



wwPDB EM Validation Summary Report ⓘ

Jul 17, 2025 – 10:09 PM JST

PDB ID : 9JMJ / pdb_00009jmj
EMDB ID : EMD-61604
Title : Cryo-EM structure of the GD-BatCoV (BtCoV/Ii/GD/2014-422) RBD in complex with human DPP4
Authors : Yuan, H.; Xiong, X.
Deposited on : 2024-09-20
Resolution : 3.40 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

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 Phenix2.0rc1
buster-report	: 1.1.7 (2018)
Percentile statistics	: 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	: FAILED
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.44

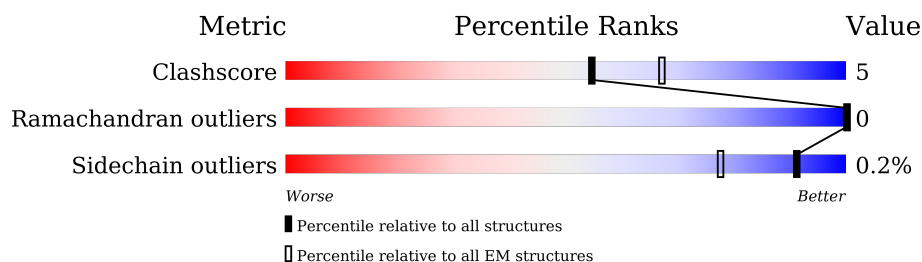
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 ≥ 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	998	63% 10% 27%
1	C	998	65% 8% 27%
2	B	502	32% 7% 60%
3	D	2	50% 50%
3	F	2	100%
3	G	2	100%
3	H	2	100%
3	I	2	100%
3	J	2	100%

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Mol	Chain	Length	Quality of chain
3	K	2	 100%
4	E	3	 67% 33%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13813 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 Dipeptidyl peptidase 4 soluble form,Isoform 1 of Immunoglobulin heavy constant gamma 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	728	Total	C	N	O	S	0	0
			5963	3827	982	1128	26		
1	C	728	Total	C	N	O	S	0	0
			5963	3827	982	1128	26		

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MET	-	initiating methionine	UNP P27487
A	16	PRO	-	expression tag	UNP P27487
A	17	MET	-	expression tag	UNP P27487
A	18	GLY	-	expression tag	UNP P27487
A	19	SER	-	expression tag	UNP P27487
A	20	LEU	-	expression tag	UNP P27487
A	21	GLN	-	expression tag	UNP P27487
A	22	PRO	-	expression tag	UNP P27487
A	23	LEU	-	expression tag	UNP P27487
A	24	ALA	-	expression tag	UNP P27487
A	25	THR	-	expression tag	UNP P27487
A	26	LEU	-	expression tag	UNP P27487
A	27	TYR	-	expression tag	UNP P27487
A	28	LEU	-	expression tag	UNP P27487
A	29	LEU	-	expression tag	UNP P27487
A	30	GLY	-	expression tag	UNP P27487
A	31	MET	-	expression tag	UNP P27487
A	32	LEU	-	expression tag	UNP P27487
A	33	VAL	-	expression tag	UNP P27487
A	34	ALA	-	expression tag	UNP P27487
A	35	SER	-	expression tag	UNP P27487
A	36	VAL	-	expression tag	UNP P27487
A	37	LEU	-	expression tag	UNP P27487
A	38	ALA	-	expression tag	UNP P27487
A	767	ASP	-	linker	UNP P27487

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Chain	Residue	Modelled	Actual	Comment	Reference
A	768	PRO	-	linker	UNP P27487
A	769	LEU	-	linker	UNP P27487
A	770	VAL	-	linker	UNP P27487
A	771	PRO	-	linker	UNP P27487
A	772	ARG	-	linker	UNP P27487
A	773	GLY	-	linker	UNP P27487
A	774	SER	-	linker	UNP P27487
A	775	GLY	-	linker	UNP P27487
A	776	GLY	-	linker	UNP P27487
A	777	GLY	-	linker	UNP P27487
A	778	GLY	-	linker	UNP P27487
A	779	ASP	-	linker	UNP P27487
A	780	PRO	-	linker	UNP P27487
C	15	MET	-	initiating methionine	UNP P27487
C	16	PRO	-	expression tag	UNP P27487
C	17	MET	-	expression tag	UNP P27487
C	18	GLY	-	expression tag	UNP P27487
C	19	SER	-	expression tag	UNP P27487
C	20	LEU	-	expression tag	UNP P27487
C	21	GLN	-	expression tag	UNP P27487
C	22	PRO	-	expression tag	UNP P27487
C	23	LEU	-	expression tag	UNP P27487
C	24	ALA	-	expression tag	UNP P27487
C	25	THR	-	expression tag	UNP P27487
C	26	LEU	-	expression tag	UNP P27487
C	27	TYR	-	expression tag	UNP P27487
C	28	LEU	-	expression tag	UNP P27487
C	29	LEU	-	expression tag	UNP P27487
C	30	GLY	-	expression tag	UNP P27487
C	31	MET	-	expression tag	UNP P27487
C	32	LEU	-	expression tag	UNP P27487
C	33	VAL	-	expression tag	UNP P27487
C	34	ALA	-	expression tag	UNP P27487
C	35	SER	-	expression tag	UNP P27487
C	36	VAL	-	expression tag	UNP P27487
C	37	LEU	-	expression tag	UNP P27487
C	38	ALA	-	expression tag	UNP P27487
C	767	ASP	-	linker	UNP P27487
C	768	PRO	-	linker	UNP P27487
C	769	LEU	-	linker	UNP P27487
C	770	VAL	-	linker	UNP P27487
C	771	PRO	-	linker	UNP P27487

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Chain	Residue	Modelled	Actual	Comment	Reference
C	772	ARG	-	linker	UNP P27487
C	773	GLY	-	linker	UNP P27487
C	774	SER	-	linker	UNP P27487
C	775	GLY	-	linker	UNP P27487
C	776	GLY	-	linker	UNP P27487
C	777	GLY	-	linker	UNP P27487
C	778	GLY	-	linker	UNP P27487
C	779	ASP	-	linker	UNP P27487
C	780	PRO	-	linker	UNP P27487

- Molecule 2 is a protein called Spike glycoprotein,Isoform 1 of Immunoglobulin heavy constant gamma 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	200	Total	C	N	O	S	0	0
			1540	981	247	299	13		

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	355	MET	-	initiating methionine	UNP A0A2R4KP93
B	356	ARG	-	expression tag	UNP A0A2R4KP93
B	357	LEU	-	expression tag	UNP A0A2R4KP93
B	358	SER	-	expression tag	UNP A0A2R4KP93
B	359	VAL	-	expression tag	UNP A0A2R4KP93
B	360	CYS	-	expression tag	UNP A0A2R4KP93
B	361	LEU	-	expression tag	UNP A0A2R4KP93
B	362	LEU	-	expression tag	UNP A0A2R4KP93
B	363	MET	-	expression tag	UNP A0A2R4KP93
B	364	PHE	-	expression tag	UNP A0A2R4KP93
B	365	LEU	-	expression tag	UNP A0A2R4KP93
B	366	LEU	-	expression tag	UNP A0A2R4KP93
B	367	THR	-	expression tag	UNP A0A2R4KP93
B	368	PRO	-	expression tag	UNP A0A2R4KP93
B	369	ILE	-	expression tag	UNP A0A2R4KP93
B	370	LYS	-	expression tag	UNP A0A2R4KP93
B	611	ASP	-	linker	UNP A0A2R4KP93
B	612	PRO	-	linker	UNP A0A2R4KP93
B	613	LEU	-	linker	UNP A0A2R4KP93
B	614	VAL	-	linker	UNP A0A2R4KP93
B	615	PRO	-	linker	UNP A0A2R4KP93
B	616	ARG	-	linker	UNP A0A2R4KP93

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Chain	Residue	Modelled	Actual	Comment	Reference
B	617	GLY	-	linker	UNP A0A2R4KP93
B	618	SER	-	linker	UNP A0A2R4KP93
B	619	GLY	-	linker	UNP A0A2R4KP93
B	620	GLY	-	linker	UNP A0A2R4KP93
B	621	GLY	-	linker	UNP A0A2R4KP93
B	622	GLY	-	linker	UNP A0A2R4KP93
B	623	ASP	-	linker	UNP A0A2R4KP93
B	624	PRO	-	linker	UNP A0A2R4KP93

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



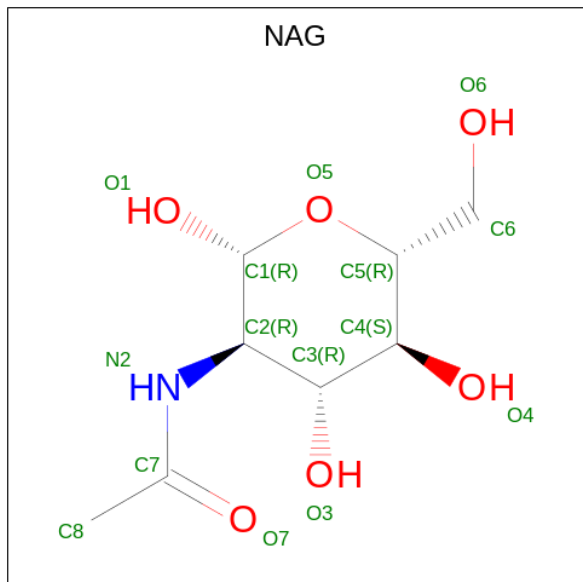
Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 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
4	E	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

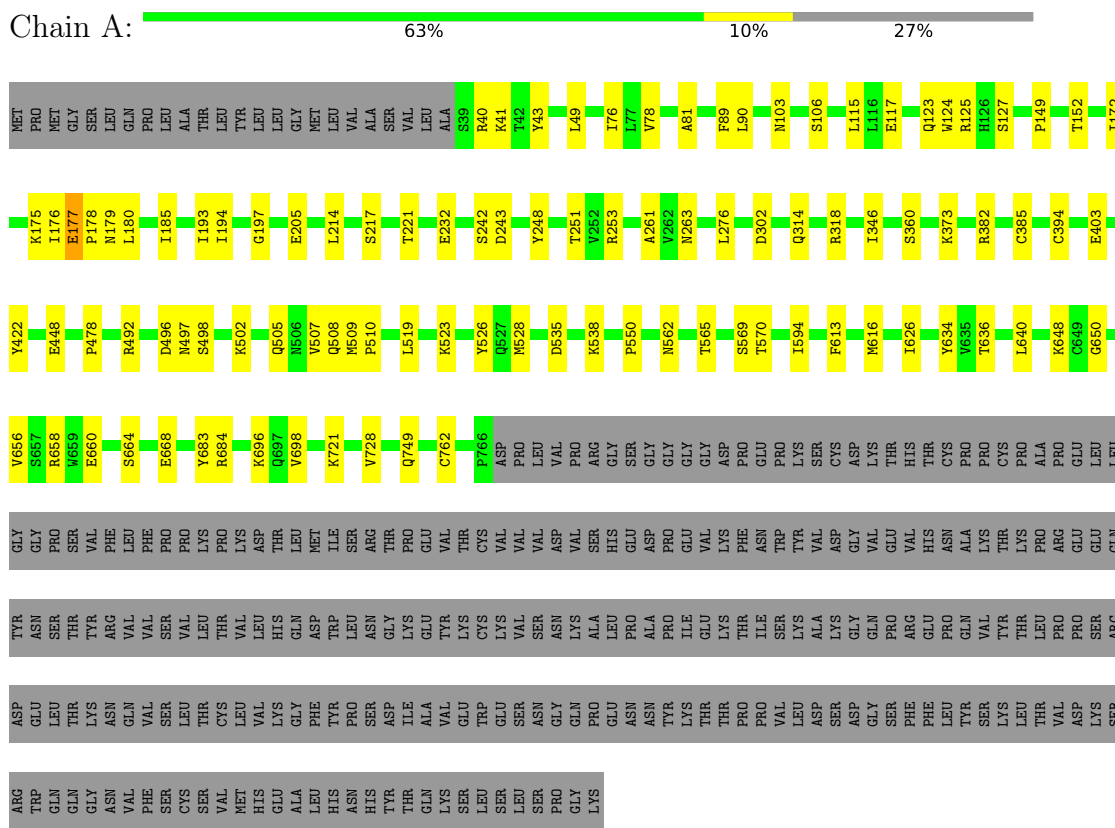


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	

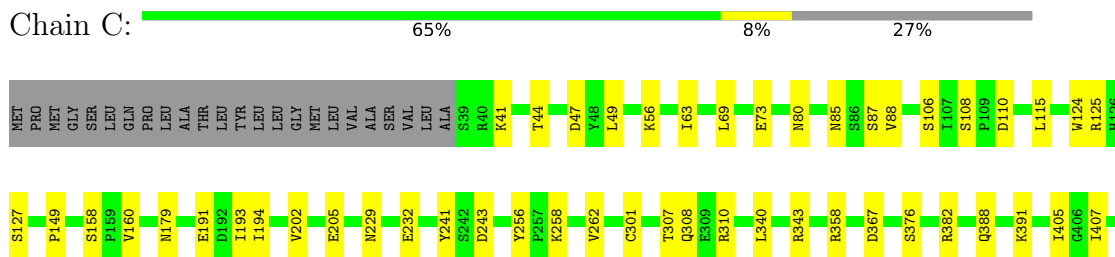
3 Residue-property plots

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: Dipeptidyl peptidase 4 soluble form,Isoform 1 of Immunoglobulin heavy constant gamma 1



- Molecule 1: Dipeptidyl peptidase 4 soluble form,Isoform 1 of Immunoglobulin heavy constant gamma 1





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%



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

Chain E:  67% 33%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72715	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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: NAG, BMA

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	0.14	0/6135	0.35	0/8344
1	C	0.13	0/6135	0.34	0/8344
2	B	0.24	0/1576	0.52	2/2141 (0.1%)
All	All	0.15	0/13846	0.37	2/18829 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	551	GLN	N-CA-C	-9.03	99.31	110.41
2	B	552	LEU	N-CA-C	-5.65	106.33	113.23

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	5963	0	5677	62	0
1	C	5963	0	5677	48	0
2	B	1540	0	1485	24	0
3	D	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
4	E	39	0	34	1	0
5	A	56	0	52	1	0
5	C	56	0	52	2	0
All	All	13813	0	13152	131	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 5.

The worst 5 of 131 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)
1:A:172:ILE:HD11	1:A:197:GLY:HA3	1.77	0.65
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.80	0.63
2:B:461:GLN:HB2	2:B:464:SER:HB3	1.80	0.63
1:A:660:GLU:OE2	1:A:684:ARG:NH1	2.35	0.60
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.84	0.59

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	726/998 (73%)	705 (97%)	21 (3%)	0	100	100
1	C	726/998 (73%)	699 (96%)	27 (4%)	0	100	100
2	B	194/502 (39%)	182 (94%)	12 (6%)	0	100	100
All	All	1646/2498 (66%)	1586 (96%)	60 (4%)	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	653/896 (73%)	652 (100%)	1 (0%)	92	96
1	C	653/896 (73%)	652 (100%)	1 (0%)	92	96
2	B	177/452 (39%)	176 (99%)	1 (1%)	84	90
All	All	1483/2244 (66%)	1480 (100%)	3 (0%)	91	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	GLU
1	C	202	VAL
2	B	429	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	126	HIS
1	C	586	GLN
2	B	491	ASN
1	C	595	ASN
1	A	430	ASN

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

17 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	D	1	1,3	14,14,15	0.66	0	17,19,21	1.96	2 (11%)
3	NAG	D	2	3	14,14,15	0.26	0	17,19,21	0.48	0
4	NAG	E	1	1,4	14,14,15	0.26	0	17,19,21	0.46	0
4	NAG	E	2	4	14,14,15	0.23	0	17,19,21	0.46	0
4	BMA	E	3	4	11,11,12	0.64	0	15,15,17	0.78	0
3	NAG	F	1	1,3	14,14,15	0.22	0	17,19,21	0.39	0
3	NAG	F	2	3	14,14,15	0.30	0	17,19,21	0.43	0
3	NAG	G	1	1,3	14,14,15	0.24	0	17,19,21	0.50	0
3	NAG	G	2	3	14,14,15	0.31	0	17,19,21	0.40	0
3	NAG	H	1	1,3	14,14,15	0.21	0	17,19,21	0.38	0
3	NAG	H	2	3	14,14,15	0.36	0	17,19,21	0.40	0
3	NAG	I	1	1,3	14,14,15	0.34	0	17,19,21	0.56	0
3	NAG	I	2	3	14,14,15	0.30	0	17,19,21	0.42	0
3	NAG	J	1	1,3	14,14,15	0.24	0	17,19,21	0.47	0
3	NAG	J	2	3	14,14,15	0.26	0	17,19,21	0.41	0
3	NAG	K	1	1,3	14,14,15	0.24	0	17,19,21	0.48	0
3	NAG	K	2	3	14,14,15	0.27	0	17,19,21	0.46	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
3	NAG	D	1	1,3	-	5/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	NAG	C2-N2-C7	6.85	132.66	122.90
3	D	1	NAG	C1-C2-N2	3.18	115.92	110.49

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

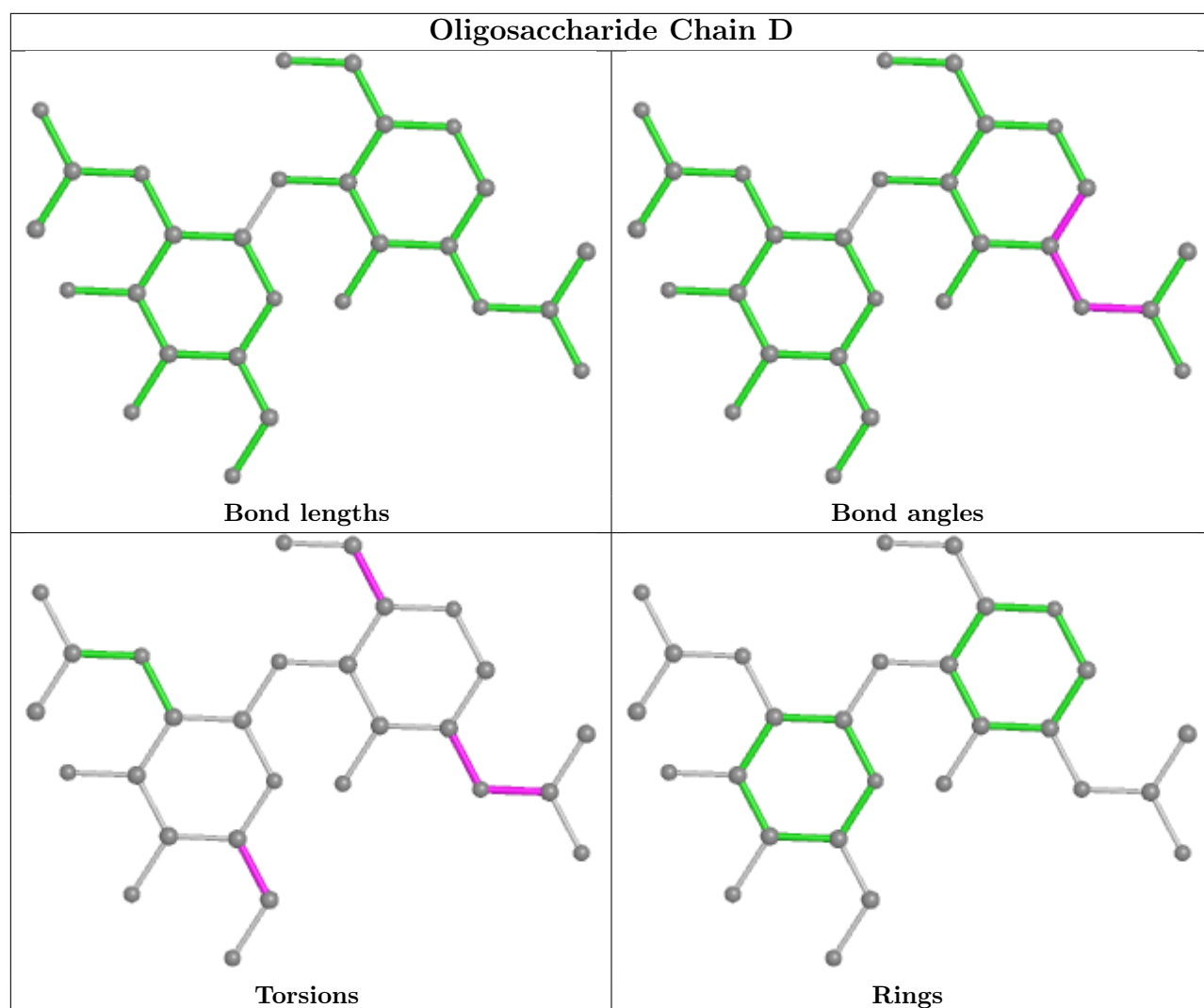
Mol	Chain	Res	Type	Atoms
3	D	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6

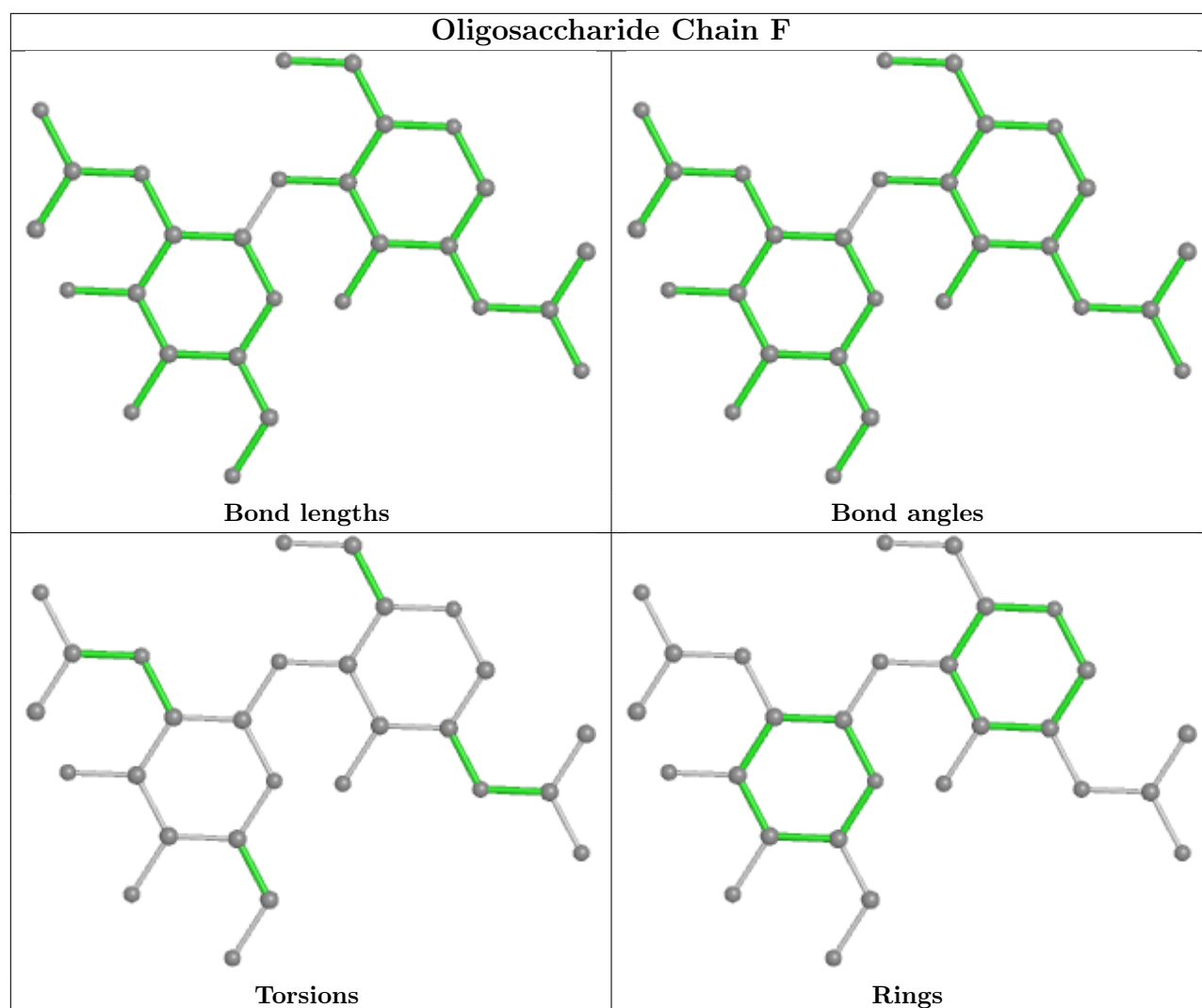
There are no ring outliers.

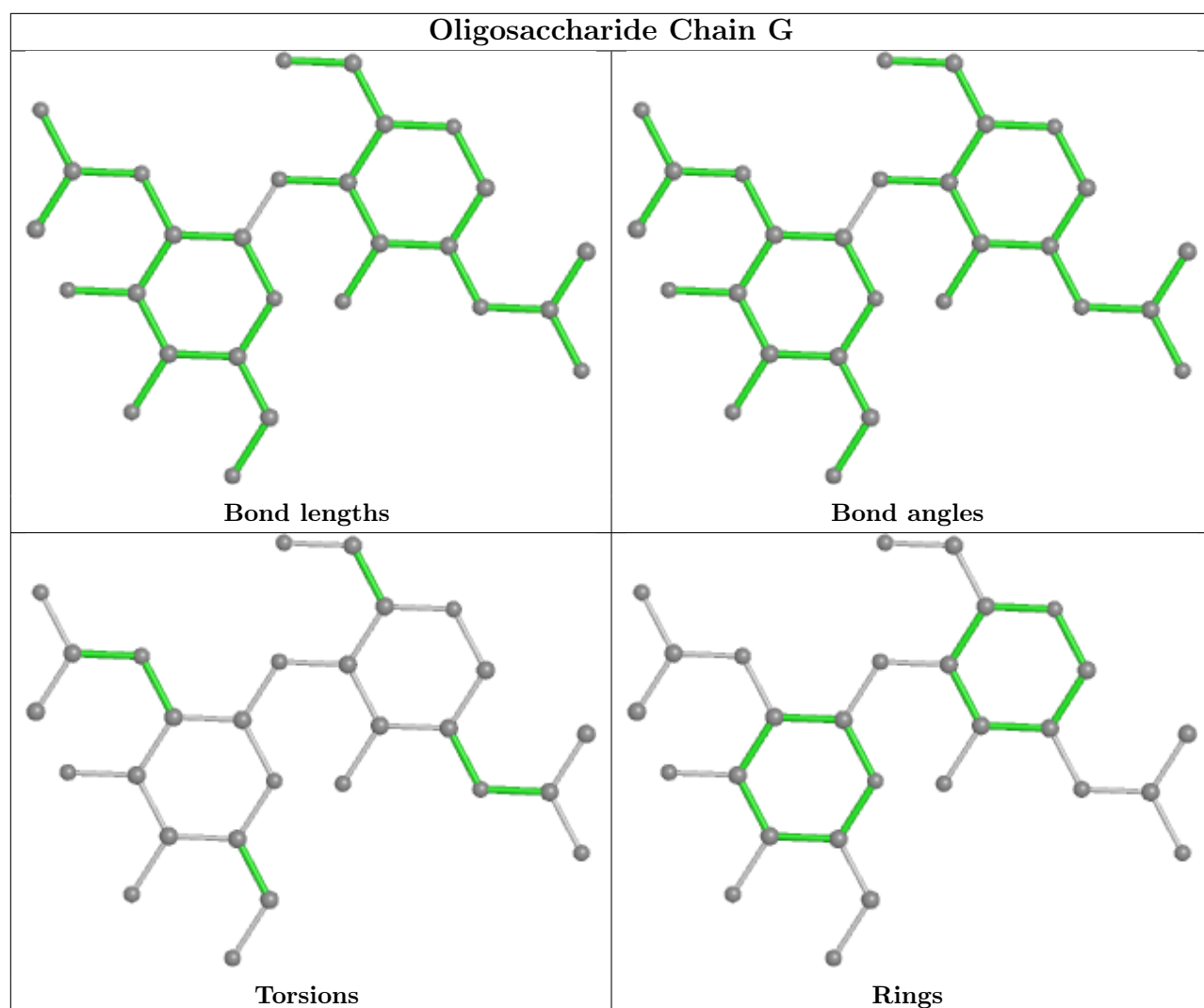
1 monomer is involved in 1 short contact:

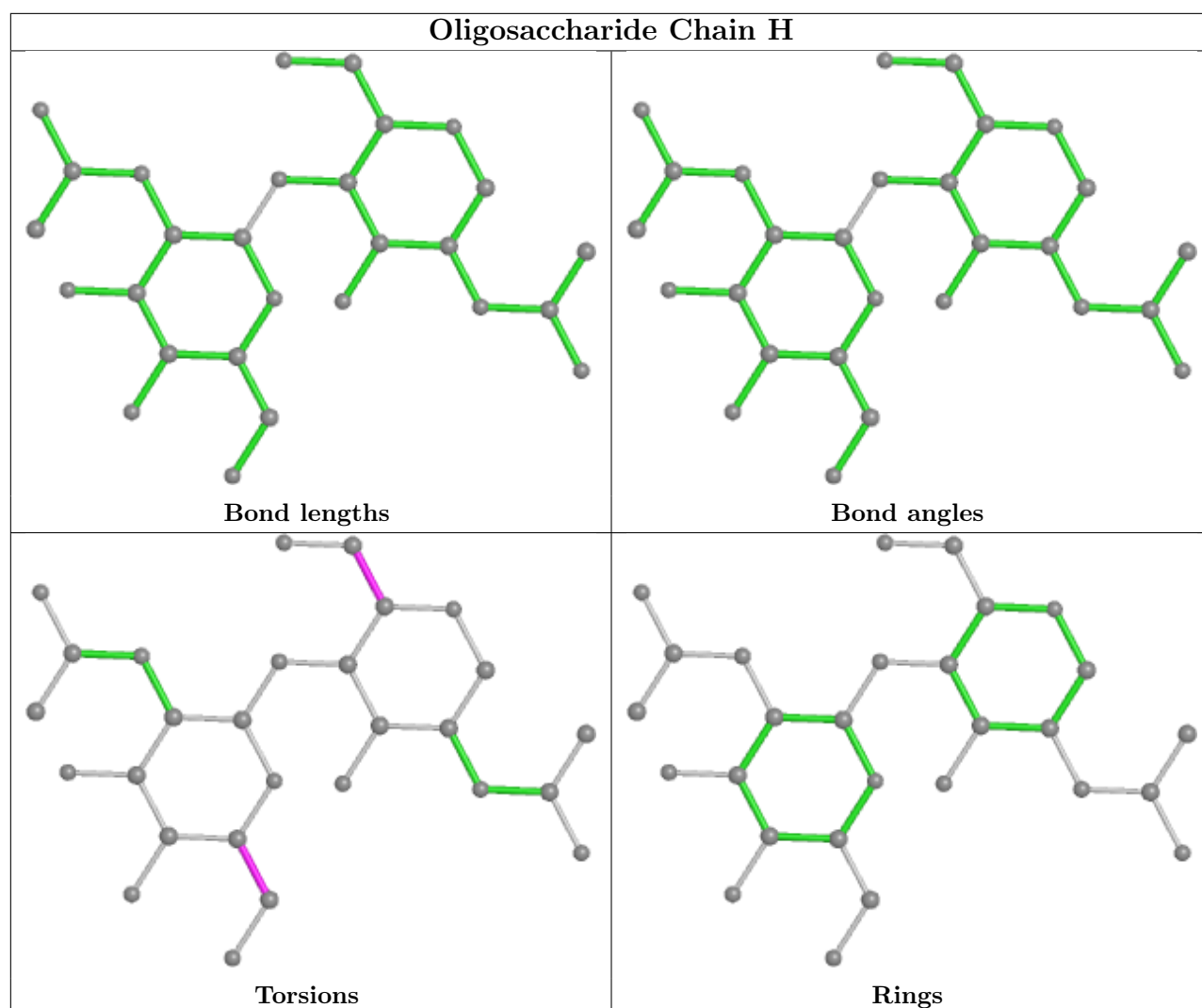
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	1	0

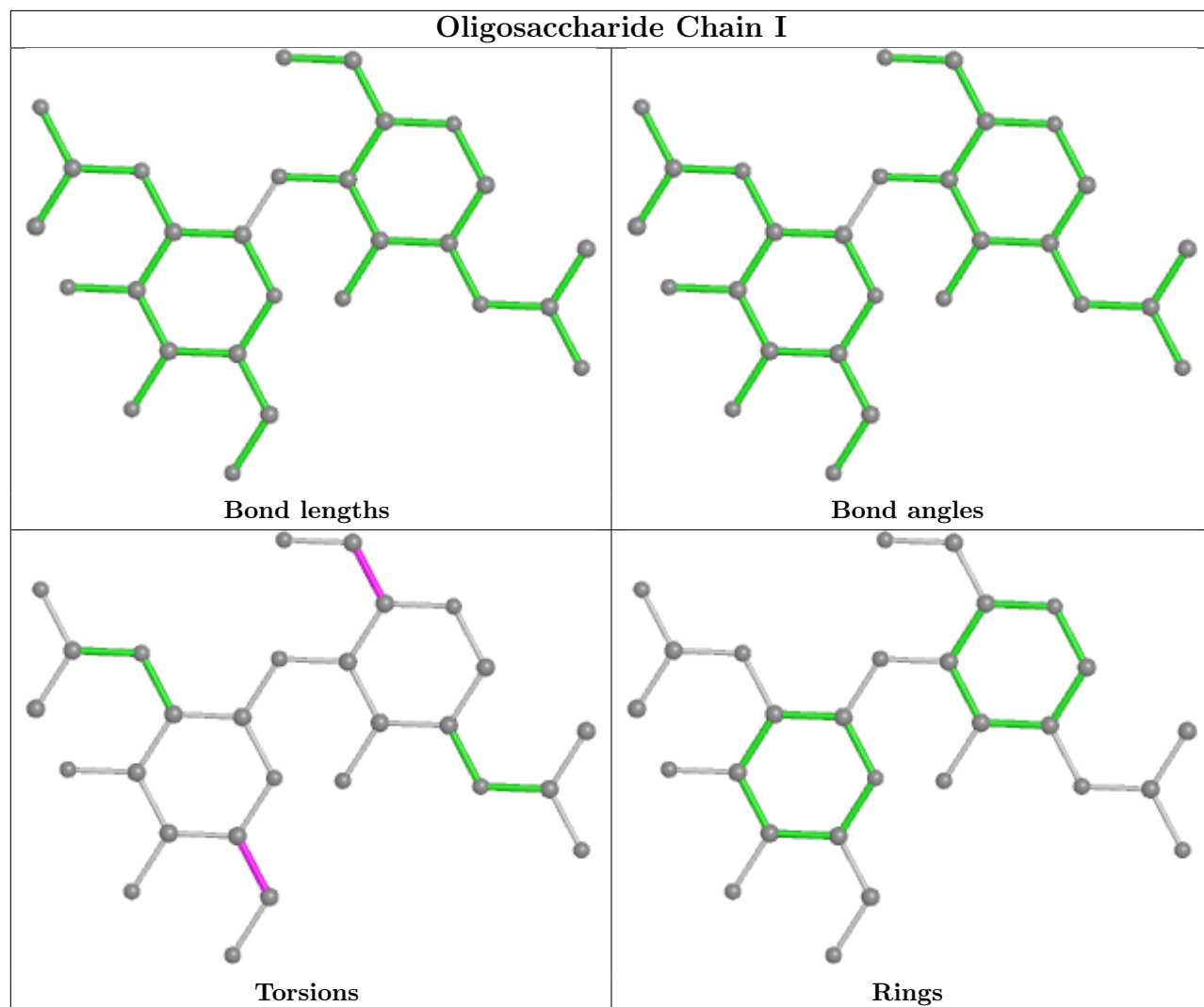
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

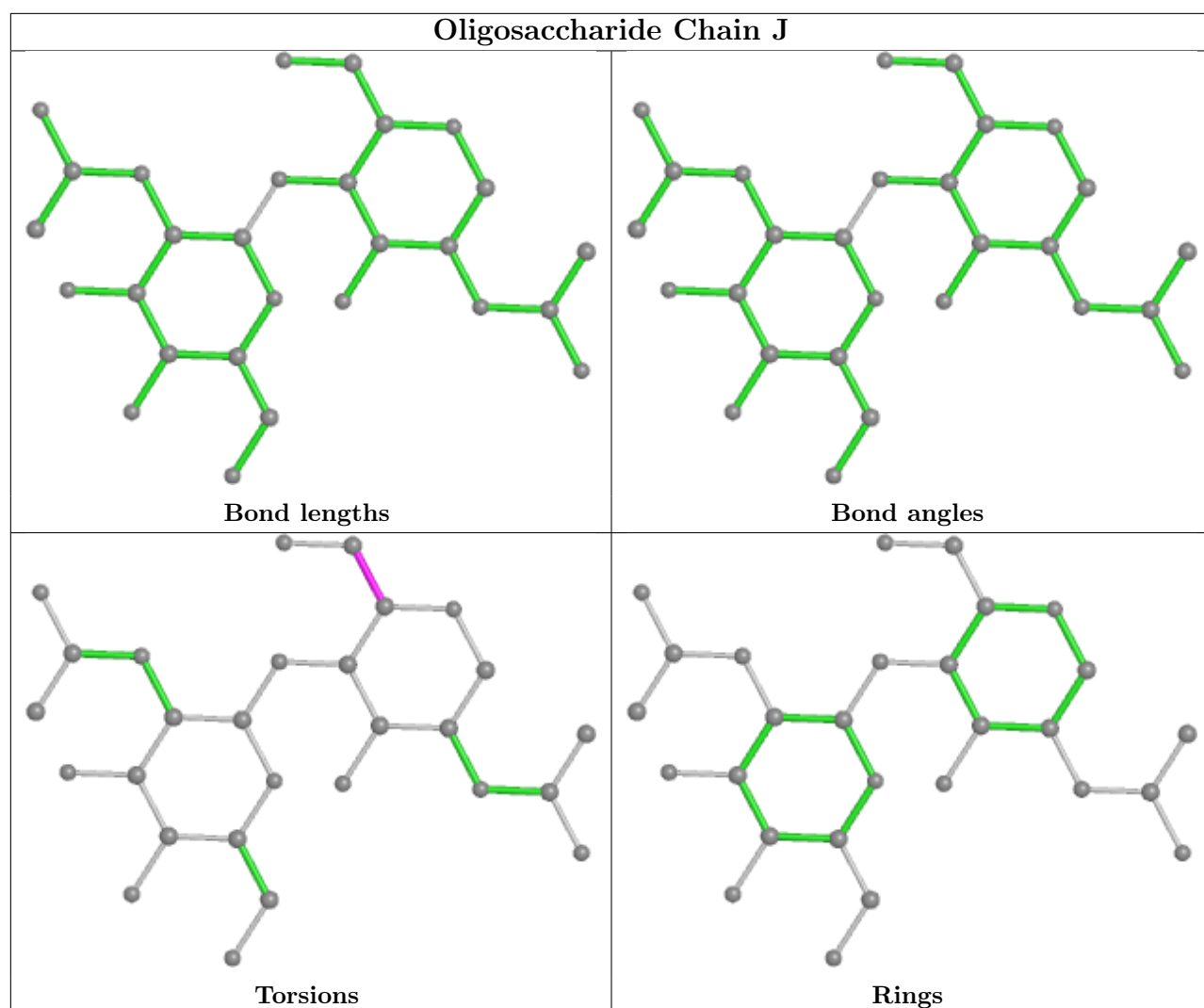


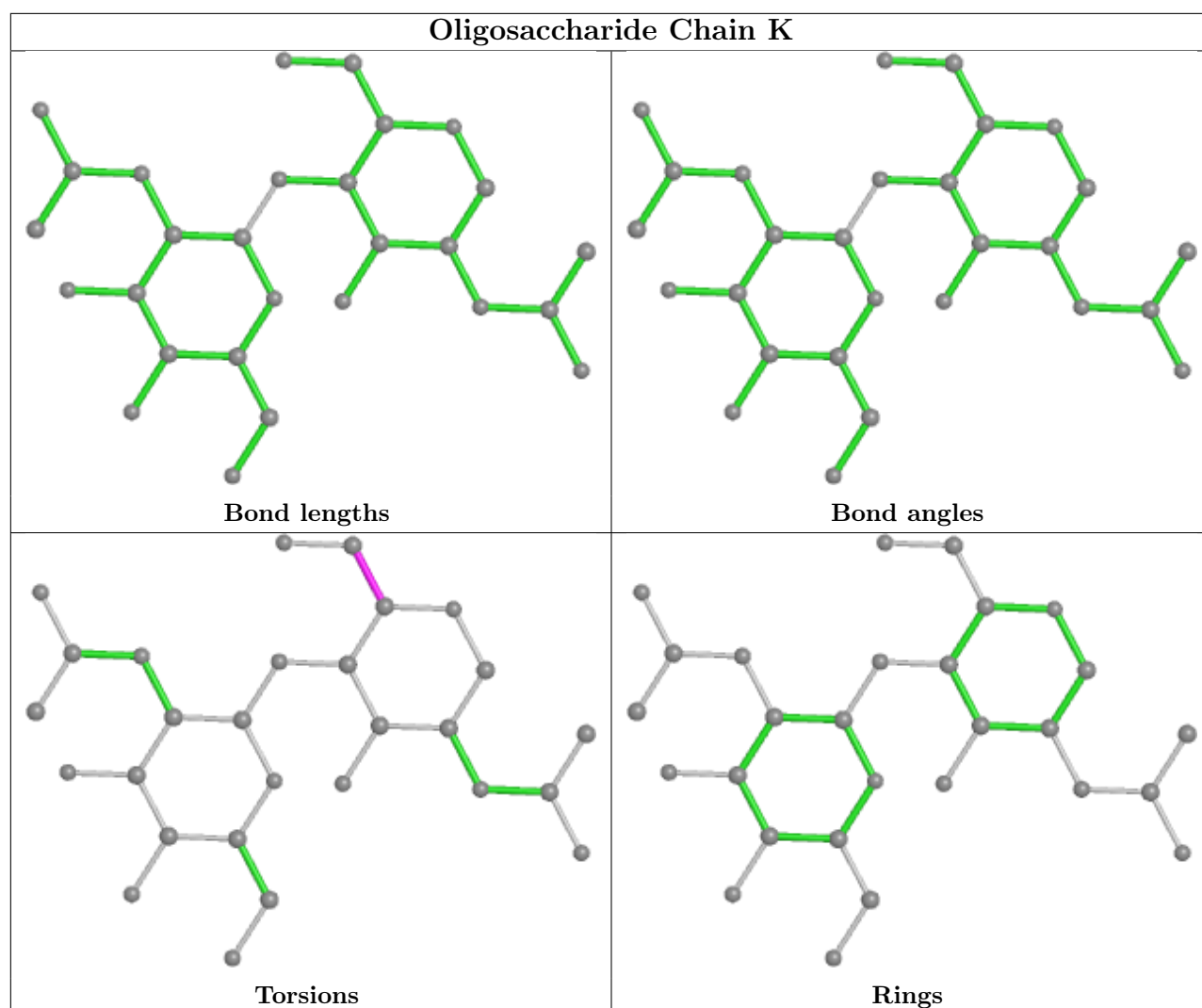


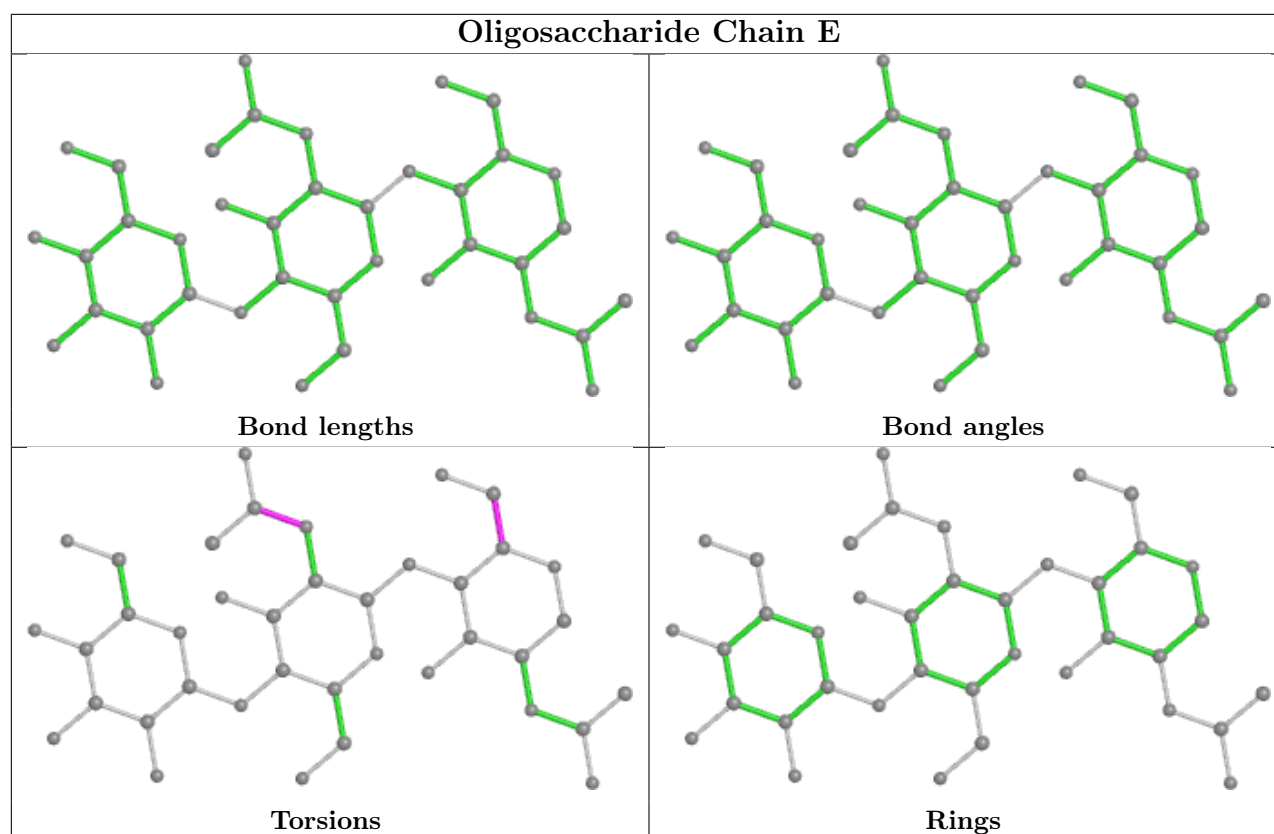












5.6 Ligand geometry [i](#)

8 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	A	1101	1	14,14,15	0.40	0	17,19,21	0.84	1 (5%)
5	NAG	A	1102	1	14,14,15	0.28	0	17,19,21	0.50	0
5	NAG	C	1101	1	14,14,15	0.31	0	17,19,21	0.48	0
5	NAG	A	1104	1	14,14,15	0.27	0	17,19,21	0.47	0
5	NAG	C	1104	1	14,14,15	0.22	0	17,19,21	0.45	0
5	NAG	C	1102	1	14,14,15	0.26	0	17,19,21	0.57	0
5	NAG	A	1103	1	14,14,15	0.27	0	17,19,21	0.44	0
5	NAG	C	1103	1	14,14,15	0.26	0	17,19,21	0.50	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
5	NAG	A	1101	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1102	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1101	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1104	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1104	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1102	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1103	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1103	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1101	NAG	C2-N2-C7	2.44	126.37	122.90

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1101	NAG	O5-C5-C6-O6
5	C	1103	NAG	O5-C5-C6-O6
5	A	1104	NAG	O5-C5-C6-O6
5	C	1102	NAG	O5-C5-C6-O6
5	C	1104	NAG	O5-C5-C6-O6

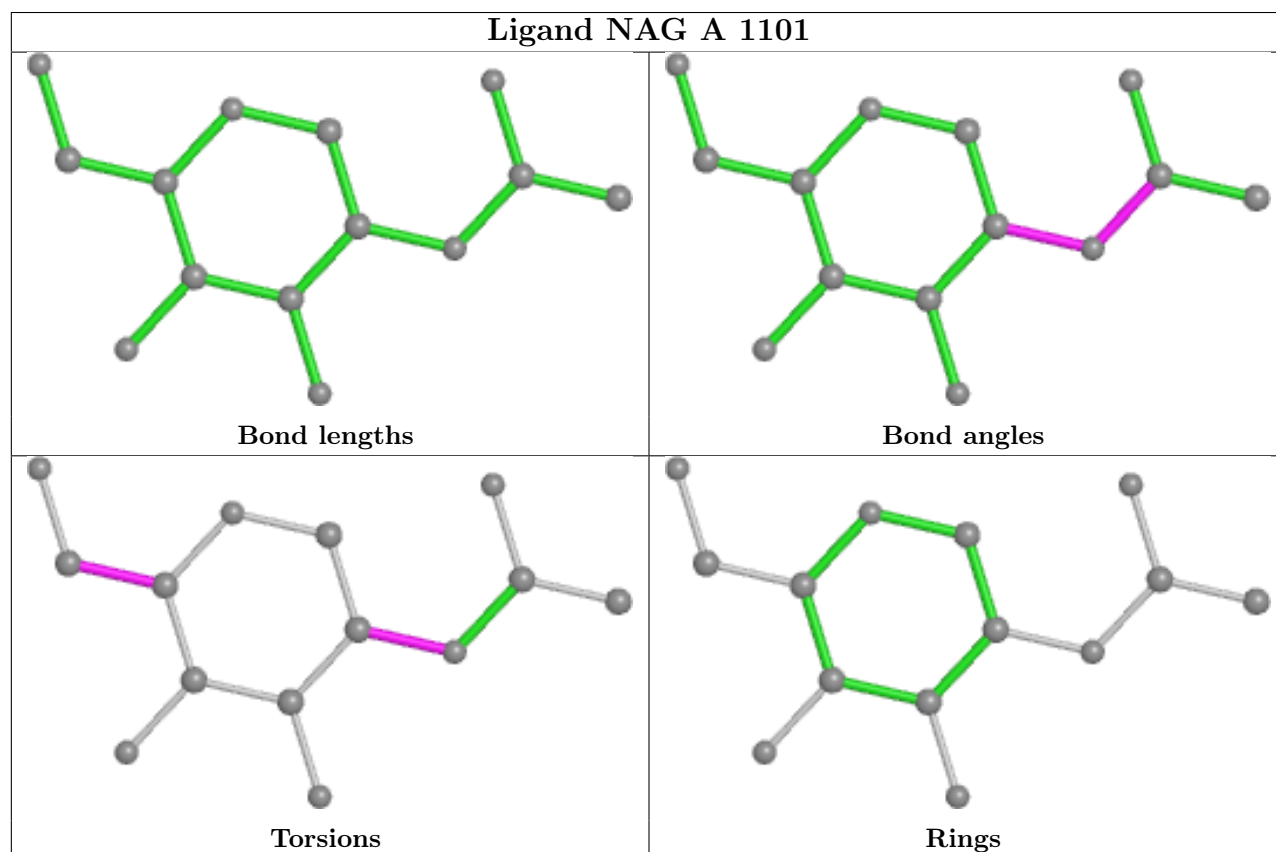
There are no ring outliers.

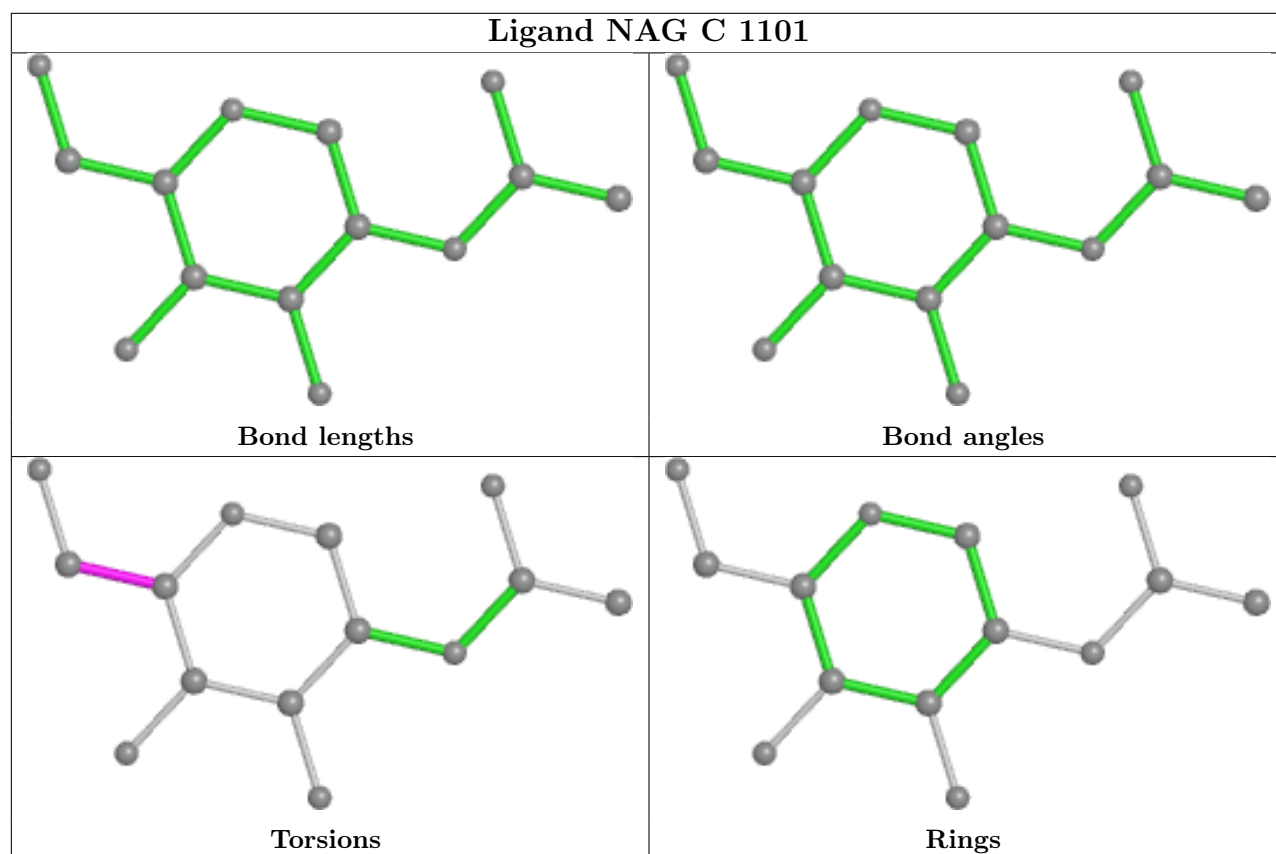
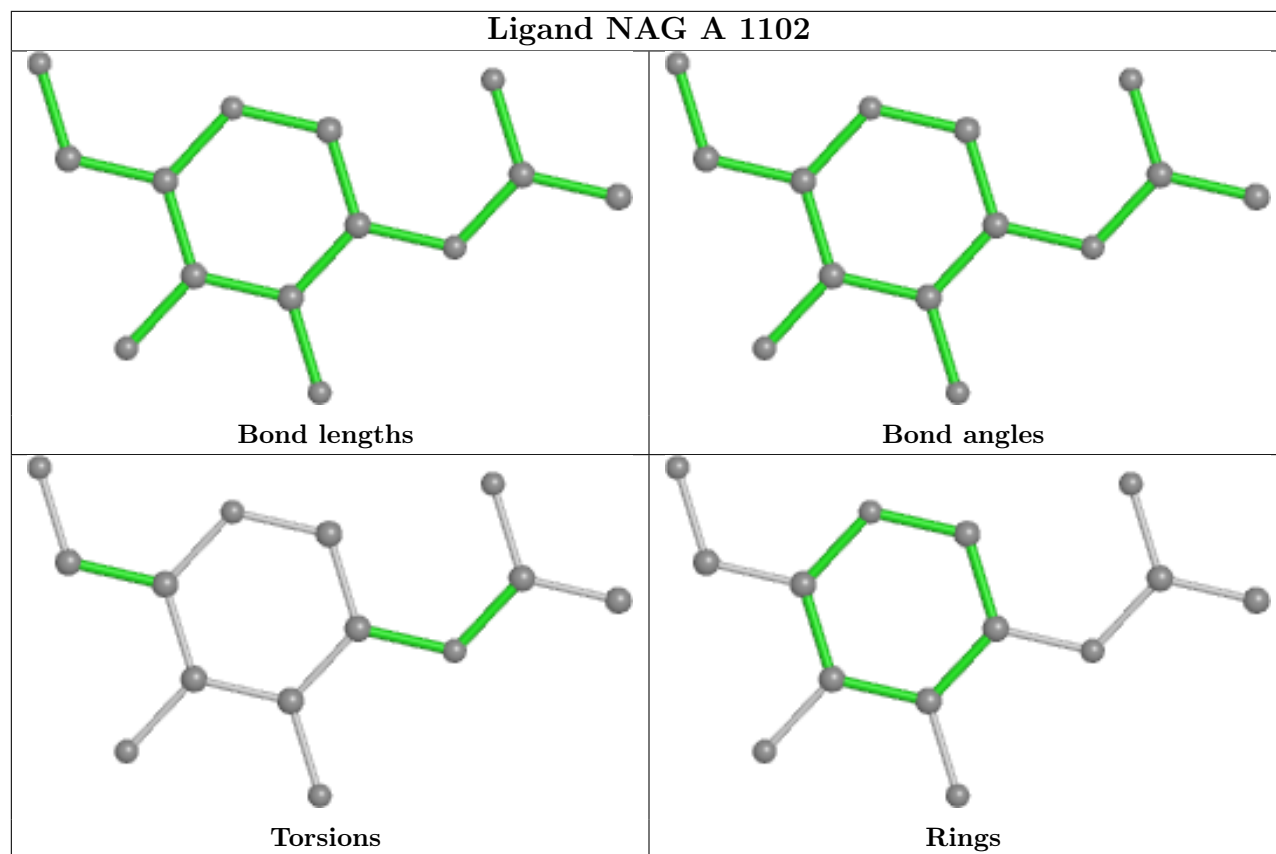
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1101	NAG	1	0
5	C	1104	NAG	1	0
5	A	1103	NAG	1	0

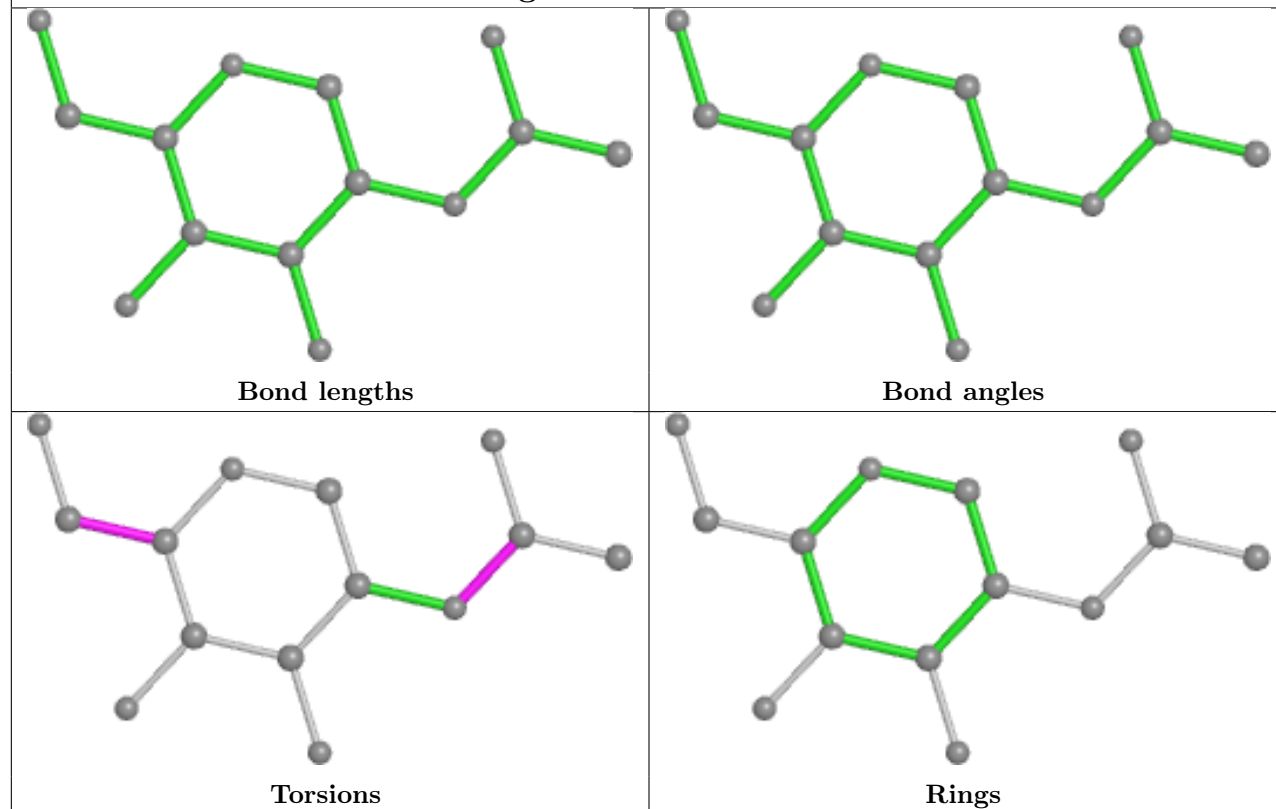
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

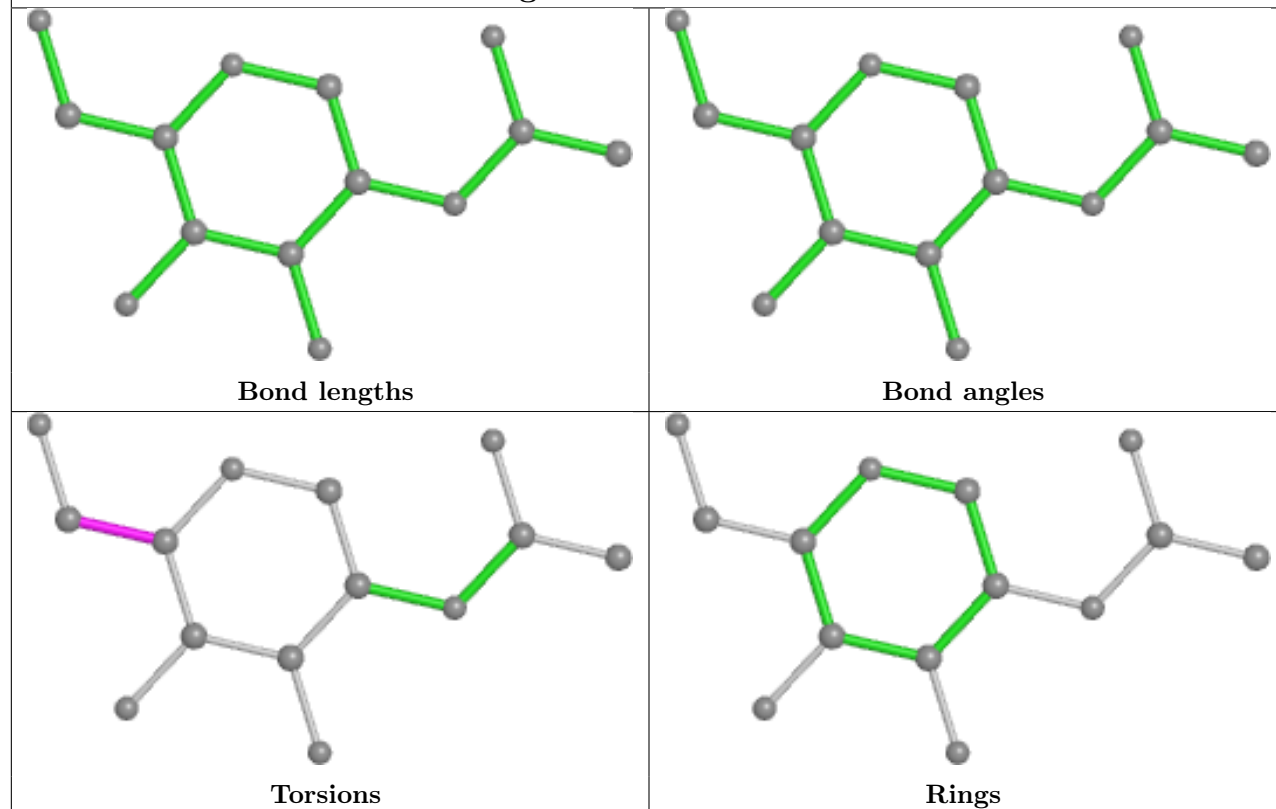




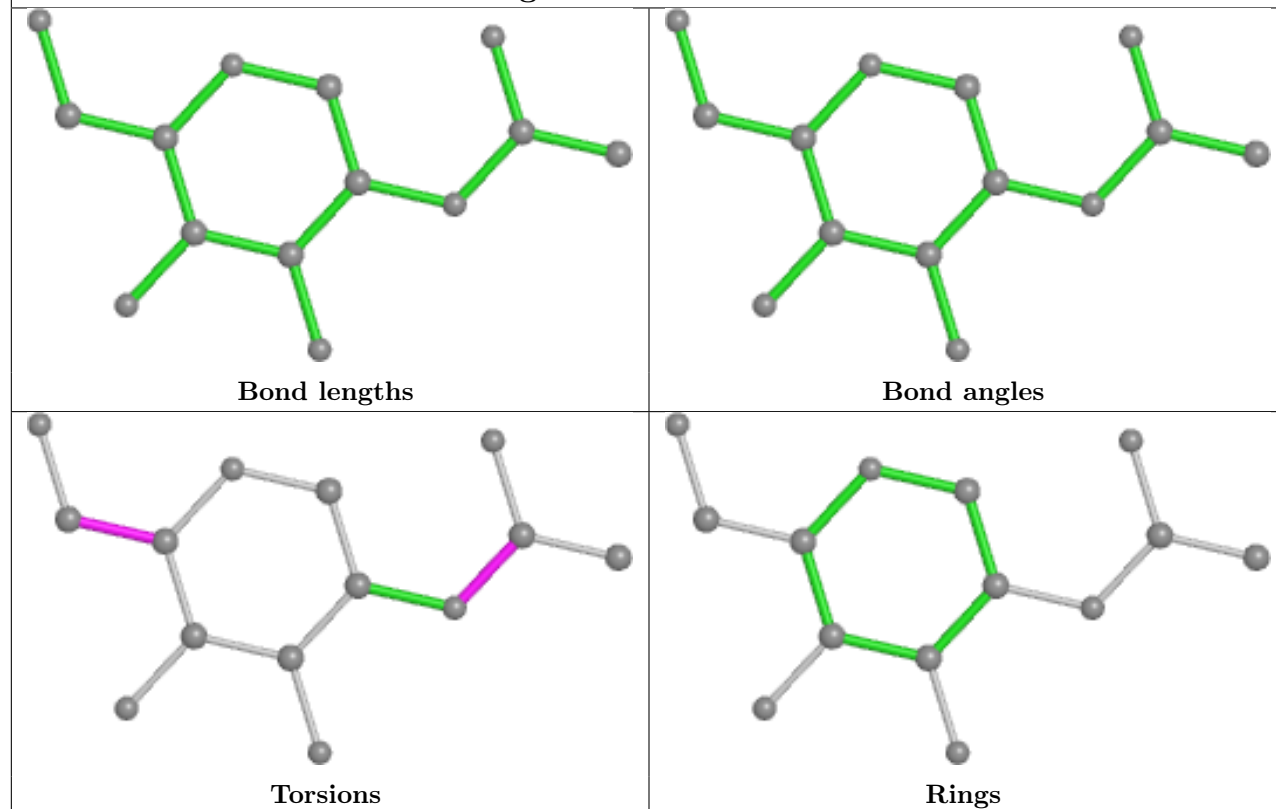
Ligand NAG A 1104



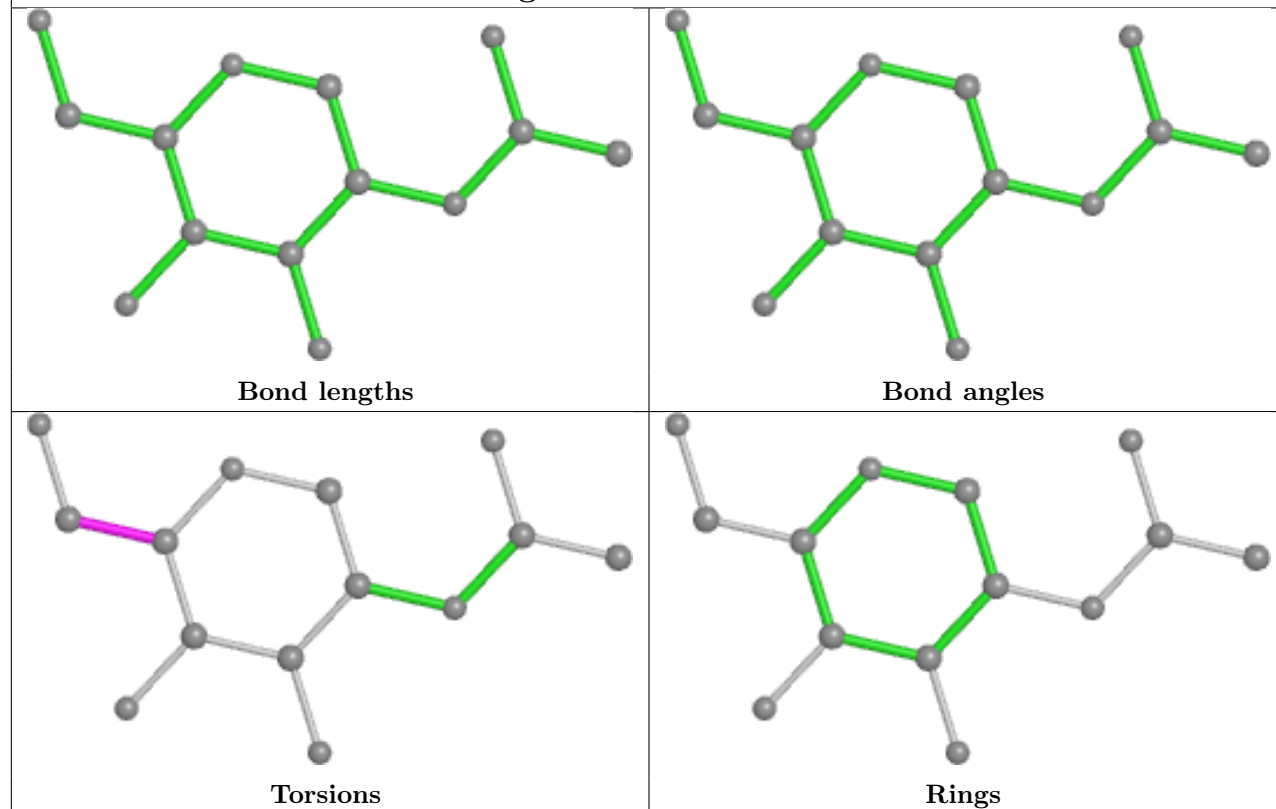
Ligand NAG C 1104

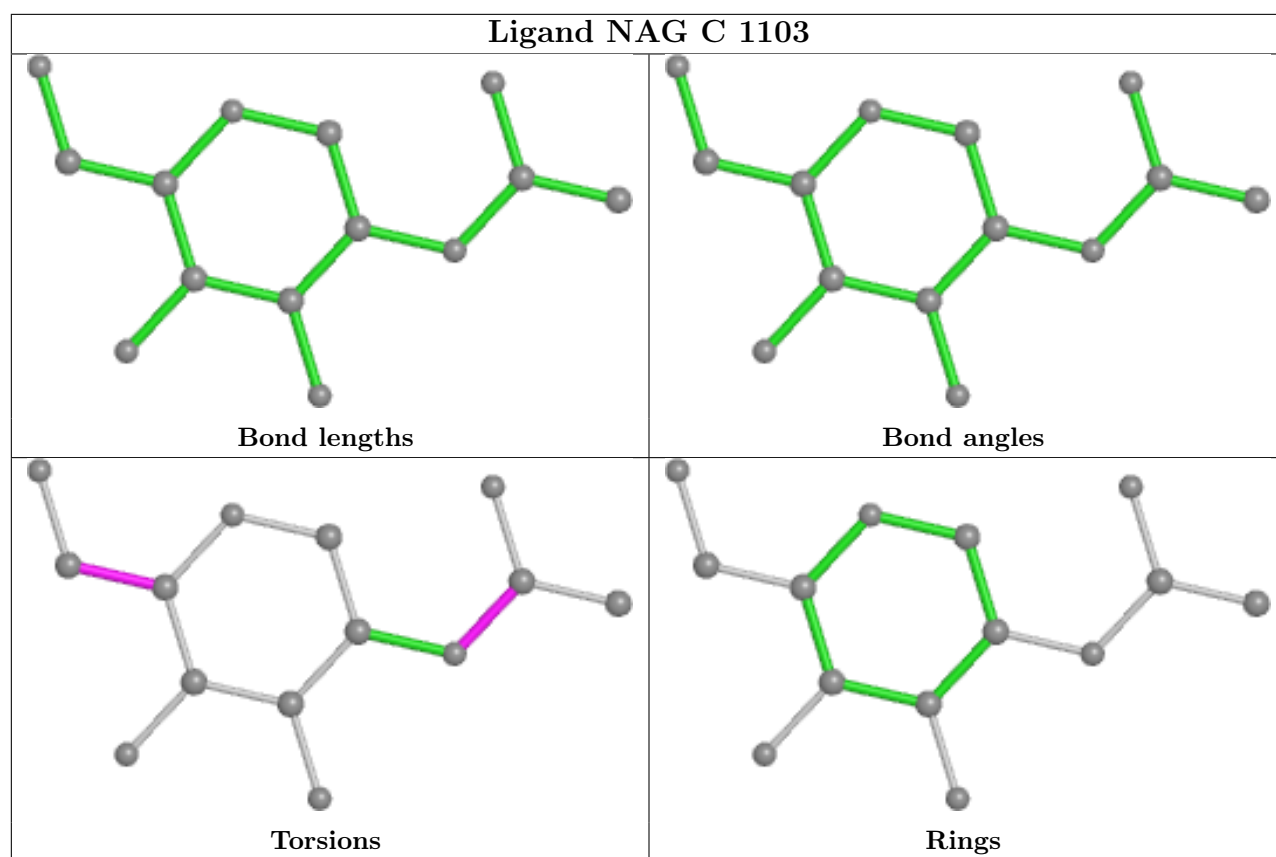


Ligand NAG C 1102



Ligand NAG A 1103





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.