



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 2, 2025 – 01:18 pm BST

PDB ID : 9S80 / pdb\_00009s80  
Title : Crystal structure of the BRL3 ectodomain from Arabidopsis thaliana in complex with brassinolide.  
Authors : Hohmann, U.; Hothorn, M.  
Deposited on : 2025-08-05  
Resolution : 2.45 Å(reported)

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

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

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<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  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

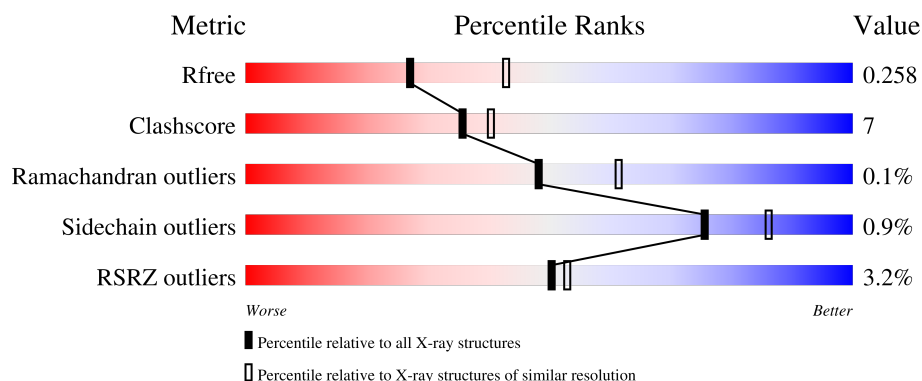
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	1096 (2.46-2.46)
Clashscore	180529	1178 (2.46-2.46)
Ramachandran outliers	177936	1170 (2.46-2.46)
Sidechain outliers	177891	1170 (2.46-2.46)
RSRZ outliers	164620	1096 (2.46-2.46)

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	A	770	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>13%</div> <div>6%</div> </div> </div>
1	B	770	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>6%</div> </div> </div>
2	C	2	<div> <div>50%</div> <div>50%</div> </div>
2	D	2	<div> <div>50%</div> <div>50%</div> </div>
2	E	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	2	 100%
2	J	2	 100%
2	K	2	 50% 50%
2	L	2	 100%
2	M	2	 100%
2	P	2	 50% 50%
2	R	2	 100%
2	S	2	 100%
2	T	2	 100%
3	F	11	 9% 73% 18%
3	N	11	 18% 82%
4	G	3	 33% 67%
4	O	3	 33% 67%
5	I	3	 33% 67%
5	Q	3	 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
12	ACT	B	808	-	-	X	-

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 23739 atoms, of which 11699 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 BRI1-like 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	721	Total	C	H	N	O	S	0	4	0
			10775	3396	5367	909	1075	28			
1	B	727	Total	C	H	N	O	S	0	7	0
			10908	3436	5436	924	1083	29			

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



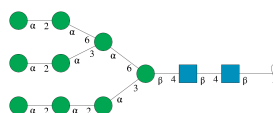
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
2	D	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
2	E	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
2	H	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
2	J	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
2	K	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
2	L	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
2	M	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
2	P	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
2	R	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

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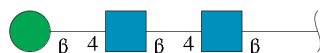
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
2	T	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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.



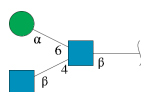
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	11	Total	C	H	N	O	0	0	0
			233	70	106	2	55			
3	N	11	Total	C	H	N	O	0	0	0
			233	70	106	2	55			

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



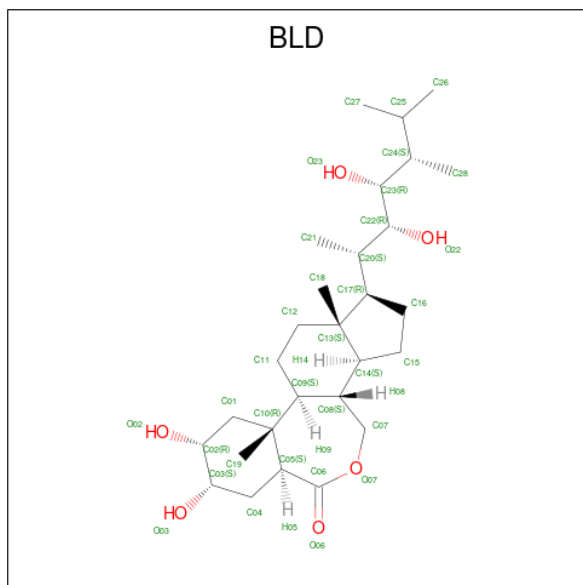
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	3	Total	C	H	N	O	0	0	0
			73	22	34	2	15			
4	O	3	Total	C	H	N	O	0	0	0
			73	22	34	2	15			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-D-mannopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	3	Total	C	H	N	O	0	0	0
			73	22	34	2	15			
5	Q	3	Total	C	H	N	O	0	0	0
			73	22	34	2	15			

- Molecule 6 is Brassinolide (CCD ID: BLD) (formula:  $C_{28}H_{48}O_6$ ).



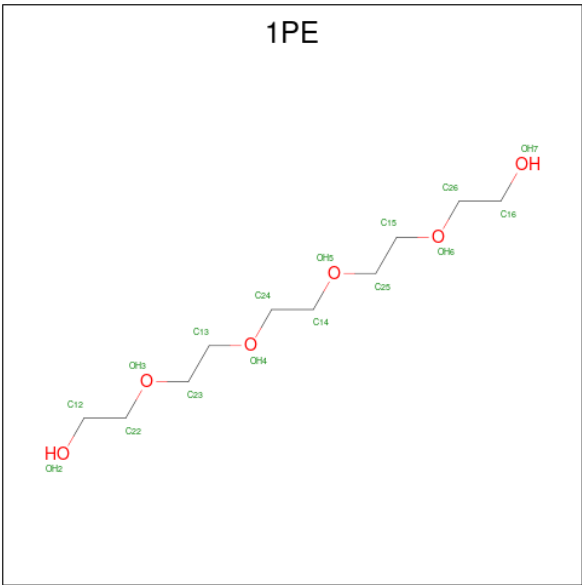
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	O		0	0
			82	28	48	6			
6	B	1	Total	C	H	O		0	0
			82	28	48	6			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



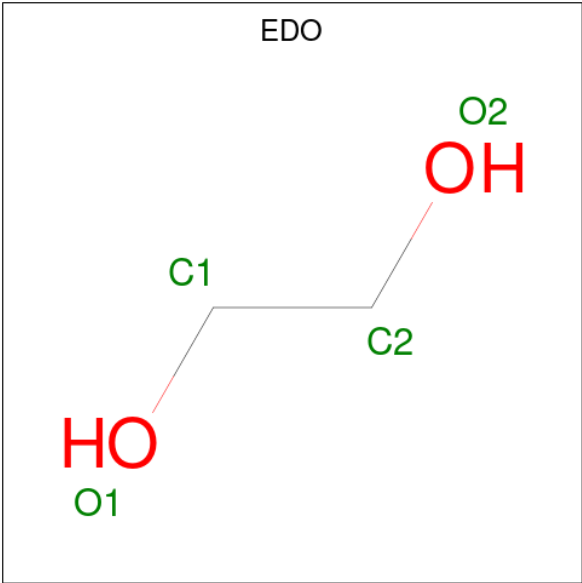
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
7	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
7	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
7	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
7	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
7	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
7	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 8 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			38	10	22	6		
8	B	1	Total	C	H	O	0	0
			38	10	22	6		

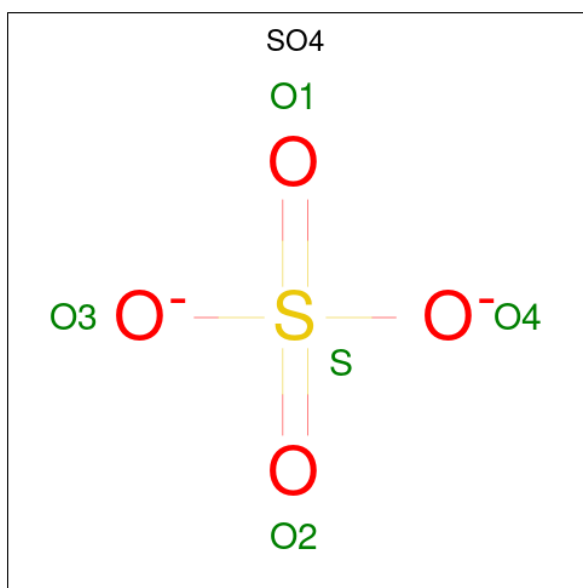
- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			10	2	6	2		
9	B	1	Total	C	H	O	0	0
			10	2	6	2		

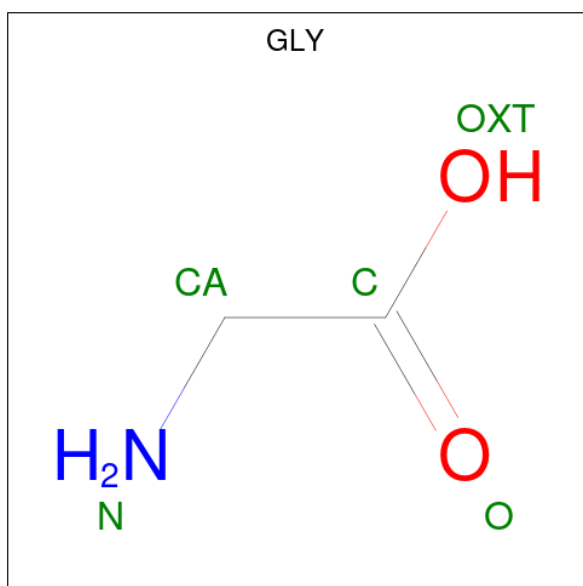


- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



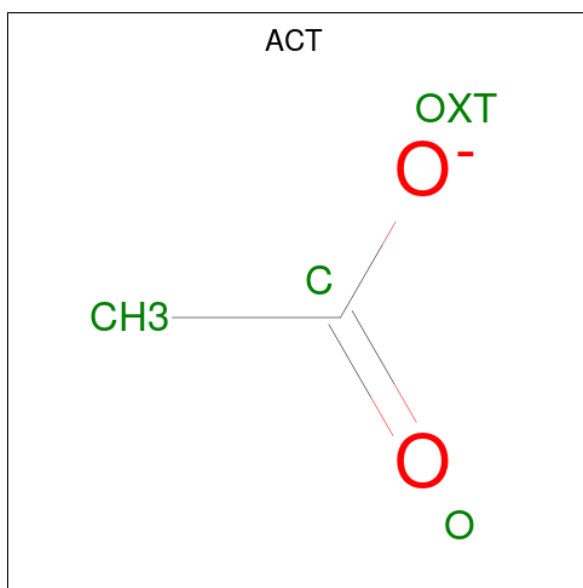
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 11 is GLYCINE (CCD ID: GLY) (formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	H	N	O	0	0
			6	2	2	1	1		

- Molecule 12 is ACETATE ION (CCD ID: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	H	O	0	0
			7	2	3	2		

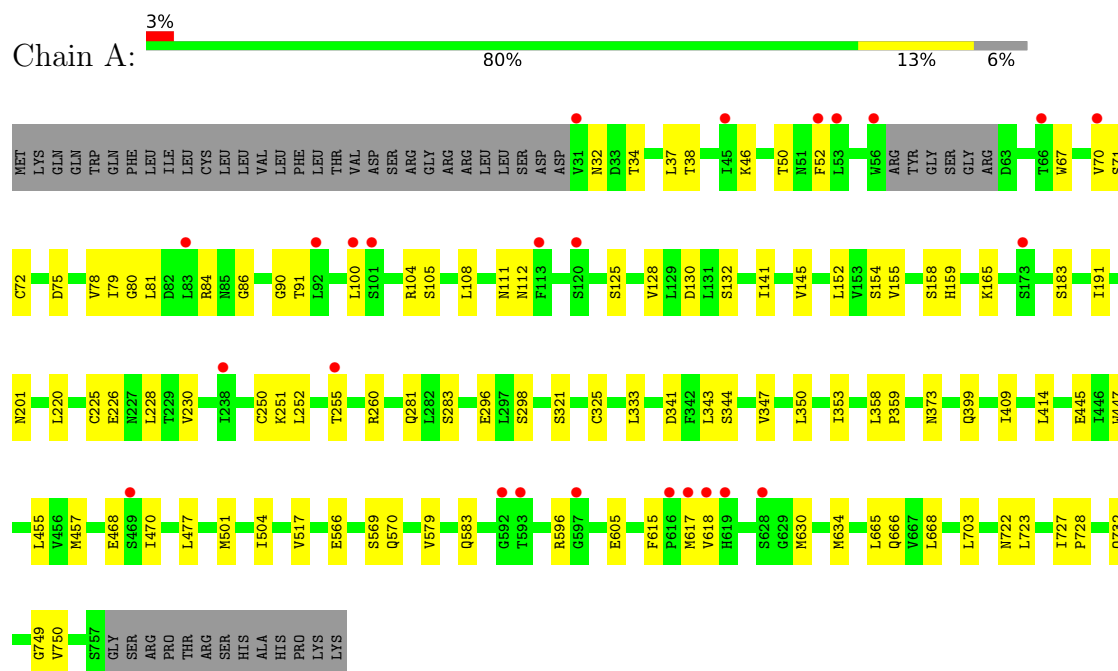
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	94	Total	O	0	0
			94	94		
13	B	96	Total	O	0	0
			96	96		

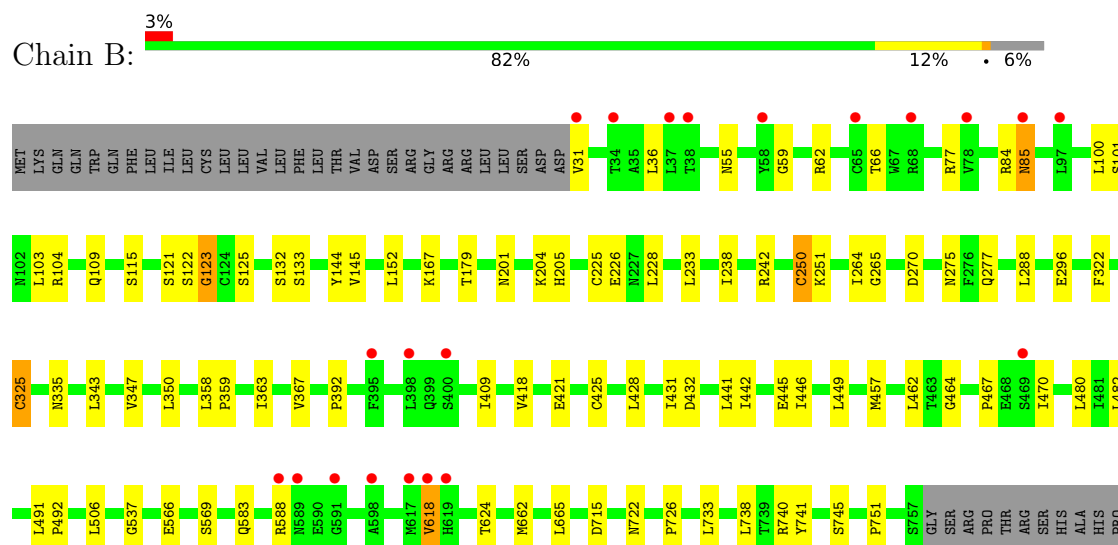
### 3 Residue-property plots [i](#)

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 BRI1-like 3



- Molecule 1: Receptor-like protein kinase BRI1-like 3



LYS  
LYS

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

Chain C:  50% 50%NAG1  
NAG2

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

Chain D:  50% 50%NAG1  
NAG2

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

Chain E:  50% 50%NAG1  
NAG2

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

Chain H:  100%NAG1  
NAG2

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

Chain J:  100%NAG1  
NAG2

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

Chain K:  50% 50%NAG1  
NAG2

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

Chain L:  100%

MAG1  
MAG2

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

Chain M:  100%

MAG1  
MAG2

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

Chain P:  50%  50%

MAG1  
MAG2

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

Chain R:  100%

MAG1  
MAG2

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

Chain S:  100%

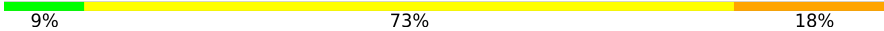
MAG1  
MAG2

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

Chain T:  100%

MAG1  
MAG2

- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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 F:  9% 73% 18%



- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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 N:  18% 82%




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

Chain G:  33% 67%



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

Chain O:  33% 67%



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

Chain I:  33% 67%



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

Chain Q:  100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.46Å 81.76Å 122.19Å 107.24° 91.94° 112.39°	Depositor
Resolution (Å)	48.66 – 2.45 48.66 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.66-2.45) 98.0 (48.66-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.222 , 0.258 0.222 , 0.258	Depositor DCC
$R_{free}$ test set	3668 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.8	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 38.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	23739	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4, 1PE, MAN, BLD, ACT, BMA, EDO

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	A	0.16	0/5516	0.35	0/7495
1	B	0.16	0/5588	0.35	0/7592
All	All	0.16	0/11104	0.35	0/15087

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

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	A	5408	5367	5355	84	0
1	B	5472	5436	5432	79	0
2	C	28	25	25	1	0
2	D	28	25	25	1	0
2	E	28	25	25	0	0
2	H	28	25	25	2	0
2	J	28	25	25	0	0
2	K	28	25	25	1	0
2	L	28	25	25	0	0
2	M	28	25	25	0	0
2	P	28	25	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	28	25	25	1	0
2	S	28	25	25	0	0
2	T	28	25	25	0	0
3	F	127	106	106	2	0
3	N	127	106	106	0	0
4	G	39	34	34	0	0
4	O	39	34	34	0	0
5	I	39	34	34	1	0
5	Q	39	34	34	0	0
6	A	34	48	48	0	0
6	B	34	48	48	1	0
7	A	56	52	52	2	0
7	B	42	39	39	3	0
8	A	16	22	22	1	0
8	B	16	22	22	0	0
9	A	4	6	6	0	0
9	B	4	6	6	0	0
10	A	5	0	0	0	0
10	B	5	0	0	0	0
11	B	4	2	2	0	0
12	B	4	3	3	2	0
13	A	94	0	0	8	0
13	B	96	0	0	8	0
All	All	12040	11699	11683	170	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 7.

The worst 5 of 170 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:A:32:ASN:OD1	1:A:34:THR:OG1	1.81	0.97
1:B:343:LEU:HD11	1:B:358:LEU:HD13	1.60	0.82
1:A:296:GLU:N	1:A:296:GLU:OE1	2.13	0.81
1:B:77:ARG:NH1	1:B:101:SER:OG	2.13	0.81
1:B:715:ASP:OD1	1:B:740:ARG:NH2	2.14	0.81

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	A	721/770 (94%)	663 (92%)	58 (8%)	0	100	100
1	B	732/770 (95%)	661 (90%)	70 (10%)	1 (0%)	48	61
All	All	1453/1540 (94%)	1324 (91%)	128 (9%)	1 (0%)	48	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	123	GLY

### 5.3.2 Protein sidechains [i](#)

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	A	633/673 (94%)	630 (100%)	3 (0%)	86	92
1	B	639/673 (95%)	629 (98%)	10 (2%)	58	72
All	All	1272/1346 (94%)	1259 (99%)	13 (1%)	75	83

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	250[B]	CYS
1	B	325[A]	CYS
1	B	722	ASN
1	B	409	ILE
1	B	618	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	589	ASN
1	B	614	HIS
1	A	538	ASN
1	A	583	GLN
1	B	278	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

58 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	$\# Z  > 2$
2	NAG	C	1	1,2	14,14,15	0.66	0	17,19,21	0.84	0
2	NAG	C	2	2	14,14,15	0.73	0	17,19,21	1.49	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.72	0	17,19,21	1.13	1 (5%)
2	NAG	D	2	2	14,14,15	0.66	0	17,19,21	0.96	0
2	NAG	E	1	1,2	14,14,15	0.66	0	17,19,21	1.02	0
2	NAG	E	2	2	14,14,15	0.65	0	17,19,21	1.18	1 (5%)
3	NAG	F	1	3,1	14,14,15	0.65	0	17,19,21	1.48	3 (17%)
3	MAN	F	10	3	11,11,12	0.84	1 (9%)	15,15,17	0.98	1 (6%)
3	MAN	F	11	3	11,11,12	0.78	0	15,15,17	1.14	1 (6%)
3	NAG	F	2	3	14,14,15	0.80	1 (7%)	17,19,21	1.23	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BMA	F	3	3	11,11,12	0.76	0	15,15,17	2.39	5 (33%)
3	MAN	F	4	3	11,11,12	0.81	0	15,15,17	0.91	1 (6%)
3	MAN	F	5	3	11,11,12	0.99	1 (9%)	15,15,17	1.17	1 (6%)
3	MAN	F	6	3	11,11,12	0.77	0	15,15,17	1.01	0
3	MAN	F	7	3	11,11,12	0.85	1 (9%)	15,15,17	1.07	1 (6%)
3	MAN	F	8	3	11,11,12	1.00	1 (9%)	15,15,17	0.92	0
3	MAN	F	9	3	11,11,12	0.85	1 (9%)	15,15,17	1.02	1 (6%)
4	NAG	G	1	4,1	14,14,15	0.66	0	17,19,21	0.95	0
4	NAG	G	2	4	14,14,15	0.72	0	17,19,21	1.03	1 (5%)
4	BMA	G	3	4	11,11,12	0.72	0	15,15,17	2.60	5 (33%)
2	NAG	H	1	1,2	14,14,15	0.75	0	17,19,21	1.06	1 (5%)
2	NAG	H	2	2	14,14,15	0.69	0	17,19,21	1.12	1 (5%)
5	NAG	I	1	1,5	14,14,15	0.79	0	17,19,21	1.04	0
5	NAG	I	2	5	14,14,15	0.81	0	17,19,21	1.00	1 (5%)
5	MAN	I	3	5	11,11,12	0.80	0	15,15,17	0.97	1 (6%)
2	NAG	J	1	1,2	14,14,15	0.65	0	17,19,21	1.61	4 (23%)
2	NAG	J	2	2	14,14,15	0.71	0	17,19,21	1.19	2 (11%)
2	NAG	K	1	1,2	14,14,15	0.64	0	17,19,21	1.35	2 (11%)
2	NAG	K	2	2	14,14,15	0.70	0	17,19,21	1.18	3 (17%)
2	NAG	L	1	1,2	14,14,15	0.66	0	17,19,21	1.18	1 (5%)
2	NAG	L	2	2	14,14,15	0.65	0	17,19,21	1.14	1 (5%)
2	NAG	M	1	1,2	14,14,15	0.69	0	17,19,21	1.05	1 (5%)
2	NAG	M	2	2	14,14,15	0.68	0	17,19,21	1.10	1 (5%)
3	NAG	N	1	3,1	14,14,15	0.68	0	17,19,21	1.34	2 (11%)
3	MAN	N	10	3	11,11,12	0.76	0	15,15,17	1.43	1 (6%)
3	MAN	N	11	3	11,11,12	0.81	0	15,15,17	0.93	0
3	NAG	N	2	3	14,14,15	0.65	0	17,19,21	1.24	2 (11%)
3	BMA	N	3	3	11,11,12	0.87	0	15,15,17	2.04	5 (33%)
3	MAN	N	4	3	11,11,12	0.84	1 (9%)	15,15,17	1.24	3 (20%)
3	MAN	N	5	3	11,11,12	0.86	0	15,15,17	1.15	2 (13%)
3	MAN	N	6	3	11,11,12	0.71	0	15,15,17	1.09	0
3	MAN	N	7	3	11,11,12	0.90	1 (9%)	15,15,17	1.10	2 (13%)
3	MAN	N	8	3	11,11,12	0.80	0	15,15,17	1.20	1 (6%)
3	MAN	N	9	3	11,11,12	0.86	1 (9%)	15,15,17	0.90	0
4	NAG	O	1	4,1	14,14,15	0.69	0	17,19,21	1.04	1 (5%)
4	NAG	O	2	4	14,14,15	0.73	0	17,19,21	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BMA	O	3	4	11,11,12	0.70	0	15,15,17	2.67	6 (40%)
2	NAG	P	1	1,2	14,14,15	0.67	0	17,19,21	0.99	0
2	NAG	P	2	2	14,14,15	0.65	0	17,19,21	1.05	1 (5%)
5	NAG	Q	1	1,5	14,14,15	0.79	0	17,19,21	0.91	1 (5%)
5	NAG	Q	2	5	14,14,15	0.77	0	17,19,21	1.10	1 (5%)
5	MAN	Q	3	5	11,11,12	0.80	1 (9%)	15,15,17	0.85	0
2	NAG	R	1	1,2	14,14,15	0.84	1 (7%)	17,19,21	1.22	2 (11%)
2	NAG	R	2	2	14,14,15	0.70	0	17,19,21	1.32	1 (5%)
2	NAG	S	1	1,2	14,14,15	0.88	1 (7%)	17,19,21	1.93	5 (29%)
2	NAG	S	2	2	14,14,15	0.74	0	17,19,21	1.14	1 (5%)
2	NAG	T	1	1,2	14,14,15	0.62	0	17,19,21	1.19	1 (5%)
2	NAG	T	2	2	14,14,15	0.76	0	17,19,21	1.32	2 (11%)

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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	MAN	F	10	3	-	0/2/19/22	0/1/1/1
3	MAN	F	11	3	-	0/2/19/22	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
3	MAN	F	6	3	-	0/2/19/22	0/1/1/1
3	MAN	F	7	3	-	0/2/19/22	0/1/1/1
3	MAN	F	8	3	-	2/2/19/22	0/1/1/1
3	MAN	F	9	3	-	0/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	H	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	H	2	2	-	1/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	MAN	I	3	5	-	0/2/19/22	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	NAG	L	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	0/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	2/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	2/6/23/26	0/1/1/1
3	MAN	N	10	3	-	2/2/19/22	0/1/1/1
3	MAN	N	11	3	-	0/2/19/22	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	BMA	N	3	3	-	0/2/19/22	0/1/1/1
3	MAN	N	4	3	-	2/2/19/22	0/1/1/1
3	MAN	N	5	3	-	0/2/19/22	0/1/1/1
3	MAN	N	6	3	-	0/2/19/22	0/1/1/1
3	MAN	N	7	3	-	0/2/19/22	0/1/1/1
3	MAN	N	8	3	-	2/2/19/22	0/1/1/1
3	MAN	N	9	3	-	2/2/19/22	0/1/1/1
4	NAG	O	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	BMA	O	3	4	-	0/2/19/22	0/1/1/1
2	NAG	P	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	P	2	2	-	1/6/23/26	0/1/1/1
5	NAG	Q	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/23/26	0/1/1/1
5	MAN	Q	3	5	-	1/2/19/22	0/1/1/1
2	NAG	R	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	R	2	2	-	2/6/23/26	0/1/1/1
2	NAG	S	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	S	2	2	-	0/6/23/26	0/1/1/1
2	NAG	T	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	T	2	2	-	1/6/23/26	0/1/1/1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	5	MAN	O5-C1	-2.61	1.39	1.43
3	F	8	MAN	O5-C1	-2.57	1.39	1.43
3	F	2	NAG	O5-C1	-2.33	1.40	1.43
2	R	1	NAG	O5-C1	-2.25	1.40	1.43
3	F	7	MAN	O5-C1	-2.19	1.40	1.43

The worst 5 of 84 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	3	BMA	C1-O5-C5	7.92	122.93	112.19
4	G	3	BMA	C1-O5-C5	7.55	122.42	112.19
3	F	3	BMA	C1-O5-C5	6.67	121.23	112.19
3	N	3	BMA	C1-O5-C5	5.30	119.37	112.19
2	C	2	NAG	C2-N2-C7	4.79	129.72	122.90

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

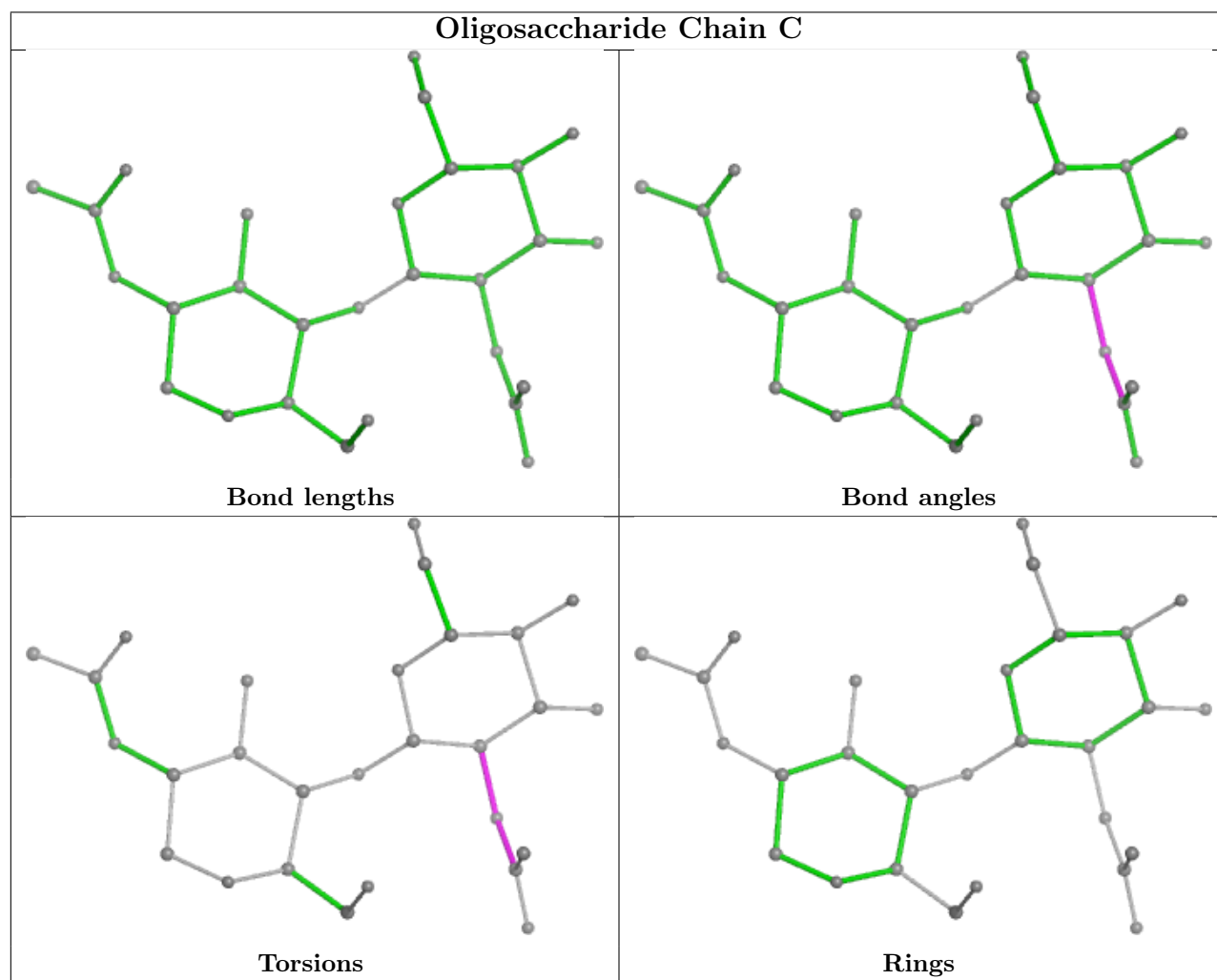
Mol	Chain	Res	Type	Atoms
2	R	1	NAG	O5-C5-C6-O6
3	N	4	MAN	O5-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	N	10	MAN	O5-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6

There are no ring outliers.

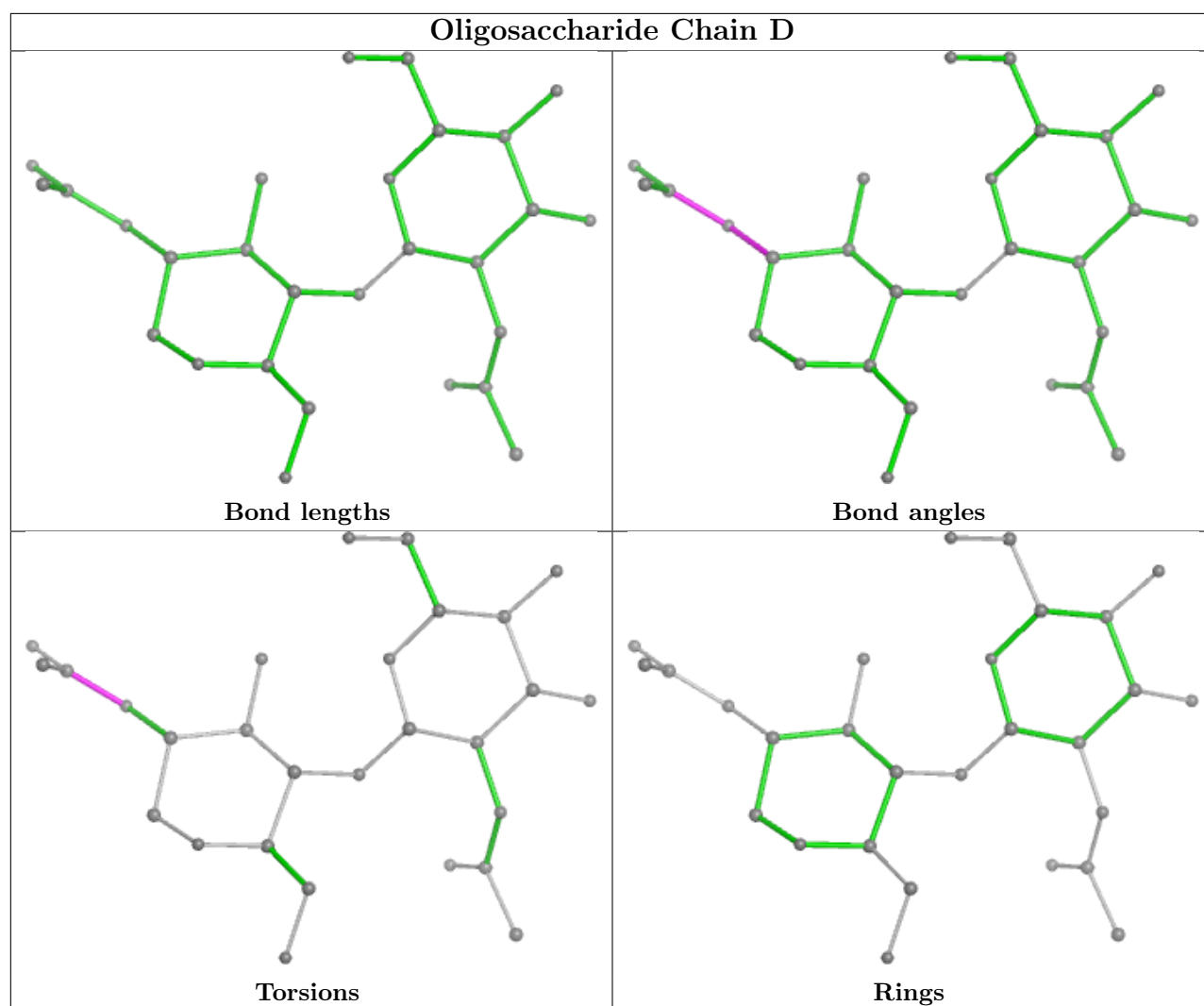
11 monomers are involved in 9 short contacts:

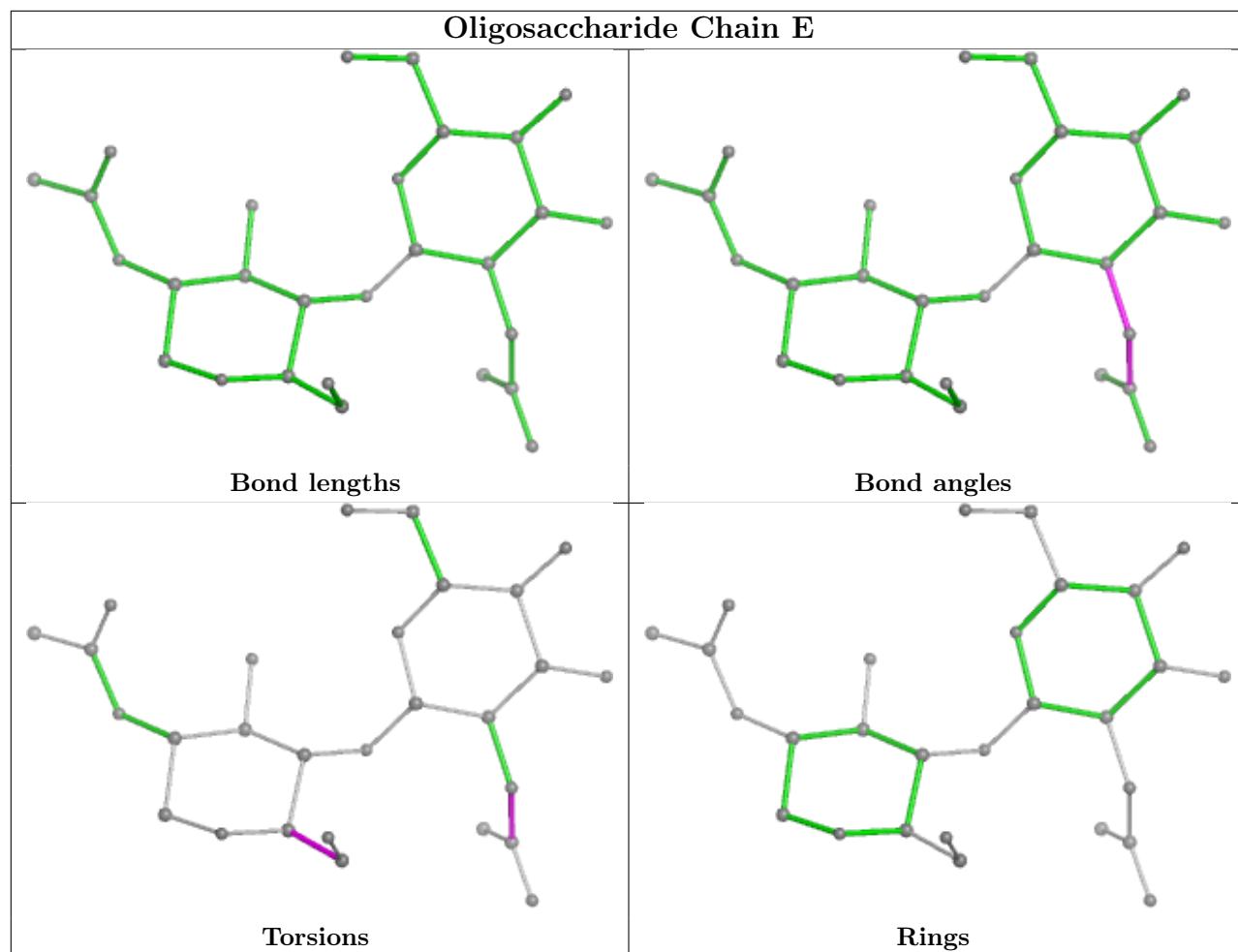
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	1	0
3	F	2	NAG	1	0
5	I	3	MAN	1	0
2	C	2	NAG	1	0
2	H	2	NAG	1	0
2	R	2	NAG	1	0
5	I	2	NAG	1	0
2	H	1	NAG	2	0
2	D	1	NAG	1	0
2	R	1	NAG	1	0
2	K	1	NAG	1	0

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

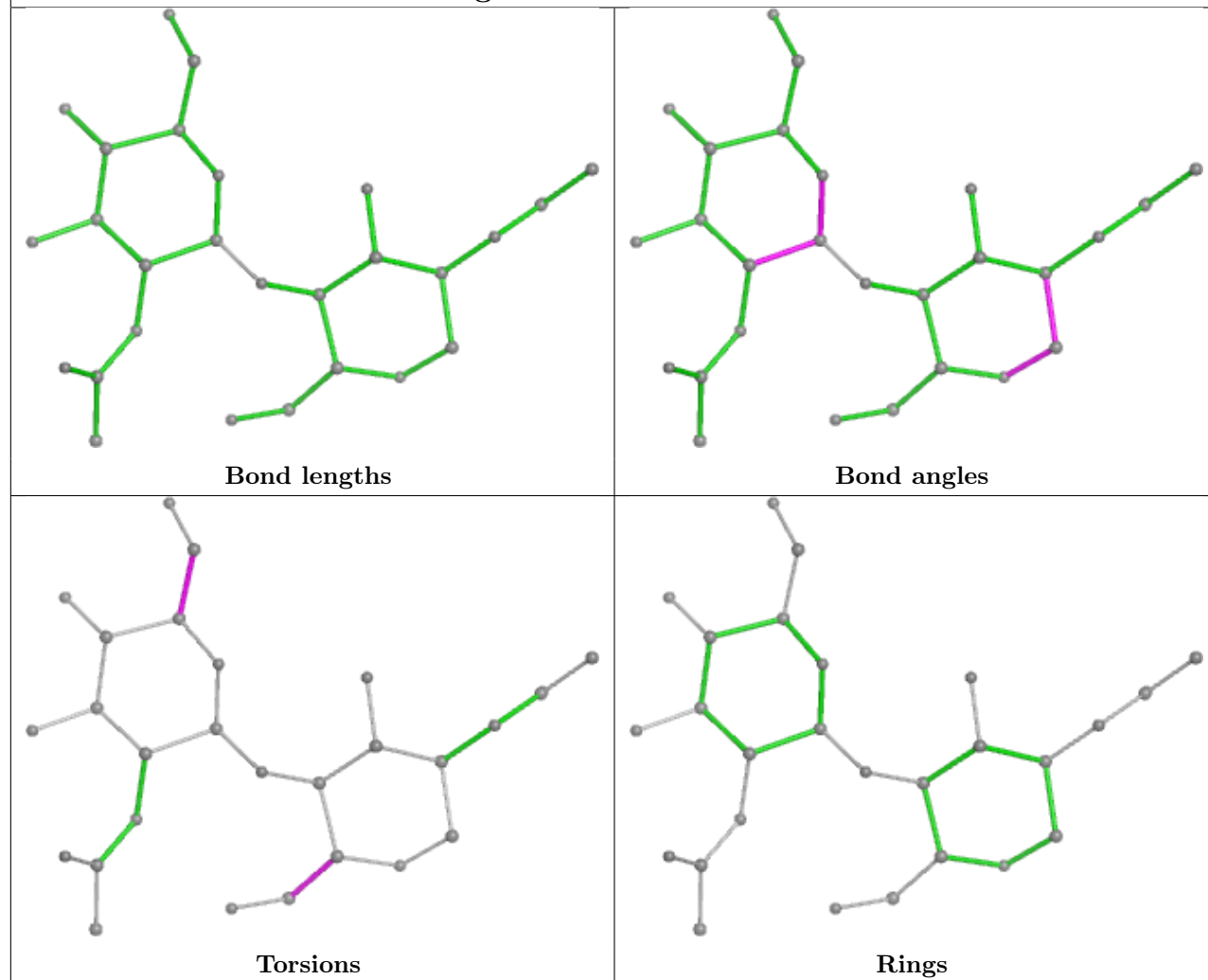


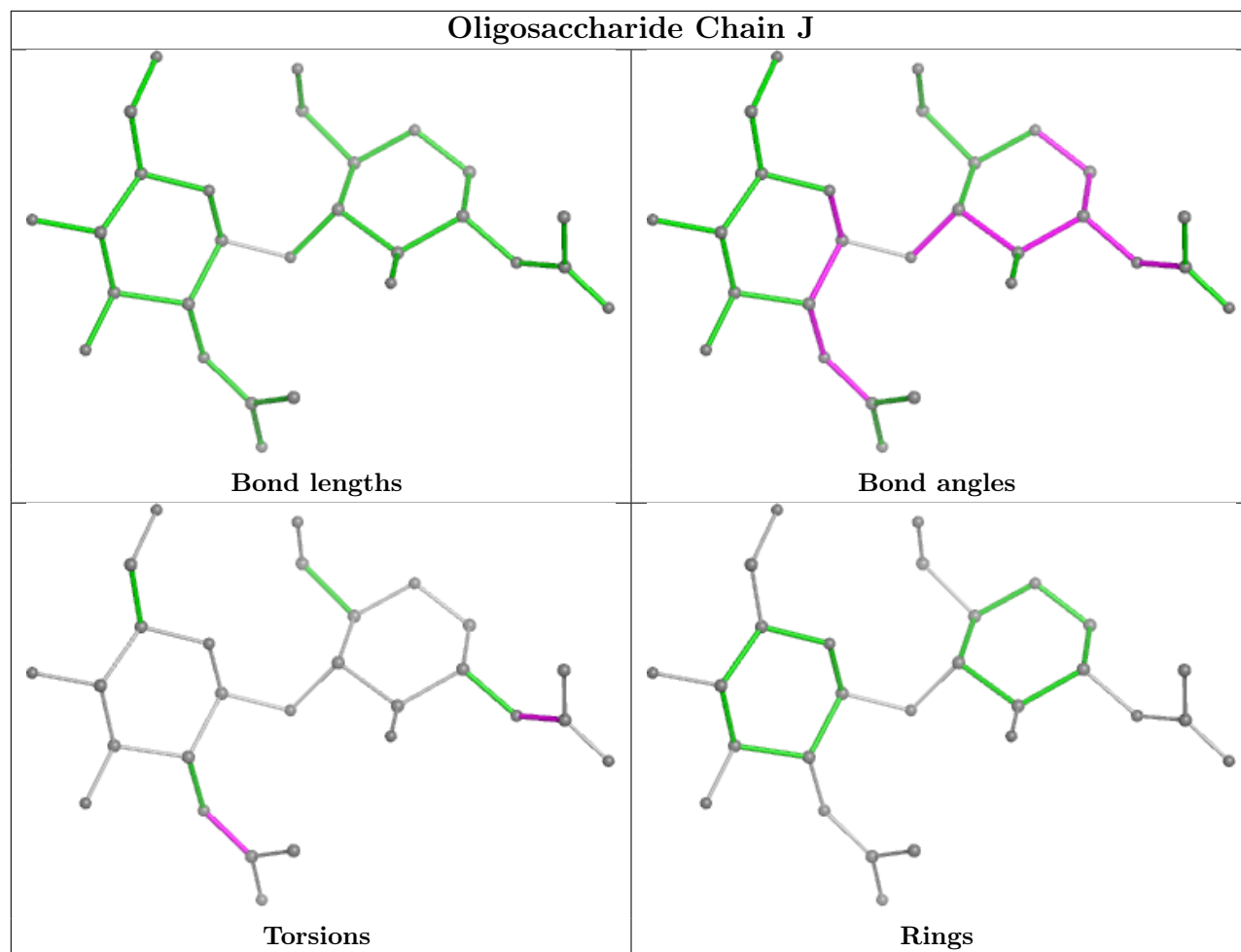


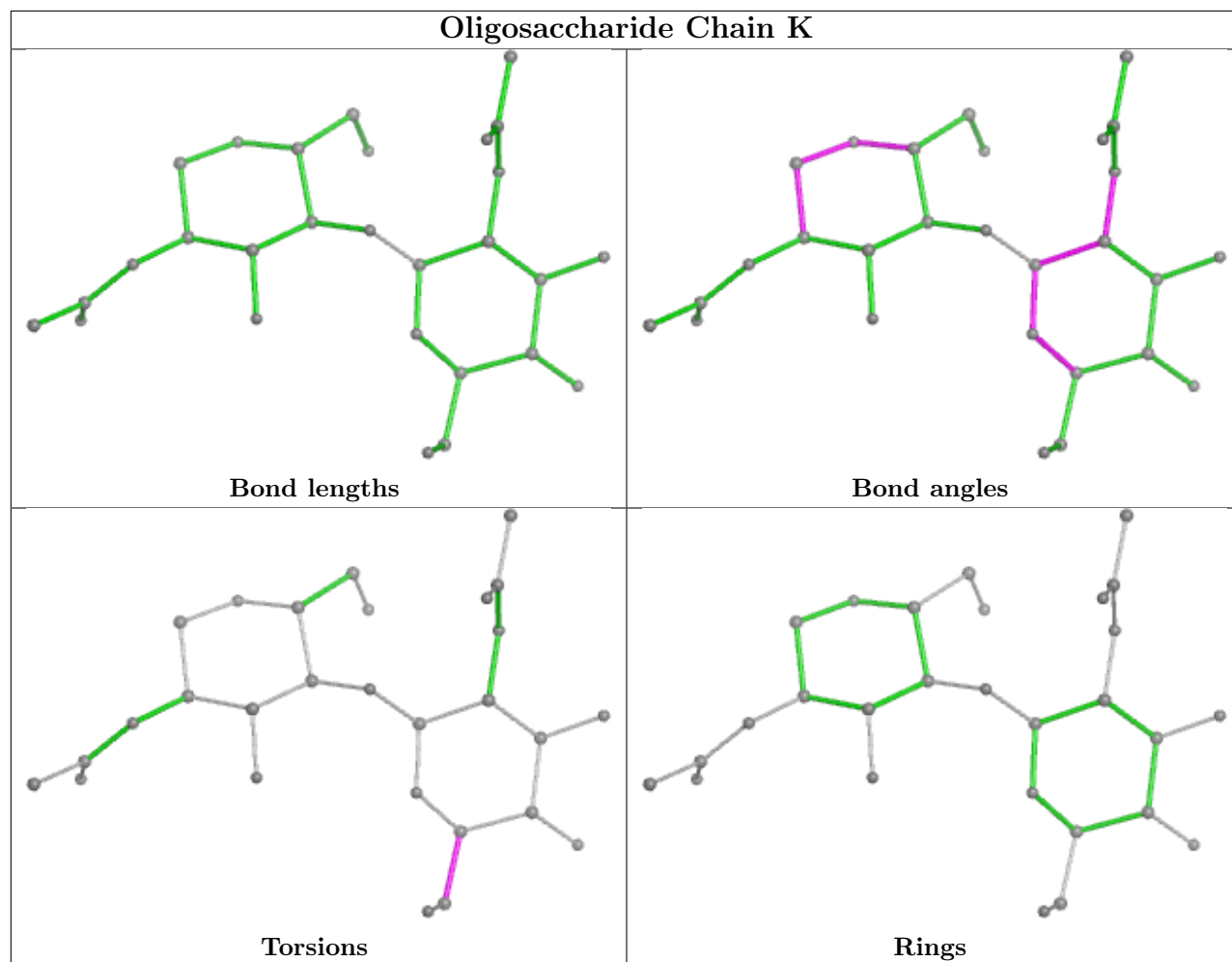




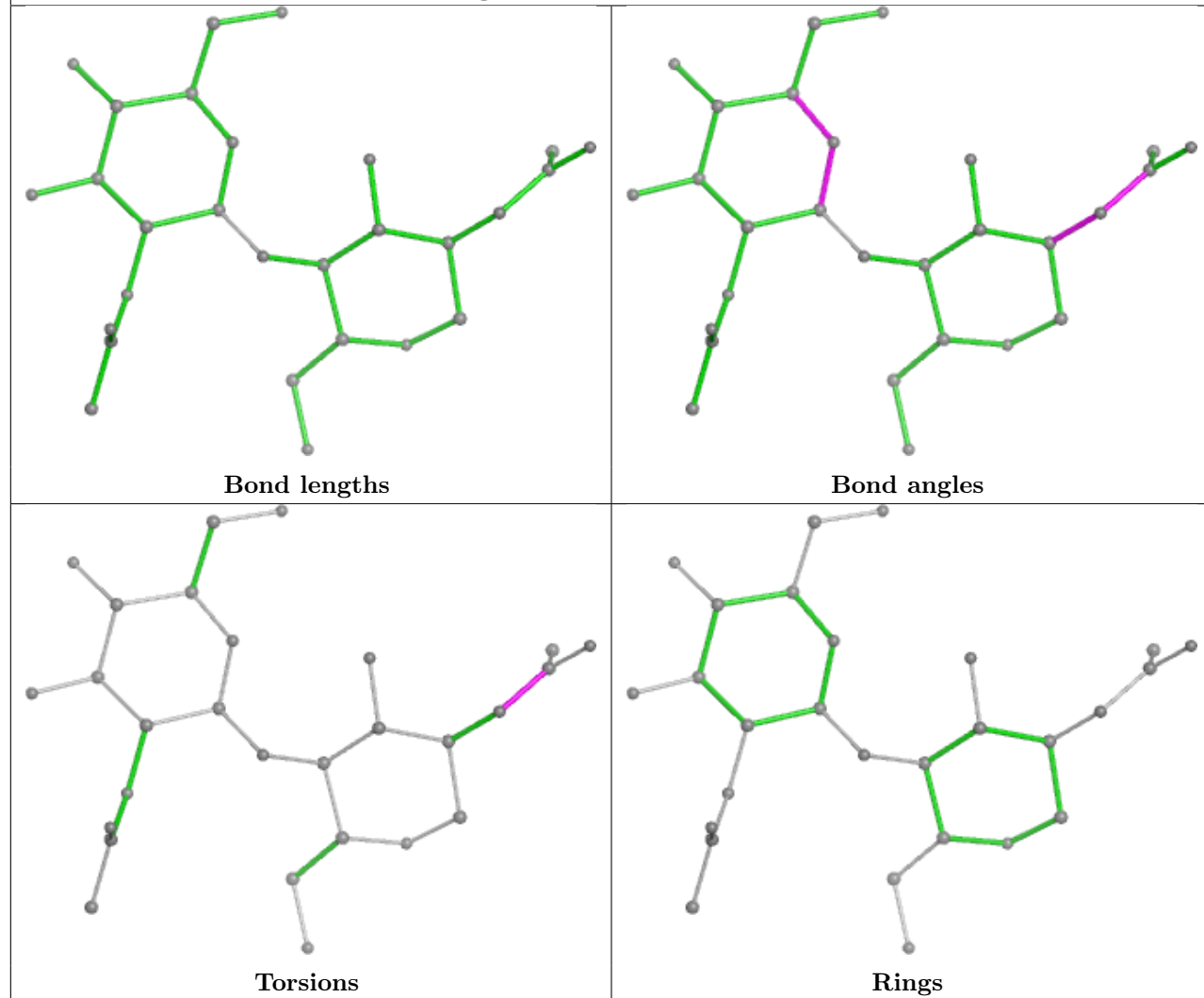
## Oligosaccharide Chain H

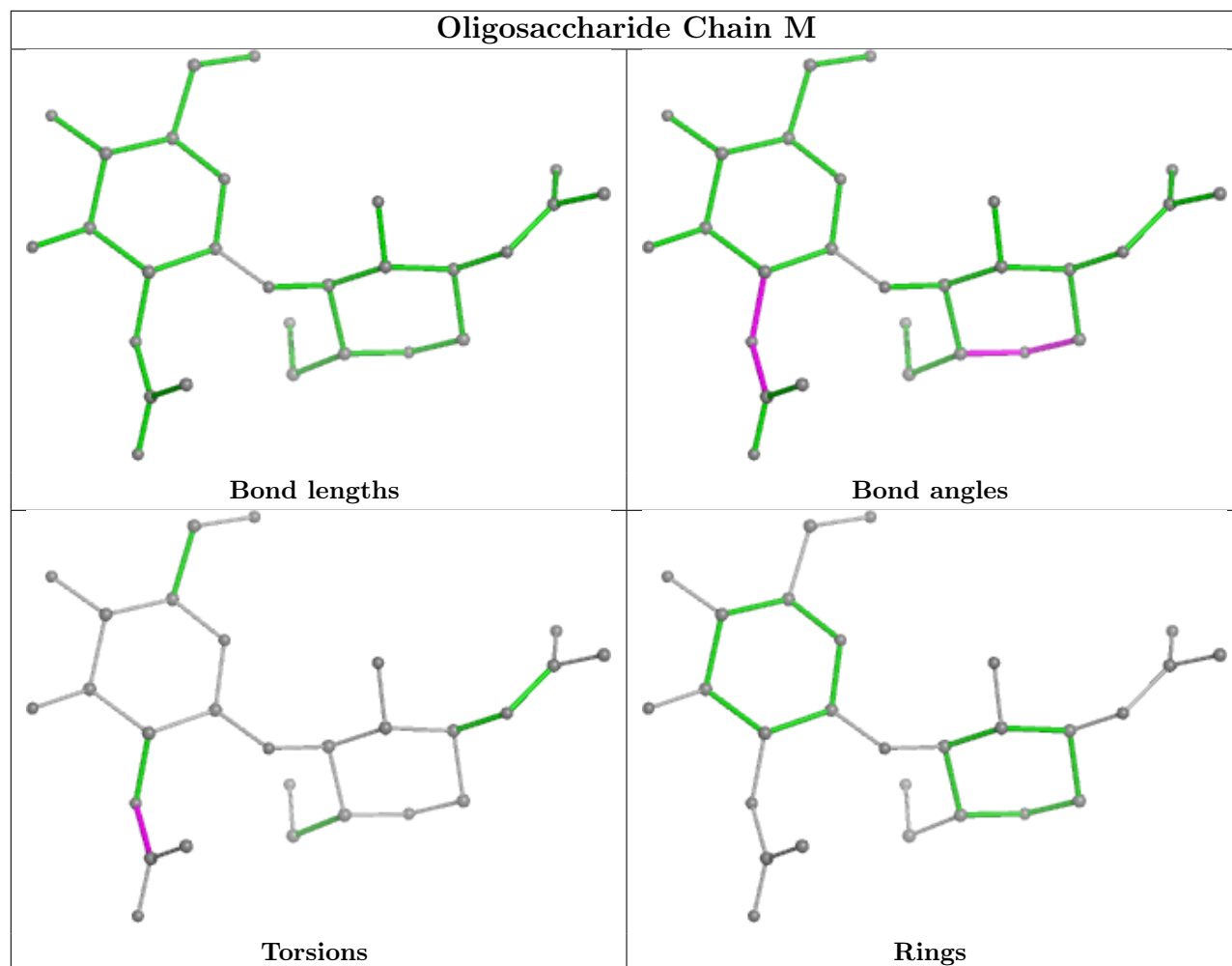




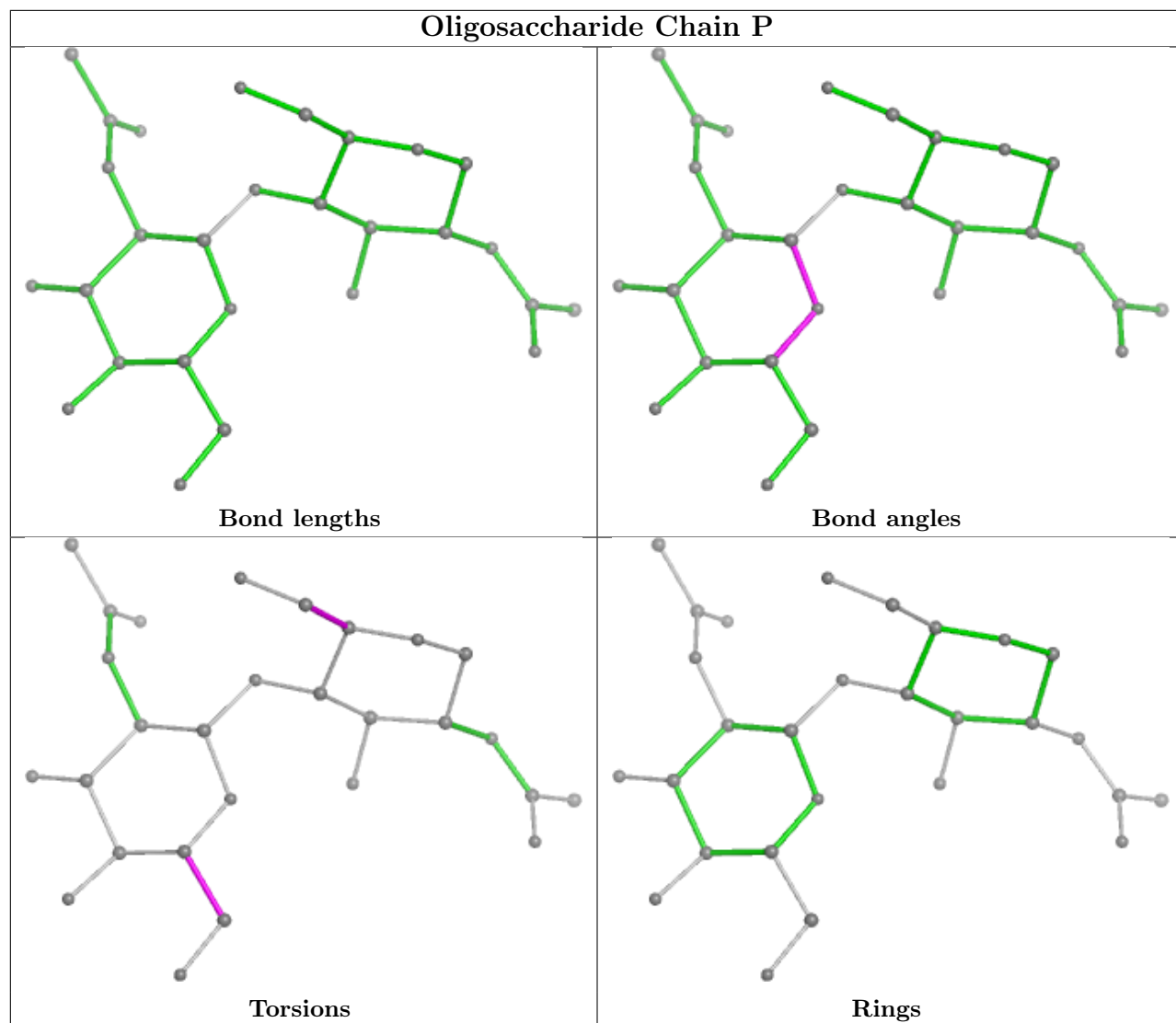


## Oligosaccharide Chain L



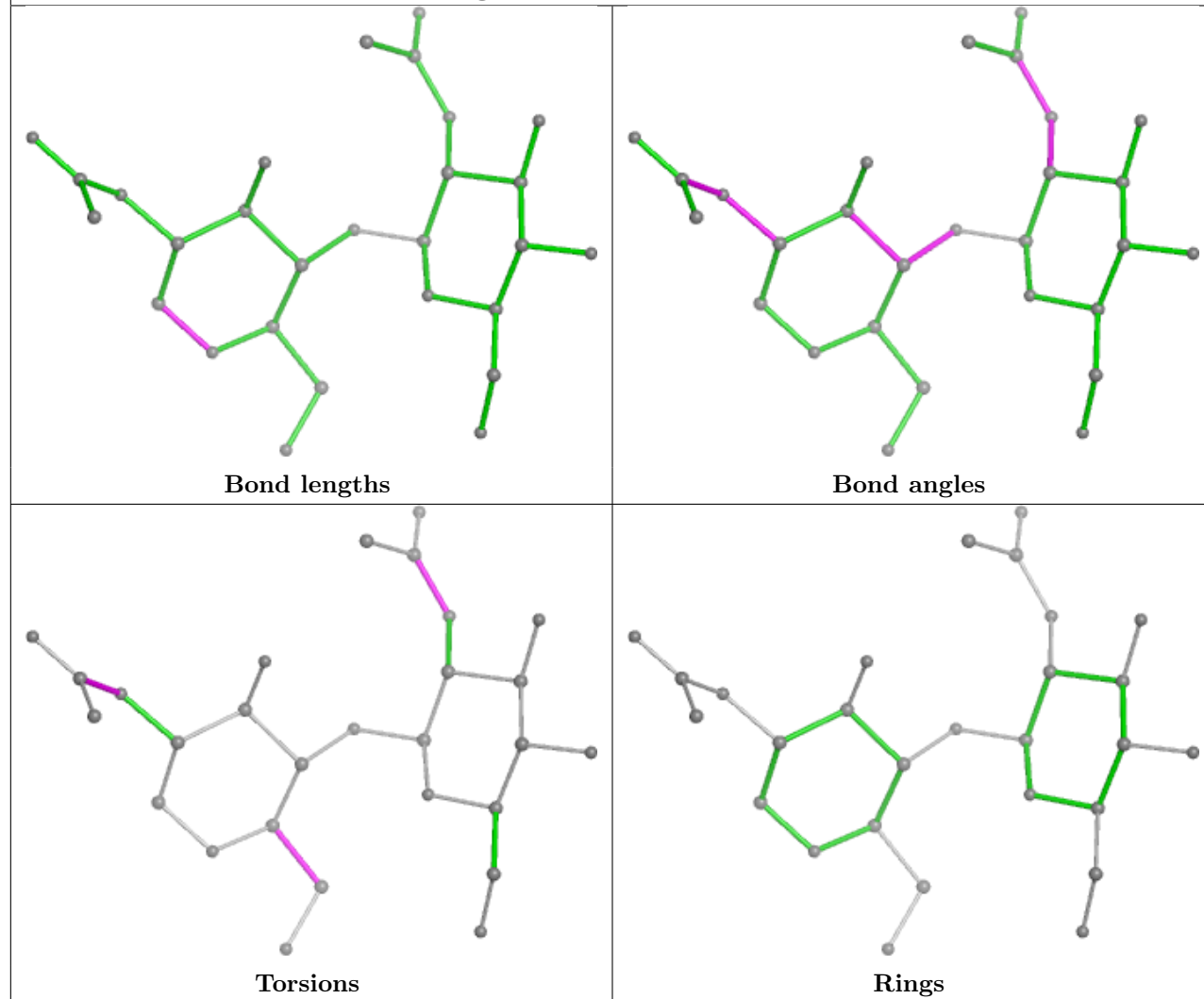


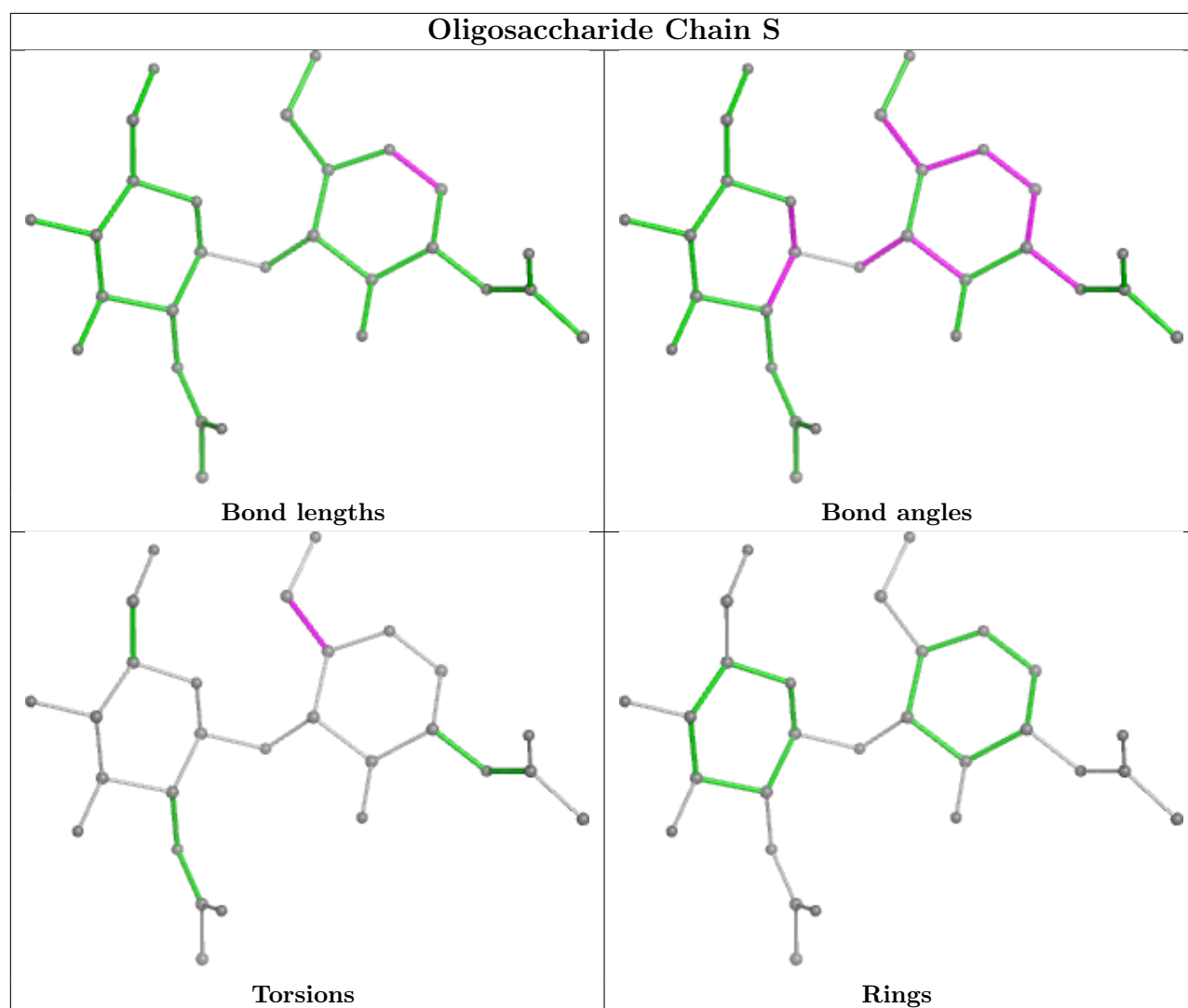
## Oligosaccharide Chain P

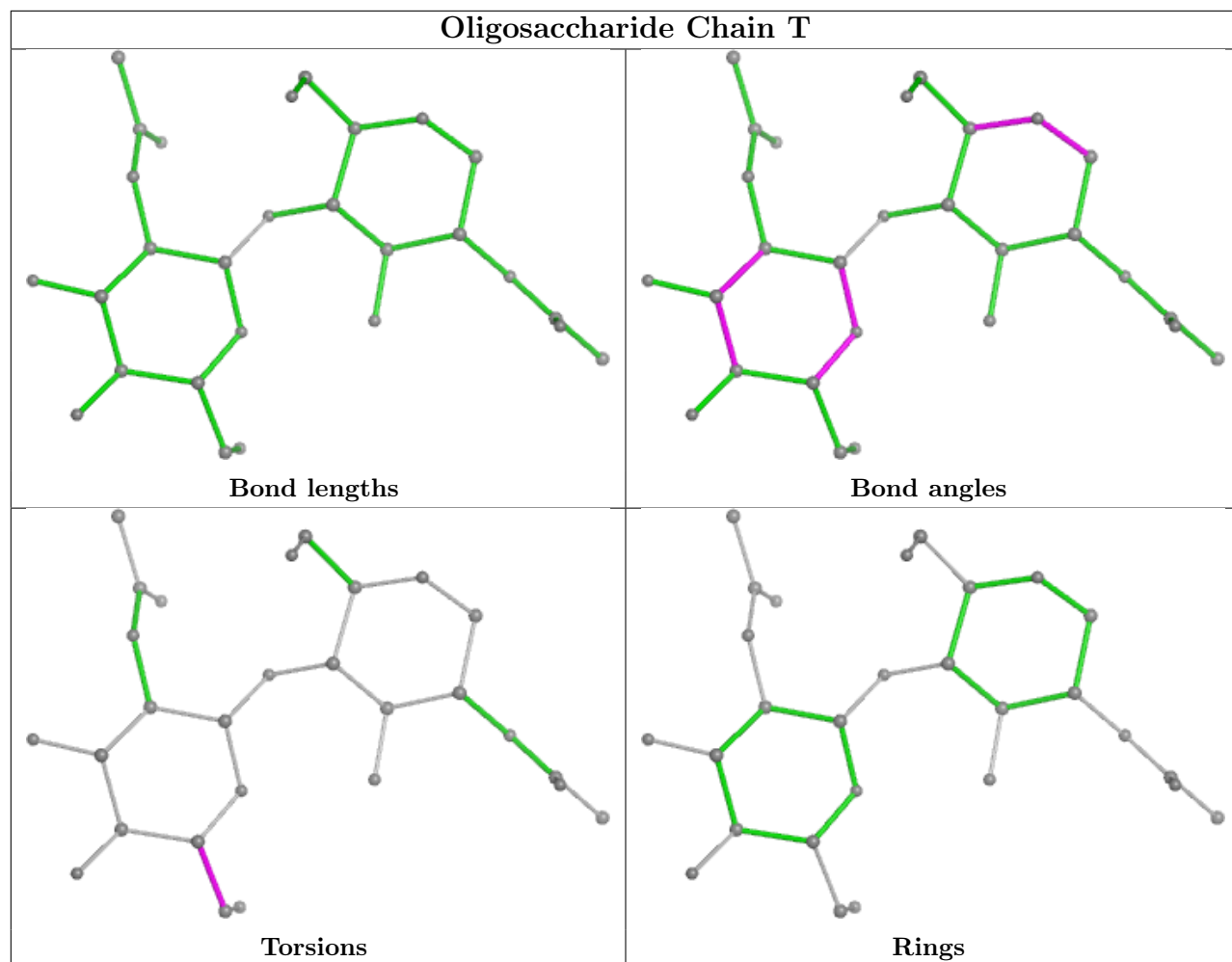


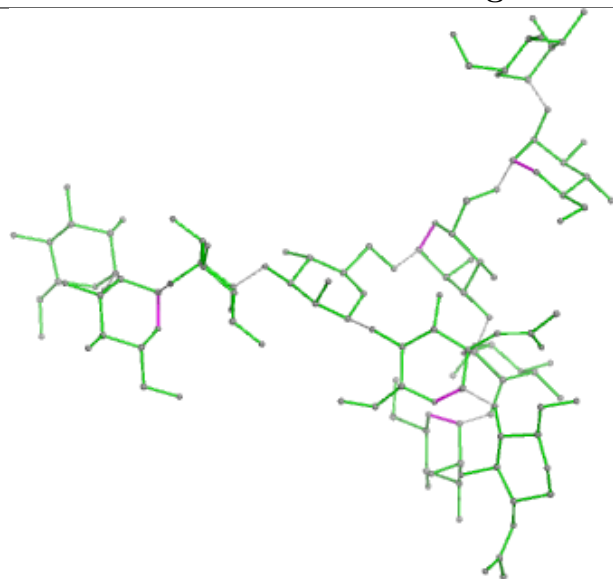
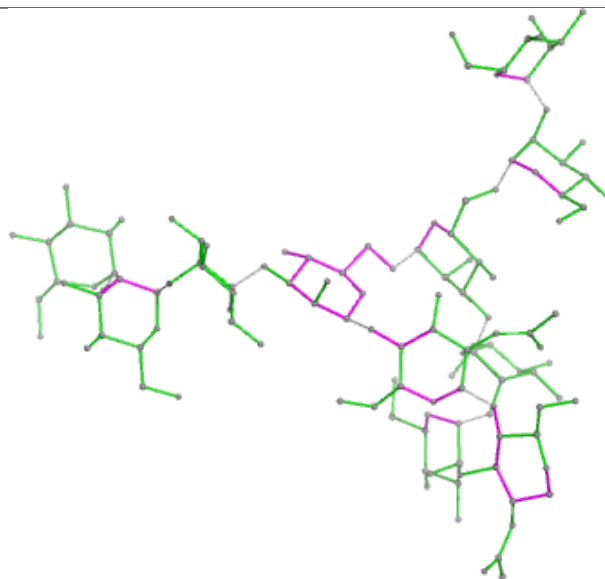
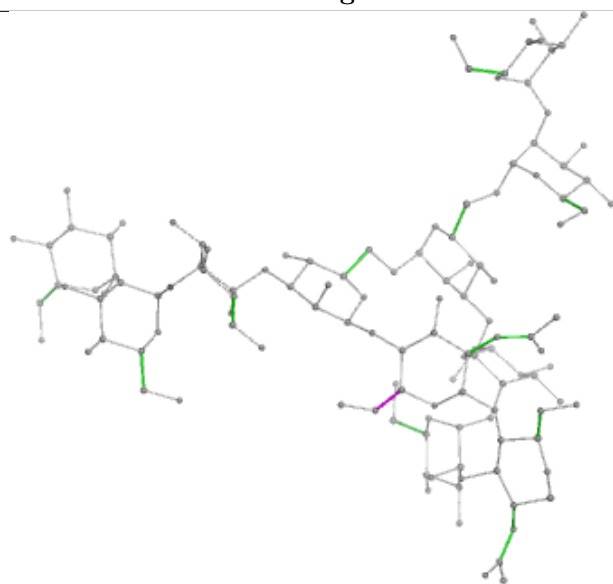
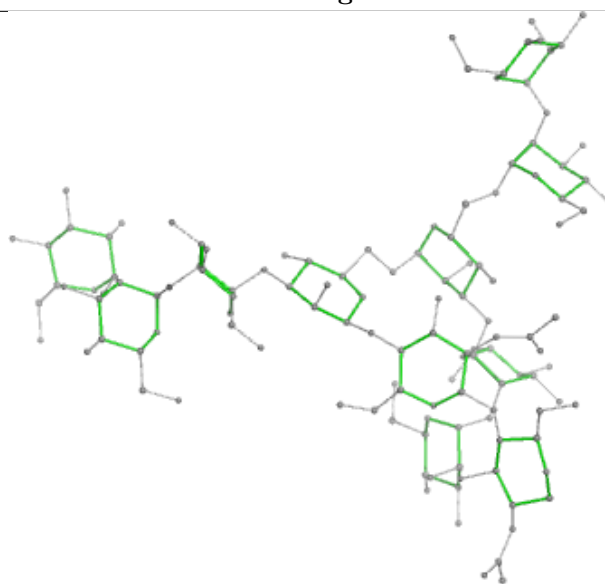


## Oligosaccharide Chain R

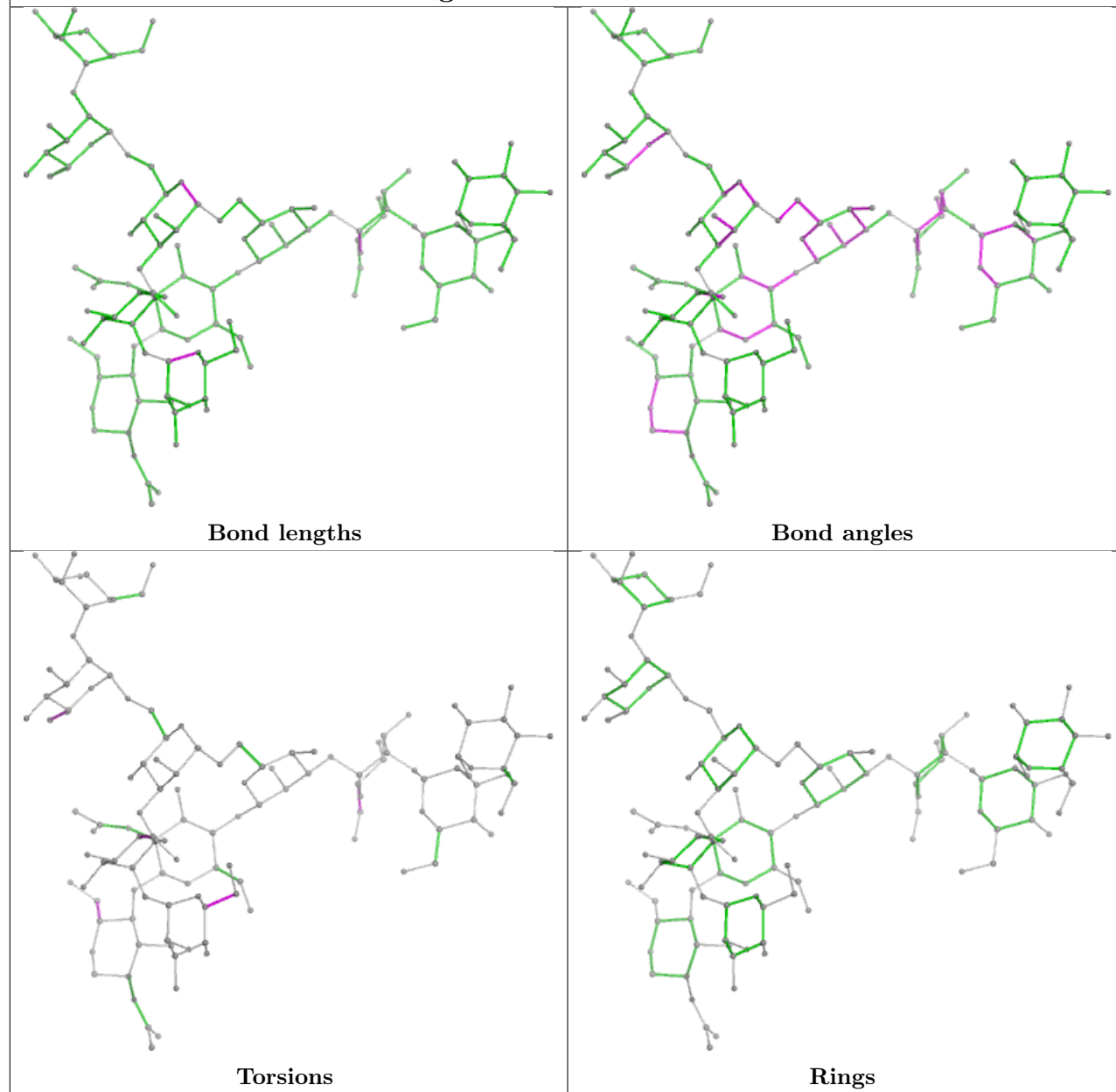


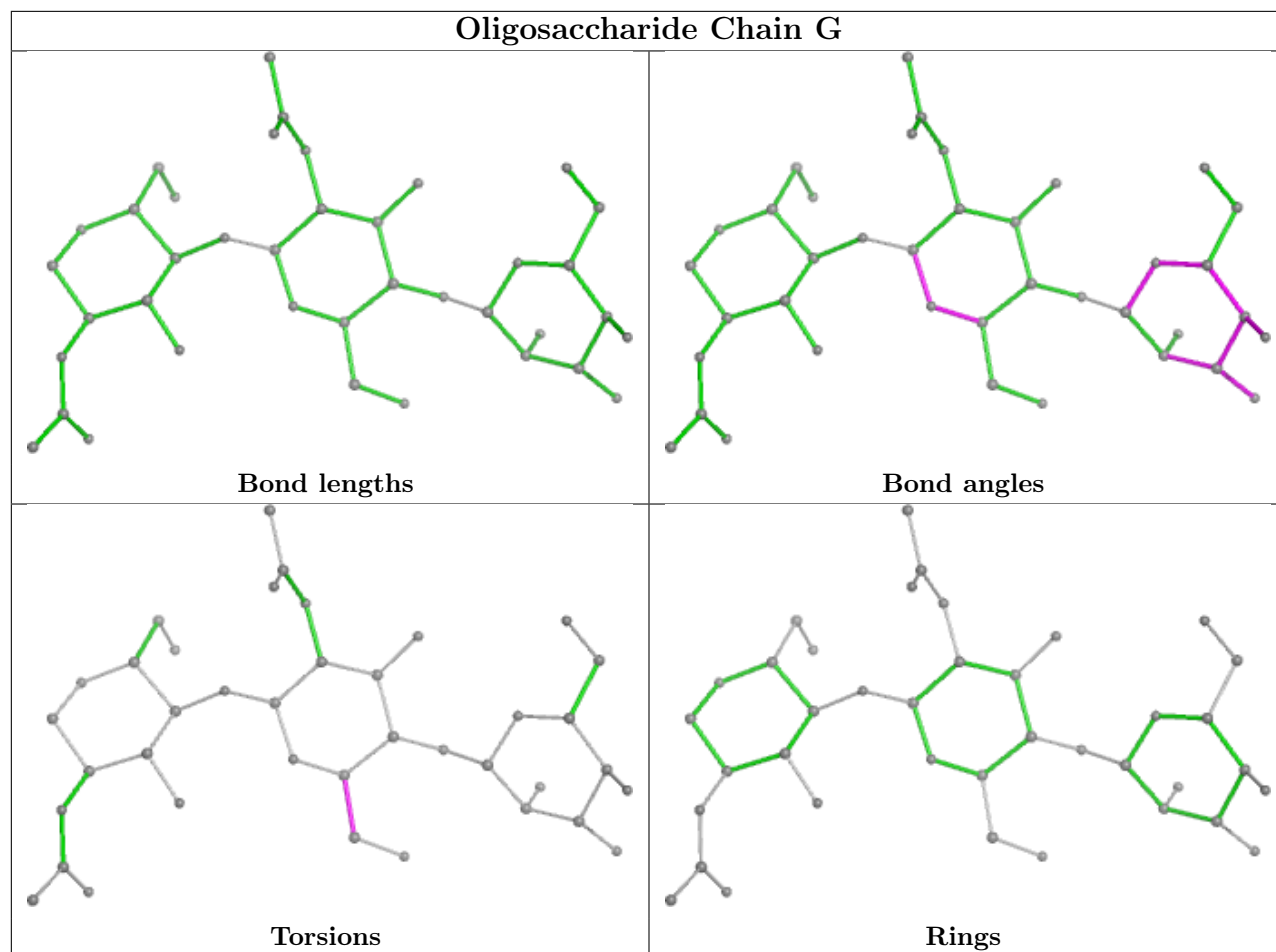


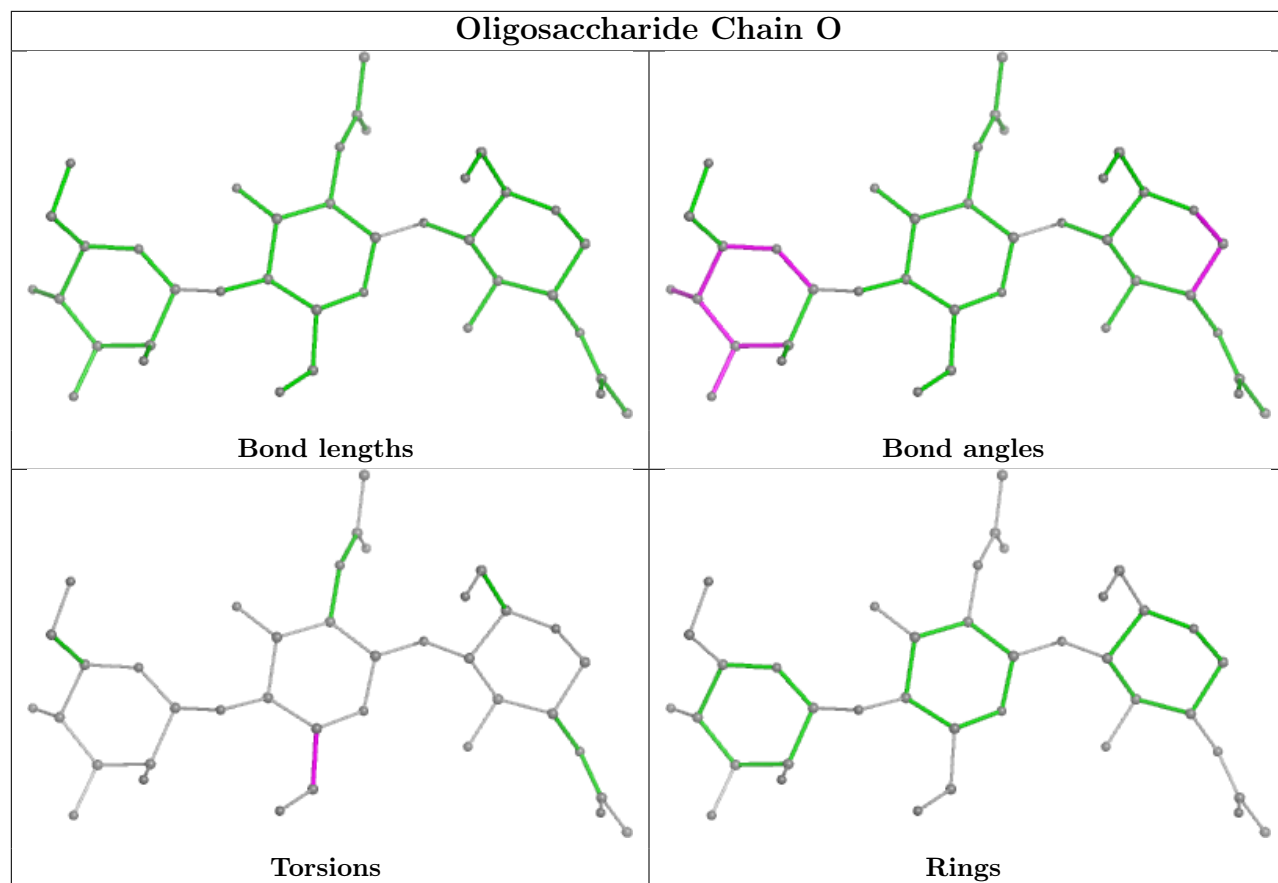


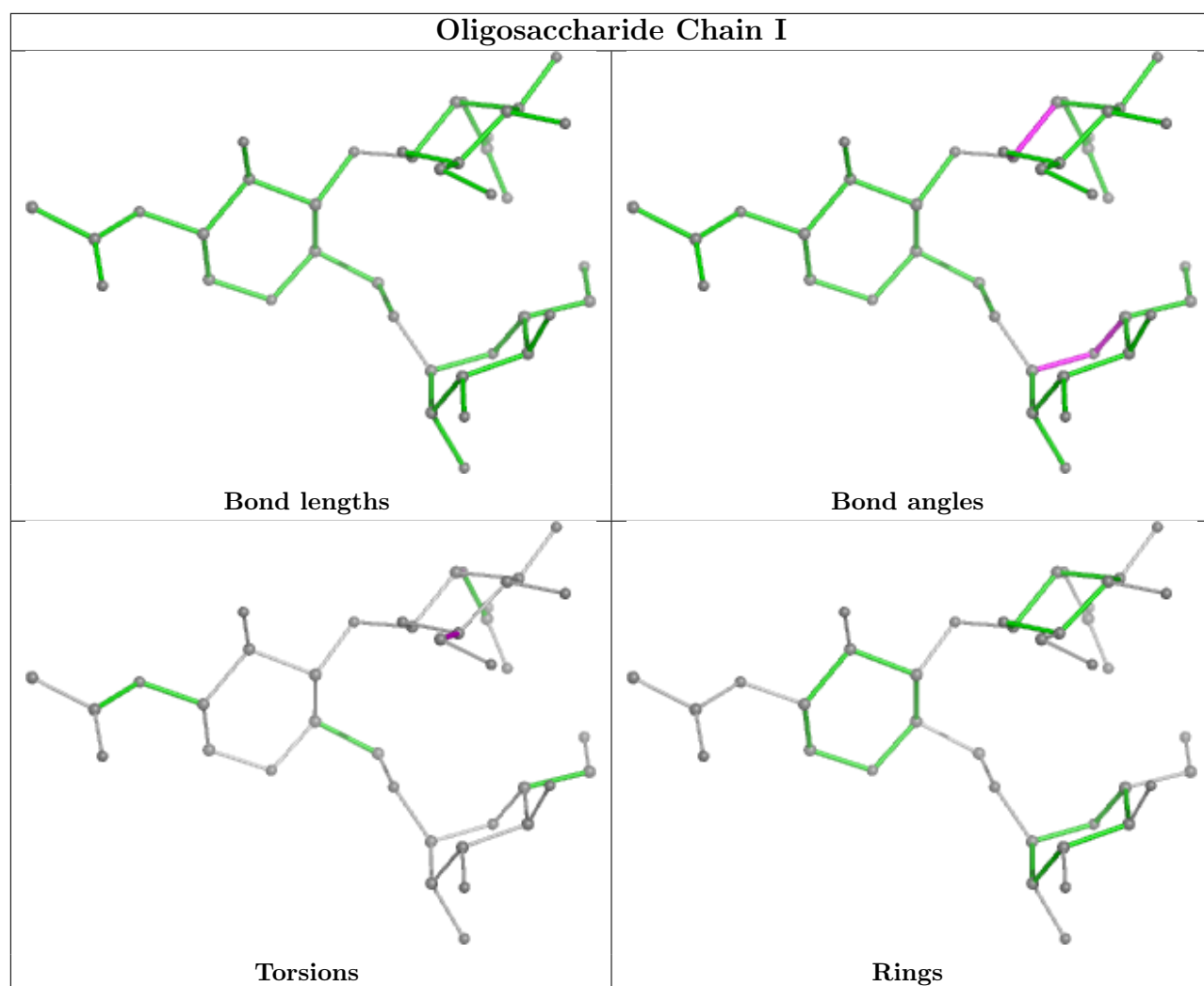
**Oligosaccharide Chain F****Bond lengths****Bond angles****Torsions****Rings**

## Oligosaccharide Chain N

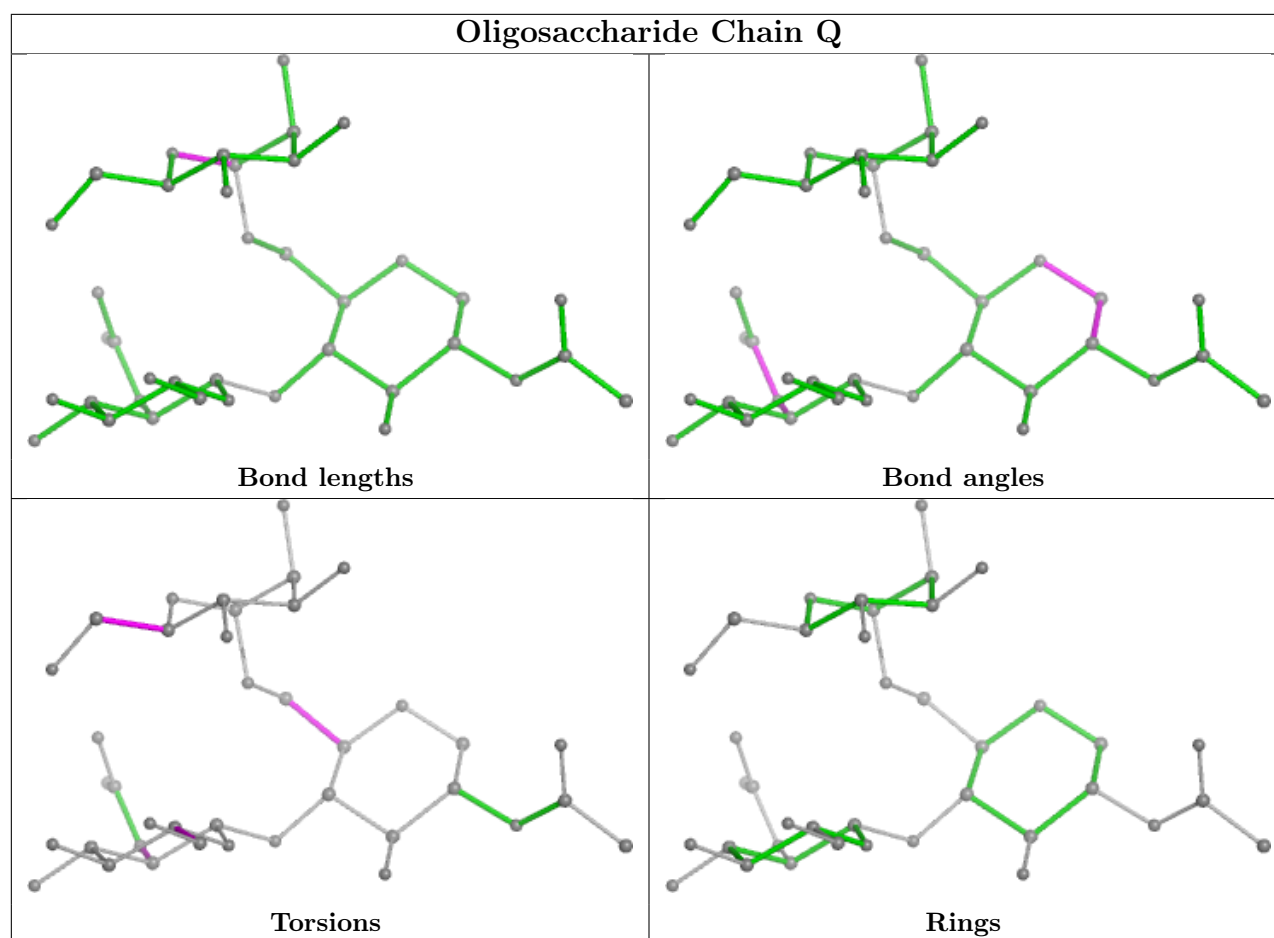












## 5.6 Ligand geometry [i](#)

17 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	$\# Z  > 2$
7	NAG	A	803	1	14,14,15	0.69	0	17,19,21	0.86	0
6	BLD	A	801	-	36,37,37	0.91	2 (5%)	46,59,59	0.99	3 (6%)
10	SO4	A	808	-	4,4,4	0.62	0	6,6,6	0.11	0
11	GLY	B	801	-	3,3,4	0.60	0	0,2,4	-	-
6	BLD	B	802	-	36,37,37	0.83	1 (2%)	46,59,59	0.92	1 (2%)
7	NAG	A	805	1	14,14,15	0.61	0	17,19,21	1.66	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	1PE	A	806	-	15,15,15	0.28	0	14,14,14	0.20	0
9	EDO	B	807	-	3,3,3	0.27	0	2,2,2	0.27	0
12	ACT	B	808	-	3,3,3	1.30	0	3,3,3	1.05	0
7	NAG	A	804	1	14,14,15	0.64	0	17,19,21	1.02	1 (5%)
7	NAG	B	804	1	14,14,15	0.77	0	17,19,21	0.94	0
8	1PE	B	806	-	15,15,15	0.29	0	14,14,14	0.19	0
9	EDO	A	807	-	3,3,3	0.28	0	2,2,2	0.31	0
10	SO4	B	809	-	4,4,4	0.63	0	6,6,6	0.18	0
7	NAG	A	802	1	14,14,15	0.72	0	17,19,21	1.23	1 (5%)
7	NAG	B	805	1	14,14,15	0.65	0	17,19,21	1.07	1 (5%)
7	NAG	B	803	1	14,14,15	0.70	0	17,19,21	1.17	2 (11%)

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	A	803	1	-	0/6/23/26	0/1/1/1
6	BLD	A	801	-	-	1/20/85/85	0/4/4/4
11	GLY	B	801	-	-	0/0/1/2	-
6	BLD	B	802	-	-	2/20/85/85	0/4/4/4
7	NAG	A	805	1	-	4/6/23/26	0/1/1/1
8	1PE	A	806	-	-	8/13/13/13	-
9	EDO	B	807	-	-	0/1/1/1	-
7	NAG	A	804	1	-	1/6/23/26	0/1/1/1
7	NAG	B	804	1	-	0/6/23/26	0/1/1/1
8	1PE	B	806	-	-	8/13/13/13	-
9	EDO	A	807	-	-	0/1/1/1	-
7	NAG	A	802	1	-	2/6/23/26	0/1/1/1
7	NAG	B	805	1	-	1/6/23/26	0/1/1/1
7	NAG	B	803	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	802	BLD	O07-C07	-2.72	1.41	1.45
6	A	801	BLD	O07-C07	-2.70	1.41	1.45
6	A	801	BLD	O07-C06	-2.56	1.31	1.34

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	805	NAG	C2-N2-C7	4.67	129.56	122.90
6	A	801	BLD	C11-C09-C08	-3.93	106.09	111.75
7	A	805	NAG	C1-O5-C5	3.39	116.78	112.19
7	A	802	NAG	C2-N2-C7	3.37	127.71	122.90
6	B	802	BLD	O23-C23-C24	3.05	116.28	109.49

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

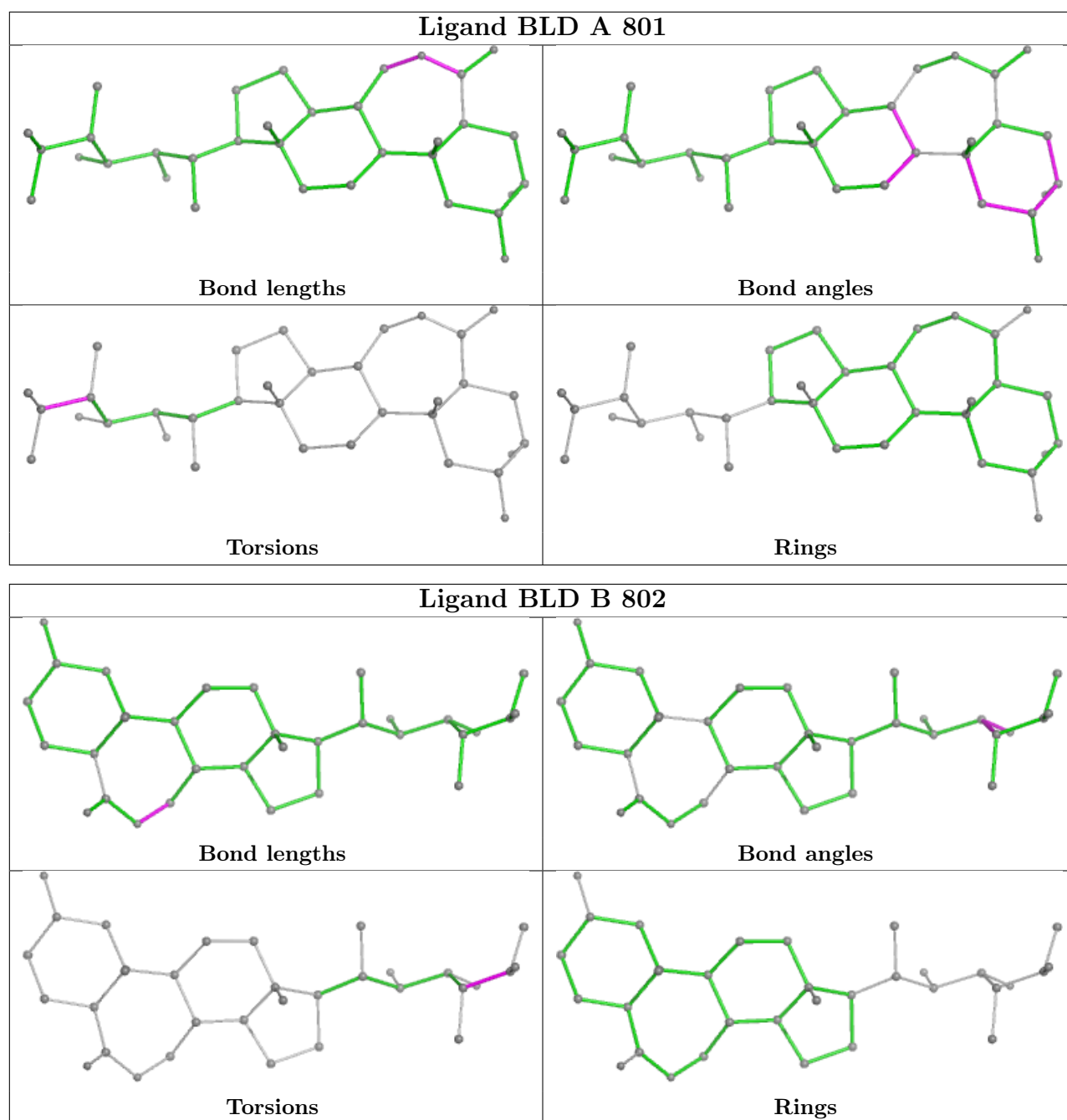
Mol	Chain	Res	Type	Atoms
6	B	802	BLD	C23-C24-C25-C26
7	A	805	NAG	O5-C5-C6-O6
7	A	805	NAG	C4-C5-C6-O6
7	A	802	NAG	C8-C7-N2-C2
7	A	802	NAG	O7-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	802	BLD	1	0
7	A	805	NAG	1	0
8	A	806	1PE	1	0
12	B	808	ACT	2	0
7	A	802	NAG	1	0
7	B	803	NAG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	A	721/770 (93%)	0.28	25 (3%)	47 49	38, 67, 130, 160	3 (0%)
1	B	727/770 (94%)	0.26	21 (2%)	54 56	29, 65, 124, 160	6 (0%)
All	All	1448/1540 (94%)	0.27	46 (3%)	50 53	29, 66, 127, 160	9 (0%)

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	LEU	3.9
1	B	618	VAL	3.9
1	A	617	MET	3.8
1	A	52	PHE	3.6
1	B	58	TYR	3.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	NAG	J	2	14/15	0.31	0.14	117,129,154,156	0
2	NAG	C	2	14/15	0.38	0.14	127,134,157,162	0
4	BMA	O	3	11/12	0.39	0.14	120,127,152,154	0
2	NAG	R	2	14/15	0.41	0.15	127,134,160,164	0
2	NAG	P	2	14/15	0.44	0.18	122,135,160,162	0

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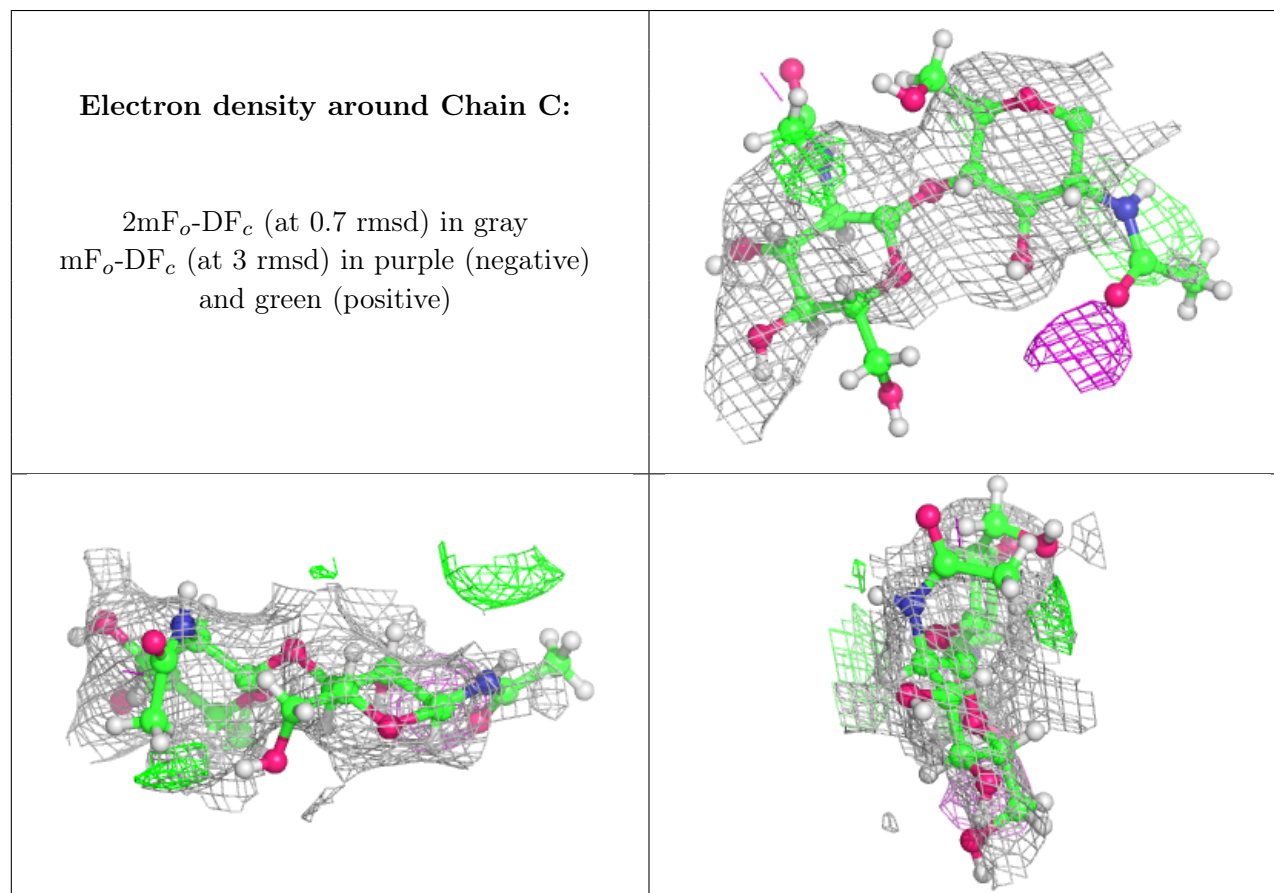
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	S	1	14/15	0.45	0.20	87,121,147,149	0
5	MAN	Q	3	11/12	0.45	0.17	120,129,153,154	0
2	NAG	C	1	14/15	0.50	0.17	113,129,153,157	0
4	BMA	G	3	11/12	0.52	0.14	99,116,139,142	0
2	NAG	S	2	14/15	0.53	0.17	110,134,161,164	0
2	NAG	L	2	14/15	0.55	0.12	113,123,148,148	0
5	MAN	I	3	11/12	0.57	0.13	106,118,142,147	0
3	MAN	F	6	11/12	0.59	0.22	87,96,113,115	0
3	MAN	N	5	11/12	0.59	0.12	94,106,125,128	0
5	NAG	Q	2	14/15	0.59	0.13	115,125,149,151	0
2	NAG	H	2	14/15	0.59	0.15	109,123,148,166	0
3	MAN	N	6	11/12	0.63	0.18	101,113,133,137	0
2	NAG	D	2	14/15	0.63	0.12	116,123,148,151	0
2	NAG	K	2	14/15	0.68	0.13	94,105,125,126	0
2	NAG	M	2	14/15	0.69	0.14	83,91,109,112	0
4	NAG	O	2	14/15	0.70	0.12	86,108,142,149	0
5	NAG	I	2	14/15	0.71	0.12	111,120,139,145	0
2	NAG	R	1	14/15	0.72	0.14	102,122,146,147	0
2	NAG	E	2	14/15	0.73	0.11	104,112,134,136	0
2	NAG	D	1	14/15	0.74	0.10	107,115,137,138	0
2	NAG	T	2	14/15	0.74	0.14	96,105,125,126	0
2	NAG	J	1	14/15	0.74	0.12	82,107,129,139	0
2	NAG	P	1	14/15	0.77	0.14	83,106,130,149	0
3	MAN	F	5	11/12	0.77	0.10	76,83,99,104	0
2	NAG	H	1	14/15	0.77	0.14	74,93,116,127	0
2	NAG	L	1	14/15	0.77	0.12	99,116,135,138	0
2	NAG	E	1	14/15	0.79	0.12	88,107,120,128	0
3	MAN	N	4	11/12	0.81	0.13	77,86,103,104	0
5	NAG	Q	1	14/15	0.82	0.14	99,119,139,143	0
4	NAG	G	2	14/15	0.82	0.12	92,105,125,129	0
5	NAG	I	1	14/15	0.82	0.14	84,101,124,131	0
2	NAG	T	1	14/15	0.84	0.12	63,83,105,105	0
3	MAN	F	11	11/12	0.85	0.10	54,67,77,82	0
2	NAG	K	1	14/15	0.85	0.12	62,88,109,119	0
3	NAG	F	2	14/15	0.86	0.12	46,57,68,73	0
3	BMA	F	3	11/12	0.88	0.11	51,61,73,82	0
3	MAN	F	10	11/12	0.88	0.11	50,59,71,74	0
3	MAN	F	4	11/12	0.89	0.08	64,74,89,90	0
3	NAG	N	2	14/15	0.89	0.09	38,53,64,80	0
2	NAG	M	1	14/15	0.89	0.08	67,80,92,98	0
4	NAG	O	1	14/15	0.90	0.10	67,81,95,100	0
3	MAN	N	10	11/12	0.90	0.10	54,63,76,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MAN	N	11	11/12	0.90	0.09	53,62,71,77	0
4	NAG	G	1	14/15	0.91	0.10	65,81,96,97	0
3	BMA	N	3	11/12	0.91	0.09	44,58,73,78	0
3	NAG	F	1	14/15	0.92	0.10	51,63,80,80	0
3	MAN	F	9	11/12	0.93	0.08	40,49,56,61	0
3	MAN	N	9	11/12	0.94	0.07	36,43,50,54	0
3	NAG	N	1	14/15	0.94	0.08	41,51,67,67	0
3	MAN	F	7	11/12	0.94	0.07	48,53,64,64	0
3	MAN	N	7	11/12	0.95	0.06	40,47,57,58	0
3	MAN	F	8	11/12	0.96	0.06	40,46,54,55	0
3	MAN	N	8	11/12	0.97	0.07	40,47,56,58	0

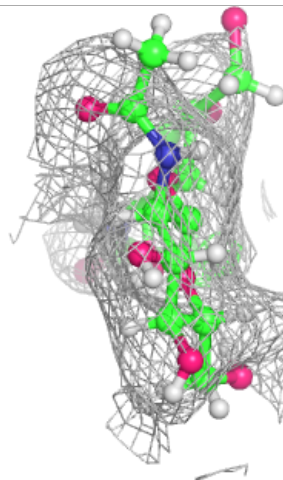
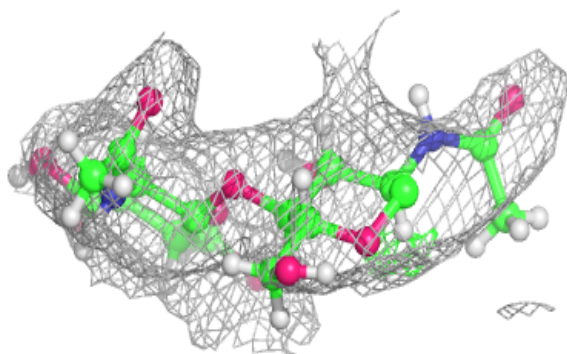
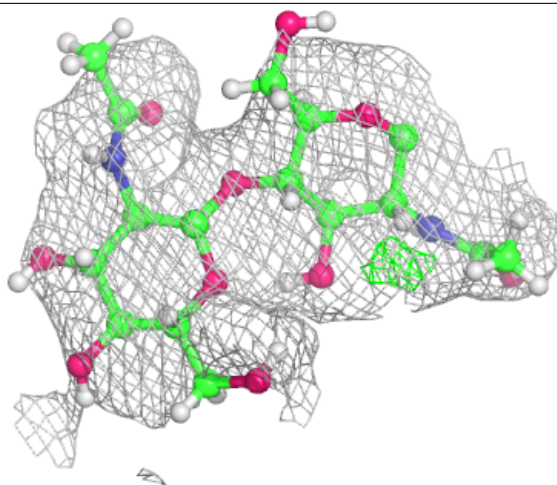
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





**Electron density around Chain D:**

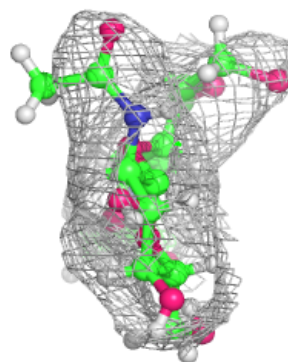
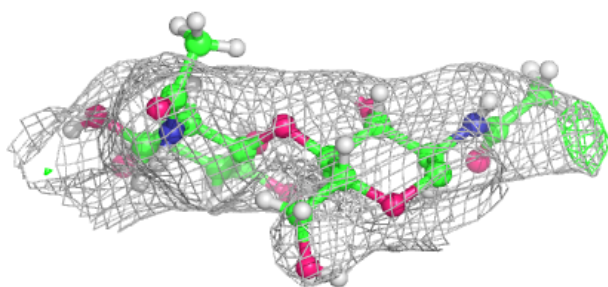
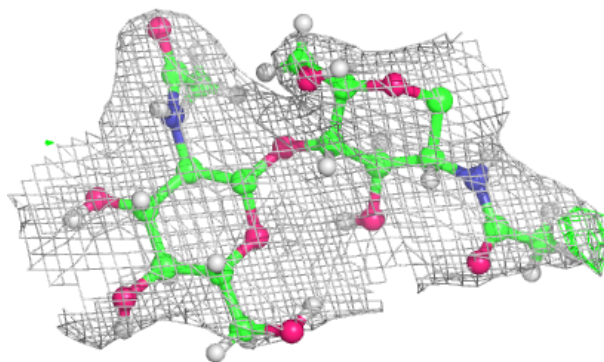
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



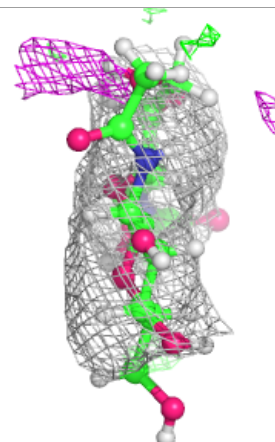
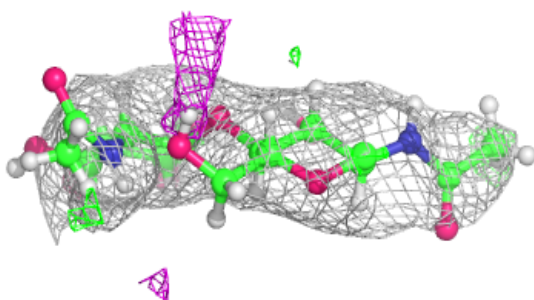
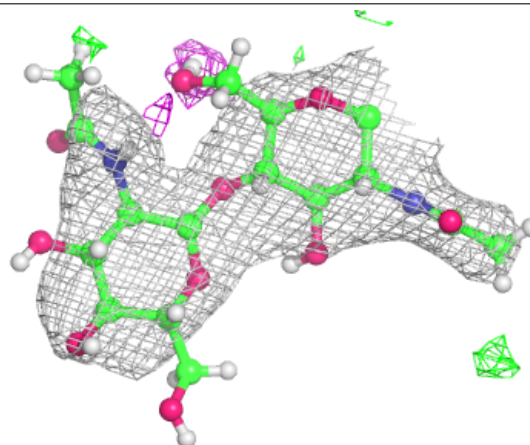


**Electron density around Chain E:**

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and green (positive)

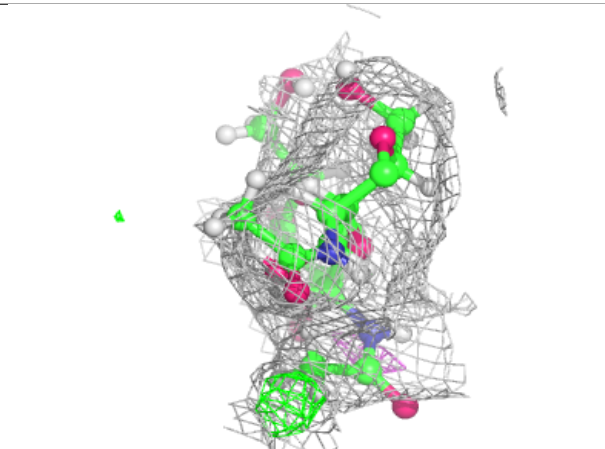
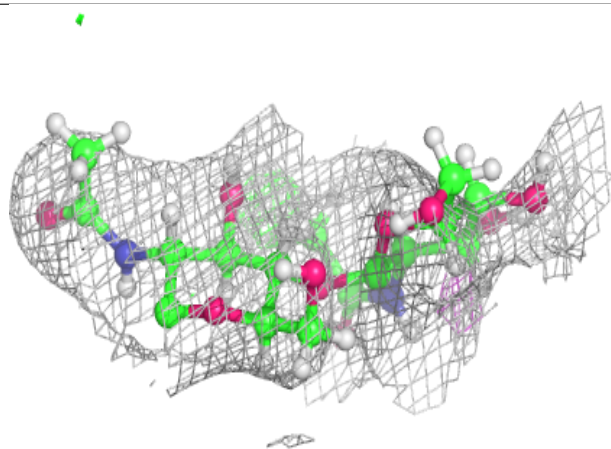
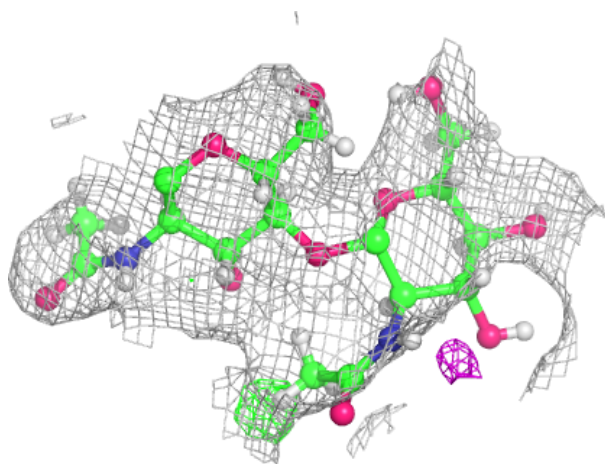
**Electron density around Chain H:**

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and green (positive)



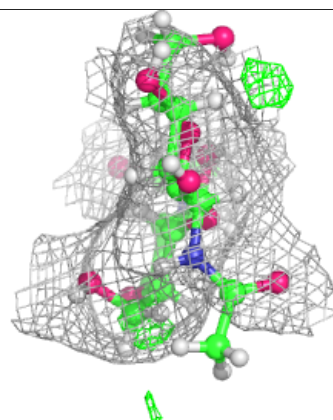
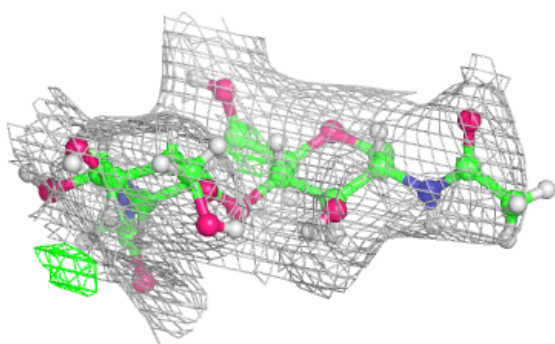
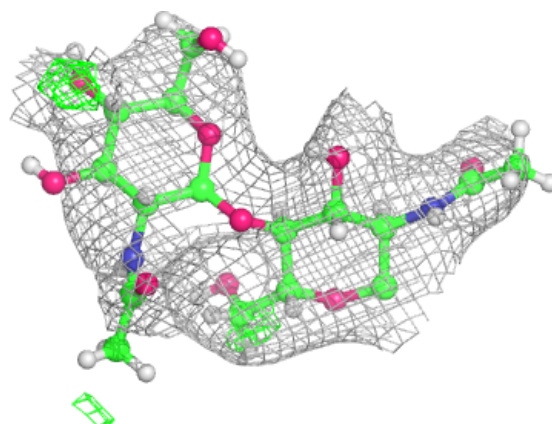
**Electron density around Chain J:**

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and green (positive)



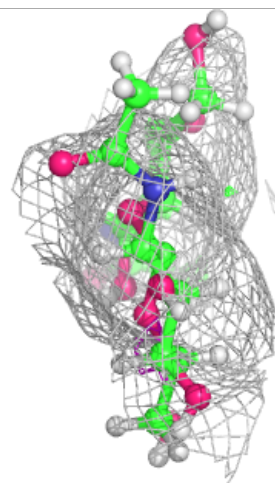
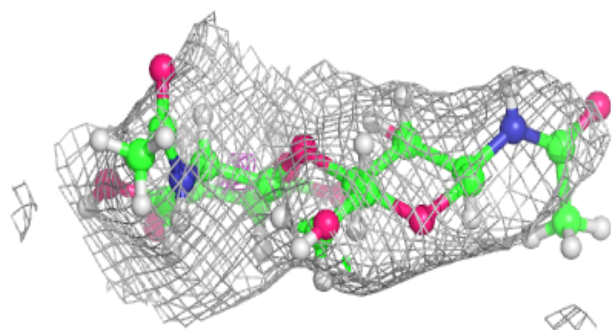
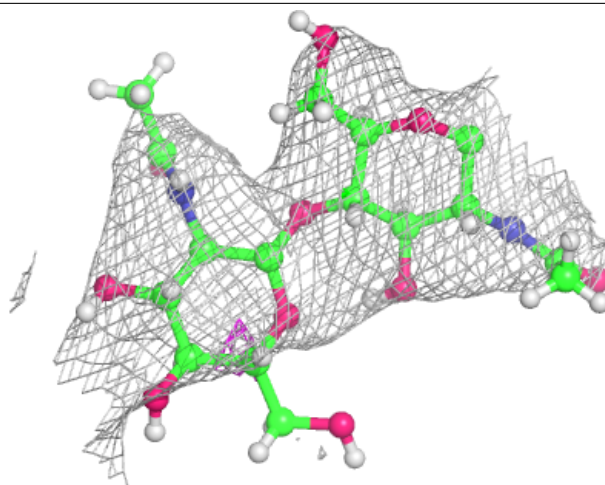
**Electron density around Chain K:**

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



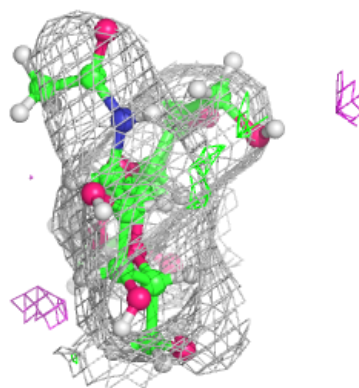
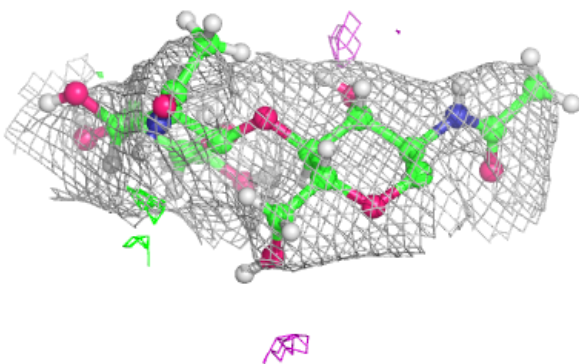
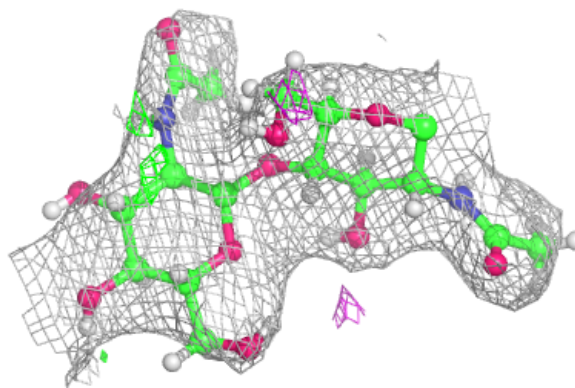
**Electron density around Chain L:**

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and green (positive)



**Electron density around Chain M:**

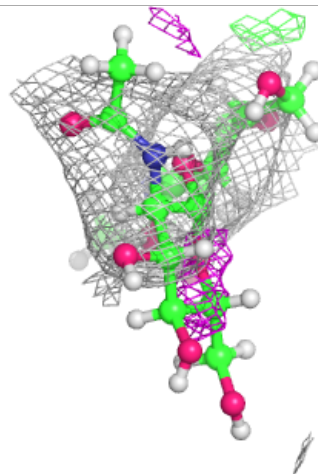
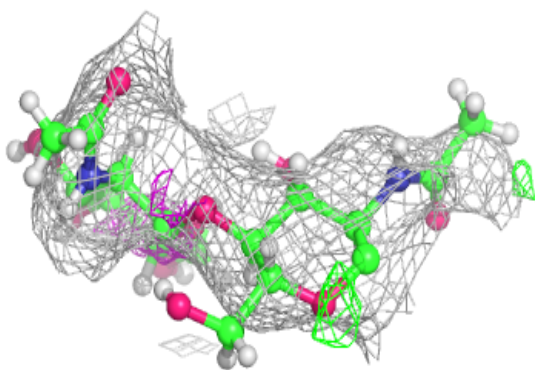
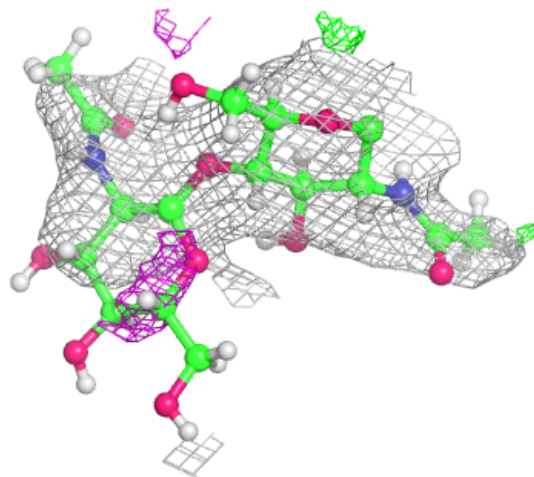
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 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





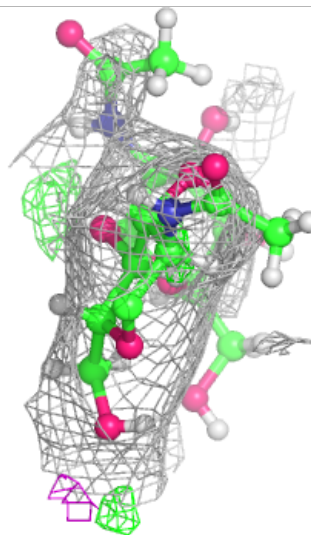
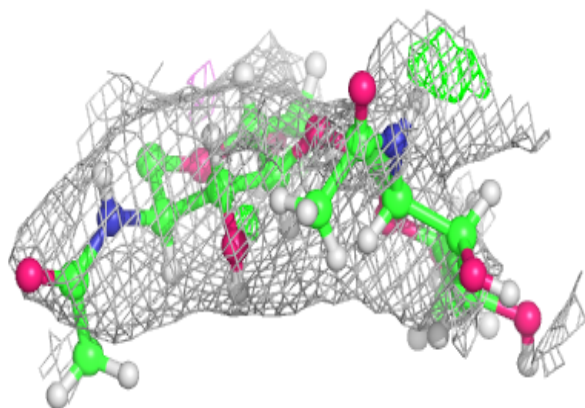
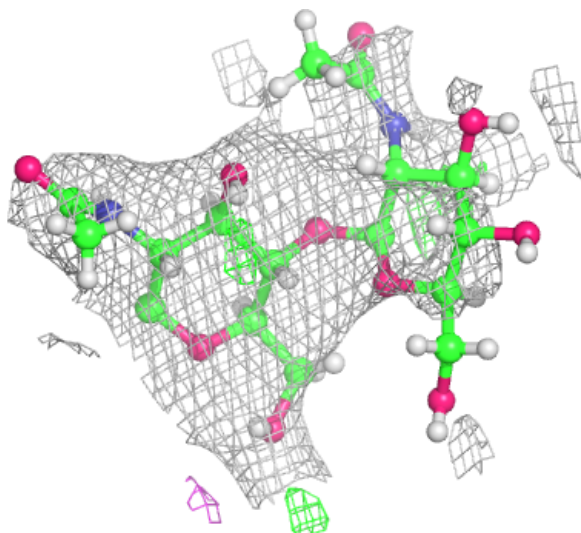
**Electron density around Chain P:**

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



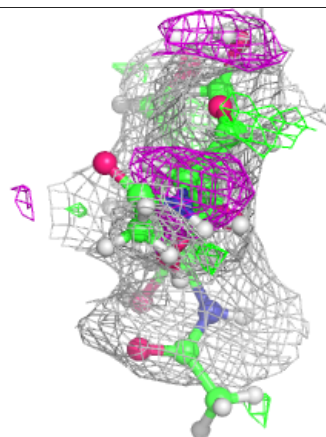
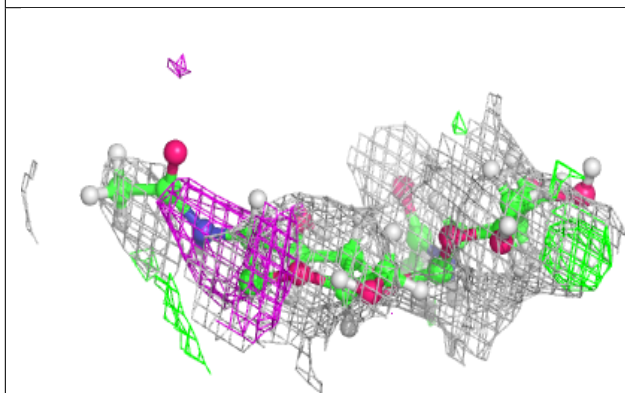
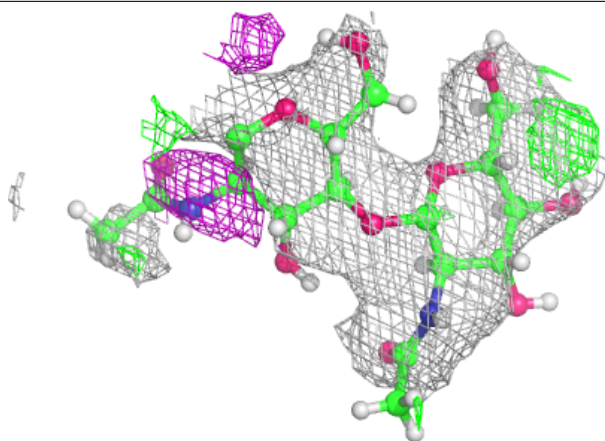
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and green (positive)



**Electron density around Chain S:**

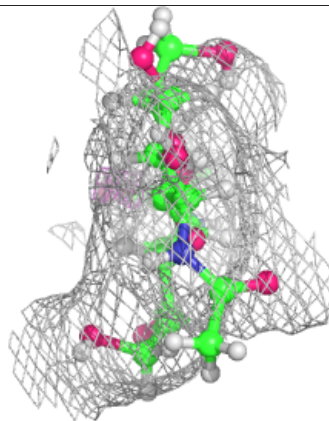
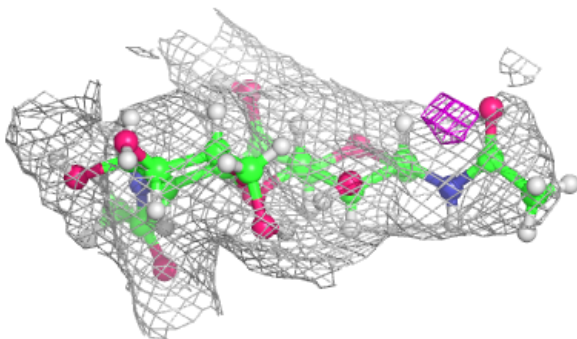
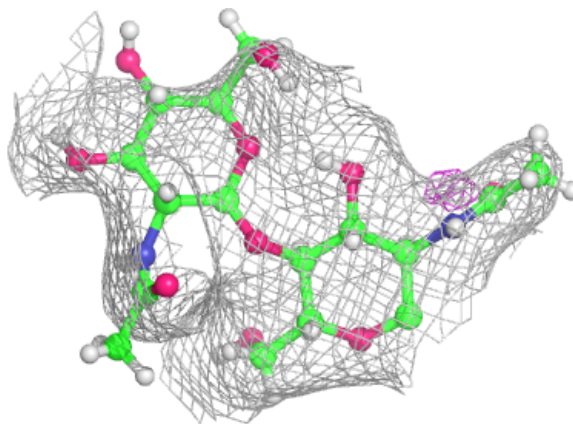
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





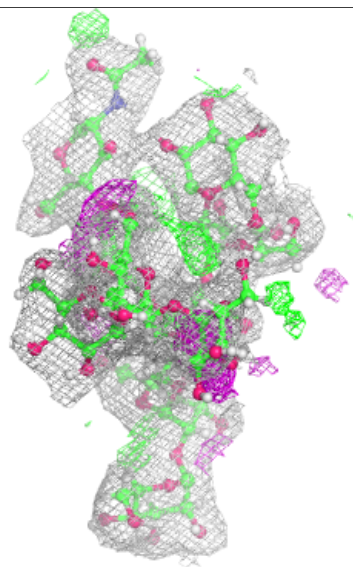
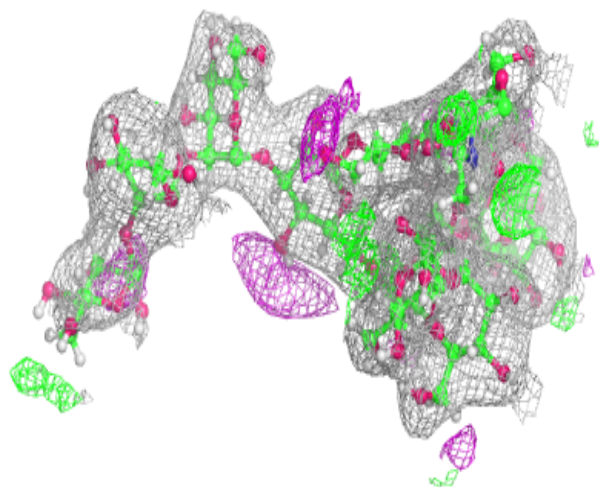
**Electron density around Chain T:**

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



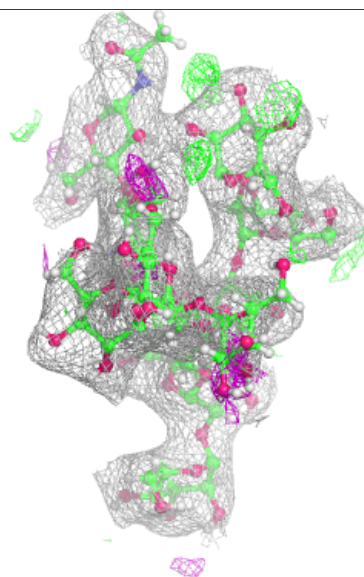
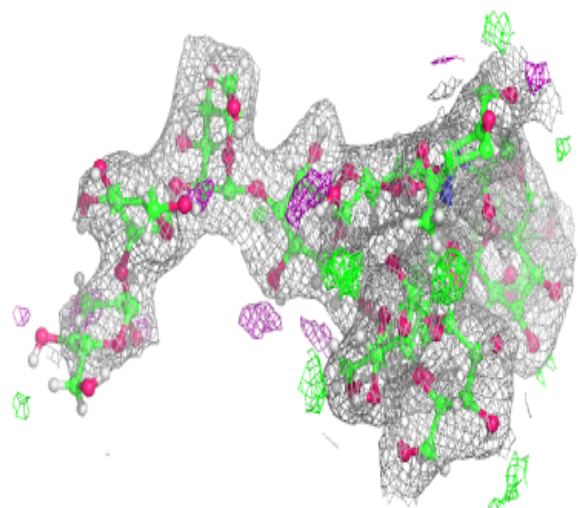
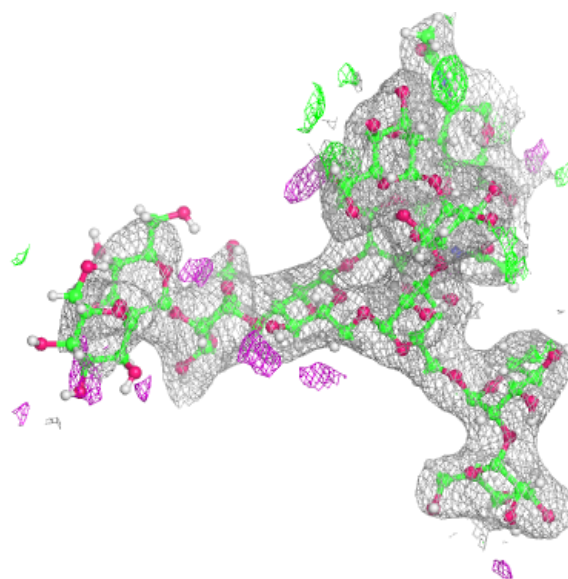
**Electron density around Chain F:**

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



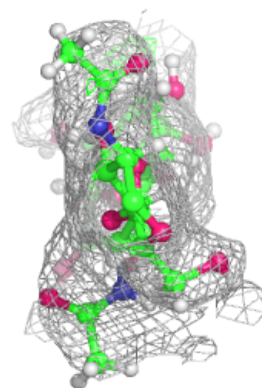
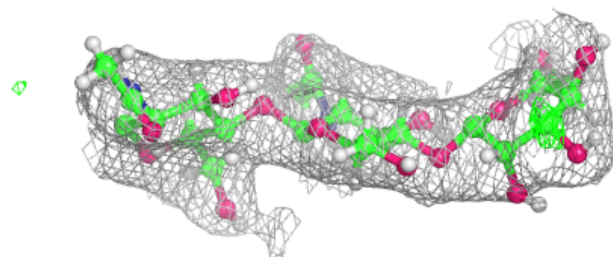
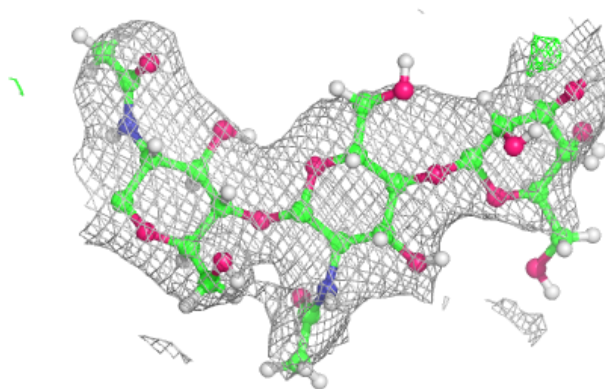
**Electron density around Chain N:**

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



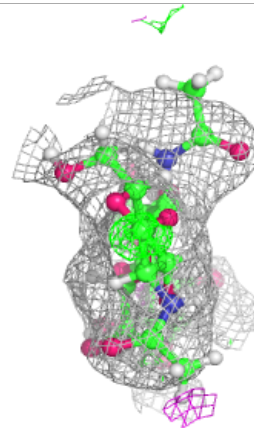
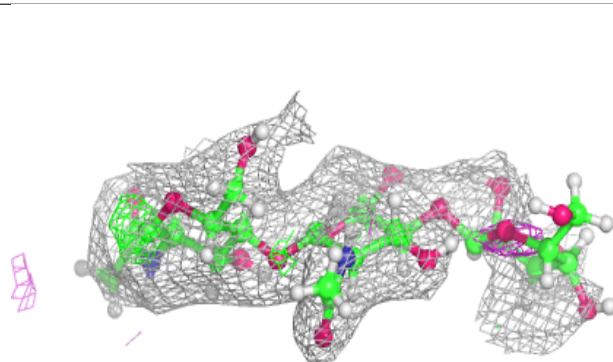
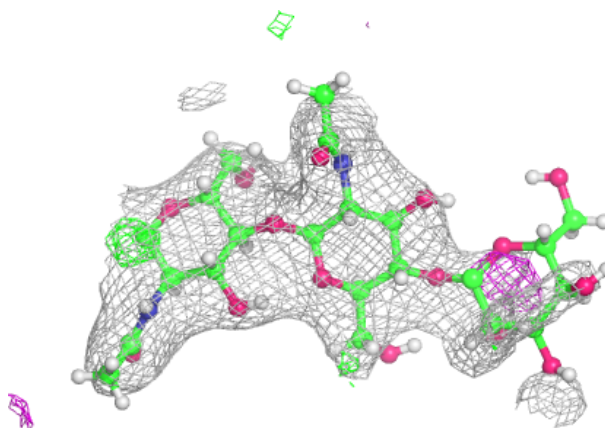
**Electron density around Chain G:**

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



**Electron density around Chain O:**

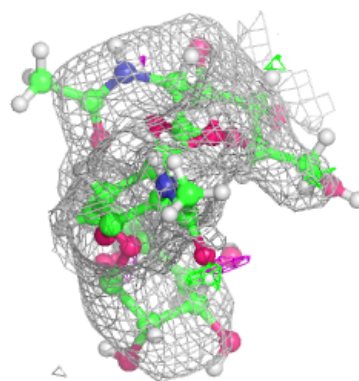
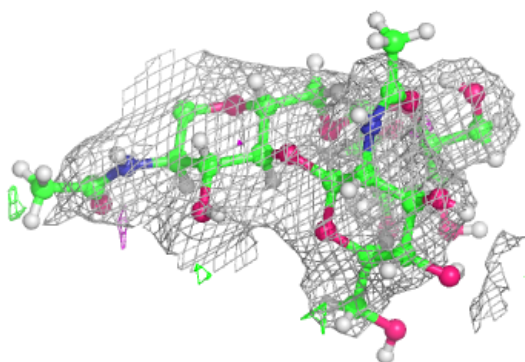
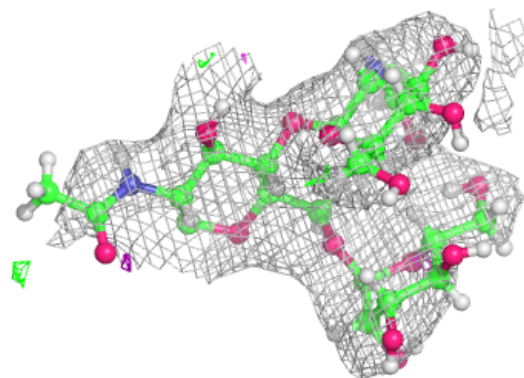
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



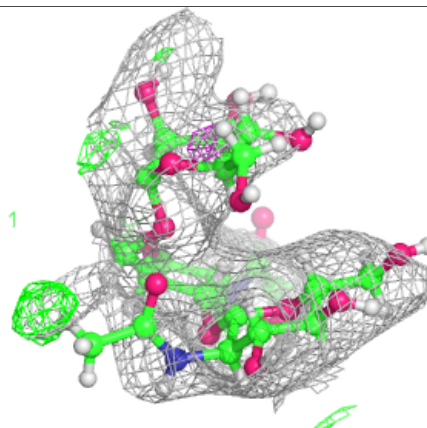
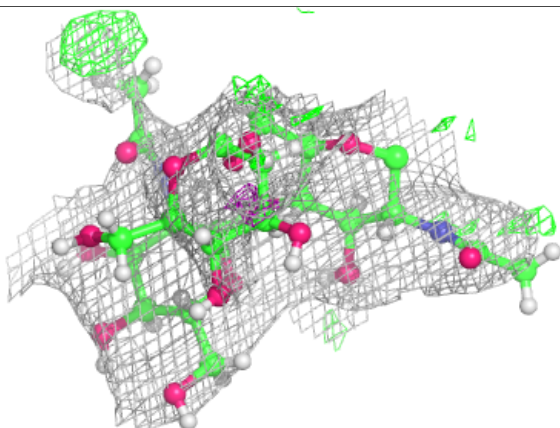
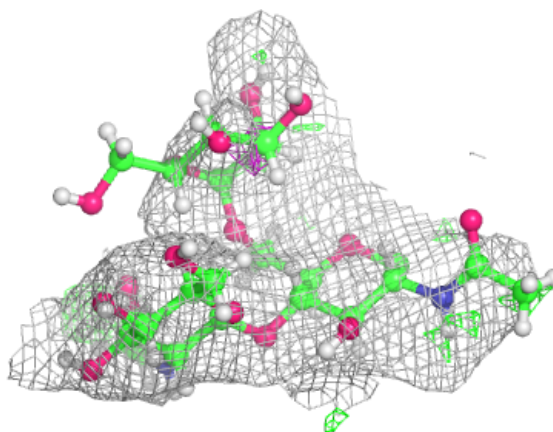


**Electron density around Chain I:**

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

**Electron density around Chain Q:**

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



## 6.4 Ligands ⓘ

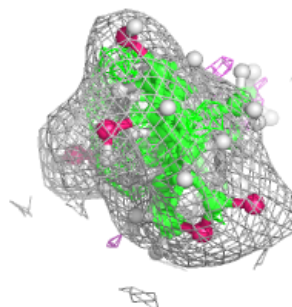
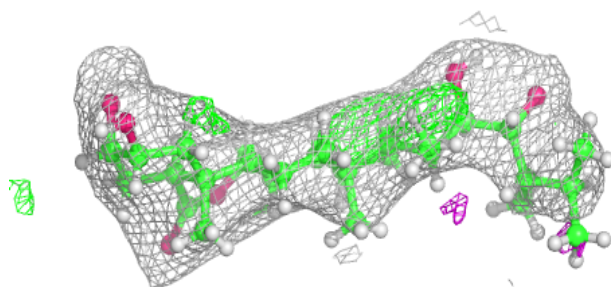
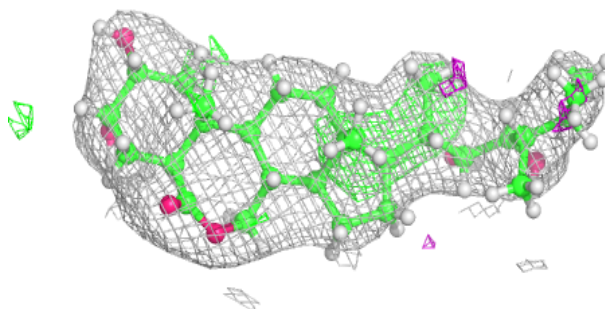
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
7	NAG	A	805	14/15	0.44	0.14	100,110,132,136	0
11	GLY	B	801	4/5	0.46	0.22	67,71,100,100	0
7	NAG	A	802	14/15	0.49	0.15	107,129,154,165	0
7	NAG	B	803	14/15	0.57	0.15	90,108,129,131	0
7	NAG	B	805	14/15	0.66	0.14	75,87,104,112	0
12	ACT	B	808	4/4	0.69	0.21	69,71,83,83	0
7	NAG	B	804	14/15	0.72	0.12	84,97,116,121	0
8	1PE	A	806	16/16	0.74	0.19	59,77,93,95	0
7	NAG	A	804	14/15	0.75	0.12	70,86,105,120	0
7	NAG	A	803	14/15	0.76	0.13	88,100,120,127	0
10	SO4	A	808	5/5	0.82	0.11	79,84,99,116	0
8	1PE	B	806	16/16	0.82	0.16	57,72,87,89	0
9	EDO	A	807	4/4	0.82	0.16	70,84,96,97	0
10	SO4	B	809	5/5	0.83	0.22	62,65,74,82	0
9	EDO	B	807	4/4	0.85	0.16	50,60,70,71	0
6	BLD	B	802	34/34	0.90	0.15	49,61,68,73	0
6	BLD	A	801	34/34	0.92	0.12	44,61,75,76	0

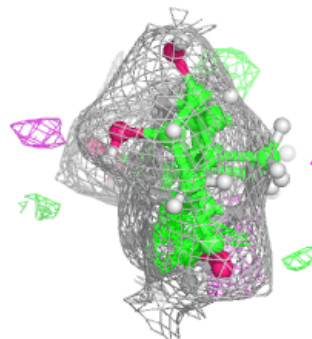
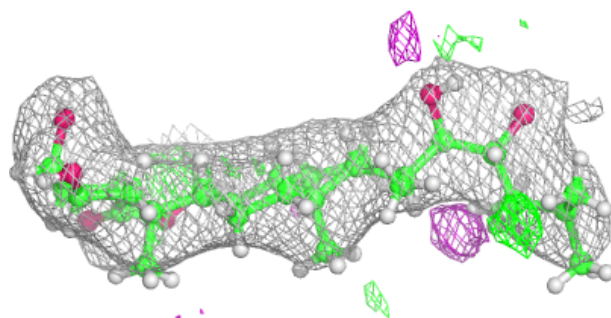
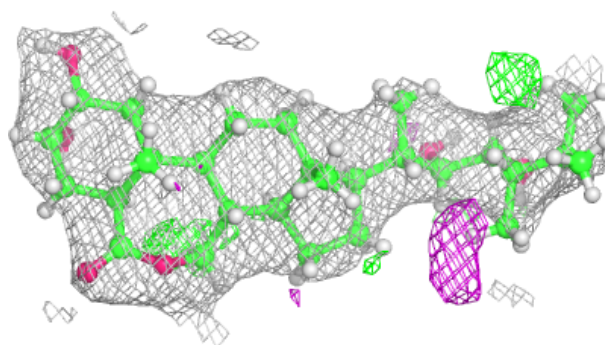
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around BLD B 802:**

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

**Electron density around BLD A 801:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.