



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 18, 2021 – 08:06 AM BST

PDB ID : 7OVW  
Title : Binding domain of botulinum neurotoxin E in complex with GD1a  
Authors : Masuyer, G.; Stenmark, P.  
Deposited on : 2021-06-15  
Resolution : 2.20 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.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.1

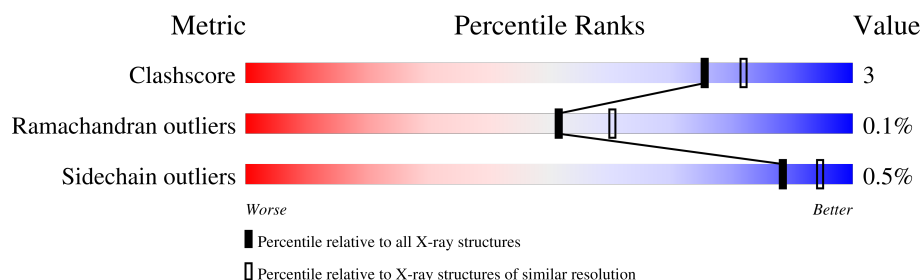
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	AAA	468	80% 6% 14%
1	BBB	468	80% 6% 14%
2	GGG	5	60% 20% 20%
3	HHH	4	50% 50%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13614 atoms, of which 6551 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 Neurotoxin type E.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	404	Total	C	H	N	O	S	97	1	0
			6548	2101	3223	574	641	9			
1	BBB	404	Total	C	H	N	O	S	97	0	0
			6534	2097	3217	572	639	9			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	785	MET	-	initiating methionine	UNP A5H0J8
AAA	786	GLY	-	expression tag	UNP A5H0J8
AAA	787	SER	-	expression tag	UNP A5H0J8
AAA	788	SER	-	expression tag	UNP A5H0J8
AAA	789	HIS	-	expression tag	UNP A5H0J8
AAA	790	HIS	-	expression tag	UNP A5H0J8
AAA	791	HIS	-	expression tag	UNP A5H0J8
AAA	792	HIS	-	expression tag	UNP A5H0J8
AAA	793	HIS	-	expression tag	UNP A5H0J8
AAA	794	HIS	-	expression tag	UNP A5H0J8
AAA	795	SER	-	expression tag	UNP A5H0J8
AAA	796	SER	-	expression tag	UNP A5H0J8
AAA	797	GLY	-	expression tag	UNP A5H0J8
AAA	798	LEU	-	expression tag	UNP A5H0J8
AAA	799	VAL	-	expression tag	UNP A5H0J8
AAA	800	PRO	-	expression tag	UNP A5H0J8
AAA	801	ARG	-	expression tag	UNP A5H0J8
AAA	802	GLY	-	expression tag	UNP A5H0J8
AAA	803	SER	-	expression tag	UNP A5H0J8
AAA	804	HIS	-	expression tag	UNP A5H0J8
AAA	805	MET	-	expression tag	UNP A5H0J8
AAA	806	ALA	-	expression tag	UNP A5H0J8
AAA	807	SER	-	expression tag	UNP A5H0J8
AAA	808	MET	-	expression tag	UNP A5H0J8
AAA	809	TYR	-	expression tag	UNP A5H0J8

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	810	PRO	-	expression tag	UNP A5H0J8
AAA	811	TYR	-	expression tag	UNP A5H0J8
AAA	812	ASP	-	expression tag	UNP A5H0J8
AAA	813	VAL	-	expression tag	UNP A5H0J8
AAA	814	PRO	-	expression tag	UNP A5H0J8
AAA	815	ASP	-	expression tag	UNP A5H0J8
AAA	816	TYR	-	expression tag	UNP A5H0J8
AAA	817	ALA	-	expression tag	UNP A5H0J8
AAA	818	GLY	-	expression tag	UNP A5H0J8
AAA	819	SER	-	expression tag	UNP A5H0J8
BBB	785	MET	-	initiating methionine	UNP A5H0J8
BBB	786	GLY	-	expression tag	UNP A5H0J8
BBB	787	SER	-	expression tag	UNP A5H0J8
BBB	788	SER	-	expression tag	UNP A5H0J8
BBB	789	HIS	-	expression tag	UNP A5H0J8
BBB	790	HIS	-	expression tag	UNP A5H0J8
BBB	791	HIS	-	expression tag	UNP A5H0J8
BBB	792	HIS	-	expression tag	UNP A5H0J8
BBB	793	HIS	-	expression tag	UNP A5H0J8
BBB	794	HIS	-	expression tag	UNP A5H0J8
BBB	795	SER	-	expression tag	UNP A5H0J8
BBB	796	SER	-	expression tag	UNP A5H0J8
BBB	797	GLY	-	expression tag	UNP A5H0J8
BBB	798	LEU	-	expression tag	UNP A5H0J8
BBB	799	VAL	-	expression tag	UNP A5H0J8
BBB	800	PRO	-	expression tag	UNP A5H0J8
BBB	801	ARG	-	expression tag	UNP A5H0J8
BBB	802	GLY	-	expression tag	UNP A5H0J8
BBB	803	SER	-	expression tag	UNP A5H0J8
BBB	804	HIS	-	expression tag	UNP A5H0J8
BBB	805	MET	-	expression tag	UNP A5H0J8
BBB	806	ALA	-	expression tag	UNP A5H0J8
BBB	807	SER	-	expression tag	UNP A5H0J8
BBB	808	MET	-	expression tag	UNP A5H0J8
BBB	809	TYR	-	expression tag	UNP A5H0J8
BBB	810	PRO	-	expression tag	UNP A5H0J8
BBB	811	TYR	-	expression tag	UNP A5H0J8
BBB	812	ASP	-	expression tag	UNP A5H0J8
BBB	813	VAL	-	expression tag	UNP A5H0J8
BBB	814	PRO	-	expression tag	UNP A5H0J8
BBB	815	ASP	-	expression tag	UNP A5H0J8
BBB	816	TYR	-	expression tag	UNP A5H0J8

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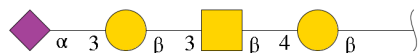
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	817	ALA	-	expression tag	UNP A5H0J8
BBB	818	GLY	-	expression tag	UNP A5H0J8
BBB	819	SER	-	expression tag	UNP A5H0J8

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	GGG	5	Total	C	H	N	O	16	0	0
			129	37	61	2	29			

- 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-(1-4)-beta-D-galactopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	HHH	4	Total	C	H	N	O	12	0	0
			106	31	50	2	23			

- Molecule 4 is water.

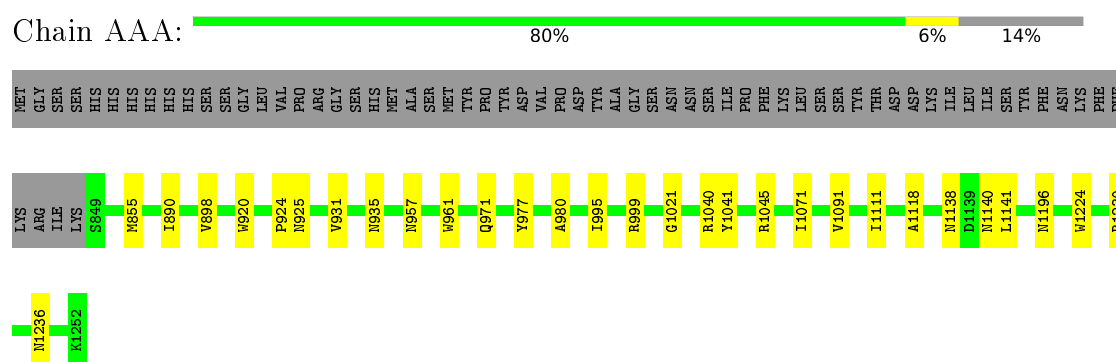
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	169	Total	O	0	0
			169	169		
4	BBB	128	Total	O	0	0
			128	128		

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

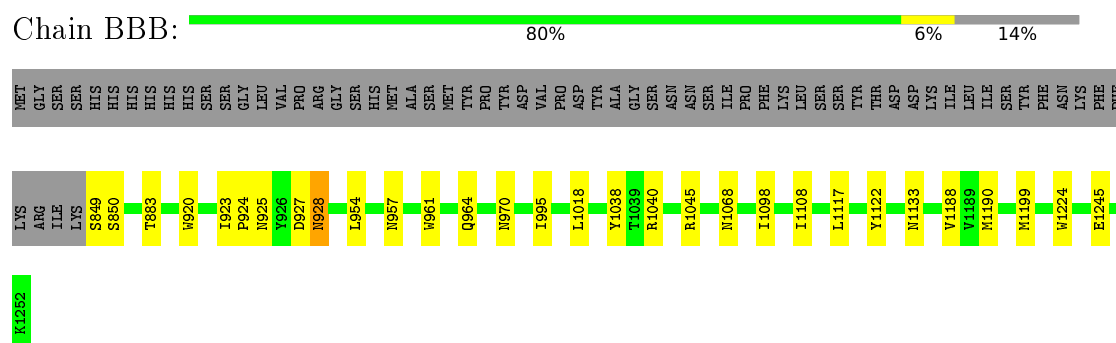
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

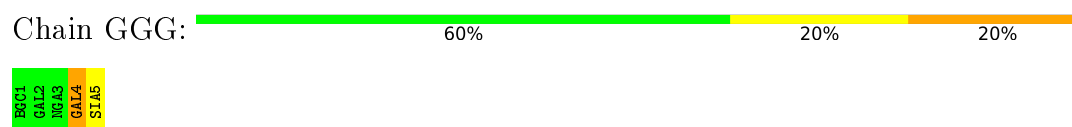
- Molecule 1: Neurotoxin type E



- Molecule 1: Neurotoxin type E



- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-beta-D-galactopyranose





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.37Å 84.92Å 79.90Å 90.00° 91.56° 90.00°	Depositor
Resolution (Å)	53.77 – 2.20	Depositor
% Data completeness (in resolution range)	95.2 (53.77-2.20)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.216 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13614	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP



## 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: BGC, 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	AAA	0.63	0/3395	0.72	0/4603
1	BBB	0.64	0/3387	0.72	0/4592
All	All	0.64	0/6782	0.72	0/9195

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 [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	3325	3223	3215	21	0
1	BBB	3317	3217	3210	19	0
2	GGG	68	61	58	1	0
3	HHH	56	50	47	3	0
4	AAA	169	0	0	1	0
4	BBB	128	0	0	1	0
All	All	7063	6551	6530	41	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 41 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:BBB:925:ASN:HD21	1:BBB:957:ASN:HD21	1.12	0.98
1:AAA:925:ASN:HD21	1:AAA:957:ASN:HD21	1.28	0.81
1:BBB:924:PRO:O	1:BBB:1040:ARG:NH2	2.30	0.64
1:AAA:1230:ARG:H	1:AAA:1236:ASN:HD21	1.45	0.64
1:AAA:925:ASN:HD21	1:AAA:957:ASN:ND2	1.96	0.63

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	403/468 (86%)	384 (95%)	19 (5%)	0	100	100
1	BBB	402/468 (86%)	384 (96%)	17 (4%)	1 (0%)	47	55
All	All	805/936 (86%)	768 (95%)	36 (4%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	1068	ASN

### 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	376/433 (87%)	374 (100%)	2 (0%)	88	94
1	BBB	375/433 (87%)	373 (100%)	2 (0%)	88	94
All	All	751/866 (87%)	747 (100%)	4 (0%)	88	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	935	ASN
1	AAA	1138	ASN
1	BBB	928	ASN
1	BBB	1133	ASN

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	BGC	GGG	1	2	12,12,12	0.48	0	17,17,17	0.49	0
2	GAL	GGG	2	2	11,11,12	0.37	0	15,15,17	0.93	0
2	NGA	GGG	3	2	14,14,15	0.41	0	17,19,21	0.55	0
2	GAL	GGG	4	2	11,11,12	0.29	0	15,15,17	0.85	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SIA	GGG	5	2	17,20,21	0.26	0	21,28,31	0.99	2 (9%)
3	GAL	HHH	1	3	11,11,12	0.51	0	15,15,17	0.91	1 (6%)
3	NGA	HHH	2	3	14,14,15	0.39	0	17,19,21	1.39	3 (17%)
3	GAL	HHH	3	3	11,11,12	0.39	0	15,15,17	1.03	2 (13%)
3	SIA	HHH	4	3	17,20,21	0.31	0	21,28,31	1.15	1 (4%)

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	GGG	1	2	-	0/2/22/22	0/1/1/1
2	GAL	GGG	2	2	-	1/2/19/22	0/1/1/1
2	NGA	GGG	3	2	-	1/6/23/26	0/1/1/1
2	GAL	GGG	4	2	-	0/2/19/22	0/1/1/1
2	SIA	GGG	5	2	-	5/14/34/38	0/1/1/1
3	GAL	HHH	1	3	-	2/2/19/22	0/1/1/1
3	NGA	HHH	2	3	-	2/6/23/26	0/1/1/1
3	GAL	HHH	3	3	-	0/2/19/22	0/1/1/1
3	SIA	HHH	4	3	-	7/14/34/38	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	HHH	4	SIA	C8-C7-C6	3.87	120.36	113.03
3	HHH	2	NGA	C2-N2-C7	2.84	126.95	122.90
3	HHH	2	NGA	O5-C5-C6	2.78	111.56	107.20
3	HHH	2	NGA	C8-C7-N2	2.64	120.57	116.10
3	HHH	3	GAL	C1-O5-C5	2.58	115.69	112.19

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	GGG	5	SIA	C5-C6-C7-C8
2	GGG	5	SIA	C5-C6-C7-O7
2	GGG	5	SIA	O6-C6-C7-C8

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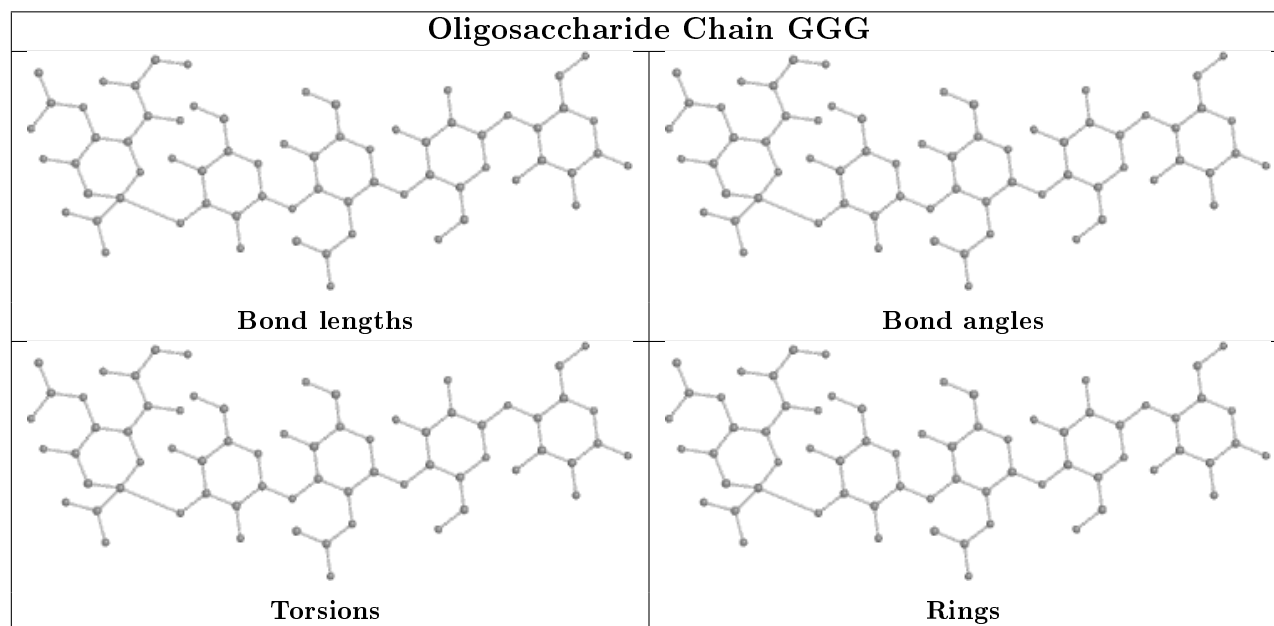
Mol	Chain	Res	Type	Atoms
3	HHH	4	SIA	C4-C5-N5-C10
3	HHH	4	SIA	C5-C6-C7-C8

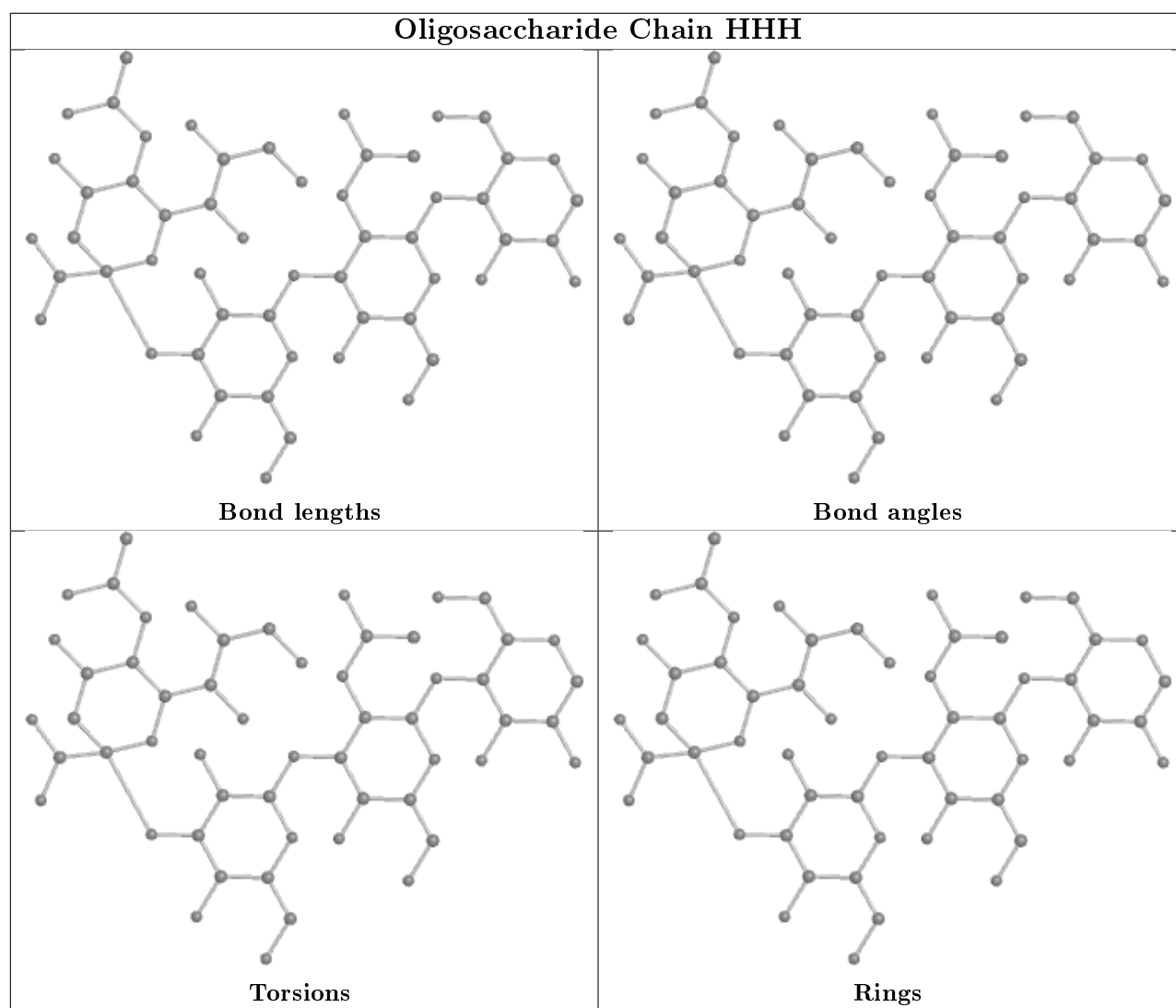
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	HHH	3	GAL	1	0
3	HHH	4	SIA	2	0
2	GGG	4	GAL	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.