



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 27, 2023 – 05:24 PM EDT

PDB ID : 3IJE  
Title : Crystal structure of the complete integrin alphaVbeta3 ectodomain plus an Alpha/beta transmembrane fragment  
Authors : Xiong, J.-P.; Mahalingam, B.; Rui, X.; Hyman, B.T.; Goodman, S.L.; Arnaout, M.A.  
Deposited on : 2009-08-04  
Resolution : 2.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

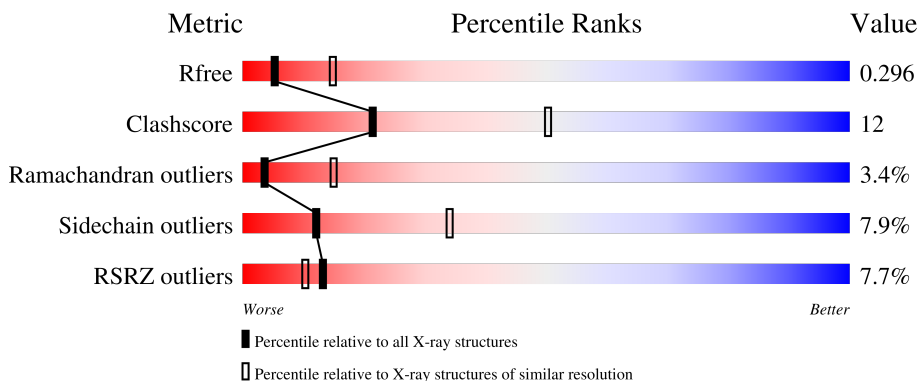
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	967	 6% 71% 23%
2	B	695	 9% 70% 26%
3	C	5	 40% 60%
4	D	2	 50% 50%
4	F	2	 50% 50%

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Mol	Chain	Length	Quality of chain
4	G	2	 100%
4	H	2	 50% 50%
4	I	2	 100%
4	K	2	 100%
5	E	6	 33% 67%
6	J	3	 33% 67%
6	L	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
3	NAG	C	2	-	-	X	-
6	BMA	J	3	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 13087 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.

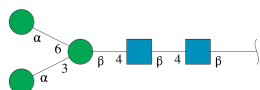
- Molecule 1 is a protein called Integrin alpha-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	938	7300	4628	1236	1400	36	0	0	0

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	695	5332	3276	909	1077	70	0	0	0

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



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

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



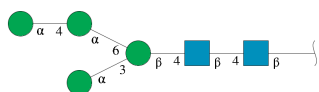
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	2	28	16	2	10	0	0	0

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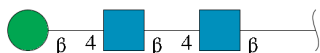
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-6)-[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
5	E	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 6 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
6	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	L	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

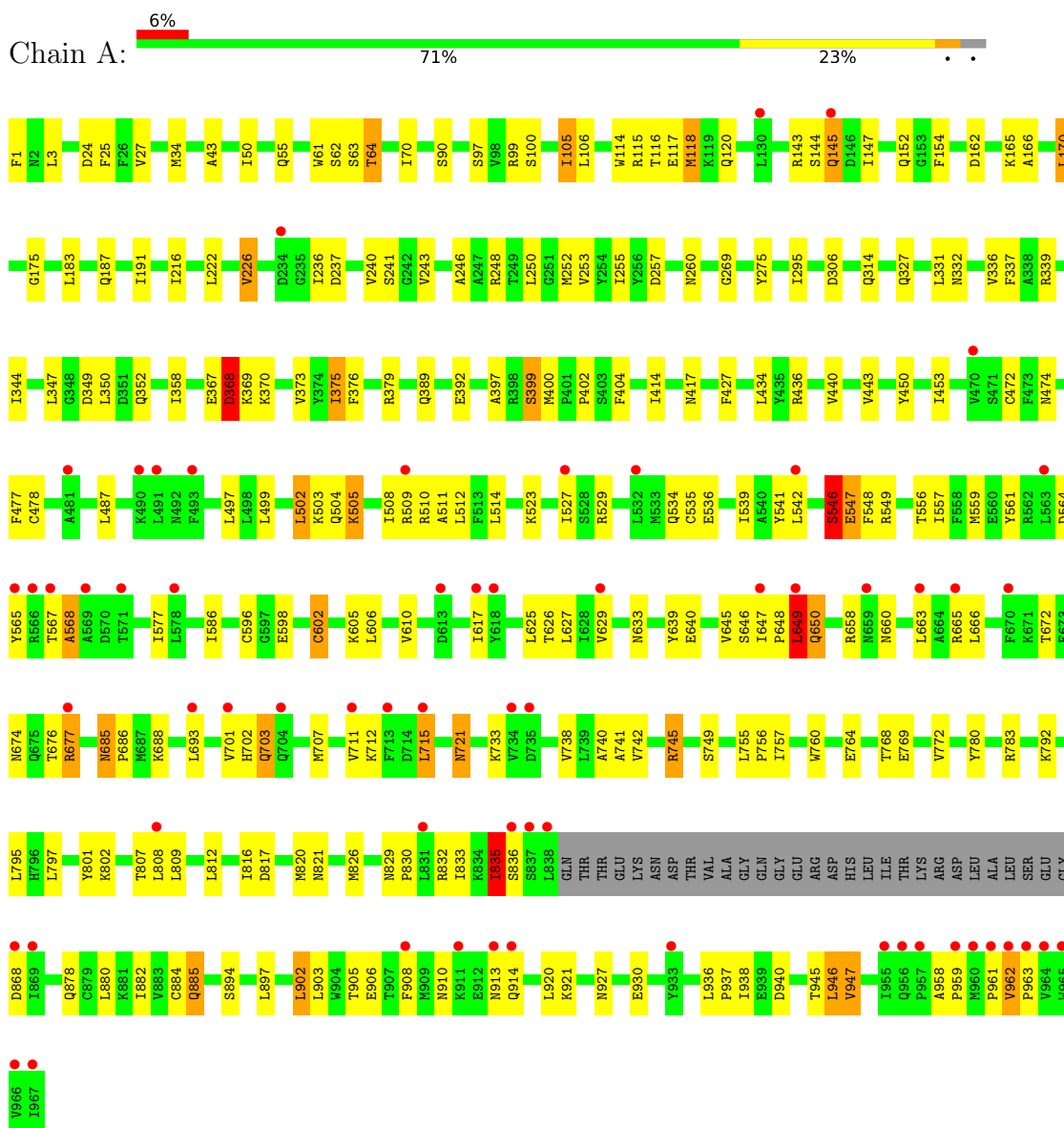
- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	5	Total Ca 5 5	0	0
8	B	1	Total Ca 1 1	0	0

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

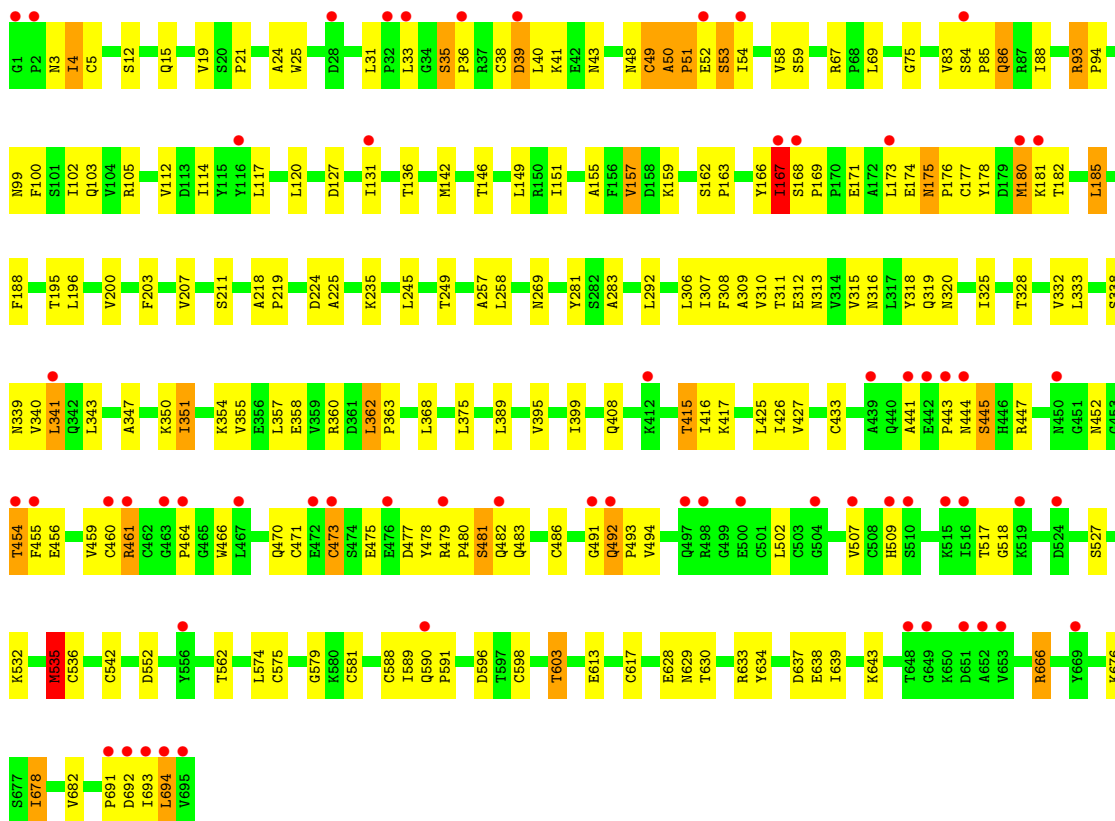
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Integrin alpha-V



- Molecule 2: Integrin beta-3





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

Chain C:



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

Chain D:




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

Chain F:




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



Chain G:  100%


MAG1  
MAG2

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

Chain H:  50% 50%


MAG1  
MAG2

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

Chain I:  100%

MAG1  
MAG2

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

Chain K:  100%

MAG1  
MAG2

- Molecule 5: alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose-(1-6)-[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 E:  33% 67%

MAG1  
MAG2  
EMAS  
MAN4  
MAN5  
MAN6

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  33% 67%

MAG1  
MAG2  
EMAS

- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%

MAG1  
MAG2  
BMA3

## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.87Å 129.87Å 305.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 64.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.90) 92.7 (64.94-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, $R_{free}$	0.244 , 0.285 0.244 , 0.296	Depositor DCC
$R_{free}$ test set	2924 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	82.4	Xtrriage
Anisotropy	0.191	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 63.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% 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: MAN, CA, 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	0.33	0/7462	0.54	0/10123
2	B	0.35	0/5429	0.54	0/7344
All	All	0.34	0/12891	0.54	0/17467

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	546	SER	Peptide

### 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	7300	0	7126	164	0
2	B	5332	0	5071	139	0
3	C	61	0	52	7	0
4	D	28	0	25	0	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	H	28	0	25	2	0
4	I	28	0	25	0	0
4	K	28	0	25	0	0
5	E	72	0	61	0	0
6	J	39	0	34	0	0
6	L	39	0	34	0	0
7	A	28	0	26	0	0
7	B	42	0	39	5	0
8	A	5	0	0	0	0
8	B	1	0	0	0	0
All	All	13087	0	12593	306	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 12.

The worst 5 of 306 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:3:LEU:HD11	1:A:350:LEU:HD11	1.58	0.85
2:B:249:THR:HG22	2:B:309:ALA:HB3	1.59	0.82
2:B:281:TYR:CE1	2:B:283:ALA:HB3	2.14	0.82
1:A:639:TYR:H	1:A:721:ASN:HD21	1.30	0.80
1:A:546:SER:O	1:A:547:GLU:HB2	1.82	0.77

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	934/967 (97%)	843 (90%)	68 (7%)	23 (2%)	5	21
2	B	693/695 (100%)	579 (84%)	82 (12%)	32 (5%)	2	9
All	All	1627/1662 (98%)	1422 (87%)	150 (9%)	55 (3%)	3	15

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	A	505	LYS
1	A	547	GLU
1	A	568	ALA
1	A	703	GLN

### 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	797/821 (97%)	727 (91%)	70 (9%)	10	30
2	B	617/617 (100%)	575 (93%)	42 (7%)	16	42
All	All	1414/1438 (98%)	1302 (92%)	112 (8%)	12	34

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	817	ASP
2	B	692	ASP
2	B	86	GLN
2	B	678	ILE
2	B	486	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	301	GLN

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Mol	Chain	Res	Type
2	B	470	GLN
2	B	303	ASN
2	B	376	ASN
1	A	623	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](#)

29 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	C	1	1,3	14,14,15	0.63	0	17,19,21	1.25	2 (11%)
3	NAG	C	2	3	14,14,15	0.42	0	17,19,21	1.51	3 (17%)
3	BMA	C	3	3	11,11,12	0.51	0	15,15,17	2.55	2 (13%)
3	MAN	C	4	3	11,11,12	0.56	0	15,15,17	1.03	2 (13%)
3	MAN	C	5	3	11,11,12	0.60	0	15,15,17	1.06	1 (6%)
4	NAG	D	1	1,4	14,14,15	0.52	0	17,19,21	0.73	0
4	NAG	D	2	4	14,14,15	0.47	0	17,19,21	0.85	1 (5%)
5	NAG	E	1	5,1	14,14,15	0.55	0	17,19,21	1.20	2 (11%)
5	NAG	E	2	5	14,14,15	0.54	0	17,19,21	0.67	0
5	BMA	E	3	5	11,11,12	0.25	0	15,15,17	0.86	1 (6%)
5	MAN	E	4	5	11,11,12	0.62	0	15,15,17	1.22	1 (6%)
5	MAN	E	5	5	11,11,12	0.65	0	15,15,17	0.95	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MAN	E	6	5	11,11,12	0.63	0	15,15,17	0.78	0
4	NAG	F	1	1,4	14,14,15	0.58	0	17,19,21	1.27	1 (5%)
4	NAG	F	2	4	14,14,15	0.50	0	17,19,21	0.79	0
4	NAG	G	1	1,4	14,14,15	0.65	0	17,19,21	1.43	2 (11%)
4	NAG	G	2	4	14,14,15	0.69	0	17,19,21	0.96	1 (5%)
4	NAG	H	1	4	14,14,15	0.68	0	17,19,21	1.65	2 (11%)
4	NAG	H	2	4	14,14,15	0.68	0	17,19,21	1.00	1 (5%)
4	NAG	I	1	1,4	14,14,15	0.68	0	17,19,21	1.25	1 (5%)
4	NAG	I	2	4	14,14,15	0.51	0	17,19,21	1.23	1 (5%)
6	NAG	J	1	1,6	14,14,15	0.50	0	17,19,21	0.99	2 (11%)
6	NAG	J	2	6	14,14,15	0.68	0	17,19,21	1.20	1 (5%)
6	BMA	J	3	6	11,11,12	0.32	0	15,15,17	0.68	0
4	NAG	K	1	2,4	14,14,15	0.47	0	17,19,21	1.91	2 (11%)
4	NAG	K	2	4	14,14,15	0.52	0	17,19,21	1.39	2 (11%)
6	NAG	L	1	2,6	14,14,15	0.51	0	17,19,21	1.10	2 (11%)
6	NAG	L	2	6	14,14,15	0.57	0	17,19,21	1.25	2 (11%)
6	BMA	L	3	6	11,11,12	0.45	0	15,15,17	0.88	1 (6%)

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	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	1/2/19/22	0/1/1/1
3	MAN	C	5	3	-	2/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
5	NAG	E	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	2/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1
5	MAN	E	5	5	-	2/2/19/22	0/1/1/1
5	MAN	E	6	5	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	1	4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	3/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
6	NAG	J	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	6/6/23/26	0/1/1/1
6	BMA	J	3	6	-	2/2/19/22	0/1/1/1
4	NAG	K	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	K	2	4	-	4/6/23/26	0/1/1/1
6	NAG	L	1	2,6	-	4/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1
6	BMA	L	3	6	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	BMA	C1-O5-C5	7.77	122.72	112.19
4	K	1	NAG	C1-O5-C5	5.58	119.76	112.19
3	C	3	BMA	C1-C2-C3	4.84	115.61	109.67
4	G	1	NAG	C4-C3-C2	4.49	117.59	111.02
4	H	1	NAG	C3-C4-C5	4.39	118.07	110.24

There are no chirality outliers.

5 of 69 torsion outliers are listed below:

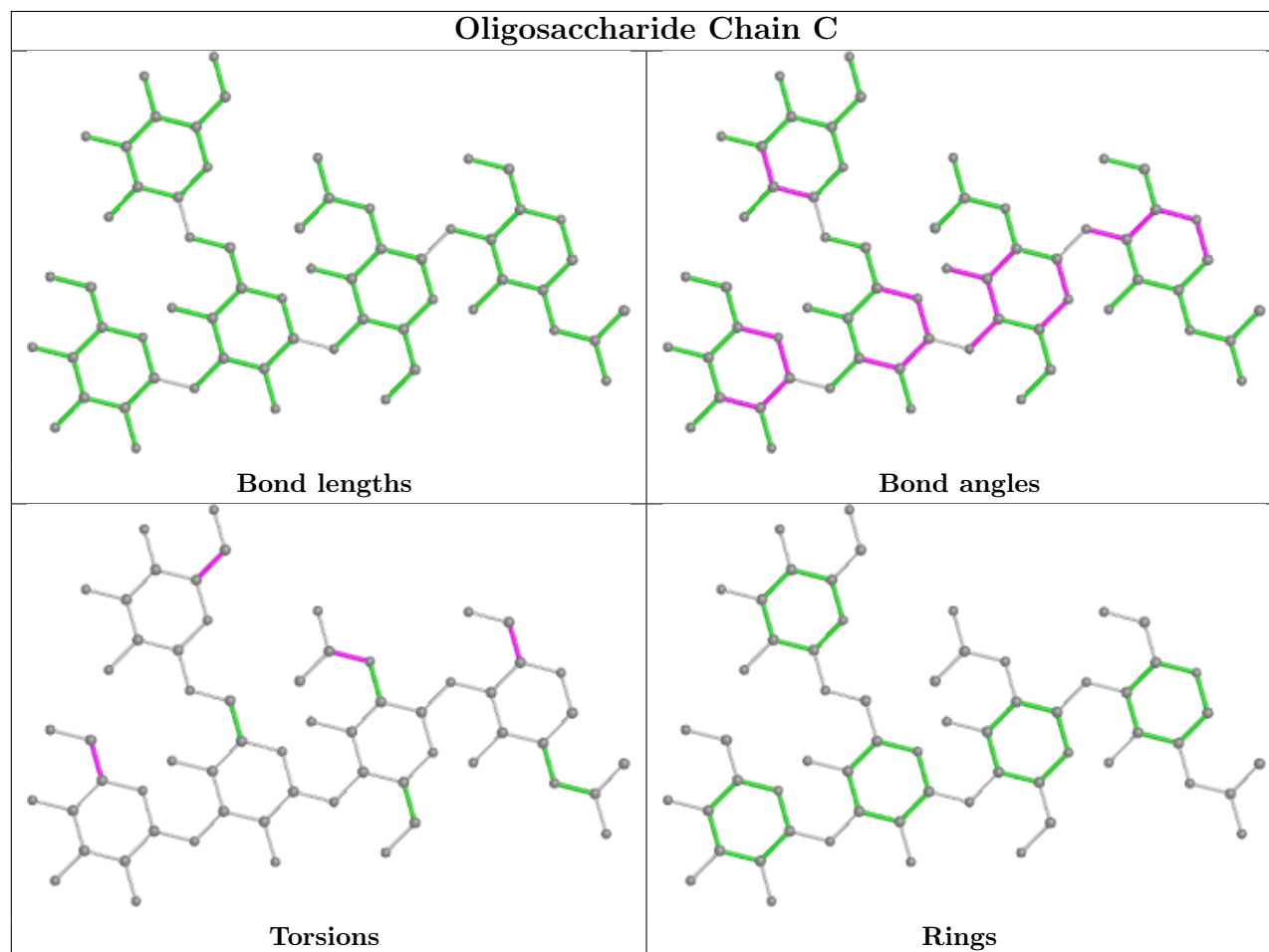
Mol	Chain	Res	Type	Atoms
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	F	1	NAG	C3-C2-N2-C7

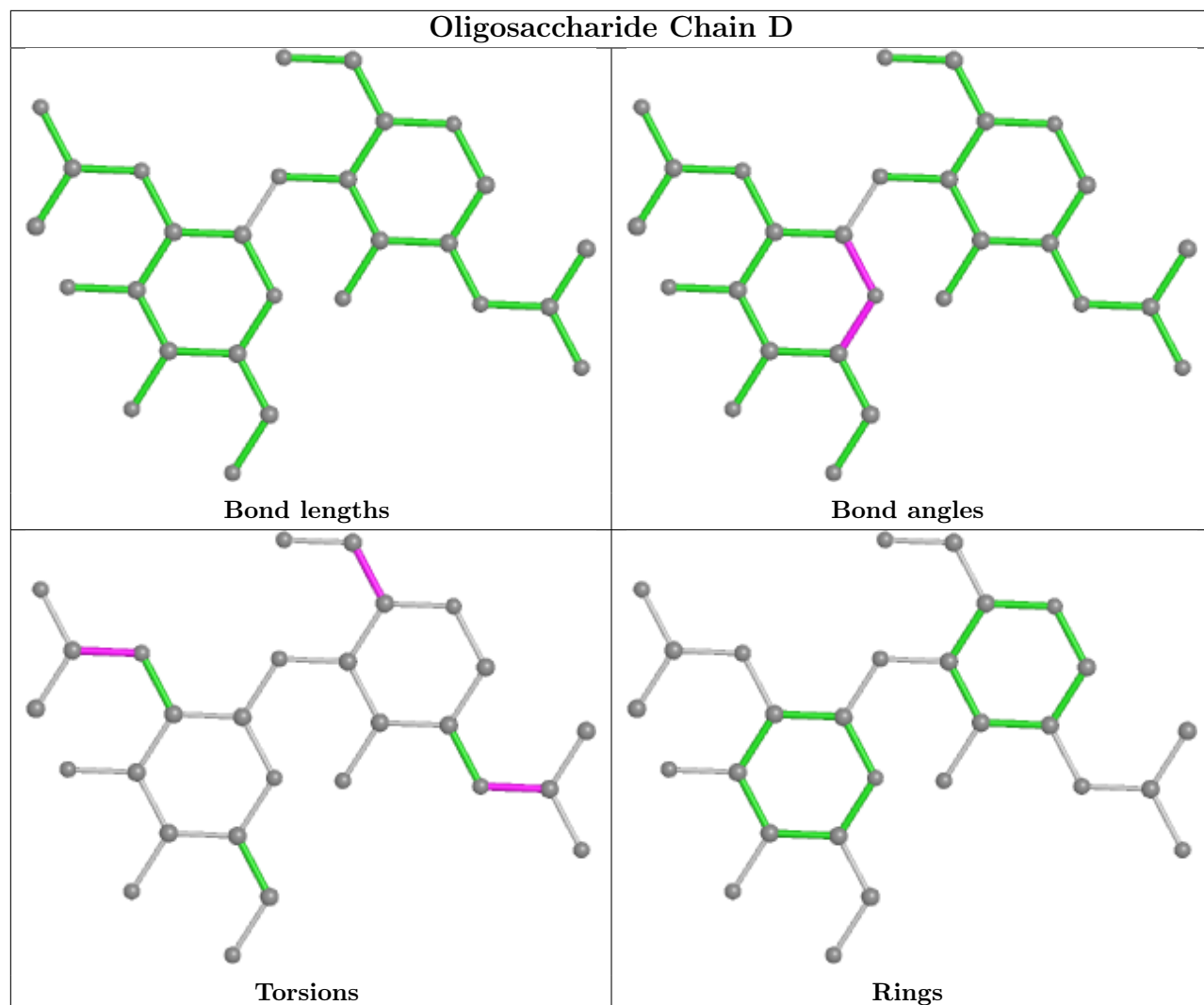
There are no ring outliers.

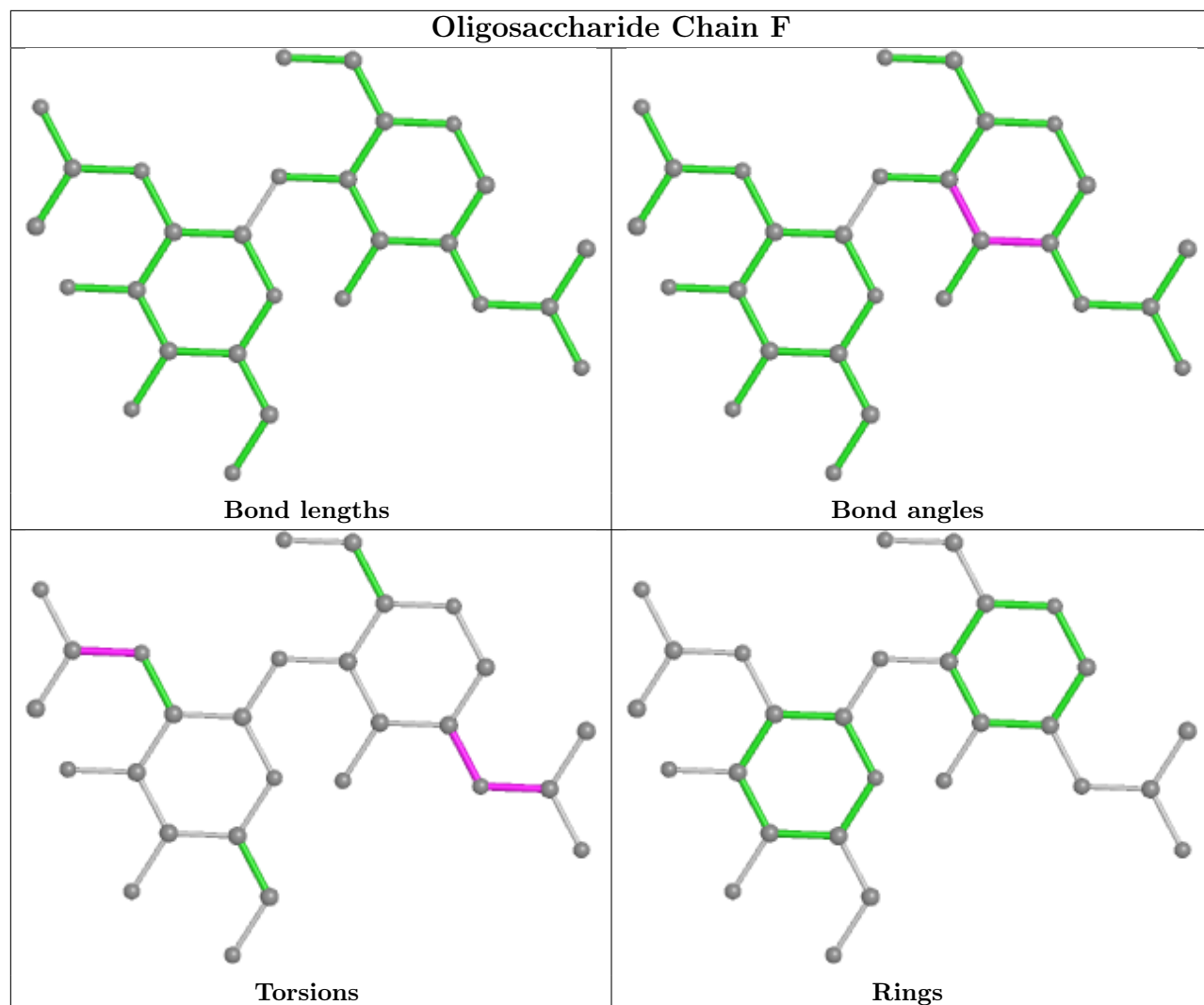
4 monomers are involved in 9 short contacts:

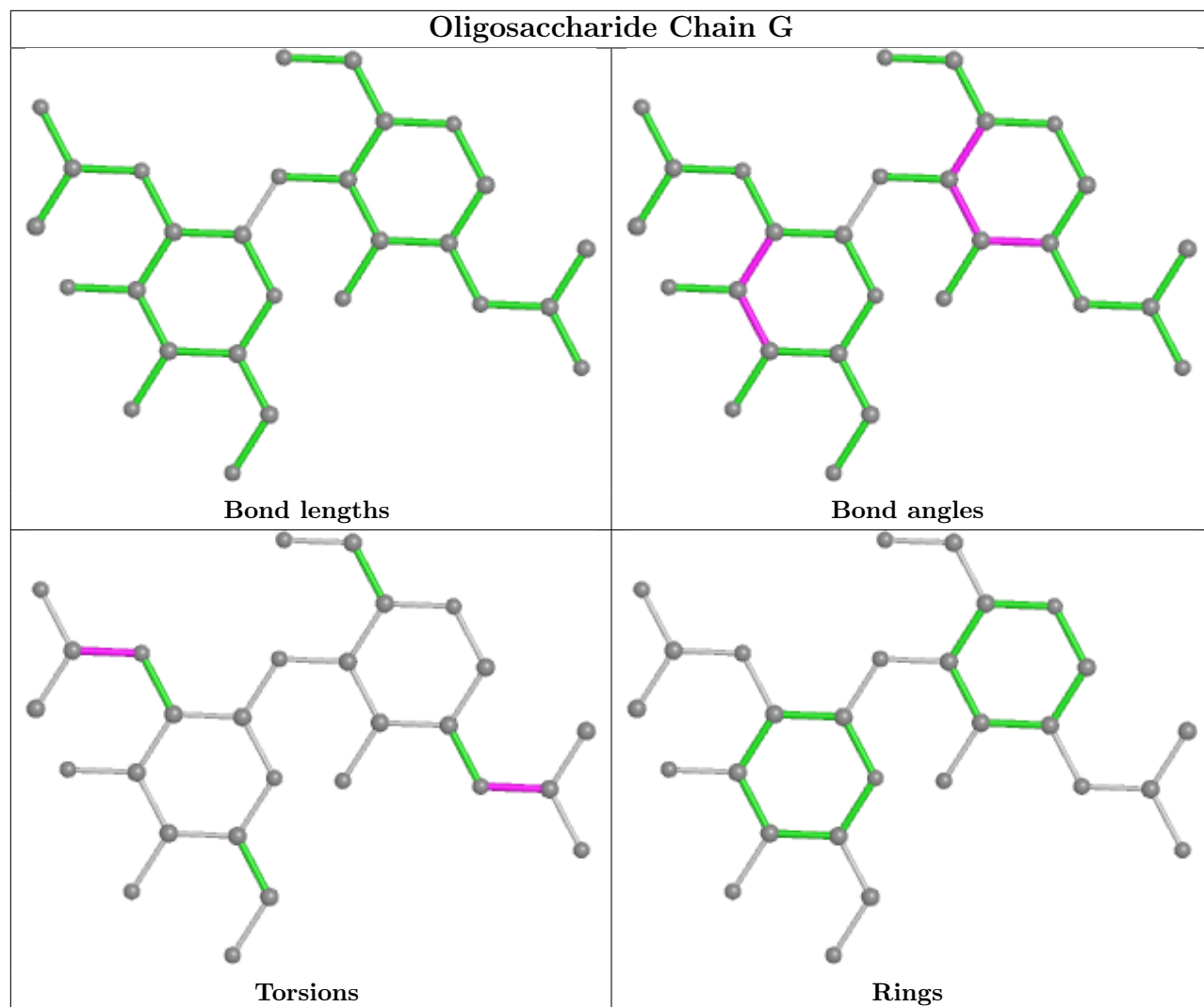
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	NAG	2	0
3	C	2	NAG	7	0
3	C	4	MAN	2	0
3	C	3	BMA	5	0

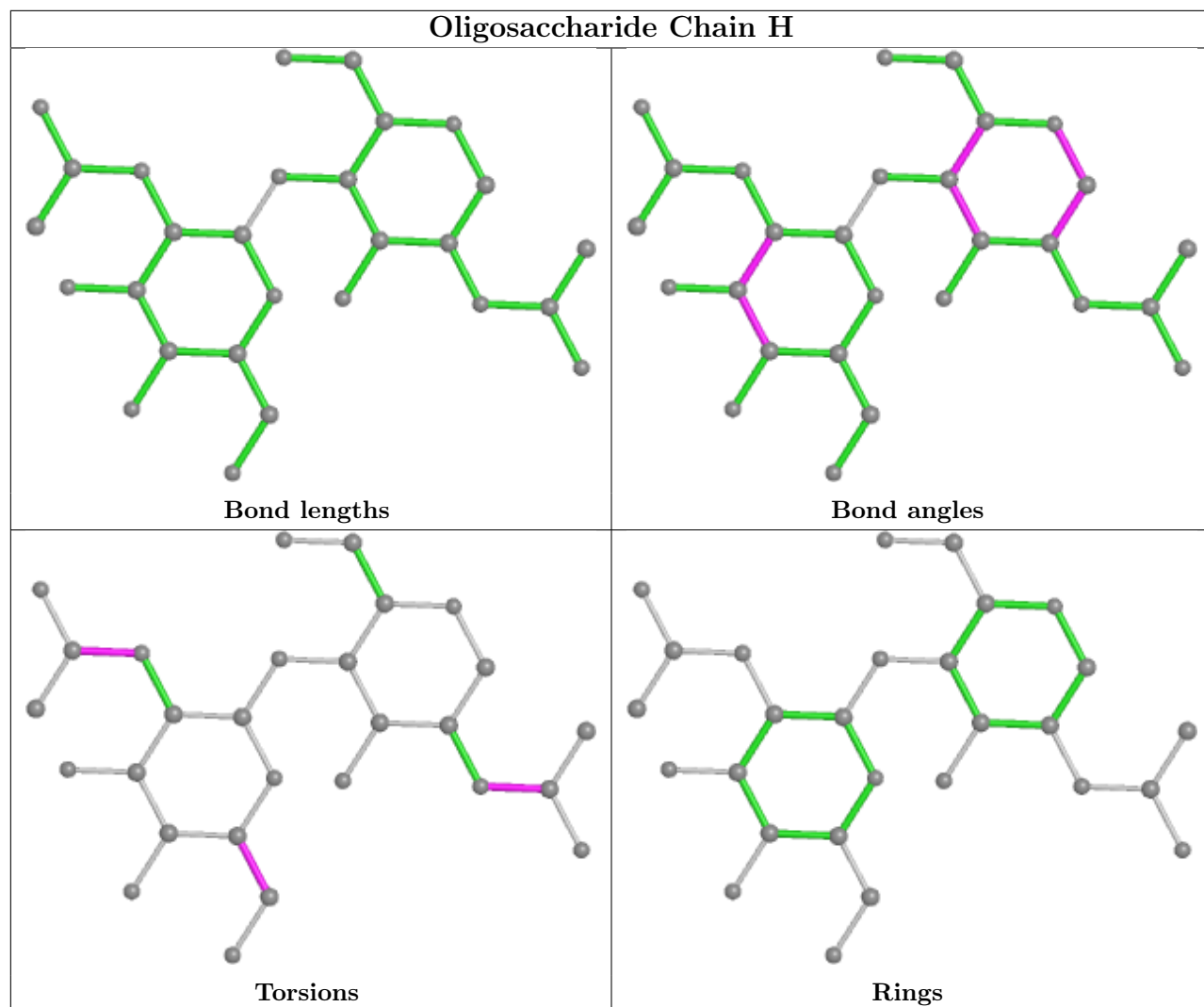
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

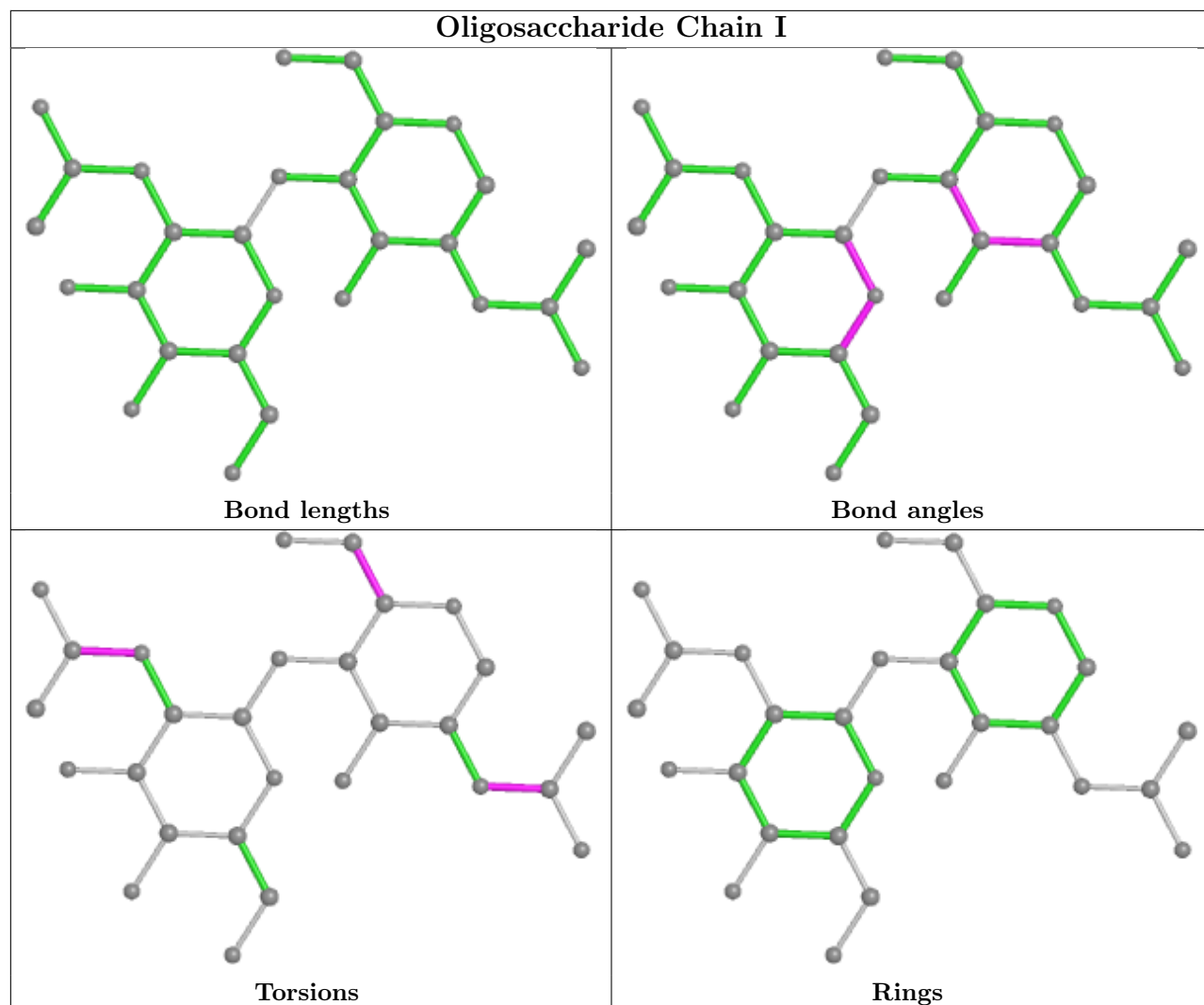


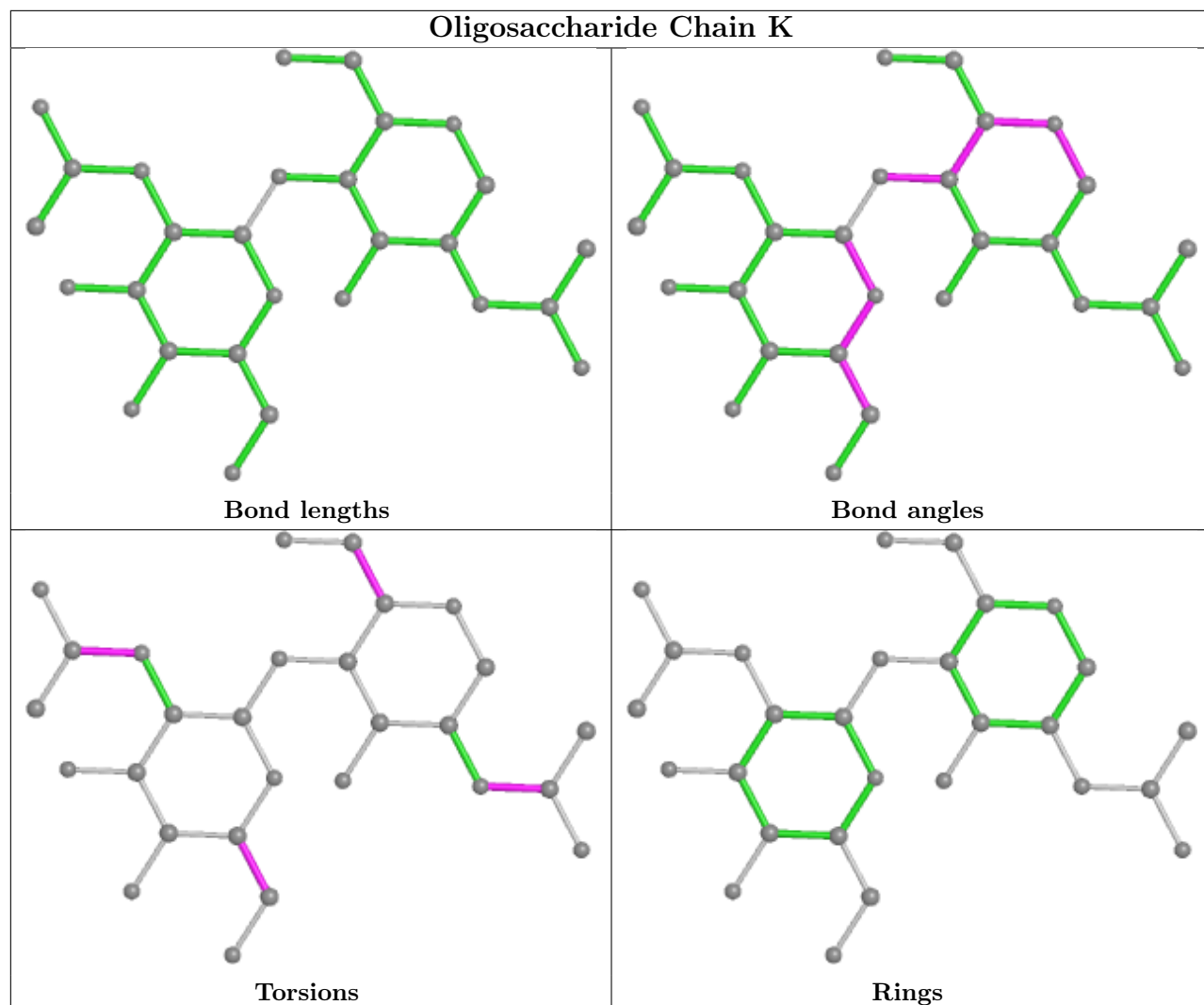




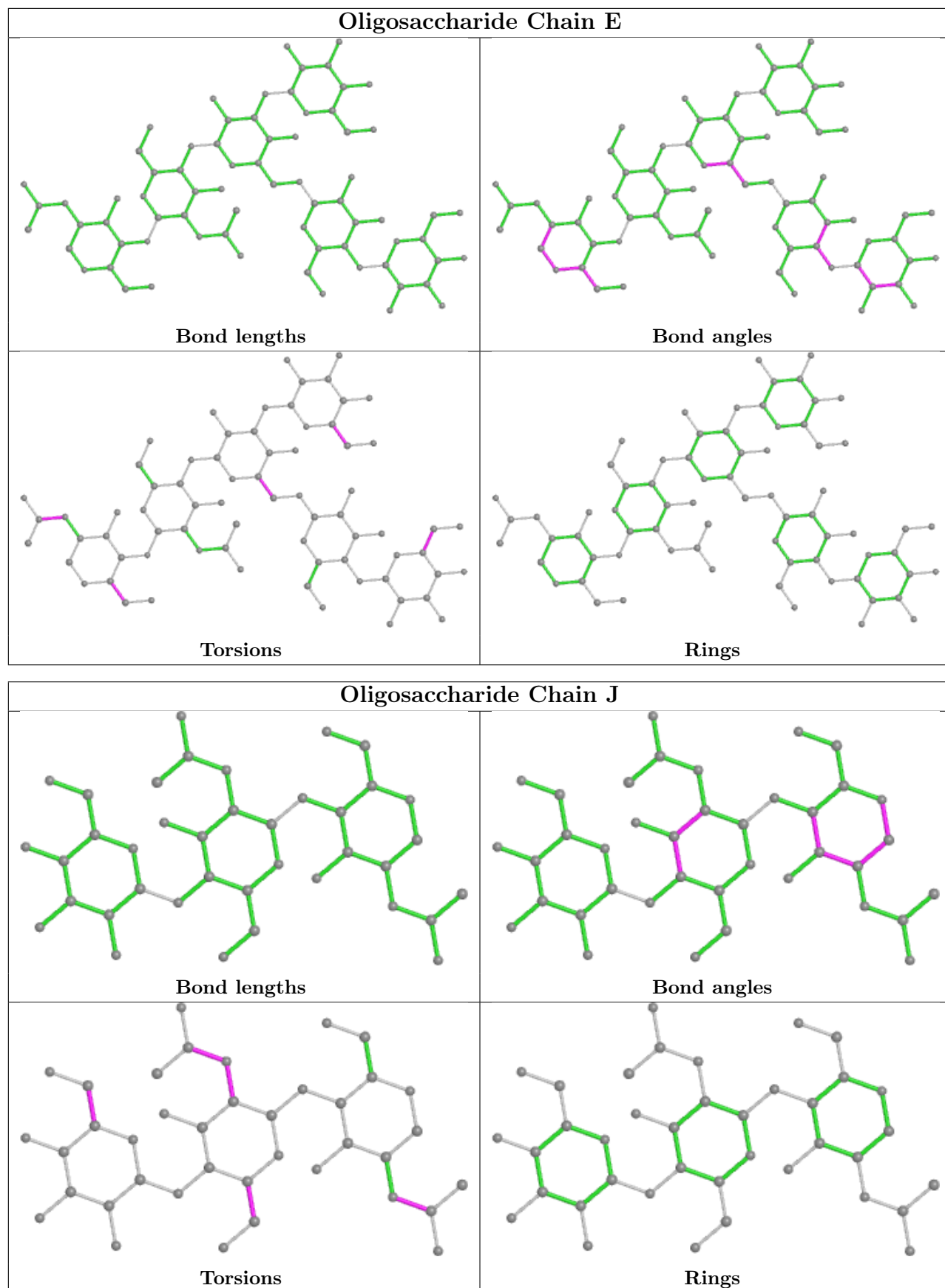


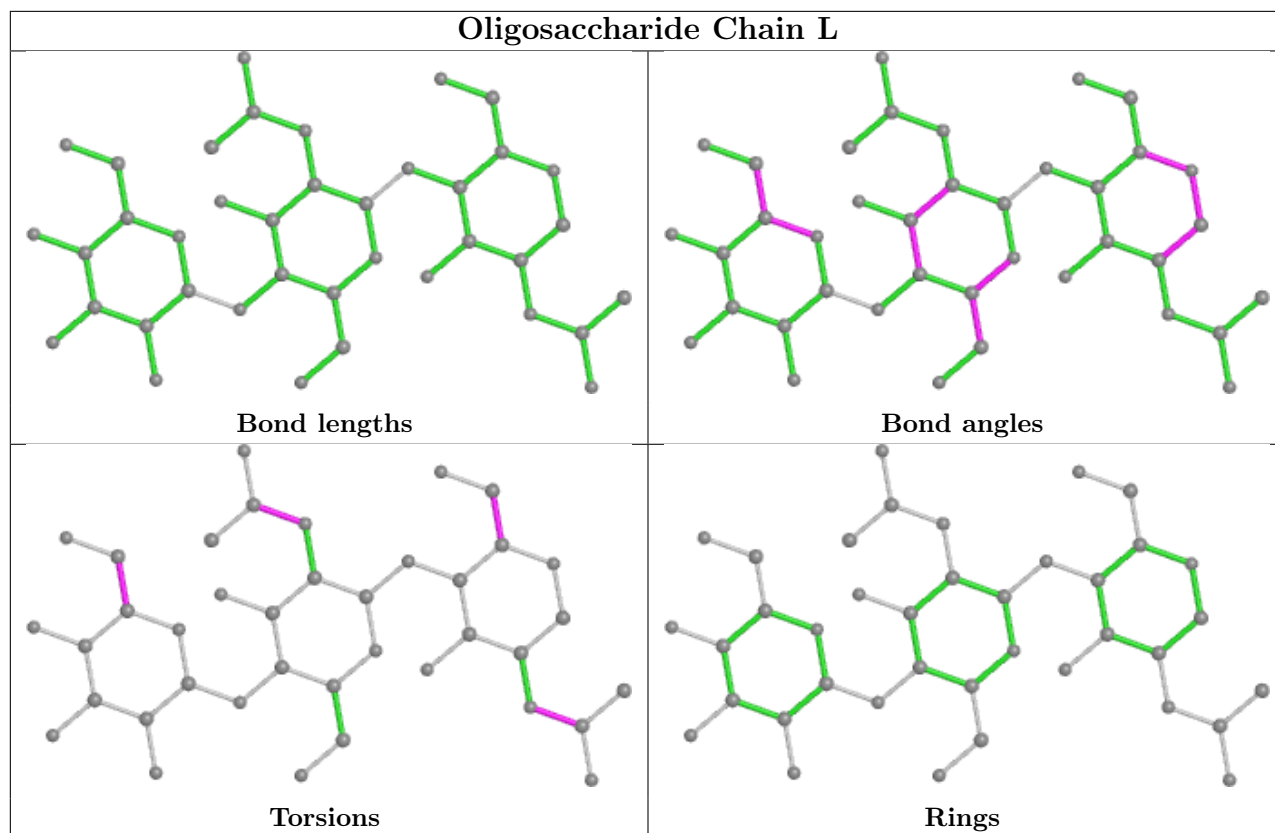












## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	B	3320	2	14,14,15	0.68	0	17,19,21	1.71	4 (23%)
7	NAG	A	2805	1	14,14,15	0.57	0	17,19,21	0.94	0
7	NAG	B	3452	2	14,14,15	0.62	0	17,19,21	0.84	1 (5%)
7	NAG	B	3099	2	14,14,15	0.49	0	17,19,21	1.33	2 (11%)
7	NAG	A	2524	1	14,14,15	0.44	0	17,19,21	1.02	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	3320	2	-	4/6/23/26	0/1/1/1
7	NAG	A	2805	1	-	2/6/23/26	0/1/1/1
7	NAG	B	3452	2	-	4/6/23/26	0/1/1/1
7	NAG	B	3099	2	-	4/6/23/26	0/1/1/1
7	NAG	A	2524	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	3320	NAG	C4-C3-C2	4.26	117.25	111.02
7	B	3320	NAG	O5-C5-C6	3.77	113.11	107.20
7	B	3099	NAG	C1-O5-C5	3.74	117.26	112.19
7	A	2524	NAG	C1-O5-C5	2.74	115.91	112.19
7	B	3452	NAG	C1-O5-C5	2.54	115.64	112.19

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2524	NAG	C8-C7-N2-C2
7	A	2524	NAG	O7-C7-N2-C2
7	B	3099	NAG	C8-C7-N2-C2
7	B	3099	NAG	O7-C7-N2-C2
7	B	3320	NAG	C8-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	3320	NAG	3	0
7	B	3452	NAG	1	0
7	B	3099	NAG	1	0

## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	938/967 (97%)	0.60	62 (6%) 18 14	42, 51, 60, 123	0
2	B	695/695 (100%)	0.66	63 (9%) 9 6	44, 51, 61, 94	0
All	All	1633/1662 (98%)	0.62	125 (7%) 13 10	42, 51, 60, 123	0

The worst 5 of 125 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	868	ASP	14.4
1	A	965	TRP	9.1
1	A	967	ILE	7.8
1	A	963	PRO	7.6
2	B	693	ILE	7.6

### 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
4	NAG	H	2	14/15	0.63	0.34	110,111,111,111	0
3	MAN	C	4	11/12	0.74	0.30	104,105,105,105	0
6	BMA	J	3	11/12	0.76	0.40	105,106,106,107	0
4	NAG	G	2	14/15	0.79	0.35	91,93,93,94	0
4	NAG	K	1	14/15	0.80	0.20	71,76,78,80	0

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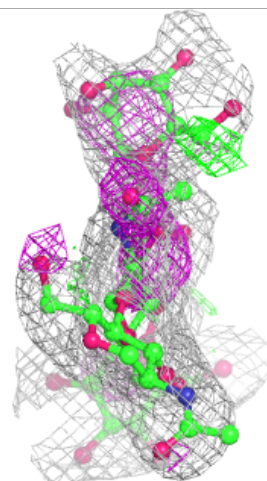
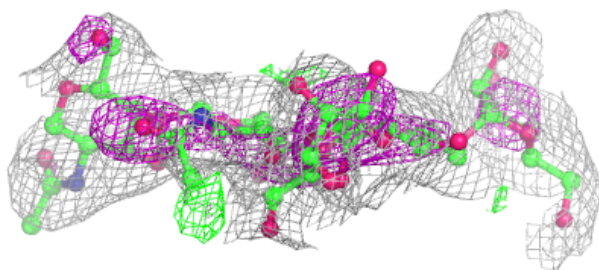
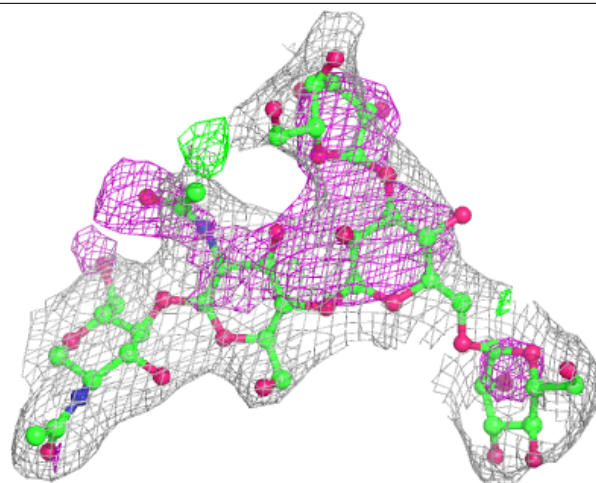
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	K	2	14/15	0.80	0.19	83,85,86,86	0
5	MAN	E	5	11/12	0.80	0.28	97,98,98,98	0
4	NAG	I	2	14/15	0.80	0.35	92,93,94,94	0
4	NAG	D	2	14/15	0.81	0.28	85,87,88,88	0
3	BMA	C	3	11/12	0.81	0.25	97,100,102,103	0
6	NAG	J	2	14/15	0.81	0.36	98,101,102,104	0
4	NAG	H	1	14/15	0.81	0.20	106,107,108,110	0
5	MAN	E	6	11/12	0.82	0.26	91,92,93,93	0
4	NAG	F	1	14/15	0.82	0.23	72,77,79,81	0
3	MAN	C	5	11/12	0.82	0.20	104,104,104,104	0
4	NAG	I	1	14/15	0.83	0.19	80,83,86,89	0
3	NAG	C	2	14/15	0.84	0.24	81,85,88,93	0
5	MAN	E	4	11/12	0.85	0.15	93,95,95,97	0
4	NAG	D	1	14/15	0.86	0.17	74,78,80,82	0
4	NAG	F	2	14/15	0.86	0.29	84,86,86,86	0
4	NAG	G	1	14/15	0.90	0.19	79,84,86,89	0
6	NAG	L	2	14/15	0.90	0.17	82,84,86,87	0
6	BMA	L	3	11/12	0.90	0.10	88,90,90,90	0
6	NAG	J	1	14/15	0.91	0.21	85,89,91,95	0
5	BMA	E	3	11/12	0.93	0.11	83,87,89,91	0
6	NAG	L	1	14/15	0.93	0.15	69,73,75,78	0
5	NAG	E	1	14/15	0.94	0.13	58,59,62,65	0
3	NAG	C	1	14/15	0.95	0.15	61,64,69,75	0
5	NAG	E	2	14/15	0.95	0.13	65,69,74,79	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.

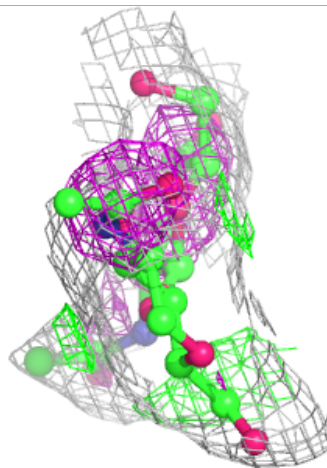
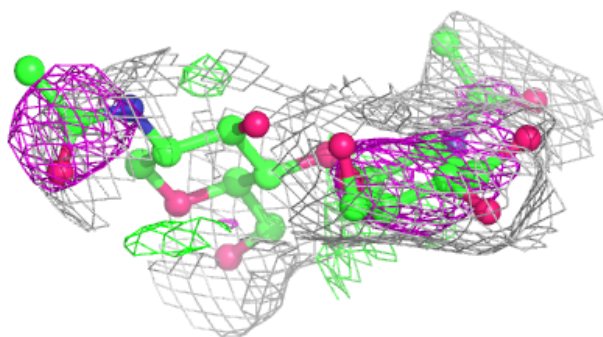
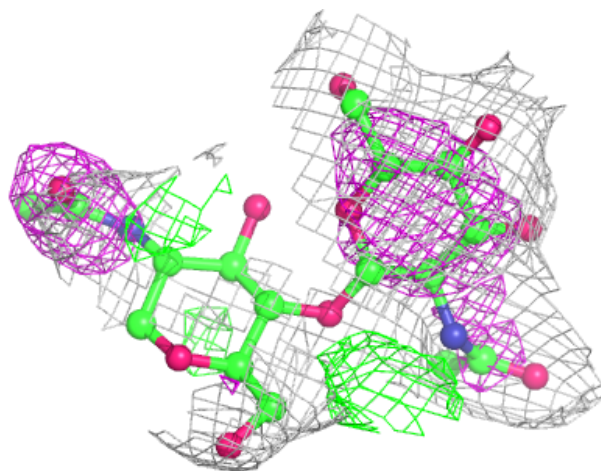
**Electron density around Chain C:**

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



**Electron density around Chain D:**

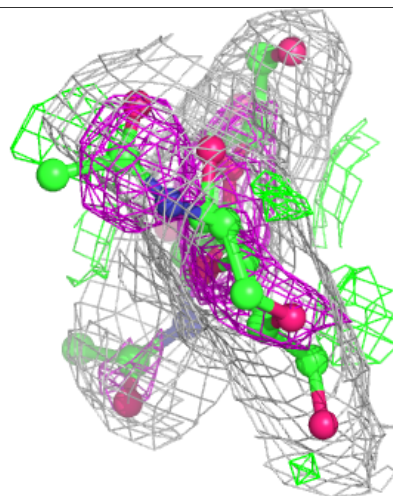
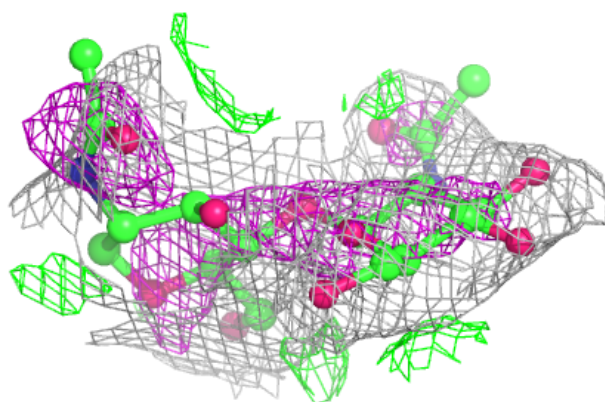
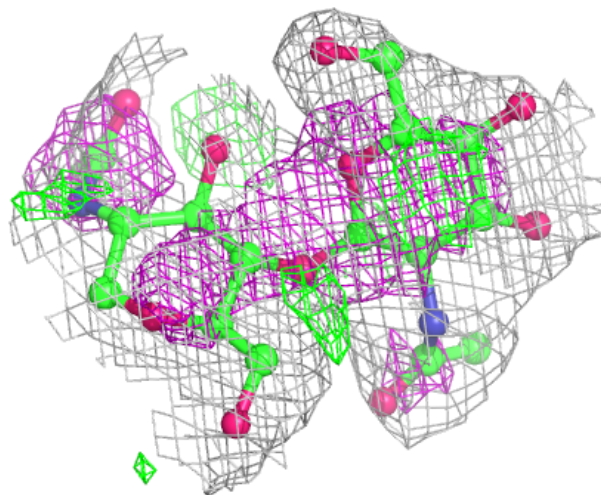
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





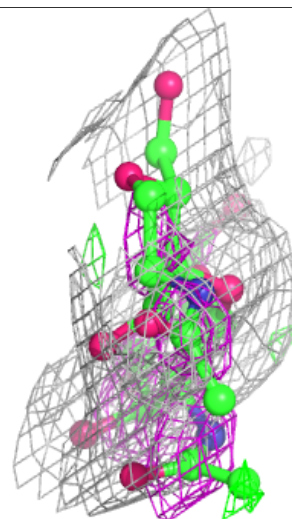
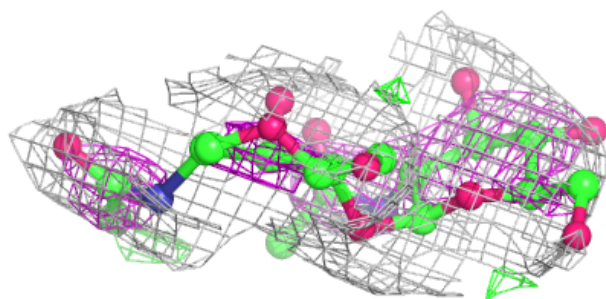
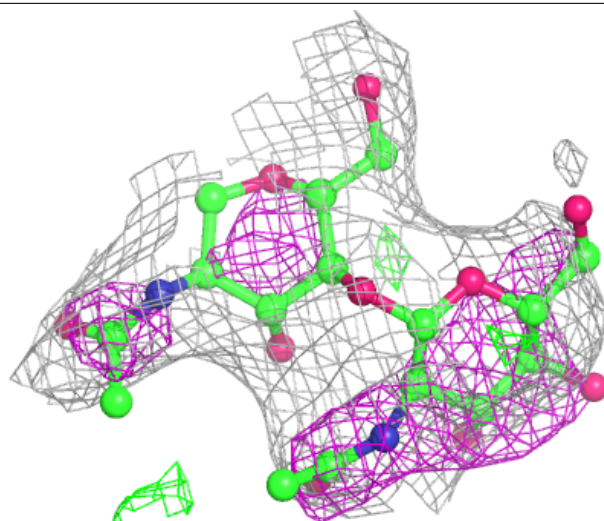
**Electron density around Chain F:**

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



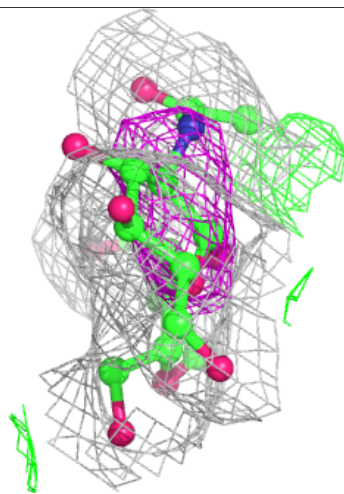
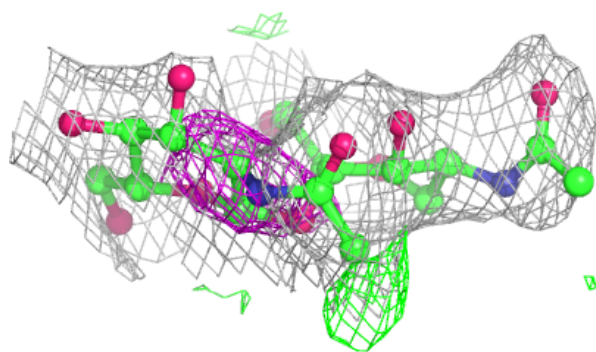
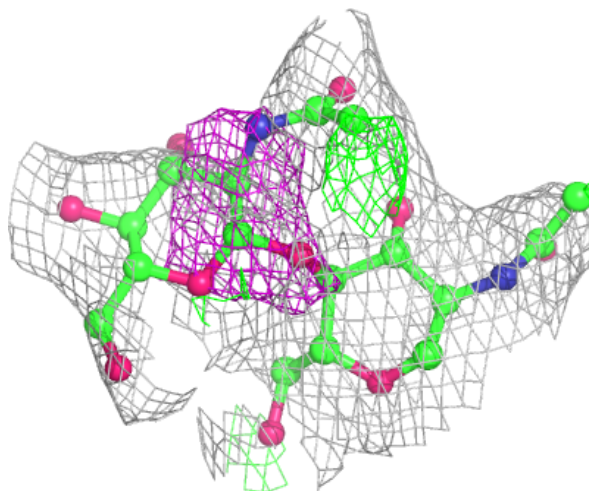
**Electron density around Chain G:**

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



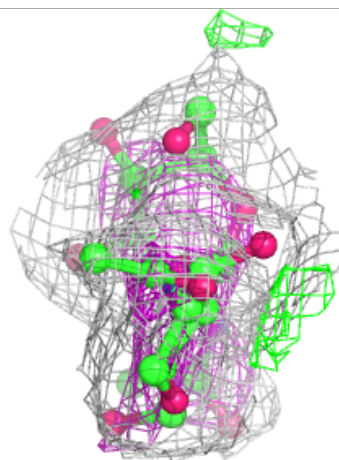
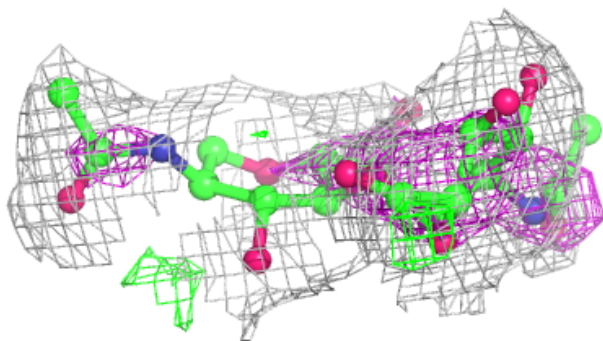
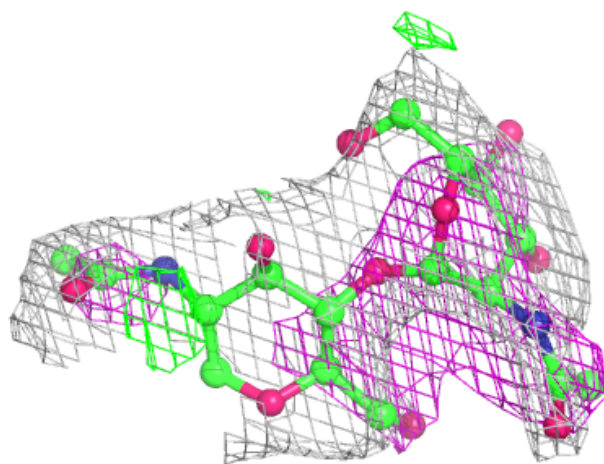
**Electron density around Chain H:**

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



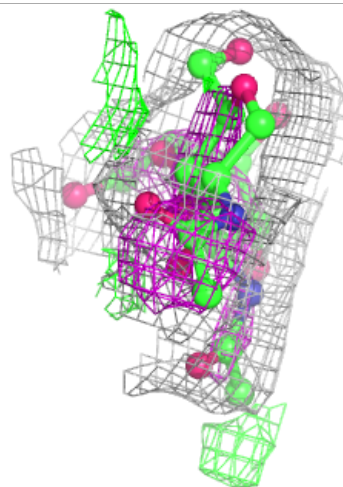
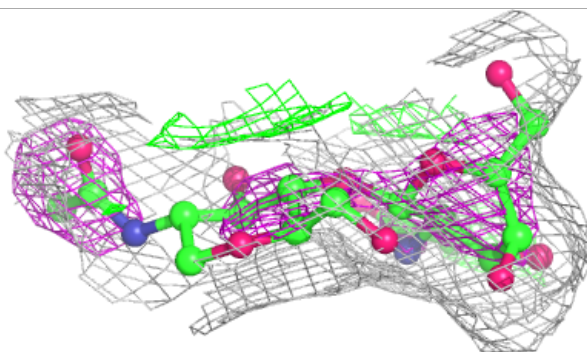
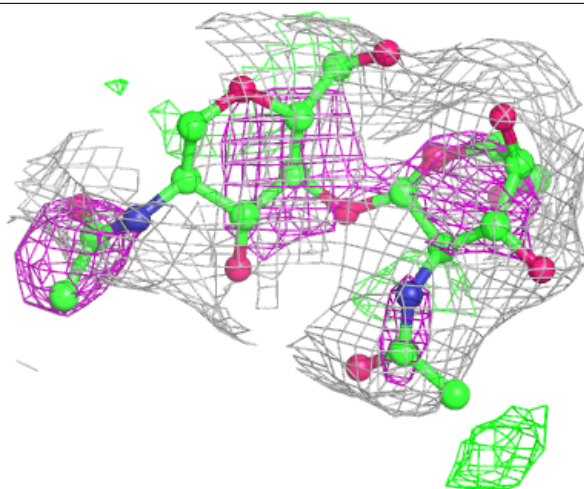
**Electron density around Chain I:**

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



**Electron density around Chain K:**

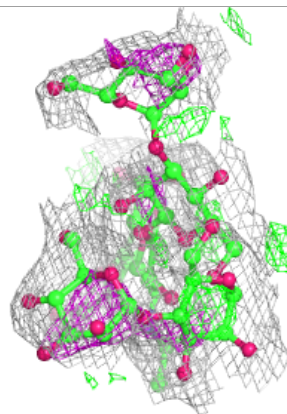
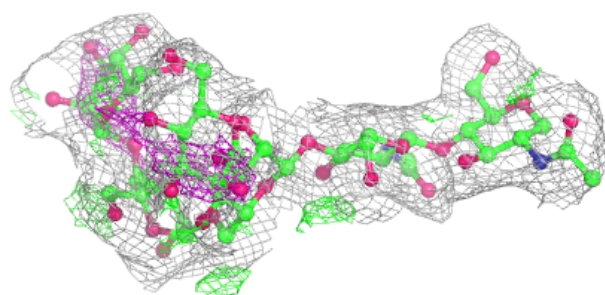
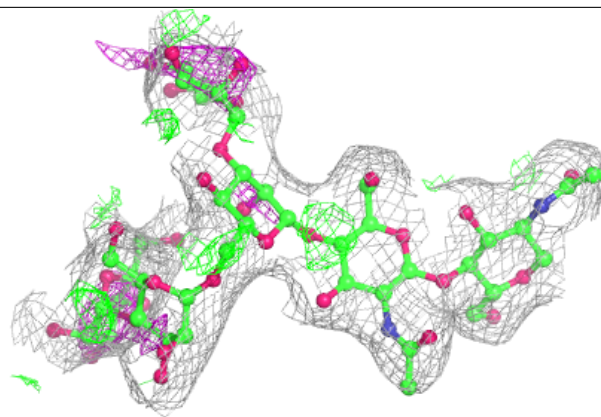
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



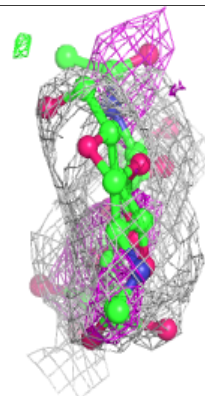
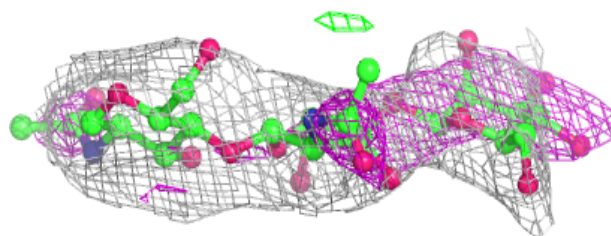
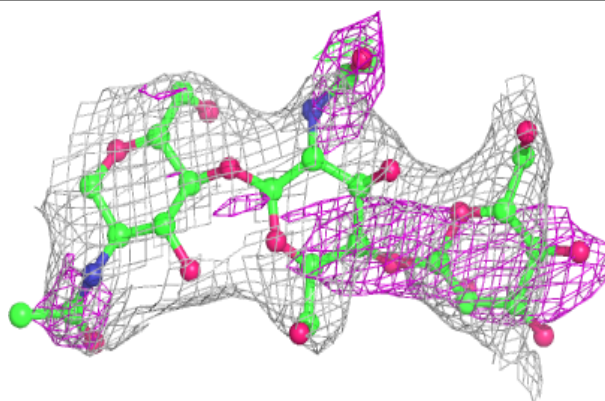


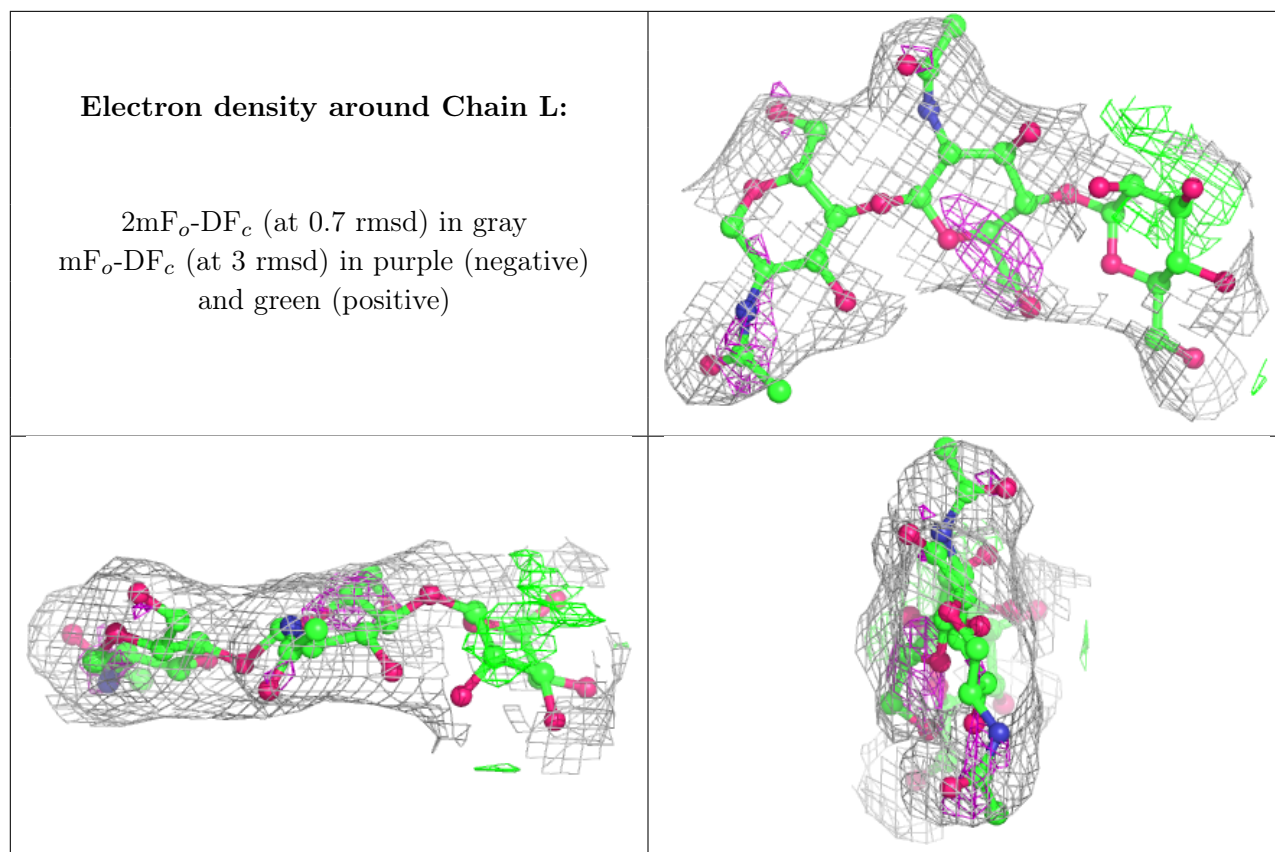
**Electron density around Chain E:**

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

**Electron density around Chain J:**

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





## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	B	3452	14/15	0.58	0.35	86,90,91,91	0
7	NAG	A	2524	14/15	0.66	0.30	81,86,87,87	0
7	NAG	A	2805	14/15	0.72	0.34	74,79,79,80	0
7	NAG	B	3320	14/15	0.73	0.22	68,71,72,73	0
7	NAG	B	3099	14/15	0.78	0.37	74,79,80,81	0
8	CA	B	4002	1/1	0.91	0.17	55,55,55,55	0
8	CA	A	4005	1/1	0.92	0.21	46,46,46,46	0
8	CA	A	4004	1/1	0.92	0.16	78,78,78,78	0
8	CA	A	4007	1/1	0.93	0.26	34,34,34,34	0
8	CA	A	4008	1/1	0.94	0.22	32,32,32,32	0
8	CA	A	4006	1/1	0.96	0.28	59,59,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.