



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2025 – 02:44 pm BST

PDB ID : 7OGO / pdb\_00007ogo  
Title : Plant peptide hormone receptor H1I1S1  
Authors : Roman, A.O.; Jimenez-Sandoval, P.; Santiago, J.  
Deposited on : 2021-05-07  
Resolution : 2.38 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

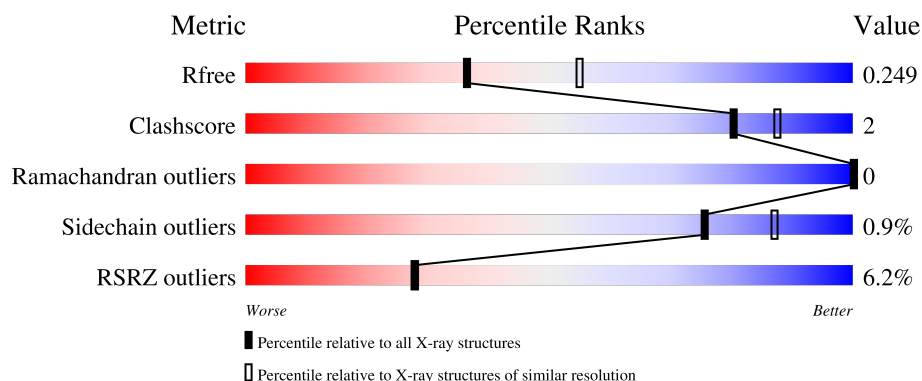
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	6699 (2.40-2.36)
Clashscore	180529	7414 (2.40-2.36)
Ramachandran outliers	177936	7337 (2.40-2.36)
Sidechain outliers	177891	7338 (2.40-2.36)
RSRZ outliers	164620	6699 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	617	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>
1	DDD	617	<div> <div>7%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>
2	BBB	203	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>9%</div> </div> </div>
2	EEE	203	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>7%</div> <div>9%</div> </div> </div>
3	CCC	14	<div> <div>7%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	FFF	14	
4	AaA	4	
5	AeA	3	
5	DkD	3	
6	AhA	2	
6	AkA	2	
6	AnA	2	
6	BaB	2	
6	BcB	2	
6	DaD	2	
6	DeD	2	
6	DgD	2	
6	EaE	2	
6	EeE	2	
7	ArA	5	
7	DqD	5	
8	DnD	3	

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	MAN	AaA	4	X	-	-	-
5	NAG	AeA	2	X	-	-	-
5	NAG	DkD	2	X	-	-	-
6	NAG	AhA	2	X	-	-	-
6	NAG	AnA	2	X	-	-	-
6	NAG	BaB	2	X	-	-	-
6	NAG	BcB	2	X	-	-	-
6	NAG	DaD	2	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	DgD	2	X	-	-	-
6	NAG	EaE	2	X	-	-	-
6	NAG	EeE	2	X	-	-	-
7	BMA	ArA	3	X	-	-	-
7	NAG	DqD	2	X	-	-	-
7	BMA	DqD	3	X	-	-	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12777 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	586	Total	C	N	O	S	0	0	0
			4384	2779	720	871	14			
1	DDD	587	Total	C	N	O	S	0	0	0
			4388	2781	720	872	15			

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	5	5	0
			1412	896	237	274	5			
2	EEE	185	Total	C	N	O	S	0	0	0
			1392	879	238	270	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-LIKE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CCC	14	Total	C	N	O	S	0	0	0
			110	69	20	20	1			
3	FFF	14	Total	C	N	O	S	0	0	0
			108	67	20	20	1			

There are 2 discrepancies between the modelled and reference sequences:

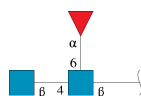
Chain	Residue	Modelled	Actual	Comment	Reference
CCC	65	TYR	ARG	conflict	UNP Q29PV4
FFF	65	TYR	ARG	conflict	UNP Q29PV4

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



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

- Molecule 5 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.



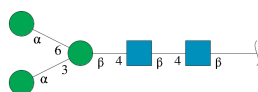
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	AeA	3	Total	C	N	O	0	0	0
			38	22	2	14			
5	DkD	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	AhA	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	AkA	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	AnA	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	BaB	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	BcB	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	DaD	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	DeD	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	DgD	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	EaE	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	EeE	2	Total	C	N	O	0	0	0
			28	16	2	10			

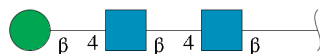
- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.





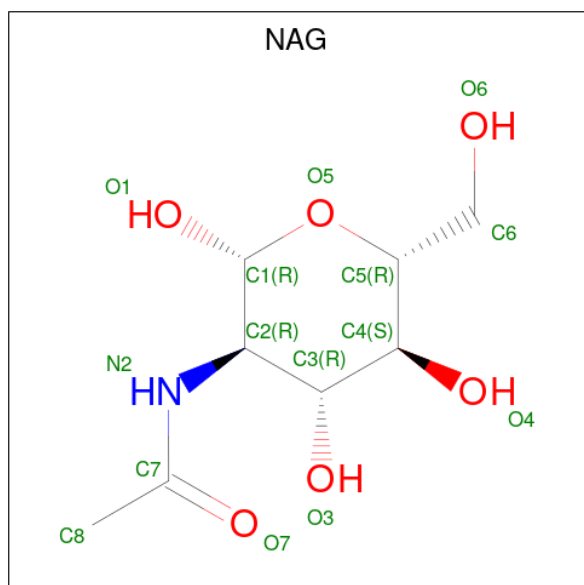
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	ArA	5	Total	C	N	O	0	0	0
			61	34	2	25			
7	DqD	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 8 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
8	DnD	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
9	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
9	AAA	1	Total	C	N	O	0	0
			14	8	1	5		

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

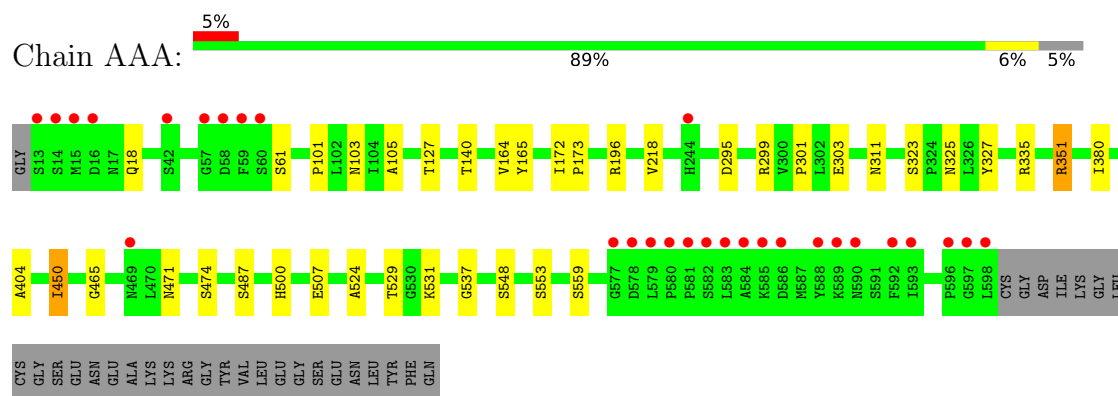
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	AAA	128	Total	O	0	0
			128	128		
10	BBB	27	Total	O	0	0
			27	27		
10	CCC	2	Total	O	0	0
			2	2		
10	DDD	86	Total	O	0	0
			86	86		
10	EEE	31	Total	O	0	0
			31	31		
10	FFF	2	Total	O	0	0
			2	2		

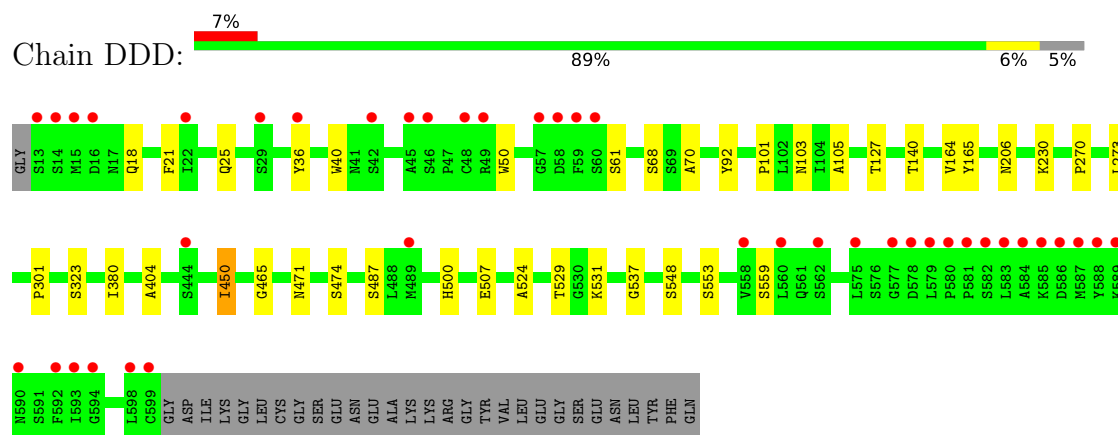
### 3 Residue-property plots [i](#)

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.

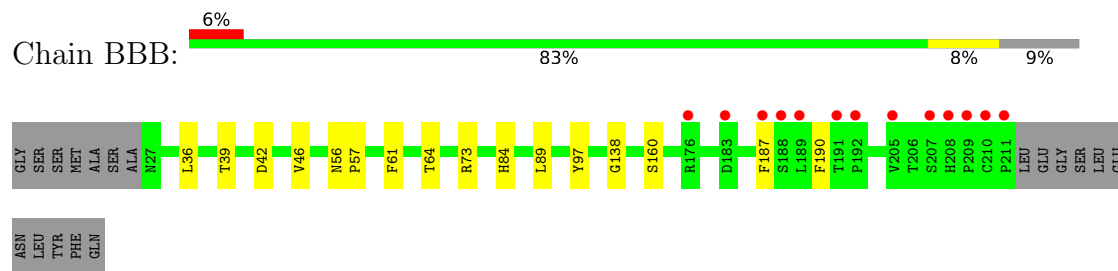
- Molecule 1: Receptor-like protein kinase HSL1



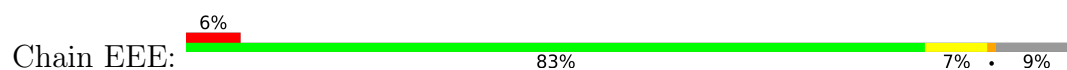
- Molecule 1: Receptor-like protein kinase HSL1



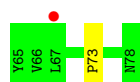
- Molecule 2: Somatic embryogenesis receptor kinase 1



- Molecule 2: Somatic embryogenesis receptor kinase 1



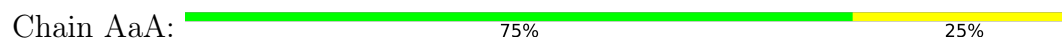
- Molecule 3: Protein IDA-LIKE 1



- Molecule 3: Protein IDA-LIKE 1



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



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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





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

Chain AkA:  100%



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

Chain AnA:  50% 50%



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

Chain BaB:  100%



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

Chain BcB:  50% 50%



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

Chain DaD:  50% 50%



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

Chain DeD:  100%



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

Chain DgD:  50% 50%

MAG1  
MAG2

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

Chain EaE:  100%

MAG1  
MAG2

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

Chain EeE:  50% 50%


MAG1  
MAG2

- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain ArA:  40% 60%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DqD:  20% 80%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain DnD:  100%

MAG1  
MAG2  
BMA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.73Å 146.41Å 169.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	111.08 – 2.38 110.84 – 2.38	Depositor EDS
% Data completeness (in resolution range)	100.0 (111.08-2.38) 100.0 (110.84-2.38)	Depositor EDS
$R_{merge}$	0.34	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.234 , 0.248 0.234 , 0.249	Depositor DCC
$R_{free}$ test set	4974 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtriage
Anisotropy	0.747	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 26.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12777	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	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 30.06 % 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 1.3933e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0/4469	1.18	2/6096 (0.0%)
1	DDD	0.93	0/4473	1.17	0/6103
2	BBB	0.94	0/1457	1.20	0/2002
2	EEE	0.94	0/1422	1.19	0/1953
3	CCC	0.90	0/104	0.97	0/138
3	FFF	0.91	0/102	0.92	0/135
All	All	0.93	0/12027	1.17	2/16427 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	351	ARG	NE-CZ-NH2	7.69	126.12	119.20
1	AAA	351	ARG	NE-CZ-NH1	-6.37	115.13	121.50

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	4384	0	4275	20	0
1	DDD	4388	0	4270	21	0
2	BBB	1412	0	1378	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	EEE	1392	0	1342	10	0
3	CCC	110	0	106	0	0
3	FFF	108	0	99	0	0
4	AaA	50	0	43	0	0
5	AeA	38	0	34	0	0
5	DkD	38	0	34	0	0
6	AhA	28	0	25	0	0
6	AkA	28	0	25	0	0
6	AnA	28	0	25	0	0
6	BaB	28	0	25	0	0
6	BcB	28	0	25	0	0
6	DaD	28	0	25	0	0
6	DeD	28	0	25	0	0
6	DgD	28	0	25	0	0
6	EaE	28	0	25	0	0
6	EeE	28	0	25	0	0
7	ArA	61	0	52	0	0
7	DqD	61	0	52	0	0
8	DnD	39	0	34	0	0
9	AAA	56	0	52	0	0
9	DDD	56	0	52	1	0
9	EEE	28	0	26	2	0
10	AAA	128	0	0	0	0
10	BBB	27	0	0	0	0
10	CCC	2	0	0	0	0
10	DDD	86	0	0	0	0
10	EEE	31	0	0	0	0
10	FFF	2	0	0	0	0
All	All	12777	0	12099	61	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 (61) 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:EEE:138:GLY:HA3	2:EEE:160:SER:HB2	1.71	0.72
2:BBB:64:THR:HB	2:BBB:73:ARG:HB2	1.80	0.64
2:BBB:42:ASP:OD1	2:BBB:46:VAL:HG22	1.98	0.63
2:EEE:64:THR:HB	2:EEE:73:ARG:HB2	1.81	0.62
2:BBB:39[A]:THR:HG21	2:BBB:84:HIS:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:465:GLY:HA3	1:AAA:487:SER:HB2	1.87	0.57
2:BBB:187:PHE:HA	2:BBB:190:PHE:CD2	2.41	0.56
1:DDD:537:GLY:HA3	1:DDD:559:SER:HB2	1.88	0.56
2:EEE:187:PHE:HA	2:EEE:190:PHE:CD2	2.41	0.56
2:BBB:138:GLY:HA3	2:BBB:160:SER:HB2	1.90	0.54
1:DDD:36:TYR:CD2	1:DDD:70:ALA:HB1	2.44	0.53
1:AAA:537:GLY:HA3	1:AAA:559:SER:HB2	1.89	0.53
2:BBB:39[A]:THR:CG2	2:BBB:84:HIS:CE1	2.91	0.53
1:DDD:36:TYR:CD2	1:DDD:70:ALA:CB	2.92	0.53
1:DDD:471:ASN:HB3	2:EEE:61:PHE:CZ	2.44	0.52
2:BBB:36:LEU:HD22	2:BBB:89:LEU:HD21	1.90	0.52
2:EEE:36:LEU:HD22	2:EEE:89:LEU:HD21	1.91	0.52
2:EEE:73:ARG:HG2	2:EEE:97:TYR:HB2	1.93	0.51
1:DDD:465:GLY:HA3	1:DDD:487:SER:HB2	1.92	0.51
1:DDD:500:HIS:HA	1:DDD:524:ALA:O	2.11	0.51
1:AAA:531:LYS:HA	1:AAA:553:SER:O	2.11	0.50
1:AAA:500:HIS:HA	1:AAA:524:ALA:O	2.12	0.50
1:DDD:40:TRP:CD1	1:DDD:50:TRP:HB3	2.47	0.49
1:AAA:303:GLU:HB3	1:AAA:327:TYR:CE2	2.48	0.48
2:BBB:56:ASN:HB2	2:BBB:57:PRO:HD2	1.95	0.48
1:DDD:380:ILE:HA	1:DDD:404:ALA:O	2.14	0.48
1:DDD:524:ALA:HA	1:DDD:548:SER:O	2.14	0.48
2:EEE:56:ASN:HB2	2:EEE:57:PRO:HD2	1.96	0.48
1:AAA:380:ILE:HA	1:AAA:404:ALA:O	2.14	0.47
2:BBB:73:ARG:HG2	2:BBB:97:TYR:HB2	1.96	0.47
9:DDD:704:NAG:H83	9:DDD:704:NAG:H3	1.96	0.47
2:EEE:115:ASN:OD1	9:EEE:302:NAG:O5	2.26	0.47
1:AAA:524:ALA:HA	1:AAA:548:SER:O	2.15	0.47
2:BBB:39[A]:THR:HG23	2:BBB:84:HIS:NE2	2.30	0.47
1:AAA:471:ASN:HB3	2:BBB:61:PHE:CZ	2.51	0.46
1:DDD:21:PHE:O	1:DDD:25:GLN:HG2	2.15	0.46
1:AAA:301:PRO:HA	1:AAA:323:SER:HB2	1.98	0.45
1:DDD:301:PRO:HA	1:DDD:323:SER:HB2	1.97	0.45
1:AAA:450:ILE:HG23	1:AAA:474:SER:HB2	1.99	0.44
1:AAA:101:PRO:HB2	1:AAA:103:ASN:OD1	2.17	0.44
1:DDD:206:ASN:HA	1:DDD:230:LYS:HD3	1.99	0.44
1:DDD:507:GLU:HG2	1:DDD:529:THR:O	2.18	0.44
1:DDD:450:ILE:HG23	1:DDD:474:SER:HB2	2.00	0.43
1:DDD:105:ALA:HB2	1:DDD:127:THR:HB	2.00	0.43
1:DDD:140:THR:HA	1:DDD:164:VAL:O	2.18	0.43
1:DDD:531:LYS:HA	1:DDD:553:SER:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:140:THR:HA	1:AAA:164:VAL:O	2.18	0.43
1:DDD:68:SER:HB2	1:DDD:92:TYR:HD2	1.84	0.43
1:DDD:270:PRO:HG2	1:DDD:273:LEU:HG	2.02	0.42
1:AAA:196:ARG:HA	1:AAA:218:VAL:O	2.20	0.42
1:AAA:311:ASN:ND2	1:AAA:335:ARG:HE	2.18	0.42
1:AAA:295:ASP:O	1:AAA:299:ARG:HG3	2.19	0.41
1:AAA:295:ASP:OD2	1:AAA:299:ARG:NH1	2.52	0.41
1:AAA:105:ALA:HB2	1:AAA:127:THR:HB	2.02	0.41
1:DDD:101:PRO:HB2	1:DDD:103:ASN:OD1	2.20	0.41
2:EEE:111:SER:OG	9:EEE:302:NAG:O7	2.26	0.41
1:DDD:36:TYR:CD2	1:DDD:70:ALA:HB2	2.55	0.41
1:AAA:507:GLU:HG2	1:AAA:529:THR:O	2.20	0.40
2:EEE:78:ASN:HD22	2:EEE:78:ASN:HA	1.64	0.40
1:AAA:172:ILE:HA	1:AAA:173:PRO:HD3	1.86	0.40
1:AAA:303:GLU:HG2	1:AAA:325:ASN:HB3	2.03	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	584/617 (95%)	570 (98%)	14 (2%)	0	100	100
1	DDD	585/617 (95%)	573 (98%)	12 (2%)	0	100	100
2	BBB	188/203 (93%)	186 (99%)	2 (1%)	0	100	100
2	EEE	183/203 (90%)	181 (99%)	2 (1%)	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	1562/1668 (94%)	1532 (98%)	30 (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	492/540 (91%)	487 (99%)	5 (1%)	73	85
1	DDD	491/540 (91%)	487 (99%)	4 (1%)	79	89
2	BBB	164/184 (89%)	164 (100%)	0	100	100
2	EEE	160/184 (87%)	157 (98%)	3 (2%)	52	70
3	CCC	12/12 (100%)	12 (100%)	0	100	100
3	FFF	11/12 (92%)	11 (100%)	0	100	100
All	All	1330/1472 (90%)	1318 (99%)	12 (1%)	75	87

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	18	GLN
1	AAA	61	SER
1	AAA	165	TYR
1	AAA	351	ARG
1	AAA	450	ILE
1	DDD	18	GLN
1	DDD	61	SER
1	DDD	165	TYR
1	DDD	450	ILE
2	EEE	78	ASN
2	EEE	82	SER
2	EEE	160	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 ⓘ

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	73	3	6,8,9	0.48	0	5,10,12	0.93	0
3	HYP	CCC	73	3	6,8,9	0.53	0	5,10,12	0.97	1 (20%)

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	73	3	-	0/0/11/13	0/1/1/1
3	HYP	CCC	73	3	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CCC	73	HYP	O-C-CA	-2.03	119.47	124.78

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 ⓘ

43 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	14,14,15	0.33	0	17,19,21	1.10	1 (5%)
4	NAG	AaA	2	4	14,14,15	0.45	0	17,19,21	0.90	0
4	BMA	AaA	3	4	11,11,12	0.36	0	15,15,17	0.74	0
4	MAN	AaA	4	4	11,11,12	0.53	0	15,15,17	0.89	0
5	NAG	AeA	1	1,5	14,14,15	0.38	0	17,19,21	1.10	0
5	NAG	AeA	2	5	14,14,15	0.51	0	17,19,21	0.91	1 (5%)
5	FUC	AeA	3	5	10,10,11	0.34	0	14,14,16	0.61	0
6	NAG	AhA	1	6,1	14,14,15	0.35	0	17,19,21	0.63	0
6	NAG	AhA	2	6	14,14,15	0.35	0	17,19,21	0.98	1 (5%)
6	NAG	AkA	1	6,1	14,14,15	0.42	0	17,19,21	1.51	4 (23%)
6	NAG	AkA	2	6	14,14,15	0.48	0	17,19,21	1.13	1 (5%)
6	NAG	AnA	1	6,1	14,14,15	0.48	0	17,19,21	0.89	0
6	NAG	AnA	2	6	14,14,15	0.47	0	17,19,21	1.18	1 (5%)
7	NAG	ArA	1	1,7	14,14,15	0.58	0	17,19,21	1.27	2 (11%)
7	NAG	ArA	2	7	14,14,15	0.32	0	17,19,21	0.84	0
7	BMA	ArA	3	7	11,11,12	0.36	0	15,15,17	1.20	2 (13%)
7	MAN	ArA	4	7	11,11,12	0.51	0	15,15,17	0.78	0
7	MAN	ArA	5	7	11,11,12	0.62	0	15,15,17	0.92	1 (6%)
6	NAG	BaB	1	6,2	14,14,15	0.33	0	17,19,21	1.27	2 (11%)
6	NAG	BaB	2	6	14,14,15	0.36	0	17,19,21	1.33	2 (11%)
6	NAG	BcB	1	6,2	14,14,15	0.36	0	17,19,21	1.03	2 (11%)
6	NAG	BcB	2	6	14,14,15	0.38	0	17,19,21	0.83	0
6	NAG	DaD	1	6,1	14,14,15	0.36	0	17,19,21	0.88	0
6	NAG	DaD	2	6	14,14,15	0.54	0	17,19,21	1.01	1 (5%)
6	NAG	DeD	1	6,1	14,14,15	0.40	0	17,19,21	0.98	1 (5%)
6	NAG	DeD	2	6	14,14,15	0.38	0	17,19,21	0.98	1 (5%)
6	NAG	DgD	1	6,1	14,14,15	0.34	0	17,19,21	1.26	2 (11%)
6	NAG	DgD	2	6	14,14,15	0.38	0	17,19,21	0.70	0
5	NAG	DkD	1	1,5	14,14,15	0.38	0	17,19,21	0.89	0
5	NAG	DkD	2	5	14,14,15	0.36	0	17,19,21	0.73	0
5	FUC	DkD	3	5	10,10,11	0.36	0	14,14,16	0.51	0
8	NAG	DnD	1	1,8	14,14,15	0.43	0	17,19,21	1.09	0
8	NAG	DnD	2	8	14,14,15	0.29	0	17,19,21	1.07	0
8	BMA	DnD	3	8	11,11,12	0.45	0	15,15,17	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	DqD	1	1,7	14,14,15	0.30	0	17,19,21	1.03	1 (5%)
7	NAG	DqD	2	7	14,14,15	0.27	0	17,19,21	0.63	0
7	BMA	DqD	3	7	11,11,12	0.39	0	15,15,17	0.83	1 (6%)
7	MAN	DqD	4	7	11,11,12	0.38	0	15,15,17	0.95	2 (13%)
7	MAN	DqD	5	7	11,11,12	0.47	0	15,15,17	0.96	1 (6%)
6	NAG	EaE	1	6,2	14,14,15	0.57	0	17,19,21	1.73	4 (23%)
6	NAG	EaE	2	6	14,14,15	0.42	0	17,19,21	0.88	1 (5%)
6	NAG	EeE	1	6,2	14,14,15	0.26	0	17,19,21	0.87	0
6	NAG	EeE	2	6	14,14,15	0.44	0	17,19,21	1.00	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	AaA	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	AaA	2	4	-	0/6/23/26	0/1/1/1
4	BMA	AaA	3	4	-	0/2/19/22	0/1/1/1
4	MAN	AaA	4	4	1/1/4/5	1/2/19/22	0/1/1/1
5	NAG	AeA	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	AeA	2	5	1/1/5/7	0/6/23/26	0/1/1/1
5	FUC	AeA	3	5	-	-	0/1/1/1
6	NAG	AhA	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	AhA	2	6	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	AkA	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	AkA	2	6	-	0/6/23/26	0/1/1/1
6	NAG	AnA	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	AnA	2	6	1/1/5/7	1/6/23/26	0/1/1/1
7	NAG	ArA	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	ArA	2	7	-	1/6/23/26	0/1/1/1
7	BMA	ArA	3	7	1/1/4/5	0/2/19/22	0/1/1/1
7	MAN	ArA	4	7	-	0/2/19/22	0/1/1/1
7	MAN	ArA	5	7	-	0/2/19/22	0/1/1/1
6	NAG	BaB	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	BaB	2	6	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	BcB	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	BcB	2	6	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	DaD	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	DaD	2	6	1/1/5/7	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	DeD	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	DeD	2	6	-	0/6/23/26	0/1/1/1
6	NAG	DgD	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	DgD	2	6	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	DkD	1	1,5	-	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
5	FUC	DkD	3	5	-	-	0/1/1/1
8	NAG	DnD	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	DnD	2	8	-	0/6/23/26	0/1/1/1
8	BMA	DnD	3	8	-	2/2/19/22	0/1/1/1
7	NAG	DqD	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	DqD	2	7	1/1/5/7	0/6/23/26	0/1/1/1
7	BMA	DqD	3	7	1/1/4/5	0/2/19/22	0/1/1/1
7	MAN	DqD	4	7	-	2/2/19/22	0/1/1/1
7	MAN	DqD	5	7	-	0/2/19/22	0/1/1/1
6	NAG	EaE	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	EaE	2	6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	EeE	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	EeE	2	6	1/1/5/7	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	EaE	1	NAG	C1-O5-C5	3.92	117.50	112.19
6	AnA	2	NAG	O5-C5-C6	3.66	112.93	107.20
7	ArA	3	BMA	O5-C5-C6	3.58	112.81	107.20
6	BaB	2	NAG	C1-C2-N2	-3.53	104.46	110.49
6	BaB	1	NAG	C1-O5-C5	3.53	116.97	112.19
6	EaE	1	NAG	C1-C2-N2	3.47	116.41	110.49
6	EaE	1	NAG	O5-C5-C6	3.43	112.58	107.20
6	DgD	1	NAG	C1-O5-C5	3.32	116.69	112.19
6	DaD	2	NAG	O5-C5-C6	3.26	112.32	107.20
6	AkA	1	NAG	C4-C3-C2	-3.24	106.27	111.02
7	ArA	1	NAG	C4-C3-C2	-3.22	106.30	111.02
6	AkA	2	NAG	C1-O5-C5	2.86	116.06	112.19
7	ArA	5	MAN	O5-C5-C6	2.85	111.68	107.20
6	AkA	1	NAG	O5-C1-C2	-2.80	106.86	111.29
6	AhA	2	NAG	O5-C5-C6	2.68	111.41	107.20
6	BcB	1	NAG	C1-O5-C5	2.66	115.80	112.19
6	DeD	1	NAG	O5-C5-C6	2.57	111.23	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	DqD	5	MAN	C1-C2-C3	2.55	112.80	109.67
6	AkA	1	NAG	C1-C2-N2	2.54	114.82	110.49
6	EaE	2	NAG	O5-C5-C6	2.40	110.96	107.20
6	BaB	1	NAG	O5-C5-C6	2.38	110.93	107.20
6	EeE	2	NAG	O5-C5-C6	2.37	110.93	107.20
4	AaA	1	NAG	C1-O5-C5	2.36	115.39	112.19
7	DqD	4	MAN	O5-C1-C2	-2.35	107.14	110.77
6	BcB	1	NAG	C1-C2-N2	-2.34	106.49	110.49
7	ArA	1	NAG	C1-O5-C5	2.33	115.36	112.19
6	AkA	1	NAG	C2-N2-C7	2.33	126.22	122.90
7	ArA	3	BMA	O5-C5-C4	-2.24	105.37	110.83
6	BaB	2	NAG	O5-C5-C6	2.22	110.68	107.20
5	AeA	2	NAG	O5-C5-C6	2.20	110.66	107.20
7	DqD	4	MAN	C3-C4-C5	2.17	114.11	110.24
7	DqD	3	BMA	O5-C1-C2	-2.07	107.57	110.77
6	DeD	2	NAG	O5-C5-C6	2.06	110.44	107.20
7	DqD	1	NAG	C2-N2-C7	2.04	125.80	122.90
6	DgD	1	NAG	C1-C2-N2	-2.02	107.03	110.49
6	EaE	1	NAG	O5-C1-C2	-2.02	108.10	111.29

All (14) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	AaA	4	MAN	C1
5	AeA	2	NAG	C1
5	DkD	2	NAG	C1
6	AhA	2	NAG	C1
6	AnA	2	NAG	C1
6	BaB	2	NAG	C1
6	BcB	2	NAG	C1
6	DaD	2	NAG	C1
6	DgD	2	NAG	C1
6	EaE	2	NAG	C1
6	EeE	2	NAG	C1
7	ArA	3	BMA	C1
7	DqD	2	NAG	C1
7	DqD	3	BMA	C1

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	BcB	2	NAG	O5-C5-C6-O6

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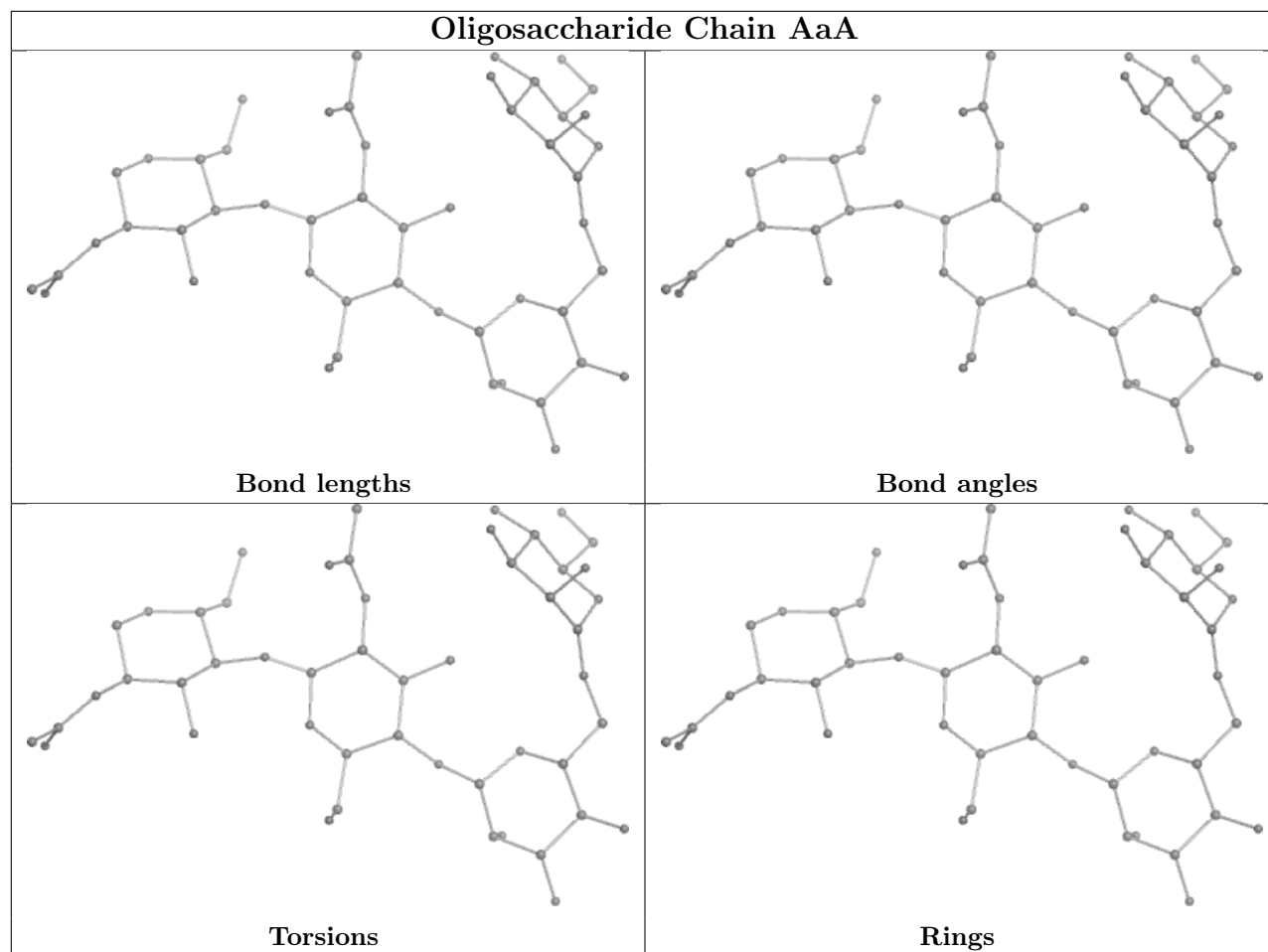
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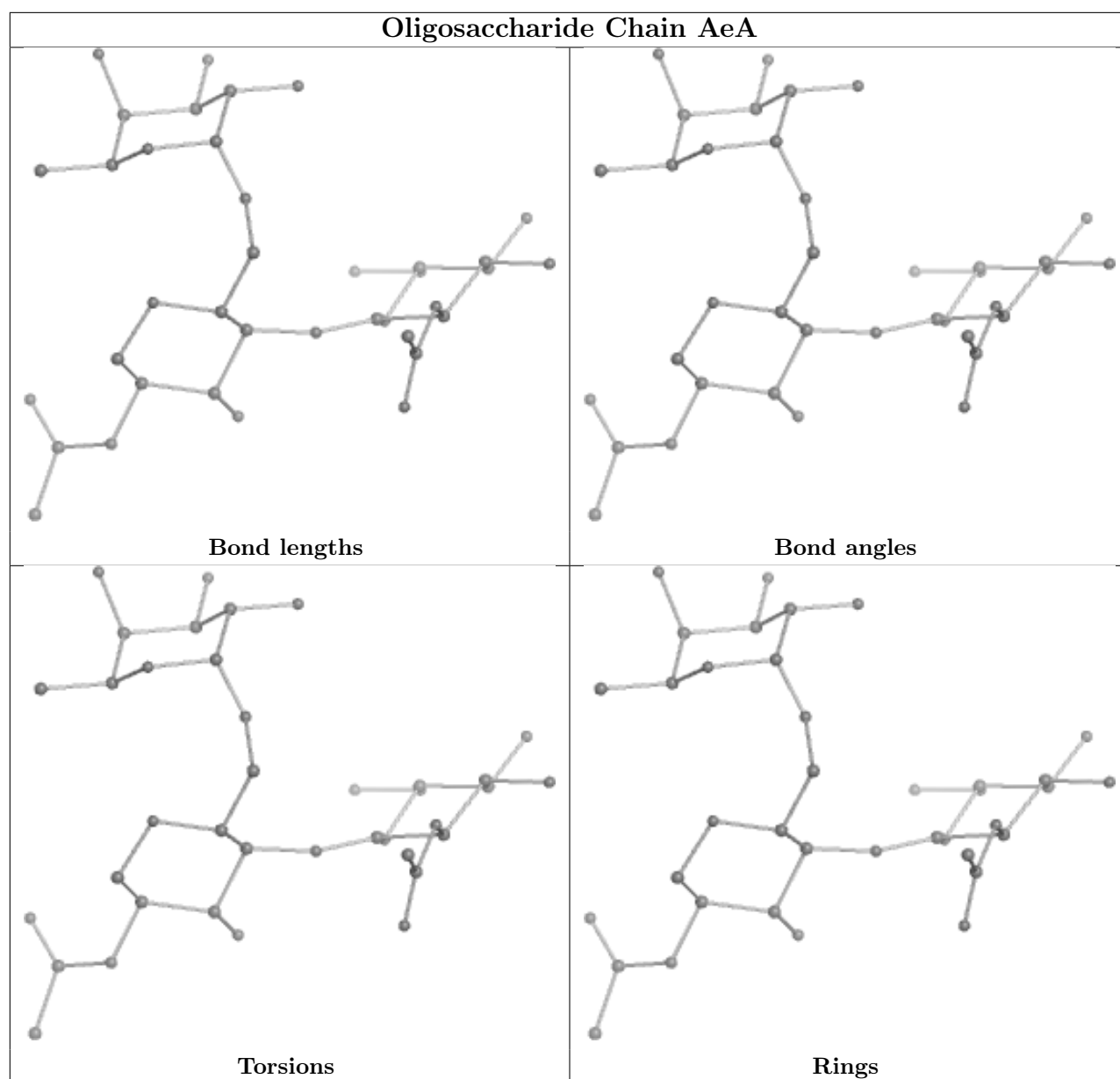
Mol	Chain	Res	Type	Atoms
6	BaB	2	NAG	O5-C5-C6-O6
6	DeD	1	NAG	O5-C5-C6-O6
6	DaD	2	NAG	C4-C5-C6-O6
7	DqD	4	MAN	O5-C5-C6-O6
8	DnD	3	BMA	O5-C5-C6-O6
4	AaA	1	NAG	C4-C5-C6-O6
6	EeE	2	NAG	O5-C5-C6-O6
6	EeE	2	NAG	C4-C5-C6-O6
6	DeD	1	NAG	C4-C5-C6-O6
8	DnD	3	BMA	C4-C5-C6-O6
6	BaB	2	NAG	C4-C5-C6-O6
7	DqD	4	MAN	C4-C5-C6-O6
4	AaA	1	NAG	O5-C5-C6-O6
6	DaD	2	NAG	O5-C5-C6-O6
6	BcB	2	NAG	C4-C5-C6-O6
4	AaA	4	MAN	O5-C5-C6-O6
6	DaD	1	NAG	O5-C5-C6-O6
6	EaE	1	NAG	O5-C5-C6-O6
6	AkA	1	NAG	C3-C2-N2-C7
6	EaE	1	NAG	C3-C2-N2-C7
7	ArA	2	NAG	C4-C5-C6-O6
6	AhA	2	NAG	C4-C5-C6-O6
6	AhA	2	NAG	O5-C5-C6-O6
6	AnA	2	NAG	C3-C2-N2-C7

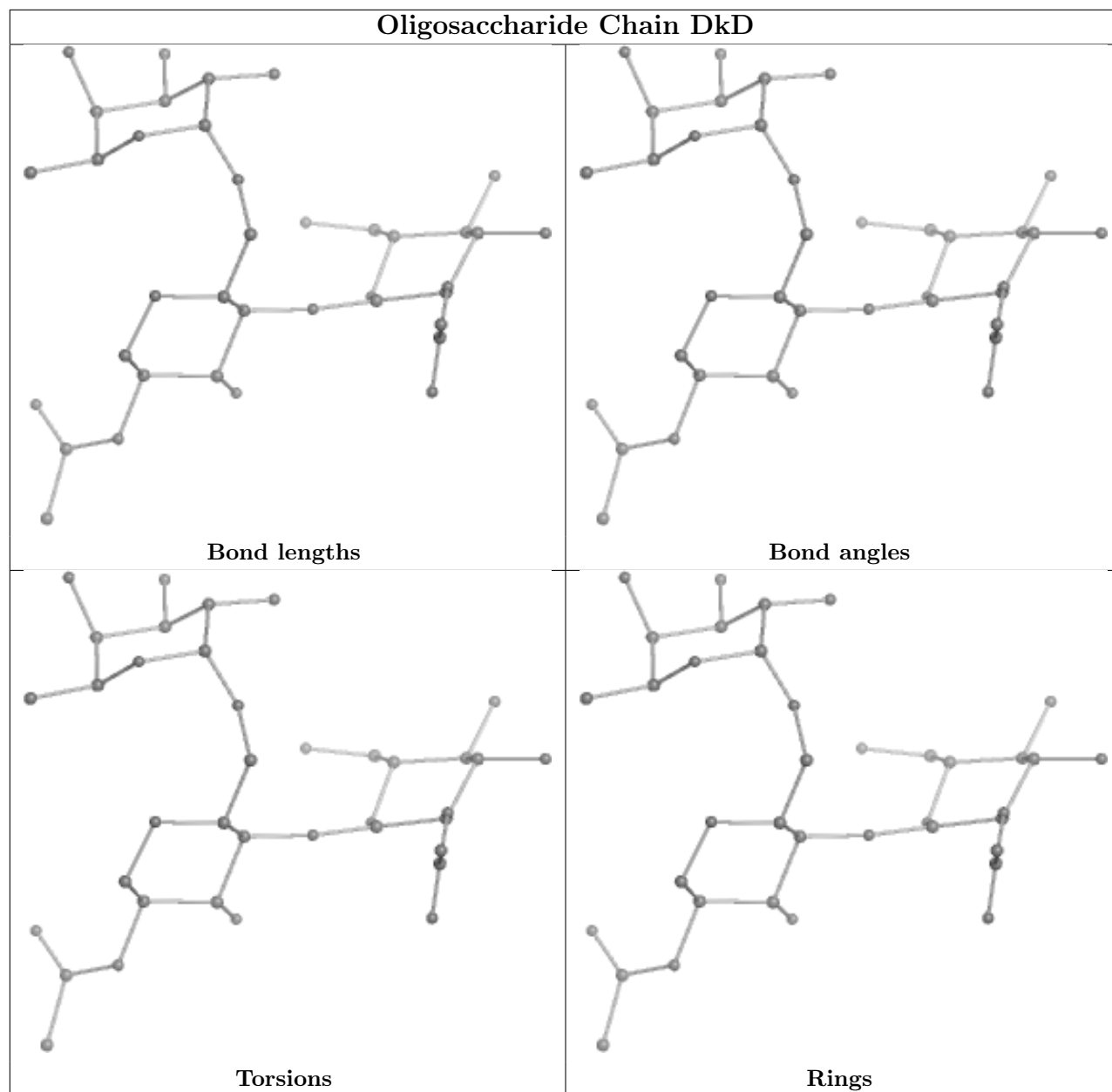
There are no ring outliers.

No monomer is involved in short contacts.

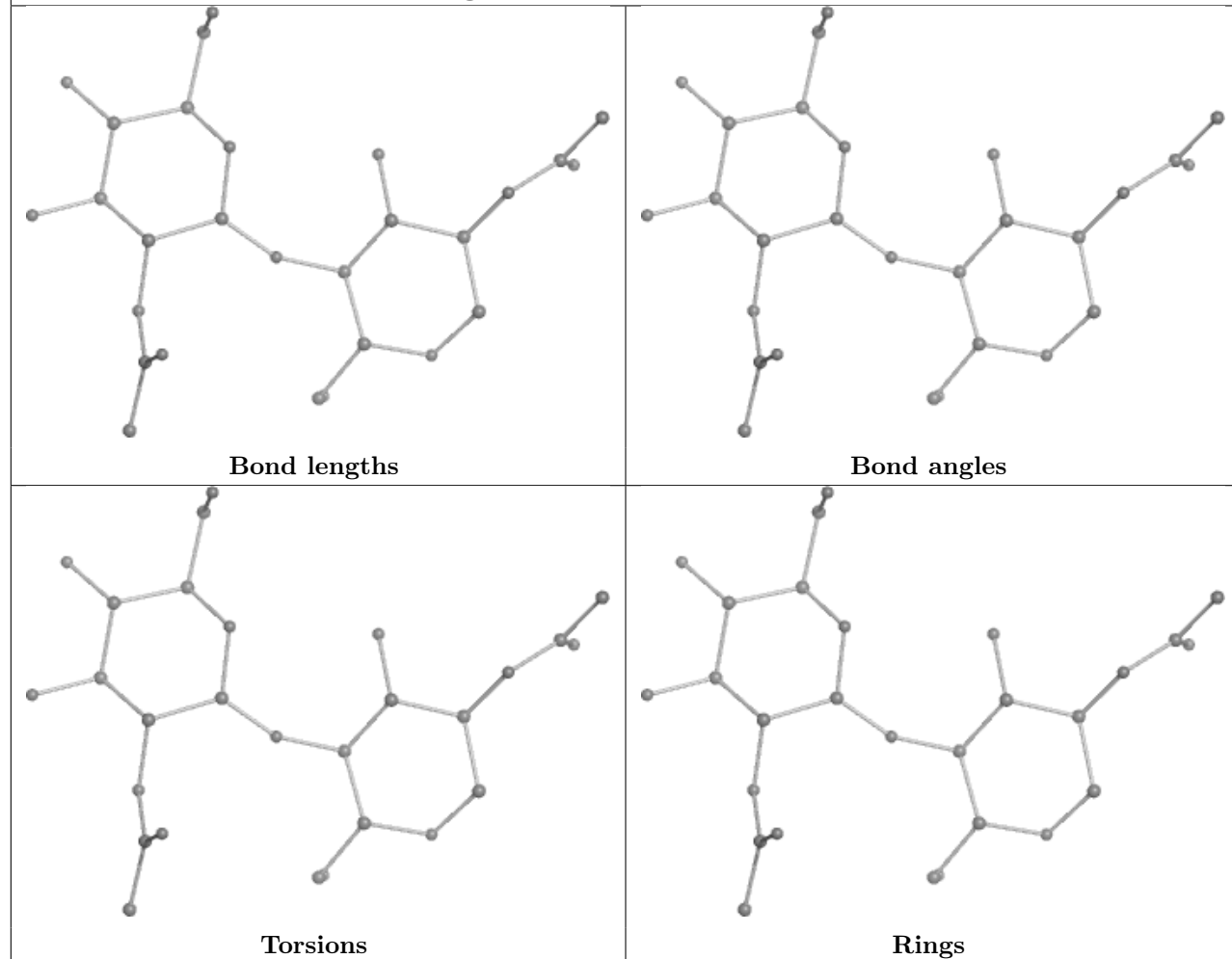
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



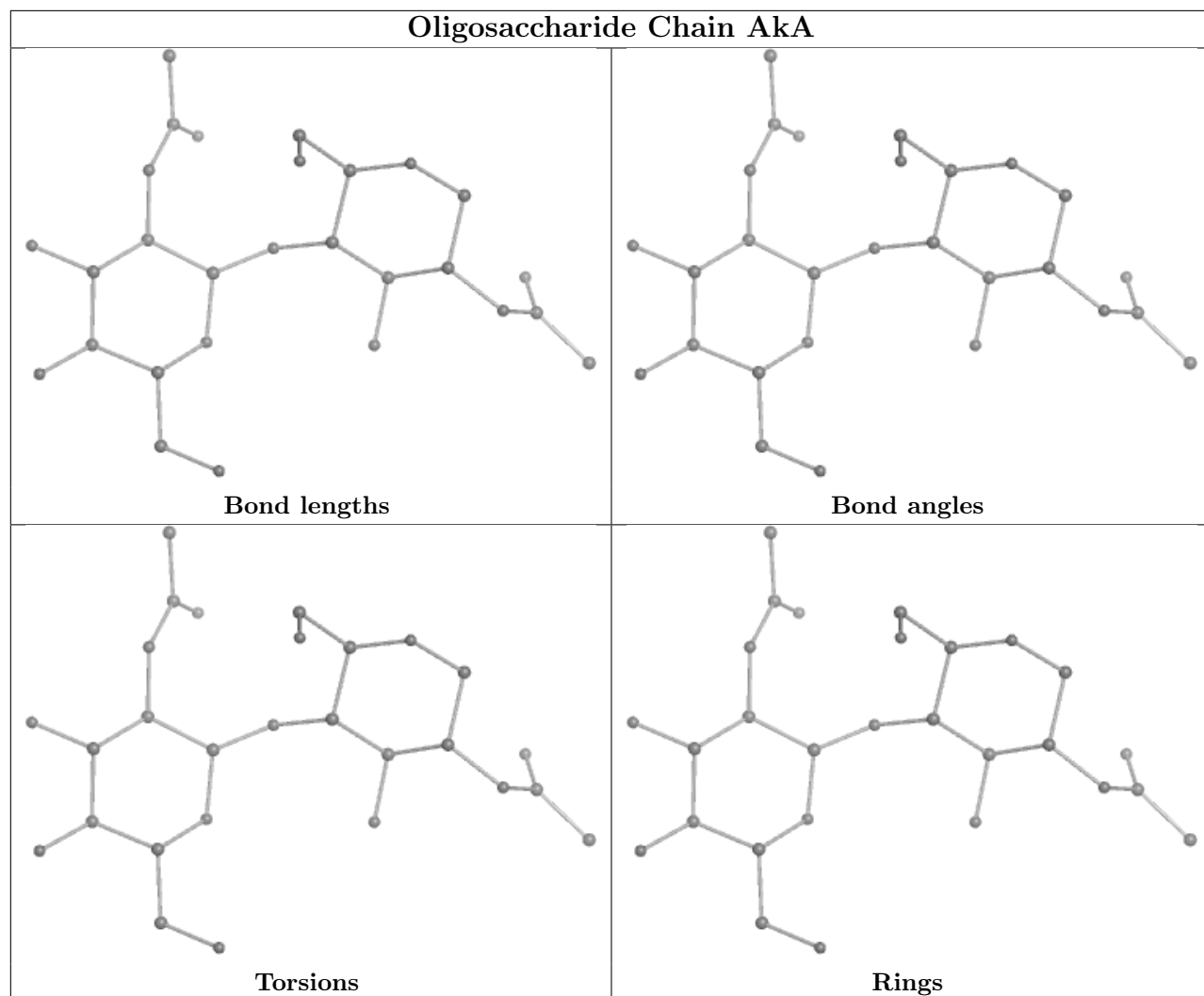


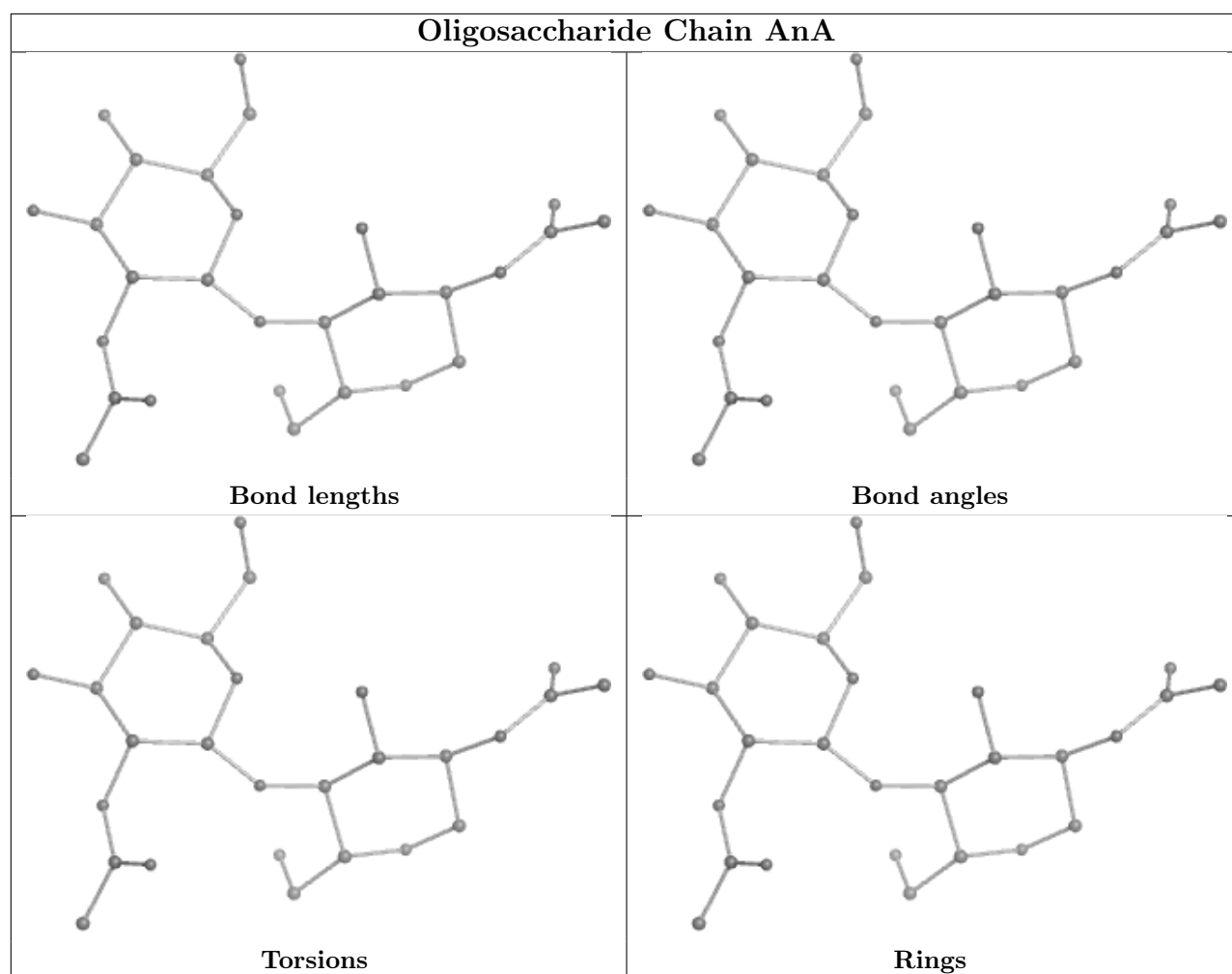


## Oligosaccharide Chain AhA

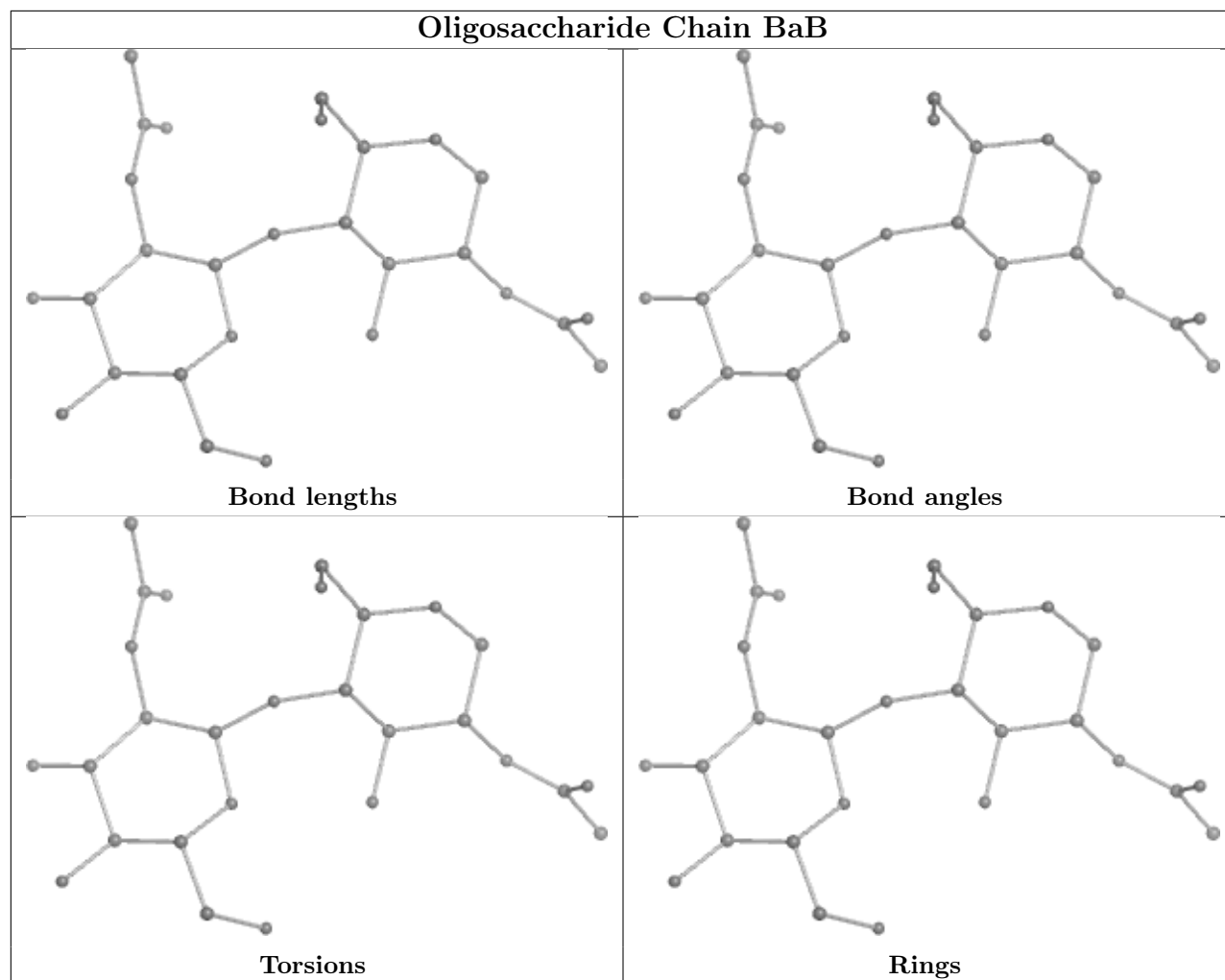


## Oligosaccharide Chain AkA

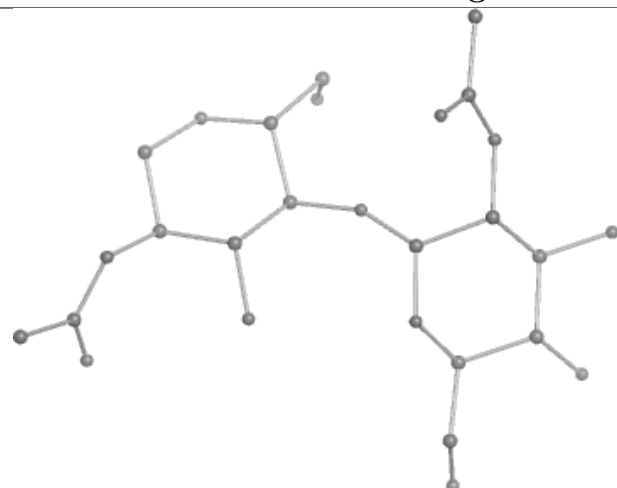




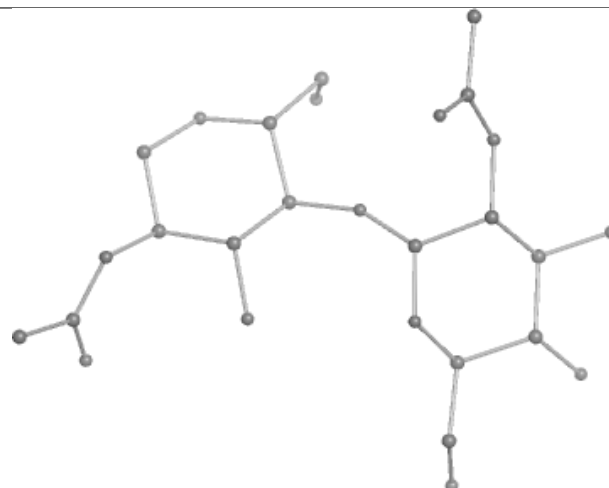




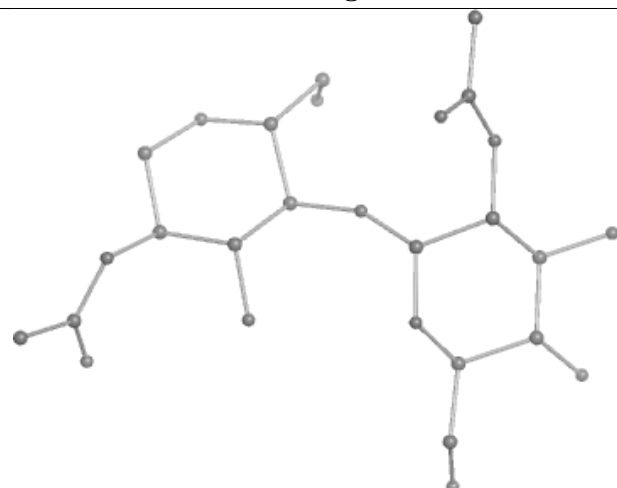
## Oligosaccharide Chain BcB



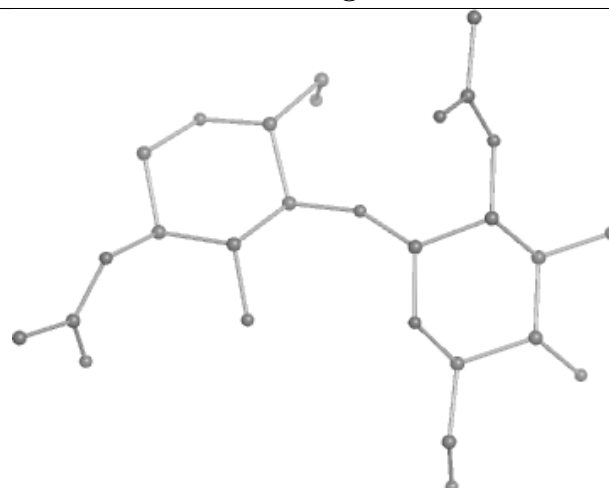
Bond lengths



Bond angles

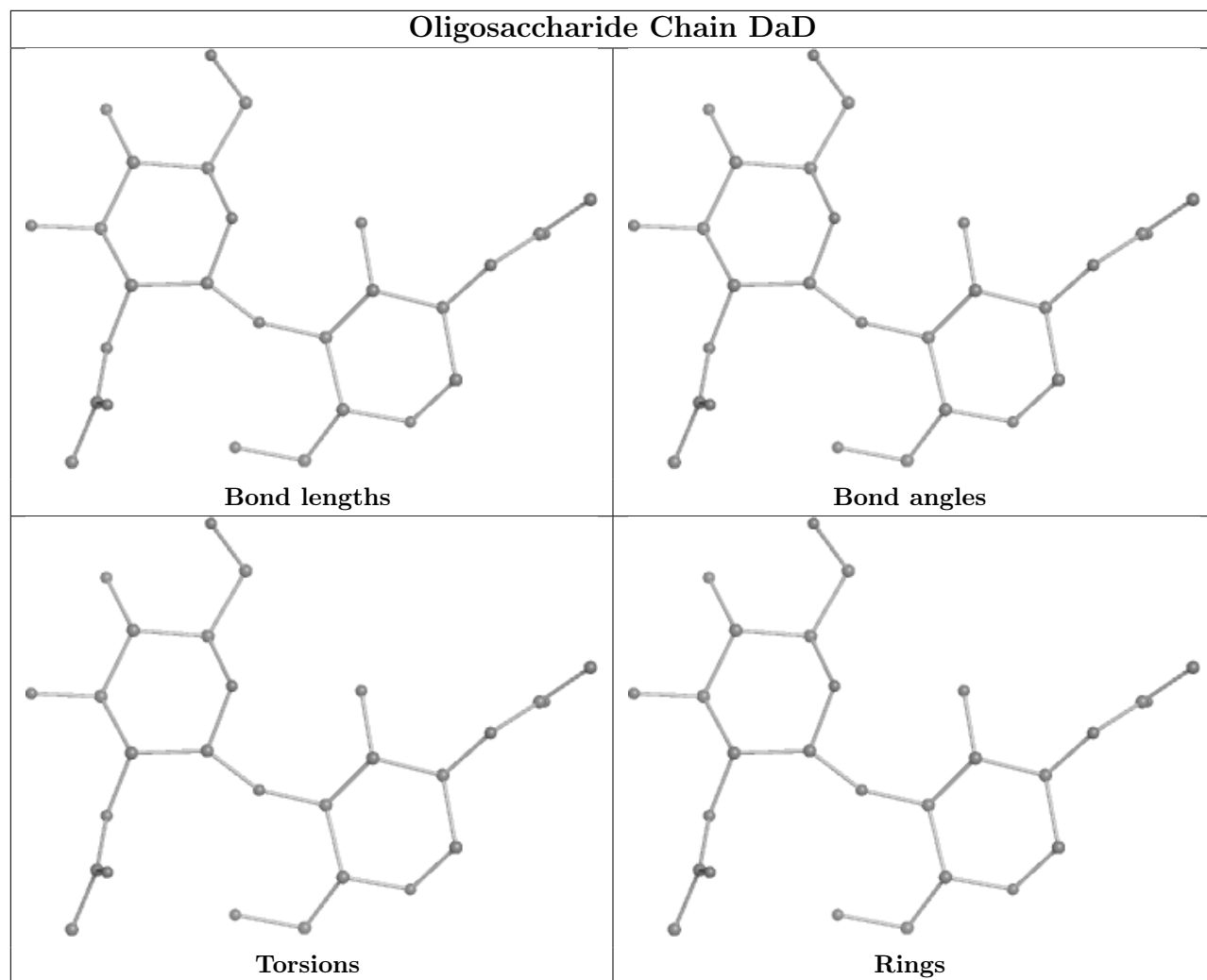


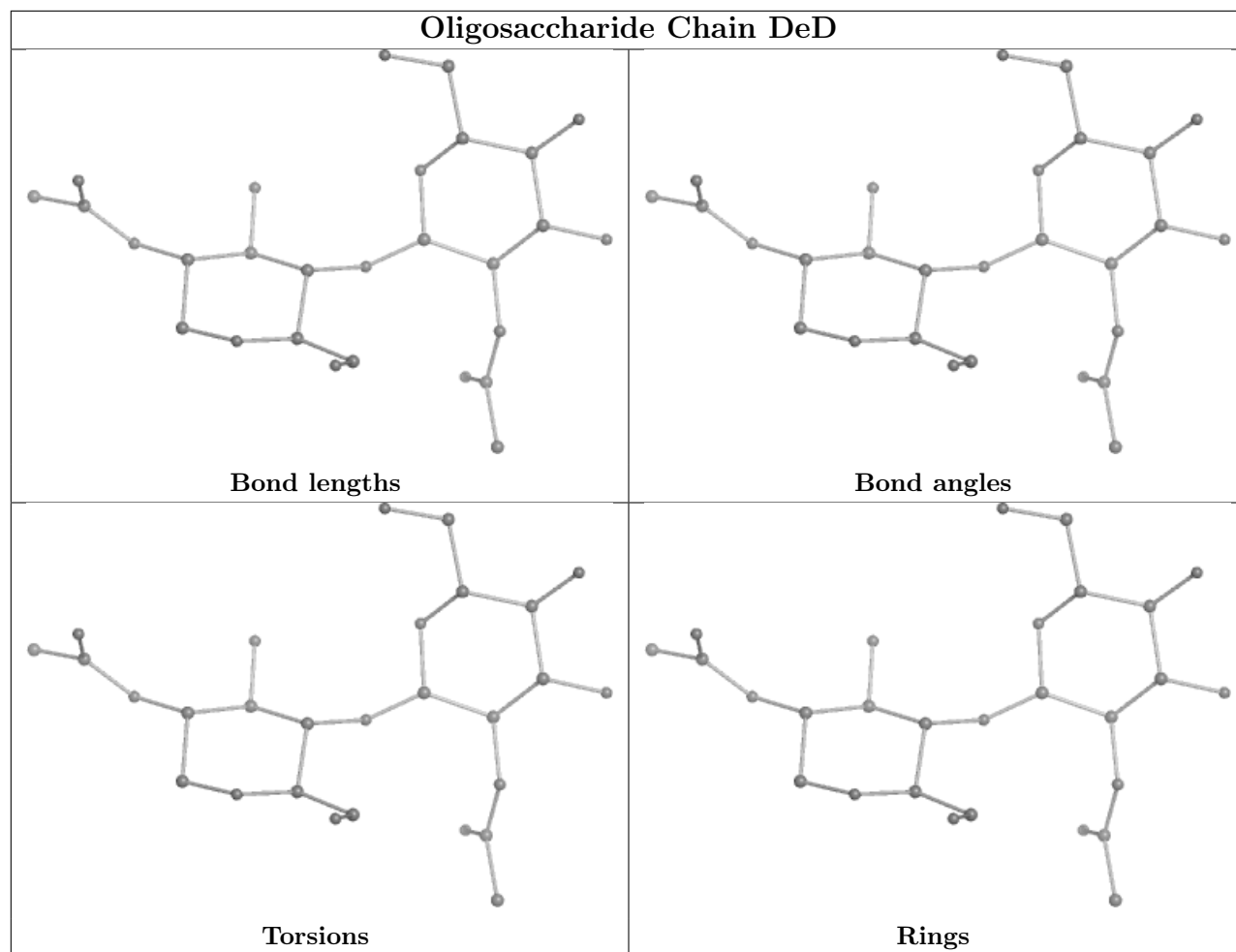
Torsions

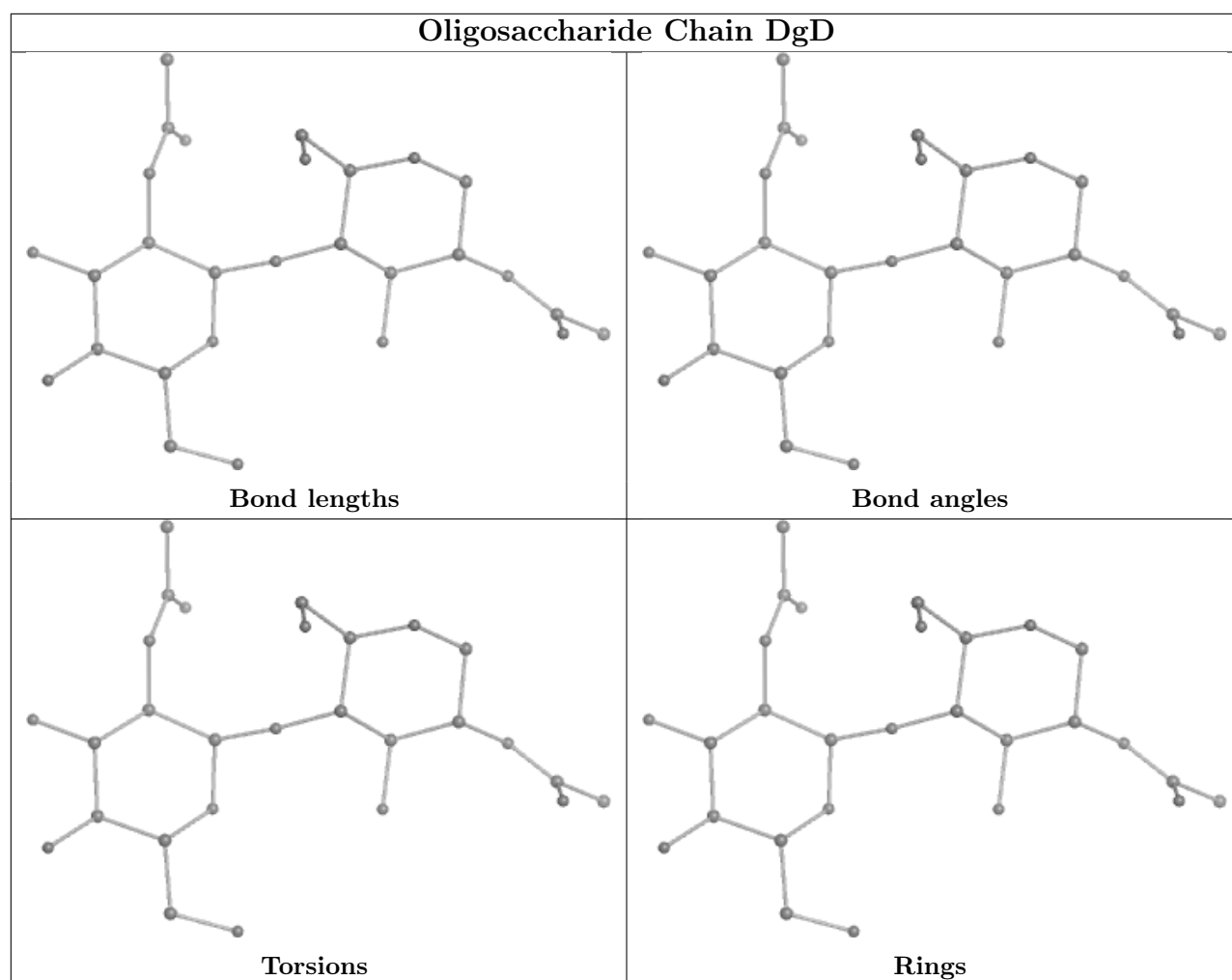


Rings

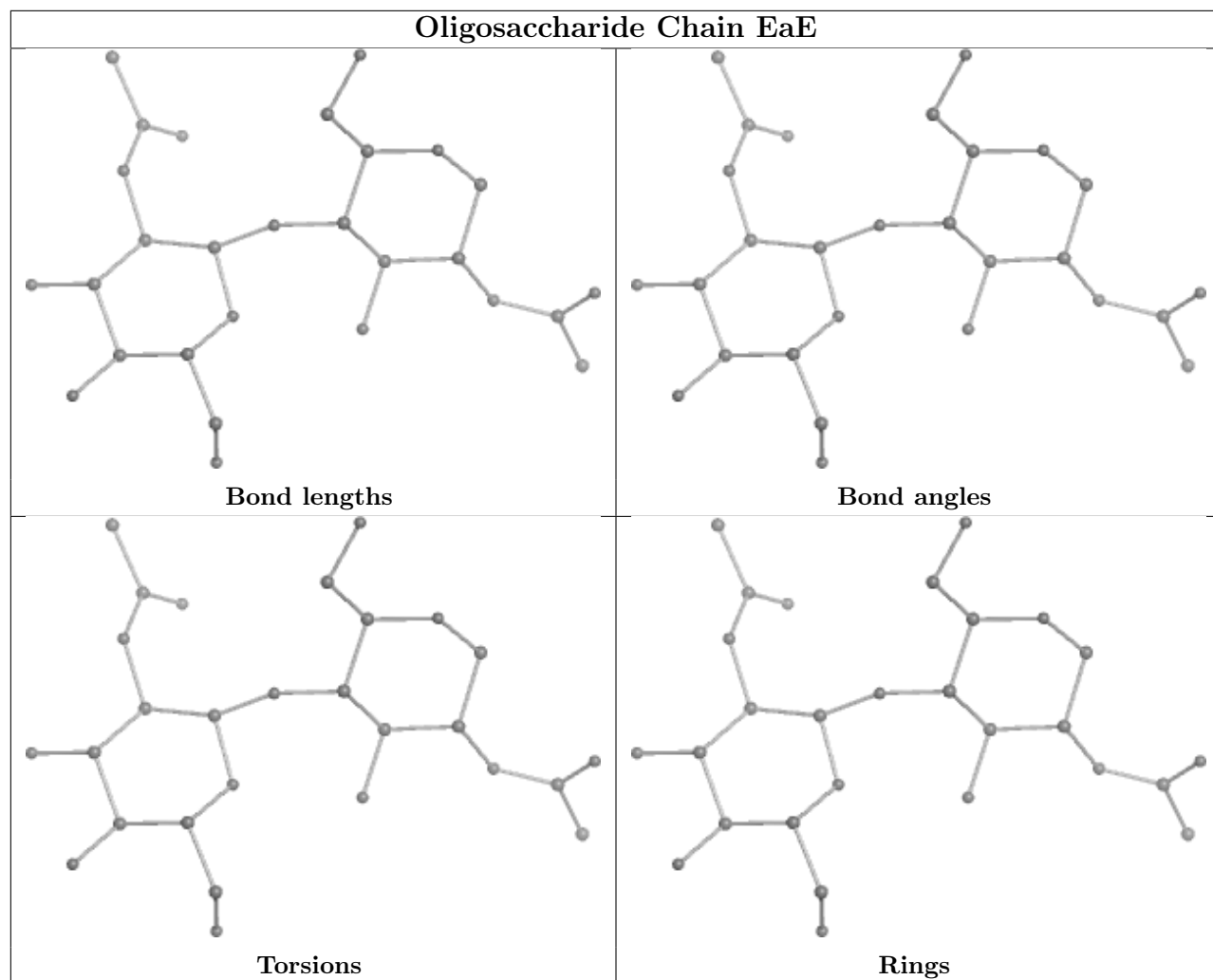
## Oligosaccharide Chain DaD

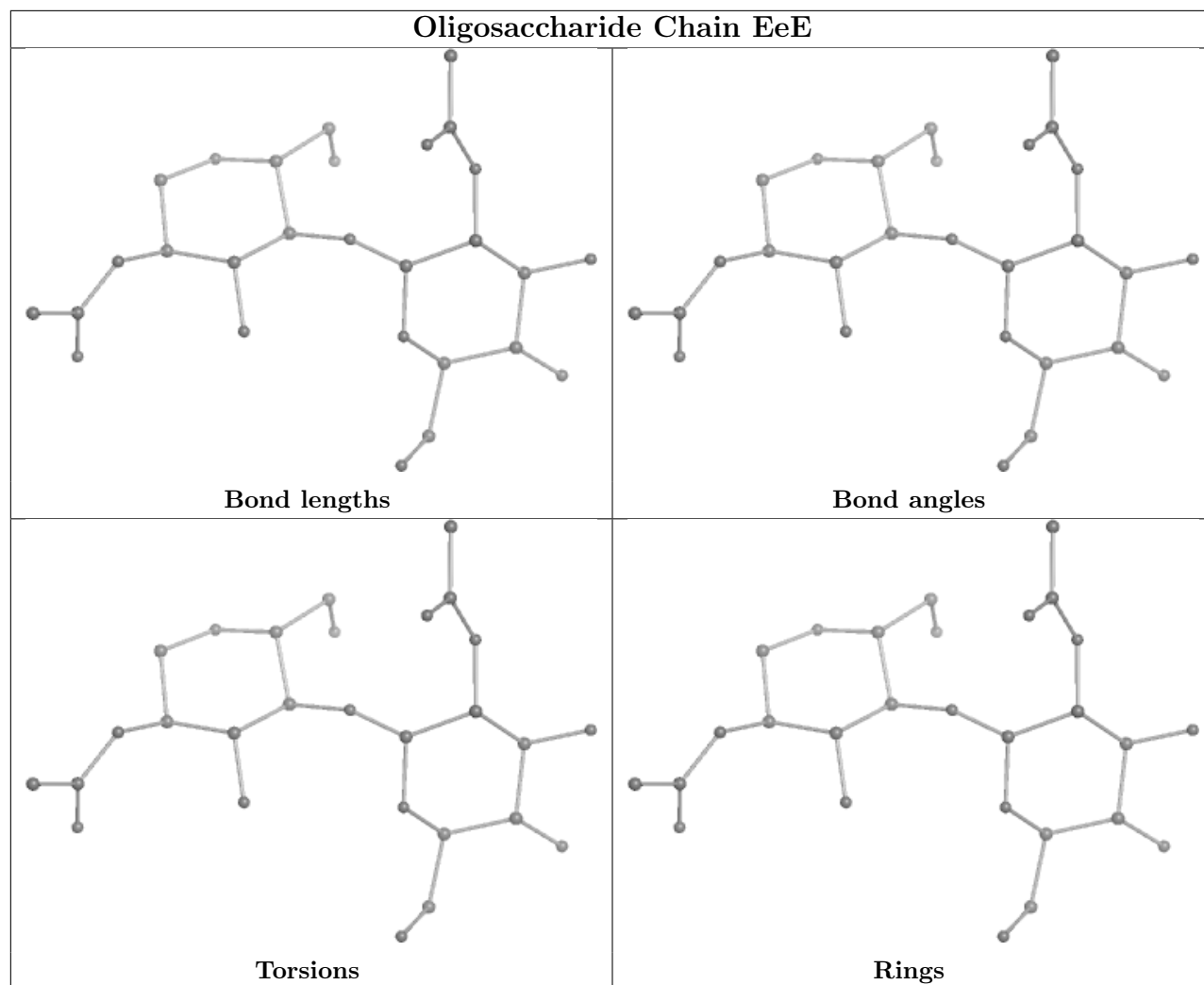




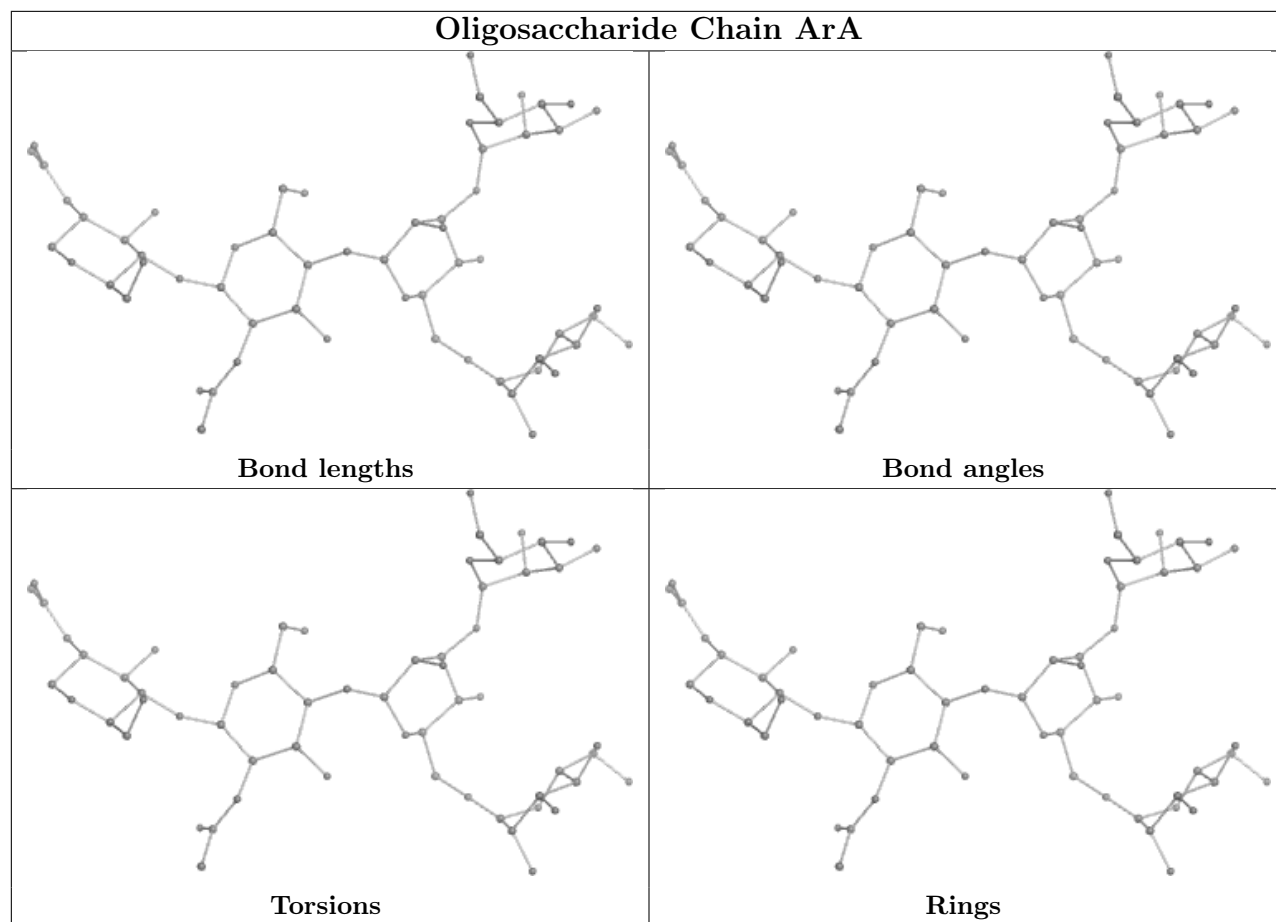


## Oligosaccharide Chain EaE

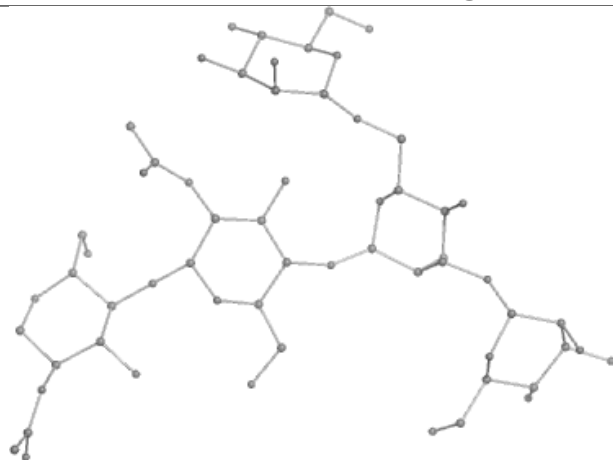
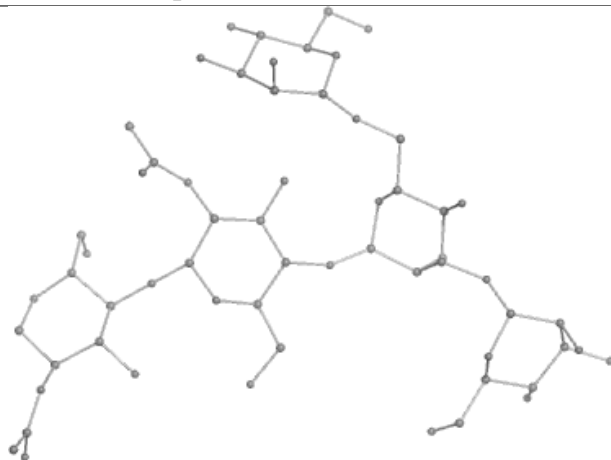
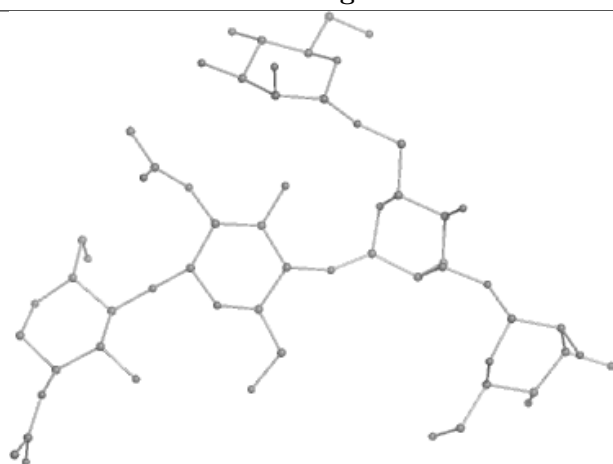
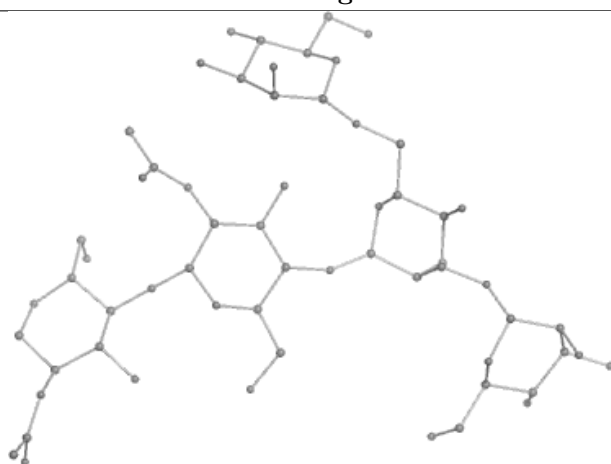


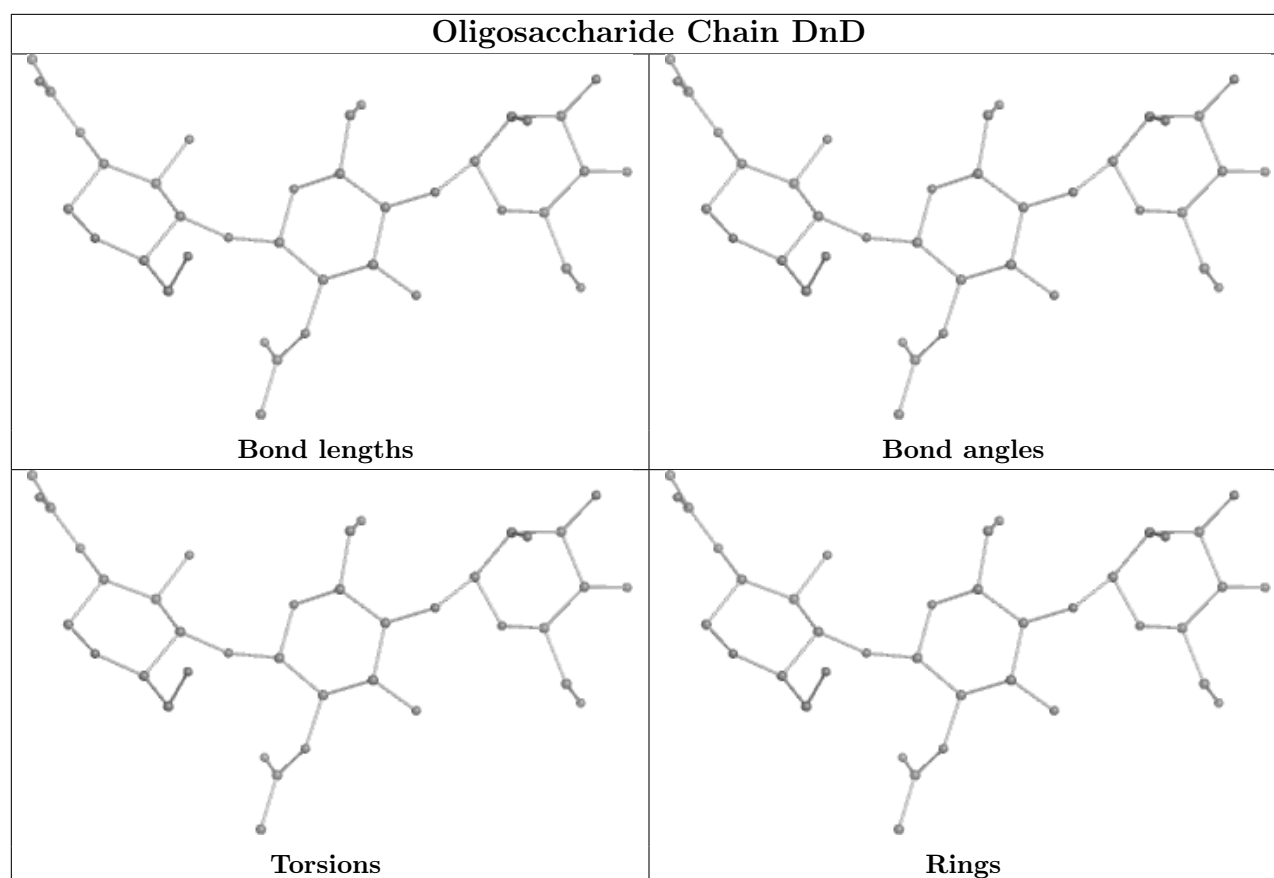


## Oligosaccharide Chain ArA





**Oligosaccharide Chain DqD****Bond lengths****Bond angles****Torsions****Rings**



## 5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
9	NAG	AAA	703	1	14,14,15	0.45	0	17,19,21	1.02	1 (5%)
9	NAG	DDD	704	1	14,14,15	0.72	0	17,19,21	1.87	4 (23%)
9	NAG	EEE	301	2	14,14,15	0.56	0	17,19,21	1.21	2 (11%)
9	NAG	EEE	302	2	14,14,15	0.65	0	17,19,21	2.98	6 (35%)
9	NAG	DDD	701	1	14,14,15	0.54	0	17,19,21	1.04	1 (5%)
9	NAG	DDD	702	1	14,14,15	0.47	0	17,19,21	1.36	3 (17%)
9	NAG	AAA	704	1	14,14,15	0.52	0	17,19,21	0.88	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	NAG	DDD	703	1	14,14,15	0.38	0	17,19,21	0.67	0
9	NAG	AAA	702	1	14,14,15	0.53	0	17,19,21	0.87	1 (5%)
9	NAG	AAA	701	1	14,14,15	0.62	0	17,19,21	1.02	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
9	NAG	AAA	703	1	-	2/6/23/26	0/1/1/1
9	NAG	DDD	704	1	-	3/6/23/26	0/1/1/1
9	NAG	EEE	301	2	-	0/6/23/26	0/1/1/1
9	NAG	EEE	302	2	-	3/6/23/26	0/1/1/1
9	NAG	DDD	701	1	-	0/6/23/26	0/1/1/1
9	NAG	DDD	702	1	-	0/6/23/26	0/1/1/1
9	NAG	AAA	704	1	-	0/6/23/26	0/1/1/1
9	NAG	DDD	703	1	-	0/6/23/26	0/1/1/1
9	NAG	AAA	702	1	-	0/6/23/26	0/1/1/1
9	NAG	AAA	701	1	-	1/6/23/26	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(°)
9	EEE	302	NAG	O5-C1-C2	-8.02	98.62	111.29
9	EEE	302	NAG	C1-O5-C5	6.61	121.15	112.19
9	DDD	704	NAG	C2-N2-C7	5.36	130.53	122.90
9	DDD	704	NAG	C8-C7-N2	3.57	122.15	116.10
9	EEE	302	NAG	C4-C3-C2	-3.23	106.29	111.02
9	EEE	301	NAG	O5-C5-C6	3.04	111.97	107.20
9	EEE	302	NAG	C8-C7-N2	2.94	121.08	116.10
9	EEE	302	NAG	C1-C2-N2	2.94	115.50	110.49
9	DDD	702	NAG	C1-O5-C5	2.85	116.06	112.19
9	DDD	702	NAG	O5-C1-C2	-2.78	106.90	111.29
9	AAA	701	NAG	C1-O5-C5	2.71	115.86	112.19
9	DDD	702	NAG	C1-C2-N2	2.60	114.92	110.49
9	AAA	704	NAG	O5-C5-C6	2.49	111.10	107.20
9	AAA	703	NAG	C1-O5-C5	2.37	115.41	112.19
9	DDD	704	NAG	O5-C5-C6	2.35	110.88	107.20
9	EEE	302	NAG	O3-C3-C2	2.34	114.31	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	DDD	704	NAG	O7-C7-C8	-2.25	117.88	122.06
9	AAA	702	NAG	C1-O5-C5	2.11	115.05	112.19
9	DDD	701	NAG	O5-C5-C6	2.10	110.50	107.20
9	EEE	301	NAG	C2-N2-C7	2.04	125.80	122.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	AAA	703	NAG	O5-C5-C6-O6
9	DDD	704	NAG	C8-C7-N2-C2
9	DDD	704	NAG	O7-C7-N2-C2
9	EEE	302	NAG	C8-C7-N2-C2
9	EEE	302	NAG	O7-C7-N2-C2
9	AAA	703	NAG	C4-C5-C6-O6
9	DDD	704	NAG	C3-C2-N2-C7
9	AAA	701	NAG	C1-C2-N2-C7
9	EEE	302	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	DDD	704	NAG	1	0
9	EEE	302	NAG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å <sup>2</sup> )	Q < 0.9
1	AAA	586/617 (94%)	0.46	29 (4%)	36 36	29, 41, 63, 101	0
1	DDD	587/617 (95%)	0.69	41 (6%)	24 24	30, 45, 74, 121	0
2	BBB	185/203 (91%)	0.65	13 (7%)	24 24	22, 44, 63, 80	5 (2%)
2	EEE	185/203 (91%)	0.71	12 (6%)	26 26	34, 45, 64, 88	0
3	CCC	13/14 (92%)	0.35	1 (7%)	21 21	31, 35, 51, 53	0
3	FFF	13/14 (92%)	0.35	1 (7%)	21 21	34, 40, 54, 56	0
All	All	1569/1668 (94%)	0.60	97 (6%)	28 28	22, 43, 67, 121	5 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	13	SER	8.1
1	DDD	14	SER	7.0
1	AAA	13	SER	6.1
1	DDD	586	ASP	5.6
1	DDD	599	CYS	5.6
1	AAA	586	ASP	5.4
1	AAA	59	PHE	5.4
2	EEE	207	SER	5.2
1	DDD	581	PRO	5.2
1	AAA	583	LEU	4.9
1	AAA	15	MET	4.8
1	DDD	578	ASP	4.8
1	AAA	578	ASP	4.7
1	DDD	58	ASP	4.6
2	BBB	207	SER	4.6
1	AAA	579	LEU	4.5
1	AAA	14	SER	4.5
1	DDD	583	LEU	4.5
1	DDD	15	MET	4.5

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Mol	Chain	Res	Type	RSRZ
1	DDD	57	GLY	4.4
1	AAA	58	ASP	4.3
1	DDD	60	SER	4.3
1	AAA	580	PRO	4.3
1	AAA	590	ASN	4.2
1	AAA	584	ALA	4.1
1	AAA	593	ILE	4.1
1	DDD	16	ASP	4.0
2	BBB	208	HIS	4.0
1	DDD	59	PHE	3.8
1	DDD	45	ALA	3.7
1	AAA	581	PRO	3.7
2	EEE	211	PRO	3.7
1	AAA	57	GLY	3.6
2	EEE	208	HIS	3.6
1	AAA	597	GLY	3.4
1	AAA	577	GLY	3.4
2	EEE	206	THR	3.4
1	DDD	589	LYS	3.3
1	AAA	60	SER	3.3
1	AAA	589	LYS	3.2
2	EEE	191	THR	3.2
1	DDD	577	GLY	3.2
1	DDD	36	TYR	3.2
1	DDD	42	SER	3.2
1	AAA	582	SER	3.2
1	DDD	587	MET	3.1
2	BBB	205	VAL	3.1
1	DDD	48	CYS	3.1
2	BBB	211	PRO	3.1
2	EEE	210	CYS	3.0
2	BBB	191	THR	3.0
1	DDD	588	TYR	3.0
1	DDD	582	SER	3.0
2	BBB	210	CYS	3.0
1	DDD	584	ALA	2.9
2	EEE	205	VAL	2.9
1	DDD	579	LEU	2.9
1	AAA	588	TYR	2.8
2	BBB	189	LEU	2.8
1	DDD	444	SER	2.7
2	EEE	188	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	DDD	562	SER	2.7
1	DDD	580	PRO	2.6
1	DDD	585	LYS	2.6
1	DDD	558	VAL	2.6
1	DDD	49	ARG	2.6
1	AAA	596	PRO	2.6
2	BBB	192	PRO	2.6
1	DDD	29	SER	2.5
2	EEE	209	PRO	2.5
2	BBB	188	SER	2.4
1	AAA	598	LEU	2.4
1	AAA	16	ASP	2.3
2	EEE	193	ILE	2.3
1	DDD	46	SER	2.3
1	AAA	585	LYS	2.3
2	BBB	209	PRO	2.3
2	EEE	176	ARG	2.3
2	EEE	189	LEU	2.2
1	DDD	593	ILE	2.2
1	DDD	594	GLY	2.2
1	DDD	598	LEU	2.2
3	FFF	66	VAL	2.2
1	DDD	592	PHE	2.2
3	CCC	67	LEU	2.2
1	AAA	592	PHE	2.2
1	DDD	560	LEU	2.2
1	DDD	22	ILE	2.1
2	BBB	176	ARG	2.1
1	AAA	469	ASN	2.1
1	DDD	590	ASN	2.1
1	DDD	489	MET	2.1
2	BBB	187	PHE	2.0
2	BBB	183	ASP	2.0
1	AAA	244	HIS	2.0
1	AAA	42	SER	2.0
1	DDD	575	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	HYP	CCC	73	8/9	0.95	0.07	33,35,35,35	0
3	HYP	FFF	73	8/9	0.97	0.06	34,37,38,38	0

### 6.3 Carbohydrates

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	AaA	1	14/15	-	-	41,45,49,52	0
4	NAG	AaA	2	14/15	-	-	49,57,62,69	0
4	BMA	AaA	3	11/12	-	-	81,85,87,87	0
4	MAN	AaA	4	11/12	-	-	84,87,93,94	0
5	NAG	AeA	1	14/15	-	-	46,51,60,62	0
5	NAG	AeA	2	14/15	-	-	70,83,87,92	0
5	FUC	AeA	3	10/11	-	-	76,79,80,82	0
5	NAG	DkD	1	14/15	-	-	53,61,74,74	0
5	NAG	DkD	2	14/15	-	-	80,87,91,91	0
5	FUC	DkD	3	10/11	-	-	89,97,99,101	0
6	NAG	AhA	1	14/15	-	-	46,51,53,58	0
6	NAG	AhA	2	14/15	-	-	64,83,87,93	0
6	NAG	AkA	1	14/15	-	-	50,57,61,73	0
6	NAG	AkA	2	14/15	-	-	74,91,97,97	0
6	NAG	AnA	1	14/15	-	-	54,64,72,81	0
6	NAG	AnA	2	14/15	-	-	86,100,109,111	0
6	NAG	BaB	1	14/15	-	-	69,76,79,80	0
6	NAG	BaB	2	14/15	-	-	89,95,101,107	0
6	NAG	BcB	1	14/15	-	-	57,62,67,72	0
6	NAG	BcB	2	14/15	-	-	75,81,85,85	0
6	NAG	DaD	1	14/15	-	-	59,65,69,74	0
6	NAG	DaD	2	14/15	-	-	96,102,106,107	0
6	NAG	DeD	1	14/15	-	-	50,53,57,65	0
6	NAG	DeD	2	14/15	-	-	87,93,98,104	0
6	NAG	DgD	1	14/15	-	-	56,61,66,76	0
6	NAG	DgD	2	14/15	-	-	86,104,106,107	0
6	NAG	EaE	1	14/15	-	-	74,79,85,87	0
6	NAG	EaE	2	14/15	-	-	86,92,95,97	0
6	NAG	EeE	1	14/15	-	-	57,65,69,77	0
6	NAG	EeE	2	14/15	-	-	83,99,105,105	0

*Continued on next page...*



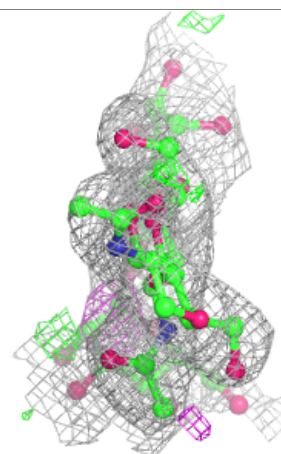
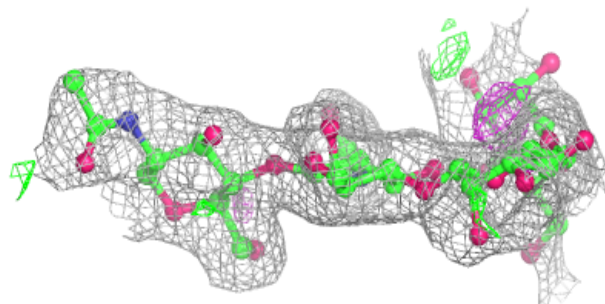
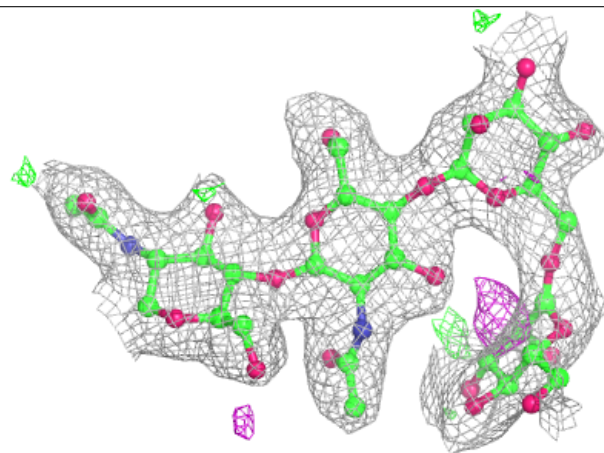
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	ArA	1	14/15	-	-	28,31,34,36	0
7	NAG	ArA	2	14/15	-	-	49,52,55,63	0
7	BMA	ArA	3	11/12	-	-	83,94,102,103	0
7	MAN	ArA	4	11/12	-	-	112,124,127,128	0
7	MAN	ArA	5	11/12	-	-	105,111,115,120	0
7	NAG	DqD	1	14/15	-	-	55,59,64,70	0
7	NAG	DqD	2	14/15	-	-	81,86,93,100	0
7	BMA	DqD	3	11/12	-	-	116,121,127,129	0
7	MAN	DqD	4	11/12	-	-	119,128,133,136	0
7	MAN	DqD	5	11/12	-	-	115,127,130,130	0
8	NAG	DnD	1	14/15	-	-	36,38,40,41	0
8	NAG	DnD	2	14/15	-	-	47,49,52,60	0
8	BMA	DnD	3	11/12	-	-	79,82,84,86	0

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

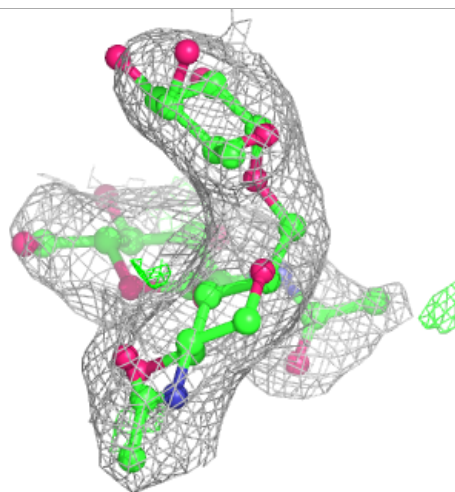
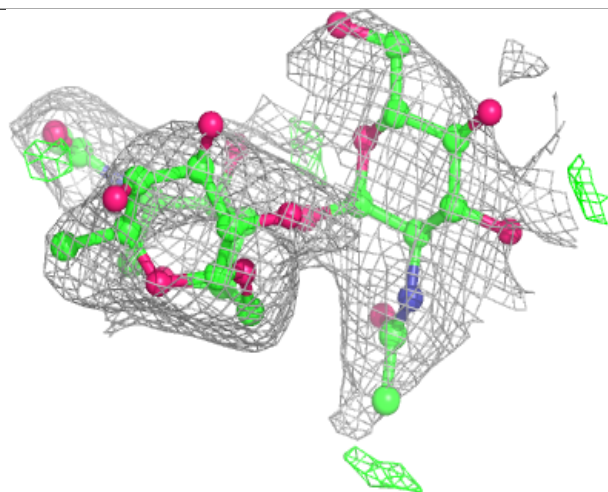
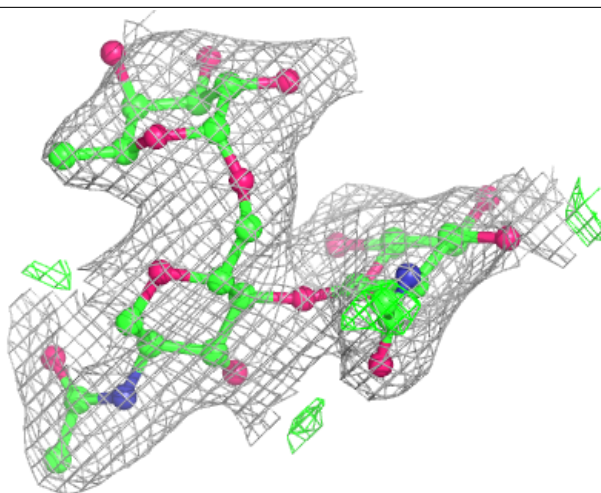
#### Electron density around Chain AaA:

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



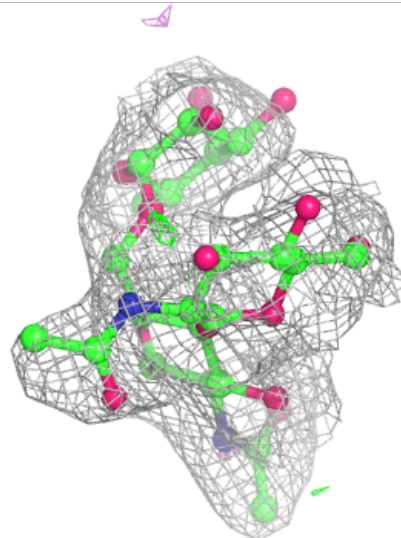
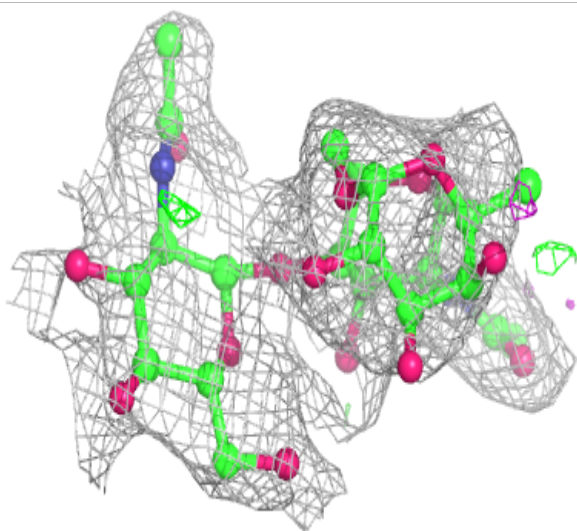
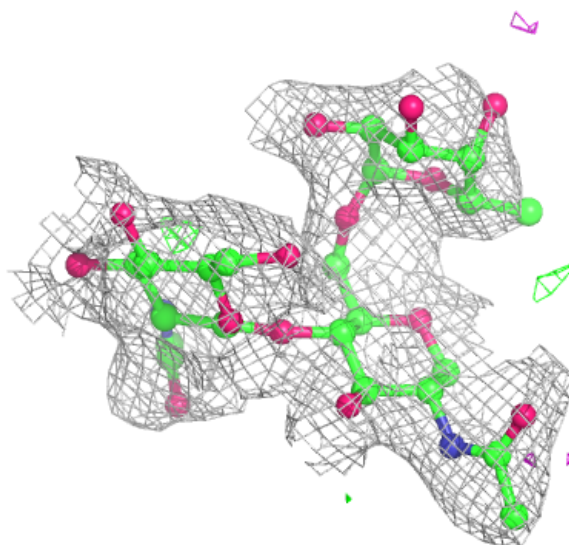
**Electron density around Chain AeA:**

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



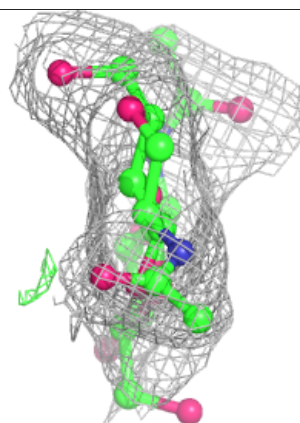
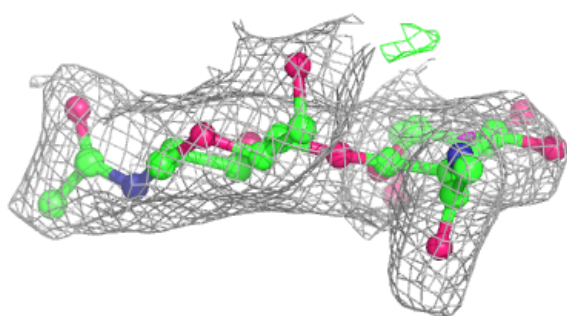
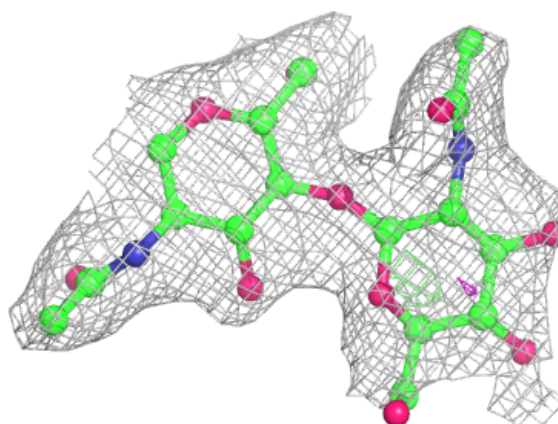
**Electron density around Chain DkD:**

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and green (positive)



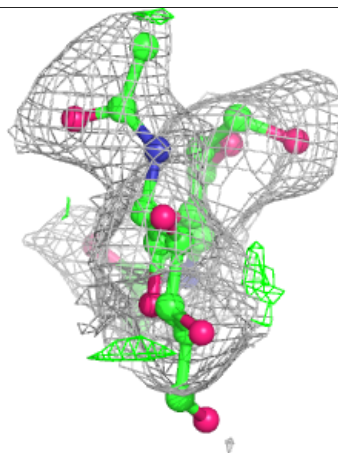
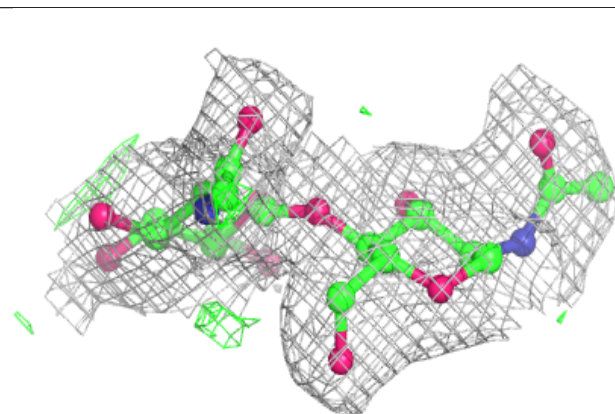
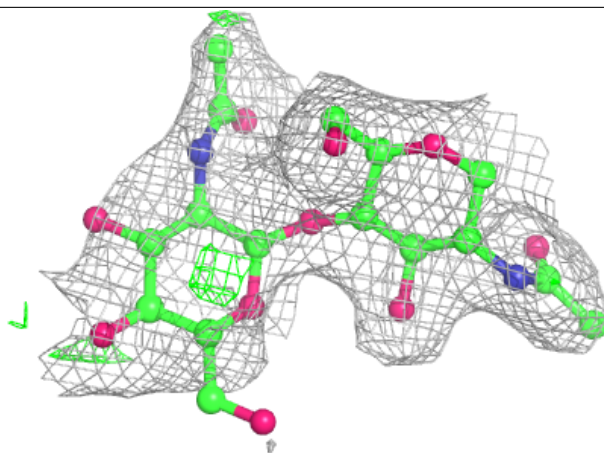
**Electron density around Chain AhA:**

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and green (positive)



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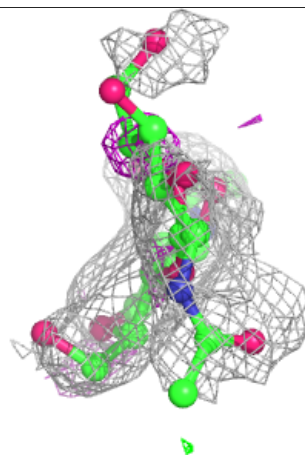
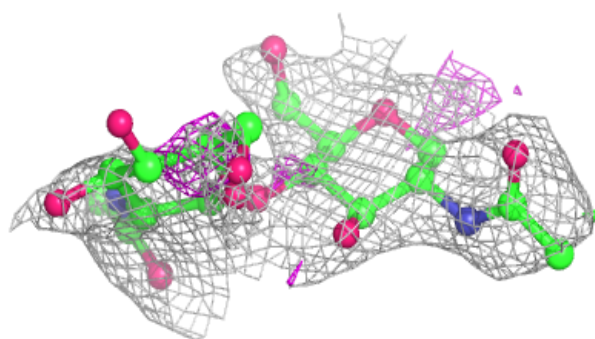
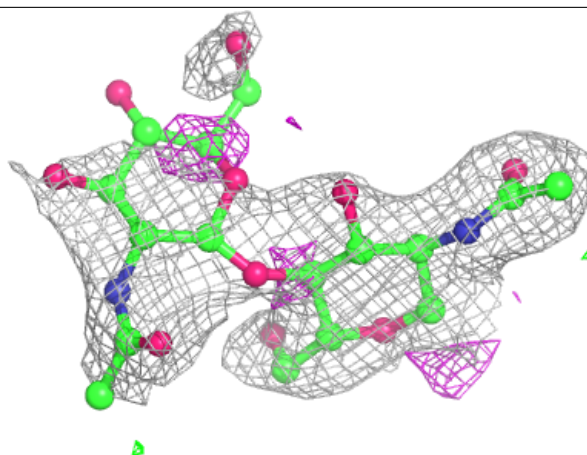
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and green (positive)





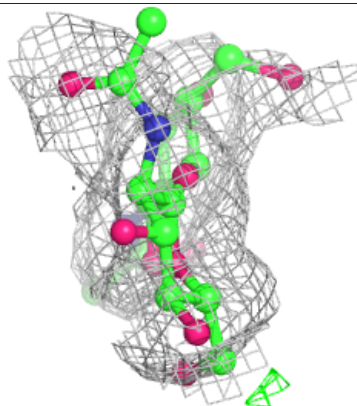
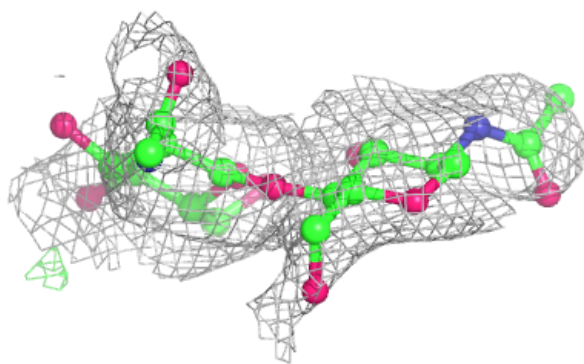
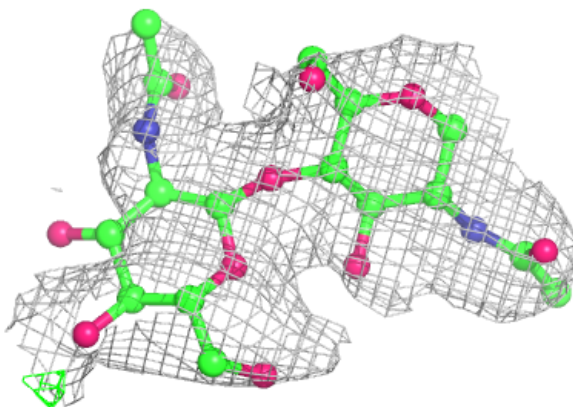
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and green (positive)



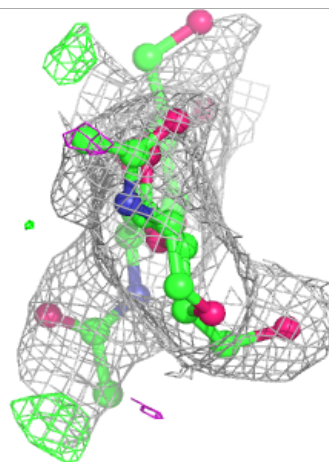
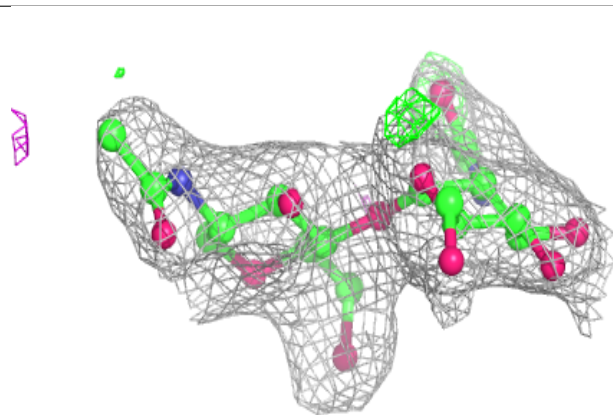
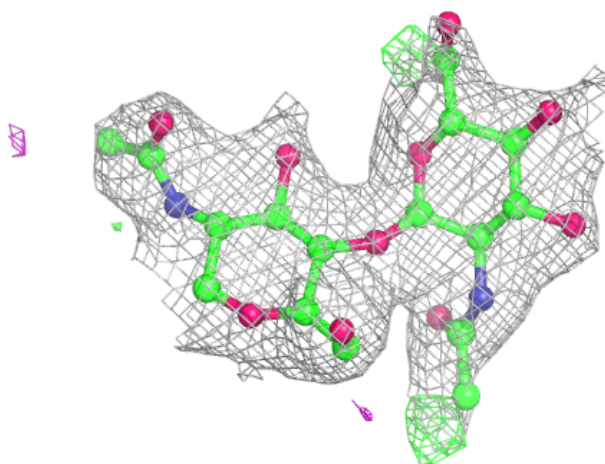
**Electron density around Chain BaB:**

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



**Electron density around Chain BcB:**

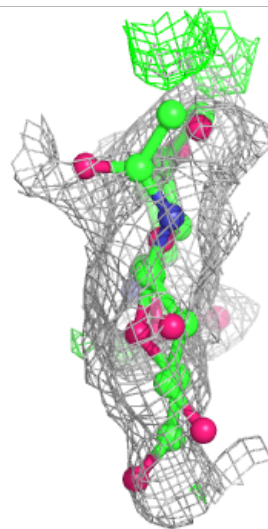
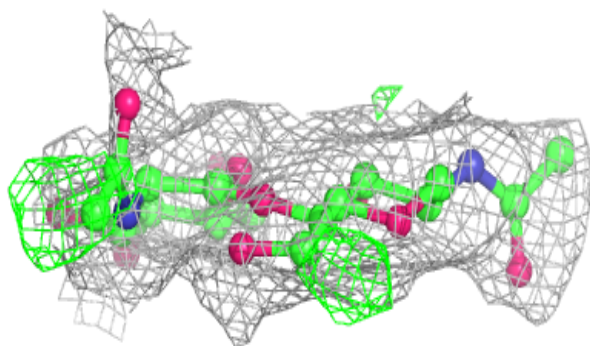
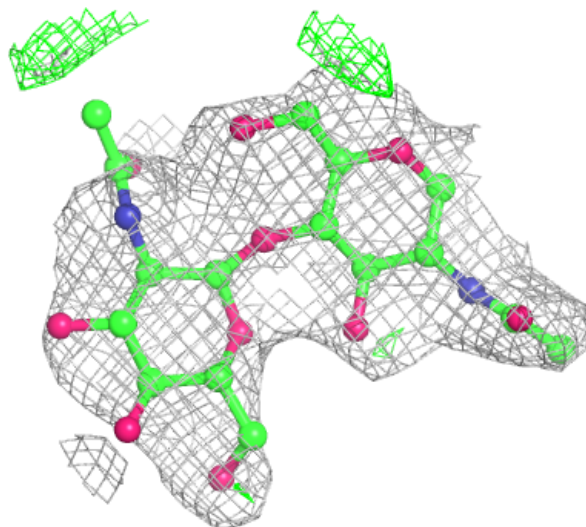
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





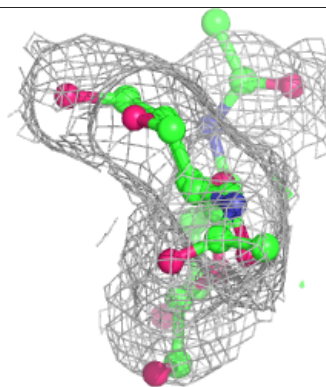
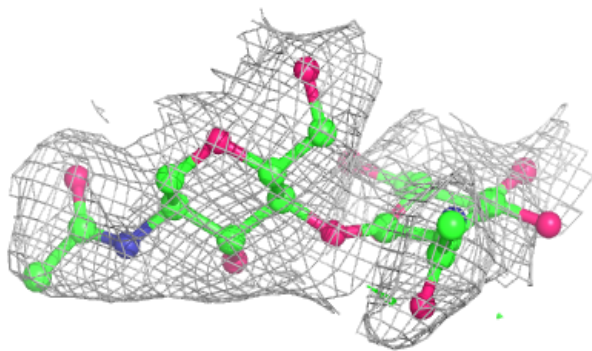
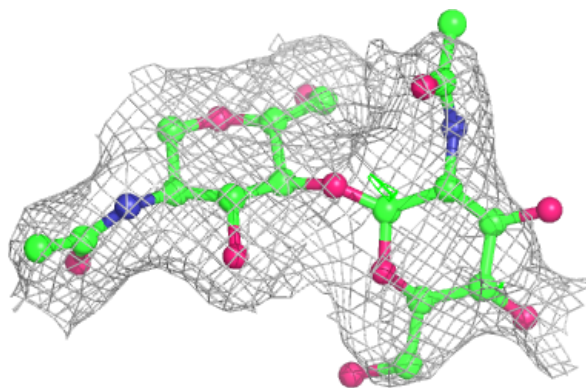
**Electron density around Chain DaD:**

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



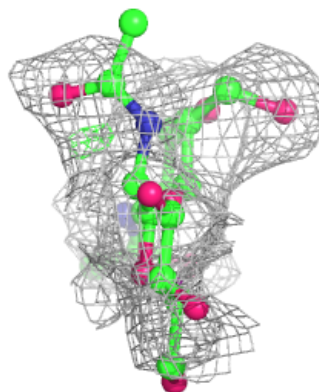
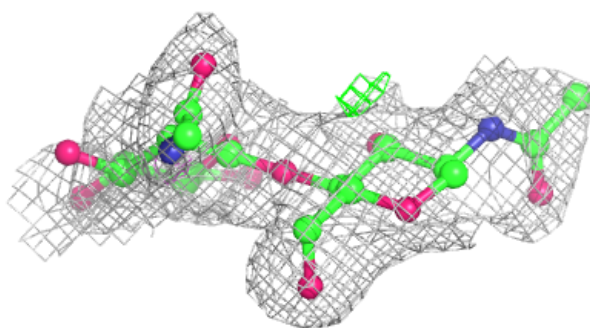
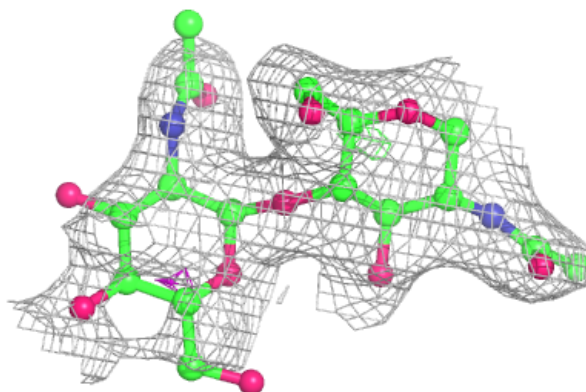
**Electron density around Chain DeD:**

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



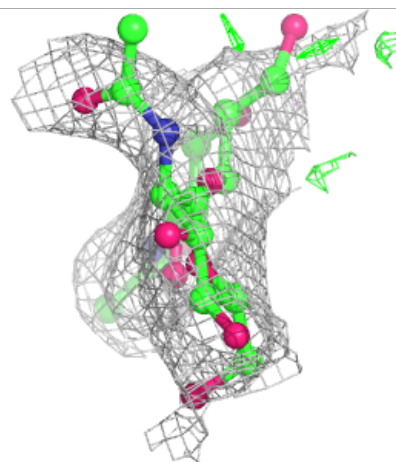
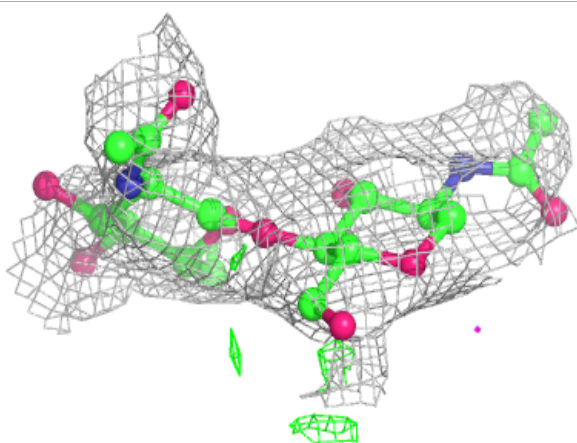
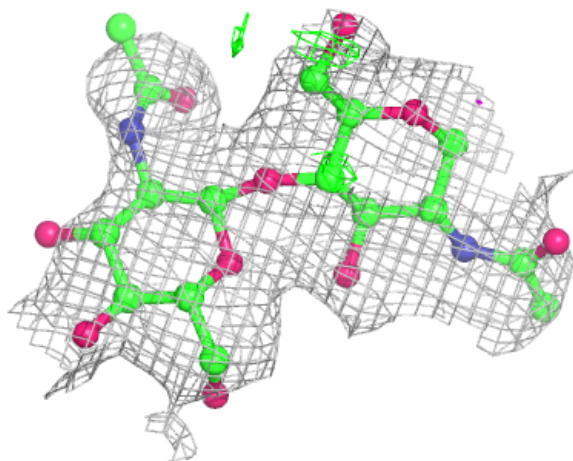
**Electron density around Chain DgD:**

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



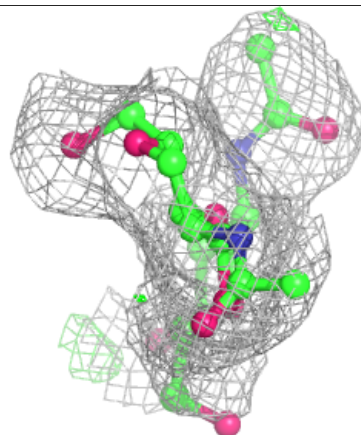
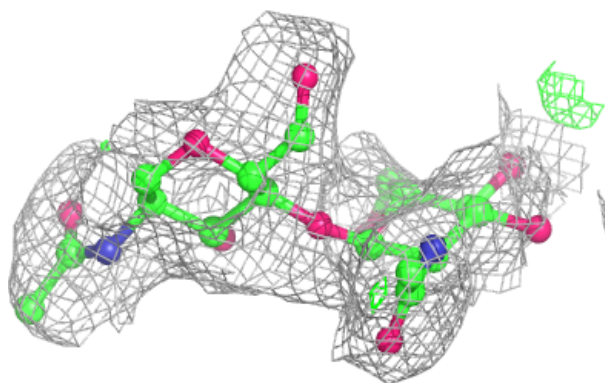
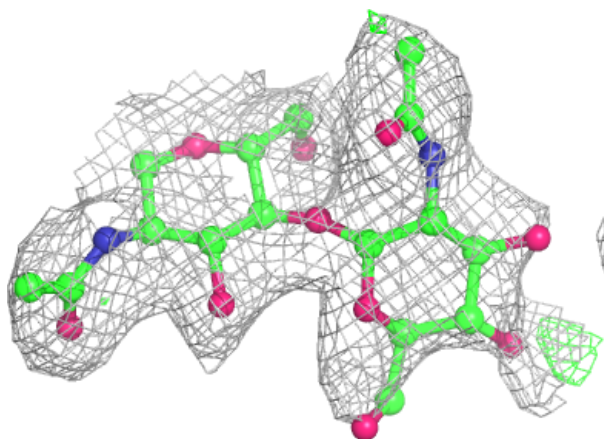
**Electron density around Chain EaE:**

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and green (positive)

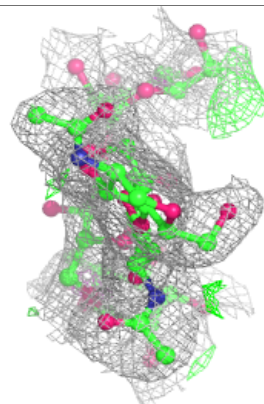
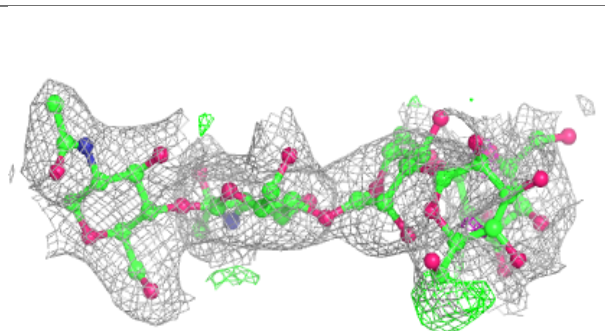
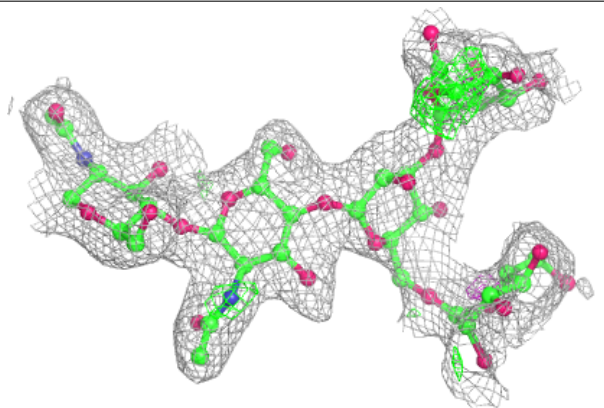


**Electron density around Chain EeE:**

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

**Electron density around Chain ArA:**

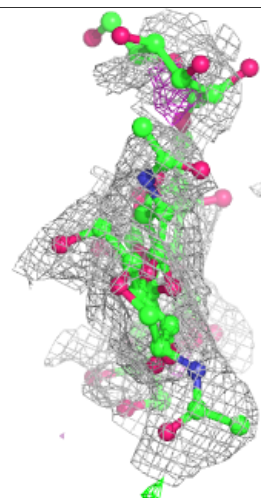
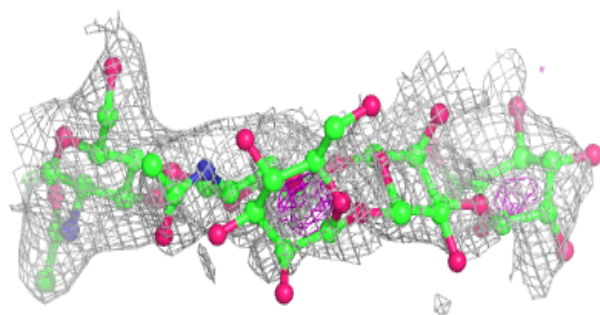
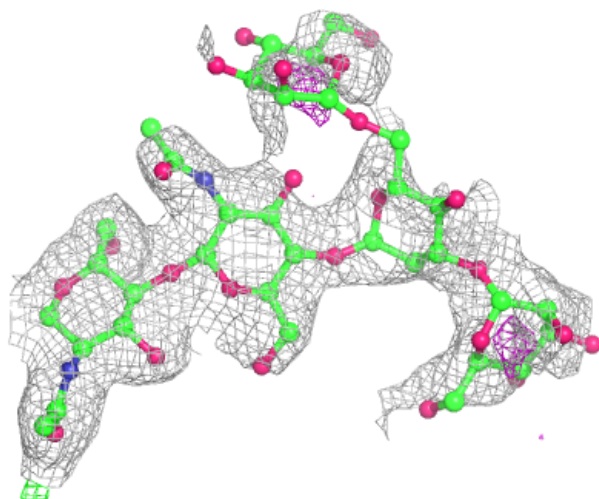
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

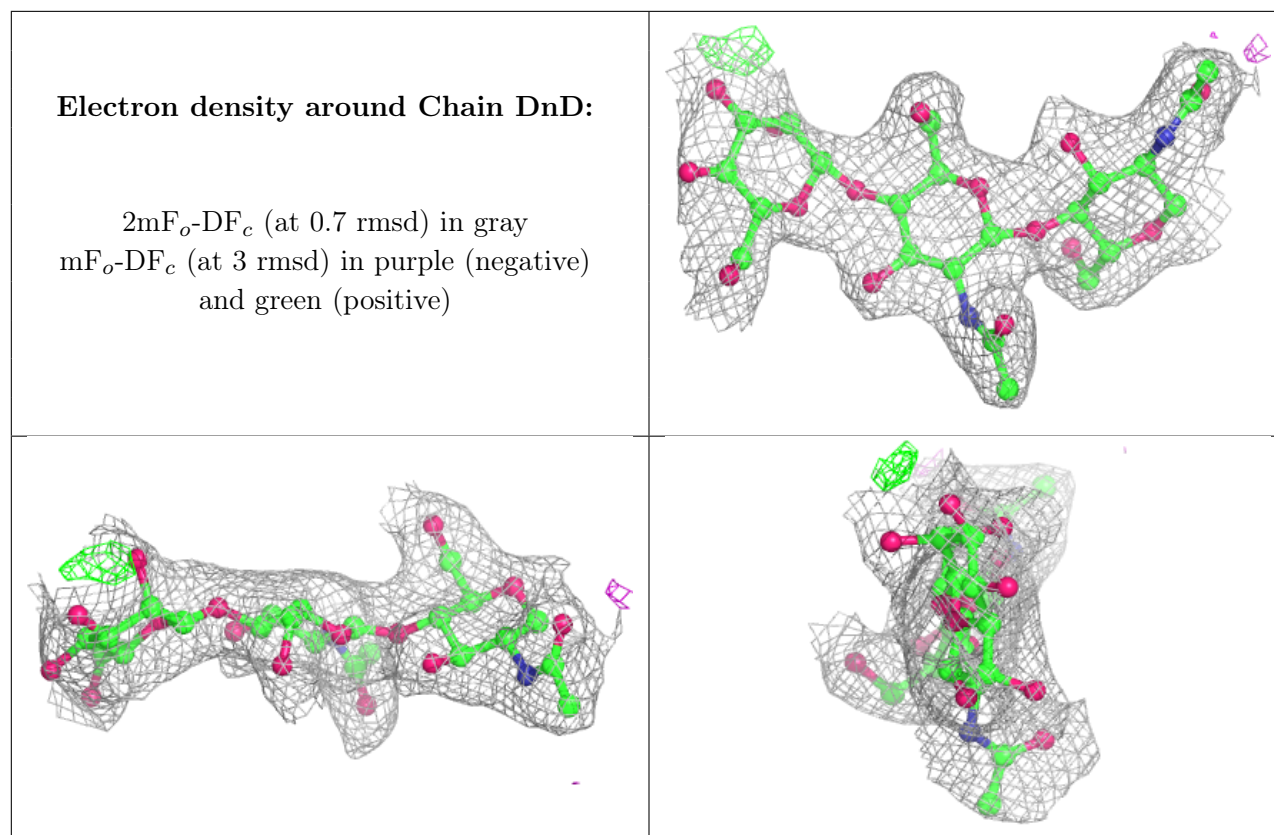




**Electron density around Chain DqD:**

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





## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	NAG	EEE	301	14/15	0.40	0.22	82,91,96,96	0
9	NAG	AAA	704	14/15	0.42	0.24	77,87,95,97	0
9	NAG	EEE	302	14/15	0.56	0.22	89,96,98,102	0
9	NAG	DDD	704	14/15	0.57	0.20	84,91,94,95	0
9	NAG	AAA	701	14/15	0.58	0.22	76,81,88,88	0
9	NAG	DDD	703	14/15	0.74	0.17	58,75,82,85	0
9	NAG	DDD	701	14/15	0.75	0.15	56,60,62,63	0
9	NAG	AAA	703	14/15	0.78	0.16	60,65,73,78	0
9	NAG	DDD	702	14/15	0.79	0.15	58,64,70,75	0
9	NAG	AAA	702	14/15	0.88	0.11	54,56,60,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.