



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 01:12 AM EDT

PDB ID : 6MKB  
Title : Crystal structure of murine 4-1BB ligand  
Authors : Bitra, A.; Zajonc, D.M.; Doukov, T.  
Deposited on : 2018-09-25  
Resolution : 2.50 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 : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : **FAILED**  
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) : 2.35.1

## 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 2.50 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5706 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 Tumor necrosis factor ligand superfamily member 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	160	1273	821	214	236	2	0	1	0
1	B	165	1313	846	219	245	3	0	0	0
1	C	165	1324	853	222	246	3	0	2	0
1	D	160	1265	816	213	234	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	4	50	28	2	20	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	F	3	39	22	2	15	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	4	50	28	2	20	0	0	0

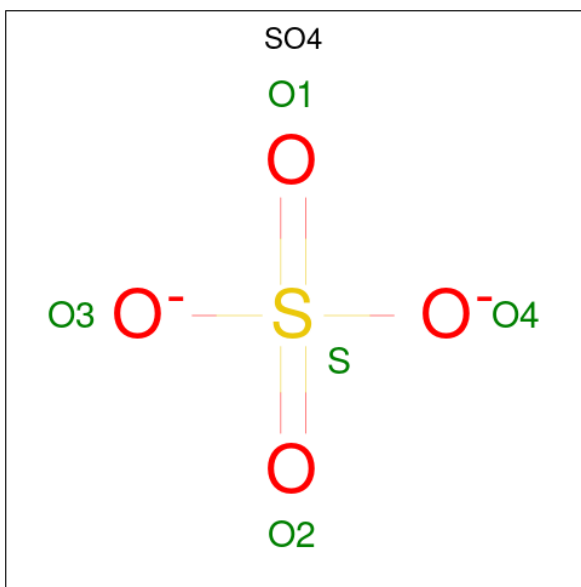
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
			Total	C	N				O
5	H	5	61	34	2	25	0	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
6	A	2	2	2	0	0
6	B	1	1	1	0	0
6	C	2	2	2	0	0
6	D	1	1	1	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
7	B	1	5	4	1	0	0
7	B	1	5	4	1	0	0
7	B	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			4	3	1		
7	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	58	Total	O	0	0
			58	58		
8	B	89	Total	O	0	0
			89	89		
8	C	78	Total	O	0	0
			78	78		
8	D	61	Total	O	0	0
			61	61		

MolProbity and EDS failed to run properly - this section is therefore empty.

### 3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.36Å 77.36Å 118.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.14 – 2.50	Depositor
% Data completeness (in resolution range)	99.7 (29.14-2.50)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.51Å)	Xtrriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.188 , 0.241	Depositor
Wilson B-factor (Å <sup>2</sup> )	58.1	Xtrriage
Anisotropy	0.006	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.011 for -h,-k,l 0.488 for h,-h-k,-l 0.011 for -k,-h,-l	Xtrriage
Total number of atoms	5706	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

### 4.5 Carbohydrates [i](#)

16 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	NAG	E	1	1,2	14,14,15	0.41	0	17,19,21	1.13	2 (11%)
2	NAG	E	2	2	14,14,15	0.50	0	17,19,21	0.95	1 (5%)
2	BMA	E	3	2	11,11,12	0.73	0	15,15,17	0.98	1 (6%)
2	MAN	E	4	2	11,11,12	0.78	0	15,15,17	1.37	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.43	0	17,19,21	1.21	1 (5%)
3	NAG	F	2	3	14,14,15	0.43	0	17,19,21	1.29	1 (5%)
3	BMA	F	3	3	11,11,12	0.67	0	15,15,17	1.11	2 (13%)
4	NAG	G	1	1,4	14,14,15	0.64	0	17,19,21	1.53	3 (17%)
4	NAG	G	2	4	14,14,15	0.32	0	17,19,21	0.75	0
4	BMA	G	3	4	11,11,12	0.24	0	15,15,17	0.93	0
4	MAN	G	4	4	11,11,12	0.24	0	15,15,17	0.88	0
5	NAG	H	1	5,1	14,14,15	0.43	0	17,19,21	1.20	1 (5%)
5	NAG	H	2	5	14,14,15	0.48	0	17,19,21	0.90	0
5	BMA	H	3	5	11,11,12	0.84	0	15,15,17	1.14	1 (6%)
5	MAN	H	4	5	11,11,12	0.68	0	15,15,17	1.19	1 (6%)
5	MAN	H	5	5	11,11,12	0.74	0	15,15,17	1.59	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	NAG	E	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	1/2/19/22	0/1/1/1
2	MAN	E	4	2	-	2/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	1/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	1/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
5	NAG	H	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	BMA	H	3	5	-	0/2/19/22	0/1/1/1
5	MAN	H	4	5	-	2/2/19/22	0/1/1/1
5	MAN	H	5	5	-	1/2/19/22	0/1/1/1



There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
5	H	5	MAN	C1-O5-C5	4.73	118.60	112.19
3	F	2	NAG	C1-O5-C5	4.66	118.50	112.19
2	E	4	MAN	C1-O5-C5	3.63	117.11	112.19
4	G	1	NAG	C8-C7-N2	3.14	121.42	116.10
5	H	4	MAN	C1-O5-C5	3.04	116.31	112.19
3	F	1	NAG	C2-N2-C7	3.04	127.23	122.90
5	H	3	BMA	O3-C3-C2	3.03	115.79	109.99
2	E	2	NAG	C1-O5-C5	2.73	115.89	112.19
4	G	1	NAG	O7-C7-N2	-2.65	117.08	121.95
2	E	3	BMA	C1-O5-C5	2.64	115.76	112.19
5	H	1	NAG	C2-N2-C7	2.63	126.65	122.90
4	G	1	NAG	O5-C5-C6	2.57	111.24	107.20
5	H	5	MAN	C1-C2-C3	2.53	112.78	109.67
3	F	3	BMA	C1-O5-C5	2.48	115.55	112.19
3	F	3	BMA	C3-C4-C5	2.19	114.15	110.24
2	E	1	NAG	C2-N2-C7	2.07	125.85	122.90
2	E	1	NAG	C8-C7-N2	-2.01	112.69	116.10

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
5	H	2	NAG	O5-C5-C6-O6
5	H	4	MAN	C4-C5-C6-O6
2	E	4	MAN	C4-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
5	H	4	MAN	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6
3	F	3	BMA	O5-C5-C6-O6
2	E	3	BMA	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
5	H	5	MAN	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
5	H	1	NAG	O7-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2

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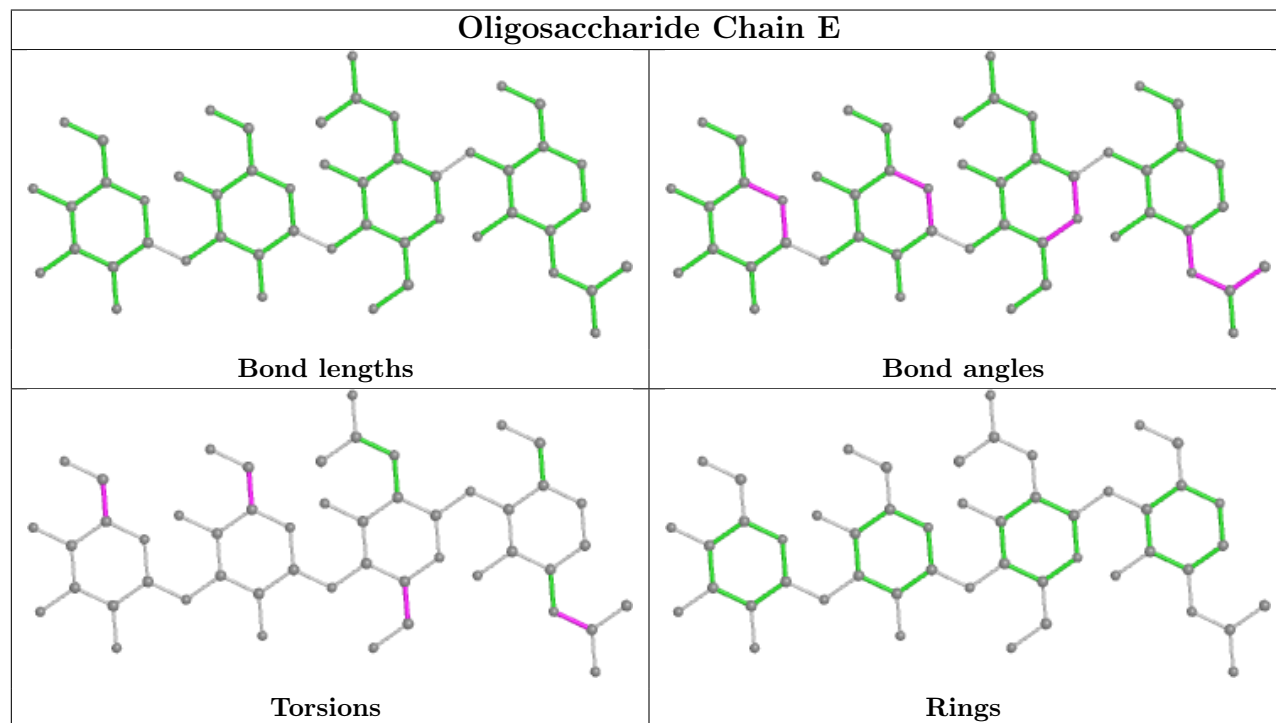
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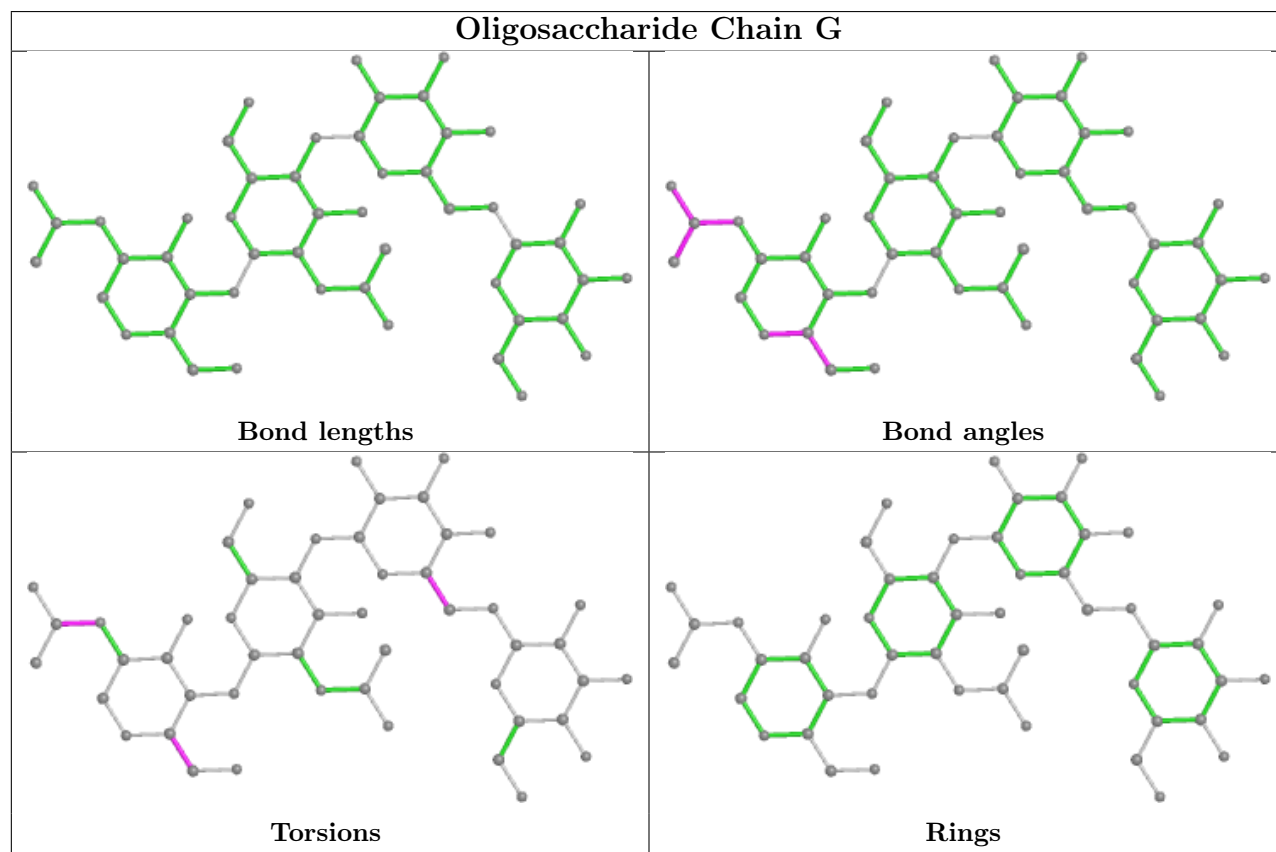
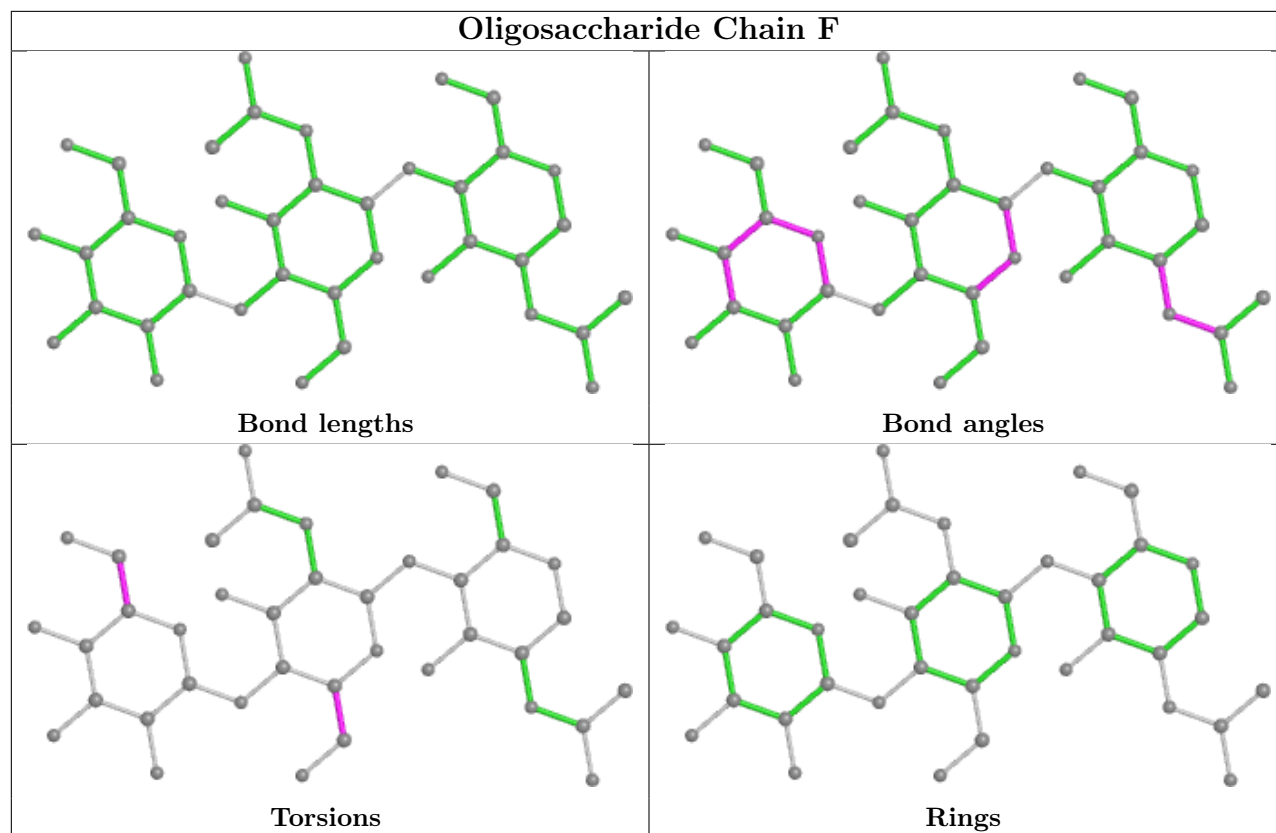
Mol	Chain	Res	Type	Atoms
4	G	3	BMA	C4-C5-C6-O6

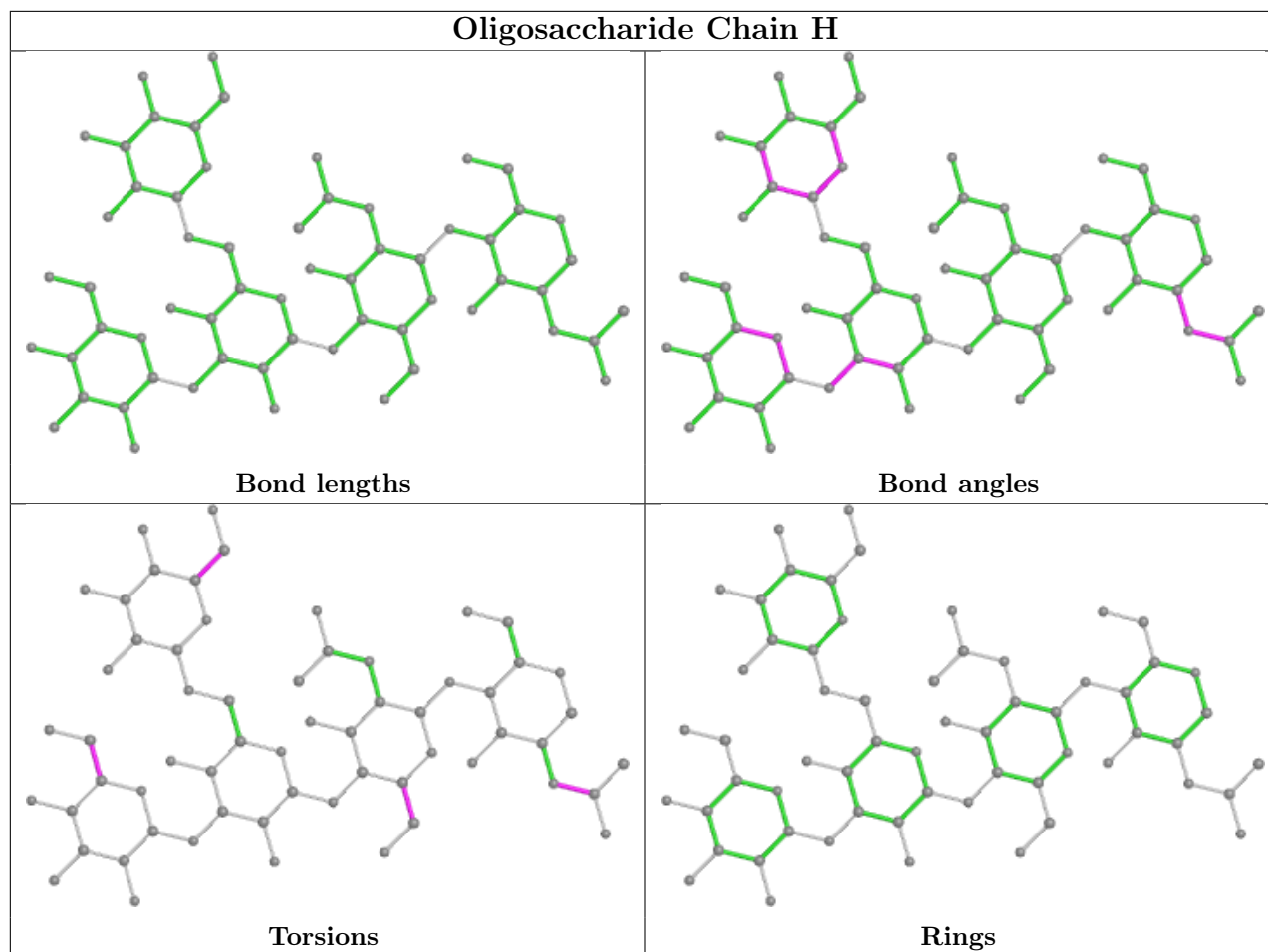
There are no ring outliers.

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.







## 4.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

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$
7	SO4	B	401	-	4,4,4	0.34	0	6,6,6	0.24	0
7	SO4	B	403	-	4,4,4	0.44	0	6,6,6	0.21	0
7	SO4	C	403	-	1,3,4	1.21	0	0,3,6	-	-
7	SO4	C	402	-	4,4,4	0.35	0	6,6,6	0.23	0
7	SO4	D	401	-	4,4,4	0.35	0	6,6,6	0.08	0
7	SO4	B	404	-	4,4,4	0.36	0	6,6,6	0.16	0
7	SO4	B	402	-	4,4,4	0.30	0	6,6,6	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	SO4	C	401	-	4,4,4	0.35	0	6,6,6	0.18	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 5 Fit of model and data [i](#)

### 5.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 5.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

### 5.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.