



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 05:20 PM BST

PDB ID : 4OIA  
Title : Crystal Structure of ICAM-5 D1-D4 ectodomain fragment, Space Group P4322  
Authors : Recacha, R.; Jimenez, D.; Tian, L.; Barredo, R.; Ghamberg, C.; Casasnovas, J.M.  
Deposited on : 2014-01-19  
Resolution : 3.70 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.

---

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

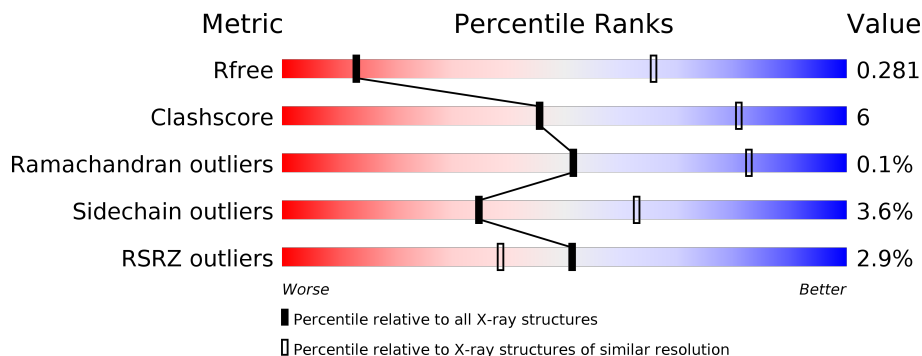
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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 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	378	
1	B	378	
2	C	2	
2	D	2	
2	G	2	
2	H	2	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	I	2	 100%
2	J	2	 100%
2	L	2	 50% 50%
3	E	3	 100%
3	F	3	 67% 33%
3	K	3	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	D	2	-	-	-	X
3	NAG	K	1	-	-	-	X
3	NAG	K	2	-	-	-	X
4	NAG	B	2303	-	-	-	X
5	EDO	A	2316	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6125 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 Intercellular adhesion molecule 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	374	2857	1772	534	539	12	0	0	0
1	B	375	2867	1780	532	543	12	0	0	0

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



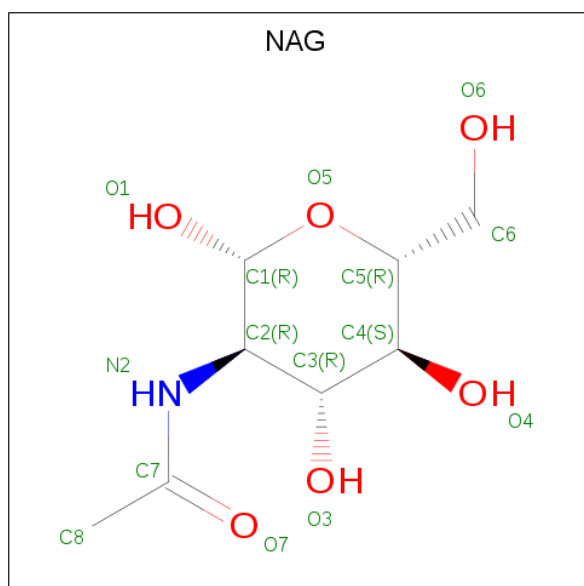
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0
2	D	2	28	16	2	10	0	0	0
2	G	2	28	16	2	10	0	0	0
2	H	2	28	16	2	10	0	0	0
2	I	2	28	16	2	10	0	0	0
2	J	2	28	16	2	10	0	0	0
2	L	2	28	16	2	10	0	0	0

- Molecule 3 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.



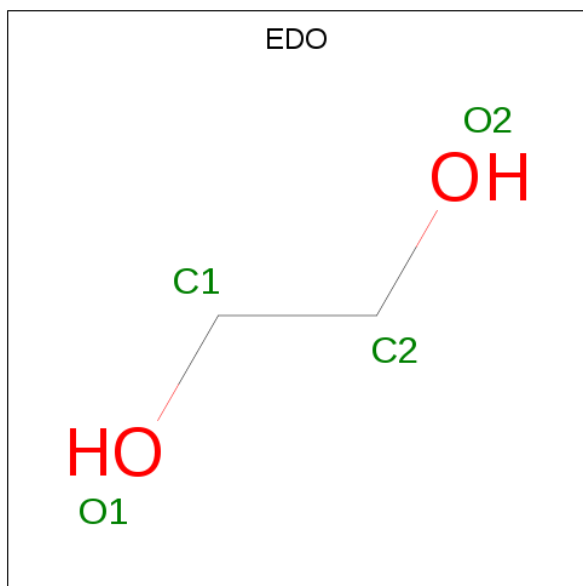
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	K	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).

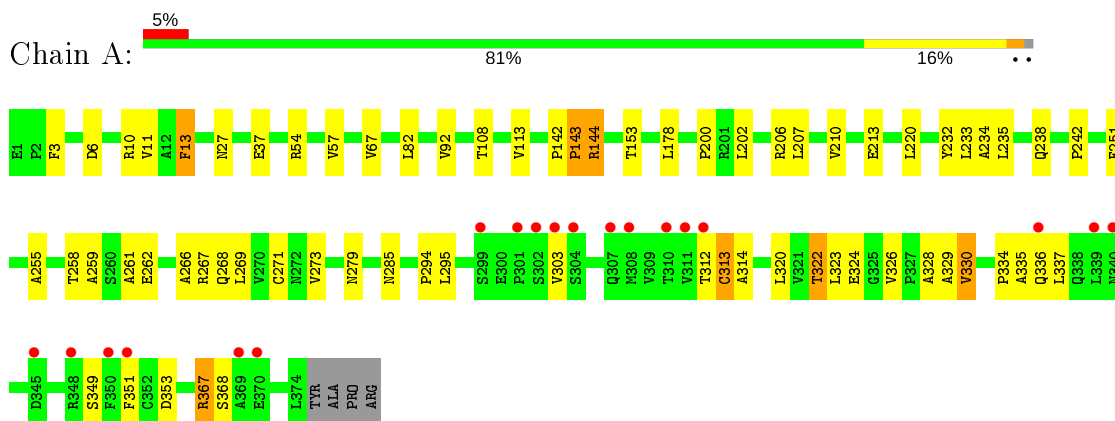


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

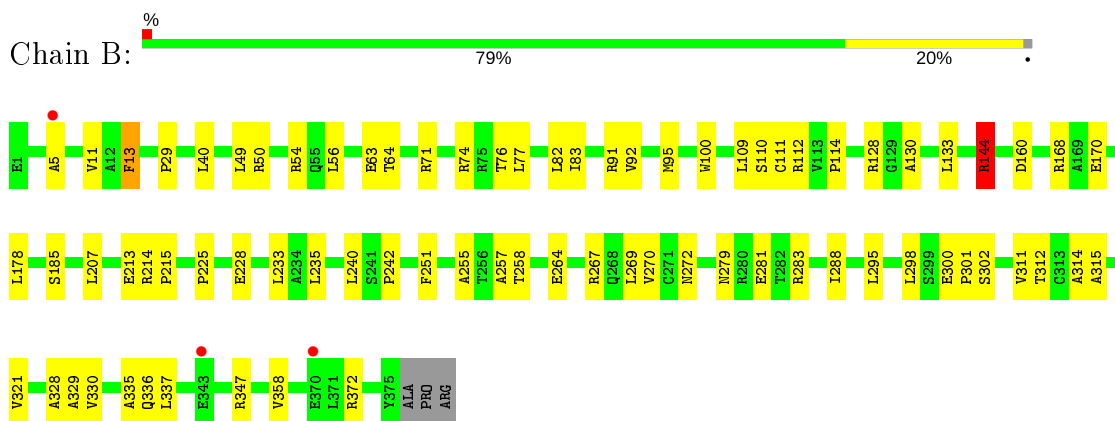
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

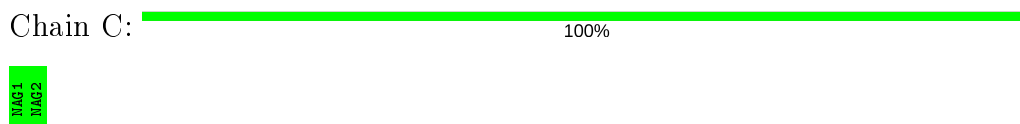
- Molecule 1: Intercellular adhesion molecule 5




- Molecule 1: Intercellular adhesion molecule 5



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

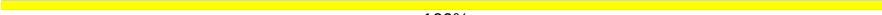


- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%

MAG1  
MAG2

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

Chain G:  100%

MAG1  
MAG2

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

Chain H:  50% 50%

MAG1  
MAG2

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

Chain I:  100%

MAG1  
MAG2

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

Chain J:  100%

MAG1  
MAG2

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

Chain L:  50% 50%

MAG1  
MAG2

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

Chain E:  100%

MAG1  
MAG2  
BVA3



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

Chain F:  67% 33%

MA01  
MA02  
B01A3

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

Chain K:  100%

MA01  
MA02  
B01A3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.07Å 96.07Å 321.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.99 – 3.70 24.99 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (24.99-3.70) 99.8 (24.99-3.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.91 (at 3.74Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.230 , 0.280 0.239 , 0.281	Depositor DCC
$R_{free}$ test set	856 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	87.4	Xtrriage
Anisotropy	0.777	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 78.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	6125	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	186.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.55% 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: BMA, NAG, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.39	1/2912 (0.0%)	0.47	3/3965 (0.1%)
1	B	0.23	0/2923	0.42	0/3981
All	All	0.32	1/5835 (0.0%)	0.45	3/7946 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	ARG	C-N	-17.69	0.93	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	PRO	O-C-N	7.17	134.17	122.70
1	A	143	PRO	CA-C-N	-5.86	104.30	117.20
1	A	143	PRO	C-N-CA	-5.25	108.56	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	130	ALA	Peptide

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	144	ARG	Sidechain

## 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	2857	0	2825	36	2
1	B	2867	0	2829	42	0
2	C	28	0	25	0	0
2	D	28	0	25	1	0
2	G	28	0	24	1	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	L	28	0	25	0	0
3	E	39	0	34	0	0
3	F	39	0	34	0	0
3	K	39	0	34	0	0
4	A	42	0	39	0	0
4	B	42	0	39	0	0
5	A	4	0	6	0	0
All	All	6125	0	6014	78	2

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 6.

The worst 5 of 78 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:328:ALA:HB1	1:A:335:ALA:HB3	1.63	0.79
1:B:63:GLU:HB3	1:B:144:ARG:HD3	1.72	0.70
1:B:112:ARG:HG2	1:B:114:PRO:HD3	1.74	0.70
1:B:63:GLU:HB3	1:B:144:ARG:CD	2.24	0.68
1:B:11:VAL:HG12	1:B:82:LEU:HB3	1.76	0.67

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:NH2	1:A:206:ARG:CD[4_565]	2.06	0.14
1:A:144:ARG:NH2	1:A:206:ARG:NE[4_565]	2.10	0.10

## 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	372/378 (98%)	347 (93%)	24 (6%)	1 (0%)	41	74
1	B	373/378 (99%)	358 (96%)	15 (4%)	0	100	100
All	All	745/756 (98%)	705 (95%)	39 (5%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	303	VAL

### 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	304/309 (98%)	294 (97%)	10 (3%)	38	64
1	B	305/309 (99%)	293 (96%)	12 (4%)	32	60
All	All	609/618 (98%)	587 (96%)	22 (4%)	35	63

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	ARG
1	B	54	ARG
1	B	300	GLU
1	B	13	PHE
1	B	49	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

23 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	0.42	0	17,19,21	0.54	0
2	NAG	C	2	2	14,14,15	0.22	0	17,19,21	0.34	0
2	NAG	D	1	1,2	14,14,15	0.39	0	17,19,21	0.45	0
2	NAG	D	2	2	14,14,15	0.62	0	17,19,21	0.76	1 (5%)
3	NAG	E	1	1,3	14,14,15	0.28	0	17,19,21	0.35	0
3	NAG	E	2	3	14,14,15	0.26	0	17,19,21	0.35	0
3	BMA	E	3	3	11,11,12	0.69	0	15,15,17	0.77	0
3	NAG	F	1	1,3	14,14,15	0.25	0	17,19,21	0.34	0
3	NAG	F	2	3	14,14,15	0.53	0	17,19,21	1.13	1 (5%)
3	BMA	F	3	3	11,11,12	0.64	0	15,15,17	0.84	0
2	NAG	G	1	1,2	14,14,15	0.49	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	G	2	2	14,14,15	0.45	0	17,19,21	0.67	1 (5%)
2	NAG	H	1	1,2	14,14,15	0.29	0	17,19,21	0.62	1 (5%)
2	NAG	H	2	2	14,14,15	0.29	0	17,19,21	0.44	0
2	NAG	I	1	1,2	14,14,15	0.47	0	17,19,21	0.54	0
2	NAG	I	2	2	14,14,15	0.25	0	17,19,21	0.39	0
2	NAG	J	1	1,2	14,14,15	0.17	0	17,19,21	0.63	0
2	NAG	J	2	2	14,14,15	0.45	0	17,19,21	0.42	0
3	NAG	K	1	1,3	14,14,15	0.33	0	17,19,21	0.37	0
3	NAG	K	2	3	14,14,15	0.22	0	17,19,21	0.39	0
3	BMA	K	3	3	11,11,12	0.65	0	15,15,17	0.85	0
2	NAG	L	1	1,2	14,14,15	0.30	0	17,19,21	0.41	0
2	NAG	L	2	2	14,14,15	0.37	0	17,19,21	0.60	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
2	NAG	C	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	1/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	L	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	L	2	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	NAG	C1-O5-C5	3.86	117.43	112.19
2	D	2	NAG	C1-O5-C5	2.88	116.09	112.19
2	G	2	NAG	C1-O5-C5	2.22	115.20	112.19
2	L	2	NAG	C1-O5-C5	2.19	115.16	112.19
2	H	1	NAG	C1-O5-C5	2.11	115.05	112.19

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2

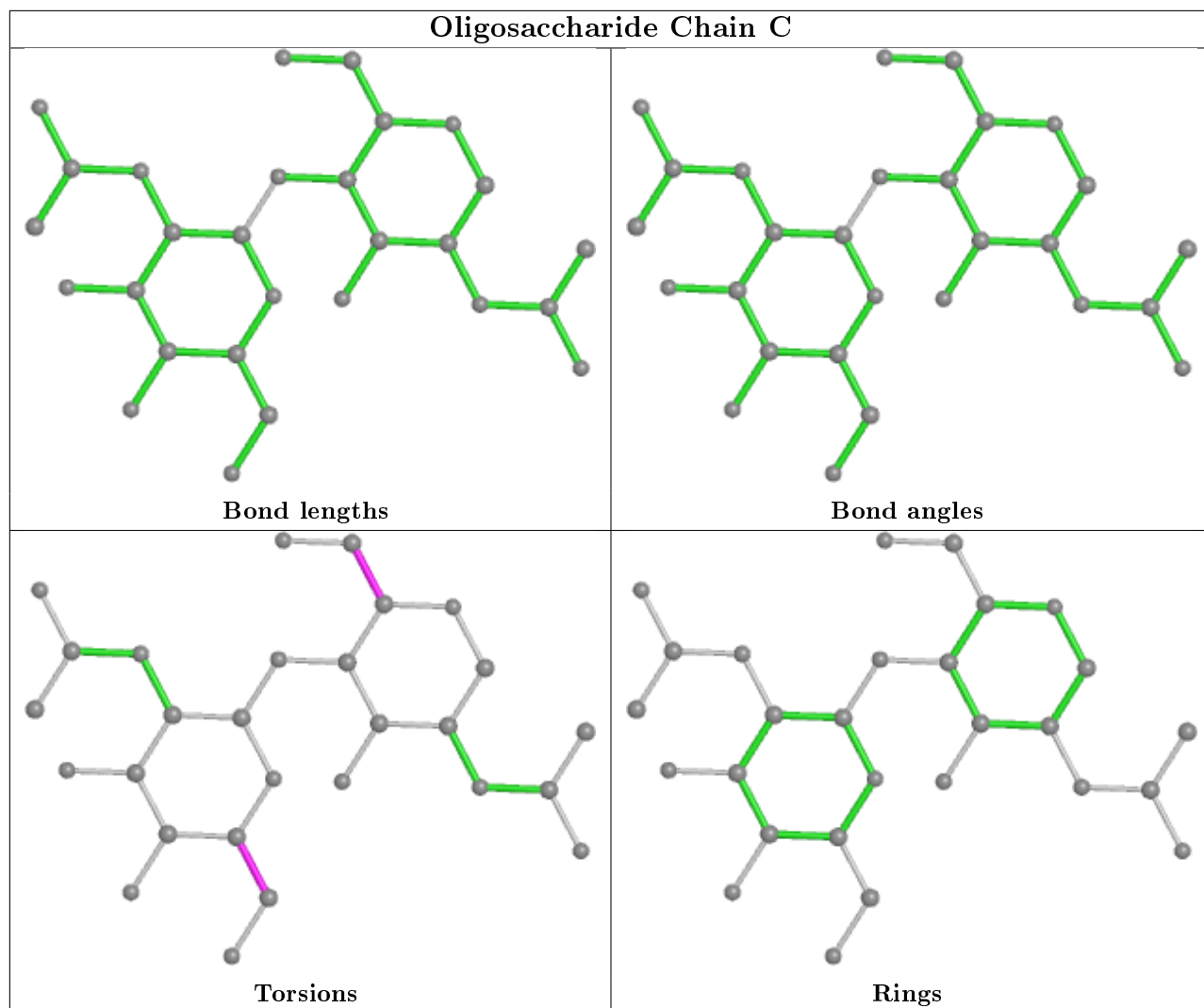
There are no ring outliers.

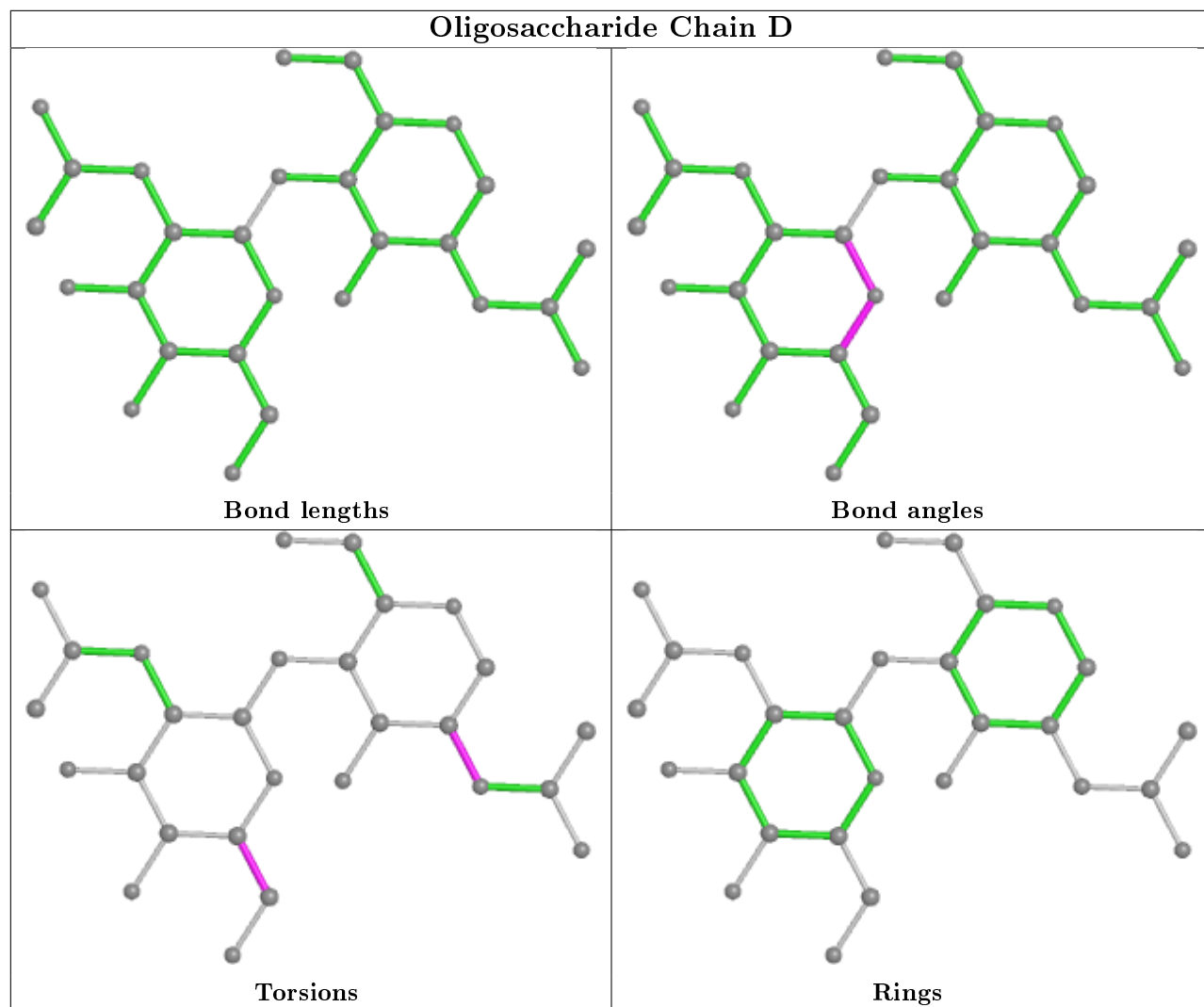
2 monomers are involved in 2 short contacts:

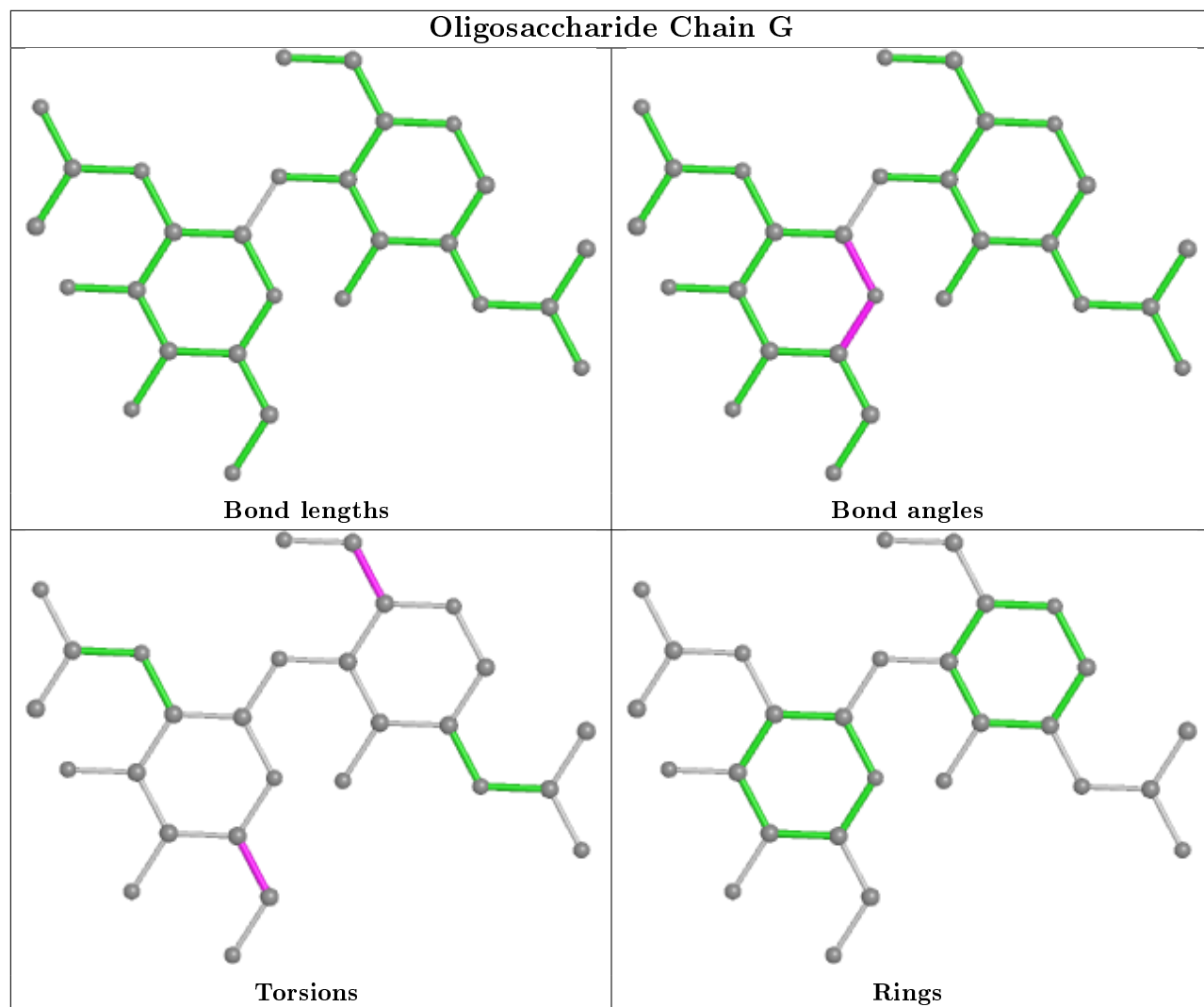
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	1	0
2	G	1	NAG	1	0

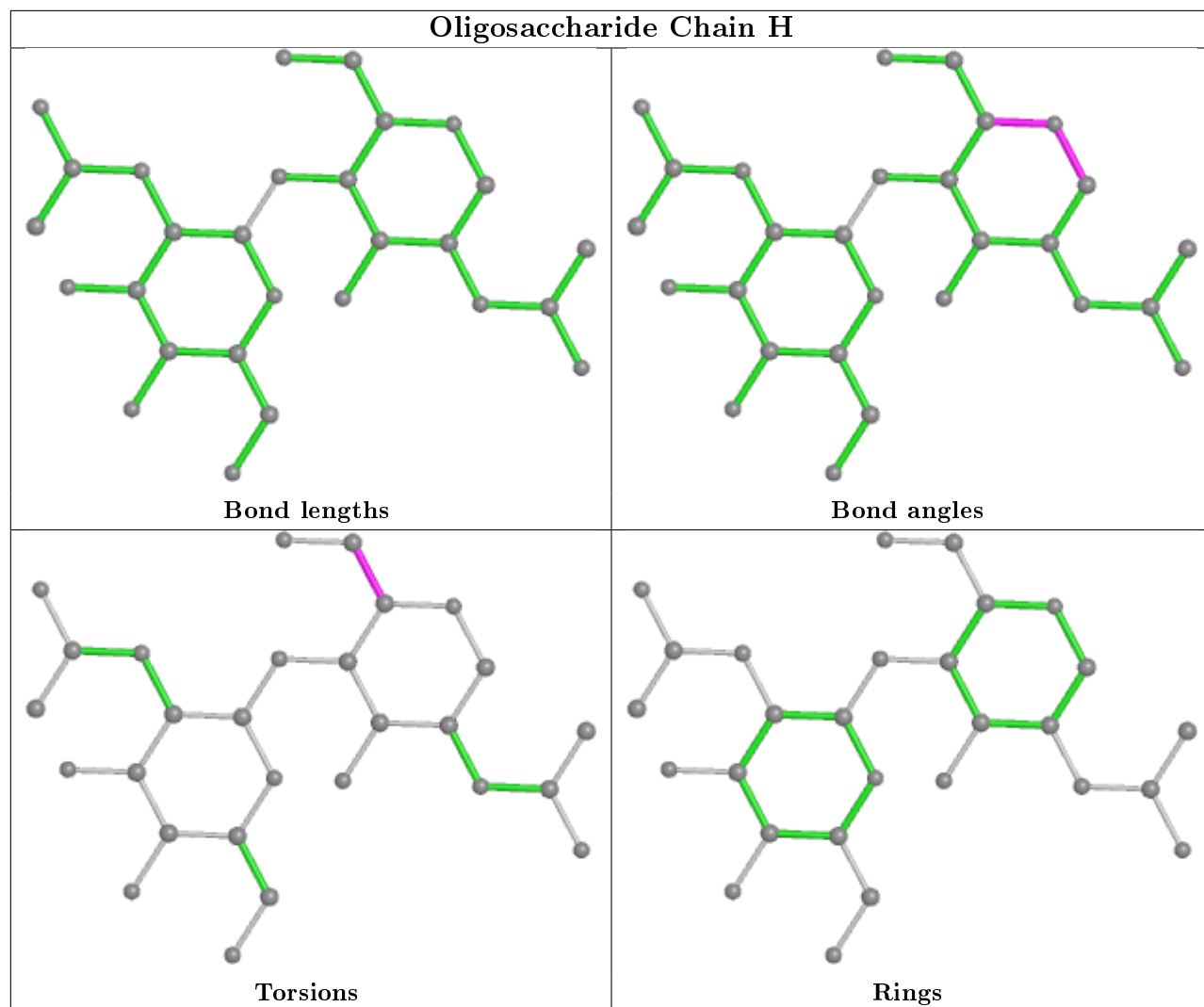
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

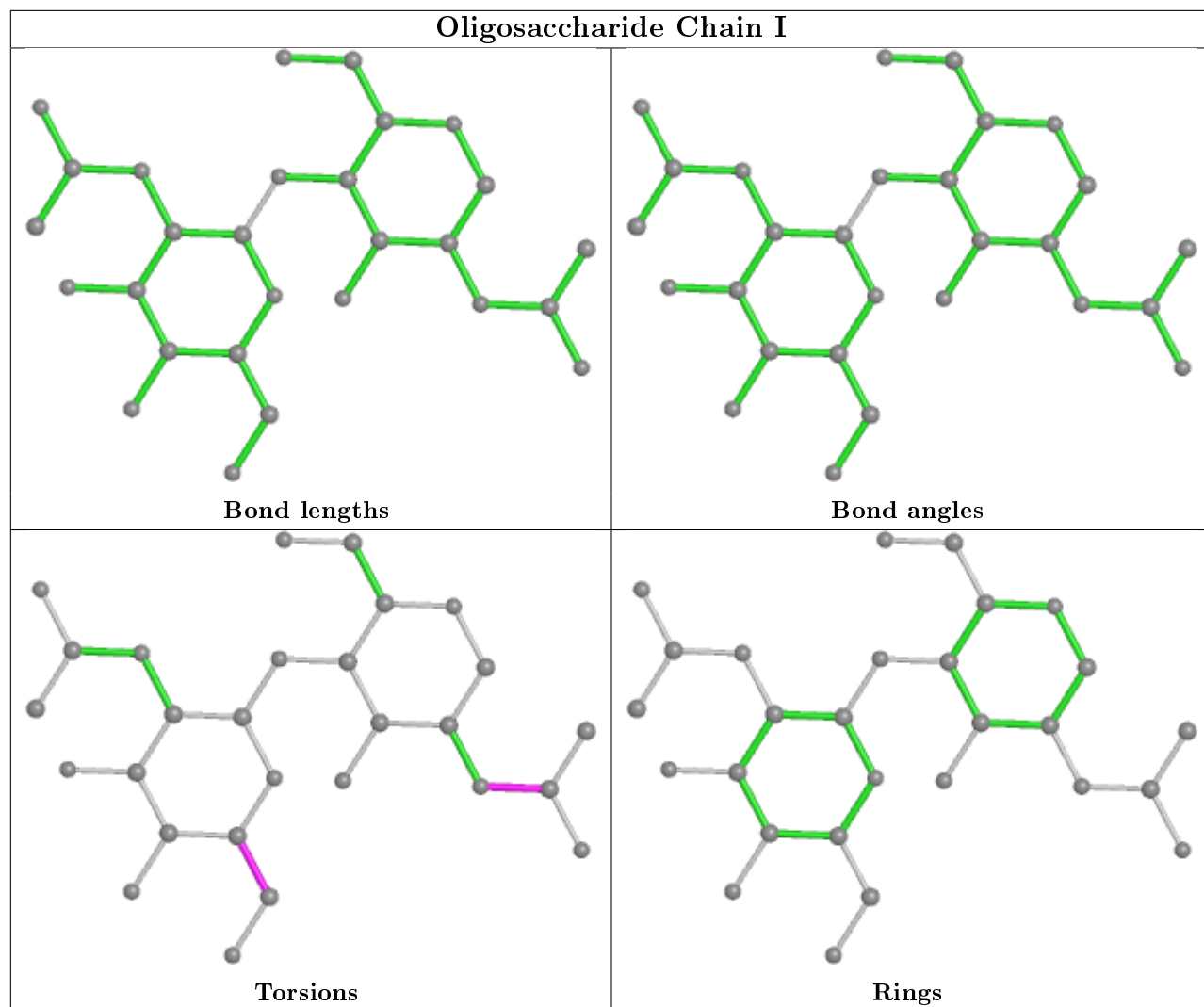


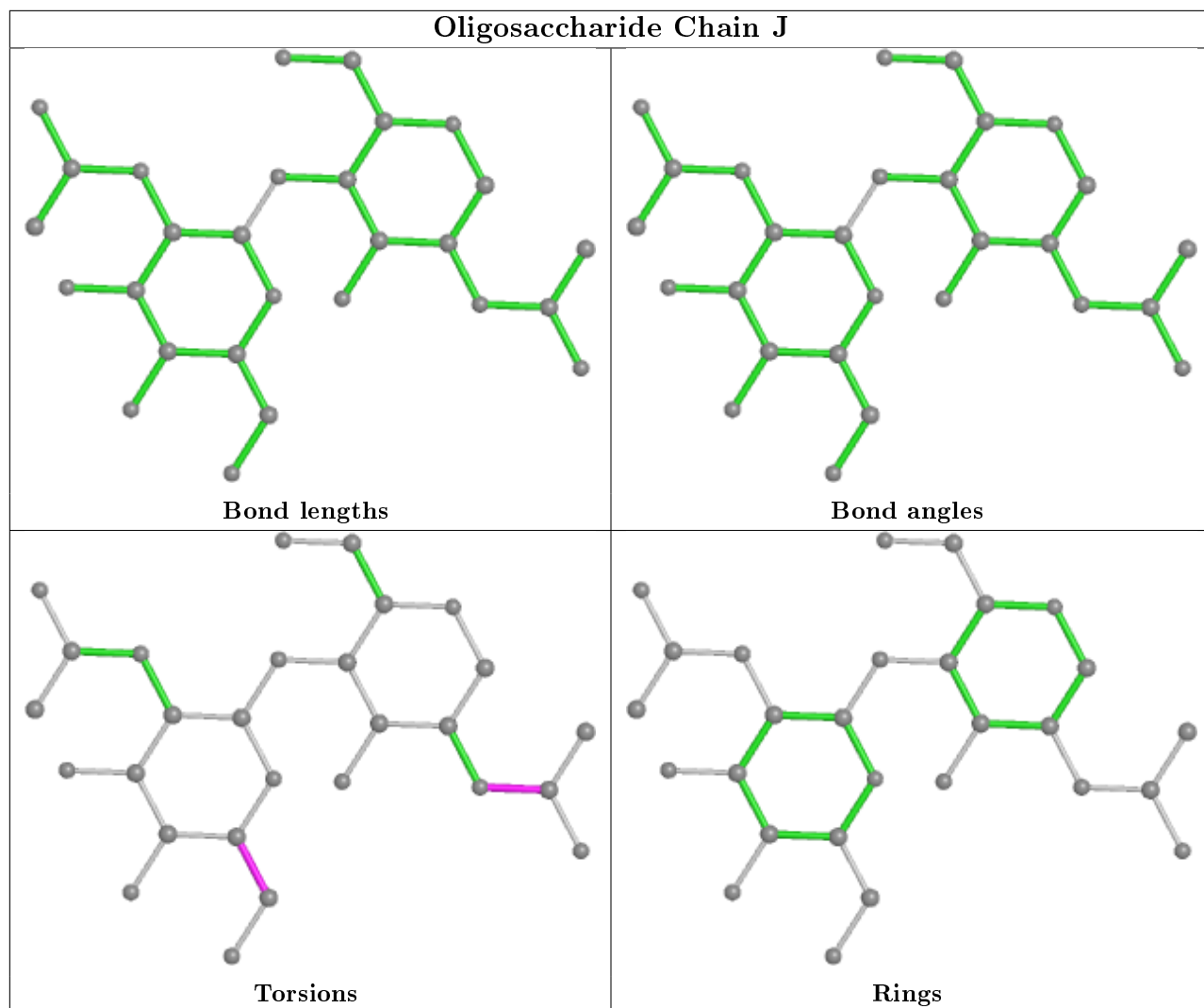


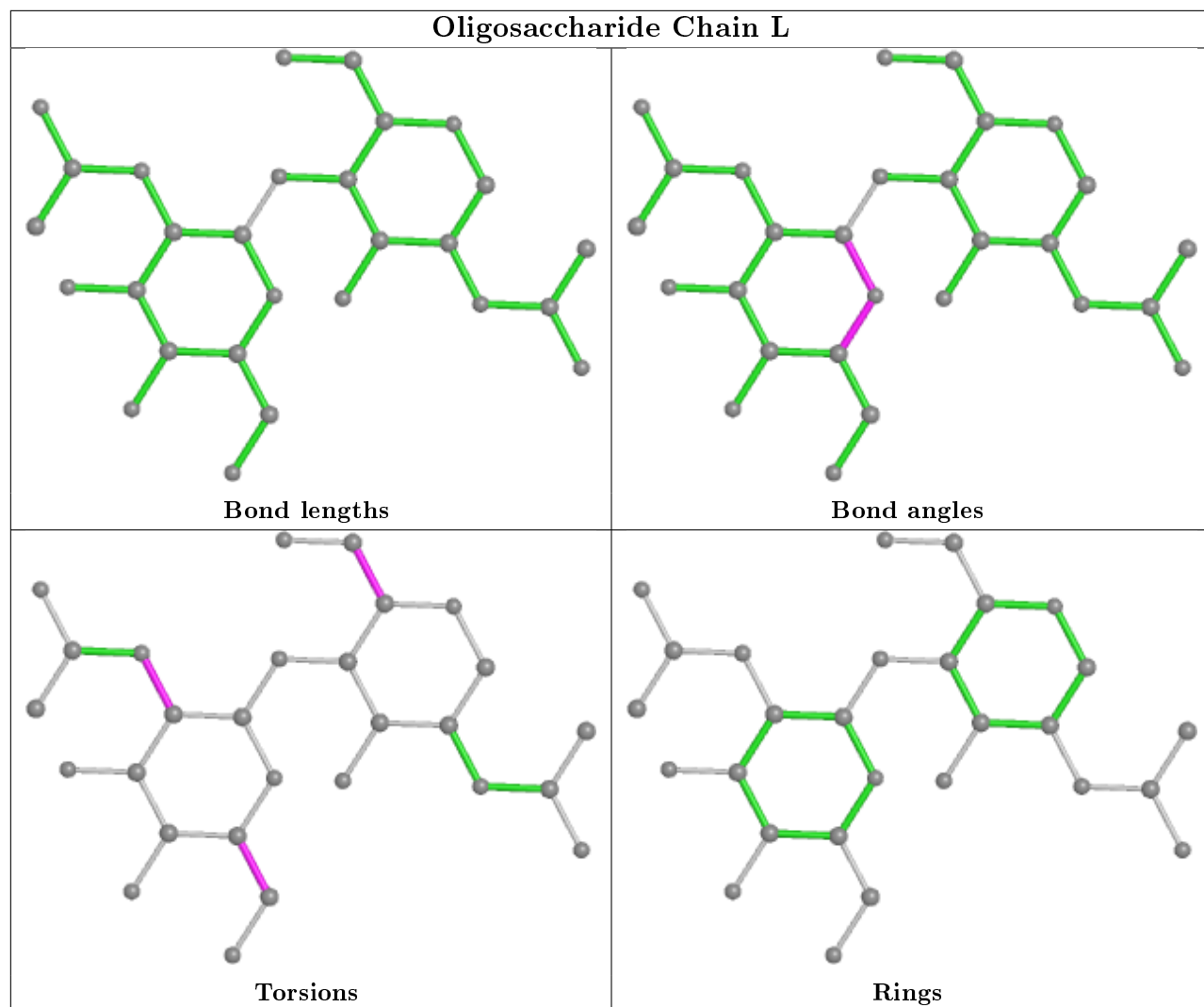


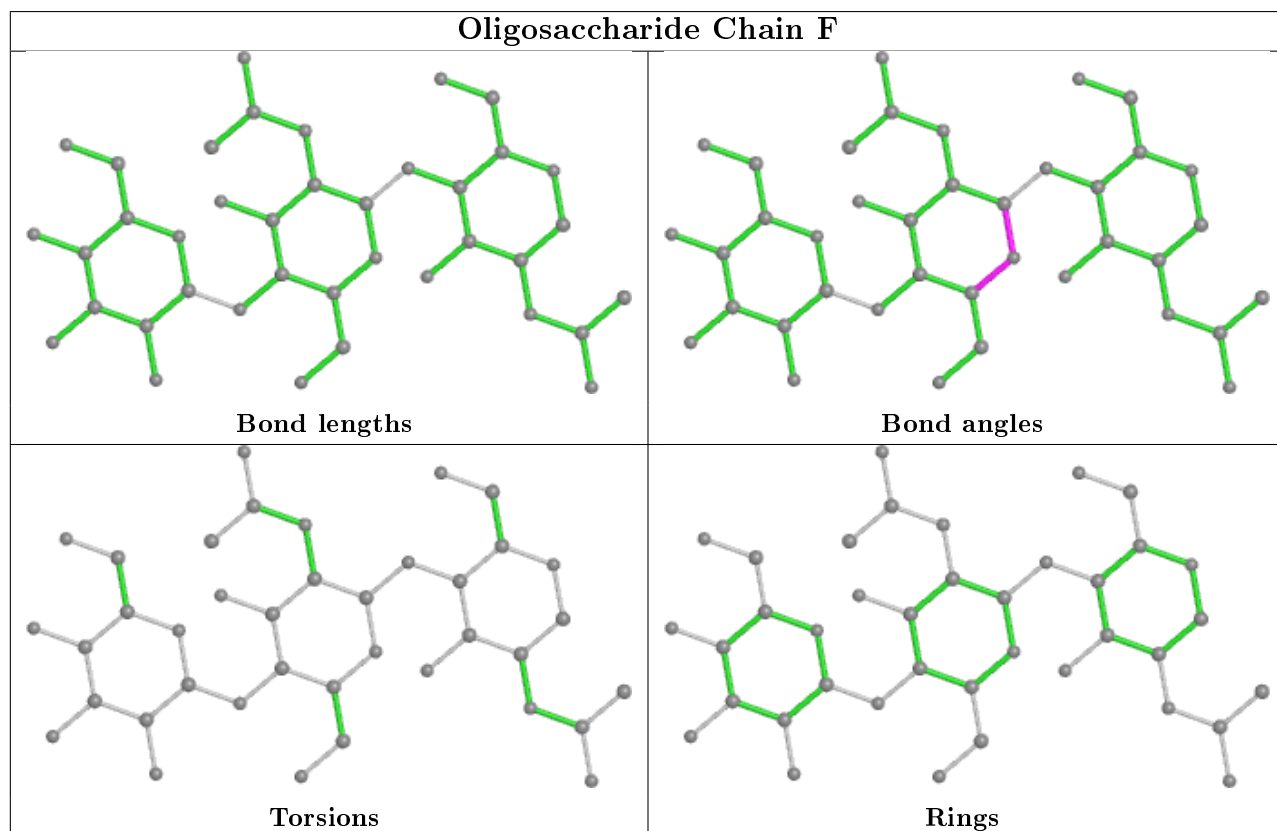
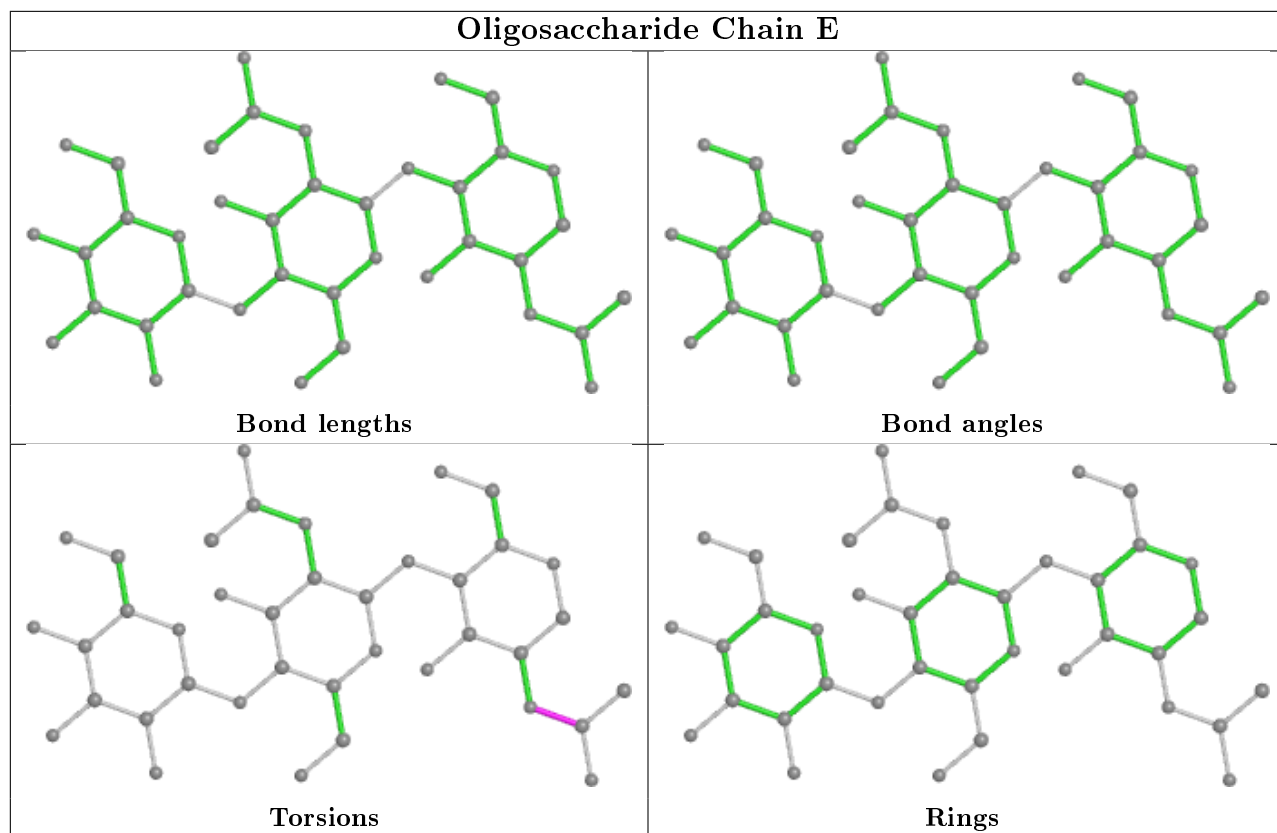




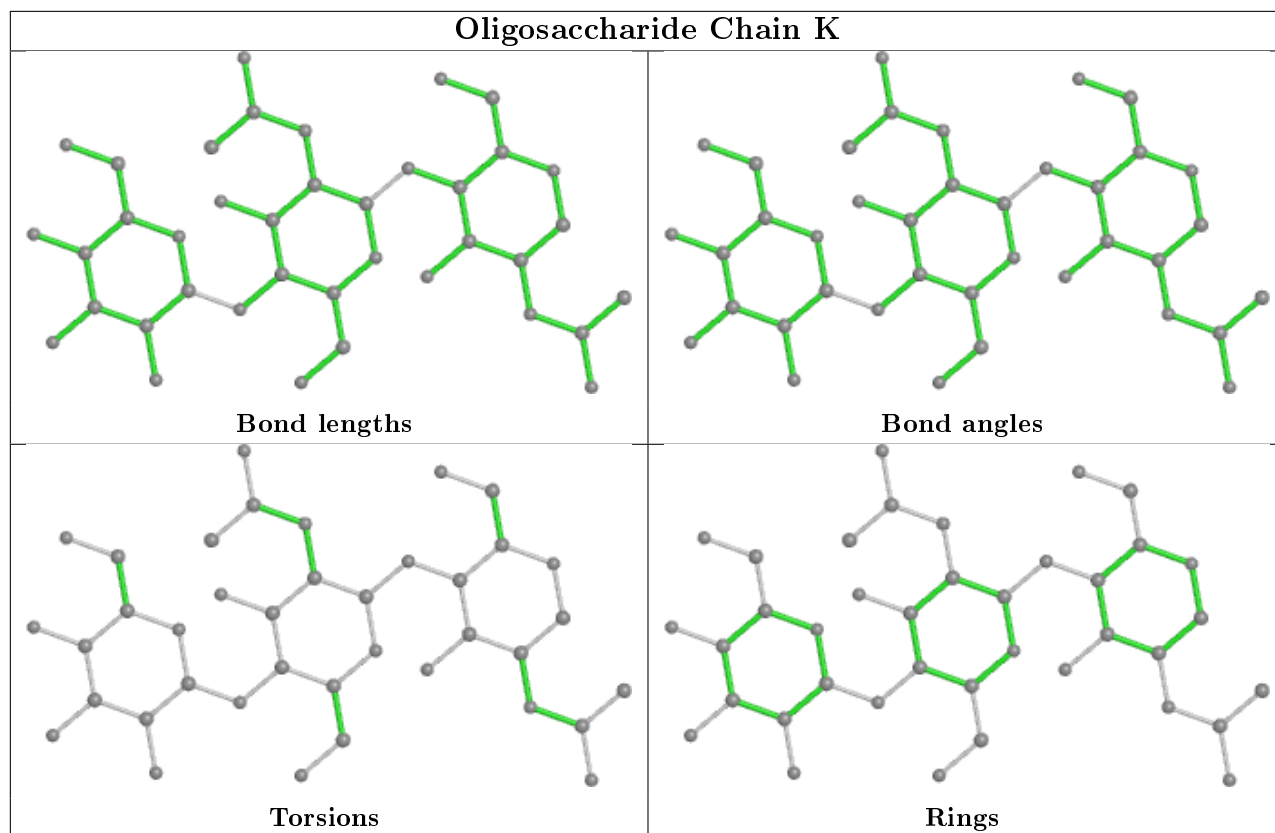












## 5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	A	2314	1	14,14,15	0.21	0	17,19,21	0.39	0
4	NAG	A	2315	1	14,14,15	0.25	0	17,19,21	0.37	0
4	NAG	A	2311	1	14,14,15	0.28	0	17,19,21	0.42	0
4	NAG	B	2303	1	14,14,15	0.29	0	17,19,21	0.41	0
4	NAG	B	2313	1	14,14,15	0.23	0	17,19,21	0.47	0
5	EDO	A	2316	-	3,3,3	0.46	0	2,2,2	0.32	0
4	NAG	B	2314	1	14,14,15	0.28	0	17,19,21	0.40	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
4	NAG	A	2314	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2315	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2311	1	-	1/6/23/26	0/1/1/1
4	NAG	B	2303	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2313	1	-	2/6/23/26	0/1/1/1
5	EDO	A	2316	-	-	0/1/1/1	-
4	NAG	B	2314	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2314	NAG	O5-C5-C6-O6
4	B	2314	NAG	C4-C5-C6-O6
4	B	2313	NAG	C8-C7-N2-C2
4	B	2313	NAG	O7-C7-N2-C2
4	A	2311	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	144:ARG	C	145:ALA	N	0.93

## 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	374/378 (98%)	0.07	19 (5%) 28 21	112, 164, 320, 402	0
1	B	375/378 (99%)	-0.08	3 (0%) 86 78	107, 169, 290, 339	0
All	All	749/756 (99%)	-0.01	22 (2%) 51 39	107, 167, 309, 402	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	302	SER	5.3
1	A	369	ALA	5.2
1	A	304	SER	4.0
1	A	303	VAL	3.9
1	A	307	GLN	3.8

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

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

### 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	D	2	14/15	0.52	0.41	218,288,302,307	0
2	NAG	I	2	14/15	0.56	0.38	143,244,274,300	0
3	BMA	F	3	11/12	0.56	0.30	229,277,299,310	0
3	NAG	K	1	14/15	0.58	0.42	131,213,243,273	0
3	BMA	K	3	11/12	0.71	0.29	228,273,294,306	0

*Continued on next page...*

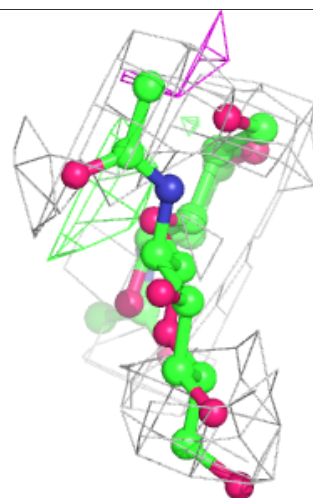
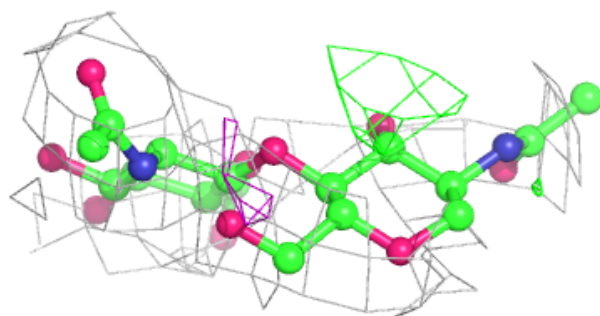
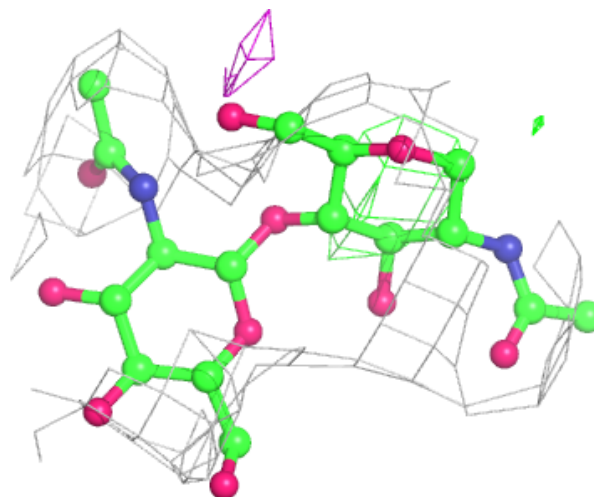
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	K	2	14/15	0.73	0.73	265,291,325,343	0
2	NAG	D	1	14/15	0.76	0.34	183,254,281,309	0
2	NAG	G	2	14/15	0.77	0.32	207,258,276,292	0
2	NAG	J	2	14/15	0.78	0.38	176,255,292,299	0
3	NAG	F	2	14/15	0.79	0.37	235,264,298,300	0
2	NAG	C	1	14/15	0.81	0.23	132,186,230,238	0
2	NAG	L	2	14/15	0.81	0.24	195,244,261,293	0
3	BMA	E	3	11/12	0.82	0.21	219,251,269,282	0
2	NAG	C	2	14/15	0.82	0.24	133,194,229,253	0
2	NAG	G	1	14/15	0.82	0.24	165,238,267,295	0
2	NAG	H	1	14/15	0.84	0.20	136,175,196,197	0
2	NAG	I	1	14/15	0.85	0.38	163,218,254,265	0
3	NAG	E	1	14/15	0.87	0.25	153,209,235,236	0
2	NAG	H	2	14/15	0.87	0.37	148,218,245,251	0
3	NAG	E	2	14/15	0.88	0.23	148,229,265,272	0
2	NAG	L	1	14/15	0.89	0.19	129,195,205,212	0
2	NAG	J	1	14/15	0.92	0.25	154,193,222,250	0
3	NAG	F	1	14/15	0.93	0.19	168,201,248,262	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.

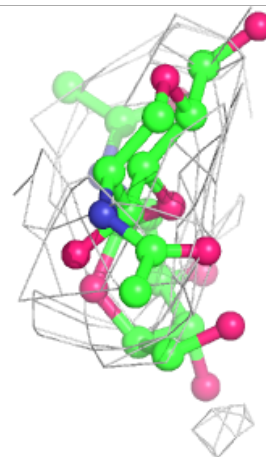
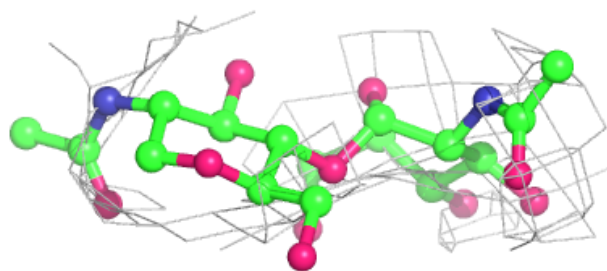
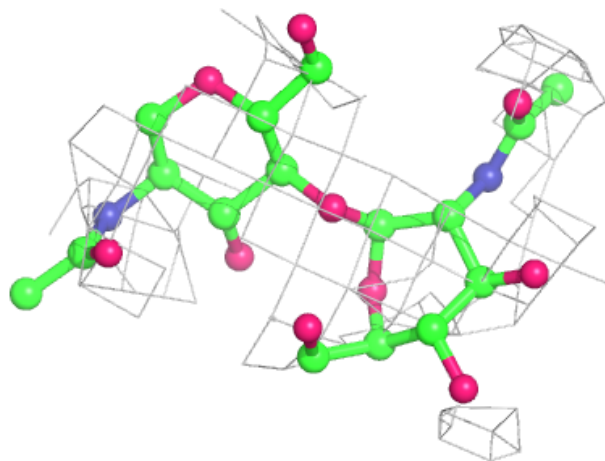
**Electron density around Chain C:**

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



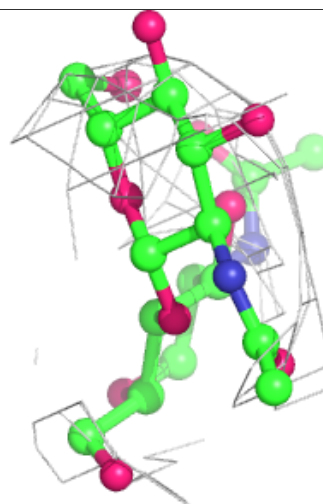
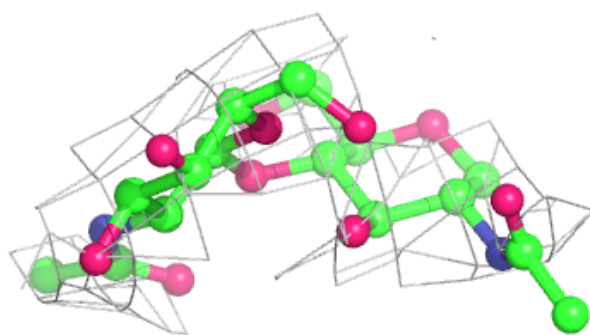
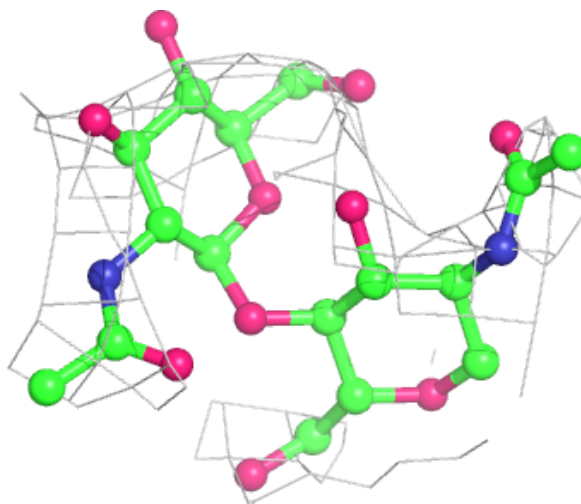
**Electron density around Chain D:**

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



**Electron density around Chain G:**

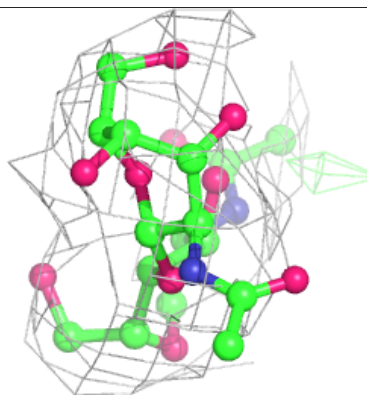
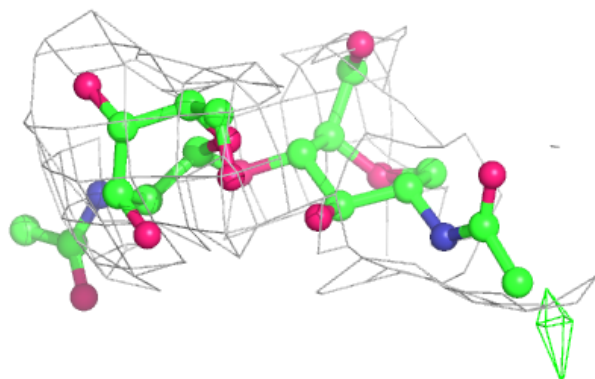
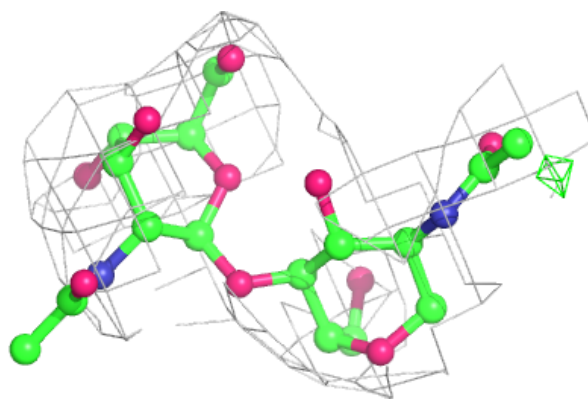
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





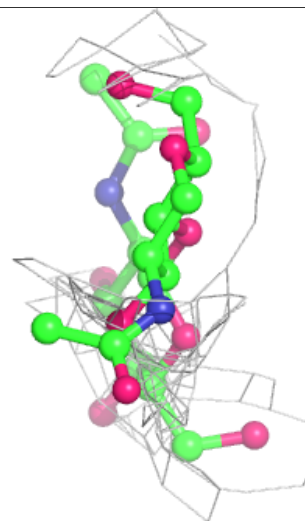
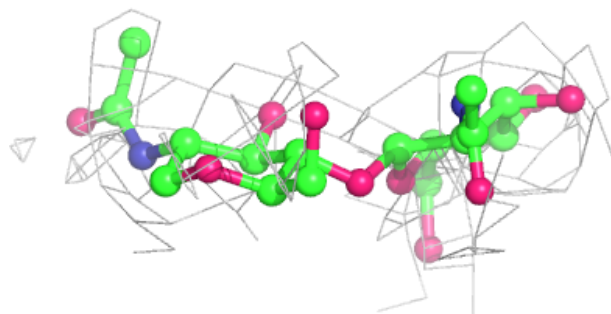
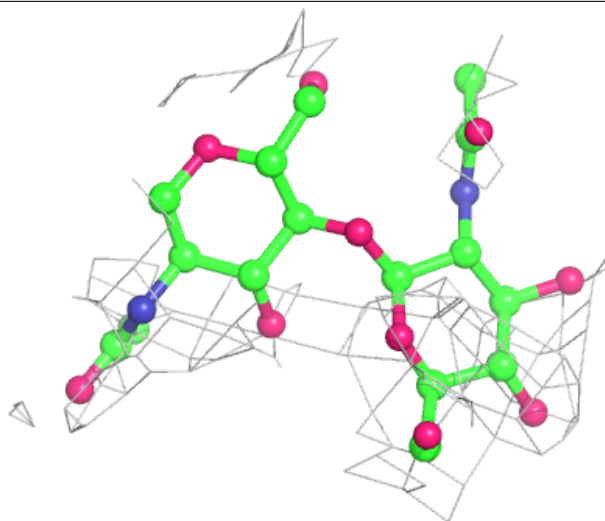
**Electron density around Chain H:**

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



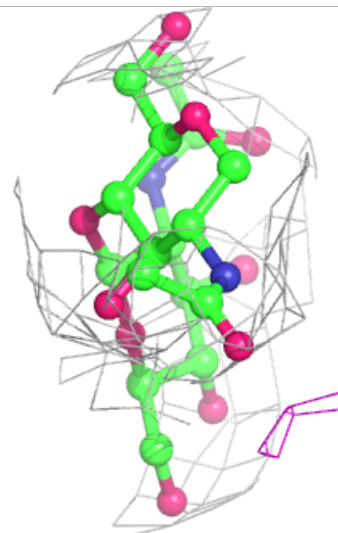
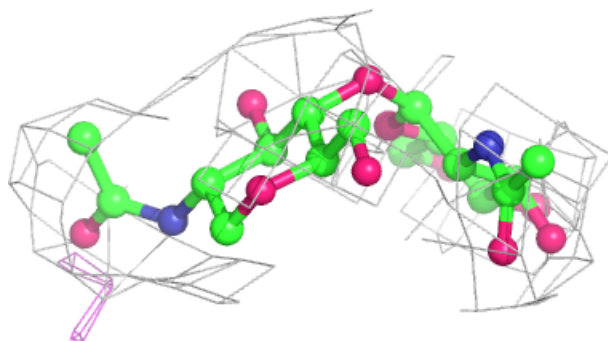
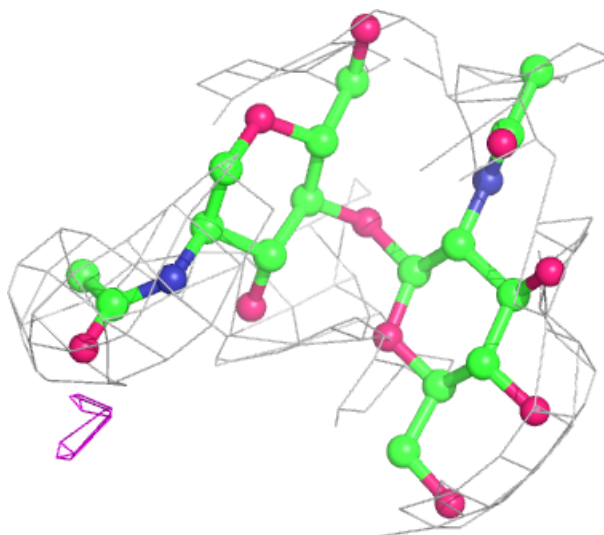
**Electron density around Chain I:**

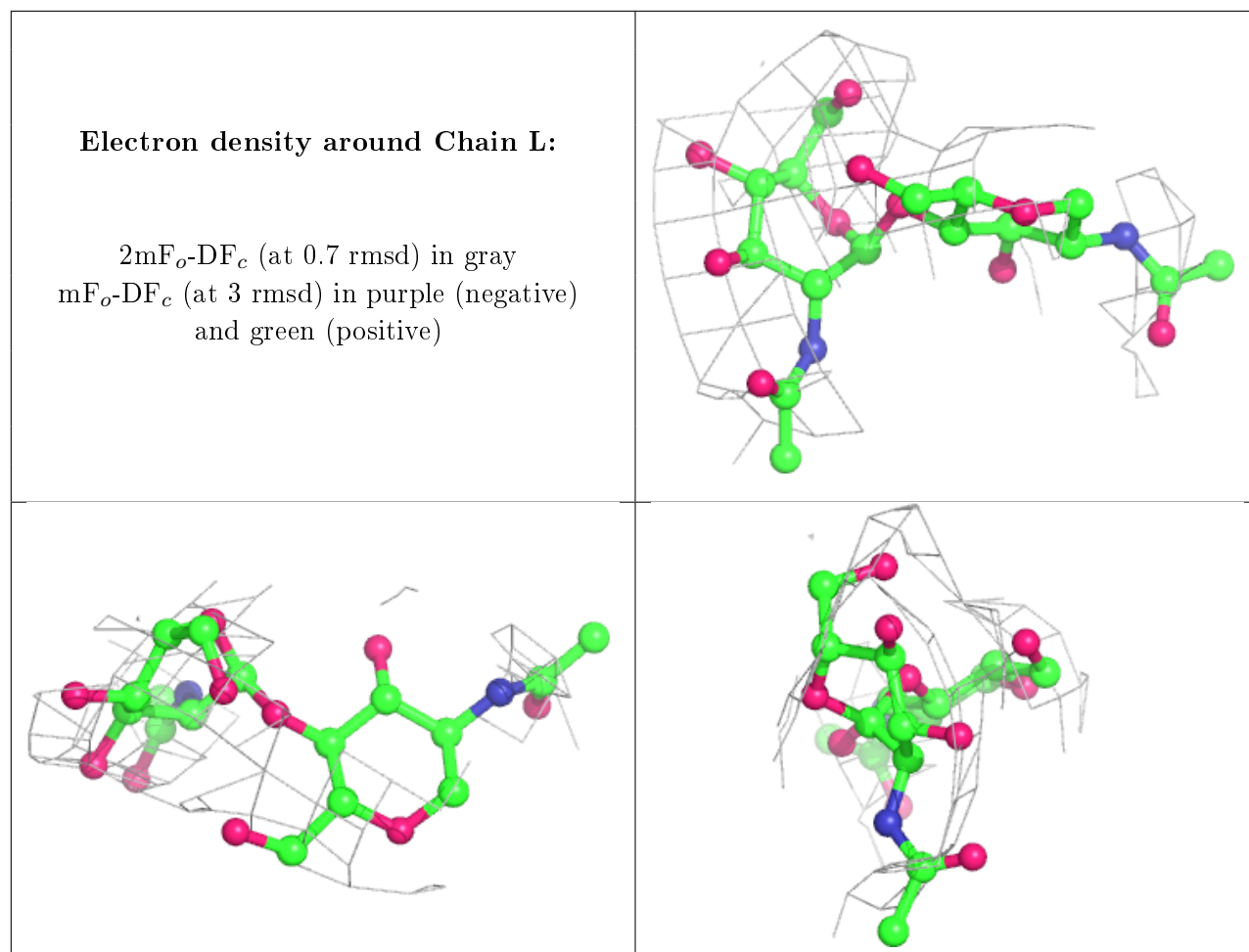
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain J:**

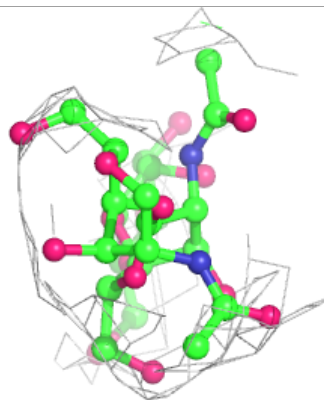
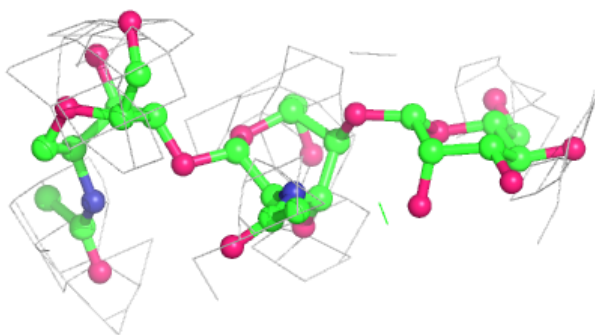
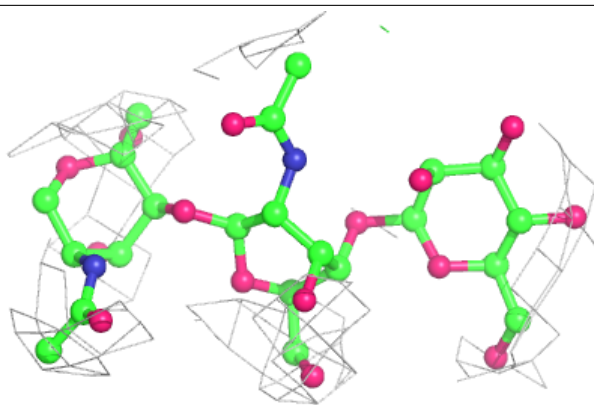
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



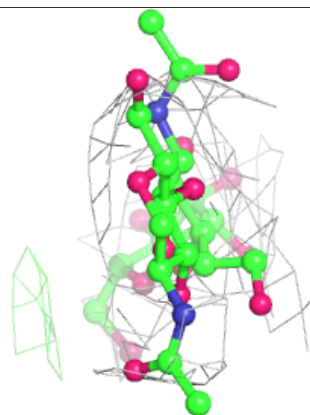
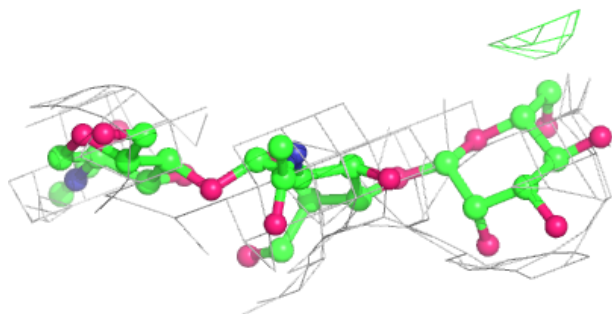
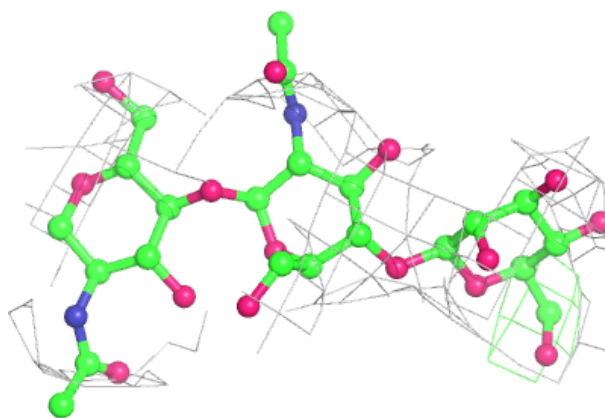


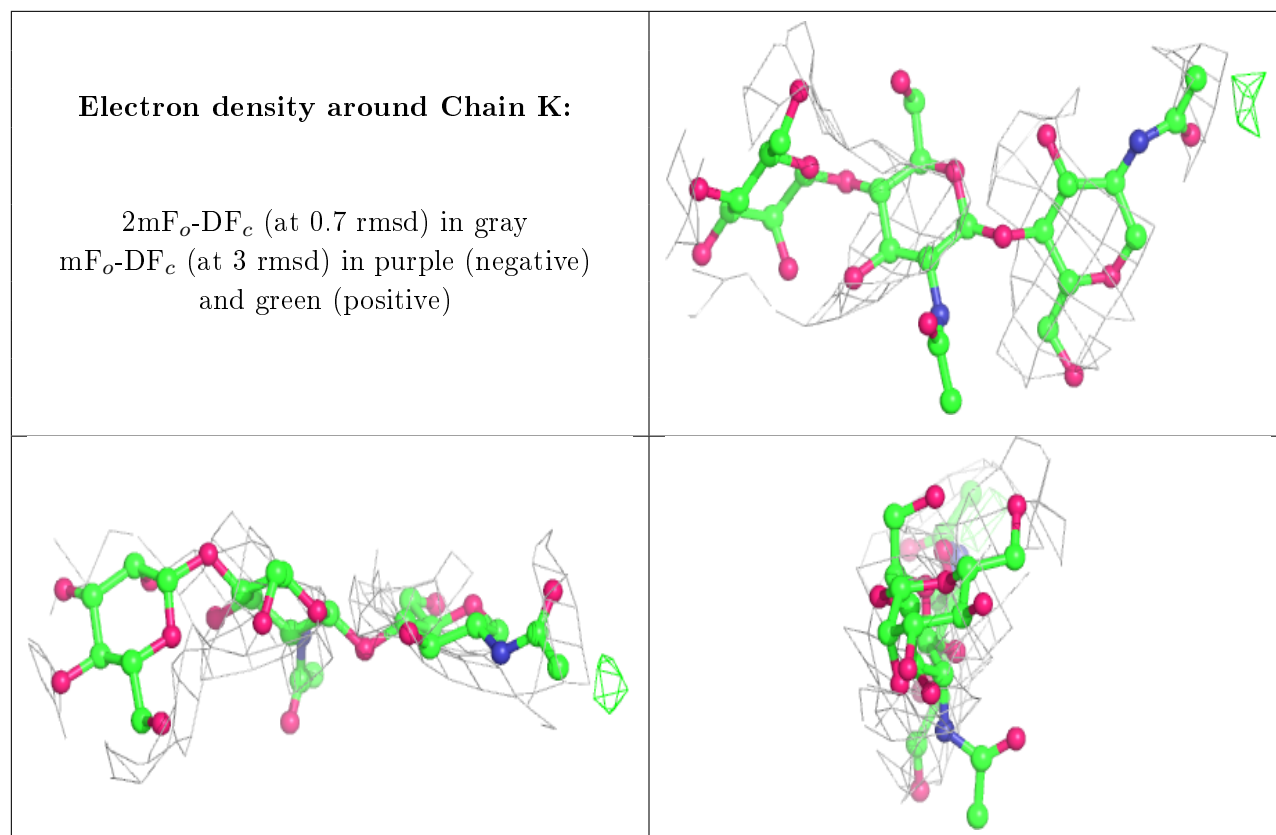
**Electron density around Chain E:**

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

**Electron density around Chain F:**

$2mF_o-DF_c$  (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(Å <sup>2</sup> )	Q<0.9
4	NAG	B	2314	14/15	0.49	0.34	168,225,247,255	0
4	NAG	B	2303	14/15	0.68	0.54	168,245,277,299	0
4	NAG	A	2311	14/15	0.70	0.33	147,220,257,261	0
5	EDO	A	2316	4/4	0.76	0.53	135,182,192,200	0
4	NAG	B	2313	14/15	0.76	0.27	183,228,250,257	0
4	NAG	A	2315	14/15	0.77	0.39	149,215,238,242	0
4	NAG	A	2314	14/15	0.81	0.21	127,197,230,234	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.