



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 04:49 PM EDT

PDB ID : 7KV7  
Title : Surface glycan-binding protein B from *Bacteroides fluxus* in complex with laminaritriose  
Authors : Tamura, K.; Brumer, H.; Van Petegem, F.  
Deposited on : 2020-11-26  
Resolution : 1.76 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

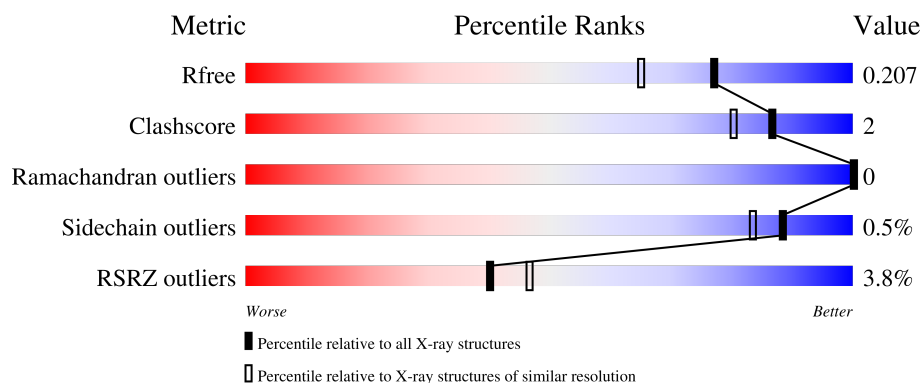
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


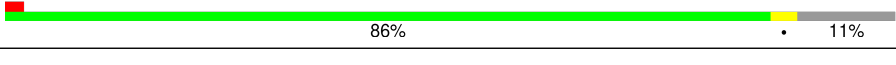
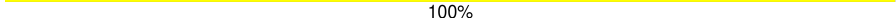
The reported resolution of this entry is 1.76 Å.

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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	290	
1	BBB	290	
2	BbB	2	

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8307 atoms, of which 3717 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 PKD domain protein.

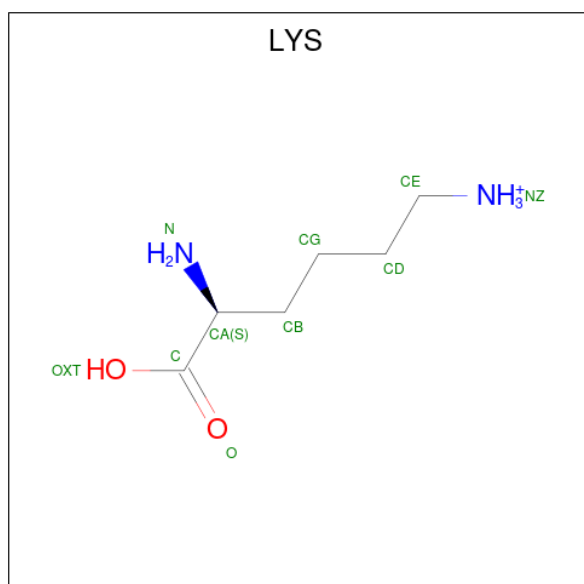
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	248	Total	C	H	N	O	S	107	3	0
			3680	1205	1784	306	379	6			
1	BBB	258	Total	C	H	N	O	S	110	2	0
			3822	1249	1856	317	394	6			

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



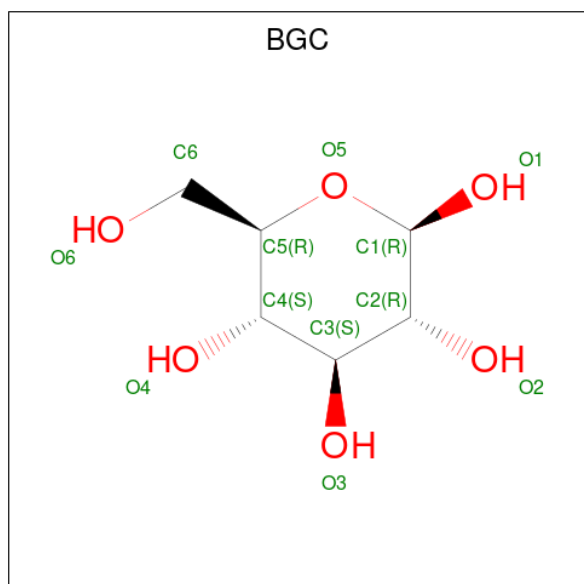
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	BbB	2	Total	C	H	O	5	0	0
			46	12	23	11			

- Molecule 3 is LYSINE (three-letter code: LYS) (formula: C<sub>6</sub>H<sub>15</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total	C	H	N	O	0	0
			10	3	5	1	1		

- Molecule 4 is beta-D-glucopyranose (three-letter code: BGC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	H	O	3	0
			22	6	11	5		
4	AAA	1	Total	C	H	O	4	0
			23	6	11	6		
4	BBB	1	Total	C	H	O	3	0
			22	6	11	5		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	AAA	1	Total	C	H	O	1	0
			17	4	10	3		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AAA	1	Total	O	S	0	0
			5	4	1		
6	BBB	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	BBB	1	Total	C	H	O	1	0
			10	2	6	2		

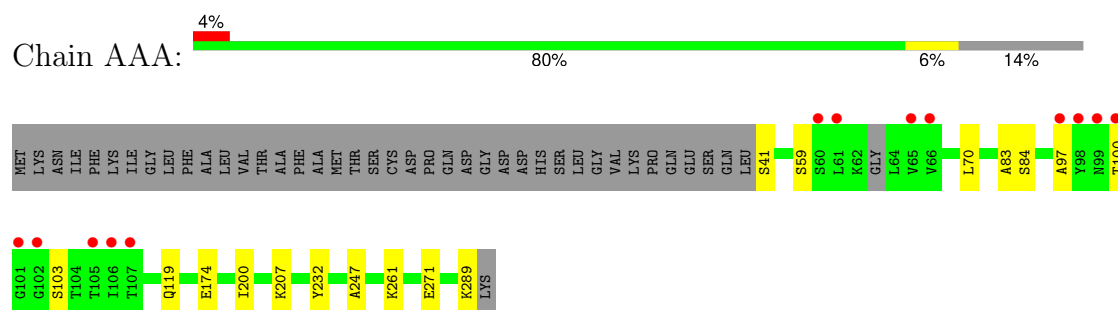
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	309	Total	O	0	0
			309	309		
8	BBB	336	Total	O	0	0
			336	336		

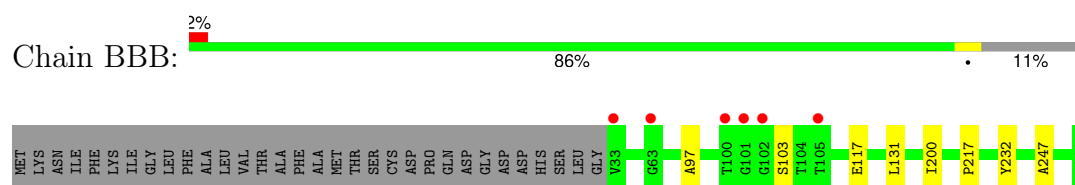
### 3 Residue-property plots [i](#)

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: PKD domain protein



- Molecule 1: PKD domain protein



- Molecule 2: beta-D-glucopyranose-(1-3)-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.27 Å   59.25 Å   148.14 Å 90.00°   102.61°   90.00°	Depositor
Resolution (Å)	35.66 – 1.76 35.66 – 1.76	Depositor EDS
% Data completeness (in resolution range)	92.7 (35.66-1.76) 92.7 (35.66-1.76)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.23 (at 1.76 Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.159   ,   0.202 0.170   ,   0.207	Depositor DCC
$R_{free}$ test set	2864 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 62.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8307	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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: SO4, BGC, PEG, EDO

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	1/1948 (0.1%)	0.87	0/2657
1	BBB	0.79	0/2020	0.85	0/2756
All	All	0.79	1/3968 (0.0%)	0.86	0/5413

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	271	GLU	CD-OE2	-6.99	1.18	1.25

There are no bond angle outliers.

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	AAA	1896	1784	1770	10	1
1	BBB	1966	1856	1844	4	0
2	BbB	23	23	20	0	0
3	AAA	5	5	1	3	0
4	AAA	23	22	21	0	0
4	BBB	11	11	10	0	0
5	AAA	7	10	10	0	0
6	AAA	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	BBB	5	0	0	0	0
7	BBB	4	6	6	1	0
8	AAA	309	0	0	2	1
8	BBB	336	0	0	1	0
All	All	4590	3717	3682	16	2

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 2.

All (16) 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:AAA:289:LYS:C	3:AAA:301:LYS:N	1.91	1.23
3:AAA:301:LYS:CB	8:AAA:644:HOH:O	2.31	0.79
1:BBB:117:GLU:HB3	1:BBB:131:LEU:HD11	1.68	0.76
1:AAA:289:LYS:C	3:AAA:301:LYS:CA	2.73	0.57
1:AAA:41:SER:N	1:AAA:59:SER:HG	2.09	0.50
1:AAA:70:LEU:HD13	1:AAA:83:ALA:HB2	1.96	0.47
1:BBB:232:TYR:CE2	1:BBB:247:ALA:HB2	2.51	0.45
1:AAA:261:LYS:HE2	8:AAA:520:HOH:O	2.18	0.44
1:AAA:97:ALA:O	1:AAA:103:SER:HA	2.19	0.43
1:BBB:200:ILE:C	1:BBB:200:ILE:HD12	2.39	0.43
1:AAA:232:TYR:CE1	1:AAA:247:ALA:HB2	2.53	0.43
1:AAA:70:LEU:HD13	1:AAA:83:ALA:CB	2.50	0.42
1:BBB:97:ALA:O	1:BBB:103:SER:HA	2.20	0.41
1:AAA:200:ILE:C	1:AAA:200:ILE:HD12	2.41	0.41
1:AAA:84:SER:OG	1:AAA:119:GLN:OE1	2.36	0.40
7:BBB:302:EDO:O1	8:BBB:401:HOH:O	2.20	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AAA:654:HOH:O	8:AAA:670:HOH:O[4_444]	1.63	0.57
1:AAA:100:THR:HG1	1:AAA:174:GLU:OE1[3_555]	1.59	0.01

## 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	AAA	247/290 (85%)	238 (96%)	9 (4%)	0	100	100
1	BBB	258/290 (89%)	250 (97%)	8 (3%)	0	100	100
All	All	505/580 (87%)	488 (97%)	17 (3%)	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	AAA	198/233 (85%)	197 (100%)	1 (0%)	88	83
1	BBB	206/233 (88%)	205 (100%)	1 (0%)	88	83
All	All	404/466 (87%)	402 (100%)	2 (0%)	88	83

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	207	LYS
1	BBB	217	PRO

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 ⓘ

2 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	BGC	BbB	1	2	12,12,12	0.61	0	17,17,17	1.20	1 (5%)
2	BGC	BbB	2	2	11,11,12	0.53	0	15,15,17	1.13	2 (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	BGC	BbB	1	2	-	1/2/22/22	0/1/1/1
2	BGC	BbB	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BbB	1	BGC	O3-C3-C2	-3.03	103.23	110.38
2	BbB	2	BGC	C1-O5-C5	-2.32	109.07	112.19
2	BbB	2	BGC	C1-C2-C3	2.10	112.70	109.64

There are no chirality outliers.

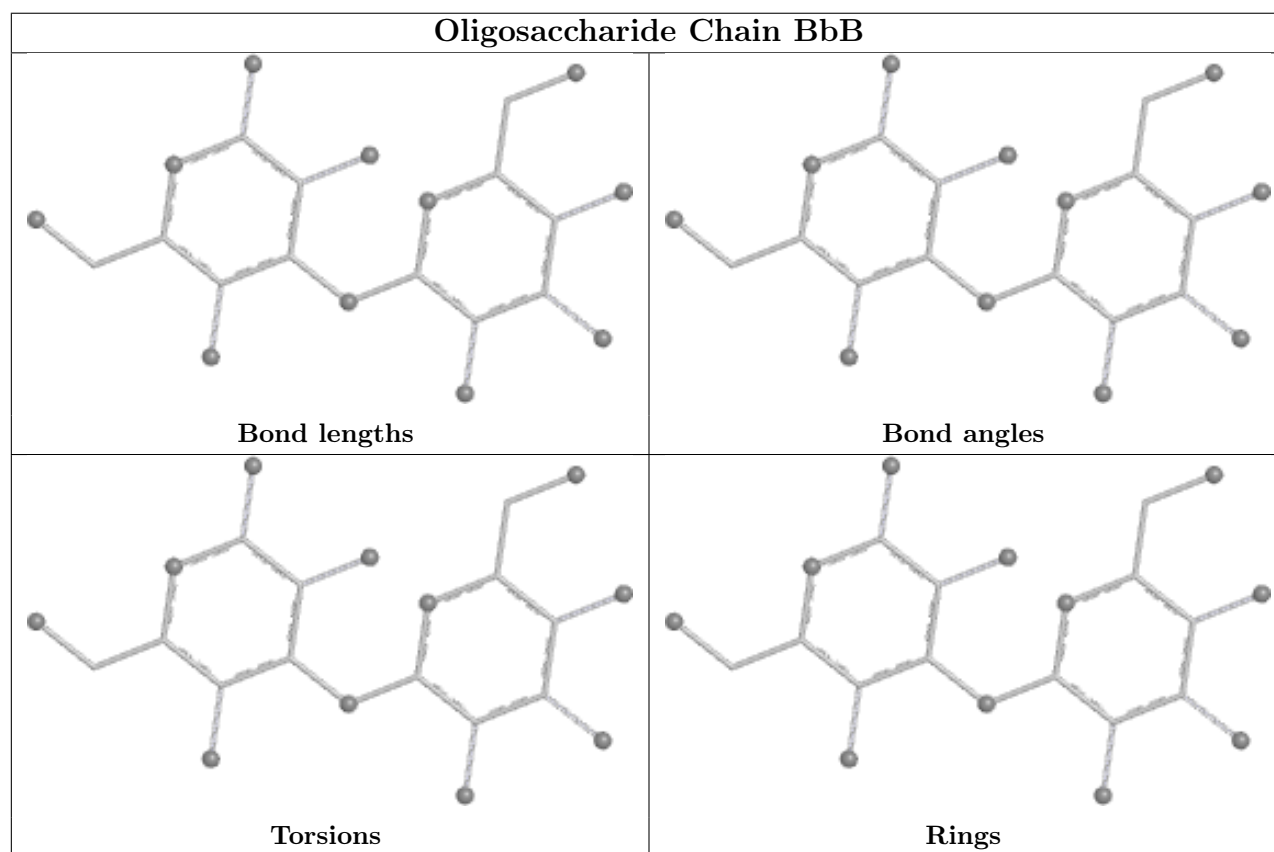
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BbB	1	BGC	O5-C5-C6-O6

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.



## 5.6 Ligand geometry [i](#)

8 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
4	BGC	AAA	302	-	11,11,12	0.92	1 (9%)	14,15,17	1.92	6 (42%)
3	LYS	AAA	301	-	3,4,9	1.06	0	2,4,10	0.28	0
4	BGC	BBB	301	-	11,11,12	0.86	0	14,15,17	0.87	0
5	PEG	AAA	304	-	6,6,6	0.48	0	5,5,5	0.19	0
6	SO4	BBB	303	-	4,4,4	0.30	0	6,6,6	0.15	0
7	EDO	BBB	302	-	3,3,3	0.16	0	2,2,2	0.14	0
6	SO4	AAA	305	-	4,4,4	0.36	0	6,6,6	0.19	0
4	BGC	AAA	303	-	12,12,12	0.44	0	17,17,17	0.81	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
4	BGC	AAA	302	-	-	0/2/18/22	0/1/1/1
3	LYS	AAA	301	-	-	0/1/2/9	-
4	BGC	BBB	301	-	-	0/2/18/22	0/1/1/1
5	PEG	AAA	304	-	-	2/4/4/4	-
7	EDO	BBB	302	-	-	0/1/1/1	-
4	BGC	AAA	303	-	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AAA	302	BGC	C1-C2	2.24	1.54	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AAA	302	BGC	C6-C5-C4	-3.33	108.97	113.53
4	AAA	302	BGC	O2-C2-C1	3.23	114.99	108.94
4	AAA	302	BGC	C4-C3-C2	-3.10	107.90	111.50
4	AAA	302	BGC	C3-C4-C5	-2.49	107.58	110.76
4	AAA	302	BGC	O5-C5-C6	2.05	111.52	106.44
4	AAA	302	BGC	C1-O5-C5	-2.02	109.75	113.65

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	AAA	304	PEG	O1-C1-C2-O2
5	AAA	304	PEG	C1-C2-O2-C3

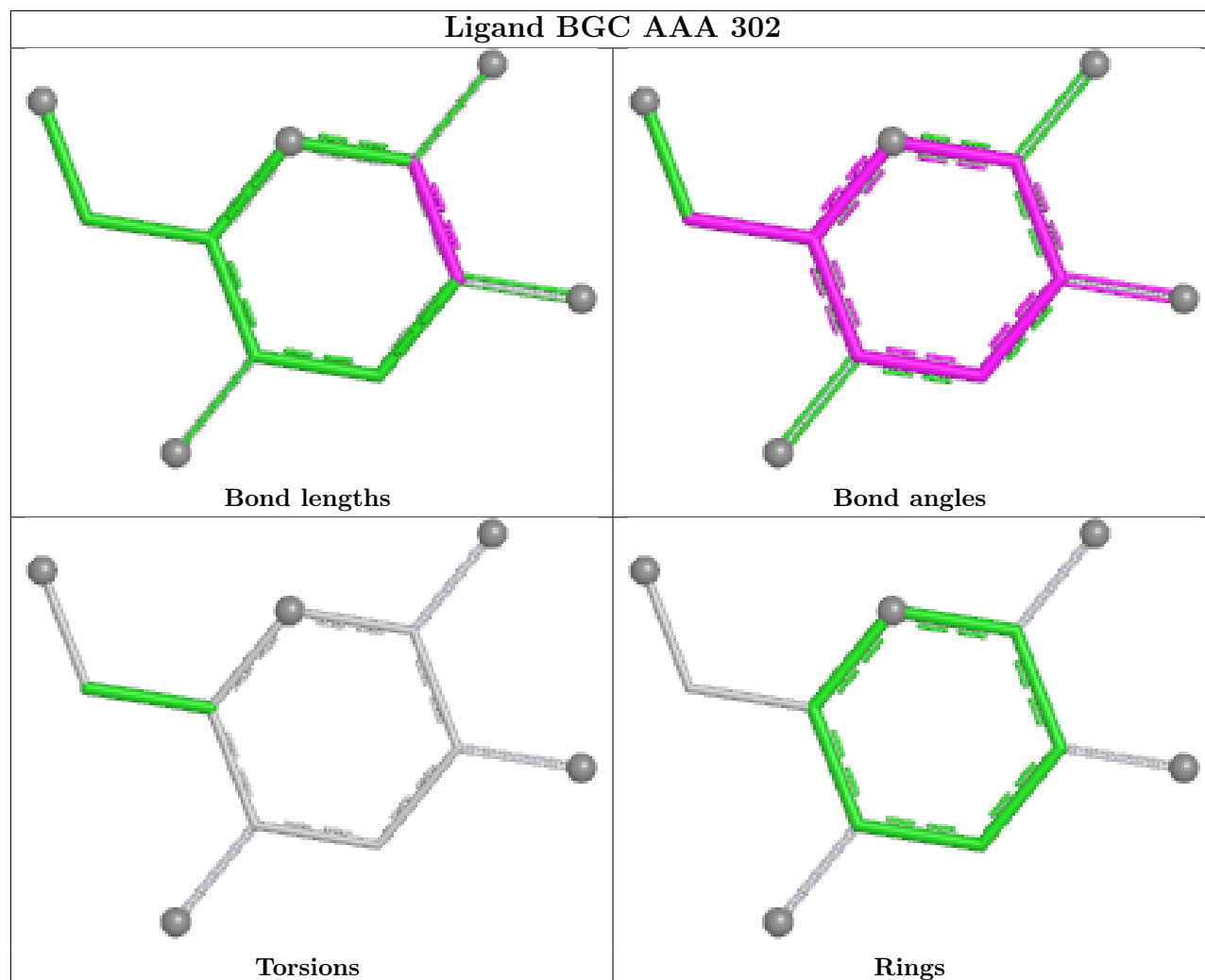
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	301	LYS	3	0
7	BBB	302	EDO	1	0

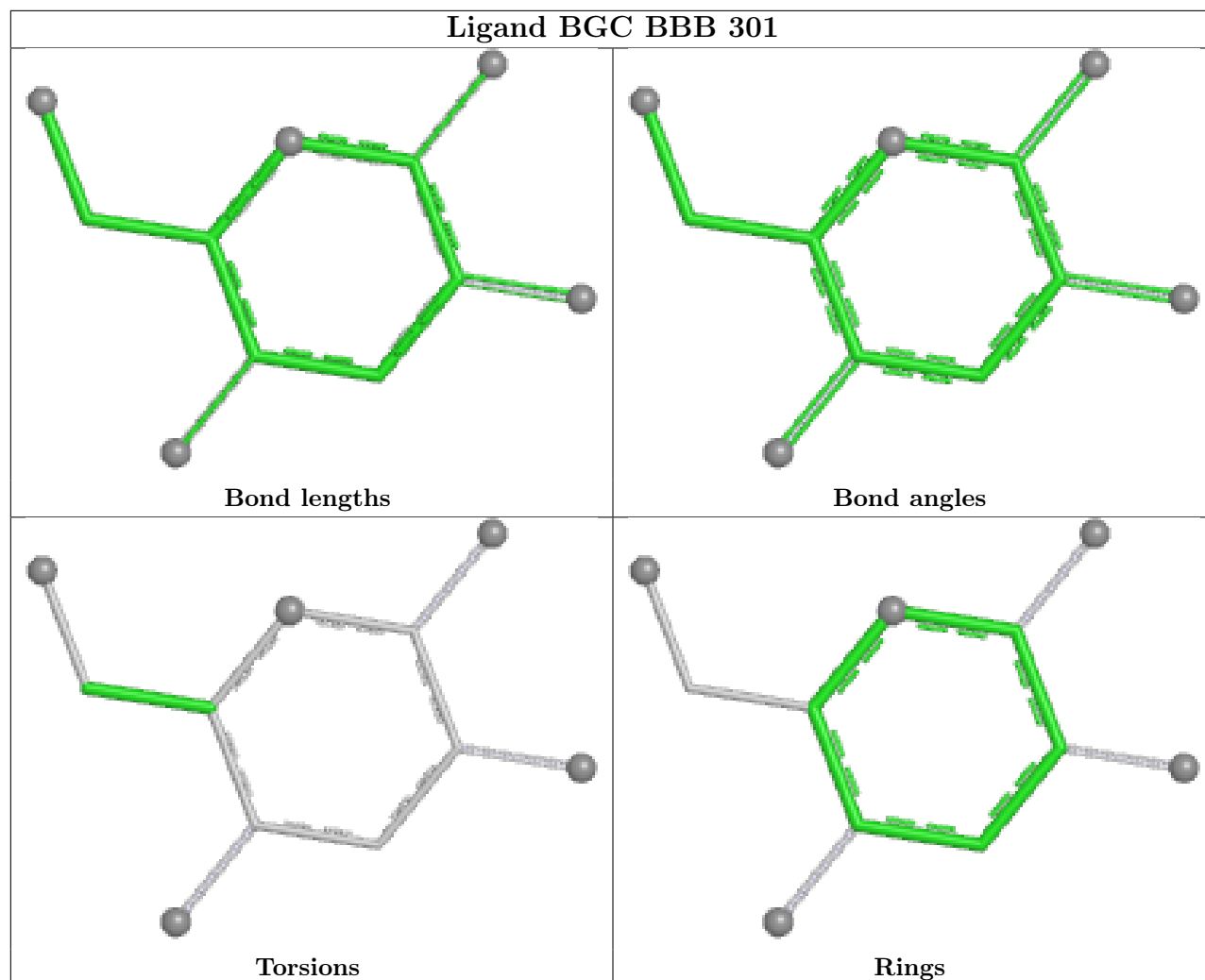
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

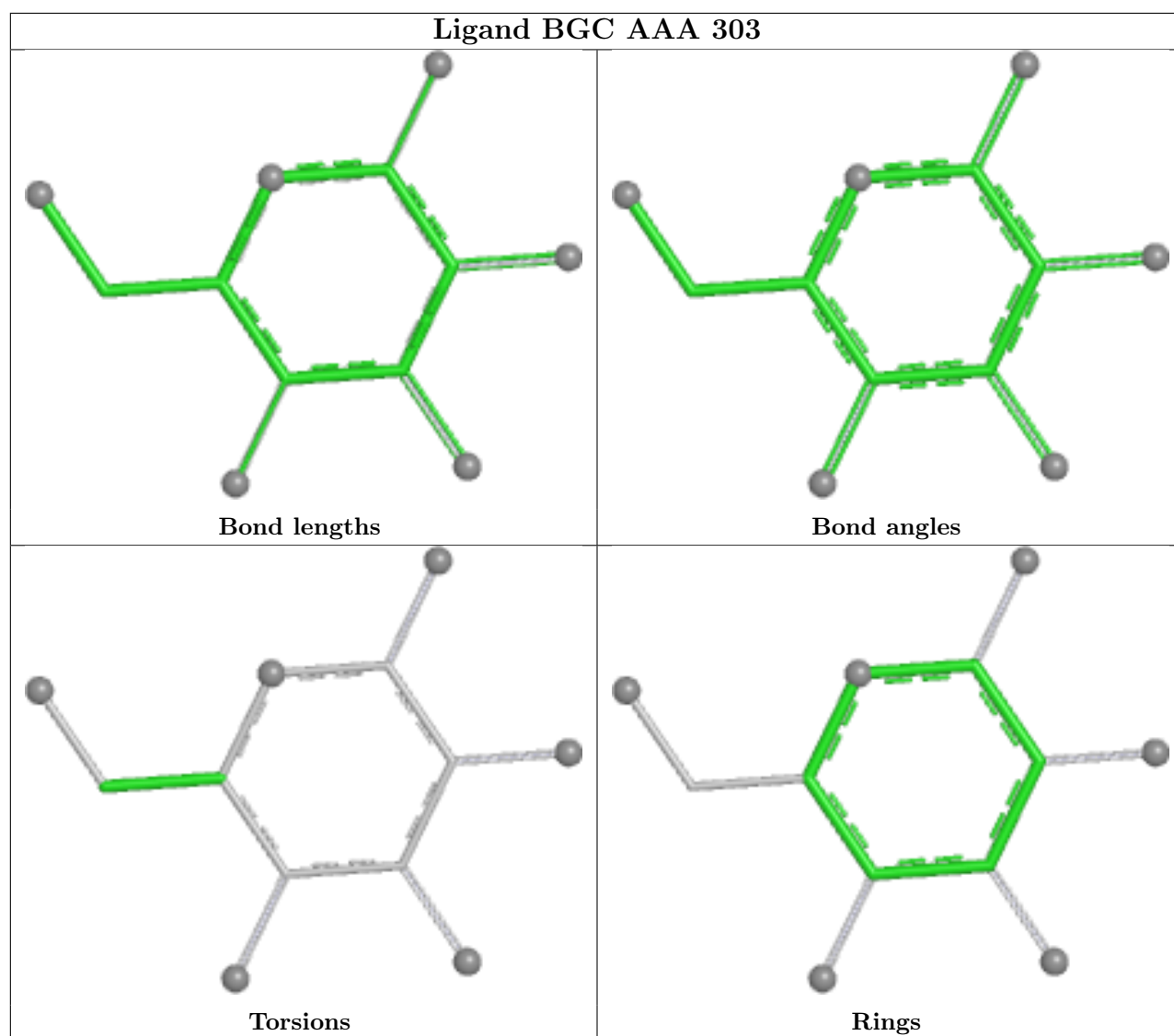
## Ligand BGC AAA 302





## Ligand BGC BBB 301





## 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	248/290 (85%)	-0.10	13 (5%) 27 33	16, 23, 41, 54	0
1	BBB	258/290 (88%)	-0.18	6 (2%) 60 67	15, 23, 44, 60	0
All	All	506/580 (87%)	-0.14	19 (3%) 40 47	15, 23, 42, 60	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	100	THR	5.0
1	AAA	100	THR	3.7
1	AAA	60	SER	3.5
1	BBB	101	GLY	3.4
1	AAA	61	LEU	3.2
1	BBB	63	GLY	3.2
1	BBB	33	VAL	3.2
1	AAA	106	ILE	3.1
1	AAA	101	GLY	3.1
1	BBB	105	THR	3.0
1	AAA	98	TYR	2.9
1	AAA	102	GLY	2.9
1	BBB	102	GLY	2.8
1	AAA	99	ASN	2.5
1	AAA	107	THR	2.5
1	AAA	105	THR	2.4
1	AAA	97	ALA	2.4
1	AAA	66	VAL	2.3
1	AAA	65	VAL	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 ⓘ

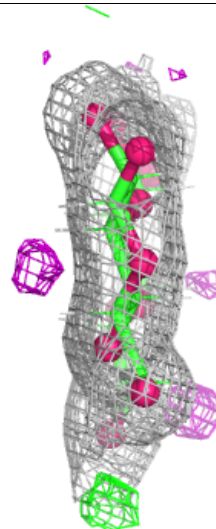
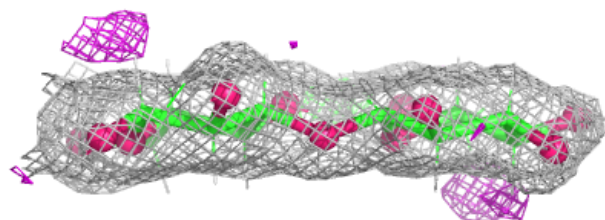
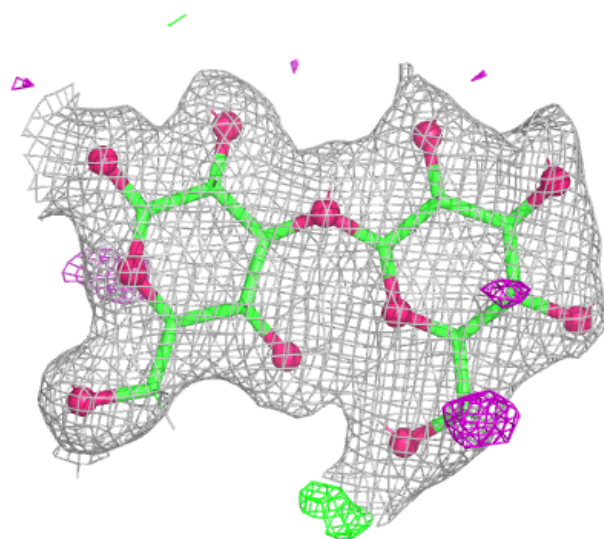
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	BGC	BbB	2	11/12	0.85	0.22	0,46,58,59	0
2	BGC	BbB	1	12/12	0.96	0.12	26,33,38,41	5

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 BbB:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.4 Ligands

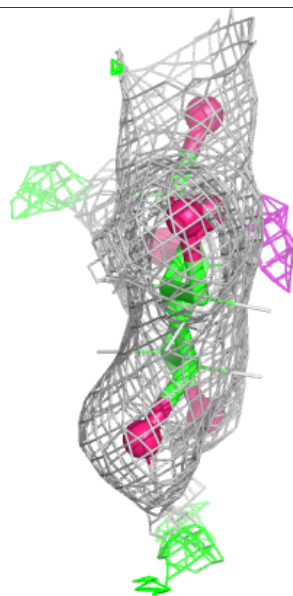
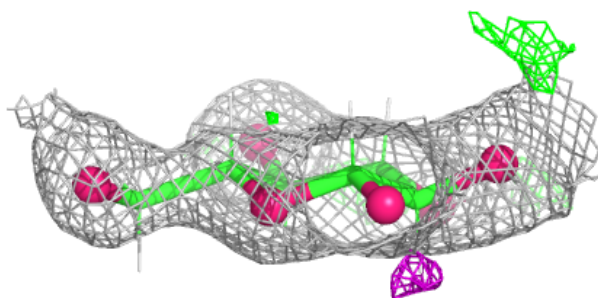
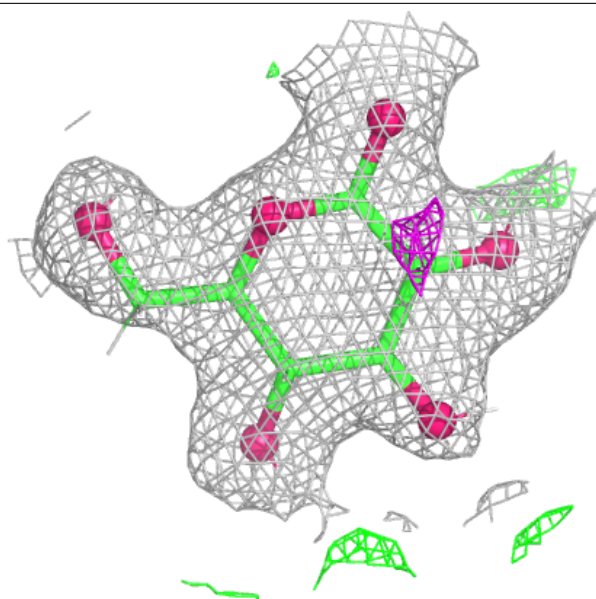
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	LYS	AAA	301	5/10	0.85	0.12	43,53,54,54	0
5	PEG	AAA	304	7/7	0.89	0.15	37,39,57,57	1
4	BGC	AAA	303	12/12	0.92	0.20	0,42,46,48	4
4	BGC	AAA	302	11/12	0.93	0.12	0,35,40,43	3
7	EDO	BBB	302	4/4	0.95	0.10	38,44,46,46	1
6	SO4	AAA	305	5/5	0.96	0.10	45,52,52,63	0
4	BGC	BBB	301	11/12	0.96	0.11	0,24,28,37	3
6	SO4	BBB	303	5/5	0.98	0.10	43,47,54,58	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.

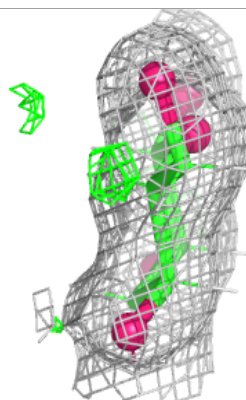
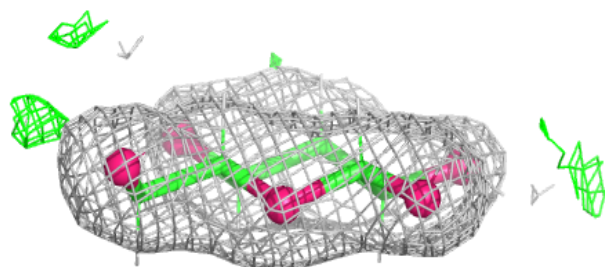
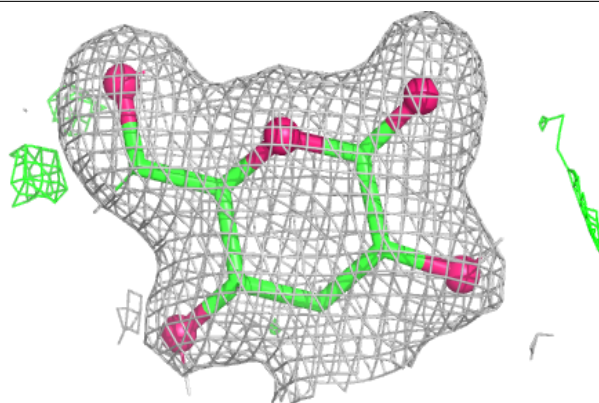
**Electron density around BGC AAA 303:**

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

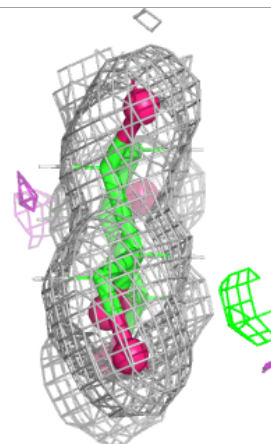
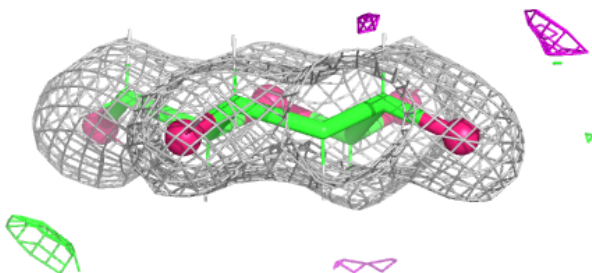
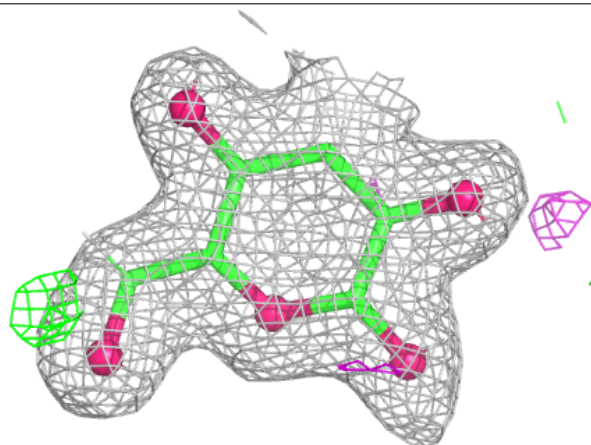


**Electron density around BGC AAA 302:**

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

**Electron density around BGC BBB 301:**

$2mF_o-DF_c$  (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.