



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 28, 2024 – 01:46 am GMT

PDB ID : 6T2S  
Title : Prominent members of the human gut microbiota express endo-acting O-glycanases to initiate mucin breakdown  
Authors : Crouch, L.I.; Liberato, M.V.; Ubranowicz, P.A.; Basle, A.; Lamb, C.A.; Cooke, K.; Doona, M.; Needham, S.; Brady, R.R.; Berrington, J.E.; Madubic, K.; Chater, P.; Zhang, F.; Linhardt, R.J.; Spence, D.I.R.; Bolam, D.N.  
Deposited on : 2019-10-09  
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

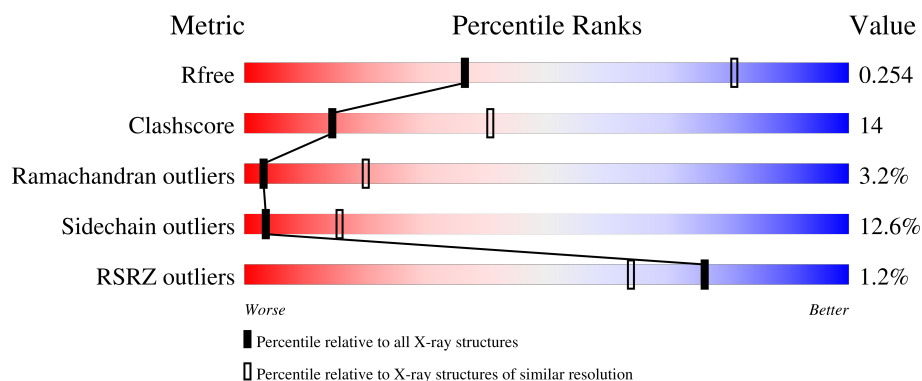
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)

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	AAA	241	<div> <div>2%</div> <div>60% 37% .</div> </div>
1	BBB	241	<div> <div>65% 28% 7%</div> </div>
1	CCC	241	<div> <div>2%</div> <div>61% 31% 7% .</div> </div>
2	A	3	<div> <div>67% 33%</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	3	<div><div></div><div>33%</div><div>67%</div></div>
2	C	3	<div><div>67%</div><div>33%</div></div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GAL	A	1	X	-	-	-
2	NAG	C	2	X	-	-	-

## 2 Entry composition [i](#)

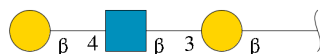
There are 2 unique types of molecules in this entry. The entry contains 5922 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycoside hydrolase family 16 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	241	Total	C	N	O	S	0	0	0
			1937	1244	322	362	9			
1	BBB	241	Total	C	N	O	S	0	0	0
			1937	1244	322	362	9			
1	CCC	241	Total	C	N	O	S	0	0	0
			1937	1244	322	362	9			

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose.

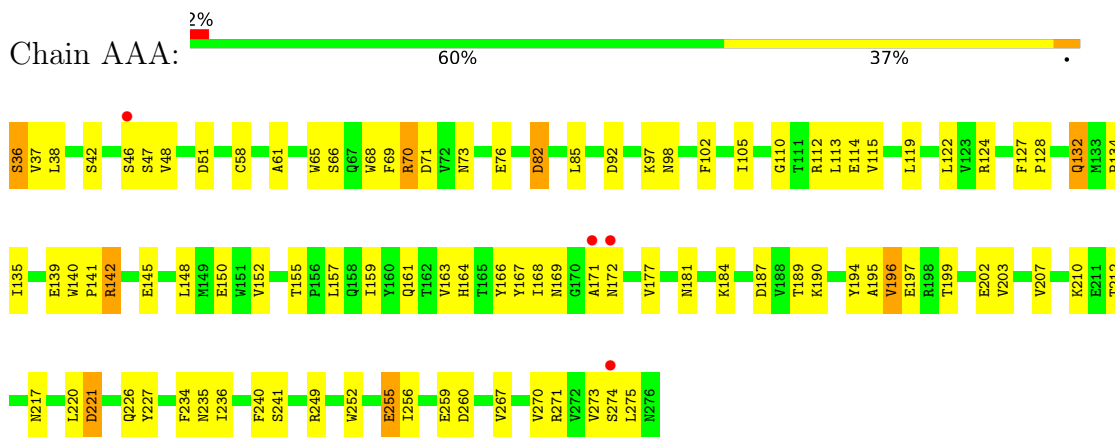


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	3	Total	C	N	O	0	0	0
			37	20	1	16			
2	B	3	Total	C	N	O	0	0	0
			37	20	1	16			
2	C	3	Total	C	N	O	0	0	0
			37	20	1	16			

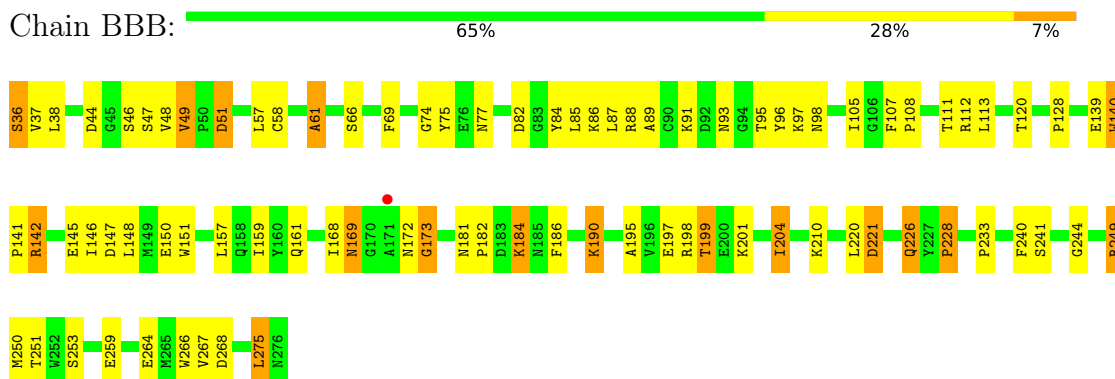
### 3 Residue-property plots

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.

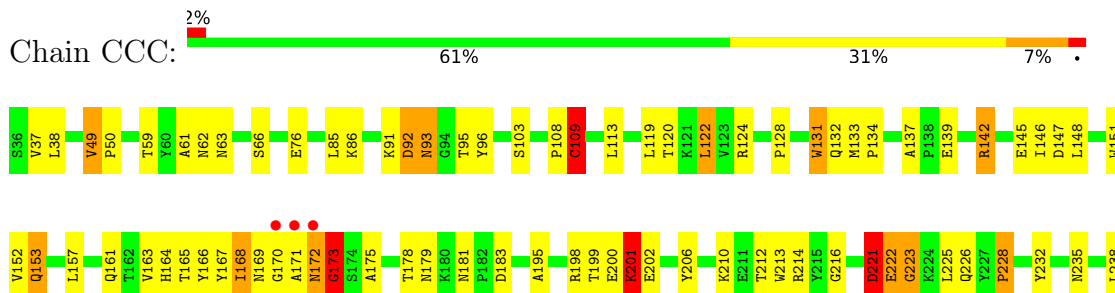
- Molecule 1: Glycoside hydrolase family 16 protein



- Molecule 1: Glycoside hydrolase family 16 protein



- Molecule 1: Glycoside hydrolase family 16 protein





- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



- Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-beta-D-galactopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.62Å 156.62Å 197.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	135.64 – 3.30 135.64 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (135.64-3.30) 99.9 (135.64-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, $R_{free}$	0.199 , 0.253 0.202 , 0.254	Depositor DCC
$R_{free}$ test set	1097 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.6	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 54.5	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	0.90	EDS
Total number of atoms	5922	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.30% 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: GAL, 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	AAA	0.79	0/1993	1.14	2/2711 (0.1%)
1	BBB	0.77	0/1993	1.04	2/2711 (0.1%)
1	CCC	0.75	0/1993	1.09	5/2711 (0.2%)
All	All	0.77	0/5979	1.09	9/8133 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AAA	0	3
1	BBB	0	1
1	CCC	0	4
All	All	0	8

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	51	ASP	CB-CA-C	6.58	123.57	110.40
1	CCC	95	THR	CA-CB-OG1	-6.32	95.72	109.00
1	AAA	142	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	AAA	194	TYR	CB-CG-CD2	6.13	124.68	121.00
1	CCC	142	ARG	NE-CZ-NH1	5.87	123.24	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	AAA	169	ASN	Peptide
1	AAA	36	SER	Peptide
1	AAA	46	SER	Peptide
1	BBB	169	ASN	Peptide
1	CCC	168	ILE	Peptide

## 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	AAA	1937	0	1844	57	0
1	BBB	1937	0	1844	45	0
1	CCC	1937	0	1844	59	0
2	A	37	0	32	3	0
2	B	37	0	32	2	0
2	C	37	0	32	2	0
All	All	5922	0	5628	159	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 14.

The worst 5 of 159 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:CCC:200:GLU:N	1:CCC:200:GLU:OE2	2.11	0.83
1:CCC:202:GLU:HB3	1:CCC:216:GLY:HA2	1.64	0.79
1:AAA:119:LEU:HD11	1:AAA:128:PRO:HG3	1.64	0.77
1:AAA:132:GLN:HG3	1:AAA:235:ASN:O	1.87	0.74
1:AAA:132:GLN:CG	1:AAA:235:ASN:O	2.36	0.73

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	AAA	239/241 (99%)	204 (85%)	31 (13%)	4 (2%)	7	31
1	BBB	239/241 (99%)	203 (85%)	28 (12%)	8 (3%)	3	19
1	CCC	239/241 (99%)	203 (85%)	25 (10%)	11 (5%)	2	13
All	All	717/723 (99%)	610 (85%)	84 (12%)	23 (3%)	3	20

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	259	GLU
1	CCC	109	CYS
1	CCC	172	ASN
1	CCC	201	LYS
1	CCC	259	GLU

### 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	AAA	206/206 (100%)	179 (87%)	27 (13%)	3	14
1	BBB	206/206 (100%)	179 (87%)	27 (13%)	3	14
1	CCC	206/206 (100%)	182 (88%)	24 (12%)	4	17
All	All	618/618 (100%)	540 (87%)	78 (13%)	3	16

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	59	THR
1	CCC	228	PRO
1	CCC	85	LEU
1	CCC	157	LEU
1	CCC	253	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

9 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	A	1	2	12,12,12	0.96	0	17,17,17	2.82	7 (41%)
2	NAG	A	2	2	14,14,15	0.76	0	17,19,21	1.80	5 (29%)
2	GAL	A	3	2	11,11,12	0.84	0	15,15,17	1.59	3 (20%)
2	GAL	B	1	2	12,12,12	0.67	0	17,17,17	1.29	1 (5%)
2	NAG	B	2	2	14,14,15	0.93	0	17,19,21	3.47	7 (41%)
2	GAL	B	3	2	11,11,12	0.64	0	15,15,17	1.78	3 (20%)
2	GAL	C	1	2	12,12,12	0.74	0	17,17,17	1.64	1 (5%)
2	NAG	C	2	2	14,14,15	0.87	0	17,19,21	3.45	7 (41%)
2	GAL	C	3	2	11,11,12	0.89	0	15,15,17	1.71	4 (26%)

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	A	1	2	1/1/5/5	1/2/22/22	0/1/1/1
2	NAG	A	2	2	-	0/6/23/26	0/1/1/1
2	GAL	A	3	2	-	0/2/19/22	0/1/1/1
2	GAL	B	1	2	-	0/2/22/22	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	GAL	B	3	2	-	1/2/19/22	0/1/1/1
2	GAL	C	1	2	-	2/2/22/22	0/1/1/1
2	NAG	C	2	2	1/1/5/7	2/6/23/26	0/1/1/1
2	GAL	C	3	2	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	NAG	O4-C4-C5	12.68	140.77	109.30
2	B	2	NAG	O4-C4-C3	10.46	134.53	110.35
2	A	1	GAL	O3-C3-C4	8.69	130.44	110.35
2	B	2	NAG	O4-C4-C5	-6.74	92.57	109.30
2	C	1	GAL	O3-C3-C4	5.23	122.44	110.35

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1	GAL	C3
2	C	2	NAG	C4

5 of 10 torsion outliers are listed below:

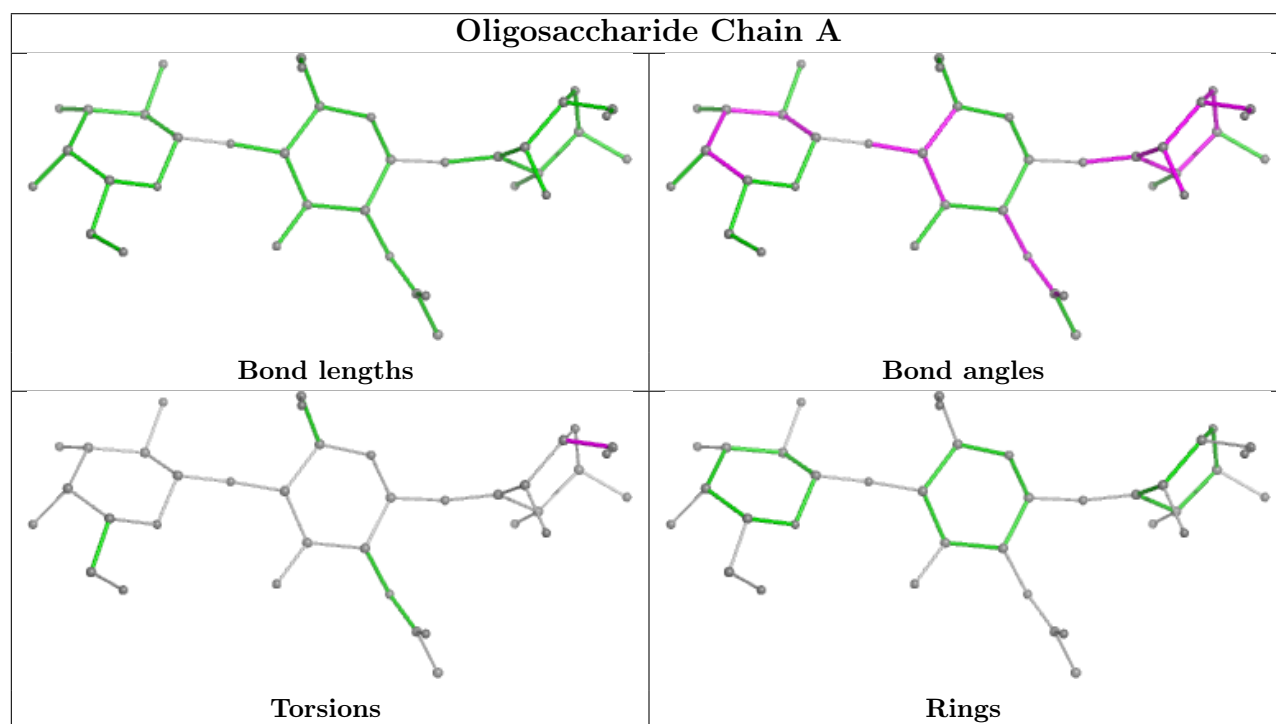
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	C	3	GAL	C4-C5-C6-O6
2	C	3	GAL	O5-C5-C6-O6
2	A	1	GAL	O5-C5-C6-O6

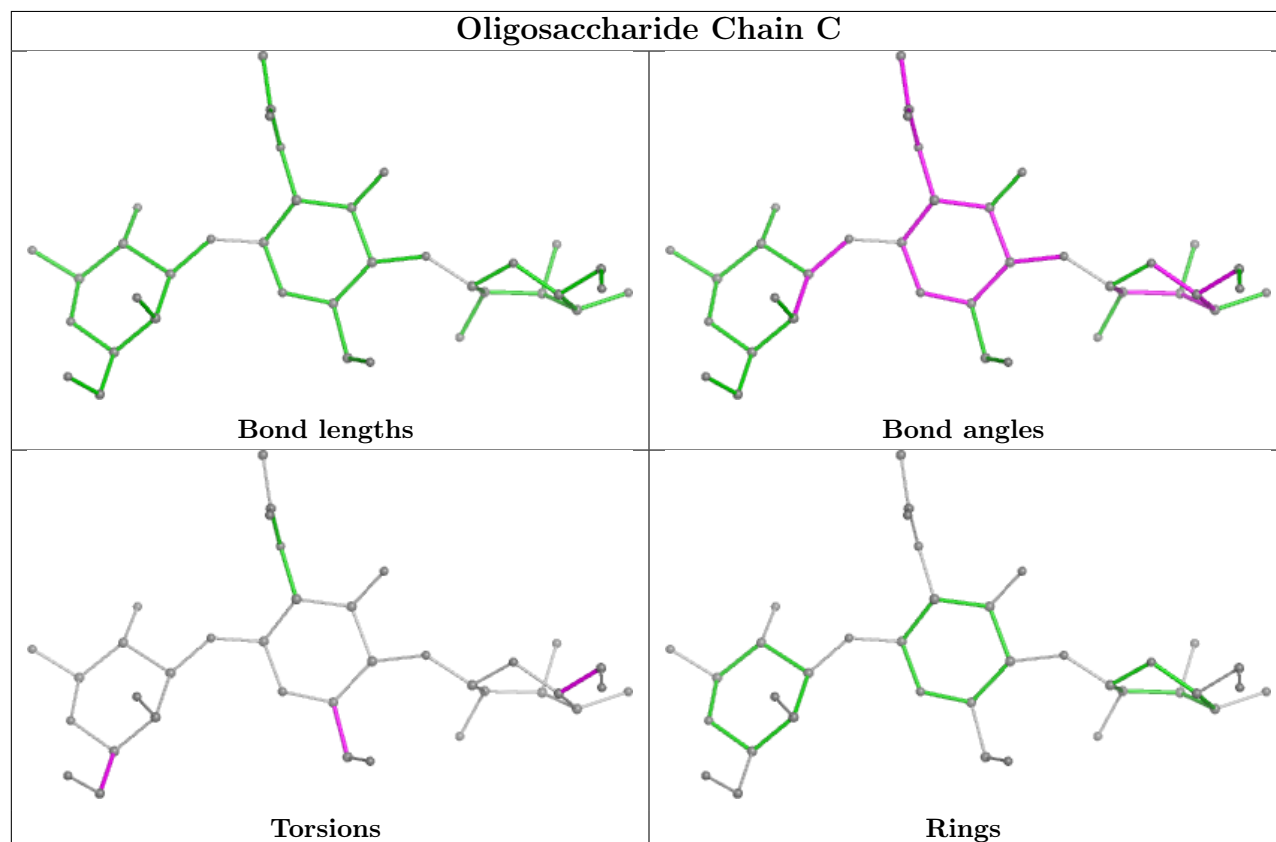
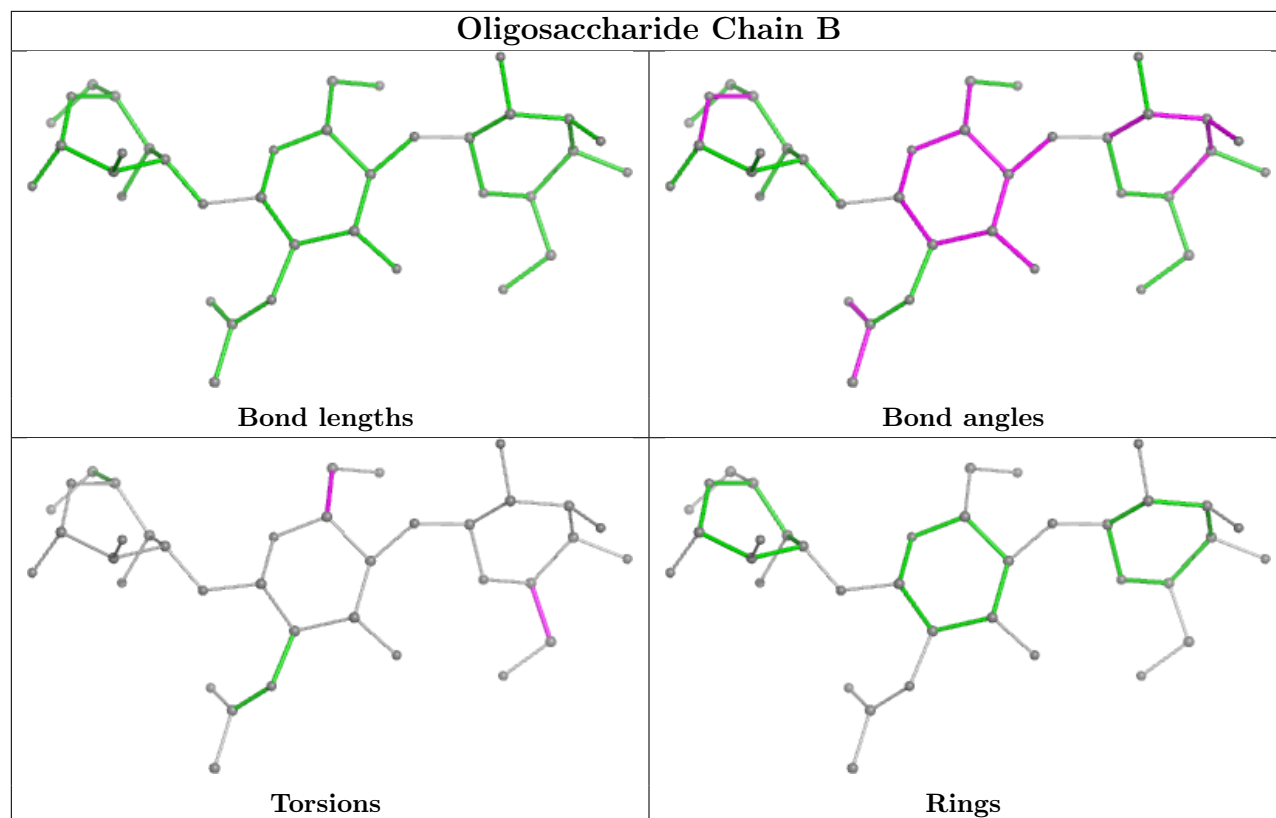
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	2	0
2	B	1	GAL	1	0
2	A	1	GAL	3	0
2	B	2	NAG	1	0

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





## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	AAA	241/241 (100%)	-0.36	4 (1%) 69 55	36, 53, 78, 117	0
1	BBB	241/241 (100%)	-0.18	1 (0%) 89 83	44, 70, 96, 123	0
1	CCC	241/241 (100%)	-0.19	4 (1%) 69 55	46, 67, 114, 147	0
All	All	723/723 (100%)	-0.24	9 (1%) 76 64	36, 63, 102, 147	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	171	ALA	5.7
1	AAA	172	ASN	5.0
1	CCC	172	ASN	3.7
1	CCC	276	ASN	2.4
1	AAA	274	SER	2.4

### 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](#)

SUGAR-RSR INFOmissingINFO

### 6.4 Ligands [i](#)

There are no ligands in this entry.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.