



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 06:04 pm GMT

PDB ID : 6FAT  
Title : The crystal structure of a feruloyl esterase C from *Fusarium oxysporum*.  
Authors : Dimarogona, M.; Chrysina, E.D.  
Deposited on : 2017-12-17  
Resolution : 2.30 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.

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 : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

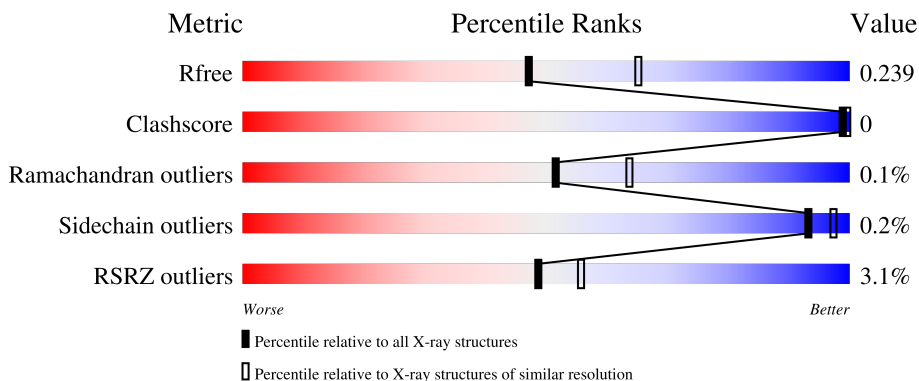
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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.





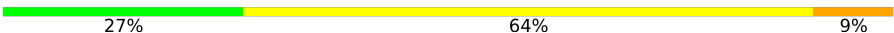
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	528	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 95%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4%      95%      . .</p>
1	B	528	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 95%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2%      95%      . .</p>
2	C	3	<div style="display: flex; align-items: center;"> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> </div> <p style="text-align: center;">67%      33%</p>
2	D	3	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 10px; background-color: green; margin-right: 5px;"></div> </div> <p style="text-align: center;">100%</p>
3	E	5	<div style="display: flex; align-items: center;"> <div style="width: 80%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">80%      20%</p>

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Mol	Chain	Length	Quality of chain
4	F	2	 50% 50%
5	G	7	 43% 57%
6	H	11	 27% 64% 9%

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 8677 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 Carboxylic ester hydrolase.

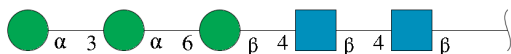
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	508	Total 3955	C 2501	N 686	O 748	S 20	0	0	0
1	B	508	Total 3958	C 2503	N 686	O 749	S 20	0	1	0

- Molecule 2 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			
2	C	3	Total 39	C 22	N 2	O 15	0	0	0
2	D	3	Total 39	C 22	N 2	O 15	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.



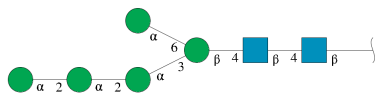
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	5	Total 61	C 34	N 2	O 25	0	0	0

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



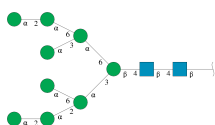
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	F	2	28	16	2	10	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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			
5	G	7	83	46	2	35	0	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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			
6	H	11	127	70	2	55	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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

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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	160	Total	O	0	0
			160	160		
9	B	197	Total	O	0	0
			197	197		



MAG1  
MAG2  
BMA3  
MAN4  
MAN5

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

Chain F:  50% 50%

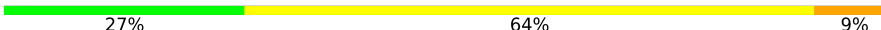
MAG1  
MAG2

- Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-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 G:  43% 57%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7

- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]-[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 H:  27% 64% 9%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9  
MAN10  
MAN11



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.54Å 87.47Å 106.56Å 90.00° 106.18° 90.00°	Depositor
Resolution (Å)	102.35 – 2.30 64.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.2 (102.35-2.30) 98.2 (64.86-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.207 , 0.235 0.217 , 0.239	Depositor DCC
$R_{free}$ test set	2634 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.3	Xtrriage
Anisotropy	0.082	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 35.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.034 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8677	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: CA, NAG, BMA, 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	0.36	0/4068	0.53	0/5527
1	B	0.36	0/4074	0.53	0/5535
All	All	0.36	0/8142	0.53	0/11062

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	3955	0	3759	3	0
1	B	3958	0	3764	4	0
2	C	39	0	34	0	0
2	D	39	0	34	0	0
3	E	61	0	52	1	0
4	F	28	0	25	1	0
5	G	83	0	70	0	0
6	H	127	0	106	1	0
7	A	14	0	13	0	0
7	B	14	0	13	0	0
8	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	1	0	0	0	0
9	A	160	0	0	0	0
9	B	197	0	0	0	0
All	All	8677	0	7870	7	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 0.

All (7) 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:222:VAL:HG23	1:A:482:LEU:HD22	1.86	0.58
1:B:222:VAL:HG23	1:B:482:LEU:HD22	1.84	0.58
1:B:82:ILE:HD11	4:F:1:NAG:H82	1.91	0.52
1:B:222:VAL:CG2	1:B:482:LEU:HD22	2.45	0.47
1:A:378:LYS:HE2	3:E:1:NAG:H83	1.99	0.43
1:B:378:LYS:HE2	6:H:1:NAG:H83	2.02	0.41
1:A:87:ILE:HD13	1:A:107:TRP:CE3	2.57	0.40

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	506/528 (96%)	487 (96%)	18 (4%)	1 (0%)	47	58
1	B	507/528 (96%)	492 (97%)	15 (3%)	0	100	100
All	All	1013/1056 (96%)	979 (97%)	33 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	527	LYS

### 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	419/438 (96%)	417 (100%)	2 (0%)	88	95
1	B	420/438 (96%)	420 (100%)	0	100	100
All	All	839/876 (96%)	837 (100%)	2 (0%)	93	97

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

Mol	Chain	Res	Type
1	A	300	GLN
1	A	303	ASN

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

31 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	C	1	2,1	14,14,15	0.49	0	17,19,21	1.09	2 (11%)
2	NAG	C	2	2	14,14,15	0.45	0	17,19,21	0.81	0
2	BMA	C	3	2	11,11,12	0.59	0	15,15,17	0.59	0
2	NAG	D	1	2,1	14,14,15	0.48	0	17,19,21	0.78	0
2	NAG	D	2	2	14,14,15	0.51	0	17,19,21	0.94	0
2	BMA	D	3	2	11,11,12	0.59	0	15,15,17	0.67	0
3	NAG	E	1	1,3	14,14,15	0.44	0	17,19,21	1.26	2 (11%)
3	NAG	E	2	3	14,14,15	0.53	0	17,19,21	1.04	1 (5%)
3	BMA	E	3	3	11,11,12	0.59	0	15,15,17	0.83	1 (6%)
3	MAN	E	4	3	11,11,12	0.45	0	15,15,17	0.92	1 (6%)
3	MAN	E	5	3	11,11,12	0.33	0	15,15,17	0.90	1 (6%)
4	NAG	F	1	1,4	14,14,15	0.48	0	17,19,21	0.98	0
4	NAG	F	2	4	14,14,15	0.47	0	17,19,21	0.90	0
5	NAG	G	1	1,5	14,14,15	0.51	0	17,19,21	0.85	0
5	NAG	G	2	5	14,14,15	0.50	0	17,19,21	1.00	0
5	BMA	G	3	5	11,11,12	0.65	0	15,15,17	0.62	0
5	MAN	G	4	5	11,11,12	0.32	0	15,15,17	1.11	1 (6%)
5	MAN	G	5	5	11,11,12	0.30	0	15,15,17	0.98	1 (6%)
5	MAN	G	6	5	11,11,12	0.26	0	15,15,17	0.81	1 (6%)
5	MAN	G	7	5	11,11,12	0.34	0	15,15,17	0.97	1 (6%)
6	NAG	H	1	6,1	14,14,15	0.51	0	17,19,21	1.37	3 (17%)
6	MAN	H	10	6	11,11,12	0.23	0	15,15,17	0.85	1 (6%)
6	MAN	H	11	6	11,11,12	0.28	0	15,15,17	0.85	1 (6%)
6	NAG	H	2	6	14,14,15	0.55	0	17,19,21	0.91	0
6	BMA	H	3	6	11,11,12	0.66	0	15,15,17	0.61	0
6	MAN	H	4	6	11,11,12	0.37	0	15,15,17	0.96	1 (6%)
6	MAN	H	5	6	11,11,12	0.31	0	15,15,17	0.85	1 (6%)
6	MAN	H	6	6	11,11,12	0.31	0	15,15,17	0.79	1 (6%)
6	MAN	H	7	6	11,11,12	0.59	0	15,15,17	1.41	1 (6%)
6	MAN	H	8	6	11,11,12	0.27	0	15,15,17	0.99	0
6	MAN	H	9	6	11,11,12	0.34	0	15,15,17	0.83	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
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	BMA	D	3	2	-	0/2/19/22	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	2/2/19/22	0/1/1/1
3	MAN	E	4	3	-	2/2/19/22	0/1/1/1
3	MAN	E	5	3	-	0/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	0/2/19/22	0/1/1/1
5	MAN	G	6	5	-	0/2/19/22	0/1/1/1
5	MAN	G	7	5	-	0/2/19/22	0/1/1/1
6	NAG	H	1	6,1	-	1/6/23/26	0/1/1/1
6	MAN	H	10	6	-	0/2/19/22	0/1/1/1
6	MAN	H	11	6	-	0/2/19/22	0/1/1/1
6	NAG	H	2	6	-	1/6/23/26	0/1/1/1
6	BMA	H	3	6	-	0/2/19/22	0/1/1/1
6	MAN	H	4	6	-	2/2/19/22	0/1/1/1
6	MAN	H	5	6	-	0/2/19/22	0/1/1/1
6	MAN	H	6	6	-	0/2/19/22	0/1/1/1
6	MAN	H	7	6	-	0/2/19/22	0/1/1/1
6	MAN	H	8	6	-	0/2/19/22	0/1/1/1
6	MAN	H	9	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	7	MAN	C1-C2-C3	4.27	114.92	109.67
5	G	4	MAN	C1-O5-C5	3.48	116.91	112.19
6	H	1	NAG	O5-C1-C2	-3.16	106.29	111.29
3	E	1	NAG	O5-C1-C2	-2.83	106.81	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	6	MAN	C1-O5-C5	2.70	115.85	112.19
3	E	3	BMA	C1-O5-C5	2.65	115.78	112.19
3	E	4	MAN	C1-C2-C3	2.56	112.82	109.67
5	G	7	MAN	C1-O5-C5	2.36	115.39	112.19
2	C	1	NAG	C1-O5-C5	2.27	115.26	112.19
6	H	10	MAN	C1-O5-C5	2.26	115.25	112.19
3	E	5	MAN	C1-O5-C5	2.25	115.24	112.19
3	E	2	NAG	O5-C1-C2	-2.25	107.74	111.29
6	H	1	NAG	C3-C4-C5	2.20	114.17	110.24
5	G	5	MAN	C1-O5-C5	2.14	115.09	112.19
6	H	5	MAN	C1-O5-C5	2.14	115.09	112.19
6	H	6	MAN	C1-O5-C5	2.11	115.05	112.19
2	C	1	NAG	O5-C1-C2	-2.10	107.97	111.29
6	H	4	MAN	C1-O5-C5	2.08	115.02	112.19
6	H	11	MAN	C1-O5-C5	2.08	115.01	112.19
6	H	1	NAG	O7-C7-C8	-2.02	118.31	122.06
3	E	1	NAG	O7-C7-C8	-2.01	118.32	122.06
6	H	9	MAN	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

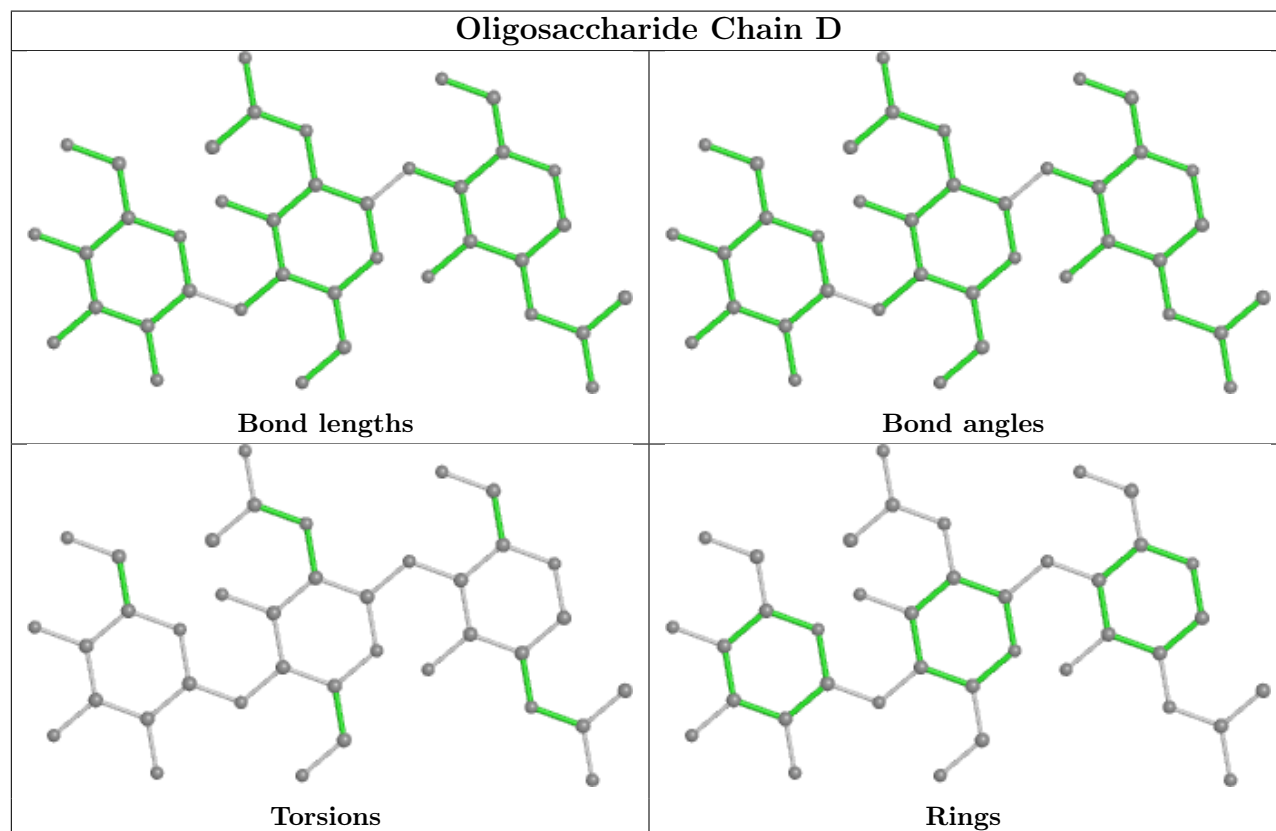
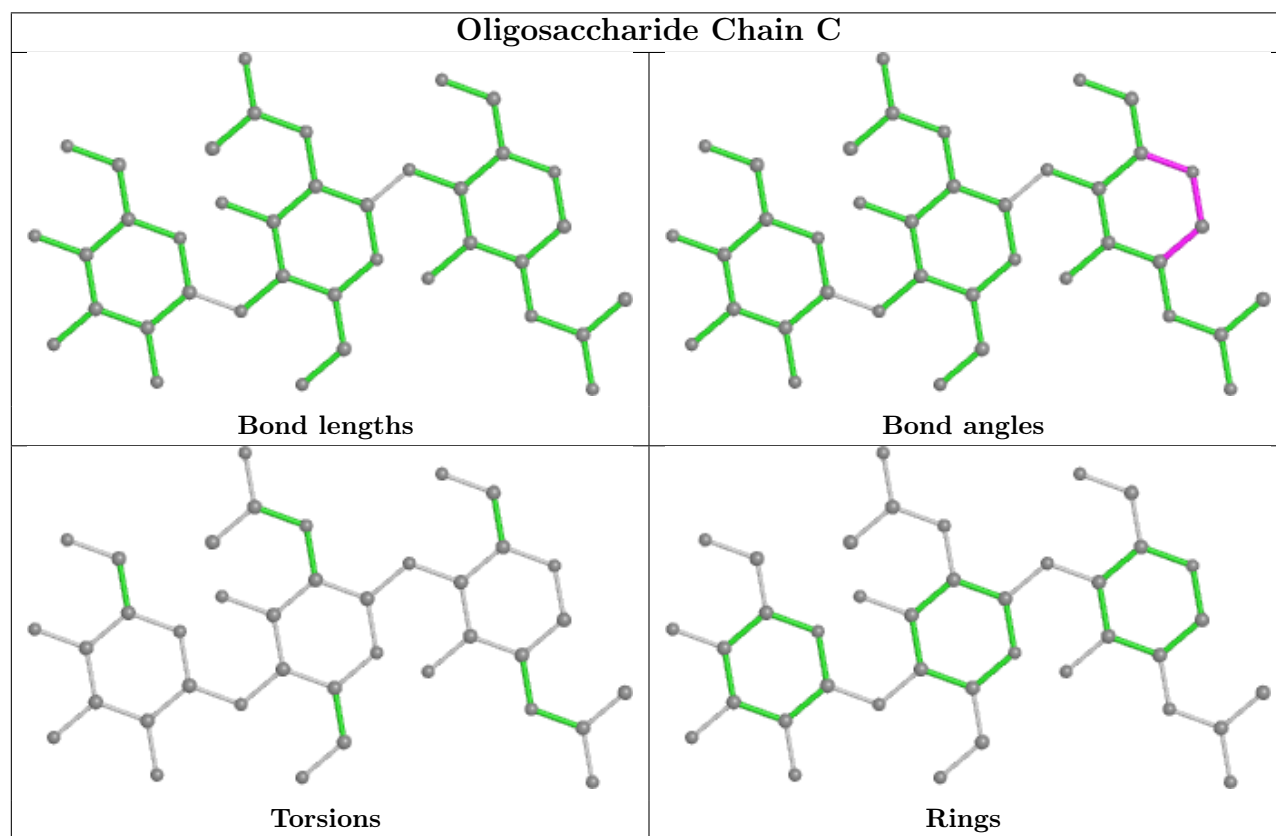
Mol	Chain	Res	Type	Atoms
5	G	3	BMA	C4-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
3	E	3	BMA	C4-C5-C6-O6
6	H	4	MAN	O5-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
3	E	3	BMA	O5-C5-C6-O6
6	H	4	MAN	C4-C5-C6-O6
6	H	1	NAG	C4-C5-C6-O6
6	H	2	NAG	O5-C5-C6-O6

There are no ring outliers.

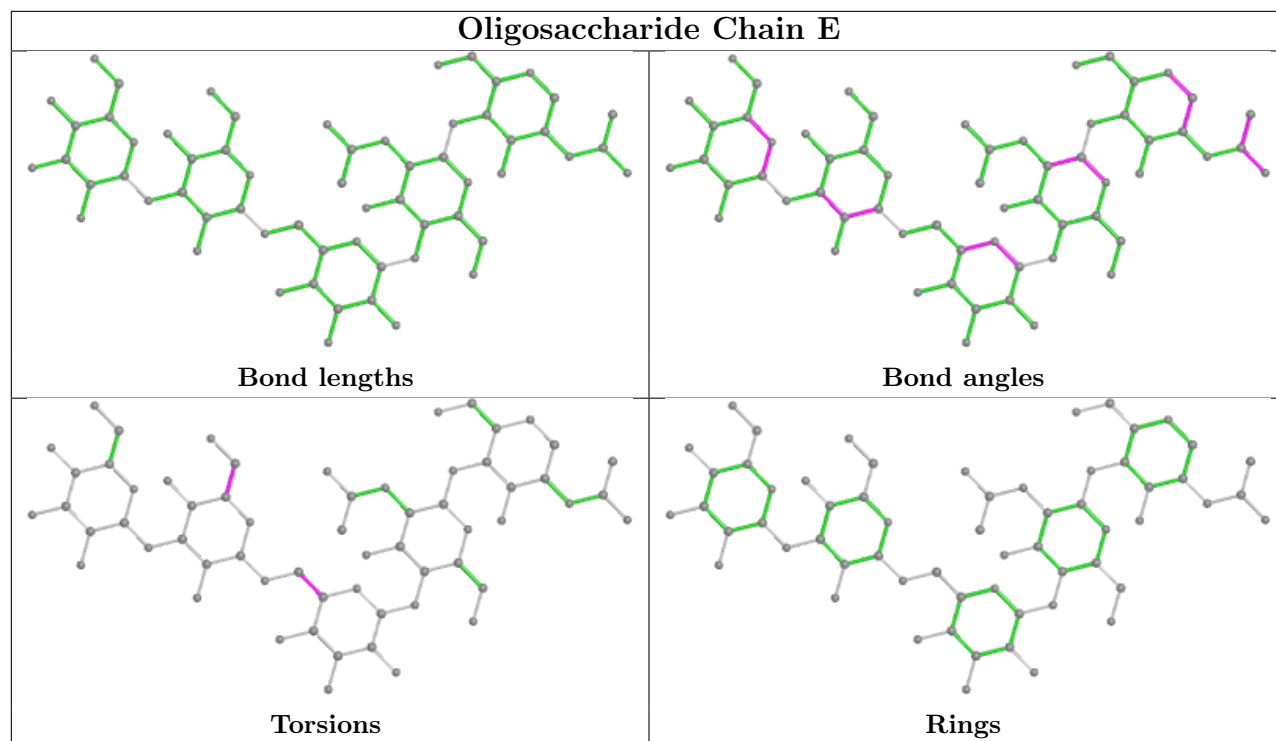
3 monomers are involved in 3 short contacts:

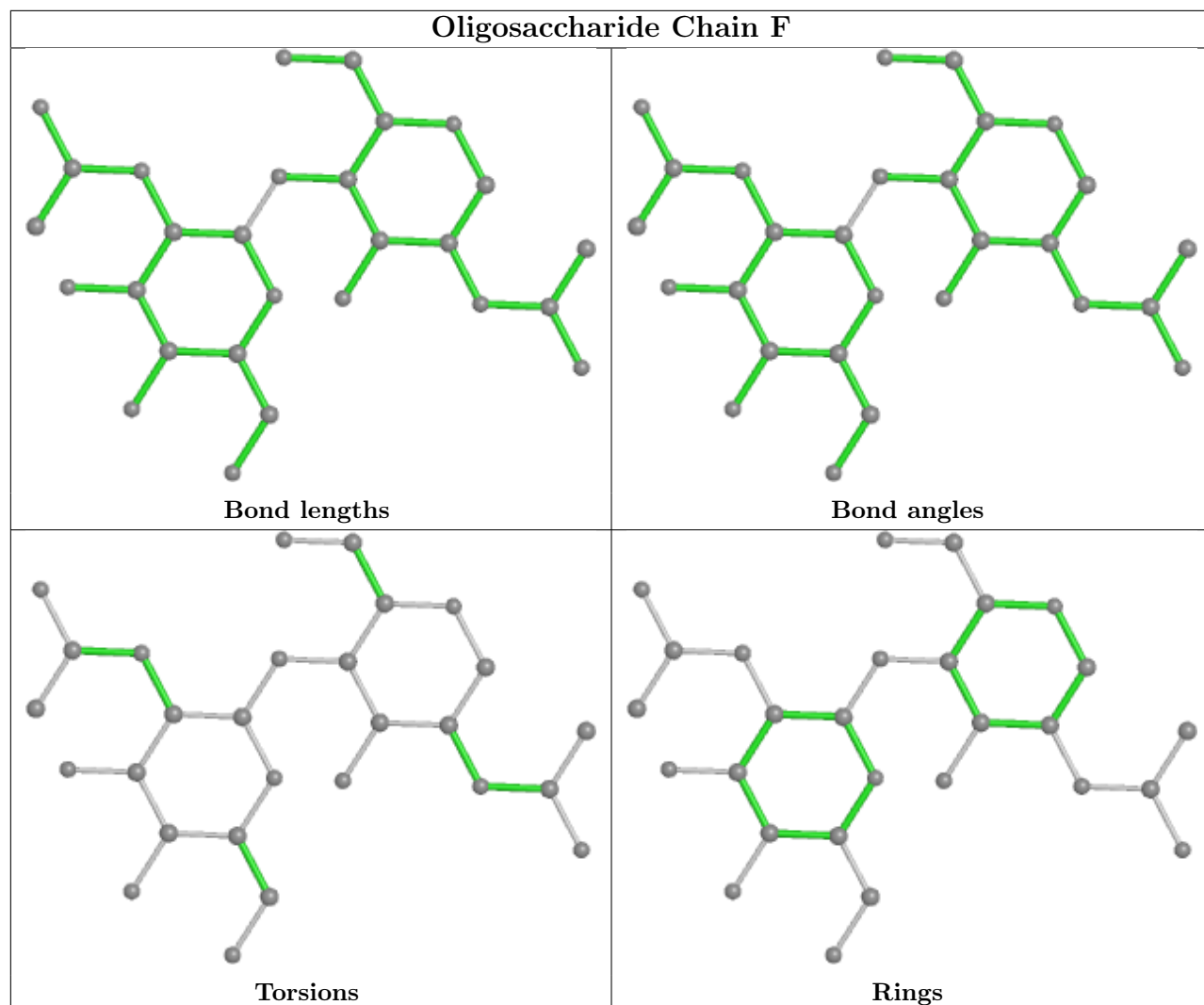
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	1	NAG	1	0
4	F	1	NAG	1	0
3	E	1	NAG	1	0

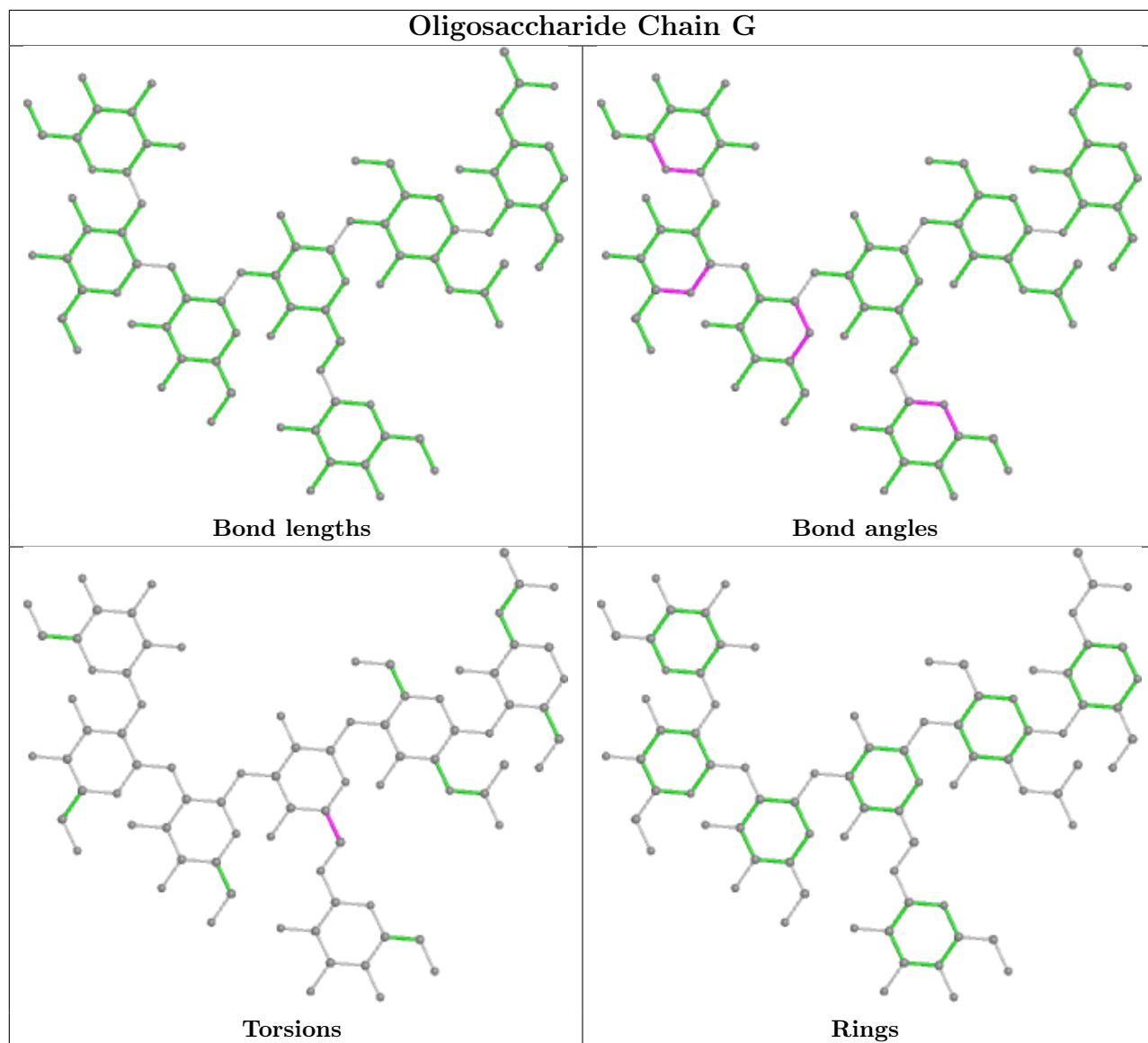
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

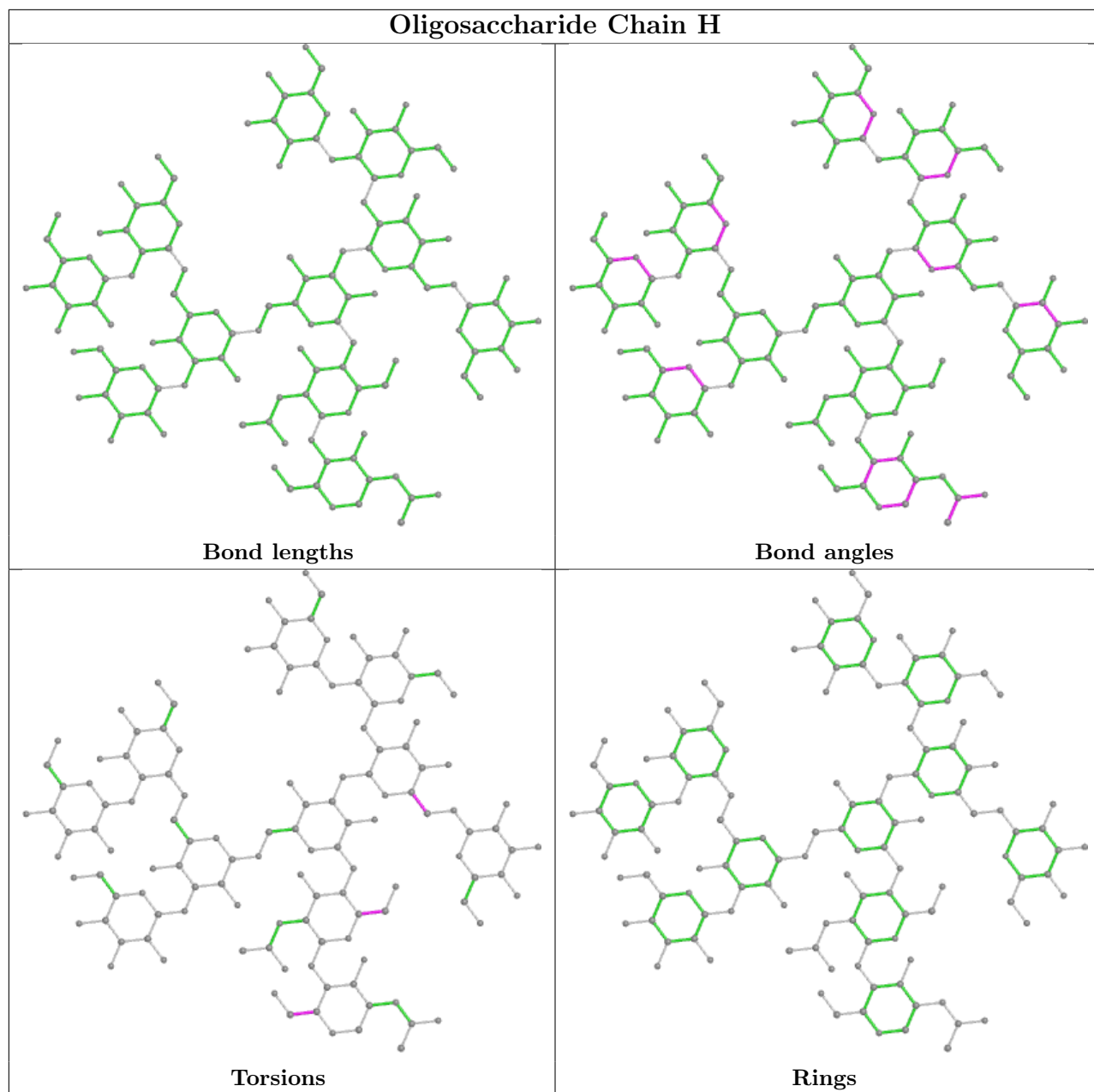












## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	603	1	14,14,15	0.54	0	17,19,21	1.16	1 (5%)
7	NAG	A	604	1	14,14,15	0.46	0	17,19,21	1.06	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
7	NAG	B	603	1	-	0/6/23/26	0/1/1/1
7	NAG	A	604	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
7	A	604	NAG	O5-C1-C2	-2.40	107.50	111.29
7	B	603	NAG	C4-C3-C2	2.22	114.27	111.02

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	508/528 (96%)	0.45	20 (3%) 39 46	25, 36, 54, 83	0
1	B	508/528 (96%)	0.24	11 (2%) 62 69	23, 32, 46, 64	0
All	All	1016/1056 (96%)	0.35	31 (3%) 49 56	23, 34, 51, 83	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	299	GLY	8.9
1	A	299	GLY	7.7
1	A	300	GLN	6.3
1	A	302	LYS	5.6
1	A	248	GLY	4.3
1	B	301	THR	4.1
1	A	351	TYR	3.8
1	A	347	GLN	3.7
1	A	298	LYS	2.9
1	A	74	PRO	2.8
1	A	159	TYR	2.8
1	A	56	TRP	2.7
1	A	342	PHE	2.7
1	A	502	ASN	2.7
1	B	509	VAL	2.7
1	A	57	PHE	2.5
1	A	85	VAL	2.5
1	A	543	GLU	2.4
1	B	300	GLN	2.4
1	B	248	GLY	2.4
1	B	503	GLY	2.3
1	A	41	CYS	2.3
1	B	502	ASN	2.3
1	B	342	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	346	GLU	2.2
1	B	510	GLU	2.2
1	A	54	LYS	2.1
1	B	351	TYR	2.1
1	A	364	THR	2.1
1	A	301	THR	2.0
1	B	49	LYS	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.

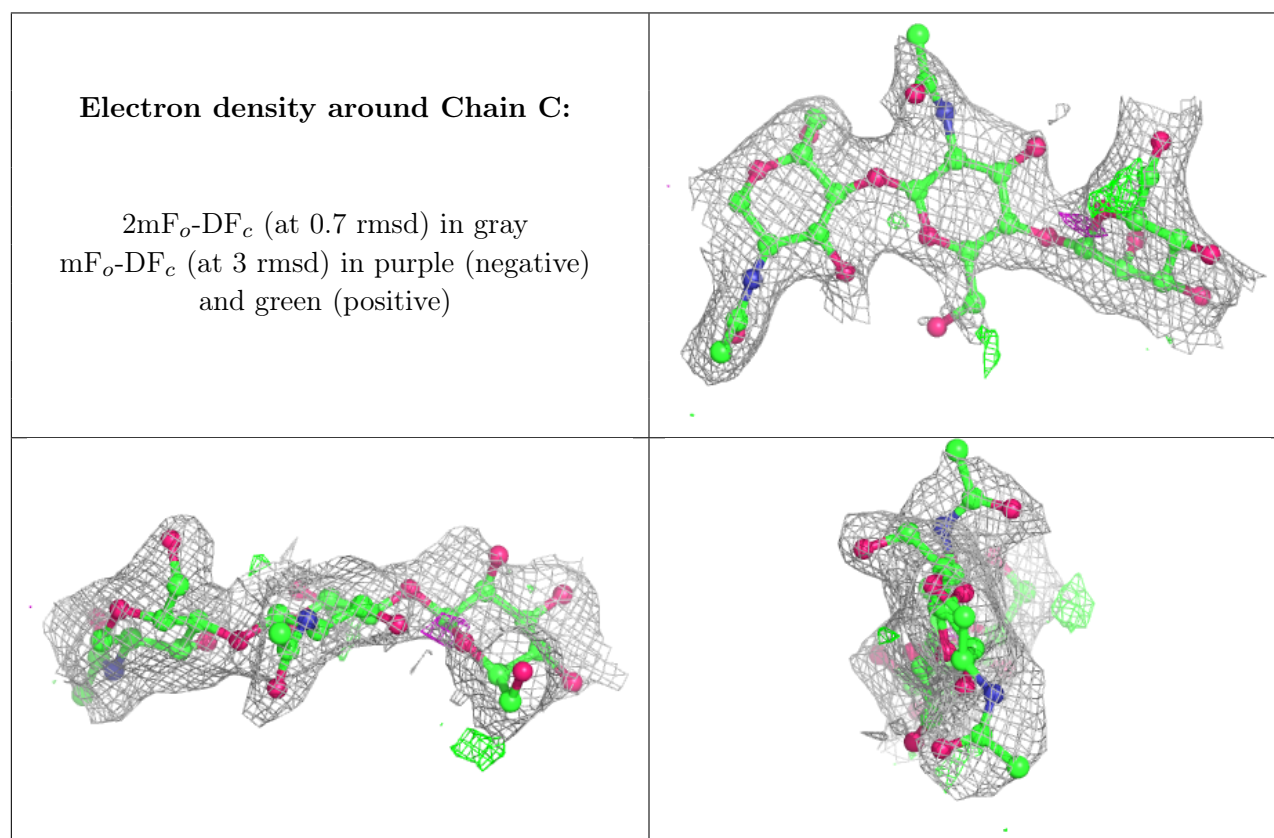
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BMA	D	3	11/12	0.67	0.28	54,56,56,57	0
5	MAN	G	7	11/12	0.70	0.19	49,50,51,51	0
3	MAN	E	4	11/12	0.73	0.23	60,62,62,63	0
6	MAN	H	7	11/12	0.74	0.31	45,47,48,49	0
2	BMA	C	3	11/12	0.78	0.16	63,64,65,65	0
2	NAG	C	2	14/15	0.83	0.20	61,62,64,64	0
3	BMA	E	3	11/12	0.84	0.15	60,60,61,62	0
4	NAG	F	1	14/15	0.84	0.23	57,60,61,63	0
2	NAG	C	1	14/15	0.85	0.14	53,55,56,58	0
6	MAN	H	11	11/12	0.87	0.26	41,43,44,44	0
5	MAN	G	6	11/12	0.88	0.15	39,40,40,40	0
3	MAN	E	5	11/12	0.88	0.20	55,56,58,58	0
4	NAG	F	2	14/15	0.89	0.33	65,67,67,67	0
6	MAN	H	6	11/12	0.90	0.18	40,41,42,42	0
3	NAG	E	2	14/15	0.90	0.17	56,58,58,59	0
6	MAN	H	10	11/12	0.90	0.17	40,40,41,42	0
5	MAN	G	5	11/12	0.90	0.13	41,41,41,42	0
2	NAG	D	1	14/15	0.91	0.19	42,43,44,45	0
5	MAN	G	4	11/12	0.91	0.15	42,42,43,44	0
2	NAG	D	2	14/15	0.91	0.23	47,48,50,52	0
6	NAG	H	1	14/15	0.92	0.16	34,34,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MAN	H	4	11/12	0.92	0.13	37,38,41,44	0
3	NAG	E	1	14/15	0.92	0.13	51,52,53,54	0
6	NAG	H	2	14/15	0.93	0.16	33,33,34,35	0
5	BMA	G	3	11/12	0.93	0.12	40,42,45,48	0
6	MAN	H	8	11/12	0.95	0.13	37,37,38,40	0
5	NAG	G	1	14/15	0.95	0.15	33,34,34,36	0
5	NAG	G	2	14/15	0.95	0.15	36,37,38,39	0
6	MAN	H	9	11/12	0.96	0.12	37,37,38,39	0
6	MAN	H	5	11/12	0.96	0.13	39,39,39,40	0
6	BMA	H	3	11/12	0.96	0.11	34,34,36,36	0

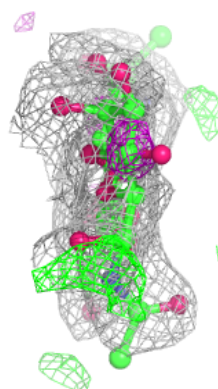
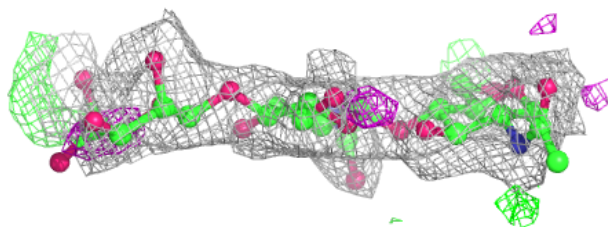
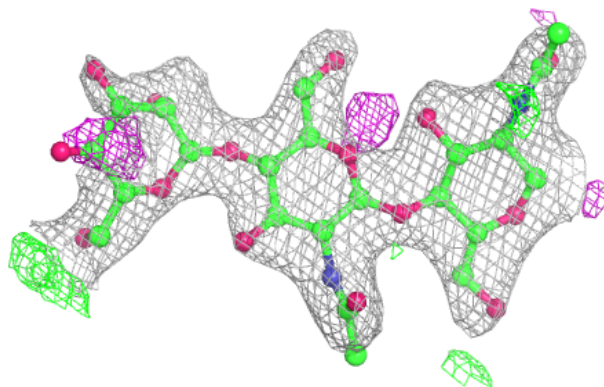
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





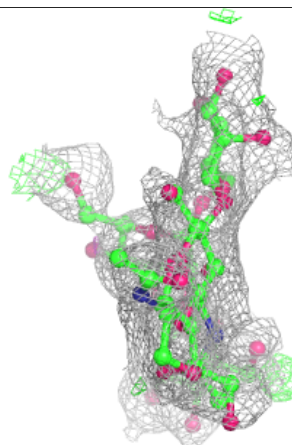
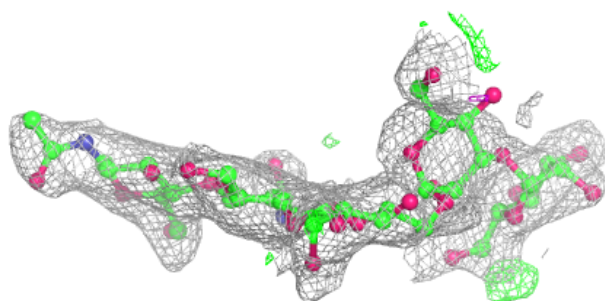
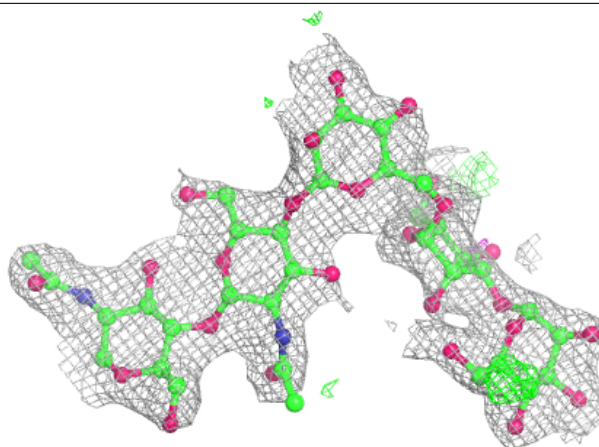
**Electron density around Chain D:**

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



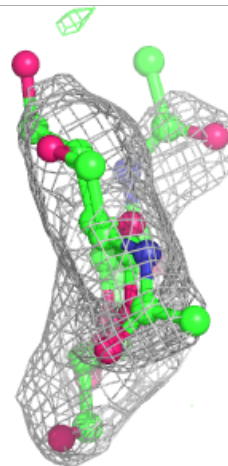
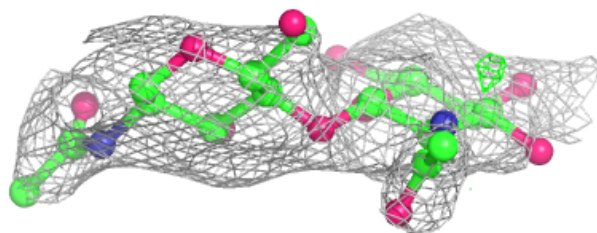
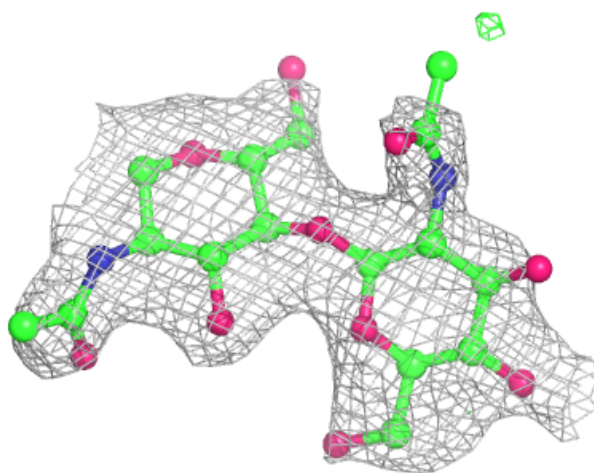
**Electron density around Chain E:**

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



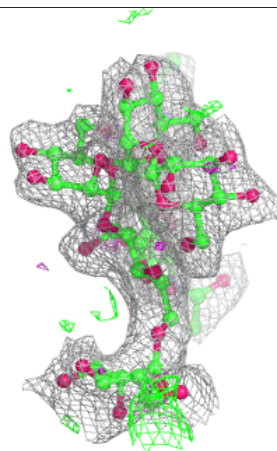
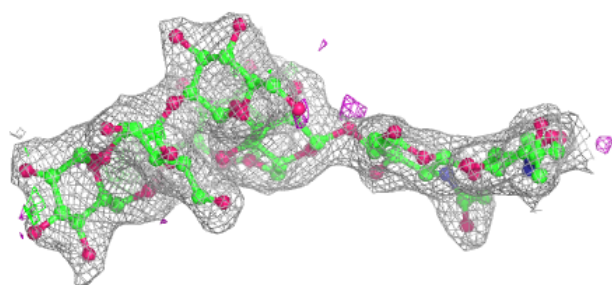
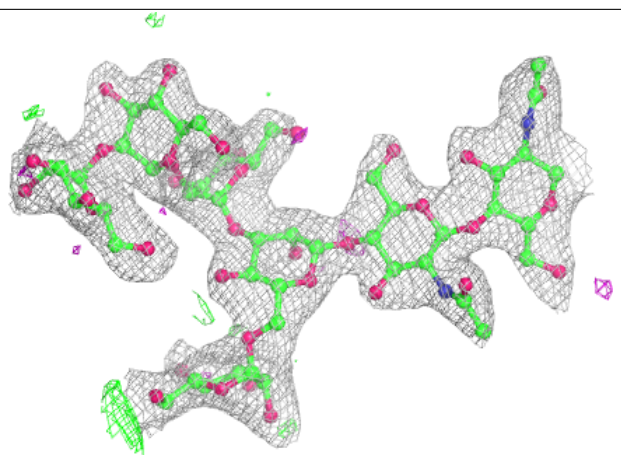
**Electron density around Chain F:**

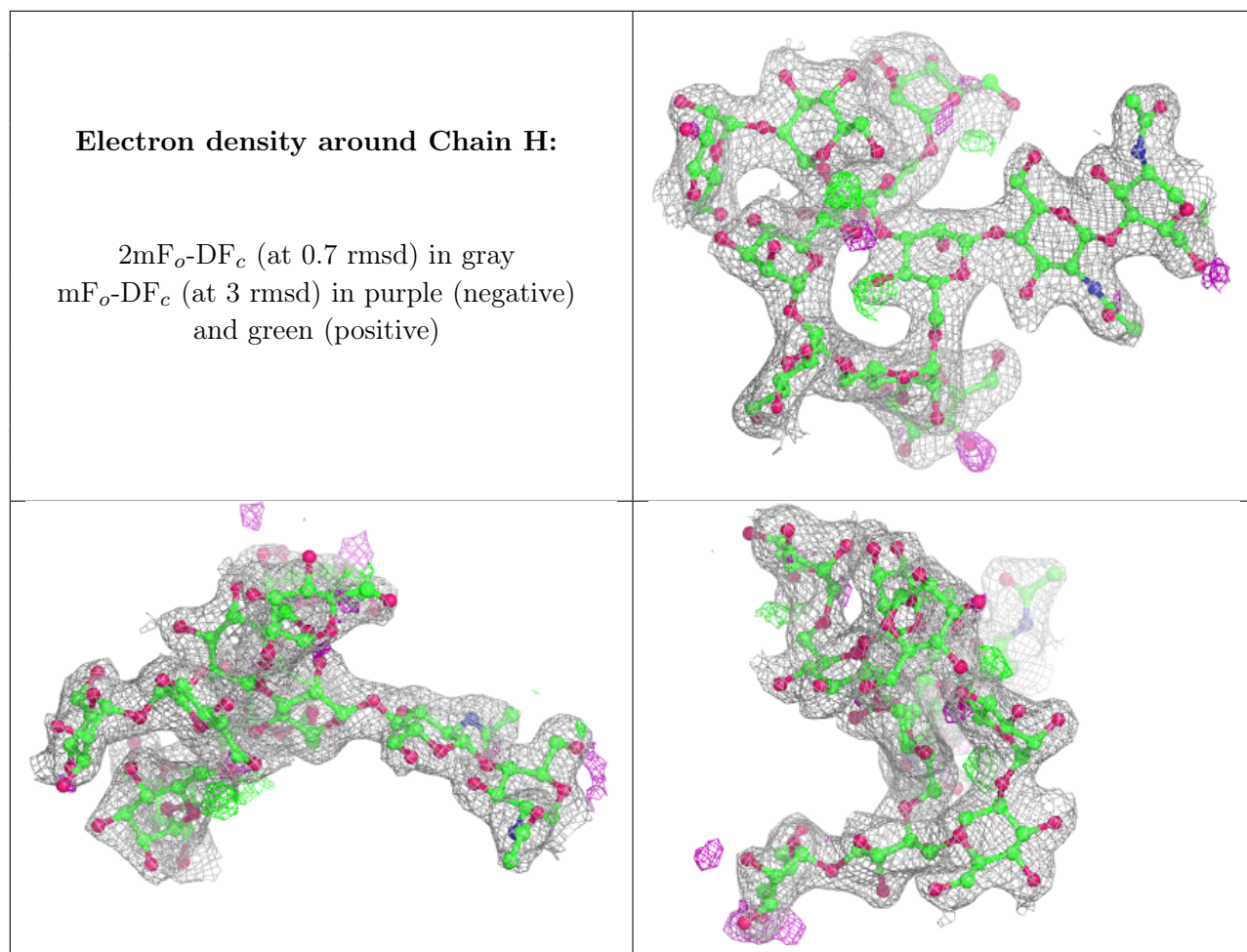
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 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
7	NAG	B	603	14/15	0.83	0.27	43,45,46,46	0
7	NAG	A	604	14/15	0.87	0.20	52,53,53,54	0
8	CA	A	613	1/1	0.91	0.09	33,33,33,33	0
8	CA	B	622	1/1	0.96	0.16	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.