



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 28, 2022 – 06:24 PM EDT

PDB ID : 7U3D  
Title : Structure of *S. venezuelae* GlgX-c-di-GMP-acarbose complex (4.6)  
Authors : Schumacher, M.A.  
Deposited on : 2022-02-27  
Resolution : 2.40 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 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 : 2.31.2  
buster-report : 1.1.7 (2018)  
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) : 2.31.2

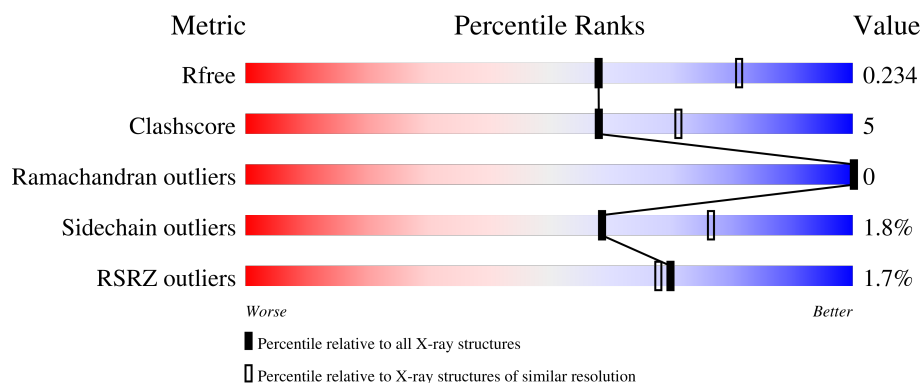
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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.



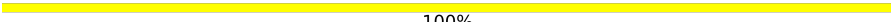
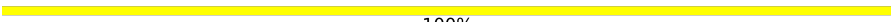

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	709	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>.</div> </div> </div>
1	B	709	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>.</div> </div> </div>
1	C	709	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>5%</div> </div> </div>
1	F	709	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>.</div> </div> </div>
2	D	3	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	3	 100%
2	I	3	 100%
2	J	3	 100%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23171 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 Glycogen debranching enzyme GlgX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	693	Total	C	N	O	S	0	0	0
			5515	3467	999	1026	23			
1	F	679	Total	C	N	O	S	0	0	1
			5400	3392	978	1006	24			
1	B	689	Total	C	N	O	S	0	0	0
			5494	3451	994	1025	24			
1	C	677	Total	C	N	O	S	0	0	0
			5386	3384	975	1003	24			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A5P2ALW6
A	-1	SER	-	expression tag	UNP A0A5P2ALW6
A	0	HIS	-	expression tag	UNP A0A5P2ALW6
A	103	VAL	ILE	conflict	UNP A0A5P2ALW6
A	192	ARG	LYS	conflict	UNP A0A5P2ALW6
A	296	ALA	SER	conflict	UNP A0A5P2ALW6
A	297	ASP	ASN	conflict	UNP A0A5P2ALW6
A	303	MET	THR	conflict	UNP A0A5P2ALW6
A	682	GLN	GLU	conflict	UNP A0A5P2ALW6
F	-2	GLY	-	expression tag	UNP A0A5P2ALW6
F	-1	SER	-	expression tag	UNP A0A5P2ALW6
F	0	HIS	-	expression tag	UNP A0A5P2ALW6
F	103	VAL	ILE	conflict	UNP A0A5P2ALW6
F	192	ARG	LYS	conflict	UNP A0A5P2ALW6
F	296	ALA	SER	conflict	UNP A0A5P2ALW6
F	297	ASP	ASN	conflict	UNP A0A5P2ALW6
F	303	MET	THR	conflict	UNP A0A5P2ALW6
F	682	GLN	GLU	conflict	UNP A0A5P2ALW6
B	-2	GLY	-	expression tag	UNP A0A5P2ALW6
B	-1	SER	-	expression tag	UNP A0A5P2ALW6
B	0	HIS	-	expression tag	UNP A0A5P2ALW6

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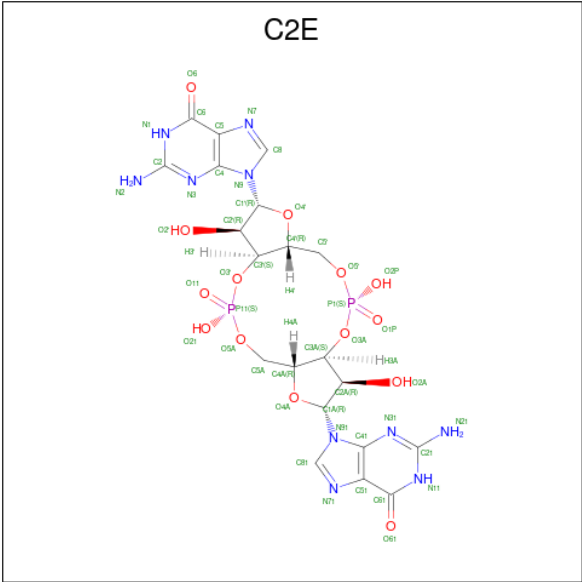
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Chain	Residue	Modelled	Actual	Comment	Reference
B	103	VAL	ILE	conflict	UNP A0A5P2ALW6
B	192	ARG	LYS	conflict	UNP A0A5P2ALW6
B	296	ALA	SER	conflict	UNP A0A5P2ALW6
B	297	ASP	ASN	conflict	UNP A0A5P2ALW6
B	303	MET	THR	conflict	UNP A0A5P2ALW6
B	682	GLN	GLU	conflict	UNP A0A5P2ALW6
C	-2	GLY	-	expression tag	UNP A0A5P2ALW6
C	-1	SER	-	expression tag	UNP A0A5P2ALW6
C	0	HIS	-	expression tag	UNP A0A5P2ALW6
C	103	VAL	ILE	conflict	UNP A0A5P2ALW6
C	192	ARG	LYS	conflict	UNP A0A5P2ALW6
C	296	ALA	SER	conflict	UNP A0A5P2ALW6
C	297	ASP	ASN	conflict	UNP A0A5P2ALW6
C	303	MET	THR	conflict	UNP A0A5P2ALW6
C	682	GLN	GLU	conflict	UNP A0A5P2ALW6

- Molecule 2 is an oligosaccharide called 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	H	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	I	3	Total	C	N	O	0	0	0
			44	25	1	18			
2	J	3	Total	C	N	O	0	0	0
			44	25	1	18			

- Molecule 3 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidoctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (three-letter code: C2E) (formula: C<sub>20</sub>H<sub>24</sub>N<sub>10</sub>O<sub>14</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	F	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	B	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	C	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

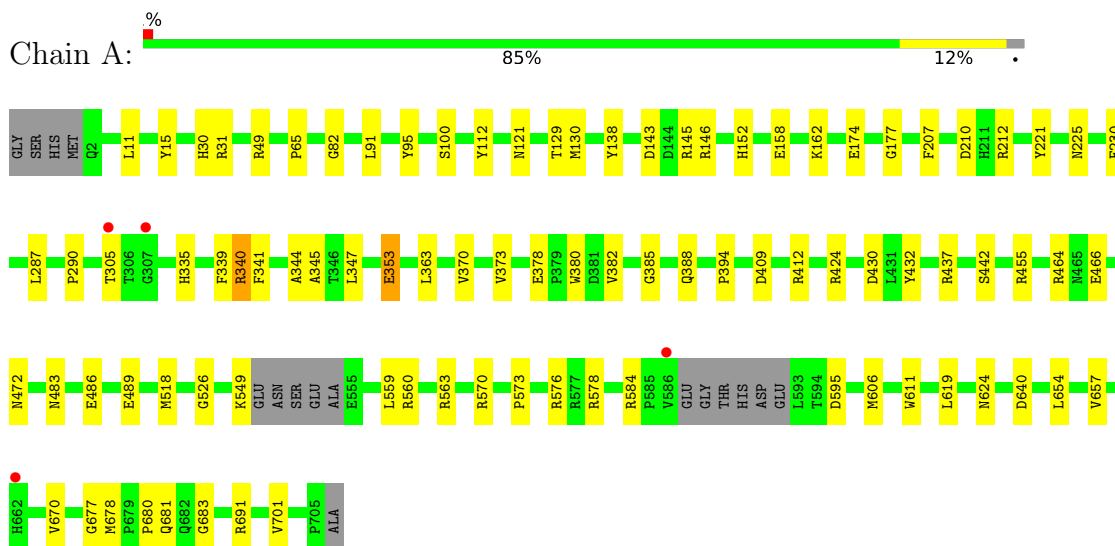
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	244	Total	O	0	0
			244	244		
4	F	266	Total	O	0	0
			266	266		
4	B	252	Total	O	0	0
			252	252		
4	C	254	Total	O	0	0
			254	254		

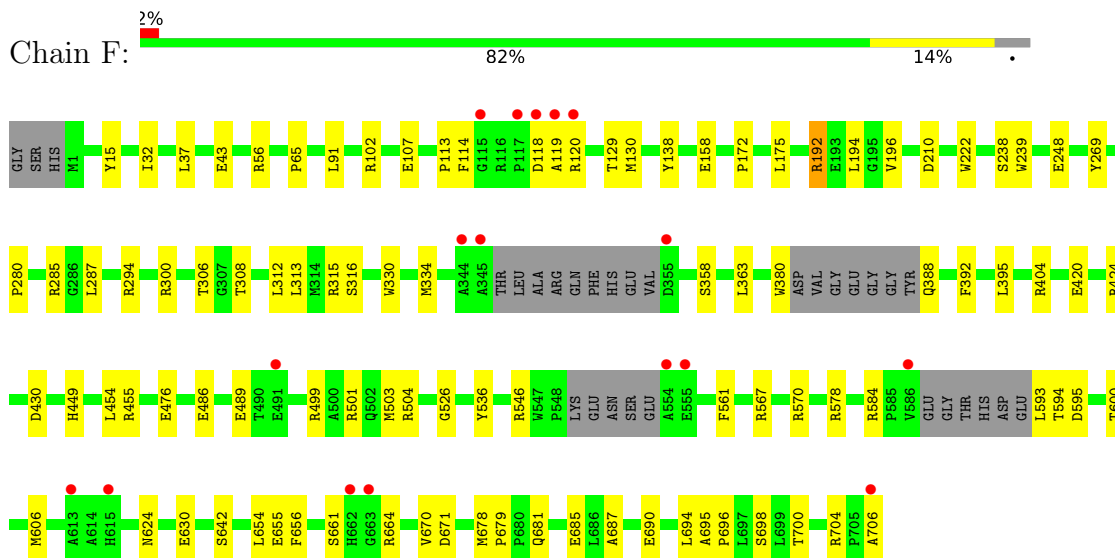
### 3 Residue-property plots [i](#)

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.

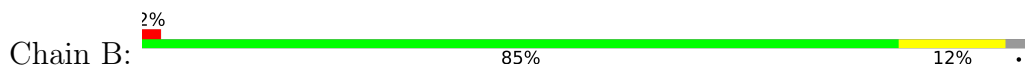
- Molecule 1: Glycogen debranching enzyme GlgX

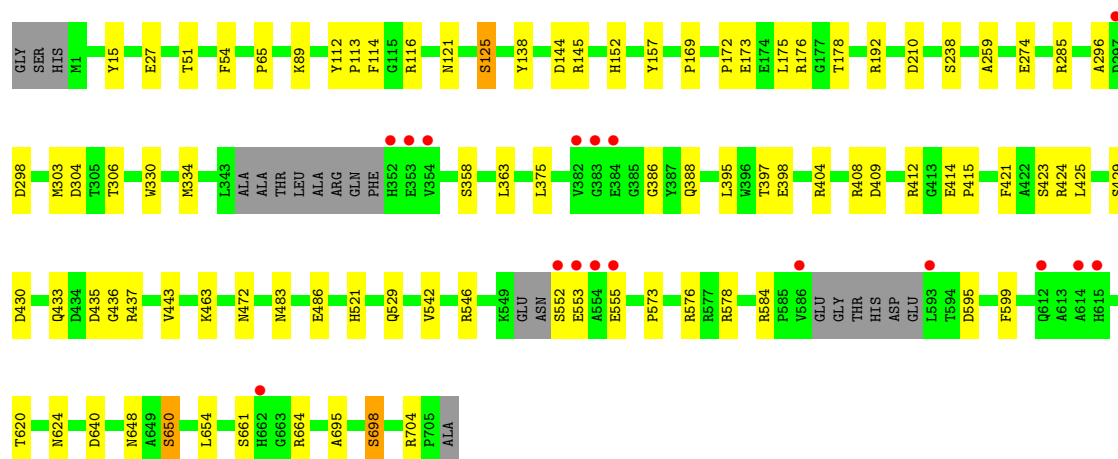


- Molecule 1: Glycogen debranching enzyme GlgX

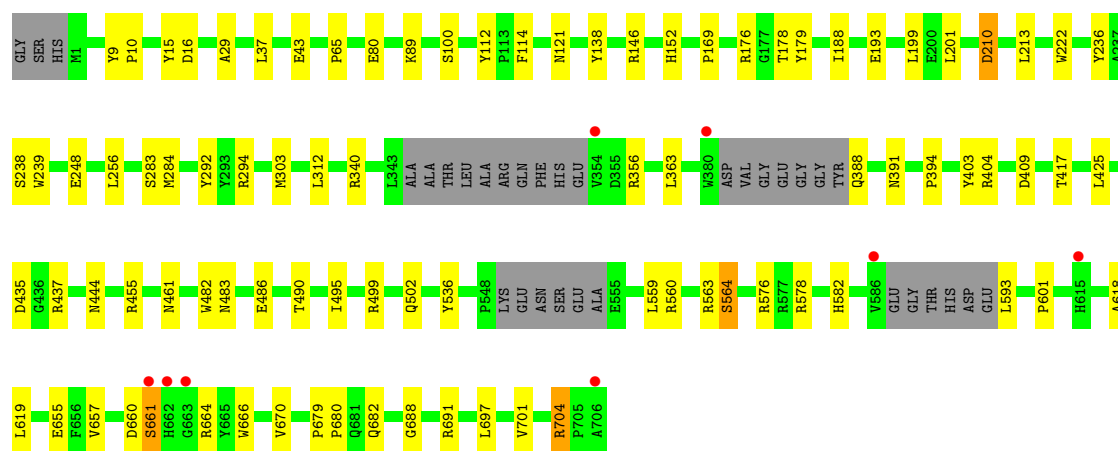
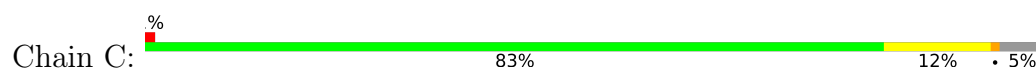


- Molecule 1: Glycogen debranching enzyme GlgX

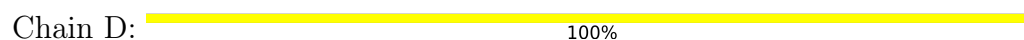




- Molecule 1: Glycogen debranching enzyme GlgX



- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino\}$ - $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose



- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino\}$ - $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose



- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino\}$ - $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose



Chain I:  100%

GLC1  
GLC2  
AC13

- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose-(1-4)- $\alpha$ -D-glucopyranose

Chain J:  100%

GLC1  
GLC2  
AC13

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.88Å 145.38Å 229.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.41 – 2.40 47.41 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.41-2.40) 99.7 (47.41-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, $R_{free}$	0.172 , 0.235 0.173 , 0.234	Depositor DCC
$R_{free}$ test set	1994 reflections (1.61%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.2	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	23171	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: GLC, C2E, AC1

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	1/5667 (0.0%)	0.60	0/7709
1	B	0.42	1/5644 (0.0%)	0.60	0/7674
1	C	0.44	0/5531	0.59	1/7521 (0.0%)
1	F	0.45	0/5545	0.60	0/7539
All	All	0.44	2/22387 (0.0%)	0.60	1/30443 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	GLU	CD-OE2	-5.32	1.19	1.25
1	B	436	GLY	C-O	-5.20	1.15	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	435	ASP	CB-CG-OD2	5.23	123.00	118.30

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	5515	0	5214	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5494	0	5200	47	0
1	C	5386	0	5099	50	0
1	F	5400	0	5122	57	0
2	D	44	0	29	0	0
2	H	44	0	29	0	0
2	I	44	0	29	0	0
2	J	44	0	29	0	0
3	A	46	0	18	0	0
3	B	46	0	18	2	0
3	C	46	0	19	2	0
3	F	46	0	20	1	0
4	A	244	0	0	5	0
4	B	252	0	0	3	0
4	C	254	0	0	4	0
4	F	266	0	0	6	0
All	All	23171	0	20826	208	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.

The worst 5 of 208 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:C:657:VAL:HG22	1:C:691:ARG:HD3	1.71	0.73
1:B:274:GLU:O	1:B:285:ARG:NH2	2.21	0.73
1:F:138:TYR:HB2	1:C:138:TYR:HB2	1.72	0.70
1:F:455:ARG:NH1	1:F:526:GLY:O	2.26	0.68
1:C:394:PRO:HA	1:C:437:ARG:HD3	1.74	0.67

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	687/709 (97%)	658 (96%)	29 (4%)	0	100	100
1	B	681/709 (96%)	655 (96%)	26 (4%)	0	100	100
1	C	667/709 (94%)	638 (96%)	29 (4%)	0	100	100
1	F	669/709 (94%)	641 (96%)	28 (4%)	0	100	100
All	All	2704/2836 (95%)	2592 (96%)	112 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	573/590 (97%)	566 (99%)	7 (1%)	71	85
1	B	574/590 (97%)	565 (98%)	9 (2%)	62	79
1	C	562/590 (95%)	547 (97%)	15 (3%)	44	65
1	F	564/590 (96%)	555 (98%)	9 (2%)	62	79
All	All	2273/2360 (96%)	2233 (98%)	40 (2%)	59	76

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

Mol	Chain	Res	Type
1	C	210	ASP
1	C	564	SER
1	C	283	SER
1	C	404	ARG
1	C	661	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	612	GLN
1	A	662	HIS
1	F	258	GLN

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Mol	Chain	Res	Type
1	C	461	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	D	1	2	12,12,12	1.15	1 (8%)	17,17,17	1.59	3 (17%)
2	GLC	D	2	2	11,11,12	2.51	4 (36%)	15,15,17	1.56	2 (13%)
2	AC1	D	3	2	21,22,23	4.27	11 (52%)	22,32,34	1.71	4 (18%)
2	GLC	H	1	2	12,12,12	1.27	1 (8%)	17,17,17	1.34	2 (11%)
2	GLC	H	2	2	11,11,12	2.70	6 (54%)	15,15,17	1.52	3 (20%)
2	AC1	H	3	2	21,22,23	4.50	11 (52%)	22,32,34	1.56	3 (13%)
2	GLC	I	1	2	12,12,12	1.29	1 (8%)	17,17,17	1.43	3 (17%)
2	GLC	I	2	2	11,11,12	2.78	5 (45%)	15,15,17	2.12	5 (33%)
2	AC1	I	3	2	21,22,23	4.44	11 (52%)	22,32,34	1.40	4 (18%)
2	GLC	J	1	2	12,12,12	1.25	1 (8%)	17,17,17	1.29	2 (11%)
2	GLC	J	2	2	11,11,12	2.74	5 (45%)	15,15,17	1.97	5 (33%)
2	AC1	J	3	2	21,22,23	4.48	10 (47%)	22,32,34	1.40	3 (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	D	1	2	-	2/2/22/22	0/1/1/1
2	GLC	D	2	2	-	1/2/19/22	0/1/1/1
2	AC1	D	3	2	-	4/6/43/46	0/2/2/2
2	GLC	H	1	2	-	2/2/22/22	0/1/1/1
2	GLC	H	2	2	-	2/2/19/22	0/1/1/1
2	AC1	H	3	2	-	3/6/43/46	0/2/2/2
2	GLC	I	1	2	-	2/2/22/22	0/1/1/1
2	GLC	I	2	2	-	0/2/19/22	0/1/1/1
2	AC1	I	3	2	-	3/6/43/46	0/2/2/2
2	GLC	J	1	2	-	2/2/22/22	0/1/1/1
2	GLC	J	2	2	-	2/2/19/22	0/1/1/1
2	AC1	J	3	2	-	4/6/43/46	0/2/2/2

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	3	AC1	C7B-C5B	17.62	1.57	1.32
2	J	3	AC1	C7B-C5B	17.40	1.57	1.32
2	I	3	AC1	C7B-C5B	17.32	1.57	1.32
2	D	3	AC1	C7B-C5B	16.78	1.56	1.32
2	I	2	GLC	O5-C5	6.13	1.55	1.43

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	3	AC1	C4A-C5B-C7B	-5.91	112.52	122.23
2	D	3	AC1	C4A-C5B-C7B	-5.22	113.66	122.23
2	I	2	GLC	C1-O5-C5	4.99	118.95	112.19
2	J	3	AC1	C4A-C5B-C7B	-4.81	114.34	122.23
2	H	2	GLC	C1-O5-C5	4.11	117.75	112.19

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3	AC1	C3-C4-N4A-C1B
2	D	3	AC1	C5-C4-N4A-C1B
2	D	3	AC1	C7B-C5B-C6B-O6B

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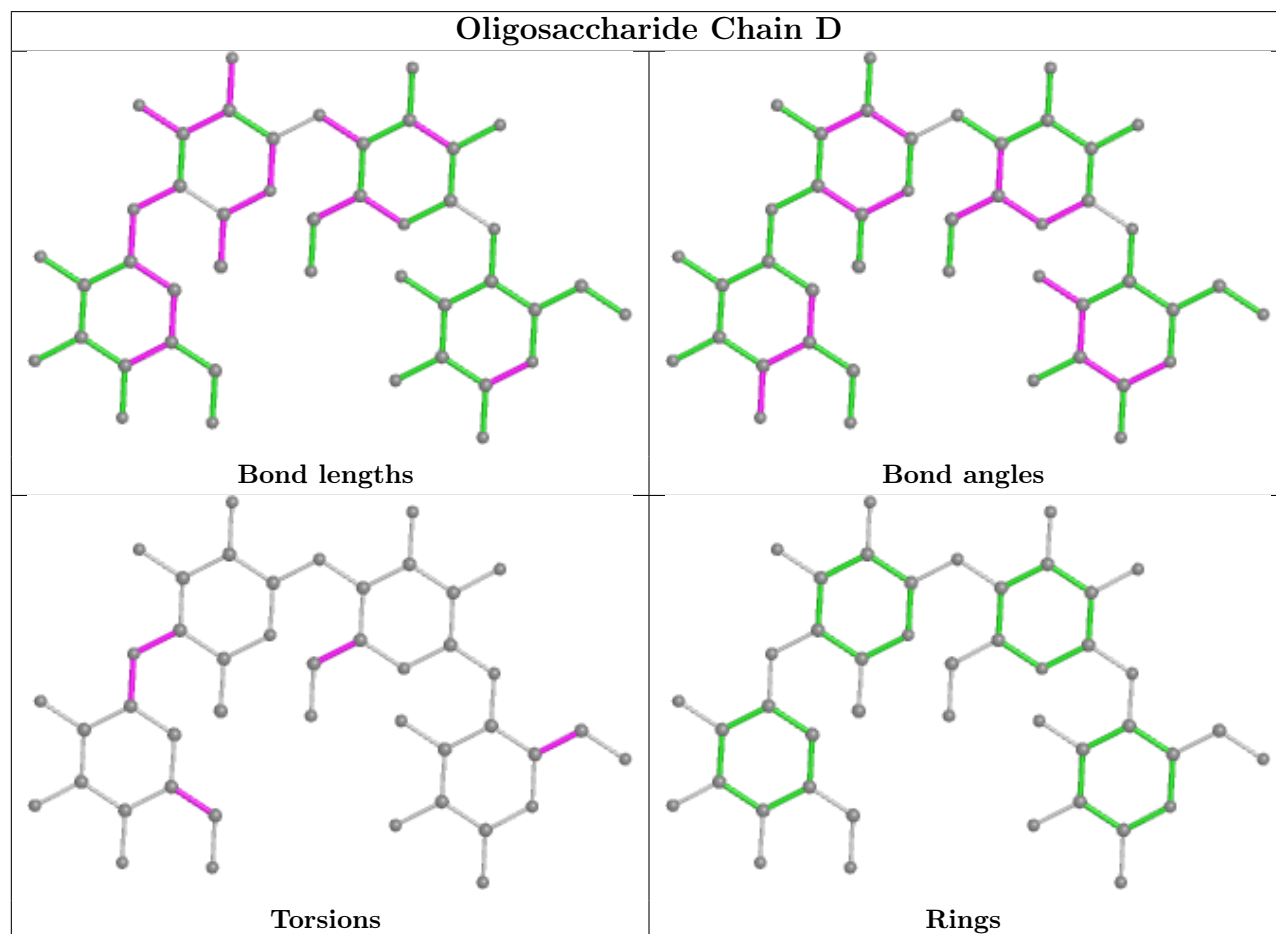
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Mol	Chain	Res	Type	Atoms
2	H	3	AC1	C3-C4-N4A-C1B
2	H	3	AC1	C5-C4-N4A-C1B

There are no ring outliers.

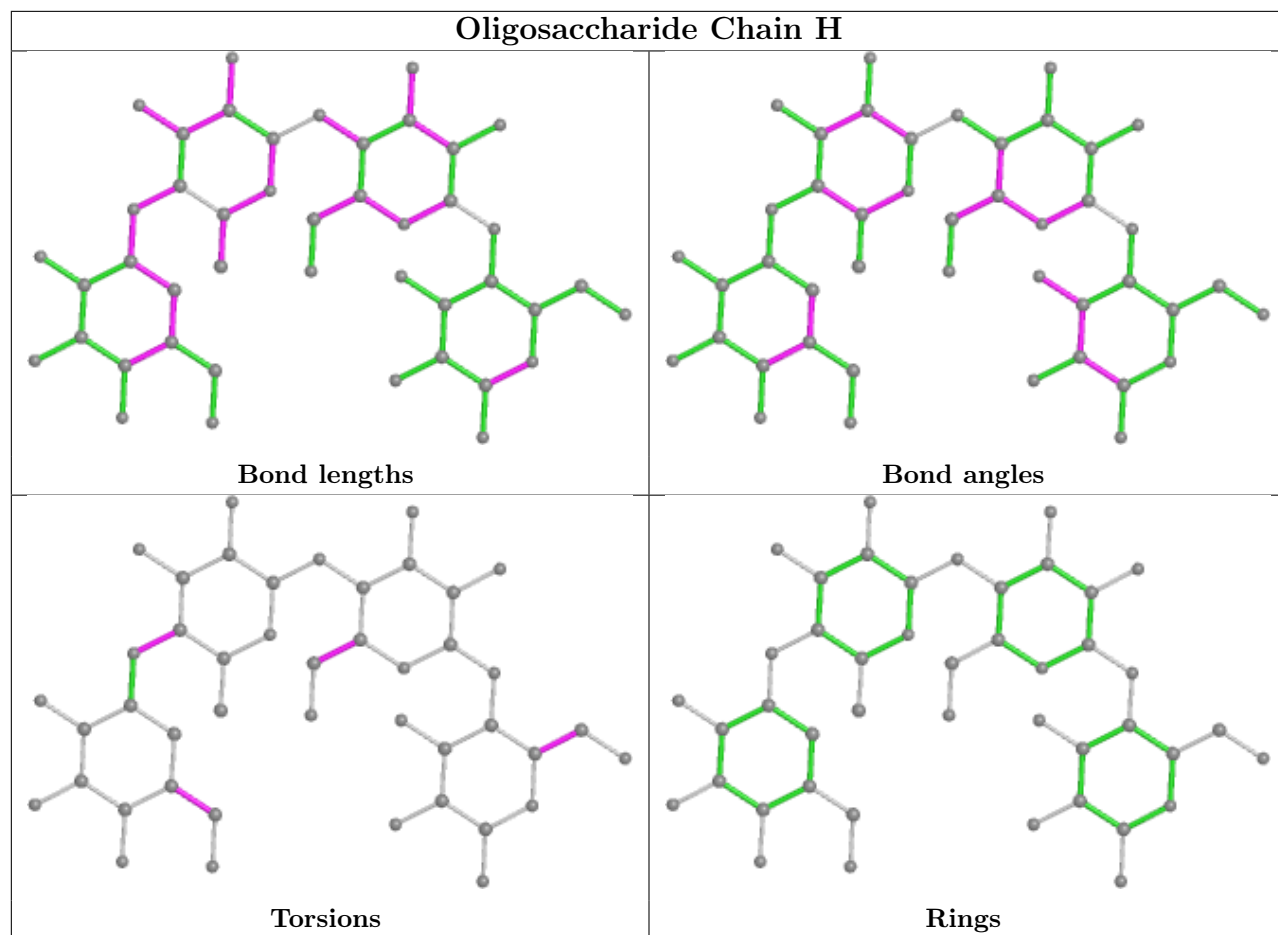
No monomer is involved in short contacts.

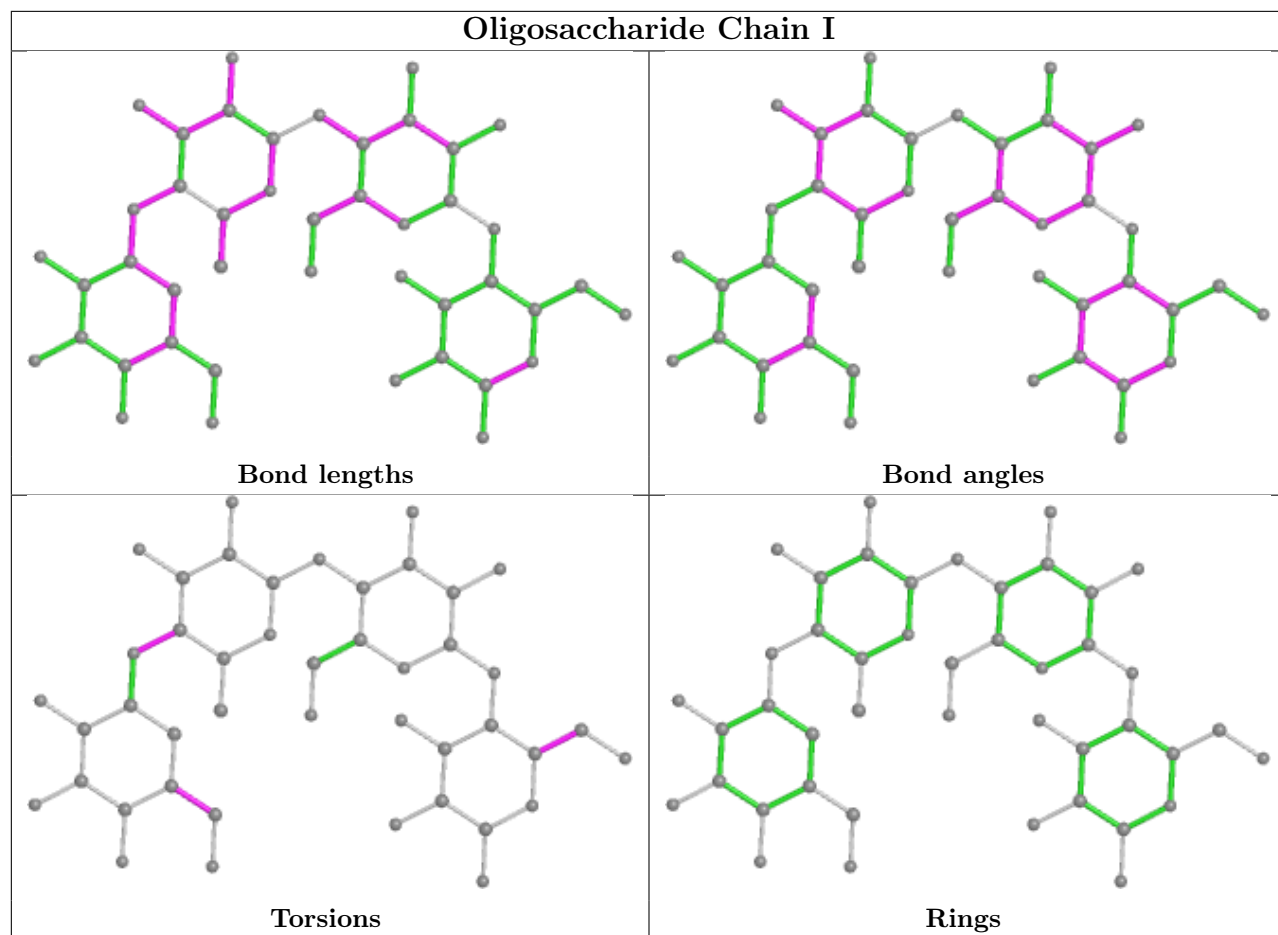
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

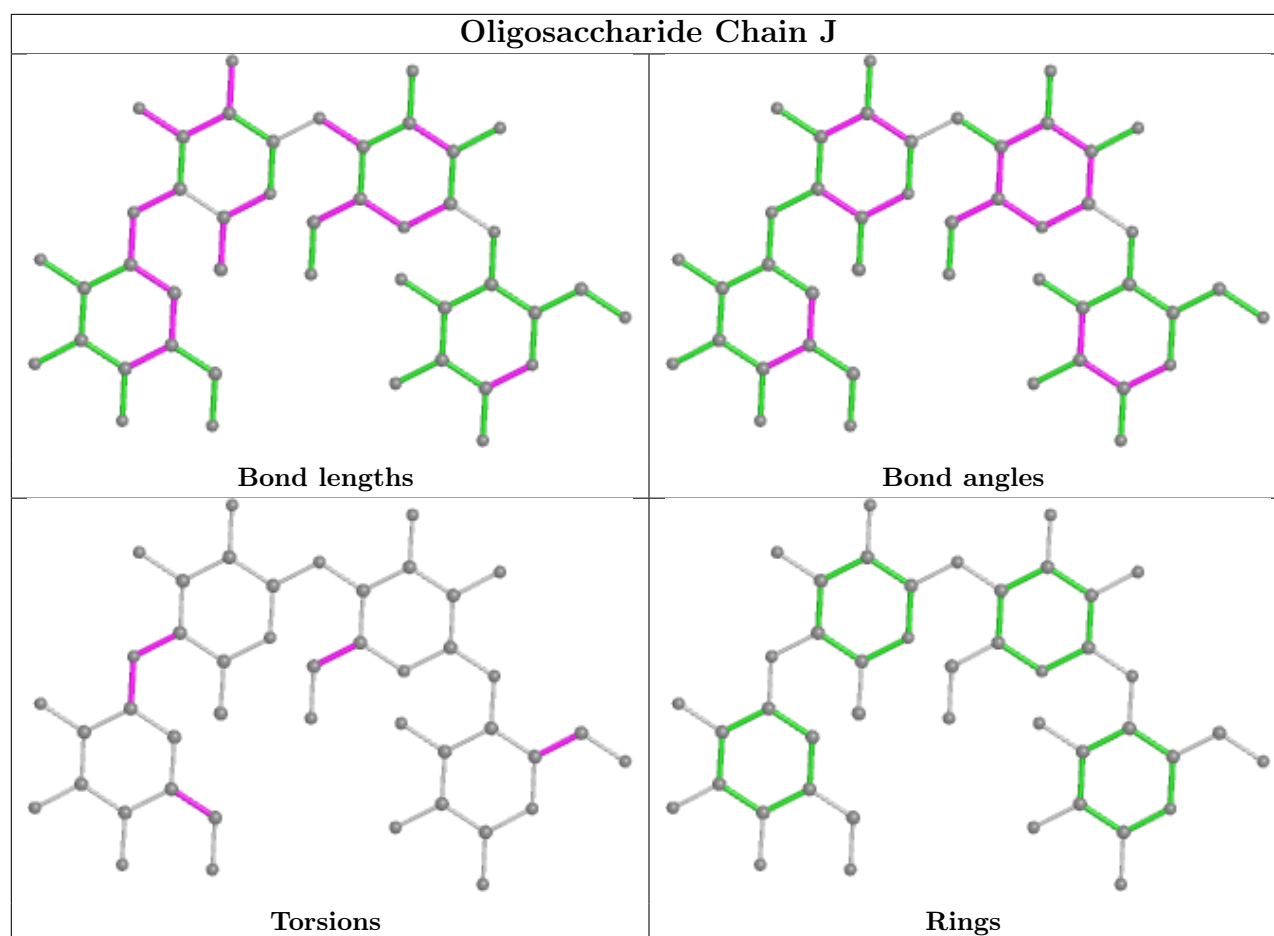




## Oligosaccharide Chain H







## 5.6 Ligand geometry [i](#)

4 ligands 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	$\# Z  > 2$
3	C2E	F	801	-	44,52,52	5.16	31 (70%)	52,82,82	1.71	14 (26%)
3	C2E	C	801	-	44,52,52	5.10	33 (75%)	52,82,82	1.51	11 (21%)
3	C2E	B	801	-	44,52,52	5.20	31 (70%)	52,82,82	1.59	13 (25%)
3	C2E	A	801	-	44,52,52	5.14	30 (68%)	52,82,82	1.62	11 (21%)

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
3	C2E	F	801	-	-	2/22/62/62	0/6/7/7
3	C2E	C	801	-	-	0/22/62/62	0/6/7/7
3	C2E	B	801	-	-	2/22/62/62	0/6/7/7
3	C2E	A	801	-	-	3/22/62/62	0/6/7/7

The worst 5 of 125 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	C2E	C2'-C1'	-17.83	1.26	1.53
3	A	801	C2E	C2'-C1'	-17.41	1.27	1.53
3	C	801	C2E	C2'-C1'	-17.21	1.27	1.53
3	F	801	C2E	C2'-C1'	-17.07	1.27	1.53
3	F	801	C2E	C2A-C3A	-13.65	1.22	1.52

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	801	C2E	N21-C21-N11	3.65	124.48	116.71
3	F	801	C2E	C5-C6-N1	3.53	120.18	113.95
3	F	801	C2E	C51-C61-N11	3.21	119.61	113.95
3	B	801	C2E	C5-C6-N1	3.19	119.59	113.95
3	C	801	C2E	O61-C61-N11	-3.08	117.01	120.65

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	801	C2E	C4'-C3'-O3'-P11
3	B	801	C2E	C5'-O5'-P1-O2P
3	F	801	C2E	C2'-C3'-O3'-P11
3	A	801	C2E	C5A-O5A-P11-O3'
3	A	801	C2E	C3'-O3'-P11-O5A

There are no ring outliers.

3 monomers are involved in 5 short contacts:

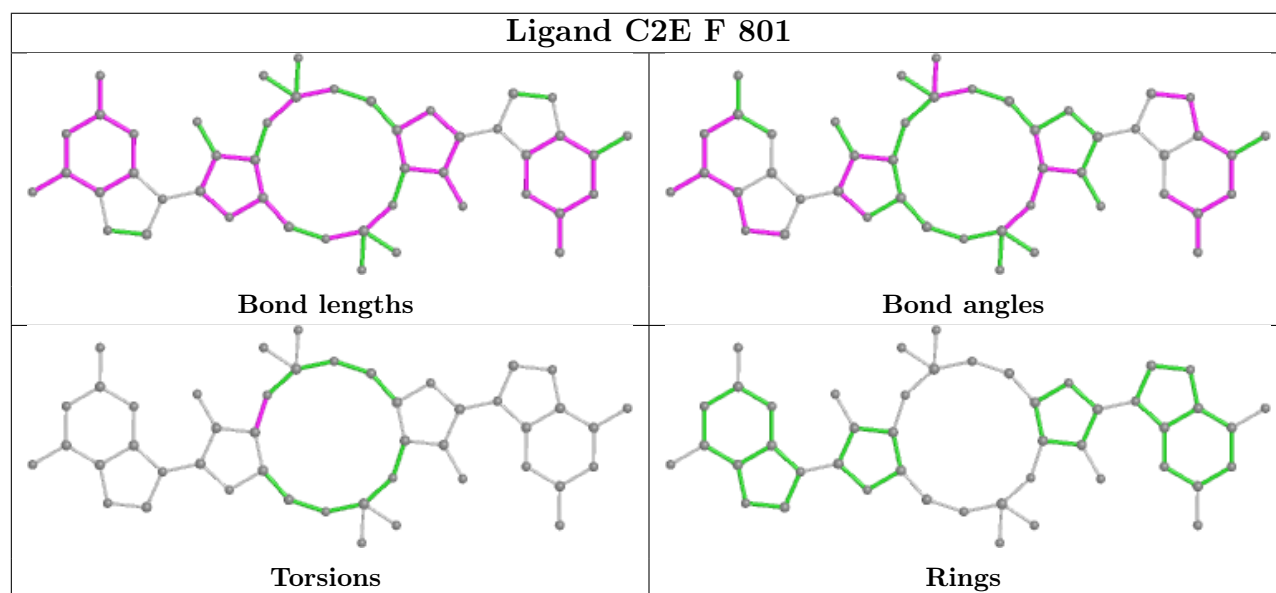
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	801	C2E	1	0

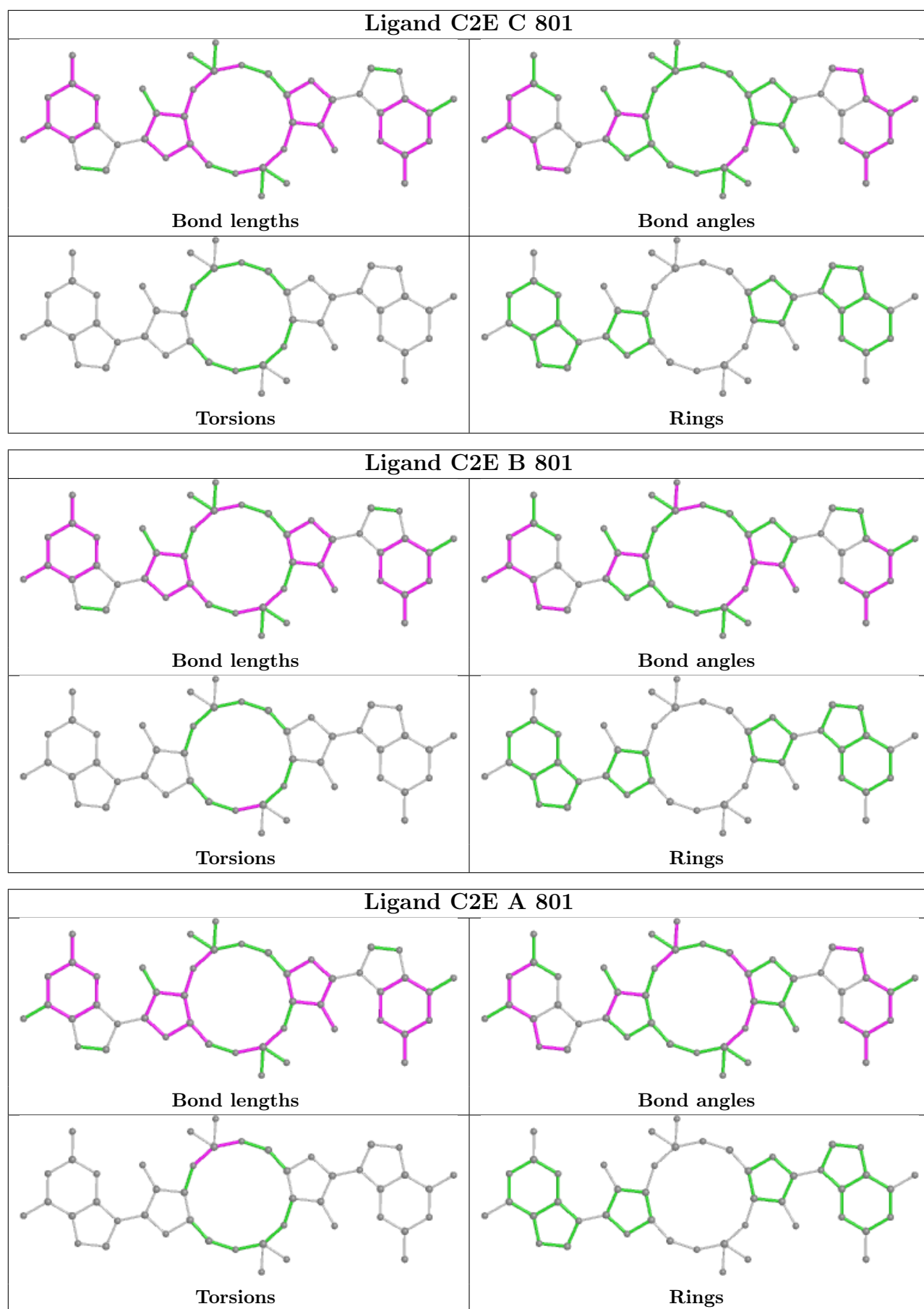
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	801	C2E	2	0
3	B	801	C2E	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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	693/709 (97%)	-0.45	4 (0%) 89 88	24, 36, 66, 121	0
1	B	689/709 (97%)	-0.38	17 (2%) 57 55	22, 34, 70, 125	0
1	C	677/709 (95%)	-0.43	8 (1%) 79 77	21, 35, 66, 110	0
1	F	679/709 (95%)	-0.33	17 (2%) 57 55	21, 35, 70, 125	0
All	All	2738/2836 (96%)	-0.40	46 (1%) 70 68	21, 35, 68, 125	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	706	ALA	8.6
1	A	586	VAL	7.6
1	B	586	VAL	5.0
1	F	345	ALA	4.9
1	F	119	ALA	4.7

### 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	AC1	I	3	21/22	0.86	0.21	27,52,86,103	0
2	AC1	J	3	21/22	0.86	0.22	37,52,86,88	0

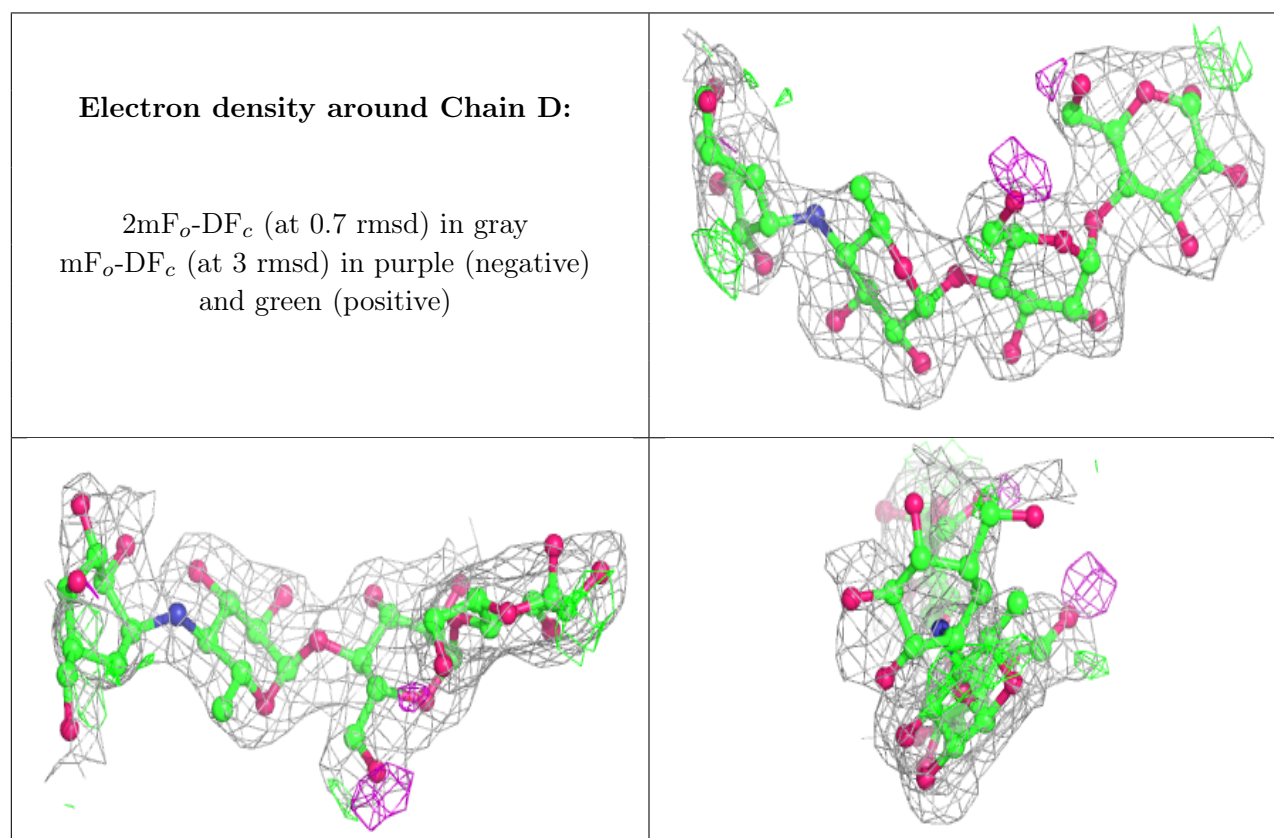
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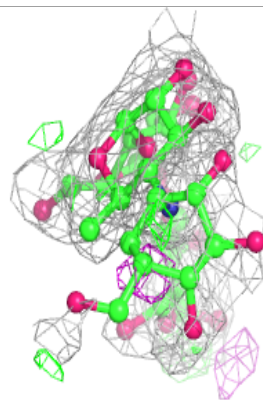
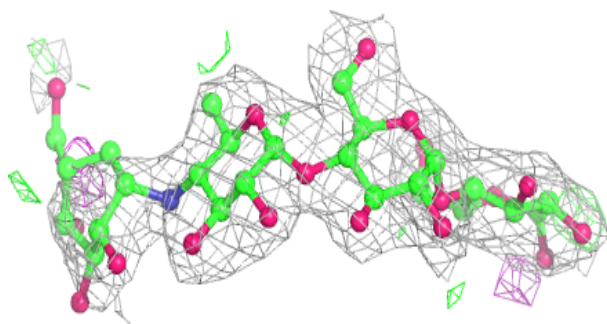
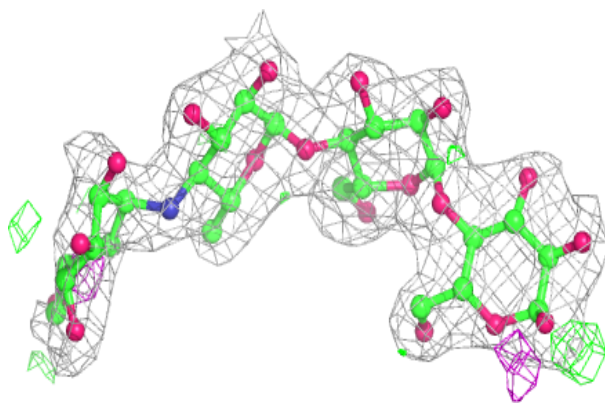
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	AC1	D	3	21/22	0.89	0.18	33,51,88,95	0
2	AC1	H	3	21/22	0.89	0.19	24,49,90,90	0
2	GLC	D	2	11/12	0.94	0.11	33,34,39,57	0
2	GLC	I	1	12/12	0.94	0.12	30,36,43,46	0
2	GLC	D	1	12/12	0.95	0.14	33,40,46,68	0
2	GLC	J	1	12/12	0.95	0.13	34,41,48,55	0
2	GLC	H	1	12/12	0.95	0.12	33,40,51,53	0
2	GLC	I	2	11/12	0.96	0.15	25,31,39,53	0
2	GLC	J	2	11/12	0.96	0.14	25,33,37,48	0
2	GLC	H	2	11/12	0.96	0.11	30,35,44,46	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.

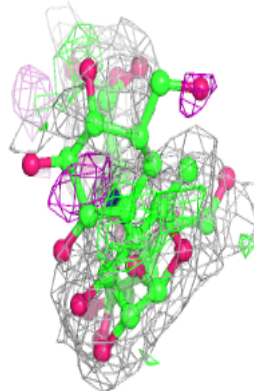
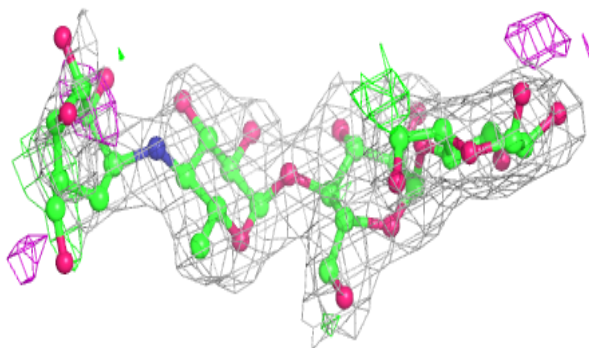
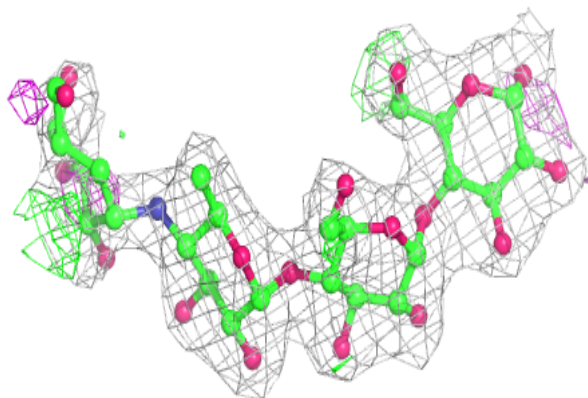


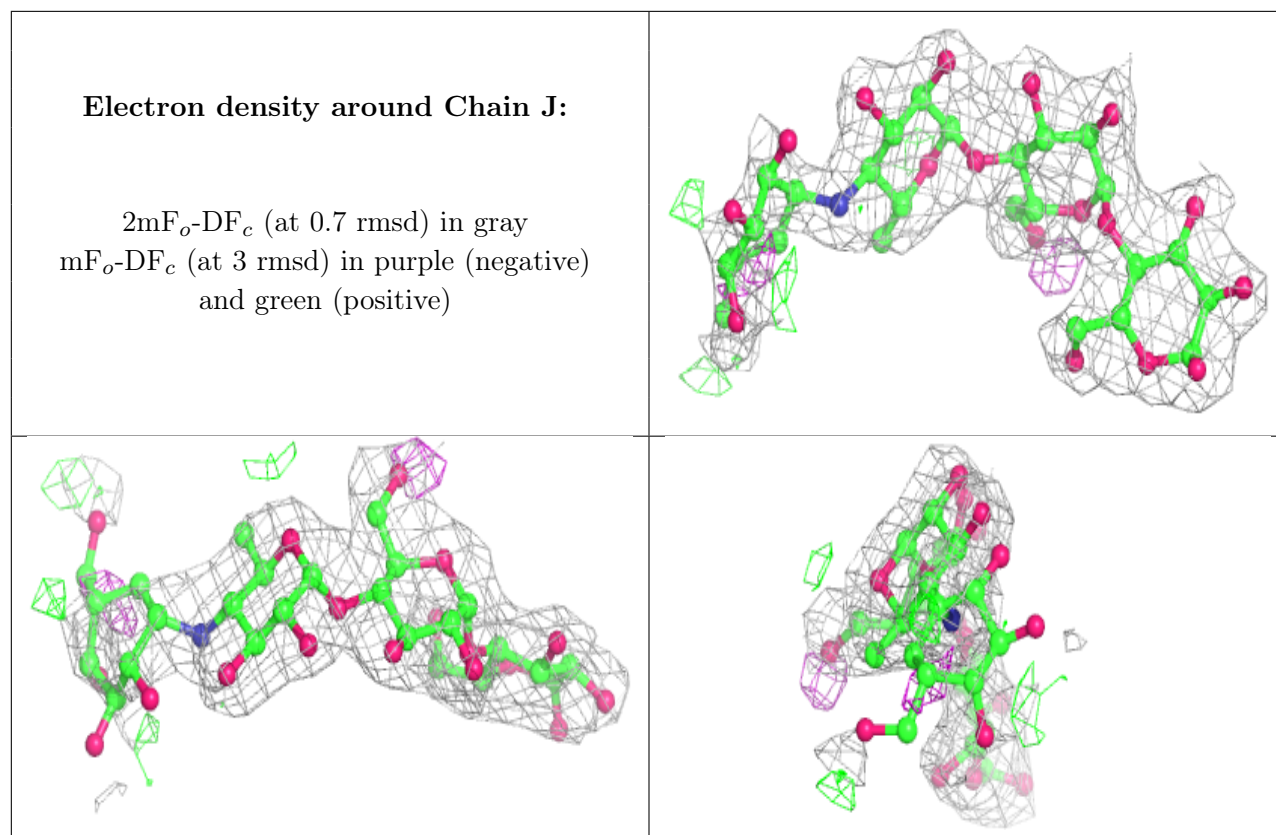
**Electron density around Chain H:**

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

**Electron density around Chain I:**

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





## 6.4 Ligands [i](#)

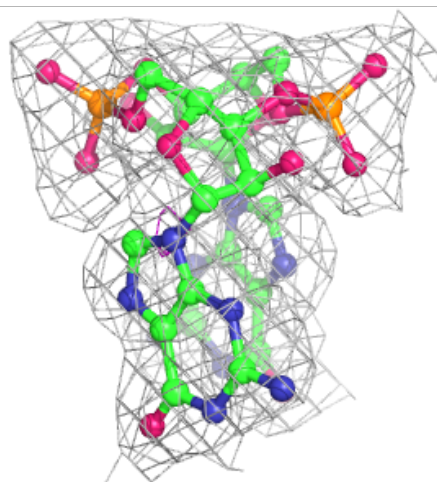
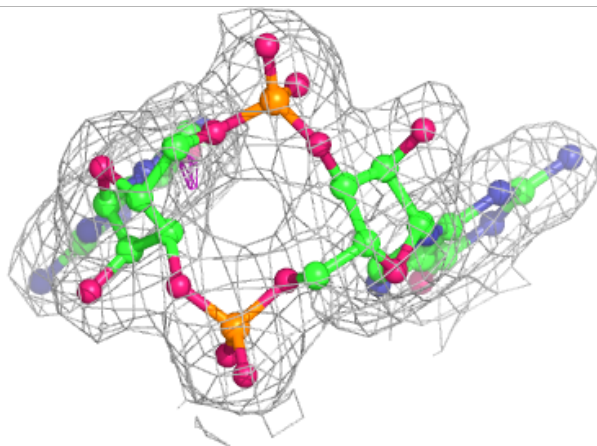
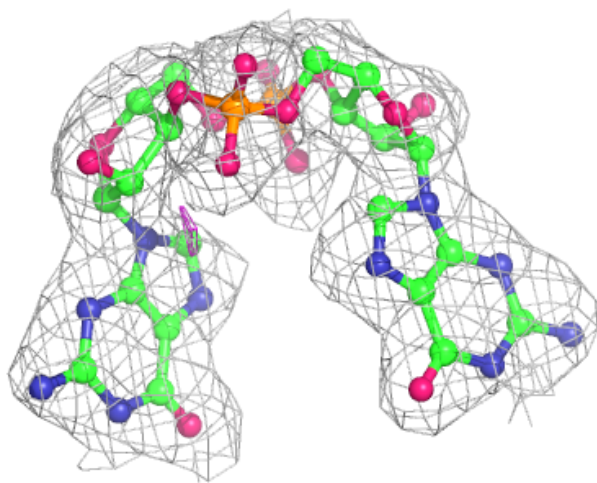
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	C2E	A	801	46/46	0.96	0.12	29,37,43,45	0
3	C2E	F	801	46/46	0.97	0.11	22,33,43,45	0
3	C2E	B	801	46/46	0.97	0.12	28,39,51,63	0
3	C2E	C	801	46/46	0.97	0.11	22,32,40,49	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around C2E A 801:**

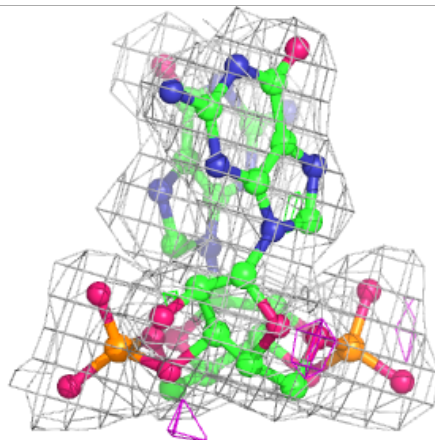
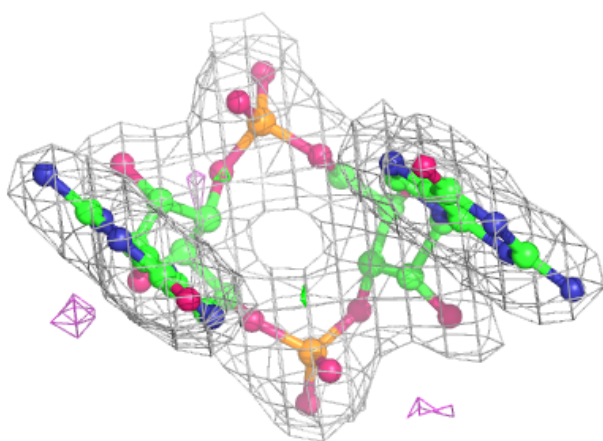
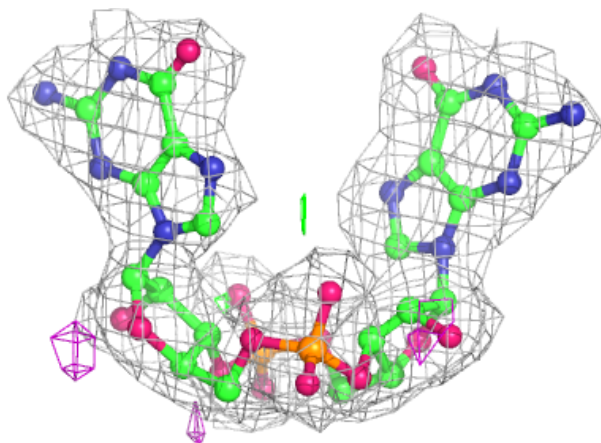
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





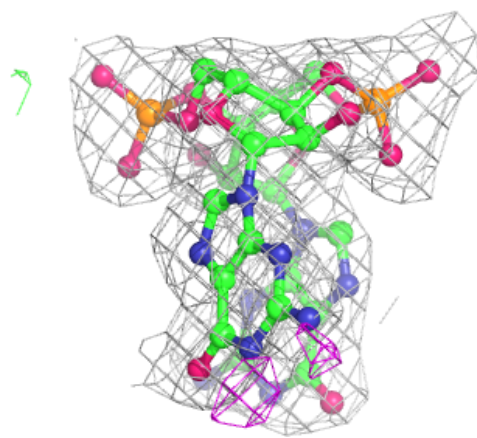
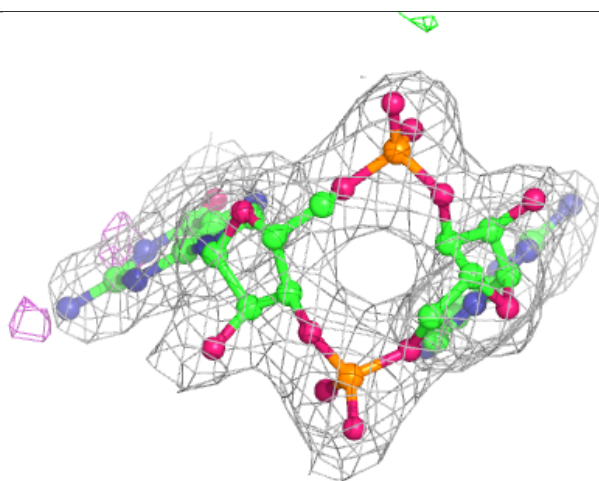
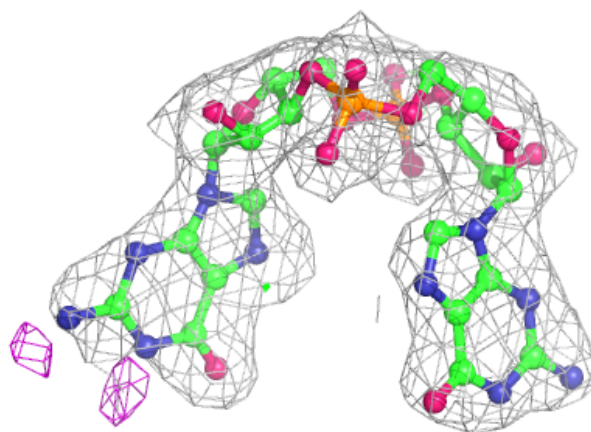
**Electron density around C2E F 801:**

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



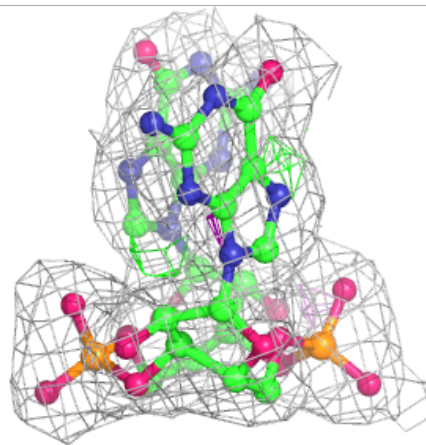
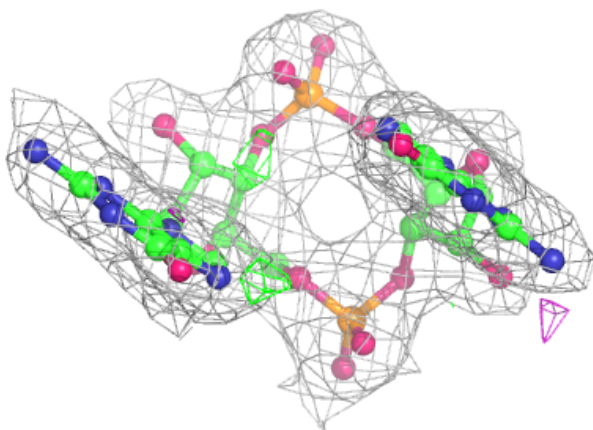
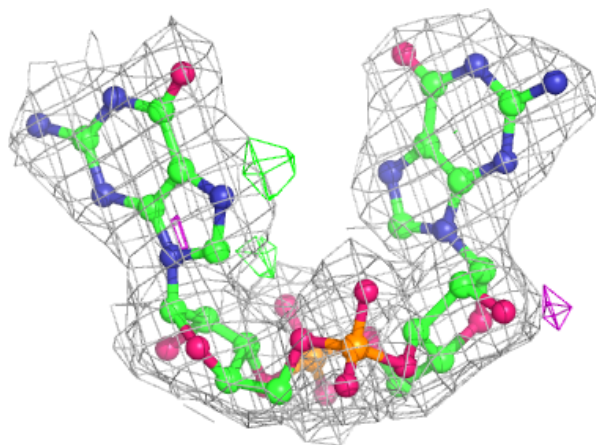
**Electron density around C2E B 801:**

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



**Electron density around C2E C 801:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.