



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 11:44 PM BST

PDB ID : 4WJK  
Title : Metal Ion and Ligand Binding of Integrin  
Authors : Xia, W.; Springer, T.A.  
Deposited on : 2014-09-30  
Resolution : 1.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

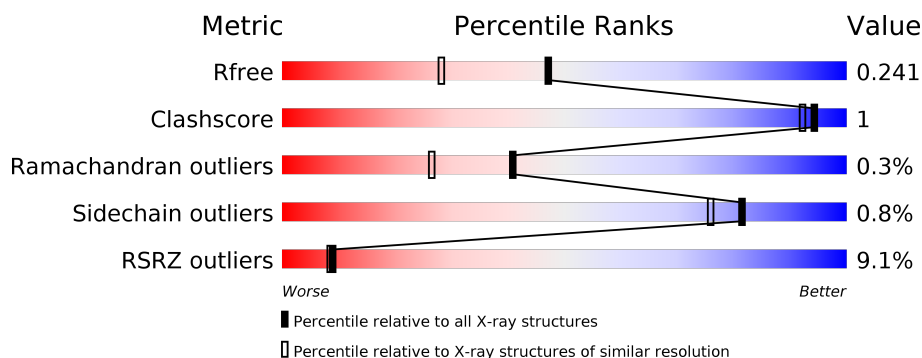
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	452	<div> <div>6%</div> <div>97%</div> <div>.</div> </div>
2	B	445	<div> <div>12%</div> <div>91%</div> <div>5%</div> <div>.</div> </div>
3	C	6	<div> <div>50%</div> <div>33%</div> <div>17%</div> </div>
4	D	3	<div> <div>67%</div> <div>33%</div> </div>
5	E	7	<div> <div>43%</div> <div>57%</div> </div>
6	F	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
6	G	2	 100%
6	H	2	 50% 50%
7	I	4	 75% 25%

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
6	NAG	H	2	-	-	-	X
8	CA	A	503	-	-	-	X

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 14350 atoms, of which 6729 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-5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	452	Total	C	H	N	O	S	0	1	0
			6615	2167	3207	559	674	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	451	VAL	ILE	engineered mutation	UNP P08648

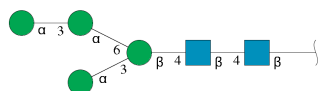
- Molecule 2 is a protein called Integrin beta-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	424	Total	C	H	N	O	S	0	1	0
			6512	2069	3208	558	652	25			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	195	THR	SER	conflict	UNP P05556

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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.



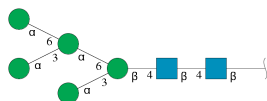
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	6	Total	C	H	N	O	0	0	0
			136	40	64	2	30			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	3	Total	C	H	N	O	0	0	0
			75	22	36	2	15			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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.



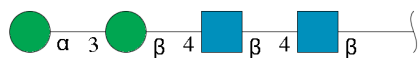
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	7	Total	C	H	N	O	0	0	0
			157	46	74	2	35			

- Molecule 6 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
6	F	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
6	G	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			
6	H	2	Total	C	H	N	O	0	0	0
			55	16	27	2	10			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	4	Total	C	H	N	O	0	0	0
			95	28	45	2	20			

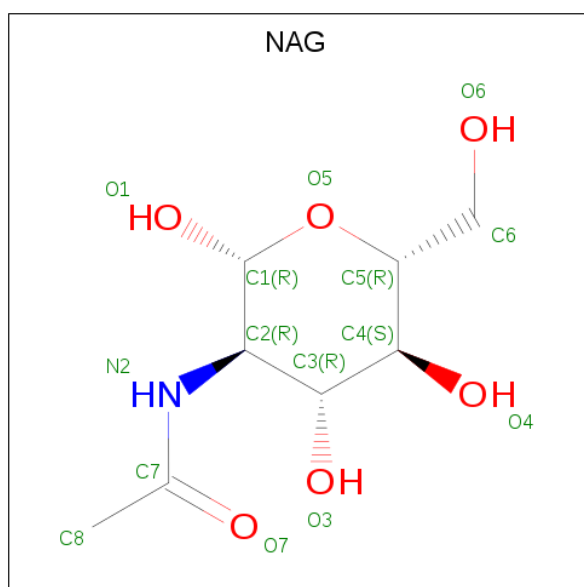
- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Ca	0	0
			2	2		
8	A	4	Total	Ca	0	0
			4	4		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Mg	0	0
			1	1		

- Molecule 10 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
10	B	1	Total	C	H	N	O	0	0
			28	8	14	1	5		

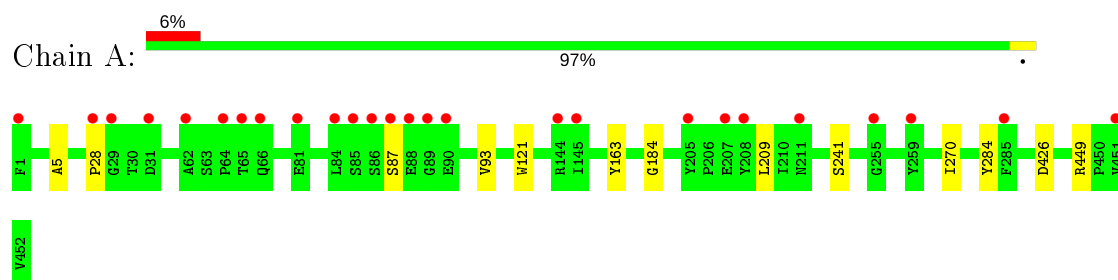
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	337	Total	O	0	0
			337	337		
11	B	223	Total	O	0	0
			223	223		

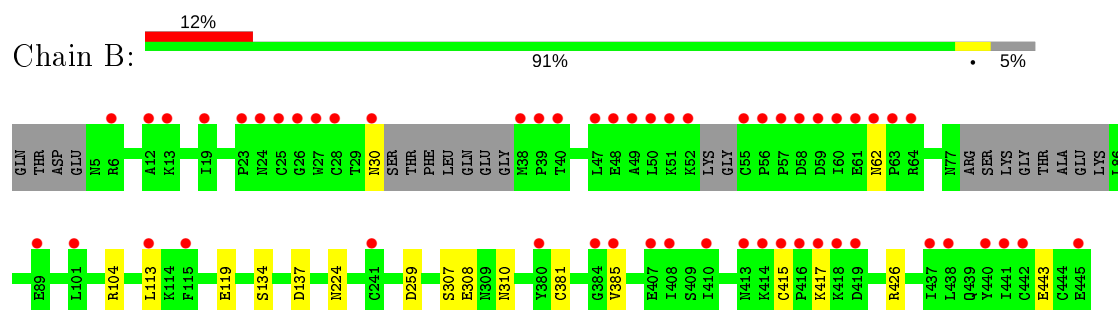
### 3 Residue-property plots

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

- Molecule 1: Integrin alpha-5



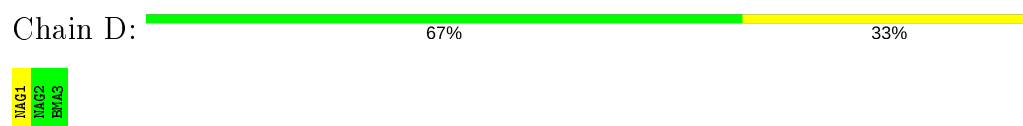
- Molecule 2: Integrin beta-1



- Molecule 3: alpha-D-mannopyranose-(1-3)-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



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





- Molecule 5:  $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-6)] $\alpha$ -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:  43% 57%

MAG1  
MAG2  
BNA3  
MAN4  
MAN5  
MAN6  
MAN7

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

Chain F:  50% 50%

MAG1  
MAG2

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

Chain G:  100%

MAG1  
MAG2

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

Chain H:  50% 50%

MAG1  
MAG2

- Molecule 7:  $\alpha$ -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 I:  75% 25%

MAG1  
MAG2  
BNA3  
MAN4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.13Å 116.75Å 159.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.10 – 1.85 47.10 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.10-1.85) 98.4 (47.10-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 1.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1760)	Depositor
R, $R_{free}$	0.191 , 0.238 0.197 , 0.241	Depositor DCC
$R_{free}$ test set	1998 reflections (2.42%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.9	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14350	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BMA, CA, NAG, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.35	0/3507	0.53	0/4785
2	B	0.33	0/3362	0.51	0/4539
All	All	0.34	0/6869	0.52	0/9324

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3408	3207	3208	7	0
2	B	3304	3208	3252	9	0
3	C	72	64	61	1	0
4	D	39	36	34	0	0
5	E	83	74	70	0	0
6	F	28	27	25	1	0
6	G	28	27	25	0	0
6	H	28	27	25	0	0
7	I	50	45	43	1	0
8	A	4	0	0	0	0
8	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	1	0	0	0	0
10	B	14	14	13	0	0
11	A	337	0	0	4	1
11	B	223	0	0	3	2
All	All	7621	6729	6756	18	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 1.

All (18) 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)
2:B:62:ASN:OD1	2:B:104:ARG:NH2	2.26	0.69
2:B:307:SER:O	2:B:426:ARG:NH2	2.26	0.68
11:B:601:HOH:O	7:I:4:MAN:O2	2.15	0.64
2:B:308:GLU:OE1	11:B:602:HOH:O	2.17	0.58
1:A:449:ARG:NH1	11:A:603:HOH:O	2.34	0.57
2:B:310:ASN:OD1	2:B:426:ARG:NH1	2.40	0.55
11:A:881:HOH:O	3:C:5:MAN:O4	2.20	0.49
2:B:443:GLU:N	2:B:443:GLU:OE1	2.45	0.49
2:B:119:GLU:O	11:B:603:HOH:O	2.20	0.48
1:A:93:VAL:HG11	1:A:209:LEU:HD11	1.97	0.47
2:B:381:CYS:HB2	2:B:385:VAL:HG13	2.00	0.43
1:A:163:TYR:O	1:A:184:GLY:HA3	2.19	0.43
1:A:28:PRO:O	11:A:776:HOH:O	2.22	0.42
1:A:5:ALA:N	11:A:867:HOH:O	2.52	0.41
1:A:426:ASP:OD1	1:A:426:ASP:N	2.52	0.41
1:A:241:SER:HB2	6:F:1:NAG:H82	2.03	0.41
2:B:137:ASP:N	2:B:137:ASP:OD1	2.54	0.40
2:B:134:SER:OG	2:B:259:ASP:OD2	2.32	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:B:601:HOH:O	11:B:610:HOH:O[1_455]	2.15	0.05
11:A:622:HOH:O	11:B:618:HOH:O[1_655]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	451/452 (100%)	432 (96%)	17 (4%)	2 (0%)	34	19
2	B	417/445 (94%)	401 (96%)	15 (4%)	1 (0%)	47	33
All	All	868/897 (97%)	833 (96%)	32 (4%)	3 (0%)	41	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	SER
1	A	270	ILE
2	B	415	CYS

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	359/358 (100%)	357 (99%)	2 (1%)	86	83
2	B	379/395 (96%)	375 (99%)	4 (1%)	73	65
All	All	738/753 (98%)	732 (99%)	6 (1%)	81	76

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	TRP
1	A	284	TYR
2	B	30	ASN

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Mol	Chain	Res	Type
2	B	113	LEU
2	B	224	ASN
2	B	417	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	GLN
2	B	30	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

26 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	C	1	1,3	14,14,15	0.19	0	17,19,21	0.49	0
3	NAG	C	2	3	14,14,15	0.29	0	17,19,21	0.60	0
3	BMA	C	3	3	11,11,12	0.80	0	15,15,17	0.98	0
3	MAN	C	4	3	11,11,12	0.60	0	15,15,17	1.07	2 (13%)
3	MAN	C	5	3	11,11,12	0.76	0	15,15,17	1.02	2 (13%)
3	MAN	C	6	3	11,11,12	0.81	1 (9%)	15,15,17	0.82	1 (6%)
4	NAG	D	1	1,4	14,14,15	0.56	0	17,19,21	0.73	1 (5%)
4	NAG	D	2	4	14,14,15	0.28	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BMA	D	3	4	11,11,12	0.75	0	15,15,17	0.66	0
5	NAG	E	1	1,5	14,14,15	0.15	0	17,19,21	0.43	0
5	NAG	E	2	5	14,14,15	0.49	0	17,19,21	0.54	0
5	BMA	E	3	5	11,11,12	0.82	0	15,15,17	0.93	0
5	MAN	E	4	5	11,11,12	0.88	1 (9%)	15,15,17	1.04	1 (6%)
5	MAN	E	5	5	11,11,12	0.81	1 (9%)	15,15,17	0.96	2 (13%)
5	MAN	E	6	5	11,11,12	0.82	1 (9%)	15,15,17	0.97	1 (6%)
5	MAN	E	7	5	11,11,12	0.90	1 (9%)	15,15,17	0.91	0
6	NAG	F	1	1,6	14,14,15	0.45	0	17,19,21	0.57	0
6	NAG	F	2	6	14,14,15	0.26	0	17,19,21	0.52	0
6	NAG	G	1	2,6	14,14,15	0.26	0	17,19,21	0.42	0
6	NAG	G	2	6	14,14,15	0.24	0	17,19,21	0.46	0
6	NAG	H	1	2,6	14,14,15	0.58	1 (7%)	17,19,21	0.52	0
6	NAG	H	2	6	14,14,15	0.27	0	17,19,21	0.43	0
7	NAG	I	1	2,7	14,14,15	0.22	0	17,19,21	0.51	0
7	NAG	I	2	7	14,14,15	0.41	0	17,19,21	0.38	0
7	BMA	I	3	7	11,11,12	0.61	0	15,15,17	0.86	0
7	MAN	I	4	7	11,11,12	0.58	0	15,15,17	1.11	2 (13%)

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	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	0/2/19/22	0/1/1/1
3	MAN	C	6	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	0/6/23/26	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	-	0/2/19/22	0/1/1/1
5	MAN	E	7	5	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	F	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	NAG	G	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	1/6/23/26	0/1/1/1
6	NAG	H	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	H	2	6	-	1/6/23/26	0/1/1/1
7	NAG	I	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	I	2	7	-	0/6/23/26	0/1/1/1
7	BMA	I	3	7	-	0/2/19/22	0/1/1/1
7	MAN	I	4	7	-	1/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	6	MAN	O5-C1	-2.50	1.39	1.43
5	E	5	MAN	O5-C1	-2.19	1.40	1.43
5	E	4	MAN	O5-C1	-2.13	1.40	1.43
5	E	6	MAN	O5-C1	-2.09	1.40	1.43
5	E	7	MAN	O5-C1	-2.06	1.40	1.43
6	H	1	NAG	O5-C1	-2.01	1.40	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	4	MAN	C1-O5-C5	2.84	116.04	112.19
3	C	4	MAN	C1-O5-C5	2.76	115.94	112.19
3	C	5	MAN	C1-O5-C5	2.54	115.63	112.19
4	D	1	NAG	C1-O5-C5	2.45	115.51	112.19
5	E	6	MAN	O2-C2-C3	-2.37	105.40	110.14
7	I	4	MAN	O2-C2-C3	-2.26	105.61	110.14
5	E	5	MAN	C1-O5-C5	2.18	115.14	112.19
3	C	5	MAN	O2-C2-C3	-2.15	105.84	110.14
3	C	4	MAN	O2-C2-C3	-2.13	105.87	110.14
3	C	6	MAN	O2-C2-C3	-2.06	106.02	110.14
5	E	4	MAN	O2-C2-C3	-2.01	106.10	110.14
5	E	5	MAN	O2-C2-C3	-2.00	106.12	110.14

There are no chirality outliers.

All (16) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
6	F	2	NAG	C4-C5-C6-O6
5	E	5	MAN	O5-C5-C6-O6
6	F	2	NAG	O5-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6
7	I	1	NAG	C8-C7-N2-C2
7	I	1	NAG	O7-C7-N2-C2
5	E	5	MAN	C4-C5-C6-O6
5	E	3	BMA	C4-C5-C6-O6
6	H	2	NAG	O5-C5-C6-O6
6	G	2	NAG	O5-C5-C6-O6
7	I	4	MAN	O5-C5-C6-O6
6	H	1	NAG	C4-C5-C6-O6
4	D	1	NAG	C3-C2-N2-C7
4	D	1	NAG	C1-C2-N2-C7
6	H	1	NAG	O5-C5-C6-O6
5	E	7	MAN	C4-C5-C6-O6

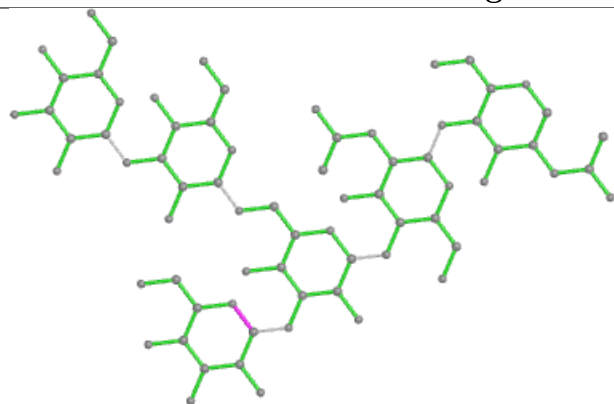
There are no ring outliers.

3 monomers are involved in 3 short contacts:

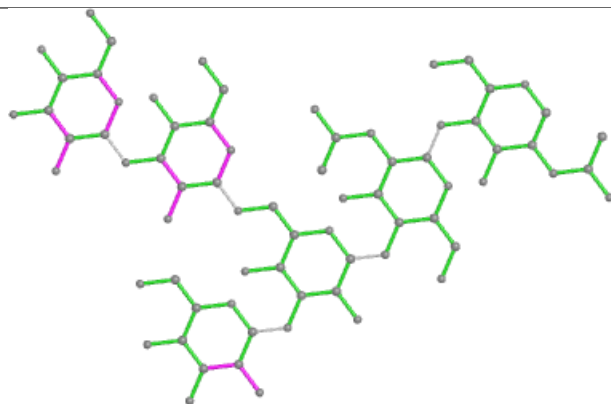
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1	NAG	1	0
7	I	4	MAN	1	0
3	C	5	MAN	1	0

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

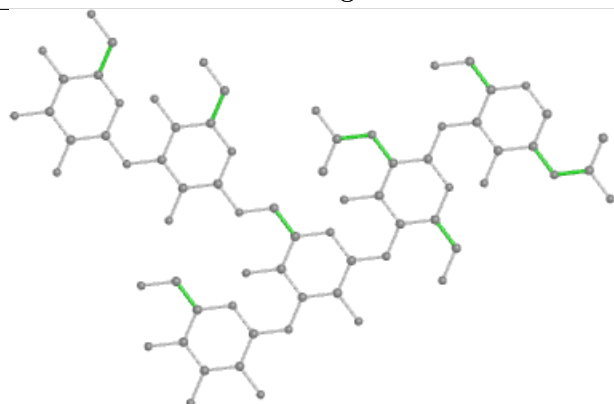
## Oligosaccharide Chain C



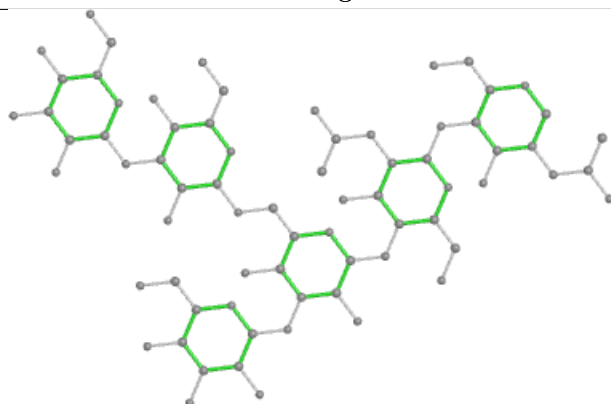
Bond lengths



Bond angles

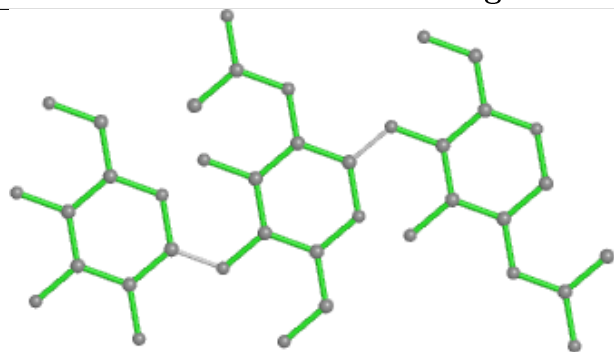


Torsions

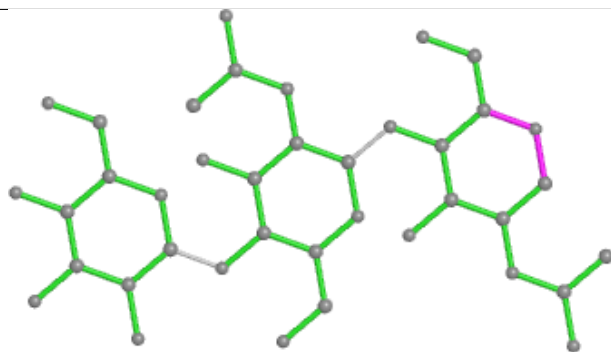


Rings

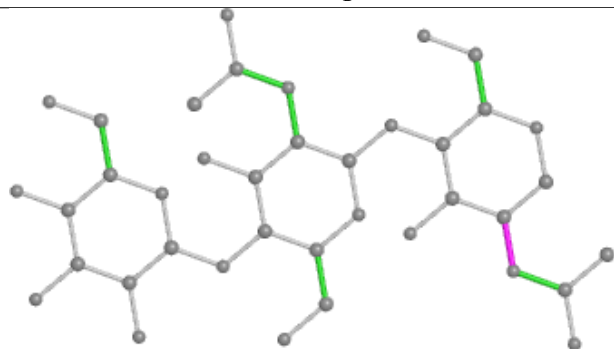
## Oligosaccharide Chain D



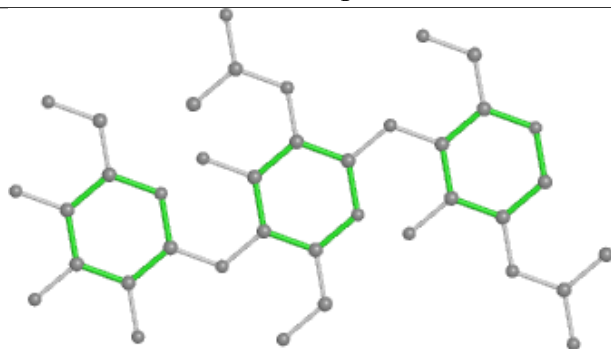
Bond lengths



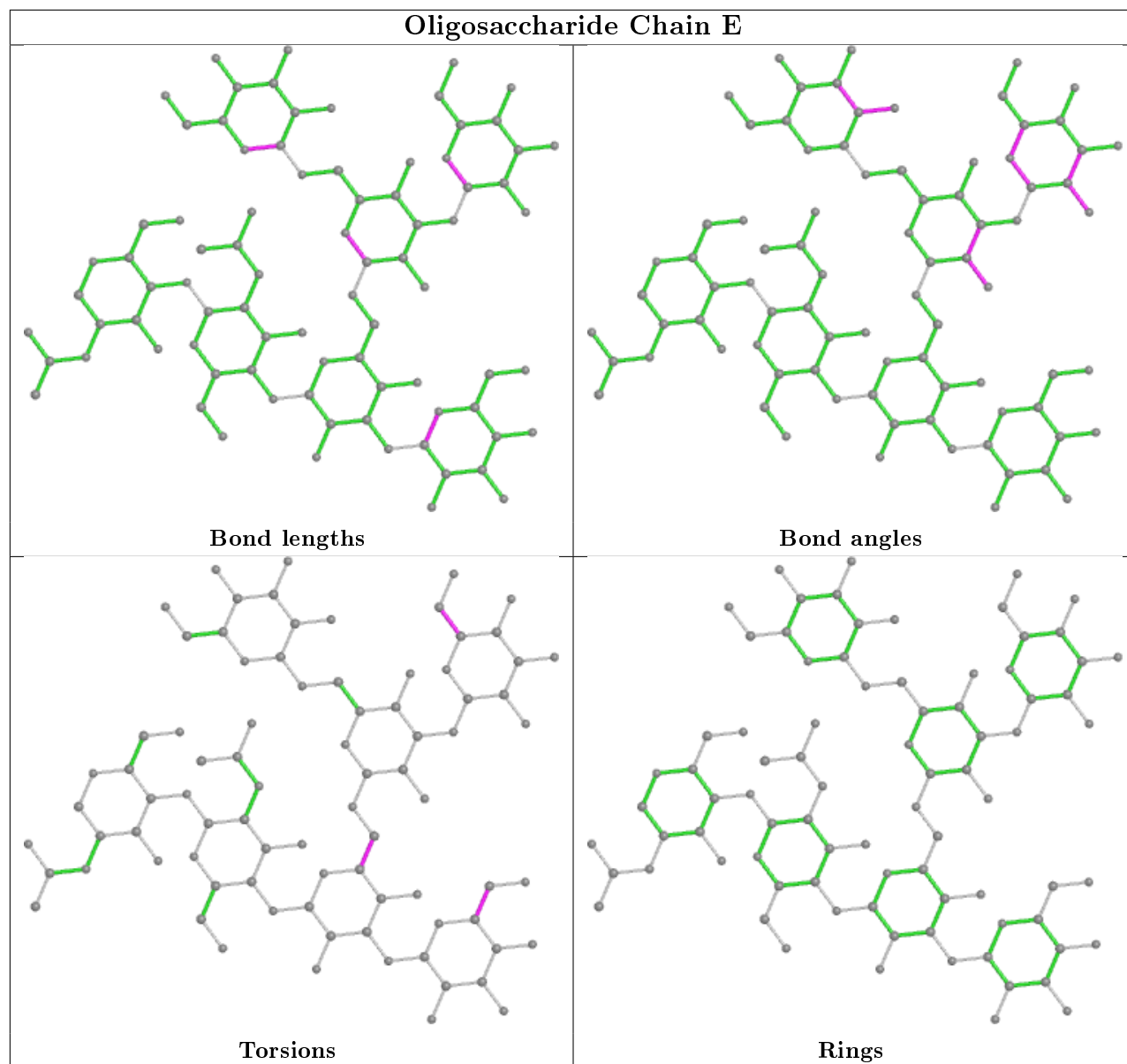
Bond angles

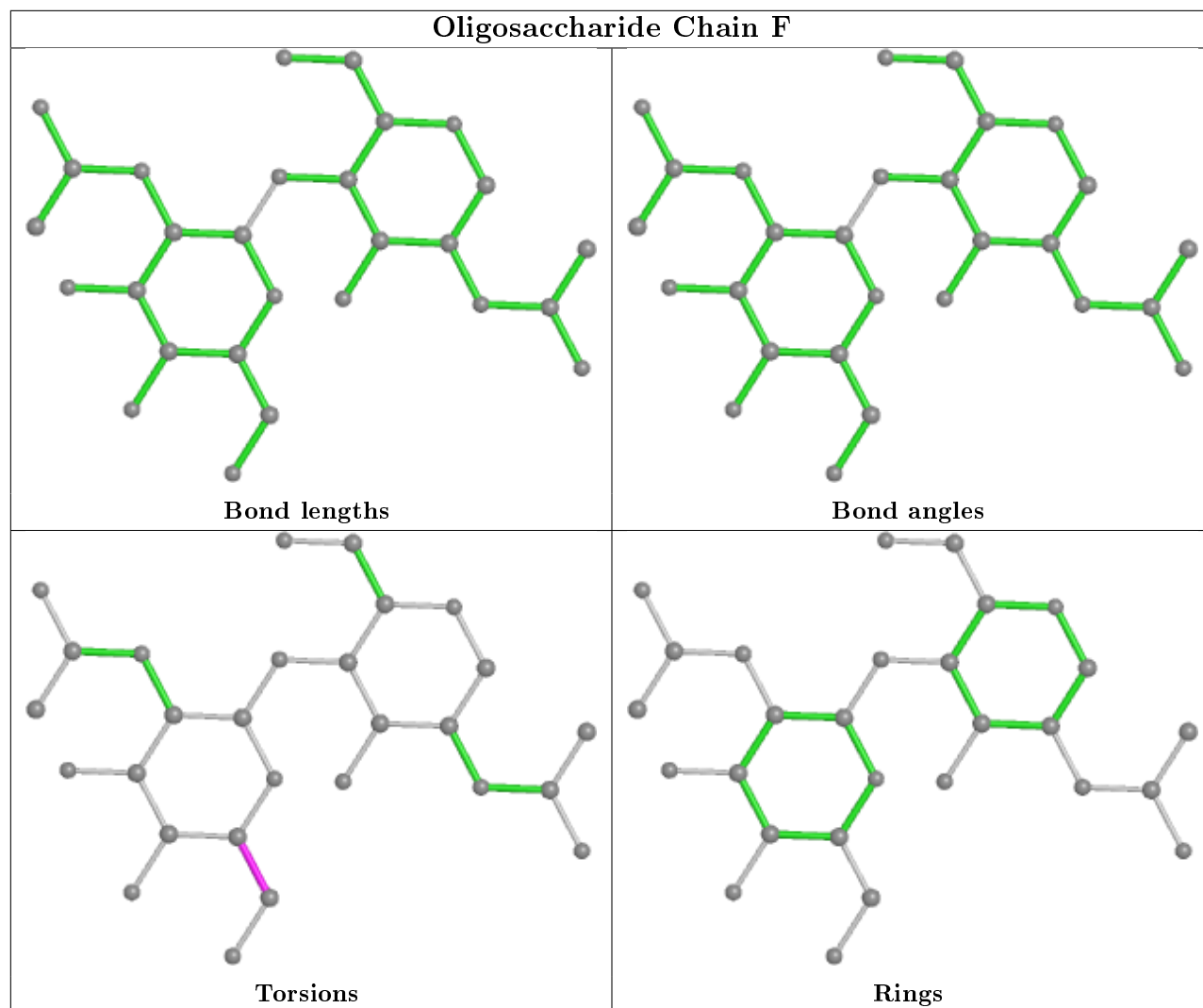


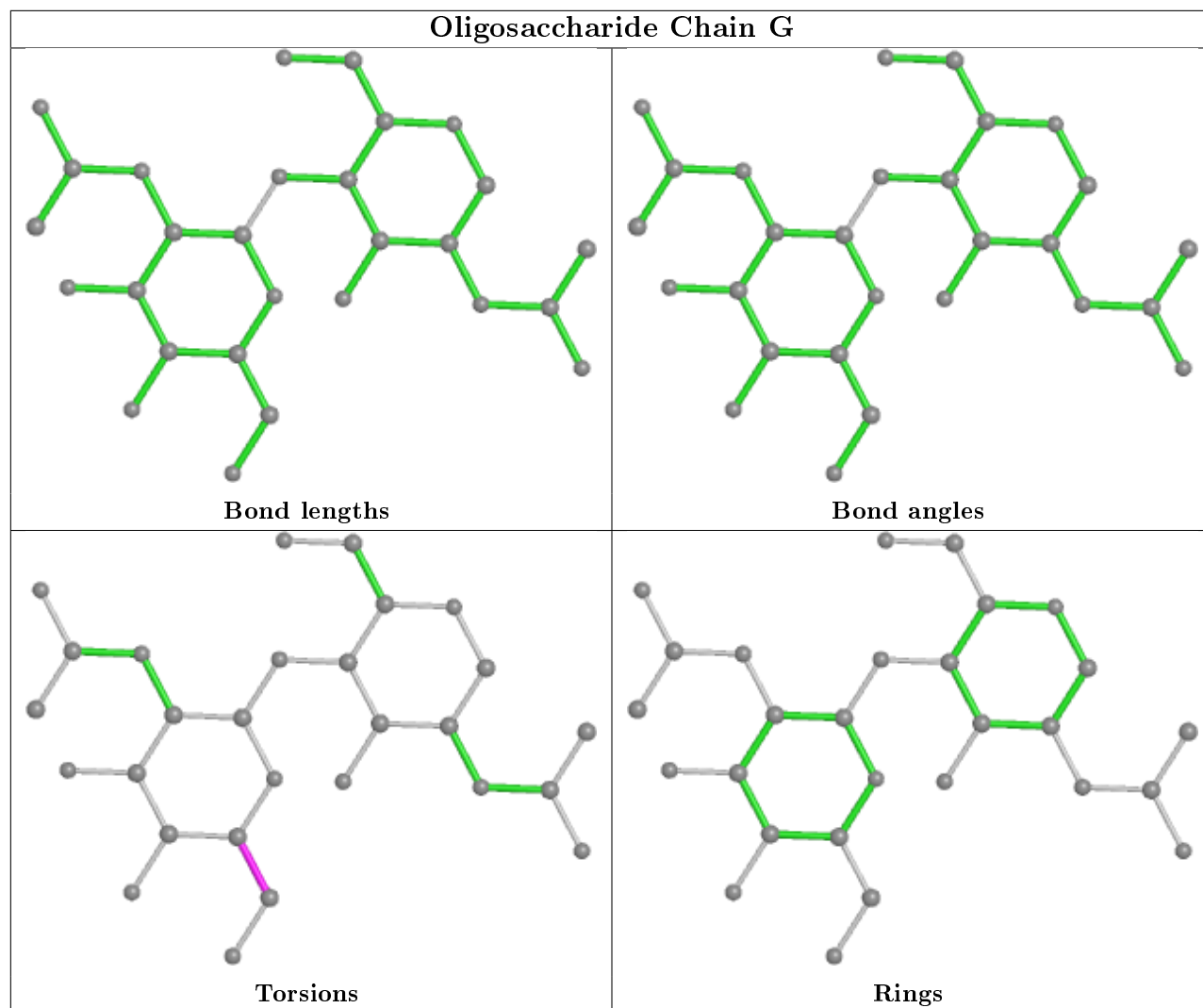
Torsions

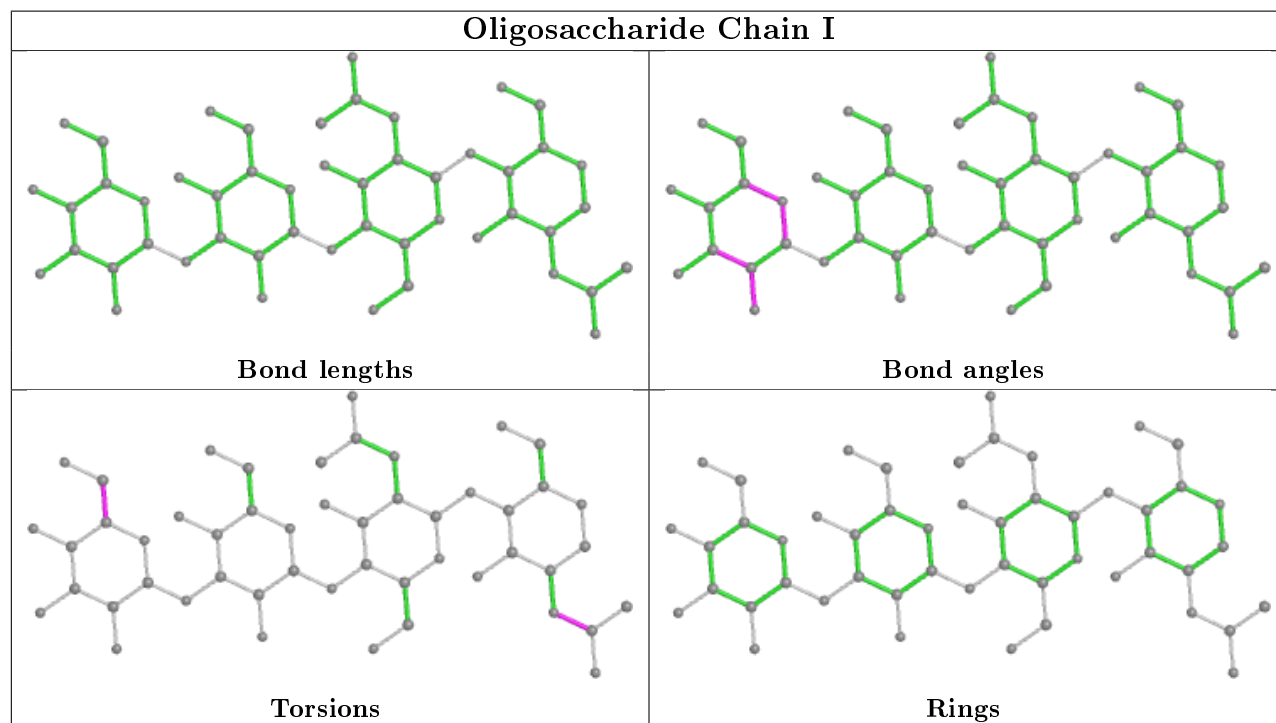
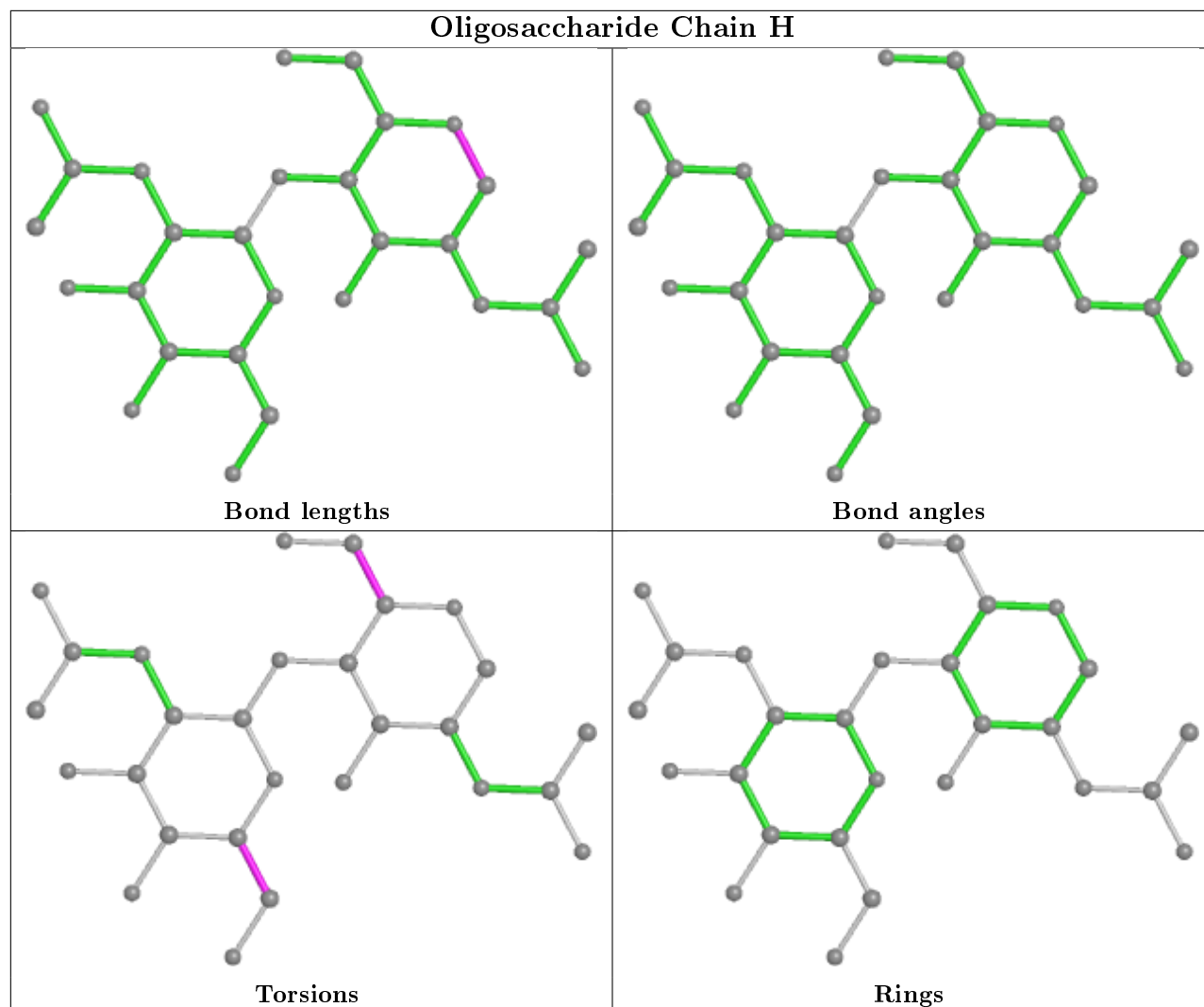


Rings









## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 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	$\# Z  > 2$
10	NAG	B	512	2	14,14,15	1.02	1 (7%)	17,19,21	0.65	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	B	512	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	512	NAG	O5-C1	-3.63	1.37	1.43

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	452/452 (100%)	0.27	26 (5%) 23 22	23, 40, 97, 180	0
2	B	424/445 (95%)	0.63	54 (12%) 3 3	21, 49, 129, 183	0
All	All	876/897 (97%)	0.45	80 (9%) 9 8	21, 42, 117, 183	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	47	LEU	7.6
2	B	417	LYS	7.2
2	B	50	LEU	7.0
2	B	416	PRO	6.4
2	B	51	LYS	6.3
2	B	48	GLU	5.8
2	B	57	PRO	5.7
2	B	445	GLU	5.4
1	A	88	GLU	5.4
2	B	415	CYS	5.4
1	A	62	ALA	5.2
1	A	29	GLY	5.1
2	B	418	LYS	5.1
1	A	84	LEU	5.0
2	B	56	PRO	4.9
2	B	414	LYS	4.7
1	A	89	GLY	4.6
2	B	89	GLU	4.6
1	A	207	GLU	4.3
2	B	52	LYS	4.3
2	B	60	ILE	4.2
1	A	31	ASP	4.1
2	B	12	ALA	4.1
2	B	19	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	6	ARG	4.0
1	A	65	THR	4.0
2	B	49	ALA	3.8
2	B	419	ASP	3.8
1	A	451	VAL	3.8
1	A	86	SER	3.7
1	A	208	TYR	3.6
1	A	87	SER	3.5
2	B	241	CYS	3.4
2	B	101	LEU	3.3
2	B	38	MET	3.2
2	B	380	TYR	3.2
2	B	410	ILE	3.2
2	B	40	THR	3.2
1	A	28	PRO	3.1
2	B	55	CYS	3.1
2	B	385	VAL	3.0
2	B	58	ASP	3.0
2	B	24	ASN	3.0
2	B	442	CYS	2.9
1	A	85	SER	2.8
2	B	59	ASP	2.8
2	B	27	TRP	2.8
2	B	438	LEU	2.8
2	B	413	ASN	2.8
2	B	63	PRO	2.7
1	A	81	GLU	2.7
2	B	113	LEU	2.7
1	A	90	GLU	2.7
1	A	144	ARG	2.6
2	B	26	GLY	2.6
2	B	115	PHE	2.5
1	A	205	TYR	2.5
1	A	64	PRO	2.4
2	B	62	ASN	2.4
1	A	66	GLN	2.4
1	A	211	ASN	2.3
2	B	407	GLU	2.3
2	B	384	GLY	2.3
2	B	437	ILE	2.3
2	B	440	TYR	2.3
1	A	1	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	259	TYR	2.2
1	A	255	GLY	2.2
2	B	64	ARG	2.2
2	B	30	ASN	2.2
2	B	39	PRO	2.2
2	B	28	CYS	2.2
2	B	441	ILE	2.1
2	B	13	LYS	2.1
2	B	61	GLU	2.1
2	B	23	PRO	2.1
1	A	285	PHE	2.1
1	A	145	ILE	2.0
2	B	25	CYS	2.0
2	B	408	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

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

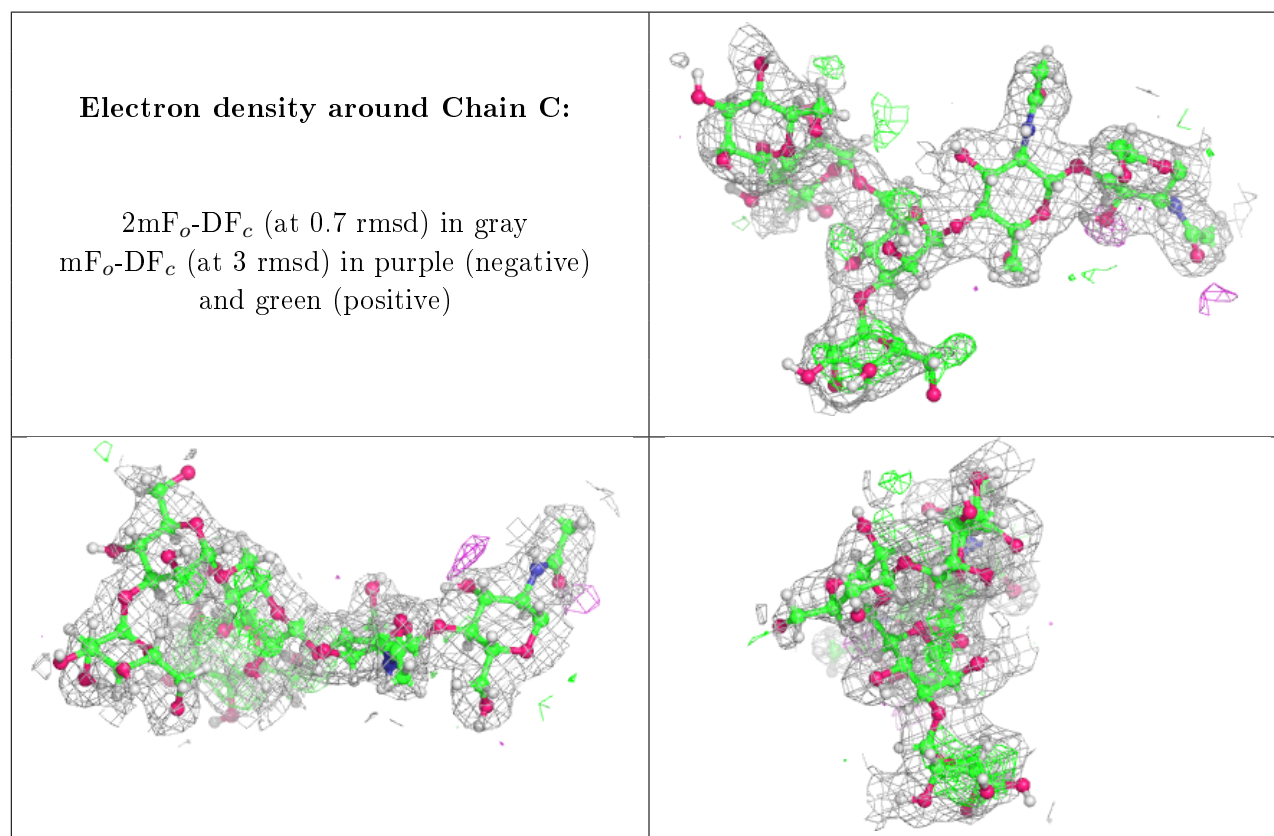
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	G	2	14/15	0.65	0.20	112,135,169,176	0
5	MAN	E	6	11/12	0.69	0.27	99,114,134,139	0
7	MAN	I	4	11/12	0.73	0.20	110,126,142,153	0
6	NAG	H	2	14/15	0.76	0.44	131,168,198,199	0
3	MAN	C	4	11/12	0.80	0.16	122,141,167,184	0
3	MAN	C	5	11/12	0.80	0.14	71,100,121,132	0
4	BMA	D	3	11/12	0.81	0.25	80,98,120,129	0
7	BMA	I	3	11/12	0.82	0.13	79,107,132,133	0
6	NAG	F	2	14/15	0.82	0.19	65,126,157,182	0
5	MAN	E	5	11/12	0.86	0.13	101,132,158,172	0
5	MAN	E	4	11/12	0.87	0.11	77,92,119,121	0
3	MAN	C	6	11/12	0.89	0.33	125,223,321,332	0
6	NAG	G	1	14/15	0.89	0.10	51,90,122,129	0
6	NAG	H	1	14/15	0.90	0.20	73,96,123,141	0

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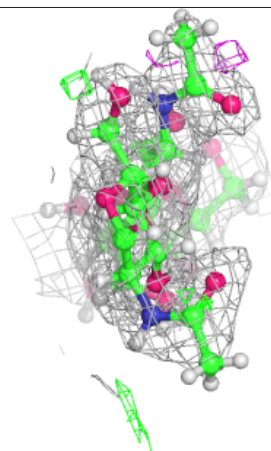
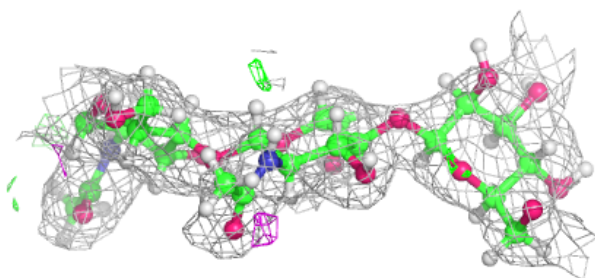
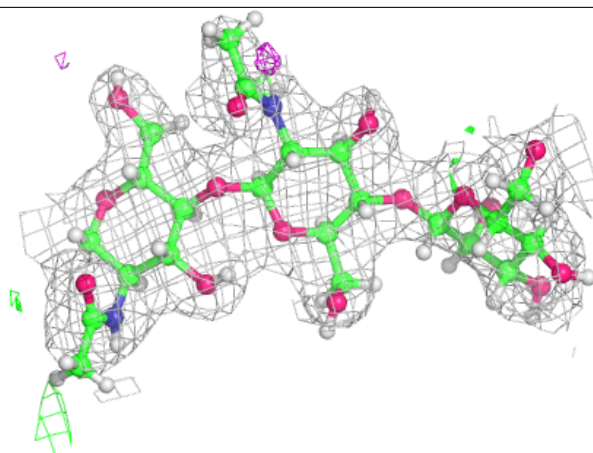
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BMA	C	3	11/12	0.91	0.09	45,74,103,103	0
7	NAG	I	1	14/15	0.91	0.14	58,83,102,107	0
5	MAN	E	7	11/12	0.92	0.10	51,68,94,94	0
7	NAG	I	2	14/15	0.92	0.15	80,106,133,133	0
5	NAG	E	2	14/15	0.92	0.09	39,68,84,101	0
4	NAG	D	2	14/15	0.93	0.15	36,57,80,94	0
6	NAG	F	1	14/15	0.94	0.13	29,60,91,104	0
5	BMA	E	3	11/12	0.94	0.10	41,63,103,103	0
3	NAG	C	2	14/15	0.95	0.10	27,48,82,107	0
5	NAG	E	1	14/15	0.96	0.08	33,45,55,55	0
3	NAG	C	1	14/15	0.96	0.10	27,37,45,52	0
4	NAG	D	1	14/15	0.97	0.18	28,40,58,58	0

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



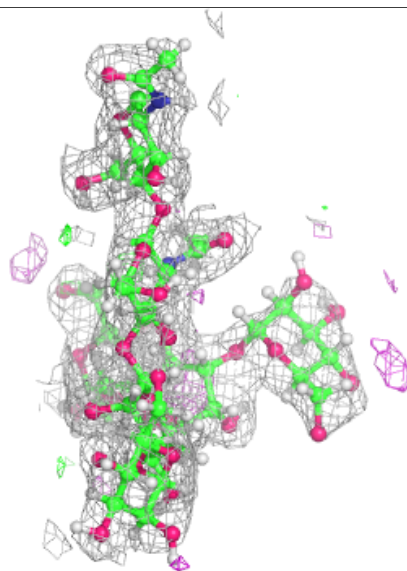
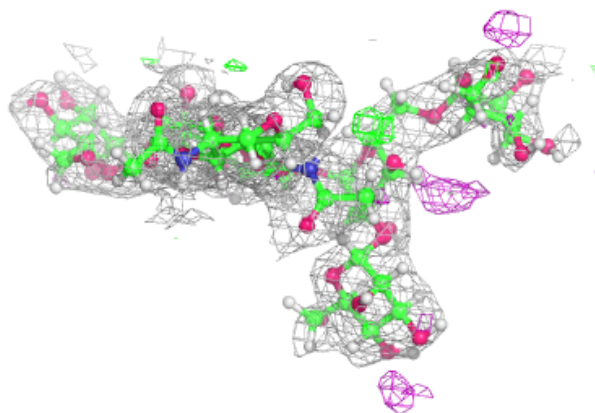
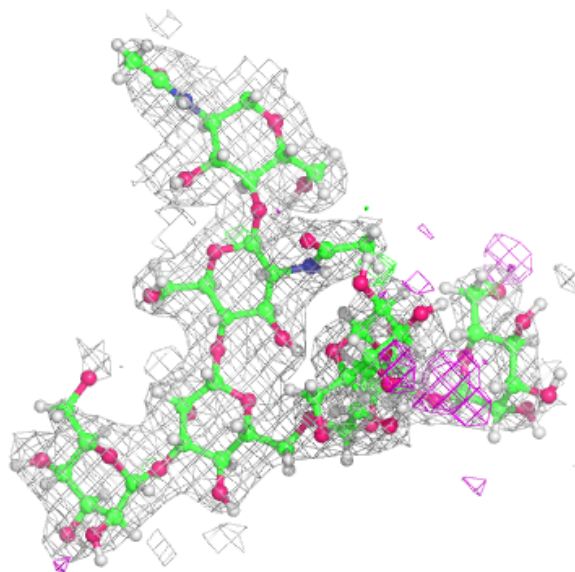
**Electron density around Chain D:**

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



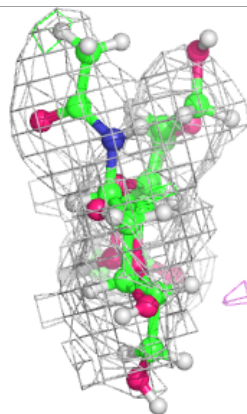
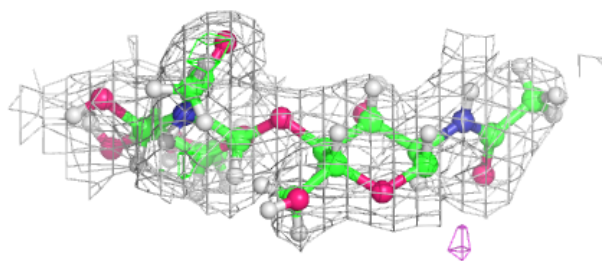
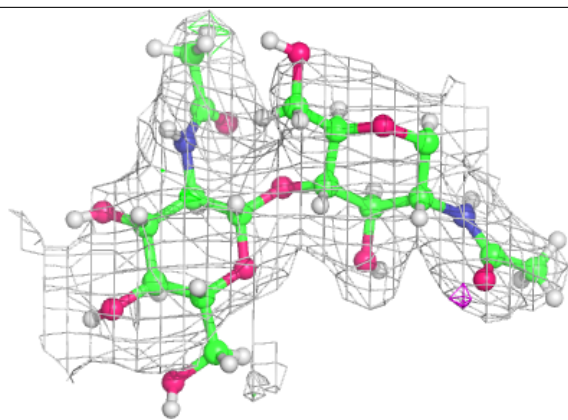
**Electron density around Chain E:**

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



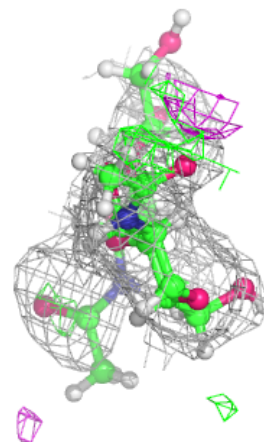
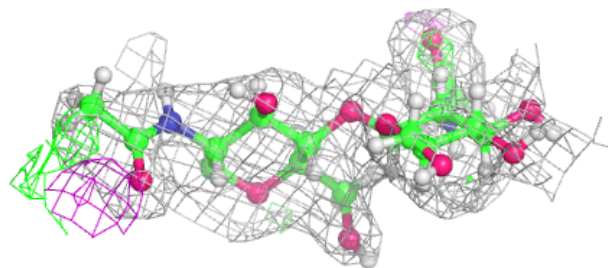
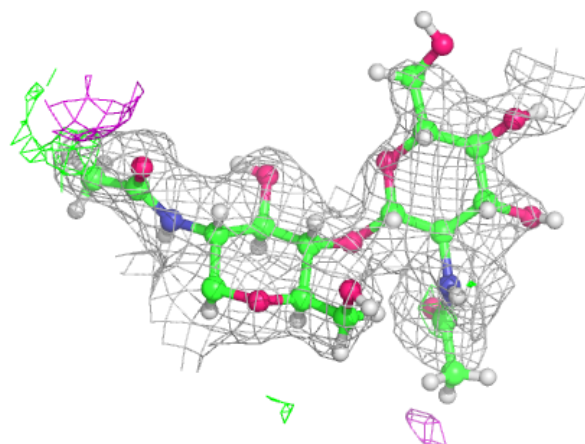
**Electron density around Chain F:**

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



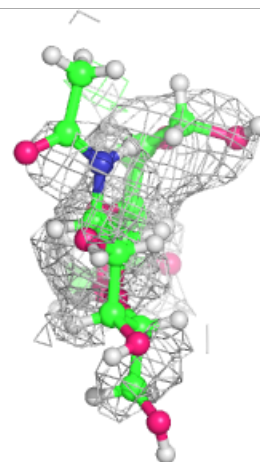
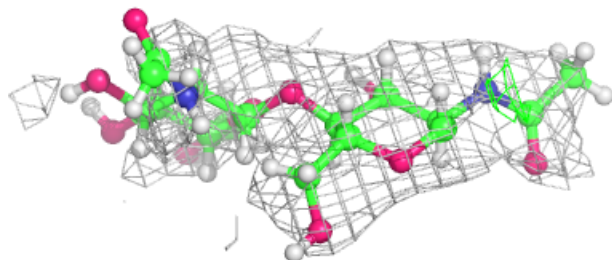
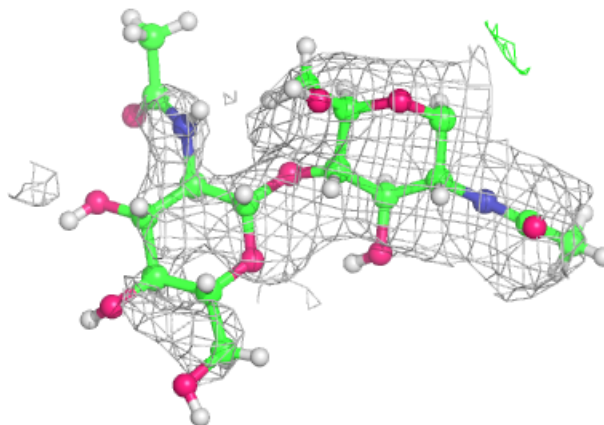
**Electron density around Chain G:**

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

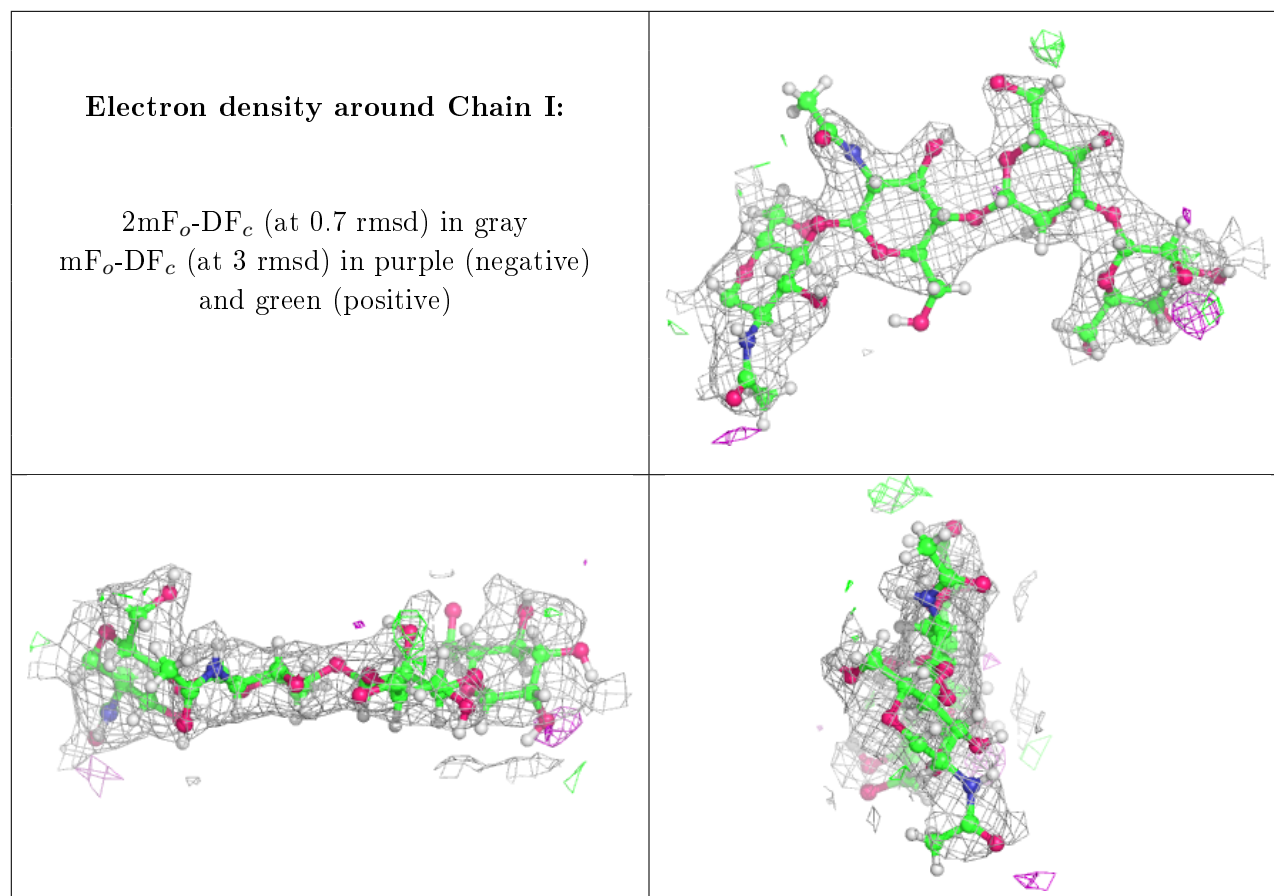


**Electron density around Chain H:**

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







## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	CA	A	503	1/1	0.54	0.60	143,143,143,143	0
10	NAG	B	512	14/15	0.74	0.20	79,115,161,161	0
9	MG	B	501	1/1	0.91	0.25	47,47,47,47	0
8	CA	A	504	1/1	0.96	0.04	42,42,42,42	0
8	CA	A	501	1/1	0.97	0.13	48,48,48,48	0
8	CA	A	502	1/1	0.99	0.04	30,30,30,30	0
8	CA	B	502	1/1	0.99	0.04	40,40,40,40	0
8	CA	B	503	1/1	0.99	0.12	26,26,26,26	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.