



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 06:18 PM BST

PDB ID : 6T18  
Title : ASR Alternansucrase in complex with oligoalternan  
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Deposited on : 2019-10-03  
Resolution : 3.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

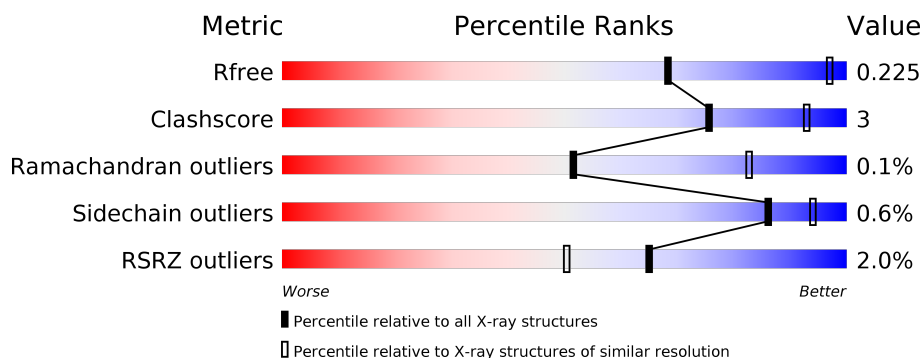
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	1278	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
1	B	1278	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>7%</div> </div> </div>
2	C	6	<div> <div>33%</div> <div>50%</div> <div>17%</div> </div>
3	D	3	<div> <div>100%</div> </div>
4	E	4	<div> <div>75%</div> <div>25%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19369 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 Alternansucrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1266	Total	C	N	O	S	0	0	0
			9921	6199	1691	2005	26			
1	B	1185	Total	C	N	O	S	0	0	0
			9300	5814	1580	1880	26			

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	6	Total	C	O	0	0	0
			67	36	31			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose.



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

- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose.



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

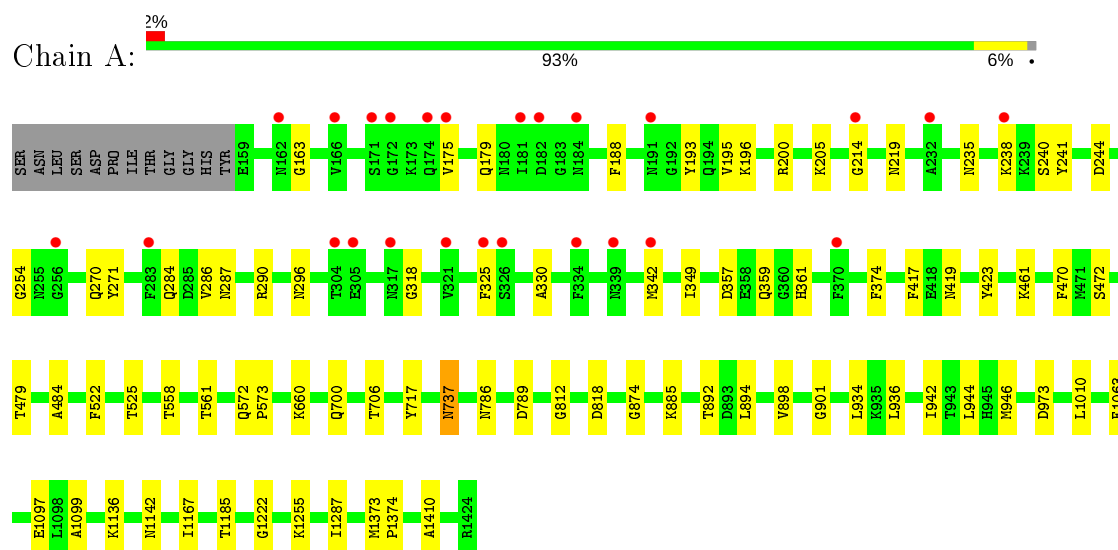
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

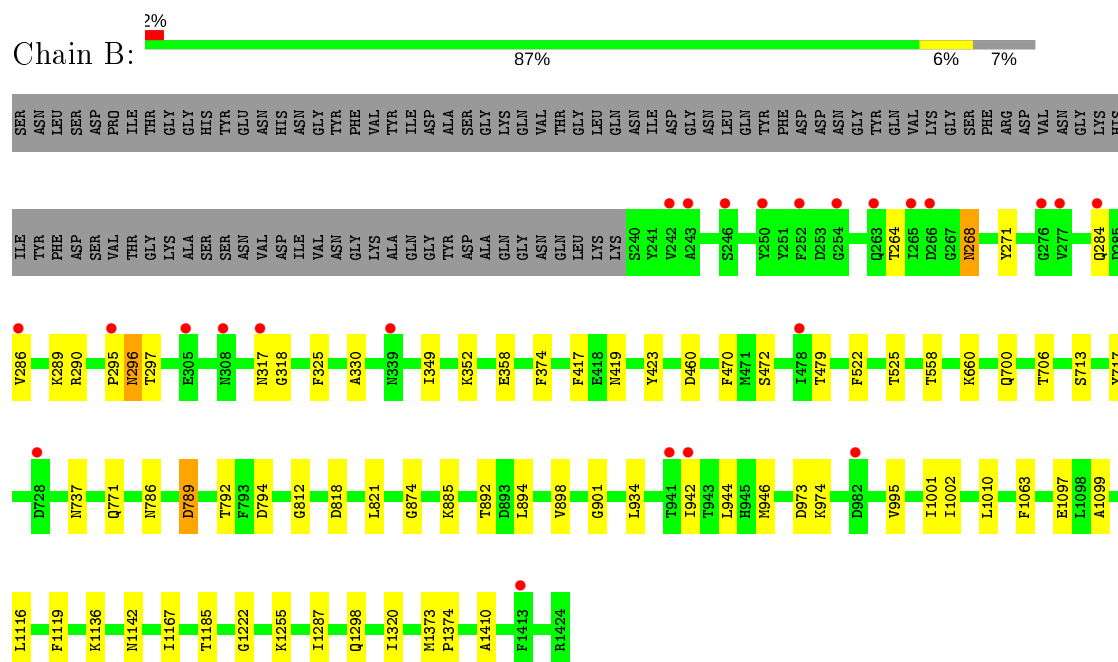
### 3 Residue-property plots [i](#)

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: Alternansucrase

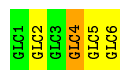


#### • Molecule 1: Alternansucrase

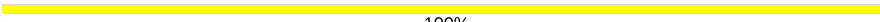


- Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain C:  33% 50% 17%

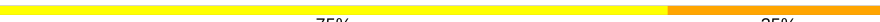


- Molecule 3: alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain D:  100%



- Molecule 4: alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-3)-alpha-D-glucopyranose

Chain E:  75% 25%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.88Å 135.65Å 239.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.15 48.13 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.15) 99.9 (48.13-3.15)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.200 , 0.226 0.198 , 0.225	Depositor DCC
$R_{free}$ test set	2769 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.5	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 34.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19369	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GLC

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	0.44	0/10130	0.62	0/13734
1	B	0.42	0/9497	0.61	0/12880
All	All	0.43	0/19627	0.62	0/26614

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	9921	0	9337	58	0
1	B	9300	0	8769	62	0
2	C	67	0	57	5	0
3	D	34	0	30	0	0
4	E	45	0	39	8	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	19369	0	18232	115	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 3.



All (115) 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:700:GLN:OE1	4:E:3:GLC:H62	0.99	1.17
1:B:700:GLN:OE1	4:E:3:GLC:C6	1.94	1.15
1:A:700:GLN:OE1	2:C:4:GLC:O6	1.84	0.93
1:A:241:TYR:OH	1:A:270:GLN:OE1	1.97	0.83
1:A:892:THR:HG23	1:A:934:LEU:HD21	1.61	0.82
1:B:296:ASN:ND2	1:B:297:THR:HG23	1.98	0.78
1:B:271:TYR:CD1	1:B:286:VAL:HG21	2.20	0.76
1:B:358:GLU:N	1:B:358:GLU:OE1	2.13	0.76
1:B:296:ASN:ND2	1:B:297:THR:N	2.37	0.73
1:A:271:TYR:CD1	1:A:286:VAL:HG21	2.25	0.71
1:B:892:THR:HG23	1:B:934:LEU:HD11	1.72	0.70
1:B:713:SER:OG	4:E:2:GLC:O3	2.06	0.70
1:B:271:TYR:CE1	1:B:286:VAL:CG2	2.75	0.69
1:A:290:ARG:O	1:A:318:GLY:HA2	1.93	0.68
1:A:717:TYR:O	2:C:4:GLC:H62	1.94	0.67
1:B:290:ARG:O	1:B:318:GLY:HA2	1.95	0.67
1:B:296:ASN:HD21	1:B:297:THR:HG23	1.59	0.67
1:B:973:ASP:OD1	1:B:974:LYS:HG3	1.95	0.66
1:A:163:GLY:O	1:B:352:LYS:CE	2.44	0.66
1:B:271:TYR:CE1	1:B:286:VAL:HG22	2.31	0.65
1:A:417:PHE:HB2	1:A:1287:ILE:HD13	1.79	0.65
1:B:973:ASP:OD1	1:B:974:LYS:N	2.30	0.64
1:A:271:TYR:CE1	1:A:286:VAL:CG2	2.82	0.62
1:B:417:PHE:HB2	1:B:1287:ILE:HD13	1.79	0.62
1:B:717:TYR:O	4:E:3:GLC:O4	2.16	0.61
1:B:296:ASN:HD22	1:B:297:THR:N	2.00	0.60
1:A:271:TYR:CE1	1:A:286:VAL:HG22	2.38	0.59
1:B:296:ASN:HD22	1:B:297:THR:H	1.49	0.59
1:A:934:LEU:HD11	1:A:936:LEU:HD12	1.85	0.59
1:A:786:ASN:O	1:A:789:ASP:HB2	2.04	0.58
1:B:786:ASN:O	1:B:789:ASP:HB2	2.05	0.56
1:B:995:VAL:HG12	1:B:1001:ILE:HG12	1.88	0.56
1:B:874:GLY:HA3	1:B:901:GLY:O	2.06	0.55
1:B:296:ASN:HD21	1:B:297:THR:CG2	2.19	0.55
1:A:934:LEU:C	1:A:934:LEU:HD13	2.27	0.55
1:B:472:SER:HB3	1:B:479:THR:HA	1.89	0.55
1:B:713:SER:CB	4:E:2:GLC:O3	2.56	0.54
1:B:284:GLN:HG3	1:B:286:VAL:HG23	1.89	0.54
1:A:472:SER:HB3	1:A:479:THR:HA	1.88	0.54
1:A:874:GLY:HA3	1:A:901:GLY:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1222:GLY:O	1:A:1255:LYS:HE2	2.08	0.54
1:A:284:GLN:HG3	1:A:286:VAL:HG23	1.90	0.53
1:B:271:TYR:CD1	1:B:286:VAL:CG2	2.91	0.53
1:B:1222:GLY:O	1:B:1255:LYS:HE2	2.09	0.53
1:B:713:SER:CB	4:E:2:GLC:HO3	2.22	0.52
1:B:522:PHE:O	1:B:525:THR:HB	2.10	0.52
1:B:296:ASN:ND2	1:B:297:THR:CG2	2.72	0.52
1:A:163:GLY:O	1:B:352:LYS:HD2	2.10	0.51
1:A:325:PHE:CE1	1:A:349:ILE:HD11	2.45	0.51
1:A:522:PHE:O	1:A:525:THR:HB	2.09	0.51
1:A:944:LEU:HB3	1:A:946:MET:HE3	1.92	0.51
1:A:885:LYS:HG3	2:C:6:GLC:H2	1.93	0.51
1:A:296:ASN:ND2	1:B:295:PRO:HB2	2.26	0.51
1:B:1097:GLU:HA	1:B:1167:ILE:HB	1.93	0.51
1:B:358:GLU:H	1:B:358:GLU:CD	2.08	0.50
1:B:894:LEU:HD23	1:B:942:ILE:HD13	1.94	0.49
1:A:357:ASP:OD1	1:A:361:HIS:N	2.46	0.49
1:B:717:TYR:O	4:E:3:GLC:H61	2.11	0.49
1:B:944:LEU:HB3	1:B:946:MET:HE3	1.94	0.49
1:A:195:VAL:HG21	1:A:200:ARG:NH2	2.27	0.49
1:A:271:TYR:CD1	1:A:286:VAL:CG2	2.96	0.49
1:A:894:LEU:HD23	1:A:942:ILE:HD13	1.94	0.49
1:A:238:LYS:HG2	1:A:254:GLY:O	2.12	0.49
1:A:1097:GLU:HA	1:A:1167:ILE:HB	1.94	0.49
1:B:325:PHE:CE1	1:B:349:ILE:HD11	2.48	0.48
1:A:163:GLY:O	1:B:352:LYS:CD	2.61	0.48
1:A:330:ALA:O	1:A:1410:ALA:HA	2.13	0.48
1:B:330:ALA:O	1:B:1410:ALA:HA	2.14	0.48
1:B:271:TYR:CE1	1:B:286:VAL:HG21	2.43	0.48
1:A:271:TYR:CE1	1:A:286:VAL:HG21	2.49	0.48
1:A:205:LYS:HE3	1:A:235:ASN:OD1	2.15	0.47
1:A:885:LYS:HG3	2:C:6:GLC:C2	2.45	0.47
1:B:1373:MET:HB3	1:B:1374:PRO:CD	2.46	0.46
1:A:342:MET:CE	1:A:359:GLN:O	2.63	0.46
1:B:1001:ILE:CG2	1:B:1002:ILE:N	2.78	0.46
1:A:1373:MET:HB3	1:A:1374:PRO:CD	2.46	0.46
1:B:268:ASN:N	1:B:268:ASN:HD22	2.13	0.45
1:A:885:LYS:HG3	2:C:6:GLC:O2	2.17	0.45
1:A:812:GLY:HA3	1:A:1010:LEU:HD23	1.99	0.45
1:B:713:SER:HG	4:E:2:GLC:HO3	1.39	0.45
1:A:419:ASN:HB2	1:A:423:TYR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:812:GLY:HA3	1:B:1010:LEU:HD23	2.00	0.44
1:A:1063:PHE:CG	1:A:1099:ALA:HB2	2.53	0.44
1:A:717:TYR:OH	1:A:885:LYS:HG2	2.18	0.43
1:A:163:GLY:O	1:B:352:LYS:HE3	2.18	0.43
1:A:219:ASN:OD1	1:A:244:ASP:HA	2.17	0.43
1:B:898:VAL:HG22	1:B:946:MET:HE1	2.01	0.43
1:B:558:THR:HG21	1:B:1185:THR:OG1	2.18	0.43
1:B:717:TYR:OH	1:B:885:LYS:HG2	2.18	0.43
1:A:558:THR:HG21	1:A:1185:THR:OG1	2.18	0.43
1:B:1063:PHE:CG	1:B:1099:ALA:HB2	2.54	0.42
1:B:264:THR:HA	1:B:268:ASN:O	2.19	0.42
1:A:737:ASN:ND2	1:A:737:ASN:O	2.39	0.42
1:B:1298:GLN:NE2	1:B:1320:ILE:O	2.53	0.42
1:B:1136:LYS:HG3	1:B:1142:ASN:HB2	2.02	0.42
1:B:419:ASN:HB2	1:B:423:TYR:O	2.19	0.42
1:B:706:THR:HG23	1:B:818:ASP:HB3	2.00	0.42
1:A:470:PHE:CE2	1:A:522:PHE:HB2	2.54	0.42
1:A:898:VAL:HG22	1:A:946:MET:HE1	2.01	0.42
1:B:470:PHE:CE2	1:B:522:PHE:HB2	2.55	0.42
1:A:461:LYS:HE2	1:A:484:ALA:O	2.20	0.41
1:B:1116:LEU:HA	1:B:1119:PHE:CE2	2.55	0.41
1:A:706:THR:HG23	1:A:818:ASP:HB3	2.02	0.41
1:A:973:ASP:OD1	1:A:973:ASP:N	2.45	0.41
1:A:196:LYS:HG2	1:A:214:GLY:CA	2.50	0.41
1:A:175:VAL:HG11	1:A:179:GLN:HG3	2.02	0.41
1:B:1373:MET:HB3	1:B:1374:PRO:HD2	2.03	0.41
1:A:1373:MET:HB3	1:A:1374:PRO:HD2	2.02	0.41
1:B:821:LEU:HD23	1:B:821:LEU:HA	1.93	0.41
1:B:289:LYS:HD3	1:B:317:ASN:O	2.21	0.41
1:A:1136:LYS:HG3	1:A:1142:ASN:HB2	2.03	0.40
1:A:572:GLN:HB2	1:A:573:PRO:HD2	2.04	0.40
1:A:188:PHE:HA	1:A:193:TYR:O	2.21	0.40
1:A:561:THR:CG2	1:A:561:THR:O	2.69	0.40
1:A:892:THR:HG21	1:A:894:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1264/1278 (99%)	1212 (96%)	51 (4%)	1 (0%)	51	83
1	B	1183/1278 (93%)	1132 (96%)	50 (4%)	1 (0%)	51	83
All	All	2447/2556 (96%)	2344 (96%)	101 (4%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	PHE
1	B	374	PHE

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1057/1079 (98%)	1053 (100%)	4 (0%)	91	96
1	B	994/1079 (92%)	985 (99%)	9 (1%)	78	91
All	All	2051/2158 (95%)	2038 (99%)	13 (1%)	86	94

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	SER
1	A	287	ASN
1	A	660	LYS
1	A	737	ASN

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Mol	Chain	Res	Type
1	B	268	ASN
1	B	296	ASN
1	B	460	ASP
1	B	660	LYS
1	B	737	ASN
1	B	771	GLN
1	B	789	ASP
1	B	792	THR
1	B	794	ASP

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

Mol	Chain	Res	Type
1	B	296	ASN
1	B	771	GLN

### 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 ⓘ

13 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	C	1	2	12,12,12	0.48	0	17,17,17	0.60	0
2	GLC	C	2	2	11,11,12	0.66	0	15,15,17	0.92	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GLC	C	3	2	11,11,12	0.59	0	15,15,17	0.74	0
2	GLC	C	4	2	11,11,12	0.69	0	15,15,17	0.96	1 (6%)
2	GLC	C	5	2	11,11,12	0.56	0	15,15,17	1.10	2 (13%)
2	GLC	C	6	2	11,11,12	0.68	0	15,15,17	0.87	0
3	GLC	D	1	3	12,12,12	0.57	0	17,17,17	1.60	2 (11%)
3	GLC	D	2	3	11,11,12	0.57	0	15,15,17	1.90	1 (6%)
3	GLC	D	3	3	11,11,12	0.58	0	15,15,17	1.28	3 (20%)
4	GLC	E	1	4	12,12,12	0.51	0	17,17,17	1.97	7 (41%)
4	GLC	E	2	4	11,11,12	0.66	0	15,15,17	0.66	0
4	GLC	E	3	4	11,11,12	0.62	0	15,15,17	1.06	1 (6%)
4	GLC	E	4	4	11,11,12	0.54	0	15,15,17	1.17	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	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	2/2/19/22	0/1/1/1
2	GLC	C	4	2	-	0/2/19/22	0/1/1/1
2	GLC	C	5	2	-	0/2/19/22	0/1/1/1
2	GLC	C	6	2	-	0/2/19/22	0/1/1/1
3	GLC	D	1	3	-	0/2/22/22	0/1/1/1
3	GLC	D	2	3	-	2/2/19/22	0/1/1/1
3	GLC	D	3	3	-	1/2/19/22	0/1/1/1
4	GLC	E	1	4	-	0/2/22/22	0/1/1/1
4	GLC	E	2	4	-	2/2/19/22	0/1/1/1
4	GLC	E	3	4	-	2/2/19/22	0/1/1/1
4	GLC	E	4	4	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	GLC	C1-O5-C5	5.71	119.93	112.19
3	D	1	GLC	C1-O5-C5	4.01	121.22	113.66
4	E	1	GLC	O1-C1-C2	3.99	120.25	109.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	GLC	C1-O5-C5	-3.55	106.96	113.66
3	D	1	GLC	O5-C1-C2	3.48	116.49	110.28
4	E	1	GLC	O5-C1-C2	2.66	115.02	110.28
4	E	3	GLC	C1-C2-C3	2.65	112.92	109.67
4	E	4	GLC	C1-O5-C5	2.64	115.77	112.19
4	E	1	GLC	C6-C5-C4	-2.60	106.92	113.00
4	E	1	GLC	O1-C1-O5	2.55	118.04	110.38
2	C	5	GLC	O5-C5-C6	2.52	111.16	107.20
3	D	3	GLC	C1-O5-C5	2.45	115.52	112.19
2	C	5	GLC	C1-O5-C5	2.39	115.43	112.19
3	D	3	GLC	O2-C2-C1	2.18	113.62	109.15
3	D	3	GLC	C2-C3-C4	-2.16	107.15	110.89
2	C	4	GLC	C1-C2-C3	2.15	112.31	109.67
4	E	1	GLC	C3-C4-C5	2.14	114.05	110.24
2	C	2	GLC	O5-C1-C2	-2.08	107.57	110.77
4	E	1	GLC	C1-C2-C3	-2.04	106.08	110.31

There are no chirality outliers.

All (11) torsion outliers are listed below:

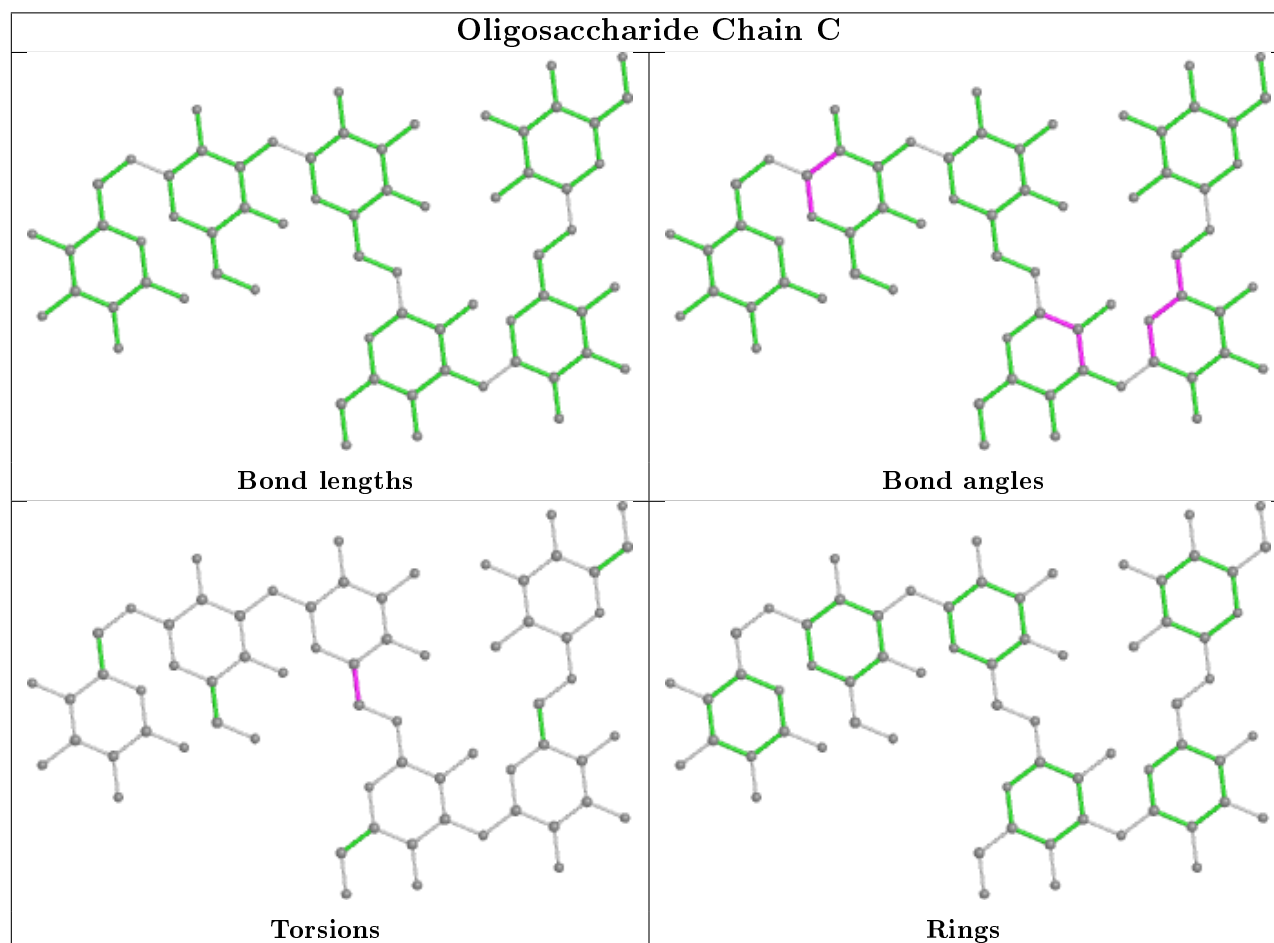
Mol	Chain	Res	Type	Atoms
3	D	2	GLC	O5-C5-C6-O6
3	D	2	GLC	C4-C5-C6-O6
4	E	3	GLC	O5-C5-C6-O6
4	E	3	GLC	C4-C5-C6-O6
4	E	4	GLC	C4-C5-C6-O6
2	C	3	GLC	C4-C5-C6-O6
2	C	3	GLC	O5-C5-C6-O6
4	E	4	GLC	O5-C5-C6-O6
4	E	2	GLC	C4-C5-C6-O6
3	D	3	GLC	O5-C5-C6-O6
4	E	2	GLC	O5-C5-C6-O6

There are no ring outliers.

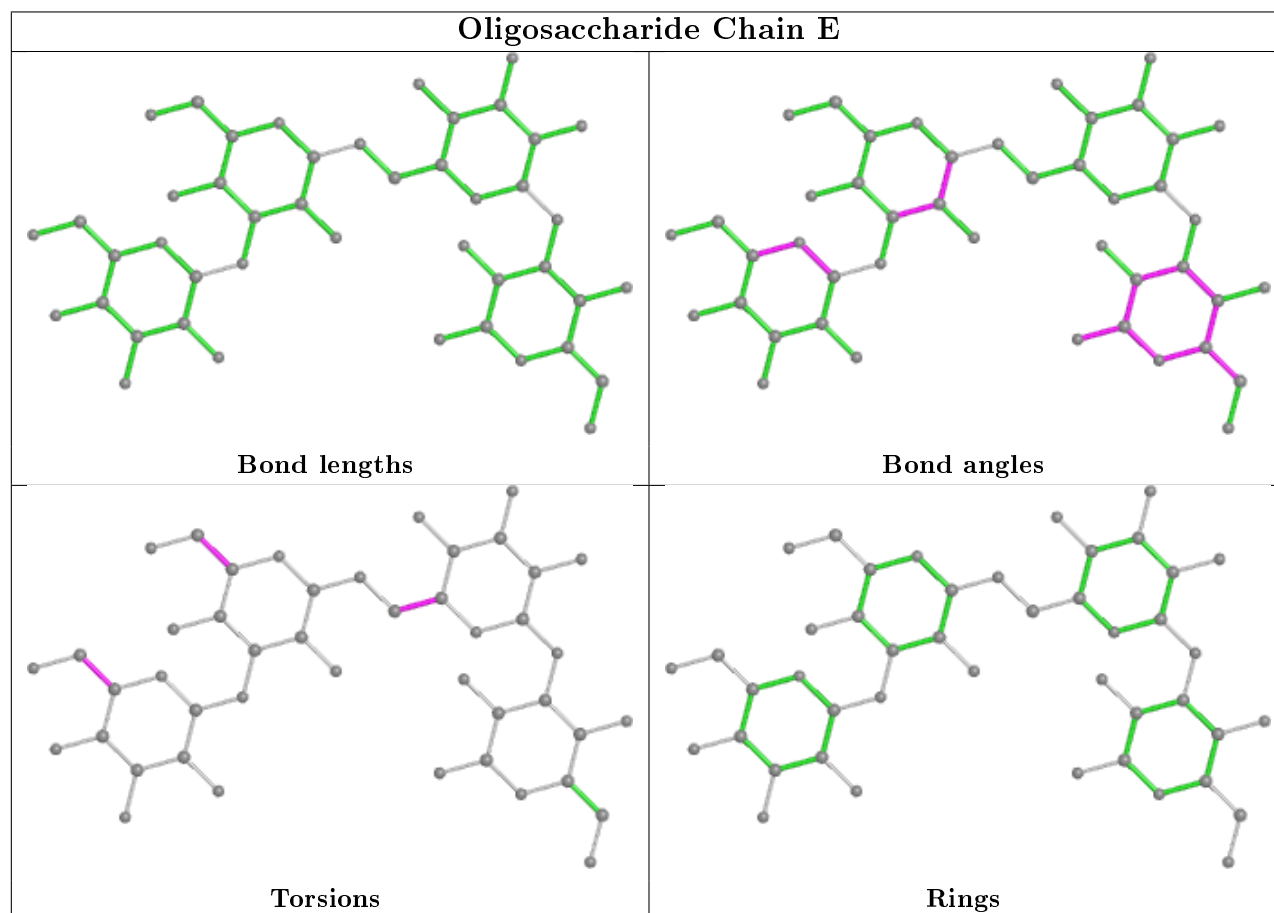
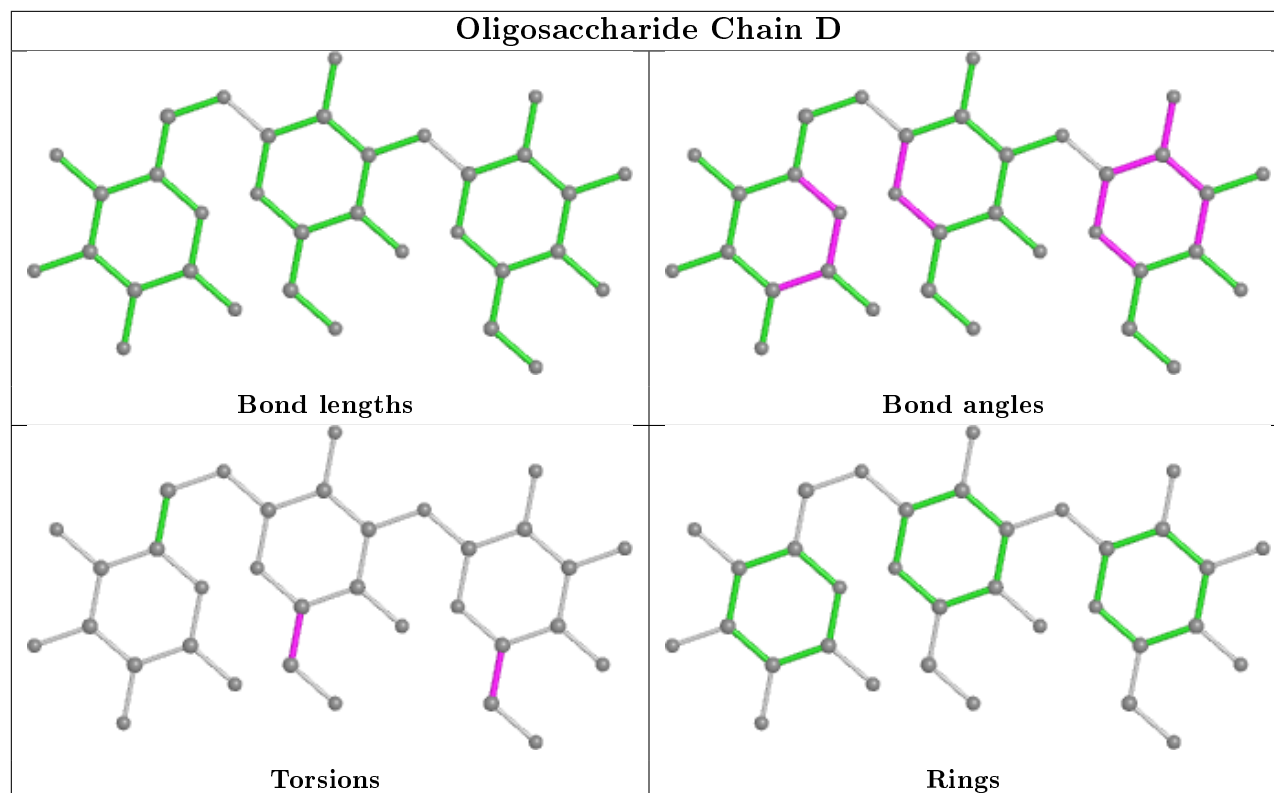
4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4	GLC	2	0
4	E	2	GLC	4	0
4	E	3	GLC	4	0
2	C	6	GLC	3	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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	1266/1278 (99%)	-0.11	25 (1%)	65 50	49, 76, 163, 202	0
1	B	1185/1278 (92%)	-0.12	24 (2%)	65 50	49, 89, 155, 230	0
All	All	2451/2556 (95%)	-0.11	49 (1%)	65 50	49, 83, 160, 230	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	GLN	7.1
1	A	184	ASN	4.3
1	A	326	SER	4.2
1	A	182	ASP	3.9
1	A	162	ASN	3.6
1	B	243	ALA	3.4
1	B	246	SER	3.4
1	B	276	GLY	3.4
1	B	284	GLN	3.2
1	B	982	ASP	3.0
1	B	308	ASN	2.9
1	B	242	VAL	2.9
1	B	317	ASN	2.9
1	A	175	VAL	2.8
1	B	266	ASP	2.8
1	B	339	ASN	2.8
1	B	295	PRO	2.7
1	A	256	GLY	2.7
1	A	317	ASN	2.6
1	B	1413	PHE	2.5
1	B	942	ILE	2.5
1	B	250	TYR	2.5
1	A	232	ALA	2.5
1	B	277	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	321	VAL	2.4
1	A	304	THR	2.4
1	B	252	PHE	2.4
1	A	214	GLY	2.4
1	A	171	SER	2.4
1	A	325	PHE	2.4
1	A	305	GLU	2.3
1	B	941	THR	2.3
1	B	254	GLY	2.3
1	A	166	VAL	2.3
1	B	286	VAL	2.2
1	B	305	GLU	2.2
1	A	172	GLY	2.2
1	A	334	PHE	2.2
1	A	191	ASN	2.2
1	B	265	ILE	2.1
1	A	283	PHE	2.1
1	A	370	PHE	2.1
1	A	339	ASN	2.1
1	B	478	ILE	2.1
1	A	238	LYS	2.0
1	B	263	GLN	2.0
1	B	728	ASP	2.0
1	A	342	MET	2.0
1	A	181	ILE	2.0

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

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

## 6.3 Carbohydrates ⓘ

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.

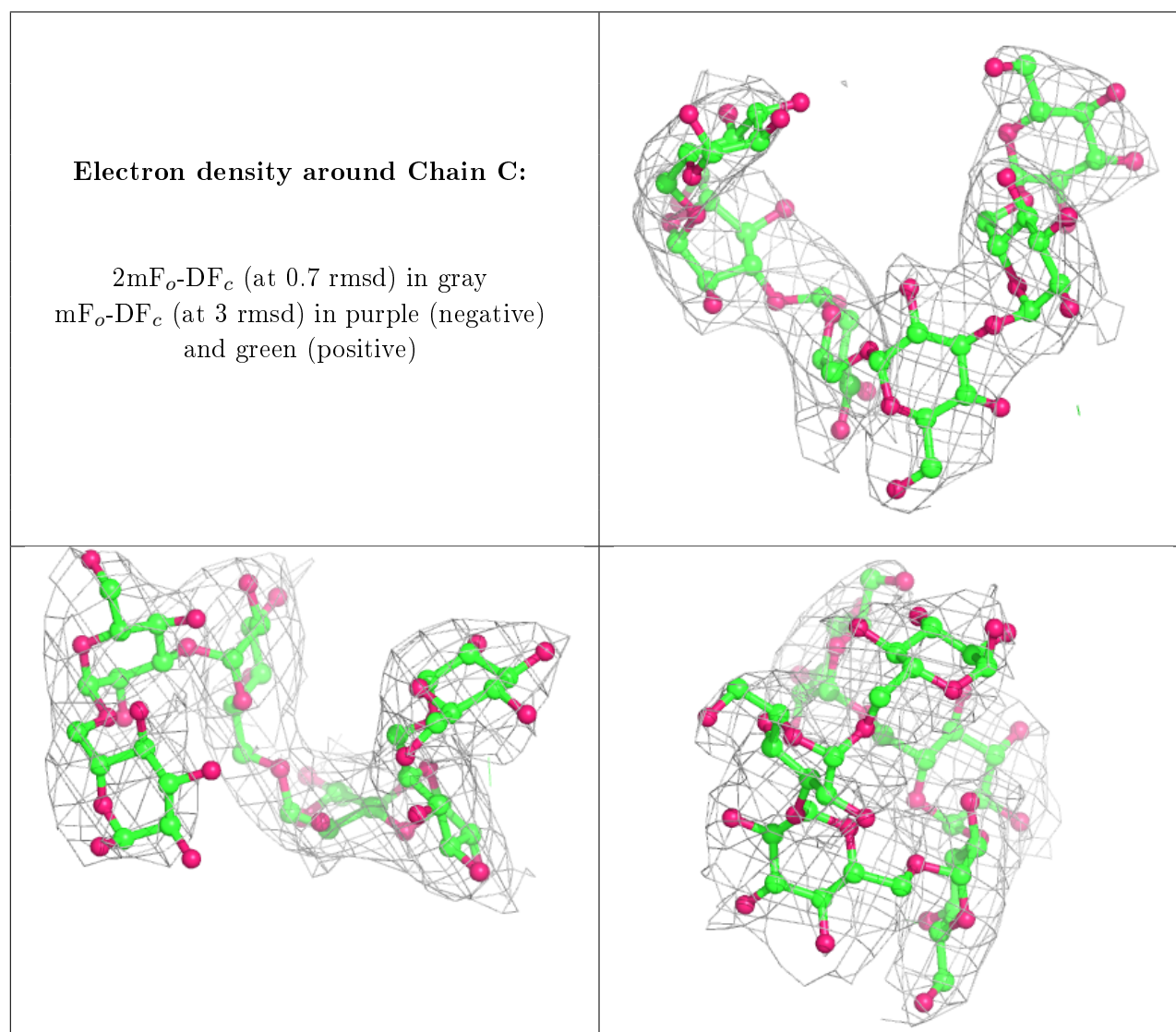
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GLC	D	2	11/12	0.79	0.25	152,160,169,172	0
2	GLC	C	1	12/12	0.79	0.29	133,139,143,149	0
4	GLC	E	1	12/12	0.80	0.28	121,129,134,134	0

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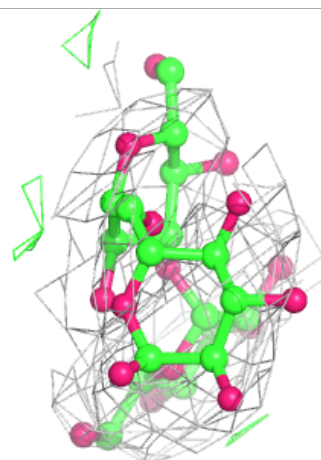
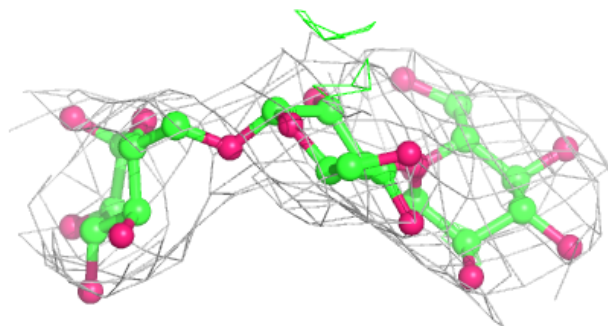
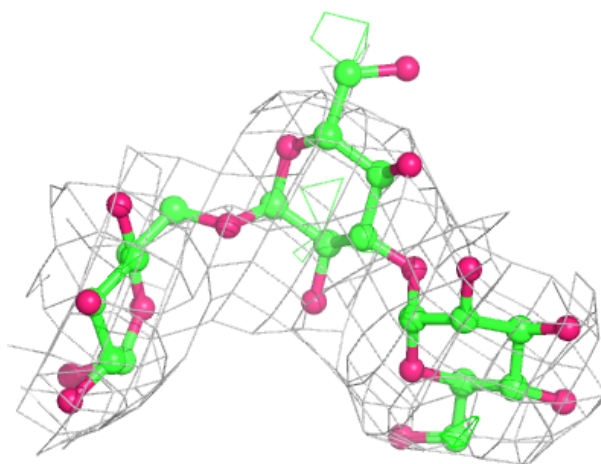
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GLC	E	4	11/12	0.81	0.27	121,124,127,131	0
3	GLC	D	1	12/12	0.83	0.21	127,139,151,160	0
2	GLC	C	6	11/12	0.87	0.29	108,116,120,121	0
4	GLC	E	3	11/12	0.87	0.23	94,104,107,114	0
3	GLC	D	3	11/12	0.88	0.18	131,139,146,146	0
2	GLC	C	2	11/12	0.93	0.14	110,117,124,126	0
2	GLC	C	3	11/12	0.94	0.12	82,93,100,104	0
4	GLC	E	2	11/12	0.94	0.13	99,106,119,120	0
2	GLC	C	4	11/12	0.94	0.17	84,91,94,104	0
2	GLC	C	5	11/12	0.96	0.17	98,101,108,111	0

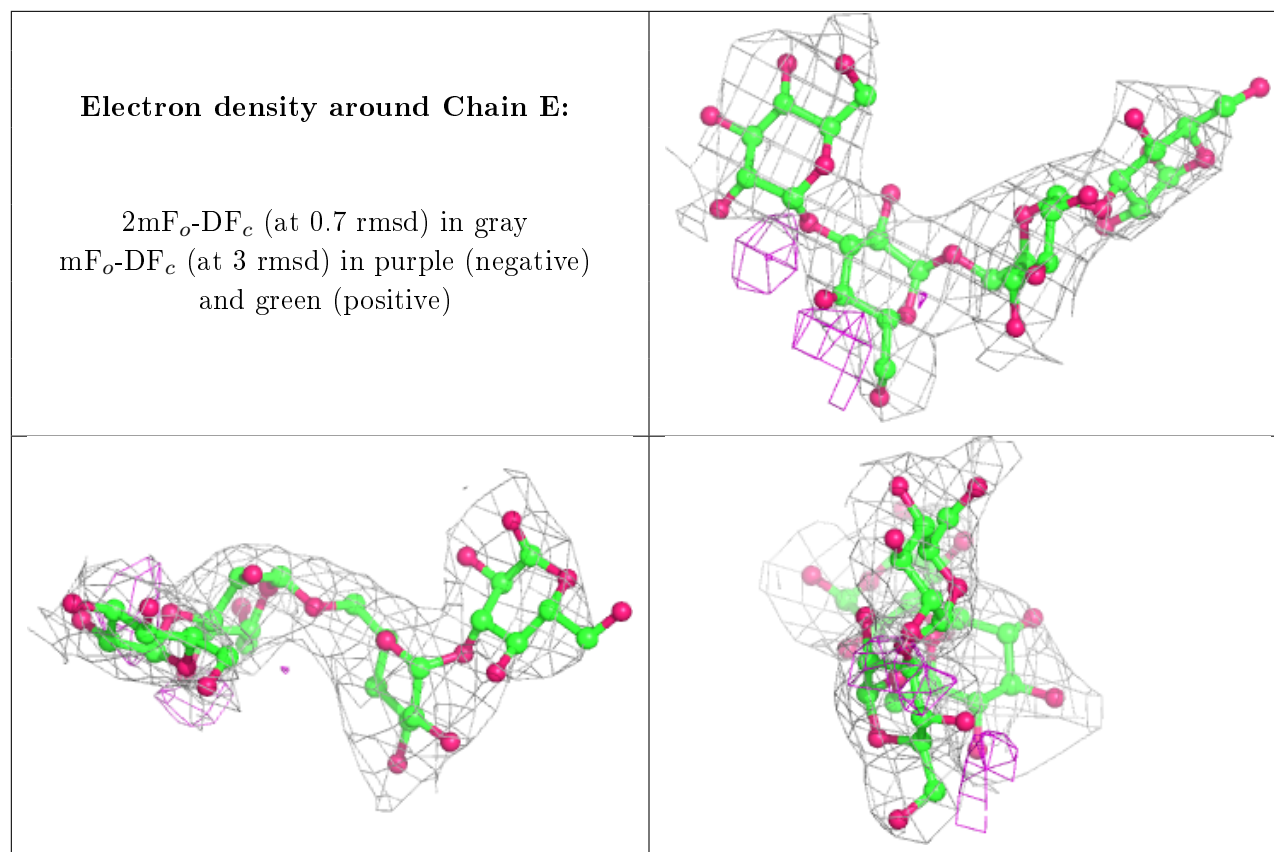
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



**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)





## 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
5	CA	A	1501	1/1	0.96	0.18	69,69,69,69	0
5	CA	B	1501	1/1	0.99	0.11	70,70,70,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.