



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 11, 2022 – 01:17 pm BST

PDB ID : 4UOJ  
Title : Structure of Fungal beta-mannosidase (GH2) from *Trichoderma harzianum*  
Authors : Muniz, J.R.C.; Aparicio, R.; Santos, J.C.; Nascimento, A.S.; Golubev, A.M.; Polikarpov, I.  
Deposited on : 2014-06-04  
Resolution : 2.50 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)

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 : 2.27  
buster-report : 1.1.7 (2018)  
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) : 2.27

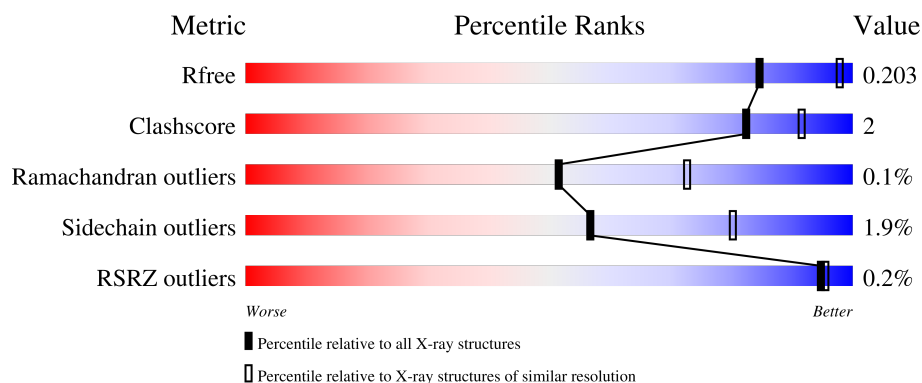
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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.



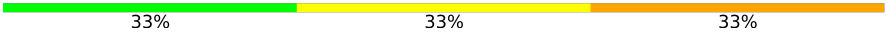
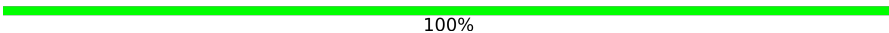



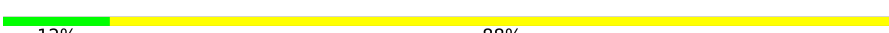



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	942	<div> <div>91%</div> <div>6%</div> <div>.</div> </div>
1	B	942	<div> <div>89%</div> <div>8%</div> <div>.</div> </div>
2	C	6	<div> <div>67%</div> <div>33%</div> </div>
2	J	6	<div> <div>33%</div> <div>67%</div> </div>
3	D	3	<div> <div>33%</div> <div>67%</div> </div>

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Mol	Chain	Length	Quality of chain
3	M	3	 33% 33% 33%
4	E	2	 100%
4	N	2	 50% 50%
5	F	11	 9% 91%
5	K	11	 27% 73%
6	G	8	 12% 88%
7	H	2	 50% 50%
7	L	2	 50% 50%
8	I	9	 22% 78%

## 2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 16996 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.

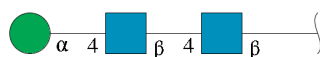
- Molecule 1 is a protein called BETA-MANNOSIDASE GH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	917	Total	C	N	O	S	0	2	0
			7259	4654	1213	1376	16			
1	B	917	Total	C	N	O	S	0	1	0
			7234	4634	1210	1374	16			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(2-6)]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
2	C	6	Total	C	N	O	0	0	0
			72	40	2	30			
2	J	6	Total	C	N	O	0	0	0
			71	40	2	29			

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



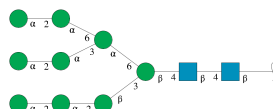
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



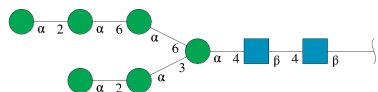
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	N	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-beta-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
5	F	11	Total	C	N	O	0	0	0
			127	70	2	55			
5	K	11	Total	C	N	O	0	0	0
			127	70	2	55			

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

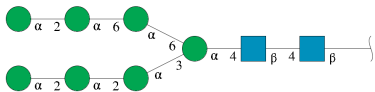


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	8	Total	C	N	O	0	0	0
			94	52	2	40			

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

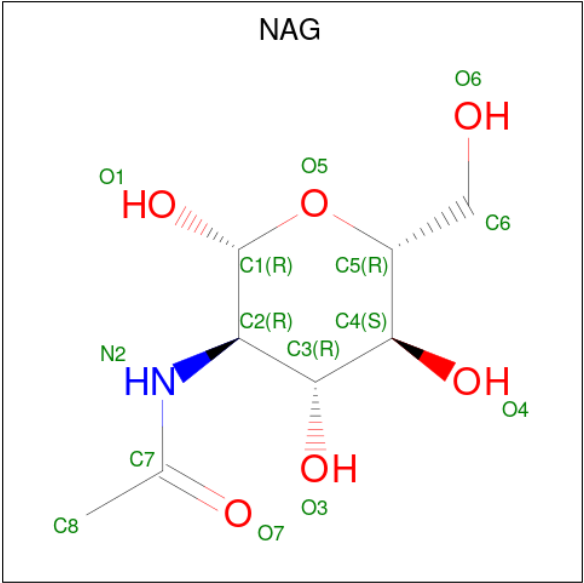
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 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-(1-6)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	I	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 9 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
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

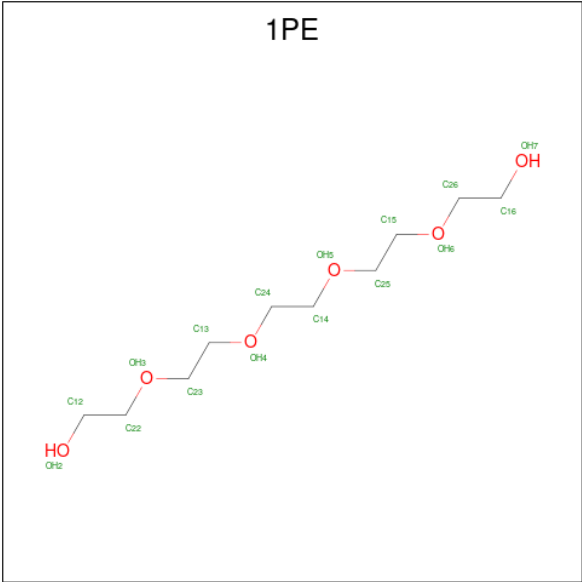
- Molecule 10 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	16	Total	Cd	0	0
			16	16		
10	B	12	Total	Cd	0	0
			12	12		

- Molecule 11 is SODIUM ION (three-letter code: NA) (formula: Na).

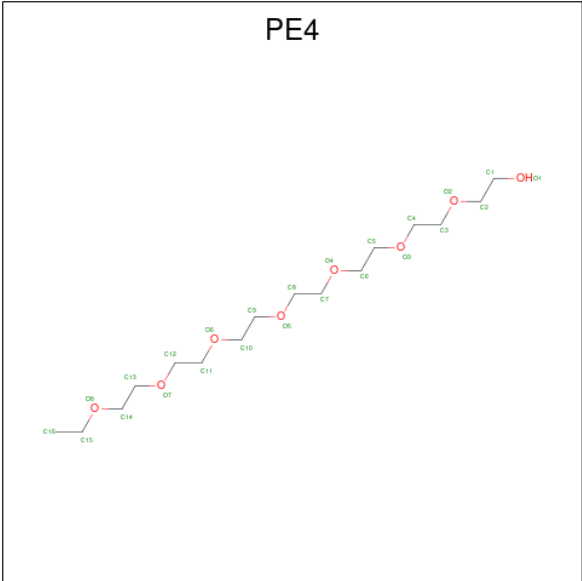
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total	Na	0	0
			2	2		
11	B	1	Total	Na	0	0
			1	1		

- Molecule 12 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			9	6	3		
12	B	1	Total	C	O	0	0
			9	6	3		

- Molecule 13 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 14 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	B	1	Total	Cl	0	0
			1	1		

- Molecule 15 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	B	1	Total	Ca	0	0
			1	1		

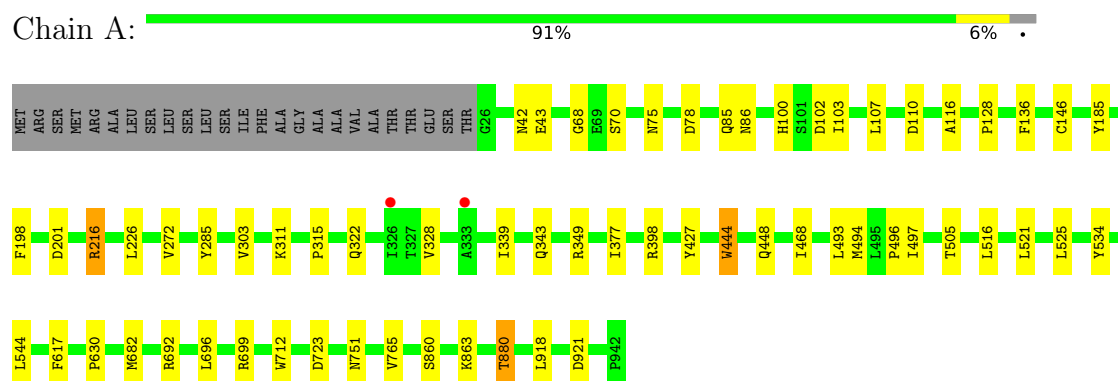
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	731	Total	O	0	0
			731	731		
16	B	769	Total	O	0	0
			769	769		

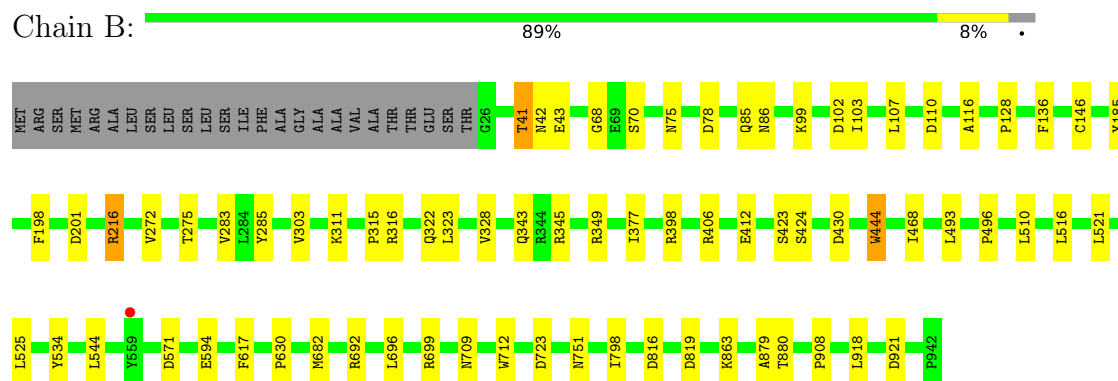
### 3 Residue-property plots

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.

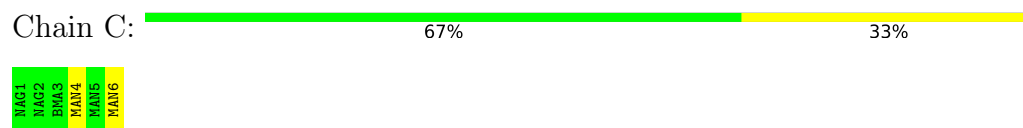
#### • Molecule 1: BETA-MANNOSIDASE GH2



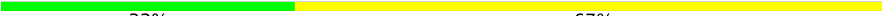
#### • Molecule 1: BETA-MANNOSIDASE GH2

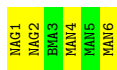


#### • Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(2-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

Chain J:  33% 67%




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

Chain D:  33% 67%



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

Chain M:  33% 33% 33%



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

Chain E:  100%



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

Chain N:  50% 50%



- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-beta-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% 91%



- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-beta-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 K:  27% 73%



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

Chain G:  12% 88%



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

Chain H:  50% 50%



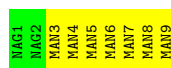
- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(3-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  50% 50%



- Molecule 8:  $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-6)- $\alpha$ -D-mannopyranose-(1-6)] $\alpha$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  22% 78%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	165.16Å 165.63Å 123.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	117.23 – 2.50 98.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (117.23-2.50) 99.1 (98.94-2.50)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.179 , 0.201 0.180 , 0.203	Depositor DCC
$R_{free}$ test set	5871 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.3	Xtriage
Anisotropy	0.625	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>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.350 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16996	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: CA, NA, CL, 1PE, BMA, MAN, CD, PE4, 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	A	0.58	0/7491	0.67	1/10260 (0.0%)
1	B	0.59	0/7459	0.67	1/10217 (0.0%)
All	All	0.59	0/14950	0.67	2/20477 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	723	ASP	CB-CG-OD1	5.94	123.65	118.30
1	B	723	ASP	CB-CG-OD1	5.76	123.48	118.30

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	A	7259	0	6837	29	0
1	B	7234	0	6809	39	0
2	C	72	0	61	0	0
2	J	71	0	59	2	0
3	D	39	0	34	2	0
3	M	39	0	34	1	0
4	E	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	28	0	25	1	0
5	F	127	0	105	0	0
5	K	127	0	106	0	0
6	G	94	0	79	0	0
7	H	28	0	25	1	0
7	L	28	0	25	1	0
8	I	105	0	88	0	0
9	A	70	0	65	0	0
9	B	70	0	65	0	0
10	A	16	0	0	0	0
10	B	12	0	0	0	0
11	A	2	0	0	0	0
11	B	1	0	0	0	0
12	A	9	0	10	0	0
12	B	9	0	10	0	0
13	A	10	0	13	2	0
13	B	16	0	21	2	0
14	B	1	0	0	0	0
15	B	1	0	0	0	0
16	A	731	0	0	3	0
16	B	769	0	0	6	0
All	All	16996	0	14496	73	0

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

The worst 5 of 73 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:B:68:GLY:HA3	16:B:1659:HOH:O	1.81	0.80
1:B:323:LEU:HD13	1:B:345:ARG:HD3	1.62	0.80
1:A:68:GLY:HA3	16:A:1645:HOH:O	1.85	0.77
1:A:42:ASN:HB2	1:A:85:GLN:OE1	1.86	0.76
1:B:43:GLU:HG3	1:B:86:ASN:HB2	1.70	0.73

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	917/942 (97%)	894 (98%)	23 (2%)	0	100	100
1	B	916/942 (97%)	889 (97%)	26 (3%)	1 (0%)	51	73
All	All	1833/1884 (97%)	1783 (97%)	49 (3%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	798	ILE

### 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	778/811 (96%)	763 (98%)	15 (2%)	57	80
1	B	774/811 (95%)	760 (98%)	14 (2%)	59	81
All	All	1552/1622 (96%)	1523 (98%)	29 (2%)	57	80

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	880	THR
1	B	712	TRP
1	B	99	LYS
1	B	444	TRP
1	B	70	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 ⓘ

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

## 5.5 Carbohydrates ⓘ

65 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	0.30	0	17,19,21	0.46	0
2	NAG	C	2	2	14,14,15	0.38	0	17,19,21	0.76	0
2	BMA	C	3	2	11,11,12	0.53	0	15,15,17	0.73	0
2	MAN	C	4	2	11,11,12	0.46	0	15,15,17	0.94	1 (6%)
2	MAN	C	5	2	11,11,12	0.52	0	15,15,17	0.58	0
2	MAN	C	6	2	11,11,12	0.59	0	13,15,17	1.09	1 (7%)
3	NAG	D	1	1,3	14,14,15	0.40	0	17,19,21	2.57	4 (23%)
3	NAG	D	2	3	14,14,15	0.71	0	17,19,21	0.88	1 (5%)
3	MAN	D	3	3	11,11,12	0.59	0	15,15,17	1.19	1 (6%)
4	NAG	E	1	1,4	14,14,15	0.58	0	17,19,21	0.83	0
4	NAG	E	2	4	14,14,15	0.60	0	17,19,21	0.70	0
5	NAG	F	1	1,5	14,14,15	0.43	0	17,19,21	0.82	1 (5%)
5	MAN	F	10	5	11,11,12	0.31	0	15,15,17	0.90	1 (6%)
5	MAN	F	11	5	11,11,12	0.56	0	15,15,17	0.83	1 (6%)
5	NAG	F	2	5	14,14,15	0.98	1 (7%)	17,19,21	1.63	2 (11%)
5	BMA	F	3	5	11,11,12	0.40	0	15,15,17	1.50	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BMA	F	4	5	11,11,12	0.35	0	15,15,17	1.66	3 (20%)
5	MAN	F	5	5	11,11,12	0.24	0	15,15,17	1.10	1 (6%)
5	MAN	F	6	5	11,11,12	0.51	0	15,15,17	0.72	1 (6%)
5	MAN	F	7	5	11,11,12	0.85	1 (9%)	15,15,17	2.43	1 (6%)
5	MAN	F	8	5	11,11,12	0.74	0	15,15,17	1.98	2 (13%)
5	MAN	F	9	5	11,11,12	0.42	0	15,15,17	0.72	0
6	NAG	G	1	1,6	14,14,15	0.64	0	17,19,21	0.72	0
6	NAG	G	2	6	14,14,15	0.92	0	17,19,21	1.30	3 (17%)
6	MAN	G	3	6	11,11,12	0.49	0	15,15,17	1.49	2 (13%)
6	MAN	G	4	6	11,11,12	0.89	0	15,15,17	0.95	1 (6%)
6	MAN	G	5	6	11,11,12	0.62	0	15,15,17	0.76	1 (6%)
6	MAN	G	6	6	11,11,12	0.50	0	15,15,17	0.91	1 (6%)
6	MAN	G	7	6	11,11,12	0.41	0	15,15,17	1.20	1 (6%)
6	MAN	G	8	6	11,11,12	0.42	0	15,15,17	1.10	1 (6%)
7	NAG	H	1	1,7	14,14,15	0.51	0	17,19,21	0.74	0
7	NAG	H	2	7	14,14,15	1.01	1 (7%)	19,19,21	2.48	3 (15%)
8	NAG	I	1	8,1	14,14,15	0.59	0	17,19,21	0.55	0
8	NAG	I	2	8	14,14,15	0.41	0	17,19,21	0.64	0
8	MAN	I	3	8	11,11,12	0.71	0	15,15,17	1.32	2 (13%)
8	MAN	I	4	8	11,11,12	0.41	0	15,15,17	0.84	1 (6%)
8	MAN	I	5	8	11,11,12	0.46	0	15,15,17	1.28	1 (6%)
8	MAN	I	6	8	11,11,12	0.62	0	15,15,17	1.67	3 (20%)
8	MAN	I	7	8	11,11,12	0.81	0	15,15,17	1.03	1 (6%)
8	MAN	I	8	8	11,11,12	0.61	0	15,15,17	0.85	1 (6%)
8	MAN	I	9	8	11,11,12	0.66	0	15,15,17	0.82	1 (6%)
2	NAG	J	1	1,2	14,14,15	0.28	0	17,19,21	0.64	0
2	NAG	J	2	2	14,14,15	0.50	0	17,19,21	0.96	0
2	BMA	J	3	2	11,11,12	0.42	0	15,15,17	0.70	0
2	MAN	J	4	2	11,11,12	0.24	0	15,15,17	1.05	1 (6%)
2	MAN	J	5	2	11,11,12	0.42	0	15,15,17	0.67	0
2	MAN	J	6	2	10,10,12	1.15	1 (10%)	13,13,17	2.10	3 (23%)
5	NAG	K	1	1,5	14,14,15	0.48	0	17,19,21	0.84	1 (5%)
5	MAN	K	10	5	11,11,12	0.35	0	15,15,17	0.68	0
5	MAN	K	11	5	11,11,12	0.47	0	15,15,17	0.77	1 (6%)
5	NAG	K	2	5	14,14,15	0.30	0	17,19,21	0.59	0
5	BMA	K	3	5	11,11,12	0.53	0	15,15,17	1.74	1 (6%)
5	BMA	K	4	5	11,11,12	0.55	0	15,15,17	1.64	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MAN	K	5	5	11,11,12	0.23	0	15,15,17	0.95	1 (6%)
5	MAN	K	6	5	11,11,12	0.39	0	15,15,17	0.83	1 (6%)
5	MAN	K	7	5	11,11,12	0.59	0	15,15,17	1.68	2 (13%)
5	MAN	K	8	5	11,11,12	0.68	0	15,15,17	0.54	0
5	MAN	K	9	5	11,11,12	0.39	0	15,15,17	0.88	1 (6%)
7	NAG	L	1	1,7	14,14,15	0.59	0	17,19,21	0.76	0
7	NAG	L	2	7	14,14,15	0.91	1 (7%)	19,19,21	2.39	3 (15%)
3	NAG	M	1	1,3	14,14,15	0.27	0	17,19,21	0.96	1 (5%)
3	NAG	M	2	3	14,14,15	0.71	0	17,19,21	0.71	0
3	MAN	M	3	3	11,11,12	0.61	0	15,15,17	1.20	2 (13%)
4	NAG	N	1	1,4	14,14,15	0.97	0	17,19,21	1.74	5 (29%)
4	NAG	N	2	4	14,14,15	0.69	0	17,19,21	0.65	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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	C	6	2	-	0/2/18/22	0/1/1/1
3	NAG	D	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	MAN	D	3	3	-	2/2/19/22	1/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	MAN	F	10	5	-	0/2/19/22	0/1/1/1
5	MAN	F	11	5	-	0/2/19/22	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	BMA	F	4	5	-	0/2/19/22	0/1/1/1
5	MAN	F	5	5	-	0/2/19/22	0/1/1/1
5	MAN	F	6	5	-	0/2/19/22	0/1/1/1
5	MAN	F	7	5	-	0/2/19/22	0/1/1/1
5	MAN	F	8	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	F	9	5	-	0/2/19/22	0/1/1/1
6	NAG	G	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	1/6/23/26	0/1/1/1
6	MAN	G	3	6	-	2/2/19/22	1/1/1/1
6	MAN	G	4	6	-	0/2/19/22	0/1/1/1
6	MAN	G	5	6	-	1/2/19/22	0/1/1/1
6	MAN	G	6	6	-	0/2/19/22	0/1/1/1
6	MAN	G	7	6	-	0/2/19/22	0/1/1/1
6	MAN	G	8	6	-	0/2/19/22	0/1/1/1
7	NAG	H	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	H	2	7	-	2/6/22/26	0/1/1/1
8	NAG	I	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	I	2	8	-	0/6/23/26	0/1/1/1
8	MAN	I	3	8	-	0/2/19/22	1/1/1/1
8	MAN	I	4	8	-	0/2/19/22	0/1/1/1
8	MAN	I	5	8	-	0/2/19/22	0/1/1/1
8	MAN	I	6	8	-	2/2/19/22	0/1/1/1
8	MAN	I	7	8	-	0/2/19/22	0/1/1/1
8	MAN	I	8	8	-	0/2/19/22	0/1/1/1
8	MAN	I	9	8	-	0/2/19/22	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	BMA	J	3	2	-	0/2/19/22	0/1/1/1
2	MAN	J	4	2	-	0/2/19/22	0/1/1/1
2	MAN	J	5	2	-	0/2/19/22	0/1/1/1
2	MAN	J	6	2	-	0/2/16/22	0/1/1/1
5	NAG	K	1	1,5	-	0/6/23/26	0/1/1/1
5	MAN	K	10	5	-	0/2/19/22	0/1/1/1
5	MAN	K	11	5	-	0/2/19/22	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	BMA	K	4	5	-	0/2/19/22	0/1/1/1
5	MAN	K	5	5	-	0/2/19/22	0/1/1/1
5	MAN	K	6	5	-	0/2/19/22	0/1/1/1
5	MAN	K	7	5	-	0/2/19/22	0/1/1/1
5	MAN	K	8	5	-	0/2/19/22	0/1/1/1
5	MAN	K	9	5	-	0/2/19/22	0/1/1/1
7	NAG	L	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	L	2	7	-	2/6/22/26	0/1/1/1
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	2	NAG	C1-C2	3.25	1.56	1.52
7	L	2	NAG	C1-C2	2.90	1.56	1.52
5	F	2	NAG	O5-C1	-2.36	1.40	1.43
2	J	6	MAN	O5-C1	2.24	1.49	1.44
5	F	7	MAN	O3-C3	-2.09	1.38	1.43

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	7	MAN	O3-C3-C4	-8.94	89.69	110.35
7	H	2	NAG	C1-C2-N2	-8.74	100.60	110.73
7	L	2	NAG	C1-C2-N2	-8.50	100.88	110.73
3	D	1	NAG	C1-O5-C5	8.09	123.15	112.19
5	F	8	MAN	O5-C1-C2	-6.52	100.71	110.77

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	N	1	NAG	C8-C7-N2-C2
8	I	6	MAN	O5-C5-C6-O6
3	D	3	MAN	C4-C5-C6-O6

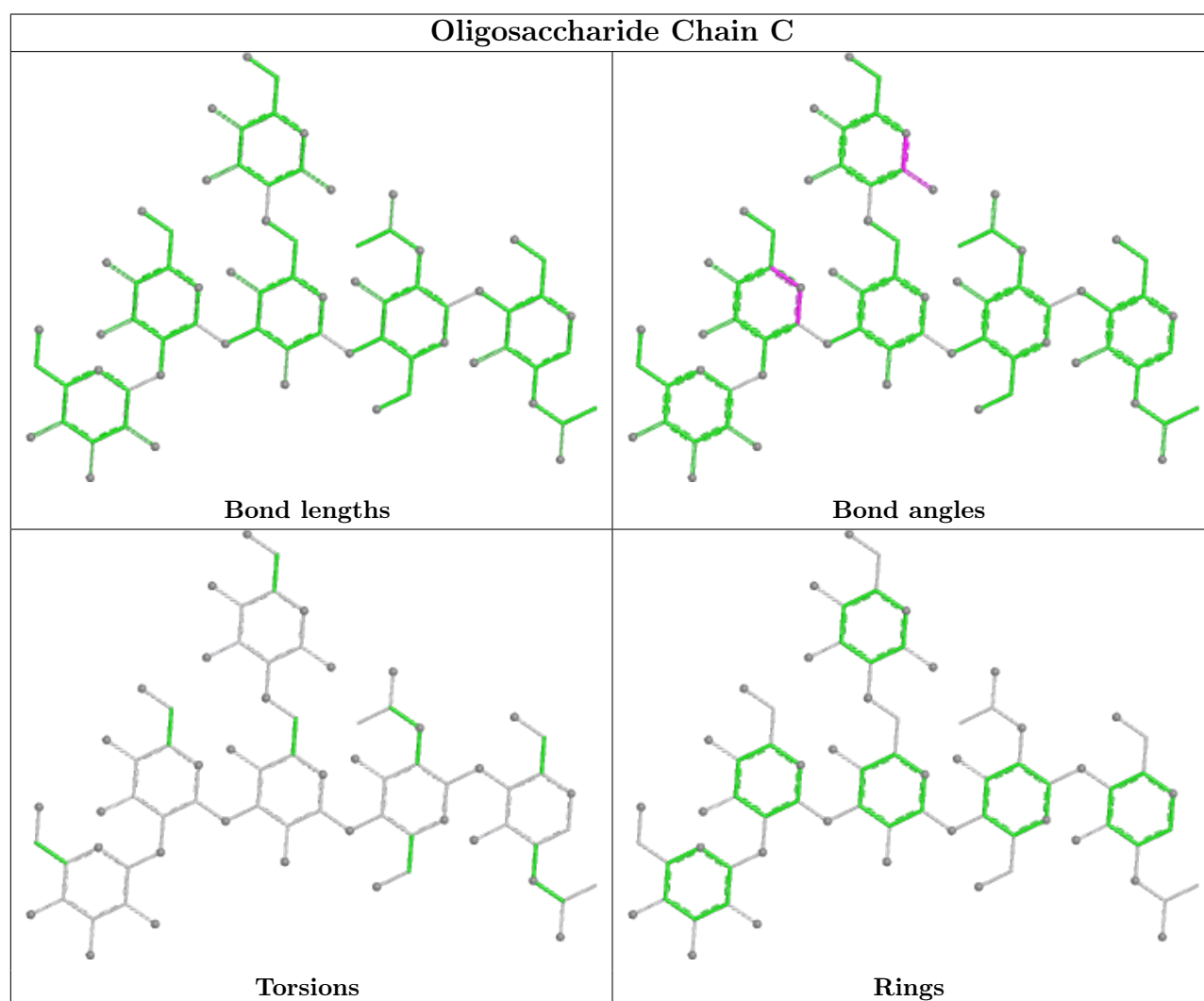
All (4) ring outliers are listed below:

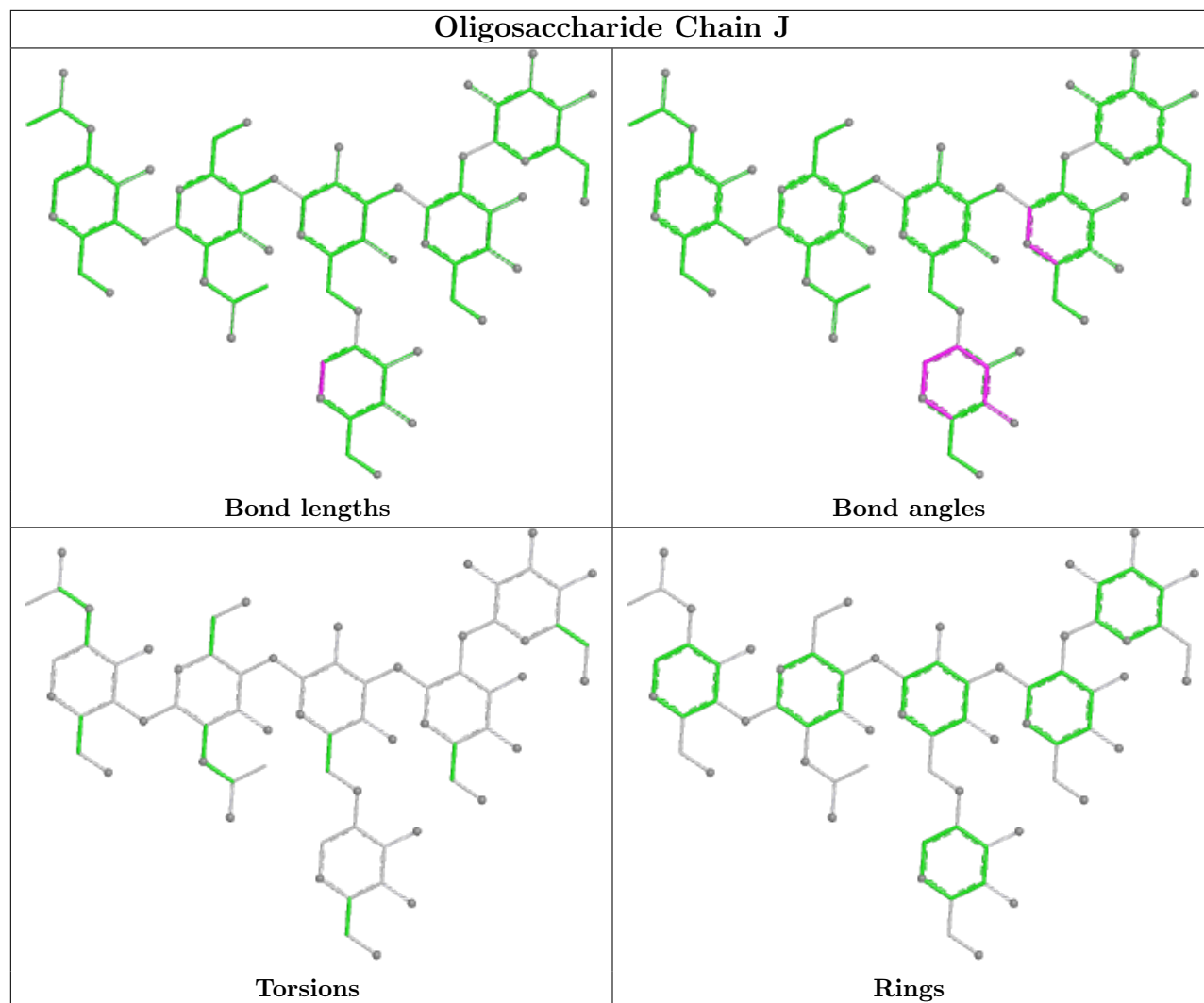
Mol	Chain	Res	Type	Atoms
3	M	3	MAN	C1-C2-C3-C4-C5-O5
8	I	3	MAN	C1-C2-C3-C4-C5-O5
3	D	3	MAN	C1-C2-C3-C4-C5-O5
6	G	3	MAN	C1-C2-C3-C4-C5-O5

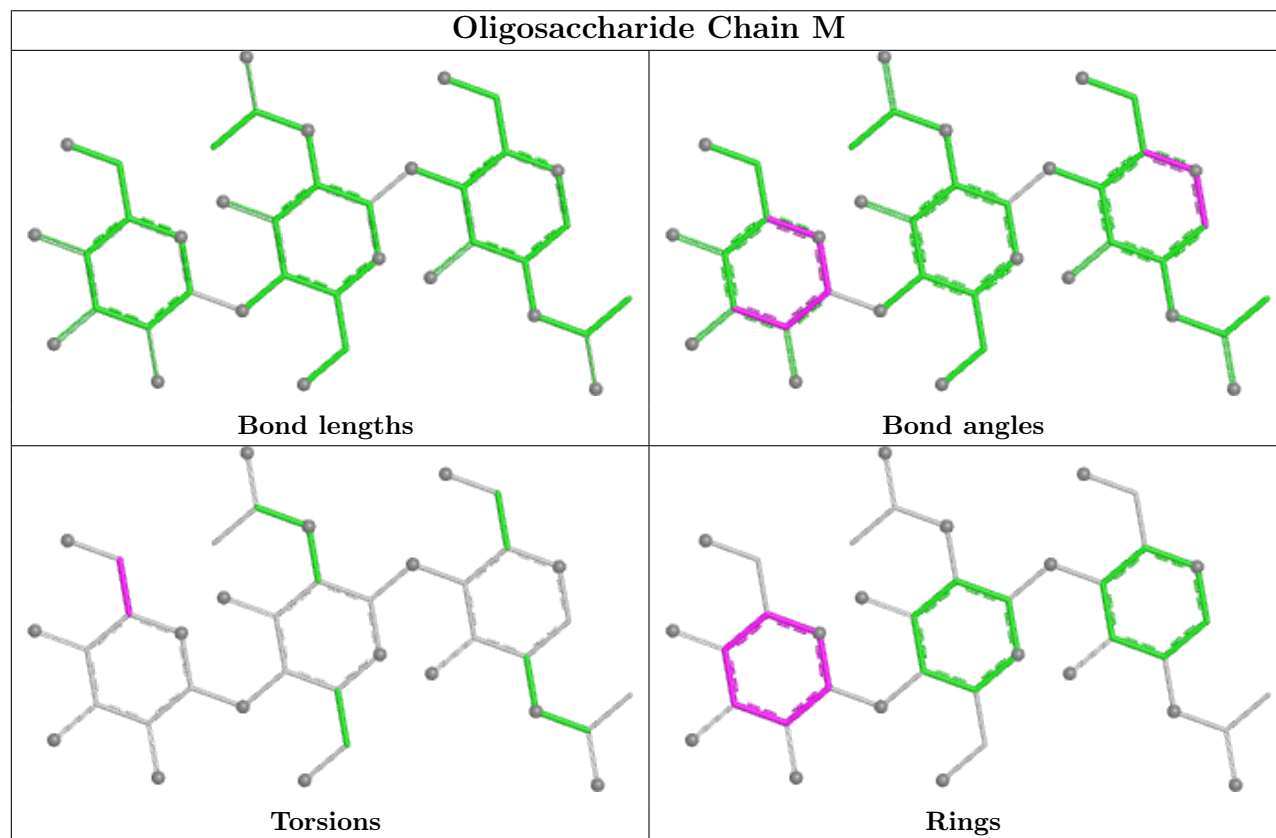
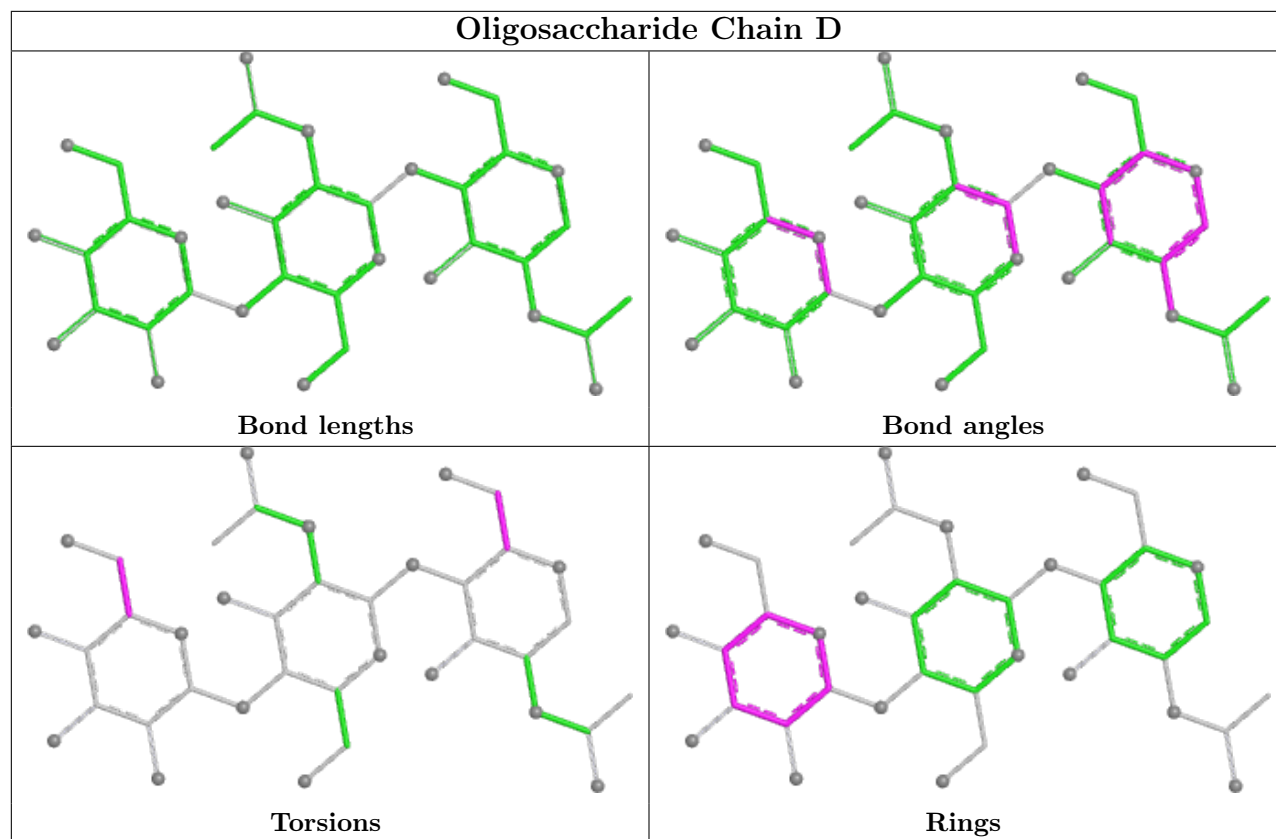
8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	1	NAG	1	0
4	N	1	NAG	1	0
7	H	2	NAG	1	0
3	D	1	NAG	1	0
2	J	2	NAG	2	0
3	M	1	NAG	1	0
7	L	2	NAG	1	0
3	D	3	MAN	1	0

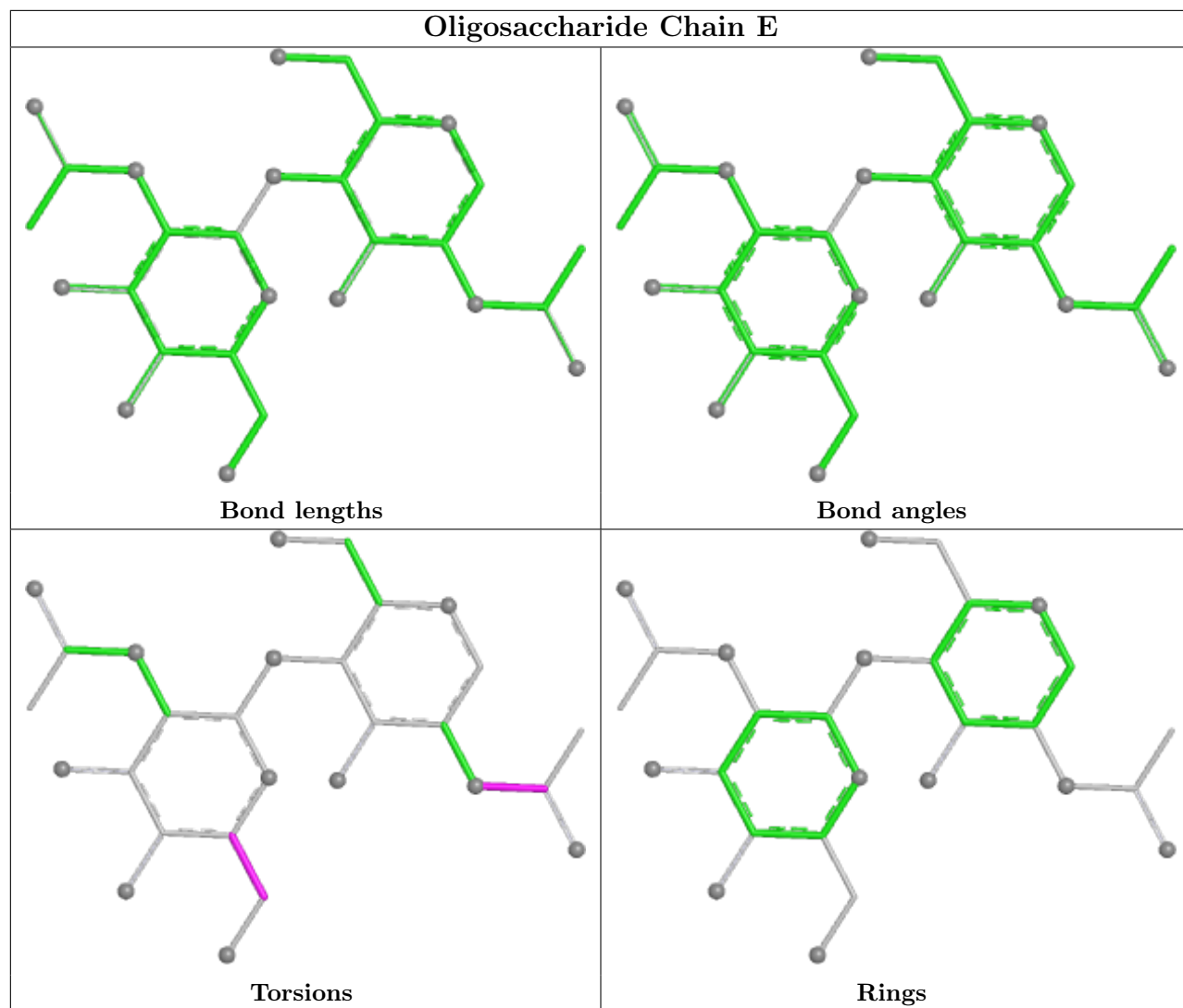
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

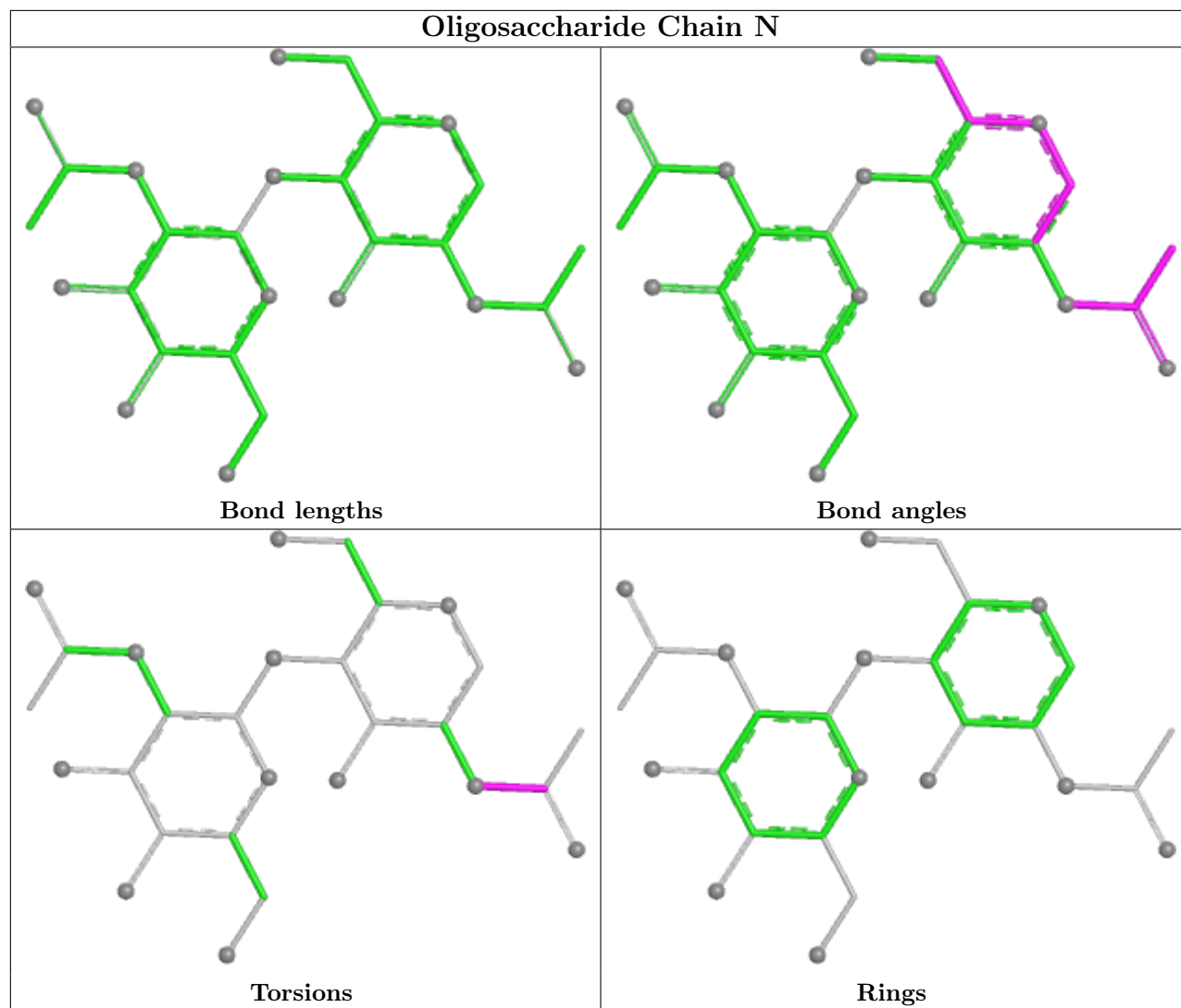


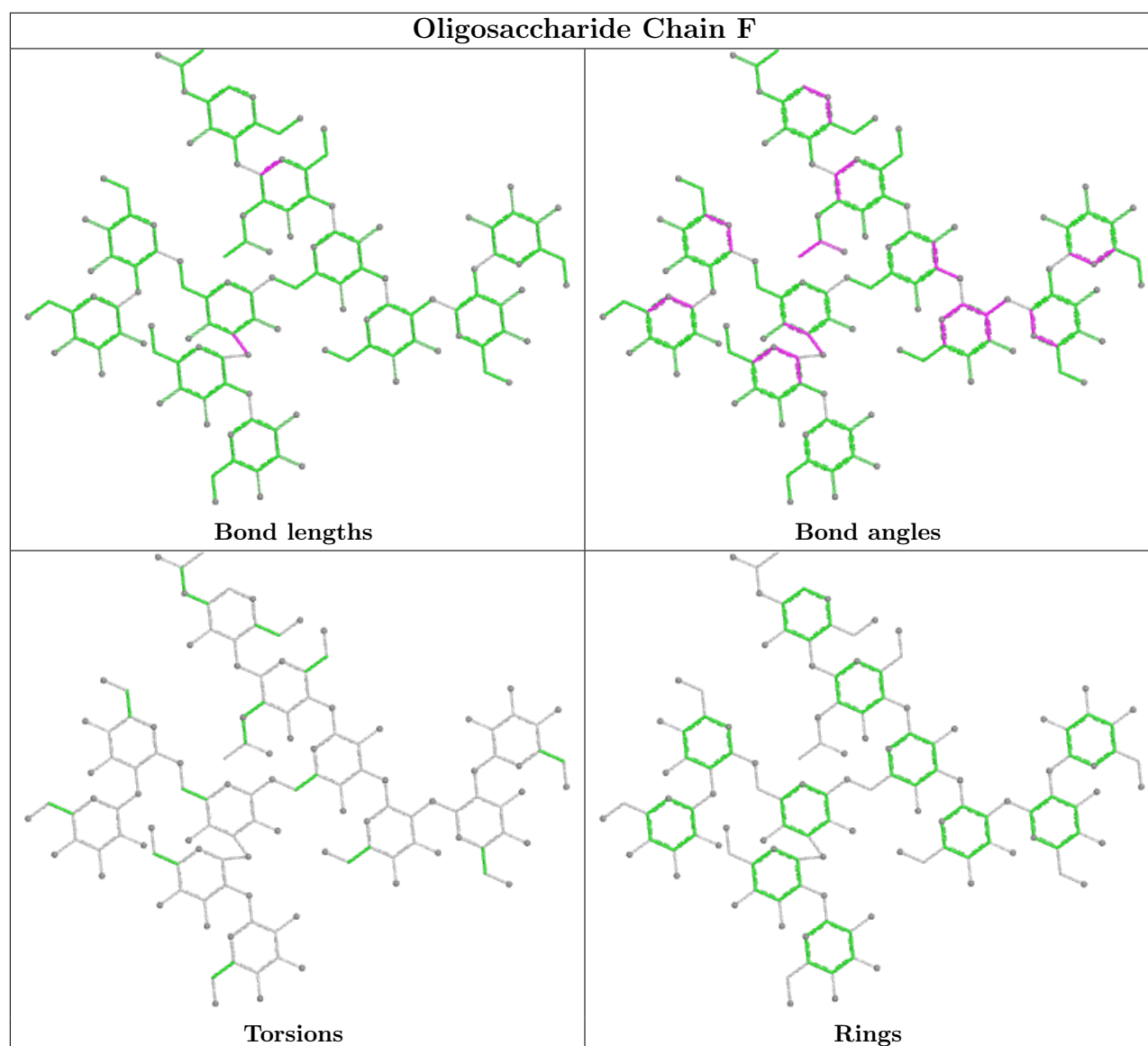


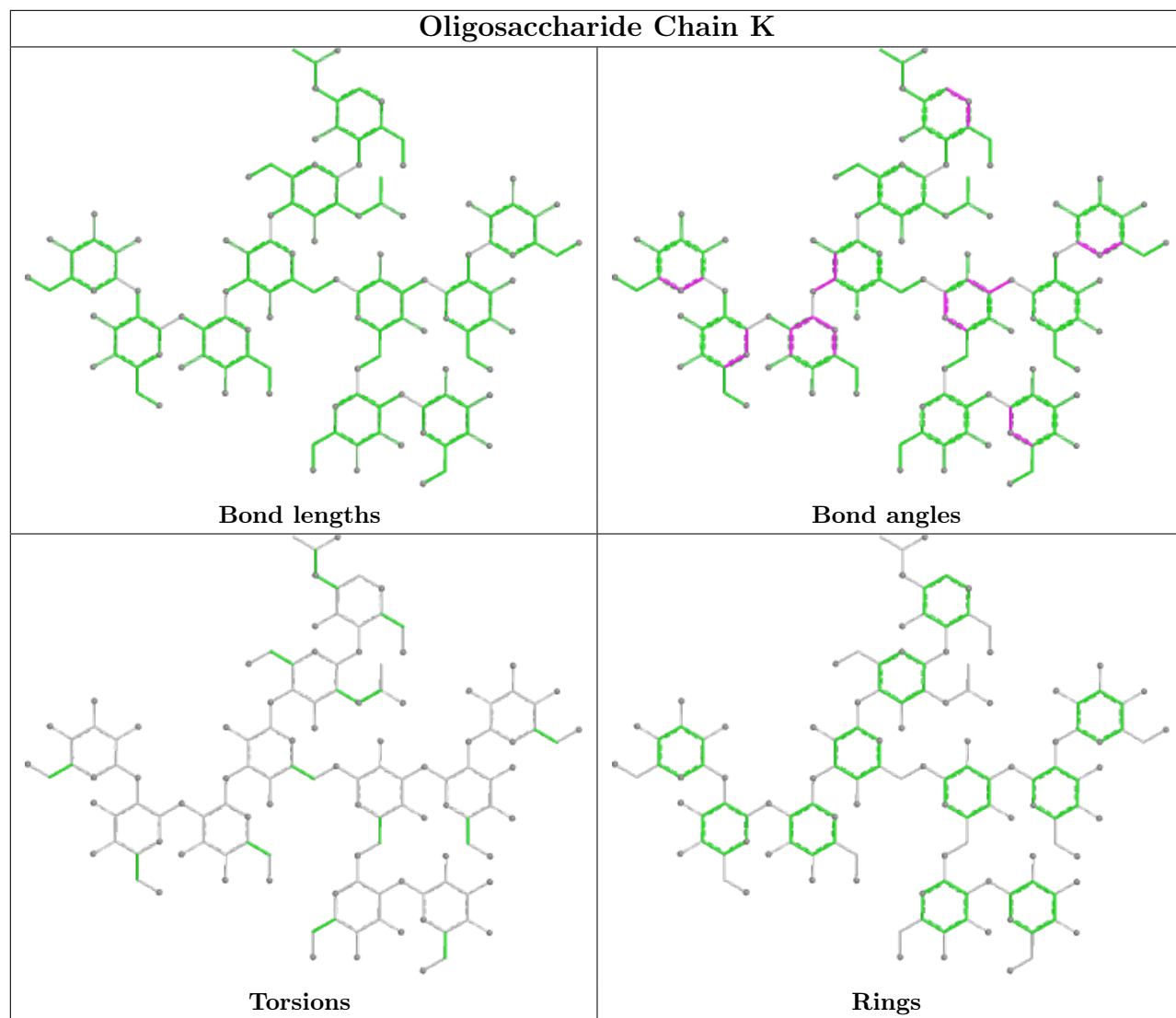


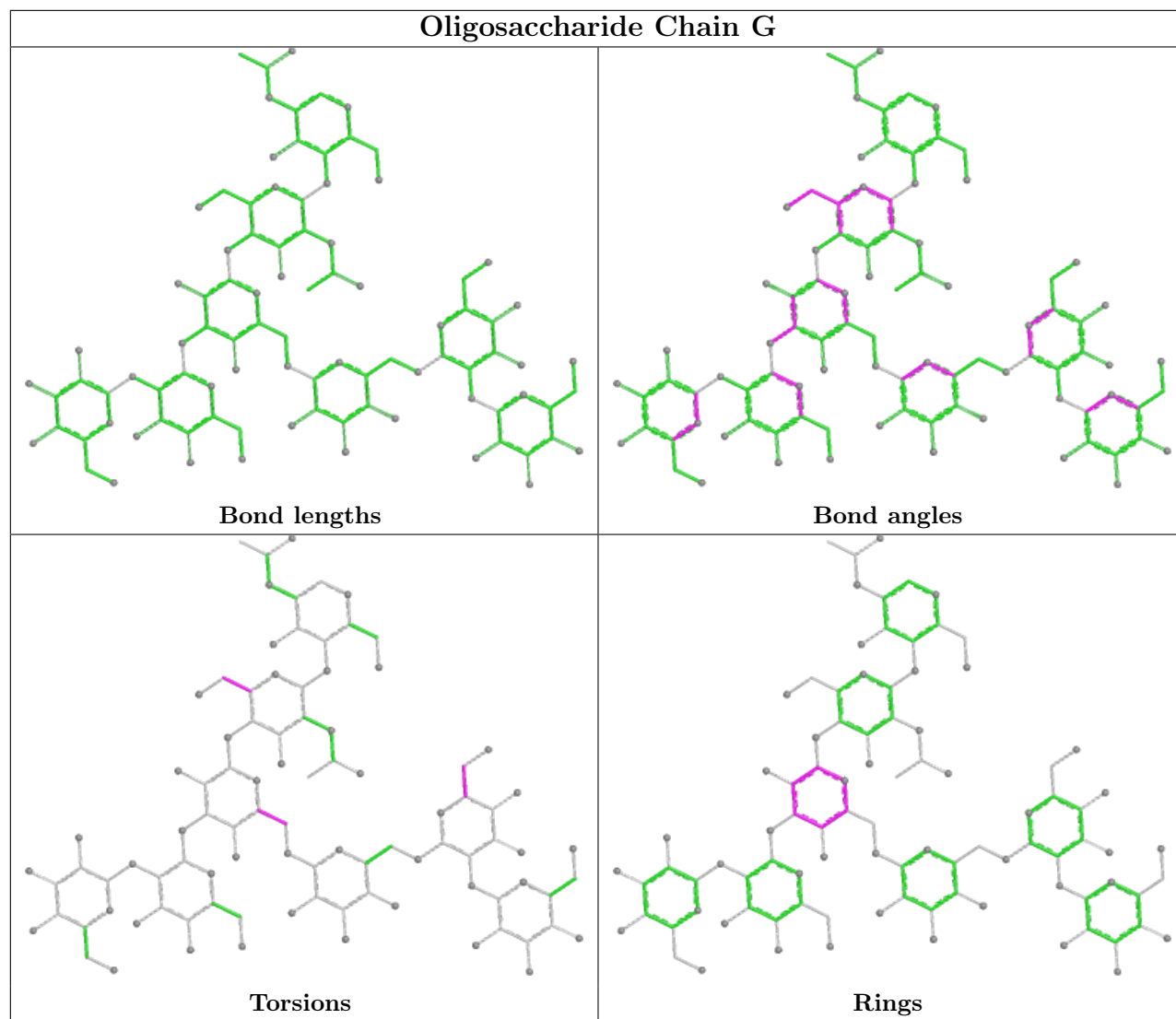


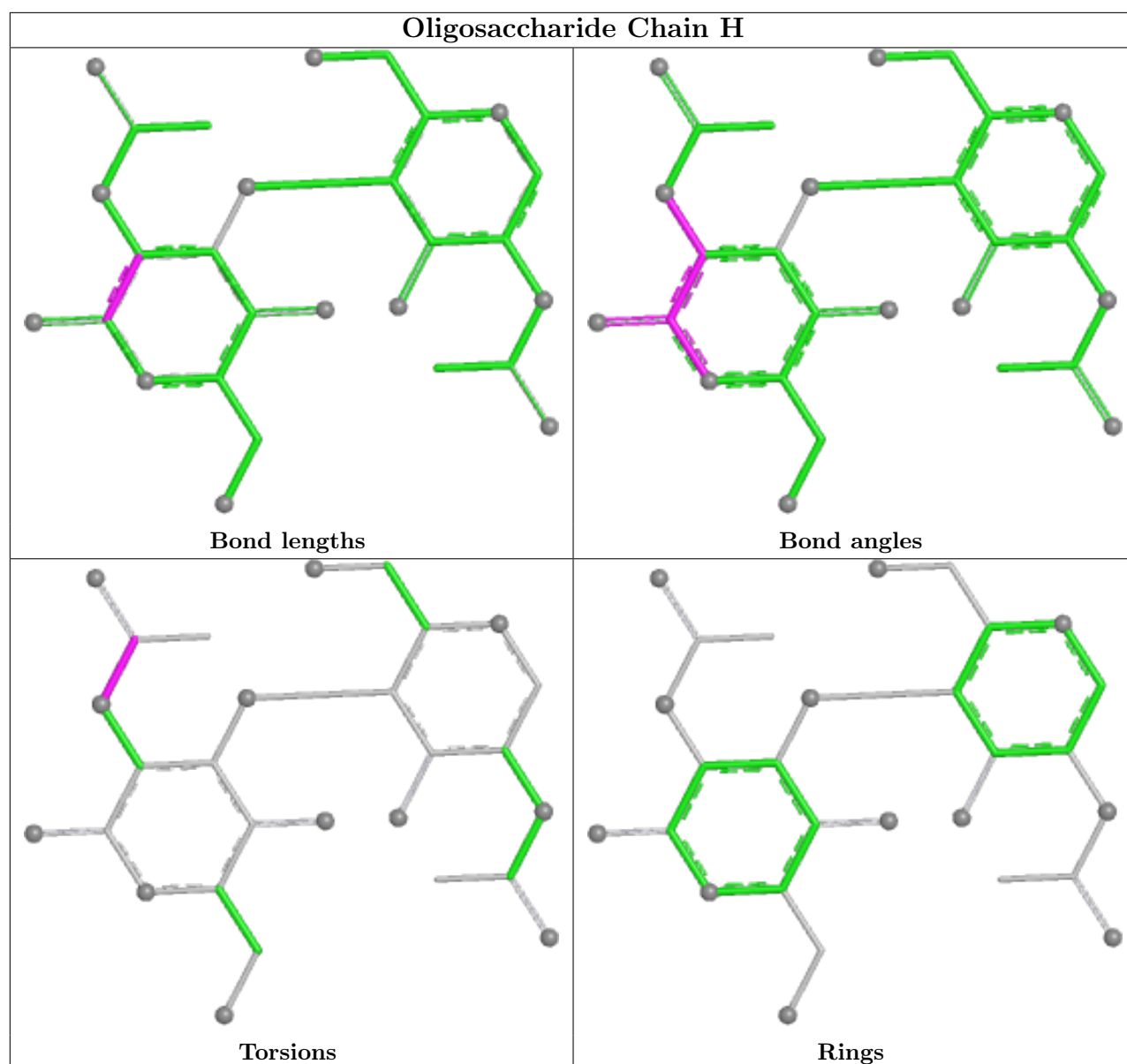


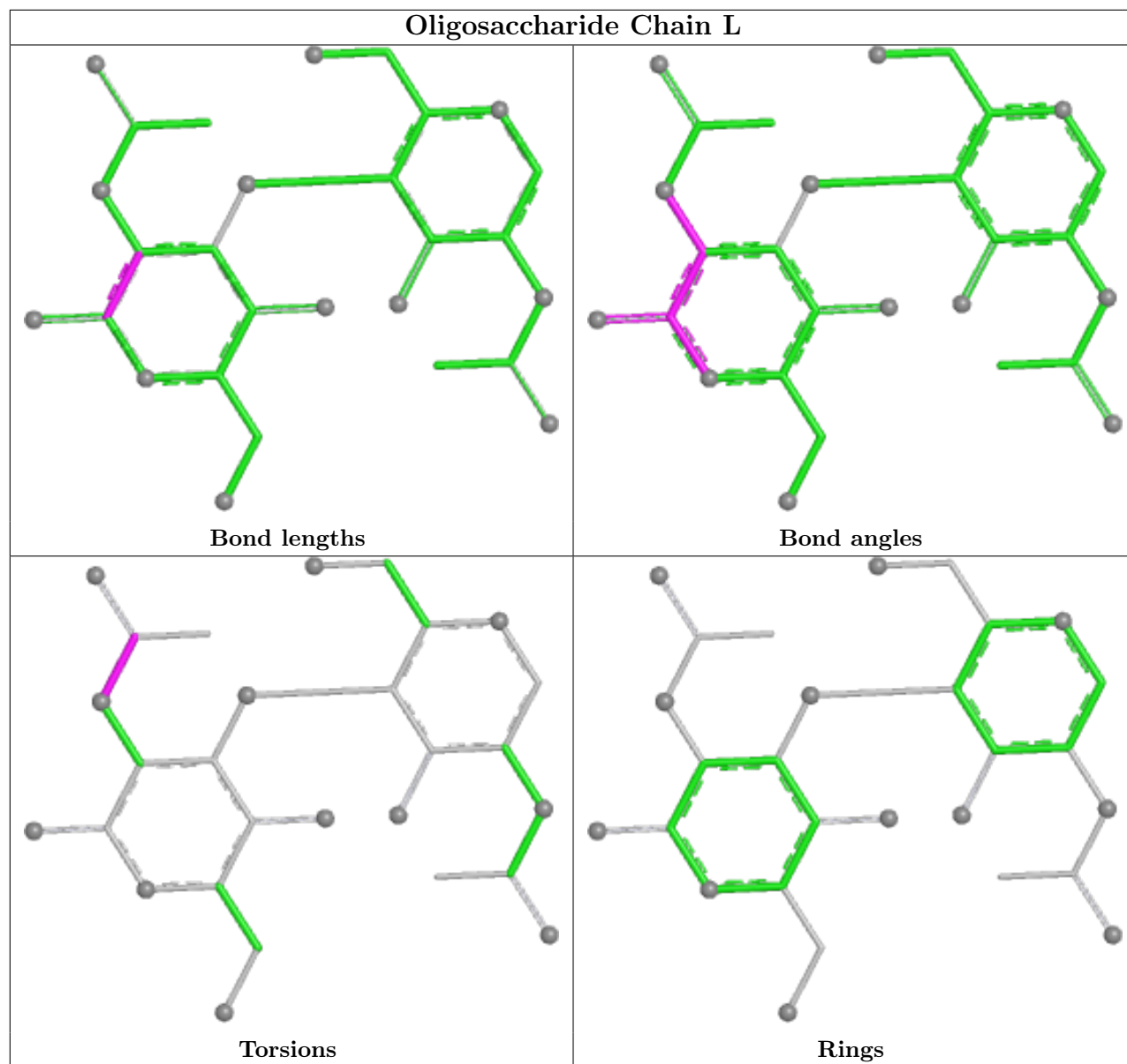


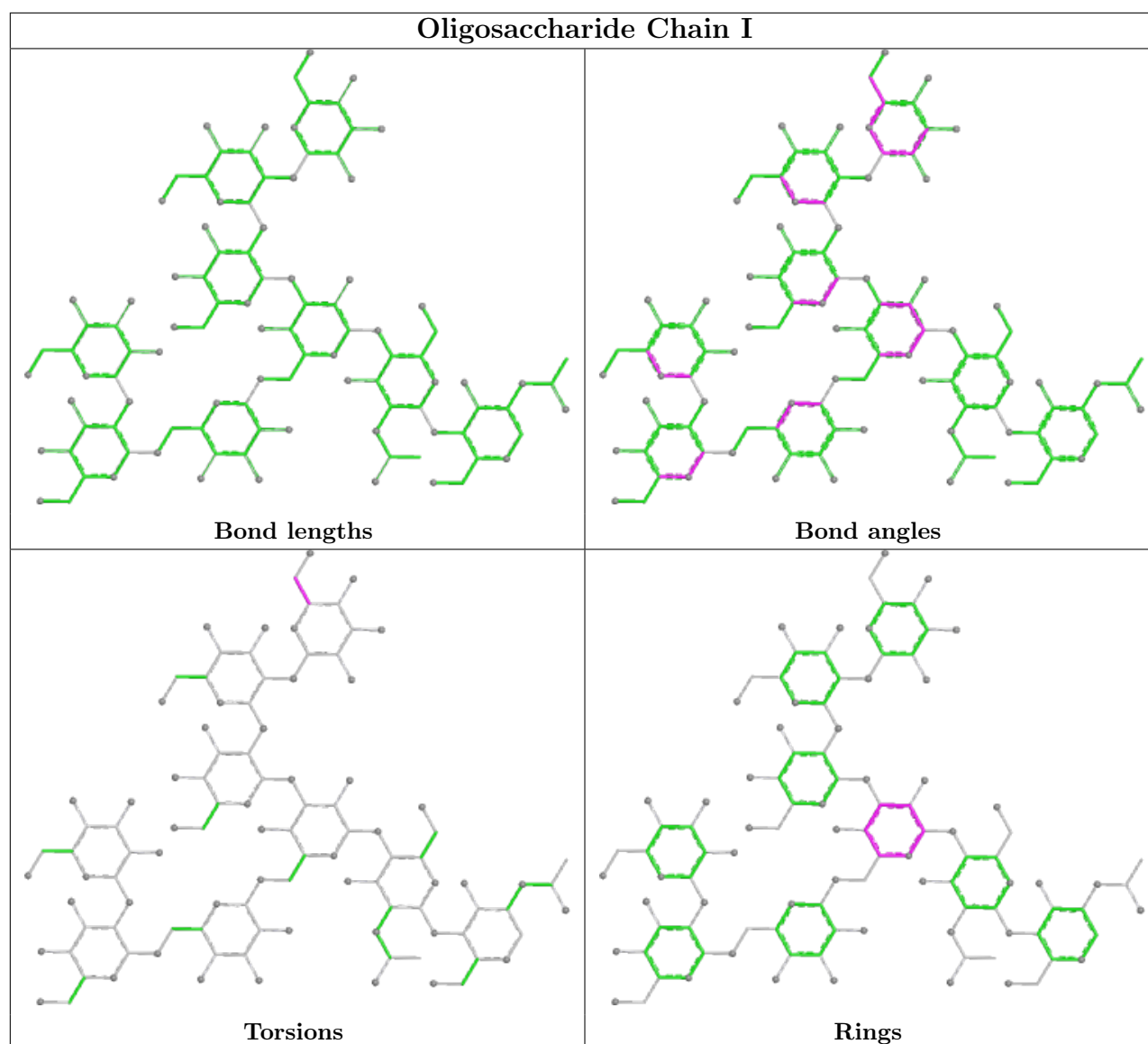












## 5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 33 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
13	PE4	A	1024	-	9,9,23	0.50	0	8,8,22	0.53	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	PE4	B	1020	-	15,15,23	0.49	0	14,14,22	0.32	0
9	NAG	B	1001	1	14,14,15	0.44	0	17,19,21	0.74	0
9	NAG	B	1002	1	14,14,15	0.59	0	17,19,21	0.73	0
9	NAG	B	1005	1	14,14,15	0.48	0	17,19,21	1.16	1 (5%)
12	1PE	A	1023	-	8,8,15	0.36	0	7,7,14	0.71	0
9	NAG	B	1003	1	14,14,15	0.61	0	17,19,21	0.48	0
9	NAG	B	1004	1	14,14,15	0.64	1 (7%)	17,19,21	0.88	1 (5%)
9	NAG	A	1001	1	14,14,15	0.52	0	17,19,21	0.85	1 (5%)
9	NAG	A	1002	1	14,14,15	0.44	0	17,19,21	0.76	1 (5%)
12	1PE	B	1018	-	8,8,15	0.37	0	7,7,14	0.82	0
9	NAG	A	1004	1	14,14,15	0.55	0	17,19,21	0.54	0
9	NAG	A	1003	1	14,14,15	0.63	0	17,19,21	0.62	0
9	NAG	A	1005	1	14,14,15	0.37	0	17,19,21	0.85	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
13	PE4	A	1024	-	-	5/7/7/21	-
13	PE4	B	1020	-	-	8/13/13/21	-
9	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
9	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
9	NAG	B	1005	1	-	0/6/23/26	0/1/1/1
12	1PE	A	1023	-	-	6/6/6/13	-
9	NAG	B	1003	1	-	0/6/23/26	0/1/1/1
9	NAG	B	1004	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1002	1	-	1/6/23/26	0/1/1/1
12	1PE	B	1018	-	-	6/6/6/13	-
9	NAG	A	1004	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1003	1	-	0/6/23/26	0/1/1/1
9	NAG	A	1005	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1004	NAG	C1-C2	2.06	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1004	NAG	C1-O5-C5	3.16	116.47	112.19
9	A	1001	NAG	C1-O5-C5	2.76	115.94	112.19
9	B	1005	NAG	C2-N2-C7	-2.71	119.04	122.90
9	A	1002	NAG	C1-O5-C5	2.37	115.41	112.19
9	A	1005	NAG	C2-N2-C7	-2.12	119.88	122.90

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

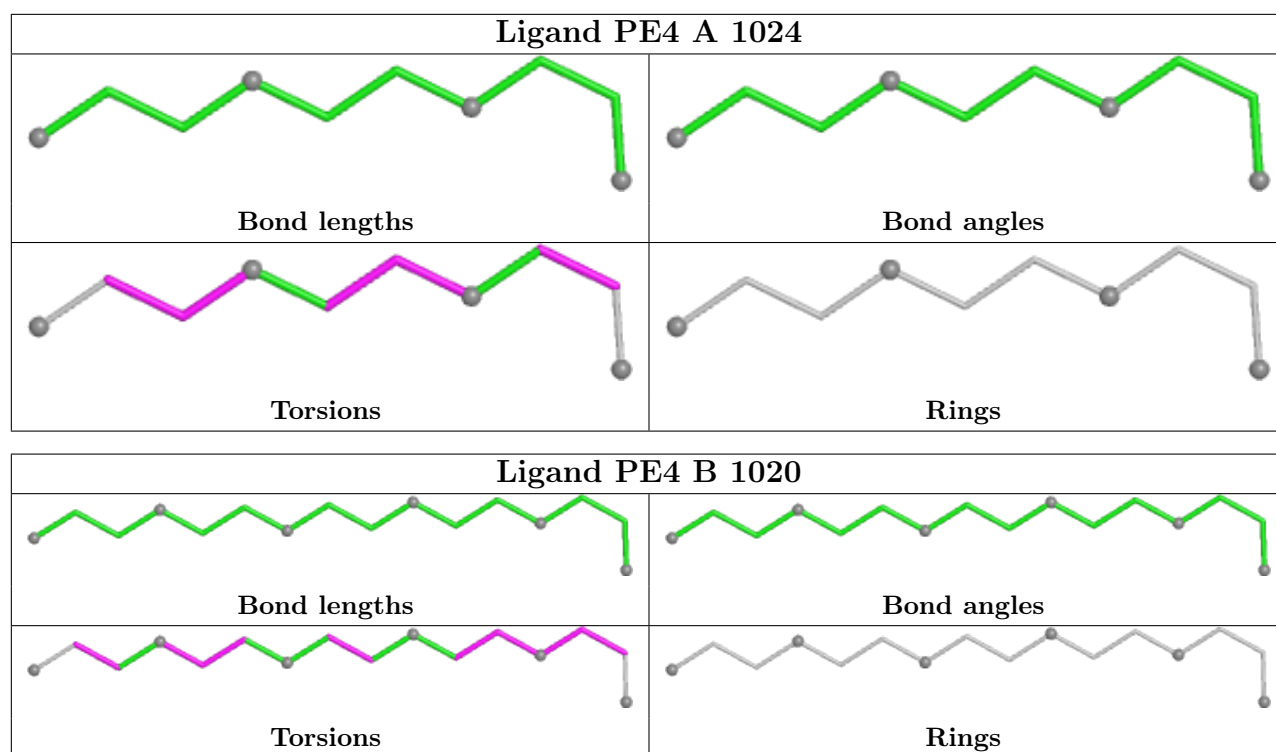
Mol	Chain	Res	Type	Atoms
13	B	1020	PE4	O2-C3-C4-O3
13	B	1020	PE4	O4-C7-C8-O5
13	A	1024	PE4	O2-C3-C4-O3
12	A	1023	1PE	OH5-C14-C24-OH4
13	A	1024	PE4	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	1024	PE4	2	0
13	B	1020	PE4	2	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	917/942 (97%)	-0.01	2 (0%) 95 95	33, 51, 85, 114	1 (0%)
1	B	917/942 (97%)	-0.06	1 (0%) 95 96	31, 48, 76, 113	0
All	All	1834/1884 (97%)	-0.04	3 (0%) 95 95	31, 49, 81, 114	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	333	ALA	3.0
1	B	559	TYR	2.2
1	A	326	ILE	2.0

### 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
8	MAN	I	6	11/12	0.62	0.29	71,74,77,77	11
7	NAG	L	2	14/15	0.80	0.19	59,66,70,71	0
2	MAN	J	6	10/12	0.83	0.16	24,26,26,27	0
7	NAG	H	2	14/15	0.83	0.17	58,67,69,73	0
6	MAN	G	4	11/12	0.85	0.21	61,65,67,67	0
6	MAN	G	6	11/12	0.87	0.25	60,63,66,68	0

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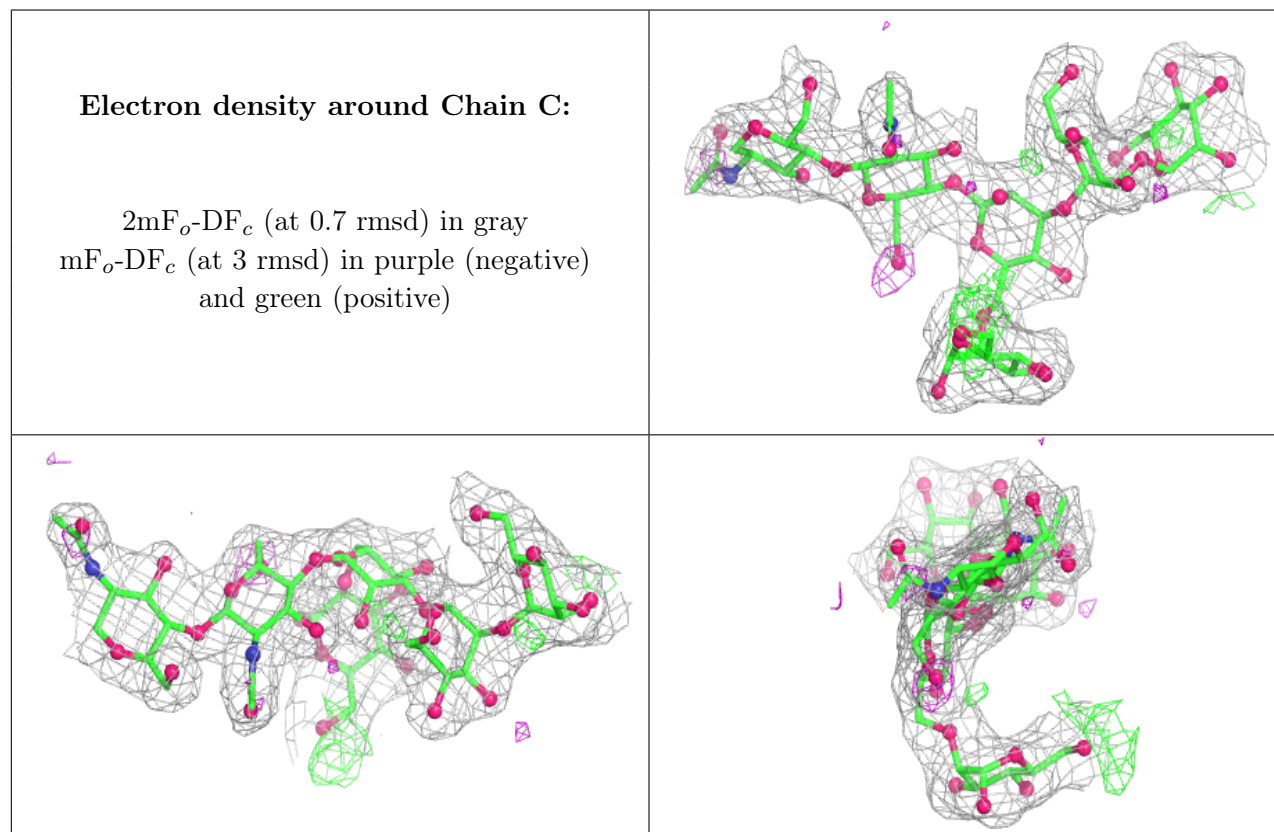
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MAN	G	3	11/12	0.87	0.14	61,62,64,67	0
8	MAN	I	9	11/12	0.87	0.38	59,66,69,71	0
3	MAN	D	3	11/12	0.88	0.14	52,56,62,63	0
2	MAN	C	6	11/12	0.88	0.13	65,67,70,71	0
3	MAN	M	3	11/12	0.89	0.15	51,56,61,62	0
8	MAN	I	5	11/12	0.89	0.15	55,61,69,73	0
4	NAG	E	2	14/15	0.90	0.12	53,58,68,72	0
6	MAN	G	7	11/12	0.90	0.15	62,64,66,67	0
8	MAN	I	3	11/12	0.90	0.16	57,61,64,68	0
4	NAG	N	2	14/15	0.91	0.13	49,55,63,63	0
5	MAN	F	8	11/12	0.91	0.15	53,55,60,61	0
8	MAN	I	7	11/12	0.91	0.26	63,67,68,68	0
8	MAN	I	8	11/12	0.91	0.21	58,62,66,67	0
6	MAN	G	8	11/12	0.91	0.14	55,61,68,71	0
8	MAN	I	4	11/12	0.92	0.17	61,63,67,67	0
5	BMA	F	4	11/12	0.92	0.14	44,45,51,51	0
5	BMA	F	3	11/12	0.92	0.17	47,47,50,51	0
6	NAG	G	2	14/15	0.93	0.13	52,56,60,65	0
5	MAN	F	7	11/12	0.93	0.13	50,52,55,59	0
5	MAN	F	6	11/12	0.93	0.20	57,62,63,64	0
6	MAN	G	5	11/12	0.93	0.16	57,58,62,64	0
7	NAG	L	1	14/15	0.94	0.15	46,50,53,55	0
5	BMA	K	4	11/12	0.94	0.15	40,46,51,52	0
5	MAN	K	6	11/12	0.94	0.18	55,60,64,64	0
4	NAG	E	1	14/15	0.95	0.12	39,43,51,54	0
5	MAN	F	5	11/12	0.95	0.14	47,50,51,54	0
5	MAN	F	9	11/12	0.95	0.13	56,57,59,59	0
5	MAN	F	11	11/12	0.95	0.12	46,50,51,52	0
5	BMA	K	3	11/12	0.95	0.16	44,46,50,50	0
2	MAN	C	5	11/12	0.95	0.12	40,50,52,55	0
2	BMA	J	3	11/12	0.96	0.10	43,47,50,50	0
2	NAG	C	2	14/15	0.96	0.15	43,45,49,53	0
8	NAG	I	1	14/15	0.96	0.14	39,47,52,52	0
4	NAG	N	1	14/15	0.96	0.12	37,44,52,59	0
2	MAN	C	4	11/12	0.96	0.13	38,47,49,50	0
2	NAG	J	2	14/15	0.96	0.17	38,43,48,53	0
5	MAN	K	9	11/12	0.96	0.12	49,52,54,54	0
5	MAN	K	11	11/12	0.96	0.12	48,51,54,55	0
7	NAG	H	1	14/15	0.96	0.16	46,50,54,56	0
6	NAG	G	1	14/15	0.96	0.12	43,53,59,61	0
3	NAG	M	1	14/15	0.97	0.13	37,39,42,43	0
5	MAN	K	7	11/12	0.97	0.12	45,47,49,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MAN	K	8	11/12	0.97	0.13	48,50,55,56	0
3	NAG	M	2	14/15	0.97	0.13	39,44,50,50	0
5	MAN	K	10	11/12	0.97	0.15	43,44,49,52	0
2	MAN	J	4	11/12	0.97	0.14	41,44,48,48	0
8	NAG	I	2	14/15	0.97	0.13	47,55,58,63	0
2	MAN	J	5	11/12	0.97	0.14	40,45,48,49	0
2	BMA	C	3	11/12	0.97	0.11	46,50,57,61	0
3	NAG	D	1	14/15	0.97	0.14	40,42,49,50	0
3	NAG	D	2	14/15	0.97	0.12	38,46,51,53	0
5	NAG	F	2	14/15	0.97	0.15	44,47,58,59	0
2	NAG	C	1	14/15	0.97	0.17	42,44,50,51	0
5	MAN	K	5	11/12	0.97	0.12	44,49,52,53	0
5	NAG	F	1	14/15	0.98	0.14	44,47,48,49	0
5	MAN	F	10	11/12	0.98	0.12	47,49,51,52	0
2	NAG	J	1	14/15	0.98	0.16	41,44,46,46	0
5	NAG	K	1	14/15	0.98	0.14	42,44,46,47	0
5	NAG	K	2	14/15	0.98	0.14	40,42,46,46	0

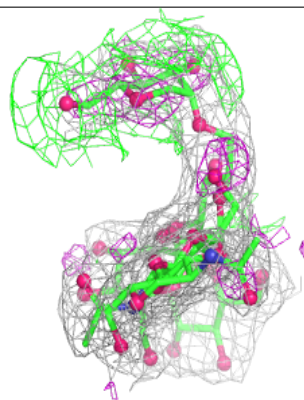
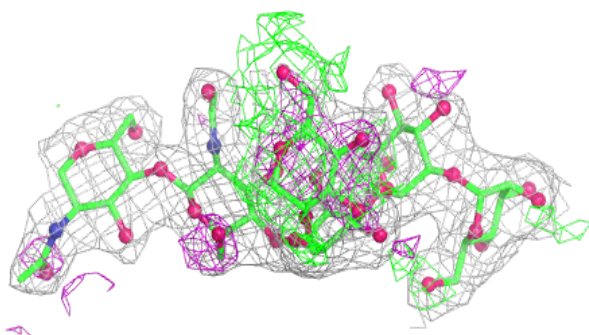
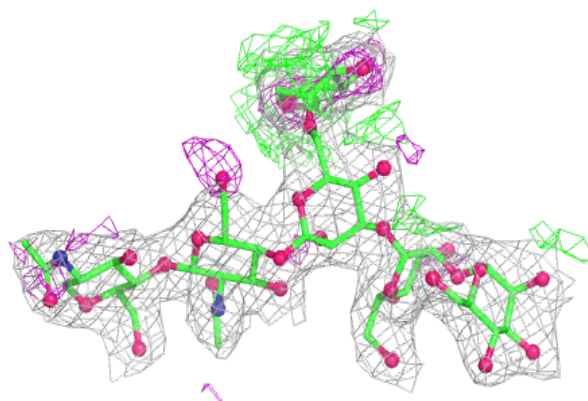
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



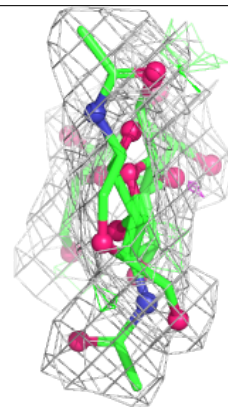
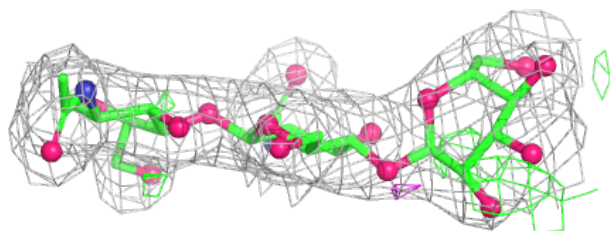
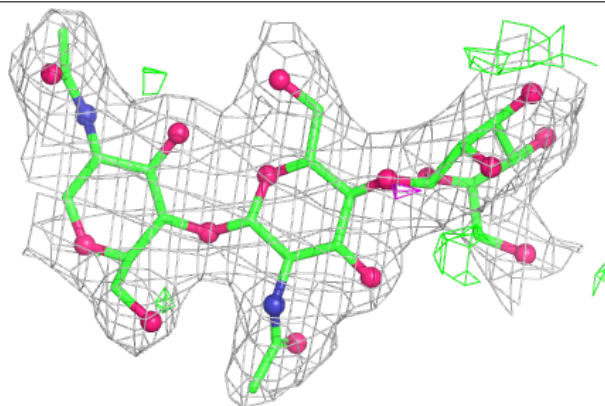


**Electron density around Chain J:**

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

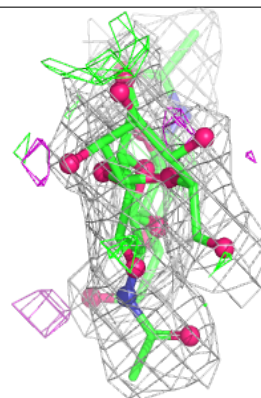
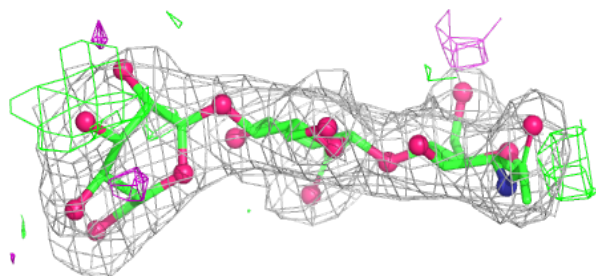
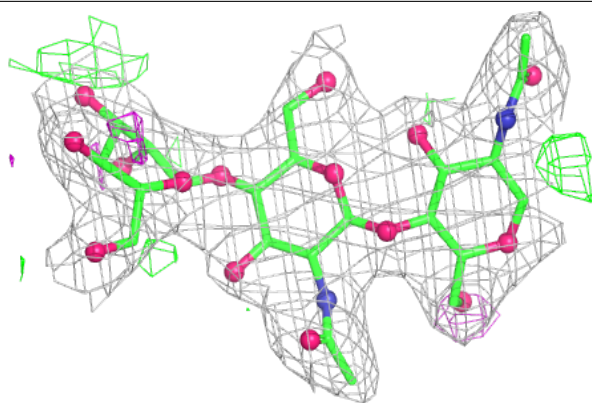
**Electron density around Chain D:**

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

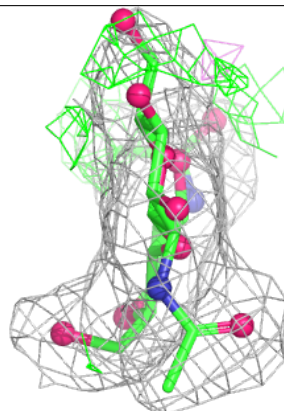
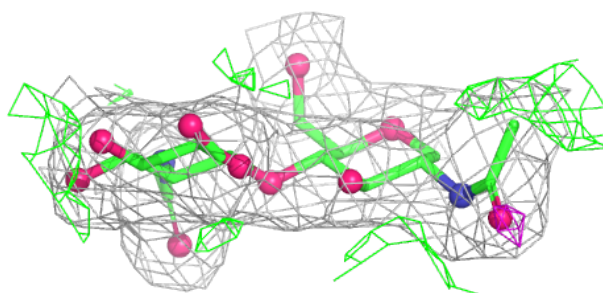
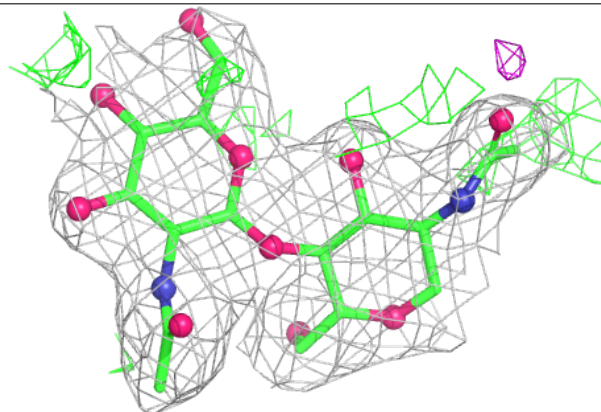


**Electron density around Chain M:**

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

**Electron density around Chain E:**

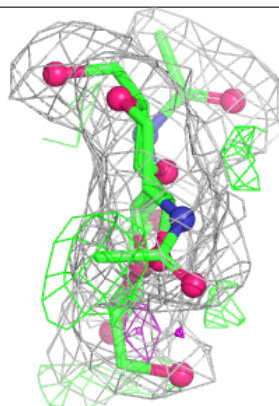
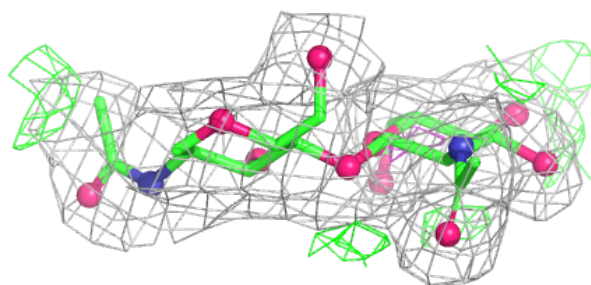
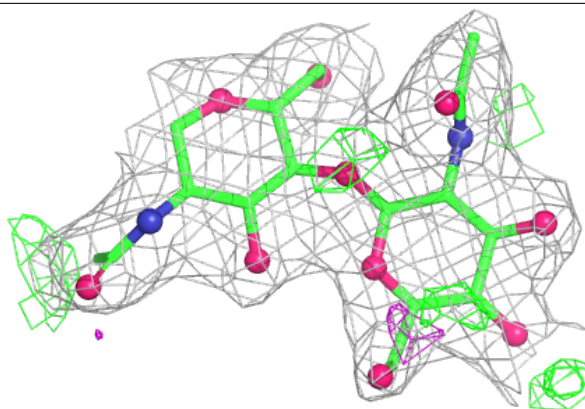
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





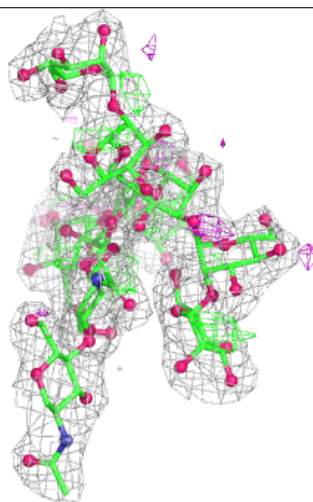
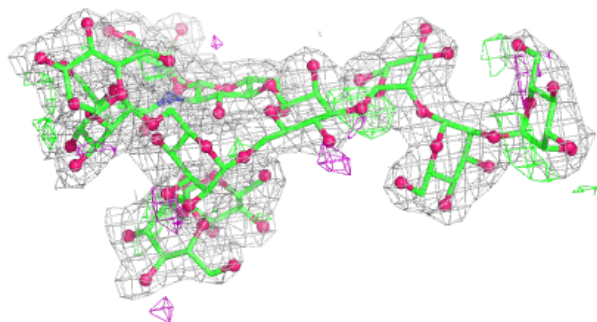
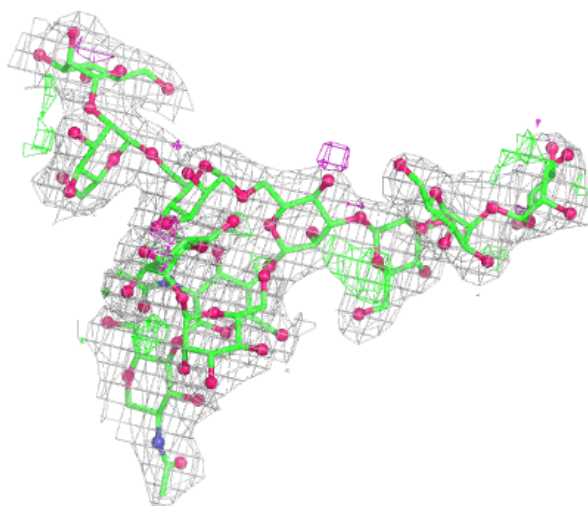
**Electron density around Chain N:**

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



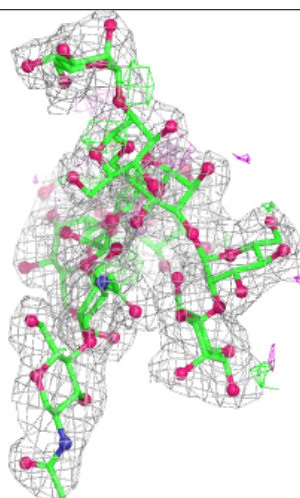
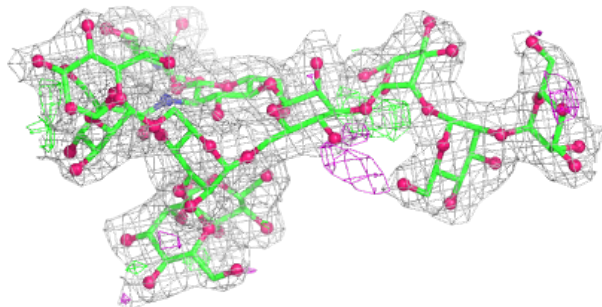
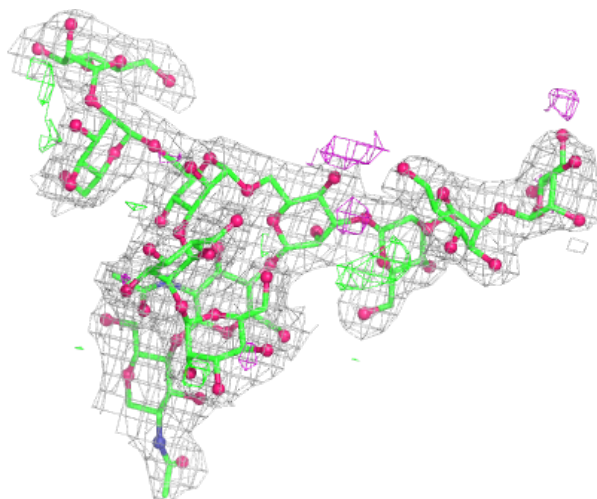
**Electron density around Chain F:**

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



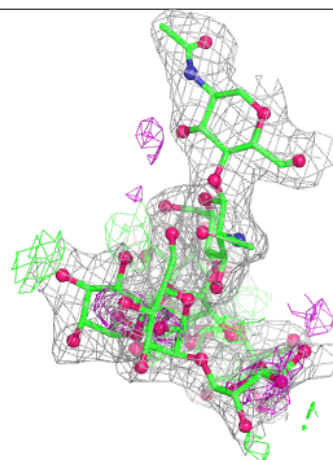
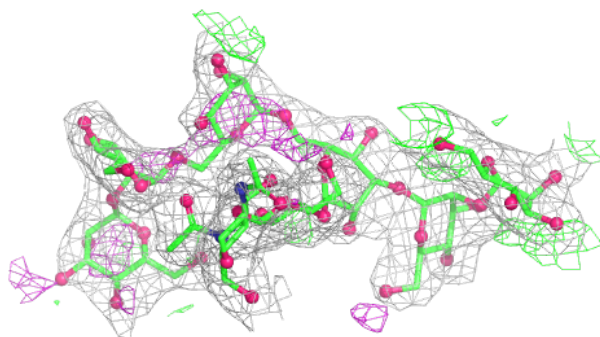
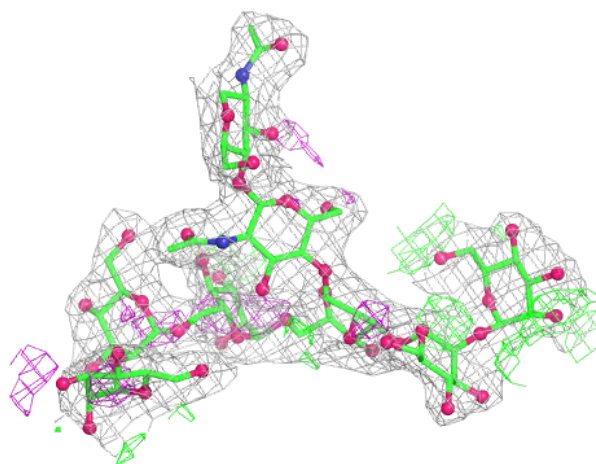
**Electron density around Chain K:**

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



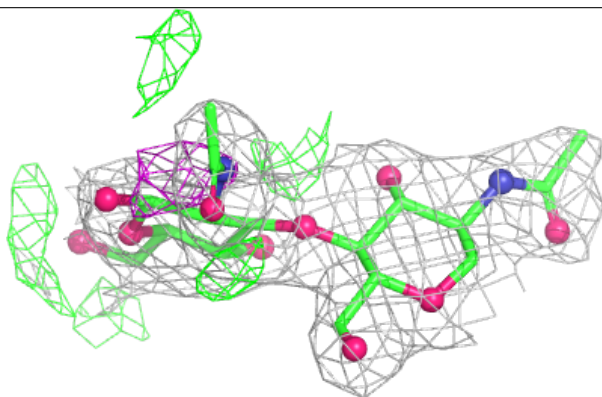
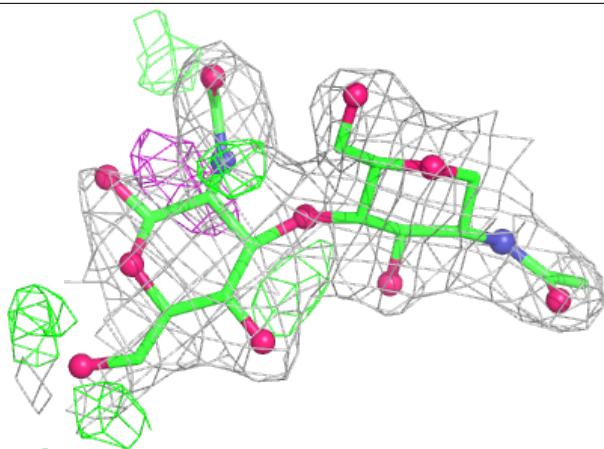
**Electron density around Chain G:**

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



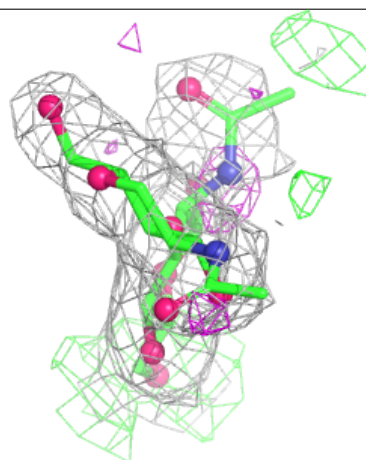
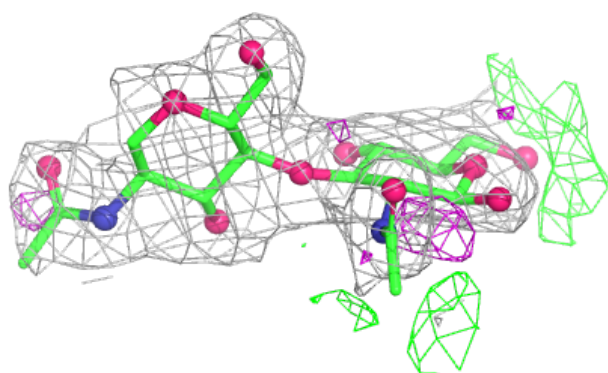
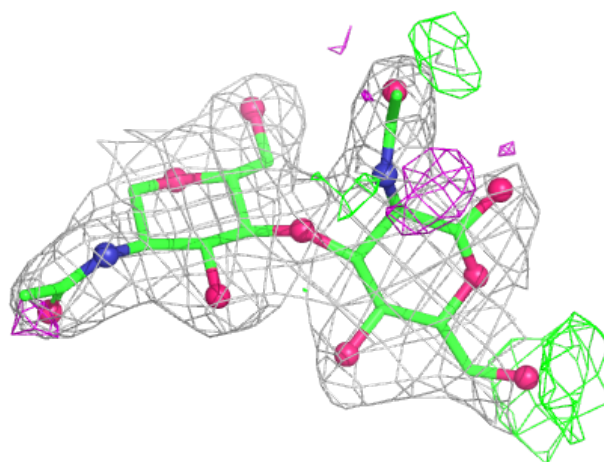
**Electron density around Chain H:**

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and green (positive)

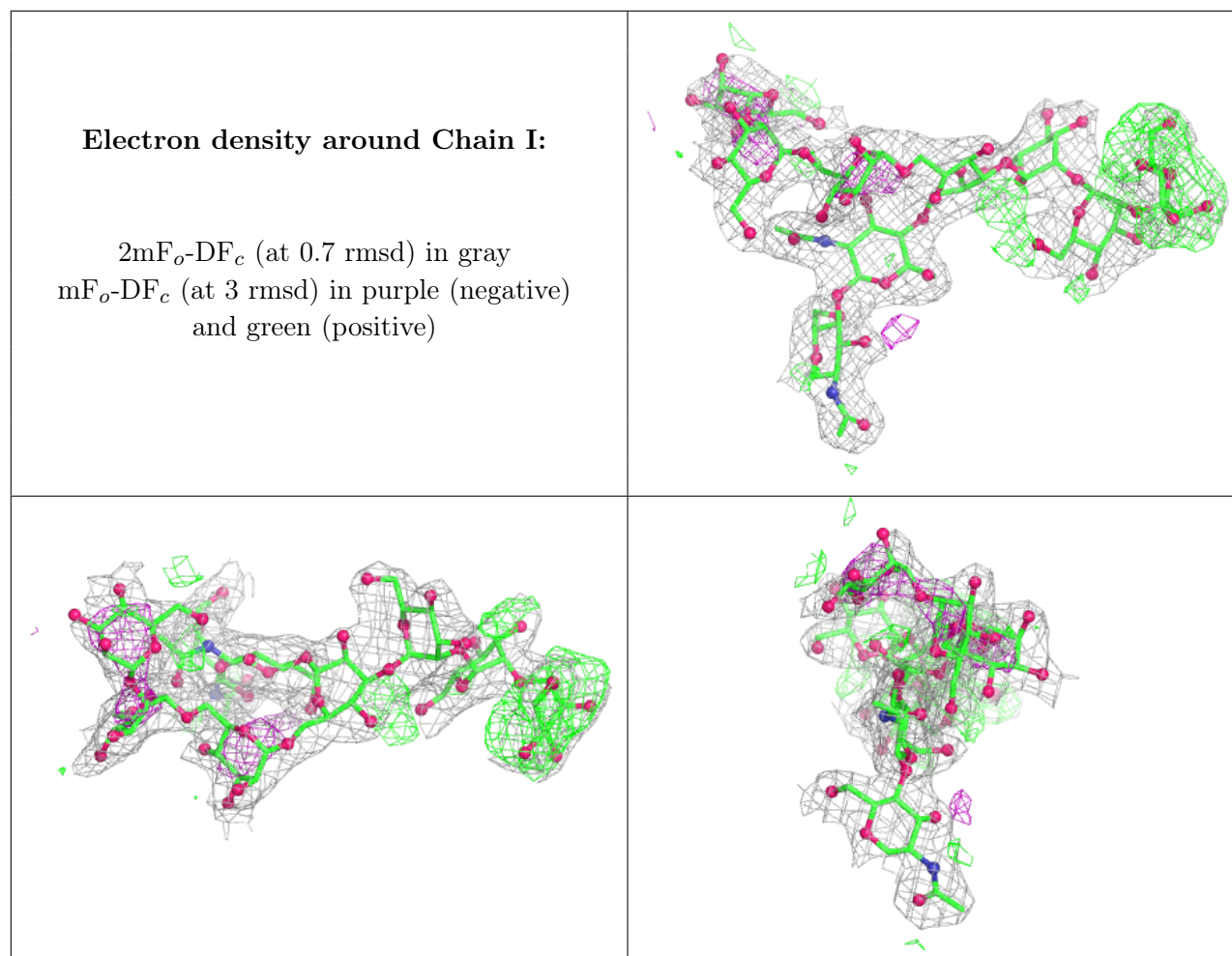


**Electron density around Chain L:**

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







## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	CD	A	1009	1/1	0.74	0.06	141,141,141,141	0
9	NAG	A	1005	14/15	0.76	0.25	24,25,26,27	14
9	NAG	B	1005	14/15	0.81	0.24	24,25,26,27	14
9	NAG	B	1002	14/15	0.87	0.16	54,57,65,65	0
9	NAG	B	1001	14/15	0.88	0.19	63,66,69,70	0
9	NAG	A	1004	14/15	0.89	0.15	51,60,63,65	0
9	NAG	B	1004	14/15	0.90	0.17	59,62,64,70	0
9	NAG	A	1002	14/15	0.91	0.18	62,65,68,70	0
11	NA	A	1021	1/1	0.91	0.31	48,48,48,48	0
11	NA	A	1022	1/1	0.91	0.22	55,55,55,55	0

*Continued on next page...*

*Continued from previous page...*

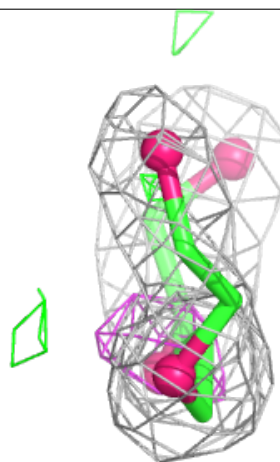
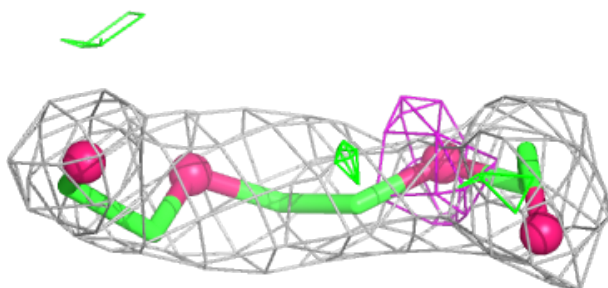
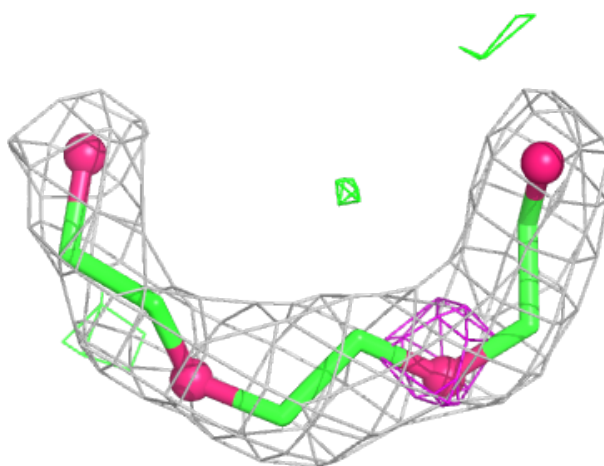
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
11	NA	B	1017	1/1	0.91	0.22	57,57,57,57	0
13	PE4	A	1024	10/24	0.91	0.33	58,63,65,67	0
9	NAG	A	1001	14/15	0.92	0.16	65,68,71,71	0
13	PE4	B	1020	16/24	0.92	0.29	56,62,69,71	0
10	CD	B	1011	1/1	0.94	0.12	35,35,35,35	1
10	CD	B	1012	1/1	0.94	0.11	56,56,56,56	1
10	CD	B	1016	1/1	0.94	0.10	79,79,79,79	0
9	NAG	B	1003	14/15	0.94	0.13	39,44,50,50	0
10	CD	A	1006	1/1	0.94	0.24	54,54,54,54	1
10	CD	A	1008	1/1	0.94	0.11	73,73,73,73	1
9	NAG	A	1003	14/15	0.94	0.13	40,46,49,52	0
10	CD	B	1008	1/1	0.94	0.05	94,94,94,94	0
12	1PE	A	1023	9/16	0.95	0.15	51,52,53,53	0
10	CD	A	1025	1/1	0.95	0.04	120,120,120,120	0
10	CD	A	1007	1/1	0.95	0.09	82,82,82,82	1
12	1PE	B	1018	9/16	0.96	0.14	51,53,54,54	0
14	CL	B	1019	1/1	0.96	0.15	53,53,53,53	0
10	CD	A	1020	1/1	0.97	0.10	102,102,102,102	0
10	CD	B	1022	1/1	0.97	0.03	114,114,114,114	0
10	CD	A	1010	1/1	0.97	0.06	94,94,94,94	0
10	CD	B	1006	1/1	0.97	0.21	58,58,58,58	1
10	CD	B	1014	1/1	0.97	0.12	95,95,95,95	0
10	CD	B	1007	1/1	0.98	0.05	127,127,127,127	0
10	CD	A	1017	1/1	0.98	0.04	63,63,63,63	1
10	CD	A	1015	1/1	0.98	0.17	47,47,47,47	1
15	CA	B	1021	1/1	0.98	0.06	54,54,54,54	0
10	CD	A	1014	1/1	0.99	0.15	55,55,55,55	0
10	CD	B	1009	1/1	0.99	0.15	54,54,54,54	0
10	CD	B	1010	1/1	0.99	0.11	59,59,59,59	0
10	CD	A	1018	1/1	0.99	0.16	47,47,47,47	0
10	CD	A	1016	1/1	0.99	0.08	58,58,58,58	1
10	CD	B	1013	1/1	0.99	0.06	83,83,83,83	1
10	CD	A	1013	1/1	1.00	0.14	39,39,39,39	0
10	CD	A	1011	1/1	1.00	0.15	41,41,41,41	0
10	CD	A	1012	1/1	1.00	0.14	40,40,40,40	0
10	CD	B	1015	1/1	1.00	0.15	47,47,47,47	0
10	CD	A	1019	1/1	1.00	0.14	39,39,39,39	0

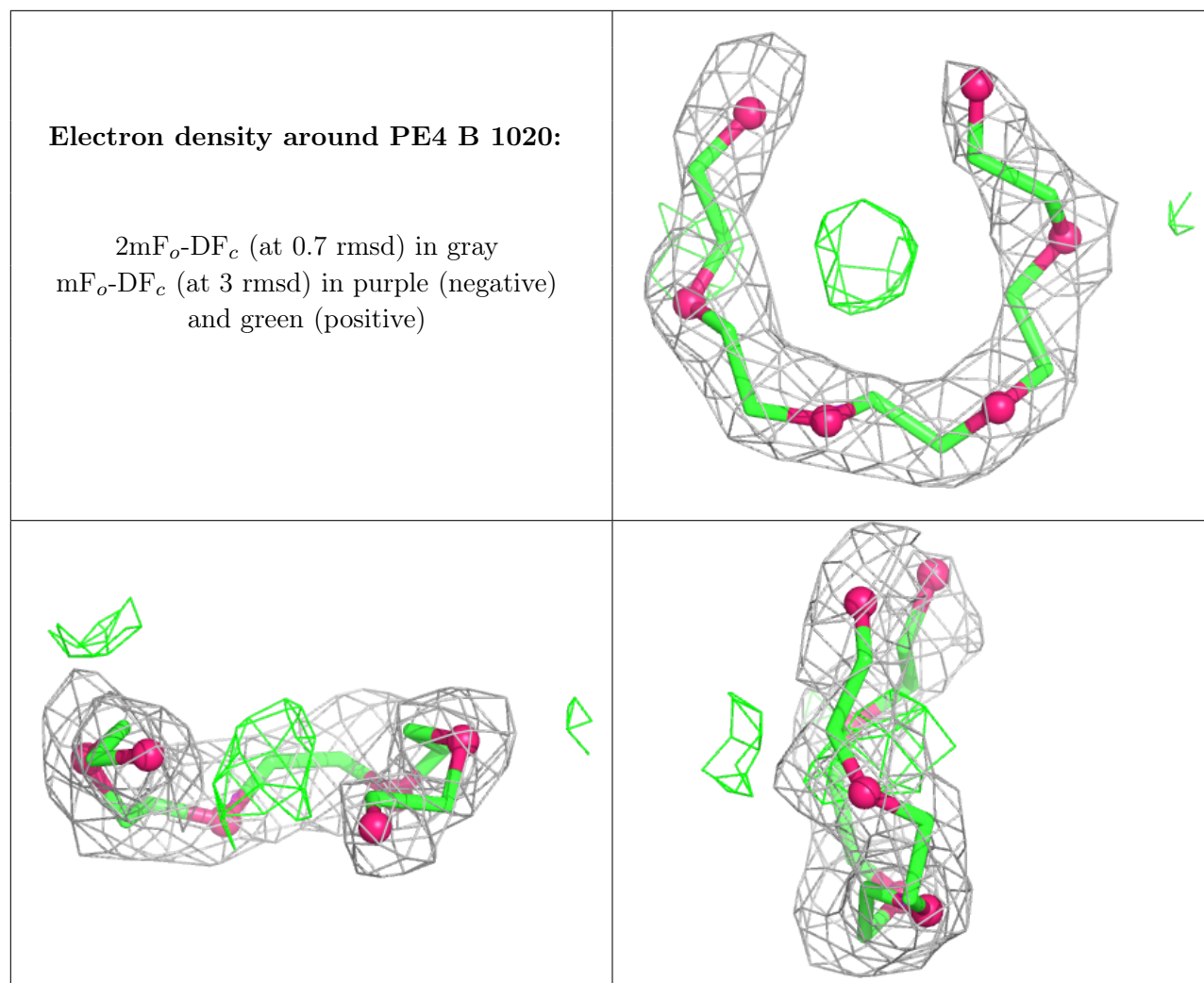
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



**Electron density around PE4 A 1024:**

$2mF_o-DF_c$  (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.