



## wwPDB EM Validation Summary Report ⓘ

Jun 11, 2026 – 10:10 PM JST

PDB ID : 9X3J / pdb\_00009x3j  
EMDB ID : EMD-66501  
Title : Glycoprotein of Mengla Virus with MR191 Fab bound  
Authors : Wang, L.; Zou, B.; Liu, B.; Xue, L.; He, J.; Xiong, X.  
Deposited on : 2025-10-09  
Resolution : 3.47 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : **NOT EXECUTED**  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

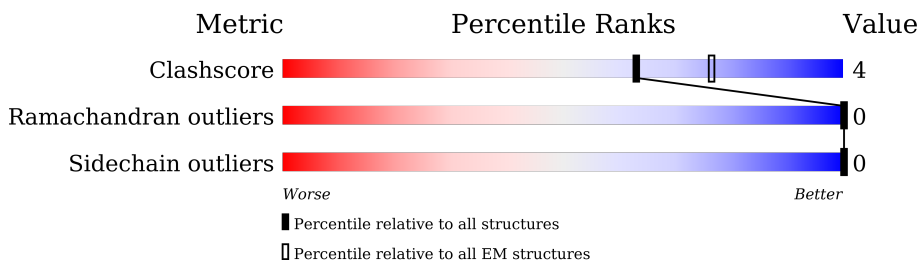
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.47 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.





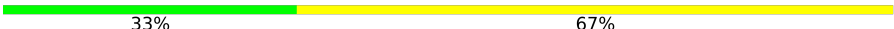



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	662	34% 62%
1	B	662	34% 5% 62%
1	E	662	35% 62%
2	C	230	49% 6% 46%
2	F	230	47% 7% 46%
2	I	230	48% 6% 46%
3	D	218	43% 8% 49%
3	G	218	42% 9% 49%
3	M	218	43% 8% 49%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
4	H	6	 33% 67%
4	K	6	 17% 83%
4	N	6	 33% 67%
5	J	3	 67% 33%
5	L	3	 67% 33%
5	O	3	 67% 33%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11679 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	252	Total 1996	C 1280	N 348	O 358	S 10	0	0
1	B	252	Total 1996	C 1280	N 348	O 358	S 10	0	0
1	E	252	Total 1996	C 1280	N 348	O 358	S 10	0	0

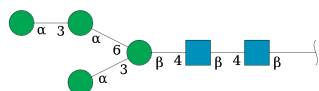
- Molecule 2 is a protein called MR191 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	125	Total 965	C 615	N 159	O 189	S 2	0	0
2	C	125	Total 965	C 615	N 159	O 189	S 2	0	0
2	F	125	Total 965	C 615	N 159	O 189	S 2	0	0

- Molecule 3 is a protein called MR191 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	111	Total 807	C 502	N 136	O 167	S 2	0	0
3	D	111	Total 807	C 502	N 136	O 167	S 2	0	0
3	G	111	Total 807	C 502	N 136	O 167	S 2	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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.



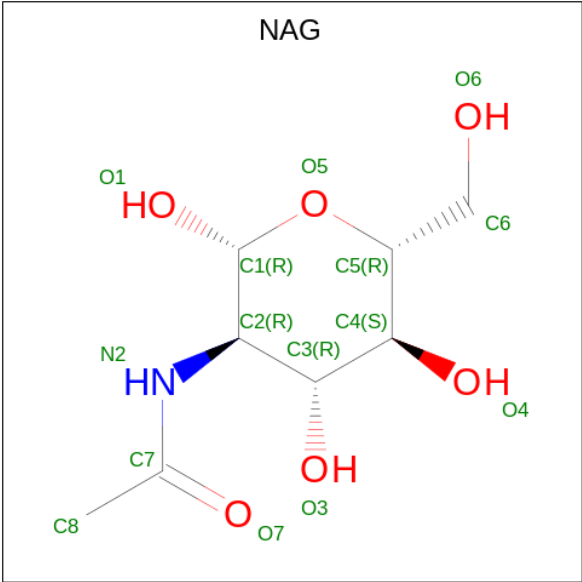
Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	6	Total	C	N	O	0	0
			72	40	2	30		
4	K	6	Total	C	N	O	0	0
			72	40	2	30		
4	N	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 5 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				AltConf	Trace
5	J	3	Total	C	N	O	0	0
			39	22	2	15		
5	L	3	Total	C	N	O	0	0
			39	22	2	15		
5	O	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).

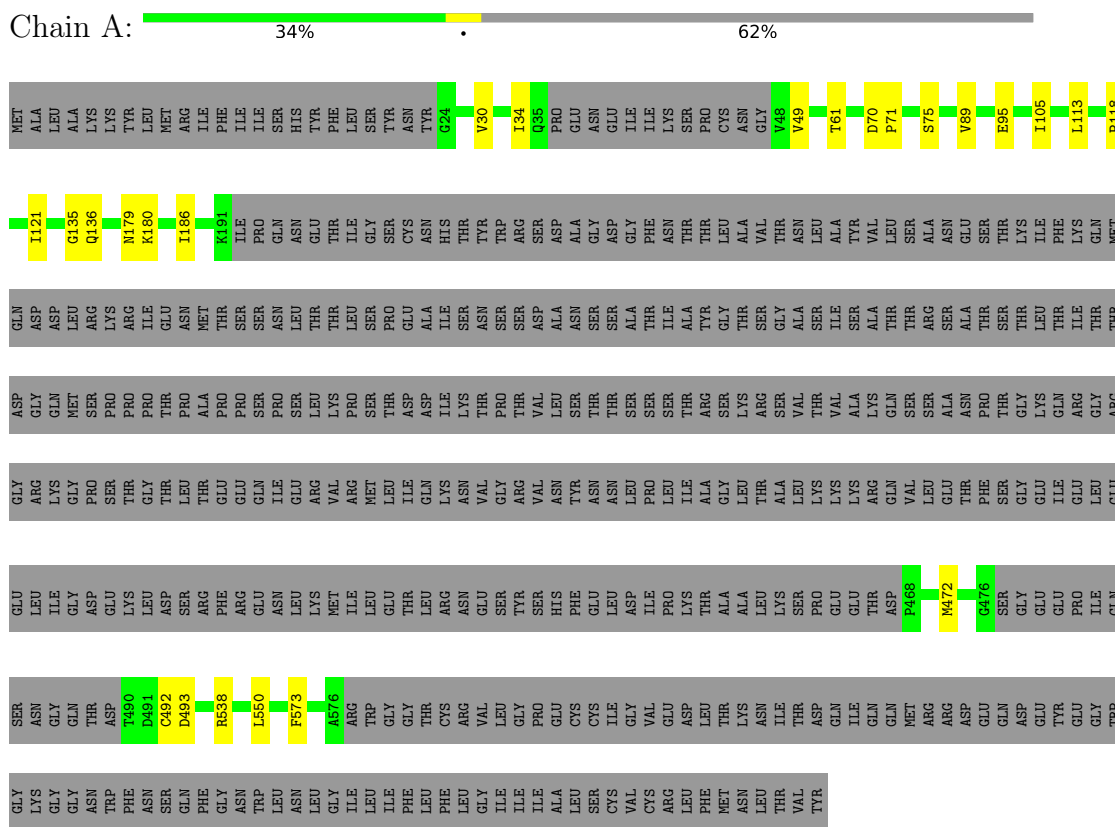


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	E	1	Total	C	N	O	0
			14	8	1	5	

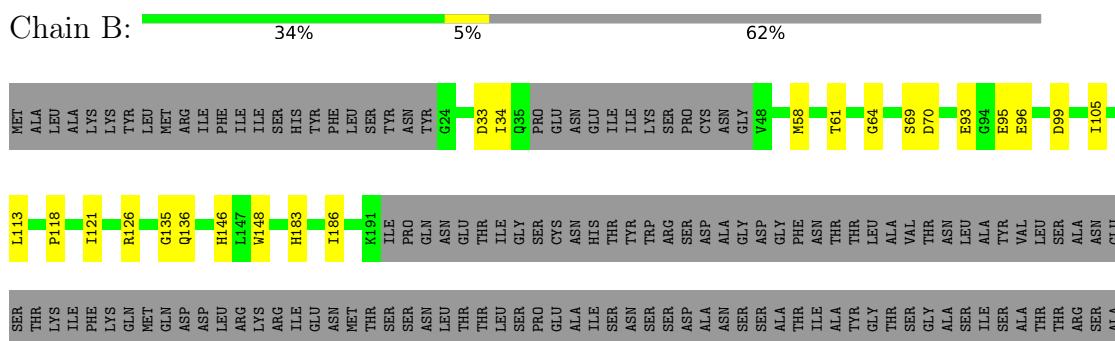
### 3 Residue-property plots

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.

- Molecule 1: Envelope glycoprotein



- Molecule 1: Envelope glycoprotein





LYS  
VAL  
ASP  
LYS  
LYS  
VAL  
GLU  
PRO  
LYS  
SER  
CYS  
ASP

● Molecule 2: MR191 Fab Heavy Chain



GLN  
L2  
Q3  
S25  
Y35  
R40  
Q41  
L47  
V69  
V84  
D91  
Q100  
V107  
S111  
K112  
S126  
ALA  
SER  
THR  
LYS  
GLY  
PRO  
SER  
VAL  
PHE  
PRO  
LEU  
ALA  
PRO  
SER  
SER  
SER  
LEU  
SER  
THR  
GLY  
GLY  
THR  
ALA  
ALA  
LEU  
CYS  
VAL  
LYS  
ASP  
THR  
PHE

VAL  
ASP  
LYS  
LYS  
VAL  
GLU  
PRO  
LYS  
SER  
CYS  
ASP

● Molecule 2: MR191 Fab Heavy Chain



GLN  
L2  
Q3  
S25  
Y35  
Q41  
P42  
P43  
L47  
E48  
S54  
N58  
N62  
V69  
V84  
Q100  
V107  
S111  
K112  
S126  
SER  
THR  
LYS  
GLY  
PRO  
SER  
VAL  
PHE  
PRO  
LEU  
ALA  
PRO  
SER  
SER  
SER  
LEU  
SER  
THR  
GLY  
THR  
ILE  
CYS  
ASN  
VAL  
LEU  
GLY  
CYS

LYS  
PRO  
SER  
ASN  
THR  
LYS  
VAL  
ASP  
GLU  
PRO  
LYS  
CYS  
ASP

● Molecule 3: MR191 Fab Light Chain



GLN  
S2  
V3  
L4  
A13  
Q16  
R17  
V18  
L48  
L49  
I50  
Y51  
R63  
T78  
G79  
L80  
Q81  
A82  
E83  
D84  
G104  
T110  
V111  
L112  
GLY  
SER  
PRO  
LYS  
ALA  
ALA  
PRO  
SER  
VAL  
SER  
THR  
LEU  
PHE  
PRO  
PRO  
SER  
SER  
PRO  
GLU  
GLU  
LEU  
TRP  
LYS  
GLN  
ALA  
ASN  
HIS  
ARG  
LYS  
SER  
THR  
LEU  
VAL  
CYS  
GLN  
VAL  
HIS

THR  
HIS  
GLU  
GLY  
SER  
THR  
VAL  
GLU  
LYS  
THR  
VAL  
VAL  
ALA  
PRO  
THR  
GLU  
CYS  
SER

● Molecule 3: MR191 Fab Light Chain

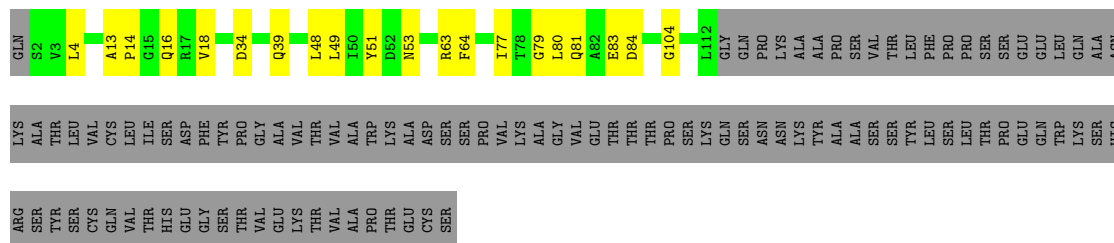


GLN  
S2  
V3  
L4  
P7  
P8  
A13  
P14  
G15  
Q16  
R17  
V18  
L41  
L48  
Y51  
F64  
I77  
L80  
Q81  
A82  
E83  
A86  
G104  
L112  
GLY  
GLN  
PRO  
LYS  
ALA  
SER  
VAL  
SER  
THR  
LEU  
PHE  
PRO  
SER  
PRO  
SER  
SER  
PRO  
GLU  
GLU  
TRP  
LYS  
SER  
HIS  
ARG  
LYS  
ALA  
THR

SER  
CYS  
GLN  
VAL  
THR  
HIS  
GLU  
GLY  
SER  
THR  
VAL  
VAL  
GLU  
LYS  
THR  
VAL  
ALA  
PRO  
THR  
GLU  
CYS  
SER

- Molecule 3: MR191 Fab Light Chain

Chain G:  42% 9% 49%



- Molecule 4: alpha-D-mannopyranose-(1-3)-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

Chain H:  33% 67%



- Molecule 4: alpha-D-mannopyranose-(1-3)-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

Chain K:  17% 83%



- Molecule 4: alpha-D-mannopyranose-(1-3)-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

Chain N:  33% 67%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  67% 33%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  67% 33%



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  67% 33%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	15563	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

## 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: BMA, MAN, NAG

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	A	0.21	0/2038	0.51	0/2753
1	B	0.20	0/2038	0.49	0/2753
1	E	0.18	0/2038	0.45	0/2753
2	C	0.20	0/990	0.51	0/1349
2	F	0.20	0/990	0.52	0/1349
2	I	0.21	0/990	0.54	0/1349
3	D	0.17	0/825	0.46	0/1126
3	G	0.18	0/825	0.49	0/1126
3	M	0.15	0/825	0.43	0/1126
All	All	0.19	0/11559	0.49	0/15684

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	A	1996	0	2014	14	0
1	B	1996	0	2014	19	0
1	E	1996	0	2014	15	0
2	C	965	0	940	8	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	965	0	940	10	0
2	I	965	0	940	8	0
3	D	807	0	773	9	0
3	G	807	0	773	11	0
3	M	807	0	773	10	0
4	H	72	0	61	0	0
4	K	72	0	61	0	0
4	N	72	0	61	0	0
5	J	39	0	34	0	0
5	L	39	0	34	0	0
5	O	39	0	34	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	E	14	0	13	0	0
All	All	11679	0	11505	97	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 4.

The worst 5 of 97 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)
3:D:48:LEU:HD11	3:D:51:TYR:HB3	1.79	0.64
1:A:472:MET:HG2	1:A:538:ARG:HH12	1.65	0.62
1:B:93:GLU:OE1	1:B:183:HIS:NE2	2.34	0.60
1:A:492:CYS:SG	1:A:493:ASP:N	2.74	0.60
1:B:492:CYS:SG	1:B:493:ASP:N	2.75	0.60

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 PDB entries followed by that with respect to all EM entries.

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	A	244/662 (37%)	233 (96%)	11 (4%)	0	100	100
1	B	244/662 (37%)	231 (95%)	13 (5%)	0	100	100
1	E	244/662 (37%)	234 (96%)	10 (4%)	0	100	100
2	C	123/230 (54%)	119 (97%)	4 (3%)	0	100	100
2	F	123/230 (54%)	117 (95%)	6 (5%)	0	100	100
2	I	123/230 (54%)	118 (96%)	5 (4%)	0	100	100
3	D	109/218 (50%)	101 (93%)	8 (7%)	0	100	100
3	G	109/218 (50%)	100 (92%)	9 (8%)	0	100	100
3	M	109/218 (50%)	100 (92%)	9 (8%)	0	100	100
All	All	1428/3330 (43%)	1353 (95%)	75 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	A	216/576 (38%)	216 (100%)	0	100	100
1	B	216/576 (38%)	216 (100%)	0	100	100
1	E	216/576 (38%)	216 (100%)	0	100	100
2	C	109/200 (54%)	109 (100%)	0	100	100
2	F	109/200 (54%)	109 (100%)	0	100	100
2	I	109/200 (54%)	109 (100%)	0	100	100
3	D	90/182 (50%)	90 (100%)	0	100	100
3	G	90/182 (50%)	90 (100%)	0	100	100
3	M	90/182 (50%)	90 (100%)	0	100	100
All	All	1245/2874 (43%)	1245 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15

such sidechains are listed below:

Mol	Chain	Res	Type
1	B	471	HIS
3	G	36	HIS
2	C	58	ASN
3	G	39	GLN
1	E	136	GLN

### 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 ⓘ

27 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	$\# Z  > 2$
4	NAG	H	1	1,4	14,14,15	0.22	0	17,19,21	0.58	0
4	NAG	H	2	4	14,14,15	0.29	0	17,19,21	0.63	1 (5%)
4	BMA	H	3	4	11,11,12	0.75	0	15,15,17	0.87	0
4	MAN	H	4	4	11,11,12	0.88	0	15,15,17	1.04	2 (13%)
4	MAN	H	5	4	11,11,12	1.17	1 (9%)	15,15,17	1.71	2 (13%)
4	MAN	H	6	4	11,11,12	0.90	1 (9%)	15,15,17	1.14	2 (13%)
5	NAG	J	1	1,5	14,14,15	0.37	0	17,19,21	0.63	0
5	NAG	J	2	5	14,14,15	0.41	0	17,19,21	0.45	0
5	BMA	J	3	5	11,11,12	0.77	0	15,15,17	0.88	1 (6%)
4	NAG	K	1	1,4	14,14,15	0.26	0	17,19,21	0.59	0
4	NAG	K	2	4	14,14,15	0.31	0	17,19,21	0.64	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BMA	K	3	4	11,11,12	0.75	0	15,15,17	0.88	1 (6%)
4	MAN	K	4	4	11,11,12	0.87	0	15,15,17	1.07	2 (13%)
4	MAN	K	5	4	11,11,12	1.12	1 (9%)	15,15,17	1.71	2 (13%)
4	MAN	K	6	4	11,11,12	0.92	1 (9%)	15,15,17	1.16	2 (13%)
5	NAG	L	1	1,5	14,14,15	0.27	0	17,19,21	0.54	0
5	NAG	L	2	5	14,14,15	0.32	0	17,19,21	0.46	0
5	BMA	L	3	5	11,11,12	0.73	0	15,15,17	0.92	1 (6%)
4	NAG	N	1	1,4	14,14,15	0.23	0	17,19,21	0.55	0
4	NAG	N	2	4	14,14,15	0.40	0	17,19,21	0.63	1 (5%)
4	BMA	N	3	4	11,11,12	0.78	0	15,15,17	0.86	0
4	MAN	N	4	4	11,11,12	0.92	0	15,15,17	1.00	2 (13%)
4	MAN	N	5	4	11,11,12	1.15	1 (9%)	15,15,17	1.72	2 (13%)
4	MAN	N	6	4	11,11,12	0.93	1 (9%)	15,15,17	1.20	2 (13%)
5	NAG	O	1	1,5	14,14,15	0.36	0	17,19,21	0.62	0
5	NAG	O	2	5	14,14,15	0.39	0	17,19,21	0.46	0
5	BMA	O	3	5	11,11,12	0.78	0	15,15,17	0.87	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
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1
4	MAN	H	4	4	-	0/2/19/22	0/1/1/1
4	MAN	H	5	4	-	0/2/19/22	0/1/1/1
4	MAN	H	6	4	-	0/2/19/22	0/1/1/1
5	NAG	J	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	BMA	J	3	5	-	2/2/19/22	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	1/6/23/26	0/1/1/1
4	BMA	K	3	4	-	2/2/19/22	0/1/1/1
4	MAN	K	4	4	-	0/2/19/22	0/1/1/1
4	MAN	K	5	4	-	0/2/19/22	0/1/1/1
4	MAN	K	6	4	-	0/2/19/22	0/1/1/1
5	NAG	L	1	1,5	-	0/6/23/26	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	L	2	5	-	2/6/23/26	0/1/1/1
5	BMA	L	3	5	-	1/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	1/6/23/26	0/1/1/1
4	BMA	N	3	4	-	2/2/19/22	0/1/1/1
4	MAN	N	4	4	-	0/2/19/22	0/1/1/1
4	MAN	N	5	4	-	0/2/19/22	0/1/1/1
4	MAN	N	6	4	-	0/2/19/22	0/1/1/1
5	NAG	O	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	BMA	O	3	5	-	2/2/19/22	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	5	MAN	C1-C2	2.83	1.58	1.52
4	H	5	MAN	C1-C2	2.82	1.58	1.52
4	K	5	MAN	C1-C2	2.71	1.58	1.52
4	N	6	MAN	C1-C2	2.42	1.57	1.52
4	K	6	MAN	C1-C2	2.30	1.57	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	5	MAN	C1-O5-C5	5.47	119.60	112.19
4	N	5	MAN	C1-O5-C5	5.40	119.51	112.19
4	K	5	MAN	C1-O5-C5	5.37	119.47	112.19
4	N	6	MAN	C1-O5-C5	2.93	116.16	112.19
4	K	6	MAN	C1-O5-C5	2.71	115.86	112.19

There are no chirality outliers.

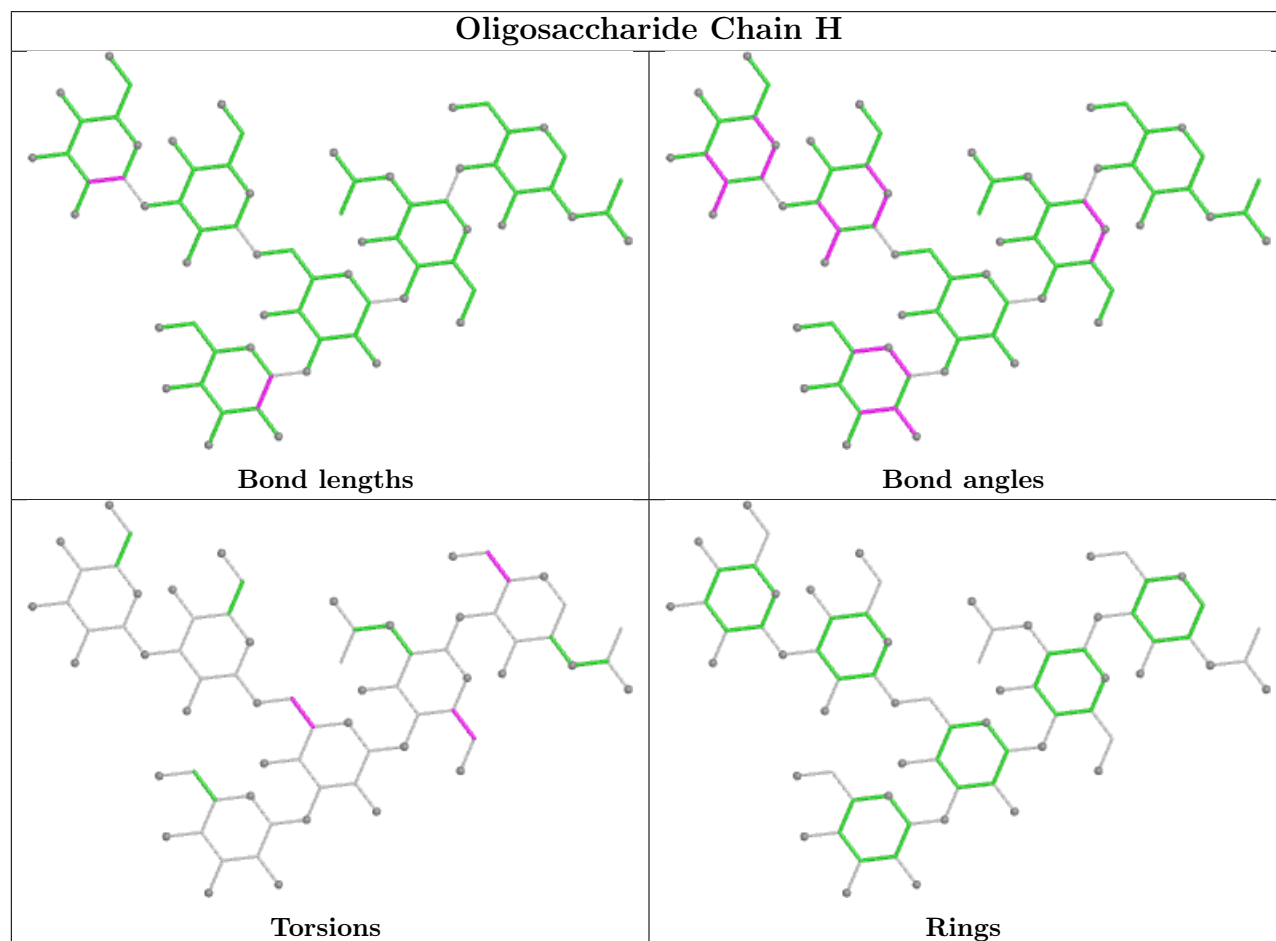
5 of 22 torsion outliers are listed below:

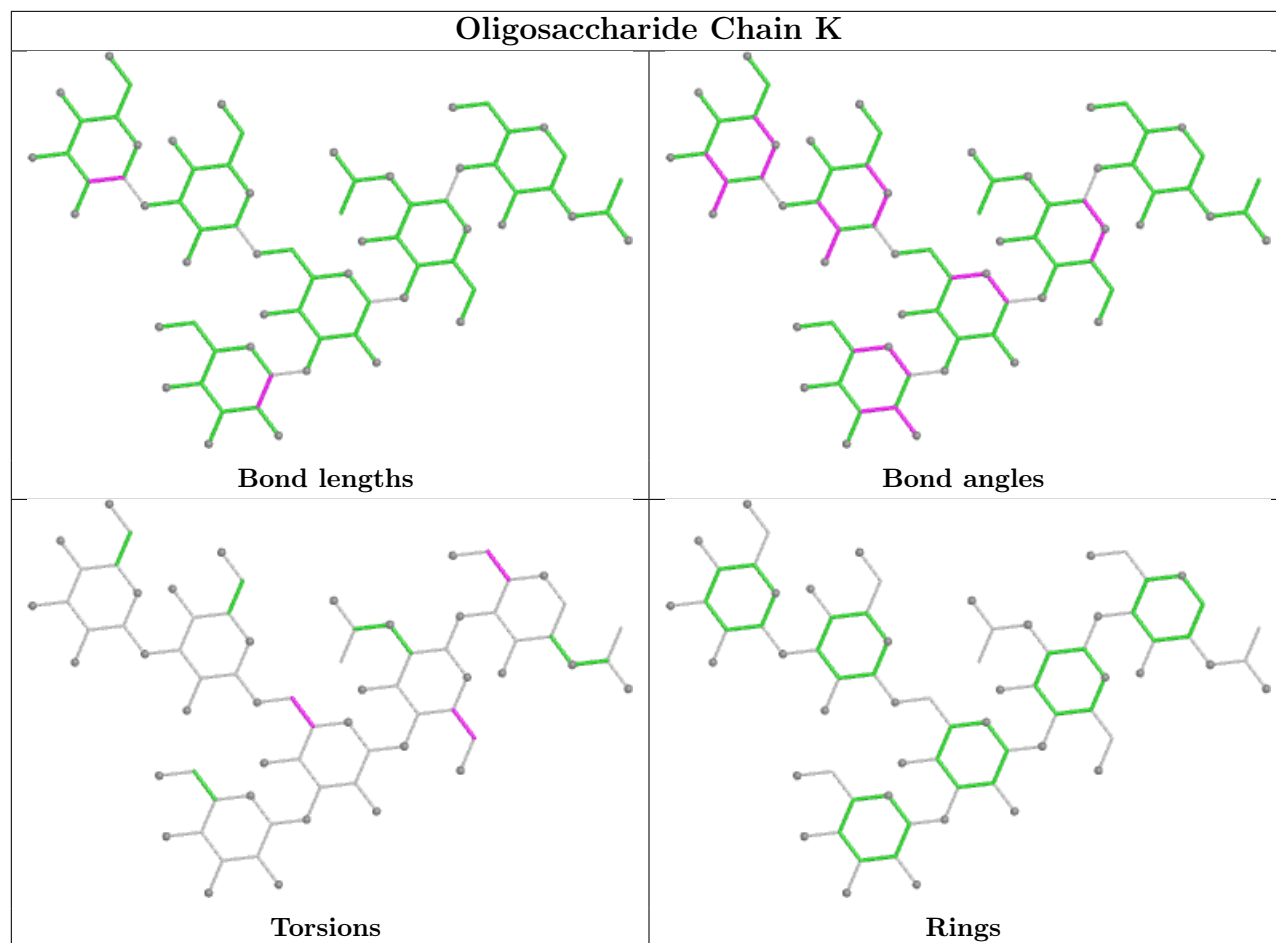
Mol	Chain	Res	Type	Atoms
4	N	1	NAG	O5-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	K	3	BMA	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6

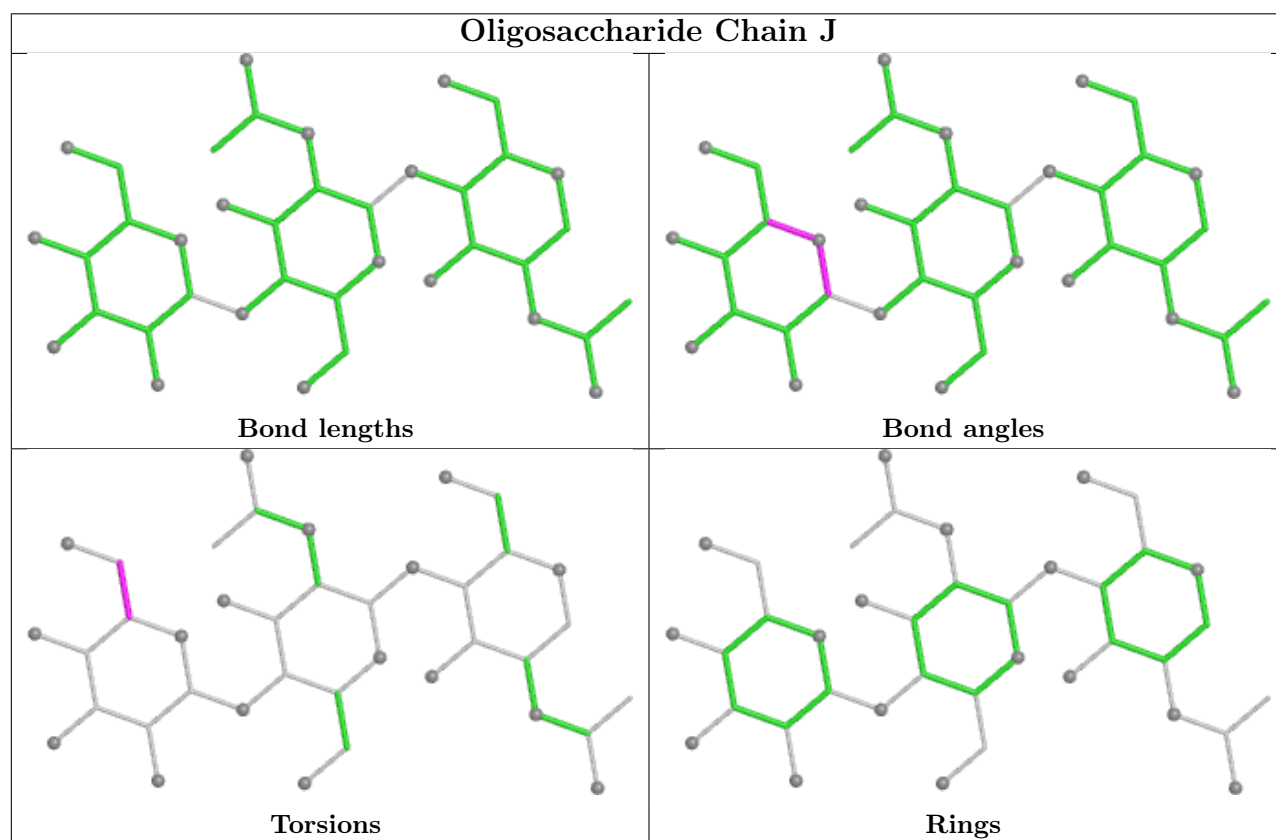
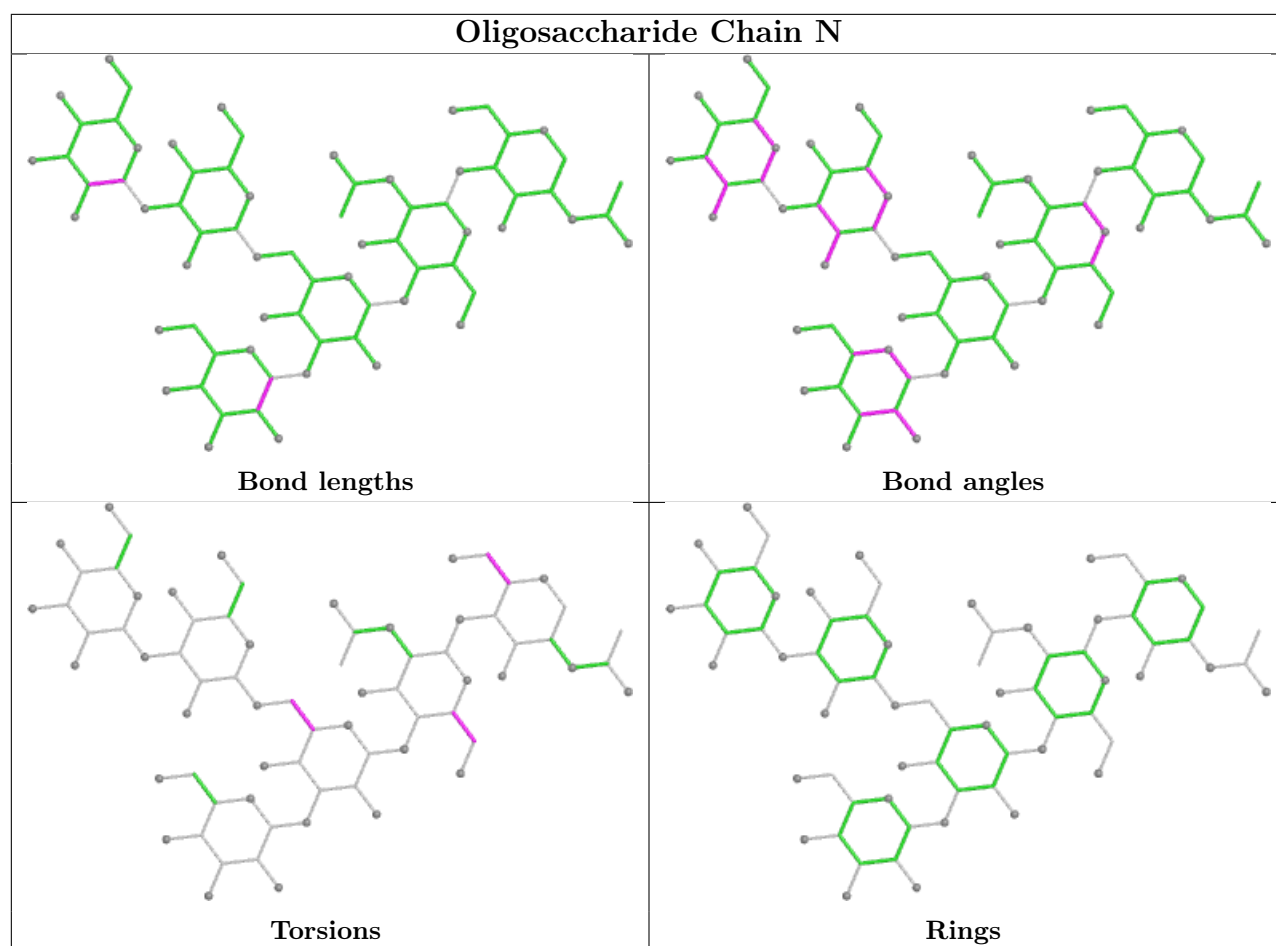
There are no ring outliers.

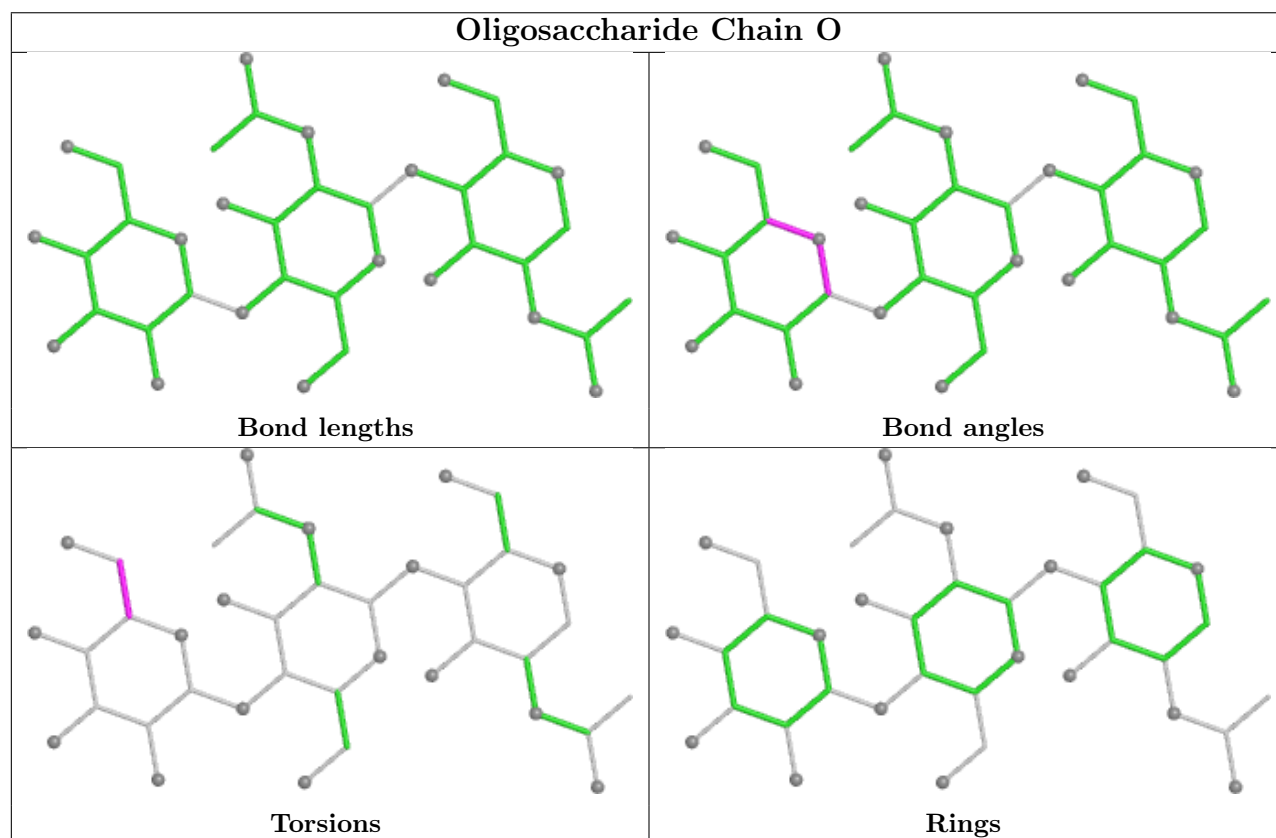
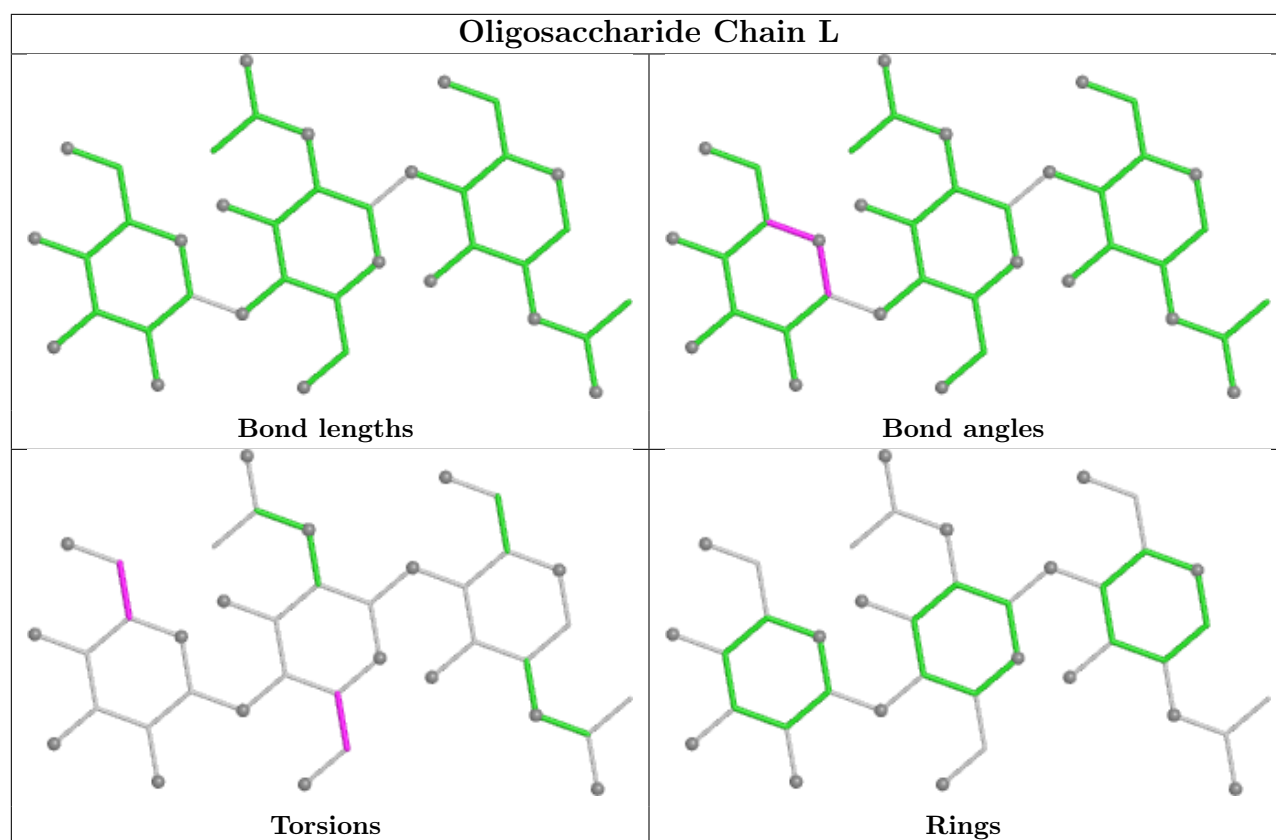
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









## 5.6 Ligand geometry

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	$\# Z  > 2$
6	NAG	B	701	1	14,14,15	0.33	0	17,19,21	0.36	0
6	NAG	A	701	1	14,14,15	0.40	0	17,19,21	0.35	0
6	NAG	E	701	1	14,14,15	0.35	0	17,19,21	0.37	0

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	B	701	1	-	2/6/23/26	0/1/1/1
6	NAG	A	701	1	-	1/6/23/26	0/1/1/1
6	NAG	E	701	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

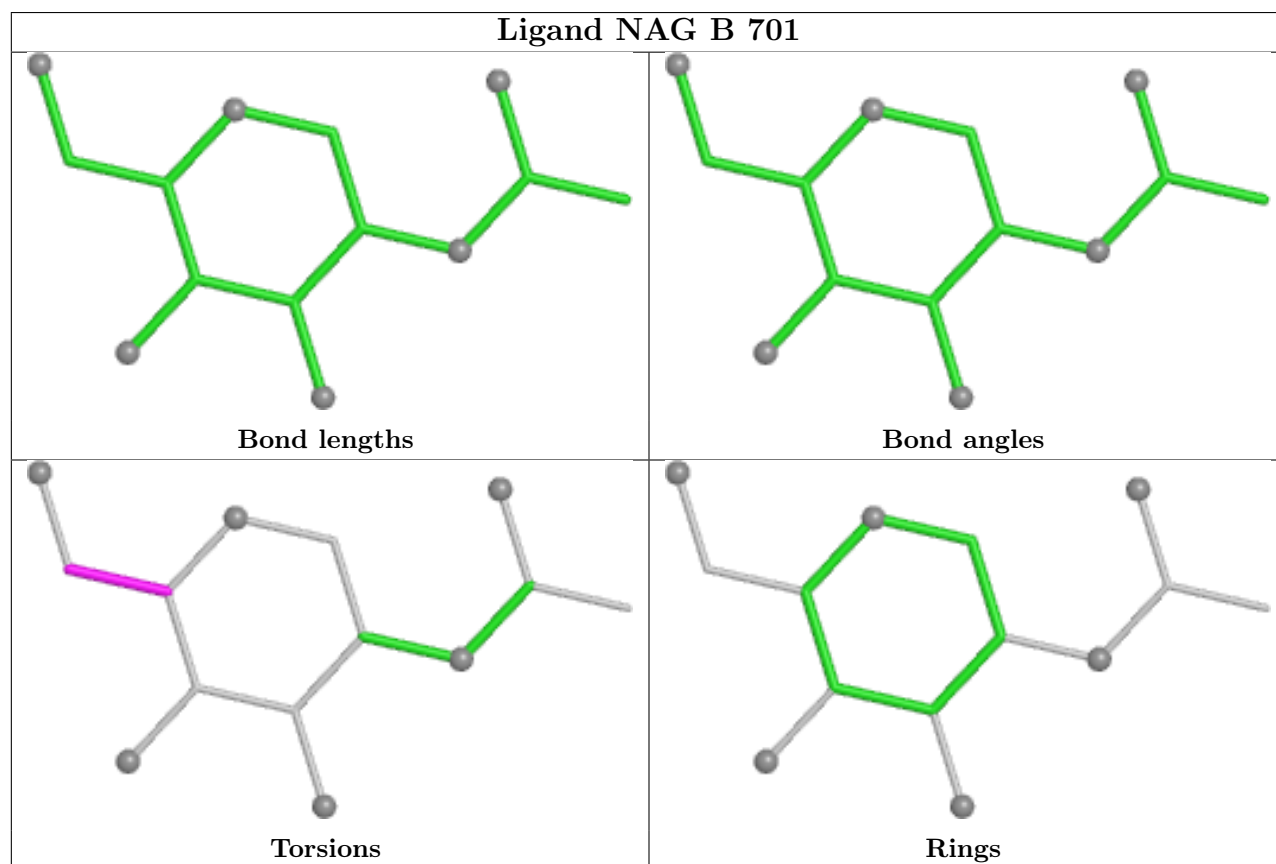
Mol	Chain	Res	Type	Atoms
6	B	701	NAG	O5-C5-C6-O6
6	E	701	NAG	O5-C5-C6-O6
6	A	701	NAG	O5-C5-C6-O6
6	B	701	NAG	C4-C5-C6-O6
6	E	701	NAG	C4-C5-C6-O6

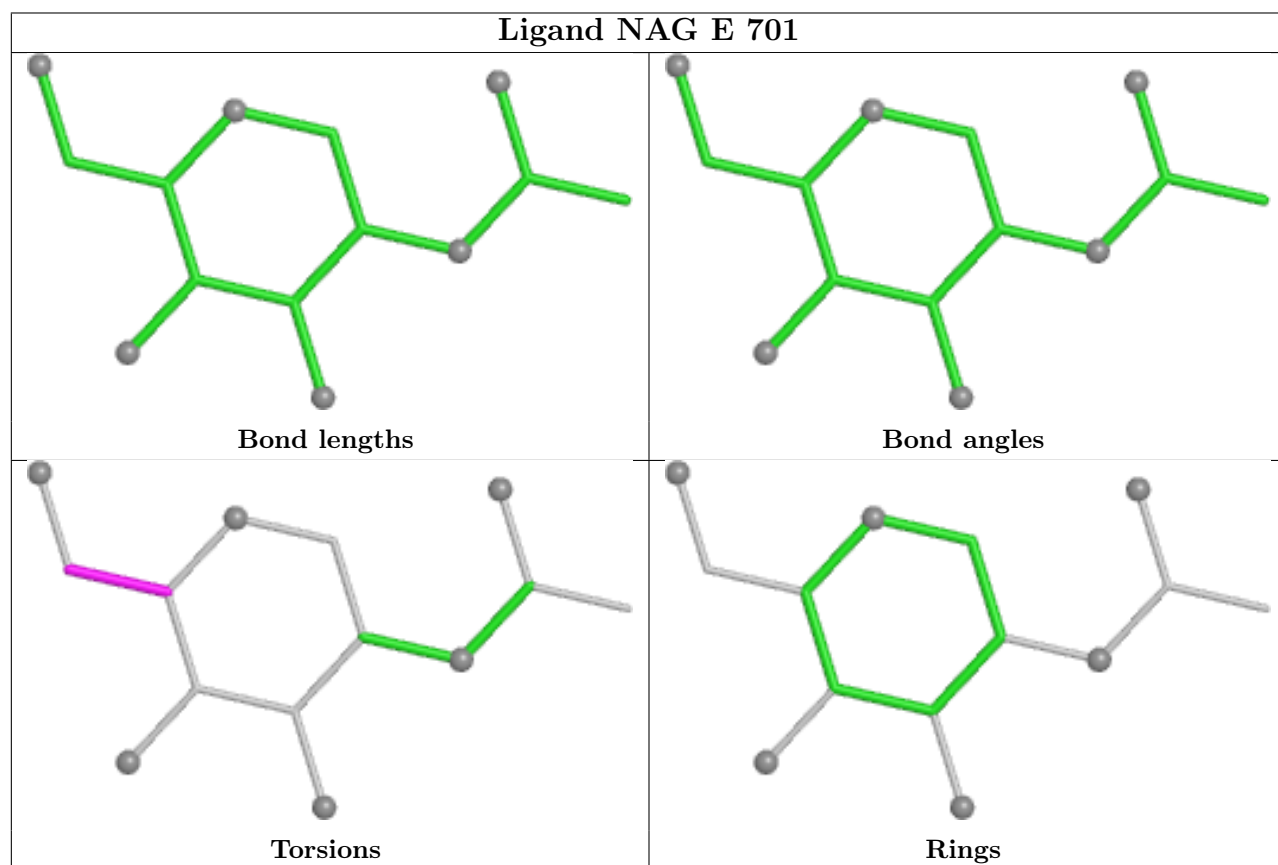
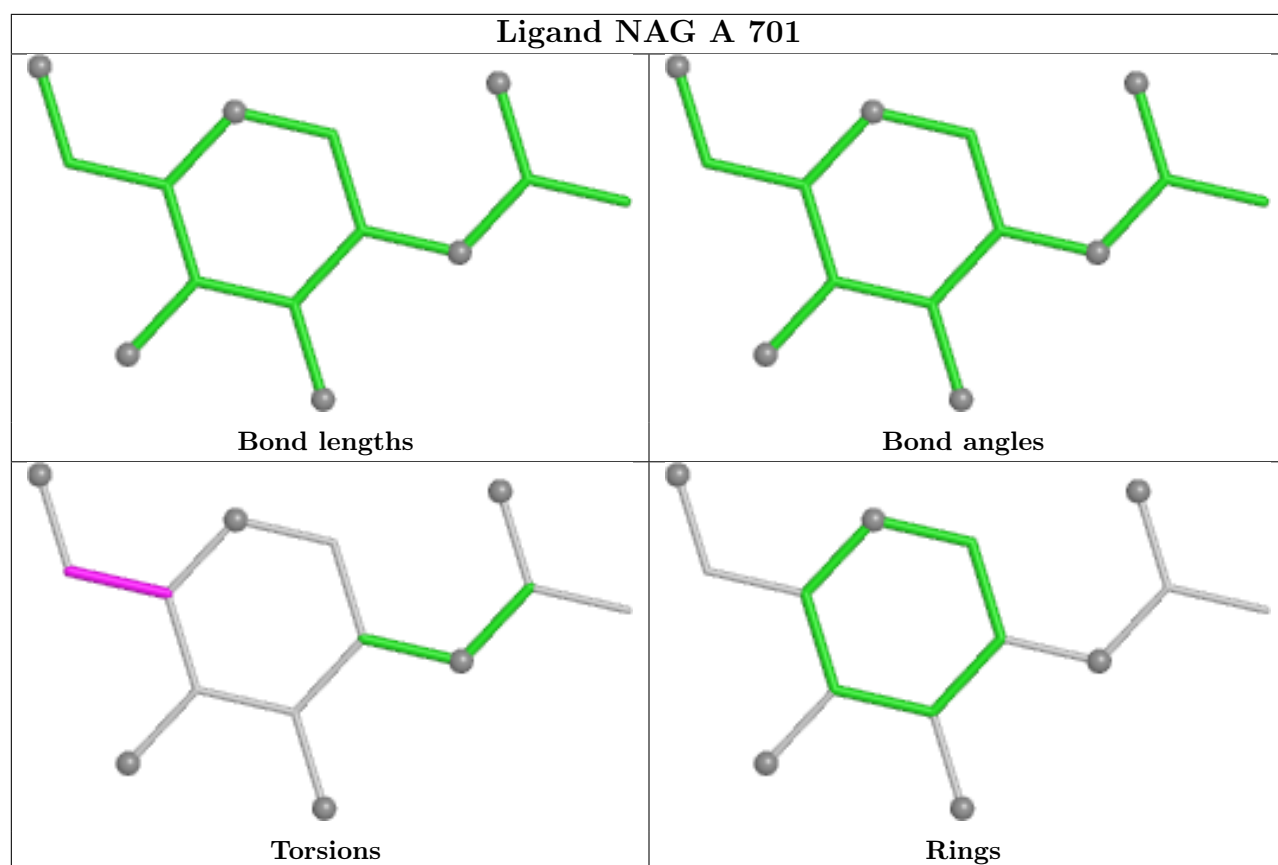
There are no ring outliers.

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 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.





## 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.