



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 08:01 PM BST

PDB ID : 5TPC  
Title : Binding domain of BoNT/A complexed with ganglioside  
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Deposited on : 2016-10-20  
Resolution : 2.00 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

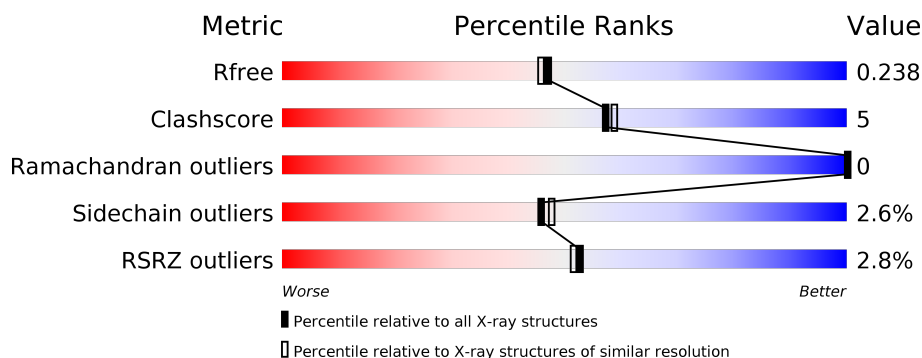
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	425	<div> <div>3%</div> <div>87%</div> <div>12%</div> </div>
2	B	2	<div> <div>50%</div> <div>50%</div> </div>
3	C	3	<div> <div>33%</div> <div>67%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3943 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.

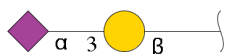
- Molecule 1 is a protein called Botulinum neurotoxin type A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	425	3540	2250	613	663	14	0	5	0

There are 4 discrepancies between the modelled and reference sequences:

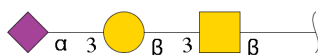
Chain	Residue	Modelled	Actual	Comment	Reference
A	873	HIS	-	expression tag	UNP P10845
A	874	MET	-	expression tag	UNP P10845
A	875	ASP	-	expression tag	UNP P10845
A	1297	GLN	-	expression tag	UNP P10845

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	32	17	1	14	0	0	0

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			45	25	2	18			

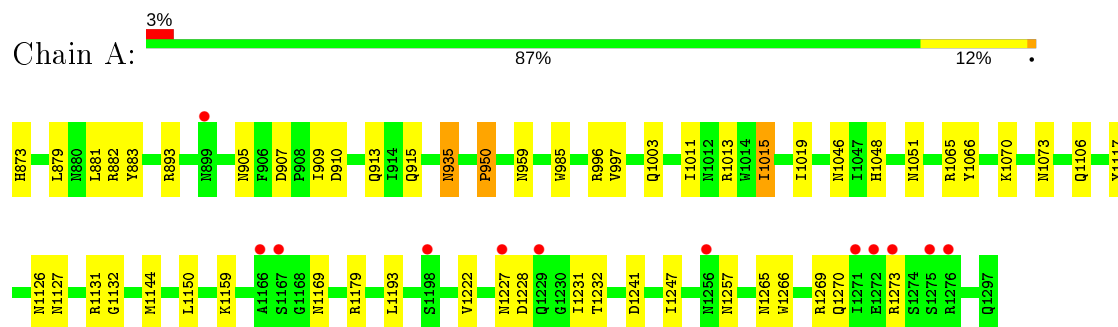
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	326	Total	O	0	0
			326	326		

### 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: Botulinum neurotoxin type A



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.97Å 114.30Å 106.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.10 – 2.00 40.42 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.7 (62.10-2.00) 97.8 (40.42-2.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.203 , 0.238 0.203 , 0.238	Depositor DCC
$R_{free}$ test set	1532 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.6	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 45.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3943	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.54% 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: SIA, GAL, NGA

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	0.45	0/3614	0.62	0/4884

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	3540	0	3489	34	0
2	B	32	0	27	0	0
3	C	45	0	38	2	0
4	A	326	0	0	9	0
All	All	3943	0	3554	35	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 (35) 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:1013[A]:ARG:HH12	1:A:1231:ILE:HD11	0.96	1.10
1:A:1013[A]:ARG:NH1	1:A:1231:ILE:HD11	1.80	0.94
1:A:1126:ASN:O	4:A:1401:HOH:O	2.05	0.75
1:A:1257:ASN:HB2	4:A:1685:HOH:O	1.86	0.74
1:A:1159:LYS:HD3	4:A:1713:HOH:O	1.97	0.64
1:A:909:ILE:HD13	1:A:1106:GLN:NE2	2.14	0.63
1:A:1013[B]:ARG:HH22	1:A:1232:THR:HG22	1.63	0.63
1:A:909:ILE:HD13	1:A:1106:GLN:HE22	1.64	0.62
1:A:1179:ARG:HG2	1:A:1222:VAL:HG22	1.84	0.59
1:A:1193:LEU:HD12	4:A:1475:HOH:O	2.05	0.56
1:A:1015:ILE:HG22	4:A:1489:HOH:O	2.09	0.53
1:A:1266:TRP:O	1:A:1270:GLN:HG2	2.10	0.52
1:A:1051[A]:ASN:O	1:A:1051[A]:ASN:OD1	2.27	0.51
1:A:1169:ASN:HB3	4:A:1583:HOH:O	2.10	0.51
1:A:935:ASN:ND2	1:A:1046:ASN:HD21	2.08	0.51
1:A:1003:GLN:HA	1:A:1011:ILE:HD11	1.95	0.48
3:C:3:SIA:H6	3:C:3:SIA:O1A	2.13	0.48
1:A:873:HIS:N	4:A:1404:HOH:O	2.47	0.47
1:A:1144:MET:HG3	1:A:1150:LEU:HD13	1.97	0.46
1:A:1241:ASP:HB3	1:A:1247:ILE:HD11	1.97	0.46
1:A:1265:ASN:O	1:A:1269:ARG:HG3	2.16	0.46
1:A:913:GLN:HG2	1:A:1070:LYS:HD3	1.96	0.46
1:A:1117:TYR:CE1	3:C:3:SIA:H4	2.49	0.45
1:A:985:TRP:O	1:A:996:ARG:HA	2.17	0.45
1:A:950:PRO:HG3	1:A:1066:TYR:CE1	2.52	0.44
1:A:985:TRP:HB3	1:A:997:VAL:HG23	1.99	0.44
1:A:1228:ASP:HB3	1:A:1273:ARG:HG2	2.00	0.43
1:A:985:TRP:CD2	1:A:1019:ILE:HG21	2.55	0.42
1:A:879:LEU:O	1:A:1073:ASN:HA	2.20	0.42
1:A:893:ARG:HD3	4:A:1442:HOH:O	2.19	0.42
1:A:1127:ASN:O	1:A:1132:GLY:HA3	2.20	0.41
1:A:883:TYR:HB2	4:A:1529:HOH:O	2.19	0.41
1:A:935:ASN:HD22	1:A:1046:ASN:HD21	1.69	0.41
1:A:905:ASN:HB3	1:A:915:GLN:HB3	2.02	0.41
1:A:907:ASP:HB3	1:A:910:ASP:O	2.20	0.41

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	428/425 (101%)	407 (95%)	21 (5%)	0	100	100

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	397/392 (101%)	387 (98%)	10 (2%)	47	49

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	881	LEU
1	A	882	ARG
1	A	935	ASN
1	A	950	PRO
1	A	959	ASN
1	A	1015	ILE
1	A	1048	HIS
1	A	1065	ARG
1	A	1131	ARG
1	A	1227	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	935	ASN
1	A	1026	ASN
1	A	1048	HIS
1	A	1052	ASN
1	A	1073	ASN
1	A	1093	ASN
1	A	1233	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 ⓘ

5 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	GAL	B	1	2	12,12,12	0.46	0	17,17,17	0.54	0
2	SIA	B	2	2	17,20,21	0.76	1 (5%)	21,28,31	0.85	1 (4%)
3	NGA	C	1	3	14,14,15	0.55	0	17,19,21	0.70	0
3	GAL	C	2	3	11,11,12	0.61	0	15,15,17	1.01	1 (6%)
3	SIA	C	3	1,3	17,20,21	0.27	0	21,28,31	0.52	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	GAL	B	1	2	-	0/2/22/22	0/1/1/1
2	SIA	B	2	2	-	0/14/34/38	0/1/1/1
3	NGA	C	1	3	-	0/6/23/26	0/1/1/1
3	GAL	C	2	3	-	1/2/19/22	0/1/1/1
3	SIA	C	3	1,3	-	7/14/34/38	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	SIA	C4-C5	-2.66	1.50	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	SIA	C6-O6-C2	3.20	118.18	111.34
3	C	2	GAL	C1-O5-C5	2.34	115.36	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

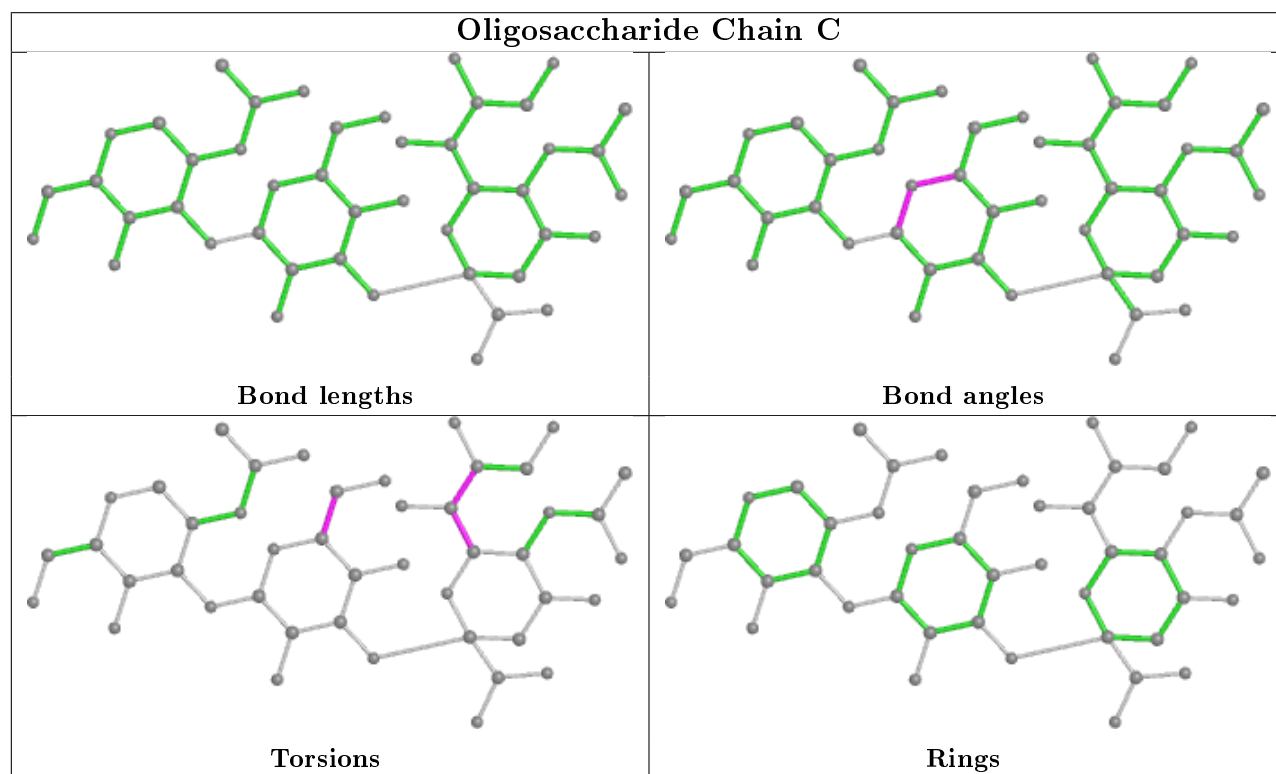
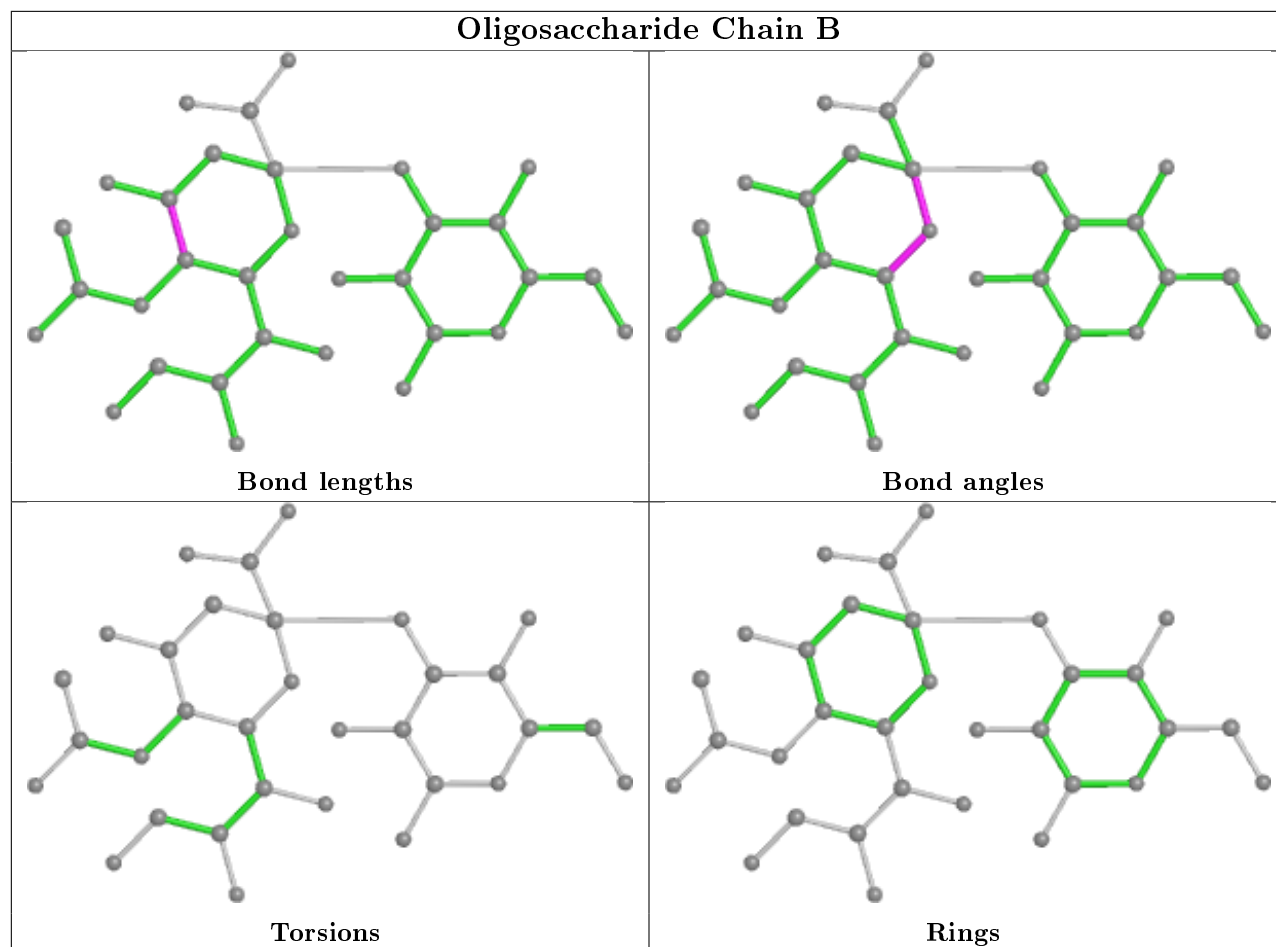
Mol	Chain	Res	Type	Atoms
3	C	3	SIA	C5-C6-C7-C8
3	C	3	SIA	C5-C6-C7-O7
3	C	3	SIA	O6-C6-C7-C8
3	C	3	SIA	O6-C6-C7-O7
3	C	2	GAL	O5-C5-C6-O6
3	C	3	SIA	O7-C7-C8-O8
3	C	3	SIA	C6-C7-C8-C9
3	C	3	SIA	O7-C7-C8-C9

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3	SIA	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

There are no ligands in this entry.

## 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 [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	425/425 (100%)	-0.06	12 (2%) 53 51	12, 24, 44, 93	4 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1272	GLU	5.0
1	A	1273	ARG	4.8
1	A	1229	GLN	4.1
1	A	1227	ASN	2.9
1	A	1198	SER	2.9
1	A	899	ASN	2.8
1	A	1167	SER	2.7
1	A	1166	ALA	2.7
1	A	1271	ILE	2.4
1	A	1276	ARG	2.4
1	A	1256	ASN	2.2
1	A	1275	SER	2.1

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

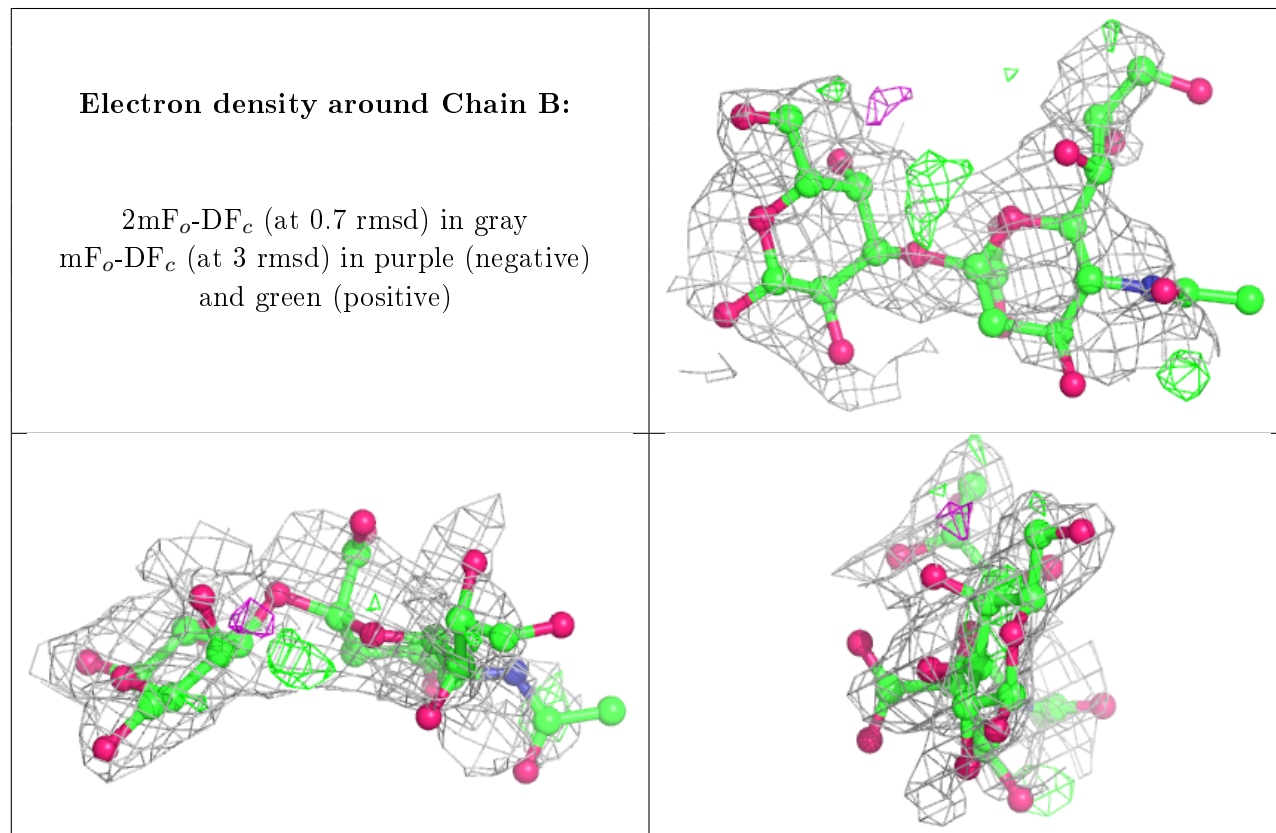
There are no non-standard protein/DNA/RNA residues in this entry.

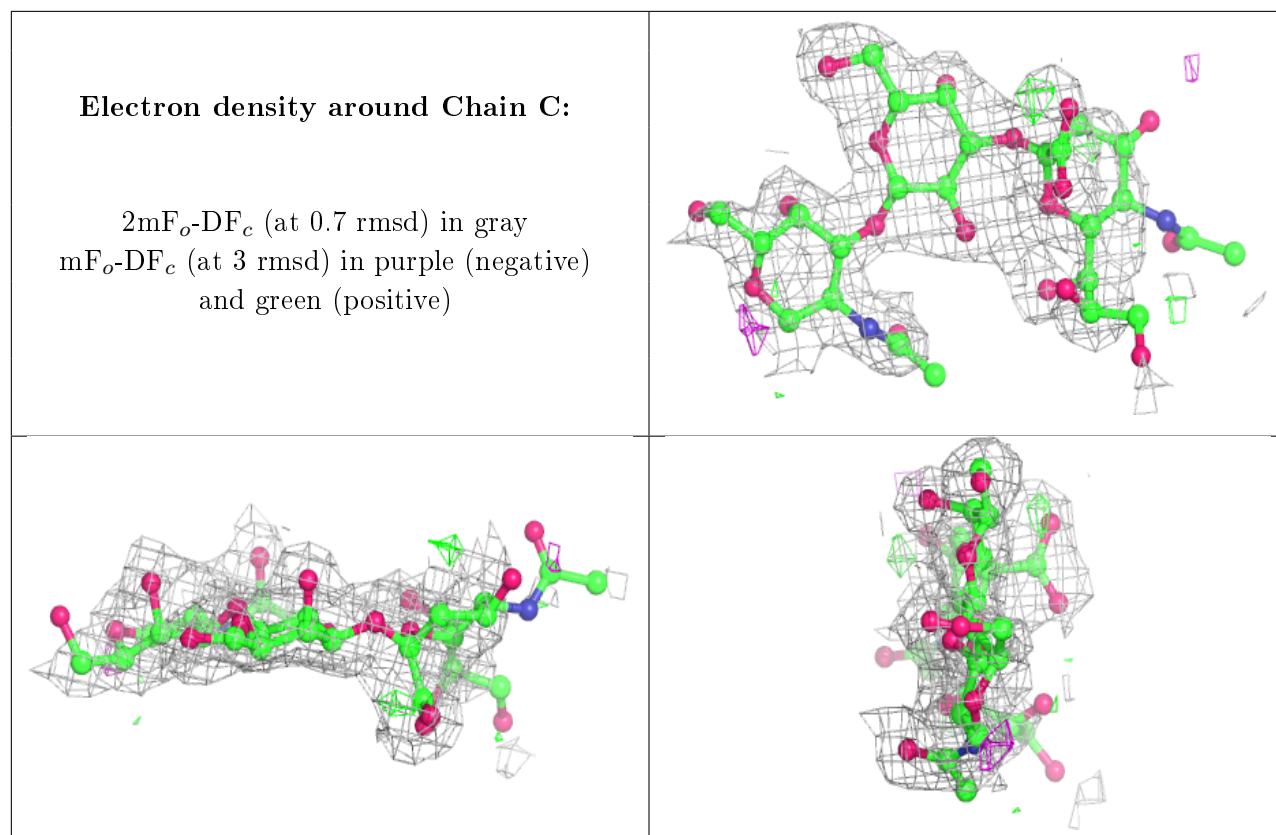
### 6.3 Carbohydrates [i](#)

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( $\text{\AA}^2$ )	Q<0.9
2	GAL	B	1	12/12	0.64	0.23	62,71,74,75	0
2	SIA	B	2	20/21	0.76	0.30	81,86,88,91	0
3	SIA	C	3	20/21	0.82	0.31	57,79,94,97	0
3	NGA	C	1	14/15	0.83	0.21	45,55,59,60	0
3	GAL	C	2	11/12	0.92	0.11	32,38,43,48	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.





## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.