



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2022 – 06:30 pm GMT

PDB ID : 7ODV
Title : Plant peptide hormone receptor complex H1LS1
Authors : Roman, A.O.; Jimenez-Sandoval, P.; Santiago, J.
Deposited on : 2021-04-30
Resolution : 2.31 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

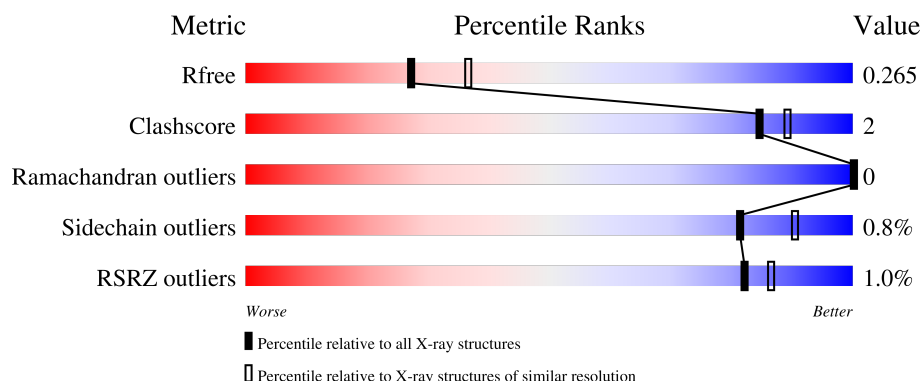
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	<div> <div>7%</div> <div>91%</div> <div>5%</div> <div>.</div> </div>
1	DDD	617	<div> <div>89%</div> <div>7%</div> <div>.</div> </div>
2	BBB	203	<div> <div>83%</div> <div>8%</div> <div>9%</div> </div>
2	EEE	203	<div> <div>88%</div> <div>.</div> <div>9%</div> </div>
3	CCC	14	<div> <div>7%</div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	FFF	14	 93% 7%
4	AdA	3	 100%
4	AmA	3	 67% 33%
4	DmD	3	 67% 33%
5	AhA	2	 50% 50%
5	AkA	2	 100%
5	BaB	2	 50% 50%
5	BeB	2	 100%
5	DbD	2	 100%
5	DdD	2	 50% 50%
5	DgD	2	 100%
5	DiD	2	 50% 50%
5	DkD	2	 50% 50%
5	EaE	2	 50% 50%
5	EcE	2	 50% 50%
6	DqD	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	BMA	AdA	3	X	-	-	-
4	NAG	AmA	2	X	-	-	-
4	BMA	AmA	3	X	-	-	-
4	NAG	DmD	2	X	-	-	-
4	BMA	DmD	3	X	-	-	-
5	NAG	AhA	2	X	-	-	-
5	NAG	AkA	2	X	-	-	-
5	NAG	BaB	2	X	-	-	-
5	NAG	BeB	2	X	-	-	-
5	NAG	DbD	2	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	DdD	2	X	-	-	-
5	NAG	DgD	2	X	-	-	-
5	NAG	DiD	2	X	-	-	-
5	NAG	DkD	2	X	-	-	-
5	NAG	EaE	2	X	-	-	-
5	NAG	EcE	2	X	-	-	-
7	NAG	BBB	301	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12821 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	0	0
			4403	2791	719	876	17			
1	DDD	595	Total	C	N	O	S	0	2	0
			4440	2812	727	885	16			

There are 30 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- 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
			1383	874	235	269	5			
2	EEE	185	Total	C	N	O	S	0	1	0
			1385	873	233	274	5			

There are 30 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

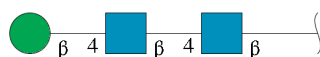
- Molecule 3 is a protein called Protein IDA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	CCC	14	Total	C	N	O	0	0	0
			112	71	21	20			
3	FFF	14	Total	C	N	O	0	0	0
			112	71	21	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CCC	56	TYR	-	expression tag	UNP Q8LAD7
FFF	56	TYR	-	expression tag	UNP Q8LAD7

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	AdA	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	AmA	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	DmD	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	AhA	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	AkA	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	BaB	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	BeB	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	DbD	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	DdD	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	DgD	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	DiD	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	DkD	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	EaE	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	EcE	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
7	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
7	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
7	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
7	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
7	BBB	1	Total	C	N	O	0	0
			14	8	1	5		
7	BBB	1	Total	C	N	O	0	0
			14	8	1	5		
7	BBB	1	Total	C	N	O	0	0
			14	8	1	5		
7	DDD	1	Total	C	N	O	0	0
			14	8	1	5		
7	DDD	1	Total	C	N	O	0	0
			14	8	1	5		
7	DDD	1	Total	C	N	O	0	0
			14	8	1	5		
7	EEE	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	1	Total Mg 1 1	1	0
8	BBB	1	Total Mg 1 1	0	0
8	DDD	1	Total Mg 1 1	1	0
8	EEE	1	Total Mg 1 1	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	AAA	1	Total Na 1 1	0	0
9	DDD	2	Total Na 2 2	0	0

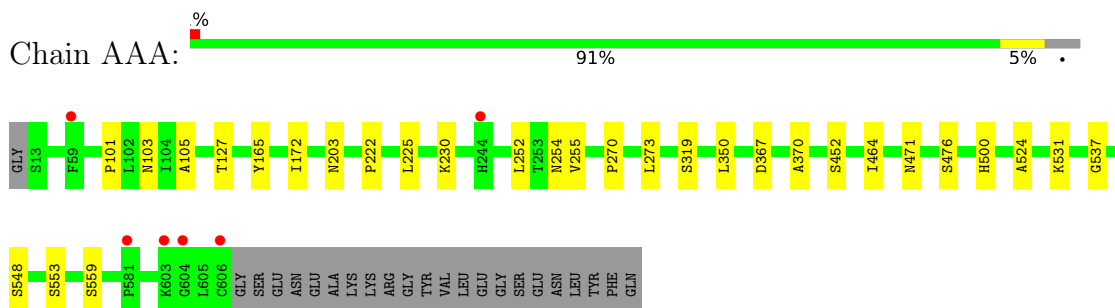
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	AAA	115	Total O 115 115	0	0
10	BBB	39	Total O 39 39	0	0
10	CCC	5	Total O 5 5	0	0
10	DDD	156	Total O 156 156	0	0
10	EEE	40	Total O 40 40	0	0
10	FFF	7	Total O 7 7	0	0

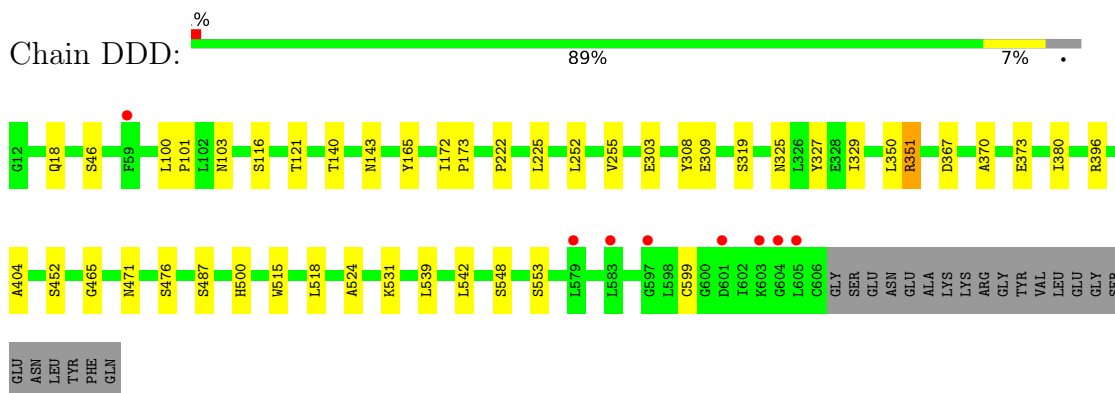
3 Residue-property plots [i](#)

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.

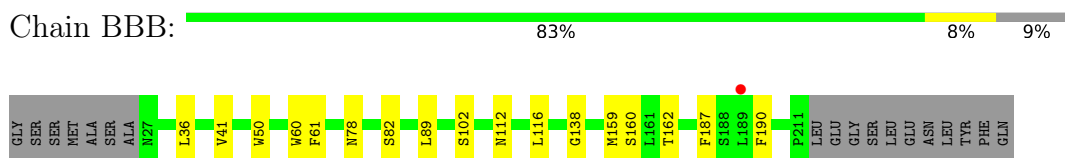
- Molecule 1: Receptor-like protein kinase HSL1



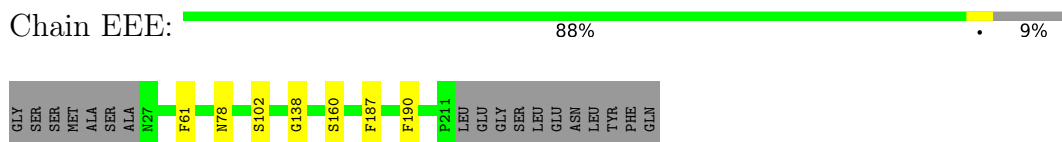
- Molecule 1: Receptor-like protein kinase HSL1



- Molecule 2: Somatic embryogenesis receptor kinase 1



- Molecule 2: Somatic embryogenesis receptor kinase 1



• Molecule 3: Protein IDA

Chain CCC:  7% 100%



• Molecule 3: Protein IDA

Chain FFF:  93% 7%



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

Chain AdA:  100%



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

Chain AmA:  67% 33%



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

Chain DmD:  67% 33%



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

Chain AhA:  50% 50%



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

Chain AkA:  100%



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

Chain BaB:  50% 50%



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

Chain BeB:  100%



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

Chain DbD:  100%



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

Chain DdD:  50% 50%



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

Chain DgD:  100%



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

Chain DiD:  50% 50%



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

Chain DkD:  50% 50%

MAG1
MAG2

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

Chain EaE:  50% 50%

MAG1
MAG2

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

Chain EcE:  50% 50%

MAG1
MAG2

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

Chain DqD:  50% 50%

MAG1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.33Å 145.88Å 169.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	110.58 – 2.31 110.58 – 2.31	Depositor EDS
% Data completeness (in resolution range)	100.0 (110.58-2.31) 99.9 (110.58-2.31)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, R_{free}	0.255 , 0.275 0.246 , 0.265	Depositor DCC
R_{free} test set	5323 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.791	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12821	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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 24.47 % 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 3.8139e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HYP, MG, NAG, FUC, NA, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AAA	0.63	0/4489	0.66	0/6130
1	DDD	0.64	0/4525	0.67	0/6175
2	BBB	0.63	0/1416	0.69	0/1946
2	EEE	0.62	0/1418	0.68	0/1949
3	CCC	0.58	0/107	0.69	0/143
3	FFF	0.57	0/107	0.68	0/143
All	All	0.63	0/12062	0.67	0/16486

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	4403	0	4227	16	0
1	DDD	4440	0	4288	25	0
2	BBB	1383	0	1325	11	0
2	EEE	1385	0	1329	5	0
3	CCC	112	0	110	0	0
3	FFF	112	0	110	1	0
4	AdA	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AmA	39	0	34	0	0
4	DmD	39	0	34	0	0
5	AhA	28	0	25	0	0
5	AkA	28	0	25	0	0
5	BaB	28	0	25	0	0
5	BeB	28	0	25	0	0
5	DbD	28	0	25	0	0
5	DdD	28	0	25	0	0
5	DgD	28	0	25	0	0
5	DiD	28	0	25	0	0
5	DkD	28	0	25	0	0
5	EaE	28	0	25	0	0
5	EcE	28	0	25	0	0
6	DqD	24	0	22	0	0
7	AAA	70	0	65	1	0
7	BBB	42	0	39	1	0
7	DDD	42	0	39	0	0
7	EEE	14	0	13	0	0
8	AAA	1	0	0	0	0
8	BBB	1	0	0	0	0
8	DDD	1	0	0	0	0
8	EEE	1	0	0	0	0
9	AAA	1	0	0	0	0
9	DDD	2	0	0	0	0
10	AAA	115	0	0	0	0
10	BBB	39	0	0	0	0
10	CCC	5	0	0	0	0
10	DDD	156	0	0	2	0
10	EEE	40	0	0	1	0
10	FFF	7	0	0	0	0
All	All	12821	0	11944	56	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 2.

All (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:112:ASN:OD1	7:BBB:301:NAG:C1	2.45	0.64
1:AAA:270:PRO:HG2	1:AAA:273:LEU:HG	1.87	0.56
1:DDD:303:GLU:HB3	1:DDD:327:TYR:CE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:222:PRO:HG2	1:AAA:225:LEU:HG	1.91	0.53
2:BBB:187:PHE:HA	2:BBB:190:PHE:CD2	2.44	0.53
2:BBB:187:PHE:HA	2:BBB:190:PHE:HD2	1.76	0.51
1:DDD:465:GLY:HA3	1:DDD:487:SER:HB2	1.92	0.51
2:EEE:187:PHE:HA	2:EEE:190:PHE:CD2	2.47	0.50
1:AAA:500:HIS:HA	1:AAA:524:ALA:O	2.13	0.49
2:EEE:138:GLY:HA3	2:EEE:160:SER:HB2	1.94	0.49
2:EEE:187:PHE:HA	2:EEE:190:PHE:HD2	1.78	0.48
10:EEE:423:HOH:O	3:FFF:67:ARG:HD3	2.12	0.48
2:BBB:138:GLY:HA3	2:BBB:160:SER:HB2	1.95	0.48
1:DDD:500:HIS:HA	1:DDD:524:ALA:O	2.15	0.46
1:DDD:524:ALA:HA	1:DDD:548:SER:O	2.16	0.46
2:BBB:159:MET:O	2:BBB:162:THR:OG1	2.34	0.46
1:DDD:396:ARG:NH1	10:DDD:804:HOH:O	2.46	0.45
1:AAA:471:ASN:HB3	2:BBB:61:PHE:CZ	2.51	0.45
1:AAA:524:ALA:HA	1:AAA:548:SER:O	2.16	0.45
1:AAA:476:SER:HA	1:AAA:500:HIS:O	2.17	0.45
1:AAA:230:LYS:HA	1:AAA:254:ASN:HD22	1.81	0.45
2:BBB:78:ASN:HA	2:BBB:102:SER:O	2.17	0.44
2:EEE:78:ASN:HA	2:EEE:102:SER:O	2.17	0.44
1:DDD:531:LYS:HA	1:DDD:553:SER:O	2.18	0.44
1:AAA:537:GLY:HA3	1:AAA:559:SER:HB2	2.00	0.44
1:DDD:101:PRO:HB2	1:DDD:103:ASN:OD1	2.18	0.44
1:AAA:105:ALA:HB2	1:AAA:127:THR:HB	1.99	0.44
1:AAA:203:ASN:OD1	7:AAA:705:NAG:O5	2.36	0.44
1:AAA:531:LYS:HA	1:AAA:553:SER:O	2.18	0.43
1:DDD:308:TYR:HD1	1:DDD:309:GLU:HG3	1.82	0.43
1:DDD:222:PRO:HG2	1:DDD:225:LEU:HG	2.01	0.43
1:DDD:252:LEU:HB3	1:DDD:255:VAL:HB	1.99	0.43
1:DDD:539:LEU:HD12	1:DDD:542:LEU:HD22	2.00	0.43
1:DDD:303:GLU:HA	1:DDD:325:ASN:O	2.19	0.43
1:DDD:351:ARG:HG2	1:DDD:373:GLU:O	2.20	0.42
1:DDD:367:ASP:HB3	1:DDD:370:ALA:HB2	2.01	0.42
2:BBB:41:VAL:HB	2:BBB:82:SER:OG	2.20	0.42
1:DDD:172:ILE:HA	1:DDD:173:PRO:HD3	1.84	0.42
2:BBB:36:LEU:HD22	2:BBB:89:LEU:HD21	2.02	0.42
1:DDD:452:SER:HA	1:DDD:476:SER:O	2.19	0.42
1:DDD:329:ILE:HG22	1:DDD:350:LEU:HD11	2.01	0.42
1:AAA:252:LEU:HB3	1:AAA:255:VAL:HB	2.01	0.42
1:DDD:380:ILE:HA	1:DDD:404:ALA:O	2.20	0.42
1:AAA:452:SER:HA	1:AAA:476:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:476:SER:HA	1:DDD:500:HIS:O	2.20	0.41
1:DDD:116:SER:HA	1:DDD:140:THR:O	2.20	0.41
1:DDD:515:TRP:HB3	1:DDD:518:LEU:HB2	2.03	0.41
1:AAA:101:PRO:HB2	1:AAA:103:ASN:OD1	2.21	0.41
1:DDD:471:ASN:HB3	2:EEE:61:PHE:CZ	2.56	0.41
1:AAA:367:ASP:HB3	1:AAA:370:ALA:HB2	2.02	0.41
2:BBB:89:LEU:O	2:BBB:116:LEU:HD21	2.21	0.40
1:DDD:599:CYS:N	10:DDD:801:HOH:O	2.46	0.40
1:AAA:350:LEU:HD12	1:AAA:350:LEU:HA	1.94	0.40
1:DDD:100:LEU:HD12	1:DDD:100:LEU:HA	1.93	0.40
2:BBB:50:TRP:HA	2:BBB:60:TRP:CD2	2.57	0.40
1:DDD:121:THR:HG22	1:DDD:143:ASN:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	592/617 (96%)	580 (98%)	12 (2%)	0	100	100
1	DDD	595/617 (96%)	584 (98%)	11 (2%)	0	100	100
2	BBB	184/203 (91%)	181 (98%)	3 (2%)	0	100	100
2	EEE	184/203 (91%)	181 (98%)	3 (2%)	0	100	100
3	CCC	11/14 (79%)	11 (100%)	0	0	100	100
3	FFF	11/14 (79%)	11 (100%)	0	0	100	100
All	All	1577/1668 (94%)	1548 (98%)	29 (2%)	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	485/540 (90%)	481 (99%)	4 (1%)	81	90
1	DDD	492/540 (91%)	487 (99%)	5 (1%)	76	87
2	BBB	158/184 (86%)	158 (100%)	0	100	100
2	EEE	161/184 (88%)	161 (100%)	0	100	100
3	CCC	12/12 (100%)	12 (100%)	0	100	100
3	FFF	12/12 (100%)	11 (92%)	1 (8%)	11	13
All	All	1320/1472 (90%)	1310 (99%)	10 (1%)	81	90

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	165	TYR
1	AAA	172	ILE
1	AAA	319	SER
1	AAA	464	ILE
1	DDD	18	GLN
1	DDD	46	SER
1	DDD	165	TYR
1	DDD	319	SER
1	DDD	351	ARG
3	FFF	67	ARG

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 ⓘ

2 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	FFF	64	3	6,8,9	0.55	0	5,10,12	0.91	0
3	HYP	CCC	64	3	6,8,9	0.61	0	5,10,12	0.89	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	FFF	64	3	-	0/0/11/13	0/1/1/1
3	HYP	CCC	64	3	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

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

33 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	AdA	1	4,1	14,14,15	0.36	0	17,19,21	1.17	2 (11%)
4	NAG	AdA	2	4	14,14,15	0.23	0	17,19,21	0.97	1 (5%)
4	BMA	AdA	3	4	11,11,12	0.45	0	15,15,17	0.73	1 (6%)
5	NAG	AhA	1	5,1	14,14,15	0.33	0	17,19,21	1.10	1 (5%)
5	NAG	AhA	2	5	14,14,15	0.35	0	17,19,21	0.65	0
5	NAG	AkA	1	5,1	14,14,15	0.32	0	17,19,21	0.66	0
5	NAG	AkA	2	5	14,14,15	0.32	0	17,19,21	0.79	0
4	NAG	AmA	1	4,1	14,14,15	0.34	0	17,19,21	1.03	2 (11%)
4	NAG	AmA	2	4	14,14,15	0.38	0	17,19,21	0.90	0
4	BMA	AmA	3	4	11,11,12	0.31	0	15,15,17	0.79	0
5	NAG	BaB	1	5,2	14,14,15	0.24	0	17,19,21	0.92	1 (5%)
5	NAG	BaB	2	5	14,14,15	0.34	0	17,19,21	0.71	0
5	NAG	BeB	1	5,2	14,14,15	0.31	0	17,19,21	1.25	3 (17%)
5	NAG	BeB	2	5	14,14,15	0.35	0	17,19,21	0.82	1 (5%)
5	NAG	DbD	1	5,1	14,14,15	0.42	0	17,19,21	0.80	0
5	NAG	DbD	2	5	14,14,15	0.24	0	17,19,21	0.69	0
5	NAG	DdD	1	5,1	14,14,15	0.34	0	17,19,21	0.92	1 (5%)
5	NAG	DdD	2	5	14,14,15	0.32	0	17,19,21	0.76	0
5	NAG	DgD	1	5,1	14,14,15	0.28	0	17,19,21	0.57	0
5	NAG	DgD	2	5	14,14,15	0.27	0	17,19,21	0.45	0
5	NAG	DiD	1	5,1	14,14,15	0.29	0	17,19,21	1.12	1 (5%)
5	NAG	DiD	2	5	14,14,15	0.31	0	17,19,21	0.99	0
5	NAG	DkD	1	5,1	14,14,15	0.32	0	17,19,21	1.10	2 (11%)
5	NAG	DkD	2	5	14,14,15	0.31	0	17,19,21	0.60	0
4	NAG	DmD	1	4,1	14,14,15	0.42	0	17,19,21	1.23	3 (17%)
4	NAG	DmD	2	4	14,14,15	0.27	0	17,19,21	0.61	0
4	BMA	DmD	3	4	11,11,12	0.33	0	15,15,17	0.79	0
6	NAG	DqD	1	1,6	14,14,15	0.48	0	17,19,21	1.01	1 (5%)
6	FUC	DqD	2	6	10,10,11	0.42	0	14,14,16	0.75	0
5	NAG	EaE	1	5,2	14,14,15	0.25	0	17,19,21	0.76	1 (5%)
5	NAG	EaE	2	5	14,14,15	0.33	0	17,19,21	0.61	0
5	NAG	EcE	1	5,2	14,14,15	0.35	0	17,19,21	1.14	2 (11%)
5	NAG	EcE	2	5	14,14,15	0.28	0	17,19,21	0.57	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	AdA	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	AdA	2	4	-	2/6/23/26	0/1/1/1
4	BMA	AdA	3	4	1/1/4/5	0/2/19/22	0/1/1/1
5	NAG	AhA	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	AhA	2	5	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	AkA	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	AkA	2	5	1/1/5/7	3/6/23/26	0/1/1/1
4	NAG	AmA	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	AmA	2	4	1/1/5/7	1/6/23/26	0/1/1/1
4	BMA	AmA	3	4	1/1/4/5	0/2/19/22	0/1/1/1
5	NAG	BaB	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	BaB	2	5	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	BeB	1	5,2	-	2/6/23/26	0/1/1/1
5	NAG	BeB	2	5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	DbD	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	DbD	2	5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	DdD	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	DdD	2	5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	DgD	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	DgD	2	5	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	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	DkD	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	DkD	2	5	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	DmD	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	DmD	2	4	1/1/5/7	0/6/23/26	0/1/1/1
4	BMA	DmD	3	4	1/1/4/5	2/2/19/22	0/1/1/1
6	NAG	DqD	1	1,6	-	2/6/23/26	0/1/1/1
6	FUC	DqD	2	6	-	-	0/1/1/1
5	NAG	EaE	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	EaE	2	5	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	EcE	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	EcE	2	5	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	DkD	1	NAG	C1-O5-C5	3.29	116.64	112.19
5	AhA	1	NAG	C1-O5-C5	3.19	116.51	112.19
5	DiD	1	NAG	C1-O5-C5	3.17	116.49	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AmA	1	NAG	C1-O5-C5	3.15	116.46	112.19
5	BeB	1	NAG	C1-O5-C5	2.93	116.16	112.19
5	EcE	1	NAG	C1-O5-C5	2.91	116.13	112.19
5	DdD	1	NAG	C1-O5-C5	2.66	115.80	112.19
4	DmD	1	NAG	C1-O5-C5	2.64	115.77	112.19
4	DmD	1	NAG	C4-C3-C2	-2.62	107.17	111.02
4	AdA	1	NAG	C4-C3-C2	-2.61	107.19	111.02
4	AdA	1	NAG	C1-O5-C5	2.52	115.61	112.19
5	BeB	2	NAG	O5-C5-C6	2.41	110.98	107.20
4	AdA	2	NAG	C4-C3-C2	-2.31	107.63	111.02
5	BaB	1	NAG	C1-O5-C5	2.24	115.22	112.19
6	DqD	1	NAG	O5-C5-C6	2.18	110.62	107.20
5	EcE	1	NAG	O5-C1-C2	-2.18	107.85	111.29
4	DmD	1	NAG	O5-C1-C2	-2.18	107.85	111.29
5	BeB	1	NAG	C2-N2-C7	2.16	125.98	122.90
5	EaE	1	NAG	C1-O5-C5	2.11	115.06	112.19
5	DkD	1	NAG	O5-C1-C2	-2.07	108.02	111.29
4	AdA	3	BMA	O5-C5-C6	2.05	110.42	107.20
5	BeB	1	NAG	C8-C7-N2	2.04	119.55	116.10
4	AmA	1	NAG	O5-C1-C2	-2.02	108.10	111.29

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	AdA	3	BMA	C1
4	AmA	2	NAG	C1
4	AmA	3	BMA	C1
4	DmD	2	NAG	C1
4	DmD	3	BMA	C1
5	AhA	2	NAG	C1
5	AkA	2	NAG	C1
5	BaB	2	NAG	C1
5	BeB	2	NAG	C1
5	DbD	2	NAG	C1
5	DdD	2	NAG	C1
5	DgD	2	NAG	C1
5	DiD	2	NAG	C1
5	DkD	2	NAG	C1
5	EaE	2	NAG	C1
5	EcE	2	NAG	C1

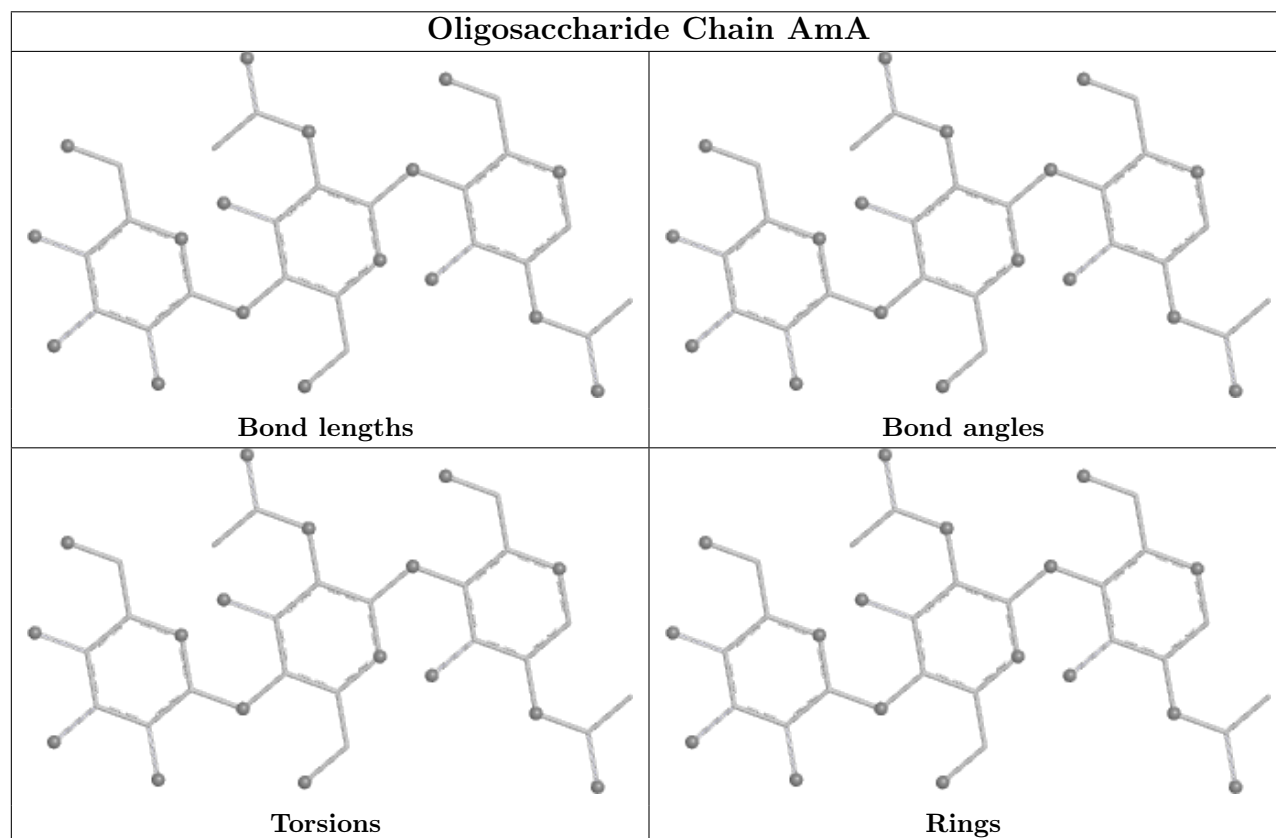
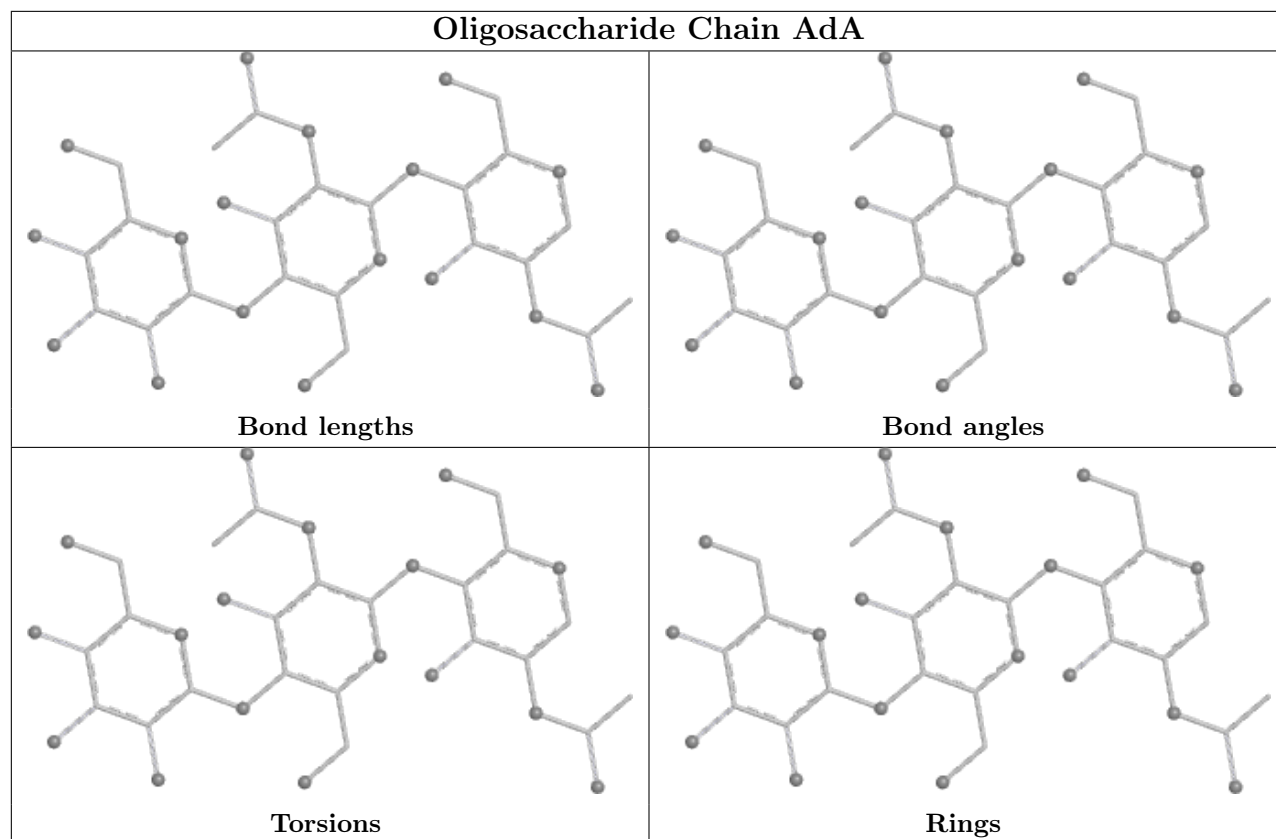
All (20) torsion outliers are listed below:

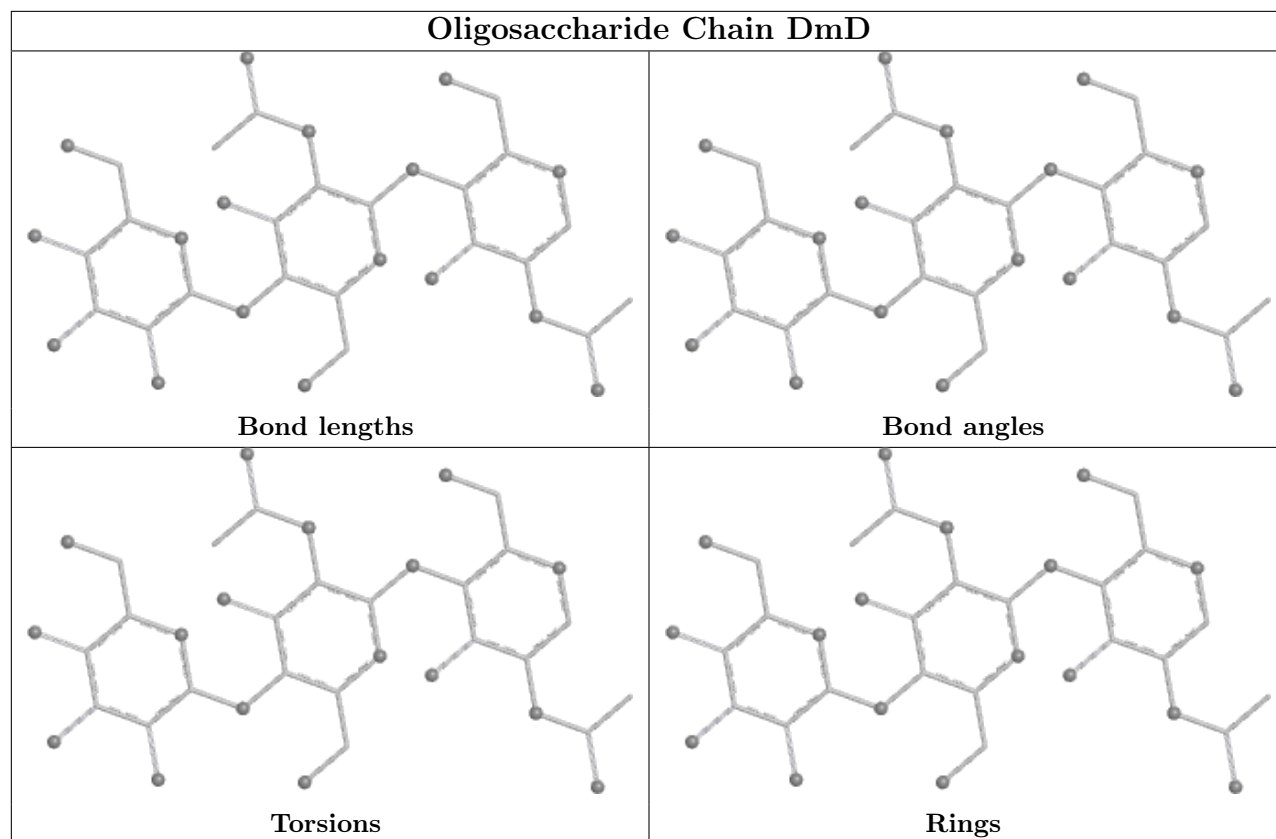
Mol	Chain	Res	Type	Atoms
4	AdA	2	NAG	O5-C5-C6-O6
5	DgD	2	NAG	O5-C5-C6-O6
5	AkA	2	NAG	O5-C5-C6-O6
5	AkA	2	NAG	C4-C5-C6-O6
5	AhA	2	NAG	O5-C5-C6-O6
5	BeB	1	NAG	C8-C7-N2-C2
5	BeB	1	NAG	O7-C7-N2-C2
5	AhA	2	NAG	C4-C5-C6-O6
4	DmD	3	BMA	C4-C5-C6-O6
4	AdA	2	NAG	C4-C5-C6-O6
5	DgD	2	NAG	C4-C5-C6-O6
4	DmD	3	BMA	O5-C5-C6-O6
6	DqD	1	NAG	C1-C2-N2-C7
5	EaE	2	NAG	C4-C5-C6-O6
5	EaE	2	NAG	O5-C5-C6-O6
5	BaB	2	NAG	C4-C5-C6-O6
4	AmA	2	NAG	C3-C2-N2-C7
5	AkA	2	NAG	C3-C2-N2-C7
5	BaB	2	NAG	O5-C5-C6-O6
6	DqD	1	NAG	C3-C2-N2-C7

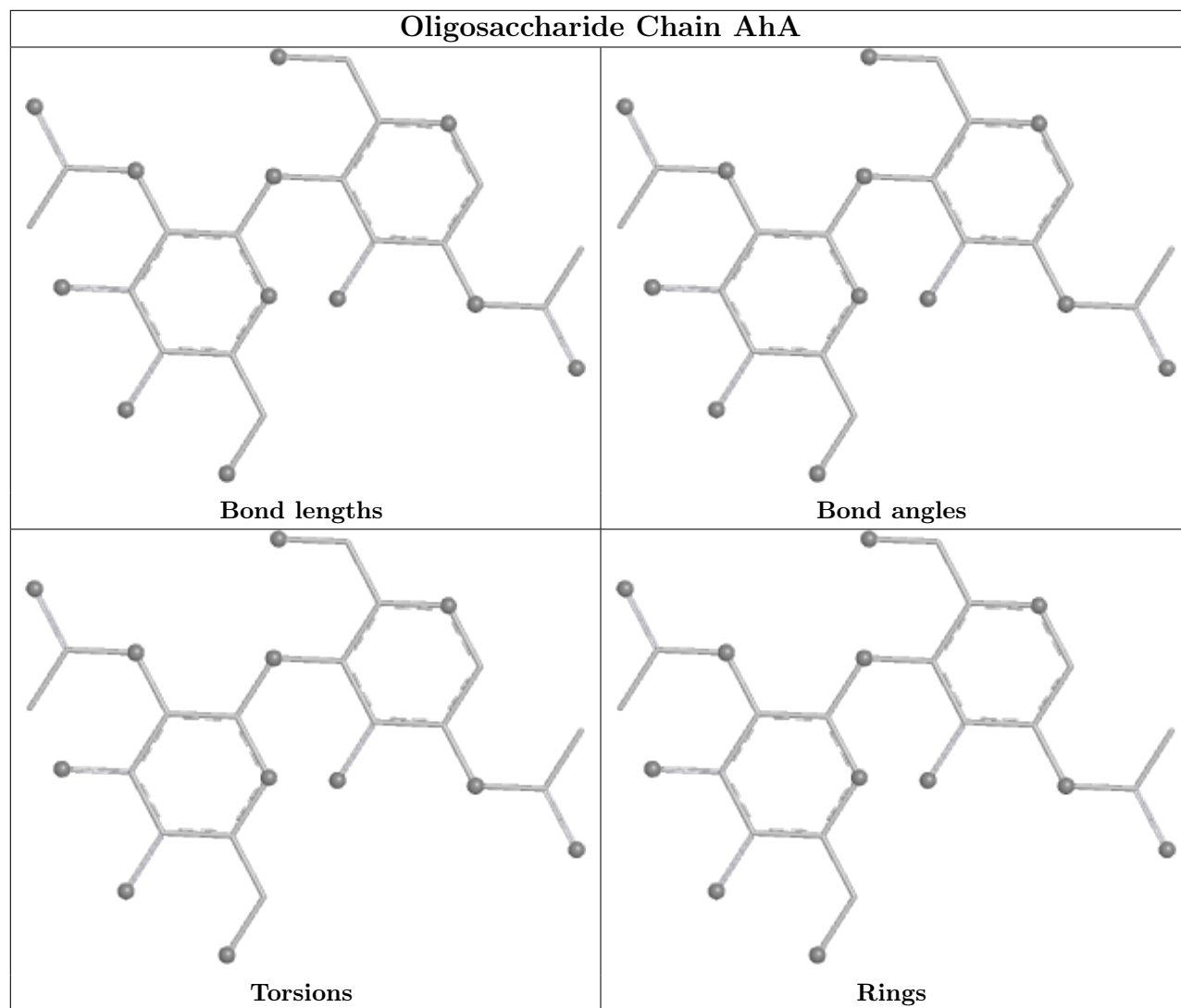
There are no ring outliers.

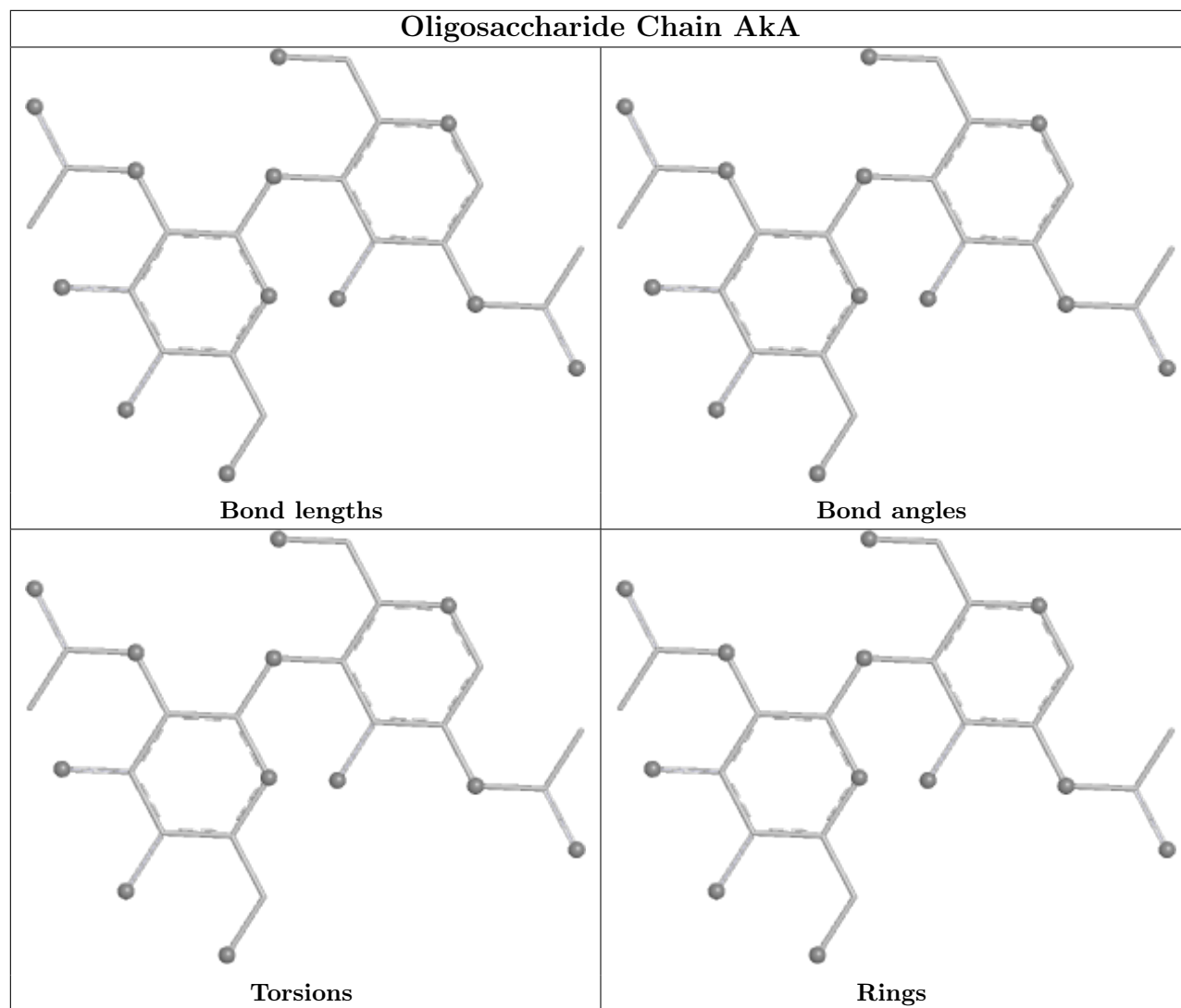
No monomer is involved in short contacts.

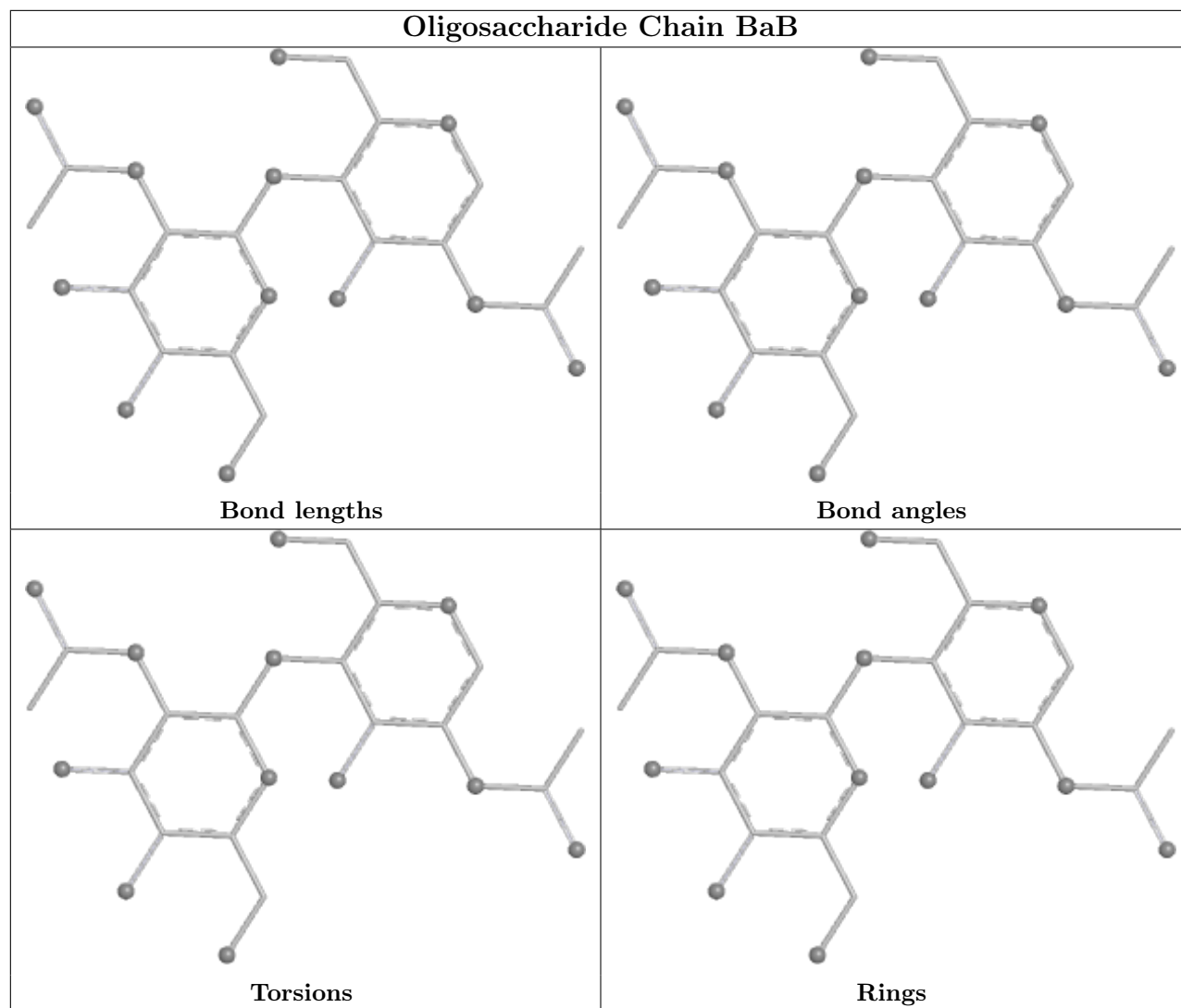
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

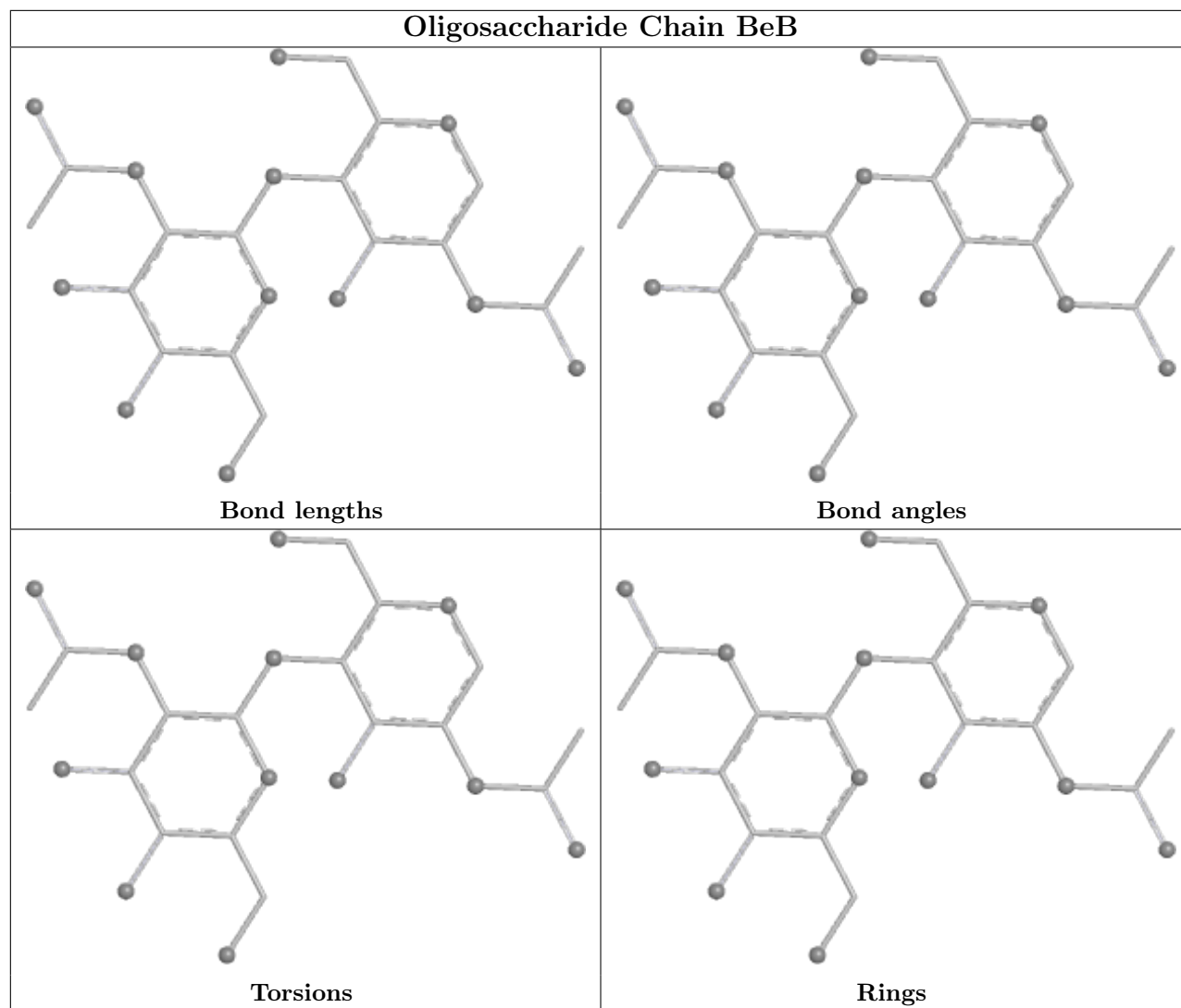


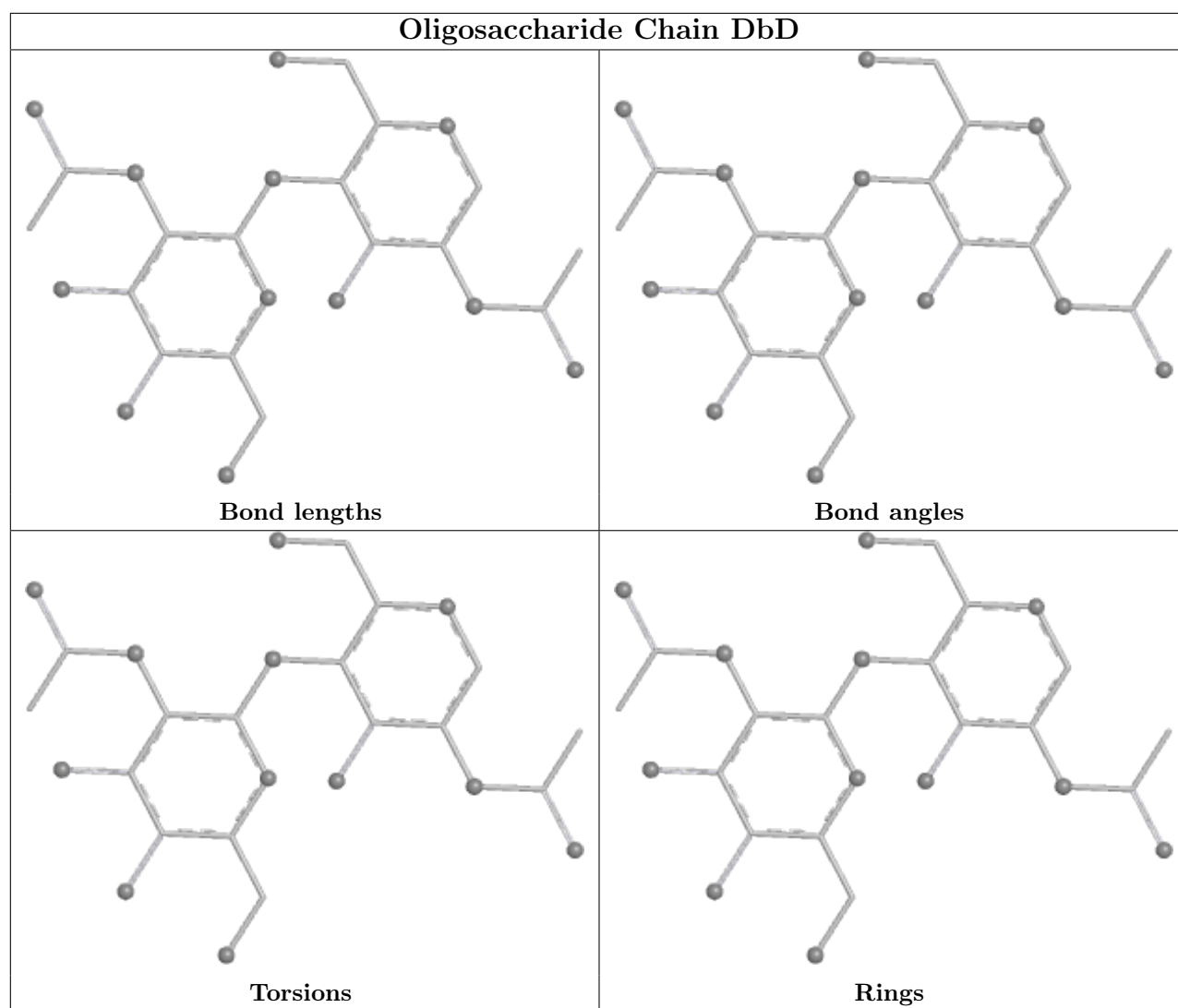


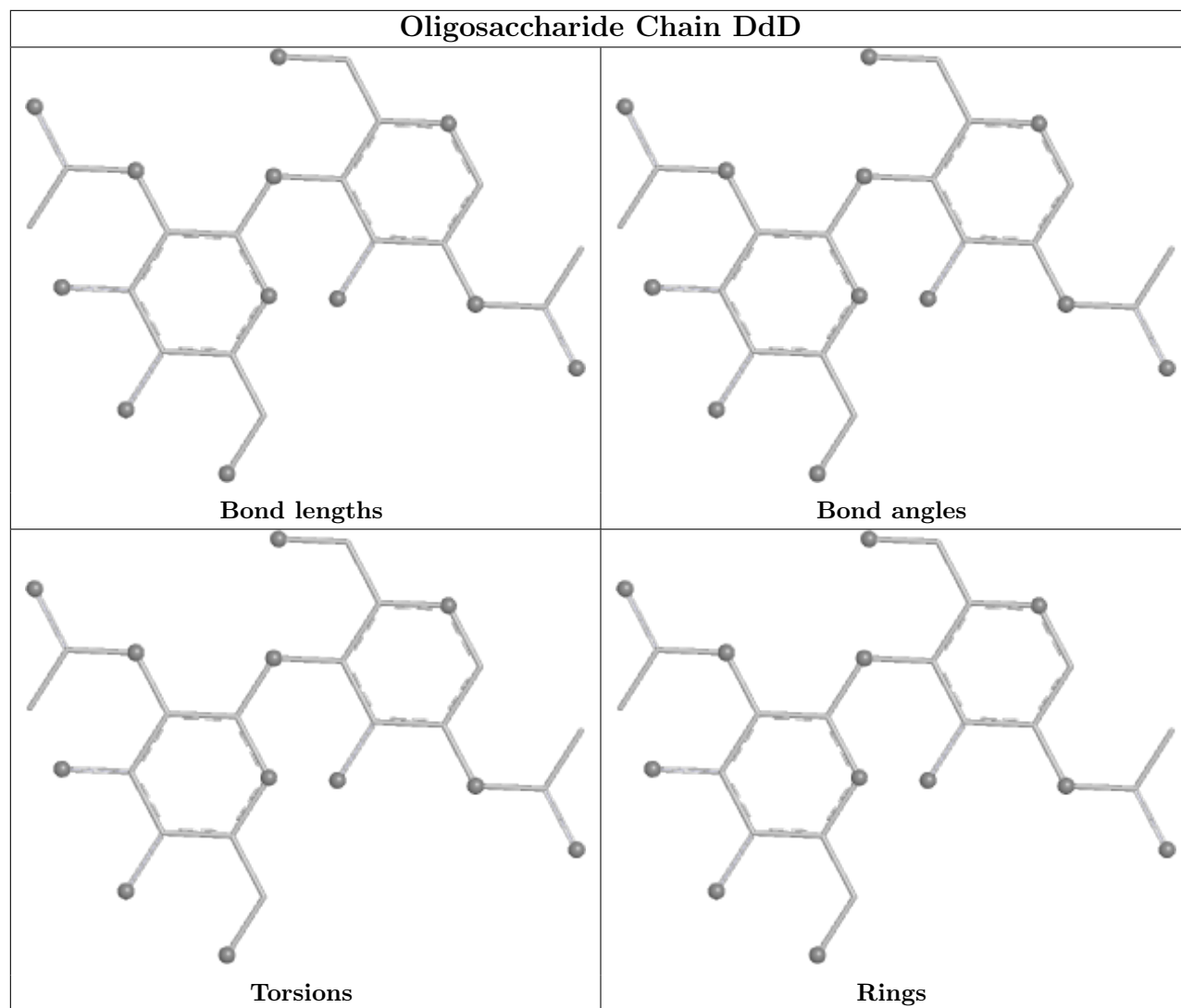


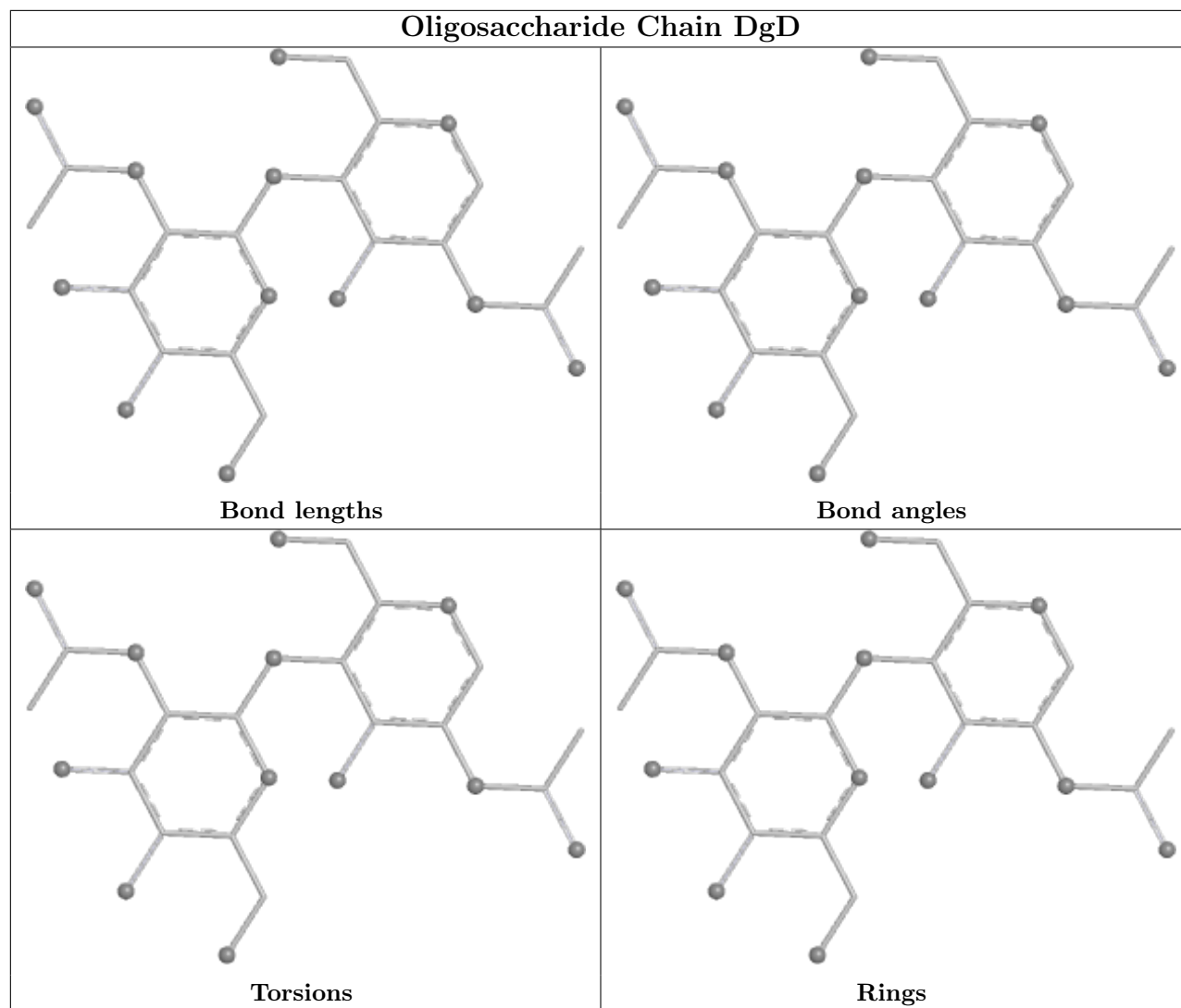


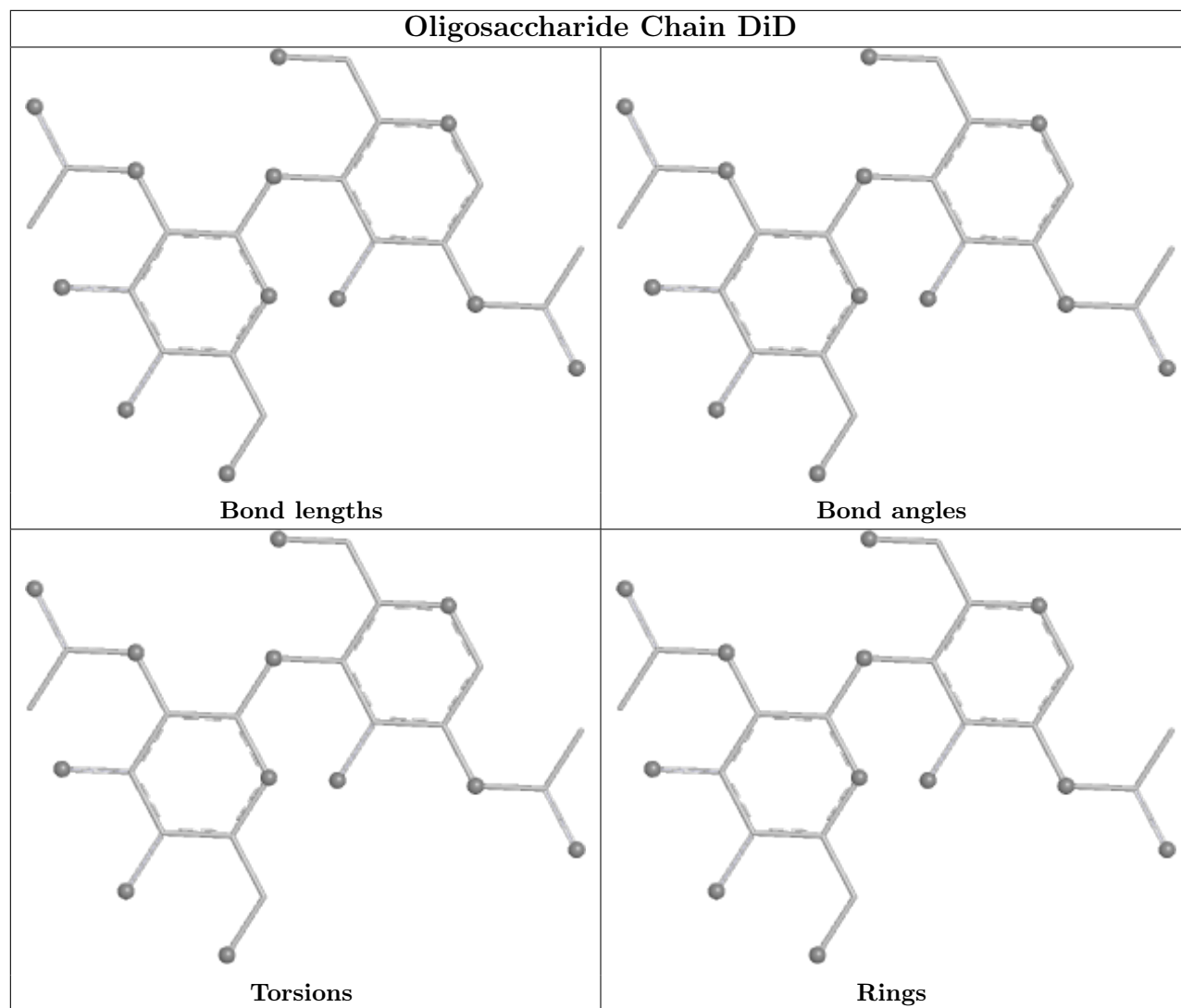


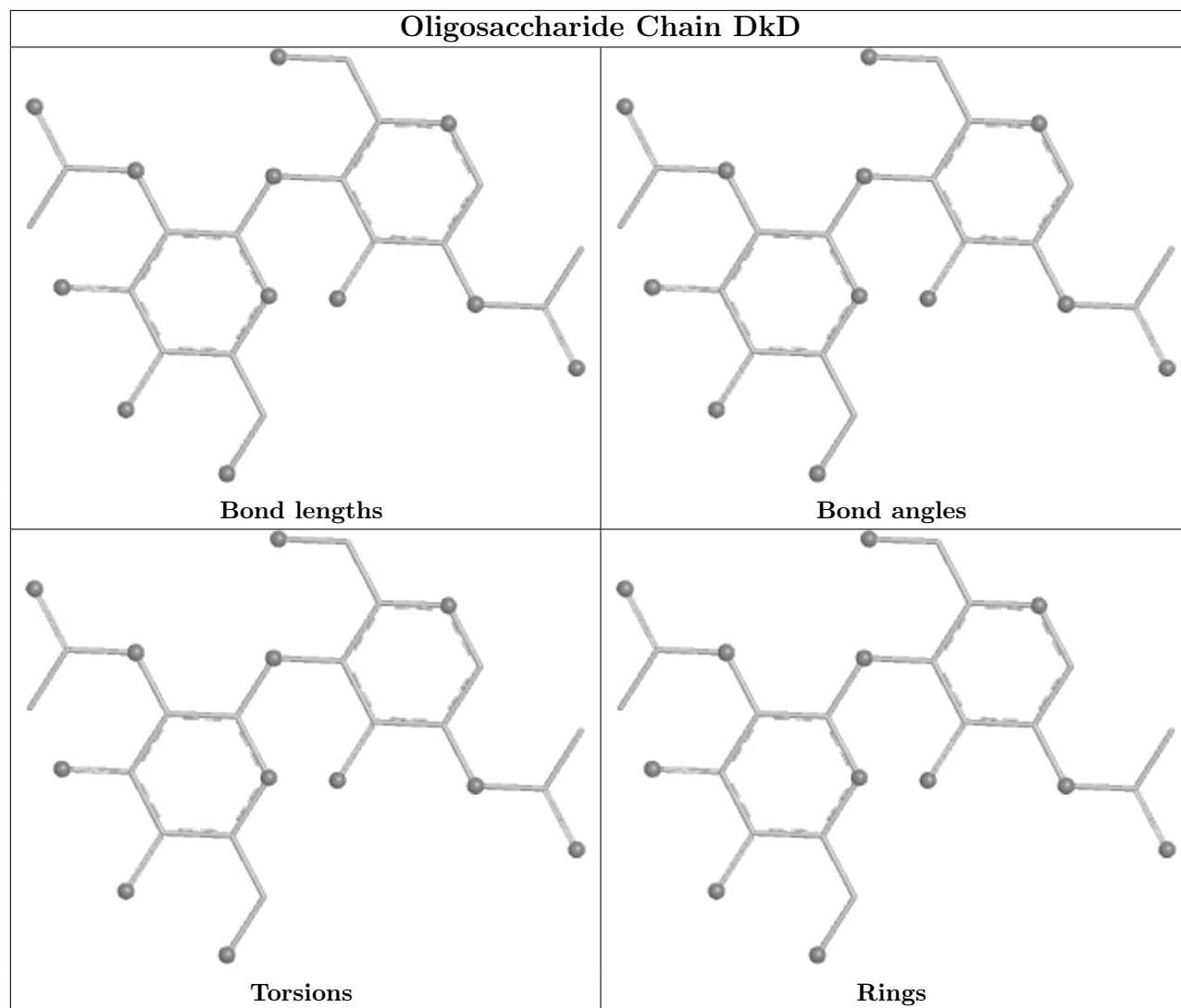


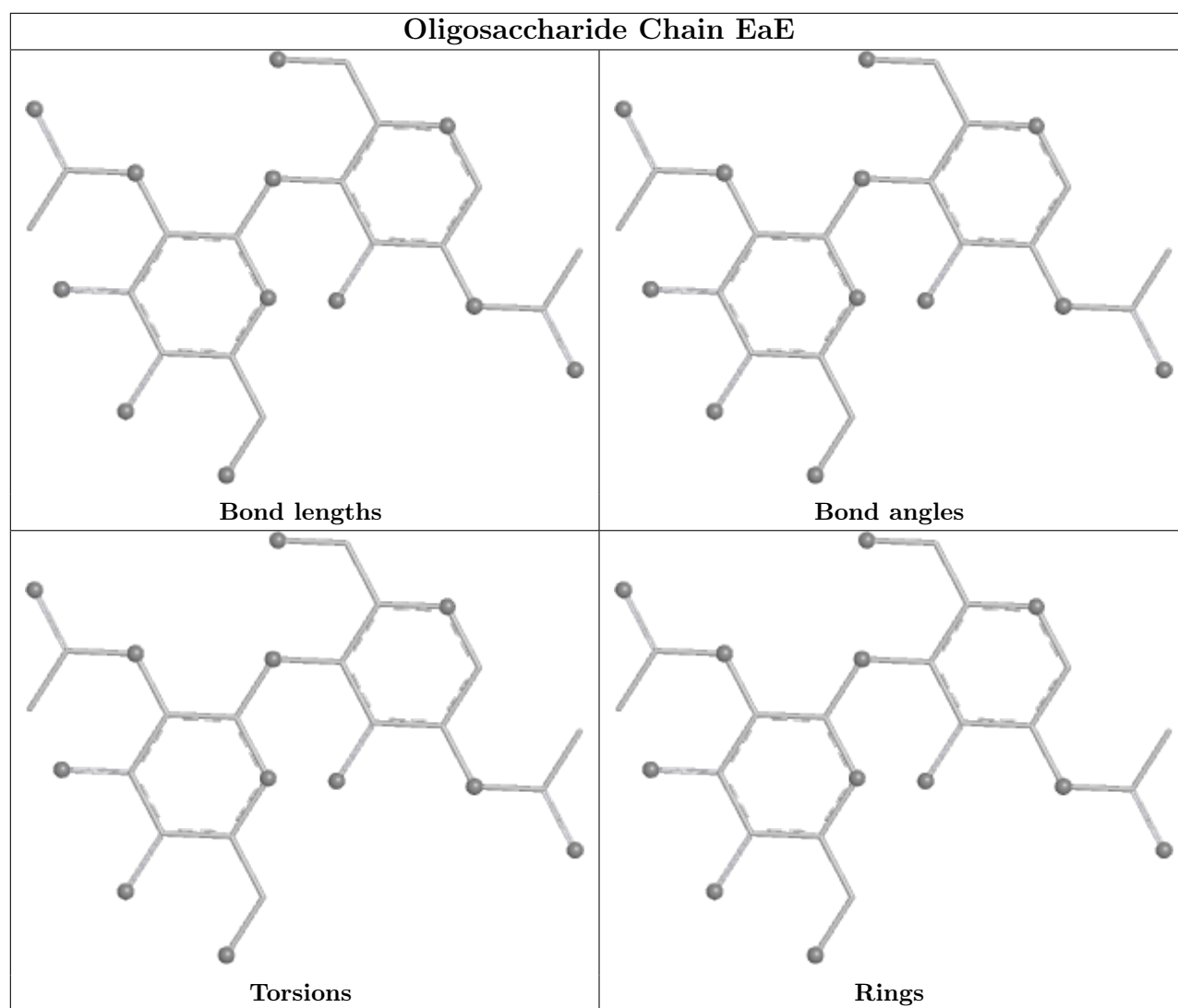


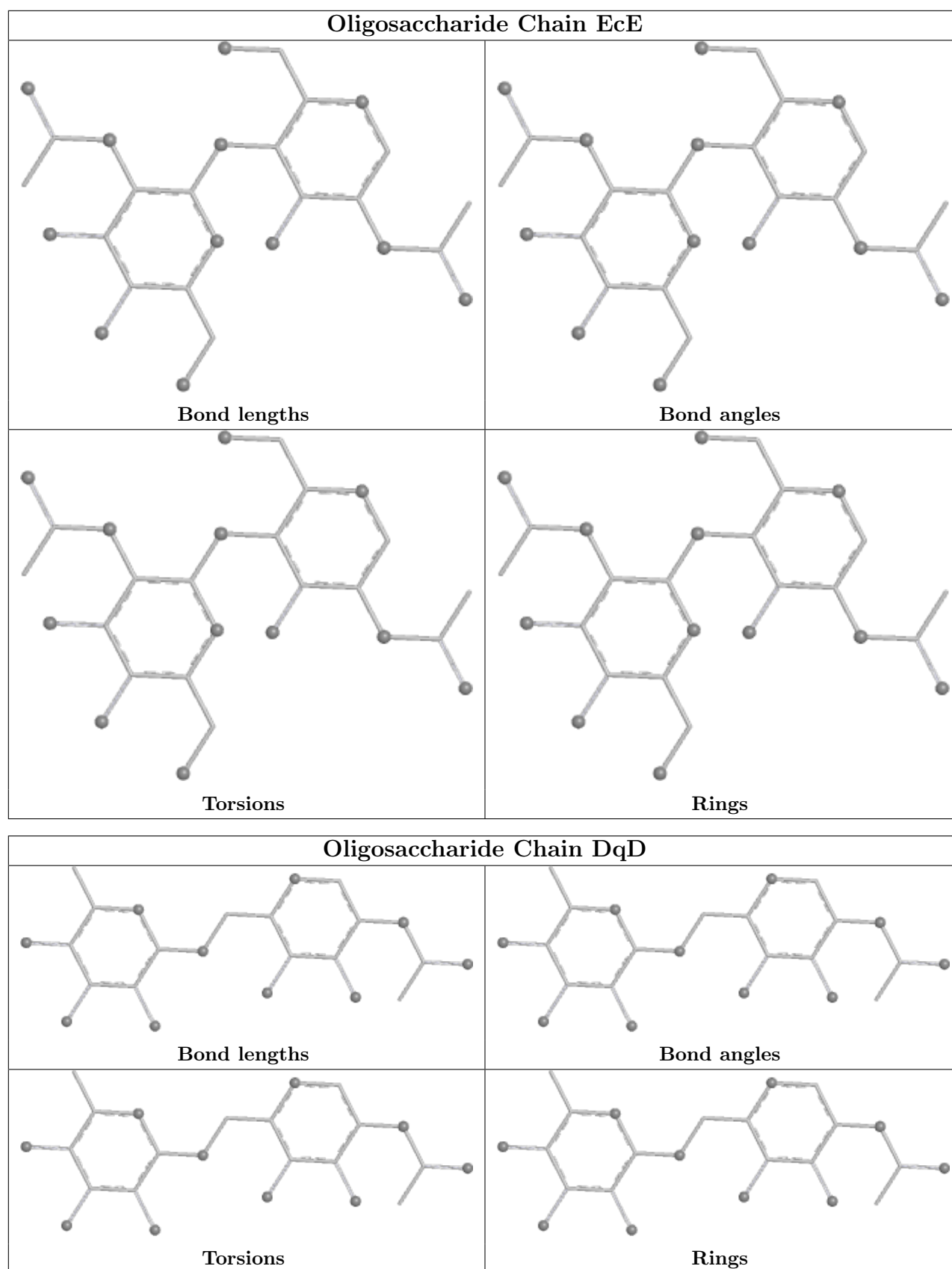












5.6 Ligand geometry

Of 19 ligands modelled in this entry, 7 are monoatomic - leaving 12 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
7	NAG	DDD	702	1	14,14,15	0.38	0	17,19,21	0.94	0
7	NAG	AAA	704	1	14,14,15	0.39	0	17,19,21	0.97	1 (5%)
7	NAG	EEE	301	2	14,14,15	0.39	0	17,19,21	0.72	0
7	NAG	AAA	703	1	14,14,15	0.38	0	17,19,21	0.86	1 (5%)
7	NAG	AAA	701	1	14,14,15	0.37	0	17,19,21	1.30	2 (11%)
7	NAG	BBB	301	2	14,14,15	0.50	0	17,19,21	1.48	2 (11%)
7	NAG	BBB	303	2	14,14,15	0.28	0	17,19,21	1.22	3 (17%)
7	NAG	DDD	701	1,9	14,14,15	0.38	0	17,19,21	0.68	0
7	NAG	DDD	703	1	14,14,15	0.40	0	17,19,21	0.95	1 (5%)
7	NAG	AAA	705	1	14,14,15	0.52	0	17,19,21	1.28	1 (5%)
7	NAG	AAA	702	1,9	14,14,15	0.36	0	17,19,21	0.77	0
7	NAG	BBB	302	2	14,14,15	0.38	0	17,19,21	0.76	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	DDD	702	1	-	2/6/23/26	0/1/1/1
7	NAG	AAA	704	1	-	1/6/23/26	0/1/1/1
7	NAG	EEE	301	2	-	0/6/23/26	0/1/1/1
7	NAG	AAA	703	1	-	0/6/23/26	0/1/1/1
7	NAG	AAA	701	1	-	3/6/23/26	0/1/1/1
7	NAG	BBB	301	2	-	0/6/23/26	0/1/1/1
7	NAG	BBB	303	2	-	2/6/23/26	0/1/1/1
7	NAG	DDD	701	1,9	-	0/6/23/26	0/1/1/1
7	NAG	DDD	703	1	-	0/6/23/26	0/1/1/1
7	NAG	AAA	705	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	AAA	702	1,9	-	0/6/23/26	0/1/1/1
7	NAG	BBB	302	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	BBB	301	NAG	C1-O5-C5	5.17	119.19	112.19
7	AAA	705	NAG	C2-N2-C7	3.49	127.88	122.90
7	AAA	701	NAG	O5-C1-C2	-2.43	107.45	111.29
7	AAA	704	NAG	C1-O5-C5	2.40	115.44	112.19
7	BBB	302	NAG	O5-C5-C6	2.33	110.85	107.20
7	AAA	703	NAG	O5-C5-C6	2.31	110.83	107.20
7	AAA	701	NAG	C8-C7-N2	2.30	119.99	116.10
7	BBB	301	NAG	O5-C1-C2	-2.23	107.77	111.29
7	BBB	303	NAG	C4-C3-C2	-2.17	107.84	111.02
7	BBB	303	NAG	O5-C1-C2	-2.16	107.87	111.29
7	BBB	303	NAG	C8-C7-N2	2.14	119.73	116.10
7	DDD	703	NAG	C2-N2-C7	2.03	125.79	122.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	AAA	705	NAG	C3-C2-N2-C7
7	AAA	701	NAG	C8-C7-N2-C2
7	AAA	701	NAG	O7-C7-N2-C2
7	BBB	303	NAG	C8-C7-N2-C2
7	BBB	303	NAG	O7-C7-N2-C2
7	DDD	702	NAG	O5-C5-C6-O6
7	DDD	702	NAG	C4-C5-C6-O6
7	AAA	701	NAG	O5-C5-C6-O6
7	AAA	704	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
7	BBB	301	NAG	1	0
7	AAA	705	NAG	1	0

5.7 Other polymers

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%)	0.18	6 (1%) 82 86	26, 45, 77, 120	0
1	DDD	595/617 (96%)	0.15	8 (1%) 77 81	27, 41, 69, 125	0
2	BBB	185/203 (91%)	0.26	1 (0%) 91 94	30, 41, 64, 85	0
2	EEE	185/203 (91%)	0.23	0 100 100	29, 42, 64, 84	0
3	CCC	13/14 (92%)	0.27	1 (7%) 13 18	29, 39, 71, 76	0
3	FFF	13/14 (92%)	0.14	0 100 100	29, 35, 64, 69	0
All	All	1585/1668 (95%)	0.18	16 (1%) 82 86	26, 43, 72, 125	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	601	ASP	3.3
1	AAA	603	LYS	3.2
1	DDD	604	GLY	3.0
1	DDD	59	PHE	3.0
1	AAA	581	PRO	3.0
1	DDD	579	LEU	2.8
1	AAA	59	PHE	2.7
1	DDD	583	LEU	2.5
1	AAA	604	GLY	2.4
1	DDD	603	LYS	2.4
3	CCC	56	TYR	2.2
1	AAA	244	HIS	2.2
2	BBB	189	LEU	2.1
1	DDD	605	LEU	2.1
1	AAA	606	CYS	2.0
1	DDD	597	GLY	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	CCC	64	8/9	0.93	0.11	35,40,42,42	0
3	HYP	FFF	64	8/9	0.96	0.11	25,33,35,36	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
6	NAG	DqD	1	14/15	0.62	0.29	95,107,121,128	0
4	BMA	AmA	3	11/12	0.70	0.25	110,137,144,154	0
5	NAG	AhA	2	14/15	0.76	0.20	66,100,107,107	0
5	NAG	DgD	2	14/15	0.77	0.24	76,92,103,103	0
4	BMA	AdA	3	11/12	0.78	0.18	76,82,87,89	0
5	NAG	AkA	2	14/15	0.78	0.23	85,104,117,132	0
5	NAG	DbD	1	14/15	0.79	0.19	68,83,98,102	0
5	NAG	DdD	2	14/15	0.79	0.16	66,100,109,111	0
5	NAG	DbD	2	14/15	0.80	0.42	103,123,132,133	0
5	NAG	BaB	2	14/15	0.80	0.21	65,94,102,102	0
5	NAG	EcE	2	14/15	0.81	0.17	82,96,105,109	0
5	NAG	BeB	2	14/15	0.82	0.24	83,107,112,115	0
6	FUC	DqD	2	10/11	0.82	0.34	102,119,125,137	0
5	NAG	EaE	2	14/15	0.84	0.25	69,100,103,107	0
4	NAG	AmA	2	14/15	0.84	0.20	100,113,128,138	0
4	BMA	DmD	3	11/12	0.85	0.17	79,86,93,101	0
5	NAG	DkD	2	14/15	0.86	0.14	70,80,86,91	0
5	NAG	AhA	1	14/15	0.87	0.15	53,69,74,88	0
5	NAG	BaB	1	14/15	0.87	0.11	60,65,71,81	0
5	NAG	DiD	2	14/15	0.87	0.17	47,70,78,78	0
4	NAG	AdA	2	14/15	0.87	0.17	51,67,71,75	0
5	NAG	EaE	1	14/15	0.89	0.15	59,64,68,75	0
5	NAG	EcE	1	14/15	0.90	0.17	70,76,83,83	0
5	NAG	AkA	1	14/15	0.90	0.10	50,56,64,74	0
4	NAG	DmD	2	14/15	0.91	0.14	58,69,77,81	0

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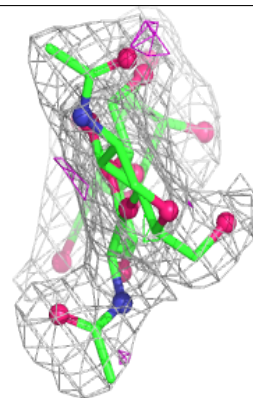
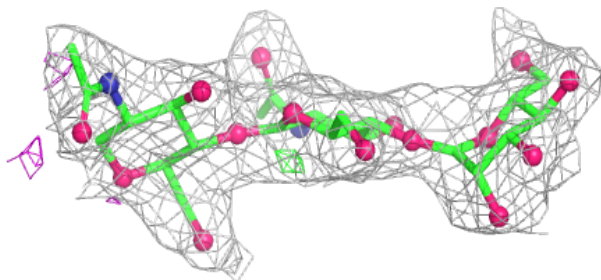
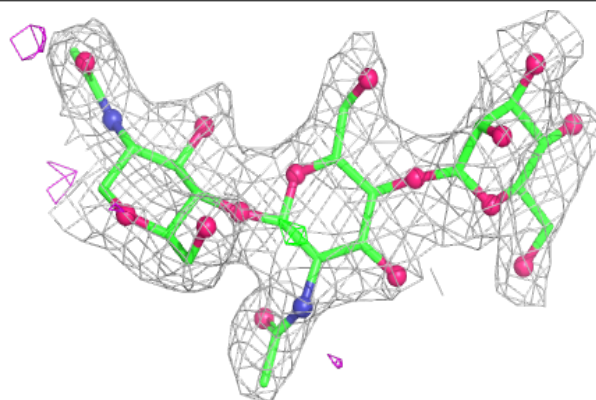
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	AmA	1	14/15	0.91	0.10	47,58,68,86	0
5	NAG	DiD	1	14/15	0.91	0.12	45,55,67,67	0
5	NAG	BeB	1	14/15	0.91	0.14	74,83,92,93	0
5	NAG	DkD	1	14/15	0.91	0.10	43,53,61,69	0
5	NAG	DdD	1	14/15	0.91	0.10	54,62,66,81	0
4	NAG	DmD	1	14/15	0.92	0.12	34,37,39,41	0
5	NAG	DgD	1	14/15	0.93	0.10	45,54,60,72	0
4	NAG	AdA	1	14/15	0.93	0.15	35,39,40,41	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.

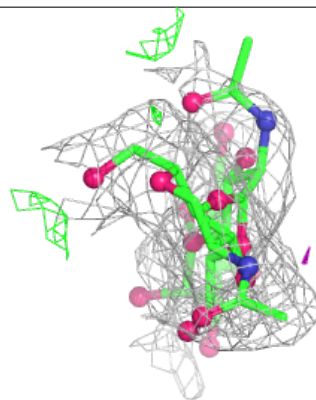
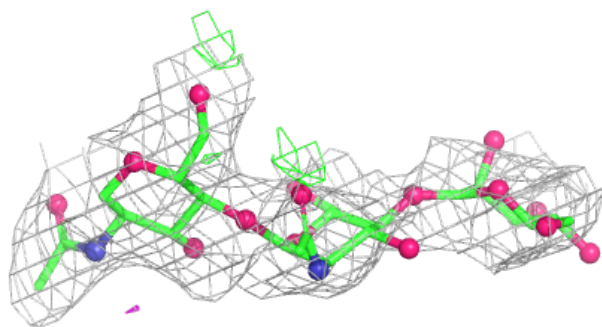
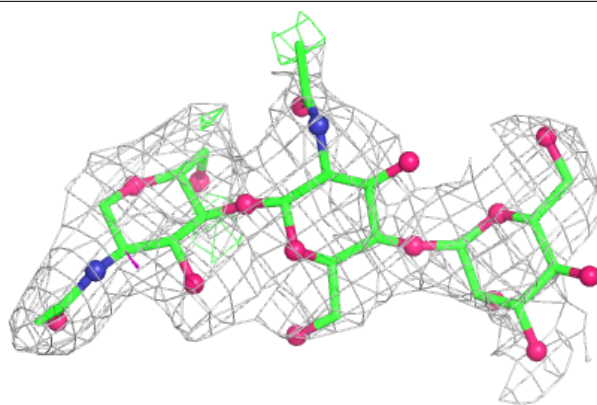
Electron density around Chain AdA:

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

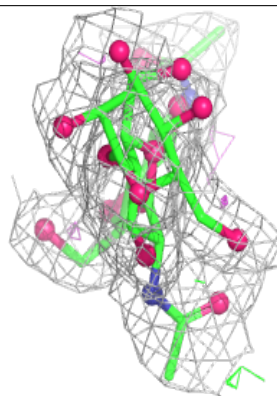
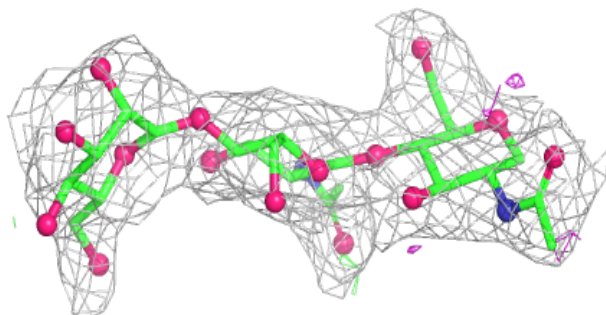
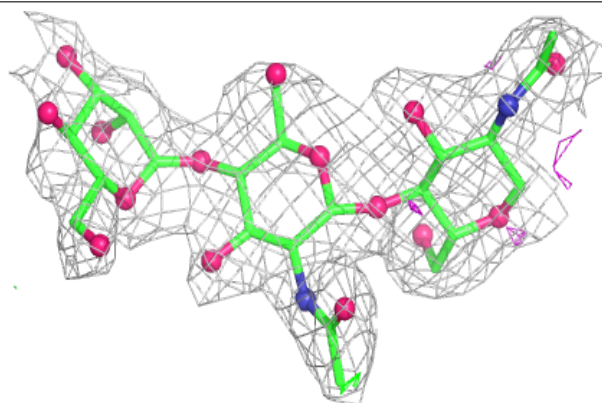


Electron density around Chain AmA:

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

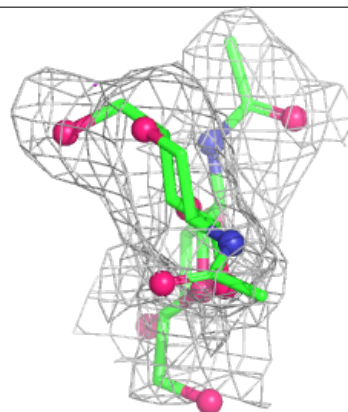
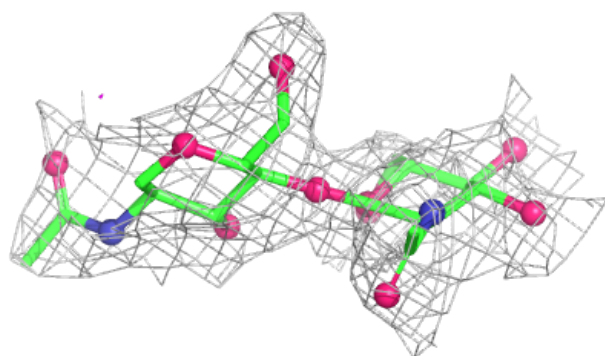
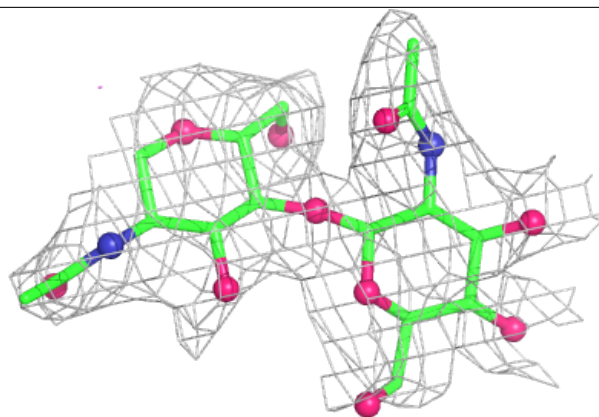
**Electron density around Chain DmD:**

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and green (positive)

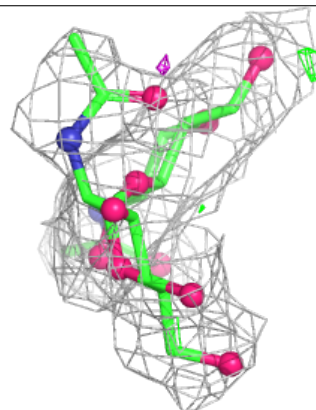
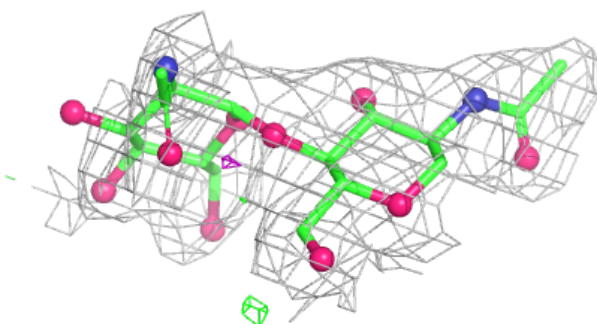
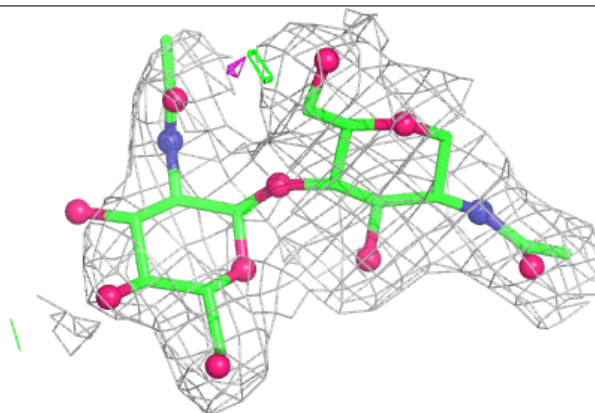


Electron density around Chain AhA:

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and green (positive)

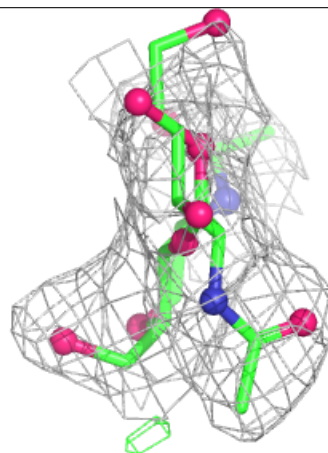
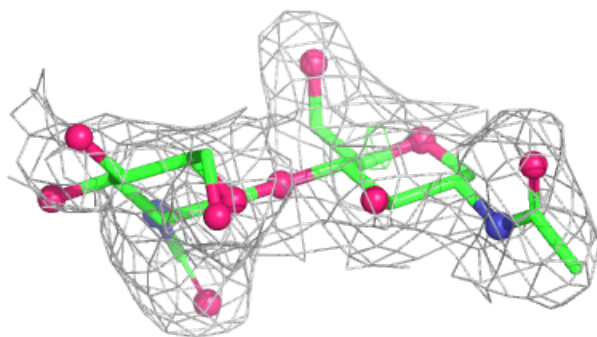
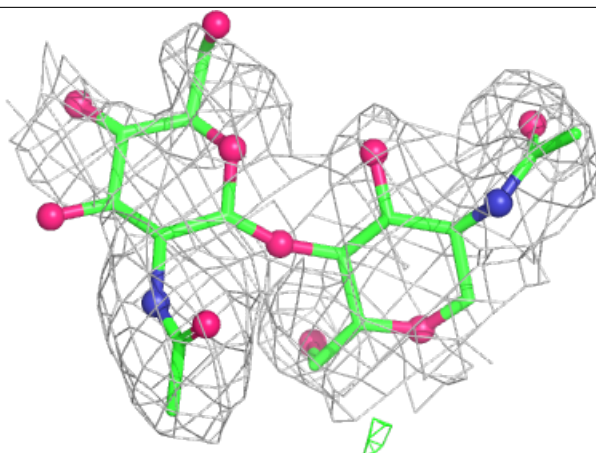
**Electron density around Chain AkA:**

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and green (positive)



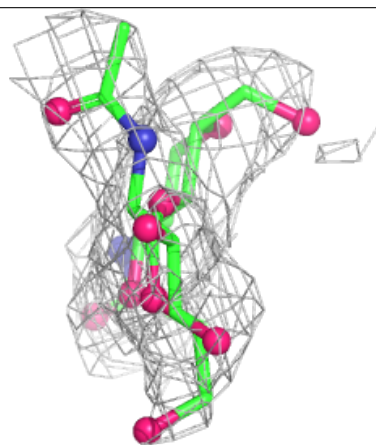
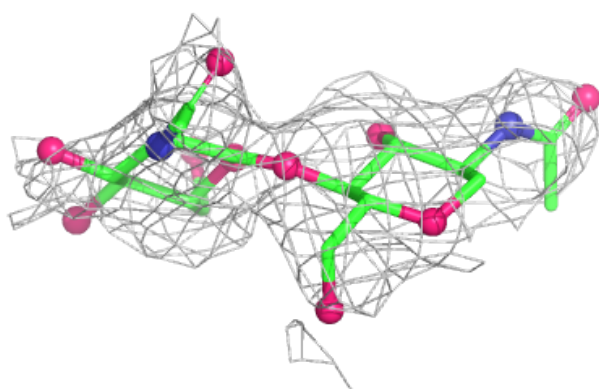
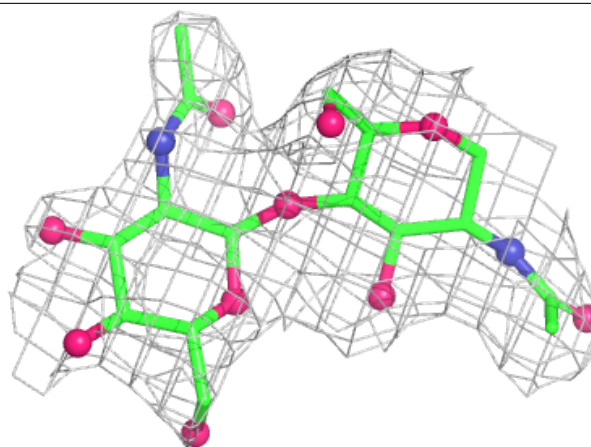
Electron density around Chain BaB:

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

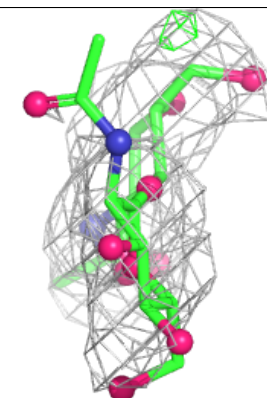
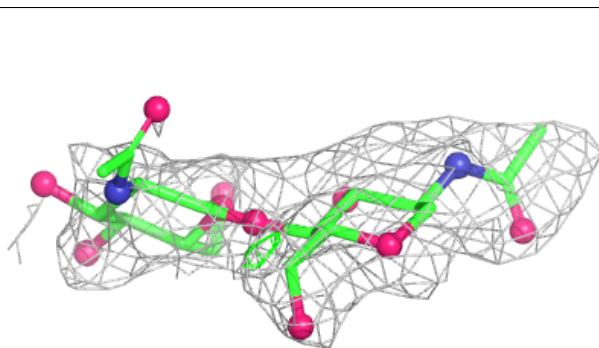
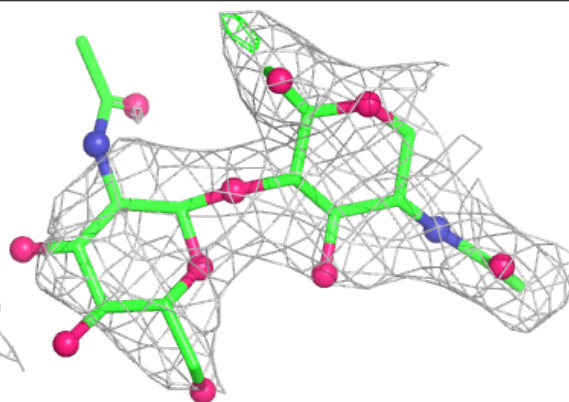


Electron density around Chain BeB:

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

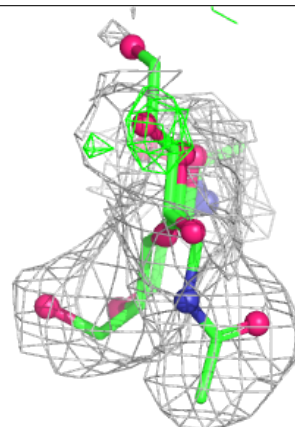
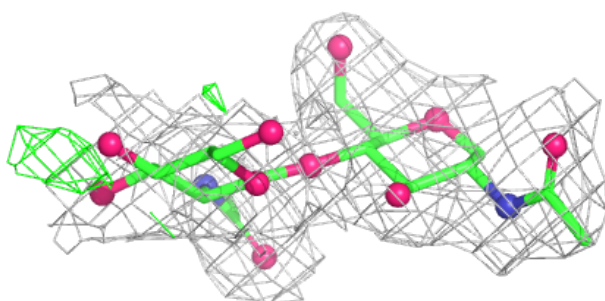
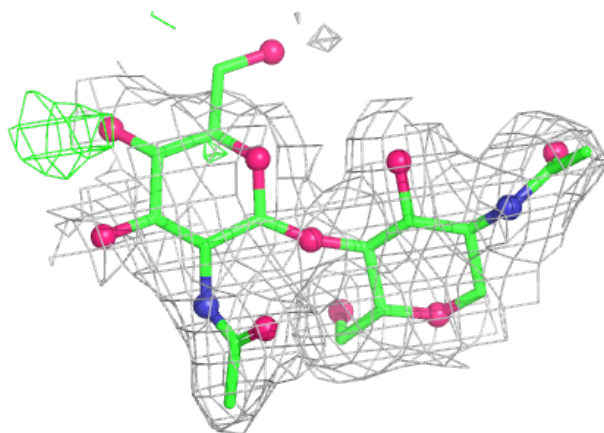
**Electron density around Chain DbD:**

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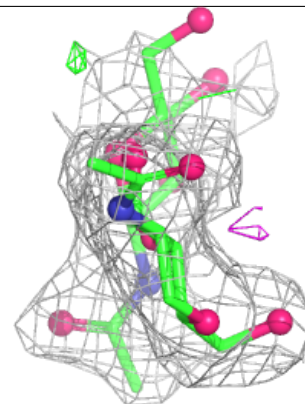
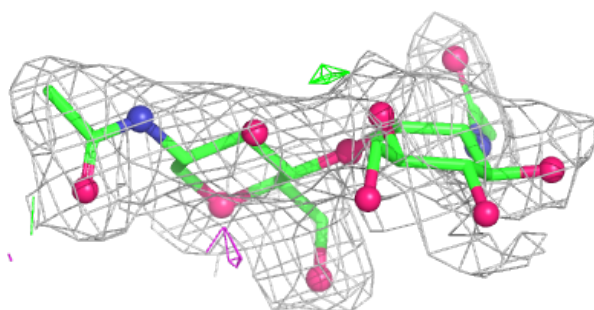
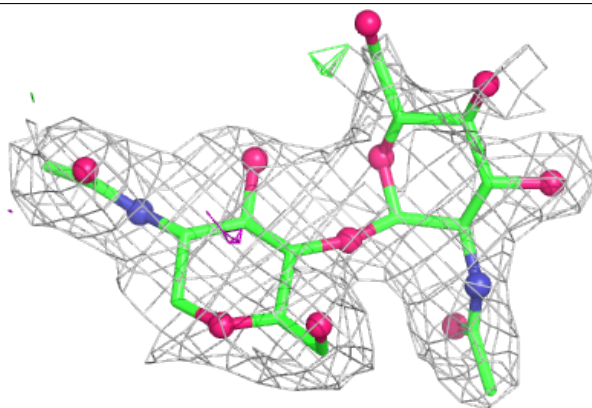


Electron density around Chain DdD:

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

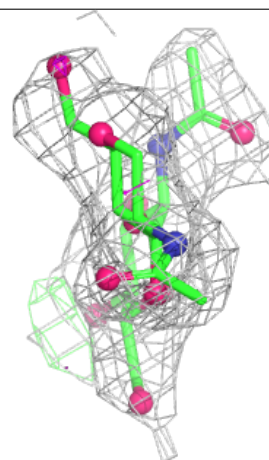
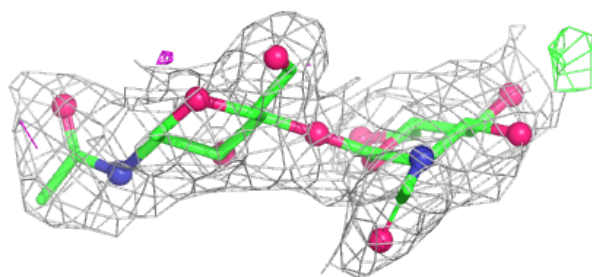
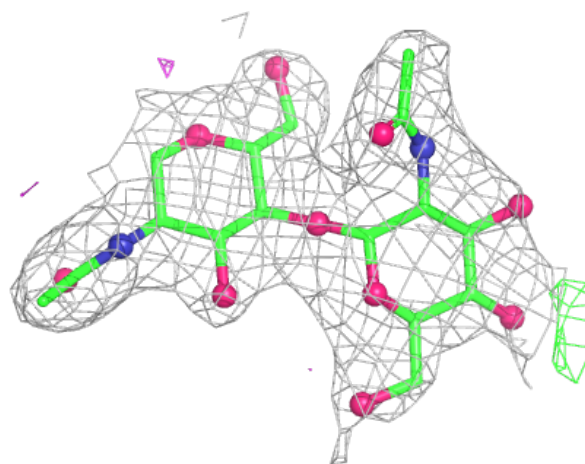
**Electron density around Chain DgD:**

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



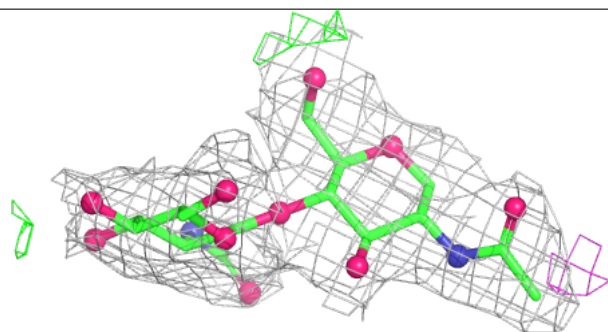
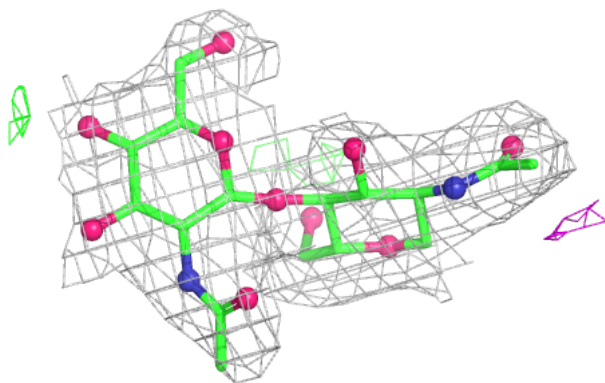
Electron density around Chain DiD:

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



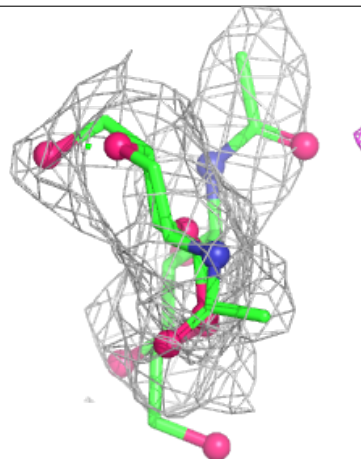
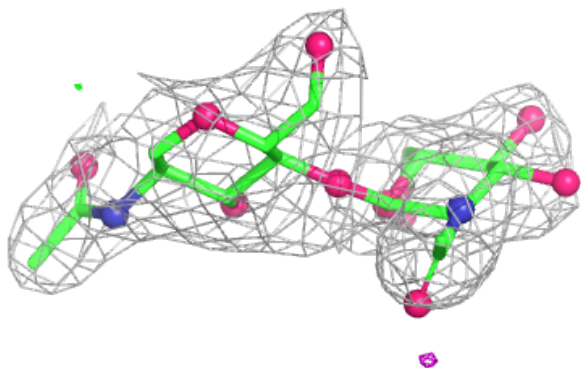
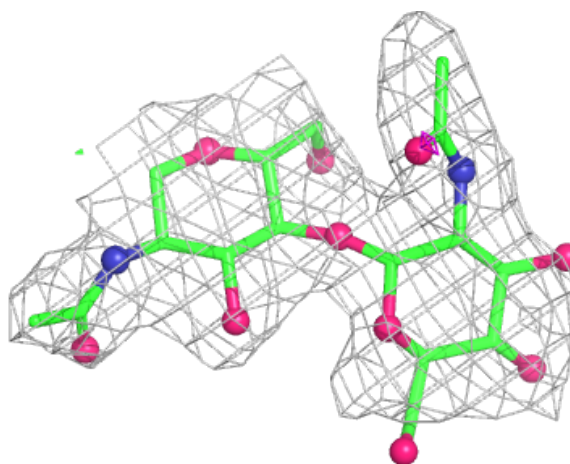
Electron density around Chain DkD:

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



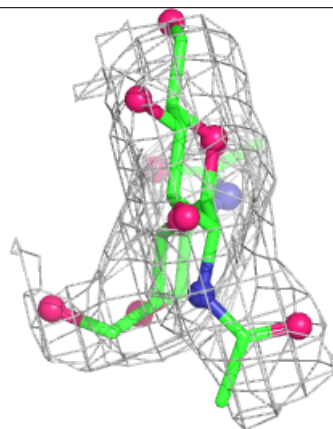
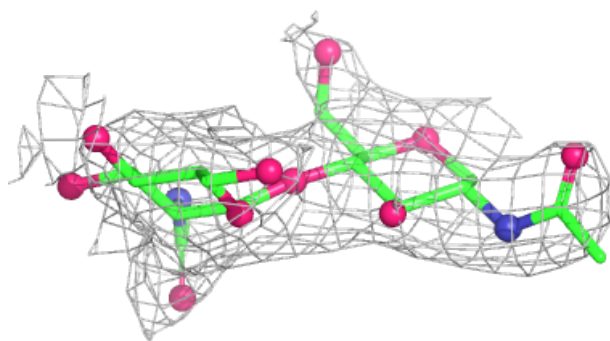
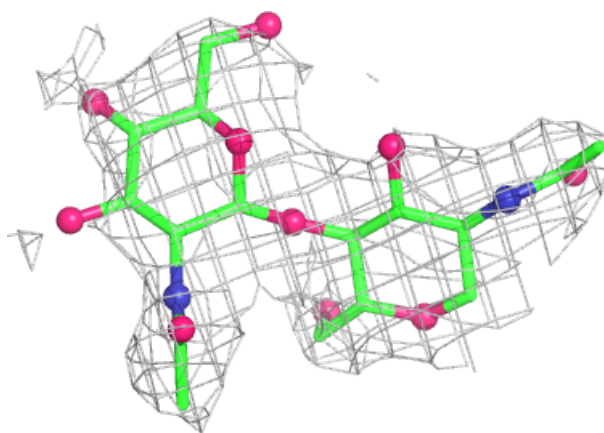
Electron density around Chain EaE:

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

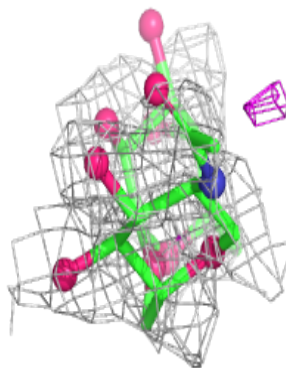
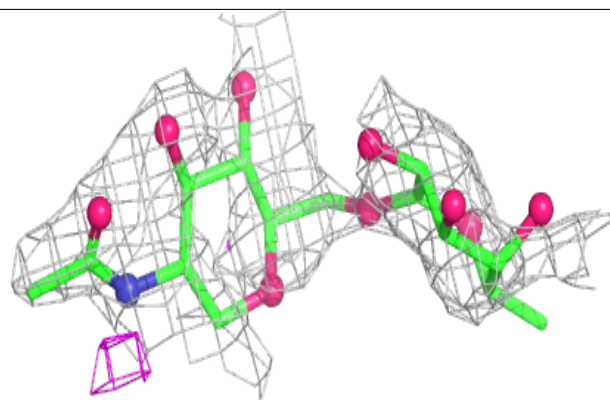
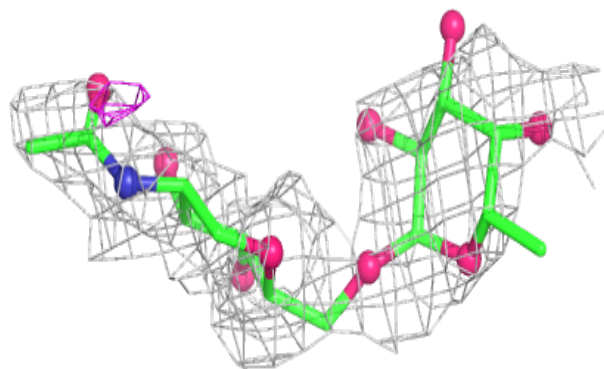


Electron density around Chain EcE:

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

**Electron density around Chain DqD:**

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



6.4 Ligands [i](#)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers [i](#)

There are no such residues in this entry.