



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 04:24 PM BST

PDB ID : 4NRJ  
Title : Structure of hemagglutinin with F95Y mutation of influenza virus B/Lee/40  
Authors : Ni, F.; Mbawuike, I.N.; Kondrashkina, E.; Wang, Q.  
Deposited on : 2013-11-26  
Resolution : 2.53 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 : 1.8.5 (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

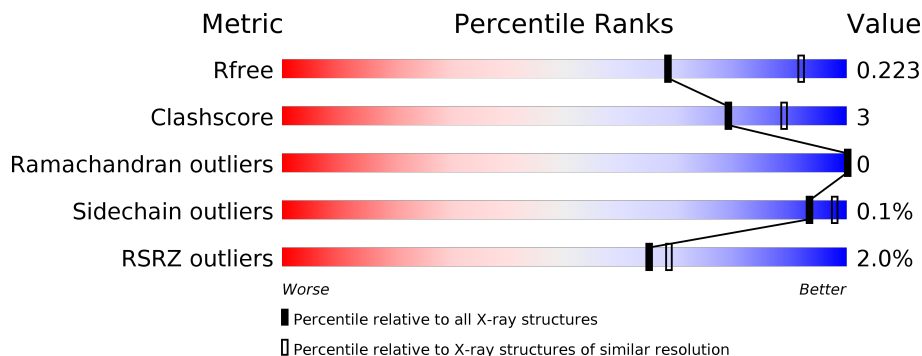
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

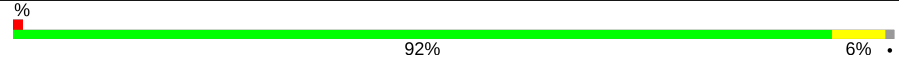
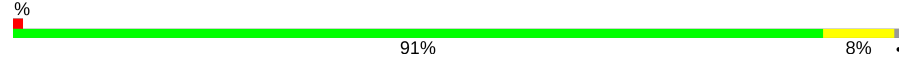
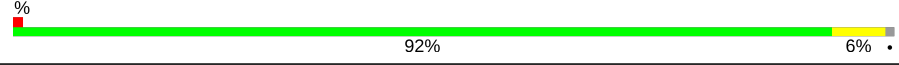
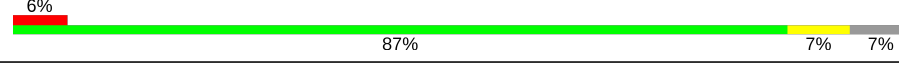

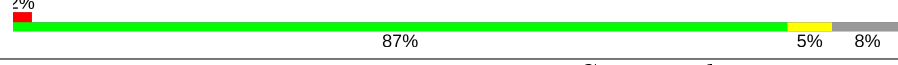
The reported resolution of this entry is 2.53 Å.

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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 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	346	
1	C	346	
1	E	346	
2	B	182	
2	D	182	
2	F	182	

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Mol	Chain	Length	Quality of chain
3	G	2	 100%
3	H	2	 50% 50%
3	I	2	 50% 50%
3	J	2	 50% 50%
3	K	2	 100%
3	M	2	 100%
3	N	2	 100%
3	O	2	 100%
3	P	2	 50% 50%
3	Q	2	 50% 50%
3	R	2	 100%
3	S	2	 50% 50%
4	L	3	 67% 33%

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	I	2	-	-	-	X
5	NAG	C	406	-	-	-	X

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 12678 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 HEMAGGLUTININ HA1 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	341	2600	1631	461	492	16	0	0	0
1	C	342	2608	1637	462	493	16	0	0	0
1	E	341	2600	1631	461	492	16	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	ARG	LYS	conflict	UNP P03460
A	76	ILE	THR	conflict	UNP P03460
A	90	VAL	ALA	conflict	UNP P03460
A	95	TYR	PHE	engineered mutation	UNP P03460
A	147	THR	ALA	conflict	UNP P03460
A	167	ILE	THR	conflict	UNP P03460
C	38	ARG	LYS	conflict	UNP P03460
C	76	ILE	THR	conflict	UNP P03460
C	90	VAL	ALA	conflict	UNP P03460
C	95	TYR	PHE	engineered mutation	UNP P03460
C	147	THR	ALA	conflict	UNP P03460
C	167	ILE	THR	conflict	UNP P03460
E	38	ARG	LYS	conflict	UNP P03460
E	76	ILE	THR	conflict	UNP P03460
E	90	VAL	ALA	conflict	UNP P03460
E	95	TYR	PHE	engineered mutation	UNP P03460
E	147	THR	ALA	conflict	UNP P03460
E	167	ILE	THR	conflict	UNP P03460

- Molecule 2 is a protein called HEMAGGLUTININ HA2 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	0	0	0
			1289	806	220	257	6			
2	D	169	Total	C	N	O	S	0	0	0
			1281	800	219	256	6			
2	F	168	Total	C	N	O	S	0	0	0
			1275	797	218	254	6			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	54	SER	TYR	conflict	UNP P03460
B	177	GLY	-	expression tag	UNP P03460
B	178	ALA	-	expression tag	UNP P03460
B	179	LEU	-	expression tag	UNP P03460
B	180	VAL	-	expression tag	UNP P03460
B	181	PRO	-	expression tag	UNP P03460
B	182	ARG	-	expression tag	UNP P03460
D	54	SER	TYR	conflict	UNP P03460
D	177	GLY	-	expression tag	UNP P03460
D	178	ALA	-	expression tag	UNP P03460
D	179	LEU	-	expression tag	UNP P03460
D	180	VAL	-	expression tag	UNP P03460
D	181	PRO	-	expression tag	UNP P03460
D	182	ARG	-	expression tag	UNP P03460
F	54	SER	TYR	conflict	UNP P03460
F	177	GLY	-	expression tag	UNP P03460
F	178	ALA	-	expression tag	UNP P03460
F	179	LEU	-	expression tag	UNP P03460
F	180	VAL	-	expression tag	UNP P03460
F	181	PRO	-	expression tag	UNP P03460
F	182	ARG	-	expression tag	UNP P03460

- 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	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	H	2	28	16	2	10	0	0	0
3	I	2	28	16	2	10	0	0	0
3	J	2	28	16	2	10	0	0	0
3	K	2	28	16	2	10	0	0	0
3	M	2	28	16	2	10	0	0	0
3	N	2	28	16	2	10	0	0	0
3	O	2	28	16	2	10	0	0	0
3	P	2	28	16	2	10	0	0	0
3	Q	2	28	16	2	10	0	0	0
3	R	2	28	16	2	10	0	0	0
3	S	2	28	16	2	10	0	0	0

- 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
			Total	C	N	O			
4	L	3	39	22	2	15	0	0	0

- Molecule 5 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
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
5	B	1	14	8	1	5	0	0
5	C	1	14	8	1	5	0	0
5	D	1	14	8	1	5	0	0
5	E	1	14	8	1	5	0	0
5	F	1	14	8	1	5	0	0

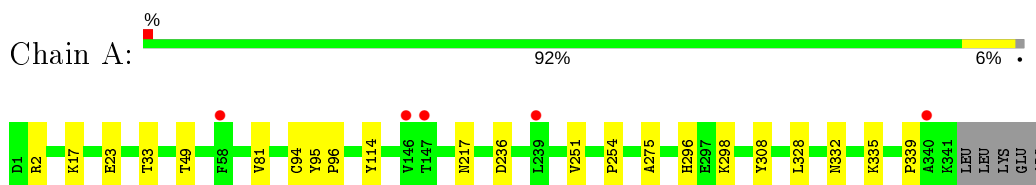
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	142	142	142	0	0
6	B	47	47	47	0	0
6	C	111	111	111	0	0
6	D	52	52	52	0	0
6	E	164	164	164	0	0
6	F	50	50	50	0	0

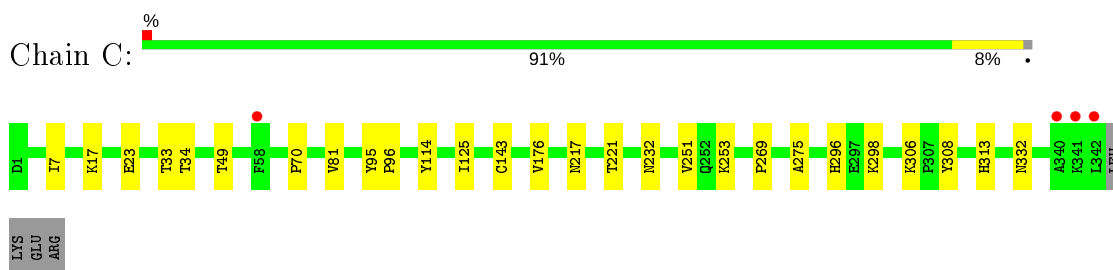
### 3 Residue-property plots [i](#)

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.

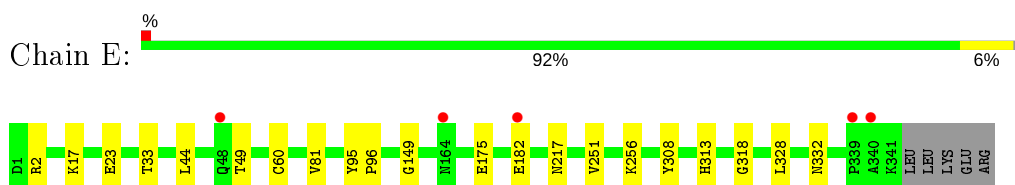
- Molecule 1: HEMAGGLUTININ HA1 CHAIN



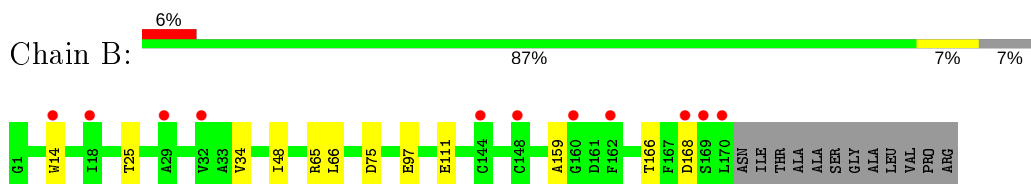
- Molecule 1: HEMAGGLUTININ HA1 CHAIN



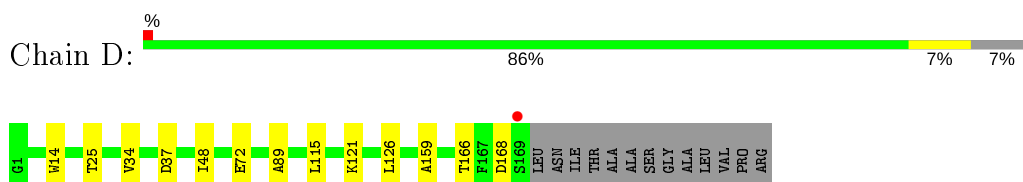
- Molecule 1: HEMAGGLUTININ HA1 CHAIN



- Molecule 2: HEMAGGLUTININ HA2 CHAIN

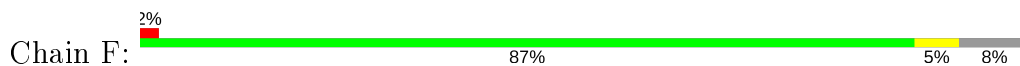


- Molecule 2: HEMAGGLUTININ HA2 CHAIN





- Molecule 2: HEMAGGLUTININ HA2 CHAIN



- 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



- 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



- 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



MAG1  
MAG2

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

Chain N:  100%MAG1  
MAG2

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

Chain O:  100%MAG1  
MAG2

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

Chain P:  50% 50%MAG1  
MAG2

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

Chain Q:  50% 50%MAG1  
MAG2

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

Chain R:  100%MAG1  
MAG2

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

Chain S:  50% 50%MAG1  
MAG2

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

Chain L:  67% 33%

HA01  
HA02  
BOA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.69Å 128.60Å 211.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.18 – 2.53 42.18 – 2.53	Depositor EDS
% Data completeness (in resolution range)	97.8 (42.18-2.53) 97.8 (42.18-2.53)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.72 (at 2.54Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_1452)	Depositor
R, $R_{free}$	0.187 , 0.222 0.190 , 0.223	Depositor DCC
$R_{free}$ test set	3772 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.7	Xtrriage
Anisotropy	0.797	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12678	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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

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	0.22	0/2659	0.43	0/3614
1	C	0.23	0/2667	0.44	0/3625
1	E	0.23	0/2659	0.44	0/3614
2	B	0.21	0/1308	0.37	0/1763
2	D	0.21	0/1300	0.36	0/1752
2	F	0.21	0/1294	0.37	0/1744
All	All	0.22	0/11887	0.42	0/16112

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2600	0	2597	15	0
1	C	2608	0	2608	16	0
1	E	2600	0	2596	15	0
2	B	1289	0	1261	10	0
2	D	1281	0	1251	10	0
2	F	1275	0	1246	8	0
3	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	1	0
3	K	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	2	0
3	O	28	0	25	0	0
3	P	28	0	25	1	0
3	Q	28	0	25	1	0
3	R	28	0	25	0	0
3	S	28	0	25	0	0
4	L	39	0	34	0	0
5	A	14	0	13	0	0
5	B	14	0	13	1	0
5	C	14	0	13	0	0
5	D	14	0	13	0	0
5	E	14	0	13	0	0
5	F	14	0	13	0	0
6	A	142	0	0	4	0
6	B	47	0	0	3	0
6	C	111	0	0	1	0
6	D	52	0	0	1	0
6	E	164	0	0	3	0
6	F	50	0	0	1	0
All	All	12678	0	11971	67	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 3.

The worst 5 of 67 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:298:LYS:NZ	6:A:632:HOH:O	2.13	0.80
1:A:254:PRO:O	6:A:536:HOH:O	2.00	0.79
1:A:339:PRO:O	6:A:607:HOH:O	2.08	0.70
2:F:65:ARG:O	6:F:315:HOH:O	2.10	0.68
1:A:335:LYS:O	6:A:583:HOH:O	2.11	0.67

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	339/346 (98%)	327 (96%)	12 (4%)	0	100	100
1	C	340/346 (98%)	327 (96%)	13 (4%)	0	100	100
1	E	339/346 (98%)	328 (97%)	11 (3%)	0	100	100
2	B	168/182 (92%)	167 (99%)	1 (1%)	0	100	100
2	D	167/182 (92%)	166 (99%)	1 (1%)	0	100	100
2	F	166/182 (91%)	165 (99%)	1 (1%)	0	100	100
All	All	1519/1584 (96%)	1480 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	293/298 (98%)	293 (100%)	0	100	100
1	C	294/298 (99%)	293 (100%)	1 (0%)	92	97
1	E	293/298 (98%)	293 (100%)	0	100	100
2	B	137/145 (94%)	137 (100%)	0	100	100
2	D	136/145 (94%)	136 (100%)	0	100	100
2	F	135/145 (93%)	135 (100%)	0	100	100
All	All	1288/1329 (97%)	1287 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	232	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	95	GLN
1	E	85	HIS
1	E	208	ASN

### 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](#)

27 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
3	NAG	G	1	1,3	14,14,15	0.26	0	17,19,21	0.37	0
3	NAG	G	2	3	14,14,15	0.26	0	17,19,21	0.37	0
3	NAG	H	1	1,3	14,14,15	1.07	1 (7%)	17,19,21	2.03	3 (17%)
3	NAG	H	2	3	14,14,15	0.25	0	17,19,21	0.45	0
3	NAG	I	1	1,3	14,14,15	1.06	1 (7%)	17,19,21	1.38	1 (5%)
3	NAG	I	2	3	14,14,15	0.26	0	17,19,21	0.41	0
3	NAG	J	1	1,3	14,14,15	0.85	1 (7%)	17,19,21	0.47	0
3	NAG	J	2	3	14,14,15	0.74	1 (7%)	17,19,21	1.99	3 (17%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	K	1	1,3	14,14,15	0.32	0	17,19,21	0.36	0
3	NAG	K	2	3	14,14,15	0.30	0	17,19,21	0.37	0
4	NAG	L	1	1,4	14,14,15	0.45	0	17,19,21	0.58	0
4	NAG	L	2	4	14,14,15	0.20	0	17,19,21	0.63	0
4	BMA	L	3	4	11,11,12	0.74	0	15,15,17	1.07	2 (13%)
3	NAG	M	1	1,3	14,14,15	0.29	0	17,19,21	0.53	0
3	NAG	M	2	3	14,14,15	0.19	0	17,19,21	0.42	0
3	NAG	N	1	1,3	14,14,15	0.59	1 (7%)	17,19,21	0.47	0
3	NAG	N	2	3	14,14,15	0.35	0	17,19,21	1.25	1 (5%)
3	NAG	O	1	1,3	14,14,15	0.27	0	17,19,21	0.40	0
3	NAG	O	2	3	14,14,15	0.29	0	17,19,21	0.35	0
3	NAG	P	1	1,3	14,14,15	1.41	1 (7%)	17,19,21	2.21	1 (5%)
3	NAG	P	2	3	14,14,15	0.25	0	17,19,21	0.51	0
3	NAG	Q	1	1,3	14,14,15	1.56	2 (14%)	17,19,21	1.92	4 (23%)
3	NAG	Q	2	3	14,14,15	0.48	0	17,19,21	0.71	1 (5%)
3	NAG	R	1	1,3	14,14,15	0.31	0	17,19,21	0.55	0
3	NAG	R	2	3	14,14,15	0.20	0	17,19,21	0.39	0
3	NAG	S	1	1,3	14,14,15	0.47	0	17,19,21	0.43	0
3	NAG	S	2	3	14,14,15	0.40	0	17,19,21	0.65	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
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	5/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	5/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	1/6/23/26	0/1/1/1
4	BMA	L	3	4	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
3	NAG	N	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	4/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	1/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	R	2	3	-	2/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1	NAG	O5-C1	5.16	1.52	1.43
3	Q	1	NAG	O5-C1	-4.27	1.36	1.43
3	I	1	NAG	O5-C1	3.87	1.49	1.43
3	H	1	NAG	O5-C1	3.82	1.49	1.43
3	Q	1	NAG	C1-C2	3.18	1.57	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1	NAG	C1-O5-C5	8.79	124.10	112.19
3	H	1	NAG	C1-O5-C5	6.08	120.43	112.19
3	J	2	NAG	C1-O5-C5	5.62	119.81	112.19
3	I	1	NAG	C1-O5-C5	5.42	119.53	112.19
3	J	2	NAG	C2-N2-C7	4.67	129.55	122.90

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	R	2	NAG	C4-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6

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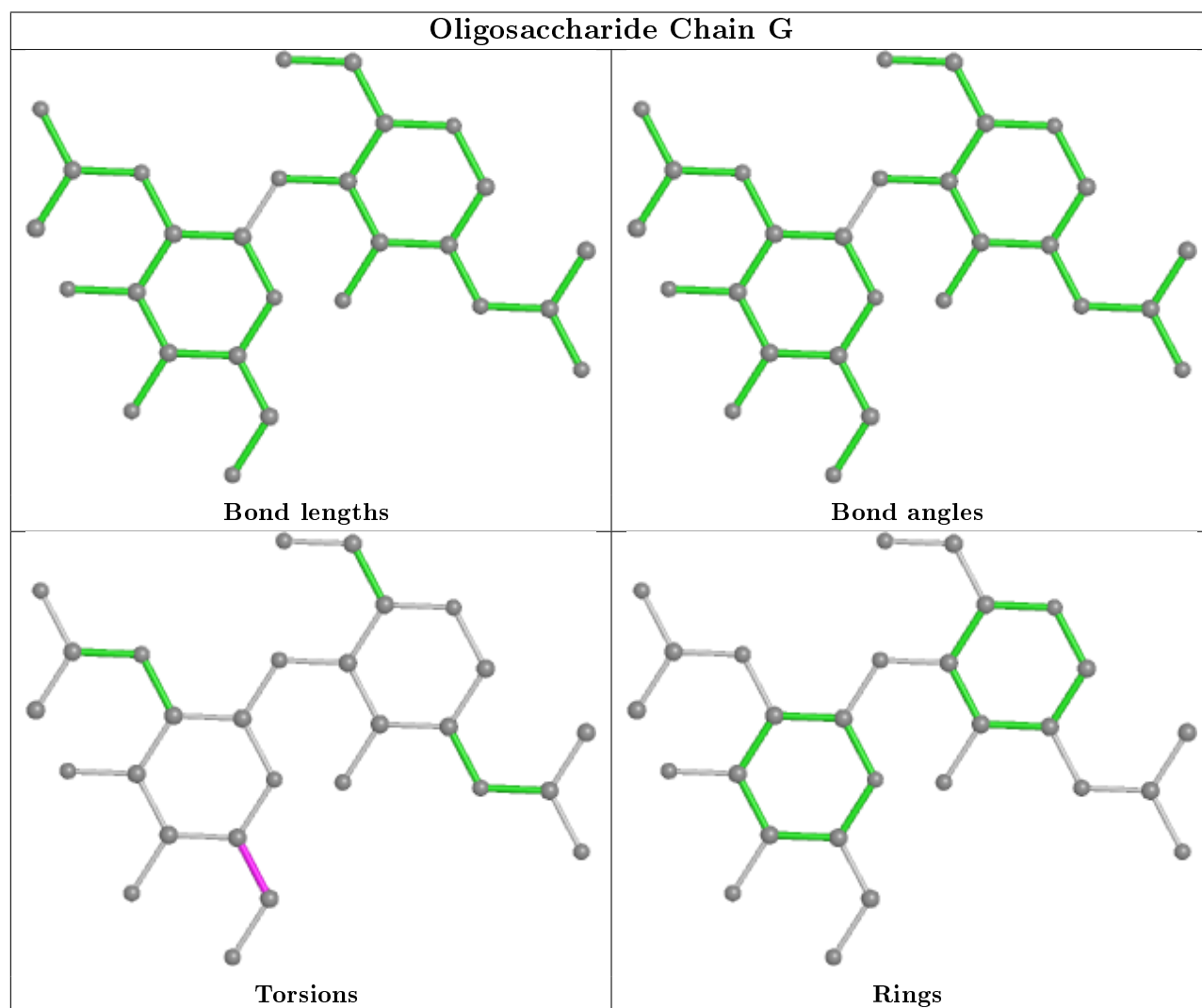
Mol	Chain	Res	Type	Atoms
3	J	1	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6

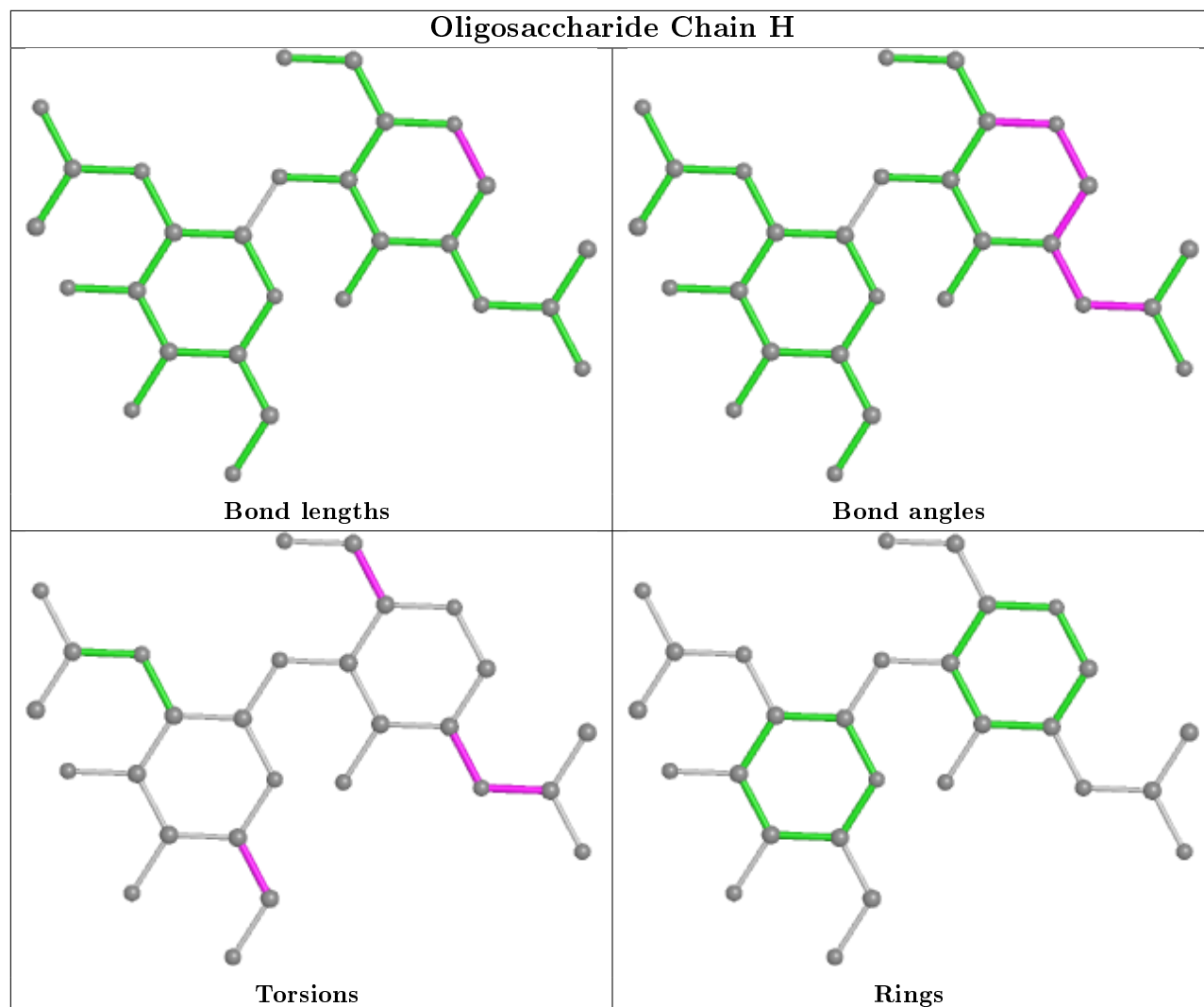
There are no ring outliers.

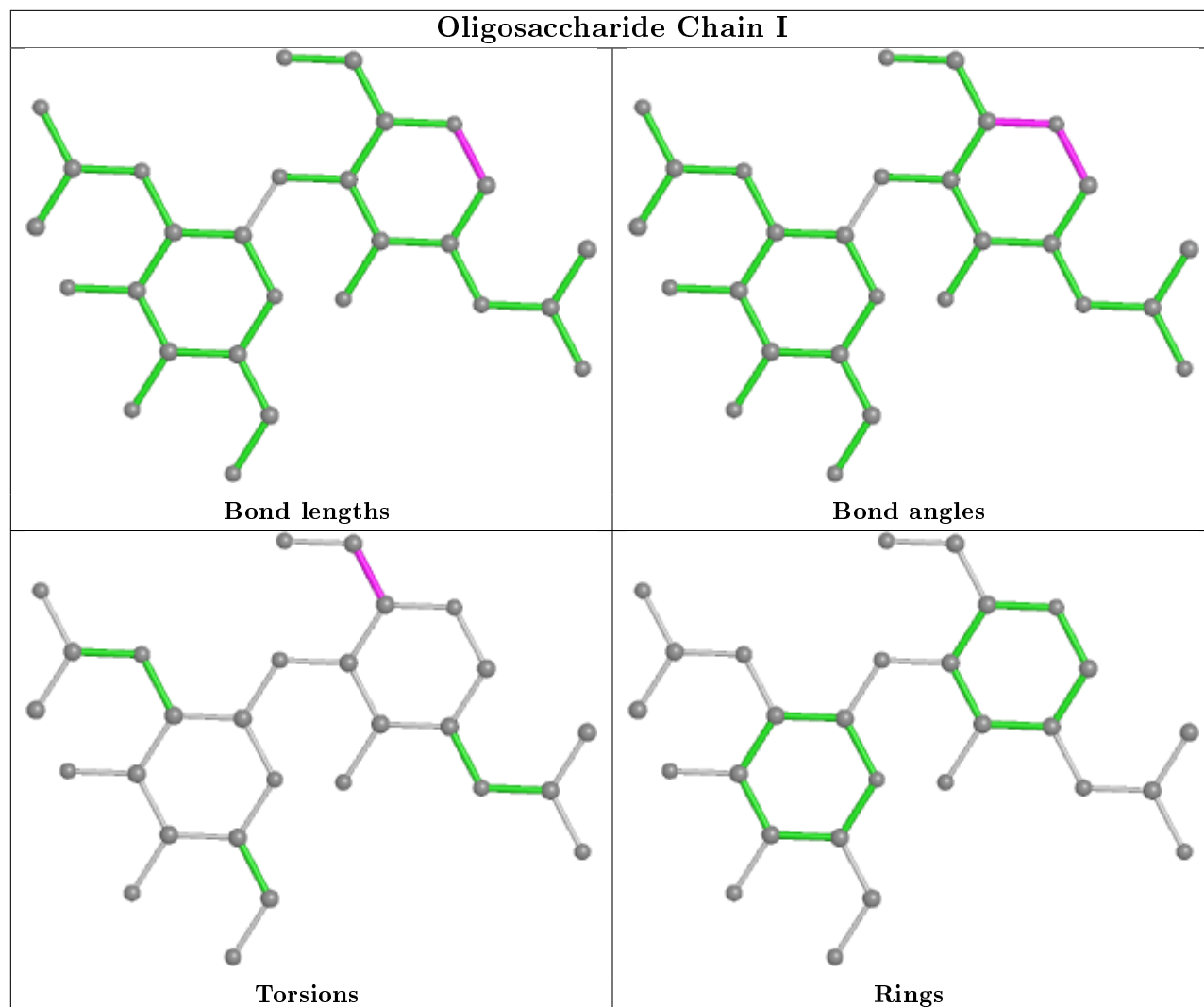
5 monomers are involved in 5 short contacts:

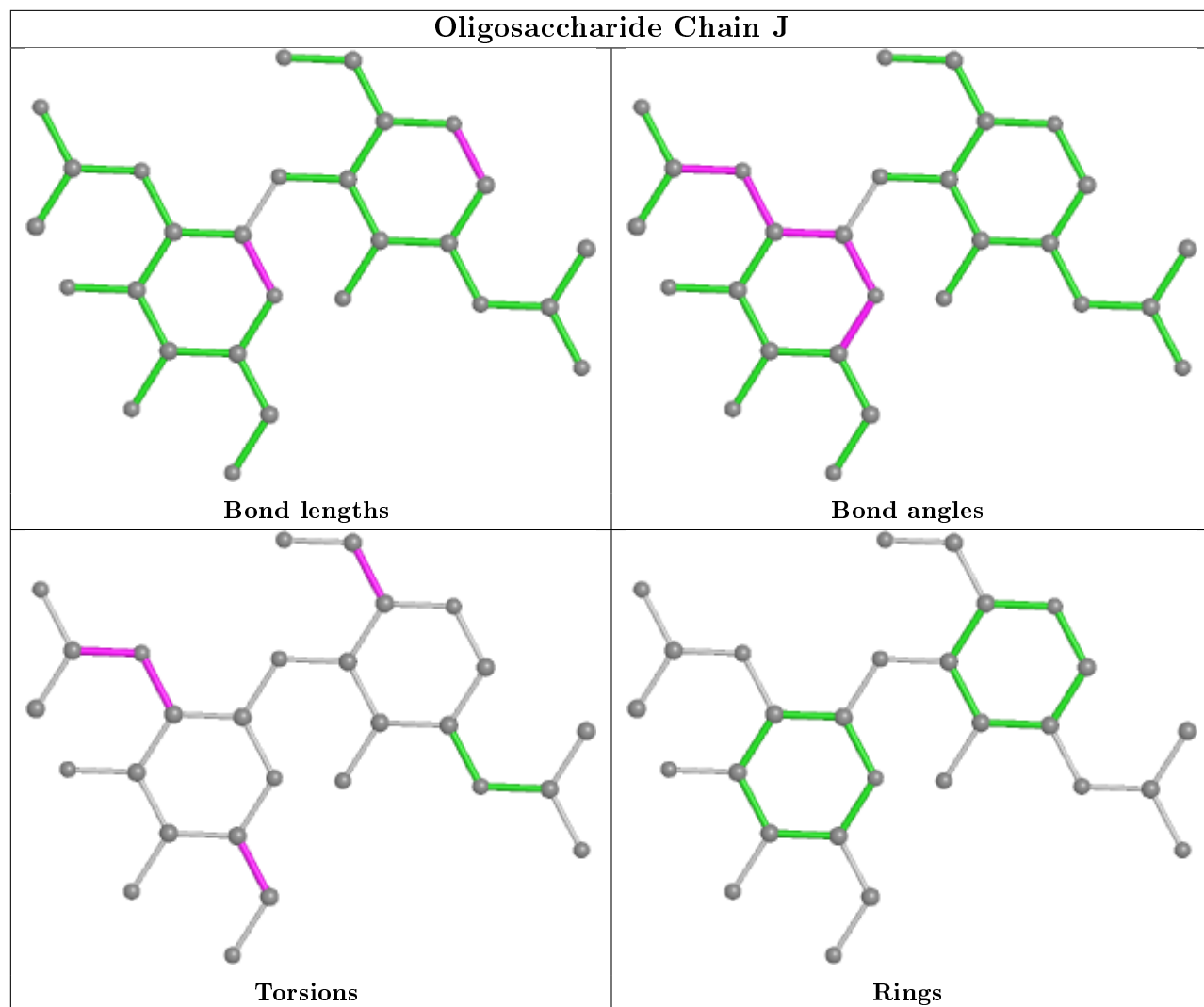
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	1	NAG	1	0
3	N	1	NAG	1	0
3	N	2	NAG	2	0
3	Q	1	NAG	1	0
3	J	2	NAG	1	0

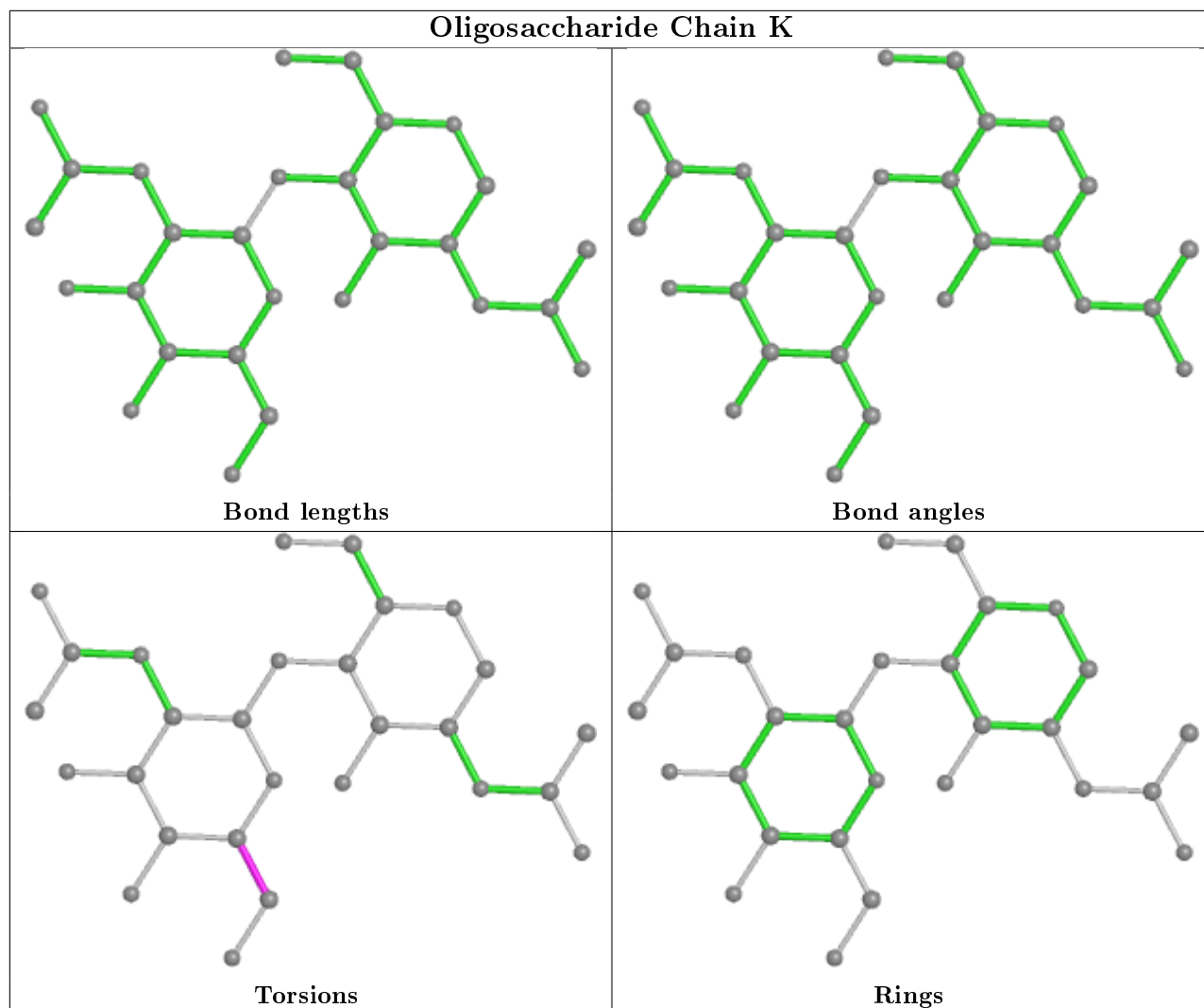
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

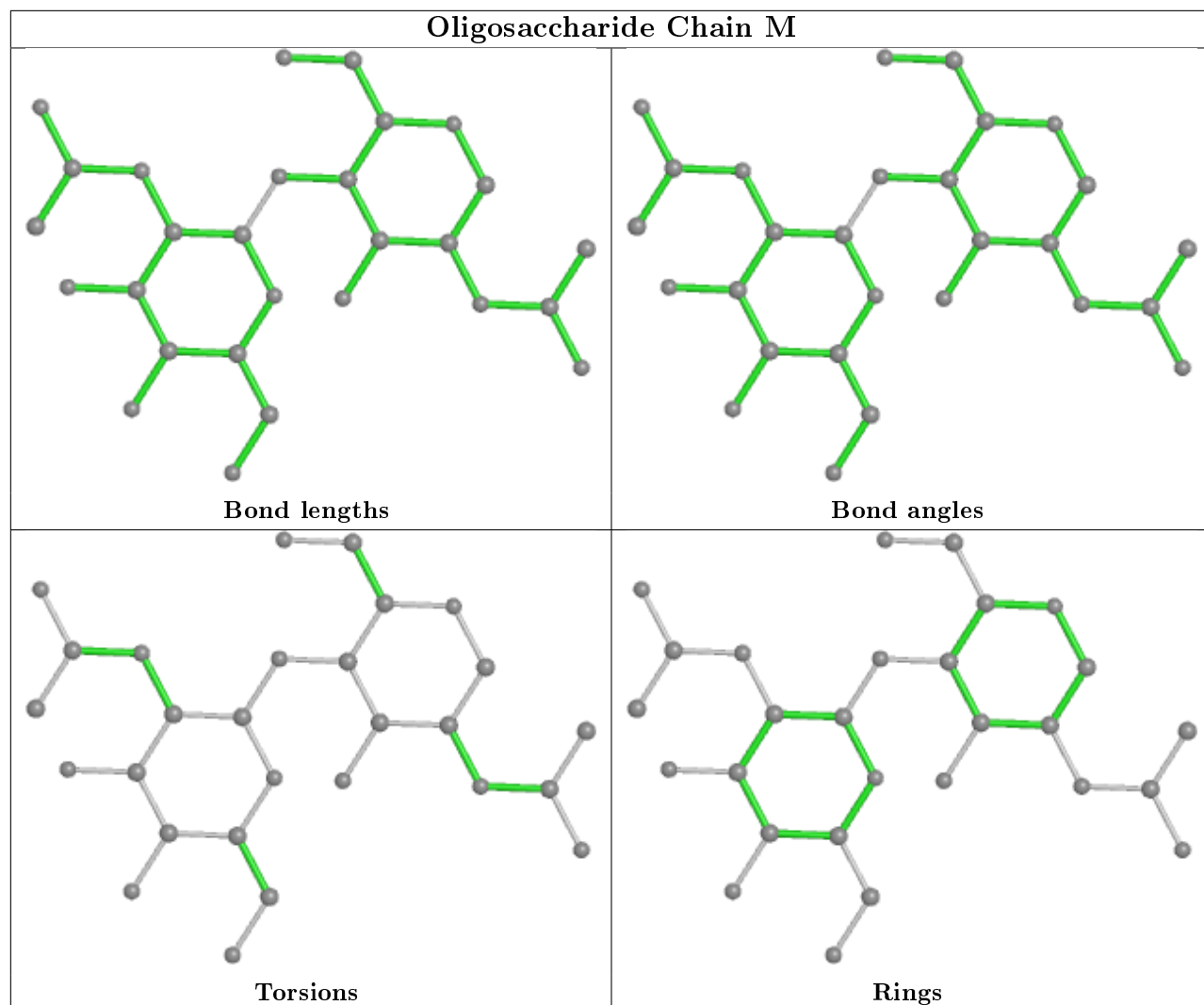




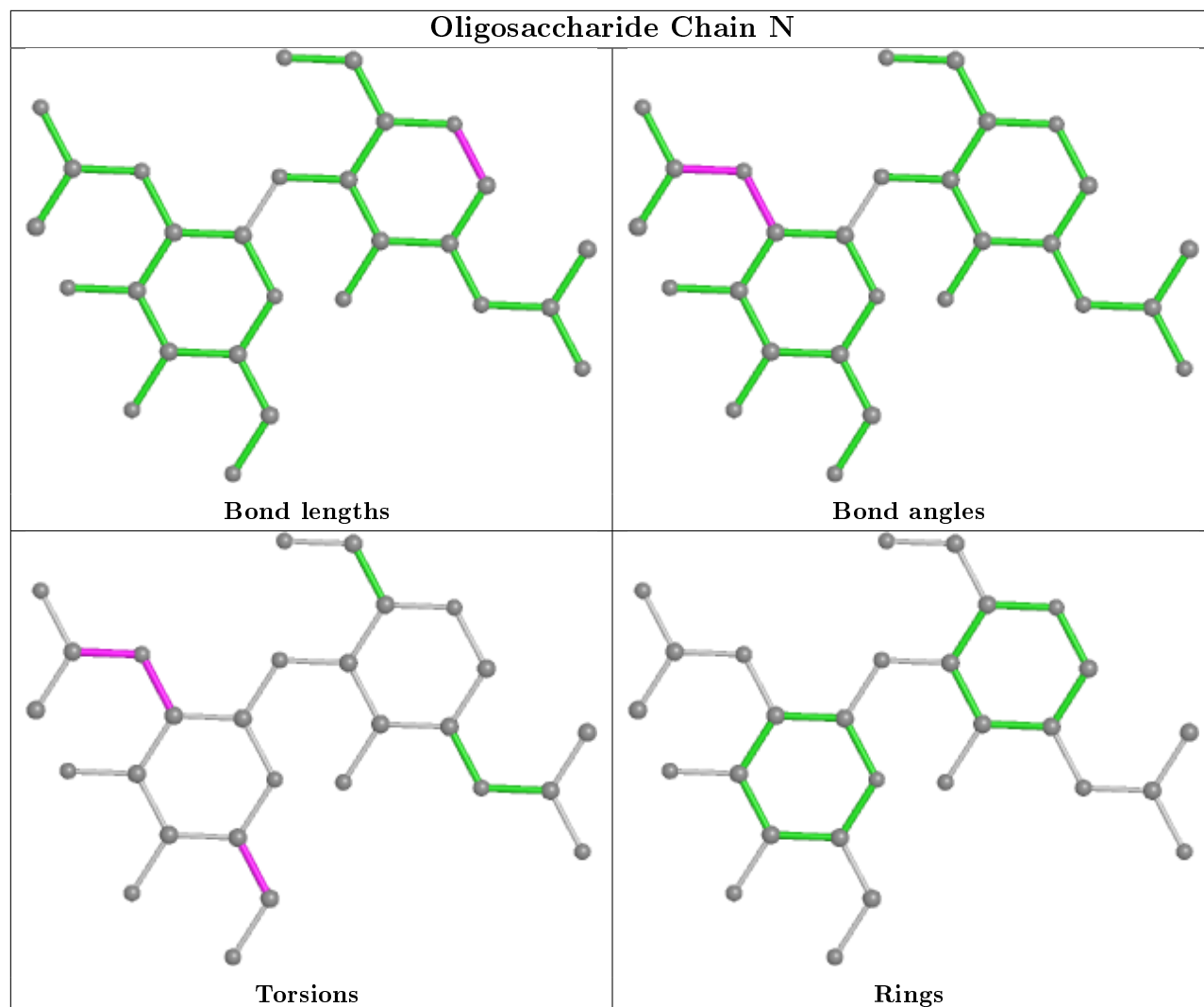


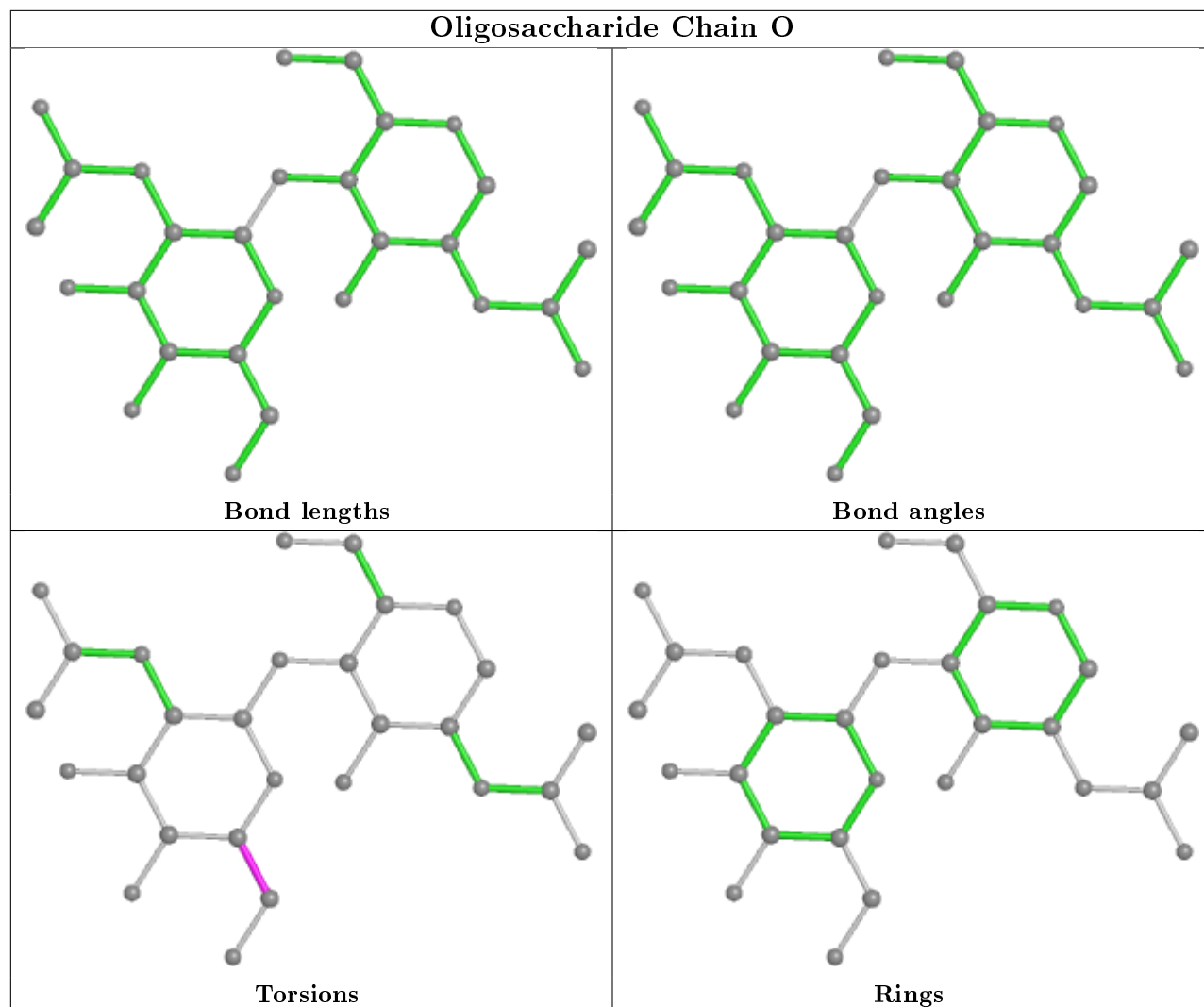


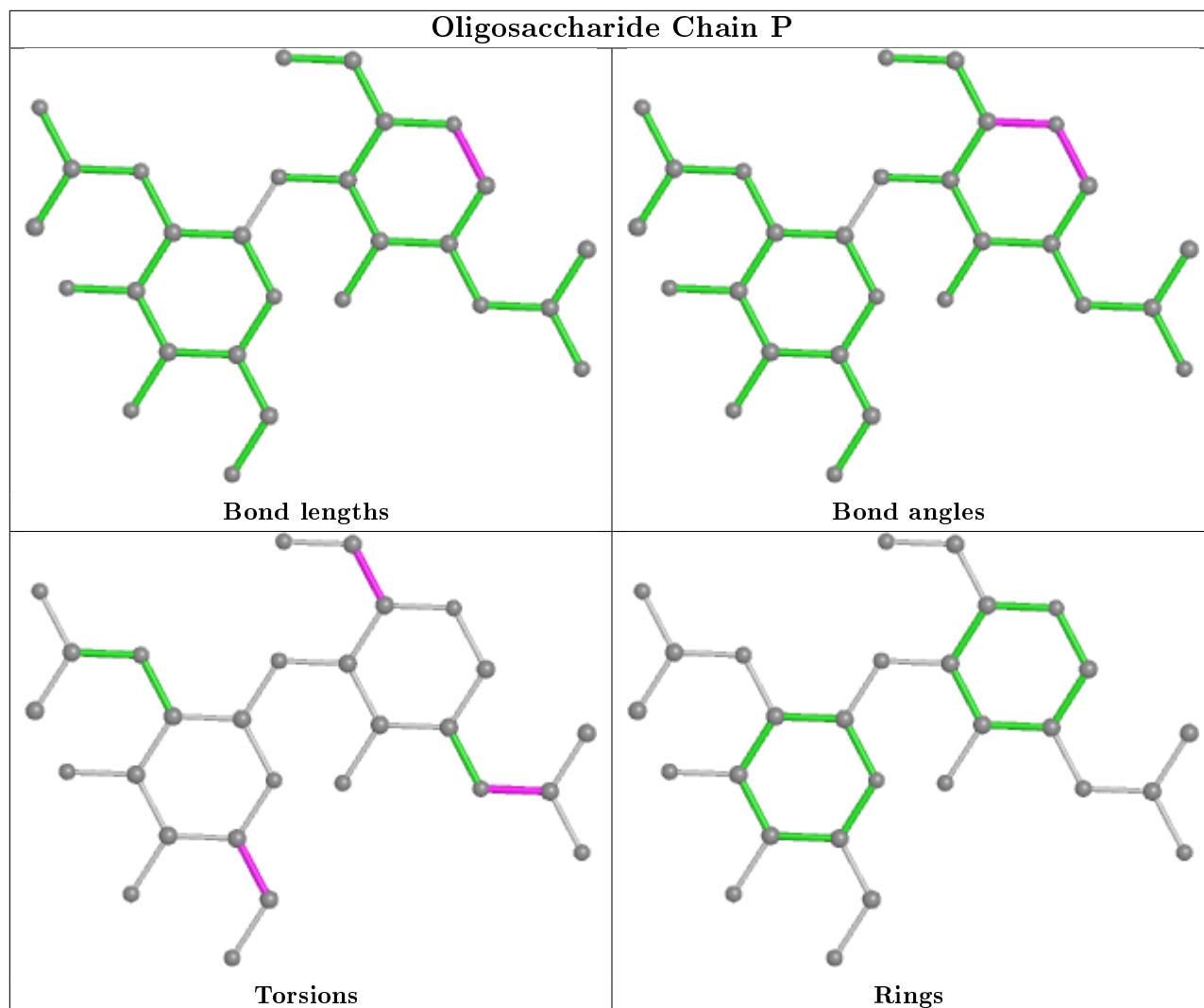


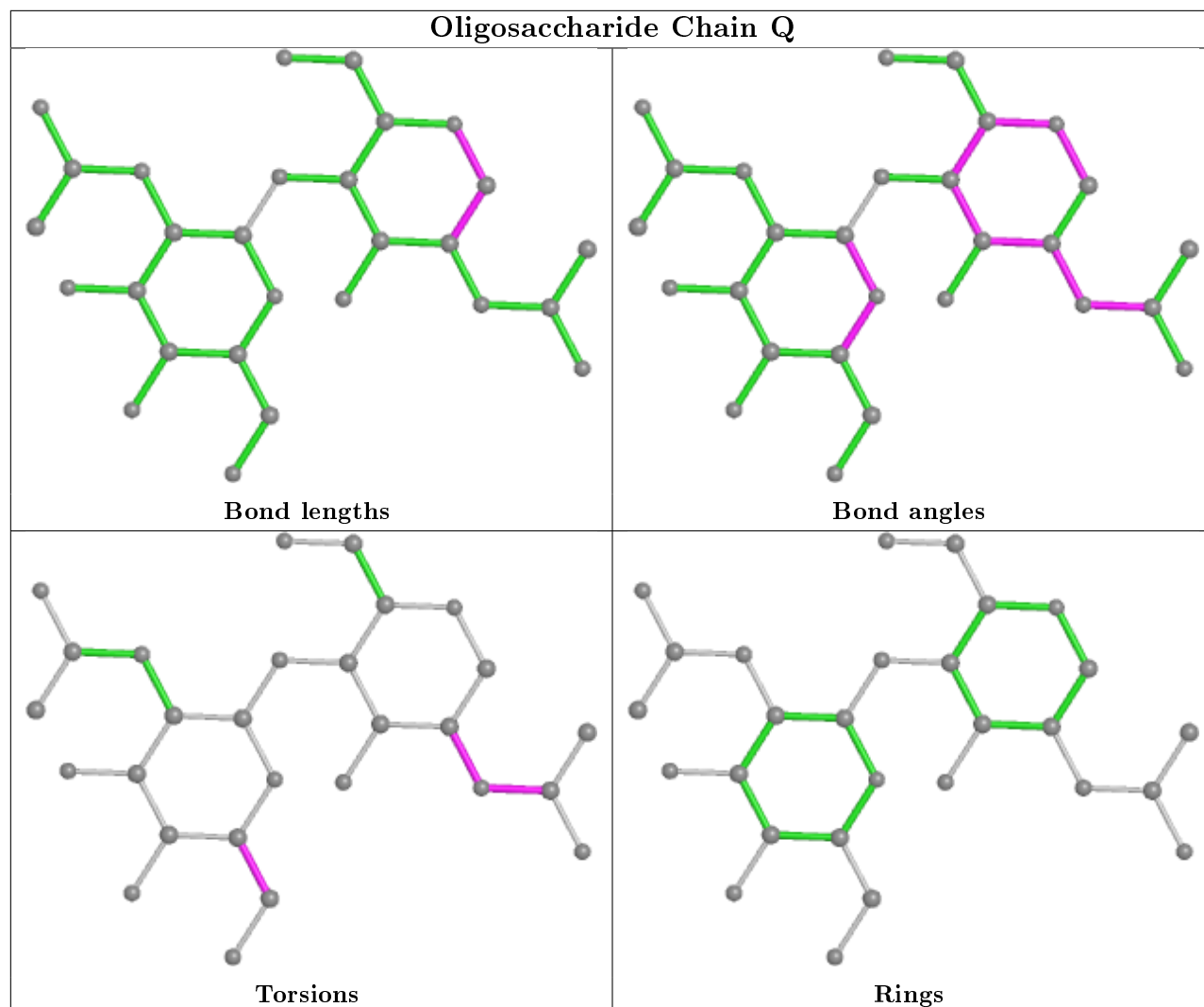


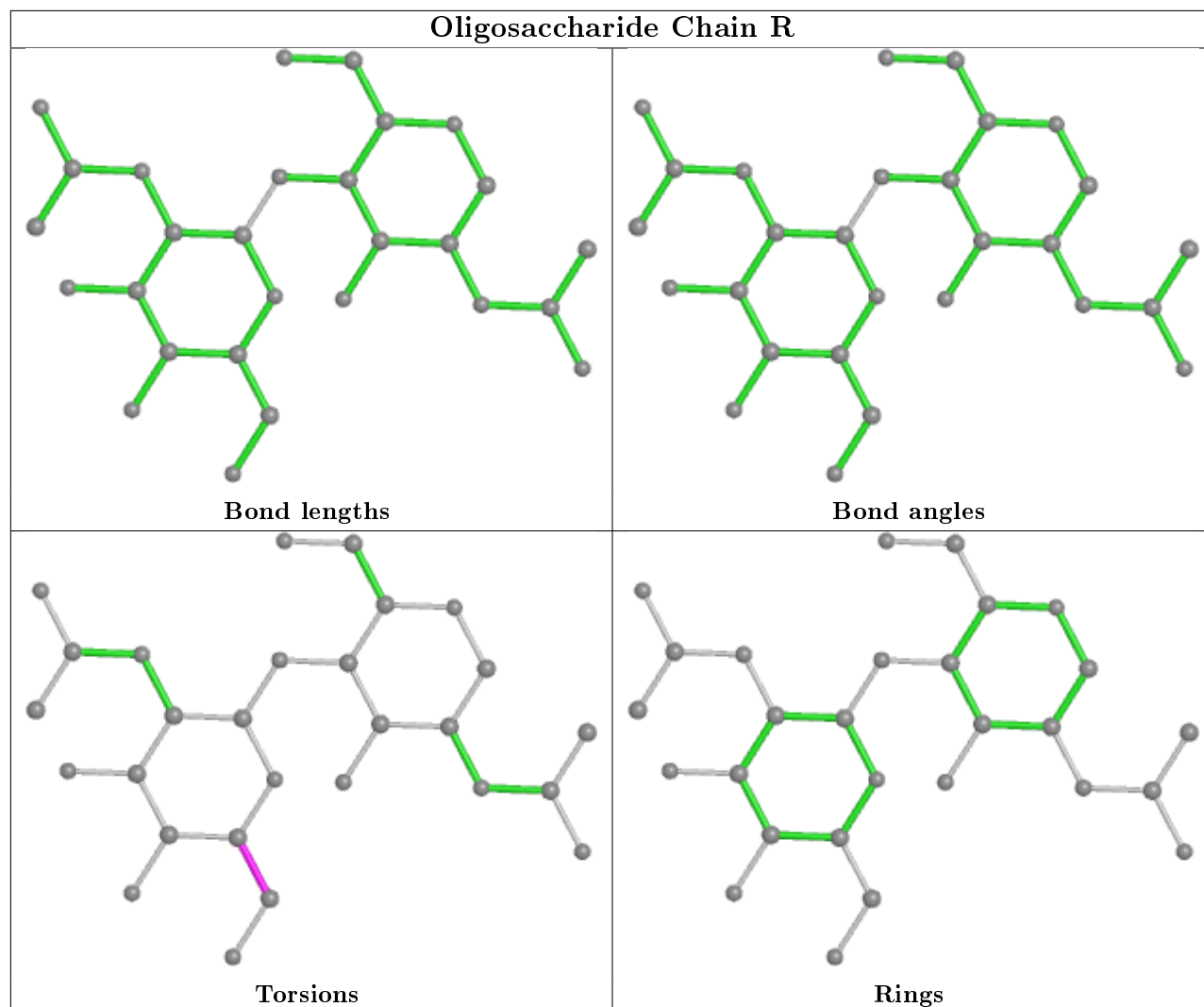


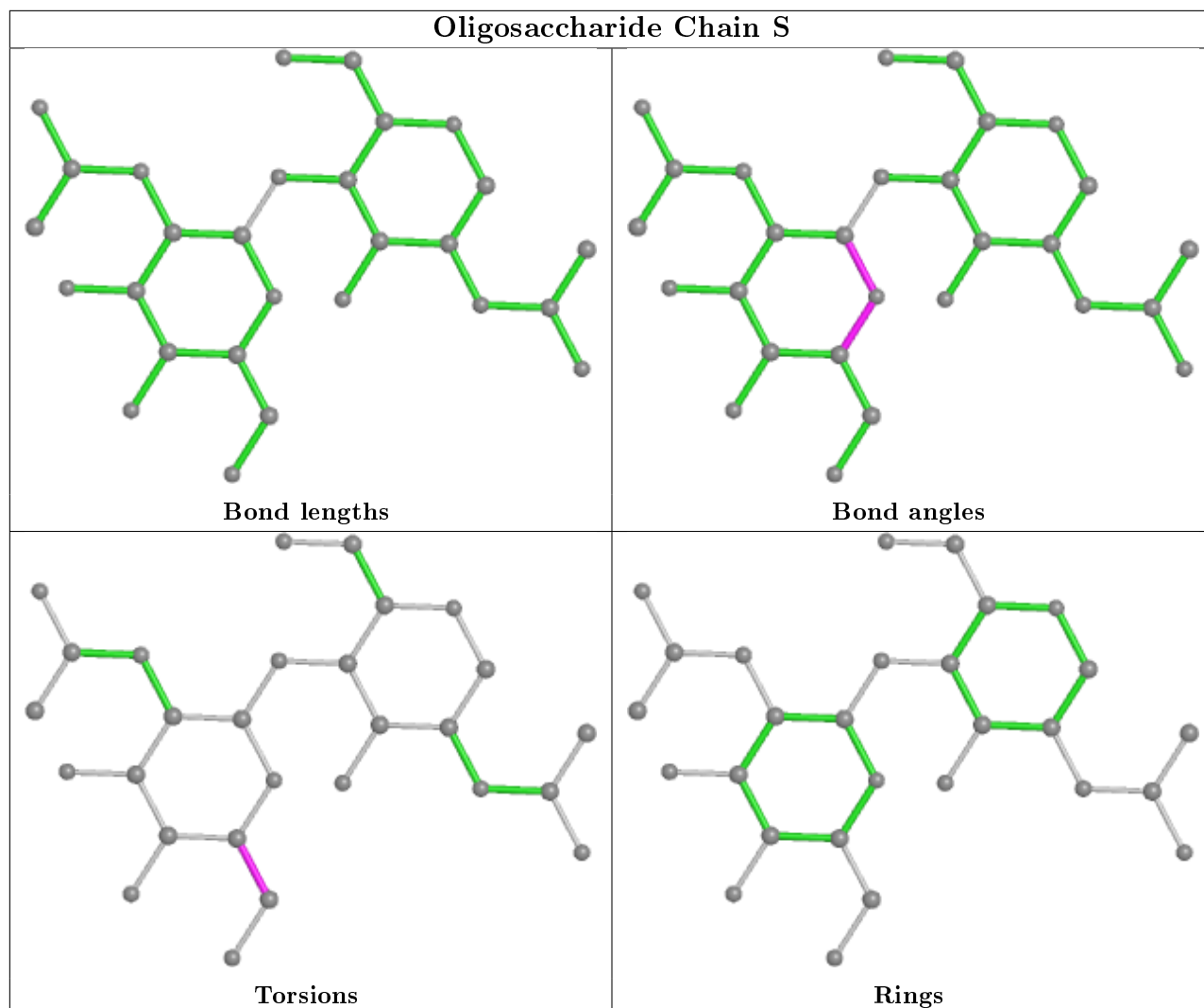


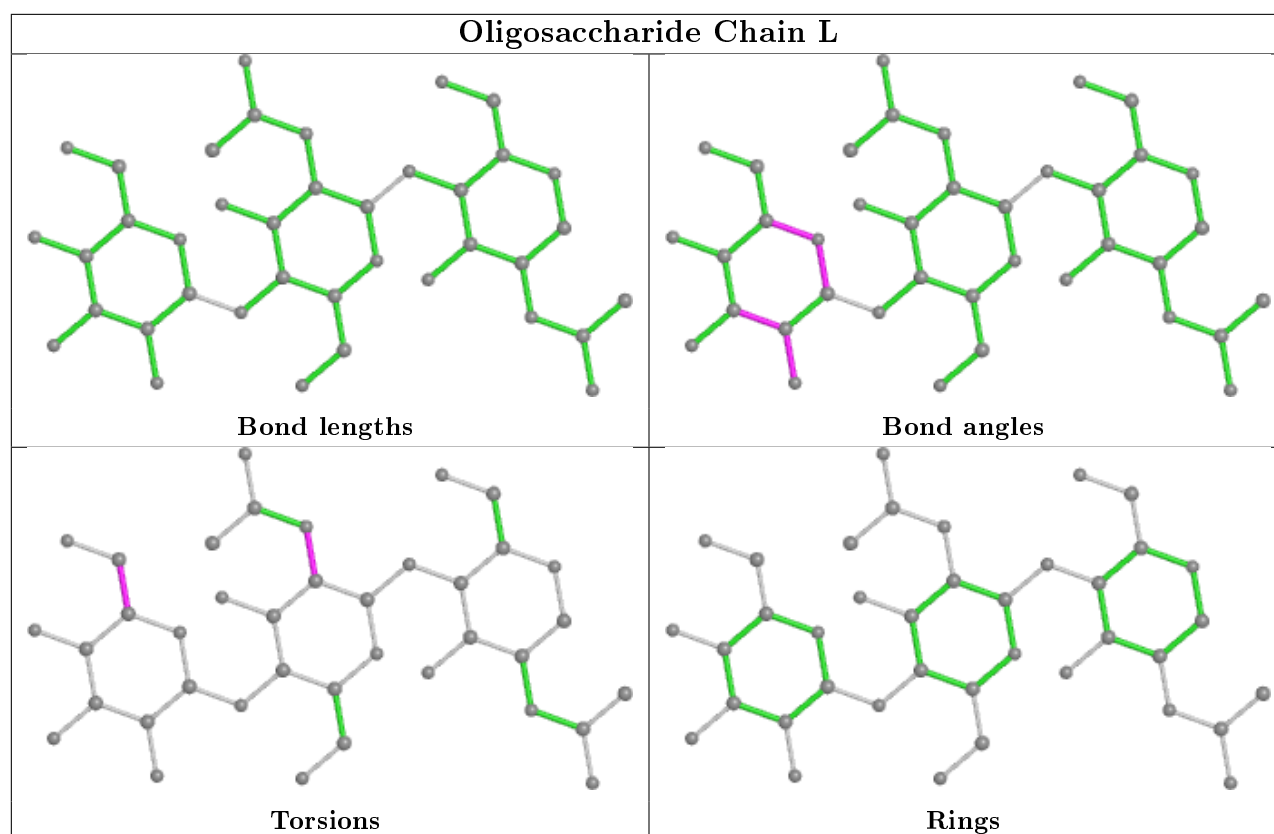












## 5.6 Ligand geometry [i](#)

6 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	$\# Z  > 2$
5	NAG	F	201	2	14,14,15	0.56	0	17,19,21	1.62	3 (17%)
5	NAG	D	201	2	14,14,15	0.20	0	17,19,21	0.41	0
5	NAG	B	201	2	14,14,15	1.25	1 (7%)	17,19,21	1.00	1 (5%)
5	NAG	A	405	1	14,14,15	0.31	0	17,19,21	0.61	1 (5%)
5	NAG	C	406	1	14,14,15	0.61	1 (7%)	17,19,21	0.70	1 (5%)
5	NAG	E	403	1	14,14,15	0.79	1 (7%)	17,19,21	0.70	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
5	NAG	F	201	2	-	3/6/23/26	0/1/1/1
5	NAG	D	201	2	-	2/6/23/26	0/1/1/1
5	NAG	B	201	2	-	2/6/23/26	0/1/1/1
5	NAG	A	405	1	-	0/6/23/26	0/1/1/1
5	NAG	C	406	1	-	2/6/23/26	0/1/1/1
5	NAG	E	403	1	-	3/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	201	NAG	O5-C1	-4.22	1.37	1.43
5	E	403	NAG	O5-C1	-2.28	1.40	1.43
5	C	406	NAG	O5-C1	-2.04	1.40	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	201	NAG	C1-O5-C5	5.34	119.43	112.19
5	B	201	NAG	C1-O5-C5	-2.66	108.59	112.19
5	F	201	NAG	C3-C4-C5	2.66	114.98	110.24
5	C	406	NAG	C1-O5-C5	-2.05	109.42	112.19
5	A	405	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	403	NAG	O5-C5-C6-O6
5	E	403	NAG	C4-C5-C6-O6
5	C	406	NAG	O5-C5-C6-O6
5	D	201	NAG	O5-C5-C6-O6
5	D	201	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
5	B	201	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 [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	341/346 (98%)	-0.01	5 (1%) 73 76	18, 30, 49, 68	0
1	C	342/346 (98%)	0.03	4 (1%) 79 81	21, 34, 53, 80	0
1	E	341/346 (98%)	-0.16	5 (1%) 73 76	18, 30, 48, 77	0
2	B	170/182 (93%)	0.20	11 (6%) 18 20	19, 42, 68, 93	0
2	D	169/182 (92%)	-0.03	1 (0%) 89 90	18, 36, 48, 86	0
2	F	168/182 (92%)	0.17	4 (2%) 59 62	17, 38, 56, 78	0
All	All	1531/1584 (96%)	0.01	30 (1%) 65 68	17, 34, 54, 93	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	170	LEU	5.0
1	A	239	LEU	4.5
2	B	169	SER	3.9
1	C	342	LEU	3.8
1	A	146	VAL	3.5

### 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](#)

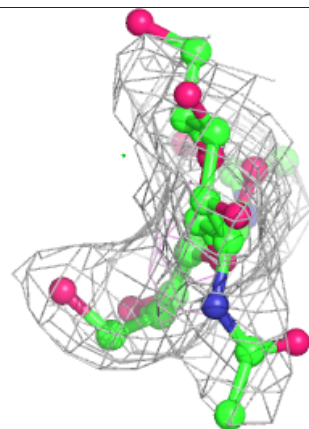
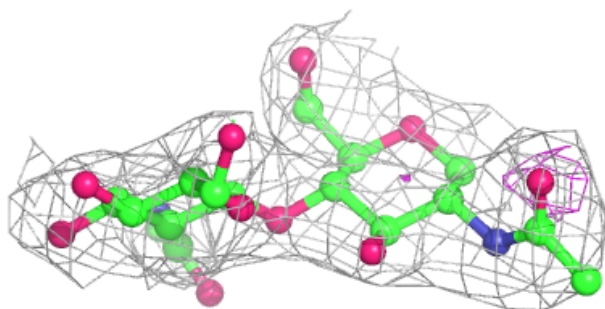
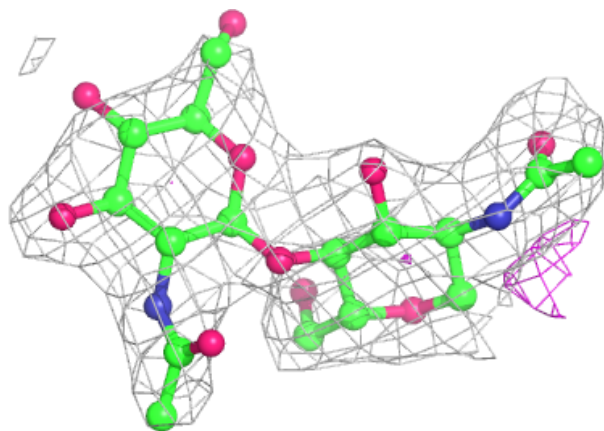
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	Q	1	14/15	0.57	0.35	64,81,96,98	0
3	NAG	S	2	14/15	0.64	0.35	66,79,89,92	0
3	NAG	Q	2	14/15	0.75	0.39	74,85,93,96	0
3	NAG	H	2	14/15	0.79	0.37	49,83,88,92	0
3	NAG	I	2	14/15	0.79	0.50	77,85,93,95	0
3	NAG	N	2	14/15	0.81	0.28	53,66,82,82	0
3	NAG	O	2	14/15	0.83	0.36	70,79,87,91	0
4	BMA	L	3	11/12	0.83	0.12	47,53,61,61	0
3	NAG	R	2	14/15	0.84	0.38	57,79,85,95	0
3	NAG	G	2	14/15	0.86	0.42	51,75,83,87	0
3	NAG	H	1	14/15	0.87	0.25	52,66,69,78	0
3	NAG	K	2	14/15	0.87	0.34	49,71,89,96	0
3	NAG	M	2	14/15	0.88	0.31	62,74,90,93	0
3	NAG	J	2	14/15	0.88	0.19	51,71,78,78	0
3	NAG	P	2	14/15	0.89	0.14	37,60,69,69	0
4	NAG	L	2	14/15	0.89	0.21	34,47,68,69	0
3	NAG	O	1	14/15	0.90	0.16	40,52,62,73	0
3	NAG	G	1	14/15	0.90	0.29	37,48,61,67	0
3	NAG	I	1	14/15	0.90	0.26	44,50,70,73	0
3	NAG	S	1	14/15	0.91	0.16	40,47,60,70	0
4	NAG	L	1	14/15	0.91	0.18	40,49,58,63	0
3	NAG	J	1	14/15	0.91	0.17	49,57,63,70	0
3	NAG	M	1	14/15	0.92	0.22	43,51,71,76	0
3	NAG	K	1	14/15	0.92	0.21	41,48,60,69	0
3	NAG	P	1	14/15	0.92	0.17	35,40,52,53	0
3	NAG	R	1	14/15	0.92	0.26	34,55,72,78	0
3	NAG	N	1	14/15	0.93	0.19	34,48,60,67	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.

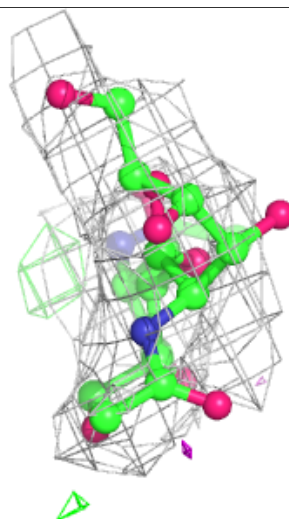
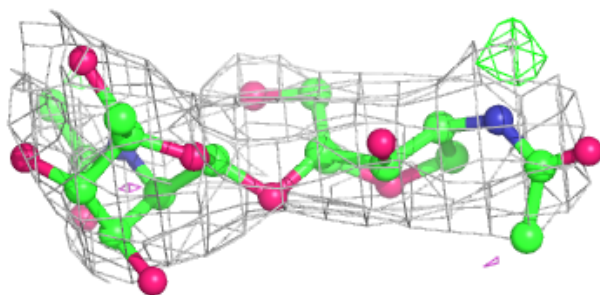
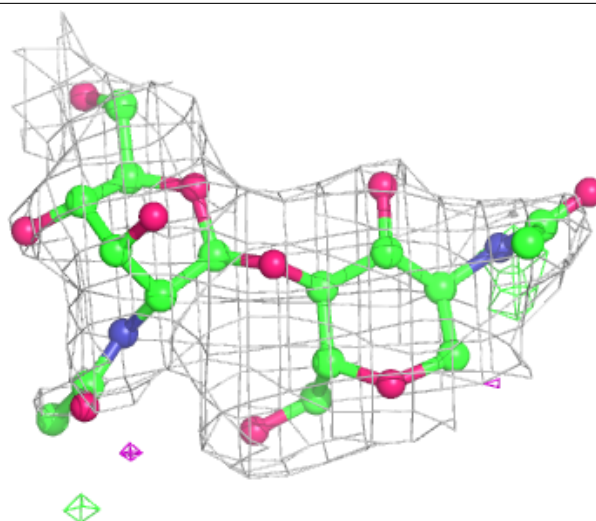
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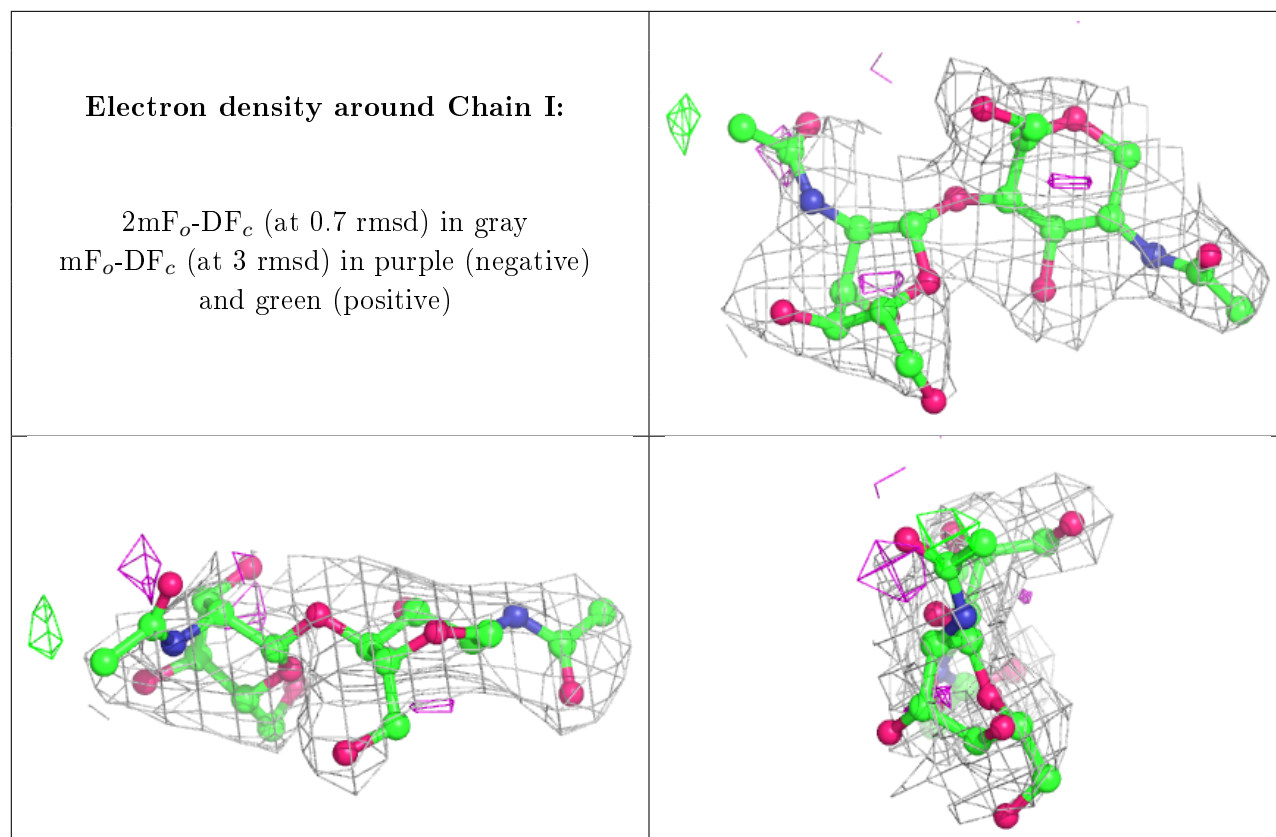
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain H:**

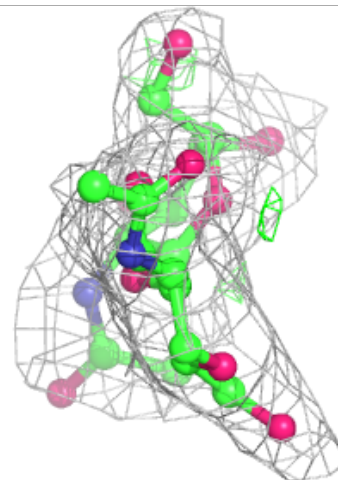
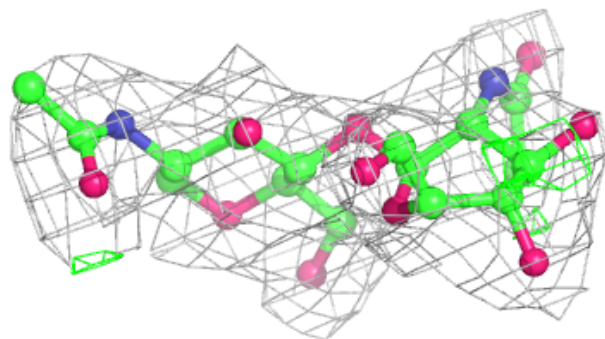
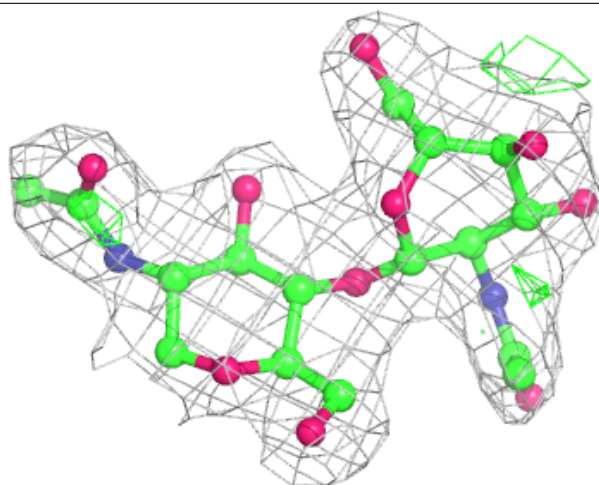
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and green (positive)





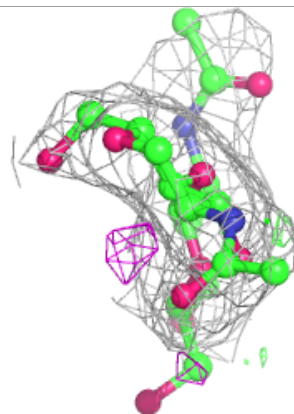
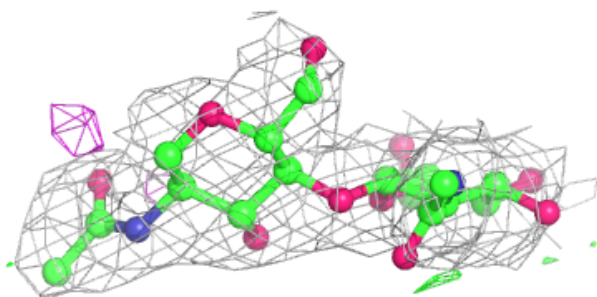
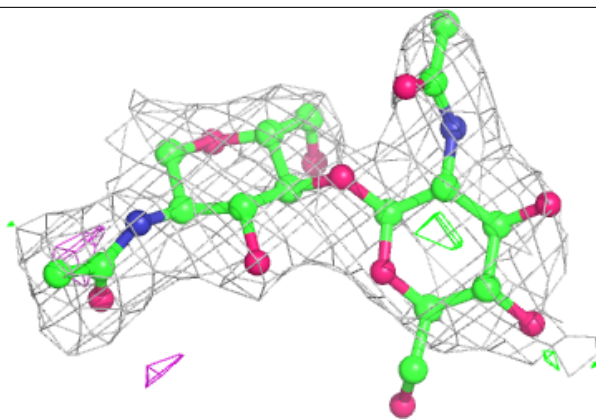
**Electron density around Chain J:**

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

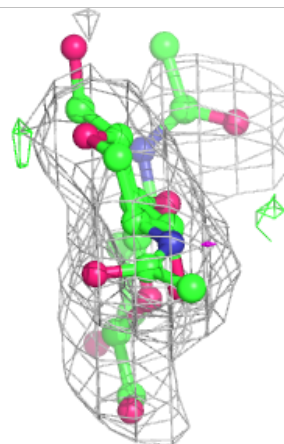
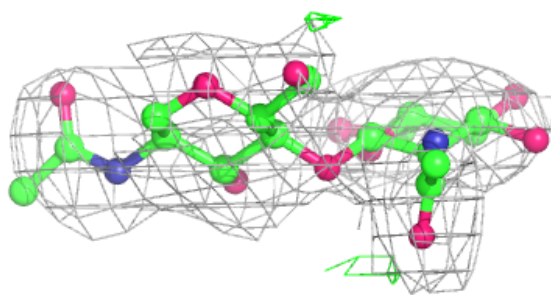
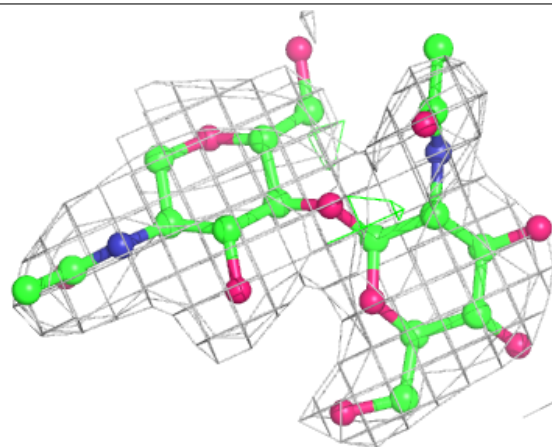


**Electron density around Chain K:**

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

**Electron density around Chain M:**

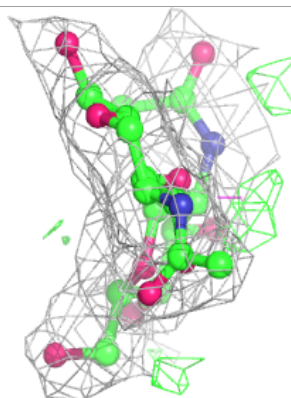
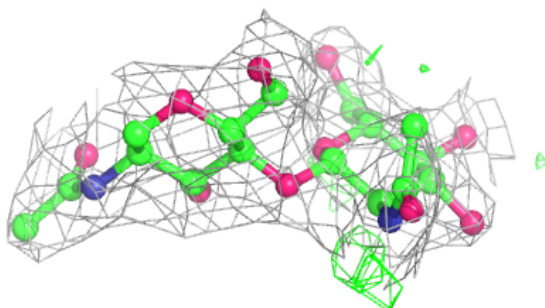
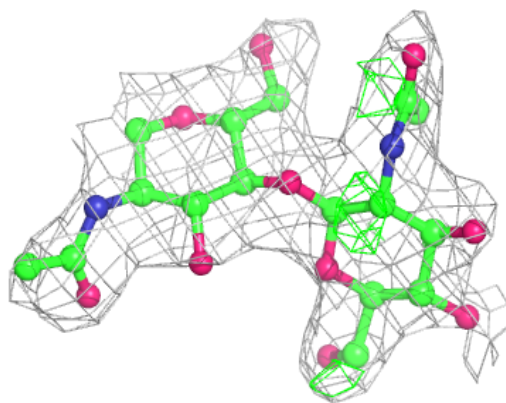
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



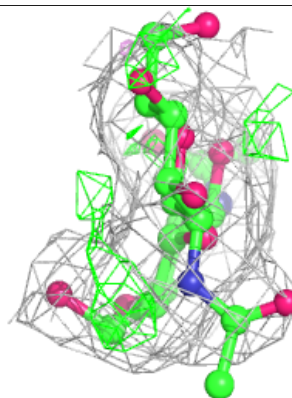
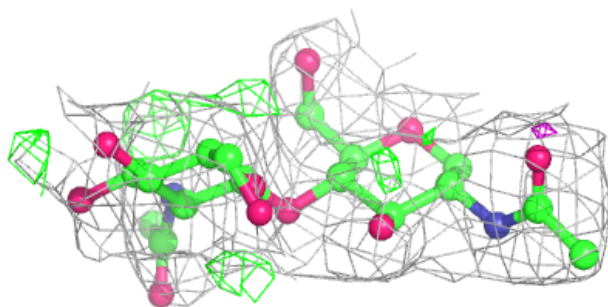
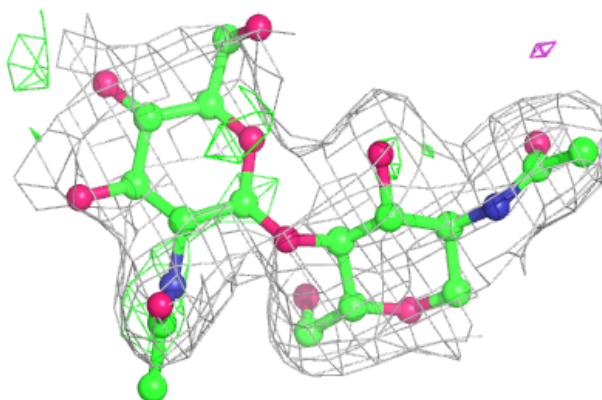


**Electron density around Chain N:**

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

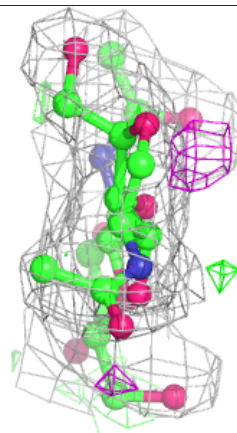
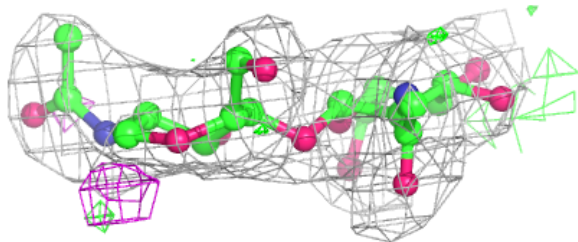
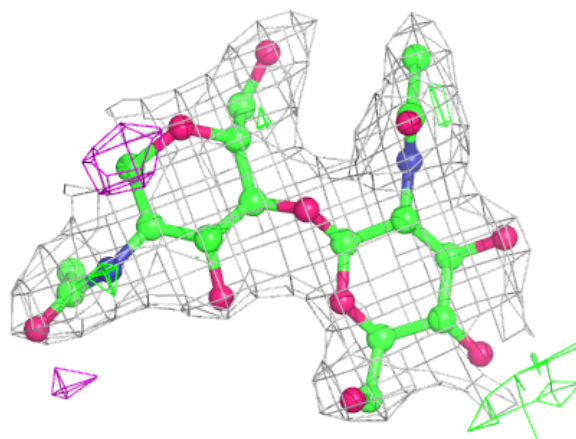
**Electron density around Chain O:**

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



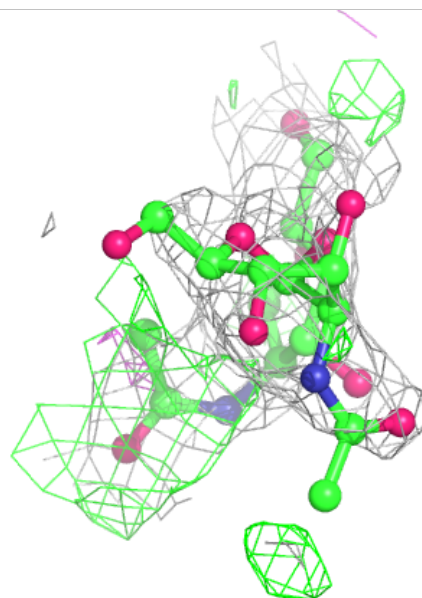
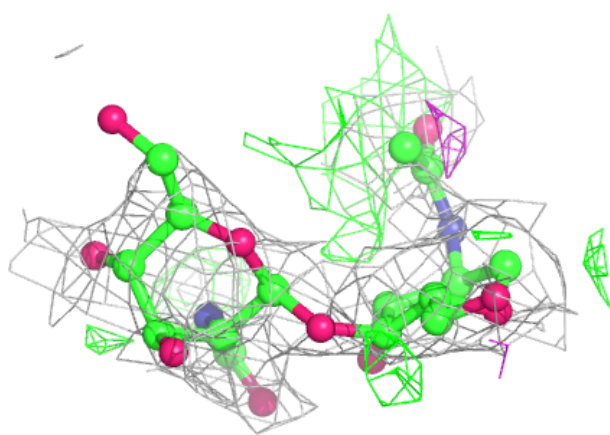
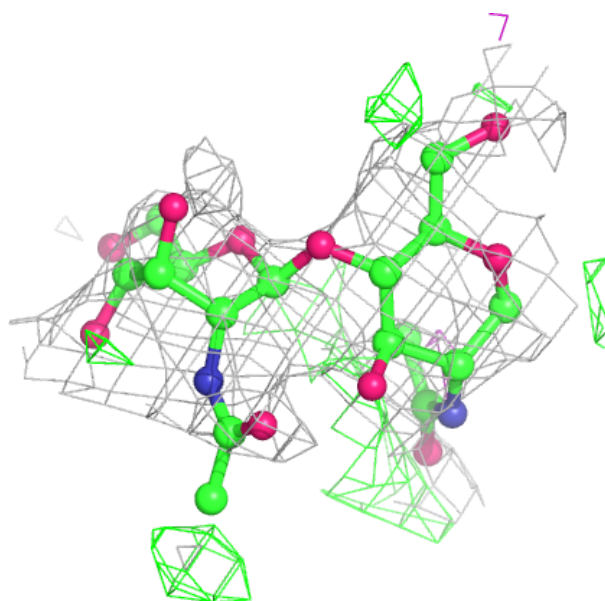
**Electron density around Chain P:**

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



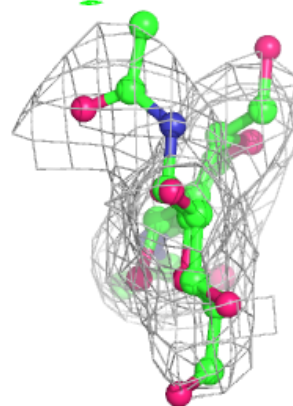
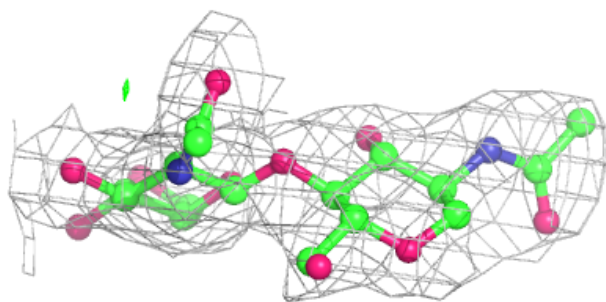
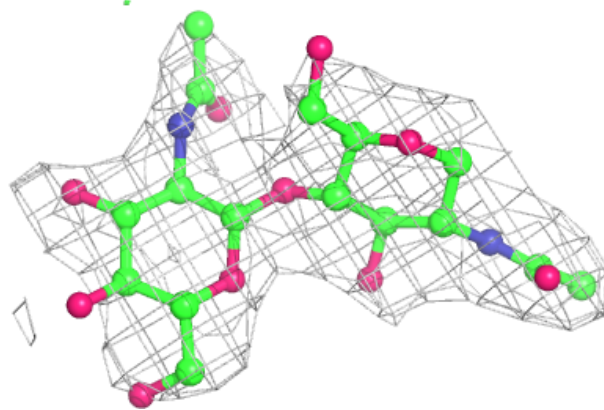
**Electron density around Chain Q:**

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

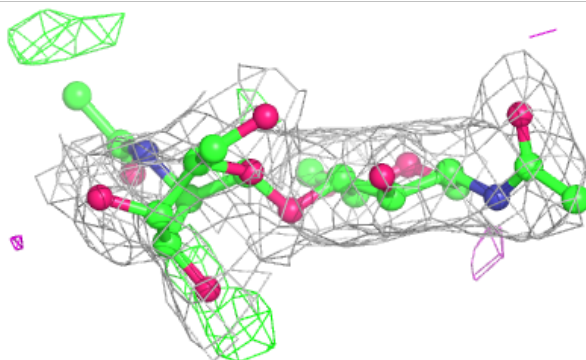
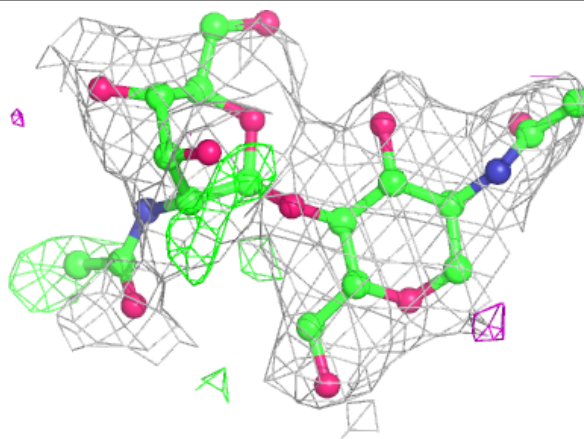


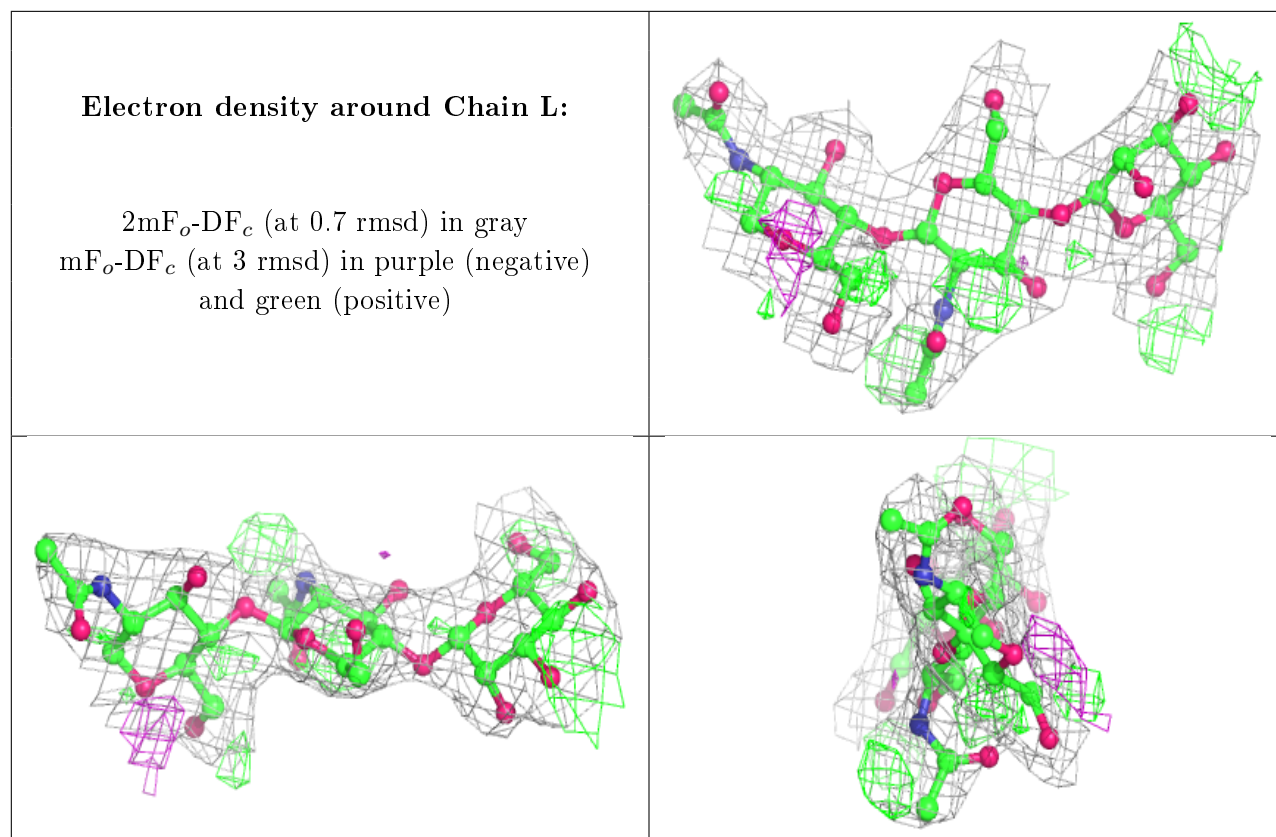
**Electron density around Chain R:**

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

**Electron density around Chain S:**

$2mF_o-DF_c$  (at 0.7 rnsd) in gray  
 $mF_o-DF_c$  (at 3 rnsd) 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
5	NAG	E	403	14/15	0.47	0.35	61,87,91,98	0
5	NAG	C	406	14/15	0.54	0.67	88,104,109,121	0
5	NAG	B	201	14/15	0.62	0.36	88,98,109,111	0
5	NAG	F	201	14/15	0.84	0.26	56,68,76,78	0
5	NAG	D	201	14/15	0.85	0.28	42,62,75,79	0
5	NAG	A	405	14/15	0.90	0.25	62,70,87,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.