



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2022 – 06:29 pm GMT

PDB ID : 7OGQ  
Title : Plant peptide hormone receptor H1I2S1  
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Deposited on : 2021-05-07  
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

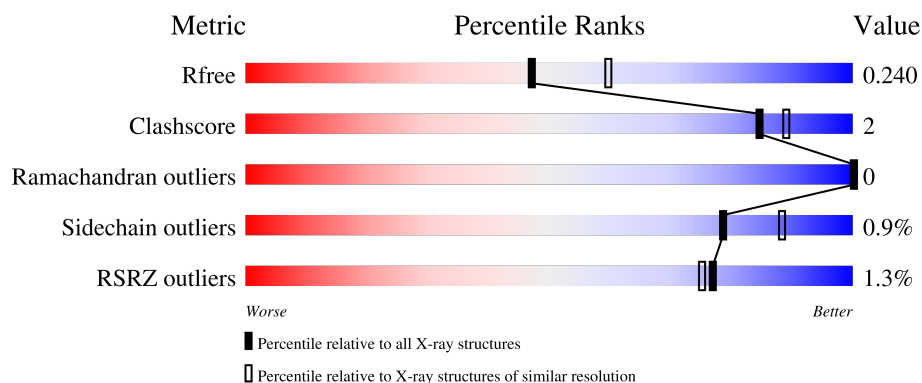
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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>%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>.</div> </div> </div>
2	BBB	203	<div> <div>84%</div> <div>7%</div> <div>9%</div> </div>
3	CCC	14	<div> <div>93%</div> <div>7%</div> </div>
4	AaA	6	<div> <div>50%</div> <div>50%</div> </div>
5	AeA	5	<div> <div>40%</div> <div>60%</div> </div>

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Mol	Chain	Length	Quality of chain
5	ApA	5	 100%
5	BaB	5	 60% 40%
6	AmA	3	 100%
7	ABA	4	 50% 50%
7	AuA	4	 50% 50%
8	AxA	3	 33% 67%
9	BbB	2	 100%
9	BfB	2	 100%

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	-	-	X
5	NAG	AeA	2	X	-	-	-
5	BMA	AeA	3	X	-	-	-
5	MAN	AeA	4	X	-	-	-
5	MAN	AeA	5	X	-	-	X
5	BMA	ApA	3	X	-	-	-
5	MAN	ApA	4	X	-	-	-
5	MAN	ApA	5	-	-	-	X
6	BMA	AmA	3	X	-	-	-
7	MAN	ABA	4	-	-	-	X
7	NAG	AuA	2	X	-	-	-
7	BMA	AuA	3	X	-	-	-
7	MAN	AuA	4	X	-	-	-
8	NAG	AxA	2	X	-	-	-
8	FUC	AxA	3	-	-	-	X
9	NAG	BbB	2	X	-	-	-

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 6812 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	595	Total	C	N	O	S	0	1	0
			4445	2810	728	890	17			

There are 15 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

- 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
			1385	872	235	273	5			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BBB	20	GLY	-	expression tag	UNP Q94AG2

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Chain	Residue	Modelled	Actual	Comment	Reference
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

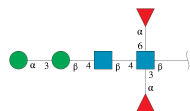
- Molecule 3 is a protein called Protein IDA-LIKE 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	CCC	14	Total	C	N	O	0	0	0
			106	65	21	20			

There are 2 discrepancies between the modelled and reference sequences:

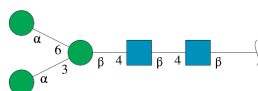
Chain	Residue	Modelled	Actual	Comment	Reference
CCC	70	TYR	HIS	conflict	UNP Q6DUW9
CCC	71	VAL	PHE	conflict	UNP Q6DUW9

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



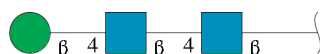
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	AaA	6	Total	C	N	O	0	0	0
			70	40	2	28			

- Molecule 5 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
5	AeA	5	Total	C	N	O	0	0	0
			61	34	2	25			
5	ApA	5	Total	C	N	O	0	0	0
			61	34	2	25			
5	BaB	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 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.



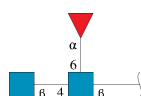
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	AmA	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



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

- Molecule 8 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.



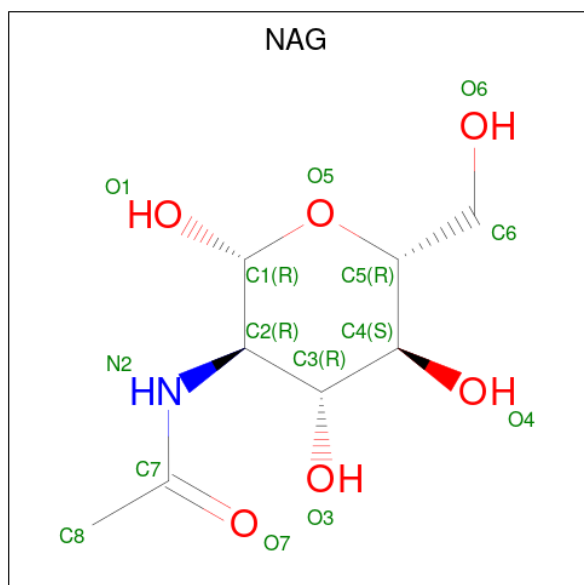
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	AxA	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



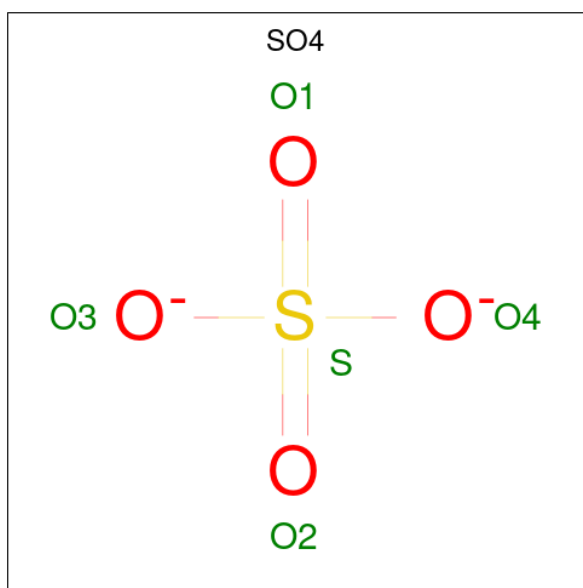
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	BbB	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	BfB	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 11 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	AAA	1	Total	O	S	0	0
			5	4	1		
11	AAA	1	Total	O	S	0	0
			5	4	1		
11	AAA	1	Total	O	S	0	0
			5	4	1		
11	AAA	1	Total	O	S	0	0
			5	4	1		
11	AAA	1	Total	O	S	0	0
			5	4	1		
11	BBB	1	Total	O	S	0	0
			5	4	1		

- Molecule 12 is water.

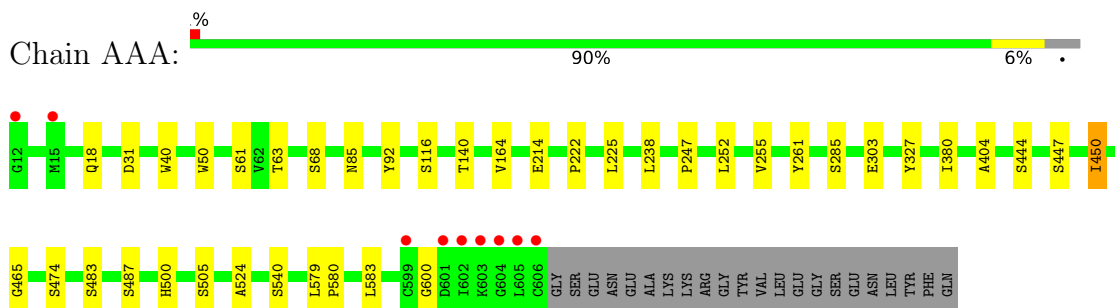
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	AAA	239	Total	O	0	0
			239	239		
12	BBB	72	Total	O	0	0
			72	72		
12	CCC	7	Total	O	0	0
			7	7		



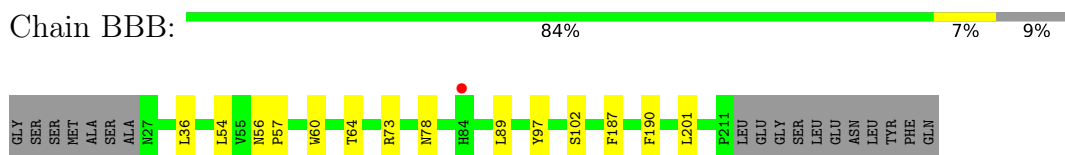
### 3 Residue-property plots [i](#)

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.

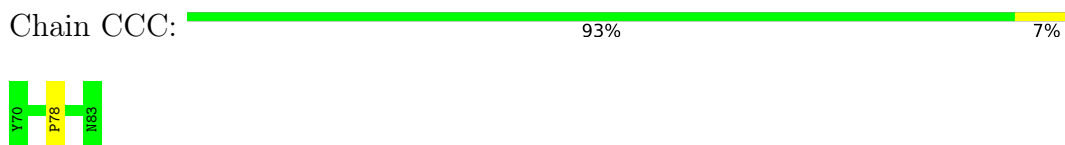
- Molecule 1: Receptor-like protein kinase HSL1



- Molecule 2: Somatic embryogenesis receptor kinase 1



- Molecule 3: Protein IDA-LIKE 2



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



- Molecule 5: 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 AeA:  40% 60%



- Molecule 5: 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 ApA:  100%



- Molecule 5: 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 BaB:  60% 40%



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

Chain AmA:  100%



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

Chain AuA:  50% 50%



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

Chain ABA:  50% 50%



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

Chain AxA:  33% 67%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BbB:  100%



- Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BfB:  100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.82Å 88.08Å 166.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.97 – 2.20 46.93 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.97-2.20) 100.0 (46.93-2.20)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.198 , 0.234 0.206 , 0.240	Depositor DCC
$R_{free}$ test set	3215 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.9	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6812	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, MAN, SO4, BMA, FUC, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	AAA	0.69	0/4529	0.73	0/6175
2	BBB	0.66	0/1414	0.75	0/1943
3	CCC	0.73	0/100	0.80	0/132
All	All	0.69	0/6043	0.73	0/8250

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	4445	0	4313	19	0
2	BBB	1385	0	1327	9	0
3	CCC	106	0	97	0	0
4	AaA	70	0	61	0	0
5	AeA	61	0	52	0	0
5	ApA	61	0	52	0	0
5	BaB	61	0	52	0	0
6	AmA	39	0	34	0	0
7	ABA	50	0	43	0	0
7	AuA	50	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AxA	38	0	34	0	0
9	BbB	28	0	25	0	0
9	BfB	28	0	25	0	0
10	AAA	28	0	26	0	0
10	BBB	14	0	13	0	0
11	AAA	25	0	0	0	0
11	BBB	5	0	0	0	0
12	AAA	239	0	0	2	1
12	BBB	72	0	0	0	0
12	CCC	7	0	0	0	0
All	All	6812	0	6197	28	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (28) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:18:GLN:OE1	12:AAA:801:HOH:O	2.09	0.69
2:BBB:64:THR:HB	2:BBB:73:ARG:HB2	1.81	0.62
1:AAA:465:GLY:HA3	1:AAA:487:SER:HB2	1.84	0.58
2:BBB:56:ASN:HB2	2:BBB:57:PRO:HD2	1.87	0.56
2:BBB:36:LEU:HD22	2:BBB:89:LEU:HD21	1.89	0.54
2:BBB:73:ARG:HG2	2:BBB:97:TYR:HB2	1.90	0.54
1:AAA:579:LEU:HD12	1:AAA:600:GLY:HA3	1.90	0.52
1:AAA:252:LEU:HB3	1:AAA:255:VAL:HB	1.92	0.52
1:AAA:483:SER:HA	1:AAA:505:SER:O	2.10	0.51
2:BBB:187:PHE:HA	2:BBB:190:PHE:HD2	1.77	0.49
1:AAA:247:PRO:HD2	12:AAA:803:HOH:O	2.13	0.48
1:AAA:303:GLU:HB3	1:AAA:327:TYR:CE2	2.52	0.45
2:BBB:187:PHE:HA	2:BBB:190:PHE:CD2	2.51	0.45
1:AAA:214:GLU:HA	1:AAA:238:LEU:O	2.17	0.45
1:AAA:222:PRO:HG2	1:AAA:225:LEU:HG	1.99	0.44
2:BBB:78:ASN:HA	2:BBB:102:SER:O	2.17	0.44
1:AAA:140:THR:HA	1:AAA:164:VAL:O	2.17	0.44
2:BBB:201:LEU:HD23	2:BBB:201:LEU:HA	1.88	0.43
2:BBB:54:LEU:HD12	2:BBB:60:TRP:HE1	1.82	0.43
1:AAA:261:TYR:HA	1:AAA:285[B]:SER:O	2.19	0.42
1:AAA:450:ILE:HG23	1:AAA:474:SER:HB2	2.01	0.42
1:AAA:68:SER:HA	1:AAA:92:TYR:O	2.20	0.42
1:AAA:380:ILE:HA	1:AAA:404:ALA:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:580:PRO:HG2	1:AAA:583:LEU:HD12	2.02	0.42
1:AAA:40:TRP:CD1	1:AAA:50:TRP:HB3	2.55	0.41
1:AAA:63:THR:HA	1:AAA:85:ASN:O	2.21	0.41
1:AAA:116:SER:HA	1:AAA:140:THR:O	2.20	0.40
1:AAA:500:HIS:HA	1:AAA:524:ALA:O	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AAA:1008:HOH:O	12:AAA:1021:HOH:O[2_595]	2.18	0.02

## 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	594/617 (96%)	582 (98%)	12 (2%)	0	100	100
2	BBB	184/203 (91%)	182 (99%)	2 (1%)	0	100	100
3	CCC	11/14 (79%)	11 (100%)	0	0	100	100
All	All	789/834 (95%)	775 (98%)	14 (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	499/540 (92%)	493 (99%)	6 (1%)	71	83
2	BBB	159/184 (86%)	159 (100%)	0	100	100
3	CCC	10/11 (91%)	10 (100%)	0	100	100
All	All	668/735 (91%)	662 (99%)	6 (1%)	78	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	31	ASP
1	AAA	61	SER
1	AAA	444	SER
1	AAA	447	SER
1	AAA	450	ILE
1	AAA	540	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 ⓘ

1 non-standard protein/DNA/RNA residue is 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	CCC	78	3	6,8,9	0.21	0	5,10,12	1.34	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	CCC	78	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	78	HYP	CB-CG-CD	-2.17	100.61	103.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

39 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	NAG	ABA	1	1,7	14,14,15	0.41	0	17,19,21	0.96	0
7	NAG	ABA	2	7	14,14,15	0.60	0	17,19,21	1.15	3 (17%)
7	BMA	ABA	3	7	11,11,12	0.42	0	15,15,17	0.92	0
7	MAN	ABA	4	7	11,11,12	0.40	0	15,15,17	0.75	1 (6%)
4	NAG	AaA	1	1,4	14,14,15	0.38	0	17,19,21	0.62	0
4	NAG	AaA	2	4	14,14,15	0.47	0	17,19,21	1.37	4 (23%)
4	BMA	AaA	3	4	11,11,12	0.59	0	15,15,17	0.97	1 (6%)
4	MAN	AaA	4	4	11,11,12	0.42	0	15,15,17	0.79	0
4	FUC	AaA	5	4	10,10,11	0.58	0	14,14,16	1.02	0
4	FUC	AaA	6	4	10,10,11	0.40	0	14,14,16	0.88	1 (7%)
5	NAG	AeA	1	1,5	14,14,15	0.47	0	17,19,21	1.12	2 (11%)
5	NAG	AeA	2	5	14,14,15	0.43	0	17,19,21	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BMA	AeA	3	5	11,11,12	0.58	0	15,15,17	0.82	0
5	MAN	AeA	4	5	11,11,12	0.87	0	15,15,17	1.19	1 (6%)
5	MAN	AeA	5	5	11,11,12	0.43	0	15,15,17	1.02	1 (6%)
6	NAG	AmA	1	6,1	14,14,15	0.33	0	17,19,21	0.83	0
6	NAG	AmA	2	6	14,14,15	0.37	0	17,19,21	0.89	0
6	BMA	AmA	3	6	11,11,12	0.42	0	15,15,17	0.78	0
5	NAG	ApA	1	1,5	14,14,15	0.53	0	17,19,21	1.55	3 (17%)
5	NAG	ApA	2	5	14,14,15	0.28	0	17,19,21	1.03	1 (5%)
5	BMA	ApA	3	5	11,11,12	0.53	0	15,15,17	0.93	1 (6%)
5	MAN	ApA	4	5	11,11,12	0.47	0	15,15,17	0.93	1 (6%)
5	MAN	ApA	5	5	11,11,12	0.57	0	15,15,17	0.84	1 (6%)
7	NAG	AuA	1	1,7	14,14,15	0.60	0	17,19,21	0.90	2 (11%)
7	NAG	AuA	2	7	14,14,15	0.40	0	17,19,21	1.12	0
7	BMA	AuA	3	7	11,11,12	0.47	0	15,15,17	0.92	2 (13%)
7	MAN	AuA	4	7	11,11,12	0.41	0	15,15,17	0.68	0
8	NAG	AxA	1	8,1	14,14,15	0.53	0	17,19,21	1.54	3 (17%)
8	NAG	AxA	2	8	14,14,15	0.38	0	17,19,21	0.79	0
8	FUC	AxA	3	8	10,10,11	0.60	0	14,14,16	1.52	1 (7%)
5	NAG	BaB	1	5,2	14,14,15	0.54	0	17,19,21	1.65	4 (23%)
5	NAG	BaB	2	5	14,14,15	0.41	0	17,19,21	0.99	1 (5%)
5	BMA	BaB	3	5	11,11,12	0.44	0	15,15,17	0.94	0
5	MAN	BaB	4	5	11,11,12	0.52	0	15,15,17	0.72	0
5	MAN	BaB	5	5	11,11,12	0.72	0	15,15,17	0.92	0
9	NAG	BbB	1	9,2	14,14,15	0.60	0	17,19,21	1.09	1 (5%)
9	NAG	BbB	2	9	14,14,15	0.27	0	17,19,21	1.11	1 (5%)
9	NAG	BfB	1	9,2	14,14,15	0.46	0	17,19,21	0.83	1 (5%)
9	NAG	BfB	2	9	14,14,15	0.40	0	17,19,21	0.98	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	ABA	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	ABA	2	7	-	2/6/23/26	0/1/1/1
7	BMA	ABA	3	7	-	2/2/19/22	0/1/1/1
7	MAN	ABA	4	7	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	AaA	1	1,4	-	0/6/23/26	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	2/2/19/22	0/1/1/1
4	FUC	AaA	5	4	-	-	0/1/1/1
4	FUC	AaA	6	4	-	-	0/1/1/1
5	NAG	AeA	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	AeA	2	5	1/1/5/7	2/6/23/26	0/1/1/1
5	BMA	AeA	3	5	1/1/4/5	1/2/19/22	0/1/1/1
5	MAN	AeA	4	5	1/1/4/5	2/2/19/22	0/1/1/1
5	MAN	AeA	5	5	1/1/4/5	2/2/19/22	0/1/1/1
6	NAG	AmA	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	AmA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	AmA	3	6	1/1/4/5	1/2/19/22	0/1/1/1
5	NAG	ApA	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	ApA	2	5	-	0/6/23/26	0/1/1/1
5	BMA	ApA	3	5	1/1/4/5	0/2/19/22	0/1/1/1
5	MAN	ApA	4	5	1/1/4/5	0/2/19/22	0/1/1/1
5	MAN	ApA	5	5	-	2/2/19/22	0/1/1/1
7	NAG	AuA	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	AuA	2	7	1/1/5/7	2/6/23/26	0/1/1/1
7	BMA	AuA	3	7	1/1/4/5	0/2/19/22	0/1/1/1
7	MAN	AuA	4	7	1/1/4/5	2/2/19/22	0/1/1/1
8	NAG	AxA	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	AxA	2	8	1/1/5/7	0/6/23/26	0/1/1/1
8	FUC	AxA	3	8	-	-	0/1/1/1
5	NAG	BaB	1	5,2	-	1/6/23/26	0/1/1/1
5	NAG	BaB	2	5	-	0/6/23/26	0/1/1/1
5	BMA	BaB	3	5	-	0/2/19/22	0/1/1/1
5	MAN	BaB	4	5	-	0/2/19/22	0/1/1/1
5	MAN	BaB	5	5	-	0/2/19/22	0/1/1/1
9	NAG	BbB	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	BbB	2	9	1/1/5/7	0/6/23/26	0/1/1/1
9	NAG	BfB	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	BfB	2	9	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	AxA	3	FUC	C1-C2-C3	4.61	115.33	109.67
5	BaB	1	NAG	C1-O5-C5	4.23	117.92	112.19
5	ApA	1	NAG	C1-O5-C5	4.07	117.71	112.19
5	ApA	1	NAG	O5-C1-C2	-3.55	105.67	111.29
5	BaB	1	NAG	C1-C2-N2	3.20	115.95	110.49
8	AxA	1	NAG	C8-C7-N2	3.04	121.25	116.10
5	BaB	2	NAG	C1-O5-C5	2.86	116.06	112.19
9	BbB	2	NAG	C1-C2-N2	-2.77	105.76	110.49
5	AeA	4	MAN	O5-C1-C2	-2.76	106.51	110.77
5	ApA	3	BMA	O5-C5-C6	2.73	111.48	107.20
9	BbB	1	NAG	O5-C5-C6	2.71	111.45	107.20
5	AeA	5	MAN	O5-C1-C2	-2.70	106.60	110.77
9	BfB	2	NAG	C1-O5-C5	2.64	115.77	112.19
5	ApA	4	MAN	O5-C5-C6	2.62	111.31	107.20
4	AaA	2	NAG	O4-C4-C5	2.59	115.72	109.30
8	AxA	1	NAG	C2-N2-C7	2.55	126.54	122.90
5	ApA	5	MAN	O5-C1-C2	-2.54	106.85	110.77
7	ABA	4	MAN	O5-C1-C2	-2.53	106.86	110.77
5	BaB	1	NAG	C4-C3-C2	-2.50	107.36	111.02
9	BfB	1	NAG	C1-O5-C5	2.47	115.53	112.19
7	ABA	2	NAG	O4-C4-C5	2.41	115.27	109.30
5	AeA	1	NAG	C1-O5-C5	2.40	115.44	112.19
7	ABA	2	NAG	C4-C3-C2	-2.34	107.58	111.02
5	BaB	1	NAG	O5-C1-C2	-2.29	107.67	111.29
4	AaA	6	FUC	C1-C2-C3	2.27	112.46	109.67
4	AaA	2	NAG	C4-C3-C2	-2.27	107.69	111.02
4	AaA	2	NAG	C1-O5-C5	2.22	115.19	112.19
5	AeA	1	NAG	C4-C3-C2	-2.20	107.79	111.02
5	ApA	2	NAG	O5-C5-C6	2.18	110.62	107.20
4	AaA	2	NAG	C3-C4-C5	-2.16	106.38	110.24
5	ApA	1	NAG	C1-C2-N2	2.16	114.18	110.49
8	AxA	1	NAG	O7-C7-C8	-2.14	118.08	122.06
7	ABA	2	NAG	C1-O5-C5	2.12	115.07	112.19
4	AaA	3	BMA	C1-O5-C5	-2.09	109.36	112.19
7	AuA	3	BMA	O5-C1-C2	-2.06	107.59	110.77
7	AuA	3	BMA	O5-C5-C6	2.04	110.40	107.20
7	AuA	1	NAG	C1-C2-N2	2.02	113.95	110.49
7	AuA	1	NAG	O5-C5-C6	2.02	110.36	107.20

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	AaA	4	MAN	C1

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Mol	Chain	Res	Type	Atom
5	AeA	2	NAG	C1
5	AeA	3	BMA	C1
5	AeA	4	MAN	C1
5	AeA	5	MAN	C1
5	ApA	3	BMA	C1
5	ApA	4	MAN	C1
6	AmA	3	BMA	C1
7	AuA	2	NAG	C1
7	AuA	3	BMA	C1
7	AuA	4	MAN	C1
8	AxA	2	NAG	C1
9	BbB	2	NAG	C1

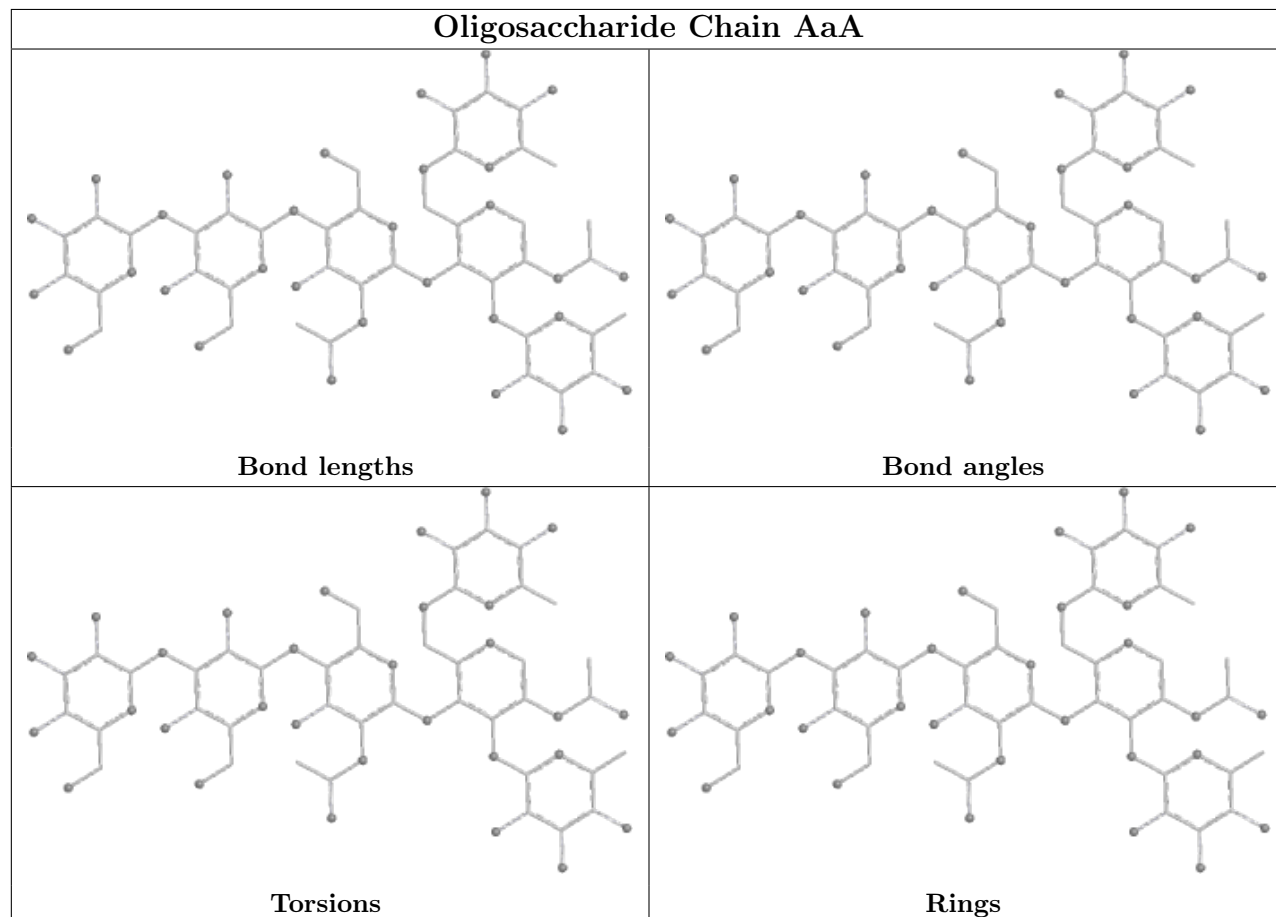
All (26) torsion outliers are listed below:

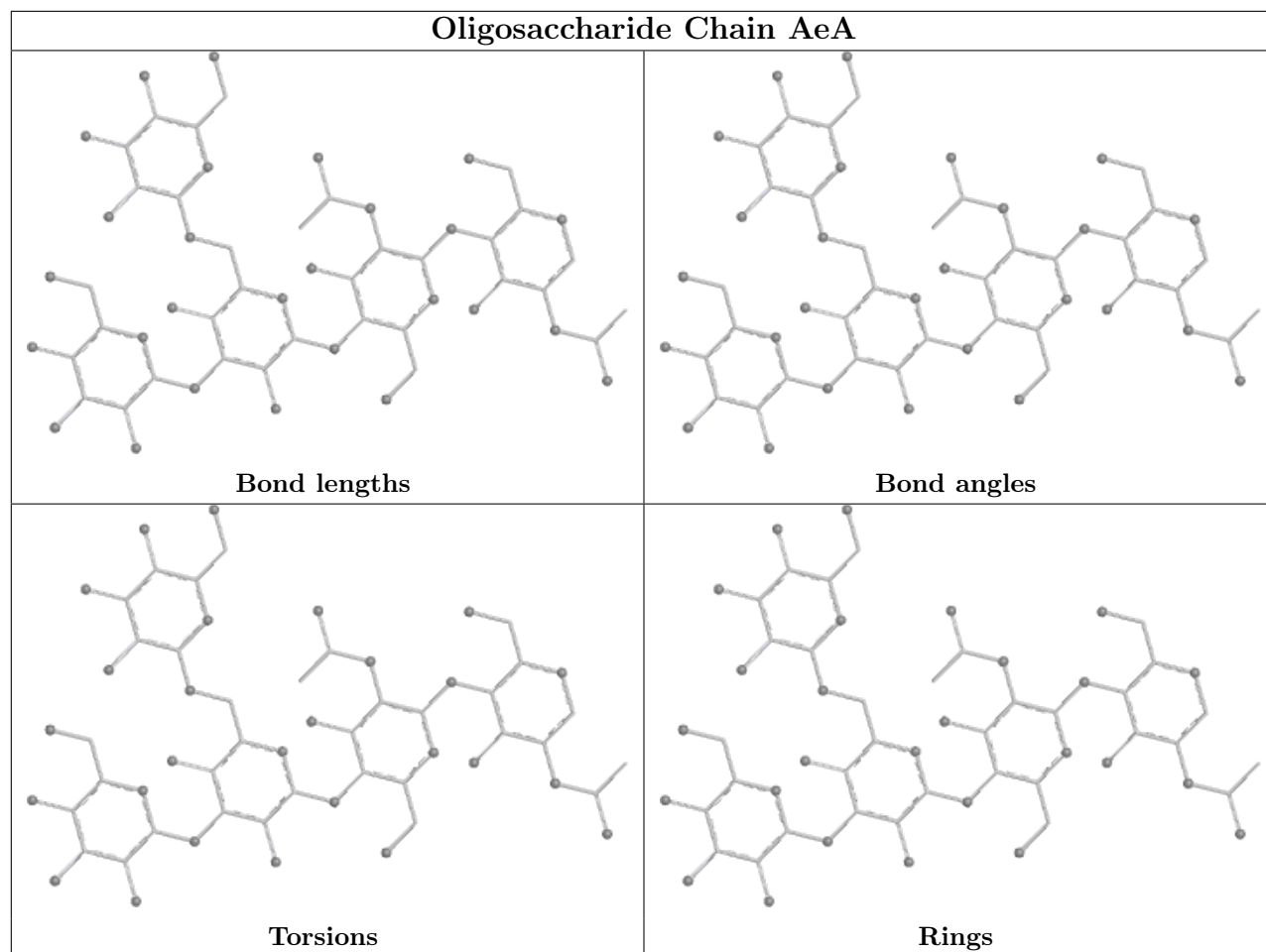
Mol	Chain	Res	Type	Atoms
5	AeA	4	MAN	C4-C5-C6-O6
5	ApA	5	MAN	C4-C5-C6-O6
4	AaA	4	MAN	O5-C5-C6-O6
5	AeA	5	MAN	C4-C5-C6-O6
5	AeA	5	MAN	O5-C5-C6-O6
5	AeA	4	MAN	O5-C5-C6-O6
5	ApA	5	MAN	O5-C5-C6-O6
5	AeA	1	NAG	C4-C5-C6-O6
8	AxA	1	NAG	C8-C7-N2-C2
8	AxA	1	NAG	O7-C7-N2-C2
5	AeA	1	NAG	O5-C5-C6-O6
7	ABA	2	NAG	O5-C5-C6-O6
7	ABA	2	NAG	C4-C5-C6-O6
7	AuA	2	NAG	O5-C5-C6-O6
4	AaA	4	MAN	C4-C5-C6-O6
7	AuA	2	NAG	C4-C5-C6-O6
7	AuA	4	MAN	O5-C5-C6-O6
6	AmA	3	BMA	O5-C5-C6-O6
7	ABA	3	BMA	C4-C5-C6-O6
7	ABA	4	MAN	O5-C5-C6-O6
7	ABA	3	BMA	O5-C5-C6-O6
5	BaB	1	NAG	C3-C2-N2-C7
5	AeA	2	NAG	O5-C5-C6-O6
5	AeA	2	NAG	C4-C5-C6-O6
5	AeA	3	BMA	C4-C5-C6-O6
7	AuA	4	MAN	C4-C5-C6-O6

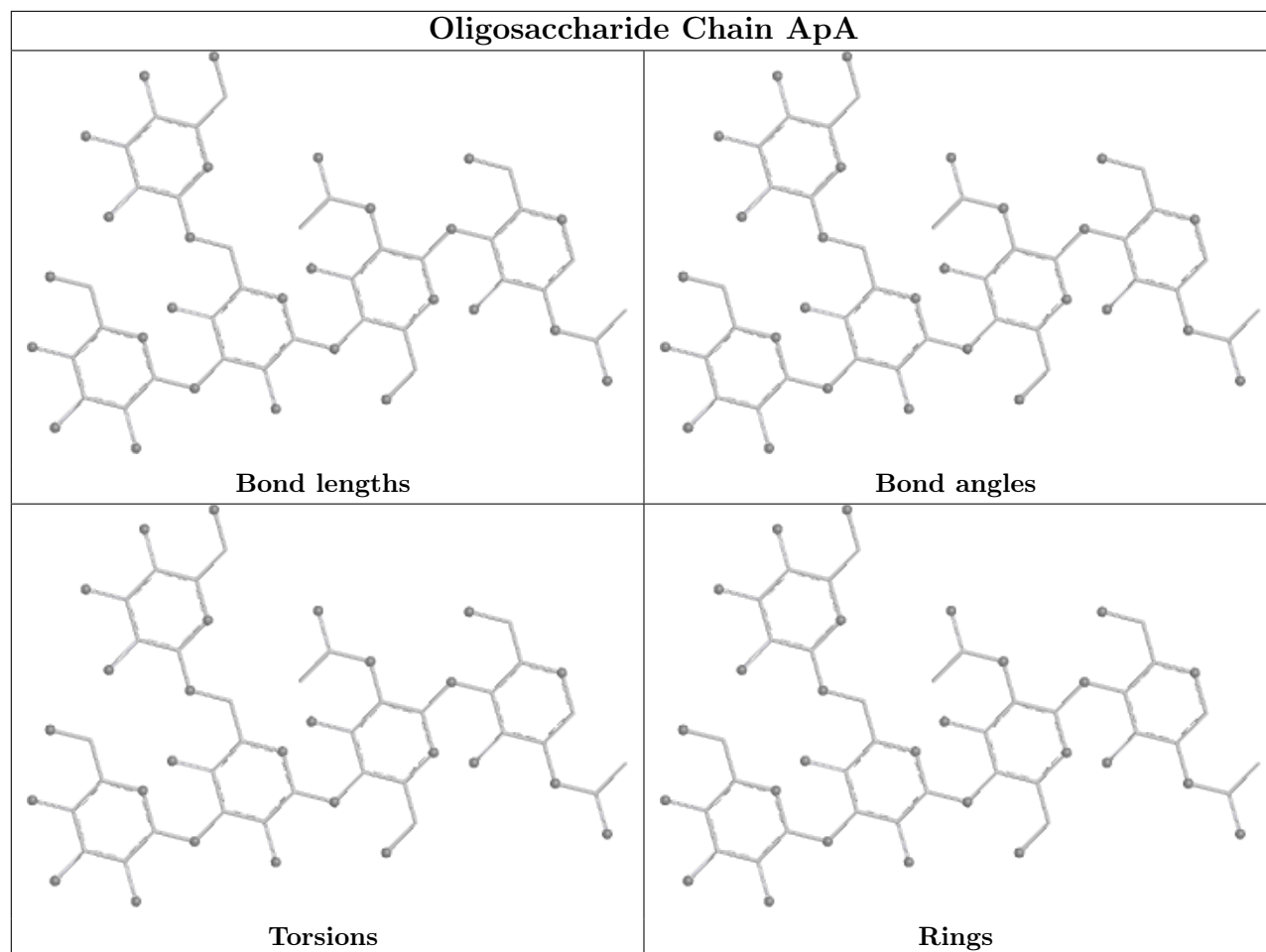
There are no ring outliers.

No monomer is involved in short contacts.

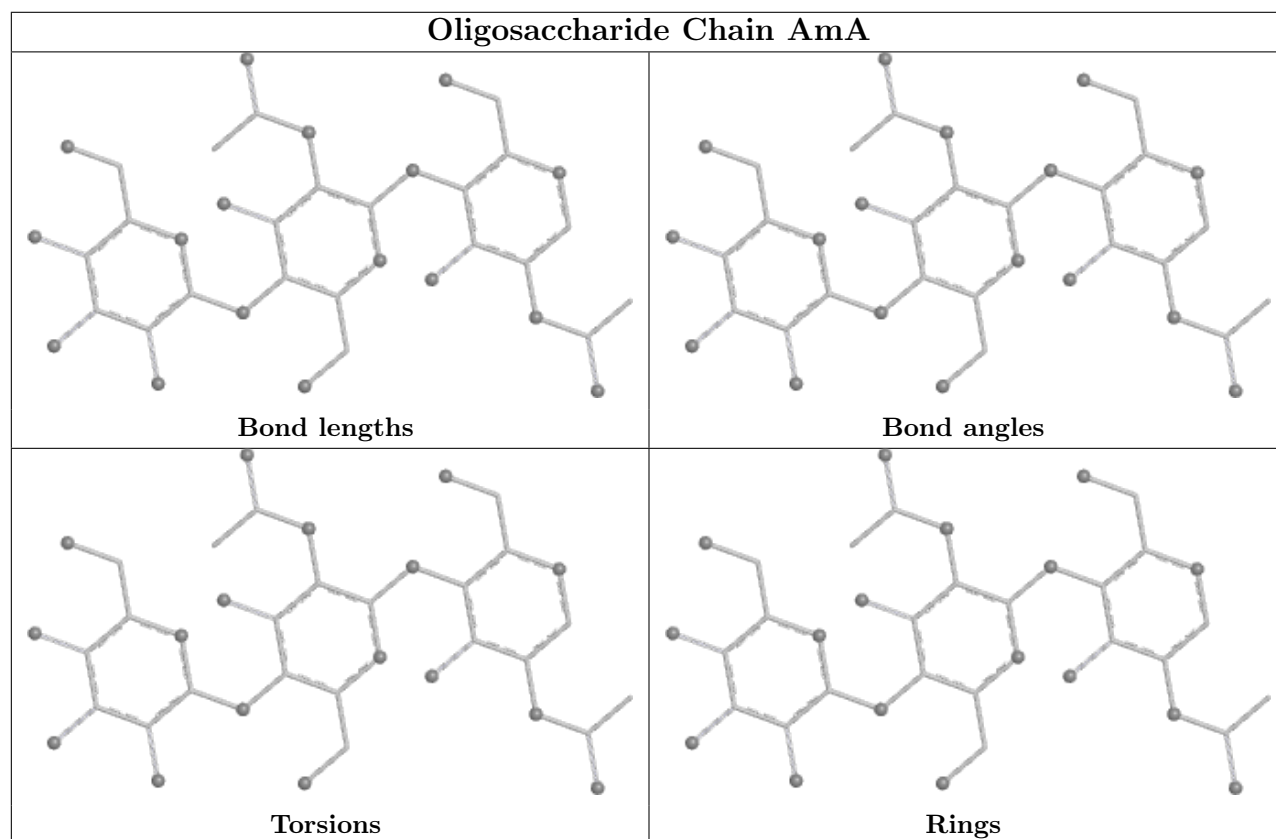
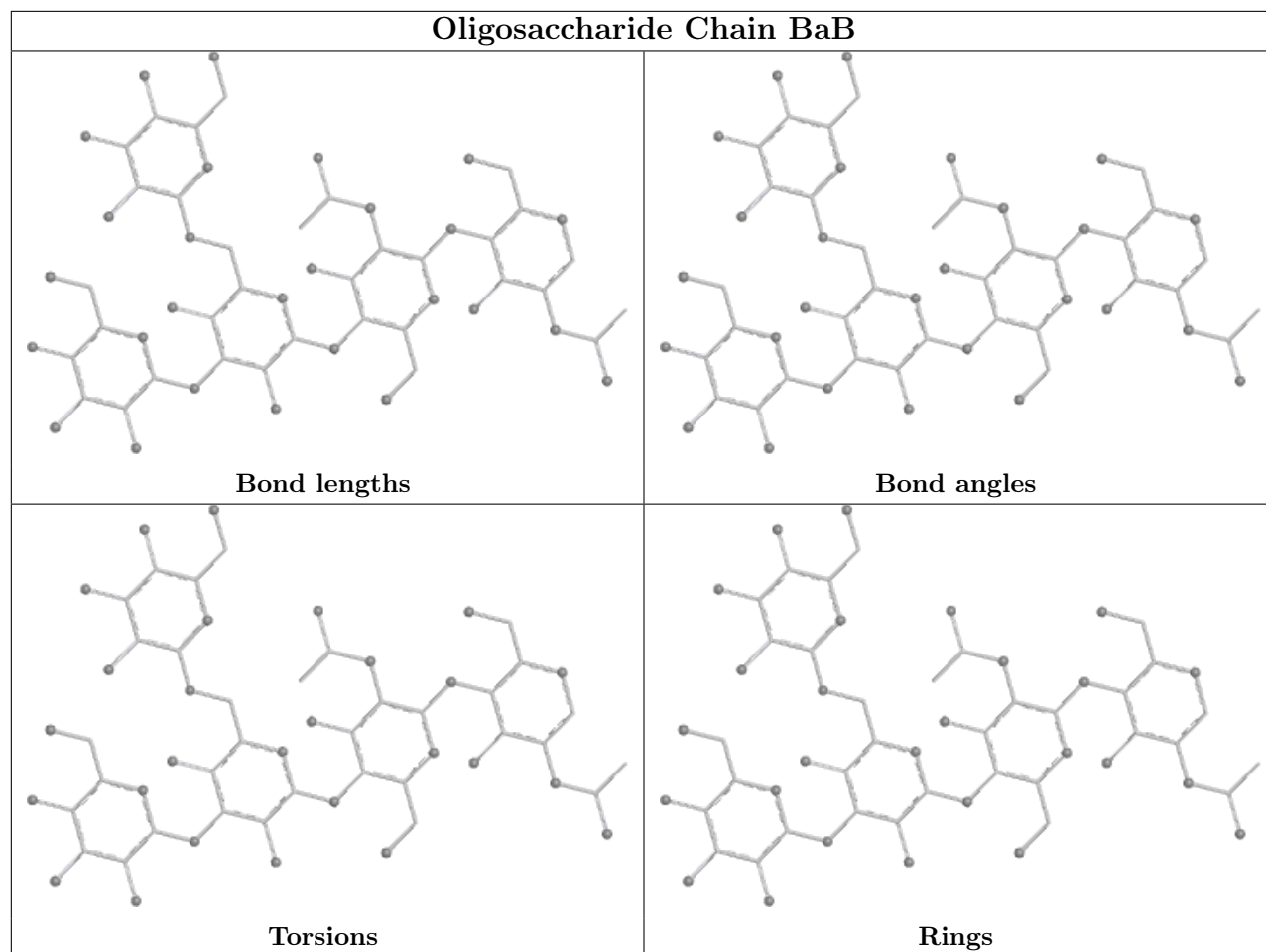
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

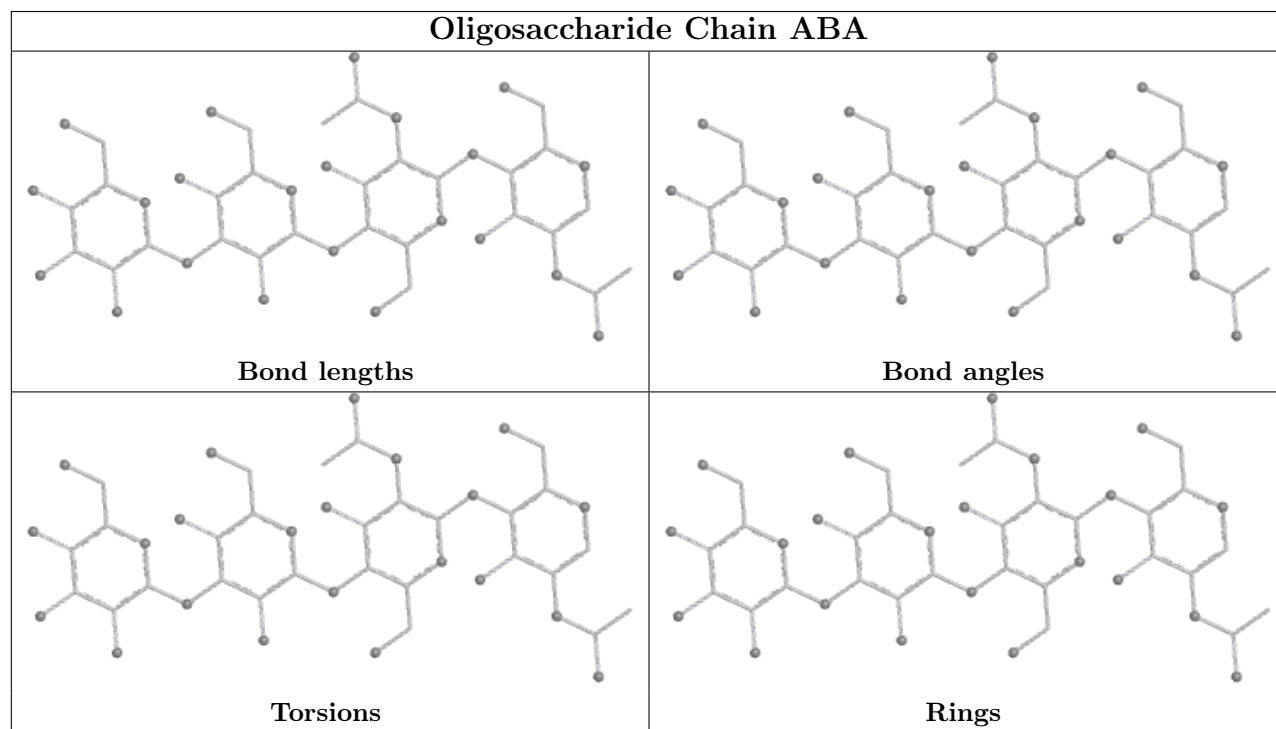
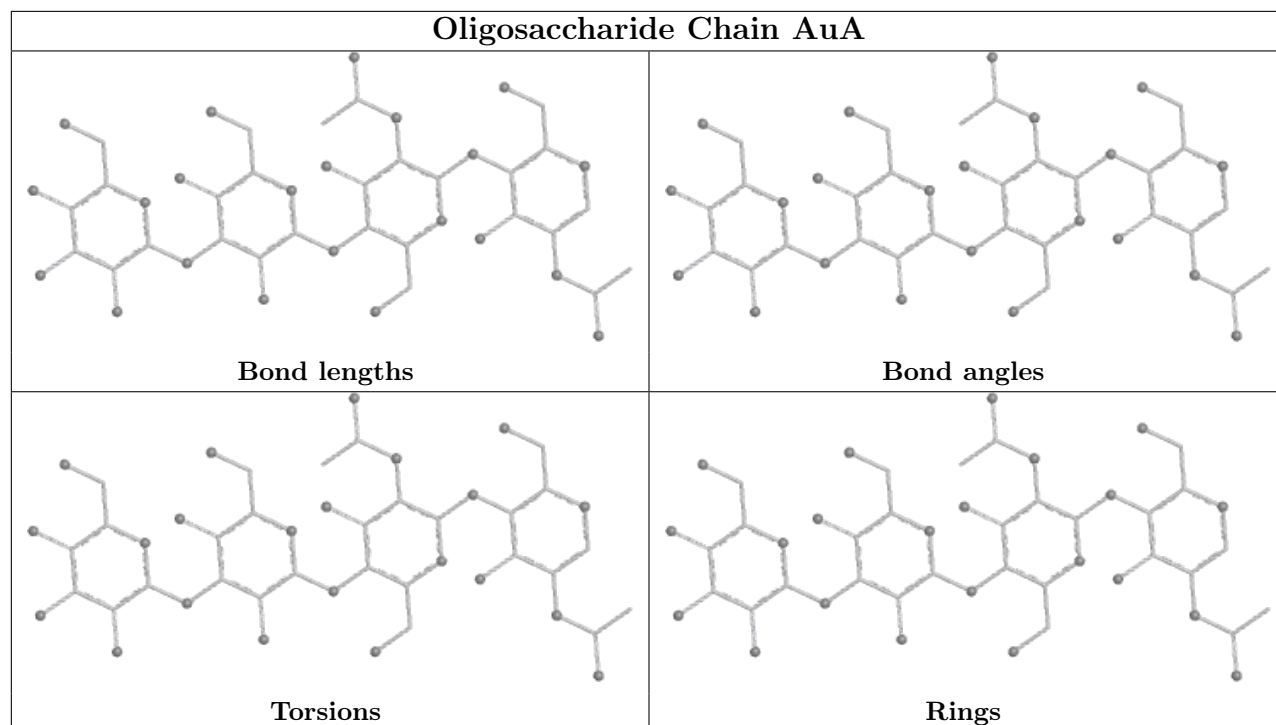


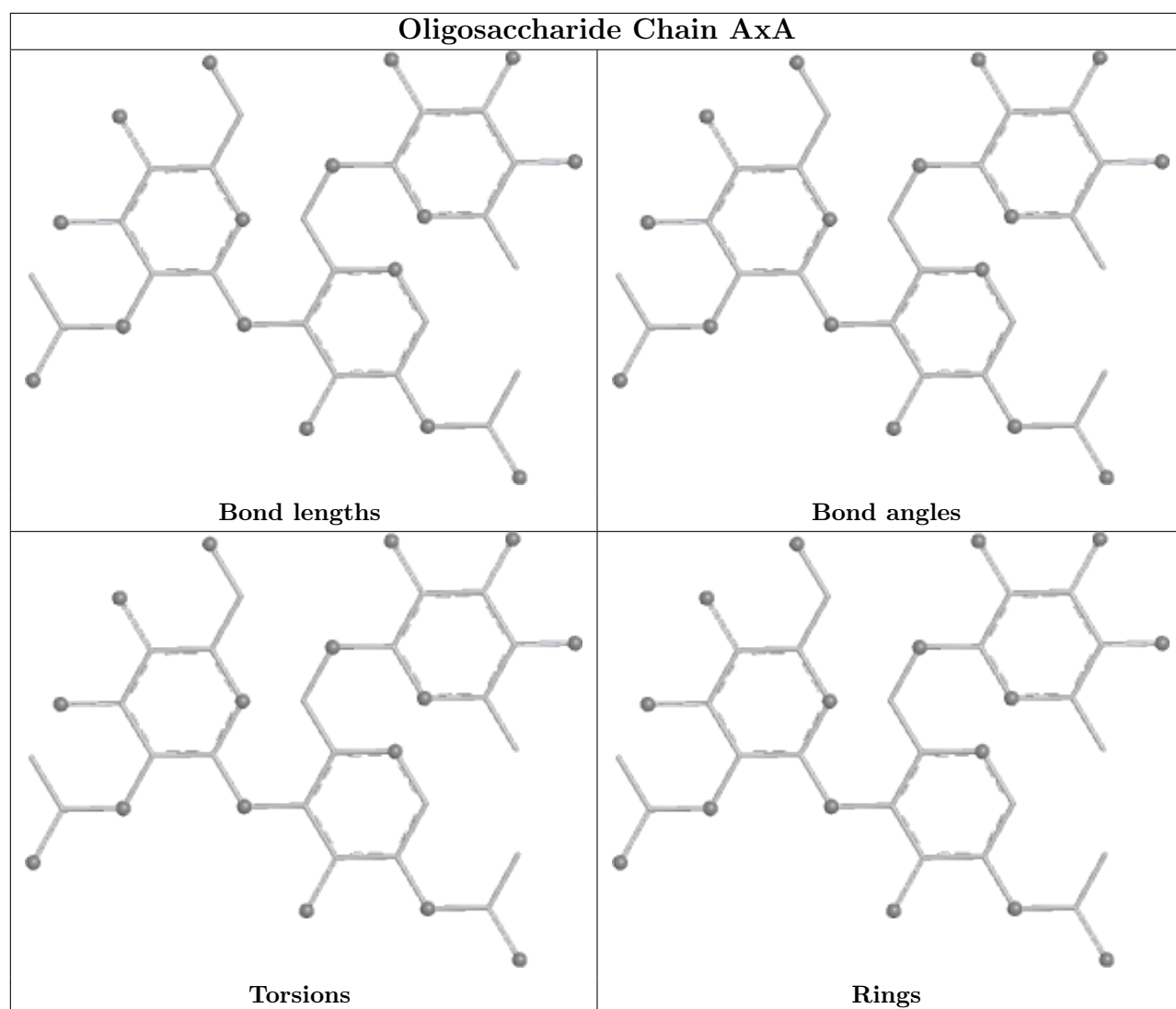


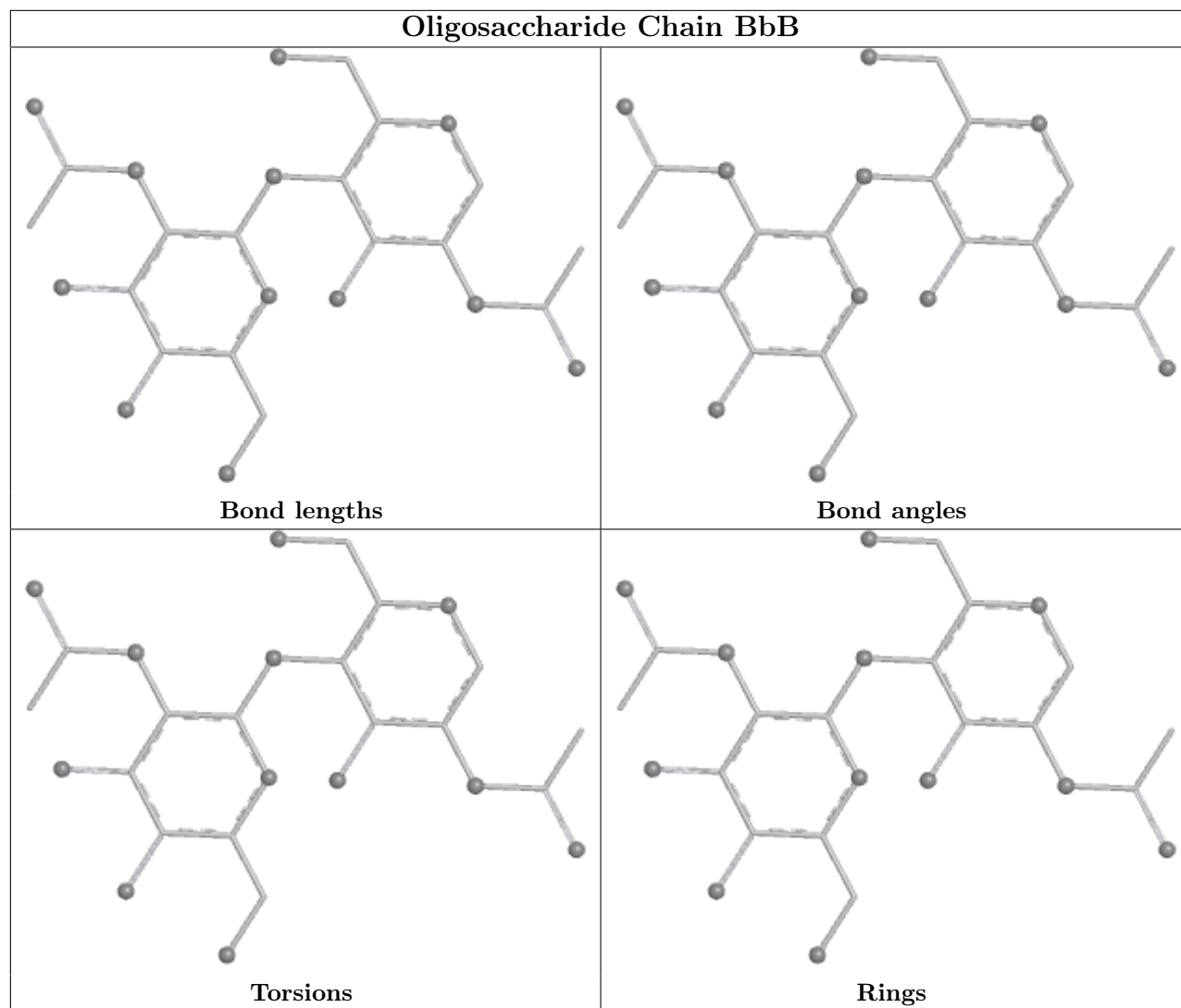


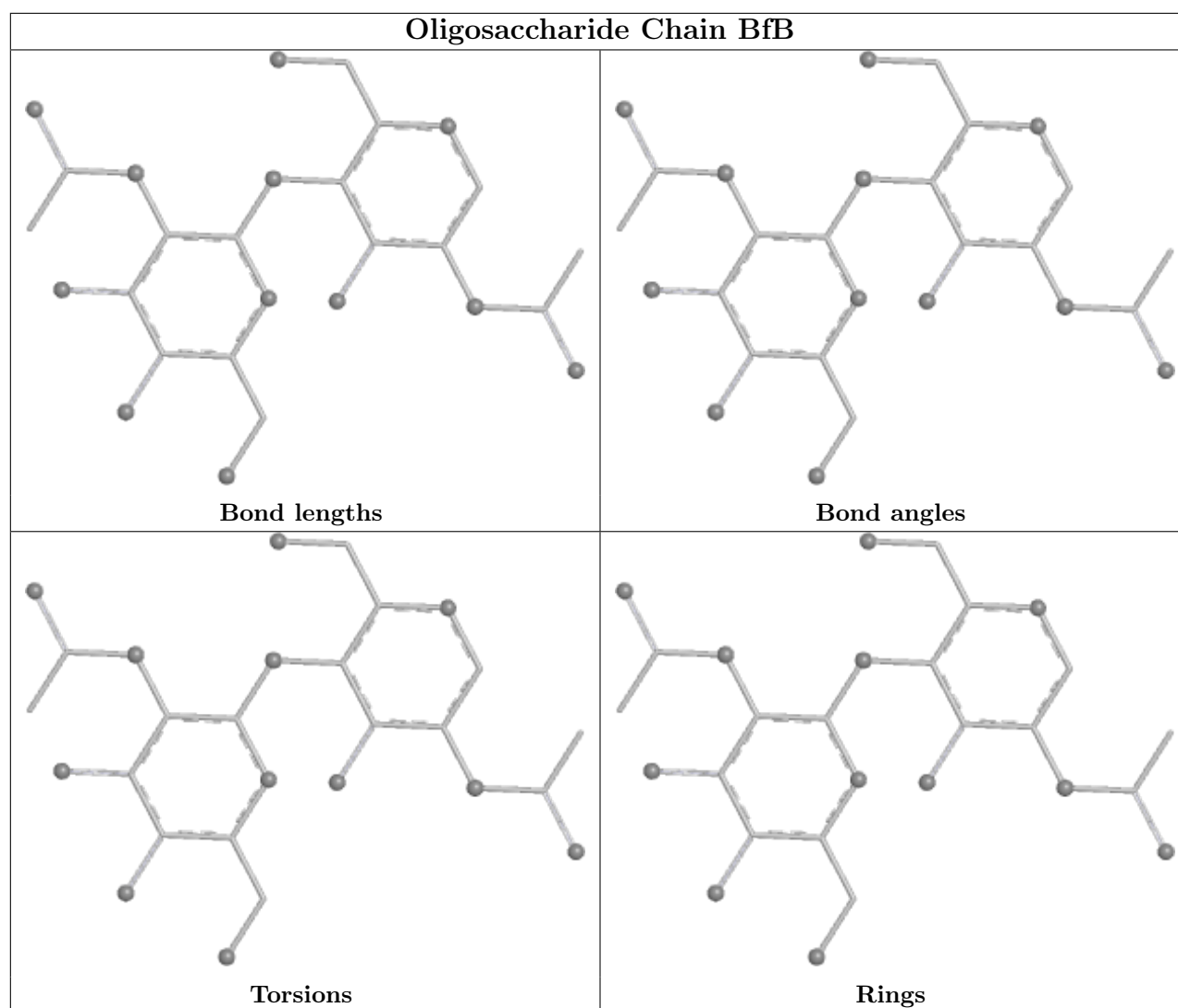












## 5.6 Ligand geometry [i](#)

9 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	$\# Z  > 2$
10	NAG	AAA	702	1	14,14,15	0.65	0	17,19,21	1.39	2 (11%)
11	SO4	AAA	703	-	4,4,4	0.35	0	6,6,6	0.06	0
10	NAG	BBB	301	2	14,14,15	0.27	0	17,19,21	1.25	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	NAG	AAA	701	1	14,14,15	0.40	0	17,19,21	1.25	2 (11%)
11	SO4	AAA	705	-	4,4,4	0.36	0	6,6,6	0.07	0
11	SO4	AAA	706	-	4,4,4	0.36	0	6,6,6	0.08	0
11	SO4	BBB	302	-	4,4,4	0.34	0	6,6,6	0.07	0
11	SO4	AAA	704	-	4,4,4	0.35	0	6,6,6	0.06	0
11	SO4	AAA	707	-	4,4,4	0.35	0	6,6,6	0.08	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
10	NAG	AAA	702	1	-	2/6/23/26	0/1/1/1
10	NAG	AAA	701	1	-	0/6/23/26	0/1/1/1
10	NAG	BBB	301	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	AAA	702	NAG	C1-C2-N2	-3.25	104.93	110.49
10	AAA	702	NAG	C2-N2-C7	3.07	127.28	122.90
10	BBB	301	NAG	C1-O5-C5	2.92	116.15	112.19
10	AAA	701	NAG	C1-C2-N2	2.81	115.28	110.49
10	BBB	301	NAG	O5-C1-C2	-2.73	106.97	111.29
10	AAA	701	NAG	C1-O5-C5	2.42	115.47	112.19
10	BBB	301	NAG	C4-C3-C2	-2.12	107.92	111.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	AAA	702	NAG	C4-C5-C6-O6
10	AAA	702	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

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	595/617 (96%)	-0.23	9 (1%) 73 72	39, 52, 79, 141	0
2	BBB	185/203 (91%)	-0.25	1 (0%) 91 90	41, 58, 74, 95	0
3	CCC	13/14 (92%)	-0.25	0 100 100	43, 46, 73, 76	0
All	All	793/834 (95%)	-0.24	10 (1%) 77 75	39, 53, 76, 141	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	606	CYS	6.2
1	AAA	602	ILE	5.1
1	AAA	604	GLY	4.8
1	AAA	603	LYS	4.6
1	AAA	605	LEU	4.0
1	AAA	12	GLY	3.6
1	AAA	601	ASP	2.5
1	AAA	15	MET	2.3
2	BBB	84[A]	HIS	2.2
1	AAA	599	CYS	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	HYP	CCC	78	8/9	0.98	0.09	40,42,43,43	0



### 6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MAN	ApA	5	11/12	0.27	0.49	127,141,146,147	0
7	MAN	ABA	4	11/12	0.29	0.40	124,140,150,152	0
4	MAN	AaA	4	11/12	0.35	0.40	129,155,163,165	0
7	BMA	AuA	3	11/12	0.47	0.24	142,160,167,169	0
5	MAN	AeA	5	11/12	0.53	0.43	118,135,139,141	0
5	MAN	ApA	4	11/12	0.55	0.29	129,153,156,157	0
5	MAN	BaB	4	11/12	0.61	0.35	119,126,130,131	0
7	MAN	AuA	4	11/12	0.62	0.36	147,166,172,180	0
6	BMA	AmA	3	11/12	0.63	0.31	118,127,132,133	0
7	BMA	ABA	3	11/12	0.64	0.31	147,160,162,167	0
5	MAN	BaB	5	11/12	0.66	0.39	83,96,100,102	0
7	NAG	AuA	2	14/15	0.68	0.28	100,114,125,139	0
5	BMA	ApA	3	11/12	0.69	0.27	133,144,146,150	0
4	BMA	AaA	3	11/12	0.71	0.22	129,156,164,168	0
5	MAN	AeA	4	11/12	0.71	0.34	73,97,106,106	0
8	NAG	AxA	2	14/15	0.71	0.38	112,131,139,142	0
7	NAG	ABA	2	14/15	0.75	0.17	80,97,113,130	0
8	NAG	AxA	1	14/15	0.78	0.20	85,103,123,132	0
5	BMA	AeA	3	11/12	0.78	0.25	110,118,122,124	0
8	FUC	AxA	3	10/11	0.80	0.43	102,112,119,121	0
4	FUC	AaA	5	10/11	0.81	0.30	109,114,117,123	0
5	BMA	BaB	3	11/12	0.81	0.39	101,107,118,128	0
9	NAG	BfB	2	14/15	0.81	0.22	78,107,116,117	0
6	NAG	AmA	2	14/15	0.84	0.18	79,92,101,114	0
4	NAG	AaA	2	14/15	0.88	0.12	87,100,113,136	0
4	FUC	AaA	6	10/11	0.88	0.20	75,88,93,94	0
9	NAG	BbB	2	14/15	0.88	0.27	81,96,100,103	0
5	NAG	AeA	2	14/15	0.88	0.16	72,99,106,114	0
7	NAG	AuA	1	14/15	0.89	0.12	66,76,82,92	0
9	NAG	BbB	1	14/15	0.89	0.14	73,77,87,91	0
9	NAG	BfB	1	14/15	0.90	0.14	63,72,78,88	0
4	NAG	AaA	1	14/15	0.90	0.08	59,67,82,86	0
5	NAG	BaB	1	14/15	0.91	0.17	70,76,92,95	0
5	NAG	ApA	2	14/15	0.92	0.18	82,89,98,108	0
6	NAG	AmA	1	14/15	0.93	0.11	56,63,68,76	0
5	NAG	ApA	1	14/15	0.94	0.13	49,53,56,60	0
5	NAG	BaB	2	14/15	0.94	0.28	84,92,98,103	0

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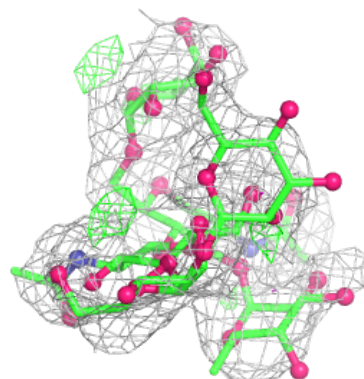
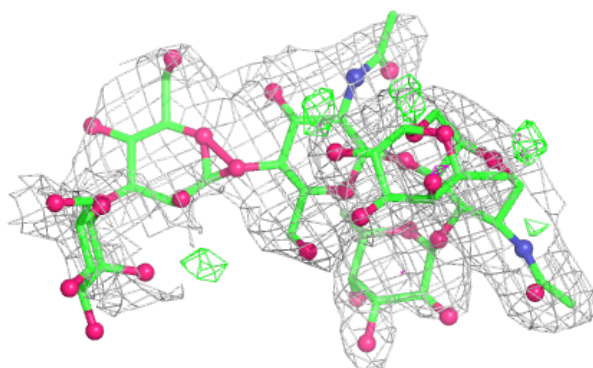
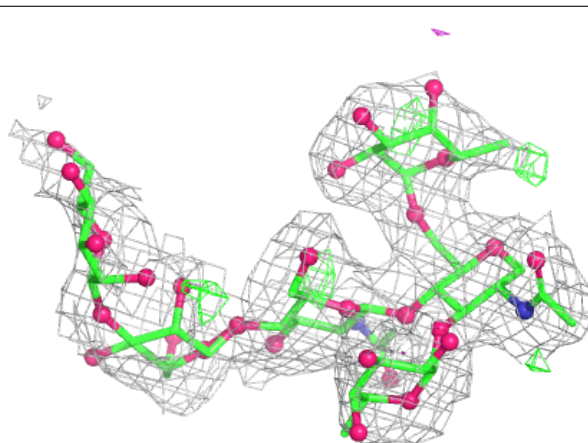
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	AeA	1	14/15	0.96	0.09	52,57,67,75	0
7	NAG	ABA	1	14/15	0.96	0.09	54,62,68,78	0

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.

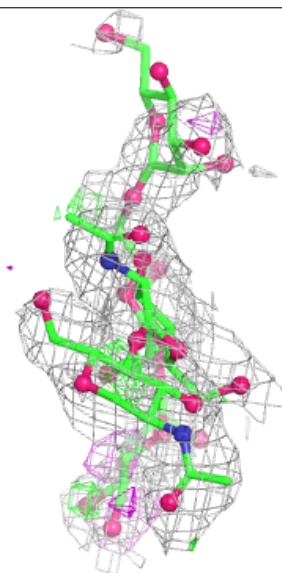
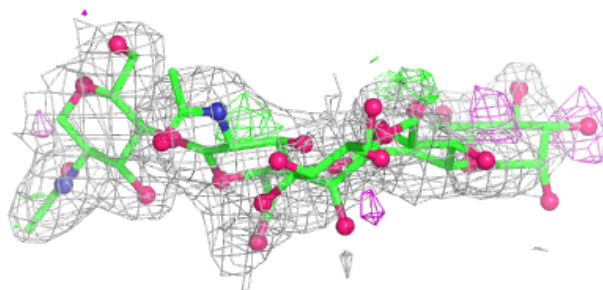
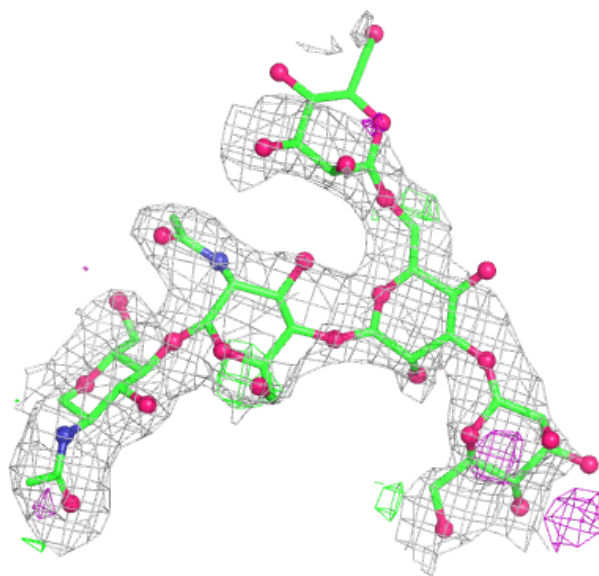
**Electron density around Chain AaA:**

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



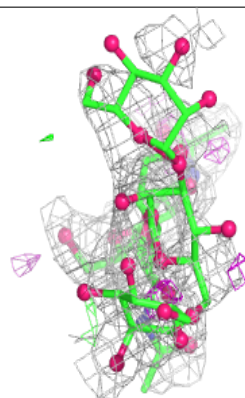
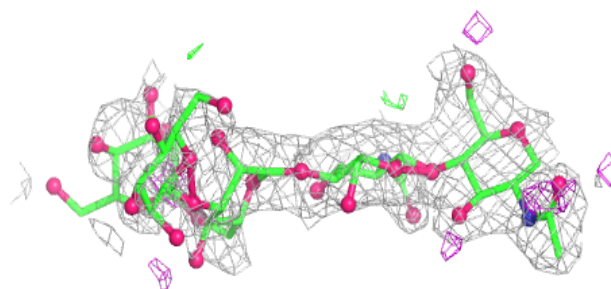
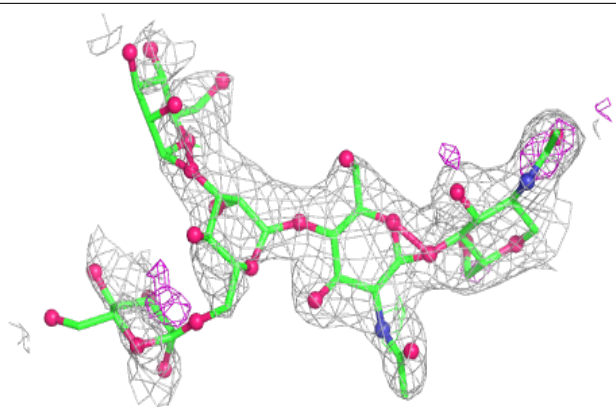
**Electron density around Chain AeA:**

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



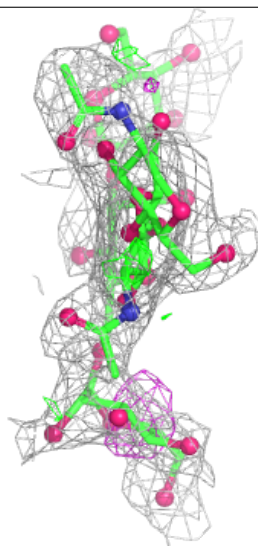
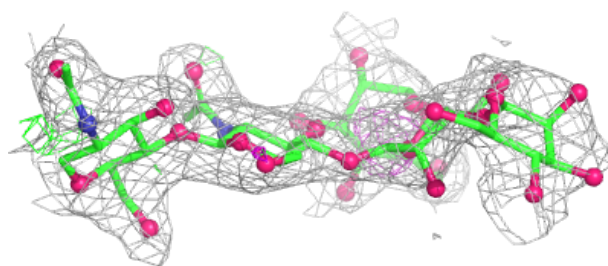
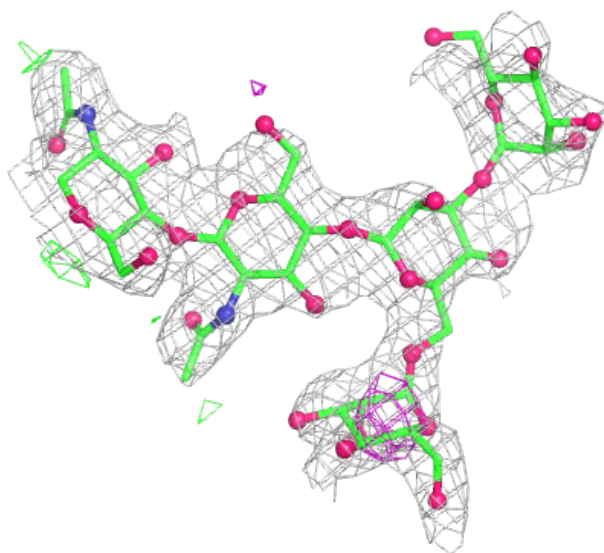
**Electron density around Chain ApA:**

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



**Electron density around Chain BaB:**

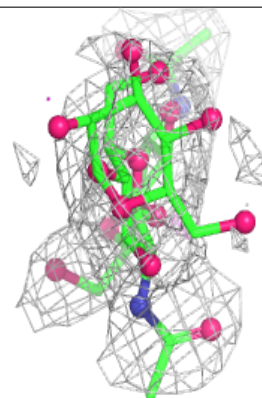
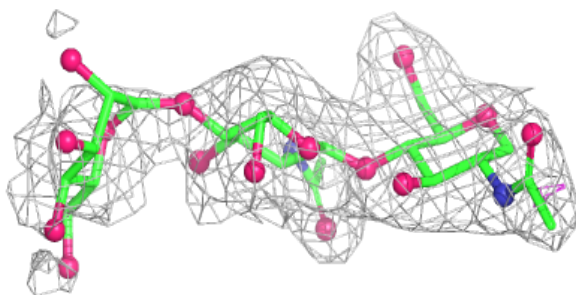
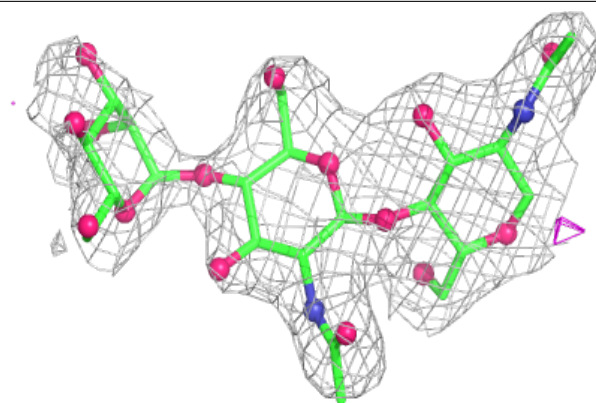
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



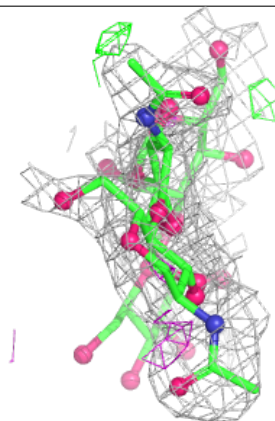
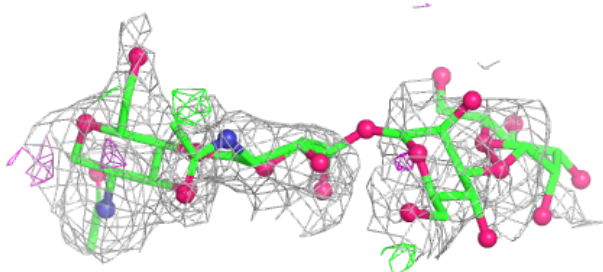
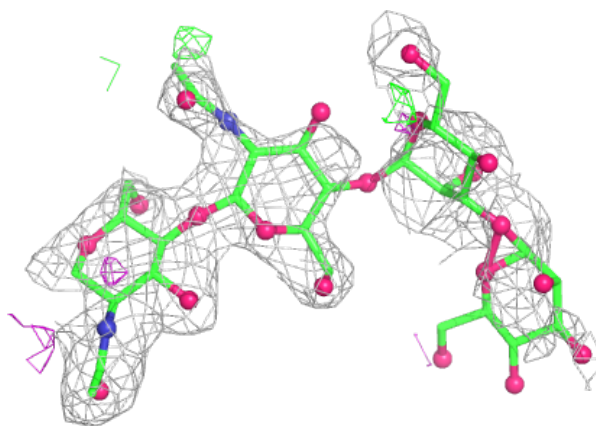


**Electron density around Chain AmA:**

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

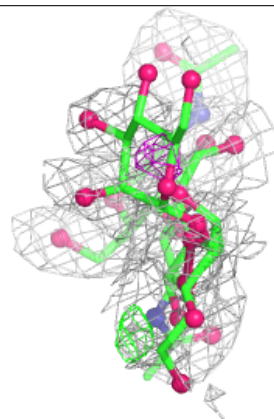
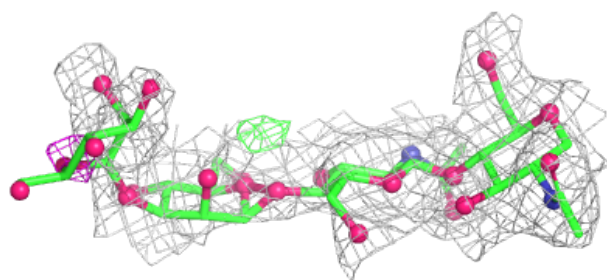
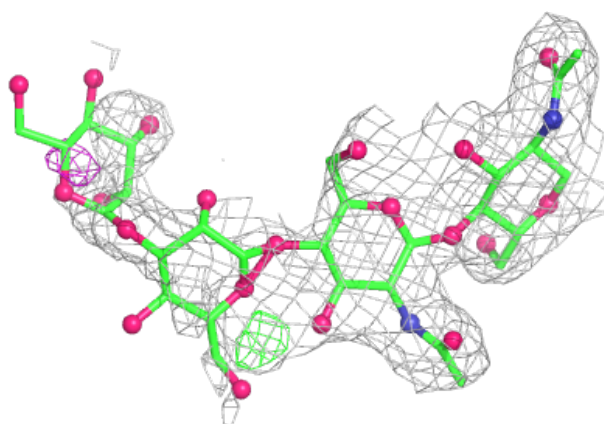
**Electron density around Chain AuA:**

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



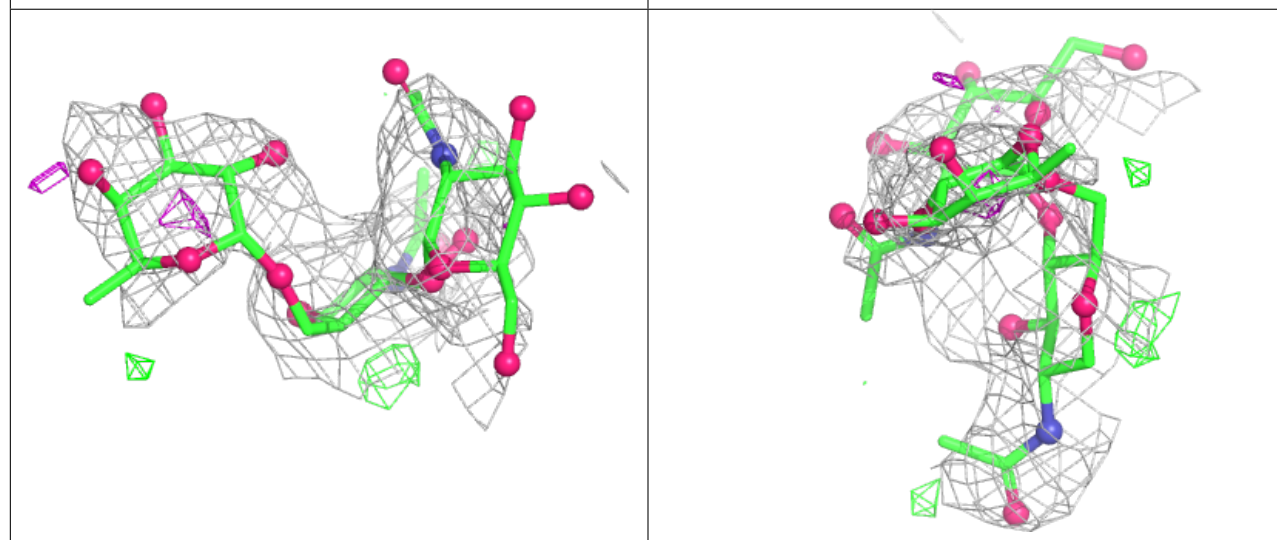
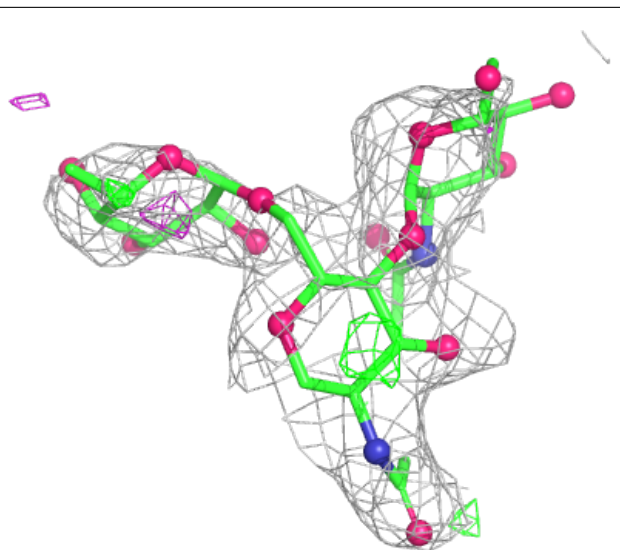
**Electron density around Chain ABA:**

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



**Electron density around Chain AxA:**

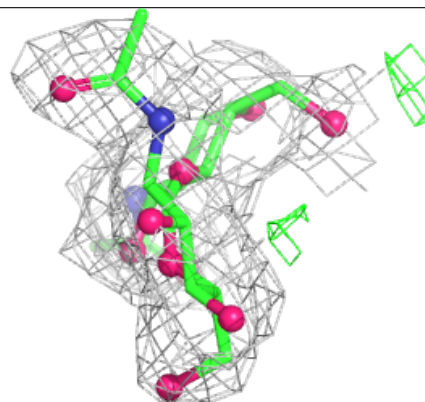
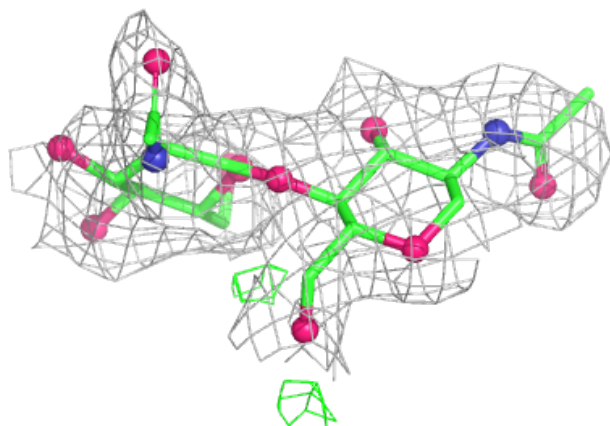
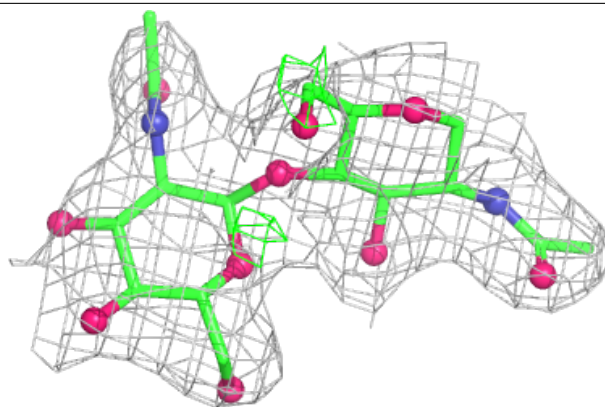
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
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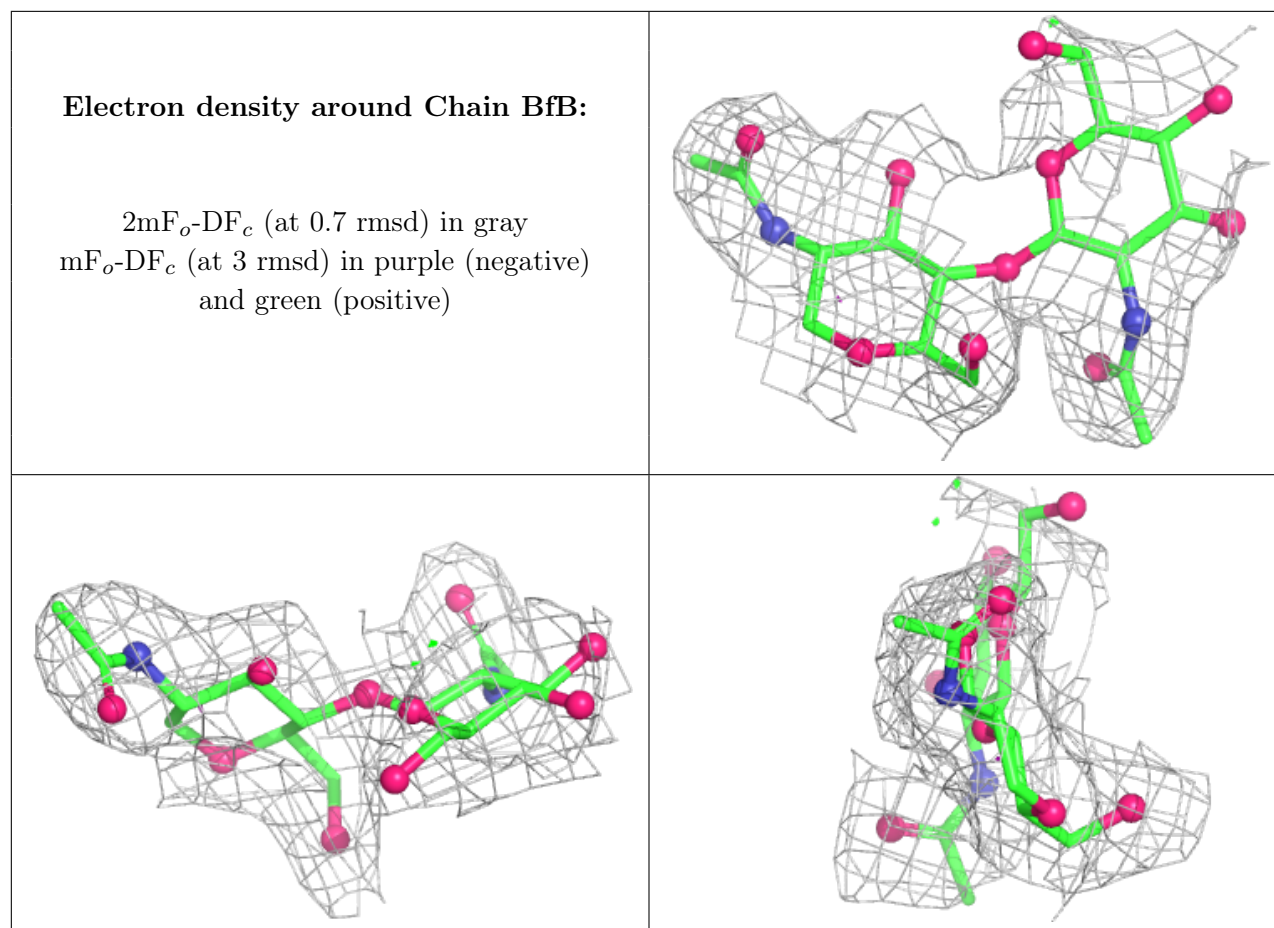




**Electron density around Chain BbB:**

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





## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
10	NAG	AAA	702	14/15	0.67	0.33	70,94,104,108	0
11	SO4	AAA	705	5/5	0.67	0.28	102,117,124,130	0
10	NAG	BBB	301	14/15	0.84	0.20	82,91,95,101	0
11	SO4	AAA	706	5/5	0.87	0.16	109,110,122,123	0
11	SO4	AAA	707	5/5	0.88	0.29	78,100,105,106	0
11	SO4	BBB	302	5/5	0.88	0.29	108,115,120,123	0
11	SO4	AAA	703	5/5	0.89	0.16	89,101,108,110	0
10	NAG	AAA	701	14/15	0.92	0.10	61,64,76,77	0
11	SO4	AAA	704	5/5	0.99	0.06	77,80,81,85	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.