



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 10:39 PM EDT

PDB ID : 3OLE  
Title : Structures of human pancreatic alpha-amylase in complex with acarviosatin II03  
Authors : Qin, X.; Ren, L.  
Deposited on : 2010-08-26  
Resolution : 1.55 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (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

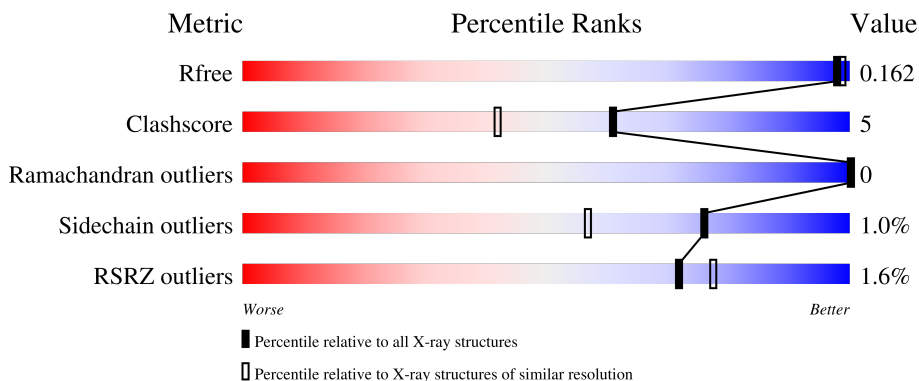
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.55 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	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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	496	 2% 93% 7%
2	B	2	 100%
3	C	3	 33% 67%
4	D	3	 100%
5	E	3	 67% 33%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
10	ACI	A	501	X	-	-	-
10	ACI	A	504	X	-	-	-
5	BGC	E	1	-	-	-	X

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 4650 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
			Total	C	N	O	S			
1	A	495	3939	2492	695	731	21	0	0	0

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
			Total	C	O			
2	B	2	20	12	8	0	0	0

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



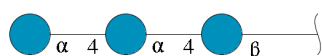
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	C	3	32	18	14	0	0	0

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace	
4	D	3	Total	C	O	0	0	0
			34	18	16			

- 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).

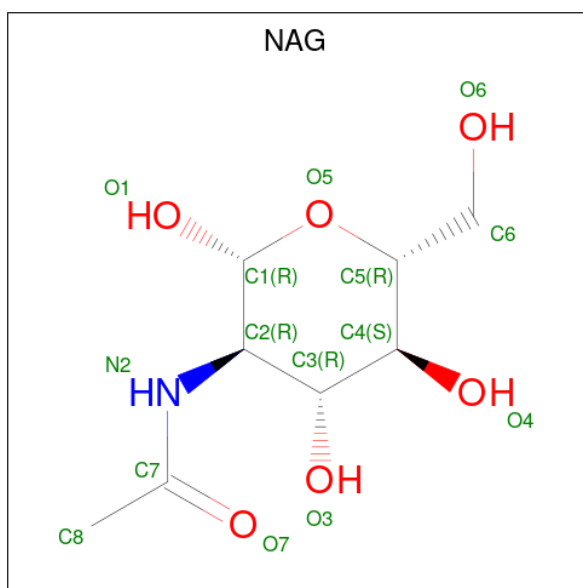
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

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



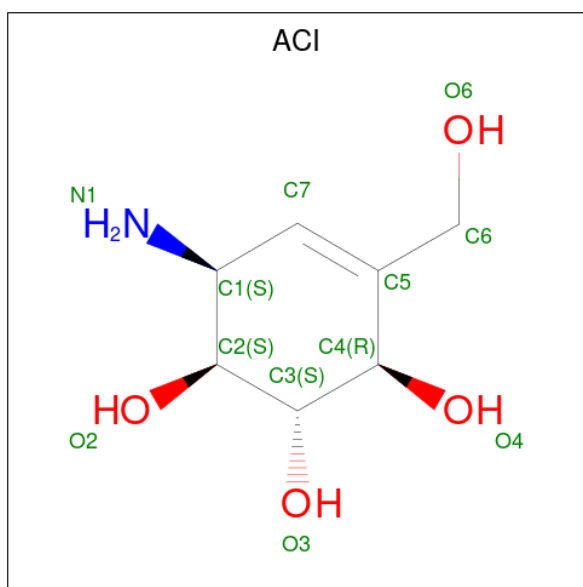
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



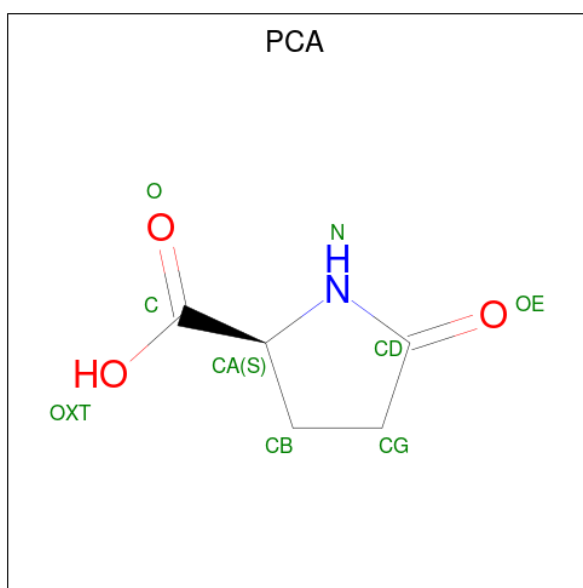
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is 6-AMINO-4-HYDROXYMETHYL-CYCLOHEX-4-ENE-1,2,3-TRIOL (three-letter code: ACI) (formula:  $C_7H_{13}NO_4$ ).



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

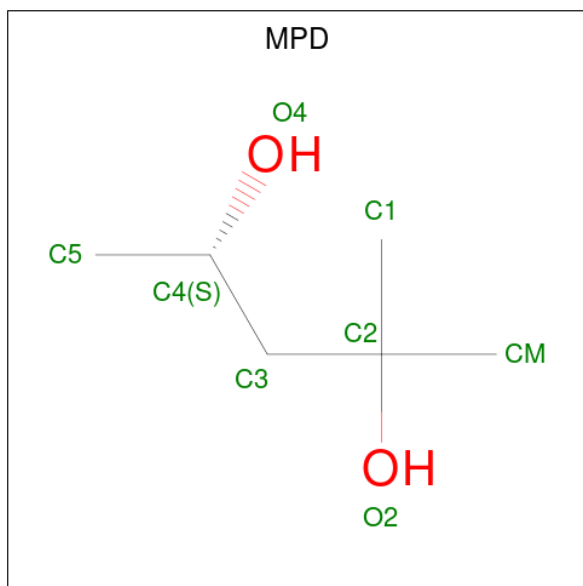
- Molecule 11 is PYROGLUTAMIC ACID (three-letter code: PCA) (formula: C<sub>5</sub>H<sub>7</sub>NO<sub>3</sub>).



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

- Molecule 12 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:

C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C O 8 6 2	0	0

- Molecule 13 is water.

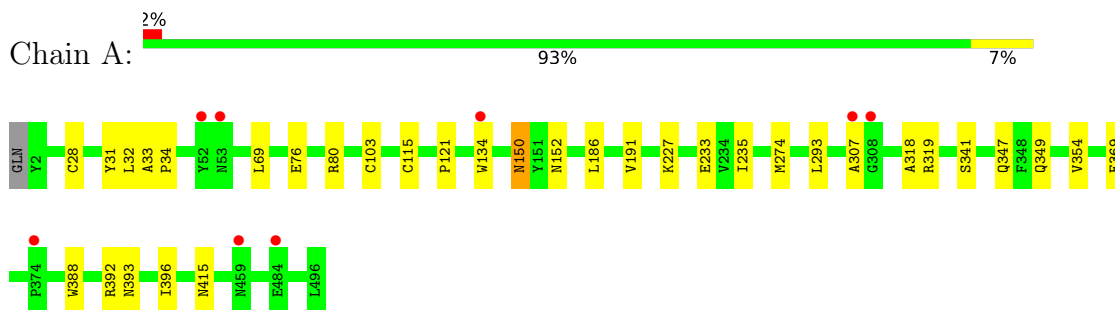
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	530	Total O 530 530	0	0



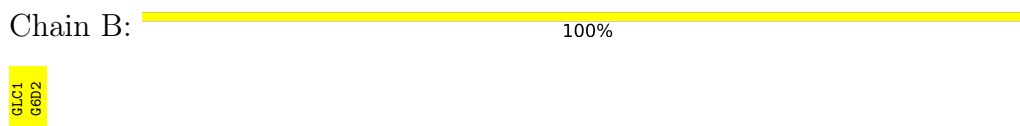
### 3 Residue-property plots [i](#)

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

- Molecule 1: Pancreatic alpha-amylase



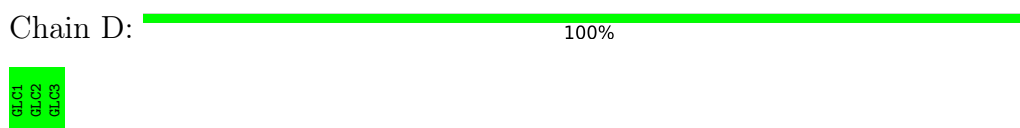
- Molecule 2: alpha-D-quinovopyranose-(1-4)-alpha-D-glucopyranose



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



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



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



BGL1  
GLC2  
GLC3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.33Å 67.88Å 130.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.16 – 1.55 26.16 – 1.55	Depositor EDS
% Data completeness (in resolution range)	98.1 (26.16-1.55) 98.1 (26.16-1.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.86 (at 1.55Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.166 , 0.178 0.162 , 0.162	Depositor DCC
$R_{free}$ test set	3387 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.6	Xtrriage
Anisotropy	0.363	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4650	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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: CL, SO4, GLC, ACI, BGC, MPD, CA, PCA, G6D, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.31	0/4053	0.62	1/5503 (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	A	293	LEU	N-CA-C	-5.01	97.47	111.00

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	3939	0	3710	32	0
2	B	20	0	10	1	0
3	C	32	0	21	0	0
4	D	34	0	30	0	0
5	E	34	0	30	3	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	5	0	0	0	0
9	A	14	0	13	0	0
10	A	24	0	21	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	8	0	5	1	0
12	A	8	0	14	3	0
13	A	530	0	0	9	0
All	All	4650	0	3854	36	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 5.

All (36) 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)
12:A:515:MPD:H13	2:B:1:GLC:O3	1.62	0.97
1:A:307:ALA:HA	13:A:674:HOH:O	1.64	0.97
12:A:515:MPD:H11	12:A:515:MPD:O4	1.89	0.72
1:A:396:ILE:HD11	13:A:1035:HOH:O	1.94	0.66
1:A:103:CYS:SG	1:A:121:PRO:HG3	2.36	0.66
1:A:347:GLN:HE21	1:A:349:GLN:HE21	1.45	0.64
1:A:150:ASN:HD22	1:A:152:ASN:H	1.47	0.61
1:A:80:ARG:HD3	13:A:925:HOH:O	2.01	0.61
1:A:150:ASN:ND2	1:A:152:ASN:H	2.02	0.57
1:A:369:GLU:HG2	13:A:1004:HOH:O	2.05	0.56
1:A:349:GLN:OE1	1:A:354:VAL:HG11	2.07	0.54
1:A:31:TYR:OH	1:A:392:ARG:HG3	2.07	0.54
1:A:318:ALA:HB3	5:E:1:BGC:H2	1.88	0.54
1:A:393:ASN:O	1:A:396:ILE:CG2	2.57	0.53
1:A:393:ASN:O	1:A:396:ILE:HG23	2.09	0.52
1:A:186:LEU:O	1:A:191:VAL:HG22	2.11	0.51
1:A:393:ASN:HA	1:A:396:ILE:HG22	1.91	0.51
1:A:69:LEU:HD12	1:A:76:GLU:HG3	1.93	0.51
1:A:274:MET:H	1:A:415:ASN:HD22	1.60	0.50
1:A:186:LEU:C	1:A:191:VAL:HG22	2.33	0.49
12:A:515:MPD:O4	12:A:515:MPD:C1	2.61	0.48
1:A:274:MET:H	1:A:415:ASN:ND2	2.13	0.47
1:A:319:ARG:NH1	13:A:616:HOH:O	2.42	0.47
1:A:150:ASN:HD22	1:A:150:ASN:C	2.21	0.45
1:A:227:LYS:HB3	1:A:227:LYS:HE3	1.86	0.44
11:A:511:PCA:HB3	13:A:979:HOH:O	2.17	0.43
1:A:396:ILE:CG2	13:A:755:HOH:O	2.66	0.43
1:A:235:ILE:HG21	1:A:307:ALA:HB3	2.00	0.43
1:A:28:CYS:HA	1:A:32:LEU:HB2	2.02	0.42
1:A:33:ALA:HB3	1:A:34:PRO:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ALA:CB	5:E:1:BGC:H2	2.50	0.41
1:A:392:ARG:CD	13:A:640:HOH:O	2.69	0.41
1:A:347:GLN:HE21	1:A:349:GLN:NE2	2.14	0.40
1:A:233:GLU:OE2	10:A:504:ACI:N1	2.54	0.40
1:A:388:TRP:CD1	5:E:2:GLC:H61	2.57	0.40
1:A:396:ILE:HG23	13:A:755:HOH:O	2.21	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	493/496 (99%)	481 (98%)	12 (2%)	0	<a href="#">100</a> <a href="#">100</a>

There are no Ramachandran outliers to report.

### 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%)	414 (99%)	4 (1%)	<a href="#">76</a> <a href="#">57</a>

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	CYS
1	A	134	TRP
1	A	150	ASN
1	A	341	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	15	HIS
1	A	150	ASN
1	A	152	ASN
1	A	216	ASN
1	A	347	GLN
1	A	415	ASN
1	A	459	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](#)

11 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	10,2	11,11,12	0.37	0	15,15,17	0.85	0
2	G6D	B	2	10,2	9,9,11	0.52	0	10,12,16	1.13	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GLC	C	1	3	12,12,12	0.42	0	17,17,17	0.68	1 (5%)
3	GLC	C	2	3	11,11,12	0.87	1 (9%)	15,15,17	0.58	0
3	G6D	C	3	10,3	9,9,11	0.53	0	10,12,16	0.88	0
4	GLC	D	1	4	12,12,12	0.38	0	17,17,17	0.35	0
4	GLC	D	2	4	11,11,12	0.46	0	15,15,17	0.54	0
4	GLC	D	3	4	11,11,12	0.48	0	15,15,17	0.29	0
5	BGC	E	1	5	12,12,12	0.82	0	17,17,17	1.74	3 (17%)
5	GLC	E	2	5	11,11,12	0.47	0	15,15,17	0.71	0
5	GLC	E	3	5	11,11,12	1.04	1 (9%)	15,15,17	0.63	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	GLC	B	1	10,2	-	0/2/19/22	0/1/1/1
2	G6D	B	2	10,2	-	-	0/1/1/1
3	GLC	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	10,3	-	-	0/1/1/1
4	GLC	D	1	4	-	0/2/22/22	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
5	BGC	E	1	5	-	2/2/22/22	0/1/1/1
5	GLC	E	2	5	-	0/2/19/22	0/1/1/1
5	GLC	E	3	5	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	3	GLC	C2-C3	-2.26	1.49	1.52
3	C	2	GLC	O5-C1	2.04	1.47	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	BGC	C4-C3-C2	-4.87	102.32	110.82
5	E	1	BGC	C6-C5-C4	2.98	119.98	113.00
5	E	1	BGC	C3-C4-C5	-2.42	105.92	110.24
3	C	1	GLC	C4-C3-C2	-2.12	107.13	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	G6D	O5-C5-C4	2.11	111.45	109.34

There are no chirality outliers.

All (4) torsion outliers are listed below:

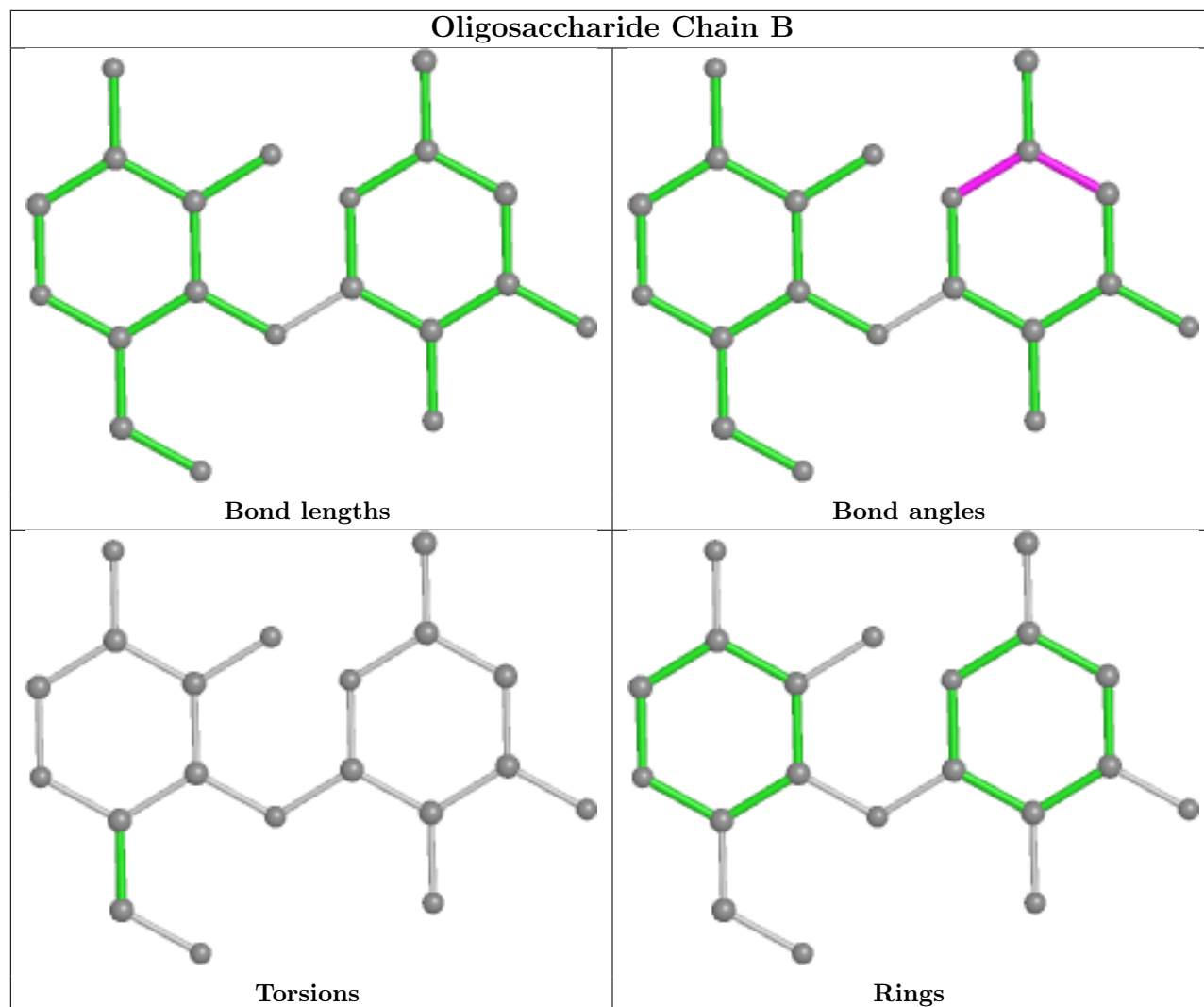
Mol	Chain	Res	Type	Atoms
3	C	1	GLC	O5-C5-C6-O6
5	E	1	BGC	C4-C5-C6-O6
5	E	1	BGC	O5-C5-C6-O6
3	C	1	GLC	C4-C5-C6-O6

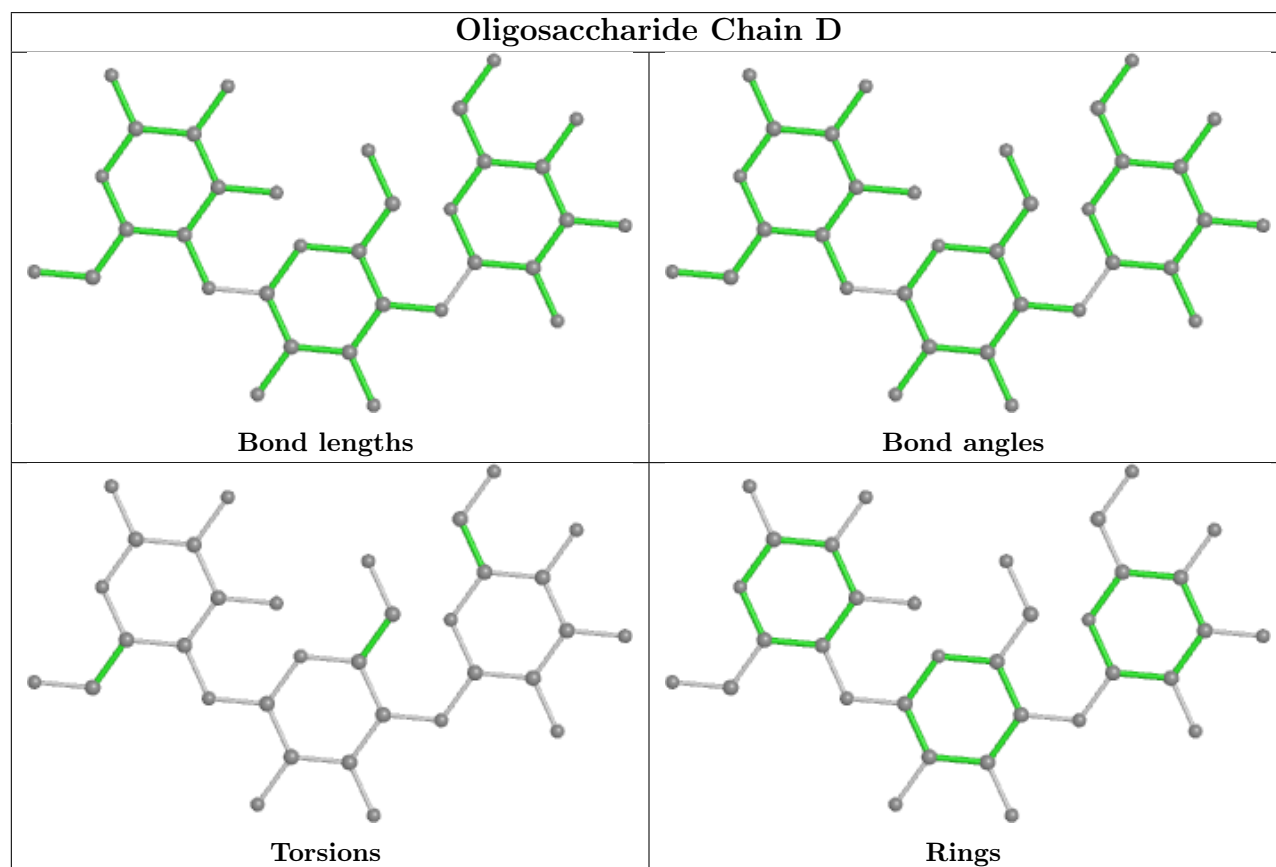
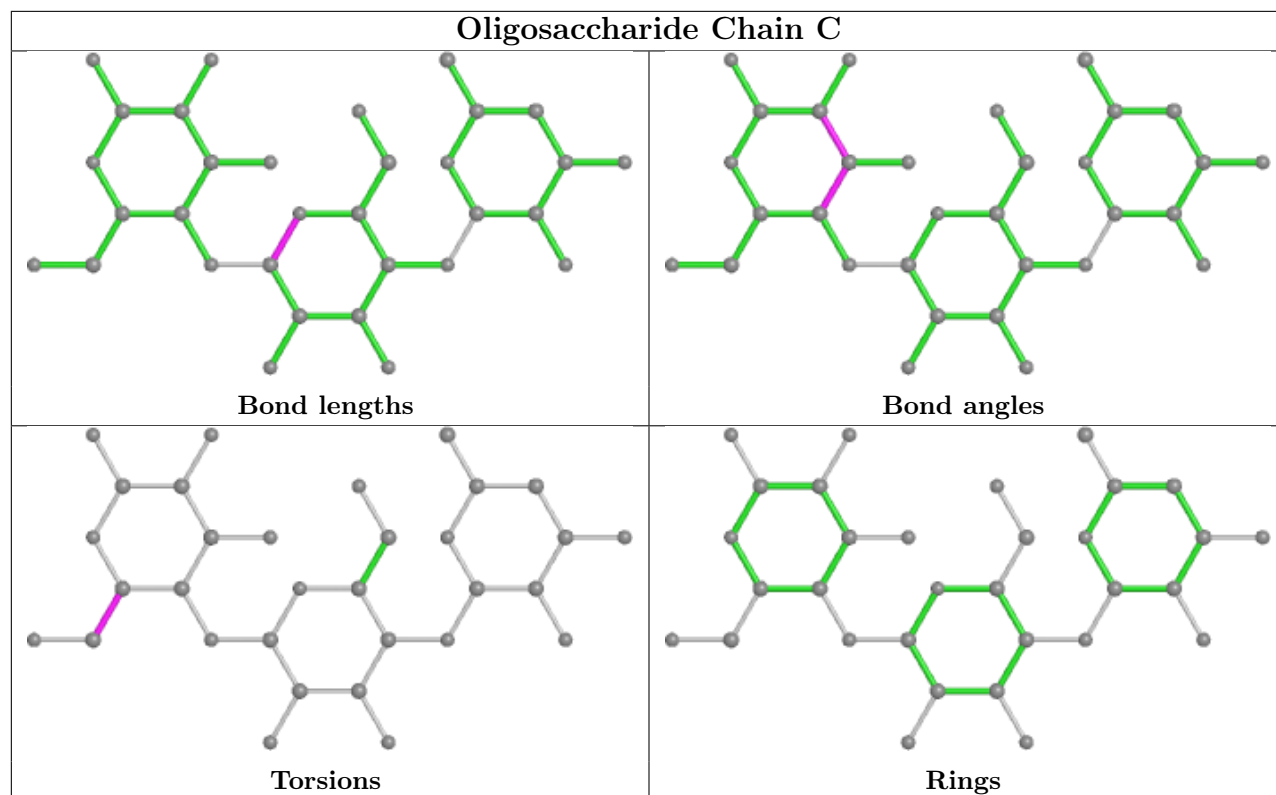
There are no ring outliers.

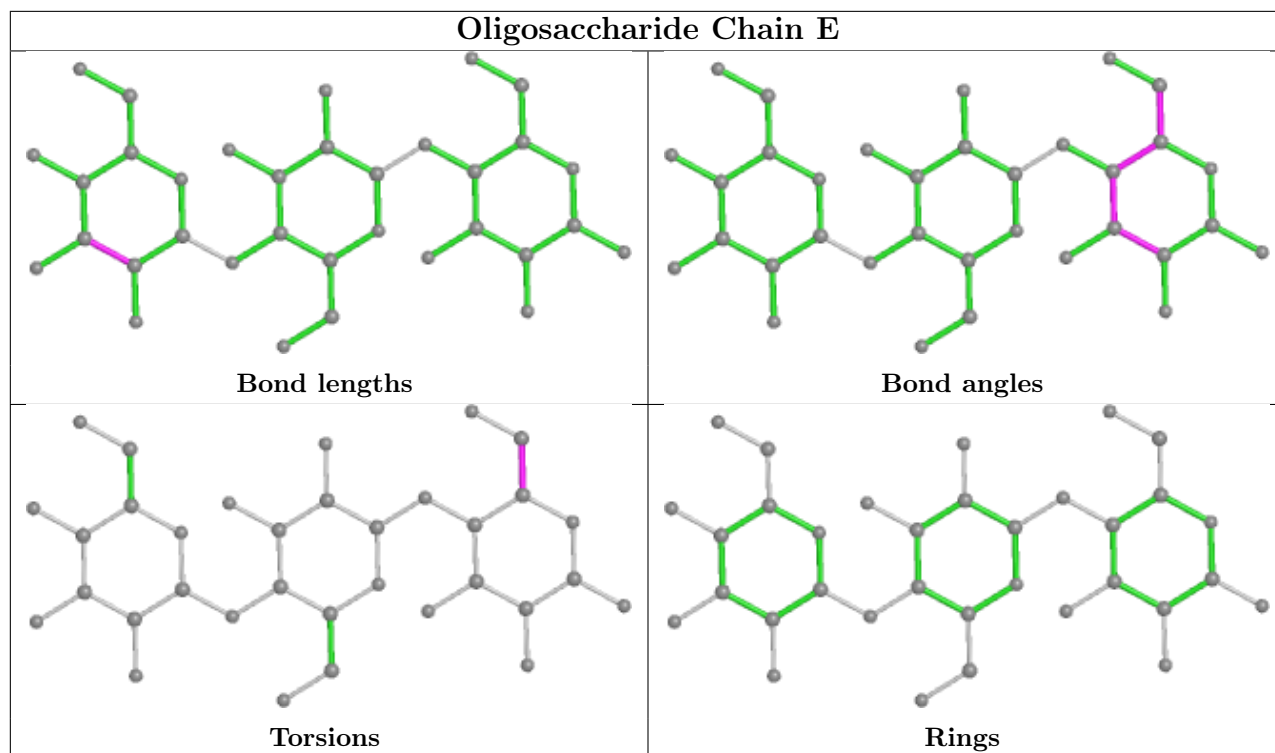
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	2	GLC	1	0
2	B	1	GLC	1	0
5	E	1	BGC	2	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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	PCA	A	511	1	7,8,9	0.76	0	9,10,12	1.90	2 (22%)
12	MPD	A	515	-	7,7,7	0.33	0	9,10,10	0.34	0
10	ACI	A	504	2,3	12,12,12	1.79	2 (16%)	11,17,17	3.48	5 (45%)
8	SO4	A	499	-	4,4,4	0.23	0	6,6,6	0.05	0
10	ACI	A	501	2	12,12,12	1.89	2 (16%)	11,17,17	3.17	4 (36%)
9	NAG	A	500	1	14,14,15	0.42	0	17,19,21	0.64	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	PCA	A	511	1	-	0/0/11/13	0/1/1/1
12	MPD	A	515	-	-	0/5/5/5	-
10	ACI	A	504	2,3	1/1/5/6	1/2/22/22	0/1/1/1
10	ACI	A	501	2	1/1/5/6	0/2/22/22	0/1/1/1
9	NAG	A	500	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	504	ACI	C7-C5	4.55	1.39	1.32
10	A	501	ACI	C7-C5	4.48	1.39	1.32
10	A	501	ACI	C4-C5	4.16	1.54	1.51
10	A	504	ACI	C4-C5	3.64	1.54	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	501	ACI	C7-C1-N1	8.84	126.63	110.71
10	A	504	ACI	C2-C1-N1	7.03	125.68	111.40
10	A	504	ACI	C7-C1-N1	6.09	121.68	110.71
10	A	504	ACI	O2-C2-C3	5.34	122.69	110.35
10	A	501	ACI	O2-C2-C3	4.10	119.83	110.35
11	A	511	PCA	CB-CG-CD	-3.80	98.27	104.40
11	A	511	PCA	O-C-CA	-2.86	117.28	124.78
10	A	501	ACI	C2-C1-N1	2.76	117.00	111.40
10	A	504	ACI	O2-C2-C1	2.54	113.81	108.96
10	A	501	ACI	O3-C3-C4	2.35	114.17	109.68
10	A	504	ACI	O4-C4-C3	-2.29	105.81	110.53

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	A	501	ACI	C1
10	A	504	ACI	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	504	ACI	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	511	PCA	1	0
12	A	515	MPD	3	0
10	A	504	ACI	1	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%)	0.01	8 (1%) 72 77	5, 10, 18, 29	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	GLY	8.4
1	A	134	TRP	4.2
1	A	52	TYR	4.1
1	A	307	ALA	3.4
1	A	459	ASN	2.9
1	A	484	GLU	2.8
1	A	374	PRO	2.6
1	A	53	ASN	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.

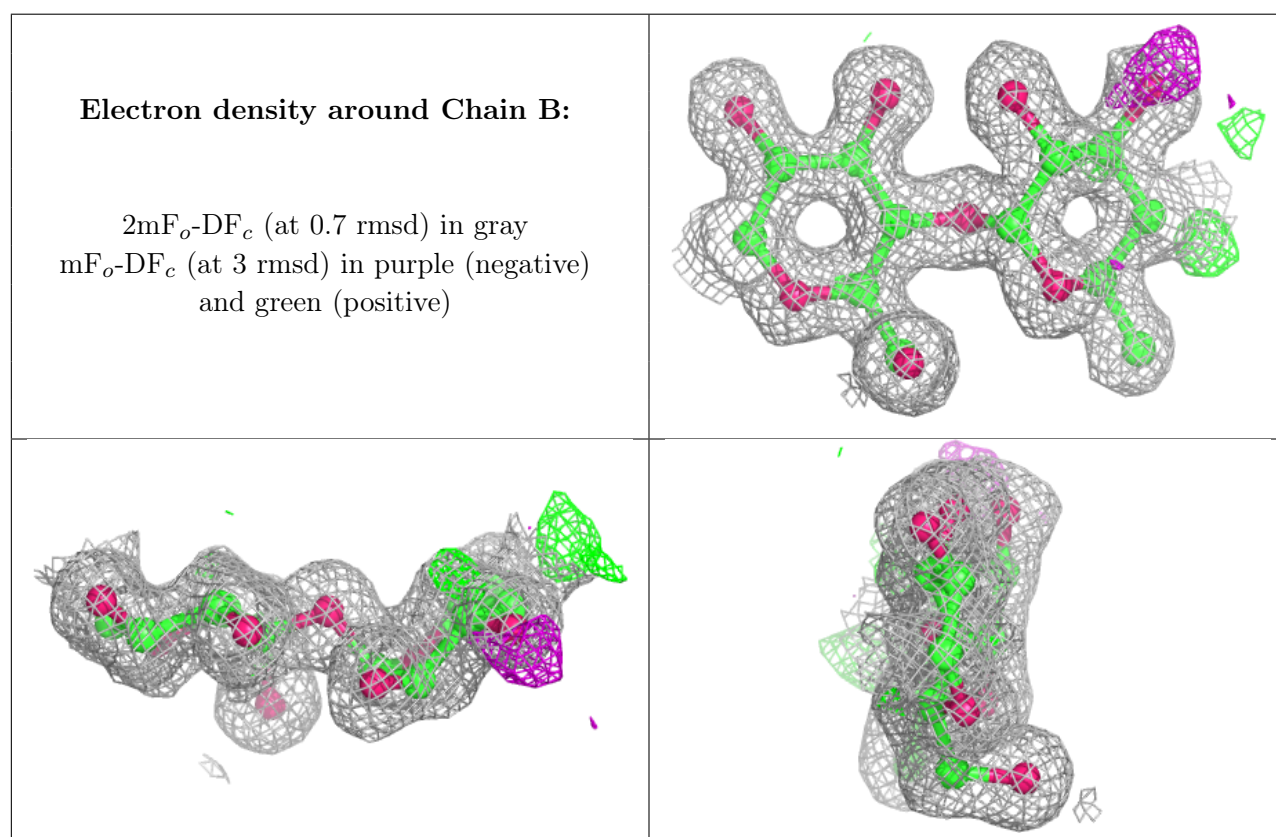
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	BGC	E	1	12/12	0.62	0.48	25,32,34,34	0
3	GLC	C	1	12/12	0.71	0.23	18,27,30,30	0
4	GLC	D	3	11/12	0.80	0.27	26,28,31,34	0
5	GLC	E	3	11/12	0.90	0.14	12,17,20,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	G6D	B	2	9/11	0.92	0.11	8,9,10,10	0
3	GLC	C	2	11/12	0.92	0.11	9,11,15,20	0
4	GLC	D	1	12/12	0.92	0.16	15,19,23,24	0
5	GLC	E	2	11/12	0.93	0.08	15,17,21,21	0
4	GLC	D	2	11/12	0.94	0.13	14,17,22,23	0
3	G6D	C	3	9/11	0.96	0.10	7,7,8,8	0
2	GLC	B	1	11/12	0.97	0.08	6,7,8,8	0

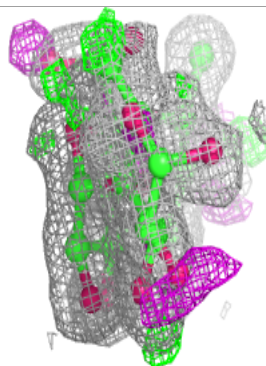
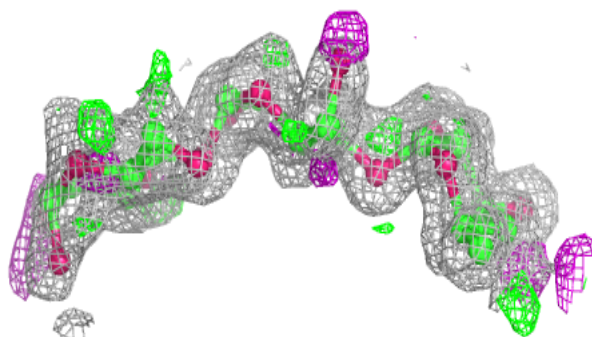
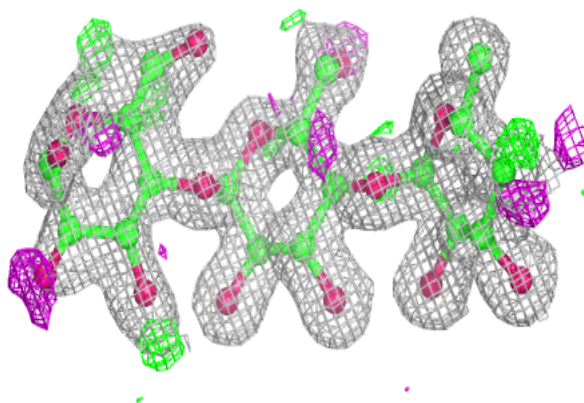
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



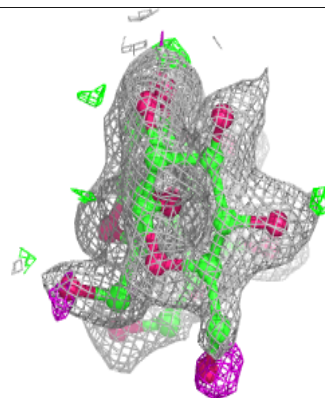
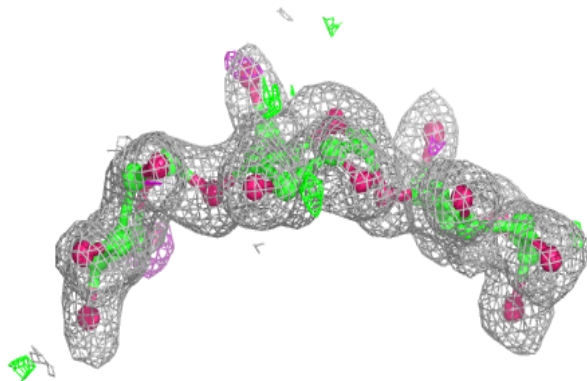
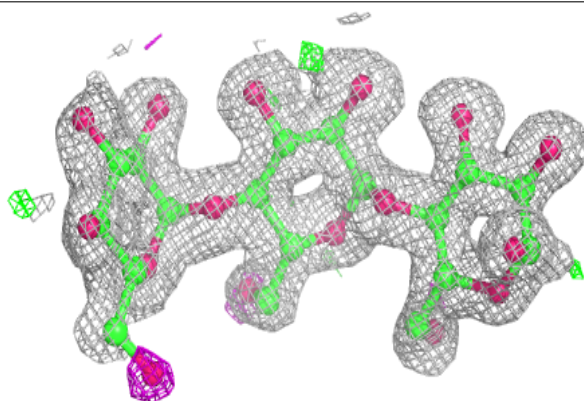


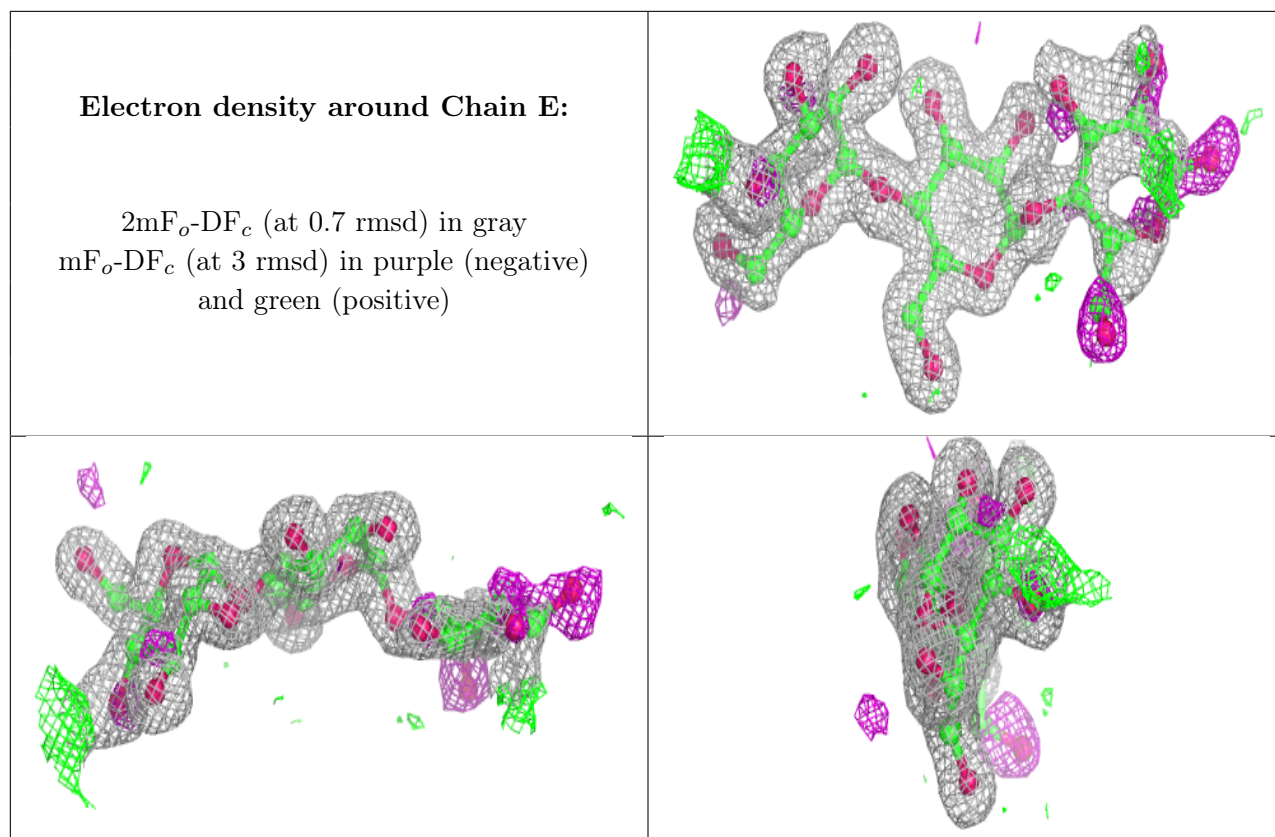
**Electron density around Chain C:**

$2mF_o-DF_c$  (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	NAG	A	500	14/15	0.61	0.23	23,25,29,31	0
12	MPD	A	515	8/8	0.62	0.28	21,23,24,25	0
8	SO4	A	499	5/5	0.82	0.22	45,45,46,46	0
10	ACI	A	504	12/12	0.83	0.17	6,9,11,12	0
10	ACI	A	501	12/12	0.83	0.12	14,21,25,26	0
11	PCA	A	511	8/9	0.91	0.12	9,13,16,22	0
6	CA	A	497	1/1	1.00	0.06	5,5,5,5	0
7	CL	A	498	1/1	1.00	0.05	6,6,6,6	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.