



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 08:11 AM EDT

PDB ID : 6VLK
Title : A varicella-zoster virus glycoprotein
Authors : Xing, Y.
Deposited on : 2020-01-24
Resolution : 2.45 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

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>.

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)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
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 2.45 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

There are 6 unique types of molecules in this entry. The entry contains 9766 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 Envelope glycoprotein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	584	4693	2961	821	889	22	0	0	0
1	B	583	4688	2958	820	888	22	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	GLY	TRP	engineered mutation	UNP Q4JR05
A	185	GLY	TYR	engineered mutation	UNP Q4JR05
A	491	GLY	ARG	engineered mutation	UNP Q4JR05
A	493	GLY	ARG	engineered mutation	UNP Q4JR05
A	494	GLY	ARG	engineered mutation	UNP Q4JR05
A	737	GLY	-	expression tag	UNP Q4JR05
A	738	SER	-	expression tag	UNP Q4JR05
A	739	HIS	-	expression tag	UNP Q4JR05
A	740	HIS	-	expression tag	UNP Q4JR05
A	741	HIS	-	expression tag	UNP Q4JR05
A	742	HIS	-	expression tag	UNP Q4JR05
A	743	HIS	-	expression tag	UNP Q4JR05
A	744	HIS	-	expression tag	UNP Q4JR05
B	180	GLY	TRP	engineered mutation	UNP Q4JR05
B	185	GLY	TYR	engineered mutation	UNP Q4JR05
B	491	GLY	ARG	engineered mutation	UNP Q4JR05
B	493	GLY	ARG	engineered mutation	UNP Q4JR05
B	494	GLY	ARG	engineered mutation	UNP Q4JR05
B	737	GLY	-	expression tag	UNP Q4JR05
B	738	SER	-	expression tag	UNP Q4JR05
B	739	HIS	-	expression tag	UNP Q4JR05
B	740	HIS	-	expression tag	UNP Q4JR05
B	741	HIS	-	expression tag	UNP Q4JR05
B	742	HIS	-	expression tag	UNP Q4JR05
B	743	HIS	-	expression tag	UNP Q4JR05

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Chain	Residue	Modelled	Actual	Comment	Reference
B	744	HIS	-	expression tag	UNP Q4JR05

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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	C	7	83	46	2	35	0	0	0

- Molecule 3 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			
3	D	5	61	34	2	25	0	0	0

- Molecule 4 is an oligosaccharide called 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	E	2	28	16	2	10	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
5	B	1	14	8	1	5	0	0
5	B	1	14	8	1	5	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	100	100	100	0	0
6	B	71	71	71	0	0

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	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	118.32Å 118.32Å 749.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.22 – 2.45	Depositor
% Data completeness (in resolution range)	100.0 (50.22-2.45)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.45Å)	Xtrriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.181 , 0.228	Depositor
Wilson B-factor (Å ²)	53.6	Xtrriage
Anisotropy	0.341	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	9766	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

14 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	C	1	1,2	14,14,15	0.62	0	17,19,21	1.13	3 (17%)
2	NAG	C	2	2	14,14,15	0.71	0	17,19,21	0.87	0
2	BMA	C	3	2	11,11,12	0.88	0	15,15,17	1.13	1 (6%)
2	MAN	C	4	2	11,11,12	0.58	0	15,15,17	0.79	0
2	MAN	C	5	2	11,11,12	0.62	0	15,15,17	1.10	1 (6%)
2	MAN	C	6	2	11,11,12	0.65	0	15,15,17	0.93	1 (6%)
2	MAN	C	7	2	11,11,12	0.68	0	15,15,17	0.92	1 (6%)
3	NAG	D	1	3,1	14,14,15	0.55	0	17,19,21	1.17	2 (11%)
3	NAG	D	2	3	14,14,15	0.57	0	17,19,21	1.24	3 (17%)
3	BMA	D	3	3	11,11,12	0.75	0	15,15,17	1.29	2 (13%)
3	MAN	D	4	3	11,11,12	0.51	0	15,15,17	1.26	2 (13%)
3	MAN	D	5	3	11,11,12	0.67	0	15,15,17	1.27	1 (6%)
4	NAG	E	1	4,1	14,14,15	0.47	0	17,19,21	1.71	1 (5%)
4	NAG	E	2	4	14,14,15	0.57	0	17,19,21	1.12	1 (5%)

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	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	MAN	C	5	2	-	1/2/19/22	0/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
2	MAN	C	7	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	2/2/19/22	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	NAG	C1-O5-C5	6.36	120.81	112.19
3	D	5	MAN	C1-C2-C3	4.09	114.69	109.67
3	D	3	BMA	C1-O5-C5	3.46	116.88	112.19
3	D	4	MAN	C1-C2-C3	-3.27	105.64	109.67
4	E	2	NAG	O5-C5-C6	2.83	111.64	107.20
3	D	2	NAG	O4-C4-C3	-2.82	103.82	110.35
2	C	5	MAN	O5-C5-C6	2.81	111.62	107.20
2	C	7	MAN	O5-C5-C6	2.53	111.18	107.20
2	C	1	NAG	O5-C1-C2	-2.43	107.44	111.29
2	C	1	NAG	O4-C4-C5	-2.39	103.36	109.30
3	D	1	NAG	C3-C4-C5	2.24	114.23	110.24
3	D	2	NAG	C4-C3-C2	2.24	114.30	111.02
3	D	4	MAN	C1-O5-C5	2.18	115.15	112.19
3	D	1	NAG	O5-C1-C2	-2.16	107.88	111.29
2	C	1	NAG	O5-C5-C6	2.15	110.57	107.20
2	C	3	BMA	C1-O5-C5	2.13	115.08	112.19
2	C	6	MAN	O5-C1-C2	-2.12	107.50	110.77
3	D	3	BMA	O2-C2-C3	-2.09	105.96	110.14
3	D	2	NAG	C2-N2-C7	-2.01	120.04	122.90

There are no chirality outliers.

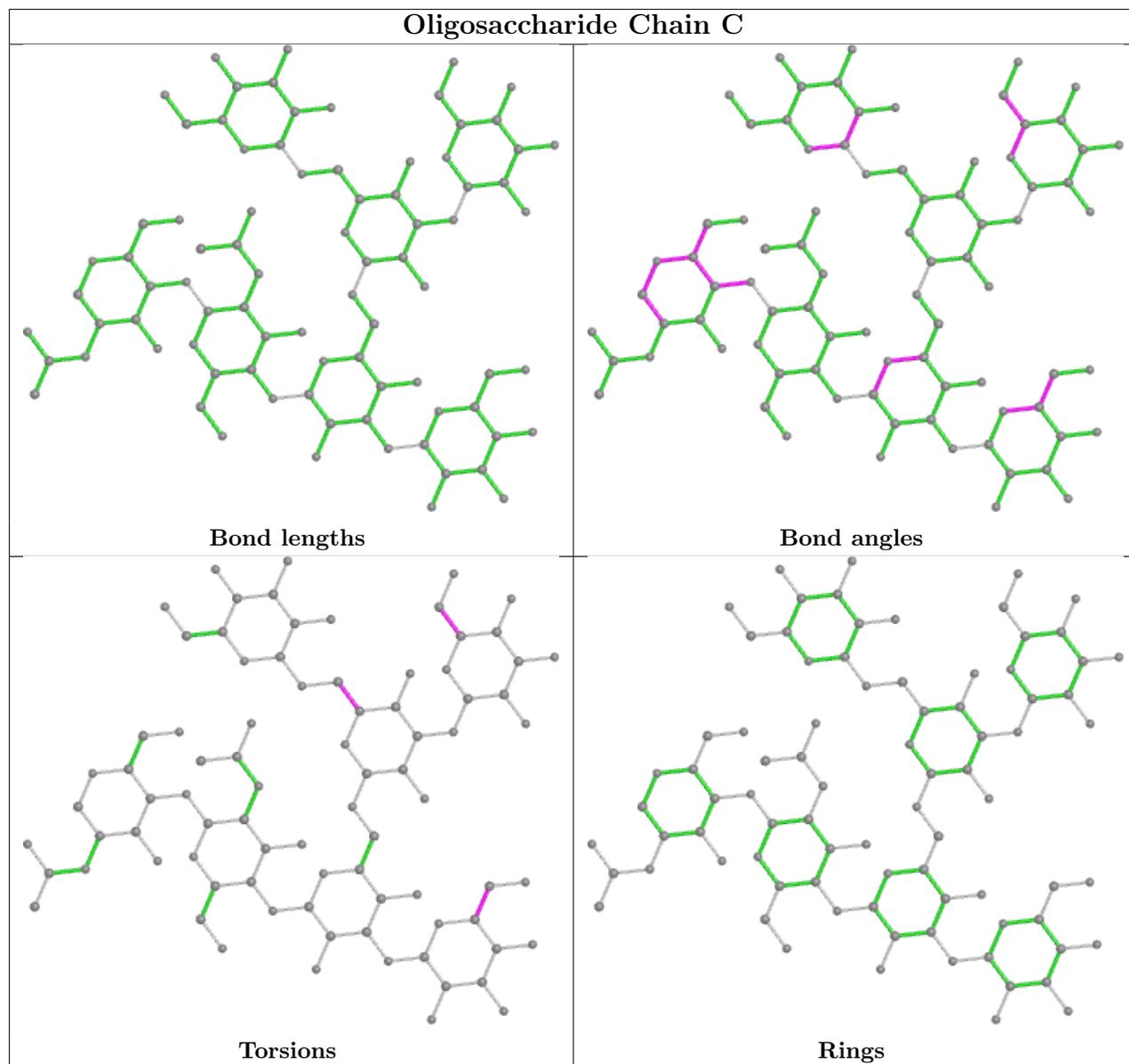
All (11) torsion outliers are listed below:

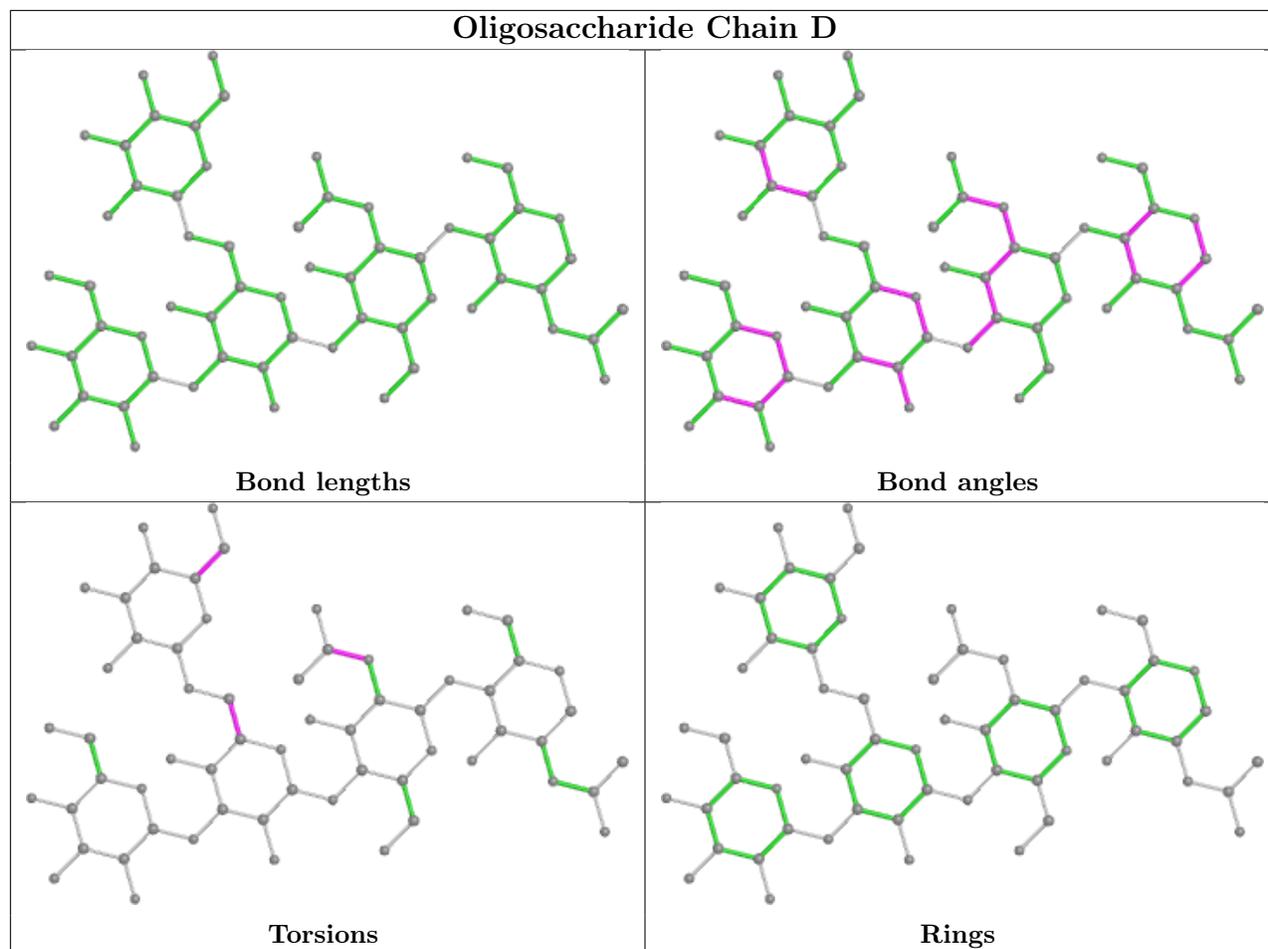
Mol	Chain	Res	Type	Atoms
2	C	4	MAN	O5-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2
3	D	3	BMA	C4-C5-C6-O6
3	D	2	NAG	O7-C7-N2-C2
3	D	3	BMA	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
3	D	5	MAN	C4-C5-C6-O6
3	D	5	MAN	O5-C5-C6-O6
2	C	5	MAN	O5-C5-C6-O6
2	C	7	MAN	C4-C5-C6-O6
2	C	7	MAN	O5-C5-C6-O6

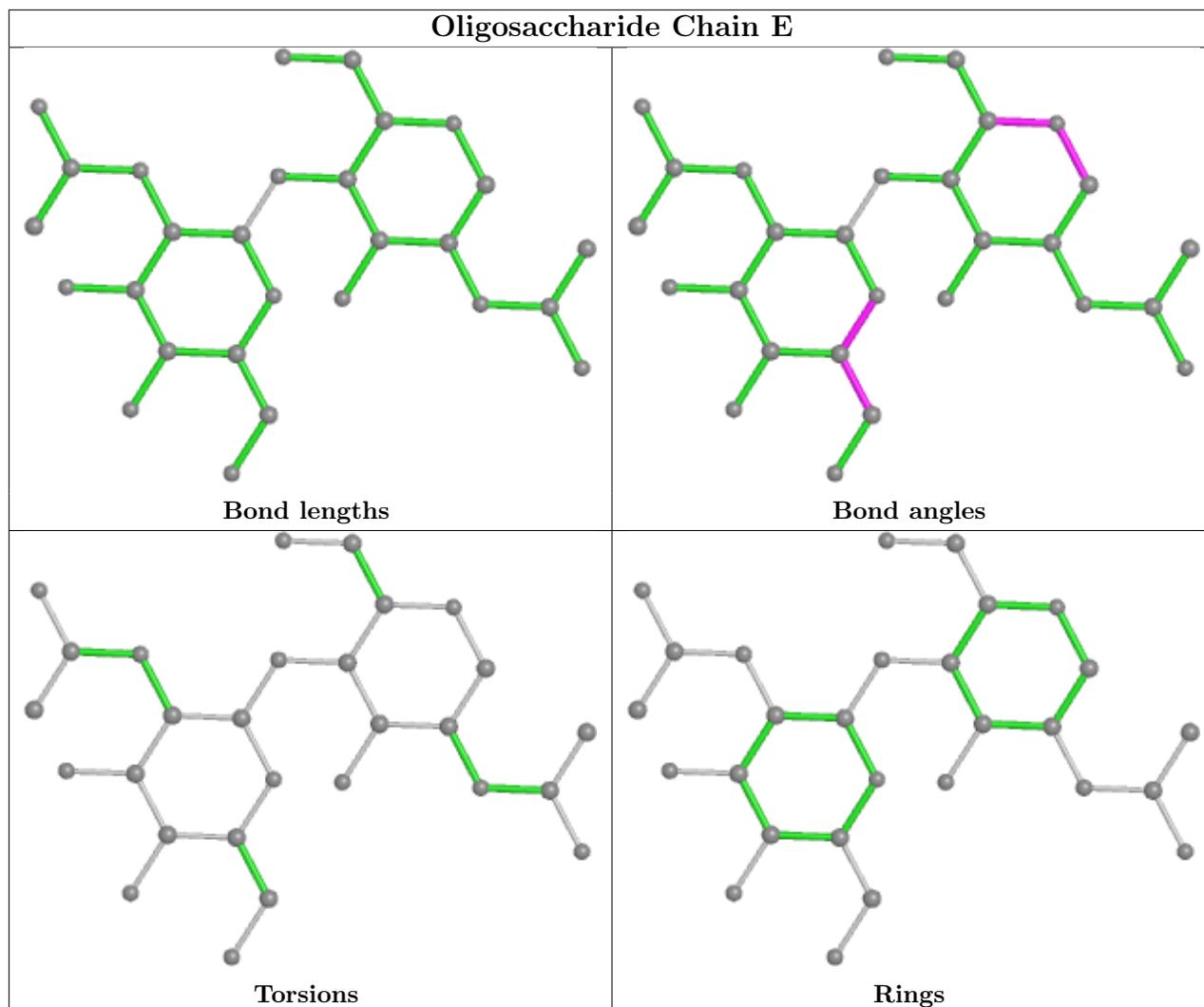
There are no ring outliers.

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.







4.6 Ligand geometry [i](#)

3 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$
5	NAG	B	804	1	14,14,15	0.45	0	17,19,21	1.23	2 (11%)
5	NAG	B	801	1	14,14,15	0.55	0	17,19,21	1.47	2 (11%)
5	NAG	A	813	1	14,14,15	0.50	0	17,19,21	1.02	2 (11%)

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
5	NAG	B	804	1	-	4/6/23/26	0/1/1/1
5	NAG	B	801	1	-	4/6/23/26	0/1/1/1
5	NAG	A	813	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	801	NAG	C4-C3-C2	3.79	116.57	111.02
5	B	804	NAG	C1-O5-C5	3.31	116.68	112.19
5	B	801	NAG	O5-C1-C2	2.88	115.83	111.29
5	A	813	NAG	O5-C5-C6	2.67	111.39	107.20
5	B	804	NAG	O5-C1-C2	2.08	114.58	111.29
5	A	813	NAG	C1-O5-C5	2.05	114.98	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

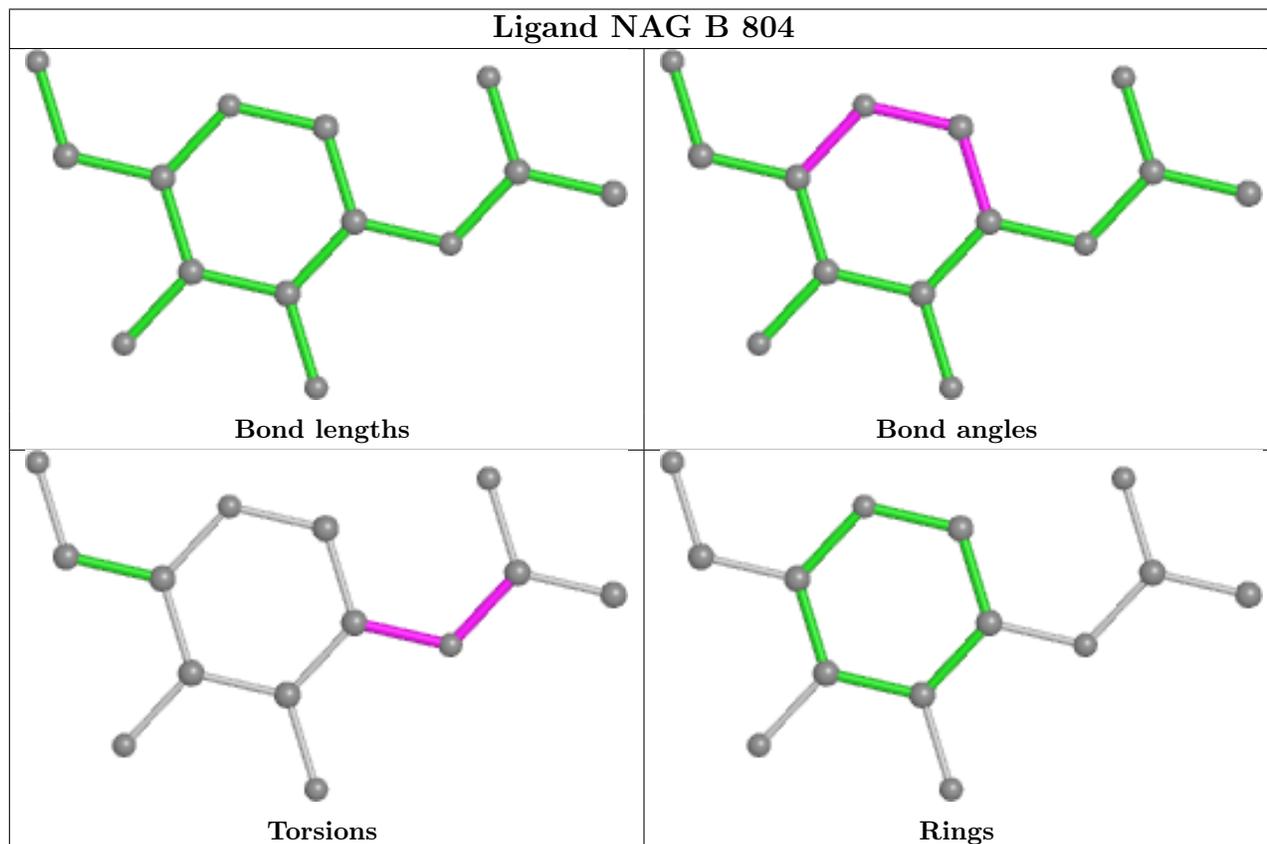
Mol	Chain	Res	Type	Atoms
5	B	801	NAG	C8-C7-N2-C2
5	B	801	NAG	O7-C7-N2-C2
5	A	813	NAG	O5-C5-C6-O6
5	A	813	NAG	C4-C5-C6-O6
5	B	804	NAG	C8-C7-N2-C2
5	B	804	NAG	O7-C7-N2-C2
5	B	804	NAG	C1-C2-N2-C7
5	B	804	NAG	C3-C2-N2-C7
5	B	801	NAG	C4-C5-C6-O6
5	B	801	NAG	O5-C5-C6-O6

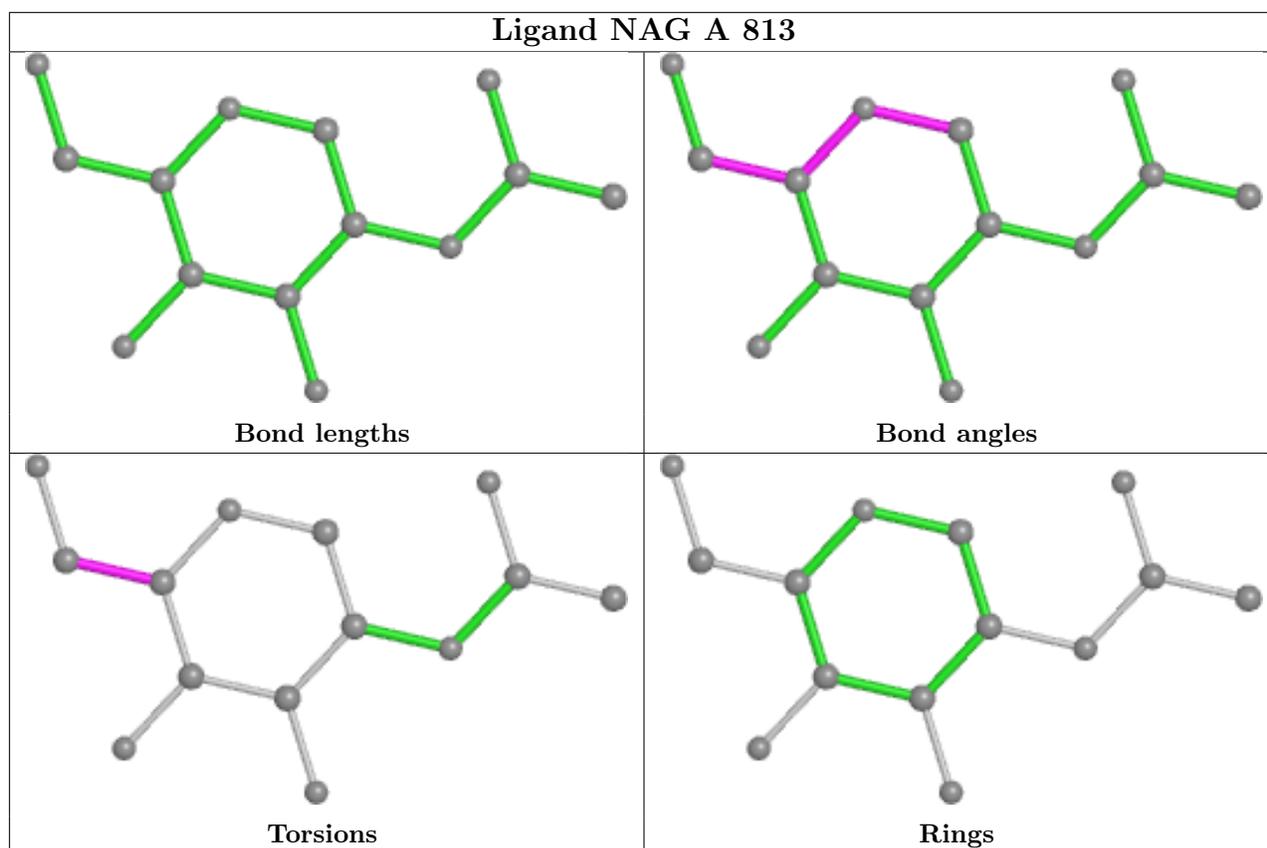
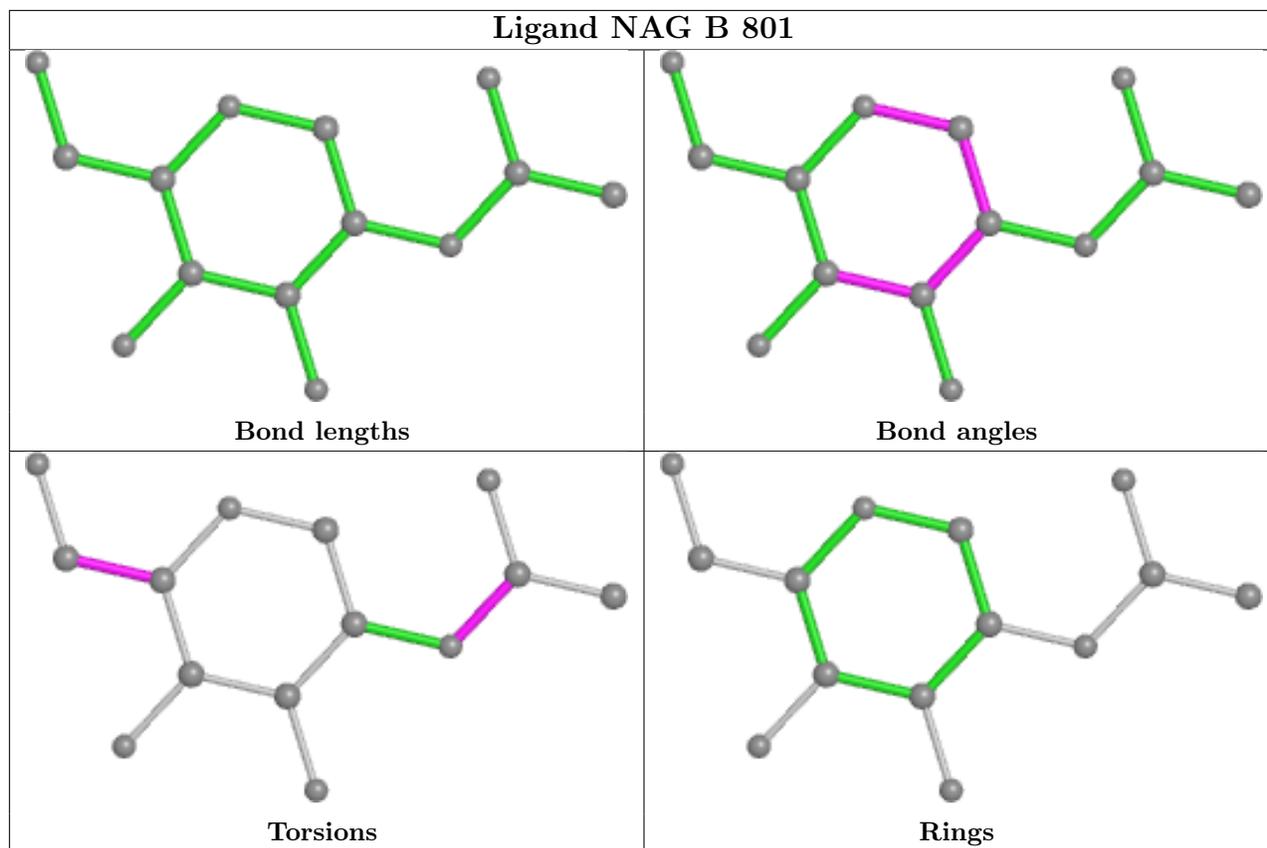
There are no ring outliers.

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 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.





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.