



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 05:29 PM BST

PDB ID : 3OLG  
Title : Structures of human pancreatic alpha-amylase in complex with acarviosatin III03  
Authors : Qin, X.; Ren, L.  
Deposited on : 2010-08-26  
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

The 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

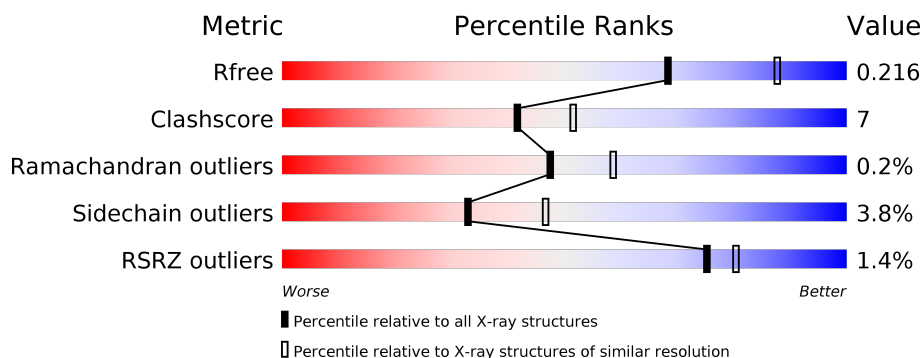
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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 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	496	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 88%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>85%</span> <span>13%</span> </div> </div>
2	B	2	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 100%);"></div> <div style="text-align: center; margin-top: 5px;">100%</div> </div>
3	C	3	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 33%, yellow 67%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>33%</span> <span>67%</span> </div> </div>
4	D	4	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 50%, orange 50%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>50%</span> <span>50%</span> </div> </div>
5	E	3	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 67%, orange 33%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>67%</span> <span>33%</span> </div> </div>

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
4	BGC	D	1	-	-	-	X
5	GLC	E	2	X	-	-	-
5	GLC	E	3	-	-	-	X

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 4384 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 Pancreatic alpha-amylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3939	2492	695	731	21			

There is a discrepancy between the modelled and reference sequences:

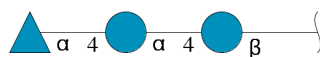
Chain	Residue	Modelled	Actual	Comment	Reference
A	287	MET	VAL	engineered mutation	UNP P04746

- Molecule 2 is an oligosaccharide called alpha-D-quinovopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	2	Total	C	O	0	0	0
			20	12	8			

- Molecule 3 is an oligosaccharide called alpha-D-quinovopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose.



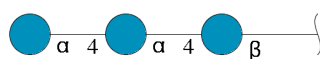
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	C	3	Total	C	O	0	0	0
			32	18	14			

- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	D	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 5 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	E	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

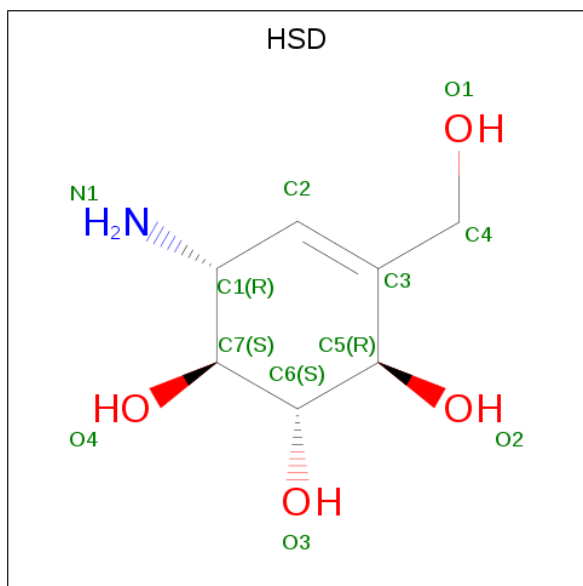
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



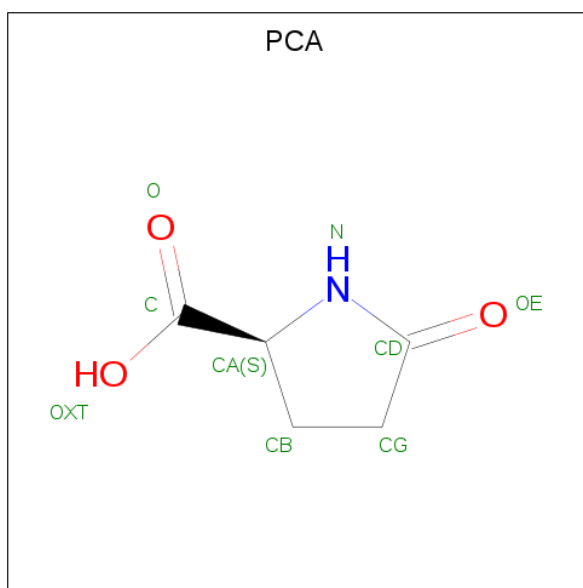
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is (1S,2S,3R,6R)-6-amino-4-(hydroxymethyl)cyclohex-4-ene-1,2,3-triol (three-letter code: HSD) (formula: C<sub>7</sub>H<sub>13</sub>NO<sub>4</sub>).



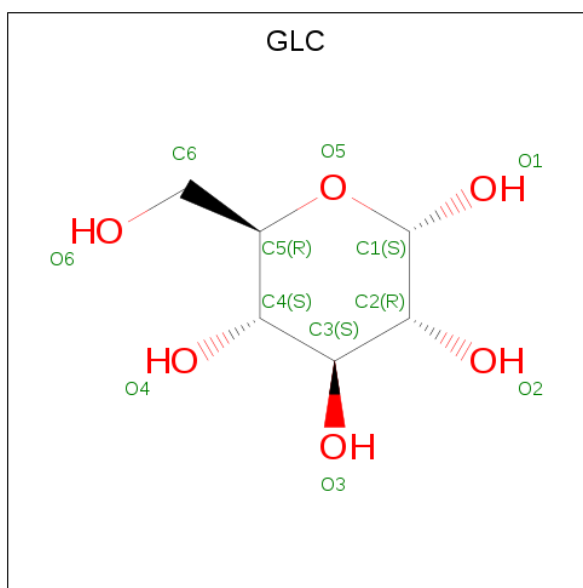
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			12	7	1	4		
9	A	1	Total	C	N	O	0	0
			12	7	1	4		

- Molecule 10 is PYROGLUTAMIC ACID (three-letter code: PCA) (formula:  $C_5H_7NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 11 is alpha-D-glucopyranose (three-letter code: GLC) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 12 is water.

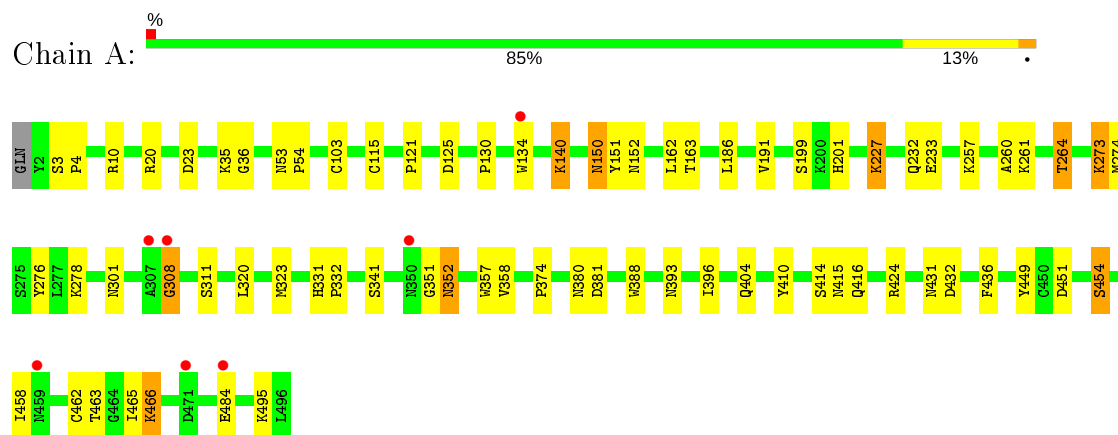
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	263	Total 263	O 263	0	0



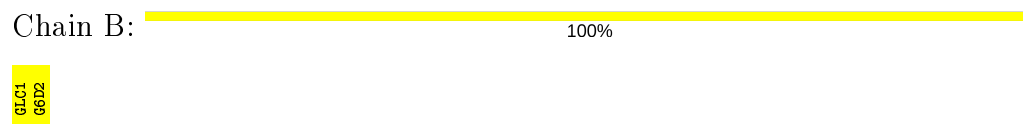
### 3 Residue-property plots

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: Pancreatic alpha-amylase



- Molecule 2: alpha-D-quinovopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 3: alpha-D-quinovopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 5: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain E:

67%

33%

BGL1  
BGL2  
BGL3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.38 Å 74.53 Å 135.74 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.87 – 2.30 40.87 – 2.29	Depositor EDS
% Data completeness (in resolution range)	94.6 (40.87-2.30) 94.0 (40.87-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.93 (at 2.29 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.193 , 0.216 0.190 , 0.216	Depositor DCC
$R_{free}$ test set	1184 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.6	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4384	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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: BGC, HSD, CL, CA, GLC, G6D, SO4, PCA

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	0.40	0/4053	0.66	0/5503

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	3939	0	3711	54	0
2	B	20	0	10	0	0
3	C	32	0	21	0	0
4	D	45	0	39	1	0
5	E	34	0	30	1	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	5	0	0	0	0
9	A	24	0	21	3	0
10	A	8	0	5	0	0
11	A	12	0	12	1	0
12	A	263	0	0	7	0
All	All	4384	0	3849	56	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 7.

The worst 5 of 56 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:163:THR:HB	9:A:500:HSD:H2	1.40	0.87
1:A:150:ASN:ND2	1:A:152:ASN:H	1.95	0.65
1:A:257:LYS:O	1:A:261:LYS:HG2	1.97	0.65
1:A:264:THR:HG22	1:A:311:SER:CB	2.28	0.63
1:A:260:ALA:O	1:A:264:THR:HG23	2.04	0.58

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	493/496 (99%)	471 (96%)	21 (4%)	1 (0%)	47 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	308	GLY

### 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	418/419 (100%)	402 (96%)	16 (4%)	33 47

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	LYS
1	A	264	THR
1	A	352	ASN
1	A	150	ASN
1	A	436	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	476	HIS
1	A	216	ASN
1	A	53	ASN
1	A	152	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 ⓘ

12 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	GLC	B	1	9,2	11,11,12	0.55	0	15,15,17	1.06	2 (13%)
2	G6D	B	2	9,2	9,9,11	0.64	0	10,12,16	2.43	5 (50%)
3	BGC	C	1	3	12,12,12	0.63	0	17,17,17	1.08	2 (11%)
3	GLC	C	2	3	11,11,12	0.57	0	15,15,17	0.87	1 (6%)
3	G6D	C	3	9,3	9,9,11	0.55	0	10,12,16	0.90	0
4	BGC	D	1	4	12,12,12	1.11	1 (8%)	17,17,17	1.91	4 (23%)
4	GLC	D	2	4	11,11,12	0.44	0	15,15,17	0.81	1 (6%)
4	GLC	D	3	4	11,11,12	0.30	0	15,15,17	0.55	0
4	GLC	D	4	4	11,11,12	0.43	0	15,15,17	0.36	0
5	BGC	E	1	5	12,12,12	1.38	3 (25%)	17,17,17	3.01	8 (47%)
5	GLC	E	2	5	11,11,12	1.21	2 (18%)	15,15,17	1.66	3 (20%)
5	GLC	E	3	5	11,11,12	0.76	0	15,15,17	1.74	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
2	GLC	B	1	9,2	-	0/2/19/22	0/1/1/1
2	G6D	B	2	9,2	-	-	0/1/1/1
3	BGC	C	1	3	-	2/2/22/22	0/1/1/1
3	GLC	C	2	3	-	0/2/19/22	0/1/1/1
3	G6D	C	3	9,3	-	-	0/1/1/1
4	BGC	D	1	4	-	1/2/22/22	0/1/1/1
4	GLC	D	2	4	-	0/2/19/22	0/1/1/1
4	GLC	D	3	4	-	0/2/19/22	0/1/1/1
4	GLC	D	4	4	-	0/2/19/22	0/1/1/1
5	BGC	E	1	5	-	2/2/22/22	0/1/1/1
5	GLC	E	2	5	1/1/4/5	0/2/19/22	0/1/1/1
5	GLC	E	3	5	-	0/2/19/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1	BGC	O5-C5	3.08	1.51	1.44
5	E	1	BGC	O5-C1	2.29	1.48	1.42
4	D	1	BGC	C4-C3	2.21	1.57	1.52
5	E	2	GLC	C4-C5	-2.12	1.48	1.53
5	E	2	GLC	C1-C2	2.10	1.57	1.52

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	BGC	C4-C3-C2	-9.49	94.26	110.82
5	E	3	GLC	O5-C1-C2	5.14	118.71	110.77
4	D	1	BGC	C1-C2-C3	-4.45	101.07	110.31
2	B	2	G6D	C3-C4-C5	4.33	118.20	111.23
2	B	2	G6D	C6-C5-C4	-3.91	107.26	113.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	E	2	GLC	C1

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1	BGC	O5-C5-C6-O6
5	E	1	BGC	C4-C5-C6-O6
3	C	1	BGC	C4-C5-C6-O6
3	C	1	BGC	O5-C5-C6-O6
4	D	1	BGC	C4-C5-C6-O6

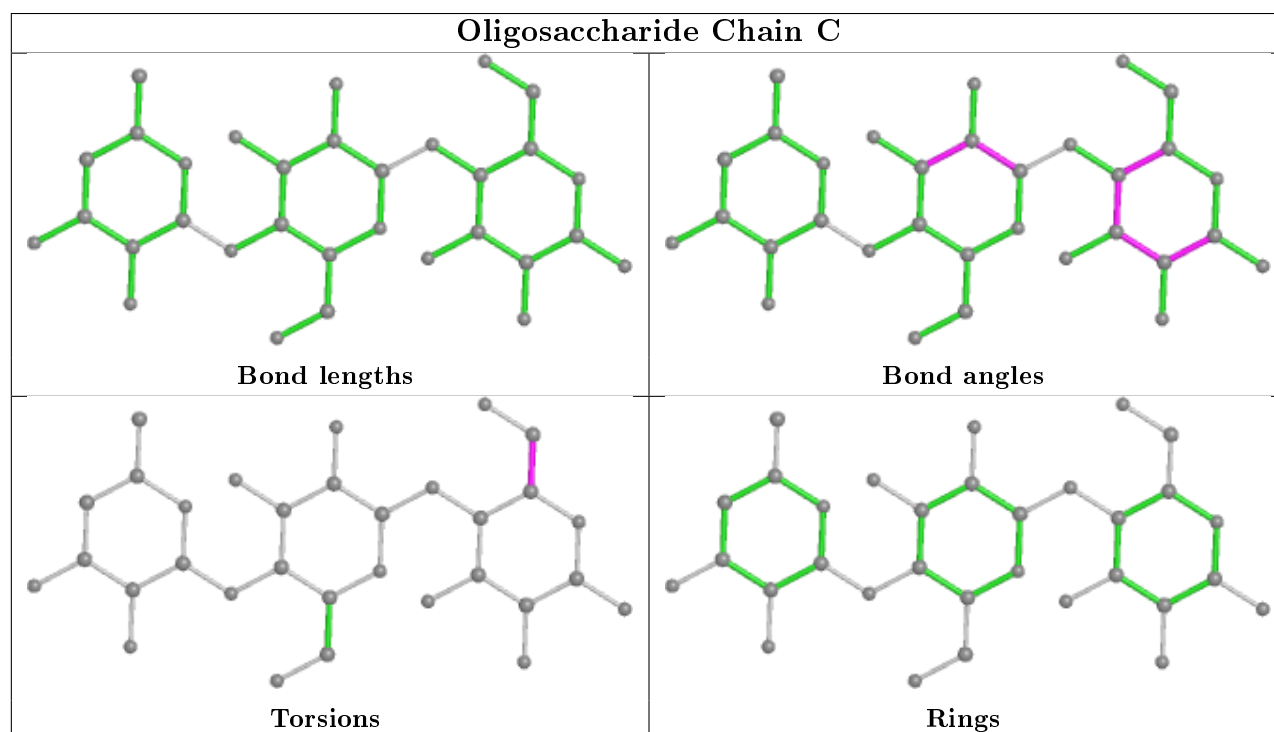
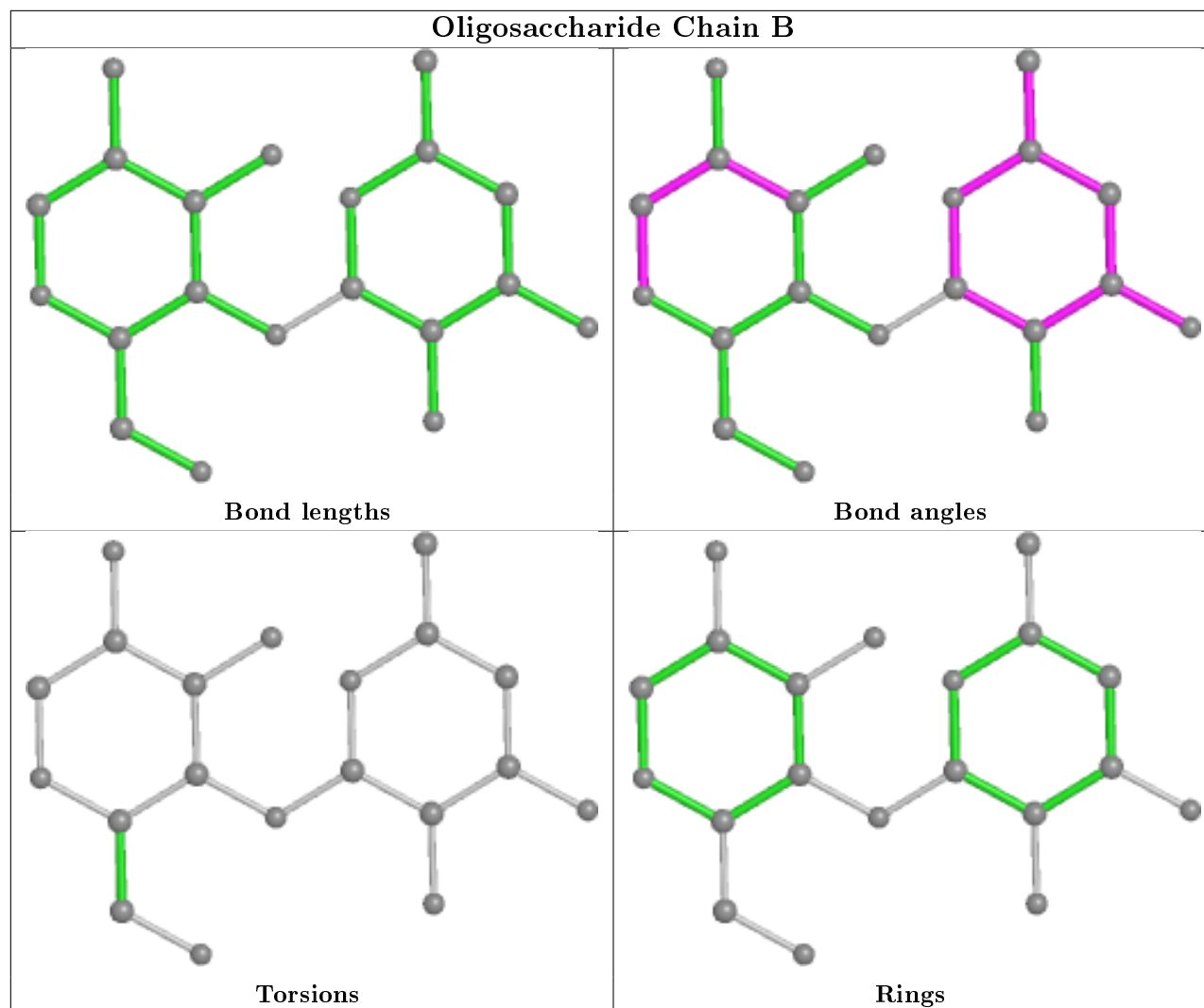
There are no ring outliers.

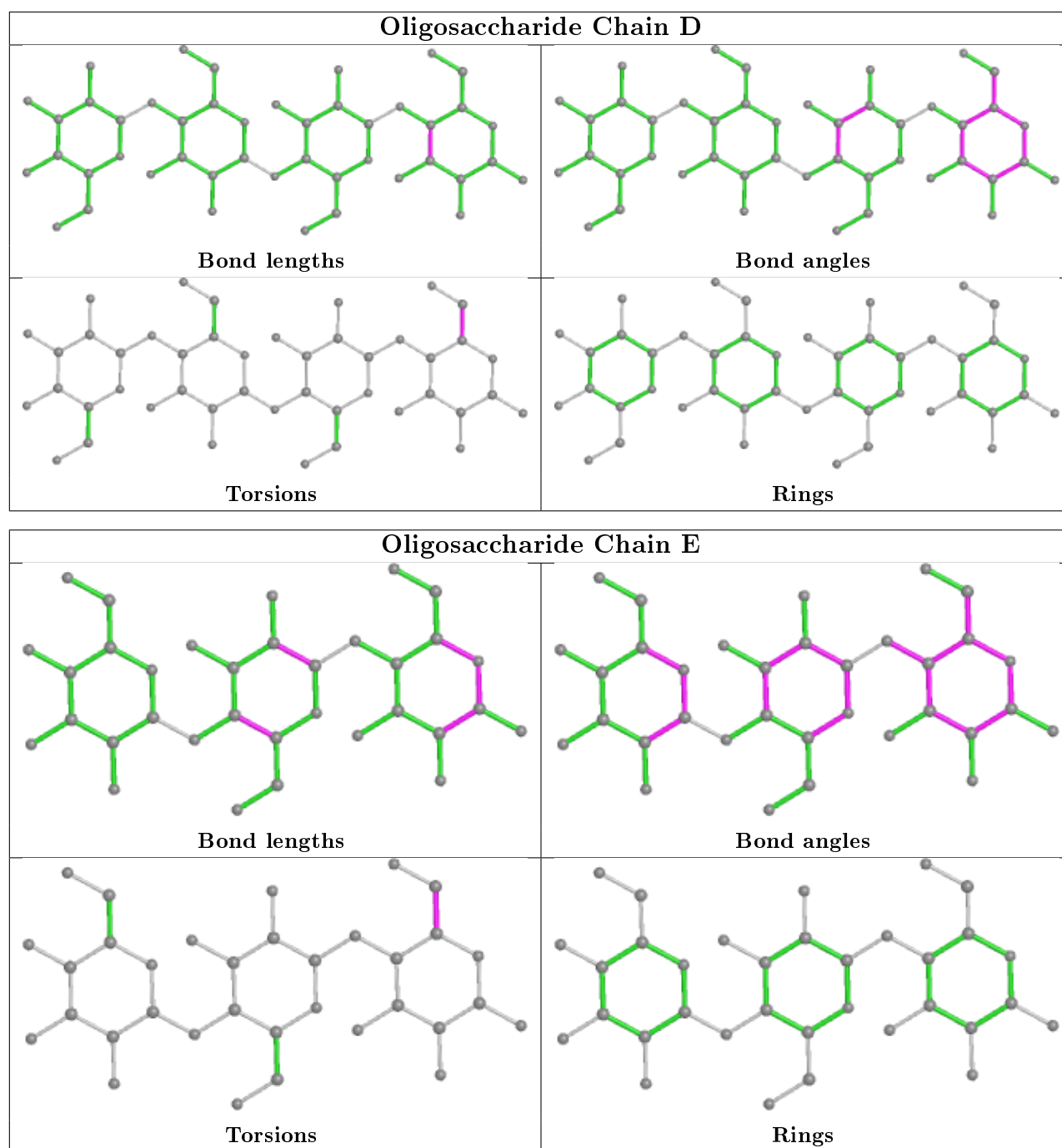
3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	BGC	1	0
5	E	1	BGC	1	0
4	D	2	GLC	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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	GLC	A	512	-	12,12,12	0.52	0	17,17,17	0.47	0
9	HSD	A	503	3,2	12,12,12	1.80	2 (16%)	11,17,17	3.18	4 (36%)
9	HSD	A	500	2	12,12,12	1.68	2 (16%)	11,17,17	3.99	8 (72%)
10	PCA	A	511	1	7,8,9	0.78	0	9,10,12	1.91	3 (33%)
8	SO4	A	499	-	4,4,4	0.27	0	6,6,6	0.05	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
11	GLC	A	512	-	-	0/2/22/22	0/1/1/1
9	HSD	A	503	3,2	-	0/2/22/22	0/1/1/1
9	HSD	A	500	2	-	0/2/22/22	0/1/1/1
10	PCA	A	511	1	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	500	HSD	C2-C3	5.06	1.39	1.32
9	A	503	HSD	C2-C3	4.79	1.39	1.32
9	A	503	HSD	C5-C3	3.40	1.54	1.51
9	A	500	HSD	C5-C3	2.23	1.53	1.51

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	500	HSD	C7-C1-N1	8.08	127.82	111.40
9	A	503	HSD	C7-C1-N1	7.45	126.55	111.40
9	A	500	HSD	O4-C7-C6	5.97	124.16	110.35
9	A	500	HSD	C2-C1-N1	5.58	120.76	110.71
9	A	503	HSD	C2-C1-N1	5.06	119.83	110.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	512	GLC	1	0
9	A	503	HSD	1	0
9	A	500	HSD	2	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	495/496 (99%)	-0.36	7 (1%) 75 80	13, 22, 33, 45	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	GLU	5.0
1	A	308	GLY	3.9
1	A	459	ASN	3.4
1	A	307	ALA	3.0
1	A	471	ASP	2.6

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

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

### 6.3 Carbohydrates [i](#)

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

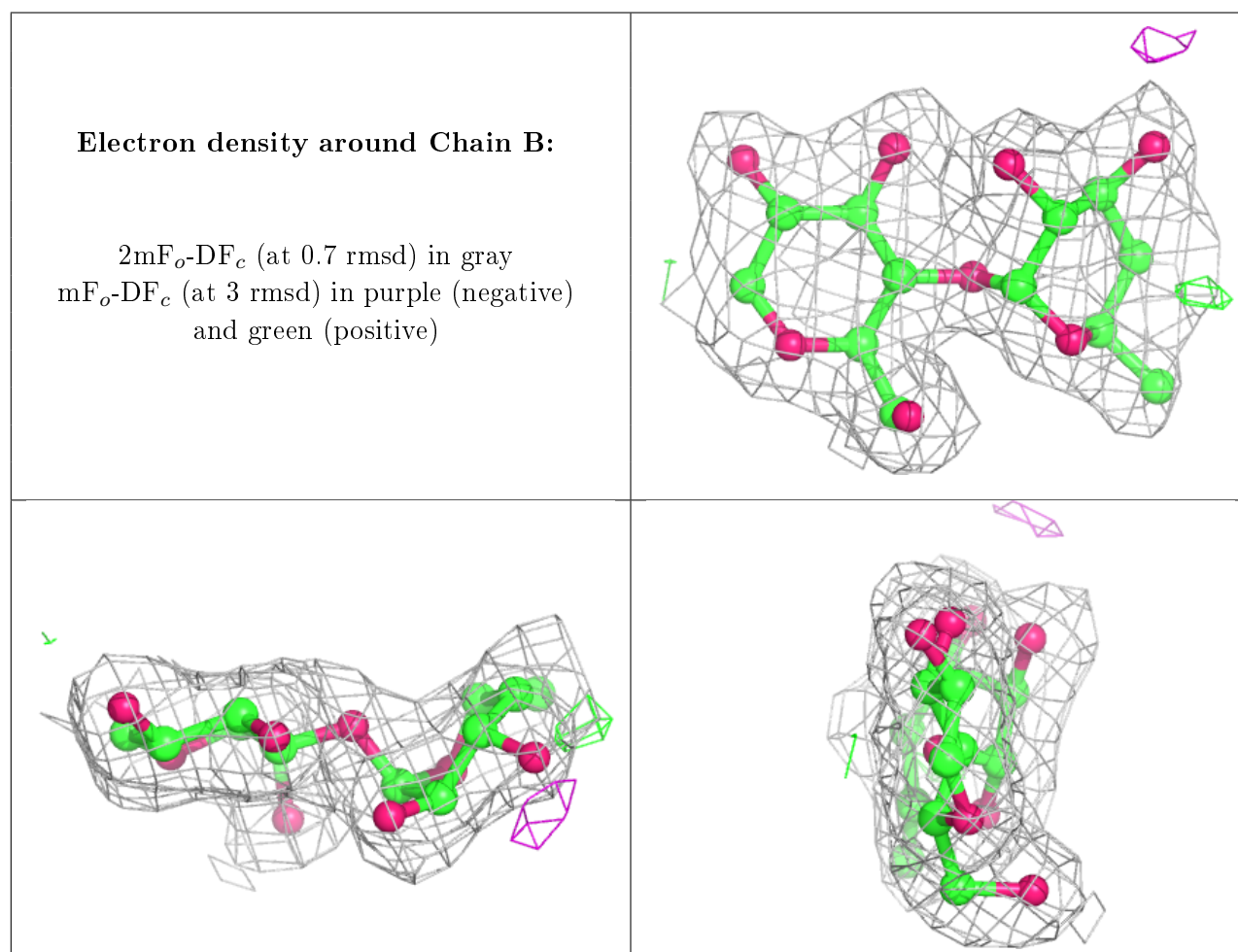
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	GLC	E	3	11/12	0.44	0.68	20,20,20,20	0
4	BGC	D	1	12/12	0.63	0.53	20,20,20,20	0
5	GLC	E	2	11/12	0.66	0.31	42,44,46,48	0
3	BGC	C	1	12/12	0.71	0.22	36,42,43,43	0
5	BGC	E	1	12/12	0.77	0.29	32,37,38,42	0
4	GLC	D	4	11/12	0.80	0.29	44,46,48,51	0
4	GLC	D	2	11/12	0.81	0.18	40,41,42,42	0

*Continued on next page...*

*Continued from previous page...*

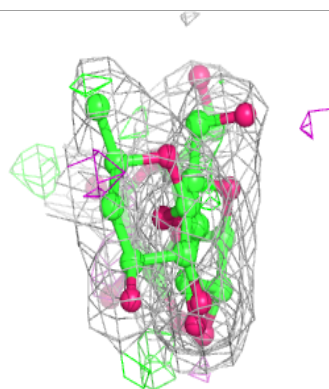
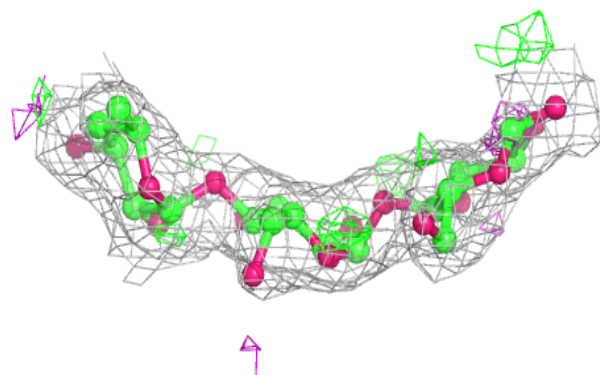
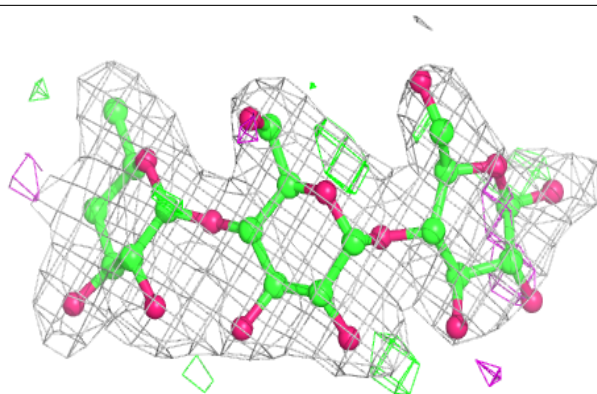
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GLC	D	3	11/12	0.91	0.18	36,40,42,45	0
3	G6D	C	3	9/11	0.92	0.14	22,24,25,25	0
2	G6D	B	2	9/11	0.93	0.13	28,29,31,33	0
3	GLC	C	2	11/12	0.94	0.15	28,32,33,34	0
2	GLC	B	1	11/12	0.96	0.11	19,22,24,26	0

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

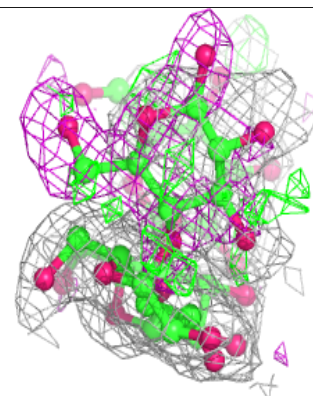
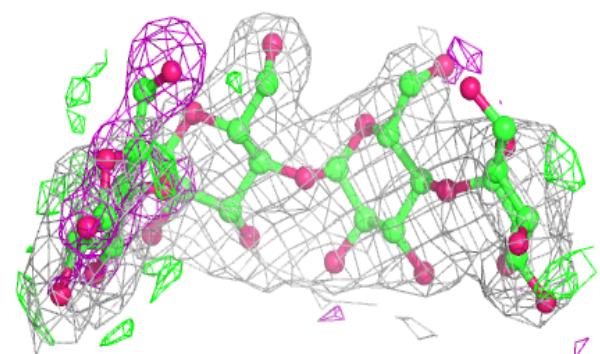
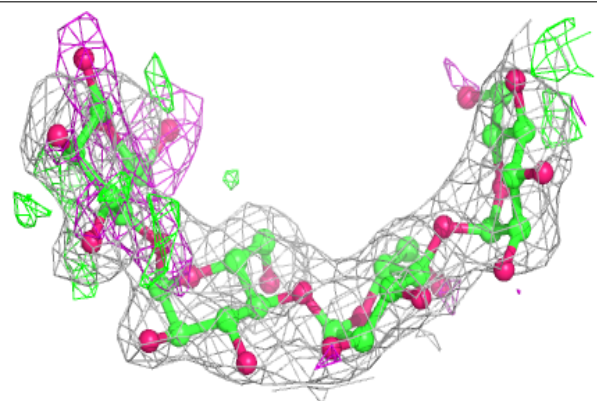


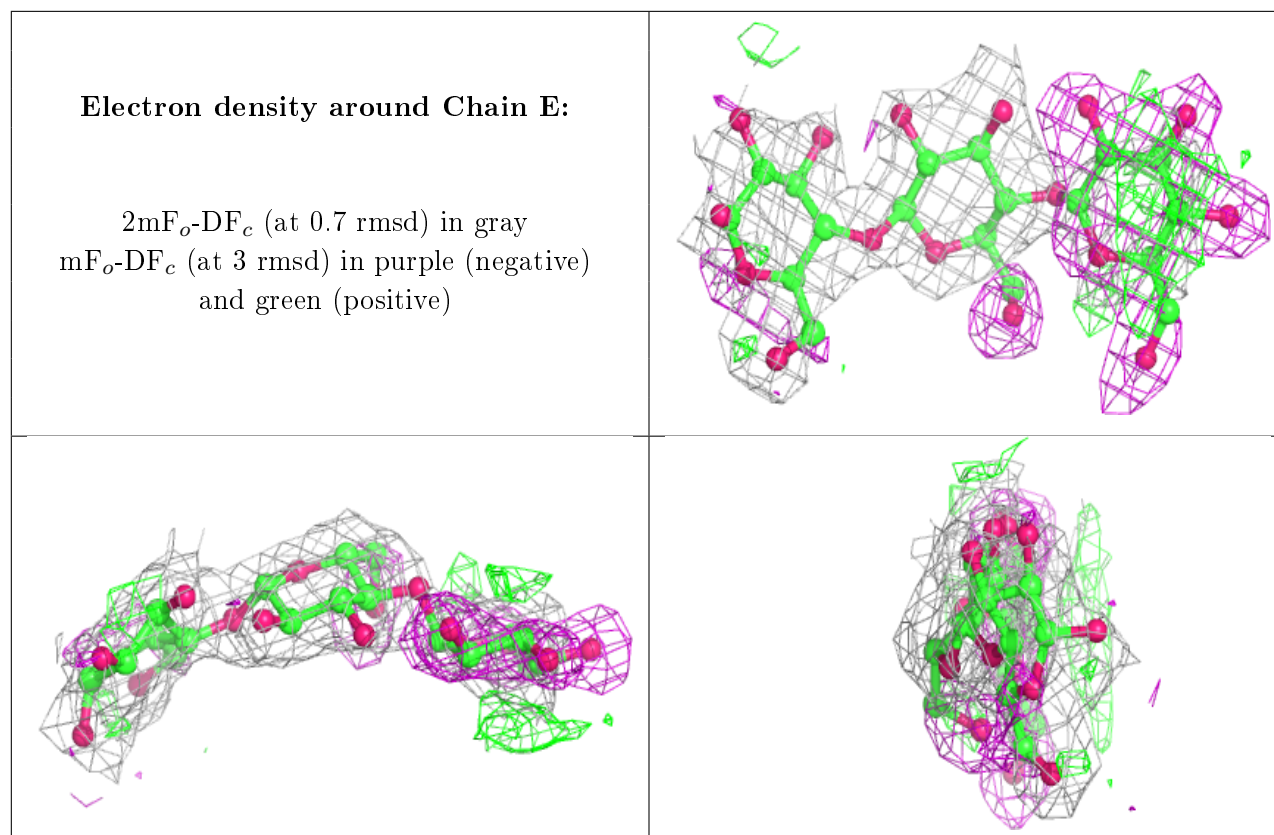
**Electron density around Chain C:**

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

**Electron density around Chain D:**

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





## 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
9	HSD	A	500	12/12	0.67	0.36	39,47,48,48	0
8	SO4	A	499	5/5	0.78	0.32	78,78,79,80	0
11	GLC	A	512	12/12	0.80	0.41	14,17,21,23	0
9	HSD	A	503	12/12	0.81	0.21	22,23,25,27	0
10	PCA	A	511	8/9	0.95	0.14	24,25,25,25	0
6	CA	A	497	1/1	0.98	0.09	29,29,29,29	0
7	CL	A	498	1/1	1.00	0.13	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.