



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 02:47 PM BST

PDB ID : 2RI8  
Title : Penicillium citrinum alpha-1,2-mannosidase complex with glycerol  
Authors : Lobsanov, Y.D.; Yoshida, T.; Desmet, T.; Nerinckx, W.; Yip, P.; Claeysens, M.; Herscovics, A.; Howell, P.L.  
Deposited on : 2007-10-10  
Resolution : 2.16 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

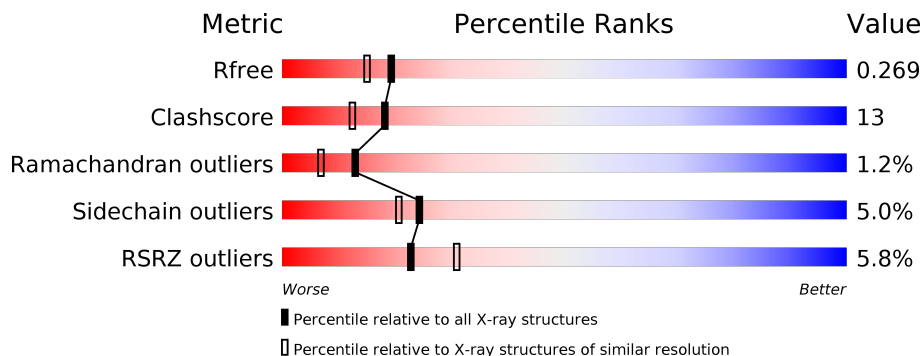
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.16 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	475	
1	B	475	
2	C	2	
2	E	2	
2	F	2	
2	H	2	

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Mol	Chain	Length	Quality of chain
3	D	5	
3	G	5	

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	MAN	D	3	X	-	-	-
3	MAN	G	3	X	-	-	-

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 8443 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 Mannosyl-oligosaccharide alpha-1,2-mannosidase.

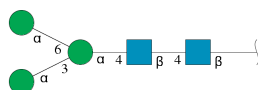
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	475	Total 3748	C 2371	N 627	O 742	S 8	0	2	0
1	B	475	Total 3725	C 2359	N 619	O 739	S 8	0	0	0

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



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

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

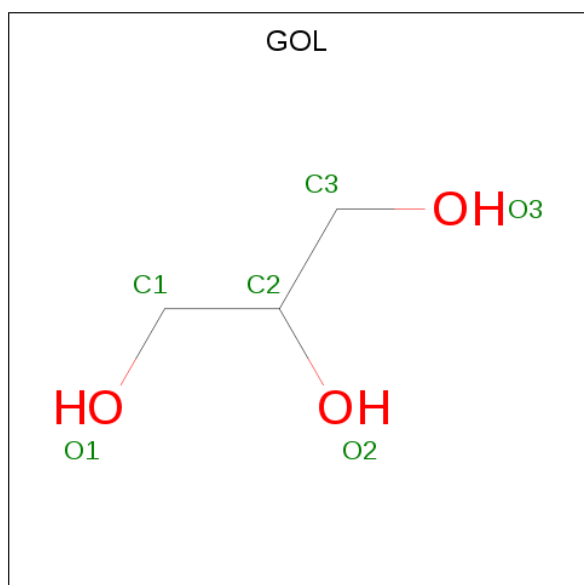


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	5	Total	C	N	O	0	0	0
			61	34	2	25			
3	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

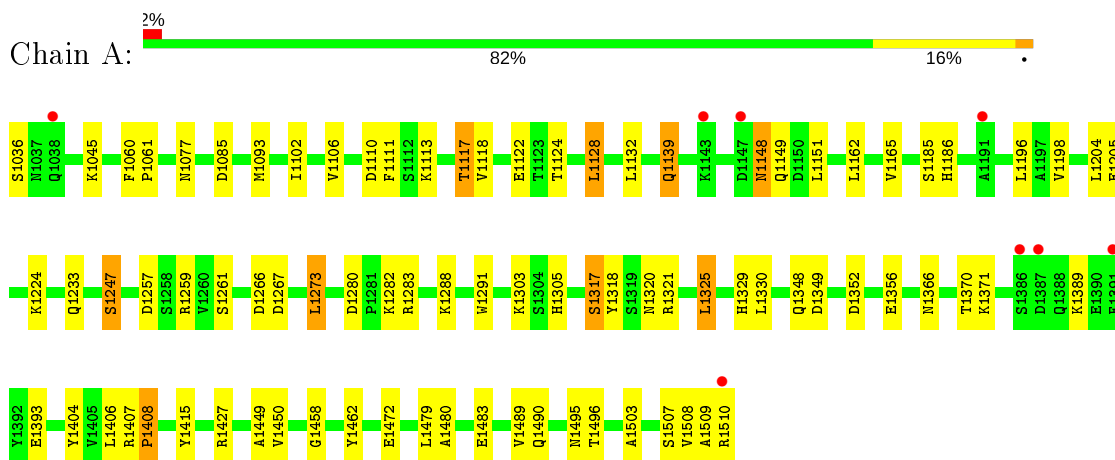
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	449	Total	O	0	0
			449	449		
6	B	243	Total	O	0	0
			243	243		

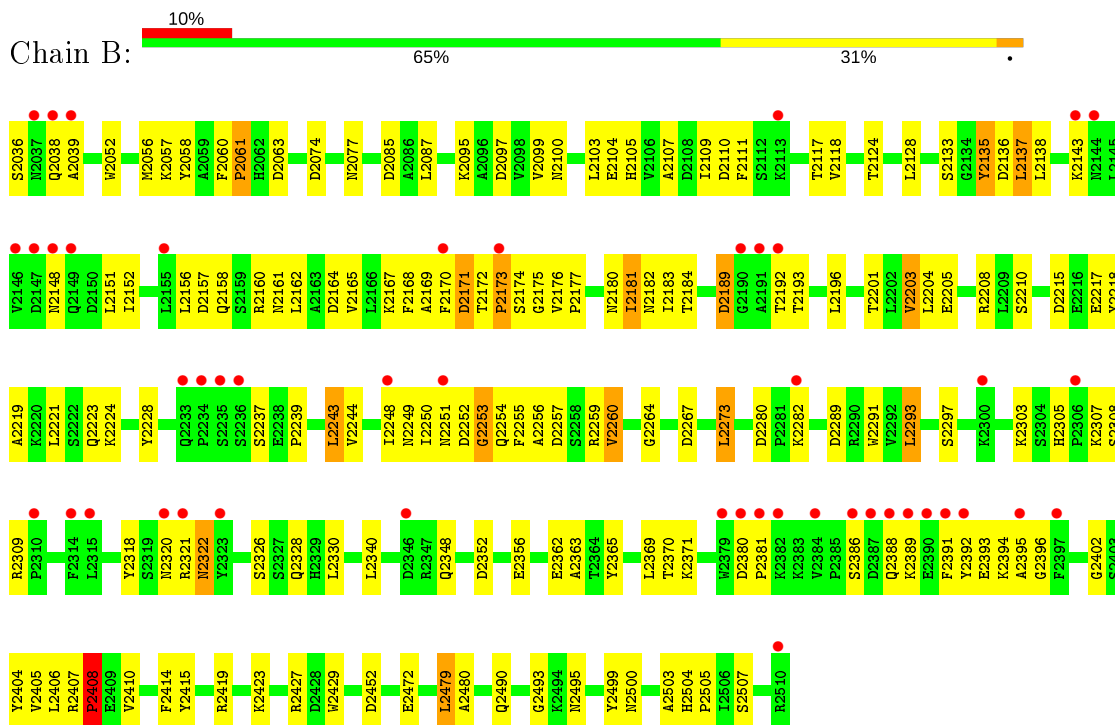
### 3 Residue-property plots [i](#)

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: Mannosyl-oligosaccharide alpha-1,2-mannosidase



- Molecule 1: Mannosyl-oligosaccharide alpha-1,2-mannosidase



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

Chain C:  50% 50%

MAG1  
MAG2

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

Chain E:  100%

MAG1  
MAG2

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

Chain F:  100%

MAG1  
MAG2

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

Chain H:  100%


MAG1  
MAG2

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

Chain D:  60% 40%

MAG1  
MAG2  
MAN3  
MAN4  
MAN5

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

Chain G:  20% 80%

MAG1  
MAG2  
MAN3  
MAN4  
MAN5



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.49Å 111.00Å 86.23Å 90.00° 99.17° 90.00°	Depositor
Resolution (Å)	20.32 – 2.16 20.32 – 2.18	Depositor EDS
% Data completeness (in resolution range)	96.6 (20.32-2.16) 96.8 (20.32-2.18)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.20 (at 2.17Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.206 , 0.274 0.200 , 0.269	Depositor DCC
$R_{free}$ test set	3759 reflections (7.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.2	Xtrriage
Anisotropy	0.249	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 72.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8443	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1269e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: GOL, 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	0.52	0/3842	0.69	0/5215
1	B	0.43	0/3820	0.66	1/5190 (0.0%)
All	All	0.48	0/7662	0.68	1/10405 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2253	GLY	N-CA-C	-5.15	100.24	113.10

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	3748	0	3548	65	0
1	B	3725	0	3523	134	0
2	C	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	H	28	0	25	0	0
3	D	61	0	52	0	0
3	G	61	0	52	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	24	0	30	6	0
5	B	18	0	23	1	0
6	A	449	0	0	12	0
6	B	243	0	0	15	0
All	All	8443	0	7328	202	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 13.

The worst 5 of 202 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:B:2264:GLY:H	1:B:2328:GLN:HE22	1.10	0.97
1:B:2158:GLN:HA	1:B:2161:ASN:HD22	1.32	0.94
1:B:2423:LYS:HE2	1:B:2423:LYS:HA	1.49	0.93
1:A:1349:ASP:HB3	5:A:1904:GOL:H11	1.50	0.90
1:B:2307:LYS:HE2	1:B:2381:PRO:HG2	1.58	0.85

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	474/475 (100%)	449 (95%)	22 (5%)	3 (1%)	25 18
1	B	473/475 (100%)	428 (90%)	37 (8%)	8 (2%)	9 3
All	All	947/950 (100%)	877 (93%)	59 (6%)	11 (1%)	13 7

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1267	ASP
1	B	2171	ASP
1	B	2189	ASP
1	B	2267	ASP
1	B	2173	PRO

### 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	402/400 (100%)	385 (96%)	17 (4%)	30	28
1	B	400/400 (100%)	377 (94%)	23 (6%)	20	15
All	All	802/800 (100%)	762 (95%)	40 (5%)	24	21

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2061	PRO
1	B	2128	LEU
1	B	2393	GLU
1	B	2087	LEU
1	B	2135	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1490	GLN
1	B	2105	HIS
1	B	2490	GLN
1	A	1495	ASN
1	B	2037	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](#)

18 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	C	1	1,2	14,14,15	0.57	0	17,19,21	0.97	0
2	NAG	C	2	2	14,14,15	0.62	0	17,19,21	0.75	1 (5%)
3	NAG	D	1	1,3	14,14,15	0.88	1 (7%)	17,19,21	0.78	0
3	NAG	D	2	3	14,14,15	0.81	1 (7%)	17,19,21	0.59	0
3	MAN	D	3	3	11,11,12	0.51	0	15,15,17	0.52	0
3	MAN	D	4	3	11,11,12	0.54	0	15,15,17	0.65	0
3	MAN	D	5	3	11,11,12	0.50	0	15,15,17	0.56	0
2	NAG	E	1	1,2	14,14,15	0.63	0	17,19,21	0.69	0
2	NAG	E	2	2	14,14,15	0.62	0	17,19,21	0.55	0
2	NAG	F	1	1,2	14,14,15	0.63	0	17,19,21	0.74	0
2	NAG	F	2	2	14,14,15	0.60	0	17,19,21	0.63	0
3	NAG	G	1	1,3	14,14,15	0.74	0	17,19,21	0.90	0
3	NAG	G	2	3	14,14,15	0.64	0	17,19,21	0.70	0
3	MAN	G	3	3	11,11,12	0.56	0	15,15,17	0.47	0
3	MAN	G	4	3	11,11,12	0.50	0	15,15,17	0.68	1 (6%)
3	MAN	G	5	3	11,11,12	0.46	0	15,15,17	0.65	1 (6%)
2	NAG	H	1	1,2	14,14,15	0.62	0	17,19,21	0.73	0
2	NAG	H	2	2	14,14,15	0.53	0	17,19,21	0.66	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
2	NAG	C	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	MAN	D	3	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
3	MAN	G	3	3	1/1/4/5	1/2/19/22	0/1/1/1
3	MAN	G	4	3	-	2/2/19/22	0/1/1/1
3	MAN	G	5	3	-	2/2/19/22	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	5/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2	NAG	C1-C2	2.52	1.56	1.52
3	D	1	NAG	C1-C2	2.20	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	4	MAN	C1-O5-C5	2.14	115.09	112.19
3	G	5	MAN	C1-O5-C5	2.07	115.00	112.19
2	C	2	NAG	C2-N2-C7	-2.01	120.04	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	3	MAN	C1
3	D	3	MAN	C1

5 of 36 torsion outliers are listed below:

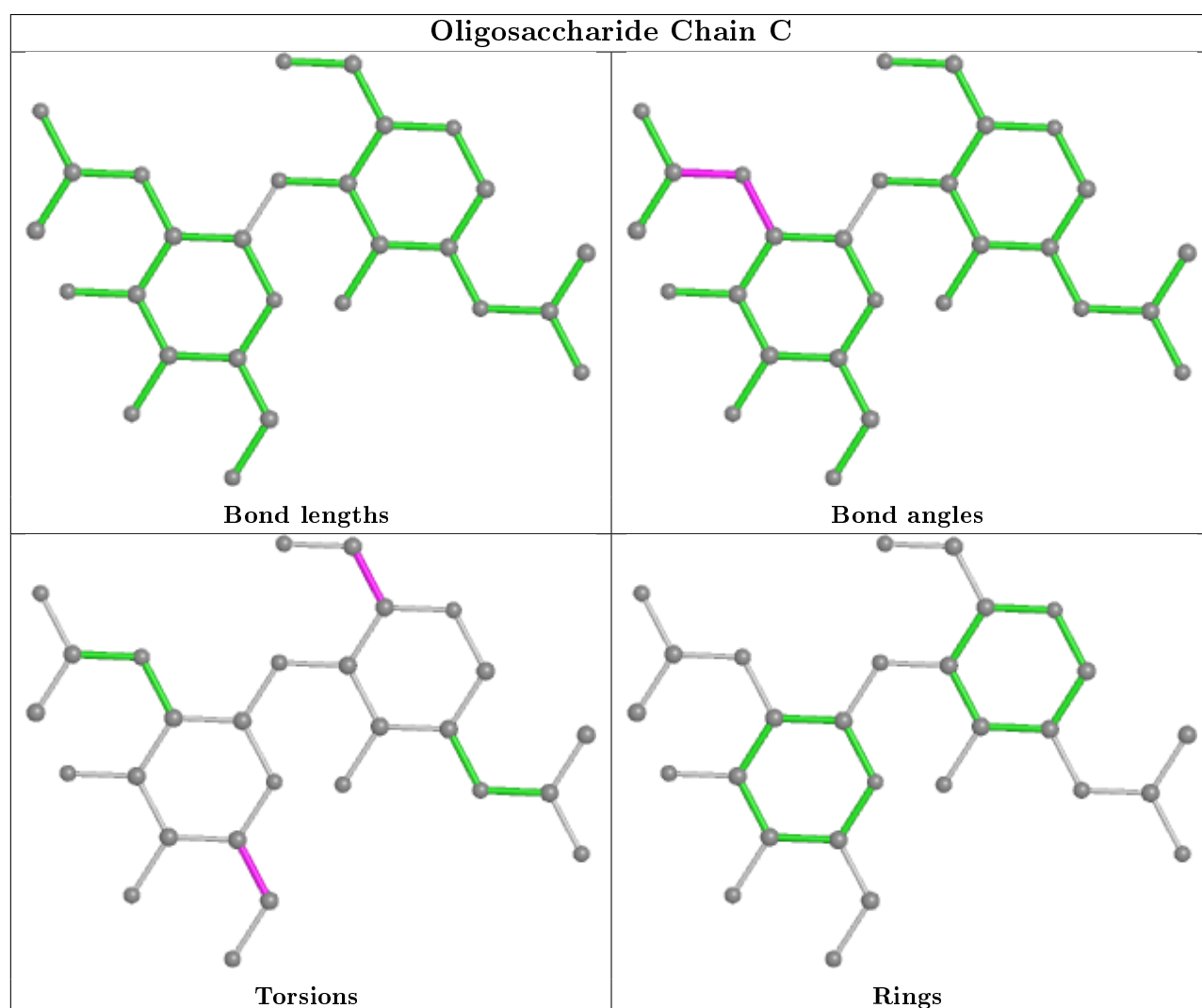
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	H	2	NAG	C3-C2-N2-C7
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2

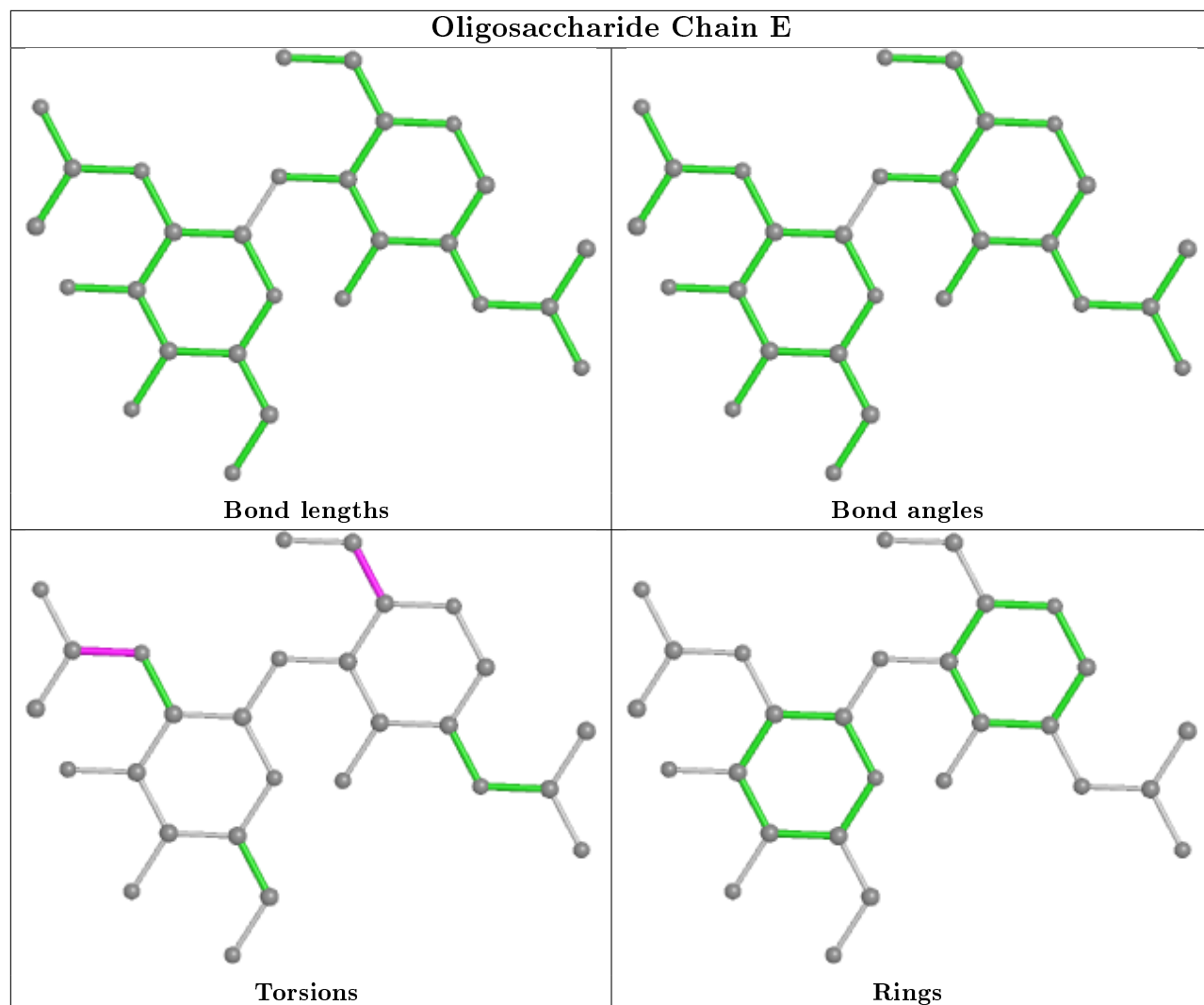
There are no ring outliers.

2 monomers are involved in 5 short contacts:

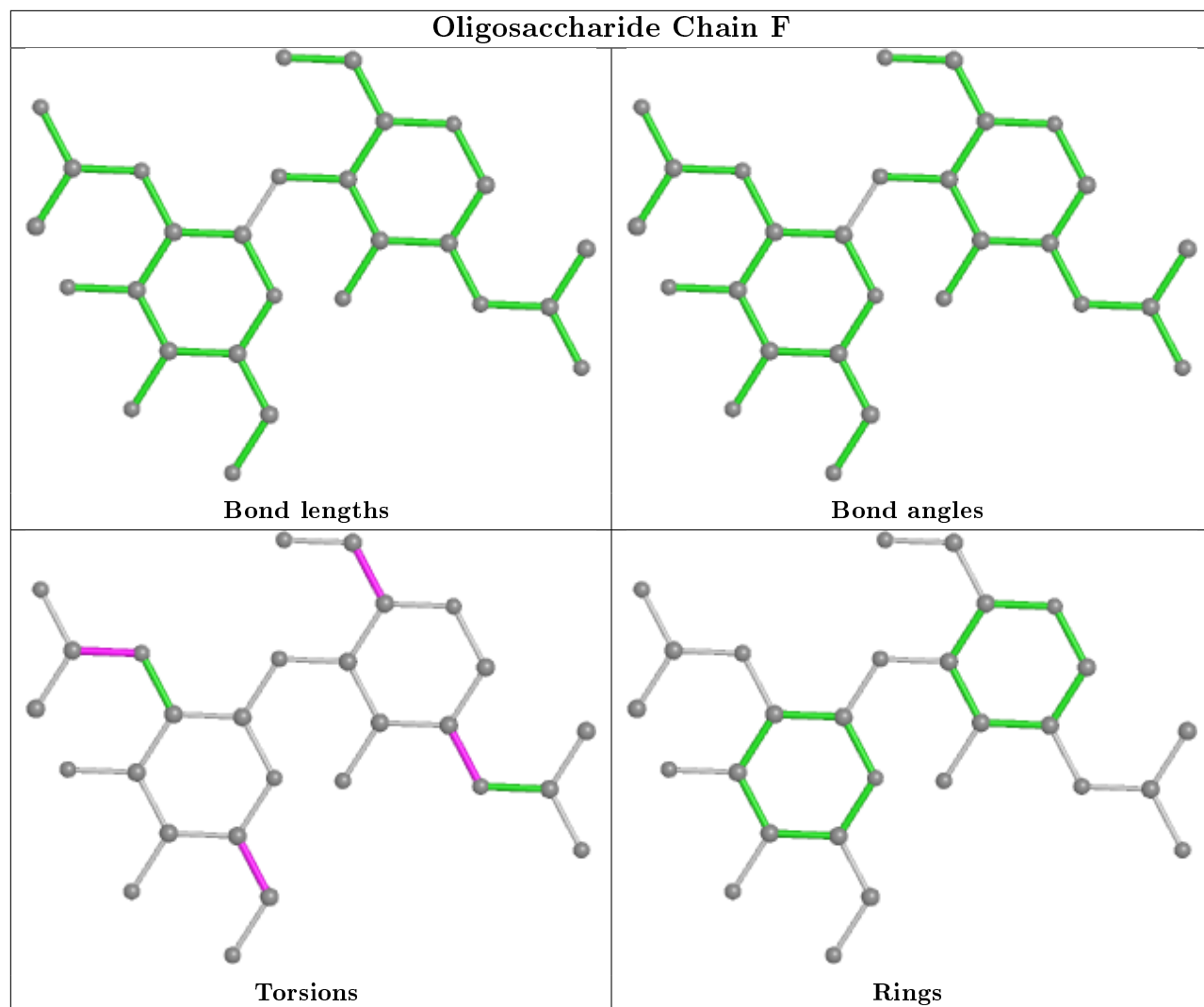
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2	NAG	2	0
3	G	1	NAG	4	0

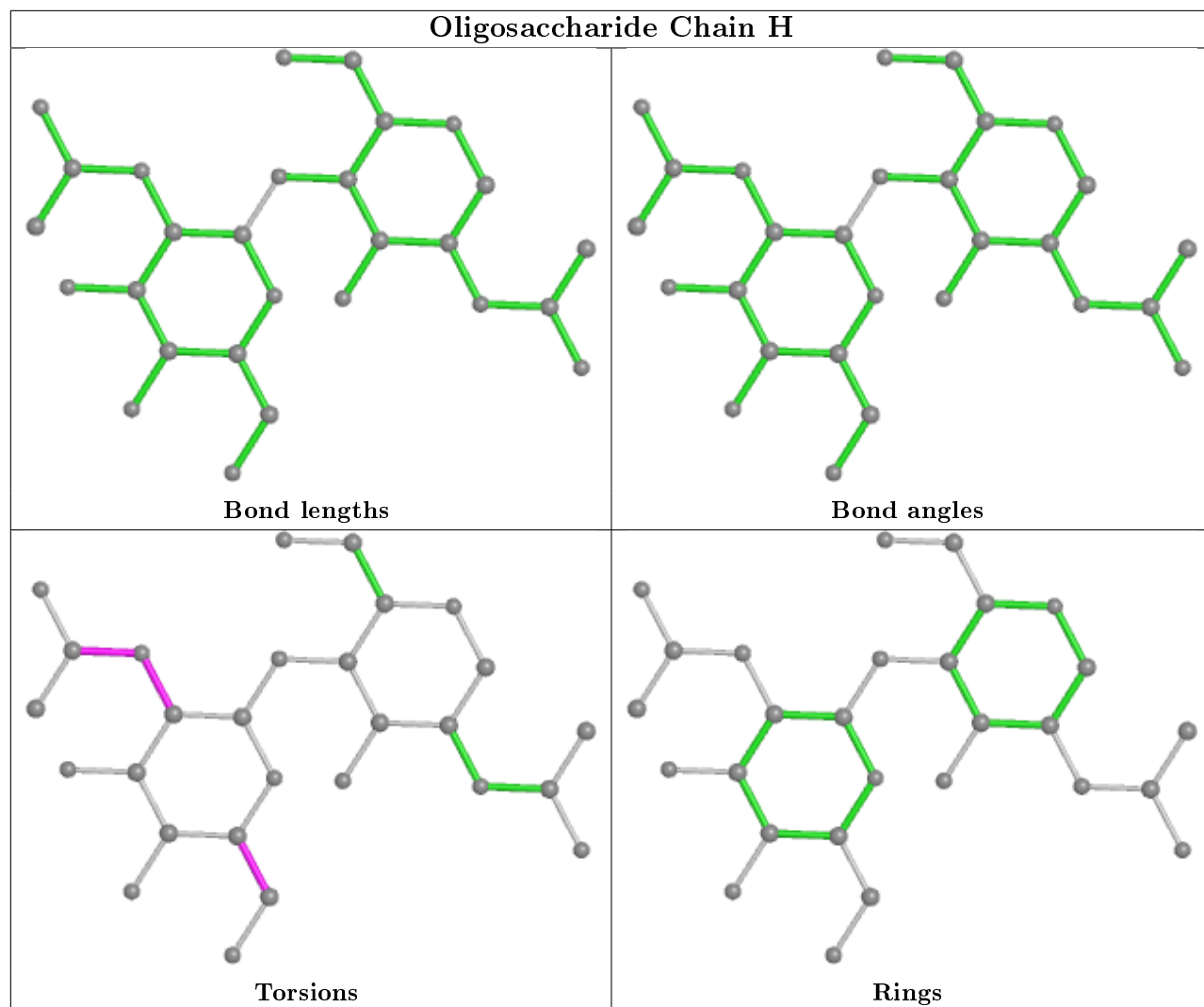
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

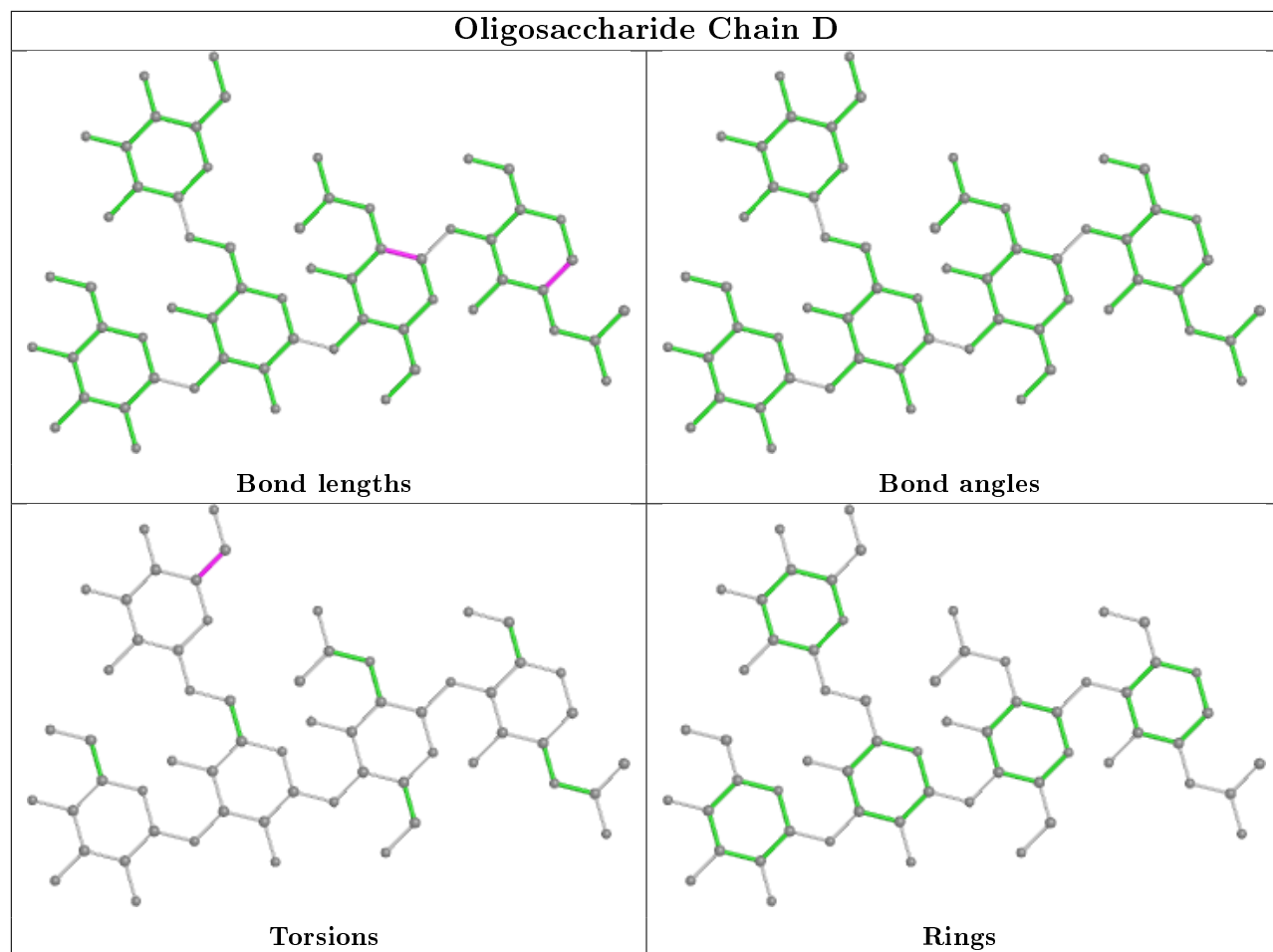


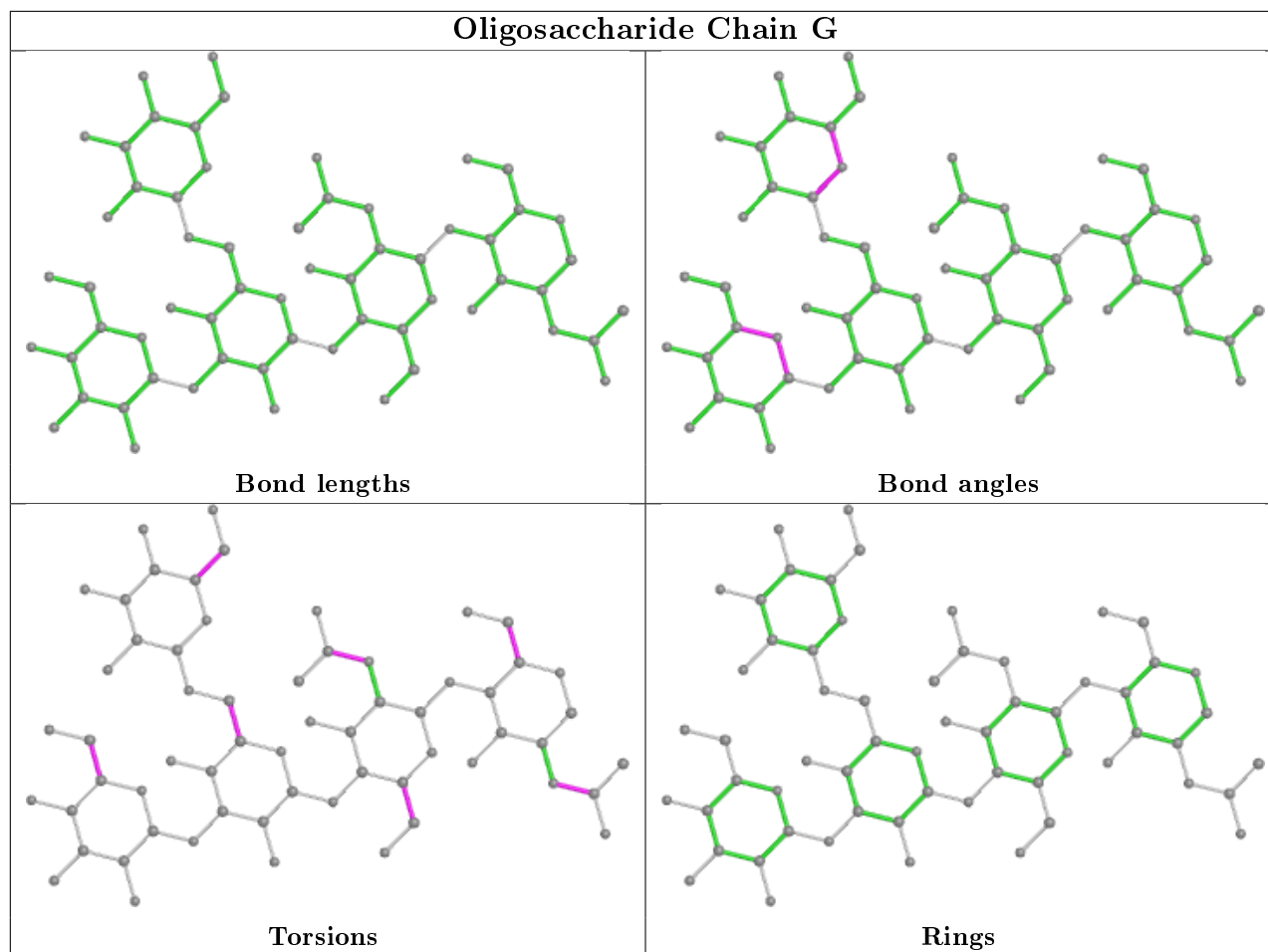












## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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
5	GOL	A	1904	-	5,5,5	0.35	0	5,5,5	0.42	0
5	GOL	A	1901	4	5,5,5	0.34	0	5,5,5	0.30	0
5	GOL	B	2903	-	5,5,5	0.35	0	5,5,5	0.43	0
5	GOL	B	2900	-	5,5,5	0.25	0	5,5,5	0.35	0
5	GOL	A	1903	-	5,5,5	0.25	0	5,5,5	0.32	0
5	GOL	A	1900	-	5,5,5	0.26	0	5,5,5	0.36	0
5	GOL	B	2901	4	5,5,5	0.39	0	5,5,5	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	1904	-	-	0/4/4/4	-
5	GOL	A	1901	4	-	0/4/4/4	-
5	GOL	B	2903	-	-	0/4/4/4	-
5	GOL	B	2900	-	-	0/4/4/4	-
5	GOL	A	1903	-	-	0/4/4/4	-
5	GOL	A	1900	-	-	0/4/4/4	-
5	GOL	B	2901	4	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1904	GOL	3	0
5	B	2903	GOL	1	0
5	A	1903	GOL	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	475/475 (100%)	-0.15	8 (1%) 70 76	7, 18, 38, 57	0
1	B	475/475 (100%)	0.49	47 (9%) 7 11	13, 30, 63, 79	0
All	All	950/950 (100%)	0.17	55 (5%) 23 31	7, 23, 52, 79	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2147	ASP	4.0
1	B	2391	PHE	3.8
1	B	2384	VAL	3.7
1	B	2320	ASN	3.6
1	A	1387	ASP	3.4

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

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

### 6.3 Carbohydrates [i](#)

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

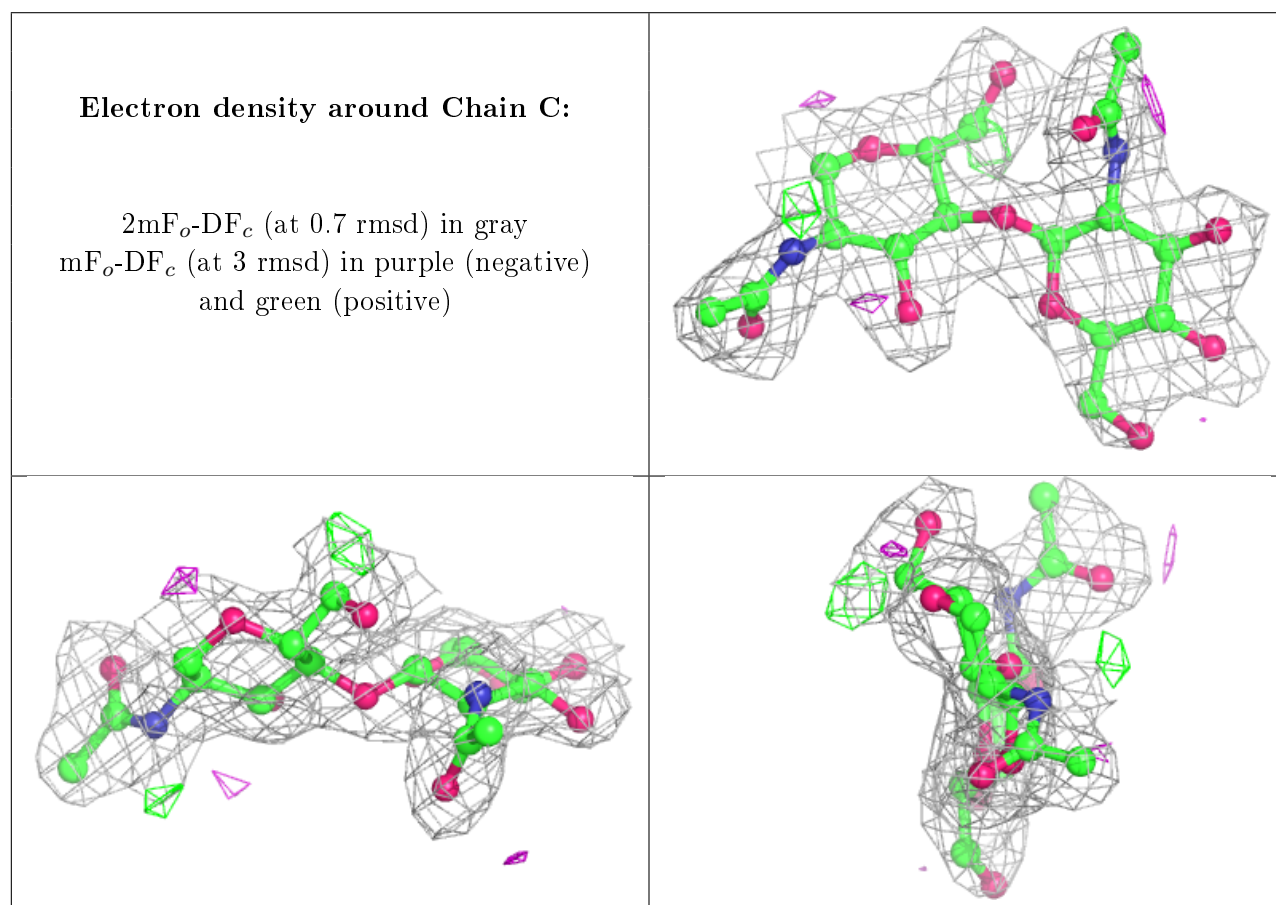
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q < 0.9
2	NAG	F	1	14/15	0.69	0.33	56,58,62,65	0
2	NAG	F	2	14/15	0.72	0.34	68,69,70,70	0
2	NAG	H	2	14/15	0.76	0.35	48,52,56,56	0
3	MAN	D	5	11/12	0.80	0.23	45,48,50,51	11
2	NAG	E	2	14/15	0.81	0.30	45,50,53,54	0

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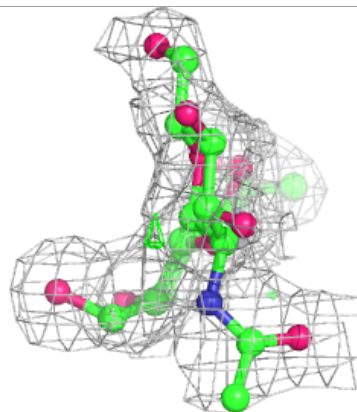
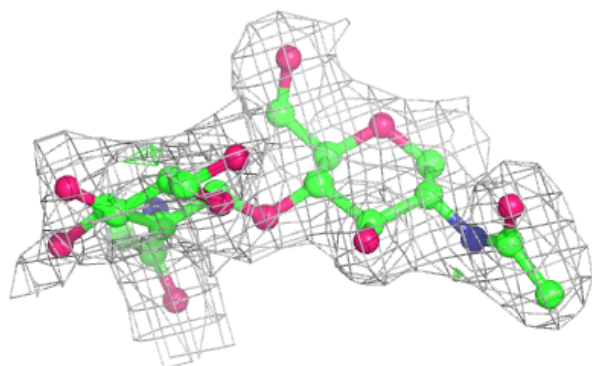
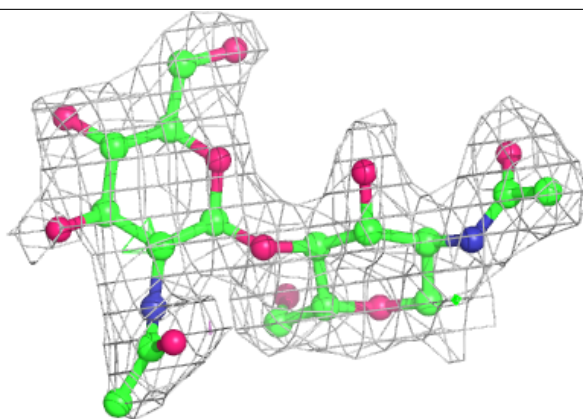
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	C	2	14/15	0.82	0.29	48,51,55,57	0
3	MAN	G	5	11/12	0.83	0.27	47,49,50,52	11
3	NAG	G	2	14/15	0.85	0.18	39,42,43,44	0
3	MAN	D	4	11/12	0.85	0.17	29,30,31,31	10
2	NAG	C	1	14/15	0.86	0.17	28,31,36,42	0
3	MAN	G	4	11/12	0.87	0.22	41,43,45,45	10
3	MAN	G	3	11/12	0.88	0.19	40,43,45,45	11
2	NAG	H	1	14/15	0.90	0.17	26,34,40,45	0
3	MAN	D	3	11/12	0.90	0.13	30,32,37,41	11
2	NAG	E	1	14/15	0.91	0.13	20,25,31,38	0
3	NAG	D	2	14/15	0.91	0.12	26,28,32,32	0
3	NAG	G	1	14/15	0.93	0.14	36,38,39,39	0
3	NAG	D	1	14/15	0.95	0.13	20,24,29,29	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.

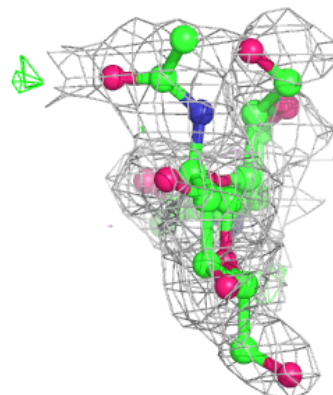
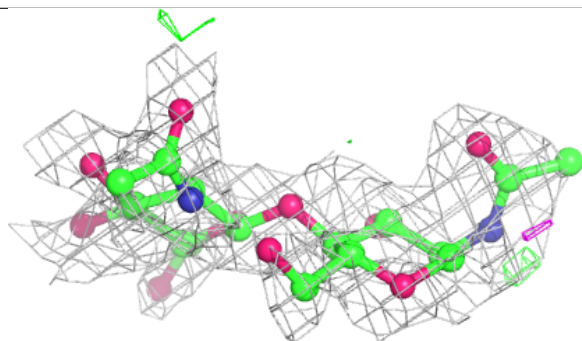
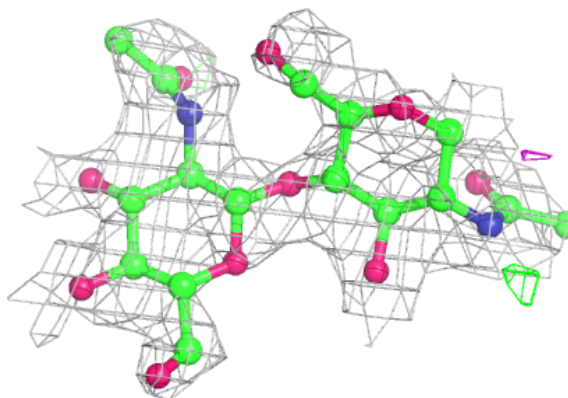


**Electron density around Chain E:**

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

**Electron density around Chain F:**

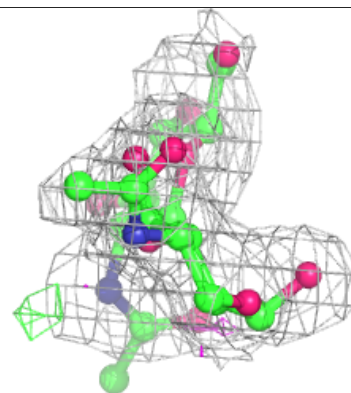
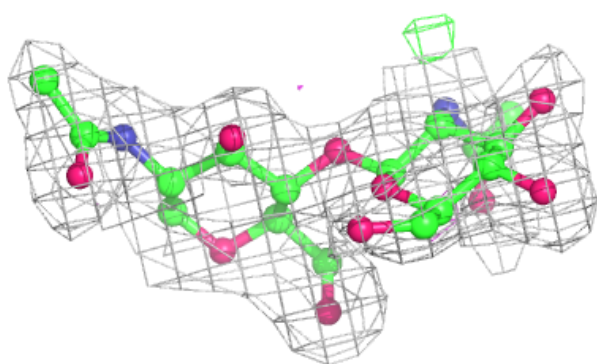
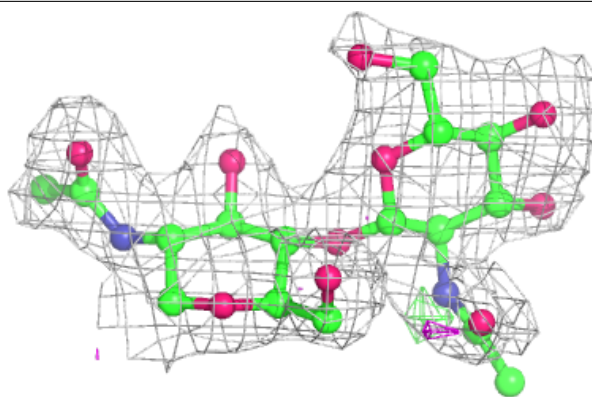
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



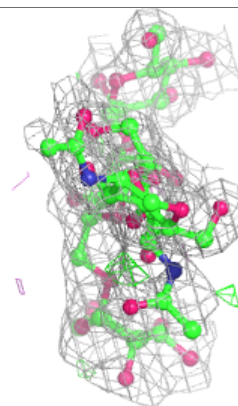
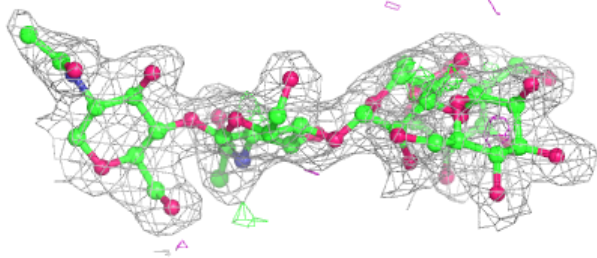
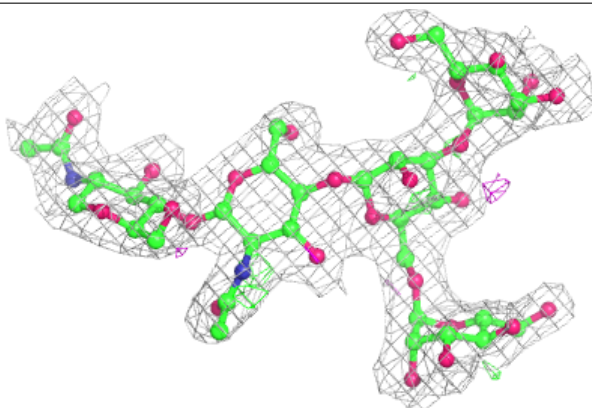


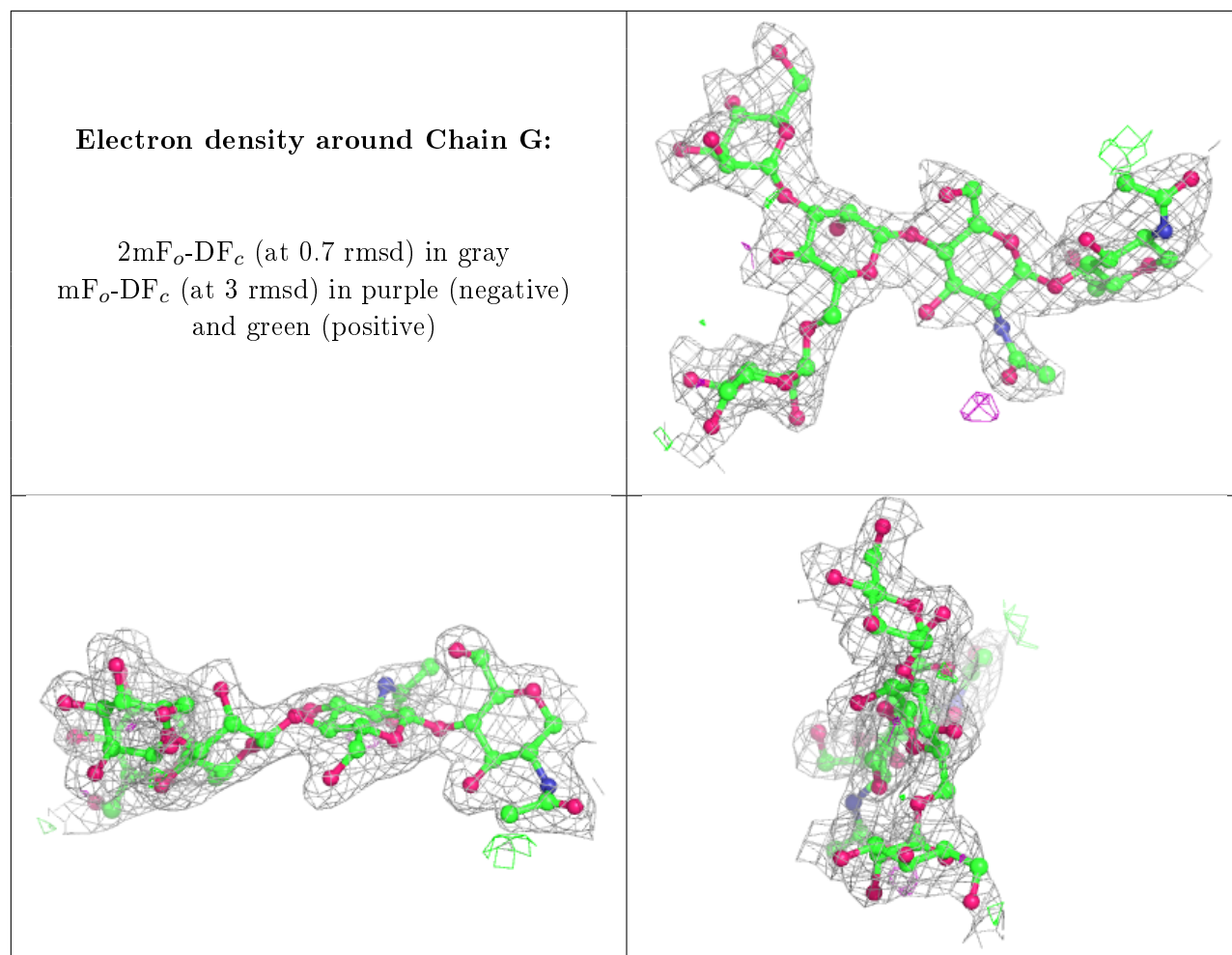
**Electron density around Chain H:**

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

**Electron density around Chain D:**

$2mF_o-DF_c$  (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
5	GOL	A	1904	6/6	0.56	0.36	62,63,64,64	0
5	GOL	B	2903	6/6	0.83	0.17	34,44,45,46	0
5	GOL	B	2900	6/6	0.87	0.14	33,34,35,36	0
5	GOL	A	1903	6/6	0.88	0.23	42,44,44,45	0
5	GOL	A	1900	6/6	0.93	0.15	21,29,30,32	0
5	GOL	B	2901	6/6	0.97	0.07	13,14,15,17	0
5	GOL	A	1901	6/6	0.98	0.06	6,11,11,12	0
4	CA	B	1551	1/1	0.99	0.06	14,14,14,14	0
4	CA	A	1550	1/1	1.00	0.04	12,12,12,12	0

## 6.5 Other polymers

There are no such residues in this entry.