



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2023 – 01:19 AM EDT

PDB ID : 6NHR
Title : Crystal structure of the A/Hong Kong/1/1968 (H3N2) influenza virus hemagglutinin HA2 I45F mutant
Authors : Wu, N.C.; Wilson, I.A.
Deposited on : 2018-12-23
Resolution : 2.10 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

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**
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 2.10 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 12724 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	321	Total 2485	C 1557	N 439	O 476	S 13	0	1	0
1	C	317	Total 2443	C 1531	N 429	O 470	S 13	0	0	0
1	E	317	Total 2443	C 1531	N 429	O 470	S 13	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	-	expression tag	UNP H9XC94
A	10	GLY	-	expression tag	UNP H9XC94
A	145	SER	UNK	variant	UNP H9XC94
A	226	LEU	MET	conflict	UNP H9XC94
C	9	PRO	-	expression tag	UNP H9XC94
C	10	GLY	-	expression tag	UNP H9XC94
C	145	SER	UNK	variant	UNP H9XC94
C	226	LEU	MET	conflict	UNP H9XC94
E	9	PRO	-	expression tag	UNP H9XC94
E	10	GLY	-	expression tag	UNP H9XC94
E	145	SER	UNK	variant	UNP H9XC94
E	226	LEU	MET	conflict	UNP H9XC94

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	172	Total 1405	C 875	N 244	O 280	S 6	0	1	0
2	D	171	Total 1385	C 861	N 241	O 277	S 6	0	0	0
2	F	171	Total 1385	C 861	N 241	O 277	S 6	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	45	PHE	ILE	engineered mutation	UNP Q91MA7
B	123	GLY	ARG	conflict	UNP Q91MA7
D	45	PHE	ILE	engineered mutation	UNP Q91MA7
D	123	GLY	ARG	conflict	UNP Q91MA7
F	45	PHE	ILE	engineered mutation	UNP Q91MA7
F	123	GLY	ARG	conflict	UNP Q91MA7

- 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
3	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	H	3	Total	C	N	O	0	0	0
			39	22	2	15			

- 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
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 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
5	J	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 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
6	L	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	186	Total 186	O 186	0	0
8	B	94	Total 94	O 94	0	0
8	C	180	Total 180	O 180	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	93	Total O 93 93	0	0
8	E	219	Total O 219 219	0	0
8	F	74	Total O 74 74	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	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.38Å 131.41Å 72.28Å 90.00° 98.07° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10	Depositor
% Data completeness (in resolution range)	97.4 (50.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.184 , 0.216	Depositor
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.152	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12724	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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](#)

18 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
3	NAG	G	1	1,3	14,14,15	0.34	0	17,19,21	1.18	1 (5%)
3	NAG	G	2	3	14,14,15	0.53	0	17,19,21	2.44	3 (17%)
3	BMA	G	3	3	11,11,12	0.50	0	15,15,17	0.80	0
3	NAG	H	1	1,3	14,14,15	0.51	0	17,19,21	1.31	2 (11%)
3	NAG	H	2	3	14,14,15	0.39	0	17,19,21	1.02	1 (5%)
3	BMA	H	3	3	11,11,12	0.50	0	15,15,17	1.21	3 (20%)
4	NAG	I	1	4,1	14,14,15	0.52	0	17,19,21	0.62	0
4	NAG	I	2	4	14,14,15	0.31	0	17,19,21	1.16	1 (5%)
5	NAG	J	1	5,1	14,14,15	0.59	0	17,19,21	0.98	1 (5%)
5	NAG	J	2	5	14,14,15	0.36	0	17,19,21	1.20	1 (5%)
5	BMA	J	3	5	11,11,12	0.36	0	15,15,17	1.20	3 (20%)
5	MAN	J	4	5	11,11,12	0.62	0	15,15,17	2.42	3 (20%)
4	NAG	K	1	4,1	14,14,15	0.33	0	17,19,21	0.86	1 (5%)
4	NAG	K	2	4	14,14,15	0.60	0	17,19,21	2.07	2 (11%)
6	NAG	L	1	6,1	14,14,15	0.37	0	17,19,21	1.12	1 (5%)
6	NAG	L	2	6	14,14,15	0.33	0	17,19,21	1.26	2 (11%)
6	BMA	L	3	6	11,11,12	0.44	0	15,15,17	1.86	3 (20%)
6	MAN	L	4	6	11,11,12	0.39	0	15,15,17	1.21	1 (6%)

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
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	1/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
4	NAG	I	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	0/6/23/26	0/1/1/1
5	NAG	J	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	1/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
5	MAN	J	4	5	-	0/2/19/22	0/1/1/1
4	NAG	K	1	4,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
6	NAG	L	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1
6	BMA	L	3	6	-	1/2/19/22	0/1/1/1
6	MAN	L	4	6	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2	NAG	C1-O5-C5	8.37	123.53	112.19
5	J	4	MAN	C1-O5-C5	7.39	122.20	112.19
4	K	2	NAG	C1-O5-C5	7.32	122.10	112.19
5	J	4	MAN	C1-C2-C3	4.64	115.37	109.67
6	L	3	BMA	C1-O5-C5	4.21	117.89	112.19

There are no chirality outliers.

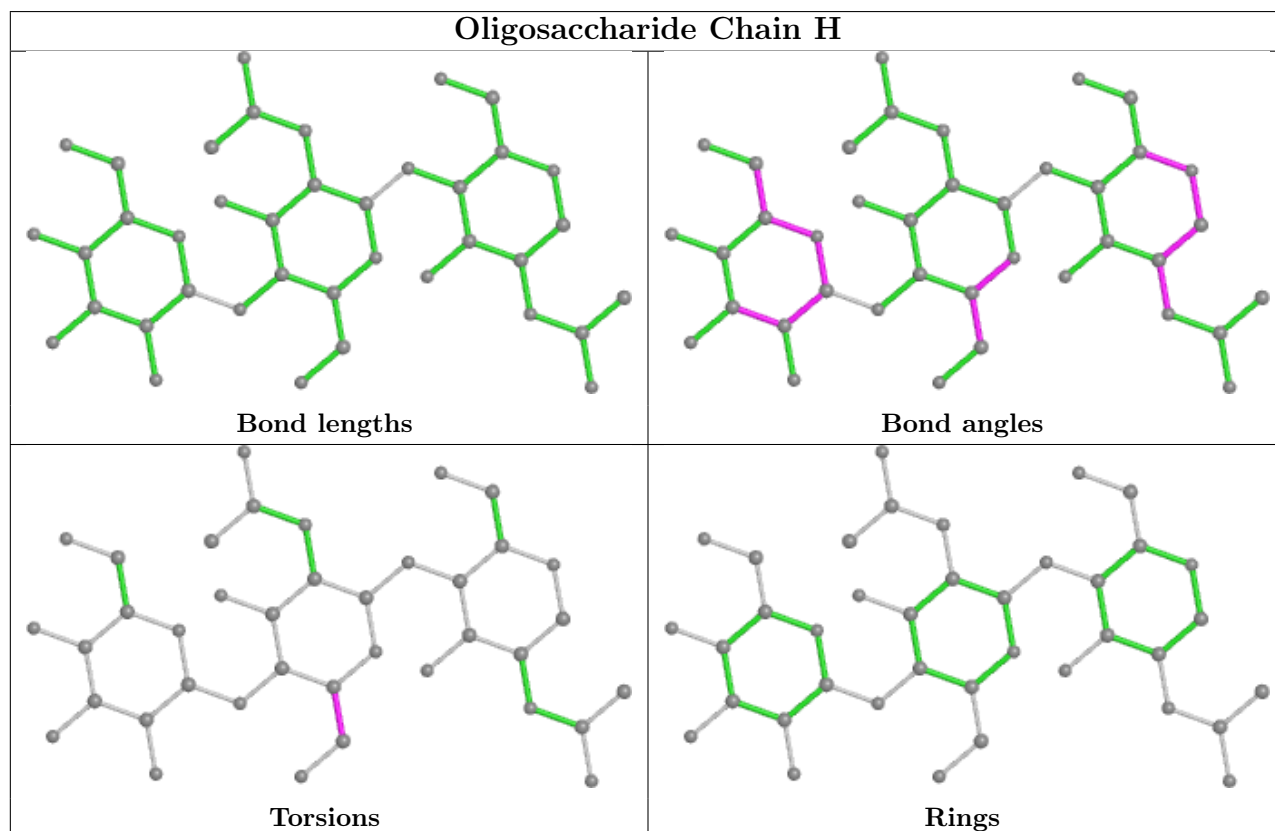
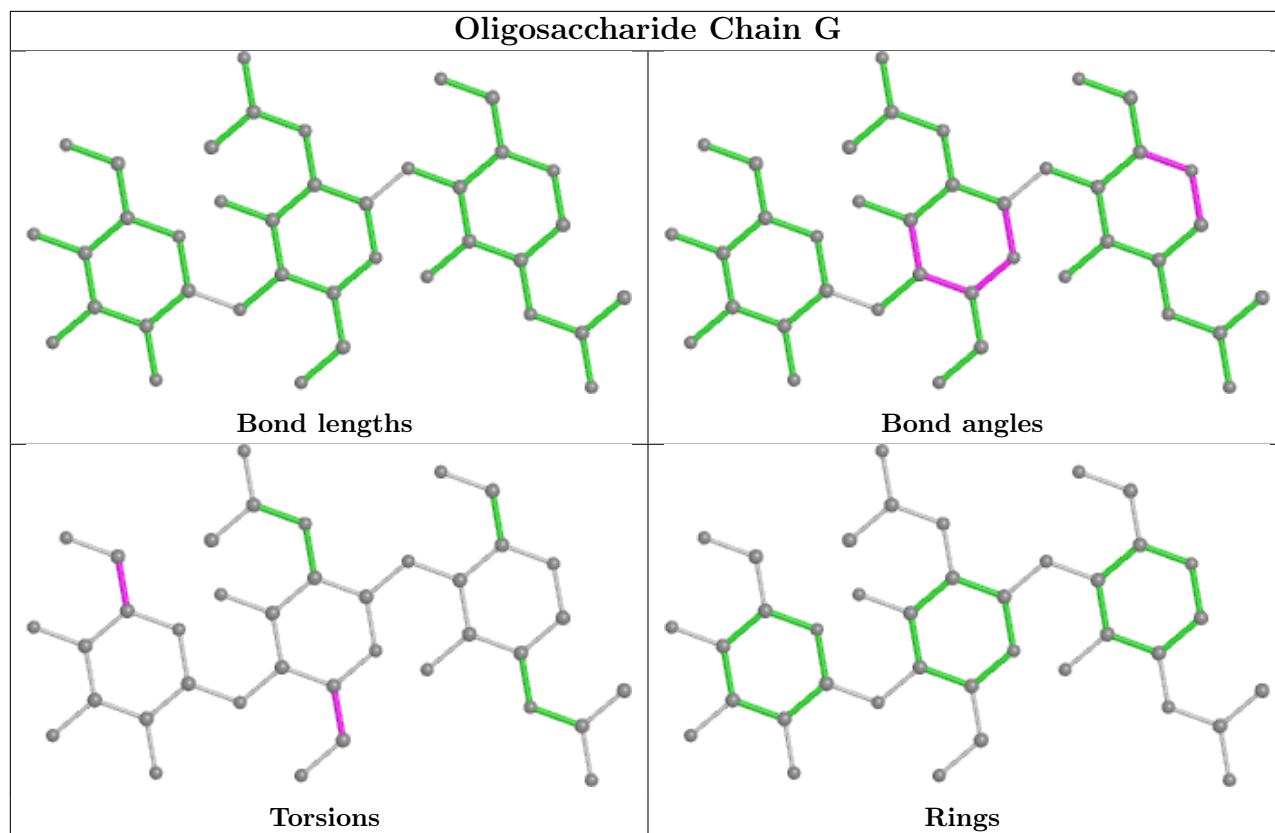
5 of 12 torsion outliers are listed below:

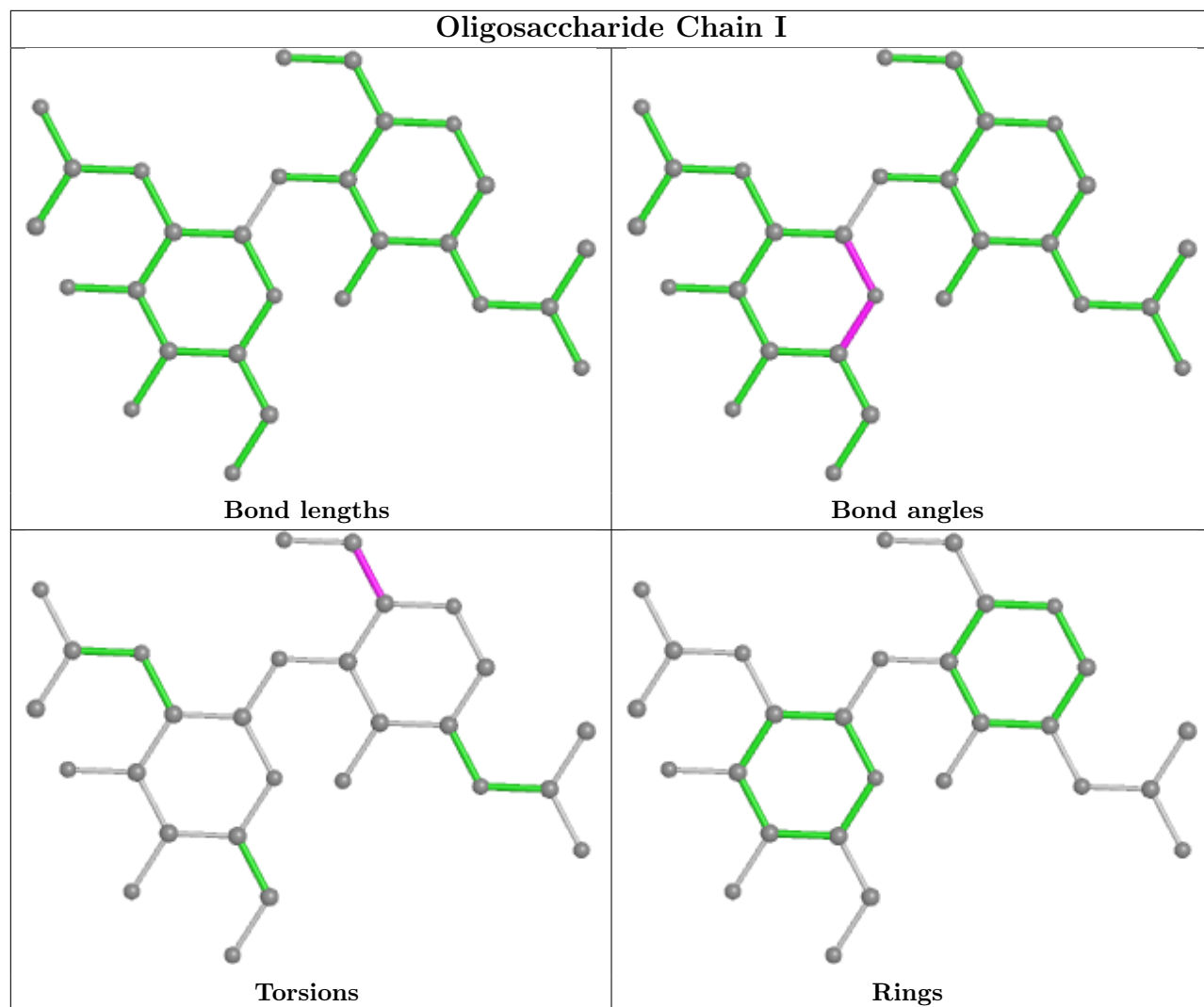
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6

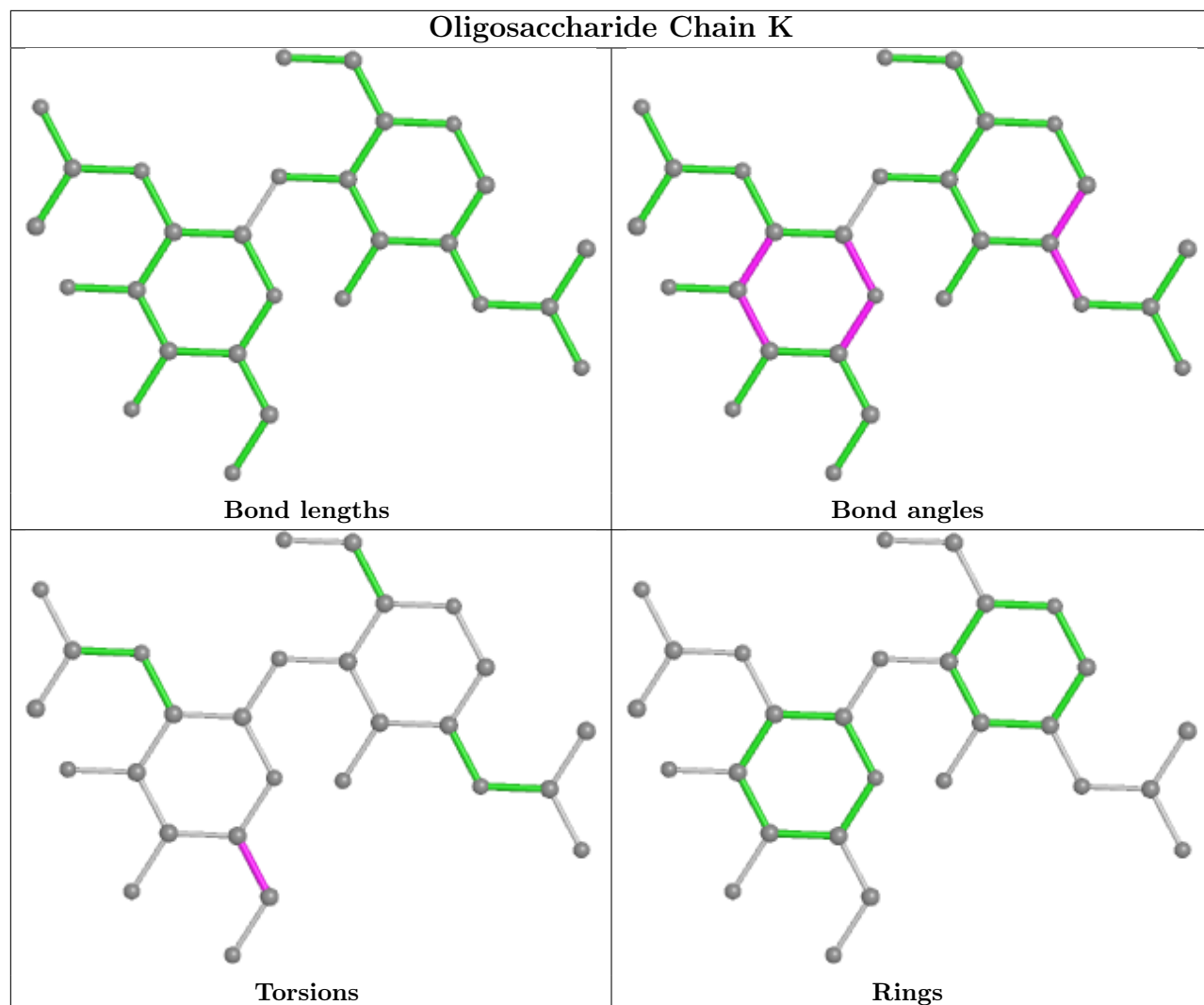
There are no ring outliers.

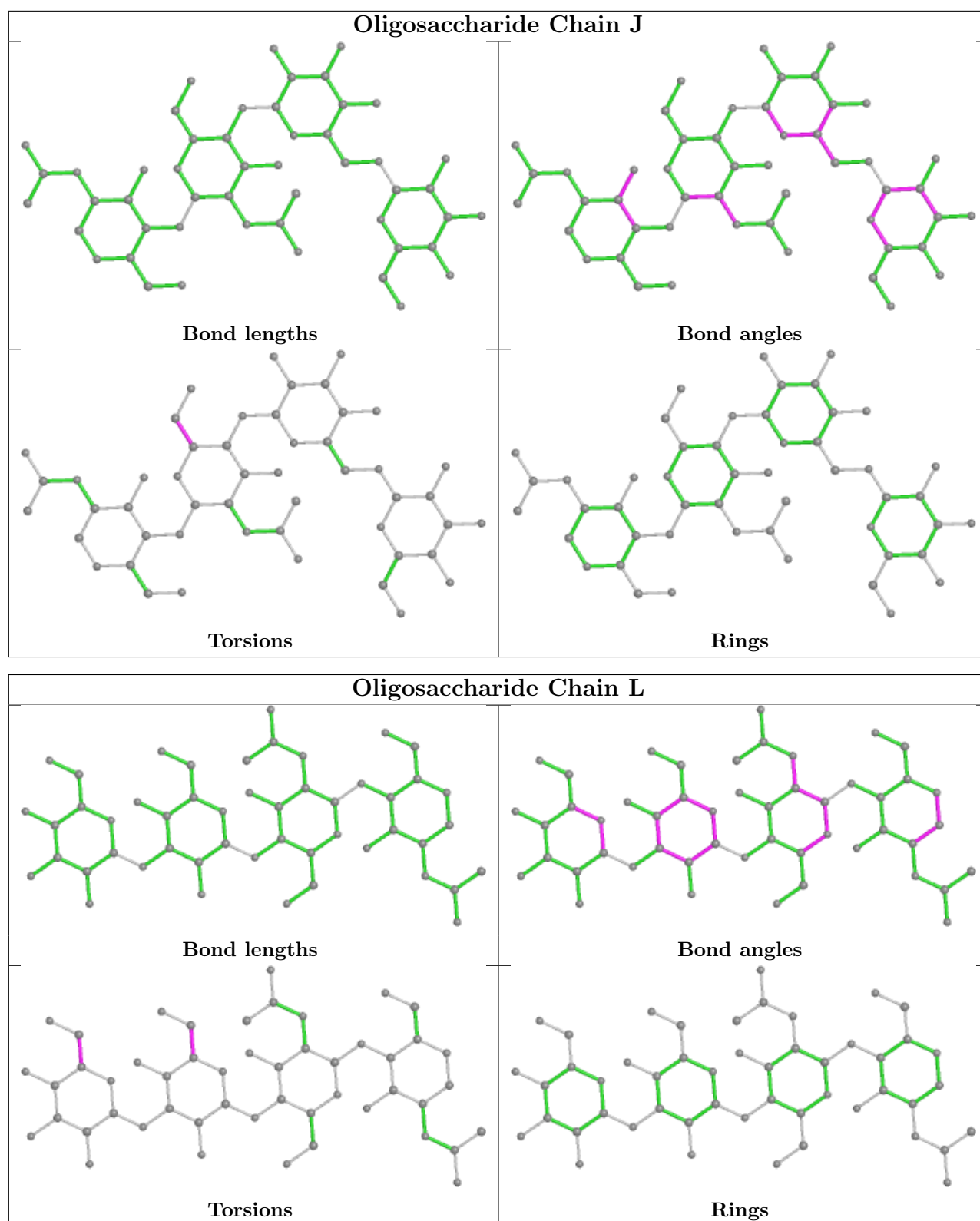
No monomer is involved in short contacts.

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](#)

7 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
7	NAG	E	501	1	14,14,15	0.58	0	17,19,21	1.49	1 (5%)
7	NAG	E	507	1	14,14,15	0.51	0	17,19,21	1.13	2 (11%)
7	NAG	C	501	1	14,14,15	0.57	0	17,19,21	2.27	3 (17%)
7	NAG	D	201	2	14,14,15	0.77	1 (7%)	17,19,21	2.17	5 (29%)
7	NAG	C	502	1	14,14,15	0.61	0	17,19,21	1.55	2 (11%)
7	NAG	A	404	1	14,14,15	0.58	0	17,19,21	1.25	3 (17%)
7	NAG	E	506	1	14,14,15	0.49	0	17,19,21	1.25	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
7	NAG	E	501	1	-	0/6/23/26	0/1/1/1
7	NAG	E	507	1	-	0/6/23/26	0/1/1/1
7	NAG	C	501	1	-	0/6/23/26	0/1/1/1
7	NAG	D	201	2	-	1/6/23/26	0/1/1/1
7	NAG	C	502	1	-	2/6/23/26	0/1/1/1
7	NAG	A	404	1	-	2/6/23/26	0/1/1/1
7	NAG	E	506	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	201	NAG	C1-C2	2.19	1.55	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	501	NAG	C1-O5-C5	8.16	123.25	112.19
7	E	501	NAG	C1-O5-C5	5.12	119.13	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	201	NAG	C2-N2-C7	5.09	130.16	122.90
7	C	502	NAG	C1-O5-C5	4.77	118.65	112.19
7	D	201	NAG	C1-O5-C5	4.03	117.66	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	201	NAG	C3-C2-N2-C7
7	A	404	NAG	O5-C5-C6-O6
7	C	502	NAG	C4-C5-C6-O6
7	A	404	NAG	C4-C5-C6-O6
7	C	502	NAG	O5-C5-C6-O6

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

5.1 Protein, DNA and RNA chains

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

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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