



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 11:55 PM BST

PDB ID : 5AE6  
Title : The structure of Hypocrea jecorina beta-xylosidase Xyl3A (Bxl1) in complex with 4-thioxylobiose  
Authors : Mikkelsen, N.E.; Gudmundsson, M.; Karkehabadi, S.; Hansson, H.; Sandgren, M.; Larenas, E.; Mitchinson, C.; Keleman, B.; Kaper, T.  
Deposited on : 2015-08-26  
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

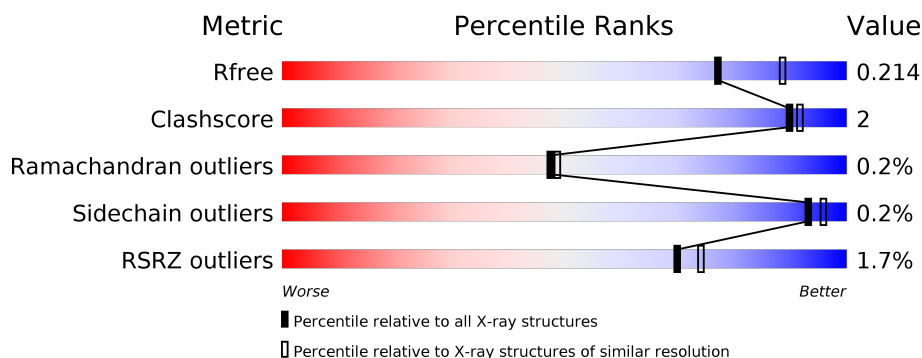
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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.



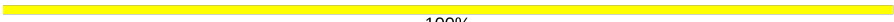



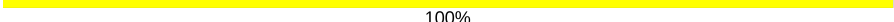

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 on 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	767	<div> <div>2%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	B	767	<div> <div>%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
2	C	4	<div> <div>25%</div> <div>75%</div> </div>
3	D	2	<div> <div>100%</div> </div>
3	F	2	<div> <div>50%</div> <div>50%</div> </div>
3	H	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	2	 100%
3	K	2	 50% 50%
4	E	3	 67% 33%
5	G	2	 50% 50%
5	L	2	 100%
6	J	5	 60% 20% 20%

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
3	NAG	F	2	-	-	-	X

## 2 Entry composition [i](#)

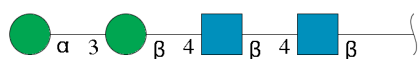
There are 9 unique types of molecules in this entry. The entry contains 13404 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-XYLOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	762	Total	C	N	O	S	0	6	0
			5947	3790	1000	1145	12			
1	B	767	Total	C	N	O	S	0	13	0
			6024	3840	1013	1159	12			

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



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

- Molecule 3 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
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called beta-D-xylopyranose-(1-4)-4-deoxy-4-thio-alpha-D-x

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	2	Total	C	O	S	0	0	0
			19	10	8	1			
5	L	2	Total	C	O	S	0	0	0
			19	10	8	1			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 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
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	7	Total	Zn	0	1
			8	8		
8	A	5	Total	Zn	0	1
			6	6		

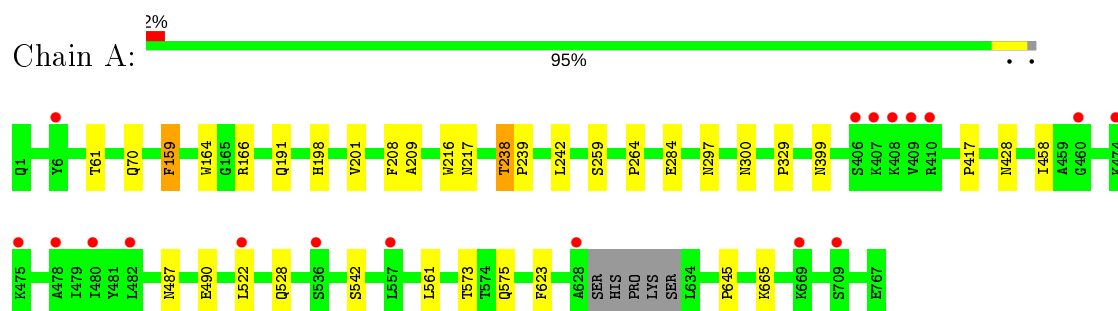
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	508	Total 509	O 509	0	5
9	B	442	Total 442	O 442	0	10

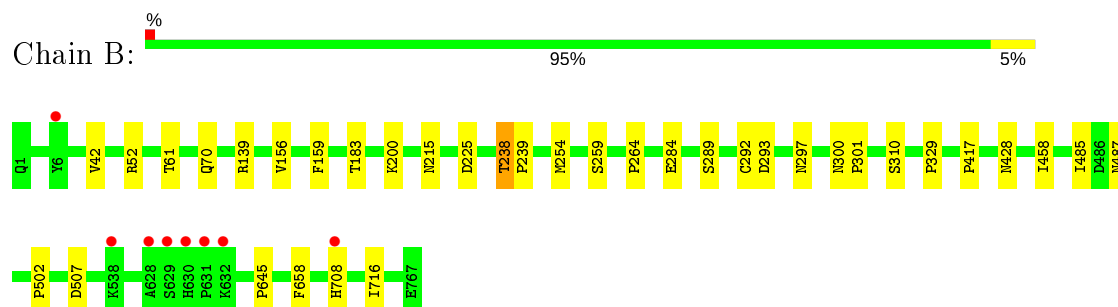
### 3 Residue-property plots

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-XYLOSIDASE



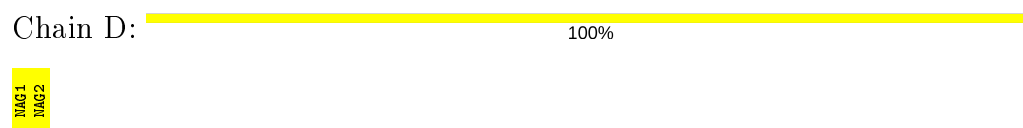
- Molecule 1: BETA-XYLOSIDASE



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



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





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

Chain F:  50% 50%

 NAG1  
NAG2

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

Chain H:  50% 50%

 NAG1  
NAG2

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

Chain I:  100%

 NAG1  
NAG2

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

Chain K:  50% 50%

 NAG1  
NAG2

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

Chain E:  67% 33%

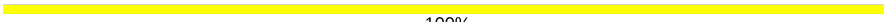
 NAG1  
NAG2  
BNA3

- Molecule 5: beta-D-xylopyranose-(1-4)-4-deoxy-4-thio-alpha-D-xylopyranose

Chain G:  50% 50%

 TYR1  
TYR2

- Molecule 5: beta-D-xylopyranose-(1-4)-4-deoxy-4-thio-alpha-D-xylopyranose

Chain L:  100%

TRF1  
XYP2

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

Chain J:



MAN1  
MAN2  
BMA3  
MAN4  
MAN5

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.24Å 202.44Å 82.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	202.44 – 2.10 29.81 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (202.44-2.10) 99.9 (29.81-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.69 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.178 , 0.214 0.178 , 0.214	Depositor DCC
$R_{free}$ test set	4912 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.4	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13404	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: XYP, ZN, BMA, NAG, TXB, PCA, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.38	0/6113	0.54	0/8331
1	B	0.38	0/6214	0.54	0/8469
All	All	0.38	0/12327	0.54	0/16800

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	5947	0	5734	25	0
1	B	6024	0	5828	23	1
2	C	50	0	43	0	0
3	D	28	0	25	0	0
3	F	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	K	28	0	25	0	0
4	E	39	0	34	0	0
5	G	19	0	0	0	0
5	L	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	61	0	52	1	0
7	A	70	0	65	1	0
7	B	70	0	65	0	0
8	A	6	0	0	0	0
8	B	8	0	0	0	0
9	A	509	0	0	1	0
9	B	442	0	0	4	1
All	All	13404	0	11946	45	1

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

All (45) 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:198[A]:HIS:NE2	9:A:2191[A]:HOH:O	2.20	0.74
1:B:708:HIS:NE2	9:B:2419:HOH:O	2.27	0.67
1:A:216:TRP:CE3	1:A:217:ASN:HB2	2.41	0.56
1:A:284:GLU:HB2	1:B:284[B]:GLU:CD	2.25	0.56
1:A:428:ASN:HB3	1:A:487:ASN:HD21	1.71	0.56
1:B:70:GLN:HB3	1:B:329:PRO:HG3	1.90	0.52
1:B:417:PRO:HB2	1:B:458:ILE:HG12	1.92	0.51
1:A:428:ASN:HB3	1:A:487:ASN:ND2	2.26	0.51
1:B:254:MET:HA	1:B:289:SER:O	2.10	0.51
1:A:284:GLU:CD	1:B:284[B]:GLU:HB2	2.32	0.50
1:A:645:PRO:HD3	1:B:61:THR:HG22	1.93	0.50
1:B:428:ASN:HB3	1:B:487:ASN:ND2	2.27	0.50
1:A:70:GLN:HB3	1:A:329:PRO:HG3	1.93	0.49
1:A:297:ASN:HA	1:A:300:ASN:O	2.13	0.49
1:A:528:GLN:HB3	1:A:575:GLN:HG3	1.94	0.48
1:A:242:LEU:C	1:A:242:LEU:HD23	2.35	0.47
1:A:159:PHE:CD2	1:A:573:THR:HG21	2.50	0.47
1:B:156:VAL:HG11	1:B:183:THR:OG1	2.15	0.47
1:B:300:ASN:HA	1:B:301:PRO:HA	1.78	0.47
1:B:225[A]:ASP:HB3	9:B:2197[A]:HOH:O	2.14	0.46
1:B:485:ILE:HG22	1:B:502:PRO:HG3	1.97	0.46
1:A:238:THR:N	1:A:239:PRO:CD	2.79	0.46
1:A:522:LEU:HD11	1:A:561:LEU:HD21	1.98	0.46
1:B:139:ARG:HD3	1:B:200:LYS:O	2.16	0.46
1:A:61:THR:HG22	1:B:645:PRO:HD3	1.98	0.46
1:A:238:THR:N	1:A:239:PRO:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ASN:HA	1:B:300:ASN:O	2.16	0.45
1:A:191:GLN:HG2	1:A:201:VAL:O	2.17	0.44
1:A:216:TRP:CZ3	1:A:217:ASN:HB2	2.53	0.44
1:A:417:PRO:HB2	1:A:458:ILE:HG12	2.00	0.44
9:B:2312:HOH:O	6:J:4:MAN:H61	2.18	0.43
7:A:1301:NAG:H5	1:B:310[B]:SER:OG	2.19	0.43
1:B:658:PHE:CZ	1:B:716[A]:ILE:HD12	2.54	0.43
1:B:428:ASN:HB3	1:B:487:ASN:HD21	1.85	0.42
1:A:399:ASN:OD1	1:A:542:SER:OG	2.36	0.42
1:A:487:ASN:HA	1:A:490:GLU:O	2.20	0.42
1:B:238:THR:N	1:B:239:PRO:CD	2.82	0.41
1:A:208:PHE:CD1	1:A:209:ALA:HB2	2.56	0.41
1:B:259:SER:HA	1:B:264:PRO:HA	2.02	0.41
1:B:292:CYS:HA	1:B:293:ASP:HA	1.85	0.41
1:A:259:SER:HA	1:A:264:PRO:HA	2.02	0.41
1:B:225[B]:ASP:HB2	9:B:2189[B]:HOH:O	2.21	0.41
1:A:623:PHE:HA	1:A:665:LYS:O	2.21	0.41
1:A:164:TRP:CE2	1:A:166:ARG:HB2	2.55	0.40
1:B:42:VAL:HA	1:B:52:ARG:HB3	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:ASP:OD2	9:B:2366:HOH:O[2_645]	2.17	0.03

## 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	764/767 (100%)	738 (97%)	25 (3%)	1 (0%)	51 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	778/767 (101%)	752 (97%)	24 (3%)	2 (0%)	41	41
All	All	1542/1534 (100%)	1490 (97%)	49 (3%)	3 (0%)	47	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	215	ASN
1	A	238	THR
1	B	238	THR

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	632/631 (100%)	631 (100%)	1 (0%)	93	96
1	B	644/631 (102%)	643 (100%)	1 (0%)	93	96
All	All	1276/1262 (101%)	1274 (100%)	2 (0%)	93	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	PHE
1	B	159	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	GLN
1	A	487	ASN
1	A	523	GLN
1	B	168	GLN
1	B	326	GLN
1	B	487	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	PCA	A	1	1	7,8,9	0.54	0	9,10,12	1.01	0
1	PCA	B	1	1	7,8,9	0.40	0	9,10,12	0.97	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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

26 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	0.57	0	17,19,21	1.17	1 (5%)
2	NAG	C	2	2	14,14,15	0.70	0	17,19,21	0.70	0
2	BMA	C	3	2	11,11,12	0.33	0	15,15,17	1.51	1 (6%)
2	MAN	C	4	2	11,11,12	0.57	0	15,15,17	1.20	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.49	0	17,19,21	1.16	1 (5%)
3	NAG	D	2	3	14,14,15	0.57	0	17,19,21	1.16	1 (5%)
4	NAG	E	1	1,4	14,14,15	0.63	0	17,19,21	0.85	1 (5%)
4	NAG	E	2	4	14,14,15	0.56	0	17,19,21	0.81	0
4	BMA	E	3	4	11,11,12	0.38	0	15,15,17	0.91	0
3	NAG	F	1	1,3	14,14,15	0.61	0	17,19,21	0.90	0
3	NAG	F	2	3	14,14,15	0.54	0	17,19,21	1.19	1 (5%)
5	TXB	G	1	5	9,10,10	1.23	0	10,14,14	0.57	0
5	XYP	G	2	5	9,9,10	0.90	0	10,12,14	1.05	1 (10%)
3	NAG	H	1	1,3	14,14,15	0.67	0	17,19,21	1.40	2 (11%)
3	NAG	H	2	3	14,14,15	0.54	0	17,19,21	0.72	0
3	NAG	I	1	1,3	14,14,15	0.60	0	17,19,21	0.96	1 (5%)
3	NAG	I	2	3	14,14,15	0.56	0	17,19,21	1.29	1 (5%)
6	NAG	J	1	1,6	14,14,15	0.58	0	17,19,21	0.71	0
6	NAG	J	2	6	14,14,15	0.44	0	17,19,21	0.99	0
6	BMA	J	3	6	11,11,12	0.57	0	15,15,17	1.10	1 (6%)
6	MAN	J	4	6	11,11,12	0.64	0	15,15,17	1.57	2 (13%)
6	MAN	J	5	6	11,11,12	0.78	0	15,15,17	0.66	0
3	NAG	K	1	1,3	14,14,15	0.59	0	17,19,21	0.85	0
3	NAG	K	2	3	14,14,15	0.47	0	17,19,21	1.32	1 (5%)
5	TXB	L	1	5	9,10,10	1.35	2 (22%)	10,14,14	0.89	0
5	XYP	L	2	5	9,9,10	1.23	1 (11%)	10,12,14	1.16	1 (10%)

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	-	2/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	2/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
5	TXB	G	1	5	-	-	0/1/1/1
5	XYP	G	2	5	-	-	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
6	NAG	J	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
6	BMA	J	3	6	-	2/2/19/22	0/1/1/1
6	MAN	J	4	6	-	2/2/19/22	0/1/1/1
6	MAN	J	5	6	-	2/2/19/22	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
5	TXB	L	1	5	-	-	0/1/1/1
5	XYP	L	2	5	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	2	XYP	C2-C3	2.87	1.56	1.52
5	L	1	TXB	O5-C5	2.18	1.47	1.43
5	L	1	TXB	O5-C1	2.01	1.45	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	BMA	C1-O5-C5	4.60	118.42	112.19
3	K	2	NAG	C1-O5-C5	4.29	118.00	112.19
3	F	2	NAG	C1-O5-C5	4.17	117.84	112.19
6	J	4	MAN	C1-C2-C3	3.96	114.54	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	4	MAN	O5-C5-C6	3.45	112.61	107.20
3	I	2	NAG	C4-C3-C2	3.40	116.00	111.02
6	J	3	BMA	C1-C2-C3	3.30	113.72	109.67
2	C	4	MAN	C1-O5-C5	3.16	116.48	112.19
5	G	2	XYP	C1-C2-C3	2.89	113.21	109.67
3	D	2	NAG	O5-C5-C6	2.87	111.70	107.20
3	D	1	NAG	C1-O5-C5	2.79	115.97	112.19
3	H	1	NAG	C1-C2-N2	-2.73	105.83	110.49
3	I	1	NAG	C1-O5-C5	2.70	115.84	112.19
5	L	2	XYP	C1-C2-C3	2.52	112.77	109.67
2	C	1	NAG	O5-C5-C6	2.28	110.78	107.20
3	H	1	NAG	O5-C5-C6	2.22	110.68	107.20
4	E	1	NAG	O5-C1-C2	-2.05	108.05	111.29

There are no chirality outliers.

All (19) torsion outliers are listed below:

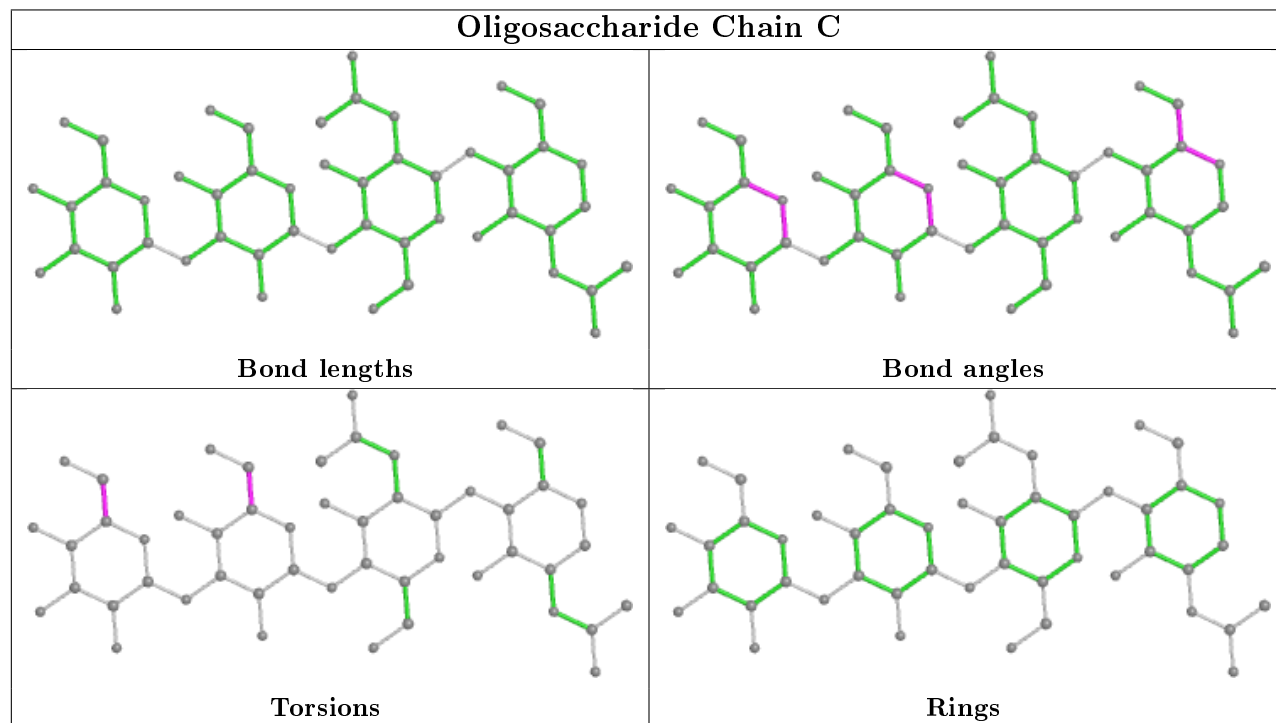
Mol	Chain	Res	Type	Atoms
6	J	4	MAN	O5-C5-C6-O6
6	J	5	MAN	O5-C5-C6-O6
6	J	4	MAN	C4-C5-C6-O6
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
6	J	5	MAN	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
2	C	3	BMA	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
2	C	3	BMA	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
6	J	3	BMA	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
6	J	3	BMA	O5-C5-C6-O6
2	C	4	MAN	O5-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6

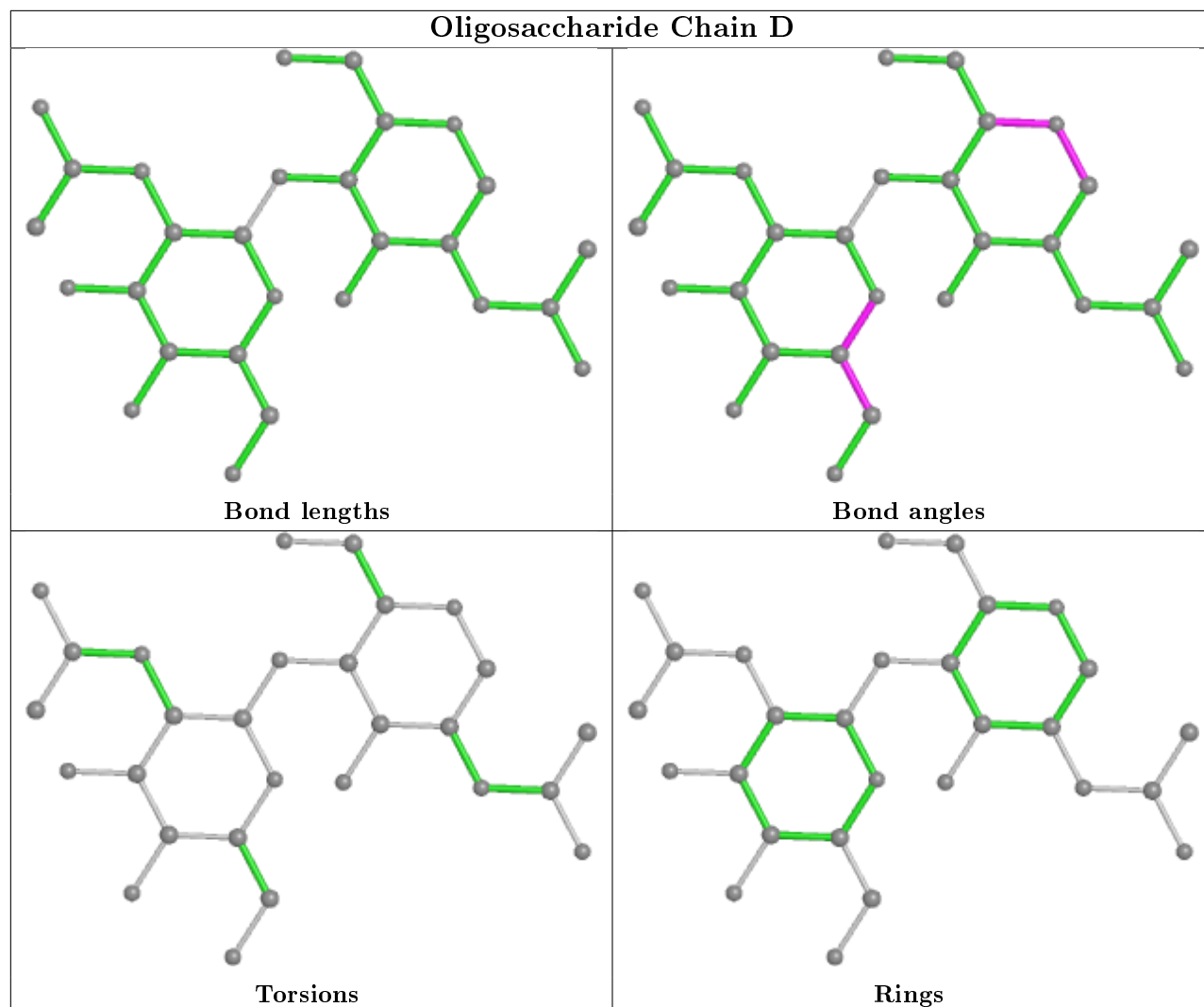
There are no ring outliers.

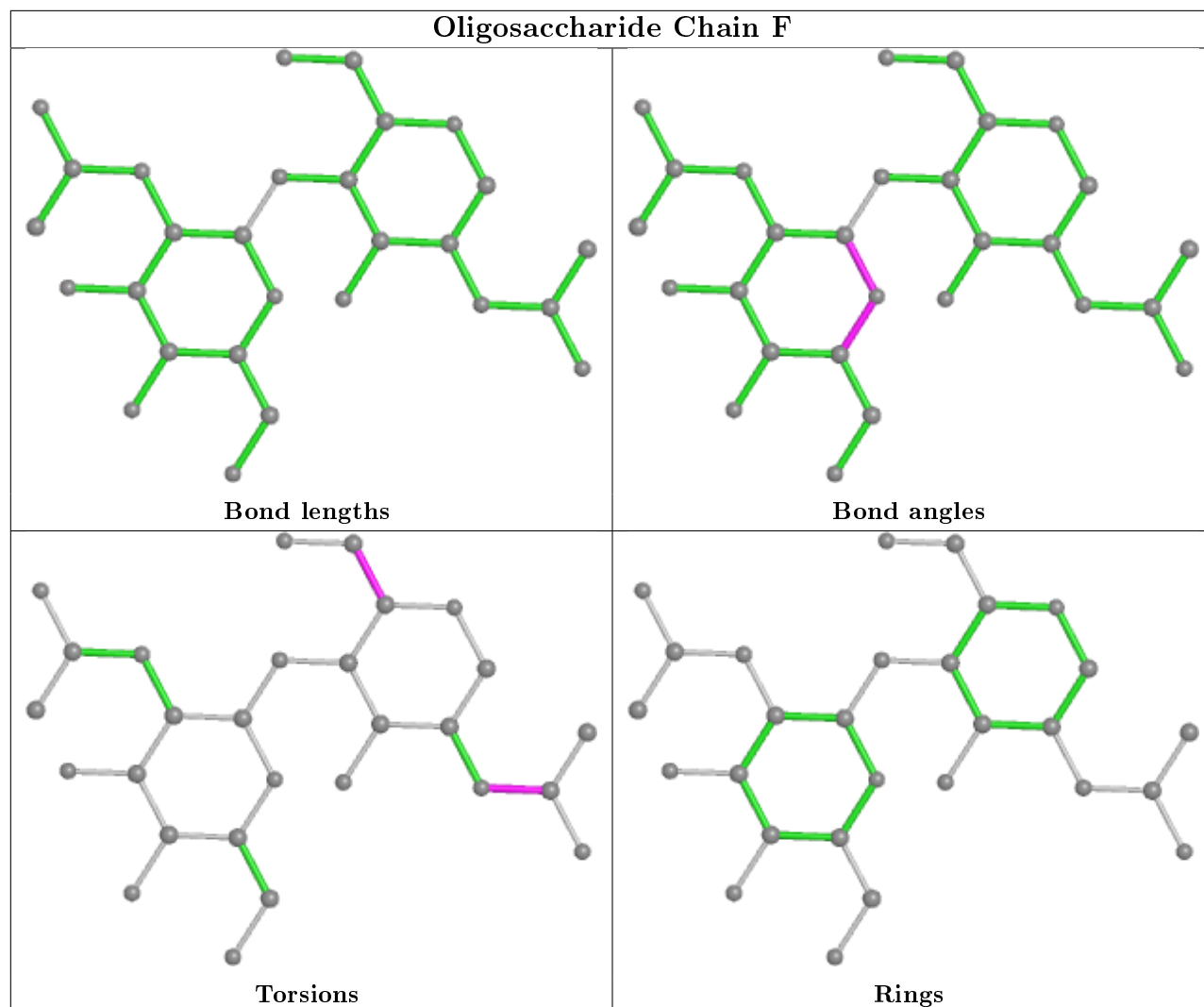
1 monomer is involved in 1 short contact:

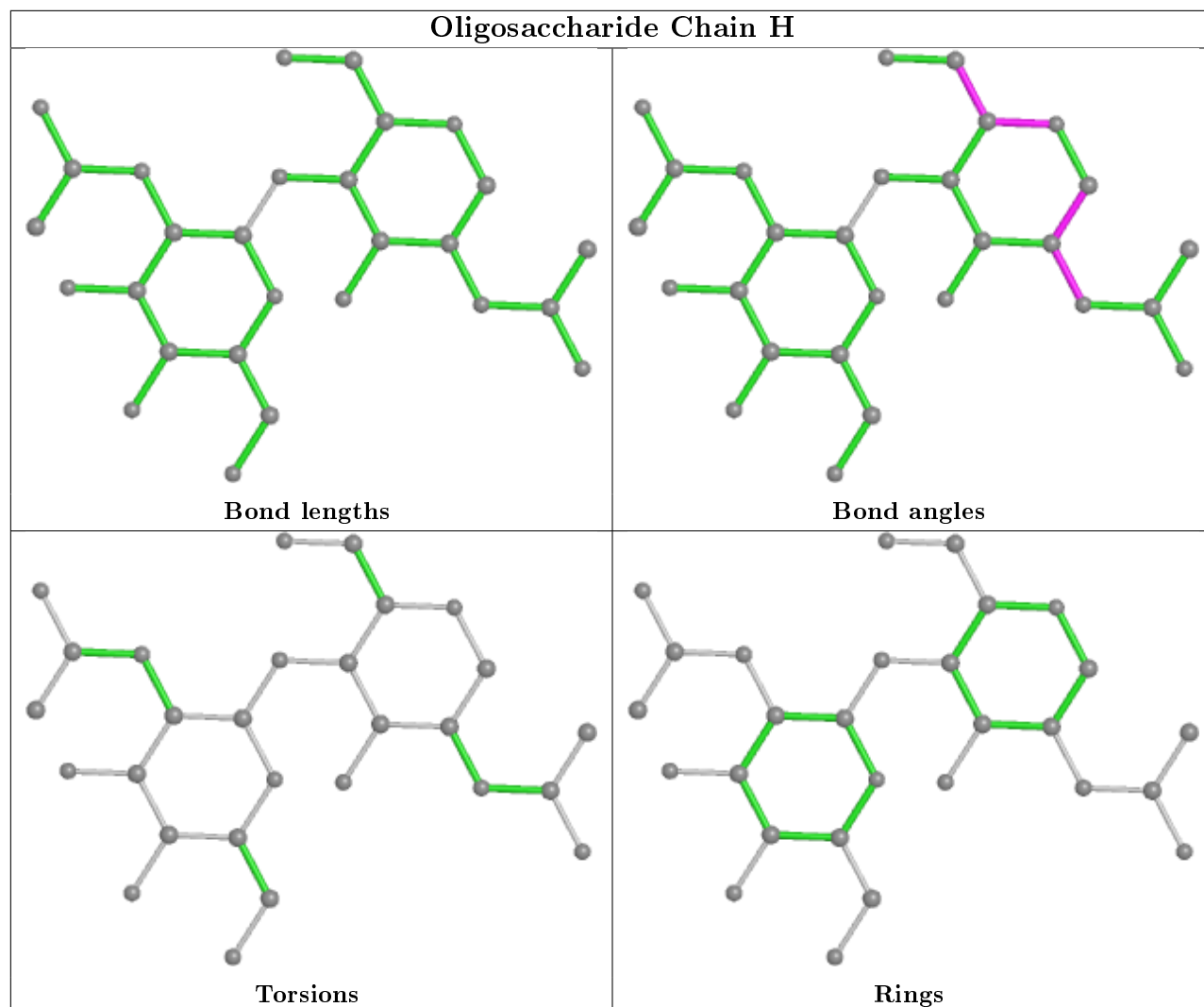
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	4	MAN	1	0

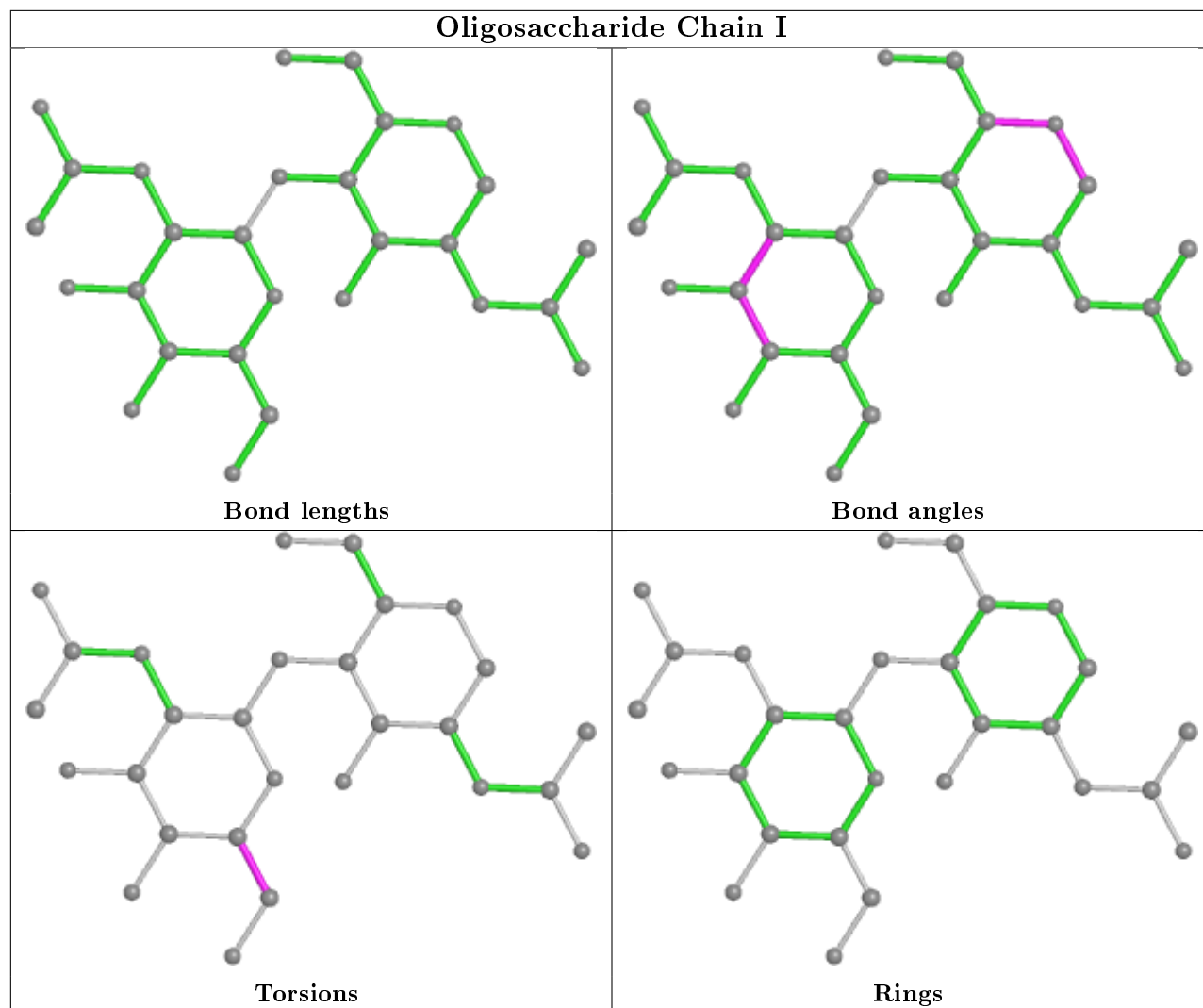
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



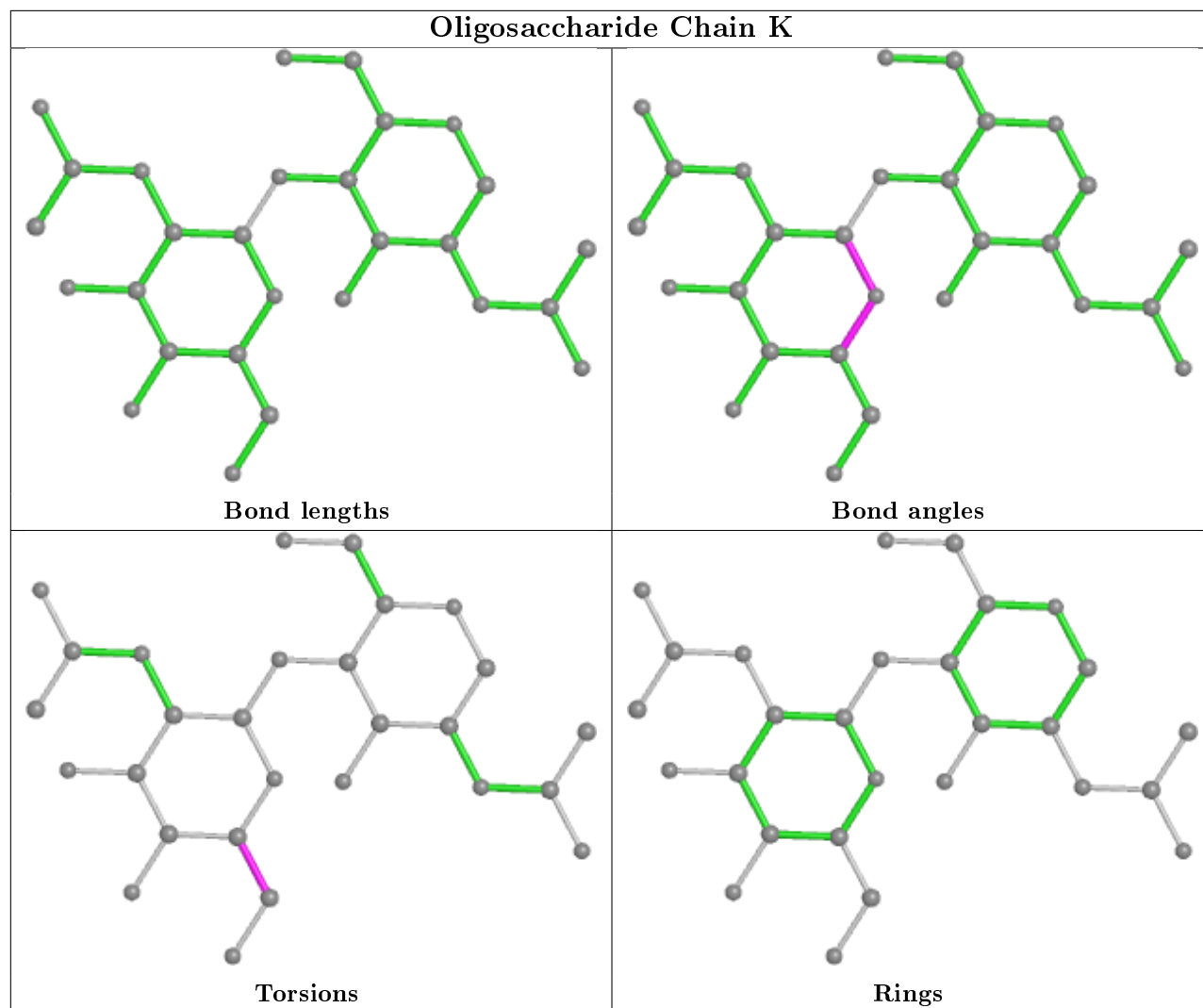


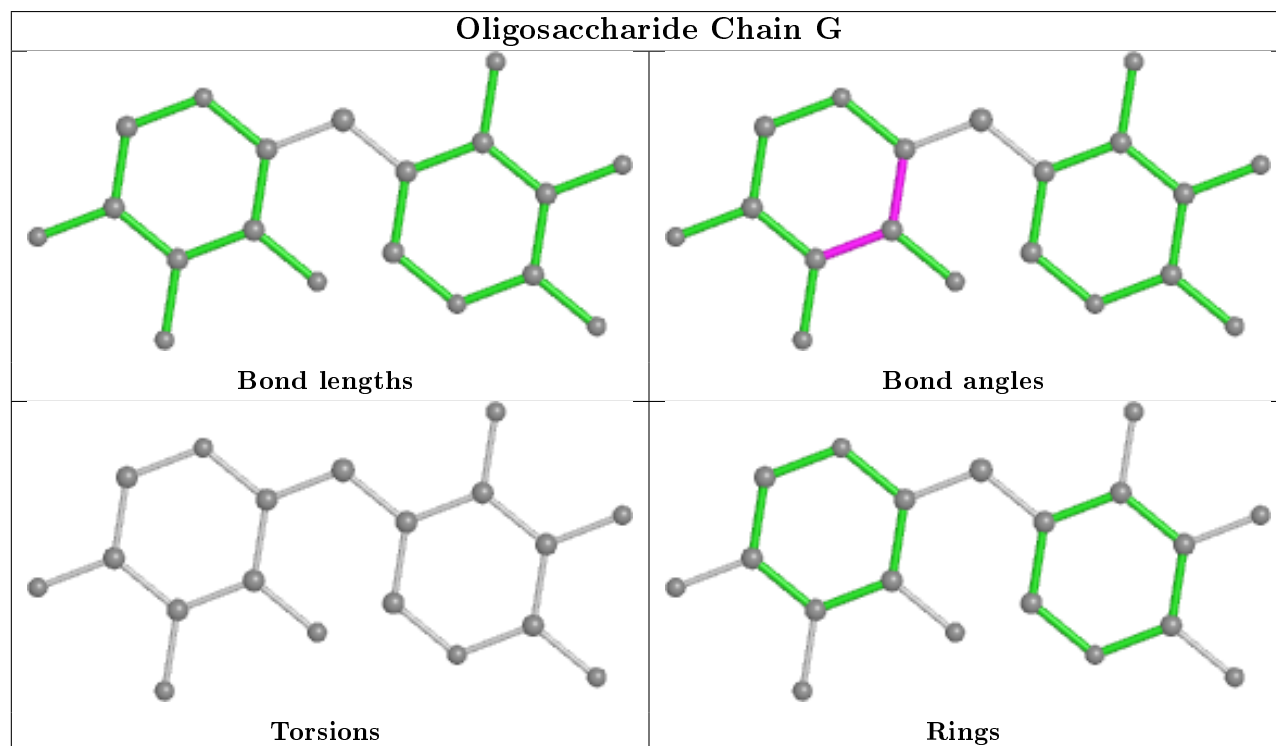
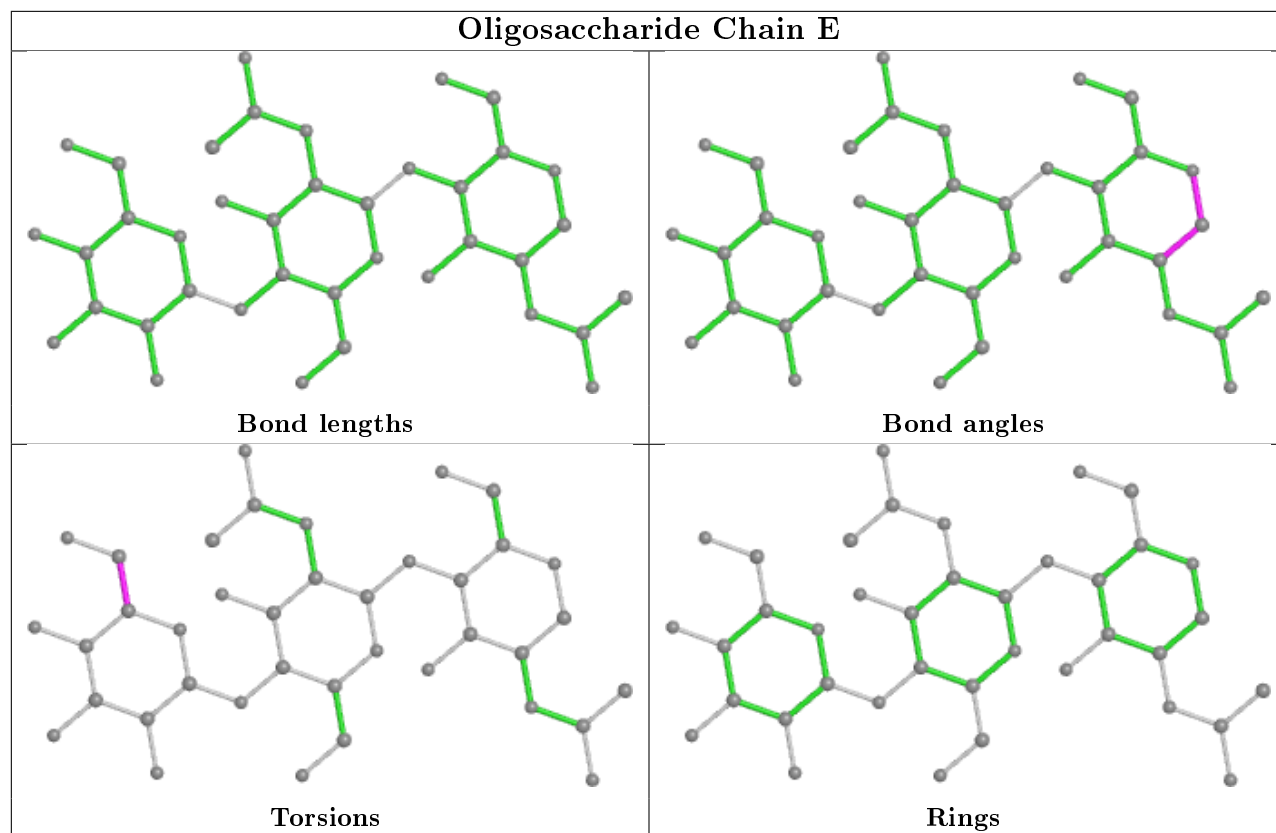


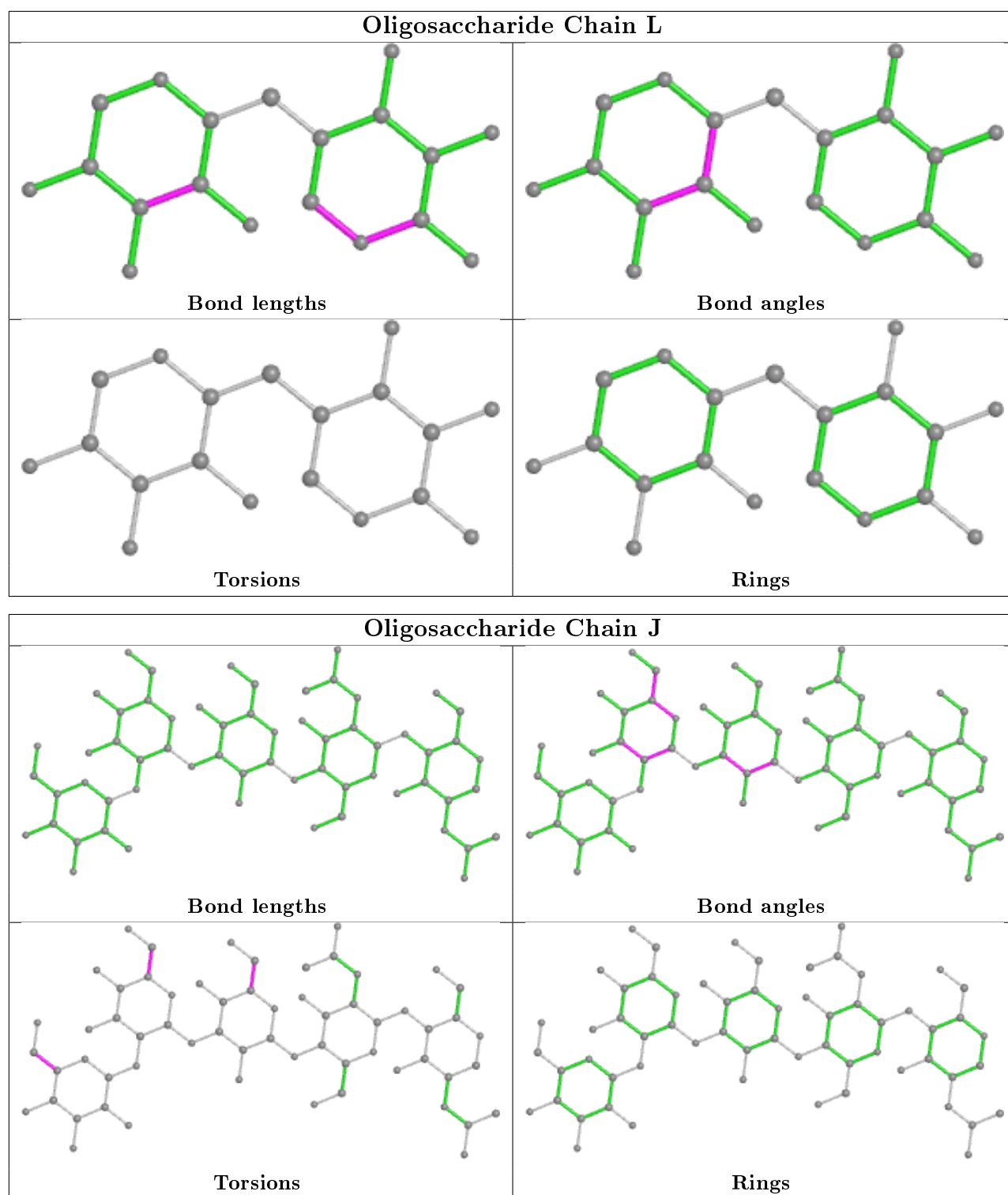












## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 14 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	NAG	A	1201	1	14,14,15	0.45	0	17,19,21	1.32	1 (5%)
7	NAG	B	1701	1	14,14,15	0.61	0	17,19,21	0.70	0
7	NAG	B	1801	1	14,14,15	0.59	0	17,19,21	0.77	1 (5%)
7	NAG	A	901	1	14,14,15	0.59	0	17,19,21	1.07	1 (5%)
7	NAG	A	1301	1	14,14,15	0.52	0	17,19,21	1.23	1 (5%)
7	NAG	B	901	1	14,14,15	0.52	0	17,19,21	1.00	1 (5%)
7	NAG	B	1301	1	14,14,15	0.45	0	17,19,21	1.39	2 (11%)
7	NAG	A	1801	1	14,14,15	0.55	0	17,19,21	0.98	1 (5%)
7	NAG	B	1001	1	14,14,15	0.60	0	17,19,21	0.76	0
7	NAG	A	1001	1	14,14,15	0.58	0	17,19,21	0.68	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
7	NAG	A	1201	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1701	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1801	1	-	0/6/23/26	0/1/1/1
7	NAG	A	901	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
7	NAG	B	901	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1801	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1001	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1301	NAG	C1-O5-C5	4.89	118.82	112.19
7	A	1201	NAG	C1-O5-C5	4.49	118.27	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1301	NAG	C1-O5-C5	4.06	117.70	112.19
7	B	1301	NAG	O5-C5-C6	2.39	110.95	107.20
7	B	1801	NAG	C1-O5-C5	2.36	115.39	112.19
7	B	901	NAG	C4-C3-C2	2.14	114.16	111.02
7	A	1801	NAG	C1-O5-C5	2.05	114.97	112.19
7	A	901	NAG	O5-C5-C6	2.04	110.40	107.20

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1801	NAG	O5-C5-C6-O6
7	A	1801	NAG	C4-C5-C6-O6
7	B	1001	NAG	C4-C5-C6-O6
7	B	1001	NAG	O5-C5-C6-O6
7	B	1701	NAG	C4-C5-C6-O6
7	B	901	NAG	O5-C5-C6-O6
7	A	1201	NAG	C4-C5-C6-O6
7	A	1001	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1301	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	761/767 (99%)	-0.14	18 (2%) 59 64	12, 21, 43, 60	0
1	B	766/767 (99%)	-0.39	8 (1%) 82 85	12, 19, 32, 67	0
All	All	1527/1534 (99%)	-0.27	26 (1%) 70 74	12, 20, 40, 67	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	630	HIS	4.6
1	A	409	VAL	3.9
1	A	407	LYS	3.9
1	A	475	LYS	3.3
1	A	410	ARG	3.2
1	B	629	SER	3.2
1	A	6	TYR	3.0
1	A	522	LEU	3.0
1	B	632	LYS	2.8
1	B	631	PRO	2.7
1	A	669	LYS	2.7
1	A	709	SER	2.5
1	A	460	GLY	2.5
1	A	557	LEU	2.5
1	A	628	ALA	2.3
1	B	628	ALA	2.3
1	A	408	LYS	2.3
1	B	6	TYR	2.2
1	A	406	SER	2.2
1	B	708	HIS	2.2
1	A	536	SER	2.1
1	A	474	LYS	2.1
1	A	478	ALA	2.1
1	A	482	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	538	LYS	2.0
1	A	480	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	PCA	A	1	8/9	0.92	0.11	21,22,23,23	0
1	PCA	B	1	8/9	0.95	0.09	22,22,23,24	0

## 6.3 Carbohydrates ⓘ

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

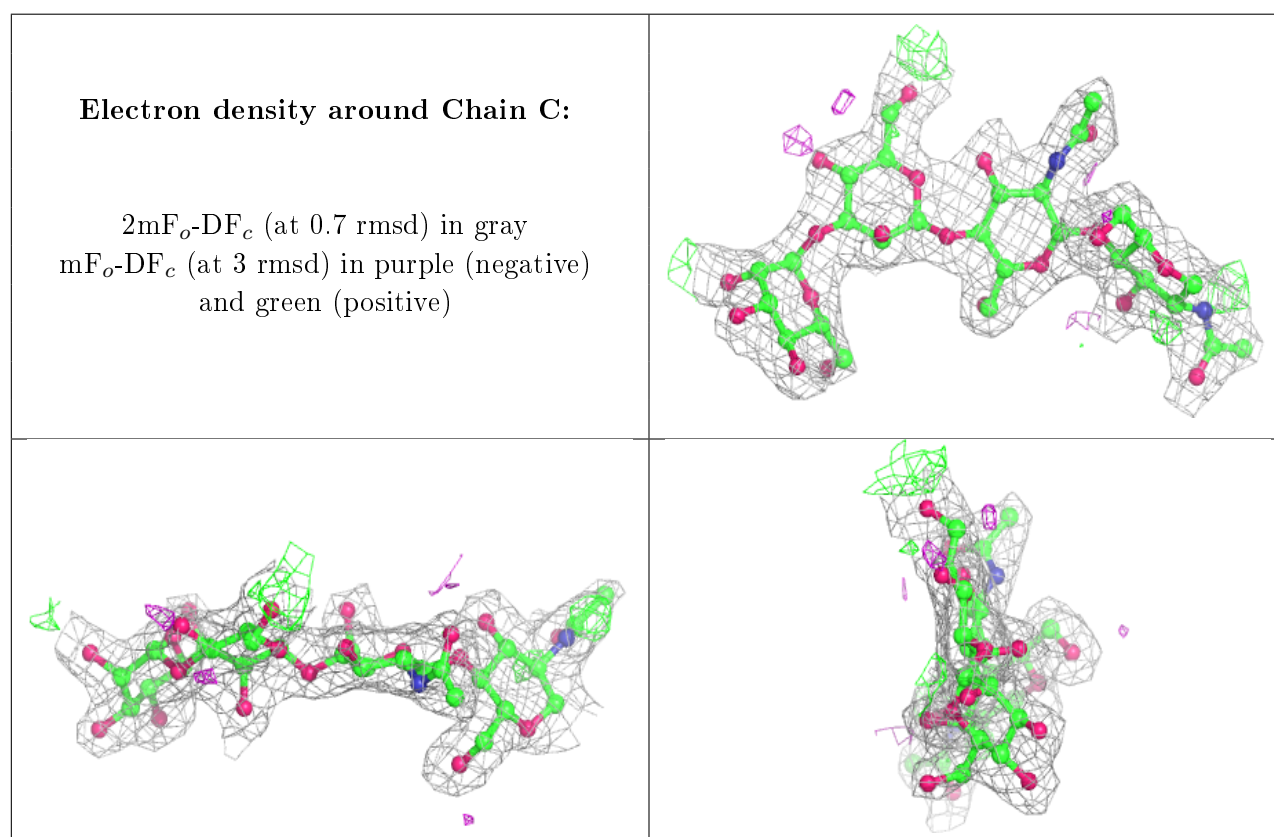
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	D	2	14/15	0.63	0.39	42,49,53,54	0
6	MAN	J	4	11/12	0.65	0.38	36,39,40,40	11
6	MAN	J	5	11/12	0.70	0.19	33,34,35,35	11
4	BMA	E	3	11/12	0.73	0.33	44,46,48,49	11
3	NAG	F	1	14/15	0.79	0.32	48,55,56,59	0
3	NAG	F	2	14/15	0.79	0.47	62,65,68,69	0
6	BMA	J	3	11/12	0.80	0.34	43,44,51,51	0
2	BMA	C	3	11/12	0.85	0.15	34,36,37,39	0
3	NAG	I	2	14/15	0.86	0.28	39,41,42,45	0
2	NAG	C	1	14/15	0.87	0.13	25,27,30,32	0
3	NAG	K	2	14/15	0.88	0.36	43,48,50,51	0
4	NAG	E	1	14/15	0.88	0.17	29,32,34,34	0
3	NAG	H	2	14/15	0.88	0.22	34,37,41,42	0
5	TXB	L	1	10/10	0.89	0.18	30,40,43,43	0
2	MAN	C	4	11/12	0.89	0.18	39,40,42,43	0
3	NAG	D	1	14/15	0.90	0.18	29,33,37,40	0
3	NAG	H	1	14/15	0.90	0.11	24,27,31,32	0
3	NAG	K	1	14/15	0.91	0.17	29,31,34,39	0
6	NAG	J	2	14/15	0.92	0.15	32,35,36,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	I	1	14/15	0.93	0.14	27,29,30,35	0
4	NAG	E	2	14/15	0.93	0.26	37,39,42,44	0
5	XYP	L	2	9/10	0.94	0.12	20,24,27,27	0
5	TXB	G	1	10/10	0.94	0.13	27,36,38,38	0
6	NAG	J	1	14/15	0.96	0.11	25,26,28,29	0
2	NAG	C	2	14/15	0.96	0.15	27,29,32,32	0
5	XYP	G	2	9/10	0.97	0.10	19,20,22,23	0

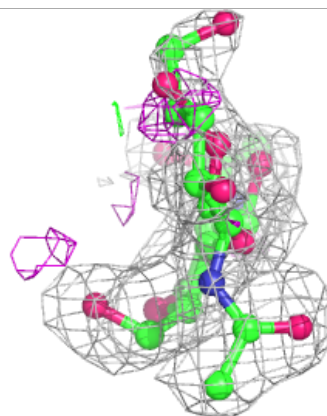
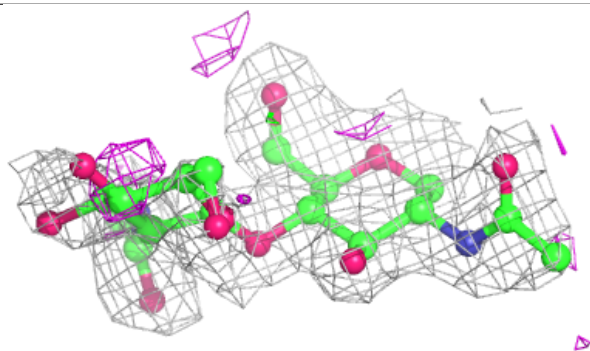
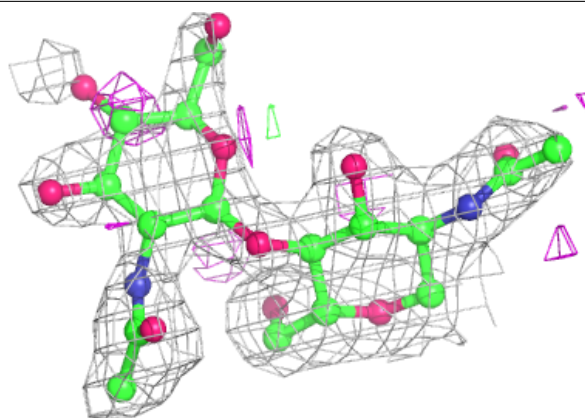
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





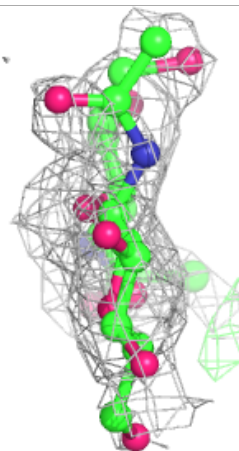
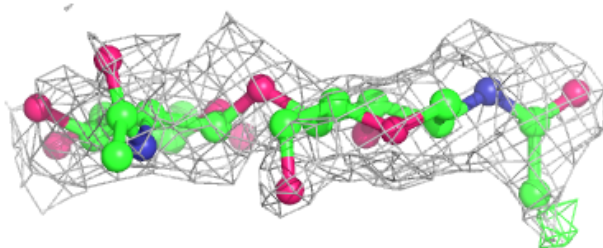
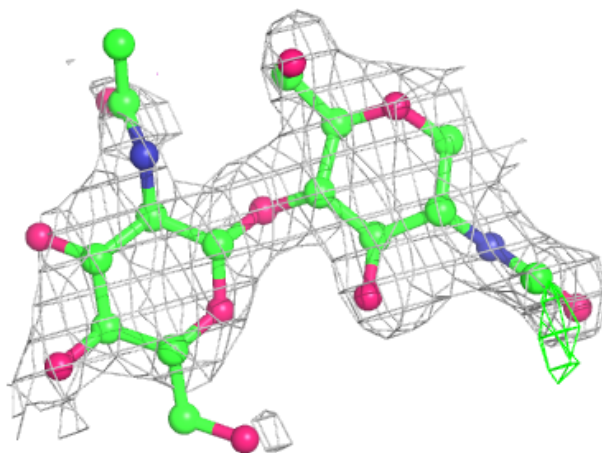
**Electron density around Chain D:**

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



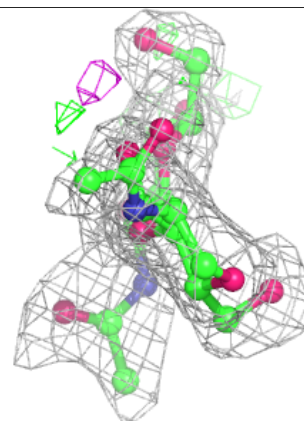
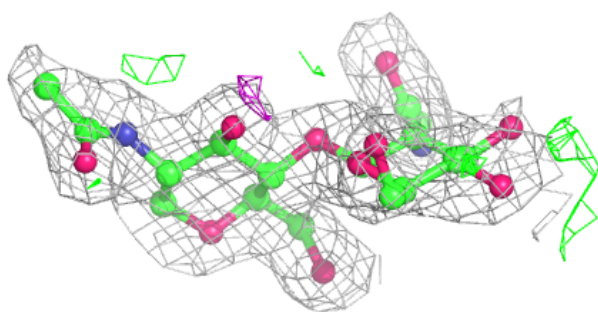
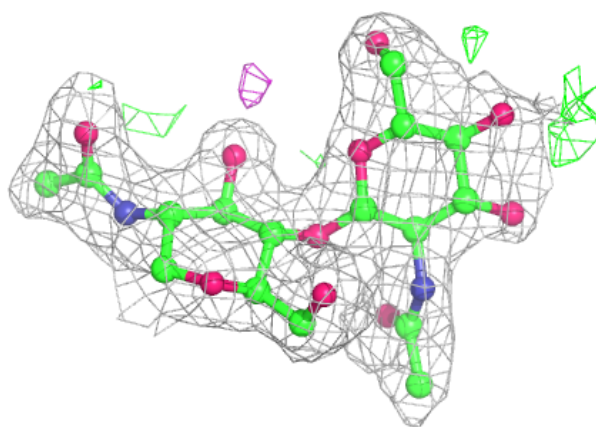
**Electron density around Chain F:**

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



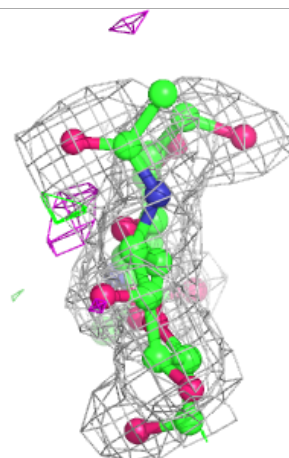
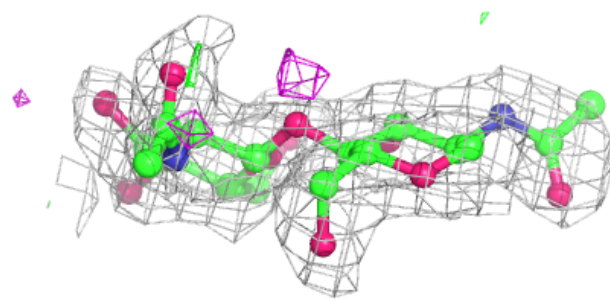
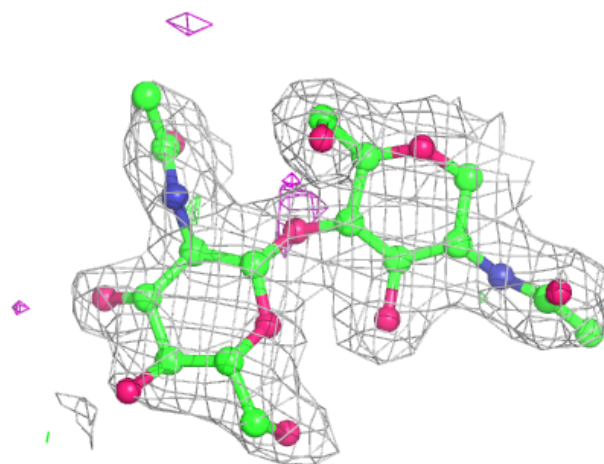
**Electron density around Chain H:**

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



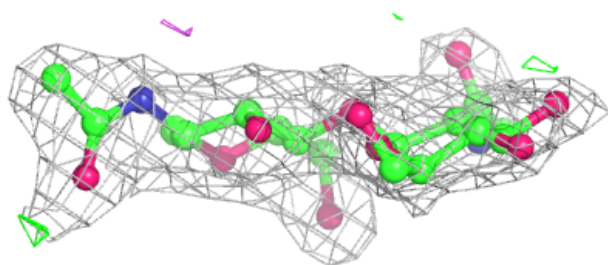
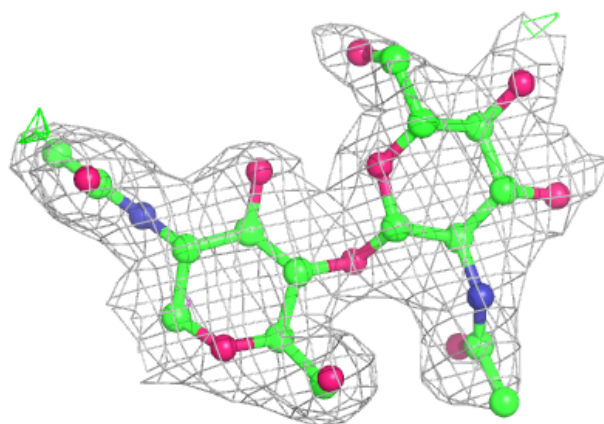
**Electron density around Chain I:**

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

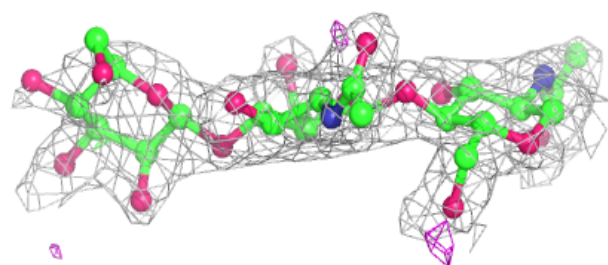
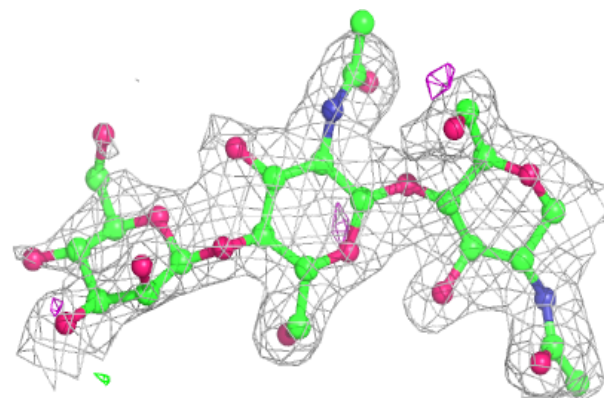


**Electron density around Chain K:**

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

**Electron density around Chain E:**

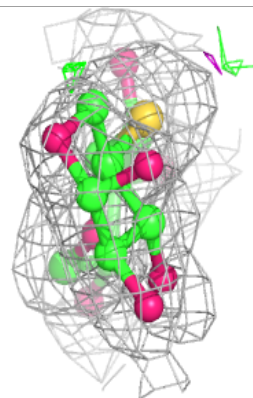
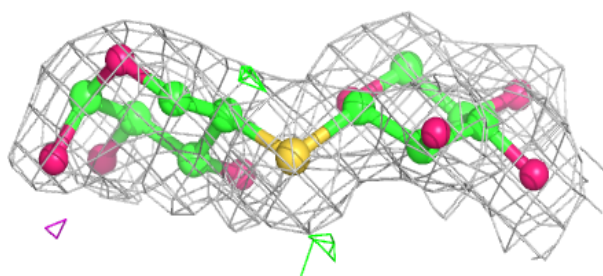
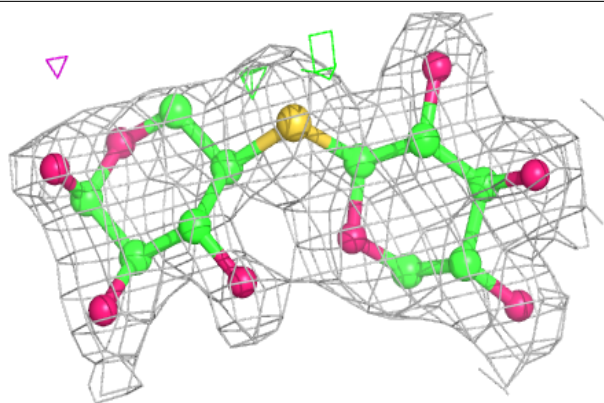
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



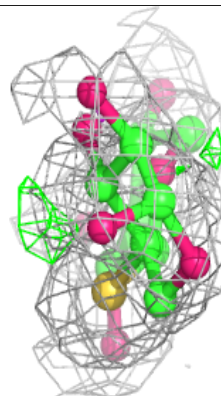
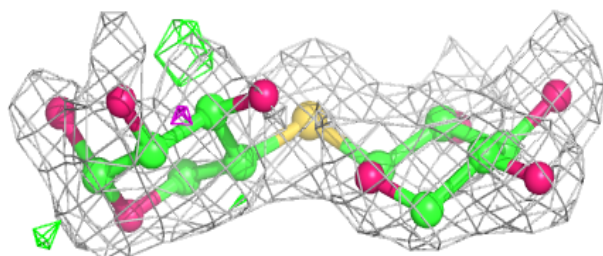
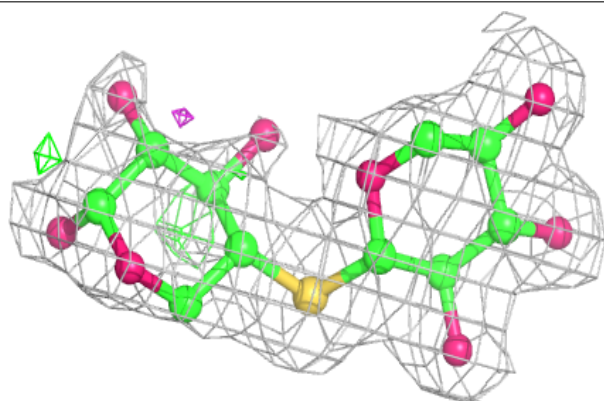


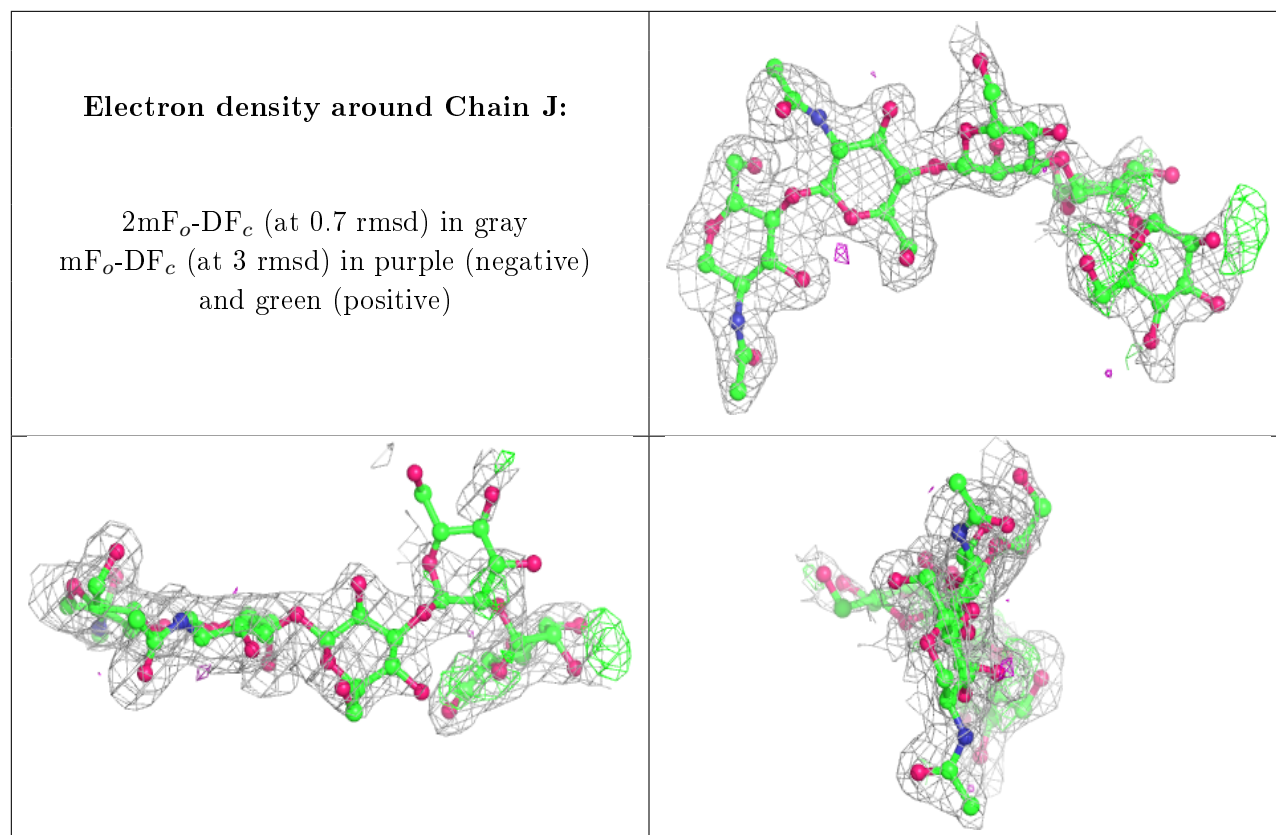
**Electron density around Chain G:**

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

**Electron density around Chain 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 ⓘ

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	B	1701	14/15	0.81	0.24	32,34,36,36	0
7	NAG	A	1201	14/15	0.82	0.29	40,44,47,52	0
7	NAG	B	1301	14/15	0.82	0.35	36,45,50,51	0
7	NAG	B	901	14/15	0.83	0.19	29,35,36,36	0
7	NAG	A	1301	14/15	0.84	0.21	31,35,39,40	0
8	ZN	A	1902	1/1	0.84	0.09	62,62,62,62	1
7	NAG	B	1001	14/15	0.89	0.18	37,41,43,44	0
7	NAG	A	901	14/15	0.91	0.14	29,31,33,34	0
8	ZN	B	1906[A]	1/1	0.92	0.12	39,39,39,39	1
8	ZN	B	1906[B]	1/1	0.92	0.12	51,51,51,51	1
7	NAG	A	1001	14/15	0.92	0.20	31,34,37,38	0
7	NAG	A	1801	14/15	0.93	0.18	40,43,45,45	0
8	ZN	B	1910	1/1	0.94	0.07	67,67,67,67	0
7	NAG	B	1801	14/15	0.94	0.13	30,32,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	ZN	A	1911	1/1	0.97	0.06	31,31,31,31	1
8	ZN	A	1906[B]	1/1	0.97	0.09	47,47,47,47	1
8	ZN	A	1906[A]	1/1	0.97	0.09	46,46,46,46	1
8	ZN	B	1911	1/1	0.98	0.05	34,34,34,34	1
8	ZN	B	1914	1/1	0.98	0.03	37,37,37,37	0
8	ZN	A	1901	1/1	0.99	0.03	25,25,25,25	0
8	ZN	B	1901	1/1	0.99	0.02	23,23,23,23	0
8	ZN	B	1907	1/1	1.00	0.10	19,19,19,19	1
8	ZN	B	1904	1/1	1.00	0.01	22,22,22,22	0
8	ZN	A	1904	1/1	1.00	0.02	21,21,21,21	0

## 6.5 Other polymers

There are no such residues in this entry.