



wwPDB EM Validation Summary Report ⓘ

Jul 14, 2025 – 06:09 PM JST

PDB ID : 9JMM / pdb_00009jmm
EMDB ID : EMD-61606
Title : Cryo-EM structure of the SE-PangolinCoV (MjHKU4r-CoV-1) RBD in complex with human DPP4
Authors : Yuan, H.; Xiong, X.
Deposited on : 2024-09-20
Resolution : 2.80 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

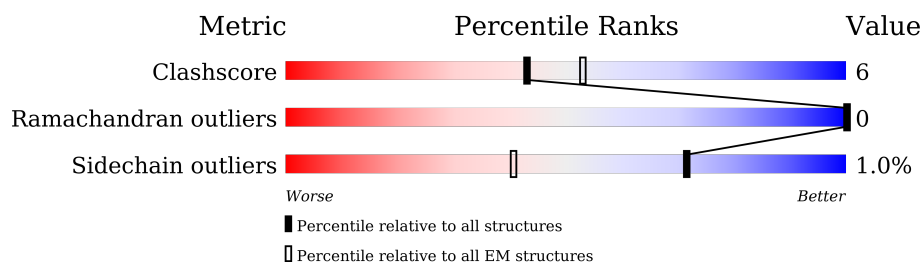
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	758	80% 15% . .
1	C	758	81% 15% .
2	B	505	25% 11% . 63%
3	D	5	60% 40%
4	E	2	100%
4	F	2	100%
4	G	2	100%
4	H	2	100%
4	I	2	100%

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Mol	Chain	Length	Quality of chain
4	J	2	 100%
4	K	2	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13761 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.

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 60 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	HIS	-	expression tag	UNP P27487
A	768	HIS	-	expression tag	UNP P27487

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Chain	Residue	Modelled	Actual	Comment	Reference
A	769	HIS	-	expression tag	UNP P27487
A	770	HIS	-	expression tag	UNP P27487
A	771	HIS	-	expression tag	UNP P27487
A	772	HIS	-	expression tag	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	HIS	-	expression tag	UNP P27487
C	768	HIS	-	expression tag	UNP P27487
C	769	HIS	-	expression tag	UNP P27487
C	770	HIS	-	expression tag	UNP P27487
C	771	HIS	-	expression tag	UNP P27487
C	772	HIS	-	expression tag	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	189	Total	C	N	O	S	0	0
			1466	942	238	275	11		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	356	MET	-	initiating methionine	UNP A0AAE8ZFM2
B	357	THR	-	expression tag	UNP A0AAE8ZFM2
B	358	CYS	-	expression tag	UNP A0AAE8ZFM2
B	359	LEU	-	expression tag	UNP A0AAE8ZFM2
B	360	THR	-	expression tag	UNP A0AAE8ZFM2
B	361	CYS	-	expression tag	UNP A0AAE8ZFM2
B	362	LEU	-	expression tag	UNP A0AAE8ZFM2
B	363	LEU	-	expression tag	UNP A0AAE8ZFM2
B	364	MET	-	expression tag	UNP A0AAE8ZFM2
B	365	PHE	-	expression tag	UNP A0AAE8ZFM2
B	366	LEU	-	expression tag	UNP A0AAE8ZFM2
B	367	LEU	-	expression tag	UNP A0AAE8ZFM2
B	368	MET	-	expression tag	UNP A0AAE8ZFM2
B	369	PHE	-	expression tag	UNP A0AAE8ZFM2
B	370	VAL	-	expression tag	UNP A0AAE8ZFM2
B	371	LYS	-	expression tag	UNP A0AAE8ZFM2
B	372	ASP	-	expression tag	UNP A0AAE8ZFM2
B	373	CYS	-	expression tag	UNP A0AAE8ZFM2
B	374	ASP	-	expression tag	UNP A0AAE8ZFM2
B	482	ALA	SER	conflict	UNP A0AAE8ZFM2
B	544	GLU	VAL	conflict	UNP A0AAE8ZFM2
B	615	ASP	-	linker	UNP A0AAE8ZFM2
B	616	PRO	-	linker	UNP A0AAE8ZFM2
B	617	LEU	-	linker	UNP A0AAE8ZFM2
B	618	VAL	-	linker	UNP A0AAE8ZFM2
B	619	PRO	-	linker	UNP A0AAE8ZFM2
B	620	ARG	-	linker	UNP A0AAE8ZFM2
B	621	GLY	-	linker	UNP A0AAE8ZFM2
B	622	SER	-	linker	UNP A0AAE8ZFM2
B	623	GLY	-	linker	UNP A0AAE8ZFM2
B	624	GLY	-	linker	UNP A0AAE8ZFM2
B	625	GLY	-	linker	UNP A0AAE8ZFM2
B	626	GLY	-	linker	UNP A0AAE8ZFM2
B	627	ASP	-	linker	UNP A0AAE8ZFM2
B	628	PRO	-	linker	UNP A0AAE8ZFM2

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



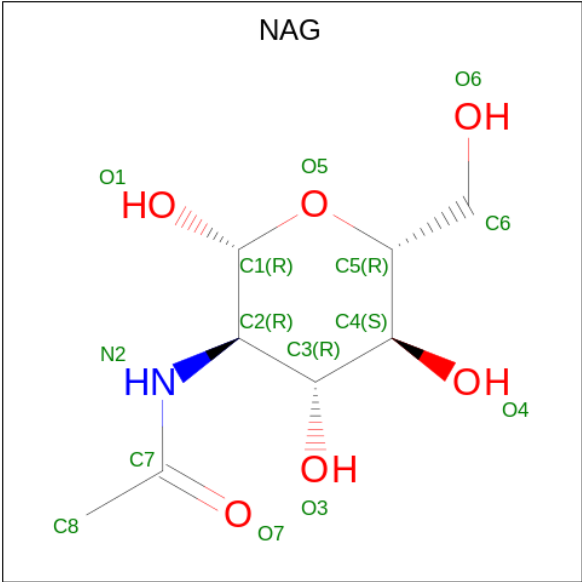
Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	5	Total	C	N	O	0	0
			61	34	2	25		

- 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				AltConf	Trace
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		

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

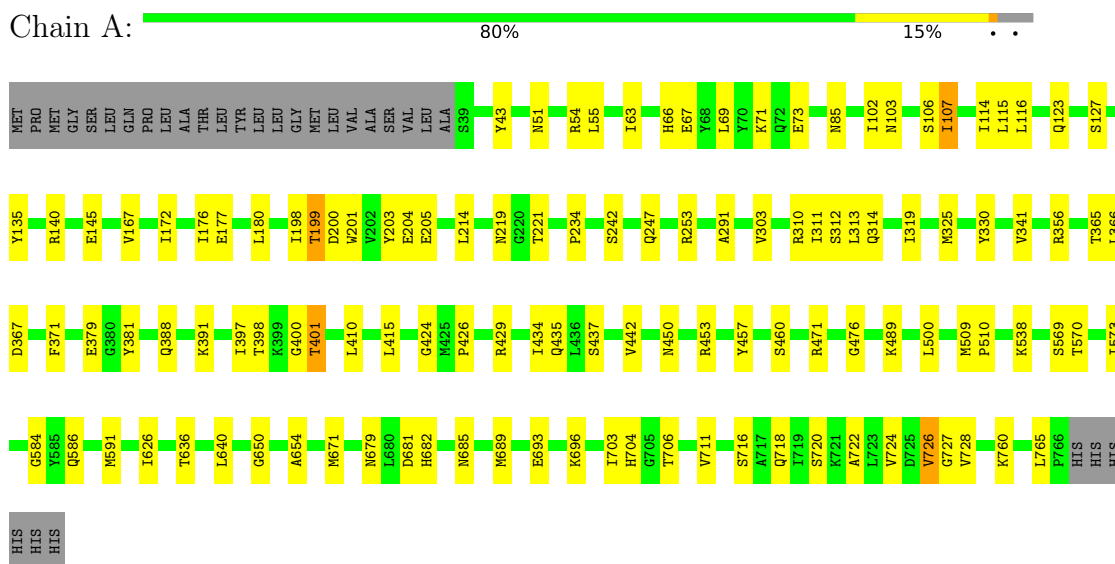


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	

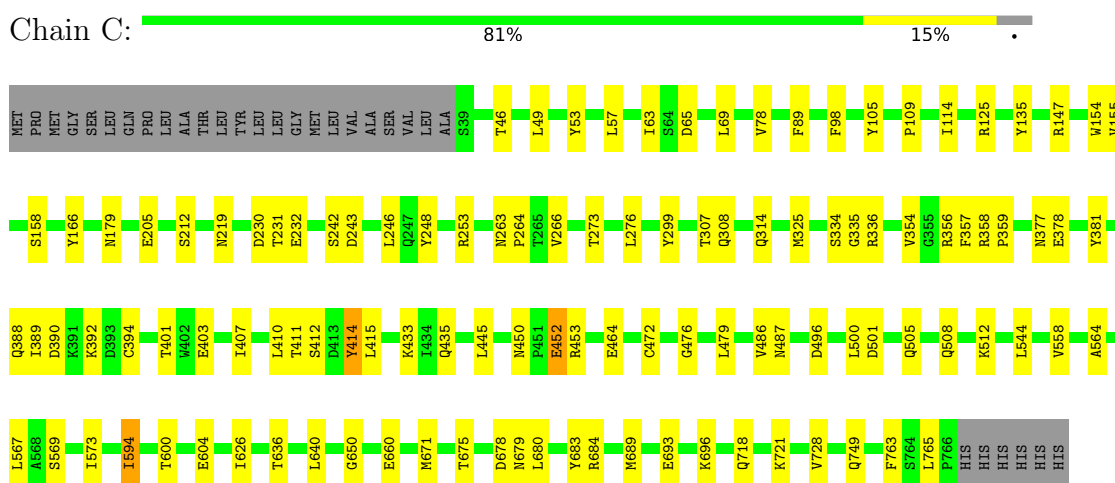
3 Residue-property plots

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

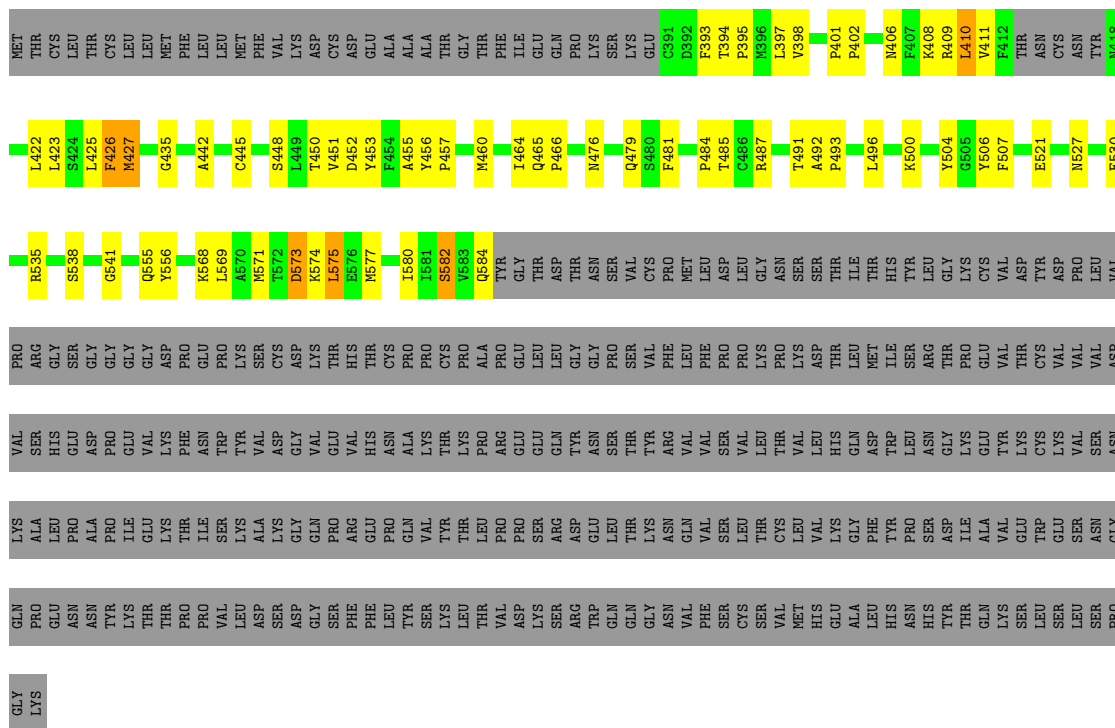


- Molecule 1: Dipeptidyl peptidase 4 soluble form



- Molecule 2: Spike glycoprotein,Isoform 1 of Immunoglobulin heavy constant gamma 1

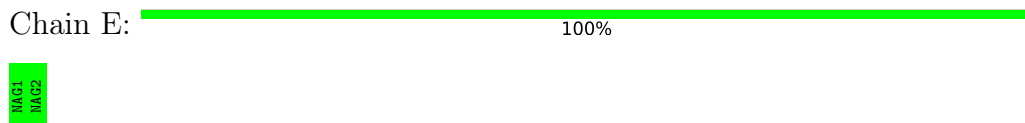




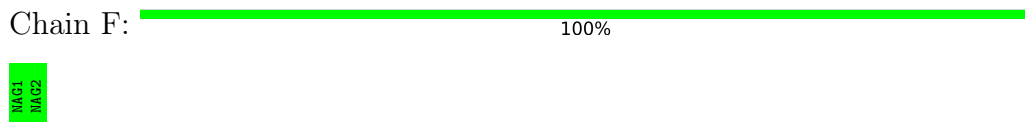
- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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





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

Chain H:  100%



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

Chain I:  100%



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

Chain J:  100%



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

Chain K:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	721281	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)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	0.63	4/6135 (0.1%)	0.55	8/8344 (0.1%)
1	C	0.55	4/6135 (0.1%)	0.59	10/8344 (0.1%)
2	B	0.46	0/1502	0.62	2/2036 (0.1%)
All	All	0.58	8/13772 (0.1%)	0.58	20/18724 (0.1%)

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	567	LEU	CA-C	-6.14	1.44	1.52
1	A	330	TYR	CA-C	-6.10	1.45	1.52
1	C	358	ARG	CA-C	-5.98	1.46	1.52
1	C	232	GLU	CA-C	-5.52	1.45	1.52
1	C	564	ALA	CA-CB	-5.49	1.44	1.53

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	266	VAL	N-CA-C	8.67	120.97	108.48
1	C	392	LYS	N-CA-C	8.00	120.00	111.28
1	C	357	PHE	N-CA-C	-7.51	105.02	114.56
1	A	727	GLY	N-CA-C	7.08	125.41	115.43
1	C	147	ARG	N-CA-C	6.99	119.59	110.43

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	71	0
1	C	5963	0	5677	64	0
2	B	1466	0	1433	43	0
3	D	61	0	52	0	0
4	E	28	0	25	0	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	H	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
5	A	56	0	52	1	0
5	C	56	0	52	0	0
All	All	13761	0	13118	173	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 6.

The worst 5 of 173 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)
2:B:422:LEU:HA	2:B:425:LEU:HD13	1.52	0.91
2:B:401:PRO:HG3	2:B:575:LEU:HD21	1.52	0.89
2:B:410:LEU:HD11	2:B:453:TYR:CE1	2.22	0.74
1:A:176:ILE:HG22	1:A:177:GLU:HG2	1.70	0.73
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.69	0.72

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	726/758 (96%)	706 (97%)	20 (3%)	0	100	100
1	C	726/758 (96%)	701 (97%)	25 (3%)	0	100	100
2	B	185/505 (37%)	170 (92%)	15 (8%)	0	100	100
All	All	1637/2021 (81%)	1577 (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	653/678 (96%)	649 (99%)	4 (1%)	84	95
1	C	653/678 (96%)	647 (99%)	6 (1%)	75	92
2	B	162/449 (36%)	157 (97%)	5 (3%)	35	69
All	All	1468/1805 (81%)	1453 (99%)	15 (1%)	71	91

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	394	CYS
2	B	573	ASP
1	C	472	CYS
2	B	582	SER
2	B	426	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	430	ASN

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Mol	Chain	Res	Type
1	C	606	GLN
1	C	592	HIS
2	B	476	ASN
1	A	606	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 ⓘ

19 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	3,1	14,14,15	0.37	0	17,19,21	0.46	0
3	NAG	D	2	3	14,14,15	0.30	0	17,19,21	0.40	0
3	BMA	D	3	3	11,11,12	0.54	0	15,15,17	0.74	0
3	MAN	D	4	3	11,11,12	0.65	0	15,15,17	1.15	2 (13%)
3	MAN	D	5	3	11,11,12	0.81	1 (9%)	15,15,17	1.19	2 (13%)
4	NAG	E	1	4,1	14,14,15	0.27	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	NAG	F	1	4,1	14,14,15	0.27	0	17,19,21	0.39	0
4	NAG	F	2	4	14,14,15	0.19	0	17,19,21	0.43	0
4	NAG	G	1	4,1	14,14,15	0.23	0	17,19,21	0.40	0
4	NAG	G	2	4	14,14,15	0.18	0	17,19,21	0.42	0
4	NAG	H	1	4,1	14,14,15	0.25	0	17,19,21	0.37	0
4	NAG	H	2	4	14,14,15	0.18	0	17,19,21	0.42	0
4	NAG	I	1	4,1	14,14,15	0.33	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	I	2	4	14,14,15	0.24	0	17,19,21	0.40	0
4	NAG	J	1	4,1	14,14,15	0.18	0	17,19,21	0.44	0
4	NAG	J	2	4	14,14,15	0.21	0	17,19,21	0.38	0
4	NAG	K	1	4,1	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	K	2	4	14,14,15	0.22	0	17,19,21	0.43	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	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	0/2/19/22	0/1/1/1
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	0/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	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)
3	D	5	MAN	C1-C2	2.41	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4	MAN	C1-O5-C5	3.12	116.42	112.19
3	D	5	MAN	C1-O5-C5	2.34	115.36	112.19
3	D	5	MAN	O2-C2-C3	-2.23	105.67	110.14
3	D	4	MAN	O2-C2-C3	-2.12	105.90	110.14

There are no chirality outliers.

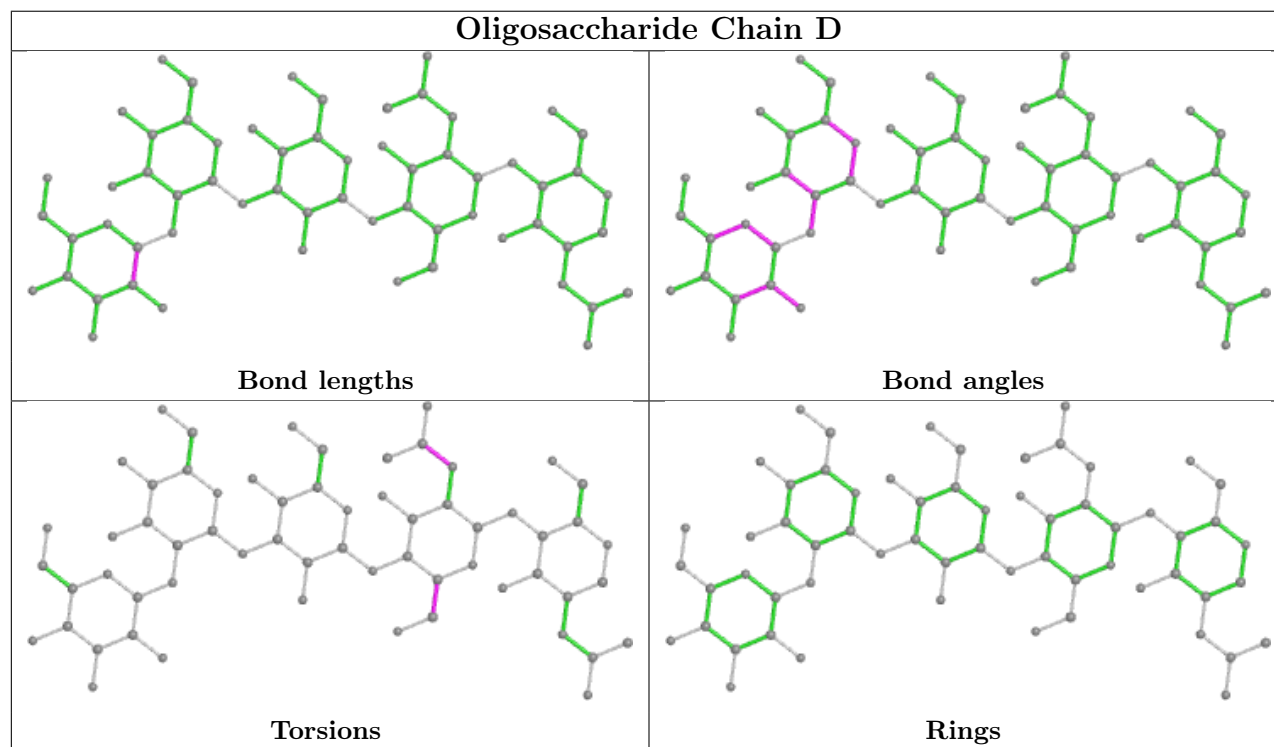
5 of 23 torsion outliers are listed below:

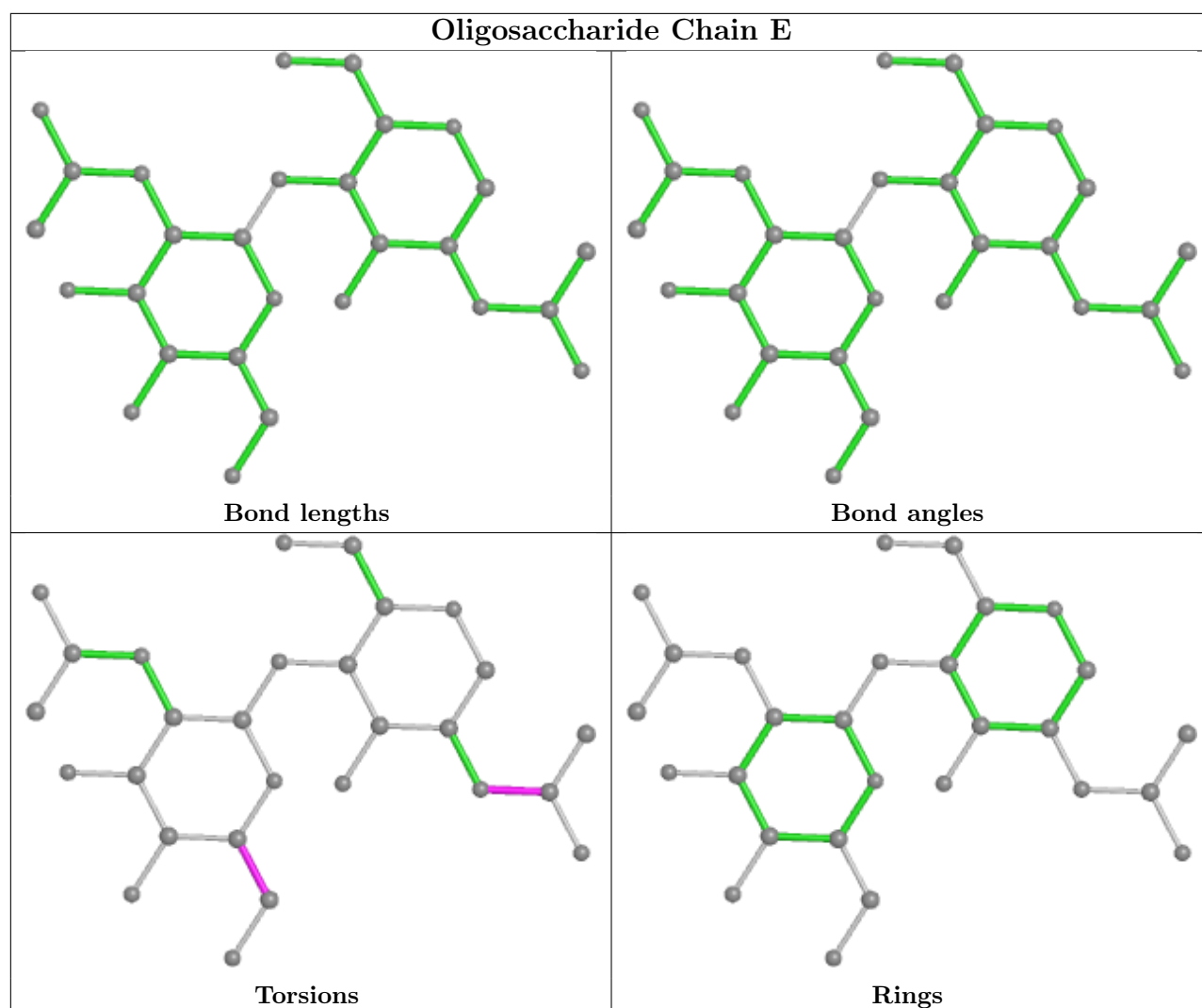
Mol	Chain	Res	Type	Atoms
4	I	1	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6

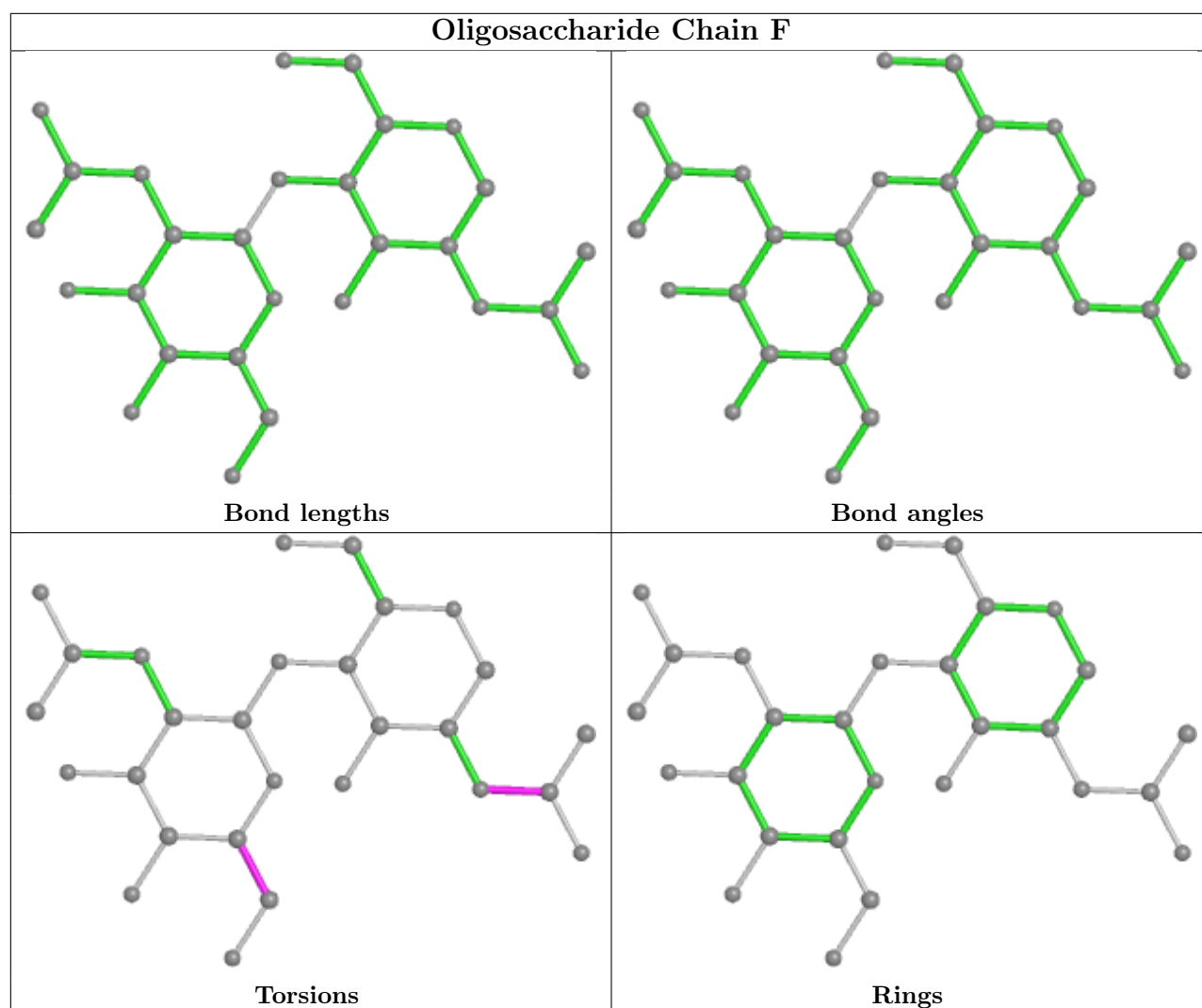
There are no ring outliers.

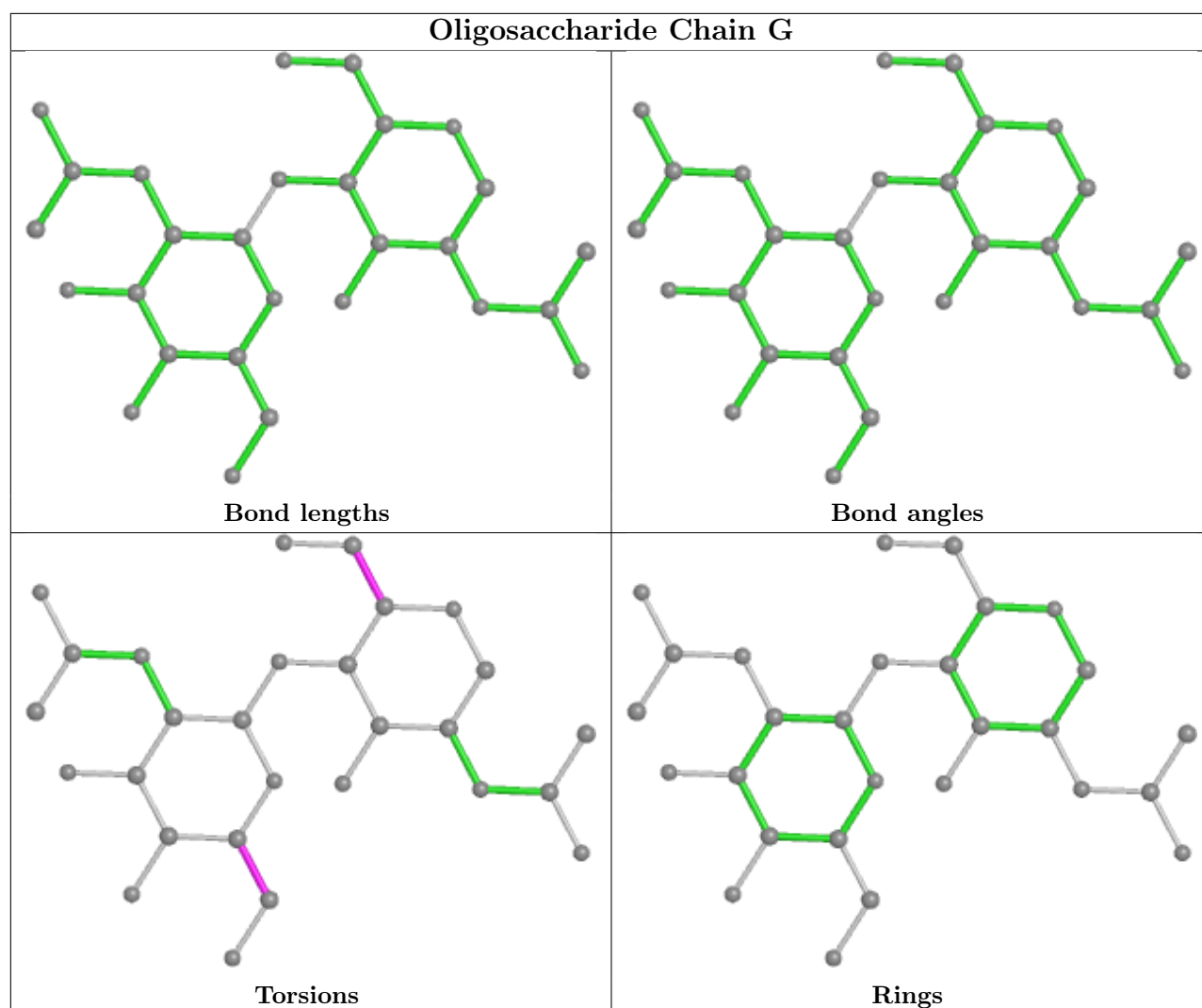
No monomer is involved in short contacts.

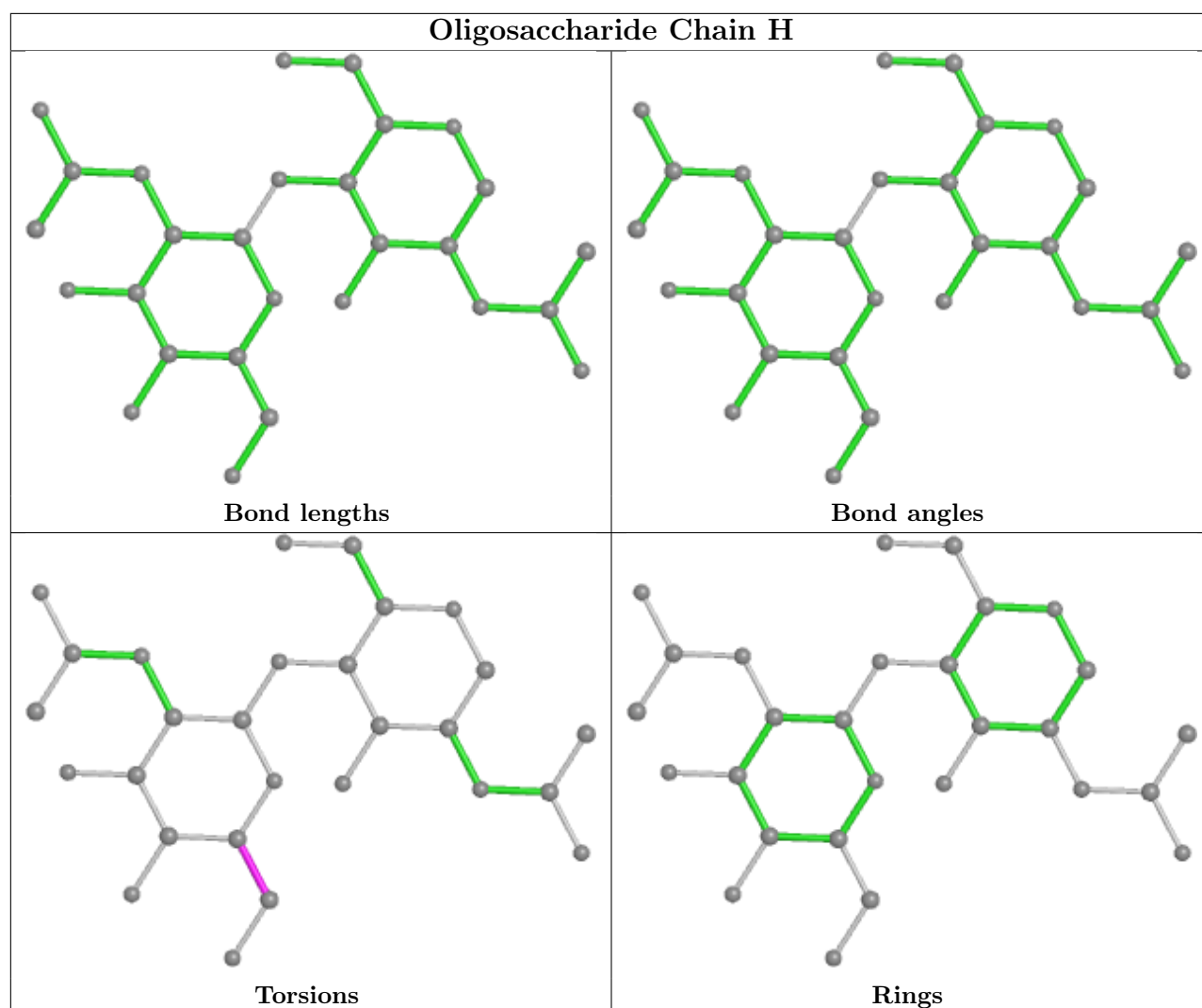
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

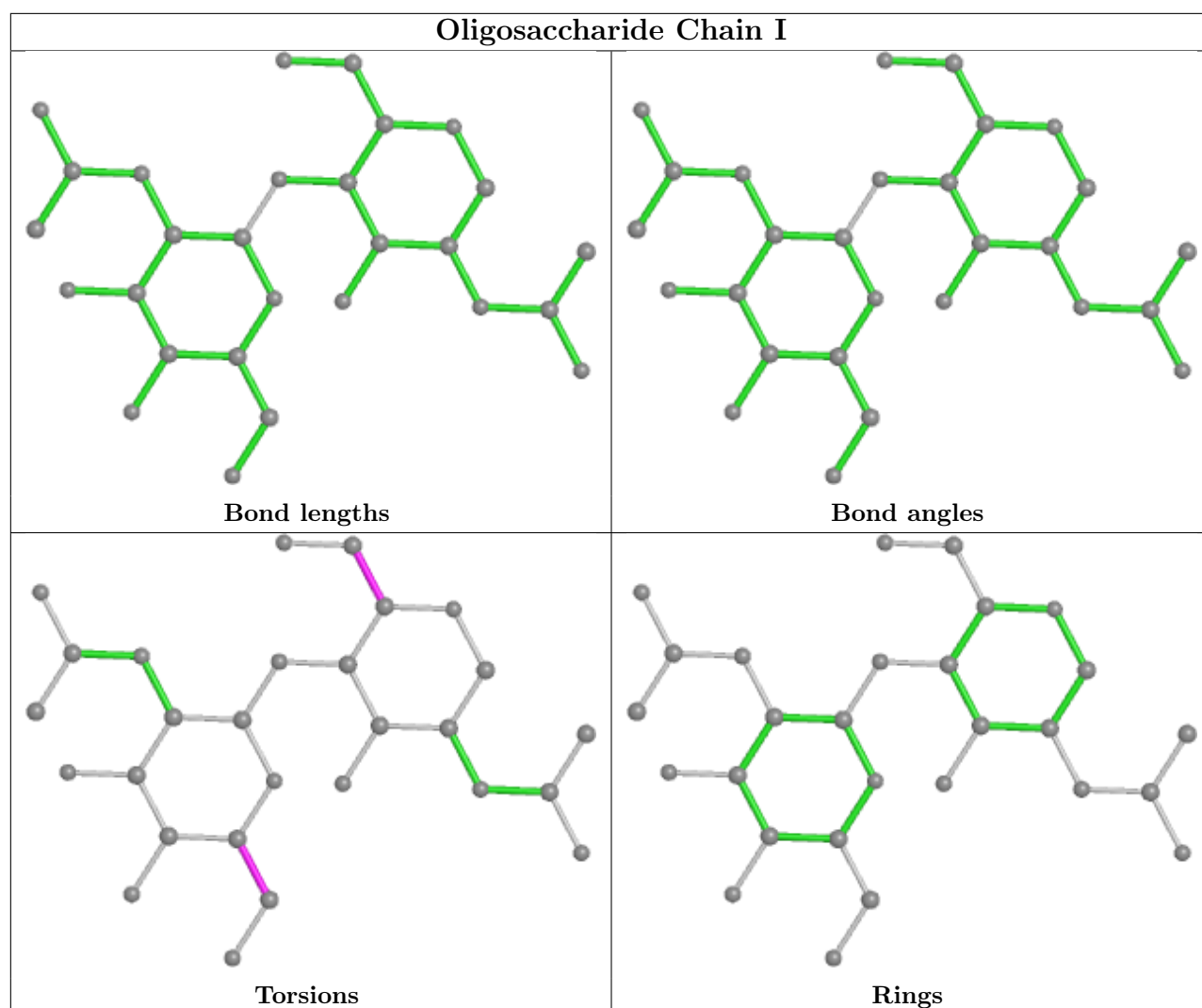


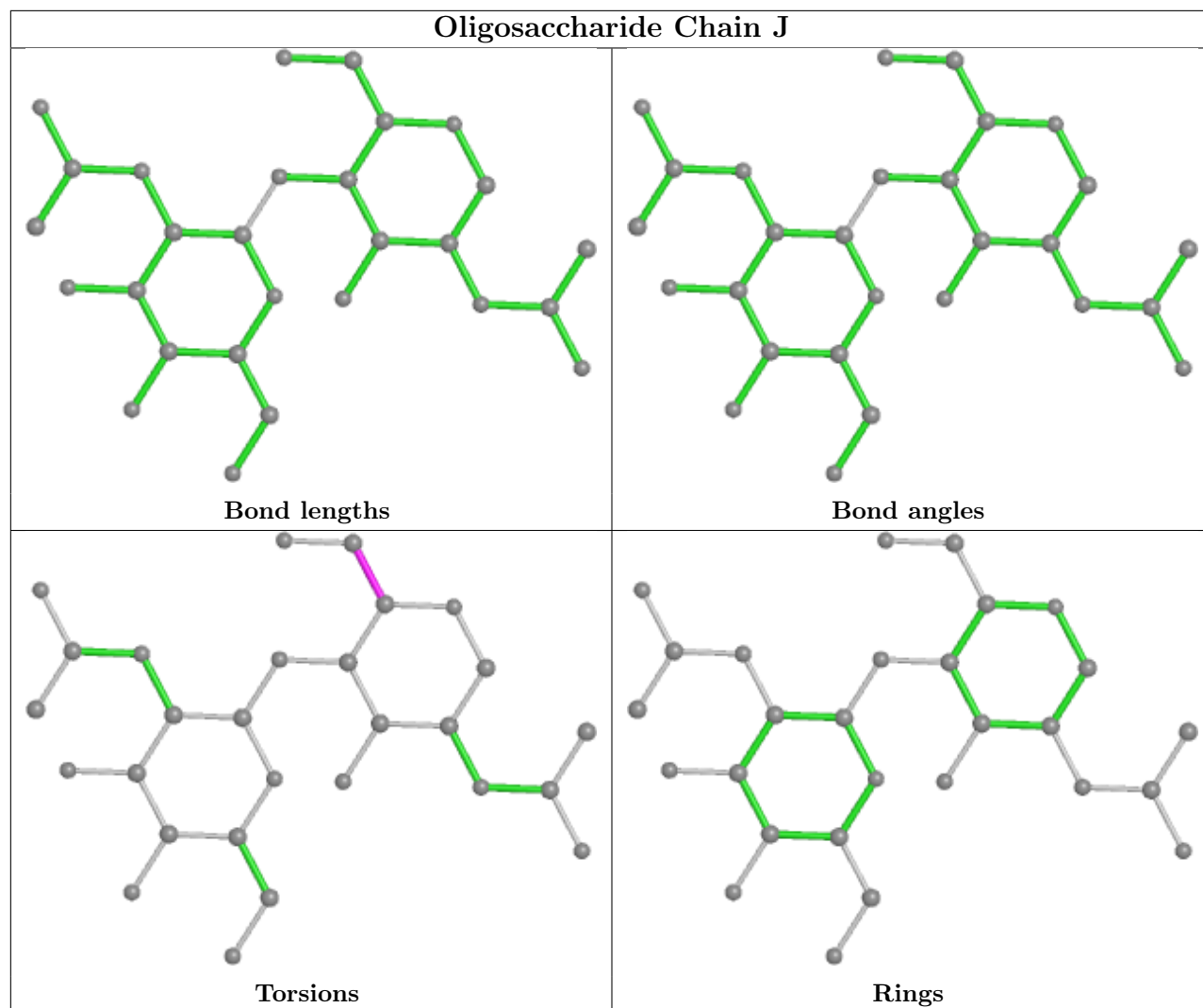


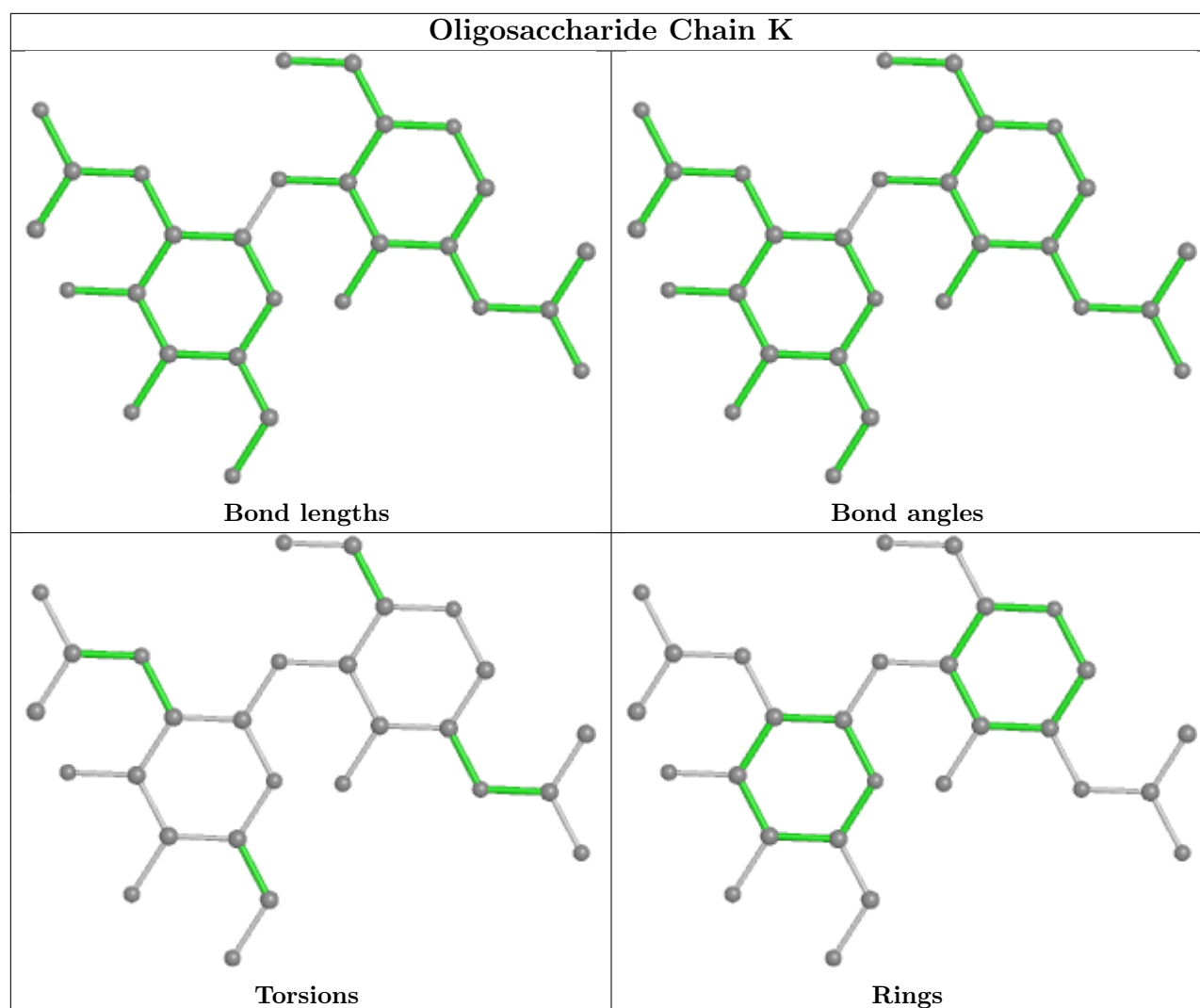












5.6 Ligand geometry [i](#)

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	801	1	14,14,15	0.20	0	17,19,21	0.47	0
5	NAG	A	802	1	14,14,15	0.20	0	17,19,21	0.45	0
5	NAG	C	802	1	14,14,15	0.28	0	17,19,21	0.46	0
5	NAG	A	804	1	14,14,15	0.19	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	803	1	14,14,15	0.28	0	17,19,21	0.47	0
5	NAG	C	801	1	14,14,15	0.22	0	17,19,21	0.40	0
5	NAG	C	804	1	14,14,15	0.24	0	17,19,21	0.44	0
5	NAG	C	803	1	14,14,15	0.21	0	17,19,21	0.43	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	801	1	-	2/6/23/26	0/1/1/1
5	NAG	A	802	1	-	2/6/23/26	0/1/1/1
5	NAG	C	802	1	-	2/6/23/26	0/1/1/1
5	NAG	A	804	1	-	2/6/23/26	0/1/1/1
5	NAG	A	803	1	-	0/6/23/26	0/1/1/1
5	NAG	C	801	1	-	2/6/23/26	0/1/1/1
5	NAG	C	804	1	-	0/6/23/26	0/1/1/1
5	NAG	C	803	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.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	801	NAG	O5-C5-C6-O6
5	A	801	NAG	C4-C5-C6-O6
5	C	801	NAG	C4-C5-C6-O6
5	C	801	NAG	O5-C5-C6-O6
5	A	804	NAG	C4-C5-C6-O6

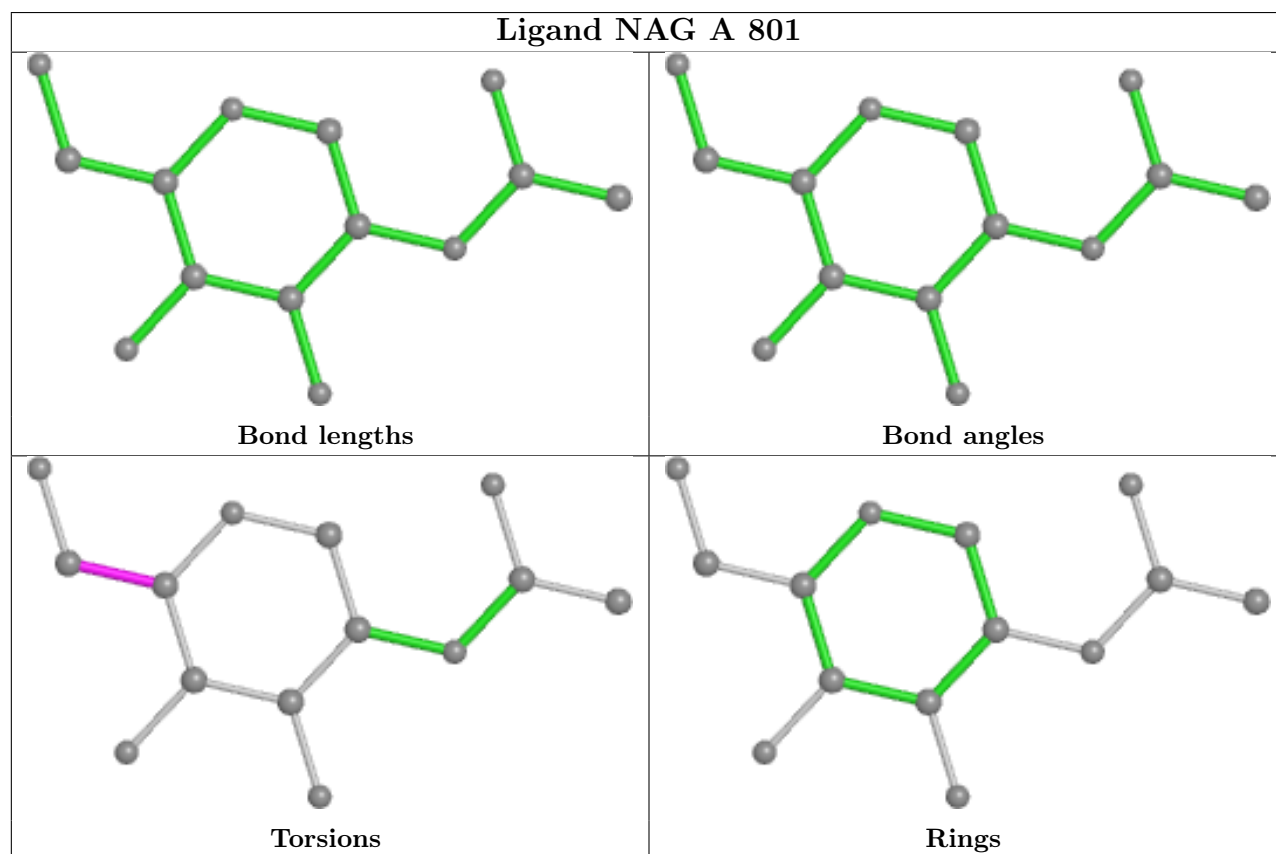
There are no ring outliers.

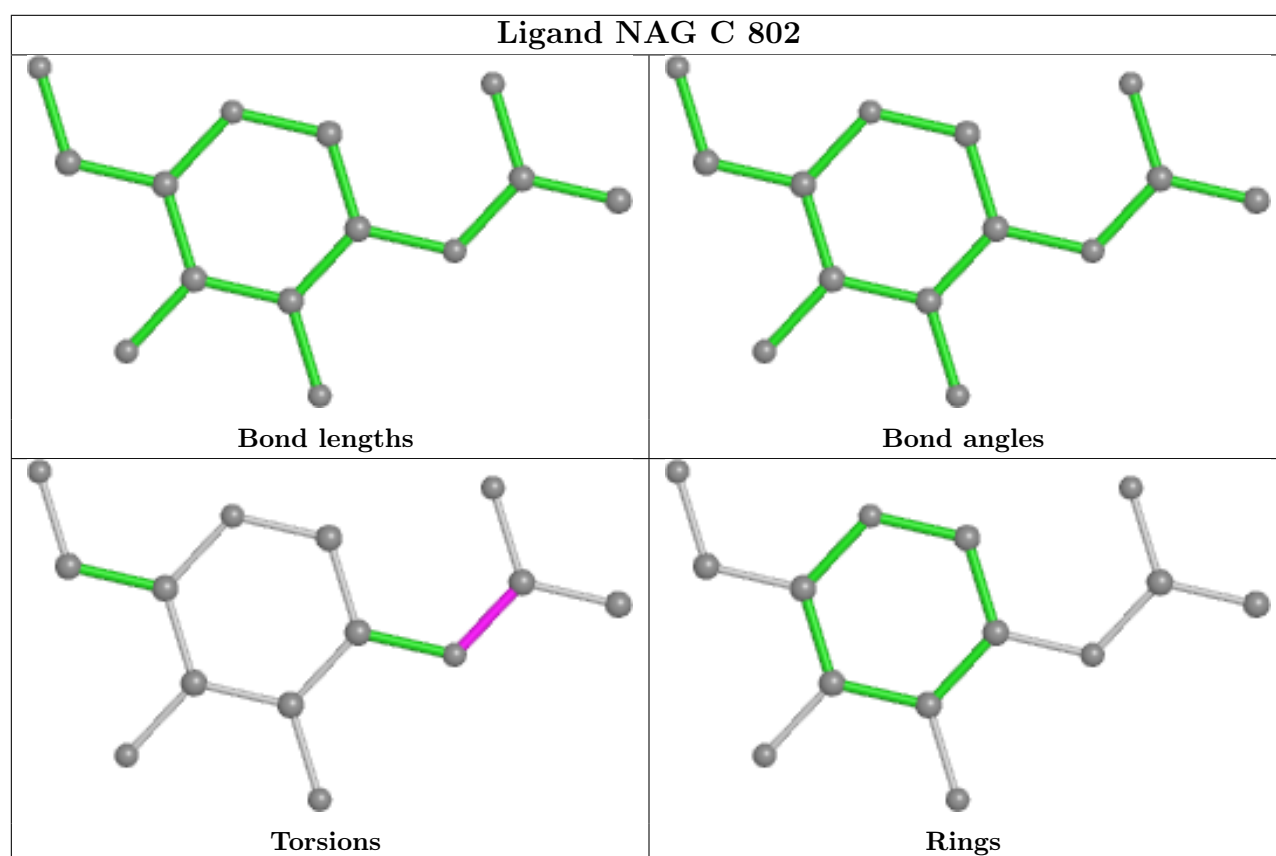
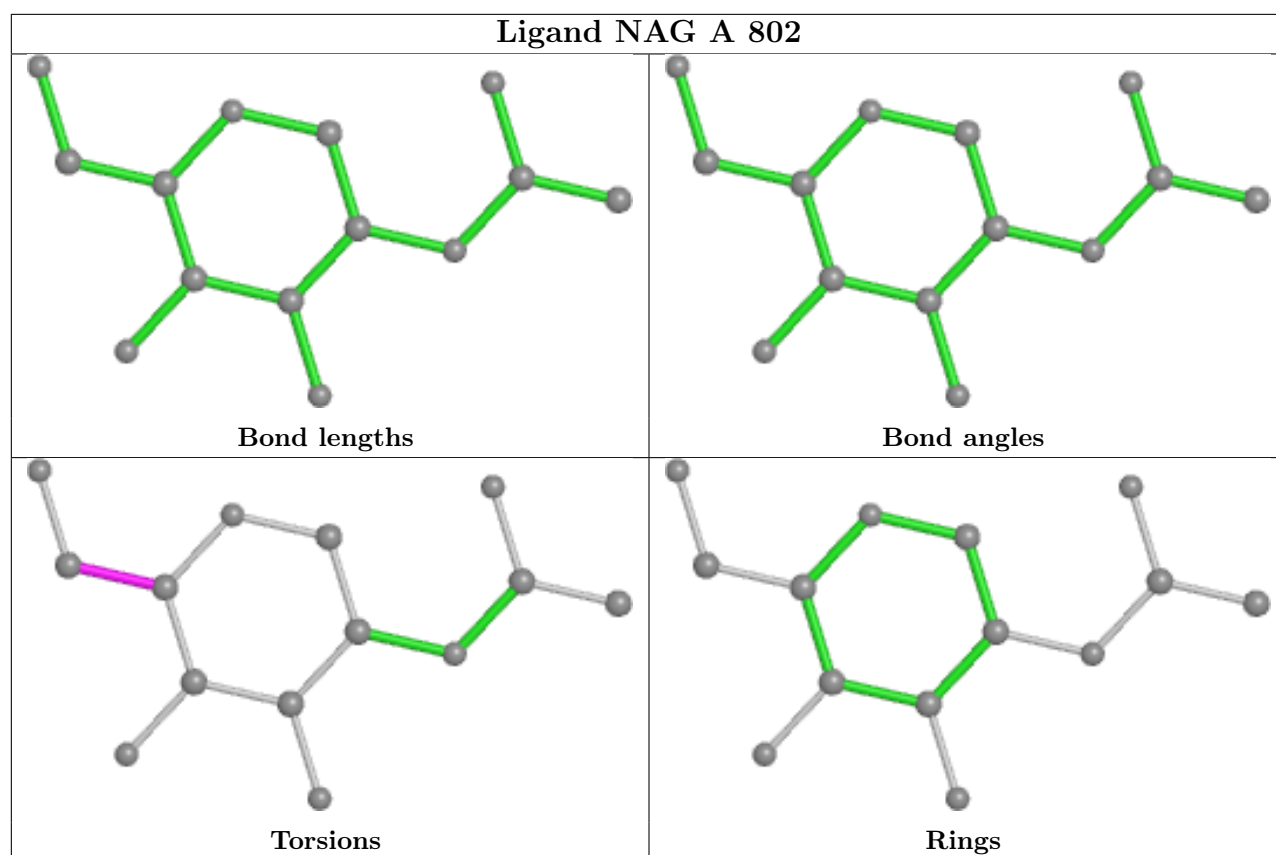
1 monomer is involved in 1 short contact:

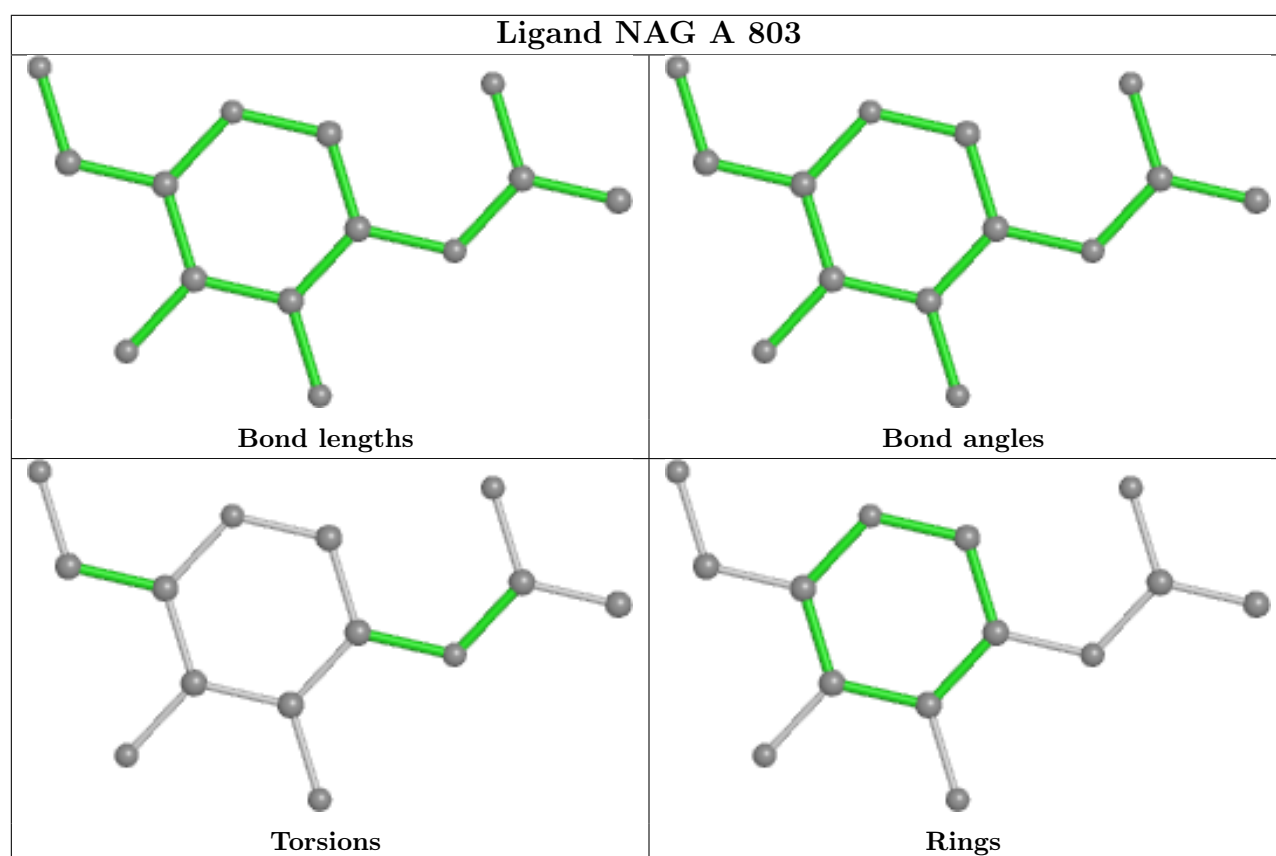
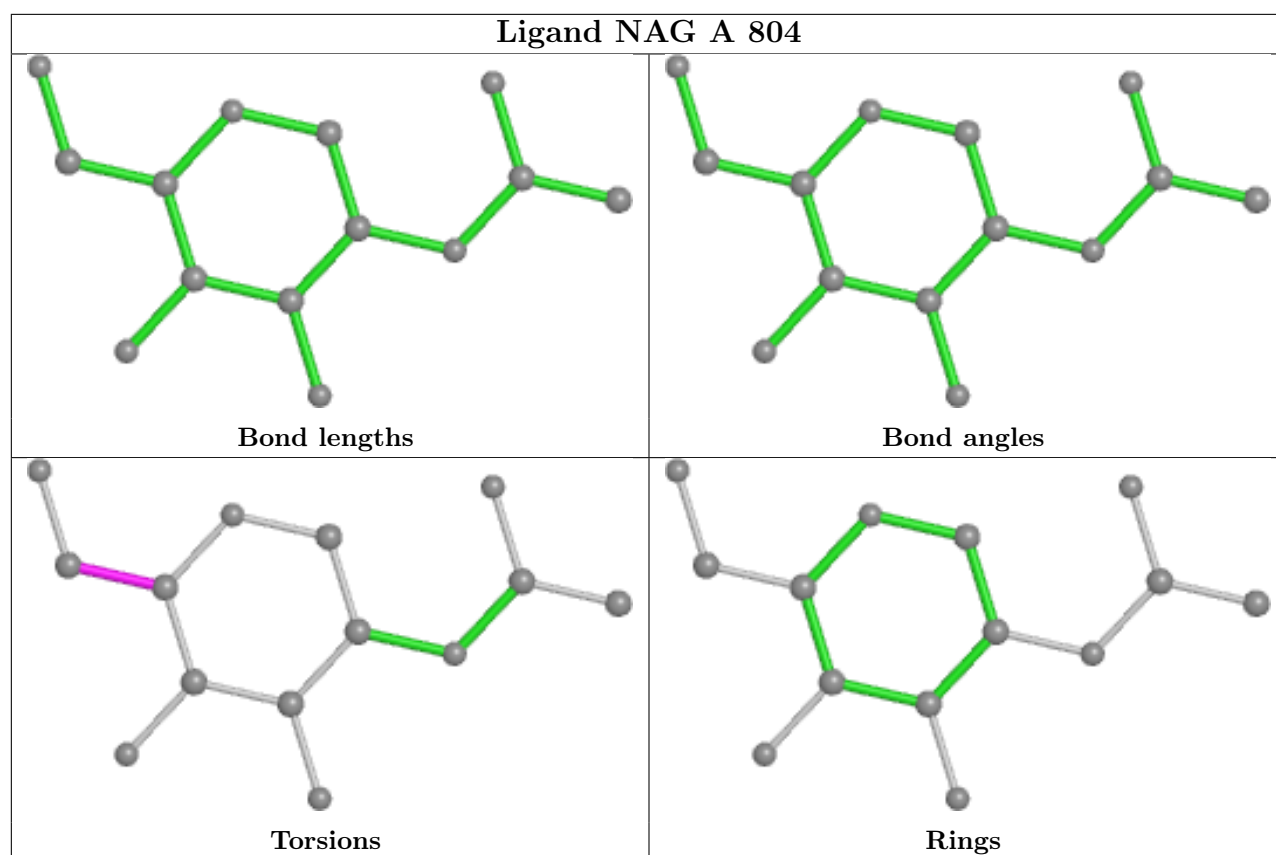
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	801	NAG	1	0

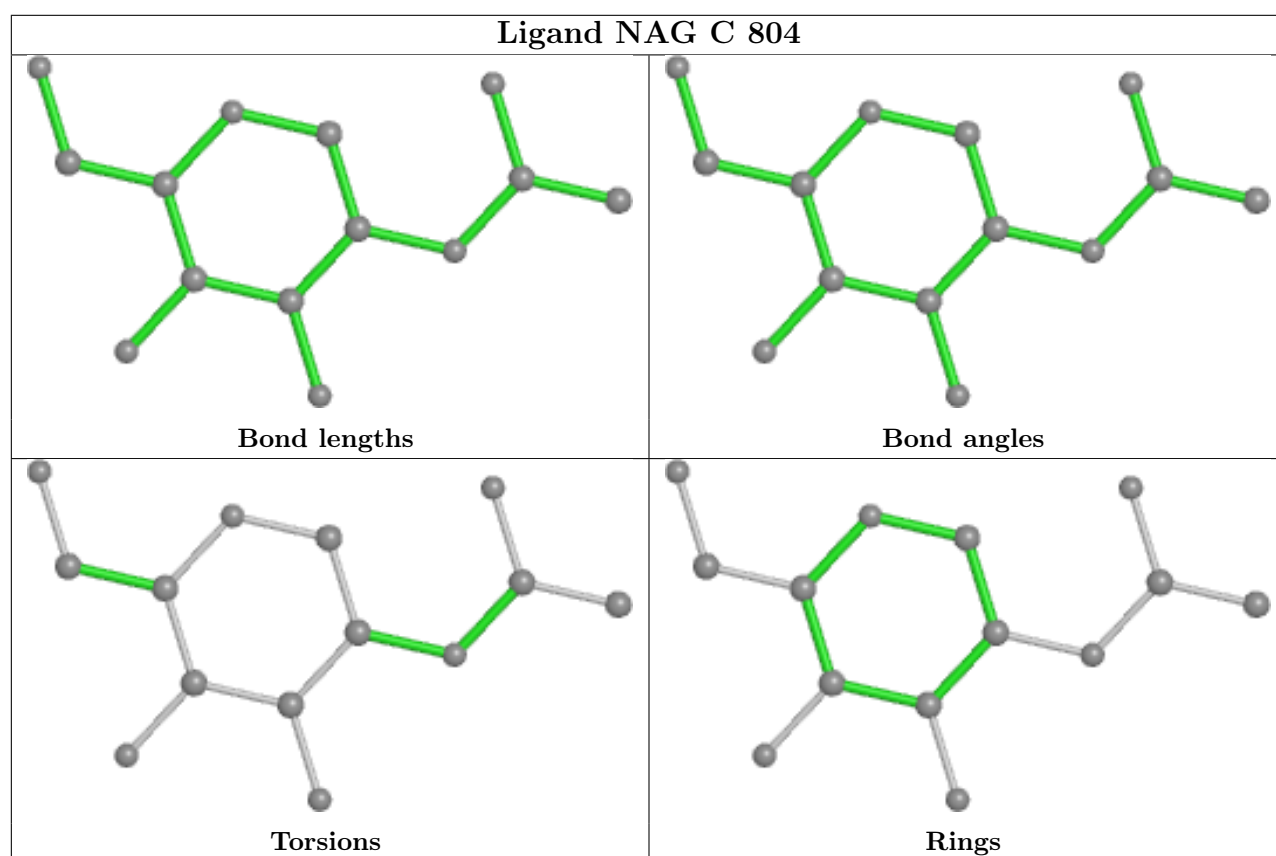
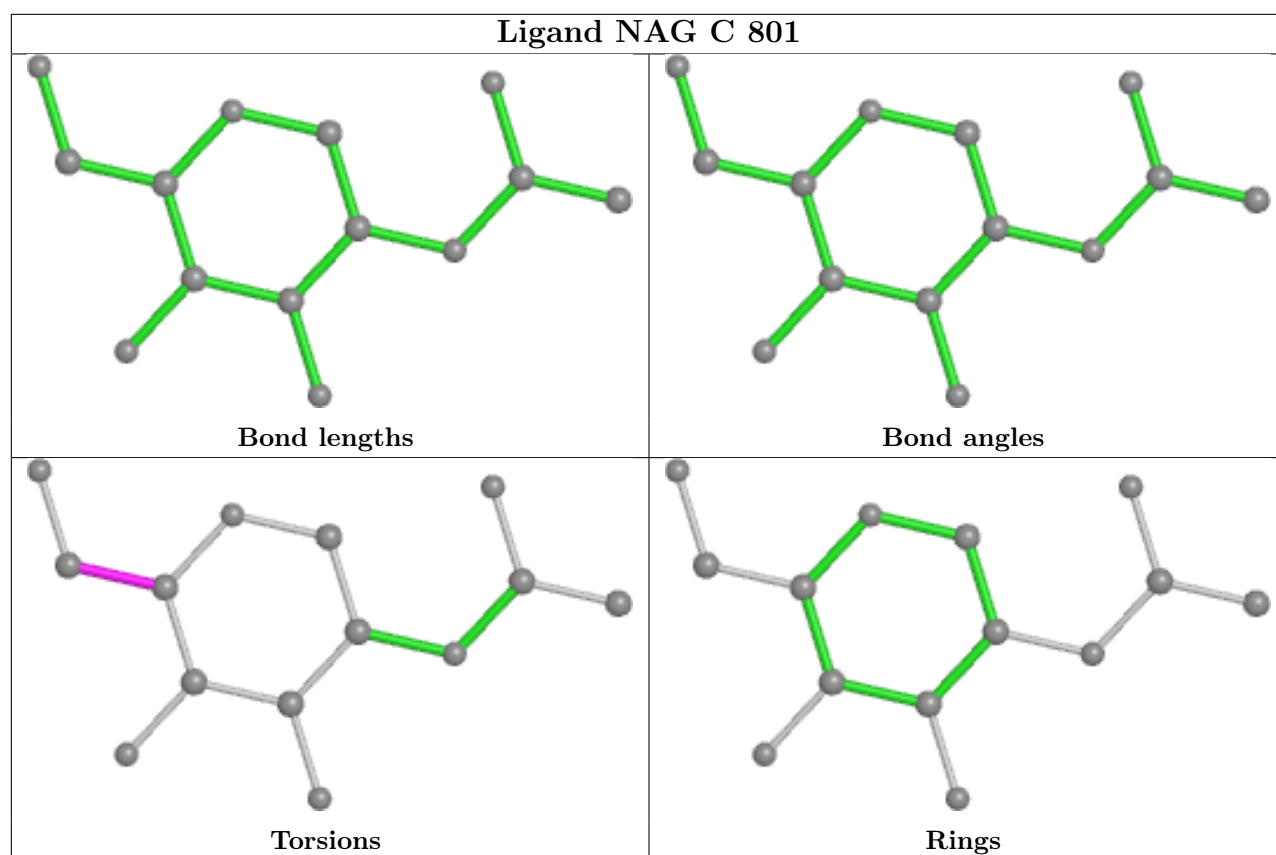
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

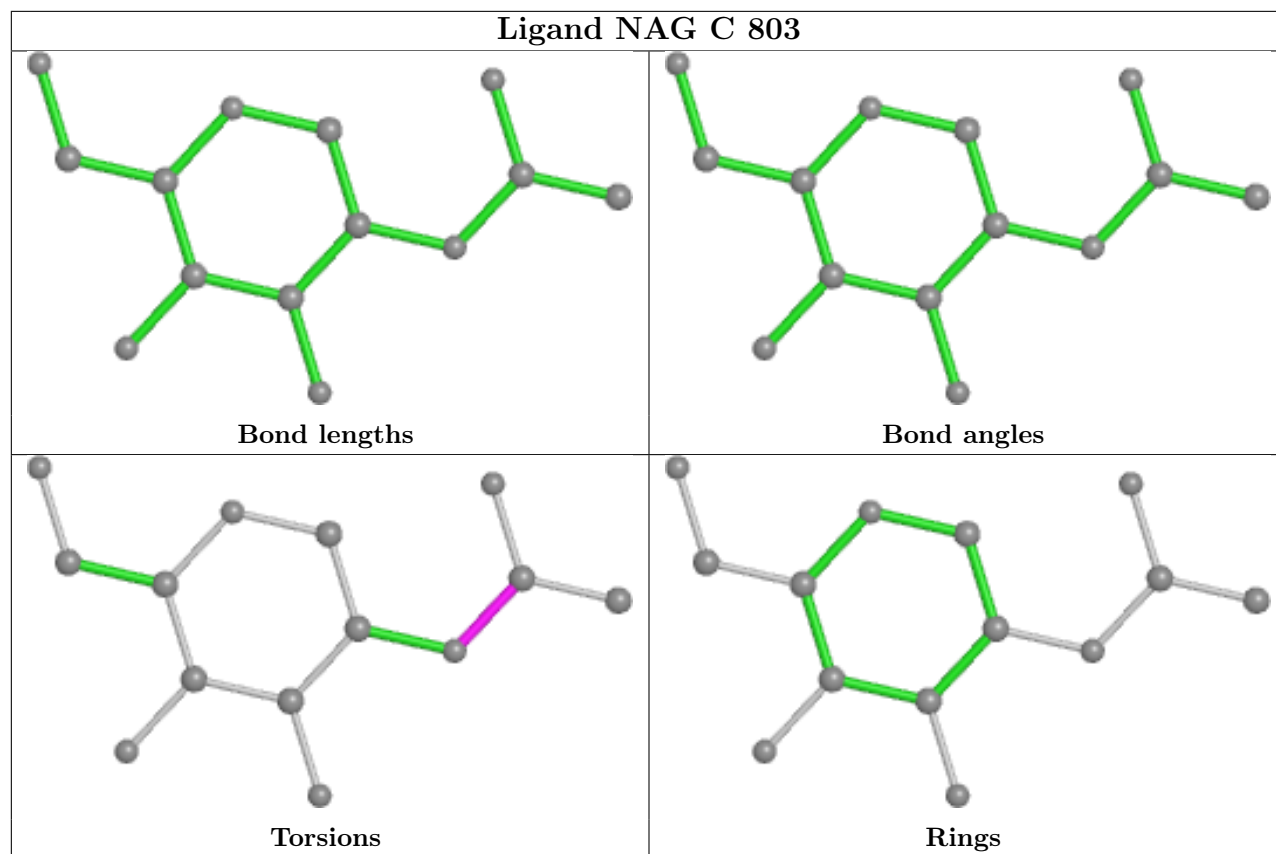
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.











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.