



Full wwPDB X-ray Structure Validation Report

Oct 3, 2023 – 02:50 AM EDT

PDB ID : 6O3O
Title : Structure of human DNAM-1 (CD226) bound to nectin-like protein-5 (necl-5)
Authors : Deuss, F.A.; Watson, G.M.; Rossjohn, J.; Berry, R.
Deposited on : 2019-02-27
Resolution : 2.80 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**
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 2.80 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 7982 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 CD226 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	218	1711	1096	290	315	10	0	1	0
1	B	196	1485	954	251	269	11	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	THR	-	expression tag	UNP Q15762
A	18	GLY	-	expression tag	UNP Q15762
A	251	GLY	-	expression tag	UNP Q15762
A	252	THR	-	expression tag	UNP Q15762
A	253	LYS	-	expression tag	UNP Q15762
A	254	HIS	-	expression tag	UNP Q15762
A	255	HIS	-	expression tag	UNP Q15762
A	256	HIS	-	expression tag	UNP Q15762
A	257	HIS	-	expression tag	UNP Q15762
A	258	HIS	-	expression tag	UNP Q15762
A	259	HIS	-	expression tag	UNP Q15762
B	17	THR	-	expression tag	UNP Q15762
B	18	GLY	-	expression tag	UNP Q15762
B	251	GLY	-	expression tag	UNP Q15762
B	252	THR	-	expression tag	UNP Q15762
B	253	LYS	-	expression tag	UNP Q15762
B	254	HIS	-	expression tag	UNP Q15762
B	255	HIS	-	expression tag	UNP Q15762
B	256	HIS	-	expression tag	UNP Q15762
B	257	HIS	-	expression tag	UNP Q15762
B	258	HIS	-	expression tag	UNP Q15762
B	259	HIS	-	expression tag	UNP Q15762

- Molecule 2 is a protein called Poliovirus receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	286	2126	1341	367	408	10	0	2	0
2	D	293	2188	1386	379	413	10	0	2	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	26	LEU	-	expression tag	UNP P15151
C	27	GLU	-	expression tag	UNP P15151
C	335	THR	-	expression tag	UNP P15151
C	336	SER	-	expression tag	UNP P15151
C	337	HIS	-	expression tag	UNP P15151
C	338	HIS	-	expression tag	UNP P15151
C	339	HIS	-	expression tag	UNP P15151
C	340	HIS	-	expression tag	UNP P15151
C	341	HIS	-	expression tag	UNP P15151
C	342	HIS	-	expression tag	UNP P15151
D	26	LEU	-	expression tag	UNP P15151
D	27	GLU	-	expression tag	UNP P15151
D	335	THR	-	expression tag	UNP P15151
D	336	SER	-	expression tag	UNP P15151
D	337	HIS	-	expression tag	UNP P15151
D	338	HIS	-	expression tag	UNP P15151
D	339	HIS	-	expression tag	UNP P15151
D	340	HIS	-	expression tag	UNP P15151
D	341	HIS	-	expression tag	UNP P15151
D	342	HIS	-	expression tag	UNP P15151

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	E	4	49	28	2	19	1	0	0
3	G	4	49	28	2	19	0	0	0

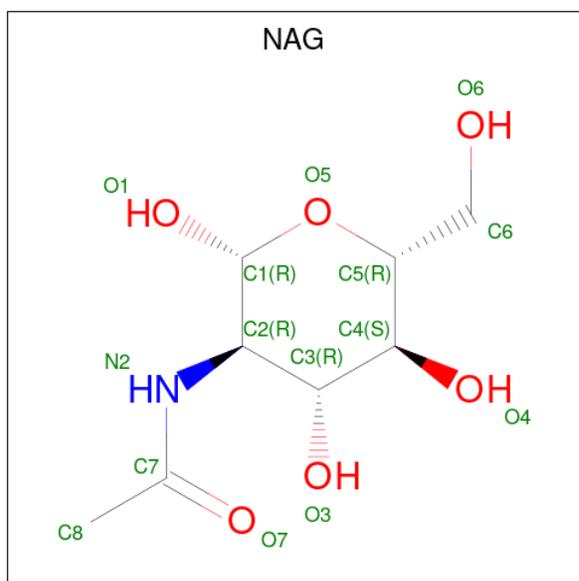
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	F	5	60	34	2	24	0	0	0

- Molecule 5 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			
5	H	2	28	16	2	10	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



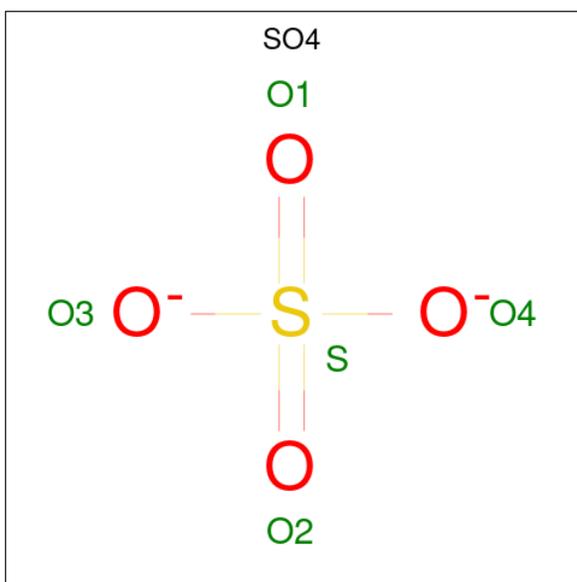
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
6	A	1	14	8	1	5	0	0
6	A	1	14	8	1	5	0	0
6	A	1	14	8	1	5	0	0
6	B	1	14	8	1	5	0	0
6	B	1	14	8	1	5	0	0
6	C	1	14	8	1	5	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	19	Total	O	0	0
			19	19		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	10	Total O 10 10	0	0
8	C	40	Total O 40 40	0	0
8	D	34	Total O 34 34	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 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	129.34Å 182.27Å 146.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.99 – 2.80	Depositor
% Data completeness (in resolution range)	99.5 (40.99-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.82Å)	Xtrriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.208 , 0.231	Depositor
Wilson B-factor (Å ²)	52.3	Xtrriage
Anisotropy	0.583	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7982	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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](#)

15 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	E	1	3,2	14,14,15	0.30	0	17,19,21	0.66	0
3	NAG	E	2	3	14,14,15	0.29	0	17,19,21	0.38	0
3	BMA	E	3	3	11,11,12	0.36	0	15,15,17	0.64	0
3	FUC	E	4	3	10,10,11	0.41	0	14,14,16	0.89	0
4	NAG	F	1	4,2	14,14,15	0.29	0	17,19,21	0.79	1 (5%)
4	NAG	F	2	4	14,14,15	0.29	0	17,19,21	0.56	0
4	BMA	F	3	4	11,11,12	0.35	0	15,15,17	0.60	0
4	MAN	F	4	4	11,11,12	0.37	0	15,15,17	0.94	1 (6%)
4	FUC	F	5	4	10,10,11	0.45	0	14,14,16	0.65	0
3	NAG	G	1	3,2	14,14,15	0.30	0	17,19,21	0.73	0
3	NAG	G	2	3	14,14,15	0.39	0	17,19,21	0.95	1 (5%)
3	BMA	G	3	3	11,11,12	0.33	0	15,15,17	0.64	1 (6%)
3	FUC	G	4	3	10,10,11	0.43	0	14,14,16	1.12	1 (7%)
5	NAG	H	1	5,2	14,14,15	0.30	0	17,19,21	0.70	1 (5%)
5	NAG	H	2	5	14,14,15	0.33	0	17,19,21	0.88	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
3	NAG	E	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	FUC	E	4	3	-	-	0/1/1/1
4	NAG	F	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	BMA	F	3	4	-	0/2/19/22	0/1/1/1
4	MAN	F	4	4	-	0/2/19/22	0/1/1/1
4	FUC	F	5	4	-	-	0/1/1/1
3	NAG	G	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
3	BMA	G	3	3	-	0/2/19/22	0/1/1/1
3	FUC	G	4	3	-	-	0/1/1/1
5	NAG	H	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	4	MAN	C1-O5-C5	3.10	116.39	112.19
4	F	1	NAG	C1-O5-C5	2.60	115.71	112.19
3	G	2	NAG	O5-C1-C2	-2.50	107.35	111.29
3	G	4	FUC	C1-O5-C5	2.40	118.22	112.78
5	H	2	NAG	C1-O5-C5	2.33	115.35	112.19
5	H	1	NAG	C1-O5-C5	2.20	115.17	112.19
5	H	2	NAG	C2-N2-C7	2.02	125.79	122.90
3	G	3	BMA	C1-O5-C5	2.01	114.91	112.19

There are no chirality outliers.

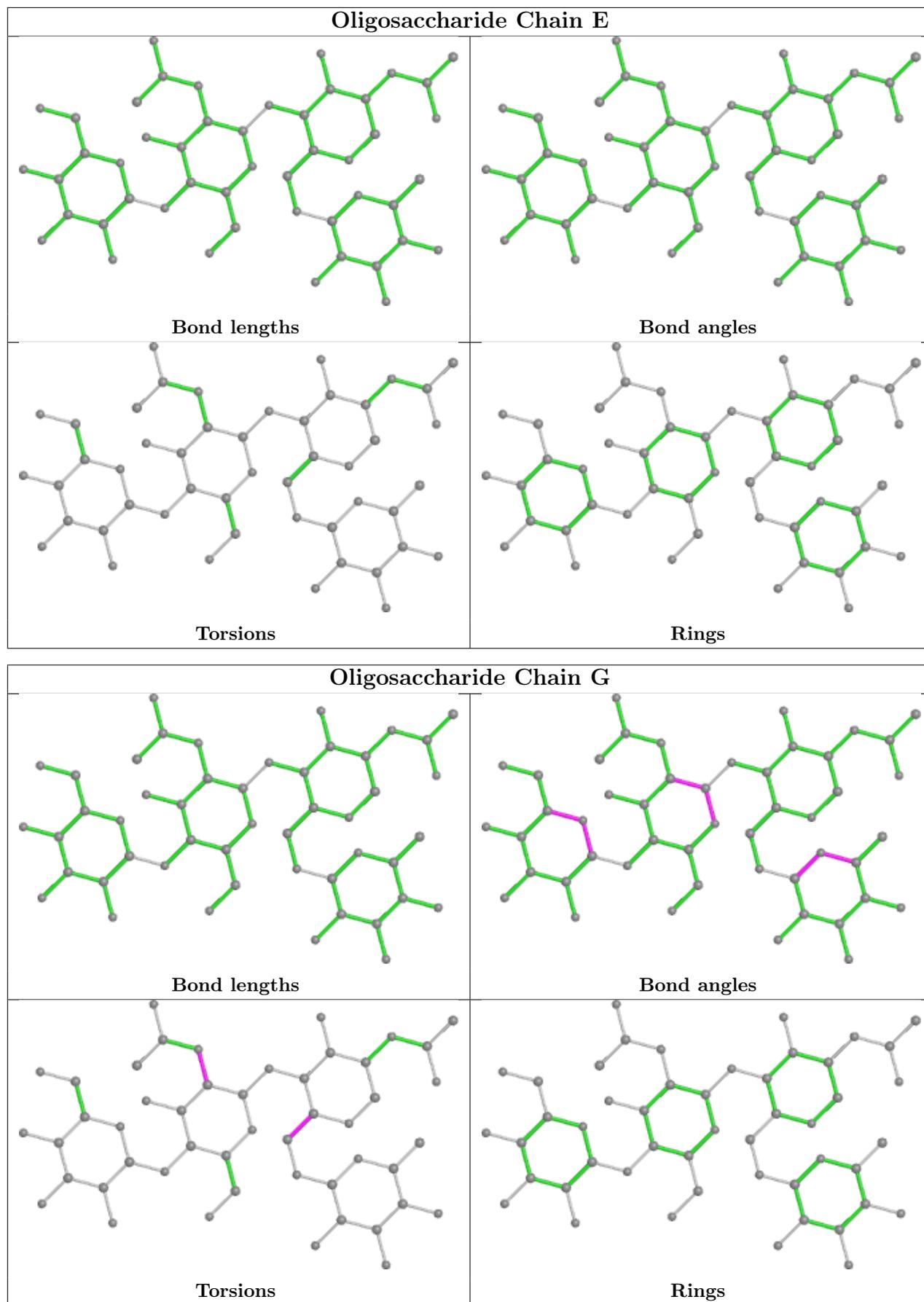
All (6) torsion outliers are listed below:

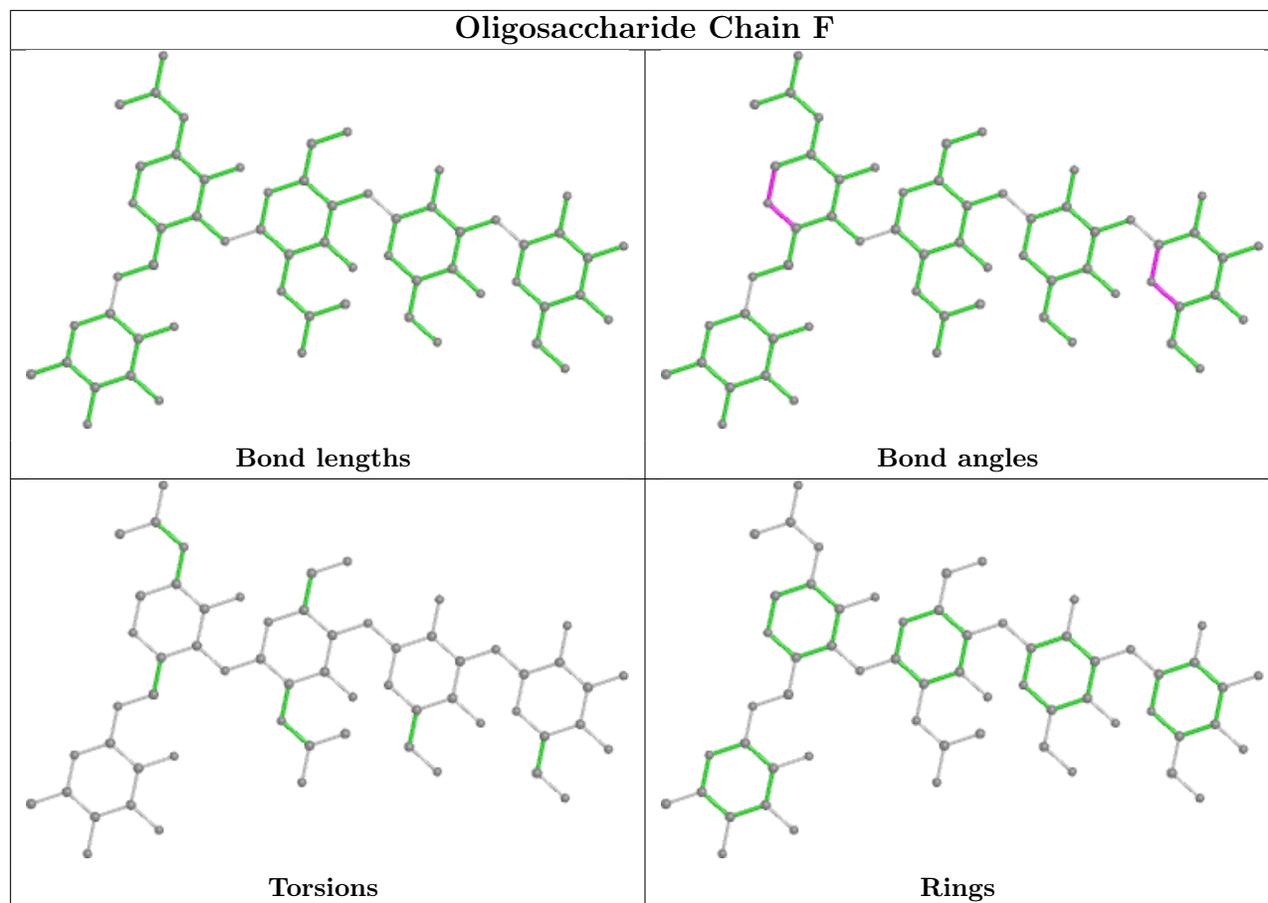
Mol	Chain	Res	Type	Atoms
5	H	2	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C3-C2-N2-C7
5	H	2	NAG	C3-C2-N2-C7

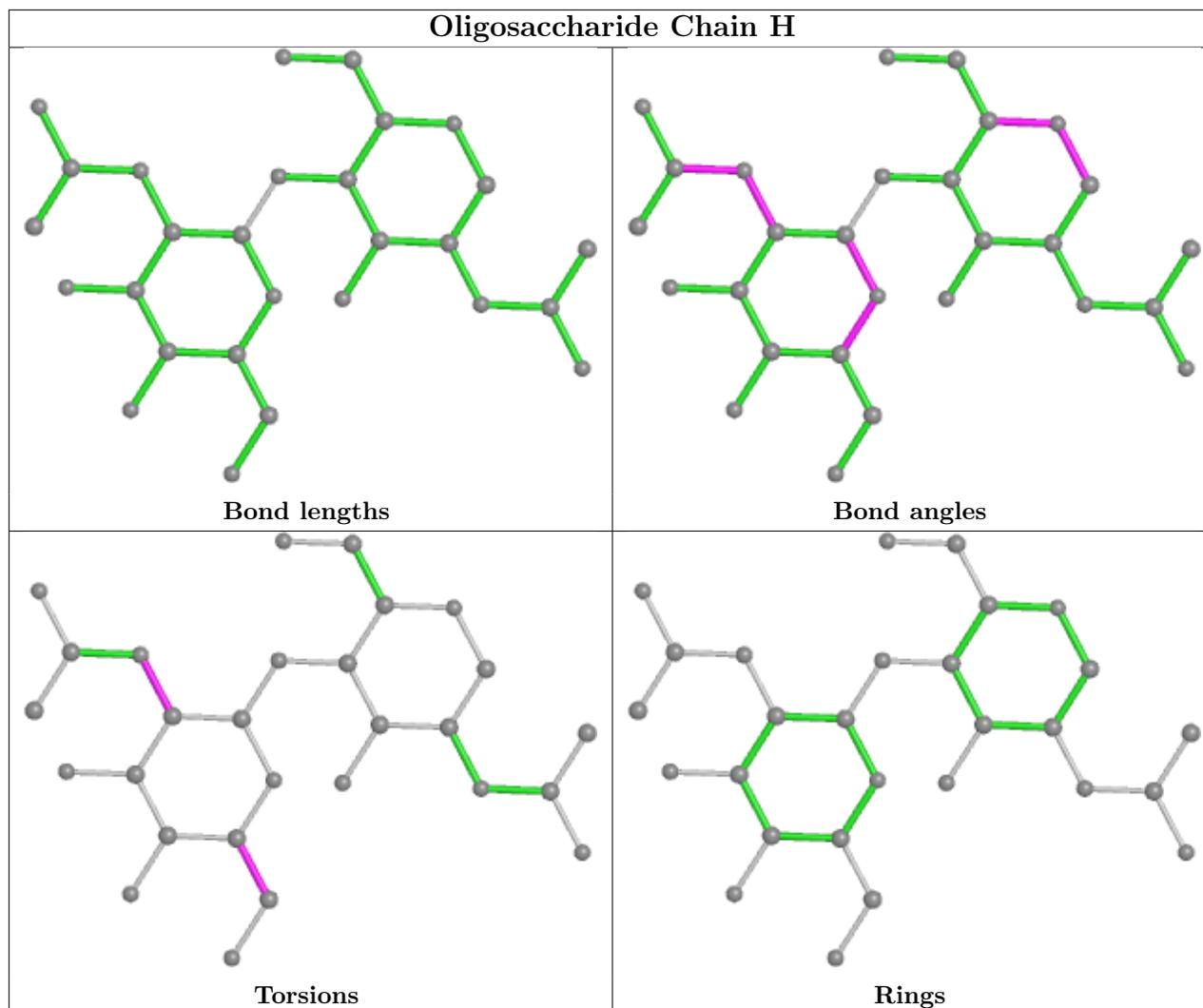
There are no ring outliers.

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](#)

15 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	$\# Z > 2$
6	NAG	C	405	2	14,14,15	0.29	0	17,19,21	0.72	0
6	NAG	B	700	1	14,14,15	0.29	0	17,19,21	1.05	2 (11%)
6	NAG	B	701	1	14,14,15	0.27	0	17,19,21	0.72	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	D	406	2	14,14,15	0.31	0	17,19,21	0.43	0
6	NAG	A	802	1	14,14,15	0.30	0	17,19,21	0.50	0
6	NAG	D	413	2	14,14,15	0.31	0	17,19,21	0.71	1 (5%)
7	SO4	D	414	-	4,4,4	0.12	0	6,6,6	0.08	0
6	NAG	A	801	1	14,14,15	0.29	0	17,19,21	0.54	0
6	NAG	C	407	2	14,14,15	0.30	0	17,19,21	0.68	1 (5%)
6	NAG	C	408	2	14,14,15	0.33	0	17,19,21	0.83	1 (5%)
7	SO4	A	806	-	4,4,4	0.14	0	6,6,6	0.06	0
6	NAG	A	804	1	14,14,15	0.29	0	17,19,21	0.82	1 (5%)
6	NAG	A	803	1	14,14,15	0.29	0	17,19,21	0.86	1 (5%)
7	SO4	A	805	-	4,4,4	0.13	0	6,6,6	0.06	0
6	NAG	C	406	2	14,14,15	0.29	0	17,19,21	0.62	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
6	NAG	C	405	2	-	0/6/23/26	0/1/1/1
6	NAG	B	700	1	-	0/6/23/26	0/1/1/1
6	NAG	B	701	1	-	0/6/23/26	0/1/1/1
6	NAG	D	406	2	-	0/6/23/26	0/1/1/1
6	NAG	A	802	1	-	0/6/23/26	0/1/1/1
6	NAG	D	413	2	-	0/6/23/26	0/1/1/1
6	NAG	A	801	1	-	1/6/23/26	0/1/1/1
6	NAG	C	407	2	-	0/6/23/26	0/1/1/1
6	NAG	C	408	2	-	0/6/23/26	0/1/1/1
6	NAG	A	804	1	-	2/6/23/26	0/1/1/1
6	NAG	A	803	1	-	0/6/23/26	0/1/1/1
6	NAG	C	406	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	803	NAG	C1-O5-C5	3.24	116.59	112.19
6	B	700	NAG	C1-O5-C5	2.99	116.25	112.19
6	D	413	NAG	C1-O5-C5	2.75	115.91	112.19
6	C	408	NAG	C1-O5-C5	2.53	115.62	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	406	NAG	C1-O5-C5	2.34	115.37	112.19
6	A	804	NAG	C1-O5-C5	2.29	115.30	112.19
6	B	700	NAG	O5-C1-C2	-2.23	107.77	111.29
6	B	701	NAG	C1-O5-C5	2.22	115.19	112.19
6	C	407	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	804	NAG	O5-C5-C6-O6
6	A	804	NAG	C4-C5-C6-O6
6	A	801	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.