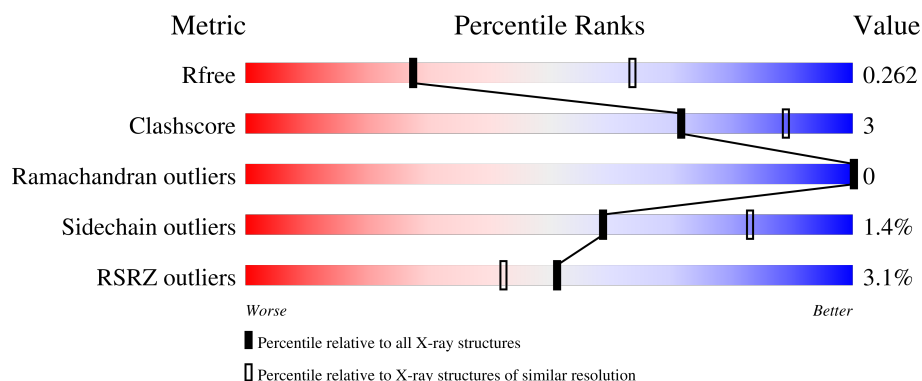
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

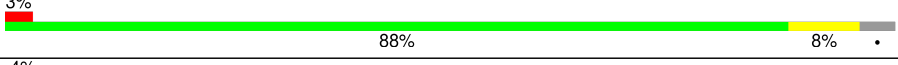
The reported resolution of this entry is 2.87 Å.

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}	180053	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (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 ≥ 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	
1	DDD	617	
1	GGG	617	
1	JJJ	617	
2	BBB	203	

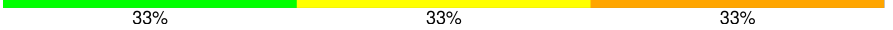
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Mol	Chain	Length	Quality of chain
2	EEE	203	
2	HHH	203	
2	KKK	203	
3	CCC	12	
3	FFF	12	
3	III	12	
3	LLL	12	
4	AaA	2	
4	AlA	2	
4	AqA	2	
4	AsA	2	
4	DeD	2	
4	DgD	2	
4	DmD	2	
4	EdE	2	
4	GgG	2	
4	GlG	2	
4	GnG	2	
4	HaH	2	
4	JaJ	2	
4	JcJ	2	
4	JeJ	2	
4	JgJ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

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Mol	Chain	Length	Quality of chain
5	AcA	4	 75%25%
5	AhA	4	 25%75%
5	DiD	4	 75%25%
6	AnA	3	 67%33%
7	BaB	3	 33%33%33%
7	DaD	3	 33%67%
7	EaE	3	 33%67%
7	GaG	3	 67%33%
7	GdG	3	 67%33%
8	DpD	4	 75%25%
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	BMA	AhA	3	X	-	-	-
5	MAN	AhA	4	X	-	-	-
5	BMA	DiD	3	X	-	-	-
7	NAG	BaB	2	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-

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			

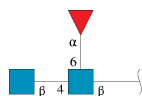
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranos

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



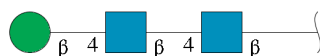
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	AcA	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	AhA	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	DiD	4	Total	C	N	O	0	0	0
			50	28	2	20			

- 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.



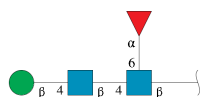
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	AnA	3	Total	C	N	O	0	0	0
			38	22	2	14			

- 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.



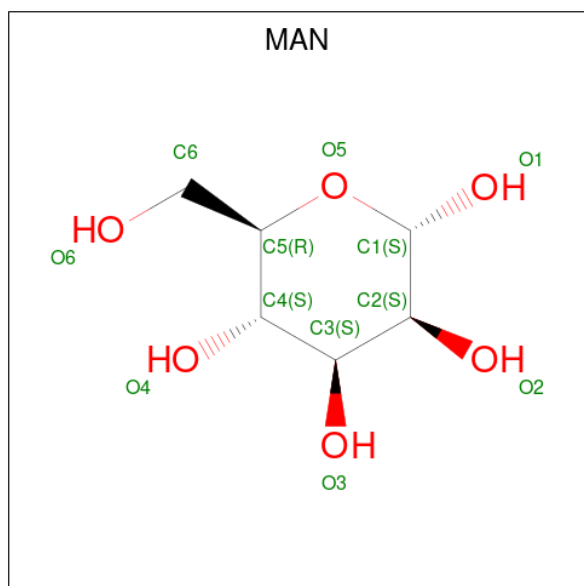
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	DpD	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



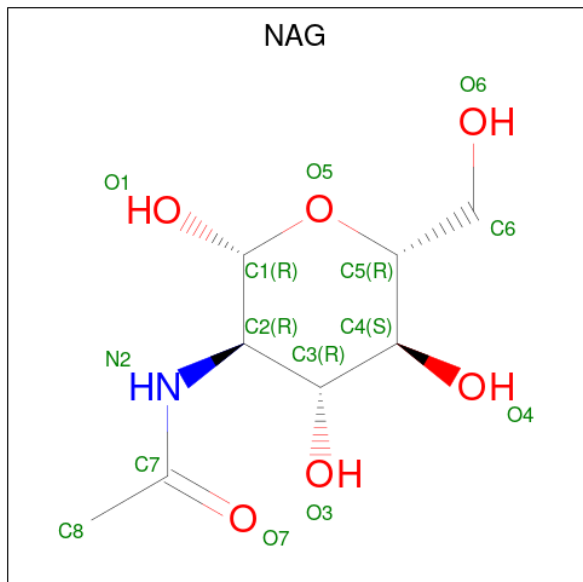
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	GjG	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 10 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆).



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 (CCD ID: 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 (CCD ID: 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

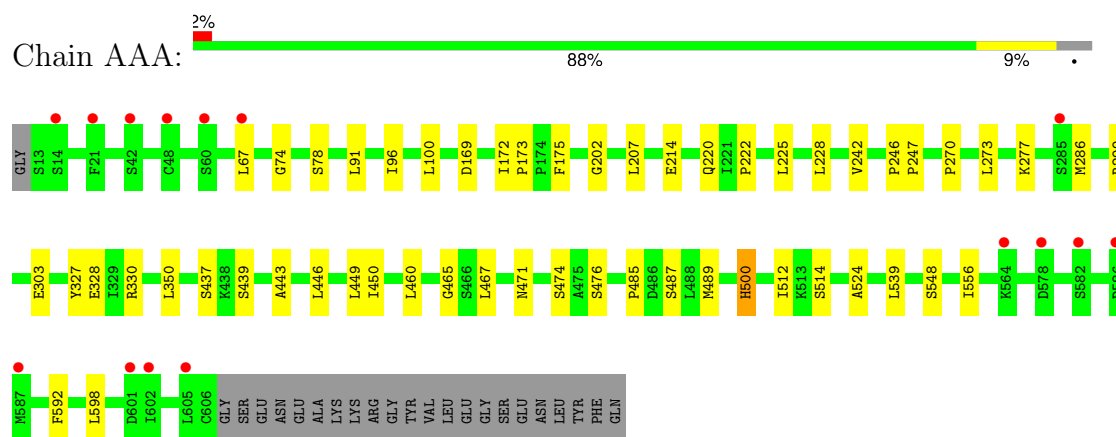
- Molecule 13 is water.

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

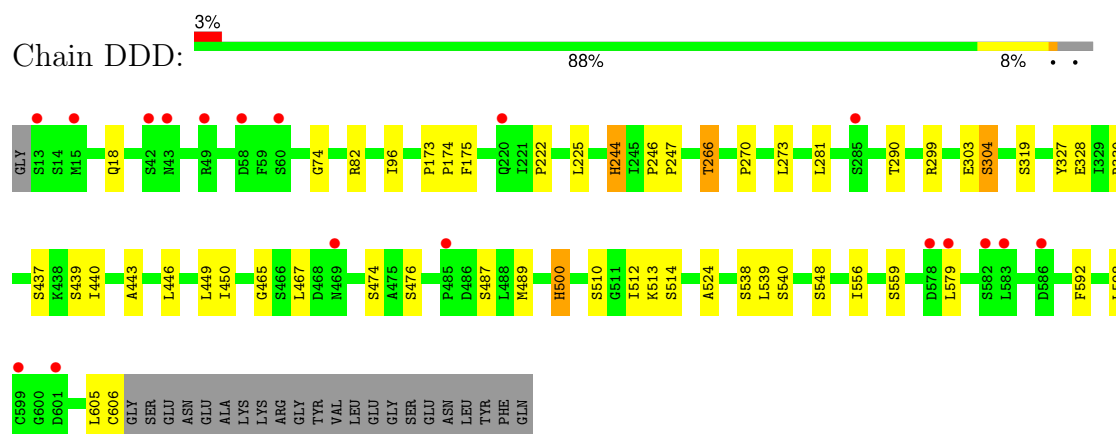
3 Residue-property plots [i](#)

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.

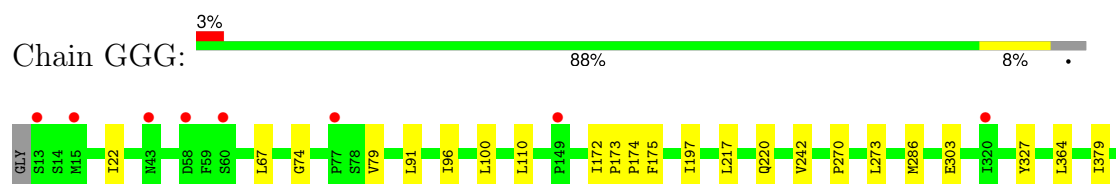
- Molecule 1: Receptor-like protein kinase HSL1

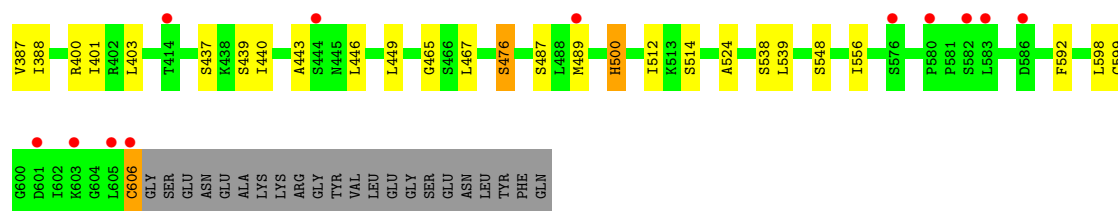


- Molecule 1: Receptor-like protein kinase HSL1

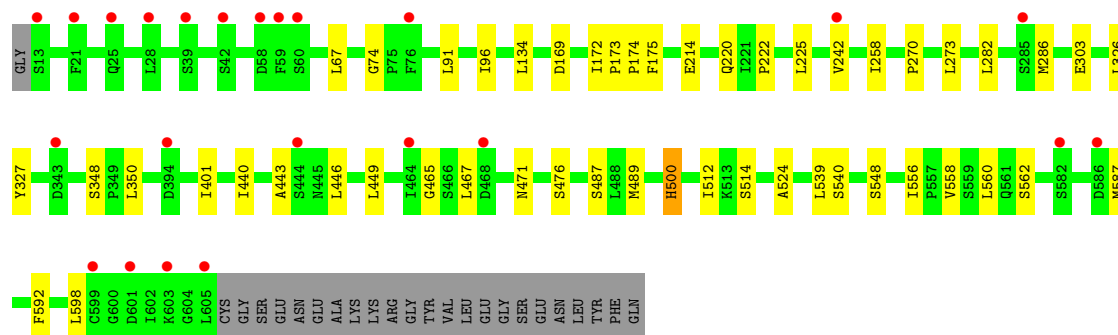
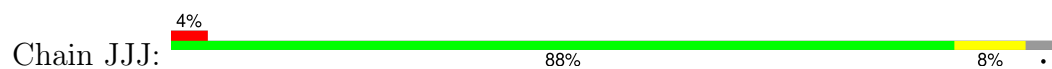


- Molecule 1: Receptor-like protein kinase HSL1

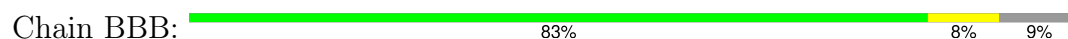




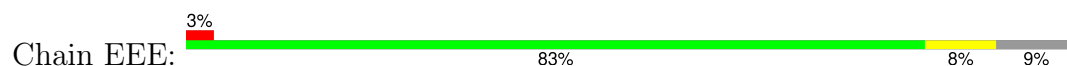
- Molecule 1: Receptor-like protein kinase HSL1



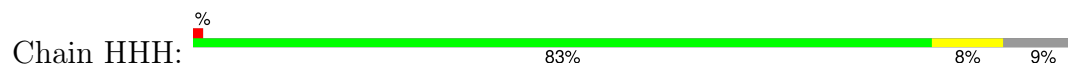
- Molecule 2: Somatic embryogenesis receptor kinase 1



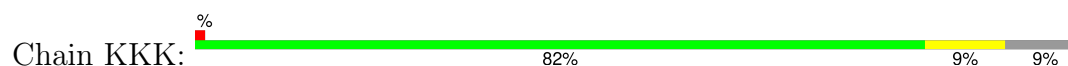
- Molecule 2: Somatic embryogenesis receptor kinase 1



- Molecule 2: Somatic embryogenesis receptor kinase 1



- Molecule 2: Somatic embryogenesis receptor kinase 1



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

Chain CCC:  25% 83% 17%



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

Chain FFF:  25% 92% 8%



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

Chain III:  17% 83% 8% 8%



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

Chain LLL:  8% 83% 8% 8%



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

Chain AaA:  50% 50%

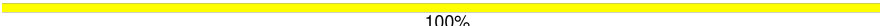


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AIA:  50% 50%



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

Chain AqA:  100%



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

Chain AsA:  50% 50%



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

Chain DeD:  100%



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

Chain DgD:  50% 50%



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

Chain DmD:  100%



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

Chain EdE:  100%



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

Chain GgG:  50% 50%

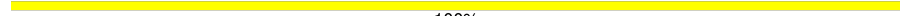


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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:  100%



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

Chain JkJ:



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

Chain KaK:



- 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:



- 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:



- 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:

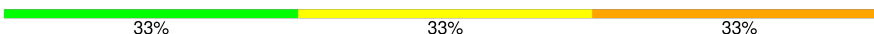


- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AnA:

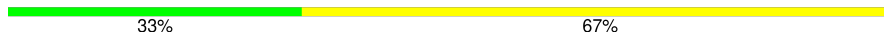


- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BaB: 



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

Chain DaD: 



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

Chain EaE: 



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

Chain GaG: 



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

Chain GdG: 



- 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

Chain DpD: 



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

Chain GjG: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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	5185 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24430	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, FUC, 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	0.93	0/4471	1.24	0/6110
1	DDD	0.93	0/4446	1.23	0/6079
1	GGG	0.93	0/4432	1.24	0/6059
1	JJJ	0.94	0/4409	1.25	0/6032
2	BBB	0.94	0/1403	1.26	0/1932
2	EEE	0.94	0/1404	1.25	0/1932
2	HHH	0.94	0/1412	1.25	0/1943
2	KKK	0.94	0/1409	1.25	0/1940
3	CCC	0.77	0/71	1.08	0/92
3	FFF	0.82	0/66	1.19	0/85
3	III	0.79	0/61	1.07	0/78
3	LLL	0.80	0/61	1.11	0/78
All	All	0.93	0/23645	1.24	0/32360

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.

There are no bond angle outliers.

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	29	0
1	JJJ	4325	0	4068	28	0
2	BBB	1371	0	1302	11	0
2	EEE	1369	0	1299	10	0
2	HHH	1377	0	1326	9	0
2	KKK	1373	0	1311	12	0
3	CCC	88	0	80	1	0
3	FFF	83	0	64	0	0
3	III	78	0	62	1	0
3	LLL	78	0	62	1	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	1	0
5	AcA	50	0	43	0	0
5	AhA	50	0	43	0	0
5	DiD	50	0	43	0	0
6	AnA	38	0	34	0	0
7	BaB	39	0	34	1	0
7	DaD	39	0	34	0	0
7	EaE	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	155	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 (155) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BaB:1:NAG:H82	7:BaB:1:NAG:O3	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
1:AAA:286:MET:HE1	3:CCC:116:ASN:HD22	1.74	0.51
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
4:KaK:1:NAG:H82	4:KaK:1:NAG:O3	2.11	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
1:JJJ:286:MET:HE1	3:LLL:116:ASN:HD22	1.78	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: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: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:EEE:210:CYS:O	2:EEE:211:PRO:C	2.62	0.43
2:BBB:64:THR:HB	2:BBB:73:ARG:HB2	2.00	0.43
2:BBB:138:GLY:HA3	2:BBB:160:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:EEE:95:LEU:HD23	2:EEE:116:LEU:HD13	2.01	0.43
2:HHH:210:CYS:O	2:HHH:211:PRO:C	2.62	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:GGG:286:MET:HE1	3:III:116:ASN:HD22	1.85	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
2:KKK:210:CYS:O	2:KKK:211:PRO:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DDD	593/617 (96%)	584 (98%)	9 (2%)	0	100	100
1	GGG	592/617 (96%)	584 (99%)	8 (1%)	0	100	100
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%)	61	84
1	DDD	465/540 (86%)	455 (98%)	10 (2%)	45	75
1	GGG	460/540 (85%)	454 (99%)	6 (1%)	61	84
1	JJJ	451/540 (84%)	444 (98%)	7 (2%)	55	81
2	BBB	155/184 (84%)	153 (99%)	2 (1%)	61	84
2	EEE	154/184 (84%)	153 (99%)	1 (1%)	78	92
2	HHH	157/184 (85%)	155 (99%)	2 (1%)	61	84
2	KKK	154/184 (84%)	152 (99%)	2 (1%)	61	84
3	CCC	8/9 (89%)	8 (100%)	0	100	100
3	FFF	6/9 (67%)	6 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	III	6/9 (67%)	6 (100%)	0	100	100
3	LLL	6/9 (67%)	6 (100%)	0	100	100
All	All	2498/2932 (85%)	2462 (99%)	36 (1%)	59	83

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

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Mol	Chain	Res	Type
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	III	115	3	7,8,9	0.63	0	5,10,12	0.82	0
3	HYP	CCC	112	3	7,8,9	0.78	0	5,10,12	1.39	1 (20%)
3	HYP	LLL	115	3	7,8,9	0.61	0	5,10,12	0.80	0
3	HYP	FFF	112	3	7,8,9	0.75	0	5,10,12	1.54	1 (20%)
3	HYP	LLL	112	3	7,8,9	0.74	0	5,10,12	0.86	0
3	HYP	III	112	3	7,8,9	0.69	0	5,10,12	0.97	0
3	HYP	CCC	115	3	7,8,9	0.62	0	5,10,12	0.93	0
3	HYP	FFF	115	3	7,8,9	0.60	0	5,10,12	0.88	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	III	115	3	-	0/0/11/13	0/1/1/1
3	HYP	CCC	112	3	-	0/0/11/13	0/1/1/1

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	FFF	112	HYP	CB-CG-CD	2.39	105.82	103.16
3	CCC	112	HYP	CB-CG-CD	2.10	105.50	103.16

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

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	4,1,12	14,14,15	0.39	0	17,19,21	0.97	0
4	NAG	AaA	2	4	14,14,15	0.38	0	17,19,21	1.10	1 (5%)
5	NAG	AcA	1	5,1	14,14,15	0.43	0	17,19,21	1.30	2 (11%)
5	NAG	AcA	2	5	14,14,15	0.24	0	17,19,21	0.96	0
5	BMA	AcA	3	5	11,11,12	0.50	0	15,15,17	1.03	0
5	MAN	AcA	4	5	11,11,12	0.41	0	15,15,17	0.81	0
5	NAG	AhA	1	5,1	14,14,15	0.37	0	17,19,21	0.95	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	AhA	2	5	14,14,15	0.42	0	17,19,21	1.18	1 (5%)
5	BMA	AhA	3	5	11,11,12	0.60	0	15,15,17	1.00	1 (6%)
5	MAN	AhA	4	5	11,11,12	0.39	0	15,15,17	0.56	0
4	NAG	AlA	1	4,1,12	14,14,15	0.50	0	17,19,21	0.88	0
4	NAG	AlA	2	4	14,14,15	0.31	0	17,19,21	0.85	1 (5%)
6	NAG	AnA	1	6,1	14,14,15	0.48	0	17,19,21	1.32	2 (11%)
6	NAG	AnA	2	6	14,14,15	0.40	0	17,19,21	0.92	0
6	FUC	AnA	3	6	10,10,11	0.40	0	14,14,16	0.71	0
4	NAG	AqA	1	4,1	14,14,15	0.45	0	17,19,21	1.30	2 (11%)
4	NAG	AqA	2	4	14,14,15	0.40	0	17,19,21	1.05	2 (11%)
4	NAG	AsA	1	4,1	14,14,15	0.48	0	17,19,21	1.21	2 (11%)
4	NAG	AsA	2	4	14,14,15	0.37	0	17,19,21	0.79	0
7	NAG	BaB	1	7,2	14,14,15	0.48	0	17,19,21	1.85	4 (23%)
7	NAG	BaB	2	7	14,14,15	0.51	0	17,19,21	1.23	2 (11%)
7	BMA	BaB	3	7	11,11,12	0.45	0	15,15,17	0.95	0
7	NAG	DaD	1	7,1	14,14,15	0.45	0	17,19,21	1.46	4 (23%)
7	NAG	DaD	2	7	14,14,15	0.33	0	17,19,21	1.21	2 (11%)
7	BMA	DaD	3	7	11,11,12	0.42	0	15,15,17	0.82	0
4	NAG	DeD	1	4,1,12	14,14,15	0.46	0	17,19,21	0.82	0
4	NAG	DeD	2	4	14,14,15	0.52	0	17,19,21	0.87	0
4	NAG	DgD	1	4,1	14,14,15	0.36	0	17,19,21	1.46	3 (17%)
4	NAG	DgD	2	4	14,14,15	0.43	0	17,19,21	0.86	0
5	NAG	DiD	1	5,1	14,14,15	0.32	0	17,19,21	0.70	0
5	NAG	DiD	2	5	14,14,15	0.39	0	17,19,21	0.98	1 (5%)
5	BMA	DiD	3	5	11,11,12	0.44	0	15,15,17	0.65	0
5	MAN	DiD	4	5	11,11,12	0.48	0	15,15,17	0.75	0
4	NAG	DmD	1	4,1	14,14,15	0.42	0	17,19,21	1.00	1 (5%)
4	NAG	DmD	2	4	14,14,15	0.39	0	17,19,21	0.88	1 (5%)
8	NAG	DpD	1	8,1	14,14,15	0.40	0	17,19,21	0.81	0
8	NAG	DpD	2	8	14,14,15	0.49	0	17,19,21	1.35	1 (5%)
8	BMA	DpD	3	8	11,11,12	0.44	0	15,15,17	0.77	0
8	FUC	DpD	4	8	10,10,11	0.39	0	14,14,16	0.85	0
7	NAG	EaE	1	7,2	14,14,15	0.40	0	17,19,21	1.22	2 (11%)
7	NAG	EaE	2	7	14,14,15	0.48	0	17,19,21	1.23	3 (17%)
7	BMA	EaE	3	7	11,11,12	0.40	0	15,15,17	0.67	0
4	NAG	EdE	1	4,2	14,14,15	0.45	0	17,19,21	0.99	1 (5%)
4	NAG	EdE	2	4	14,14,15	0.28	0	17,19,21	1.04	2 (11%)
7	NAG	GaG	1	7,1	14,14,15	0.60	0	17,19,21	1.58	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	GaG	2	7	14,14,15	0.30	0	17,19,21	1.09	0
7	BMA	GaG	3	7	11,11,12	0.47	0	15,15,17	0.78	0
7	NAG	GdG	1	7,1,12	14,14,15	0.38	0	17,19,21	1.06	1 (5%)
7	NAG	GdG	2	7	14,14,15	0.48	0	17,19,21	1.04	0
7	BMA	GdG	3	7	11,11,12	0.53	0	15,15,17	0.87	0
4	NAG	GgG	1	4,1	14,14,15	0.38	0	17,19,21	0.69	0
4	NAG	GgG	2	4	14,14,15	0.44	0	17,19,21	1.20	1 (5%)
9	NAG	GjG	1	1,9	14,14,15	0.57	0	17,19,21	1.13	1 (5%)
9	FUC	GjG	2	9	10,10,11	0.45	0	14,14,16	0.74	0
4	NAG	GlG	1	4,1	14,14,15	0.32	0	17,19,21	0.99	2 (11%)
4	NAG	GlG	2	4	14,14,15	0.34	0	17,19,21	0.59	0
4	NAG	GnG	1	4,1	14,14,15	0.45	0	17,19,21	1.68	2 (11%)
4	NAG	GnG	2	4	14,14,15	0.59	0	17,19,21	1.45	2 (11%)
4	NAG	HaH	1	4,2	14,14,15	0.49	0	17,19,21	1.41	2 (11%)
4	NAG	HaH	2	4	14,14,15	0.52	0	17,19,21	0.96	0
4	NAG	JaJ	1	4,1	14,14,15	0.44	0	17,19,21	1.21	3 (17%)
4	NAG	JaJ	2	4	14,14,15	0.30	0	17,19,21	0.87	0
4	NAG	JcJ	1	4,1	14,14,15	0.45	0	17,19,21	1.38	2 (11%)
4	NAG	JcJ	2	4	14,14,15	0.36	0	17,19,21	1.04	1 (5%)
4	NAG	JeJ	1	4,1	14,14,15	0.57	0	17,19,21	1.44	3 (17%)
4	NAG	JeJ	2	4	14,14,15	0.45	0	17,19,21	0.81	1 (5%)
4	NAG	JgJ	1	4,1	14,14,15	0.30	0	17,19,21	0.87	0
4	NAG	JgJ	2	4	14,14,15	0.49	0	17,19,21	0.85	0
4	NAG	JkJ	1	4,1	14,14,15	0.57	0	17,19,21	1.41	3 (17%)
4	NAG	JkJ	2	4	14,14,15	0.44	0	17,19,21	0.68	0
4	NAG	KaK	1	4,2	14,14,15	0.41	0	17,19,21	1.71	4 (23%)
4	NAG	KaK	2	4	14,14,15	0.33	0	17,19,21	0.88	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	AaA	1	4,1,12	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	4,1,12	-	2/6/23/26	0/1/1/1
4	NAG	AlA	2	4	-	2/6/23/26	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	4,1	-	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	4,1	-	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	-	2/6/23/26	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	4,1,12	-	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	4,1	-	1/6/23/26	0/1/1/1
4	NAG	DgD	2	4	1/1/5/7	2/6/23/26	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	4,1	-	0/6/23/26	0/1/1/1
4	NAG	DmD	2	4	-	3/6/23/26	0/1/1/1
8	NAG	DpD	1	8,1	-	1/6/23/26	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	4,2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
7	BMA	GdG	3	7	1/1/4/5	2/2/19/22	0/1/1/1
4	NAG	GgG	1	4,1	-	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	4,1	-	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	4,1	-	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	4,2	-	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	4,1	-	0/6/23/26	0/1/1/1
4	NAG	JaJ	2	4	1/1/5/7	3/6/23/26	0/1/1/1
4	NAG	JcJ	1	4,1	-	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	4,1	-	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	4,1	-	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	4,1	-	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	4,2	-	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 (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	GnG	1	NAG	C1-O5-C5	5.51	119.57	112.19
4	JcJ	1	NAG	C1-O5-C5	4.72	118.51	112.19
7	BaB	1	NAG	C2-N2-C7	4.09	128.38	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	HaH	1	NAG	C1-O5-C5	4.06	117.63	112.19
8	DpD	2	NAG	C1-O5-C5	4.01	117.56	112.19
7	BaB	1	NAG	C8-C7-N2	4.00	122.75	116.12
4	KaK	1	NAG	C8-C7-N2	3.99	122.73	116.12
7	GaG	1	NAG	C1-O5-C5	3.71	117.16	112.19
4	JeJ	1	NAG	O5-C1-C2	3.67	116.97	111.29
7	EaE	1	NAG	C1-O5-C5	3.64	117.07	112.19
4	GnG	2	NAG	C1-O5-C5	3.54	116.93	112.19
4	JkJ	1	NAG	C1-O5-C5	3.50	116.88	112.19
4	DgD	1	NAG	C1-O5-C5	3.39	116.73	112.19
7	BaB	2	NAG	C1-O5-C5	3.29	116.59	112.19
5	AhA	2	NAG	C1-O5-C5	3.20	116.48	112.19
7	GaG	1	NAG	C1-C2-N2	3.16	115.41	110.43
4	KaK	1	NAG	C2-N2-C7	3.01	126.94	122.90
7	GaG	1	NAG	O5-C1-C2	-2.99	106.66	111.29
4	AqA	1	NAG	C1-O5-C5	2.98	116.18	112.19
7	DaD	1	NAG	C1-O5-C5	2.97	116.17	112.19
6	AnA	1	NAG	C1-O5-C5	2.94	116.13	112.19
4	AsA	1	NAG	C4-C3-C2	-2.90	106.77	111.02
4	JaJ	1	NAG	C1-C2-N2	2.85	114.92	110.43
4	KaK	1	NAG	C1-C2-N2	-2.78	106.05	110.43
7	EaE	2	NAG	C8-C7-N2	2.73	120.65	116.12
4	DgD	1	NAG	C4-C3-C2	-2.72	107.03	111.02
5	AcA	1	NAG	C1-O5-C5	2.70	115.81	112.19
7	GdG	1	NAG	C1-O5-C5	2.70	115.80	112.19
4	AsA	1	NAG	C1-O5-C5	2.66	115.75	112.19
6	AnA	1	NAG	C1-C2-N2	-2.64	106.27	110.43
7	EaE	1	NAG	O5-C1-C2	-2.64	107.21	111.29
4	AqA	1	NAG	C4-C3-C2	-2.62	107.18	111.02
4	JeJ	1	NAG	O4-C4-C5	2.60	115.73	109.32
4	KaK	1	NAG	O7-C7-N2	-2.56	117.45	121.98
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
7	DaD	1	NAG	O5-C1-C2	-2.51	107.41	111.29
5	AcA	1	NAG	O5-C1-C2	-2.50	107.43	111.29
4	JcJ	2	NAG	O5-C5-C6	2.48	112.49	107.66
4	GnG	2	NAG	O5-C1-C2	-2.45	107.51	111.29
4	HaH	1	NAG	O5-C1-C2	-2.42	107.55	111.29
5	DiD	2	NAG	O4-C4-C3	-2.40	104.73	110.38
4	JaJ	1	NAG	O5-C1-C2	-2.38	107.60	111.29
4	AqA	2	NAG	C8-C7-N2	2.35	120.01	116.12
4	JkJ	1	NAG	C2-N2-C7	2.34	126.03	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	BaB	1	NAG	O7-C7-N2	-2.33	117.86	121.98
4	EdE	1	NAG	C1-C2-N2	-2.31	106.79	110.43
7	EaE	2	NAG	C2-N2-C7	2.31	125.99	122.90
7	DaD	2	NAG	C1-O5-C5	2.31	115.28	112.19
5	AhA	3	BMA	O5-C5-C6	2.30	112.14	107.66
4	AlA	2	NAG	C1-O5-C5	2.29	115.25	112.19
4	DgD	1	NAG	O5-C1-C2	-2.26	107.79	111.29
7	DaD	1	NAG	O3-C3-C4	-2.26	105.05	110.38
4	AqA	2	NAG	C2-N2-C7	2.24	125.91	122.90
7	BaB	2	NAG	O5-C1-C2	-2.24	107.83	111.29
4	GgG	2	NAG	C2-N2-C7	2.23	125.89	122.90
4	JeJ	2	NAG	C2-N2-C7	2.23	125.88	122.90
4	JaJ	1	NAG	C1-O5-C5	2.18	115.11	112.19
9	GjG	1	NAG	O5-C5-C6	2.18	111.91	107.66
7	EaE	2	NAG	C1-C2-N2	-2.15	107.05	110.43
4	JkJ	1	NAG	O7-C7-N2	2.12	125.73	121.98
4	GnG	1	NAG	O4-C4-C5	2.12	114.53	109.32
4	JeJ	1	NAG	C1-C2-N2	2.11	113.75	110.43
7	DaD	1	NAG	C6-C5-C4	-2.10	107.86	113.02
7	BaB	1	NAG	C1-C2-N2	-2.09	107.14	110.43
4	GlG	1	NAG	C1-O5-C5	2.07	114.96	112.19
4	DmD	1	NAG	O4-C4-C5	2.05	114.37	109.32
4	EdE	2	NAG	O5-C1-C2	-2.05	108.12	111.29
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
4	DmD	2	NAG	C1-O5-C5	2.03	114.90	112.19
7	DaD	2	NAG	C8-C7-N2	-2.02	112.77	116.12
4	AaA	2	NAG	O5-C5-C4	-2.01	105.94	110.83

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

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Mol	Chain	Res	Type	Atom
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 (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
4	GgG	2	NAG	O5-C5-C6-O6
4	JcJ	1	NAG	O5-C5-C6-O6
8	DpD	2	NAG	O5-C5-C6-O6
4	GgG	1	NAG	C4-C5-C6-O6
4	DmD	2	NAG	O5-C5-C6-O6
5	AhA	3	BMA	C4-C5-C6-O6
4	JgJ	2	NAG	O5-C5-C6-O6
7	BaB	2	NAG	C4-C5-C6-O6
5	AhA	1	NAG	O5-C5-C6-O6
4	JeJ	1	NAG	C4-C5-C6-O6
4	JgJ	2	NAG	C4-C5-C6-O6
4	GgG	2	NAG	C4-C5-C6-O6
4	JcJ	1	NAG	C4-C5-C6-O6
4	JeJ	2	NAG	C4-C5-C6-O6
5	DiD	2	NAG	C4-C5-C6-O6
4	JeJ	1	NAG	O5-C5-C6-O6
4	DeD	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	KaK	1	NAG	C4-C5-C6-O6
7	GdG	3	BMA	C4-C5-C6-O6
7	BaB	2	NAG	O5-C5-C6-O6
4	GnG	2	NAG	O5-C5-C6-O6
4	JgJ	1	NAG	O5-C5-C6-O6
4	HaH	2	NAG	C4-C5-C6-O6
4	AsA	2	NAG	O5-C5-C6-O6
4	AsA	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	GdG	2	NAG	O5-C5-C6-O6
7	GdG	3	BMA	O5-C5-C6-O6
7	GdG	1	NAG	O5-C5-C6-O6
4	DmD	2	NAG	C4-C5-C6-O6
4	JeJ	2	NAG	O5-C5-C6-O6
5	AcA	1	NAG	O5-C5-C6-O6
7	GdG	2	NAG	C4-C5-C6-O6
5	AhA	3	BMA	O5-C5-C6-O6
5	AcA	1	NAG	C4-C5-C6-O6
7	GaG	3	BMA	C4-C5-C6-O6
7	GaG	3	BMA	O5-C5-C6-O6
4	JkJ	2	NAG	C4-C5-C6-O6
4	HaH	1	NAG	O5-C5-C6-O6
7	DaD	3	BMA	C4-C5-C6-O6
7	EaE	2	NAG	C4-C5-C6-O6
4	KaK	1	NAG	O5-C5-C6-O6
4	AlA	1	NAG	O5-C5-C6-O6
7	EaE	2	NAG	O5-C5-C6-O6
4	GlG	2	NAG	O5-C5-C6-O6
7	DaD	3	BMA	O5-C5-C6-O6
4	AqA	1	NAG	C4-C5-C6-O6
4	JgJ	1	NAG	C4-C5-C6-O6
7	GdG	1	NAG	C4-C5-C6-O6
4	JaJ	2	NAG	O5-C5-C6-O6

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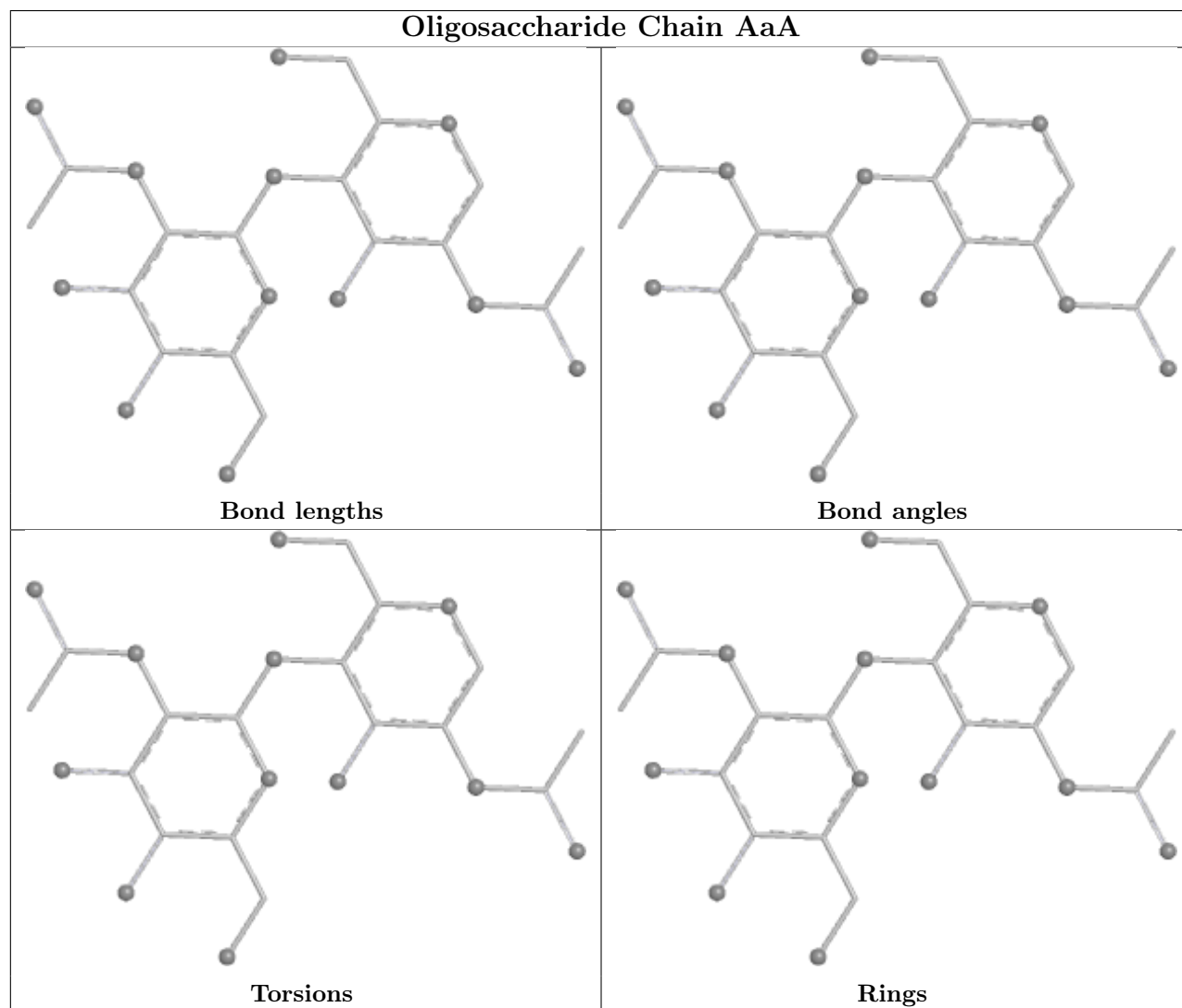
Mol	Chain	Res	Type	Atoms
5	AhA	2	NAG	O5-C5-C6-O6
4	AqA	1	NAG	O5-C5-C6-O6
5	AhA	4	MAN	O5-C5-C6-O6
4	DgD	1	NAG	C3-C2-N2-C7
4	DgD	2	NAG	C3-C2-N2-C7
4	HaH	2	NAG	C3-C2-N2-C7
4	GnG	1	NAG	O5-C5-C6-O6
5	AhA	2	NAG	C4-C5-C6-O6
7	DaD	2	NAG	O5-C5-C6-O6
4	HaH	1	NAG	C4-C5-C6-O6
5	AcA	3	BMA	C4-C5-C6-O6
4	GlG	1	NAG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

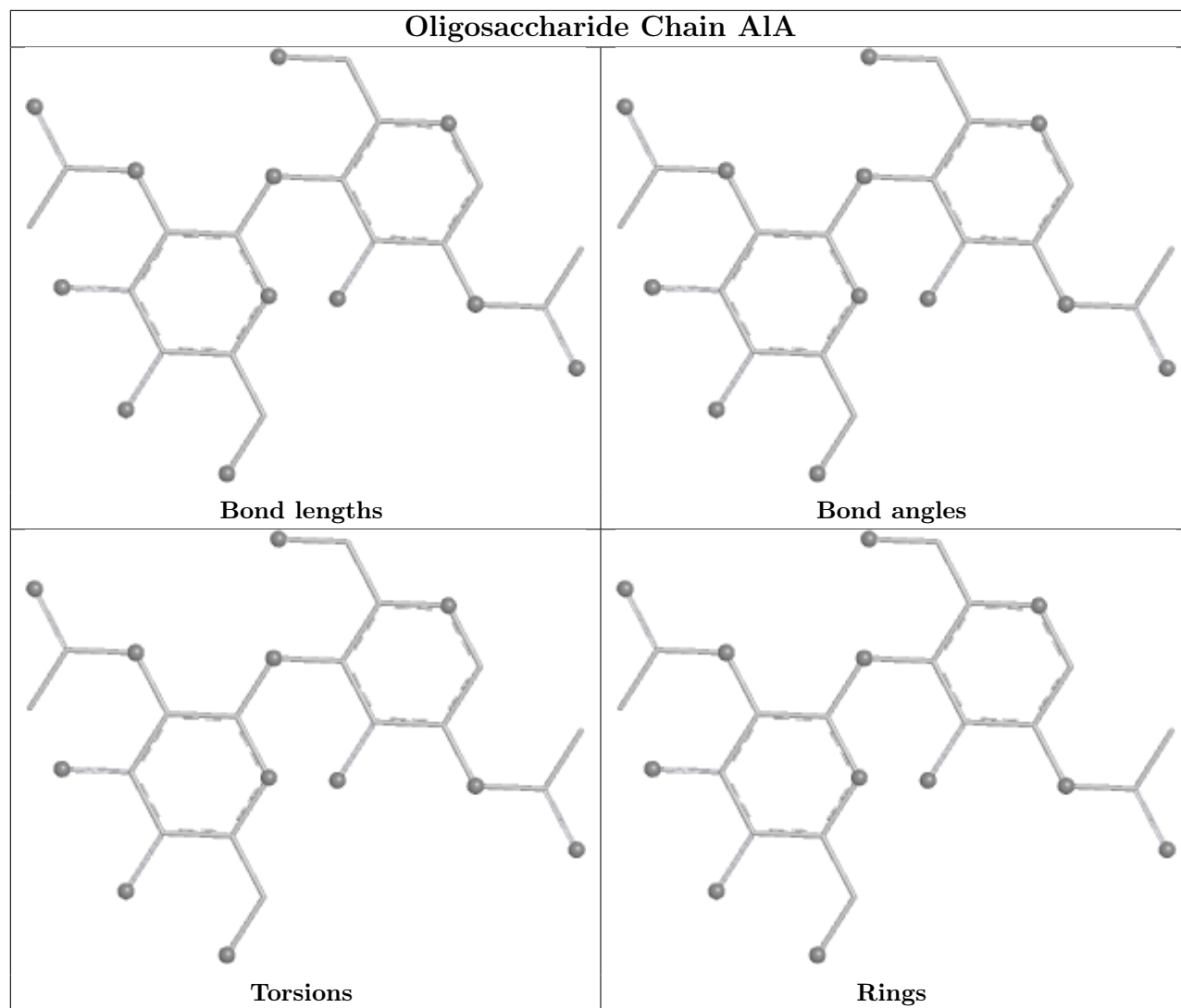
There are no ring outliers.

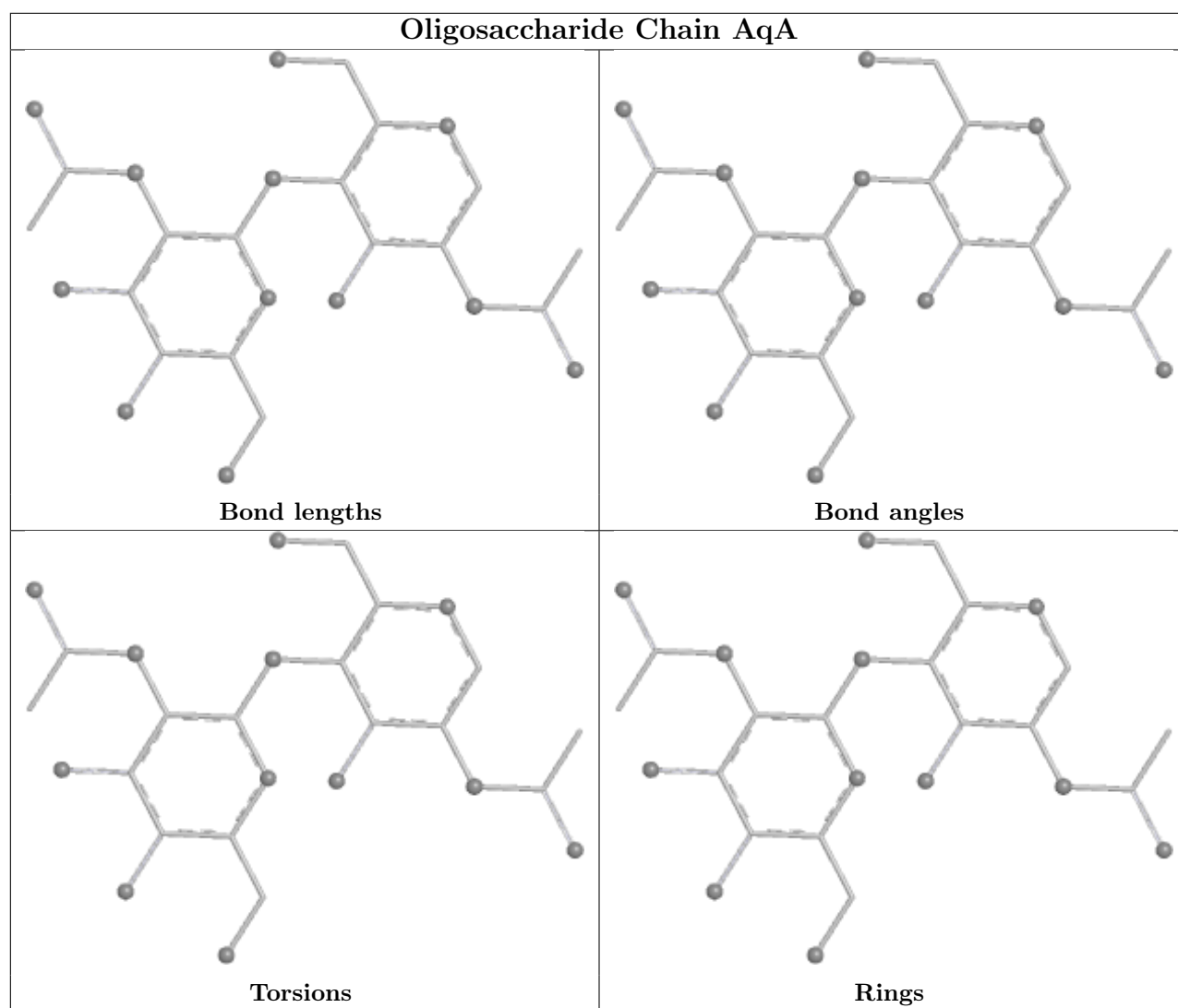
2 monomers are involved in 2 short contacts:

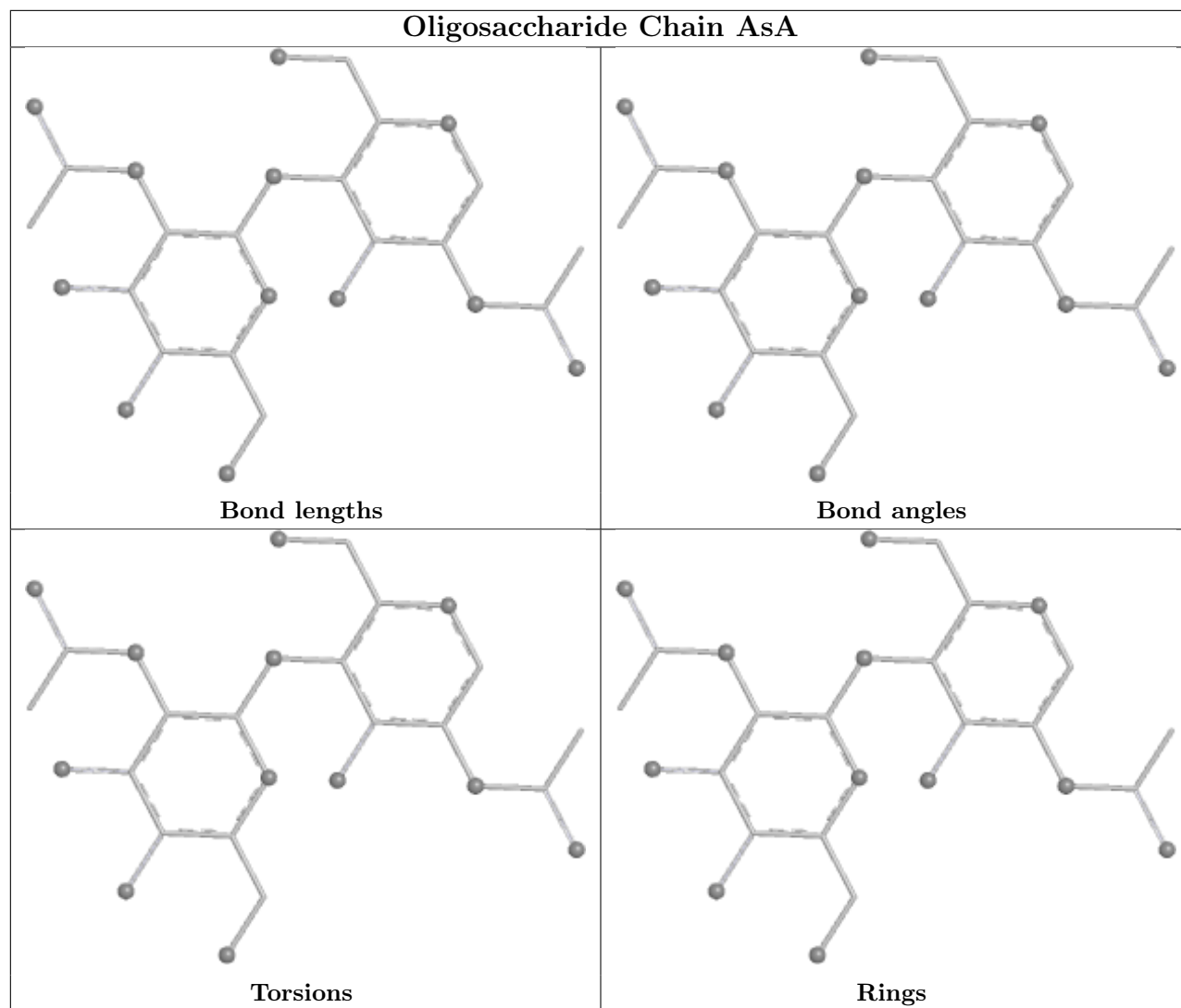
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	KaK	1	NAG	1	0
7	BaB	1	NAG	1	0

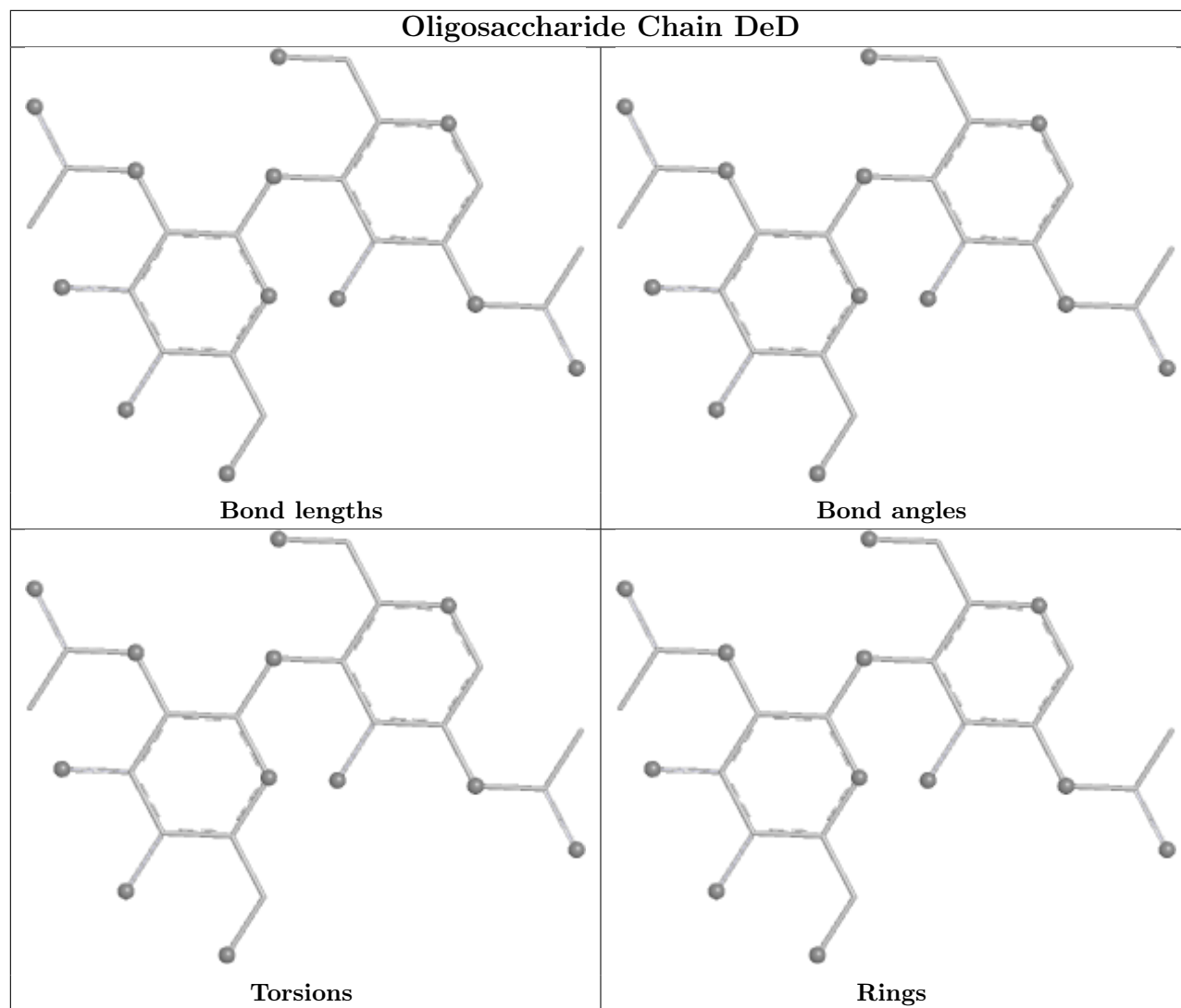
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

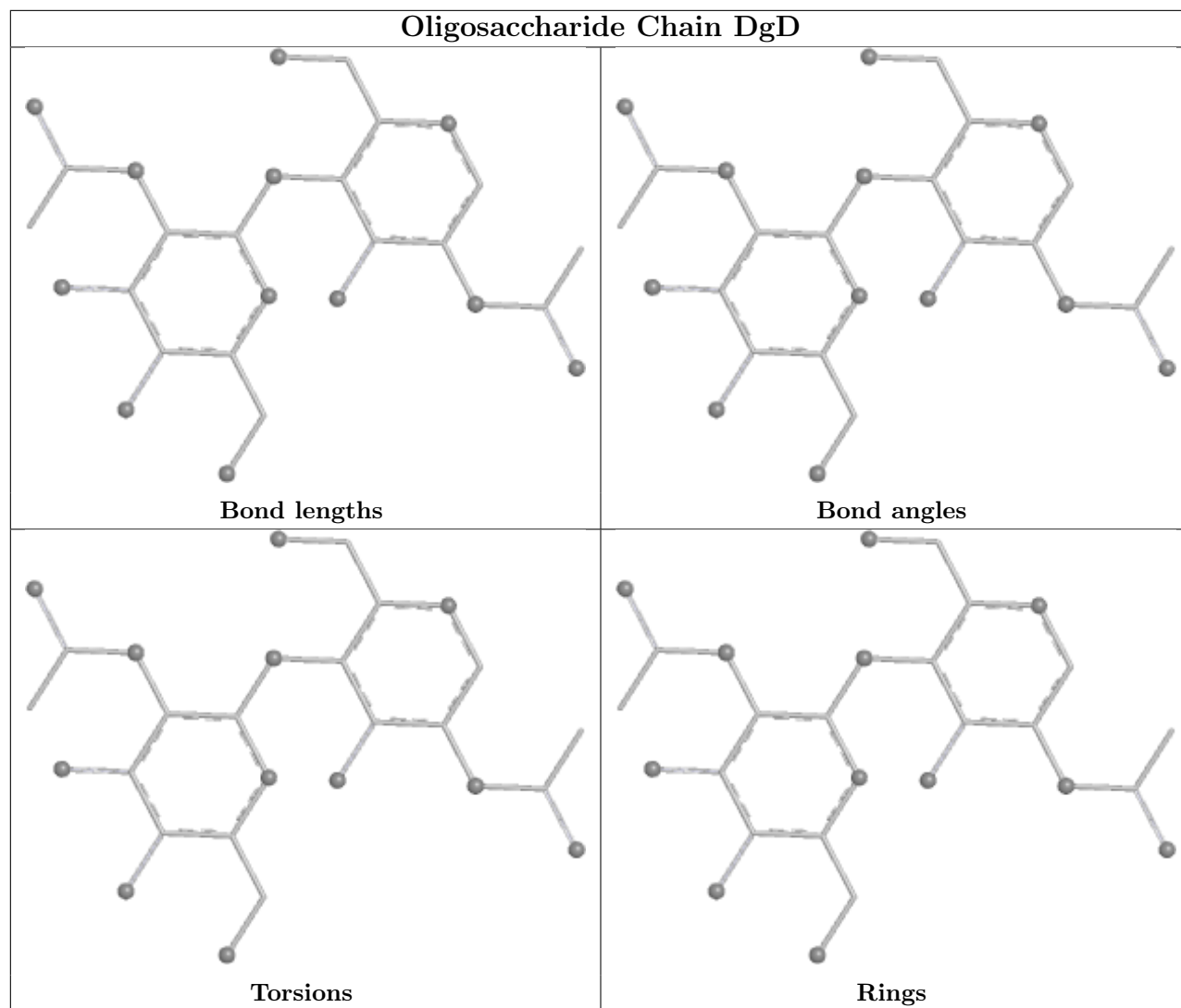


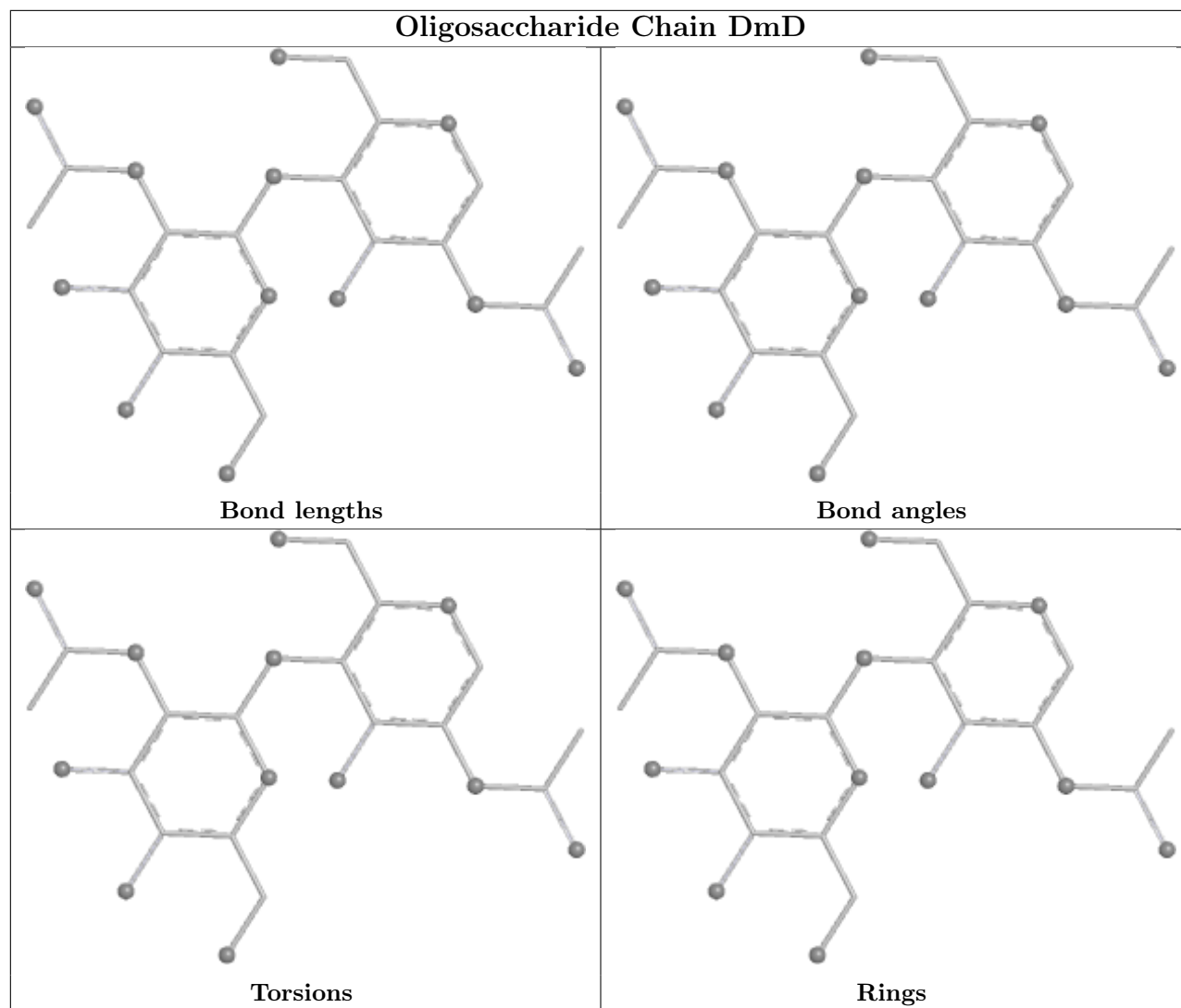


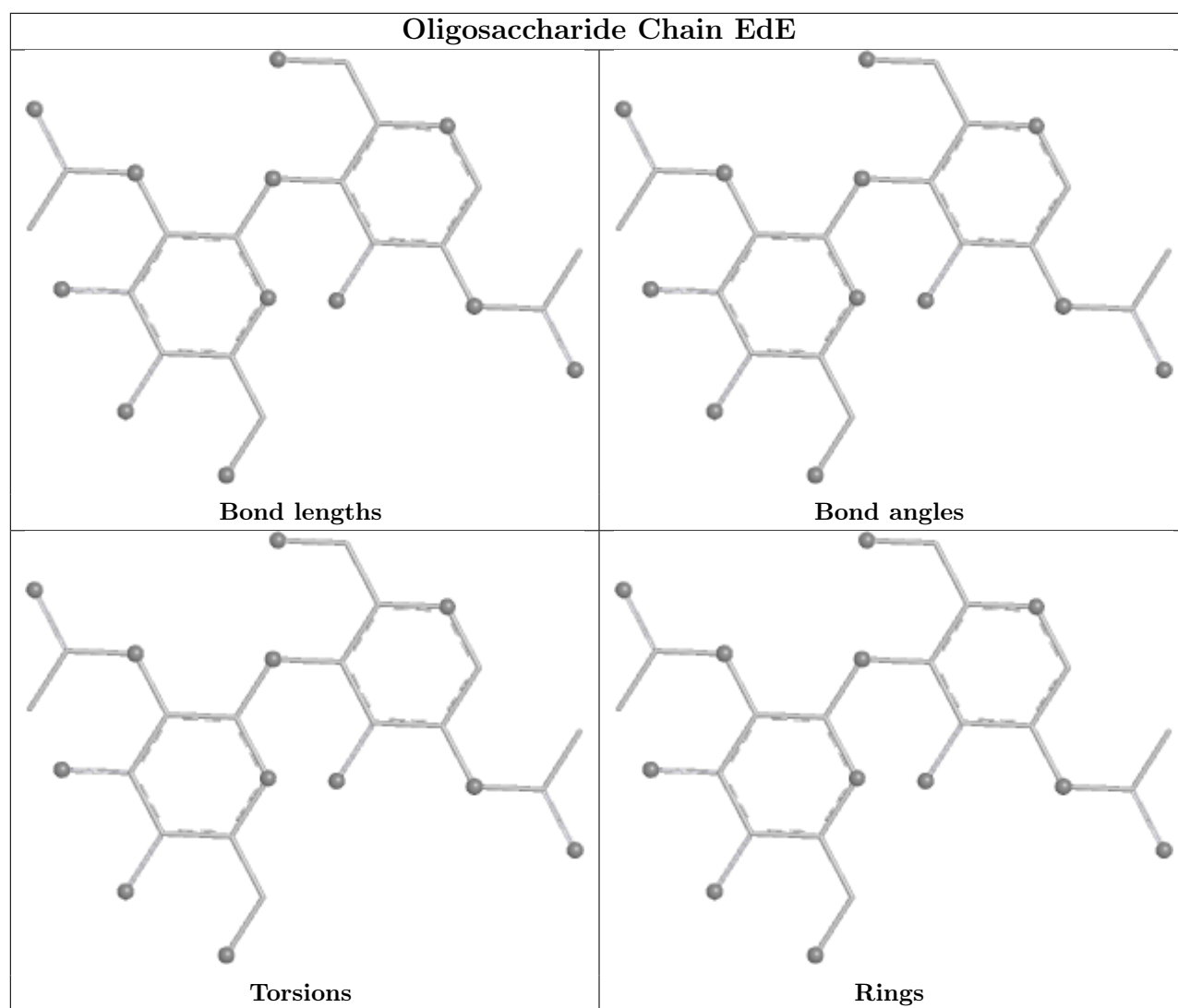


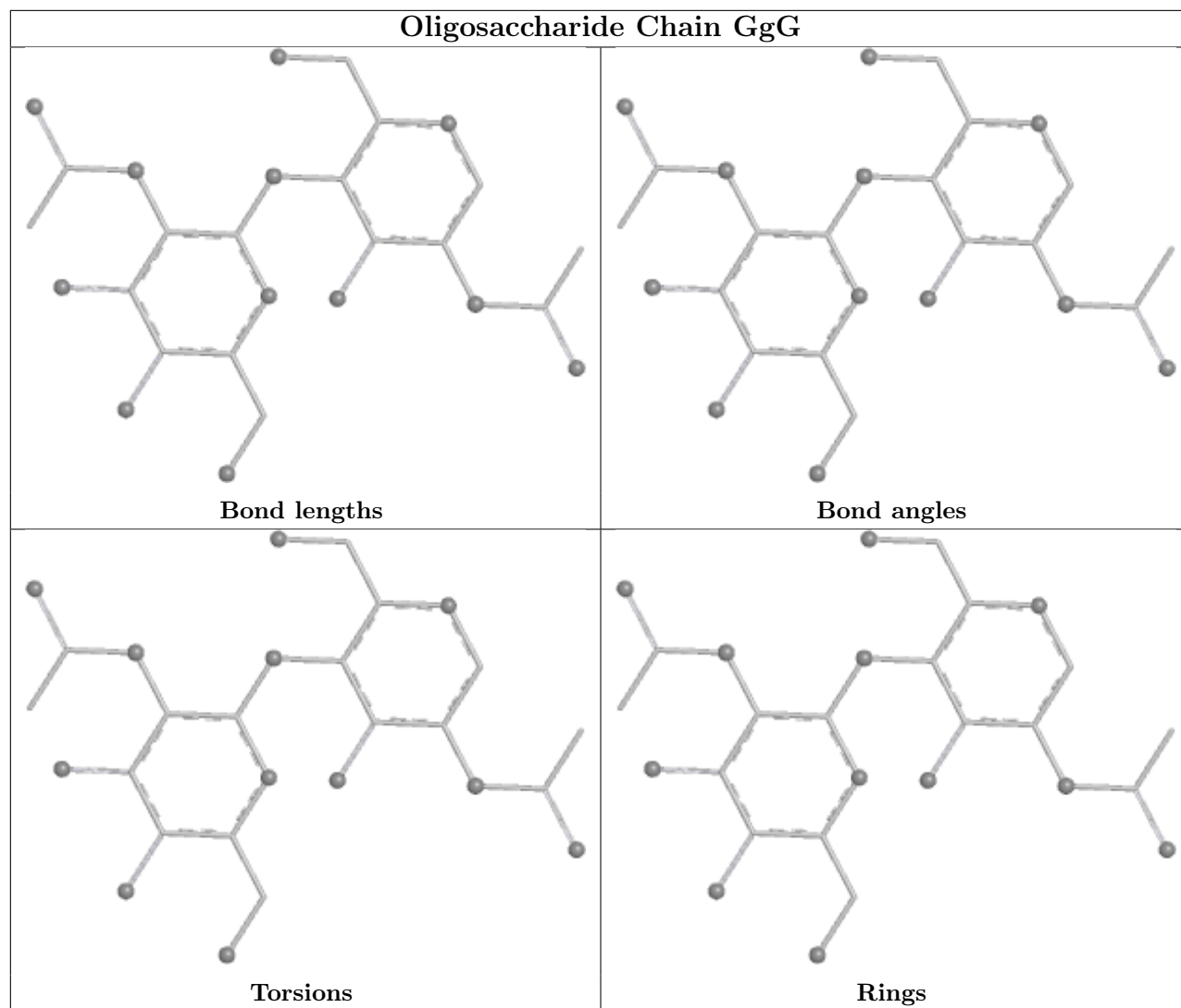


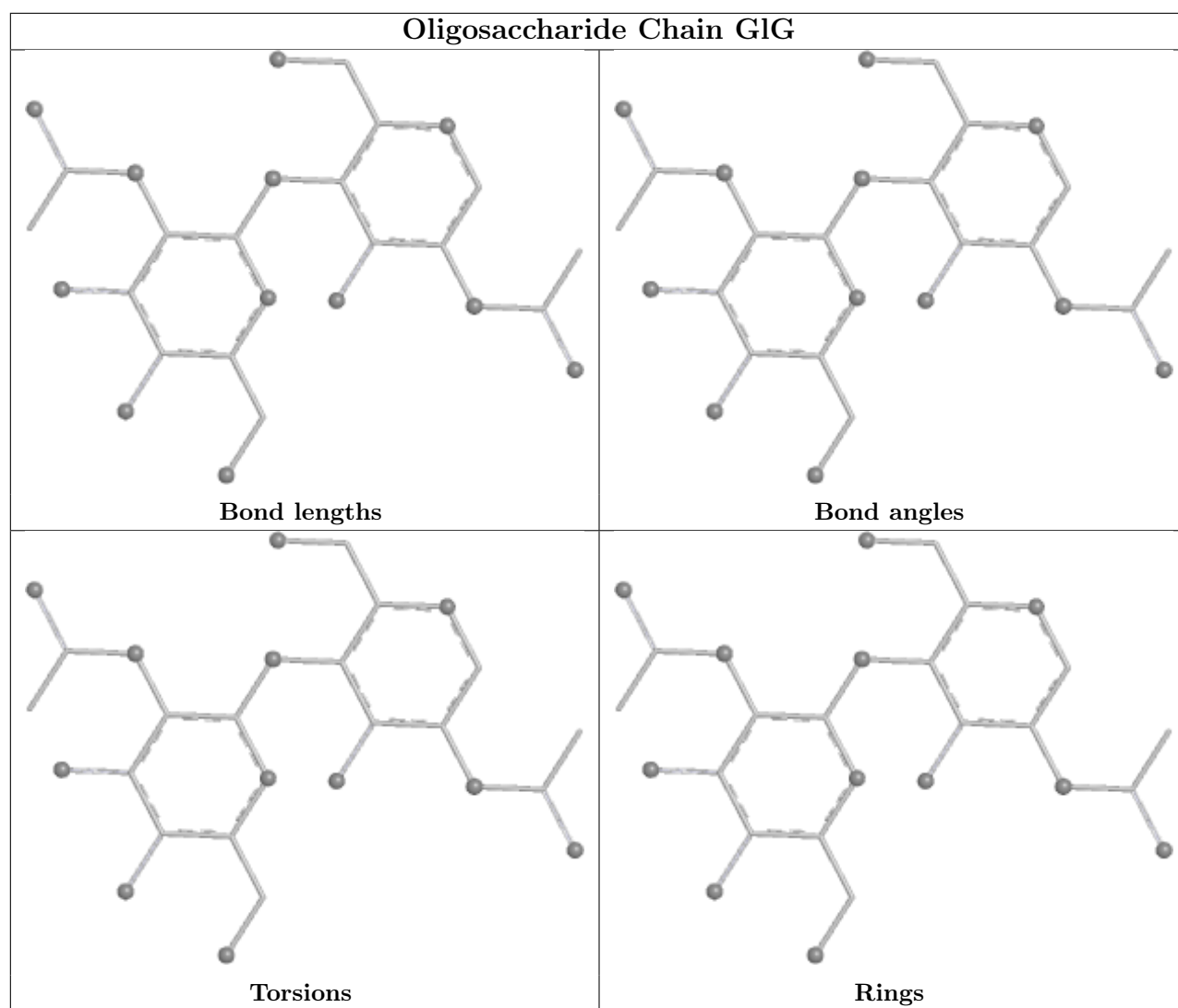


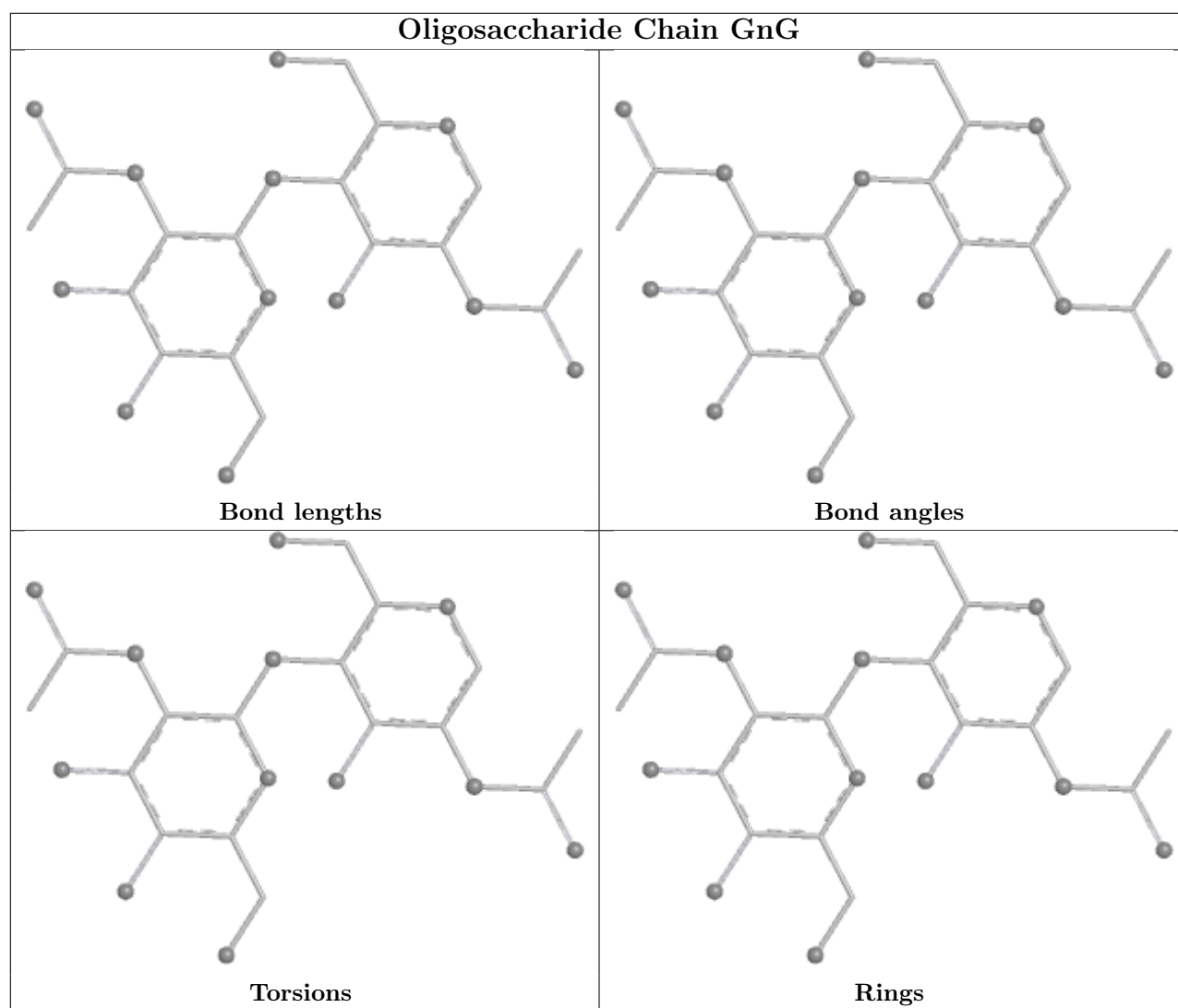


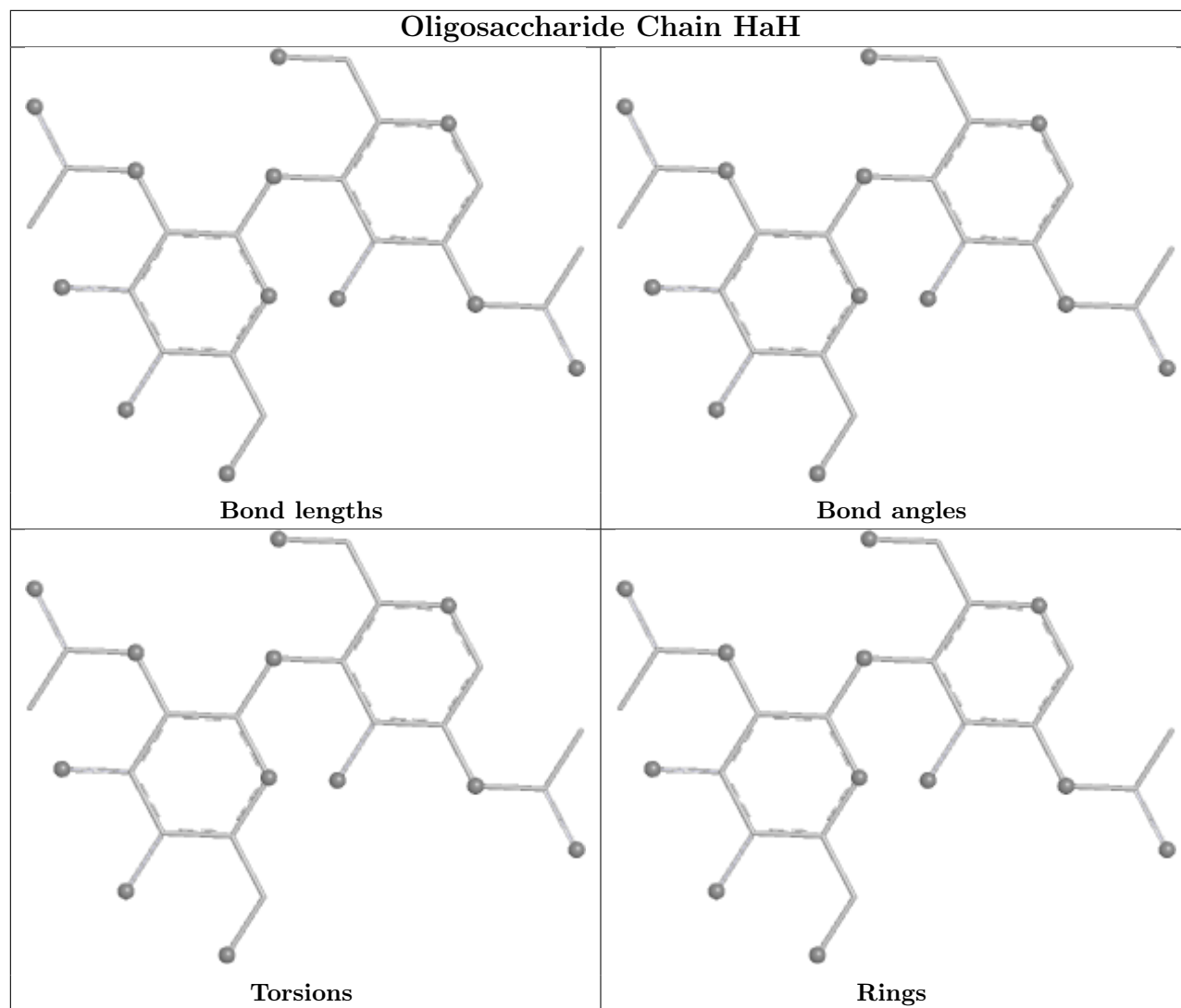




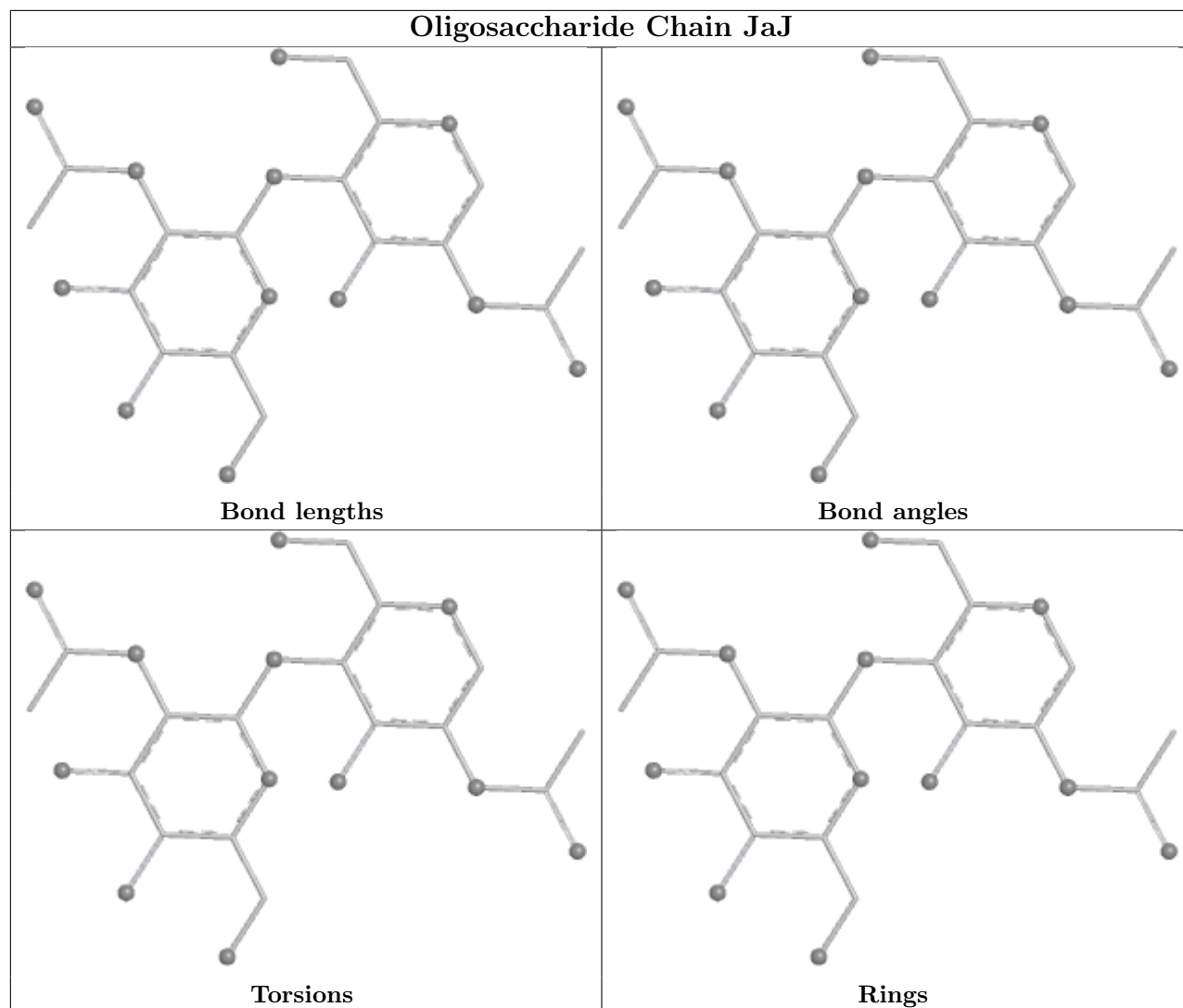




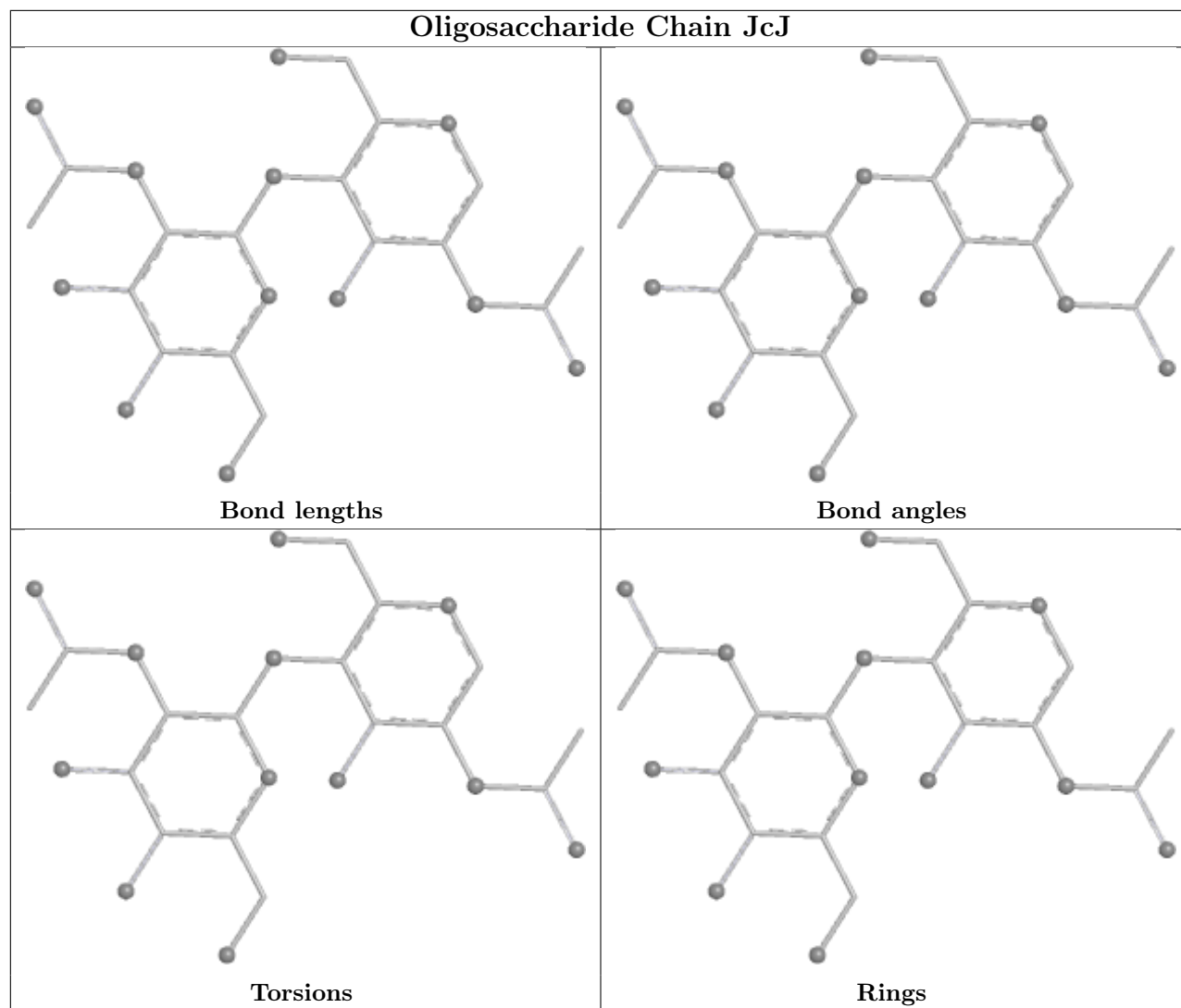




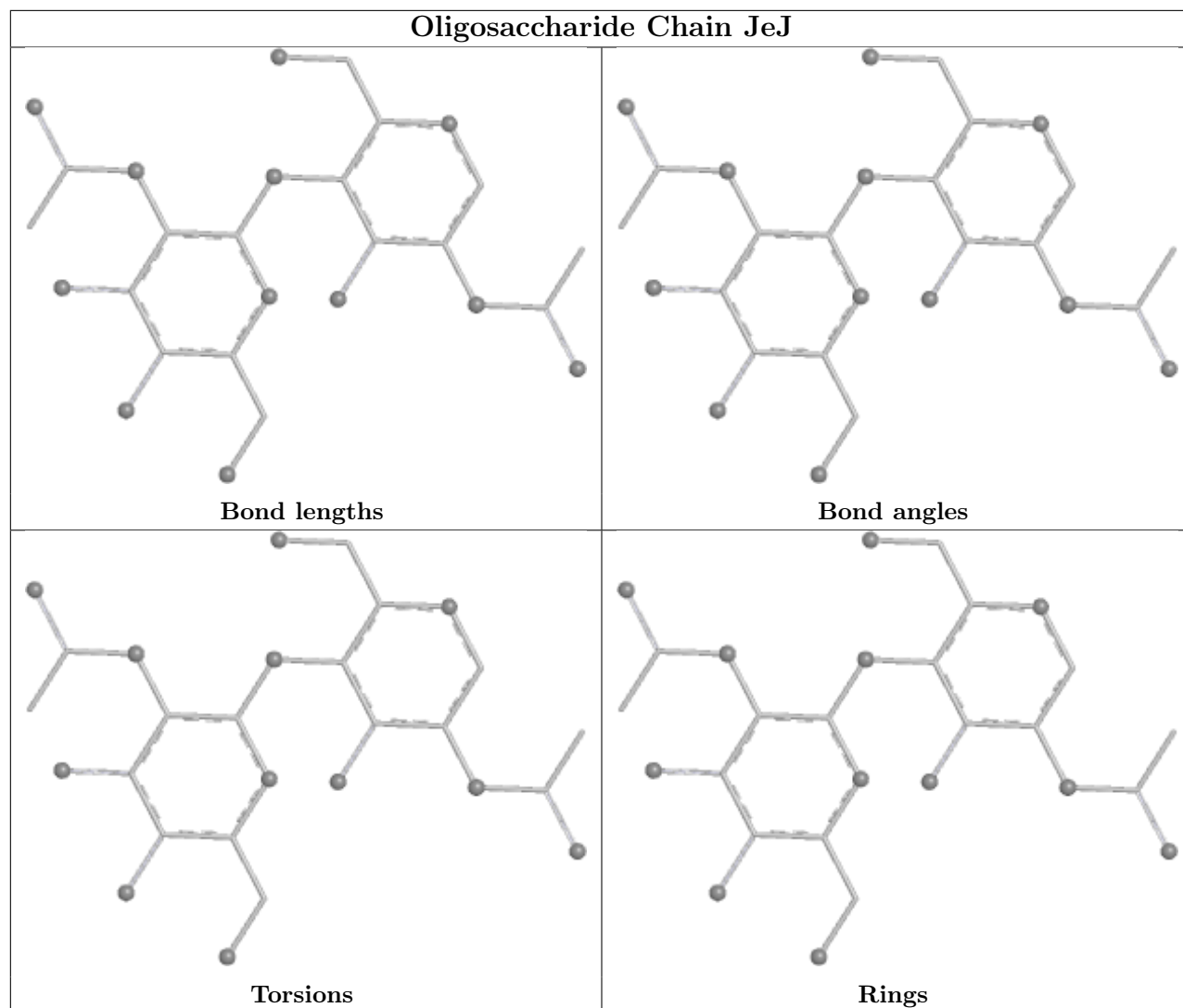
Oligosaccharide Chain JaJ



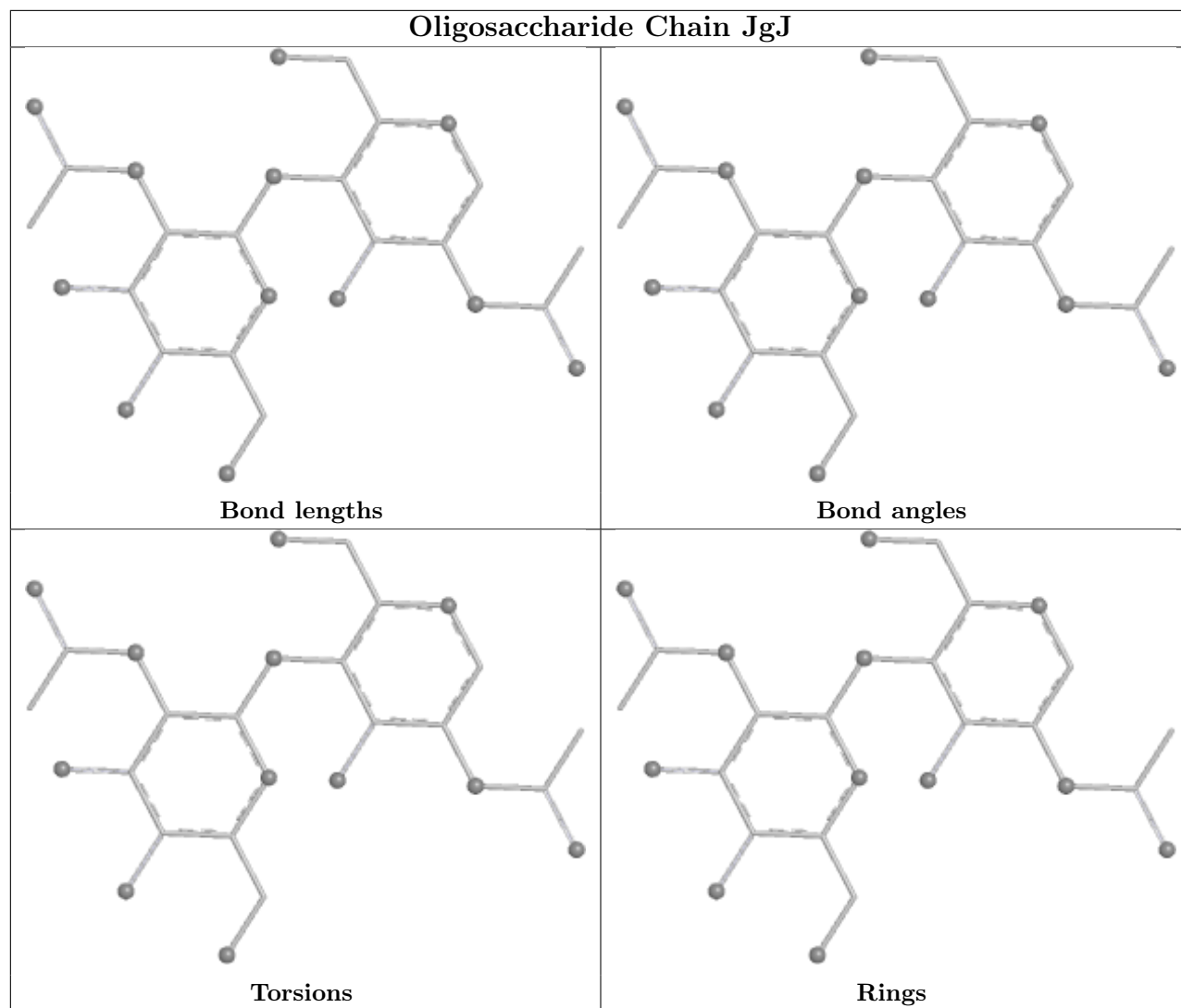
Oligosaccharide Chain JcJ



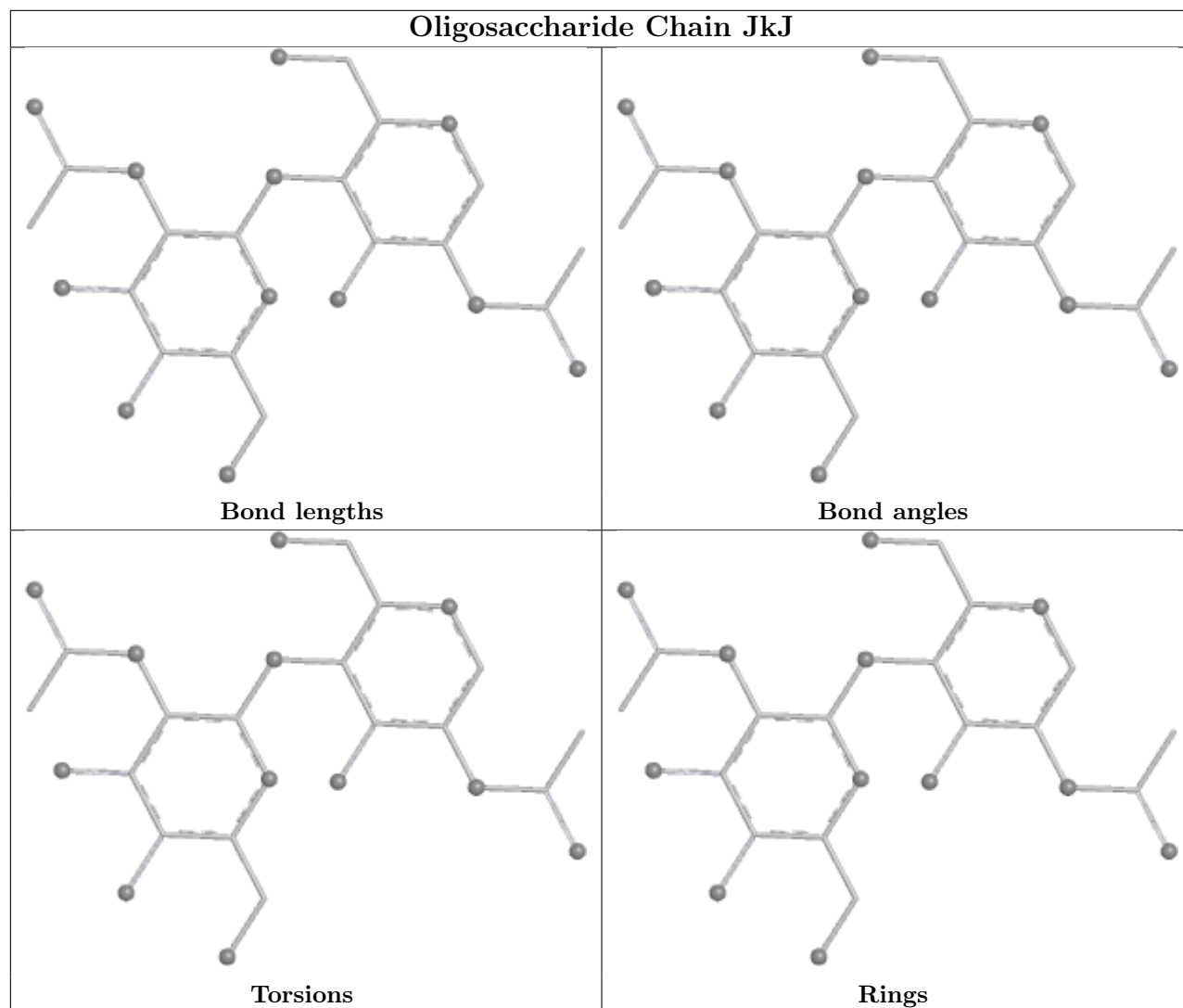
Oligosaccharide Chain JeJ

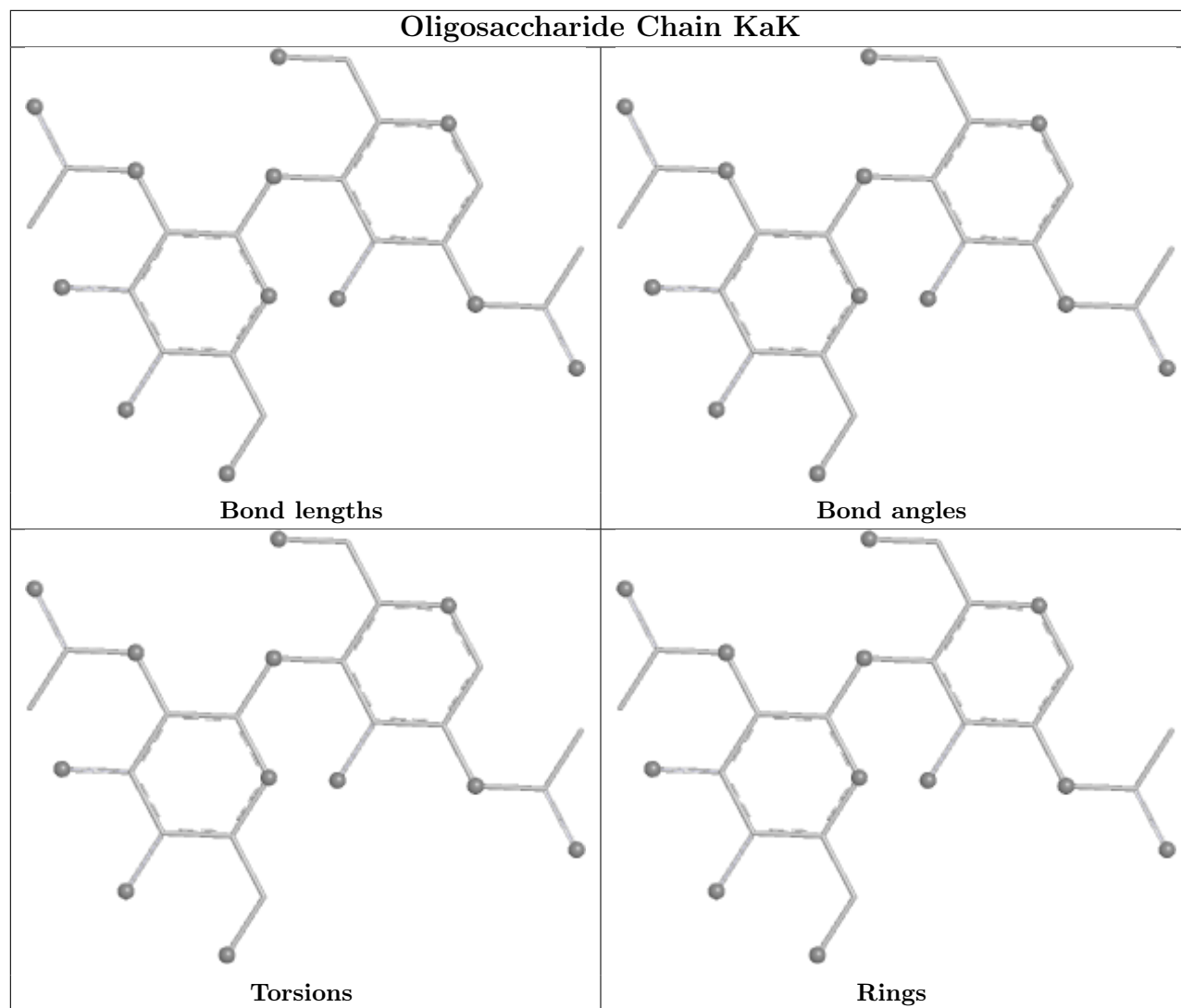


Oligosaccharide Chain JgJ

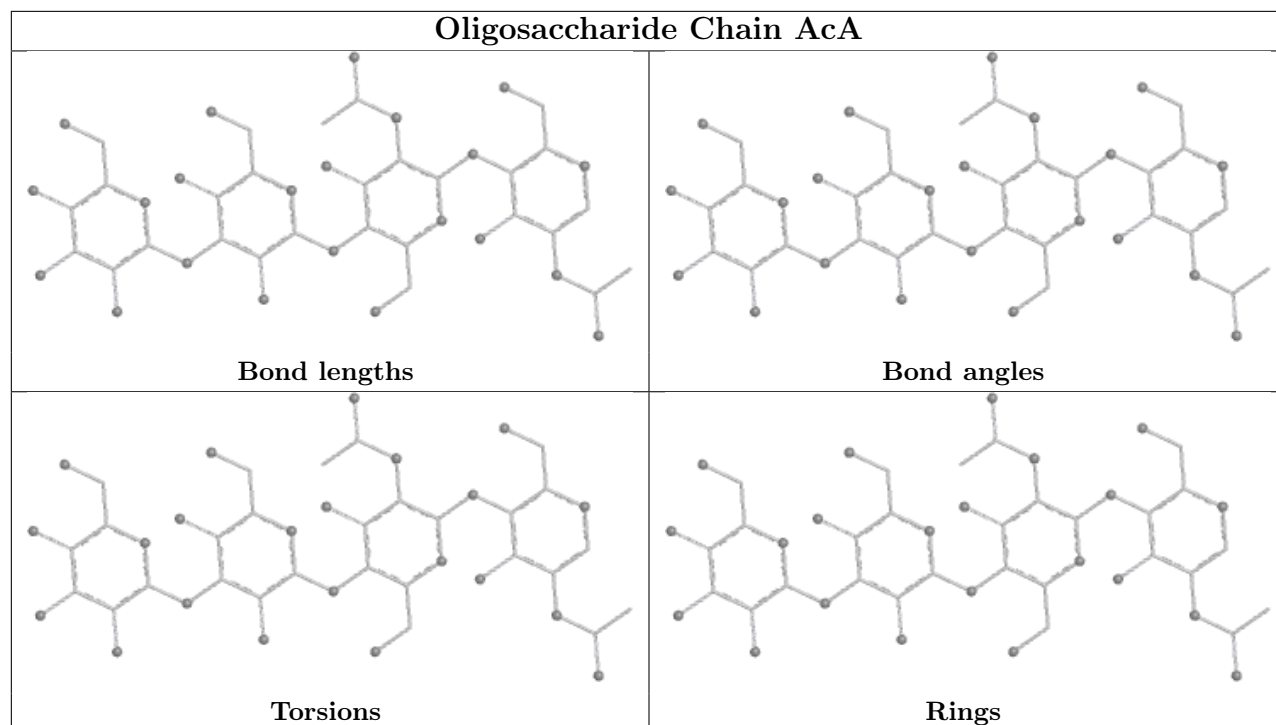


Oligosaccharide Chain JkJ

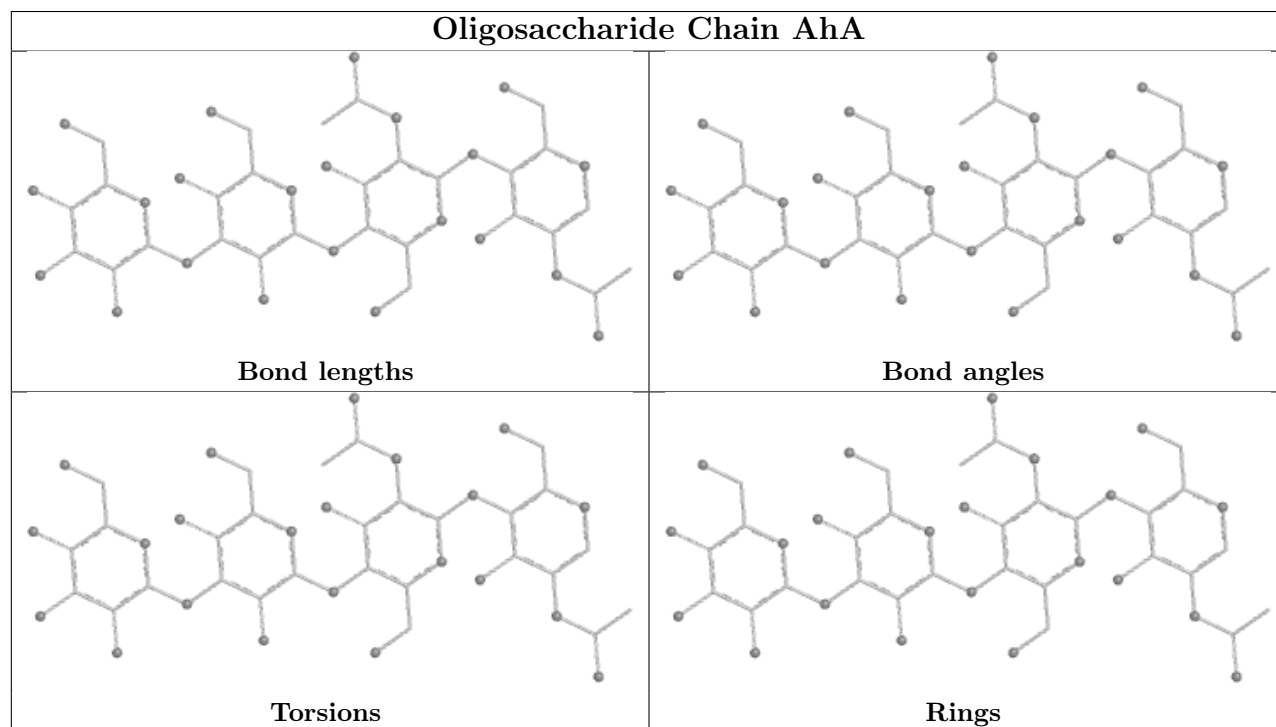


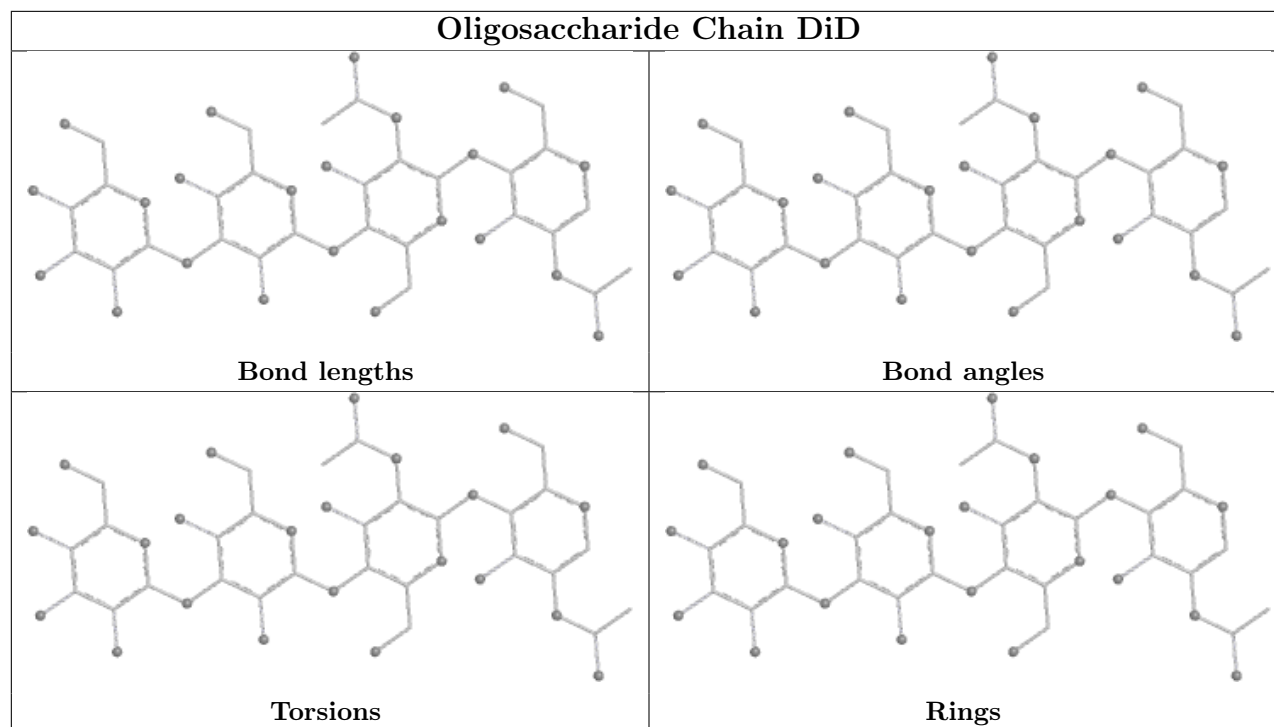


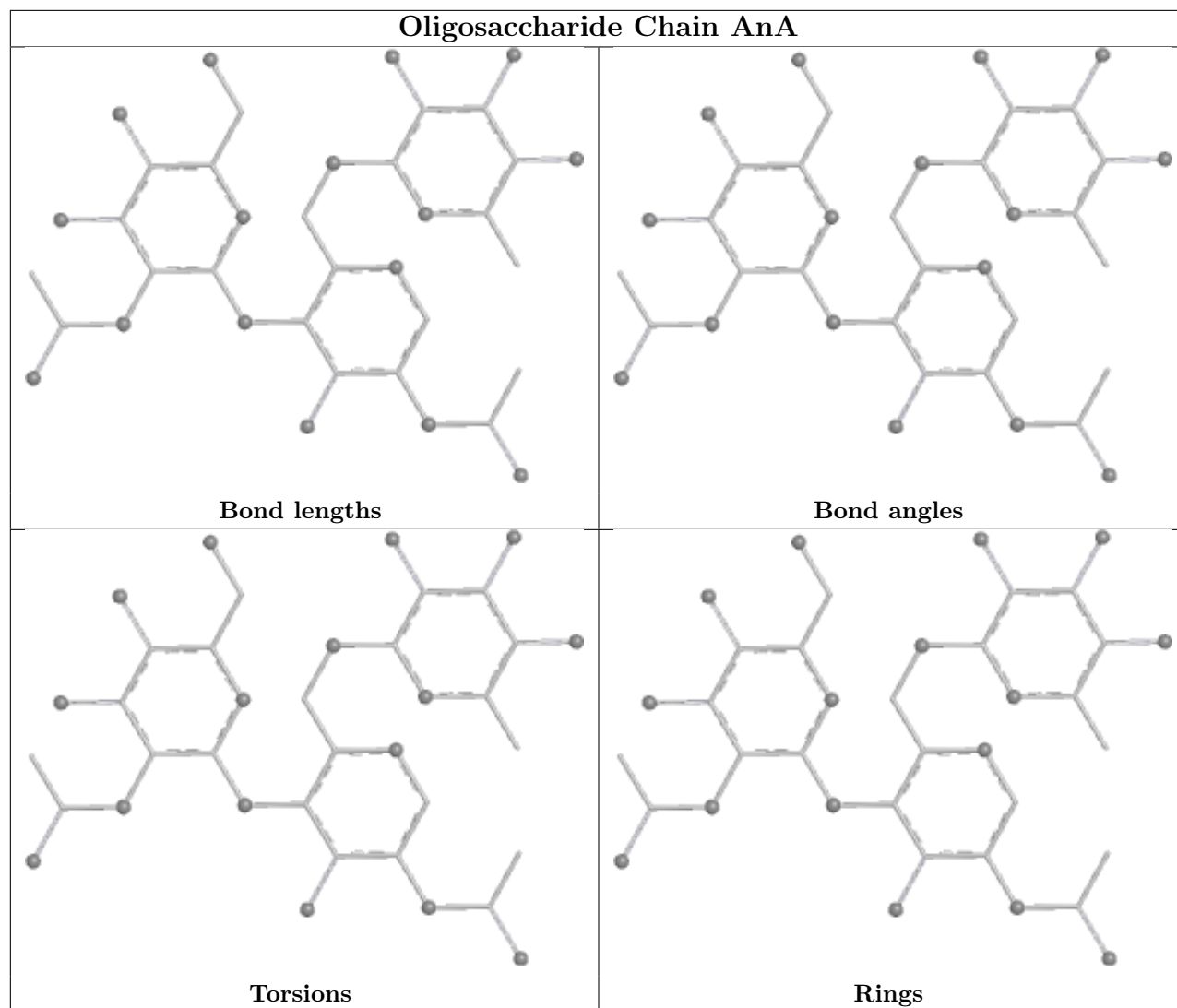
Oligosaccharide Chain AcA



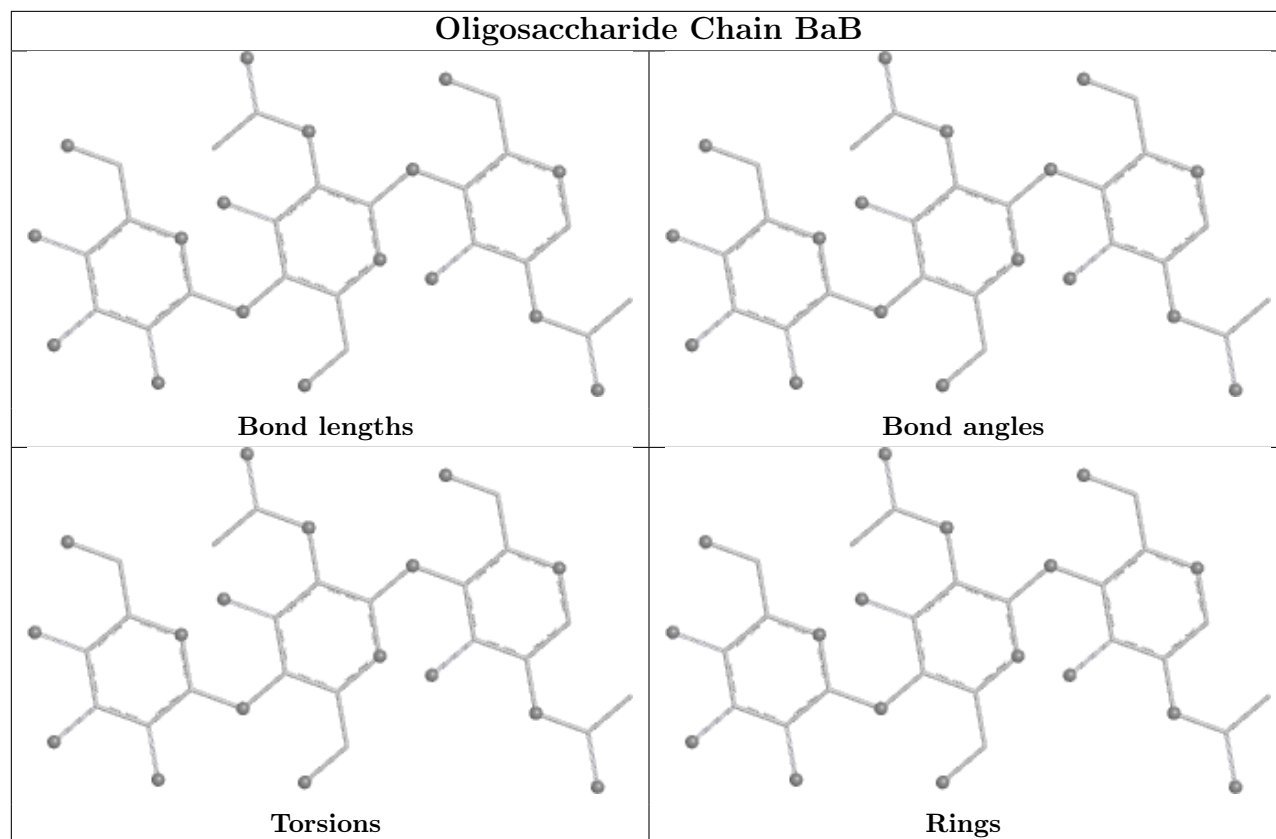
Oligosaccharide Chain AhA



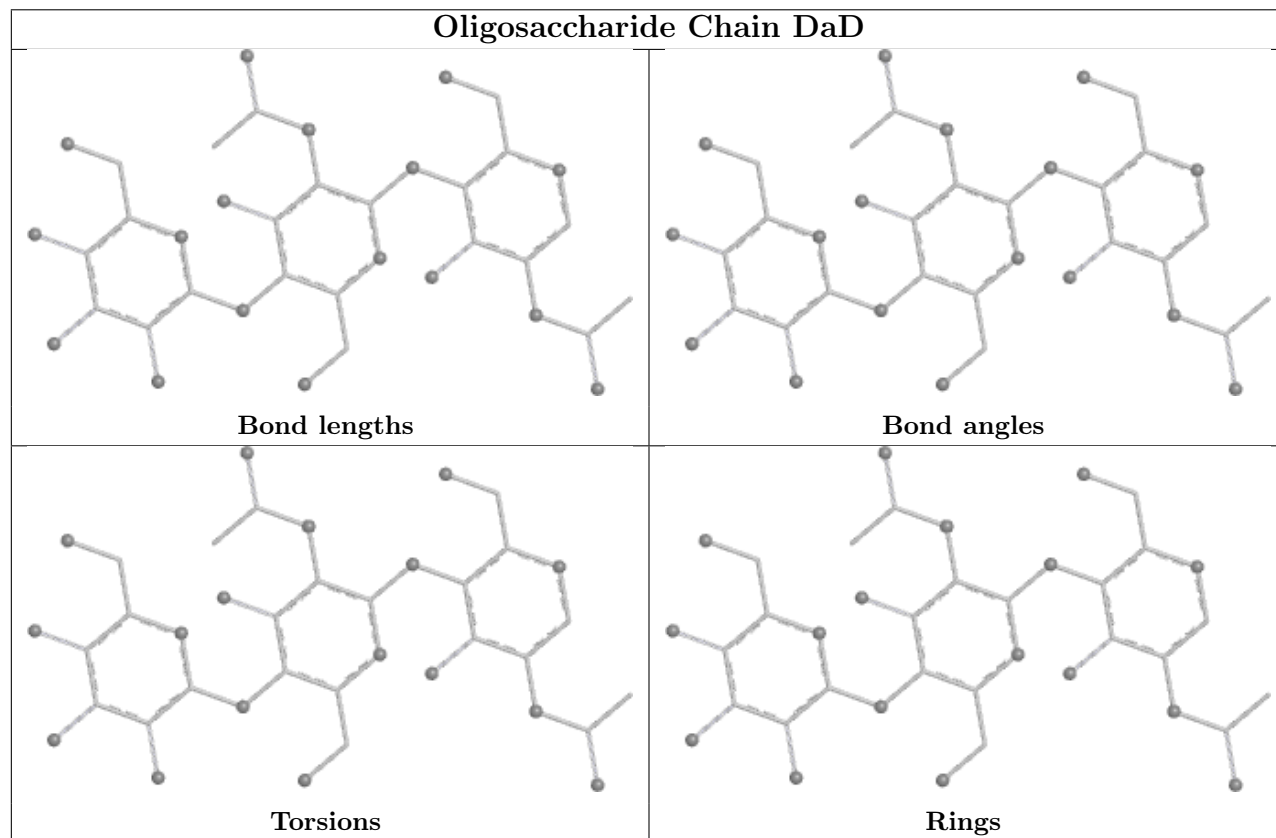




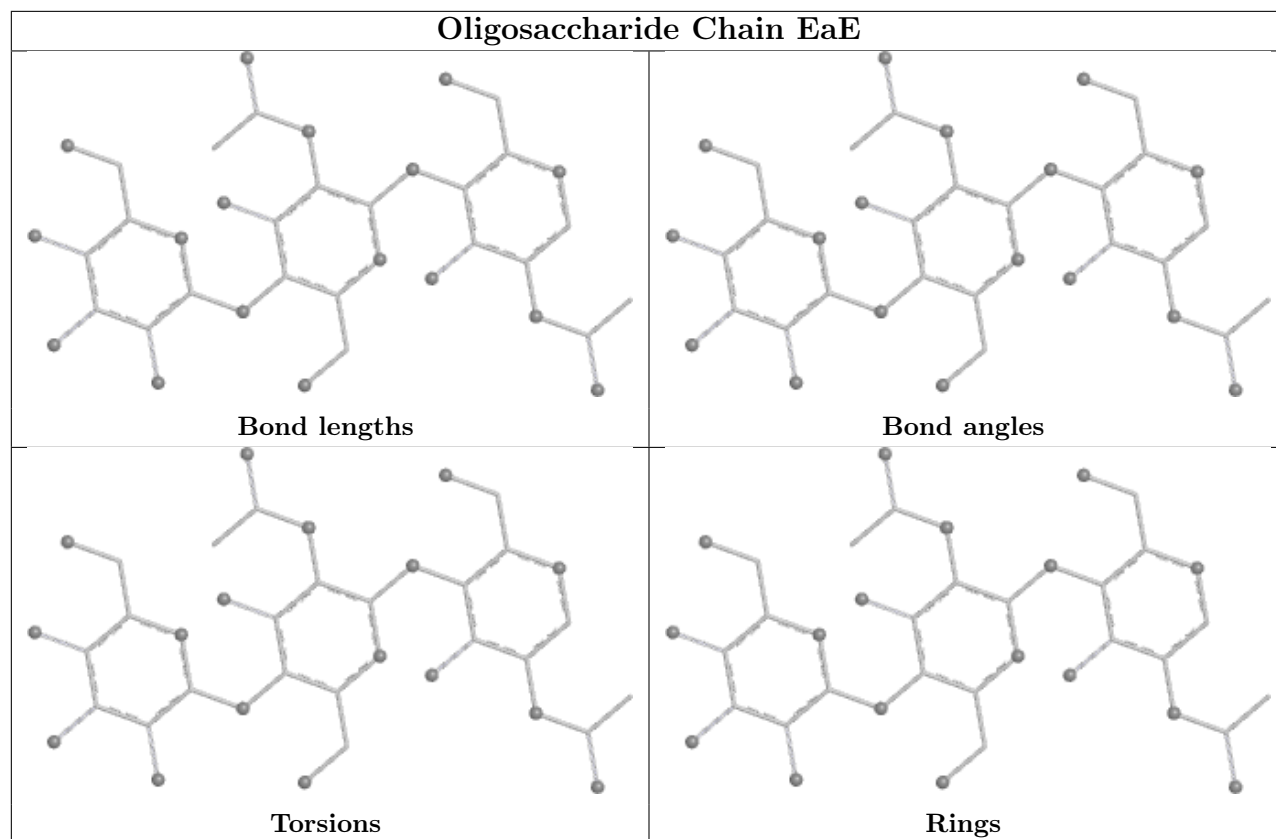
Oligosaccharide Chain BaB



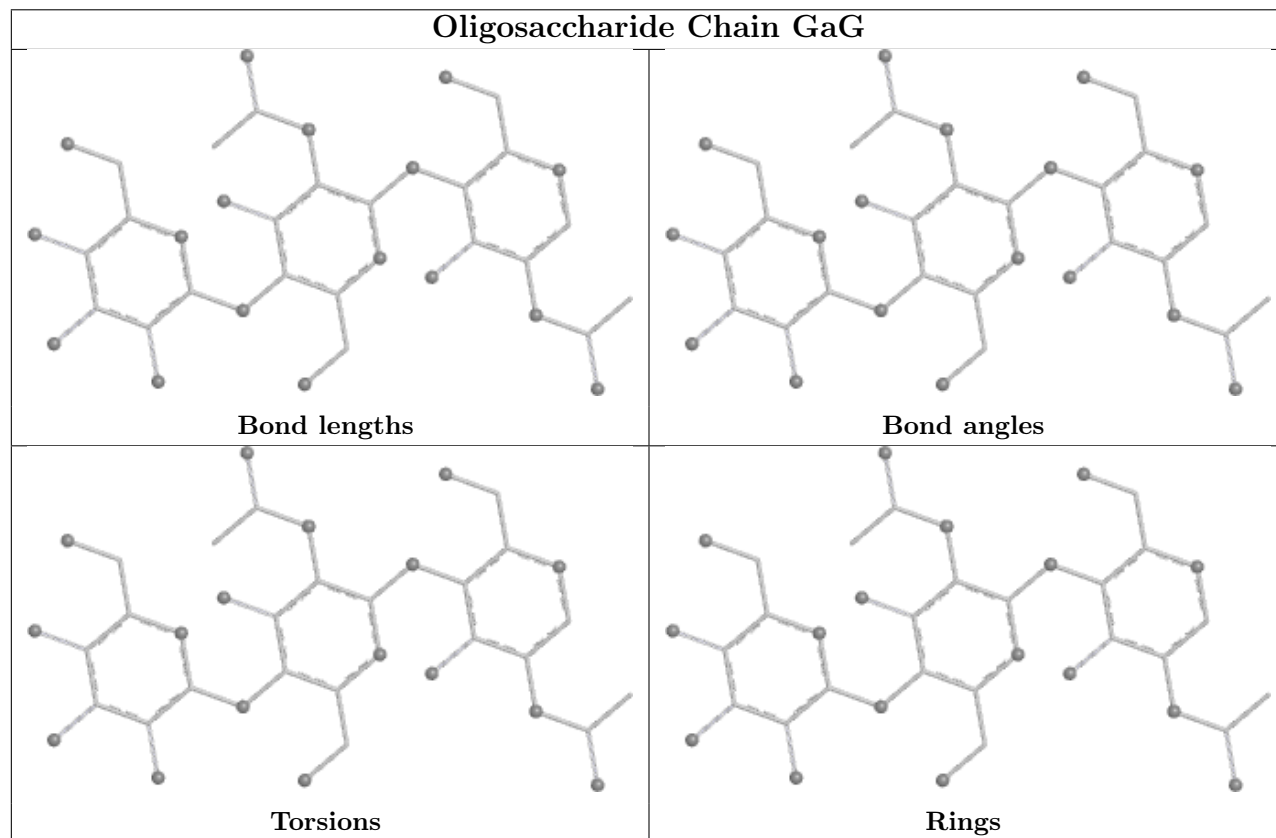
Oligosaccharide Chain DaD



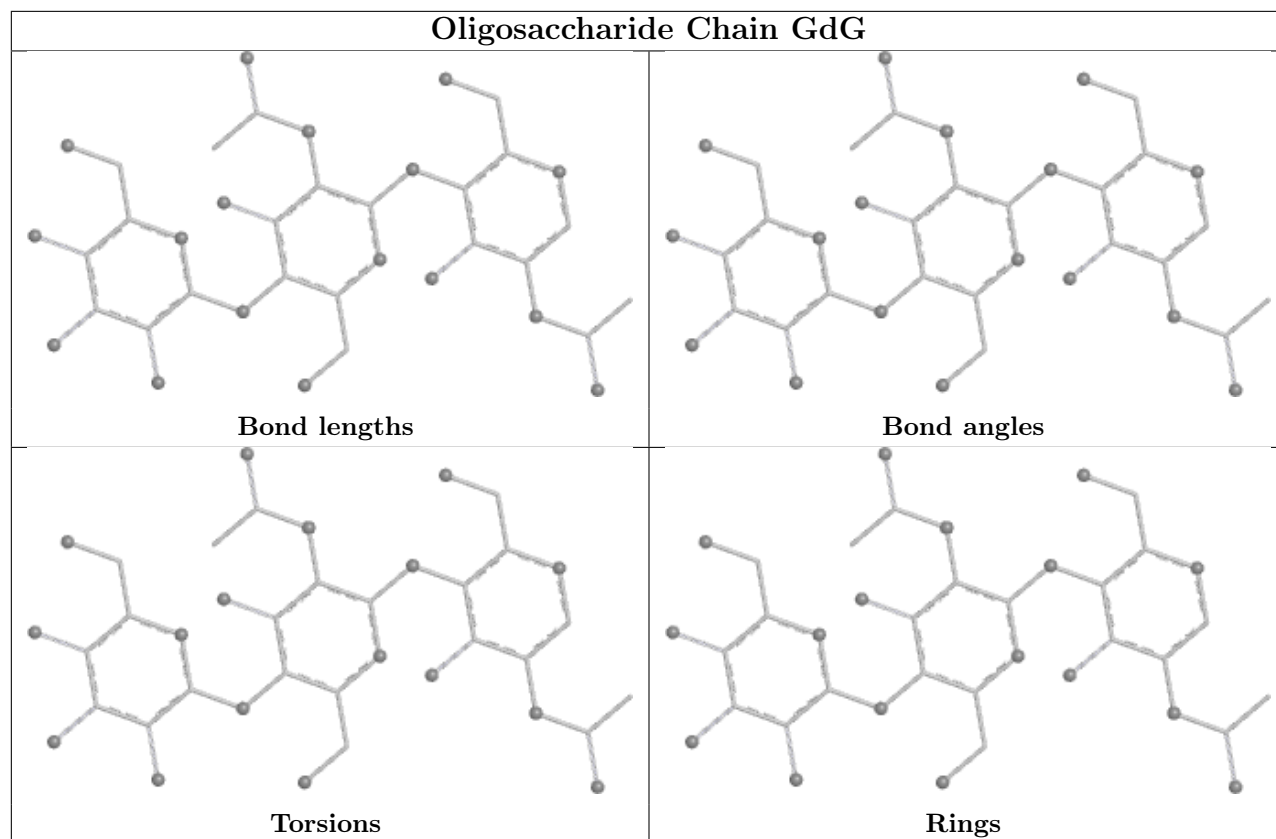
Oligosaccharide Chain EaE



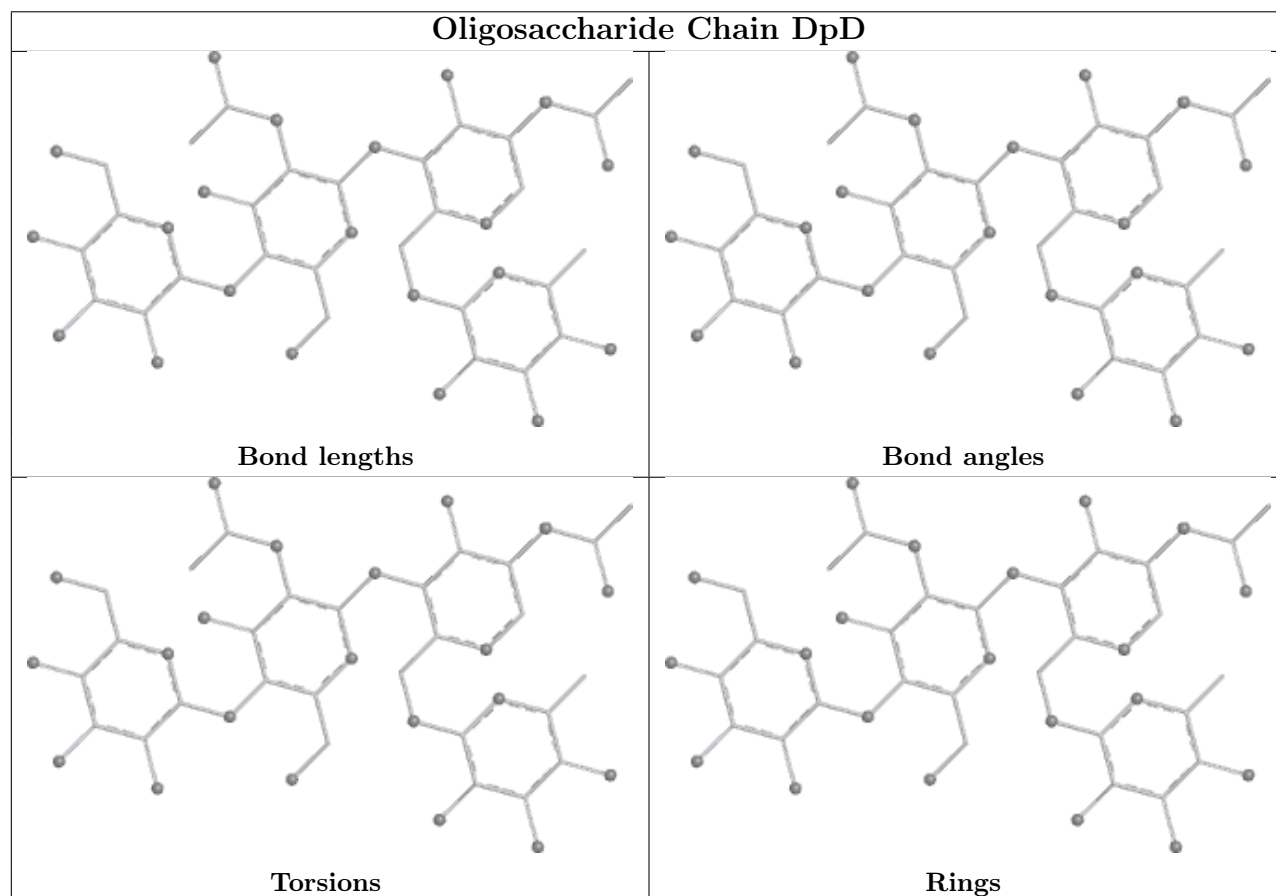
Oligosaccharide Chain GaG

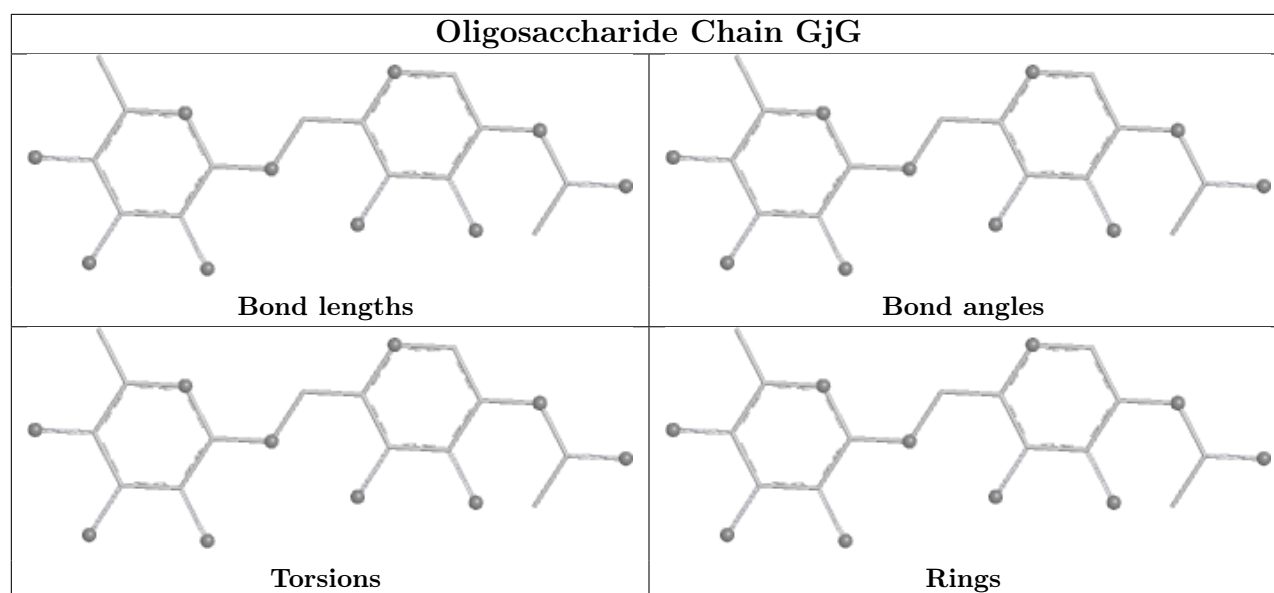


Oligosaccharide Chain GdG



Oligosaccharide Chain DpD





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	EEE	301	2	14,14,15	0.55	0	17,19,21	0.97	0
11	NAG	HHH	301	2	14,14,15	0.39	0	17,19,21	1.43	2 (11%)
11	NAG	JJJ	703	1	14,14,15	0.61	0	17,19,21	1.24	2 (11%)
11	NAG	AAA	702	1	14,14,15	0.49	0	17,19,21	1.06	1 (5%)
11	NAG	DDD	701	1	14,14,15	0.47	0	17,19,21	0.99	0
11	NAG	BBB	301	2	14,14,15	0.42	0	17,19,21	1.45	2 (11%)
11	NAG	GGG	701	1	14,14,15	0.66	0	17,19,21	1.32	2 (11%)
11	NAG	JJJ	701	1	14,14,15	0.49	0	17,19,21	1.00	0
11	NAG	JJJ	702	1	14,14,15	0.40	0	17,19,21	1.27	2 (11%)
10	MAN	AAA	701	-	11,11,12	0.53	0	15,15,17	0.48	0
11	NAG	JJJ	704	1	14,14,15	0.49	0	17,19,21	1.04	1 (5%)
11	NAG	DDD	702	1	14,14,15	0.56	0	17,19,21	1.13	2 (11%)
11	NAG	BBB	302	2	14,14,15	0.75	0	17,19,21	2.22	6 (35%)

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	EEE	301	2	-	0/6/23/26	0/1/1/1
11	NAG	HHH	301	2	-	2/6/23/26	0/1/1/1
11	NAG	JJJ	703	1	-	2/6/23/26	0/1/1/1
11	NAG	AAA	702	1	-	2/6/23/26	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	GGG	701	1	-	2/6/23/26	0/1/1/1
11	NAG	JJJ	701	1	-	1/6/23/26	0/1/1/1
11	NAG	JJJ	702	1	-	2/6/23/26	0/1/1/1
10	MAN	AAA	701	-	-	2/2/19/22	0/1/1/1
11	NAG	JJJ	704	1	-	2/6/23/26	0/1/1/1
11	NAG	DDD	702	1	-	2/6/23/26	0/1/1/1
11	NAG	BBB	302	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	BBB	302	NAG	O5-C1-C2	-5.02	103.53	111.29
11	BBB	302	NAG	C1-O5-C5	4.53	118.25	112.19
11	BBB	301	NAG	C1-C2-N2	-3.94	104.22	110.43
11	HHH	301	NAG	C1-C2-N2	-3.91	104.27	110.43
11	BBB	302	NAG	C1-C2-N2	3.57	116.06	110.43
11	JJJ	702	NAG	C1-O5-C5	3.50	116.88	112.19
11	HHH	301	NAG	C1-O5-C5	3.46	116.82	112.19
11	BBB	301	NAG	C1-O5-C5	3.02	116.23	112.19
11	JJJ	703	NAG	C1-O5-C5	3.00	116.21	112.19
11	JJJ	703	NAG	O5-C1-C2	-2.96	106.71	111.29
11	GGG	701	NAG	O5-C1-C2	-2.90	106.81	111.29
11	GGG	701	NAG	C1-O5-C5	2.89	116.06	112.19
11	DDD	702	NAG	C1-O5-C5	2.83	115.98	112.19
11	JJJ	702	NAG	O5-C1-C2	-2.51	107.41	111.29
11	JJJ	704	NAG	C1-C2-N2	2.50	114.37	110.43
11	BBB	302	NAG	C4-C3-C2	-2.49	107.37	111.02
11	BBB	302	NAG	C8-C7-N2	2.46	120.21	116.12
11	BBB	302	NAG	C6-C5-C4	-2.34	107.27	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AAA	702	NAG	C1-O5-C5	2.11	115.02	112.19
11	DDD	702	NAG	O5-C1-C2	-2.02	108.16	111.29

There are no chirality outliers.

All (24) 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	JJJ	703	NAG	O5-C5-C6-O6
11	BBB	302	NAG	O5-C5-C6-O6
11	JJJ	703	NAG	C4-C5-C6-O6
11	AAA	702	NAG	C4-C5-C6-O6
11	JJJ	702	NAG	O5-C5-C6-O6
11	DDD	702	NAG	C4-C5-C6-O6
11	HHH	301	NAG	O5-C5-C6-O6
11	DDD	701	NAG	C4-C5-C6-O6
11	GGG	701	NAG	O5-C5-C6-O6
11	GGG	701	NAG	C4-C5-C6-O6
11	BBB	302	NAG	C8-C7-N2-C2
11	BBB	302	NAG	O7-C7-N2-C2
11	HHH	301	NAG	C4-C5-C6-O6
11	JJJ	704	NAG	O5-C5-C6-O6
11	JJJ	702	NAG	C4-C5-C6-O6
11	JJJ	701	NAG	O5-C5-C6-O6
10	AAA	701	MAN	C4-C5-C6-O6
10	AAA	701	MAN	O5-C5-C6-O6
11	JJJ	704	NAG	C1-C2-N2-C7
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

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	594/617 (96%)	0.38	15 (2%) 58 49	25, 52, 79, 136	1 (0%)
1	DDD	594/617 (96%)	0.37	18 (3%) 52 44	24, 51, 73, 125	1 (0%)
1	GGG	594/617 (96%)	0.47	20 (3%) 48 39	40, 58, 83, 132	0
1	JJJ	593/617 (96%)	0.52	23 (3%) 43 35	28, 60, 87, 112	1 (0%)
2	BBB	185/203 (91%)	0.36	1 (0%) 87 83	28, 52, 73, 98	1 (0%)
2	EEE	185/203 (91%)	0.40	6 (3%) 50 41	30, 55, 75, 94	2 (1%)
2	HHH	185/203 (91%)	0.43	3 (1%) 70 63	35, 57, 80, 93	2 (1%)
2	KKK	185/203 (91%)	0.40	3 (1%) 70 63	31, 57, 77, 91	2 (1%)
3	CCC	10/12 (83%)	1.36	3 (30%) 1 1	44, 57, 95, 97	0
3	FFF	10/12 (83%)	1.31	3 (30%) 1 1	46, 55, 99, 101	0
3	III	9/12 (75%)	0.79	2 (22%) 2 2	51, 55, 74, 82	0
3	LLL	9/12 (75%)	0.76	1 (11%) 10 9	50, 59, 74, 88	0
All	All	3153/3328 (94%)	0.43	98 (3%) 51 42	24, 55, 82, 136	10 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	285[A]	SER	5.9
1	JJJ	599	CYS	4.9
3	FFF	110	LEU	4.2
1	JJJ	468	ASP	4.0
3	CCC	109	ARG	3.9
3	FFF	109	ARG	3.8
1	JJJ	21	PHE	3.6
1	AAA	42	SER	3.5
3	III	110	LEU	3.5
1	DDD	582	SER	3.4
1	GGG	582	SER	3.4

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Mol	Chain	Res	Type	RSRZ
3	CCC	110	LEU	3.3
1	AAA	587	MET	3.2
1	DDD	601	ASP	3.1
1	JJJ	444	SER	3.0
1	DDD	43	ASN	3.0
1	JJJ	586	ASP	3.0
1	JJJ	25	GLN	3.0
1	JJJ	60	SER	3.0
1	GGG	77	PRO	2.9
1	AAA	48	CYS	2.9
1	AAA	605	LEU	2.8
1	DDD	583	LEU	2.8
1	GGG	586	ASP	2.8
1	DDD	599	CYS	2.7
1	GGG	320	ILE	2.7
1	JJJ	58	ASP	2.7
1	GGG	601	ASP	2.7
1	JJJ	601	ASP	2.7
1	AAA	14	SER	2.7
2	KKK	188	SER	2.7
1	DDD	485	PRO	2.7
1	AAA	602	ILE	2.6
3	FFF	111	VAL	2.6
1	GGG	489	MET	2.6
1	GGG	583	LEU	2.6
1	JJJ	605	LEU	2.6
1	DDD	58	ASP	2.6
3	LLL	110	LEU	2.6
1	AAA	582	SER	2.6
1	JJJ	76	PHE	2.6
1	DDD	13	SER	2.5
1	GGG	13	SER	2.5
3	CCC	111	VAL	2.5
1	GGG	414	THR	2.5
1	JJJ	582	SER	2.5
1	GGG	605	LEU	2.5
1	AAA	578	ASP	2.5
1	AAA	601	ASP	2.5
1	JJJ	13	SER	2.5
2	KKK	112	ASN	2.5
1	DDD	586	ASP	2.4
1	JJJ	285[A]	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	AAA	21	PHE	2.4
1	GGG	444	SER	2.4
1	JJJ	59	PHE	2.4
1	DDD	579	LEU	2.4
1	DDD	49	ARG	2.3
1	GGG	576	SER	2.3
1	JJJ	464	ILE	2.3
1	GGG	580	PRO	2.3
1	DDD	42	SER	2.3
2	EEE	208	HIS	2.3
2	EEE	59	THR	2.3
2	EEE	207	SER	2.3
2	HHH	111	SER	2.3
2	KKK	211	PRO	2.3
1	JJJ	343	ASP	2.3
1	AAA	564	LYS	2.3
2	EEE	84	HIS	2.3
1	AAA	60	SER	2.3
2	EEE	141	SER	2.3
1	DDD	469	ASN	2.2
1	DDD	220	GLN	2.2
2	HHH	84	HIS	2.2
1	JJJ	39	SER	2.2
2	BBB	211	PRO	2.2
1	GGG	603	LYS	2.2
1	AAA	285[A]	SER	2.2
1	GGG	149	PRO	2.2
1	DDD	578	ASP	2.2
1	DDD	15	MET	2.2
1	JJJ	28	LEU	2.2
1	AAA	586	ASP	2.1
1	DDD	60	SER	2.1
2	HHH	208	HIS	2.1
1	JJJ	42	SER	2.1
1	GGG	43	ASN	2.1
2	EEE	111	SER	2.1
1	JJJ	603	LYS	2.1
1	GGG	15	MET	2.0
1	AAA	67	LEU	2.0
1	GGG	60	SER	2.0
1	JJJ	242	VAL	2.0
1	GGG	606	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	GGG	58	ASP	2.0
1	JJJ	394	ASP	2.0
3	III	111	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	HYP	FFF	112	8/9	0.77	0.15	65,69,72,73	0
3	HYP	III	112	8/9	0.85	0.12	72,73,76,79	0
3	HYP	CCC	112	8/9	0.87	0.10	63,67,69,70	0
3	HYP	III	115	8/9	0.92	0.11	63,65,67,69	0
3	HYP	FFF	115	8/9	0.93	0.10	53,54,55,56	0
3	HYP	LLL	112	8/9	0.93	0.10	67,69,71,73	0
3	HYP	LLL	115	8/9	0.94	0.09	56,63,64,65	0
3	HYP	CCC	115	8/9	0.95	0.10	55,58,59,59	0

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	AaA	1	14/15	-	-	53,64,68,76	0
4	NAG	AaA	2	14/15	-	-	82,93,99,101	0
4	NAG	AlA	1	14/15	-	-	58,69,73,81	0
4	NAG	AlA	2	14/15	-	-	101,107,109,110	0
4	NAG	AqA	1	14/15	-	-	59,67,75,86	0
4	NAG	AqA	2	14/15	-	-	90,99,103,105	0
4	NAG	AsA	1	14/15	-	-	58,64,70,77	0
4	NAG	AsA	2	14/15	-	-	77,95,99,102	0
4	NAG	DeD	1	14/15	-	-	53,61,65,72	0
4	NAG	DeD	2	14/15	-	-	79,91,98,102	0
4	NAG	DgD	1	14/15	-	-	65,72,82,84	0
4	NAG	DgD	2	14/15	-	-	96,103,113,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	DmD	1	14/15	-	-	68,73,82,83	0
4	NAG	DmD	2	14/15	-	-	77,84,87,92	0
4	NAG	EdE	1	14/15	-	-	67,71,76,90	0
4	NAG	EdE	2	14/15	-	-	92,108,115,115	0
4	NAG	GgG	1	14/15	-	-	68,80,83,86	0
4	NAG	GgG	2	14/15	-	-	90,97,105,109	0
4	NAG	GlG	1	14/15	-	-	66,70,75,83	0
4	NAG	GlG	2	14/15	-	-	103,106,108,109	0
4	NAG	GnG	1	14/15	-	-	72,80,82,89	0
4	NAG	GnG	2	14/15	-	-	99,112,119,132	0
4	NAG	HaH	1	14/15	-	-	80,90,96,97	0
4	NAG	HaH	2	14/15	-	-	112,116,117,118	0
4	NAG	JaJ	1	14/15	-	-	49,54,57,60	0
4	NAG	JaJ	2	14/15	-	-	73,77,82,85	0
4	NAG	JcJ	1	14/15	-	-	52,69,76,78	0
4	NAG	JcJ	2	14/15	-	-	75,83,88,90	0
4	NAG	JeJ	1	14/15	-	-	71,80,90,92	0
4	NAG	JeJ	2	14/15	-	-	89,104,109,112	0
4	NAG	JgJ	1	14/15	-	-	74,81,84,86	0
4	NAG	JgJ	2	14/15	-	-	83,96,104,104	0
4	NAG	JkJ	1	14/15	-	-	80,89,96,103	0
4	NAG	JkJ	2	14/15	-	-	116,126,132,135	0
4	NAG	KaK	1	14/15	-	-	86,91,94,94	0
4	NAG	KaK	2	14/15	-	-	83,91,95,95	0
5	NAG	AcA	1	14/15	-	-	54,59,62,71	0
5	NAG	AcA	2	14/15	-	-	72,85,92,94	0
5	BMA	AcA	3	11/12	-	-	105,113,117,124	0
5	MAN	AcA	4	11/12	-	-	123,142,149,152	0
5	NAG	AhA	1	14/15	-	-	48,50,57,59	0
5	NAG	AhA	2	14/15	-	-	59,66,71,83	0
5	BMA	AhA	3	11/12	-	-	93,101,105,112	0
5	MAN	AhA	4	11/12	-	-	102,110,117,117	0
5	NAG	DiD	1	14/15	-	-	63,68,75,79	0
5	NAG	DiD	2	14/15	-	-	76,78,84,95	0
5	BMA	DiD	3	11/12	-	-	106,117,123,131	0
5	MAN	DiD	4	11/12	-	-	119,132,139,139	0
6	NAG	AnA	1	14/15	-	-	58,65,75,84	0
6	NAG	AnA	2	14/15	-	-	75,88,94,99	0
6	FUC	AnA	3	10/11	-	-	84,86,91,93	0
7	NAG	BaB	1	14/15	-	-	82,85,89,92	0
7	NAG	BaB	2	14/15	-	-	88,97,102,103	0
7	BMA	BaB	3	11/12	-	-	101,104,108,108	0

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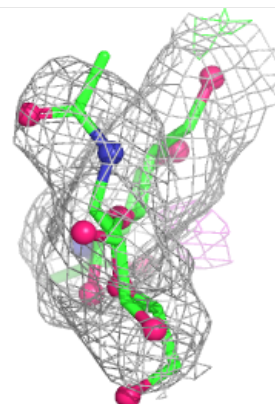
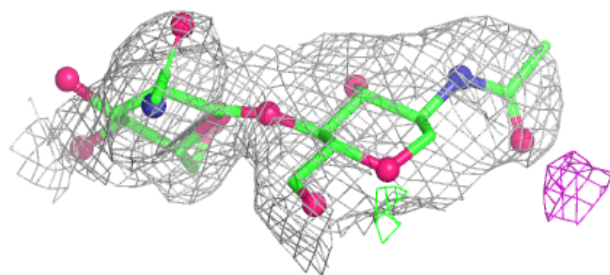
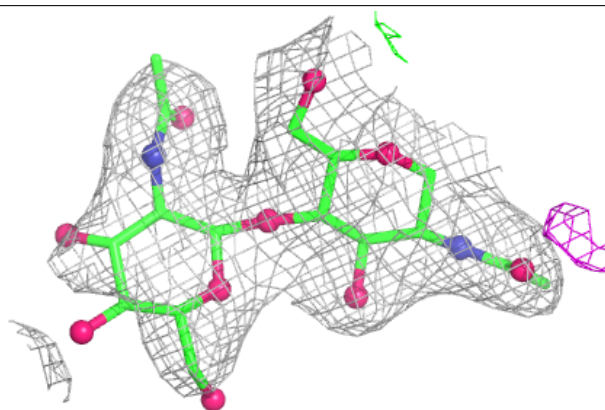
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	DaD	1	14/15	-	-	35,42,44,52	0
7	NAG	DaD	2	14/15	-	-	52,65,72,80	0
7	BMA	DaD	3	11/12	-	-	95,102,105,106	0
7	NAG	EaE	1	14/15	-	-	73,77,85,85	0
7	NAG	EaE	2	14/15	-	-	90,100,105,107	0
7	BMA	EaE	3	11/12	-	-	104,119,124,128	0
7	NAG	GaG	1	14/15	-	-	45,47,52,61	0
7	NAG	GaG	2	14/15	-	-	62,81,85,92	0
7	BMA	GaG	3	11/12	-	-	107,110,117,117	0
7	NAG	GdG	1	14/15	-	-	58,69,79,81	0
7	NAG	GdG	2	14/15	-	-	80,95,101,110	0
7	BMA	GdG	3	11/12	-	-	102,112,117,121	0
8	NAG	DpD	1	14/15	-	-	60,63,74,77	0
8	NAG	DpD	2	14/15	-	-	85,91,102,113	0
8	BMA	DpD	3	11/12	-	-	108,118,124,131	0
8	FUC	DpD	4	10/11	-	-	92,95,98,98	0
9	NAG	GjG	1	14/15	-	-	75,79,88,95	0
9	FUC	GjG	2	10/11	-	-	105,112,116,120	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.

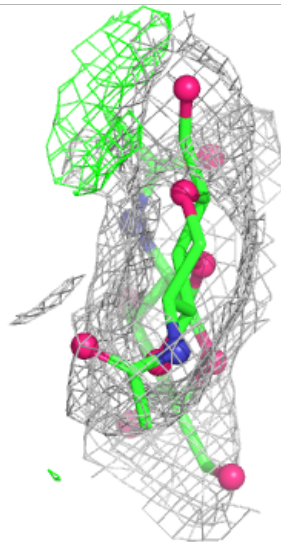
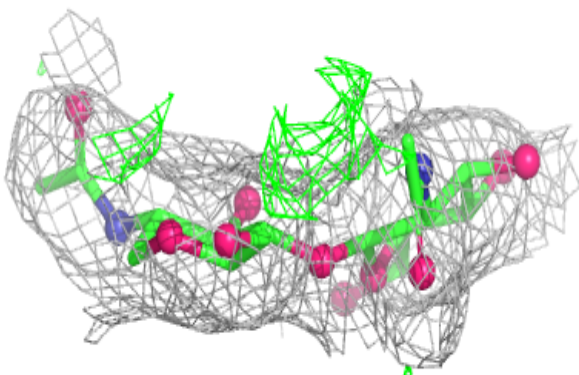
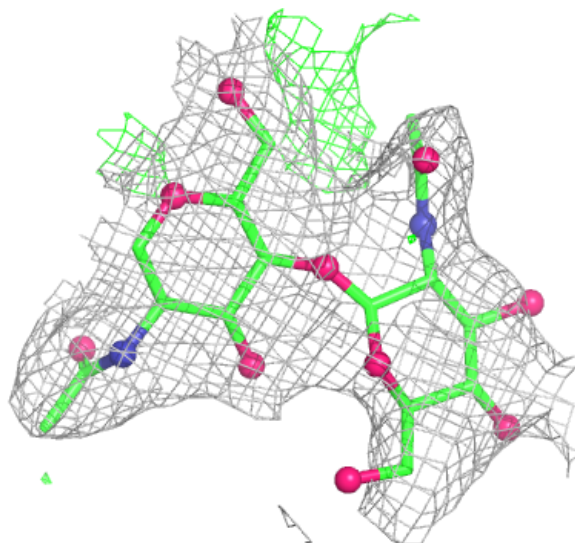
Electron density around Chain AaA:

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



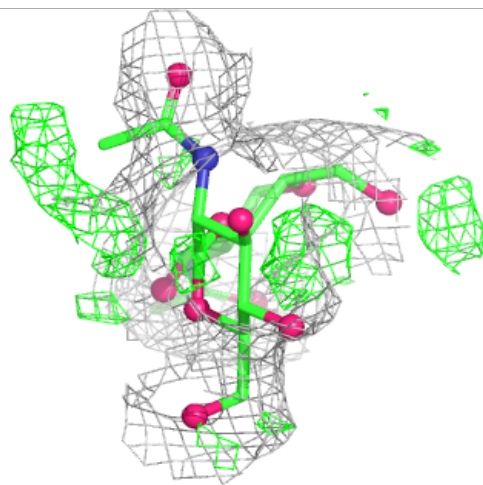
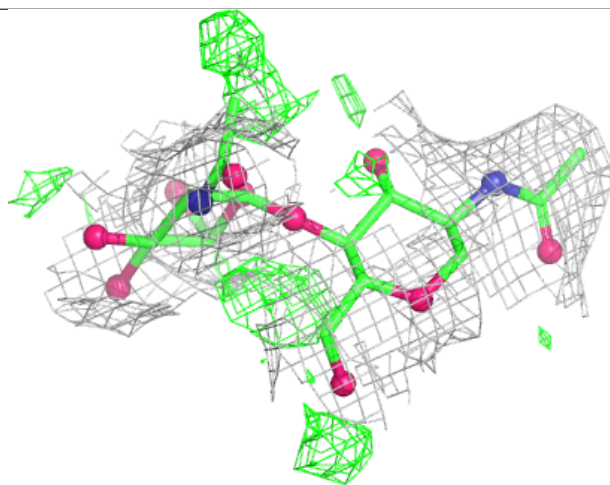
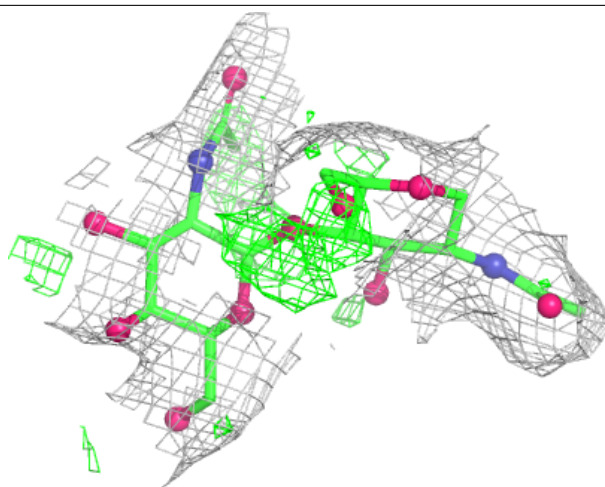
Electron density around Chain A1A:

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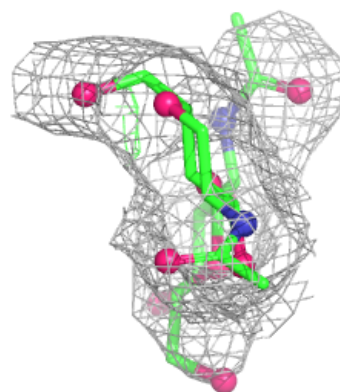
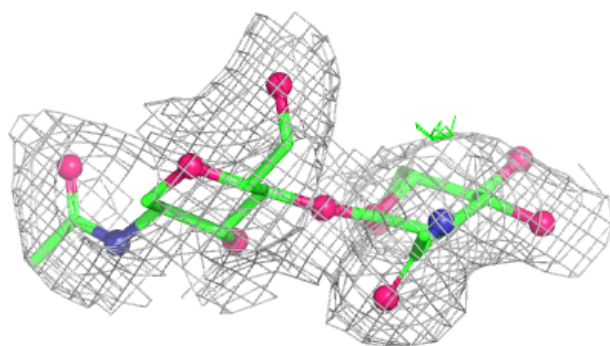
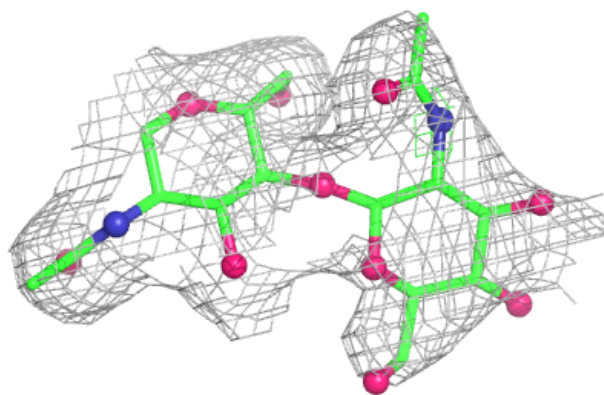
Electron density around Chain AqA:

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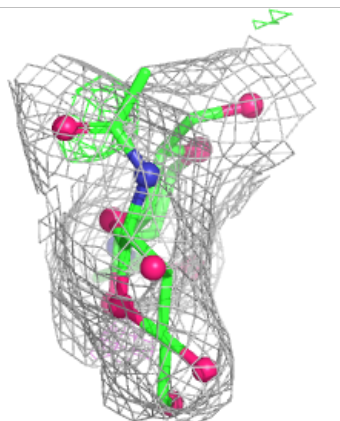
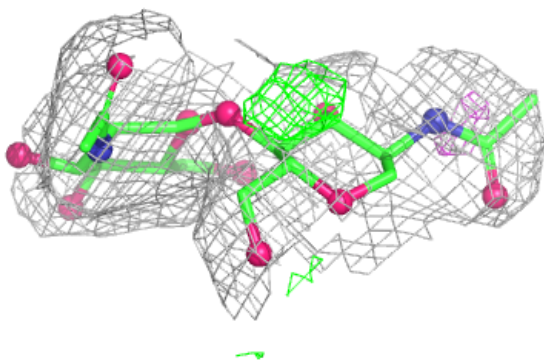
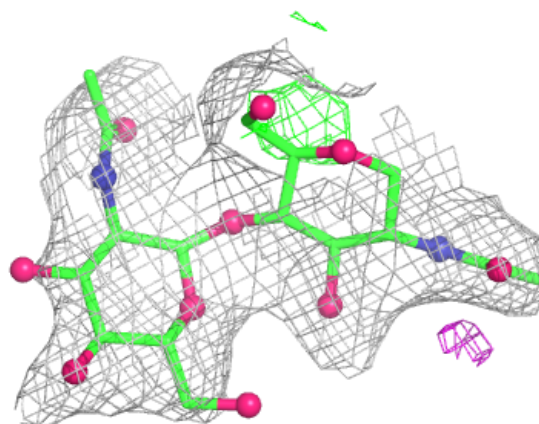


Electron density around Chain AsA:

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

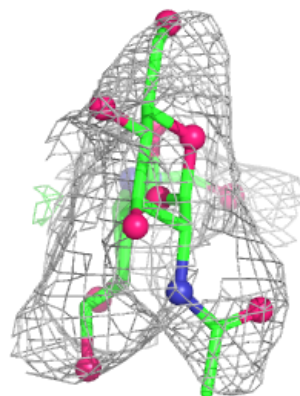
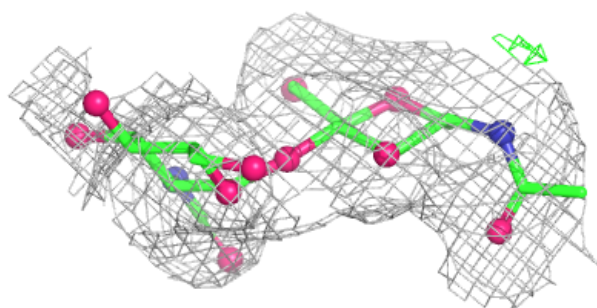
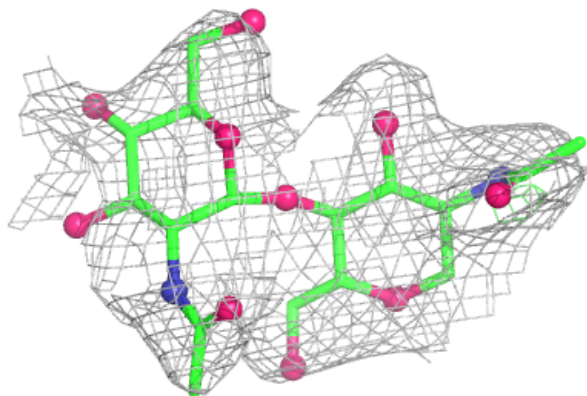
**Electron density around Chain DeD:**

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



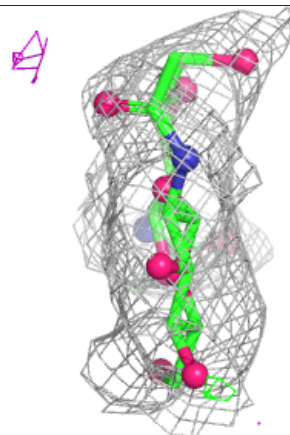
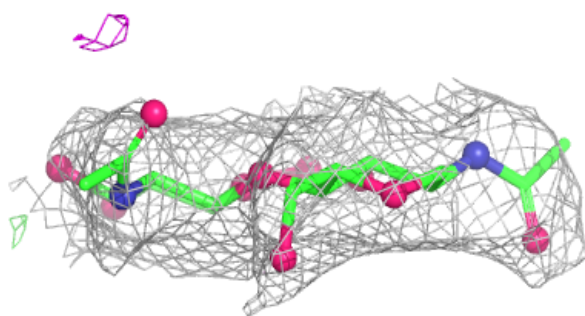
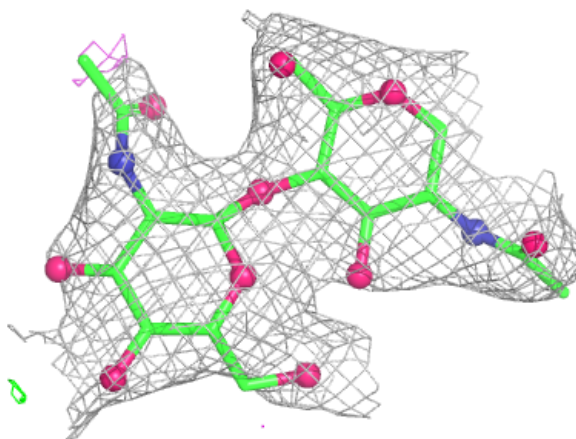
Electron density around Chain DgD:

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



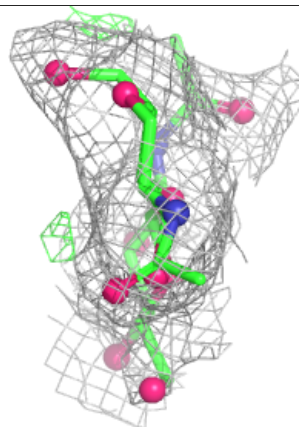
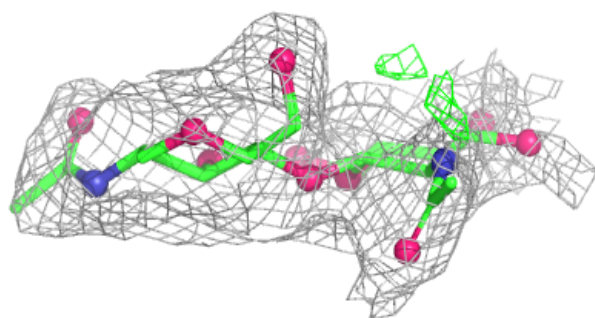
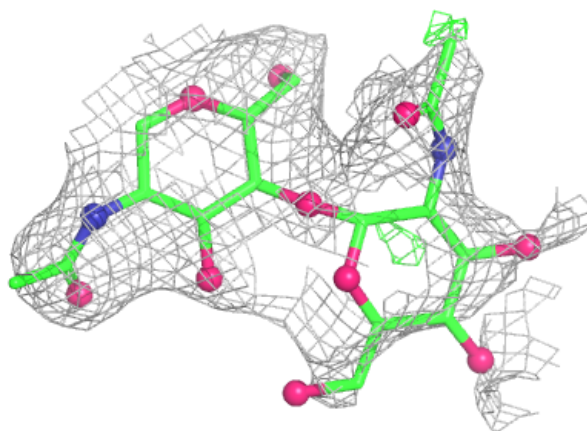
Electron density around Chain DmD:

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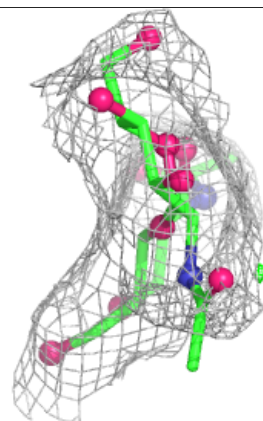
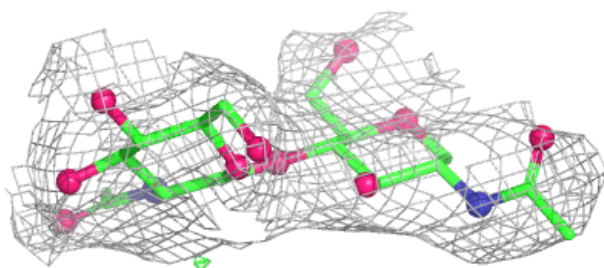
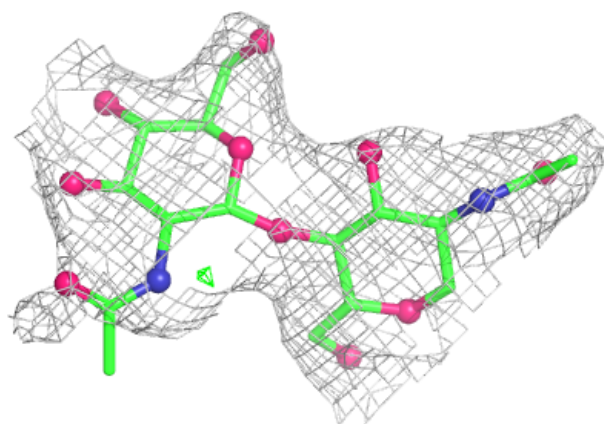
Electron density around Chain EdE:

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and green (positive)



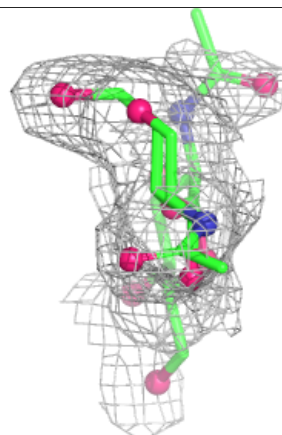
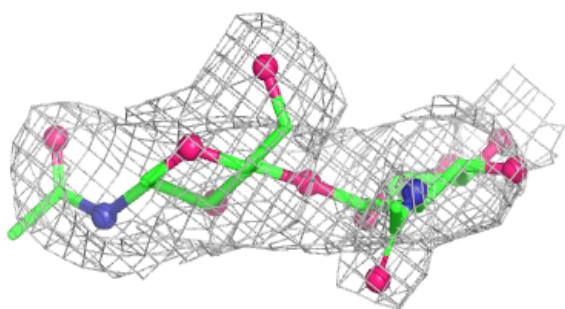
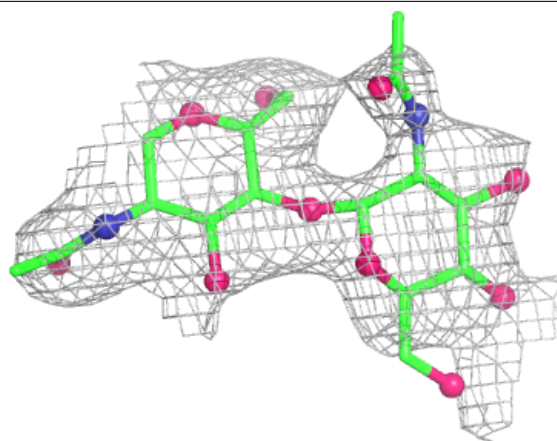
Electron density around Chain GgG:

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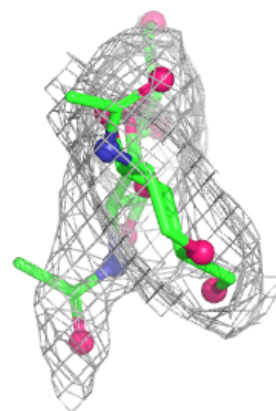
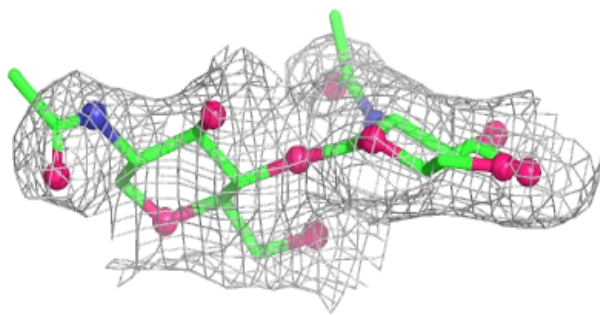
Electron density around Chain GIG:

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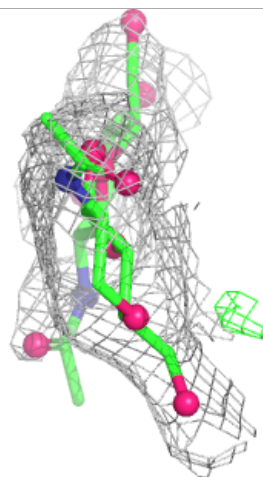
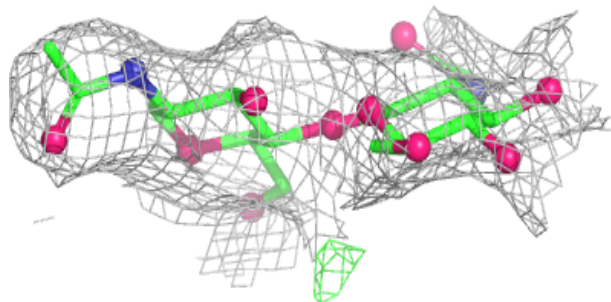
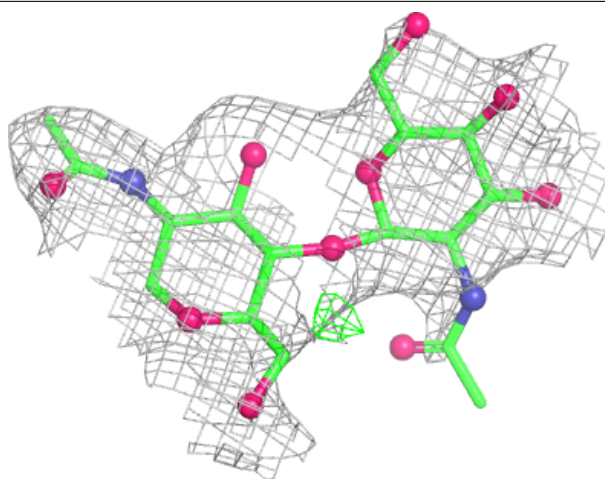
Electron density around Chain GnG:

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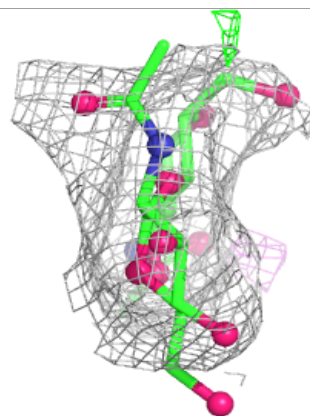
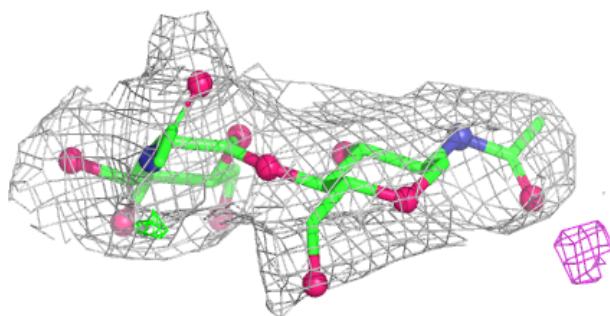
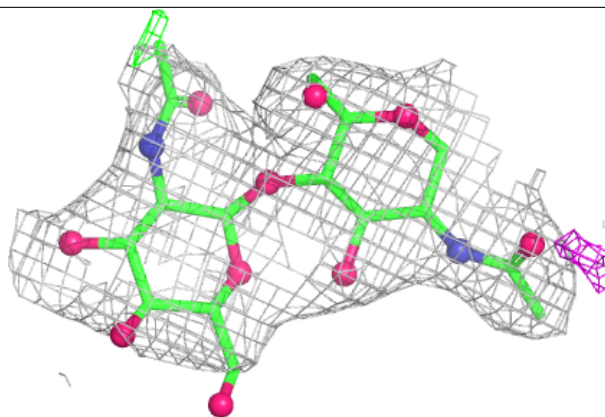
Electron density around Chain HaH:

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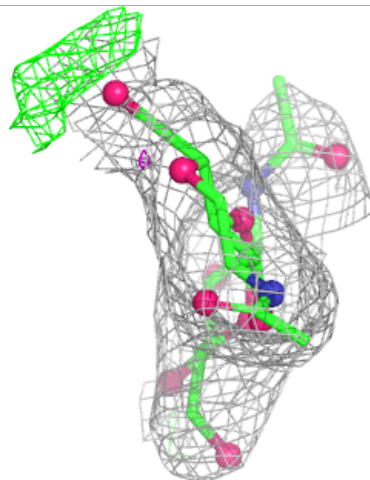
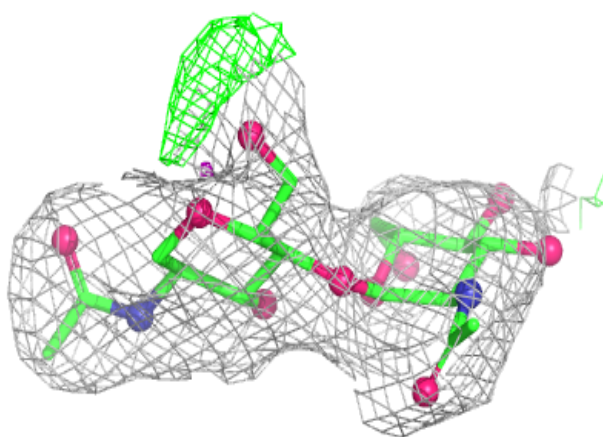
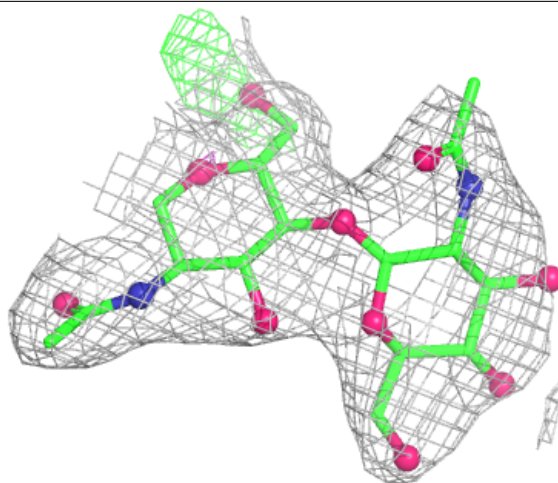
Electron density around Chain JaJ:

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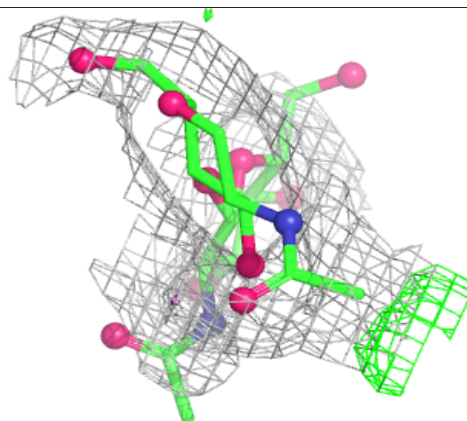
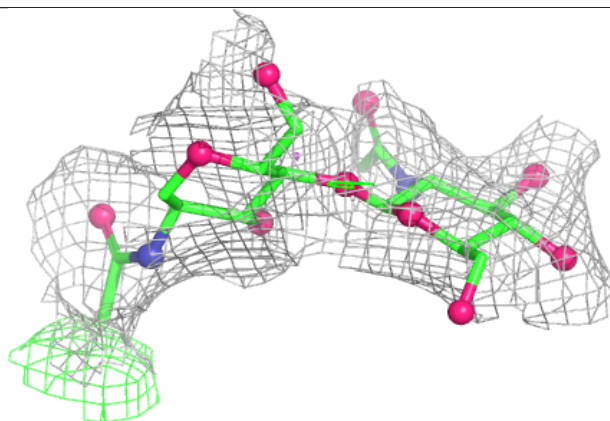
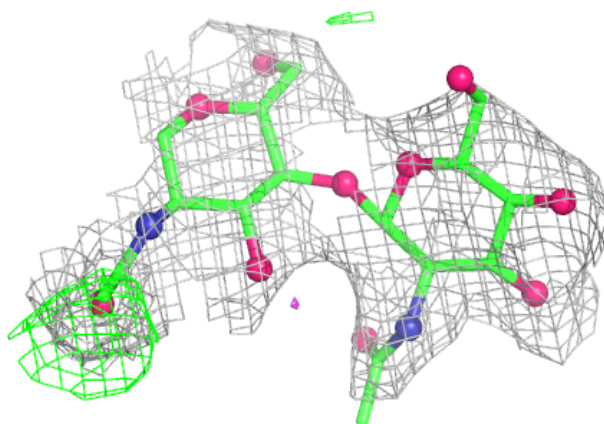
Electron density around Chain JcJ:

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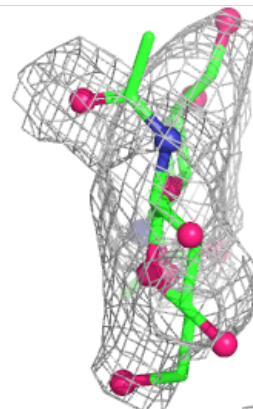
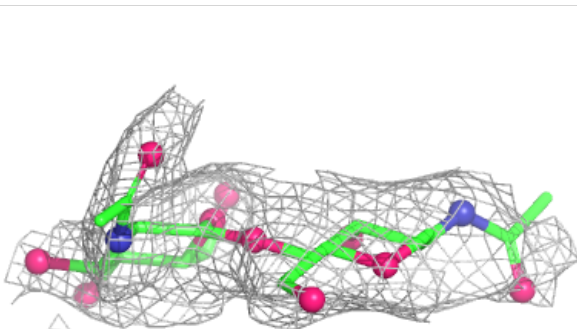
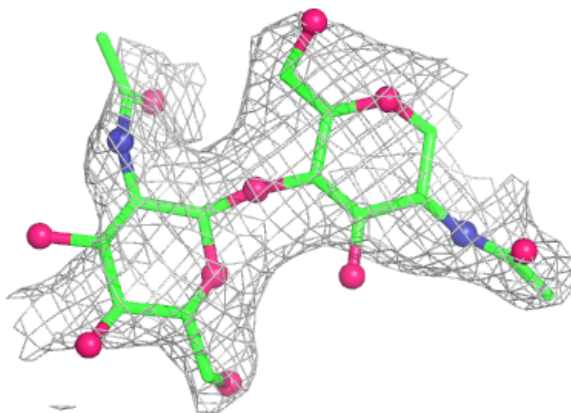


Electron density around Chain JeJ:

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and green (positive)

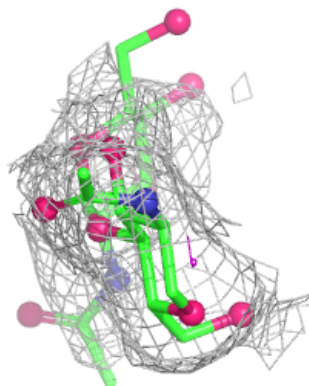
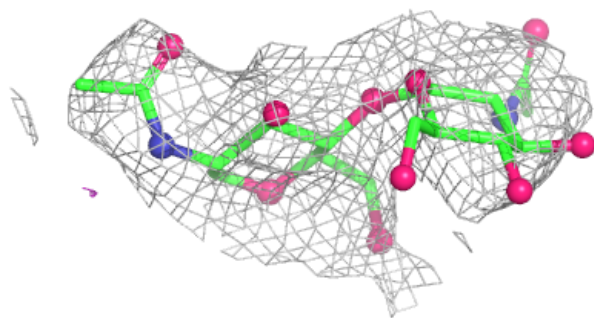
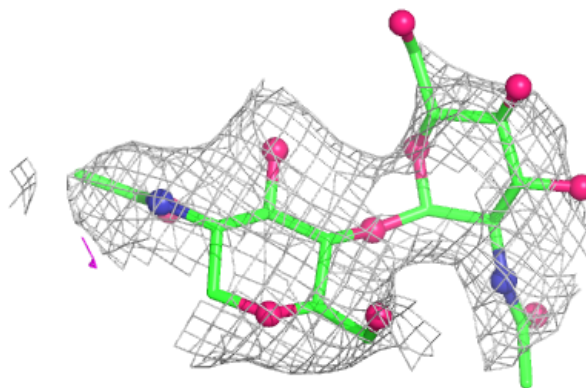
**Electron density around Chain JgJ:**

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



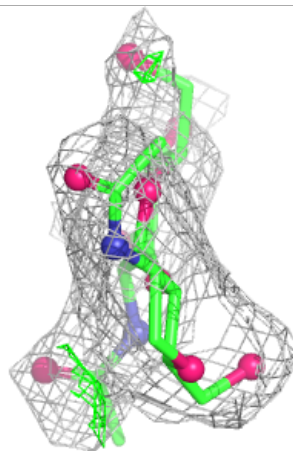
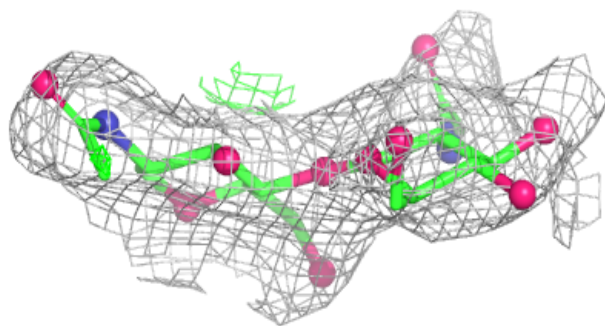
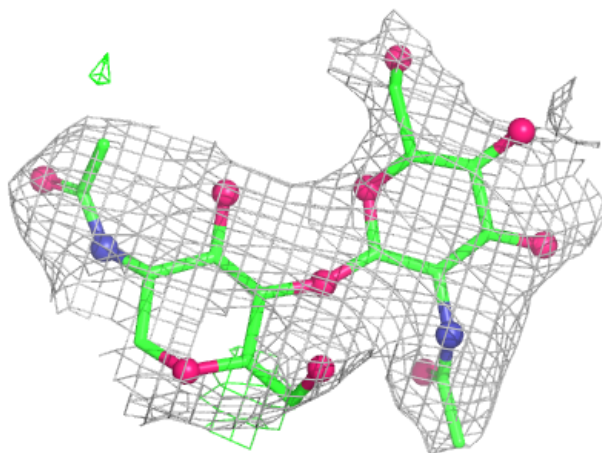
Electron density around Chain JkJ:

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



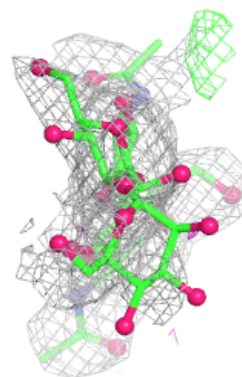
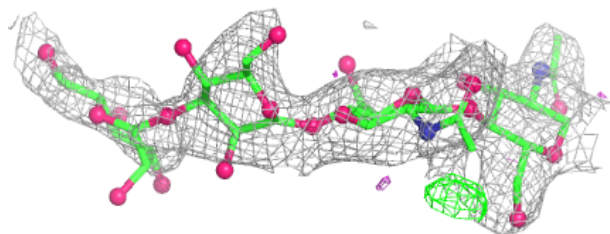
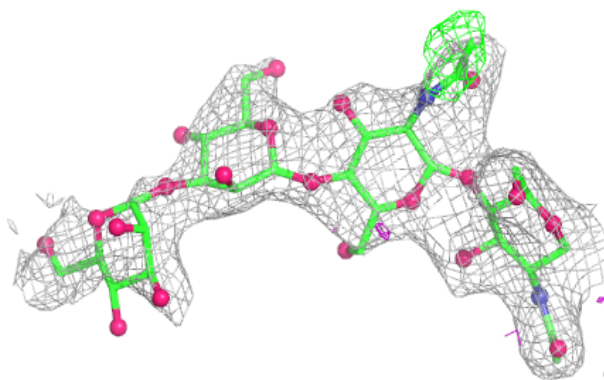
Electron density around Chain KaK:

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

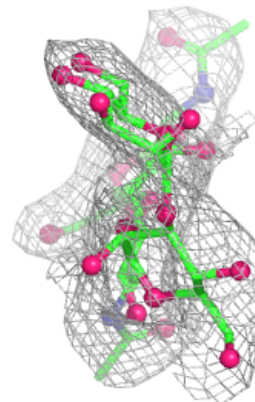
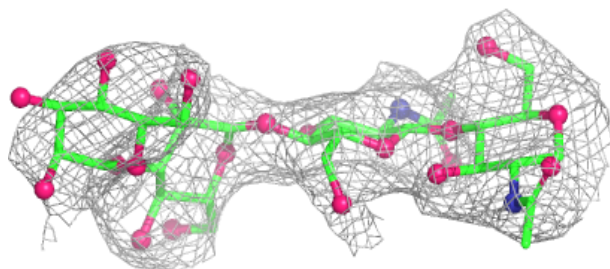
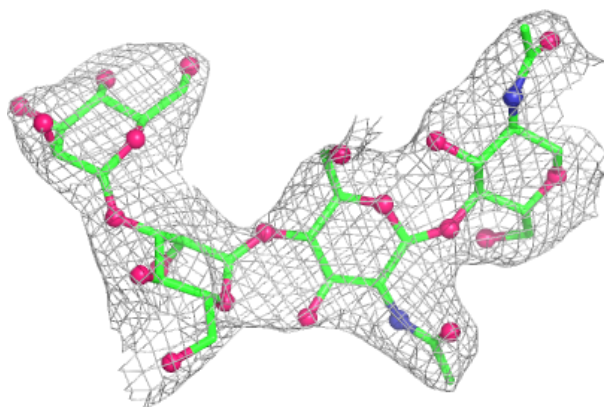


Electron density around Chain AcA:

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

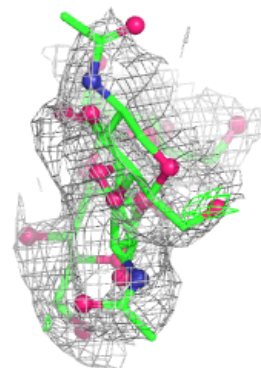
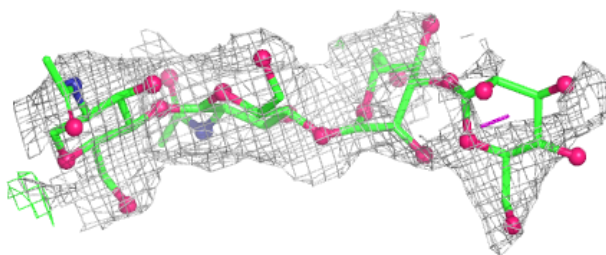
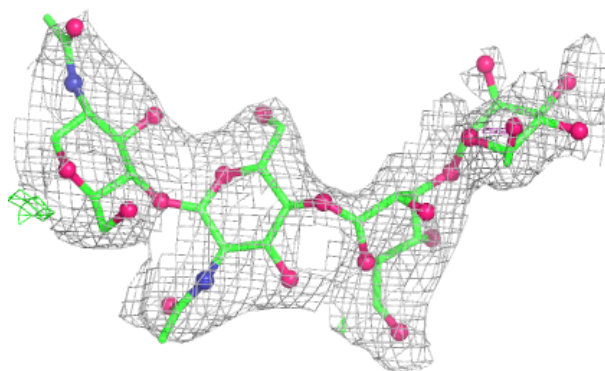
**Electron density around Chain AhA:**

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



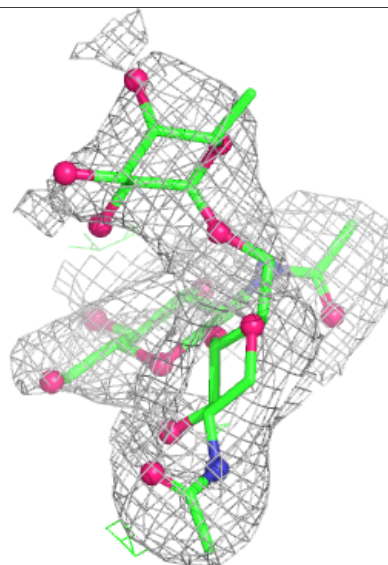
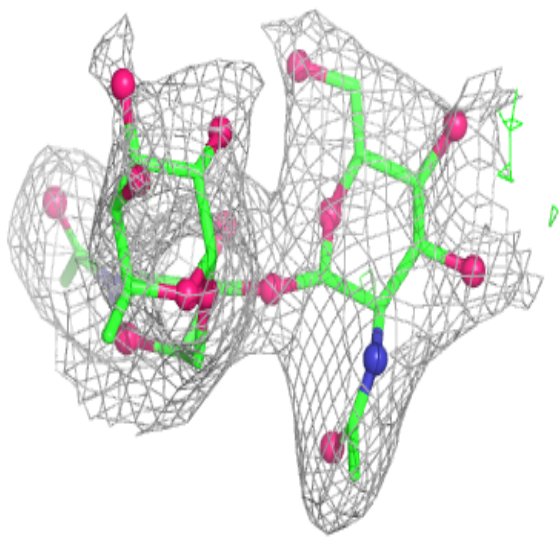
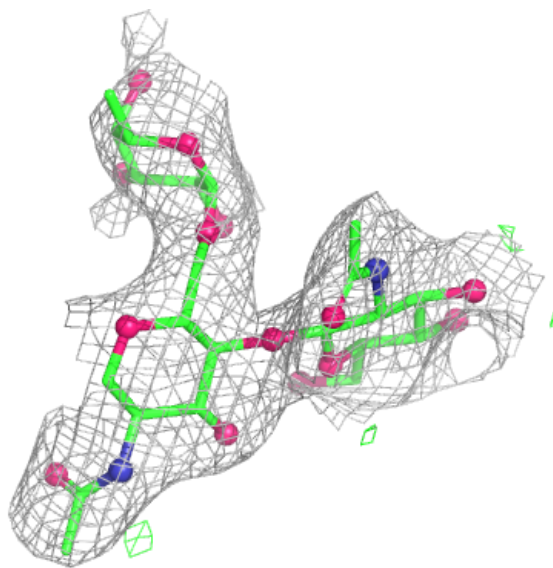
Electron density around Chain DiD:

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



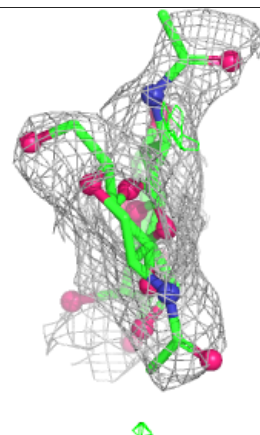
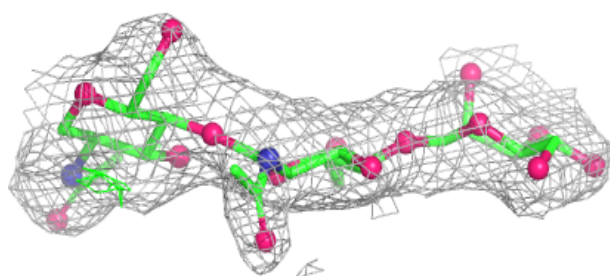
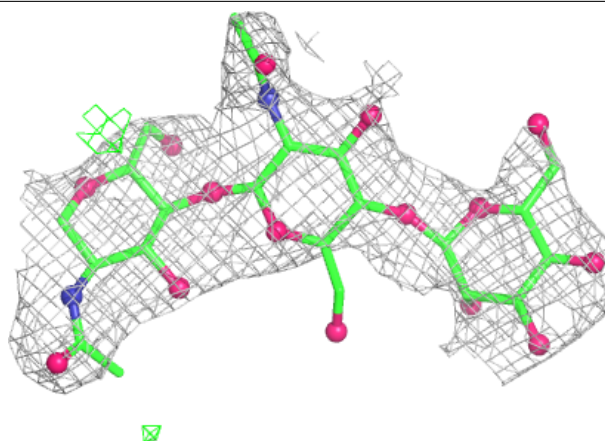
Electron density around Chain AnA:

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

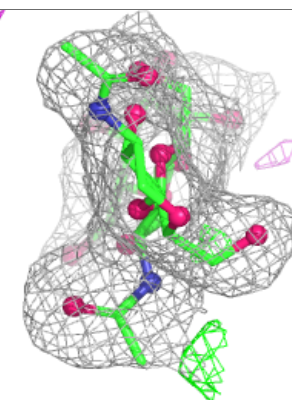
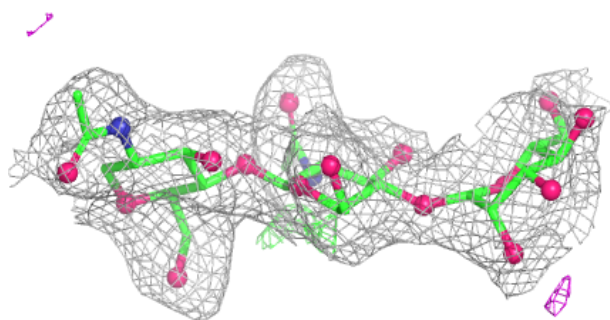
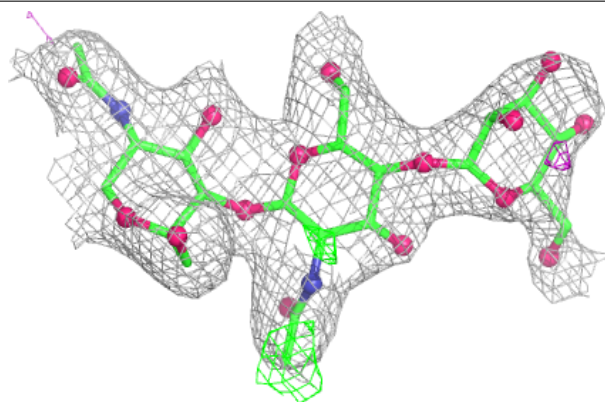


Electron density around Chain BaB:

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

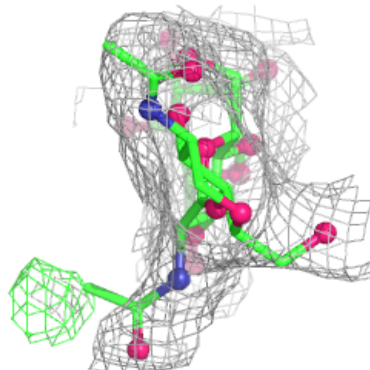
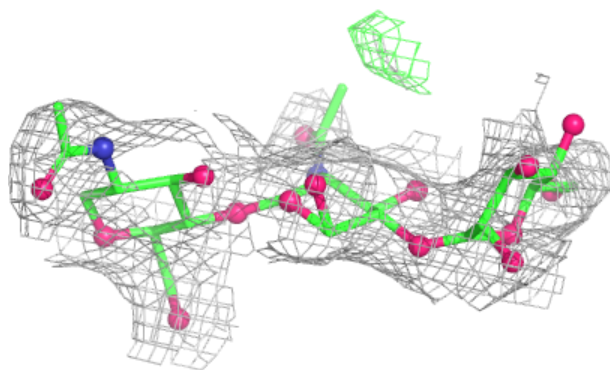
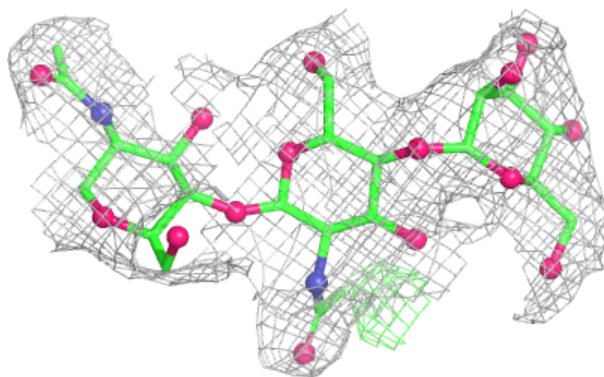
**Electron density around Chain DaD:**

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

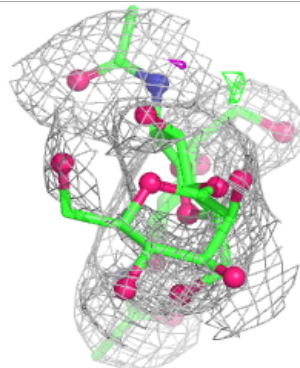
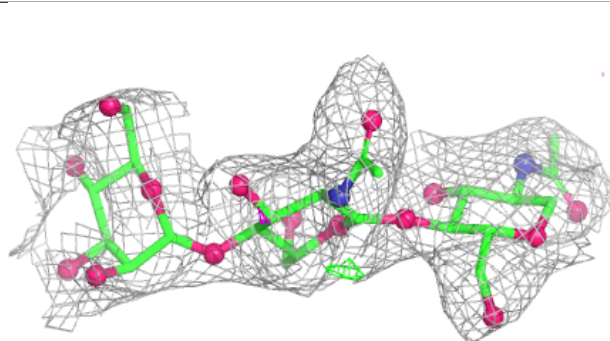
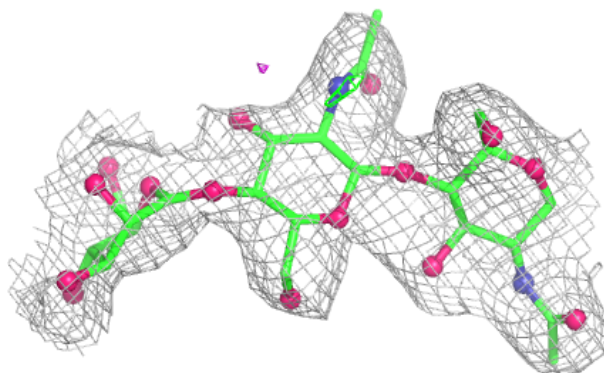


Electron density around Chain EaE:

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

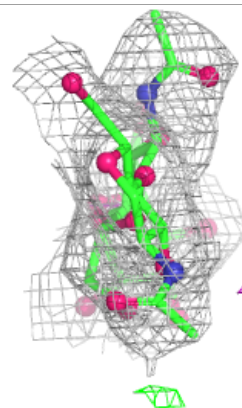
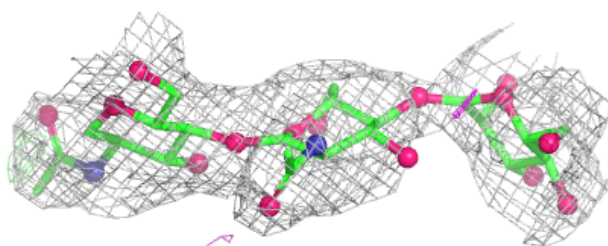
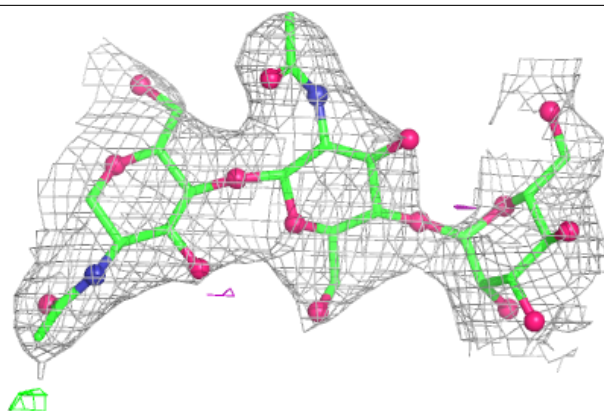
**Electron density around Chain GaG:**

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

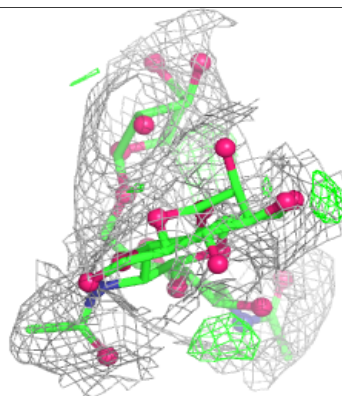
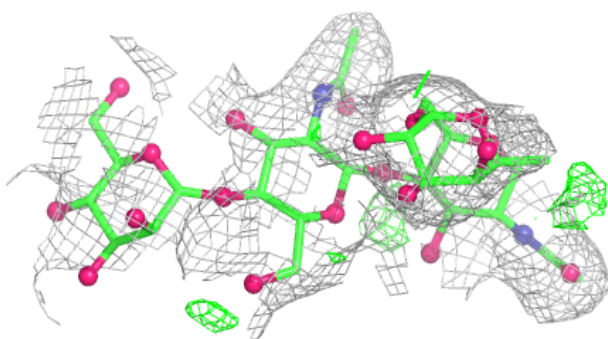
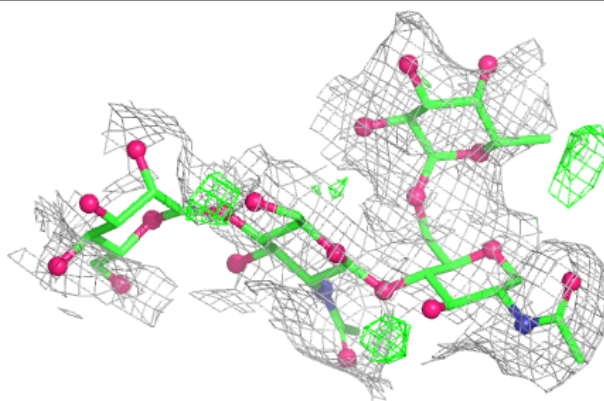


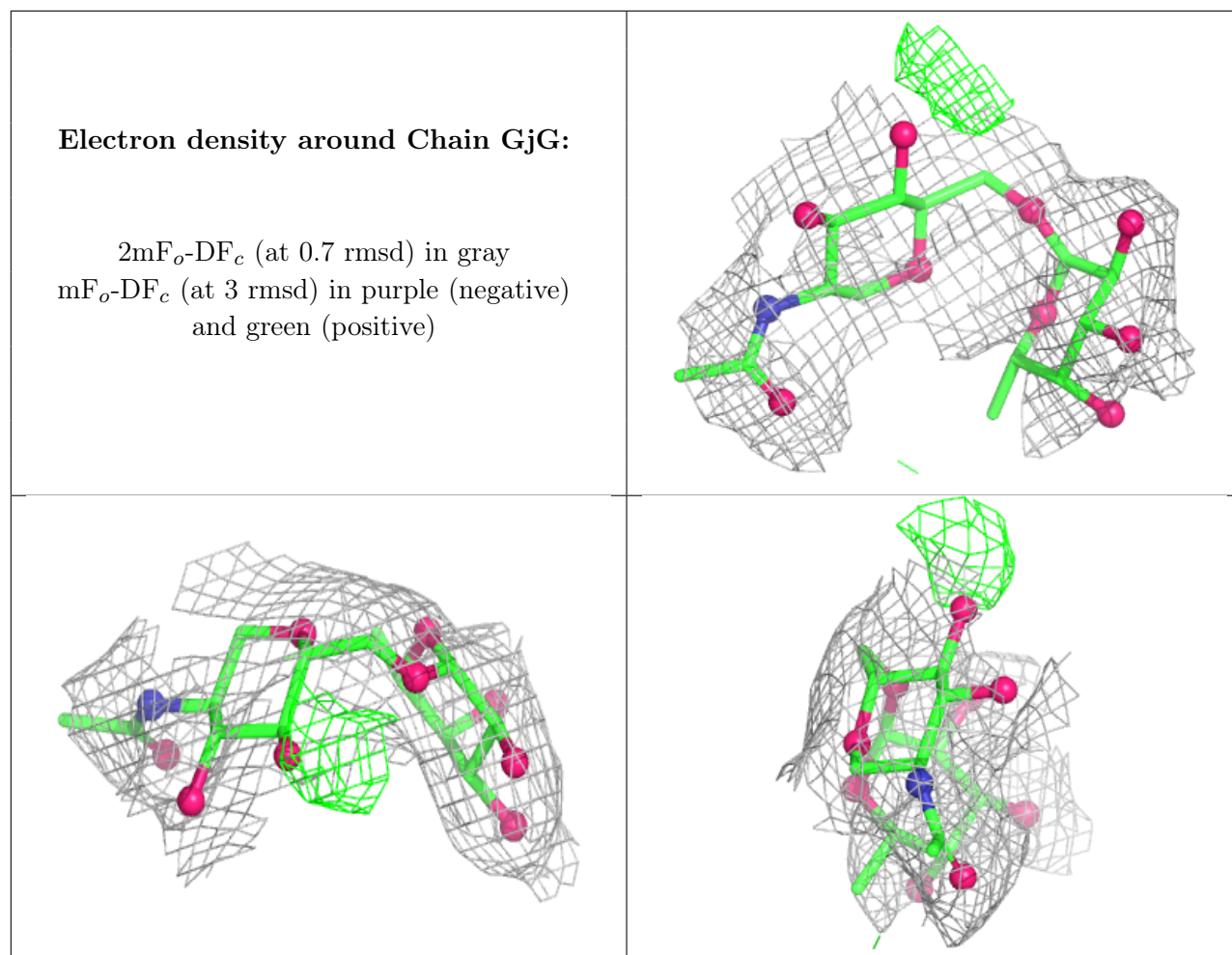
Electron density around Chain GdG:

$2mF_o - DF_c$ (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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	NAG	BBB	302	14/15	0.47	0.16	80,96,99,100	0
11	NAG	EEE	301	14/15	0.49	0.17	96,104,111,113	0
10	MAN	AAA	701	11/12	0.56	0.16	106,118,121,122	0
11	NAG	DDD	701	14/15	0.73	0.14	64,77,84,85	0
11	NAG	JJJ	703	14/15	0.73	0.14	73,75,80,80	0
11	NAG	JJJ	701	14/15	0.75	0.14	72,80,87,88	0
11	NAG	GGG	701	14/15	0.75	0.14	70,76,83,86	0
11	NAG	BBB	301	14/15	0.76	0.14	68,74,77,79	0
11	NAG	HHH	301	14/15	0.76	0.14	71,75,82,84	0
11	NAG	AAA	702	14/15	0.77	0.14	76,80,85,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	NA	AAA	704	1/1	0.77	0.14	44,44,44,44	0
12	NA	AAA	703	1/1	0.79	0.09	37,37,37,37	0
11	NAG	DDD	702	14/15	0.80	0.13	62,74,80,81	0
11	NAG	JJJ	704	14/15	0.80	0.11	72,77,81,87	0
11	NAG	JJJ	702	14/15	0.81	0.10	73,79,84,88	0
12	NA	GGG	702	1/1	0.88	0.11	52,52,52,52	0
12	NA	BBB	303	1/1	0.94	0.13	21,21,21,21	0
12	NA	HHH	302	1/1	0.94	0.10	27,27,27,27	0
12	NA	DDD	703	1/1	0.95	0.10	29,29,29,29	0
12	NA	EEE	302	1/1	0.95	0.08	22,22,22,22	0
12	NA	KKK	301	1/1	0.96	0.10	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.